



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 10:06 pm GMT

PDB ID : 7R3K
EMDB ID : EMD-14248
Title : Chlamydomonas reinhardtii TSP9 mutant small Photosystem I complex
Authors : Klaiman, D.; Schwartz, T.; Nelson, N.
Deposited on : 2022-02-07
Resolution : 2.52 Å(reported)
Based on initial model : 6JO5

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

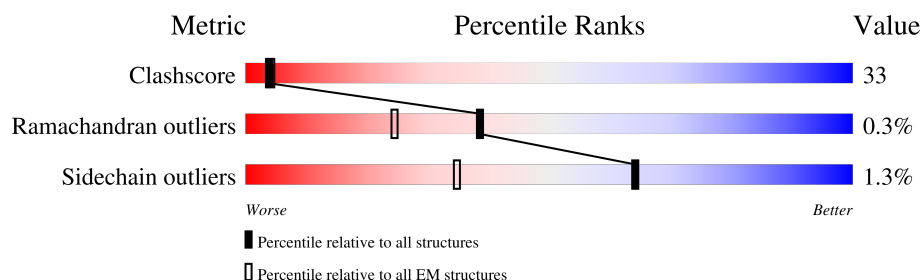
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.52 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	A	751	
2	B	735	
3	C	81	
4	D	196	
5	E	97	
6	F	227	
7	G	126	
8	I	106	

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Mol	Chain	Length	Quality of chain
9	J	41	
10	K	113	
11	1	228	
11	Z	228	
12	3	298	
13	7	241	
14	8	243	
15	4	264	
16	5	257	
17	6	257	

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	CL0	A	801	X	-	-	-
19	CLA	1	5006	X	-	-	-
19	CLA	1	5007	X	-	-	-
19	CLA	1	5008	X	-	-	-
19	CLA	1	5010	X	-	-	-
19	CLA	1	5011	X	-	-	-
19	CLA	1	5012	X	-	-	-
19	CLA	1	5013	X	-	-	-
19	CLA	1	5015	X	-	-	-
19	CLA	1	5016	X	-	X	-
19	CLA	1	5018	X	-	-	-
19	CLA	3	5008	X	-	-	-
19	CLA	3	5009	X	-	-	-
19	CLA	3	5010	X	-	-	-
19	CLA	3	5011	X	-	-	-
19	CLA	3	5012	X	-	-	-
19	CLA	3	5013	X	-	-	-
19	CLA	3	5014	X	-	-	-
19	CLA	3	5015	X	-	-	-
19	CLA	3	5016	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	3	5018	X	-	-	-
19	CLA	3	5019	X	-	-	-
19	CLA	3	5020	X	-	-	-
19	CLA	4	306	X	-	X	-
19	CLA	4	307	X	-	-	-
19	CLA	4	308	X	-	-	-
19	CLA	4	309	X	-	-	-
19	CLA	4	310	X	-	-	-
19	CLA	4	311	X	-	-	-
19	CLA	4	312	X	-	-	-
19	CLA	4	313	X	-	-	-
19	CLA	4	316	X	-	-	-
19	CLA	4	318	X	-	-	-
19	CLA	5	301	X	-	-	-
19	CLA	5	306	X	-	-	-
19	CLA	5	307	X	-	-	-
19	CLA	5	308	X	-	-	-
19	CLA	5	309	X	-	-	-
19	CLA	5	310	X	-	-	-
19	CLA	5	311	X	-	-	-
19	CLA	5	312	X	-	-	-
19	CLA	5	313	X	-	-	-
19	CLA	5	314	X	-	-	-
19	CLA	5	317	X	-	-	-
19	CLA	5	319	X	-	-	-
19	CLA	5	321	X	-	-	-
19	CLA	5	322	X	-	-	-
19	CLA	5	325	X	-	-	-
19	CLA	6	301	X	-	-	-
19	CLA	6	302	X	-	-	-
19	CLA	6	309	X	-	-	-
19	CLA	6	310	X	-	X	-
19	CLA	6	311	X	-	-	-
19	CLA	6	312	X	-	-	-
19	CLA	6	313	X	-	X	-
19	CLA	6	314	X	-	-	-
19	CLA	6	318	X	-	-	-
19	CLA	6	320	X	-	-	-
19	CLA	6	322	X	-	-	-
19	CLA	6	323	X	-	-	-
19	CLA	7	306	X	-	-	-
19	CLA	7	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	7	308	X	-	-	-
19	CLA	7	309	X	-	-	-
19	CLA	7	310	X	-	-	-
19	CLA	7	311	X	-	-	-
19	CLA	7	312	X	-	-	-
19	CLA	7	313	X	-	-	-
19	CLA	7	316	X	-	-	-
19	CLA	7	317	X	-	-	-
19	CLA	7	318	X	-	-	-
19	CLA	7	319	X	-	-	-
19	CLA	7	324	X	-	-	-
19	CLA	8	307	X	-	-	-
19	CLA	8	308	X	-	-	-
19	CLA	8	309	X	-	-	-
19	CLA	8	310	X	-	-	-
19	CLA	8	311	X	-	-	-
19	CLA	8	312	X	-	-	-
19	CLA	8	313	X	-	-	-
19	CLA	8	314	X	-	-	-
19	CLA	8	318	X	-	-	-
19	CLA	8	320	X	-	-	-
19	CLA	A	802	X	-	-	-
19	CLA	A	803	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	X	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	832	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	835	X	-	-	-
19	CLA	A	836	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	841	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	843	X	-	-	-
19	CLA	A	857	X	-	-	-
19	CLA	B	801	X	-	-	-
19	CLA	B	802	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	805	X	-	-	-
19	CLA	B	806	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	X	-
19	CLA	B	824	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	828	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	838	X	-	-	-
19	CLA	B	839	X	-	-	-
19	CLA	B	840	X	-	-	-
19	CLA	B	850	X	-	X	-
19	CLA	F	301	X	-	-	-
19	CLA	F	303	X	-	-	-
19	CLA	G	1601	X	-	-	-
19	CLA	G	1602	X	-	-	-
19	CLA	I	201	X	-	-	-
19	CLA	J	1901	X	-	-	-
19	CLA	K	202	X	-	-	-
19	CLA	K	203	X	-	-	-
19	CLA	K	204	X	-	-	-
19	CLA	K	205	X	-	-	-
19	CLA	Z	303	X	-	-	-
19	CLA	Z	304	X	-	-	-
19	CLA	Z	305	X	-	-	-
19	CLA	Z	306	X	-	-	-
19	CLA	Z	307	X	-	-	-
19	CLA	Z	308	X	-	-	-
19	CLA	Z	311	X	-	-	-
19	CLA	Z	312	X	-	-	-
19	CLA	Z	314	X	-	-	-
19	CLA	Z	315	X	-	-	-
21	SF4	A	845	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	SF4	C	102	-	-	X	-
22	BCR	3	5006	-	-	X	-
22	BCR	6	307	-	-	X	-
32	CHL	1	5009	X	-	-	-
32	CHL	1	5014	X	-	-	-
32	CHL	1	5017	X	-	-	-
32	CHL	3	5017	X	-	-	-
32	CHL	4	314	X	-	-	-
32	CHL	4	315	X	-	-	-
32	CHL	4	317	X	-	-	-
32	CHL	4	319	X	-	-	-
32	CHL	5	315	X	-	-	-
32	CHL	5	316	X	-	-	-
32	CHL	5	318	X	-	-	-
32	CHL	5	320	X	-	-	-
32	CHL	6	315	X	-	-	-
32	CHL	6	316	X	-	-	-
32	CHL	6	317	X	-	-	-
32	CHL	6	319	X	-	-	-
32	CHL	6	321	X	-	-	-
32	CHL	7	314	X	-	-	-
32	CHL	7	315	X	-	-	-
32	CHL	8	301	X	-	-	-
32	CHL	8	315	X	-	-	-
32	CHL	8	316	X	-	-	-
32	CHL	8	317	X	-	-	-
32	CHL	8	319	X	-	-	-
32	CHL	Z	302	X	-	-	-
32	CHL	Z	309	X	-	-	-
32	CHL	Z	310	X	-	-	-
32	CHL	Z	313	X	-	-	-
33	SPH	3	5001	-	-	X	-
38	ERG	6	326	-	-	X	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 46504 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	740	Total	C	N	O	S	0	0
			5811	3799	991	999	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5824	3825	977	1004	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			601	369	103	117	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1135	725	201	202	7		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	63	Total	C	N	O	0	0
			496	316	87	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1266	817	213	233	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	67	Total	C	N	O	0	0
			495	321	86	88		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			281	195	39	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	39	Total	C	N	O	S	0	0
			320	219	45	55	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			570	362	98	108	2		

- Molecule 11 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		
11	Z	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3	219	Total	C	N	O	S	0	0
			1673	1092	270	303	8		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	7	213	Total	C	N	O	S	0	0
			1650	1072	274	298	6		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	8	217	Total	C	N	O	S	0	0
			1650	1073	280	293	4		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic (Lhca4).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	4	210	Total	C	N	O	S	0	0
			1628	1068	262	293	5		

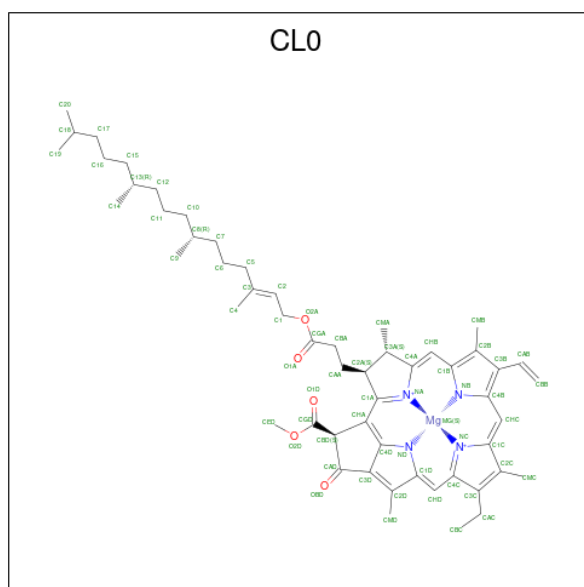
- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	5	227	Total	C	N	O	S	0	0
			1775	1154	297	316	8		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

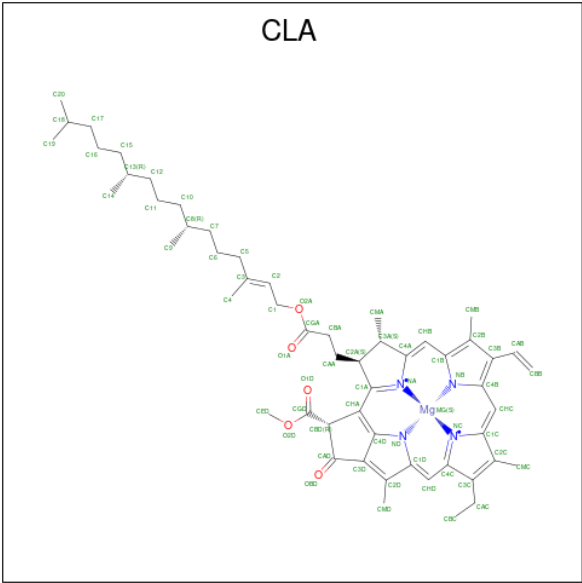
Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	229	Total	C	N	O	S	0	0
			1766	1164	292	304	6		

- Molecule 18 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
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
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	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
			56	46	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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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 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	A	1	Total 61	C 51	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 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	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	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 57	C 47	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

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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 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	A	1	Total 52	C 42	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 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 52	C 42	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
			56	46	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
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 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 52	C 42	Mg 1	N 4	O 5	0
19	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
19	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	K	1	Total 49	C 39	Mg 1	N 4	O 5	0
19	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	1	1	Total 48	C 38	Mg 1	N 4	O 5	0
19	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	Z	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	Z	1	Total 65	C 55	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 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total 65	C 55	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 65	C 55	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 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 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 55	C 45	Mg 1	N 4	O 5	0
19	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	7	1	Total 61	C 51	Mg 1	N 4	O 5	0
19	7	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
19	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	7	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
19	7	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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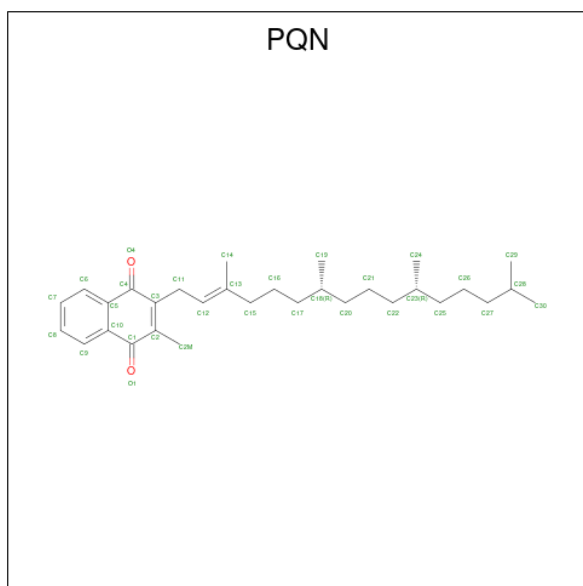
Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
19	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
19	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
19	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	6	1	Total 65	C 55	Mg 1	N 4	O 5	0

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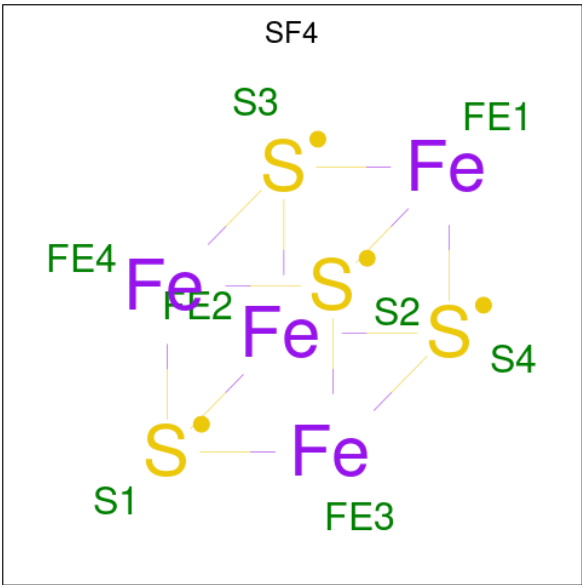
Mol	Chain	Residues	Atoms					AltConf
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



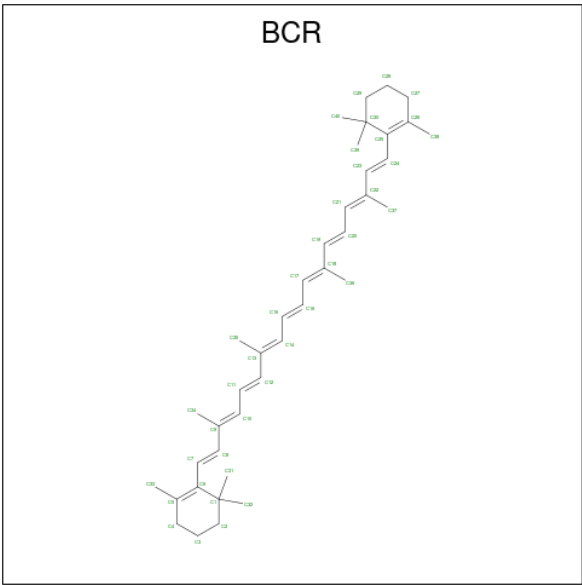
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			33	31	2	
20	B	1	Total	C	O	0
			33	31	2	

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

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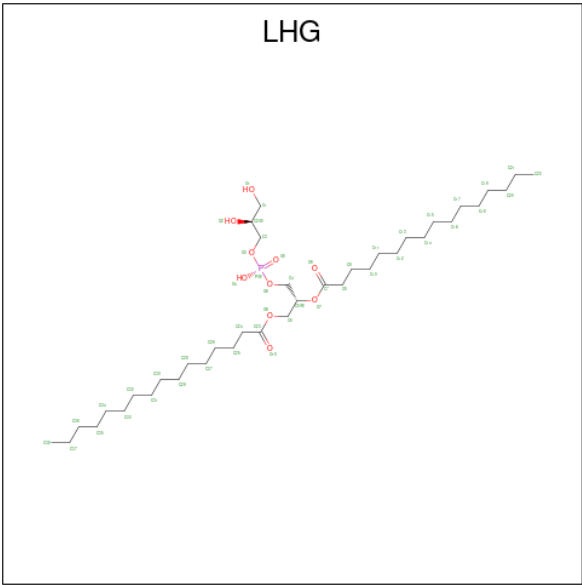
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	G	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	7	1	Total C 40 40	0
22	8	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
22	8	1	Total	C	0
			40	40	
22	4	1	Total	C	0
			40	40	
22	5	1	Total	C	0
			40	40	
22	5	1	Total	C	0
			40	40	
22	6	1	Total	C	0
			40	40	
22	6	1	Total	C	0
			40	40	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



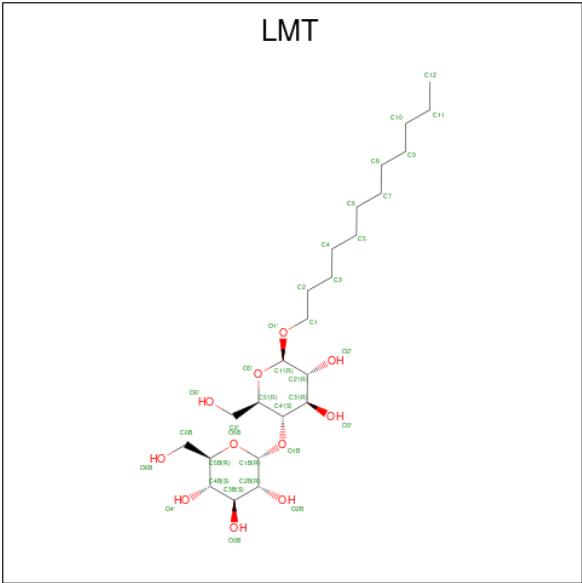
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			35	24	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			23	12	10	1	
23	1	1	Total	C	O	P	0
			43	32	10	1	
23	Z	1	Total	C	O	P	0
			43	32	10	1	

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Mol	Chain	Residues	Atoms				AltConf
23	3	1	Total	C	O	P	0
			20	9	10	1	
23	7	1	Total	C	O	P	0
			37	26	10	1	
23	8	1	Total	C	O	P	0
			38	27	10	1	
23	4	1	Total	C	O	P	0
			49	38	10	1	
23	5	1	Total	C	O	P	0
			37	26	10	1	
23	6	1	Total	C	O	P	0
			32	21	10	1	
23	6	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 24 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



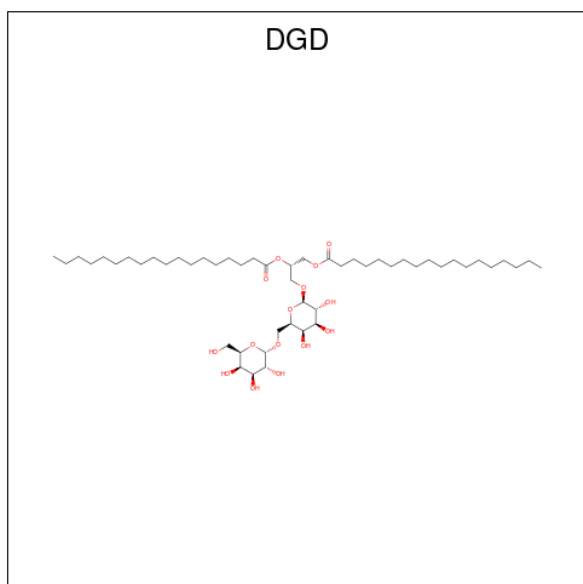
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			35	24	11	
24	A	1	Total	C	O	0
			35	24	11	
24	A	1	Total	C	O	0
			35	24	11	
24	A	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
24	F	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			35	24	11	
24	1	1	Total	C	O	0
			35	24	11	
24	Z	1	Total	C	O	0
			35	24	11	
24	Z	1	Total	C	O	0
			35	24	11	
24	3	1	Total	C	O	0
			35	24	11	
24	7	1	Total	C	O	0
			35	24	11	
24	8	1	Total	C	O	0
			35	24	11	
24	8	1	Total	C	O	0
			35	24	11	
24	4	1	Total	C	O	0
			35	24	11	
24	4	1	Total	C	O	0
			35	24	11	
24	4	1	Total	C	O	0
			35	24	11	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

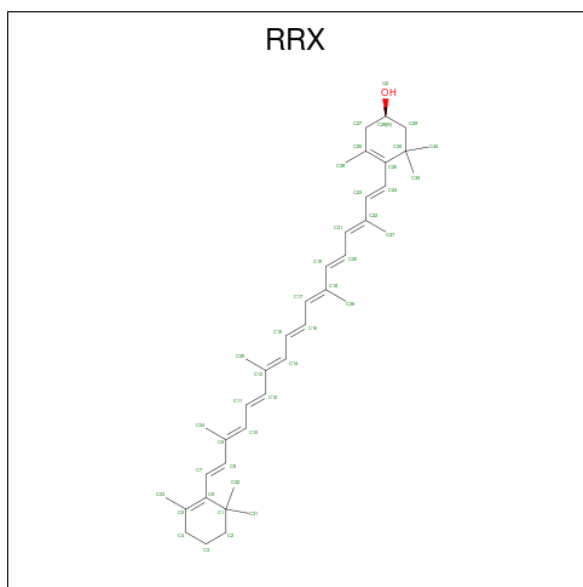


Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			66	51	15	

- Molecule 26 is CALCIUM ION (three-letter code: CA) (formula: Ca).

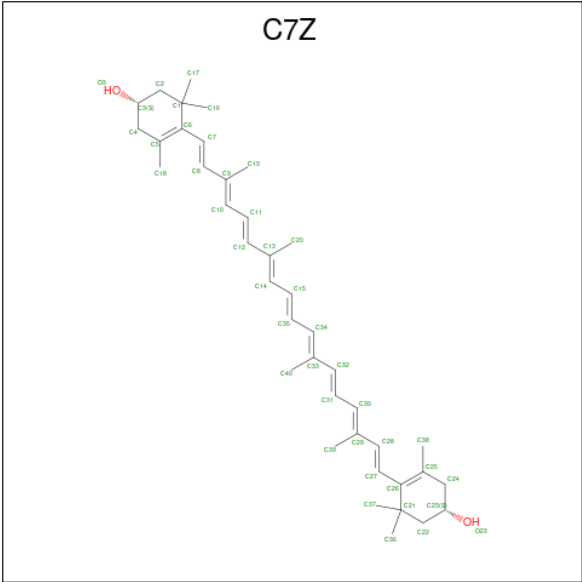
Mol	Chain	Residues	Atoms			AltConf
26	B	1	Total	Ca		0
			1	1		

- Molecule 27 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C₄₀H₅₆O).



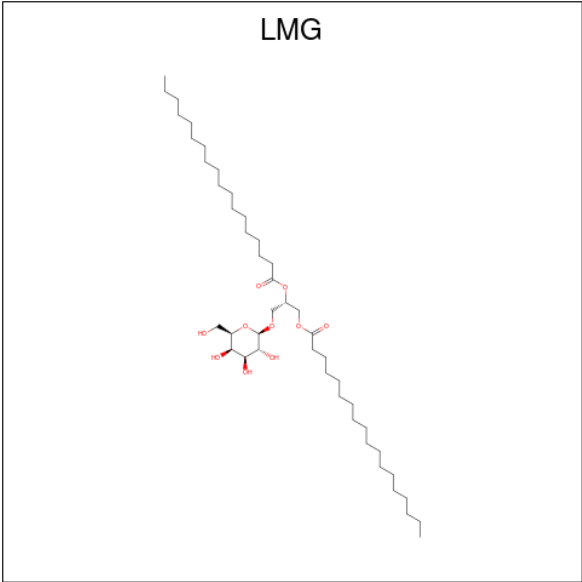
Mol	Chain	Residues	Atoms			AltConf
27	F	1	Total	C	O	0
			41	40	1	
27	4	1	Total	C	O	0
			41	40	1	
27	5	1	Total	C	O	0
			41	40	1	

- Molecule 28 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: C₄₀H₅₆O₂).



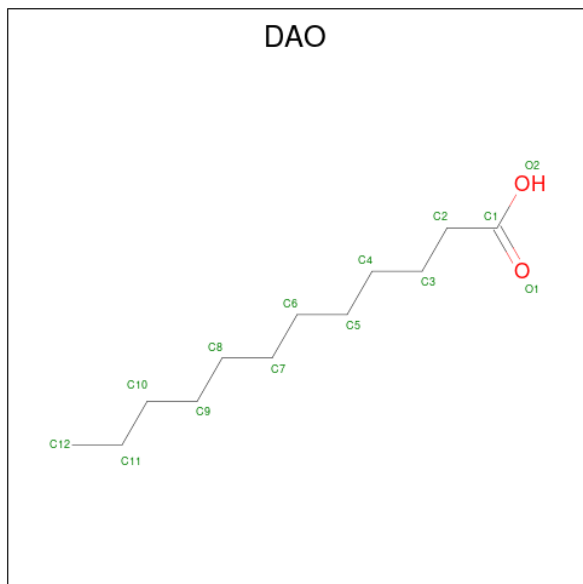
Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	6	1	Total	C	O	0
			42	40	2	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



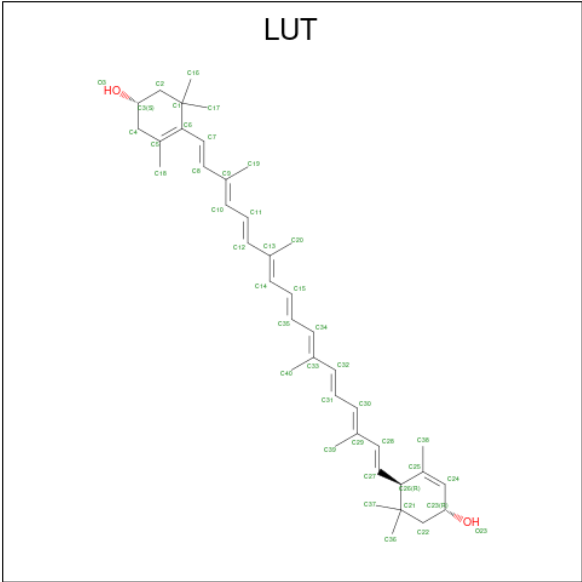
Mol	Chain	Residues	Atoms			AltConf
29	J	1	Total	C	O	0
			35	25	10	
29	J	1	Total	C	O	0
			45	35	10	
29	7	1	Total	C	O	0
			29	19	10	

- Molecule 30 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



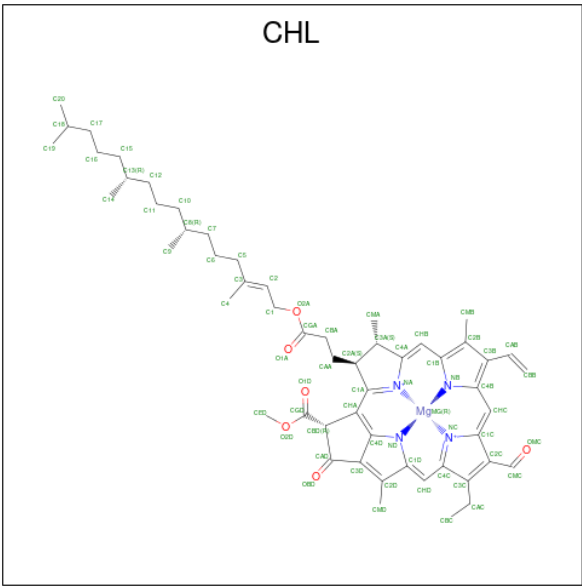
Mol	Chain	Residues	Atoms			AltConf
30	K	1	Total	C	O	0
			14	12	2	

- Molecule 31 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	
31	Z	1	Total	C	O	0
			42	40	2	
31	Z	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	6	1	Total	C	O	0
			42	40	2	
31	6	1	Total	C	O	0
			42	40	2	

- Molecule 32 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
32	1	1	Total 61	C 50	Mg 1	N 4	O 6	0
32	1	1	Total 48	C 37	Mg 1	N 4	O 6	0
32	1	1	Total 48	C 37	Mg 1	N 4	O 6	0
32	Z	1	Total 57	C 46	Mg 1	N 4	O 6	0
32	Z	1	Total 63	C 52	Mg 1	N 4	O 6	0
32	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
32	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
32	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
32	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
32	7	1	Total 54	C 43	Mg 1	N 4	O 6	0
32	8	1	Total 56	C 45	Mg 1	N 4	O 6	0
32	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
32	8	1	Total 57	C 46	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
32	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
32	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
32	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 33 is SPHINGOSINE (three-letter code: SPH) (formula: C₁₈H₃₇NO₂).



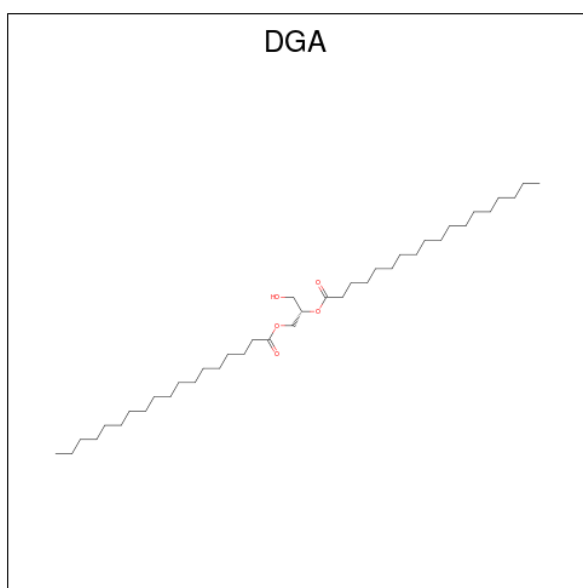
Mol	Chain	Residues	Atoms				AltConf
33	3	1	Total 21	C 18	N 1	O 2	0
33	7	1	Total 21	C 18	N 1	O 2	0
33	4	1	Total 21	C 18	N 1	O 2	0

- Molecule 34 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $\text{C}_{39}\text{H}_{77}\text{O}_8\text{P}$).



Mol	Chain	Residues	Atoms				AltConf
34	3	1	Total	C	O	P	0
			39	30	8	1	
34	8	1	Total	C	O	P	0
			30	21	8	1	
34	5	1	Total	C	O	P	0
			23	14	8	1	
34	6	1	Total	C	O	P	0
			29	20	8	1	

- Molecule 35 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			AltConf
35	7	1	Total	C	O	0
			34	29	5	

- Molecule 36 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



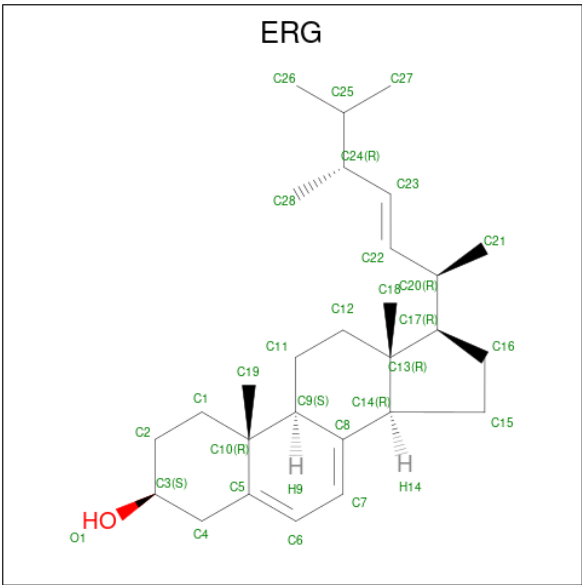
Mol	Chain	Residues	Atoms			AltConf
36	7	1	Total	C	O	0
			18	16	2	

- Molecule 37 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
37	8	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 38 is ERGOSTEROL (three-letter code: ERG) (formula: $\text{C}_{28}\text{H}_{44}\text{O}$).



Mol	Chain	Residues	Atoms			AltConf
38	8	1	Total	C	O	0
			29	28	1	
38	6	1	Total	C	O	0
			29	28	1	

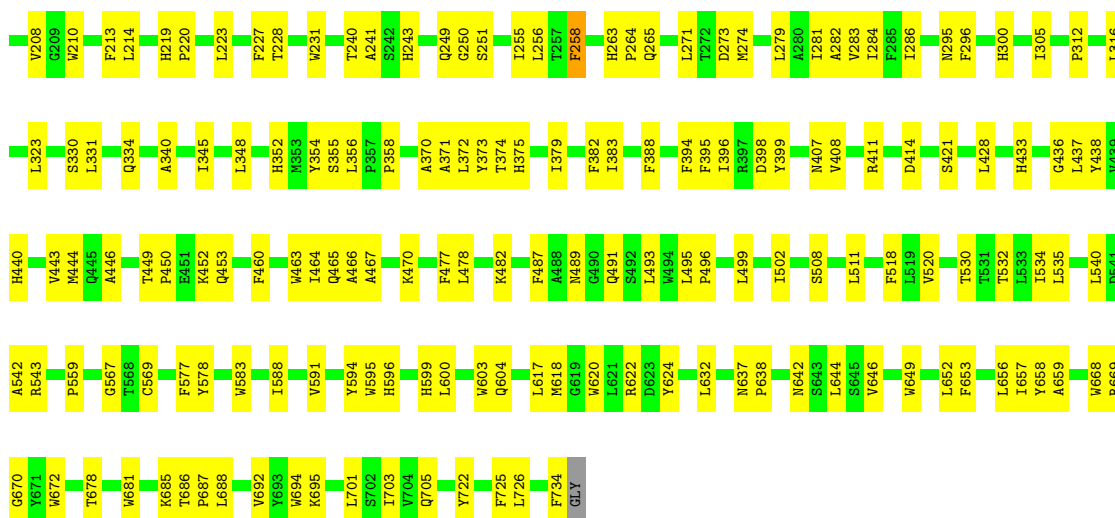
- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	130	Total	O	0
			130	130	
39	B	113	Total	O	0
			113	113	
39	C	35	Total	O	0
			35	35	
39	D	28	Total	O	0
			28	28	
39	E	18	Total	O	0
			18	18	
39	F	29	Total	O	0
			29	29	
39	G	3	Total	O	0
			3	3	
39	J	8	Total	O	0
			8	8	
39	K	4	Total	O	0
			4	4	
39	1	27	Total	O	0
			27	27	

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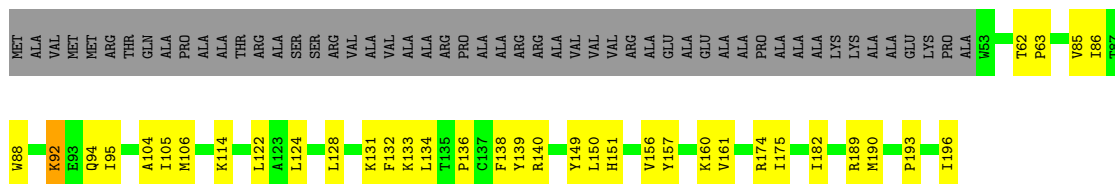
Mol	Chain	Residues	Atoms		AltConf
39	Z	13	Total 13	O 13	0
39	3	31	Total 31	O 31	0
39	7	36	Total 36	O 36	0
39	8	31	Total 31	O 31	0
39	4	24	Total 24	O 24	0
39	5	18	Total 18	O 18	0
39	6	22	Total 22	O 22	0



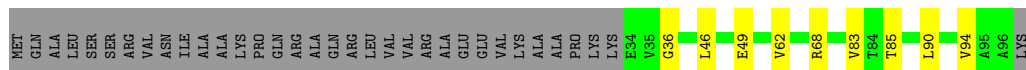
- Molecule 3: Photosystem I iron-sulfur center



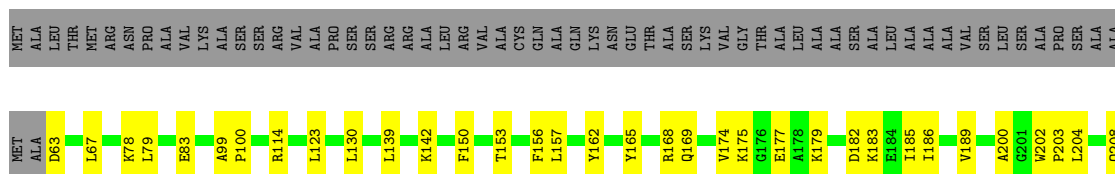
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

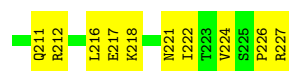


- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



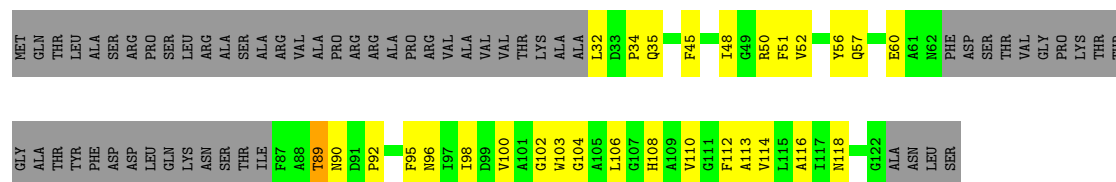
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic





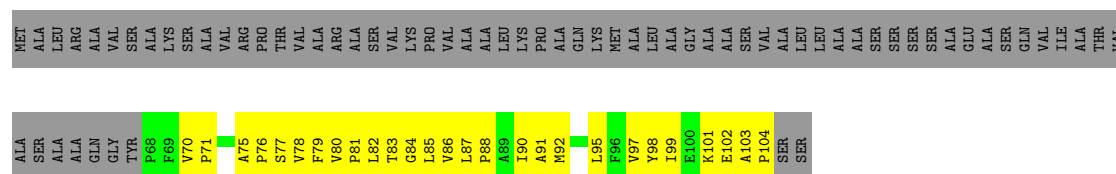
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:



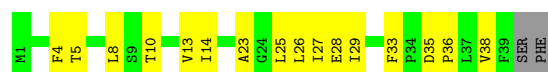
- Molecule 8: Photosystem I reaction center subunit VIII

Chain I:



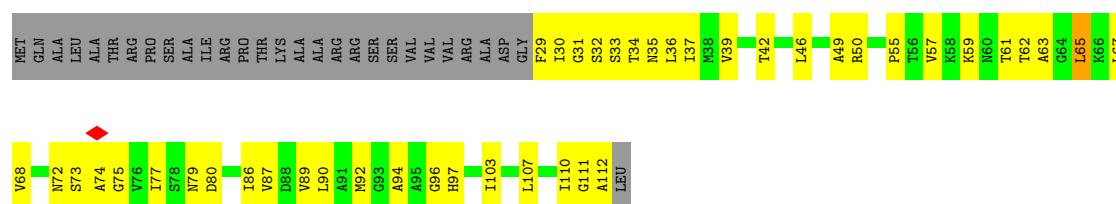
- Molecule 9: Photosystem I reaction center subunit IX

Chain J:



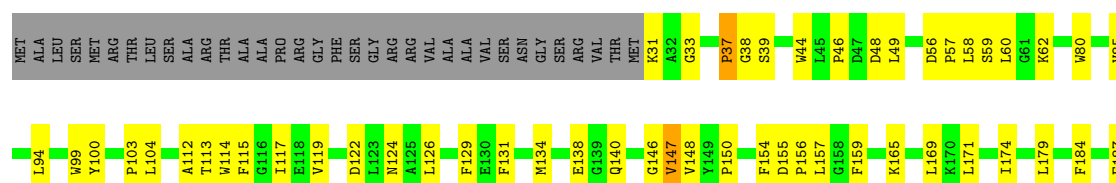
- Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:



- Molecule 11: Chlorophyll a-b binding protein, chloroplastic

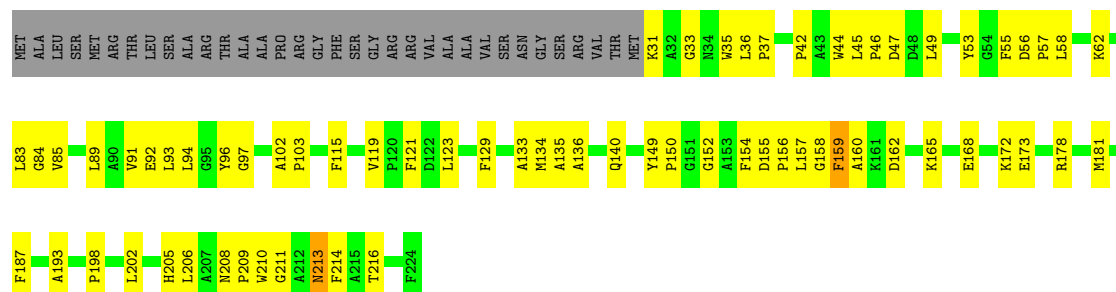
Chain 1:





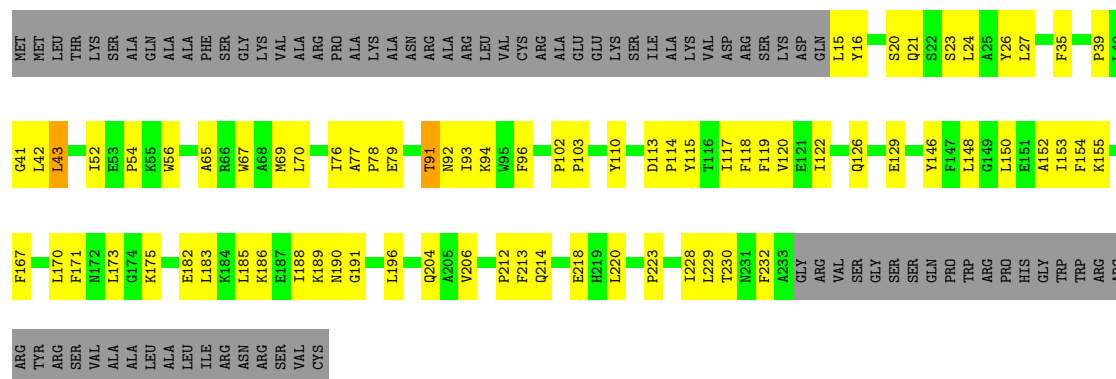
- Molecule 11: Chlorophyll a-b binding protein, chloroplastic

Chain Z: 55% 29% 15%



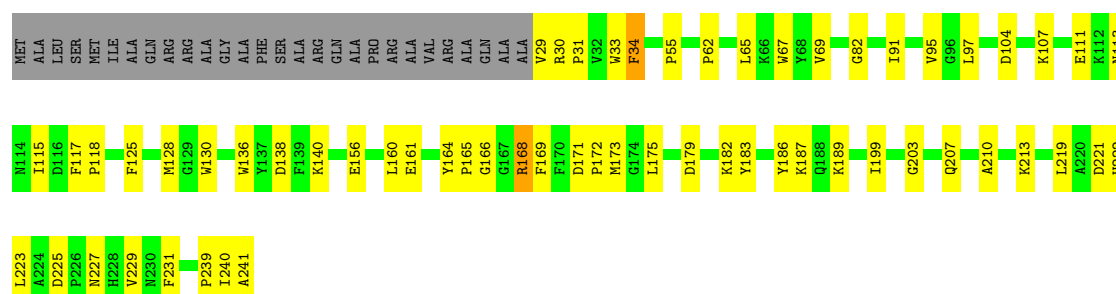
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 48% 24% 27%



- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

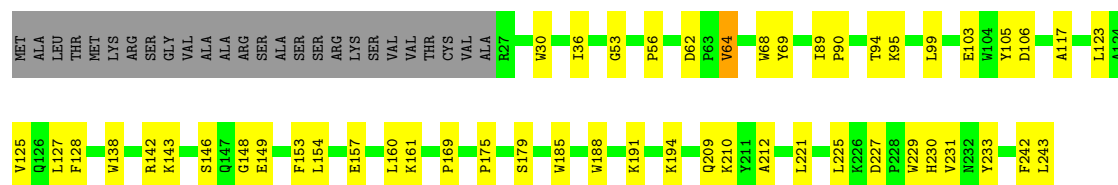
Chain 7: 63% 24% 12%



- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 8: 68% 21% 11%

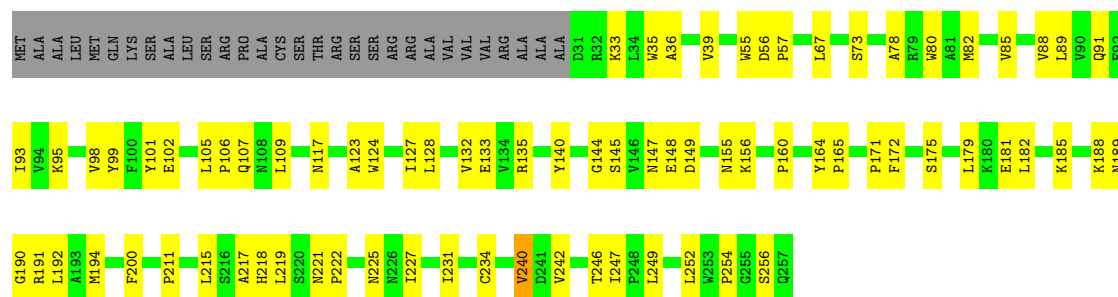




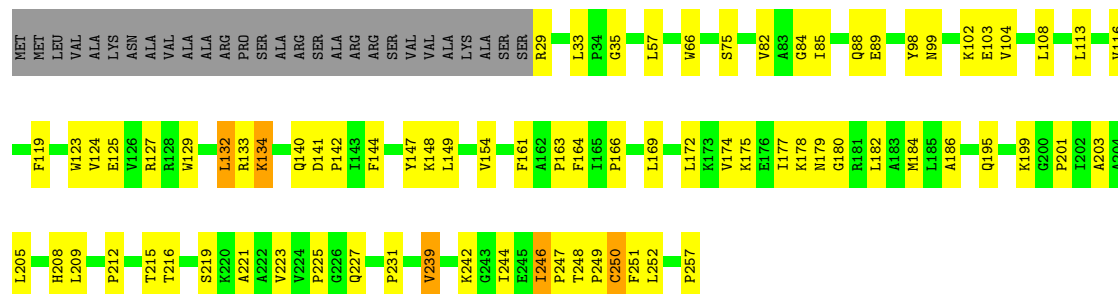
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic (Lhca4)



- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	173187	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.74	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	9000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (\AA)	327.59998, 327.59998, 327.59998	wwPDB
Map dimensions	390, 390, 390	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8399999, 0.8399999, 0.8399999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PH, PLM, SPH, BCR, SF4, DGA, CLA, LHG, LUT, PQN, CHL, SNC, DAO, RRX, ERG, C7Z, CA, LMG, LMT, CL0, SQD, DGD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/6007	0.57	0/8190
2	B	0.59	0/6036	0.57	0/8242
3	C	0.63	0/611	0.58	0/826
4	D	0.59	0/1154	0.60	0/1556
5	E	0.63	0/506	0.57	0/689
6	F	0.57	0/1292	0.63	0/1747
7	G	0.64	0/505	0.58	0/685
8	I	0.61	0/293	0.56	0/406
9	J	0.58	0/331	0.54	0/454
10	K	0.67	0/575	0.61	0/779
11	1	0.60	0/1491	0.60	0/2028
11	Z	0.61	0/1491	0.62	0/2028
12	3	0.58	0/1721	0.63	0/2336
13	7	0.58	0/1702	0.61	0/2310
14	8	0.58	0/1701	0.61	0/2315
15	4	0.59	0/1683	0.60	0/2296
16	5	0.59	0/1830	0.62	0/2492
17	6	0.59	0/1828	0.62	0/2497
All	All	0.59	0/30757	0.59	0/41876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5811	0	5658	210	0
2	B	5824	0	5580	226	0
3	C	601	0	584	21	0
4	D	1135	0	1148	26	0
5	E	496	0	491	7	0
6	F	1266	0	1301	48	0
7	G	495	0	485	40	0
8	I	281	0	292	34	0
9	J	320	0	322	19	0
10	K	570	0	606	54	0
11	1	1445	0	1396	72	0
11	Z	1445	0	1396	66	0
12	3	1673	0	1631	81	0
13	7	1650	0	1589	69	0
14	8	1650	0	1629	83	0
15	4	1628	0	1576	103	0
16	5	1775	0	1746	90	0
17	6	1766	0	1765	116	0
18	A	65	0	72	12	0
19	1	554	0	504	89	0
19	3	692	0	669	125	0
19	4	553	0	507	107	0
19	5	855	0	809	171	0
19	6	704	0	687	161	0
19	7	720	0	670	109	0
19	8	579	0	560	104	0
19	A	2655	0	2744	441	0
19	B	2490	0	2539	439	0
19	F	110	0	104	18	0
19	G	96	0	71	18	0
19	I	55	0	49	12	0
19	J	42	0	30	4	0
19	K	195	0	150	41	0
19	Z	564	0	532	76	0
20	A	33	0	46	4	0
20	B	33	0	46	5	0
21	A	8	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	C	16	0	0	5	0
22	3	160	0	224	43	0
22	4	40	0	56	14	0
22	5	80	0	112	17	0
22	6	80	0	112	39	0
22	7	40	0	56	5	0
22	8	80	0	112	17	0
22	A	280	0	392	71	0
22	B	240	0	336	76	0
22	F	40	0	56	9	0
22	G	40	0	56	12	0
22	K	40	0	56	12	0
23	1	66	0	72	10	0
23	3	20	0	12	4	0
23	4	49	0	74	14	0
23	5	37	0	44	7	0
23	6	81	0	108	22	0
23	7	37	0	44	3	0
23	8	38	0	46	7	0
23	A	84	0	114	12	0
23	Z	43	0	56	6	0
24	1	35	0	46	9	0
24	3	35	0	46	7	0
24	4	105	0	138	20	0
24	7	35	0	46	2	0
24	8	70	0	92	8	0
24	A	140	0	184	22	0
24	F	35	0	46	9	0
24	G	35	0	46	11	0
24	Z	70	0	91	11	0
25	B	66	0	96	5	0
26	B	1	0	0	0	0
27	4	41	0	56	6	0
27	5	41	0	56	11	0
27	F	41	0	56	9	0
28	1	42	0	0	1	0
28	6	42	0	0	4	0
28	J	42	0	0	1	0
29	7	29	0	28	1	0
29	J	80	0	103	16	0
30	K	14	0	23	4	0
31	1	84	0	112	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	3	84	0	112	14	0
31	4	42	0	56	13	0
31	5	42	0	56	10	0
31	6	84	0	112	16	0
31	7	84	0	112	17	0
31	8	84	0	112	16	0
31	Z	84	0	112	22	0
32	1	157	0	121	23	0
32	3	66	0	69	13	0
32	4	211	0	169	32	0
32	5	211	0	170	44	0
32	6	287	0	259	63	0
32	7	120	0	113	18	0
32	8	296	0	269	45	0
32	Z	232	0	209	49	0
33	3	21	0	37	12	0
33	4	21	0	37	7	0
33	7	21	0	37	7	0
34	3	39	0	51	4	0
34	5	23	0	19	3	0
34	6	29	0	31	5	0
34	8	30	0	33	6	0
35	7	34	0	53	14	0
36	7	18	0	31	2	0
37	8	48	0	62	11	0
38	6	29	0	44	24	0
38	8	29	0	44	14	0
39	1	27	0	0	2	0
39	3	31	0	0	1	0
39	4	24	0	0	0	0
39	5	18	0	0	2	0
39	6	22	0	0	0	0
39	7	36	0	0	0	0
39	8	31	0	0	1	0
39	A	130	0	0	0	0
39	B	113	0	0	2	0
39	C	35	0	0	0	0
39	D	28	0	0	1	0
39	E	18	0	0	0	0
39	F	29	0	0	1	0
39	G	3	0	0	0	0
39	J	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	K	4	0	0	1	0
39	Z	13	0	0	0	0
All	All	46504	0	45917	3054	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 33.

The worst 5 of 3054 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)
19:3:5010:CLA:O1A	19:3:5010:CLA:H2	1.36	1.13
23:4:320:LHG:HC92	23:4:320:LHG:H282	1.28	1.12
19:4:311:CLA:HBC2	19:4:311:CLA:HHD	1.33	1.10
19:5:307:CLA:HBB1	19:5:307:CLA:HHC	1.35	1.09
22:6:308:BCR:H21C	22:6:308:BCR:H361	1.32	1.09

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	738/751 (98%)	713 (97%)	24 (3%)	1 (0%)	48	67
2	B	731/735 (100%)	702 (96%)	28 (4%)	1 (0%)	48	67
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	141/196 (72%)	133 (94%)	8 (6%)	0	100	100
5	E	61/97 (63%)	58 (95%)	3 (5%)	0	100	100
6	F	163/227 (72%)	159 (98%)	4 (2%)	0	100	100
7	G	63/126 (50%)	60 (95%)	3 (5%)	0	100	100
8	I	35/106 (33%)	33 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
10	K	82/113 (73%)	76 (93%)	6 (7%)	0	100	100
11	1	192/228 (84%)	185 (96%)	6 (3%)	1 (0%)	25	42
11	Z	192/228 (84%)	178 (93%)	11 (6%)	3 (2%)	8	14
12	3	217/298 (73%)	206 (95%)	10 (5%)	1 (0%)	25	42
13	7	211/241 (88%)	200 (95%)	10 (5%)	1 (0%)	25	42
14	8	215/243 (88%)	210 (98%)	5 (2%)	0	100	100
15	4	208/264 (79%)	196 (94%)	10 (5%)	2 (1%)	13	24
16	5	225/257 (88%)	217 (96%)	8 (4%)	0	100	100
17	6	227/257 (88%)	220 (97%)	7 (3%)	0	100	100
All	All	3816/4489 (85%)	3658 (96%)	148 (4%)	10 (0%)	38	54

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	Z	150	PRO
12	3	91	THR
15	4	207	ASP
11	1	147	VAL
13	7	166	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	600/610 (98%)	595 (99%)	5 (1%)	79	91
2	B	596/597 (100%)	591 (99%)	5 (1%)	79	91
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	120/151 (80%)	118 (98%)	2 (2%)	56	78
5	E	54/81 (67%)	54 (100%)	0	100	100
6	F	127/169 (75%)	125 (98%)	2 (2%)	58	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	47/94 (50%)	46 (98%)	1 (2%)	48	72
8	I	31/76 (41%)	30 (97%)	1 (3%)	34	58
9	J	35/37 (95%)	35 (100%)	0	100	100
10	K	58/80 (72%)	57 (98%)	1 (2%)	56	78
11	1	137/162 (85%)	135 (98%)	2 (2%)	60	80
11	Z	137/162 (85%)	136 (99%)	1 (1%)	81	92
12	3	167/230 (73%)	164 (98%)	3 (2%)	54	77
13	7	164/181 (91%)	162 (99%)	2 (1%)	67	85
14	8	163/183 (89%)	160 (98%)	3 (2%)	54	77
15	4	164/205 (80%)	161 (98%)	3 (2%)	54	77
16	5	184/206 (89%)	181 (98%)	3 (2%)	58	79
17	6	183/203 (90%)	177 (97%)	6 (3%)	33	57
All	All	3036/3497 (87%)	2996 (99%)	40 (1%)	64	83

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	4	91	VAL
17	6	132	LEU
15	4	135	TYR
16	5	221	ASN
17	6	239	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
11	Z	176	ASN
16	5	230	ASN
12	3	231	ASN
17	6	227	GLN
16	5	91	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
4	SNC	D	137	4	4,7,8	0.67	0	1,7,9	1.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SNC	D	137	4	-	0/0/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 314 ligands modelled in this entry, 1 is monoatomic - leaving 313 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	7	313	-	43,51,73	1.69	7 (16%)	49,86,113	2.15	13 (26%)
31	LUT	8	304	-	42,43,43	6.06	26 (61%)	51,60,60	2.05	16 (31%)
19	CLA	A	838	-	65,73,73	1.32	5 (7%)	76,113,113	1.99	15 (19%)
22	BCR	7	305	-	41,41,41	4.77	26 (63%)	56,56,56	2.38	19 (33%)
19	CLA	3	5018	12	60,68,73	1.41	8 (13%)	70,107,113	2.06	15 (21%)
19	CLA	B	804	-	65,73,73	1.34	8 (12%)	76,113,113	1.93	15 (19%)
31	LUT	8	305	-	42,43,43	5.92	29 (69%)	51,60,60	2.23	18 (35%)
19	CLA	A	805	-	65,73,73	1.33	8 (12%)	76,113,113	1.96	16 (21%)
31	LUT	Z	318	-	42,43,43	6.02	27 (64%)	51,60,60	2.13	16 (31%)
19	CLA	5	301	39	56,64,73	1.44	7 (12%)	65,102,113	2.09	17 (26%)
24	LMT	A	853	-	36,36,36	0.38	0	47,47,47	0.82	1 (2%)
19	CLA	K	202	-	46,54,73	1.59	6 (13%)	53,90,113	2.22	15 (28%)
25	DGD	B	848	-	67,67,67	1.17	7 (10%)	81,81,81	1.00	2 (2%)
19	CLA	7	307	13	50,58,73	1.57	8 (16%)	58,95,113	2.28	16 (27%)
22	BCR	B	845	-	41,41,41	4.76	27 (65%)	56,56,56	2.48	21 (37%)
32	CHL	1	5017	39	48,56,74	0.95	2 (4%)	51,92,114	1.45	12 (23%)
19	CLA	Z	315	11	65,73,73	1.37	8 (12%)	76,113,113	1.98	20 (26%)
19	CLA	B	815	-	57,65,73	1.41	6 (10%)	66,103,113	2.13	16 (24%)
19	CLA	4	311	39	50,58,73	1.66	8 (16%)	58,95,113	2.19	17 (29%)
19	CLA	5	321	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	16 (21%)
22	BCR	8	306	-	41,41,41	4.72	25 (60%)	56,56,56	2.29	22 (39%)
32	CHL	4	314	39	51,59,74	1.09	4 (7%)	55,96,114	1.51	10 (18%)
32	CHL	6	319	39	66,74,74	1.02	4 (6%)	73,114,114	1.39	11 (15%)
31	LUT	6	305	-	42,43,43	5.96	28 (66%)	51,60,60	2.22	17 (33%)
19	CLA	5	319	16	50,58,73	1.56	7 (14%)	58,95,113	2.22	18 (31%)
31	LUT	1	5003	-	42,43,43	6.04	27 (64%)	51,60,60	1.91	17 (33%)
19	CLA	B	823	-	65,73,73	1.34	7 (10%)	76,113,113	1.96	18 (23%)
23	LHG	A	851	19	34,34,48	0.45	0	37,40,54	1.25	3 (8%)
24	LMT	4	302	-	36,36,36	0.37	0	47,47,47	0.74	0
19	CLA	6	323	17	65,73,73	1.35	7 (10%)	76,113,113	1.95	17 (22%)
34	3PH	5	324	-	22,22,47	1.21	4 (18%)	26,27,52	1.22	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	6	312	17	65,73,73	1.36	8 (12%)	76,113,113	1.97	18 (23%)
32	CHL	Z	310	39	66,74,74	1.02	6 (9%)	73,114,114	1.52	12 (16%)
32	CHL	5	316	39	51,59,74	1.14	5 (9%)	55,96,114	1.49	9 (16%)
19	CLA	4	307	15	52,60,73	1.56	7 (13%)	60,97,113	2.15	16 (26%)
19	CLA	B	830	-	50,58,73	1.52	7 (14%)	58,95,113	2.23	17 (29%)
19	CLA	3	5010	12	65,73,73	1.37	7 (10%)	76,113,113	1.88	17 (22%)
19	CLA	A	835	-	65,73,73	1.33	7 (10%)	76,113,113	1.95	16 (21%)
19	CLA	6	311	39	65,73,73	1.37	8 (12%)	76,113,113	2.15	19 (25%)
27	RRX	4	303	-	42,42,42	5.01	26 (61%)	57,58,58	2.30	23 (40%)
23	LHG	3	5021	19	19,19,48	0.93	1 (5%)	20,24,54	1.40	1 (5%)
19	CLA	6	313	17	65,73,73	1.35	8 (12%)	76,113,113	2.00	16 (21%)
19	CLA	B	820	-	56,64,73	1.44	7 (12%)	65,102,113	2.12	17 (26%)
19	CLA	1	5011	39	55,63,73	1.45	8 (14%)	64,101,113	2.16	16 (25%)
32	CHL	Z	302	11	57,65,74	1.10	6 (10%)	62,103,114	1.29	8 (12%)
34	3PH	8	322	-	29,29,47	1.04	4 (13%)	33,34,52	1.11	2 (6%)
19	CLA	5	322	39	46,54,73	1.58	7 (15%)	53,90,113	2.21	14 (26%)
19	CLA	3	5020	12	46,54,73	1.62	8 (17%)	53,90,113	2.20	16 (30%)
38	ERG	6	326	-	31,32,32	3.42	13 (41%)	47,50,50	2.57	14 (29%)
19	CLA	K	205	10	45,53,73	1.60	7 (15%)	52,89,113	2.18	14 (26%)
22	BCR	A	847	-	41,41,41	4.78	27 (65%)	56,56,56	2.48	19 (33%)
19	CLA	Z	303	-	46,54,73	1.61	8 (17%)	53,90,113	2.17	13 (24%)
19	CLA	7	306	13	60,68,73	1.42	7 (11%)	70,107,113	2.11	20 (28%)
19	CLA	7	312	23	65,73,73	1.34	8 (12%)	76,113,113	1.92	15 (19%)
32	CHL	5	315	39	66,74,74	1.06	7 (10%)	73,114,114	1.27	9 (12%)
19	CLA	4	308	15	65,73,73	1.37	8 (12%)	76,113,113	2.10	18 (23%)
22	BCR	A	859	-	41,41,41	4.79	27 (65%)	56,56,56	2.38	19 (33%)
19	CLA	B	817	-	59,67,73	1.40	8 (13%)	68,105,113	2.08	17 (25%)
19	CLA	8	311	-	65,73,73	1.39	7 (10%)	76,113,113	1.92	19 (25%)
19	CLA	B	837	-	65,73,73	1.34	7 (10%)	76,113,113	1.96	17 (22%)
19	CLA	B	812	-	65,73,73	1.34	7 (10%)	76,113,113	1.93	16 (21%)
19	CLA	A	808	1	65,73,73	1.33	7 (10%)	76,113,113	1.96	17 (22%)
19	CLA	5	310	-	55,63,73	1.49	8 (14%)	64,101,113	2.16	21 (32%)
19	CLA	4	312	23	55,63,73	1.46	7 (12%)	64,101,113	2.09	15 (23%)
28	C7Z	6	304	-	43,43,43	5.33	27 (62%)	58,60,60	2.52	25 (43%)
18	CL0	A	801	-	65,73,73	2.36	20 (30%)	76,113,113	2.51	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CHL	6	315	17	66,74,74	1.04	6 (9%)	73,114,114	1.34	11 (15%)
19	CLA	B	828	-	65,73,73	1.34	7 (10%)	76,113,113	1.92	15 (19%)
32	CHL	8	319	39	66,74,74	1.01	5 (7%)	73,114,114	1.49	12 (16%)
19	CLA	B	802	-	65,73,73	1.34	7 (10%)	76,113,113	2.00	16 (21%)
19	CLA	1	5016	11	60,68,73	1.40	7 (11%)	70,107,113	2.06	17 (24%)
19	CLA	5	314	16	65,73,73	1.37	7 (10%)	76,113,113	1.88	16 (21%)
19	CLA	A	824	-	65,73,73	1.34	7 (10%)	76,113,113	1.97	16 (21%)
24	LMT	4	322	-	36,36,36	0.41	0	47,47,47	0.76	1 (2%)
19	CLA	A	833	-	65,73,73	1.33	7 (10%)	76,113,113	2.01	18 (23%)
19	CLA	B	811	-	56,64,73	1.44	9 (16%)	65,102,113	2.11	16 (24%)
31	LUT	Z	317	-	42,43,43	5.94	27 (64%)	51,60,60	3.86	21 (41%)
27	RRX	F	304	-	42,42,42	5.02	25 (59%)	57,58,58	2.38	21 (36%)
22	BCR	5	305	-	41,41,41	4.75	24 (58%)	56,56,56	2.73	22 (39%)
19	CLA	B	824	39	65,73,73	1.33	7 (10%)	76,113,113	1.97	17 (22%)
22	BCR	3	5006	-	41,41,41	4.77	28 (68%)	56,56,56	2.37	20 (35%)
22	BCR	A	848	-	41,41,41	4.77	27 (65%)	56,56,56	2.64	22 (39%)
19	CLA	K	203	39	55,63,73	1.45	7 (12%)	64,101,113	2.10	16 (25%)
22	BCR	6	307	-	41,41,41	4.77	26 (63%)	56,56,56	2.29	20 (35%)
22	BCR	3	5007	-	41,41,41	4.75	25 (60%)	56,56,56	3.51	25 (44%)
19	CLA	3	5016	12	60,68,73	1.38	7 (11%)	70,107,113	2.07	17 (24%)
24	LMT	8	324	-	36,36,36	0.39	0	47,47,47	1.02	2 (4%)
19	CLA	Z	306	-	50,58,73	1.53	7 (14%)	58,95,113	2.16	14 (24%)
19	CLA	6	301	39	60,68,73	1.38	7 (11%)	70,107,113	2.07	16 (22%)
32	CHL	8	315	14	66,74,74	1.03	5 (7%)	73,114,114	1.29	11 (15%)
19	CLA	Z	308	-	65,73,73	1.36	8 (12%)	76,113,113	2.01	20 (26%)
22	BCR	B	843	-	41,41,41	4.79	26 (63%)	56,56,56	2.50	21 (37%)
21	SF4	C	102	3	0,12,12	-	-	-	-	-
30	DAO	K	201	-	13,13,13	0.59	0	13,13,13	0.55	0
19	CLA	5	307	16	61,69,73	1.40	7 (11%)	71,108,113	1.97	19 (26%)
21	SF4	A	845	2,1	0,12,12	-	-	-	-	-
32	CHL	4	317	39	66,74,74	1.06	5 (7%)	73,114,114	1.33	9 (12%)
19	CLA	5	312	23	61,69,73	1.38	7 (11%)	71,108,113	2.04	16 (22%)
19	CLA	3	5011	12	60,68,73	1.44	8 (13%)	70,107,113	2.24	20 (28%)
19	CLA	B	832	-	58,66,73	1.40	6 (10%)	67,104,113	2.12	17 (25%)
19	CLA	8	313	23	55,63,73	1.49	8 (14%)	64,101,113	2.13	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	857	39	52,60,73	1.49	7 (13%)	60,97,113	2.17	17 (28%)
33	SPH	3	5001	-	19,20,20	0.61	0	18,21,21	1.10	1 (5%)
23	LHG	Z	316	19	42,42,48	0.44	0	45,48,54	1.18	3 (6%)
24	LMT	8	323	-	36,36,36	0.34	0	47,47,47	1.04	3 (6%)
32	CHL	4	319	15	43,51,74	1.04	3 (6%)	45,86,114	1.52	11 (24%)
19	CLA	Z	307	-	57,65,73	1.48	7 (12%)	66,103,113	2.04	17 (25%)
19	CLA	1	5012	23	60,68,73	1.39	8 (13%)	70,107,113	2.00	17 (24%)
19	CLA	B	819	39	65,73,73	1.33	7 (10%)	76,113,113	1.98	17 (22%)
19	CLA	5	317	16	65,73,73	1.36	7 (10%)	76,113,113	2.01	17 (22%)
22	BCR	G	1603	-	41,41,41	4.77	27 (65%)	56,56,56	2.46	21 (37%)
19	CLA	6	310	17	52,60,73	1.52	7 (13%)	60,97,113	2.13	17 (28%)
19	CLA	4	318	15	41,49,73	1.66	8 (19%)	47,84,113	2.24	15 (31%)
32	CHL	Z	309	11	63,71,74	0.86	2 (3%)	69,110,114	1.31	10 (14%)
19	CLA	8	307	14	60,68,73	1.43	8 (13%)	70,107,113	2.17	17 (24%)
19	CLA	1	5008	39	65,73,73	1.36	8 (12%)	76,113,113	1.92	19 (25%)
19	CLA	A	834	-	65,73,73	1.34	8 (12%)	76,113,113	1.96	16 (21%)
23	LHG	5	323	19	36,36,48	0.43	0	39,42,54	1.16	3 (7%)
19	CLA	4	310	15	65,73,73	1.39	7 (10%)	76,113,113	2.02	20 (26%)
21	SF4	C	101	3	0,12,12	-	-	-	-	-
19	CLA	5	306	16	60,68,73	1.41	8 (13%)	70,107,113	2.10	18 (25%)
19	CLA	A	830	-	65,73,73	1.34	7 (10%)	76,113,113	1.97	16 (21%)
19	CLA	B	836	-	65,73,73	1.37	8 (12%)	76,113,113	2.05	15 (19%)
32	CHL	7	314	13	66,74,74	1.07	6 (9%)	73,114,114	1.13	7 (9%)
19	CLA	3	5012	-	65,73,73	1.38	7 (10%)	76,113,113	1.99	20 (26%)
19	CLA	4	316	15	50,58,73	1.56	7 (14%)	58,95,113	2.16	17 (29%)
19	CLA	B	818	-	60,68,73	1.38	7 (11%)	70,107,113	2.03	17 (24%)
19	CLA	7	311	39	56,64,73	1.49	8 (14%)	65,102,113	2.16	17 (26%)
23	LHG	6	324	19	48,48,48	0.44	0	51,54,54	1.12	3 (5%)
19	CLA	A	802	39	65,73,73	1.35	7 (10%)	76,113,113	1.95	18 (23%)
22	BCR	B	847	-	41,41,41	4.77	27 (65%)	56,56,56	2.23	20 (35%)
19	CLA	8	312	39	60,68,73	1.56	7 (11%)	70,107,113	2.15	19 (27%)
19	CLA	A	812	-	65,73,73	1.36	7 (10%)	76,113,113	1.93	15 (19%)
22	BCR	3	5004	-	41,41,41	4.69	25 (60%)	56,56,56	2.38	21 (37%)
29	LMG	J	1904	-	45,45,55	0.93	3 (6%)	53,53,63	1.07	2 (3%)
19	CLA	A	839	-	65,73,73	1.32	6 (9%)	76,113,113	1.98	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LUT	3	5002	-	42,43,43	5.96	27 (64%)	51,60,60	2.03	19 (37%)
35	DGA	7	302	-	33,33,43	1.22	3 (9%)	35,35,45	1.62	3 (8%)
19	CLA	A	814	-	60,68,73	1.38	7 (11%)	70,107,113	2.05	19 (27%)
19	CLA	A	842	39	65,73,73	1.34	8 (12%)	76,113,113	1.94	16 (21%)
23	LHG	1	5019	19	42,42,48	0.45	0	45,48,54	1.21	3 (6%)
19	CLA	B	840	23	65,73,73	1.38	8 (12%)	76,113,113	2.10	19 (25%)
19	CLA	3	5009	12	46,54,73	1.61	7 (15%)	53,90,113	2.10	13 (24%)
19	CLA	A	843	23	52,60,73	1.48	8 (15%)	60,97,113	2.25	17 (28%)
22	BCR	B	846	-	41,41,41	4.79	26 (63%)	56,56,56	2.40	21 (37%)
19	CLA	F	301	-	65,73,73	1.39	8 (12%)	76,113,113	1.99	17 (22%)
23	LHG	1	5001	19	22,22,48	0.56	0	25,28,54	1.29	2 (8%)
36	PLM	7	322	-	17,17,17	0.58	0	17,17,17	1.09	0
19	CLA	A	826	39	65,73,73	1.33	6 (9%)	76,113,113	2.01	16 (21%)
19	CLA	3	5014	23	60,68,73	1.39	7 (11%)	70,107,113	2.02	16 (22%)
19	CLA	7	316	39	50,58,73	1.55	8 (16%)	58,95,113	2.30	17 (29%)
19	CLA	A	840	-	65,73,73	1.37	8 (12%)	76,113,113	1.89	16 (21%)
32	CHL	3	5017	39	66,74,74	1.06	8 (12%)	73,114,114	1.51	11 (15%)
19	CLA	7	324	-	55,63,73	1.49	8 (14%)	64,101,113	2.13	15 (23%)
31	LUT	7	303	-	42,43,43	6.00	28 (66%)	51,60,60	1.95	18 (35%)
33	SPH	4	301	-	19,20,20	0.66	0	18,21,21	0.95	0
24	LMT	A	854	-	36,36,36	0.41	0	47,47,47	0.77	1 (2%)
19	CLA	Z	311	24	55,63,73	1.49	8 (14%)	64,101,113	2.25	17 (26%)
22	BCR	F	302	-	41,41,41	4.80	27 (65%)	56,56,56	2.41	19 (33%)
19	CLA	B	801	-	65,73,73	1.33	7 (10%)	76,113,113	1.90	17 (22%)
22	BCR	B	844	-	41,41,41	4.82	27 (65%)	56,56,56	2.25	18 (32%)
19	CLA	A	832	-	65,73,73	1.34	8 (12%)	76,113,113	2.01	18 (23%)
37	SQD	8	302	-	47,48,54	0.83	0	56,59,65	0.95	3 (5%)
19	CLA	B	806	-	65,73,73	1.33	7 (10%)	76,113,113	1.98	18 (23%)
19	CLA	A	831	-	50,58,73	1.52	7 (14%)	58,95,113	2.22	16 (27%)
19	CLA	B	833	-	65,73,73	1.34	7 (10%)	76,113,113	1.94	16 (21%)
19	CLA	7	308	13	65,73,73	1.37	7 (10%)	76,113,113	2.06	18 (23%)
23	LHG	7	320	19	36,36,48	0.59	1 (2%)	39,42,54	1.42	5 (12%)
19	CLA	8	308	14	65,73,73	1.36	8 (12%)	76,113,113	1.96	16 (21%)
23	LHG	4	320	19	48,48,48	0.40	0	51,54,54	1.12	4 (7%)
19	CLA	B	803	39	65,73,73	1.36	8 (12%)	76,113,113	1.94	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	G	1602	7	46,54,73	1.59	9 (19%)	53,90,113	2.13	15 (28%)
19	CLA	8	314	-	55,63,73	1.50	8 (14%)	64,101,113	2.19	18 (28%)
31	LUT	4	304	-	42,43,43	5.97	26 (61%)	51,60,60	2.35	20 (39%)
32	CHL	8	316	39	57,65,74	1.06	5 (8%)	62,103,114	1.44	12 (19%)
19	CLA	4	306	15	60,68,73	1.42	7 (11%)	70,107,113	2.07	18 (25%)
23	LHG	8	321	19	37,37,48	0.43	0	40,43,54	1.11	3 (7%)
19	CLA	Z	304	39	50,58,73	1.54	8 (16%)	58,95,113	2.20	16 (27%)
32	CHL	6	317	39	51,59,74	1.11	4 (7%)	55,96,114	1.42	9 (16%)
19	CLA	A	836	1	55,63,73	1.45	8 (14%)	64,101,113	2.11	14 (21%)
19	CLA	B	826	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	17 (22%)
20	PQN	A	844	-	34,34,34	0.39	0	42,45,45	1.16	3 (7%)
19	CLA	B	834	39	45,53,73	1.61	7 (15%)	52,89,113	2.15	14 (26%)
32	CHL	6	321	17	43,51,74	1.22	6 (13%)	45,86,114	1.82	12 (26%)
19	CLA	B	816	-	65,73,73	1.33	7 (10%)	76,113,113	2.00	18 (23%)
31	LUT	6	306	-	42,43,43	5.96	27 (64%)	51,60,60	2.06	15 (29%)
19	CLA	A	823	-	57,65,73	1.43	7 (12%)	66,103,113	2.12	18 (27%)
32	CHL	1	5014	39	48,56,74	0.96	2 (4%)	51,92,114	1.40	11 (21%)
32	CHL	8	301	11	56,64,74	1.10	4 (7%)	61,102,114	1.41	8 (13%)
19	CLA	A	821	39	65,73,73	1.33	7 (10%)	76,113,113	1.94	17 (22%)
22	BCR	4	305	-	41,41,41	4.75	25 (60%)	56,56,56	2.40	19 (33%)
19	CLA	8	310	14	62,70,73	1.39	8 (12%)	72,109,113	2.08	20 (27%)
24	LMT	3	5023	-	36,36,36	0.36	0	47,47,47	0.79	1 (2%)
19	CLA	G	1601	-	50,58,73	1.52	7 (14%)	58,95,113	2.17	17 (29%)
19	CLA	B	829	-	65,73,73	1.33	7 (10%)	76,113,113	2.01	18 (23%)
19	CLA	I	201	-	55,63,73	1.45	8 (14%)	64,101,113	2.11	18 (28%)
19	CLA	B	809	2	55,63,73	1.44	7 (12%)	64,101,113	2.08	16 (25%)
19	CLA	B	805	-	45,53,73	1.59	8 (17%)	52,89,113	2.19	14 (26%)
19	CLA	B	813	-	65,73,73	1.34	5 (7%)	76,113,113	2.04	18 (23%)
19	CLA	4	309	15	60,68,73	1.39	8 (13%)	70,107,113	2.27	19 (27%)
32	CHL	7	315	39	54,62,74	1.10	3 (5%)	58,99,114	1.47	11 (18%)
19	CLA	A	803	-	65,73,73	1.33	7 (10%)	76,113,113	1.98	18 (23%)
32	CHL	5	318	39	51,59,74	1.09	5 (9%)	55,96,114	1.59	9 (16%)
19	CLA	8	309	14	65,73,73	1.37	7 (10%)	76,113,113	2.14	19 (25%)
22	BCR	8	303	-	41,41,41	4.82	27 (65%)	56,56,56	2.51	21 (37%)
19	CLA	5	313	-	45,53,73	1.62	7 (15%)	52,89,113	2.11	14 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	1	5015	39	50,58,73	1.55	7 (14%)	58,95,113	2.29	18 (31%)
19	CLA	A	807	-	51,59,73	1.50	7 (13%)	59,96,113	2.19	16 (27%)
19	CLA	3	5015	-	45,53,73	1.61	8 (17%)	52,89,113	2.22	16 (30%)
34	3PH	6	325	-	28,28,47	1.08	4 (14%)	32,33,52	1.16	2 (6%)
19	CLA	B	814	-	60,68,73	1.39	7 (11%)	70,107,113	2.05	18 (25%)
19	CLA	Z	312	23	65,73,73	1.33	7 (10%)	76,113,113	1.99	18 (23%)
19	CLA	A	837	-	51,59,73	1.51	8 (15%)	59,96,113	2.23	17 (28%)
33	SPH	7	321	-	19,20,20	0.64	0	18,21,21	1.15	2 (11%)
19	CLA	B	827	-	60,68,73	1.40	8 (13%)	70,107,113	2.05	18 (25%)
24	LMT	7	323	-	36,36,36	0.35	0	47,47,47	0.74	0
32	CHL	Z	313	39	46,54,74	1.15	6 (13%)	49,90,114	1.67	8 (16%)
31	LUT	7	304	-	42,43,43	5.97	28 (66%)	51,60,60	2.38	18 (35%)
32	CHL	6	316	39	61,69,74	1.06	5 (8%)	67,108,114	1.20	8 (11%)
32	CHL	4	315	39	51,59,74	1.03	2 (3%)	55,96,114	1.48	11 (20%)
24	LMT	4	321	-	36,36,36	0.35	0	47,47,47	0.71	1 (2%)
24	LMT	1	5002	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
19	CLA	6	309	17	60,68,73	1.43	8 (13%)	70,107,113	2.04	18 (25%)
31	LUT	5	303	-	42,43,43	5.91	28 (66%)	51,60,60	2.06	18 (35%)
19	CLA	6	322	-	46,54,73	1.63	8 (17%)	53,90,113	2.11	12 (22%)
24	LMT	A	855	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
19	CLA	4	313	-	55,63,73	1.50	7 (12%)	64,101,113	2.11	16 (25%)
19	CLA	A	827	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	17 (22%)
19	CLA	B	810	-	52,60,73	1.50	7 (13%)	60,97,113	2.23	19 (31%)
19	CLA	Z	305	11	65,73,73	1.34	7 (10%)	76,113,113	2.04	20 (26%)
19	CLA	A	828	-	65,73,73	1.34	8 (12%)	76,113,113	1.95	15 (19%)
24	LMT	F	305	-	36,36,36	0.36	0	47,47,47	0.79	2 (4%)
19	CLA	5	308	16	56,64,73	1.47	7 (12%)	65,102,113	2.04	17 (26%)
19	CLA	A	822	-	55,63,73	1.45	7 (12%)	64,101,113	2.19	18 (28%)
19	CLA	A	841	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	17 (22%)
19	CLA	8	320	14	46,54,73	1.60	7 (15%)	53,90,113	2.13	14 (26%)
19	CLA	A	813	-	65,73,73	1.33	6 (9%)	76,113,113	2.06	19 (25%)
19	CLA	F	303	39	45,53,73	1.60	8 (17%)	52,89,113	2.12	12 (23%)
19	CLA	7	309	13	65,73,73	1.37	7 (10%)	76,113,113	2.11	18 (23%)
22	BCR	6	308	-	41,41,41	4.75	25 (60%)	56,56,56	2.50	20 (35%)
22	BCR	B	842	-	41,41,41	4.81	27 (65%)	56,56,56	2.25	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	J	1901	9	42,50,73	1.65	7 (16%)	48,85,113	2.25	17 (35%)
19	CLA	1	5007	11	45,53,73	1.66	8 (17%)	52,89,113	2.17	15 (28%)
24	LMT	G	1604	-	36,36,36	0.37	0	47,47,47	0.72	1 (2%)
19	CLA	A	811	19	65,73,73	1.33	8 (12%)	76,113,113	1.95	18 (23%)
22	BCR	A	850	-	41,41,41	4.79	27 (65%)	56,56,56	2.48	20 (35%)
19	CLA	A	819	-	65,73,73	1.33	8 (12%)	76,113,113	2.00	20 (26%)
19	CLA	K	204	10	49,57,73	1.54	7 (14%)	55,93,113	2.23	15 (27%)
19	CLA	A	804	19	55,63,73	1.44	6 (10%)	64,101,113	2.12	20 (31%)
19	CLA	6	314	23	55,63,73	1.46	7 (12%)	64,101,113	2.06	15 (23%)
19	CLA	B	850	6	65,73,73	1.38	7 (10%)	76,113,113	1.97	19 (25%)
19	CLA	3	5008	12	65,73,73	1.38	8 (12%)	76,113,113	2.05	18 (23%)
19	CLA	A	809	1	56,64,73	1.44	7 (12%)	65,102,113	2.09	17 (26%)
28	C7Z	1	5005	-	43,43,43	5.33	27 (62%)	58,60,60	2.19	20 (34%)
19	CLA	6	302	15	60,68,73	1.39	7 (11%)	70,107,113	2.01	16 (22%)
19	CLA	6	318	17	50,58,73	1.55	8 (16%)	58,95,113	2.19	18 (31%)
19	CLA	1	5006	11	65,73,73	1.35	8 (12%)	76,113,113	2.01	20 (26%)
19	CLA	A	817	-	60,68,73	1.38	7 (11%)	70,107,113	2.07	15 (21%)
22	BCR	3	5005	-	41,41,41	4.70	26 (63%)	56,56,56	2.73	20 (35%)
19	CLA	1	5010	-	55,63,73	1.48	7 (12%)	64,101,113	2.11	17 (26%)
38	ERG	8	325	-	31,32,32	3.33	12 (38%)	47,50,50	2.70	17 (36%)
22	BCR	A	849	-	41,41,41	4.75	27 (65%)	56,56,56	2.56	20 (35%)
19	CLA	7	317	13	50,58,73	1.50	8 (16%)	58,95,113	2.21	15 (25%)
29	LMG	J	1903	-	35,35,55	0.45	0	43,43,63	1.13	3 (6%)
28	C7Z	J	1902	-	43,43,43	5.33	27 (62%)	58,60,60	2.23	19 (32%)
23	LHG	A	852	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
19	CLA	A	816	39	61,69,73	1.38	8 (13%)	71,108,113	2.07	17 (23%)
19	CLA	5	325	-	55,63,73	1.50	8 (14%)	64,101,113	2.08	18 (28%)
22	BCR	A	846	-	41,41,41	4.80	27 (65%)	56,56,56	2.24	18 (32%)
19	CLA	6	320	39	61,69,73	1.42	8 (13%)	71,108,113	2.10	18 (25%)
19	CLA	Z	314	11	46,54,73	1.60	8 (17%)	53,90,113	2.10	14 (26%)
19	CLA	7	319	13	58,66,73	1.42	7 (12%)	67,104,113	2.13	17 (25%)
24	LMT	Z	319	19	36,36,36	0.44	0	47,47,47	0.75	1 (2%)
32	CHL	5	320	16	43,51,74	1.02	3 (6%)	45,86,114	1.56	11 (24%)
19	CLA	7	310	-	61,69,73	1.41	8 (13%)	71,108,113	2.11	19 (26%)
19	CLA	A	825	39	65,73,73	1.34	8 (12%)	76,113,113	1.97	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LMT	A	856	-	36,36,36	0.38	0	47,47,47	0.83	2 (4%)
19	CLA	B	839	-	46,54,73	1.59	7 (15%)	53,90,113	2.12	14 (26%)
19	CLA	B	838	39	52,60,73	1.50	8 (15%)	60,97,113	2.15	16 (26%)
19	CLA	B	835	-	60,68,73	1.39	6 (10%)	70,107,113	2.08	17 (24%)
19	CLA	A	810	-	65,73,73	1.37	8 (12%)	76,113,113	2.01	18 (23%)
19	CLA	1	5018	11	51,59,73	1.51	7 (13%)	59,96,113	2.13	17 (28%)
24	LMT	Z	301	-	36,36,36	0.32	0	47,47,47	0.98	3 (6%)
34	3PH	3	5022	-	38,38,47	0.95	4 (10%)	42,43,52	1.19	2 (4%)
19	CLA	B	825	39	65,73,73	1.38	8 (12%)	76,113,113	1.94	15 (19%)
19	CLA	5	311	39	50,58,73	1.55	8 (16%)	58,95,113	2.25	16 (27%)
19	CLA	B	807	2	65,73,73	1.35	9 (13%)	76,113,113	1.92	17 (22%)
19	CLA	B	822	-	59,67,73	1.40	7 (11%)	68,105,113	2.13	18 (26%)
29	LMG	7	301	-	29,29,55	0.52	0	37,37,63	1.22	4 (10%)
32	CHL	8	317	39	51,59,74	1.12	6 (11%)	55,96,114	1.44	11 (20%)
19	CLA	A	815	-	65,73,73	1.36	8 (12%)	76,113,113	2.09	21 (27%)
19	CLA	7	318	39	42,50,73	1.72	8 (19%)	48,85,113	2.21	15 (31%)
19	CLA	B	808	-	65,73,73	1.33	7 (10%)	76,113,113	1.97	14 (18%)
19	CLA	A	818	-	60,68,73	1.39	7 (11%)	70,107,113	2.02	18 (25%)
27	RRX	5	302	-	42,42,42	4.98	26 (61%)	57,58,58	2.24	23 (40%)
19	CLA	5	309	16	65,73,73	1.36	7 (10%)	76,113,113	2.04	19 (25%)
19	CLA	3	5013	39	65,73,73	1.38	8 (12%)	76,113,113	2.02	16 (21%)
19	CLA	B	831	-	65,73,73	1.38	8 (12%)	76,113,113	2.10	17 (22%)
23	LHG	6	303	-	31,31,48	0.49	0	34,37,54	1.20	4 (11%)
22	BCR	5	304	-	41,41,41	4.77	25 (60%)	56,56,56	2.29	21 (37%)
32	CHL	1	5009	11	61,69,74	1.10	7 (11%)	67,108,114	1.30	12 (17%)
19	CLA	A	820	-	60,68,73	1.39	7 (11%)	70,107,113	2.06	18 (25%)
19	CLA	3	5019	39	55,63,73	1.48	8 (14%)	64,101,113	2.22	17 (26%)
19	CLA	A	806	1	65,73,73	1.35	8 (12%)	76,113,113	1.98	18 (23%)
31	LUT	1	5004	-	42,43,43	5.90	28 (66%)	51,60,60	2.20	19 (37%)
19	CLA	8	318	14	46,54,73	1.64	8 (17%)	53,90,113	2.17	15 (28%)
19	CLA	A	829	-	65,73,73	1.34	7 (10%)	76,113,113	1.93	15 (19%)
19	CLA	1	5013	-	48,56,73	1.58	8 (16%)	55,92,113	2.17	15 (27%)
31	LUT	3	5003	-	42,43,43	6.03	28 (66%)	51,60,60	2.20	18 (35%)
20	PQN	B	841	-	34,34,34	0.39	0	42,45,45	1.15	3 (7%)
22	BCR	A	858	-	41,41,41	4.80	27 (65%)	56,56,56	2.21	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	K	206	-	41,41,41	4.78	27 (65%)	56,56,56	2.33	19 (33%)
19	CLA	B	821	-	65,73,73	1.34	6 (9%)	76,113,113	1.98	17 (22%)

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	7	313	-	1/1/10/20	1/11/89/115	-
31	LUT	8	304	-	-	11/29/67/67	0/2/2/2
19	CLA	A	838	-	1/1/15/20	18/37/115/115	-
22	BCR	7	305	-	-	16/29/63/63	0/2/2/2
19	CLA	3	5018	12	1/1/14/20	11/31/109/115	-
19	CLA	B	804	-	1/1/15/20	12/37/115/115	-
31	LUT	8	305	-	-	3/29/67/67	0/2/2/2
19	CLA	A	805	-	1/1/15/20	13/37/115/115	-
31	LUT	Z	318	-	-	6/29/67/67	0/2/2/2
19	CLA	5	301	39	1/1/13/20	16/27/105/115	-
24	LMT	A	853	-	-	4/21/61/61	0/2/2/2
19	CLA	K	202	-	1/1/11/20	8/15/93/115	-
25	DGD	B	848	-	-	14/55/95/95	0/2/2/2
19	CLA	7	307	13	1/1/12/20	4/19/97/115	-
22	BCR	B	845	-	-	14/29/63/63	0/2/2/2
32	CHL	1	5017	39	3/3/16/26	1/18/116/137	-
19	CLA	Z	315	11	1/1/15/20	13/37/115/115	-
19	CLA	B	815	-	1/1/13/20	16/28/106/115	-
19	CLA	4	311	39	1/1/12/20	7/19/97/115	-
19	CLA	5	321	-	1/1/15/20	16/37/115/115	-
22	BCR	8	306	-	-	9/29/63/63	0/2/2/2
32	CHL	4	314	39	3/3/17/26	6/21/119/137	-
32	CHL	6	319	39	3/3/20/26	13/39/137/137	-
31	LUT	6	305	-	-	5/29/67/67	0/2/2/2
19	CLA	5	319	16	1/1/12/20	9/19/97/115	-
31	LUT	1	5003	-	-	6/29/67/67	0/2/2/2
19	CLA	B	823	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	A	851	19	-	24/39/39/53	-
24	LMT	4	302	-	-	4/21/61/61	0/2/2/2
19	CLA	6	323	17	1/1/15/20	11/37/115/115	-
34	3PH	5	324	-	-	8/24/24/49	-
19	CLA	6	312	17	1/1/15/20	8/37/115/115	-
32	CHL	Z	310	39	3/3/20/26	11/39/137/137	-
32	CHL	5	316	39	3/3/17/26	2/21/119/137	-
19	CLA	4	307	15	1/1/12/20	8/22/100/115	-
19	CLA	B	830	-	1/1/12/20	9/19/97/115	-
19	CLA	3	5010	12	1/1/15/20	15/37/115/115	-
19	CLA	A	835	-	1/1/15/20	10/37/115/115	-
19	CLA	6	311	39	1/1/15/20	9/37/115/115	-
27	RRX	4	303	-	-	7/29/65/65	0/2/2/2
23	LHG	3	5021	19	-	17/22/22/53	-
19	CLA	6	313	17	1/1/15/20	18/37/115/115	-
19	CLA	B	820	-	1/1/13/20	15/27/105/115	-
19	CLA	1	5011	39	1/1/13/20	11/25/103/115	-
32	CHL	Z	302	11	3/3/18/26	5/29/127/137	-
34	3PH	8	322	-	-	15/31/31/49	-
19	CLA	5	322	39	1/1/11/20	7/15/93/115	-
19	CLA	3	5020	12	1/1/11/20	9/15/93/115	-
38	ERG	6	326	-	-	8/13/71/71	0/4/4/4
19	CLA	K	205	10	1/1/11/20	7/13/91/115	-
22	BCR	A	847	-	-	13/29/63/63	0/2/2/2
19	CLA	Z	303	-	1/1/11/20	7/15/93/115	-
19	CLA	7	306	13	1/1/14/20	12/31/109/115	-
19	CLA	7	312	23	1/1/15/20	15/37/115/115	-
32	CHL	5	315	39	3/3/20/26	15/39/137/137	-
19	CLA	4	308	15	1/1/15/20	15/37/115/115	-
22	BCR	A	859	-	-	16/29/63/63	0/2/2/2
19	CLA	B	817	-	1/1/13/20	17/30/108/115	-
19	CLA	8	311	-	1/1/15/20	17/37/115/115	-
19	CLA	B	837	-	1/1/15/20	19/37/115/115	-
19	CLA	B	812	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	808	1	1/1/15/20	17/37/115/115	-
19	CLA	5	310	-	1/1/13/20	15/25/103/115	-
19	CLA	4	312	23	1/1/13/20	12/25/103/115	-
28	C7Z	6	304	-	-	13/29/67/67	0/2/2/2
18	CL0	A	801	-	3/3/20/25	12/37/135/135	-
32	CHL	6	315	17	3/3/20/26	13/39/137/137	-
19	CLA	B	828	-	1/1/15/20	12/37/115/115	-
32	CHL	8	319	39	3/3/20/26	13/39/137/137	-
19	CLA	B	802	-	1/1/15/20	17/37/115/115	-
19	CLA	1	5016	11	1/1/14/20	14/31/109/115	-
19	CLA	5	314	16	1/1/15/20	19/37/115/115	-
19	CLA	A	824	-	1/1/15/20	15/37/115/115	-
24	LMT	4	322	-	-	4/21/61/61	0/2/2/2
19	CLA	A	833	-	1/1/15/20	16/37/115/115	-
19	CLA	B	811	-	1/1/13/20	12/27/105/115	-
31	LUT	Z	317	-	-	6/29/67/67	0/2/2/2
27	RRX	F	304	-	-	14/29/65/65	0/2/2/2
22	BCR	5	305	-	-	7/29/63/63	0/2/2/2
19	CLA	B	824	39	1/1/15/20	13/37/115/115	-
22	BCR	3	5006	-	-	16/29/63/63	0/2/2/2
22	BCR	A	848	-	-	12/29/63/63	0/2/2/2
19	CLA	K	203	39	1/1/13/20	10/25/103/115	-
22	BCR	6	307	-	-	10/29/63/63	0/2/2/2
22	BCR	3	5007	-	-	13/29/63/63	0/2/2/2
19	CLA	3	5016	12	1/1/14/20	15/31/109/115	-
24	LMT	8	324	-	-	4/21/61/61	0/2/2/2
19	CLA	Z	306	-	1/1/12/20	11/19/97/115	-
19	CLA	6	301	39	1/1/14/20	17/31/109/115	-
32	CHL	8	315	14	3/3/20/26	14/39/137/137	-
19	CLA	Z	308	-	1/1/15/20	15/37/115/115	-
22	BCR	B	843	-	-	14/29/63/63	0/2/2/2
21	SF4	C	102	3	-	-	0/6/5/5
30	DAO	K	201	-	-	2/11/11/11	-
19	CLA	5	307	16	1/1/14/20	12/33/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CHL	4	317	39	3/3/20/26	7/39/137/137	-
21	SF4	A	845	2,1	-	-	0/6/5/5
19	CLA	5	312	23	1/1/14/20	15/33/111/115	-
19	CLA	3	5011	12	1/1/14/20	4/31/109/115	-
19	CLA	B	832	-	1/1/13/20	16/29/107/115	-
19	CLA	8	313	23	1/1/13/20	14/25/103/115	-
19	CLA	A	857	39	1/1/12/20	11/22/100/115	-
33	SPH	3	5001	-	-	14/21/21/21	-
23	LHG	Z	316	19	-	27/47/47/53	-
24	LMT	8	323	-	-	4/21/61/61	0/2/2/2
32	CHL	4	319	15	3/3/15/26	1/12/110/137	-
19	CLA	Z	307	-	1/1/13/20	15/28/106/115	-
19	CLA	1	5012	23	1/1/14/20	12/31/109/115	-
19	CLA	B	819	39	1/1/15/20	21/37/115/115	-
19	CLA	5	317	16	1/1/15/20	14/37/115/115	-
22	BCR	G	1603	-	-	9/29/63/63	0/2/2/2
19	CLA	6	310	17	1/1/12/20	8/22/100/115	-
19	CLA	4	318	15	1/1/10/20	4/8/86/115	-
32	CHL	Z	309	11	3/3/19/26	17/36/134/137	-
19	CLA	8	307	14	1/1/14/20	15/31/109/115	-
19	CLA	1	5008	39	1/1/15/20	14/37/115/115	-
19	CLA	A	834	-	1/1/15/20	16/37/115/115	-
23	LHG	5	323	19	-	27/41/41/53	-
19	CLA	4	310	15	1/1/15/20	12/37/115/115	-
21	SF4	C	101	3	-	-	0/6/5/5
19	CLA	5	306	16	1/1/14/20	17/31/109/115	-
19	CLA	A	830	-	1/1/15/20	12/37/115/115	-
19	CLA	B	836	-	1/1/15/20	16/37/115/115	-
32	CHL	7	314	13	3/3/20/26	15/39/137/137	-
19	CLA	3	5012	-	1/1/15/20	7/37/115/115	-
19	CLA	4	316	15	1/1/12/20	5/19/97/115	-
19	CLA	B	818	-	1/1/14/20	15/31/109/115	-
19	CLA	7	311	39	1/1/13/20	9/27/105/115	-
23	LHG	6	324	19	-	30/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	802	39	1/1/15/20	15/37/115/115	-
22	BCR	B	847	-	-	12/29/63/63	0/2/2/2
19	CLA	8	312	39	1/1/14/20	12/31/109/115	-
19	CLA	A	812	-	1/1/15/20	12/37/115/115	-
22	BCR	3	5004	-	-	13/29/63/63	0/2/2/2
29	LMG	J	1904	-	-	8/40/60/70	0/1/1/1
19	CLA	A	839	-	1/1/15/20	18/37/115/115	-
31	LUT	3	5002	-	-	4/29/67/67	0/2/2/2
35	DGA	7	302	-	-	23/35/35/45	-
19	CLA	A	814	-	1/1/14/20	11/31/109/115	-
19	CLA	A	842	39	1/1/15/20	12/37/115/115	-
23	LHG	1	5019	19	-	32/47/47/53	-
19	CLA	B	840	23	1/1/15/20	14/37/115/115	-
19	CLA	3	5009	12	1/1/11/20	4/15/93/115	-
19	CLA	A	843	23	1/1/12/20	12/22/100/115	-
22	BCR	B	846	-	-	13/29/63/63	0/2/2/2
19	CLA	F	301	-	1/1/15/20	11/37/115/115	-
23	LHG	1	5001	19	-	15/26/26/53	-
36	PLM	7	322	-	-	4/15/15/15	-
19	CLA	A	826	39	1/1/15/20	11/37/115/115	-
19	CLA	3	5014	23	1/1/14/20	22/31/109/115	-
19	CLA	7	316	39	1/1/12/20	2/19/97/115	-
19	CLA	A	840	-	1/1/15/20	14/37/115/115	-
32	CHL	3	5017	39	3/3/20/26	9/39/137/137	-
19	CLA	7	324	-	1/1/13/20	9/25/103/115	-
31	LUT	7	303	-	-	5/29/67/67	0/2/2/2
33	SPH	4	301	-	-	12/21/21/21	-
24	LMT	A	854	-	-	2/21/61/61	0/2/2/2
19	CLA	Z	311	24	1/1/13/20	11/25/103/115	-
22	BCR	F	302	-	-	12/29/63/63	0/2/2/2
19	CLA	B	801	-	1/1/15/20	12/37/115/115	-
22	BCR	B	844	-	-	10/29/63/63	0/2/2/2
19	CLA	A	832	-	1/1/15/20	20/37/115/115	-
37	SQD	8	302	-	-	10/43/63/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	806	-	1/1/15/20	11/37/115/115	-
19	CLA	A	831	-	1/1/12/20	4/19/97/115	-
19	CLA	B	833	-	1/1/15/20	13/37/115/115	-
19	CLA	7	308	13	1/1/15/20	13/37/115/115	-
23	LHG	7	320	19	-	26/41/41/53	-
19	CLA	8	308	14	1/1/15/20	13/37/115/115	-
23	LHG	4	320	19	-	34/53/53/53	-
19	CLA	B	803	39	1/1/15/20	13/37/115/115	-
19	CLA	G	1602	7	1/1/11/20	8/15/93/115	-
19	CLA	8	314	-	1/1/13/20	14/25/103/115	-
31	LUT	4	304	-	-	7/29/67/67	0/2/2/2
32	CHL	8	316	39	3/3/18/26	10/29/127/137	-
19	CLA	4	306	15	1/1/14/20	12/31/109/115	-
23	LHG	8	321	19	-	22/42/42/53	-
19	CLA	Z	304	39	1/1/12/20	2/19/97/115	-
32	CHL	6	317	39	3/3/17/26	8/21/119/137	-
19	CLA	A	836	1	1/1/13/20	13/25/103/115	-
19	CLA	B	826	-	1/1/15/20	18/37/115/115	-
20	PQN	A	844	-	-	6/23/43/43	0/2/2/2
19	CLA	B	834	39	1/1/11/20	5/13/91/115	-
32	CHL	6	321	17	3/3/15/26	2/12/110/137	-
19	CLA	B	816	-	1/1/15/20	14/37/115/115	-
31	LUT	6	306	-	-	8/29/67/67	0/2/2/2
19	CLA	A	823	-	1/1/13/20	17/28/106/115	-
32	CHL	1	5014	39	3/3/16/26	4/18/116/137	-
32	CHL	8	301	11	3/3/18/26	10/27/125/137	-
19	CLA	A	821	39	1/1/15/20	11/37/115/115	-
22	BCR	4	305	-	-	16/29/63/63	0/2/2/2
19	CLA	8	310	14	1/1/14/20	8/34/112/115	-
24	LMT	3	5023	-	-	6/21/61/61	0/2/2/2
19	CLA	G	1601	-	1/1/12/20	10/19/97/115	-
19	CLA	B	829	-	1/1/15/20	16/37/115/115	-
19	CLA	I	201	-	1/1/13/20	15/25/103/115	-
19	CLA	B	809	2	1/1/13/20	14/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	805	-	1/1/11/20	5/13/91/115	-
19	CLA	B	813	-	1/1/15/20	18/37/115/115	-
19	CLA	4	309	15	1/1/14/20	11/31/109/115	-
32	CHL	7	315	39	3/3/17/26	6/25/123/137	-
19	CLA	A	803	-	1/1/15/20	14/37/115/115	-
32	CHL	5	318	39	3/3/17/26	2/21/119/137	-
19	CLA	8	309	14	1/1/15/20	8/37/115/115	-
22	BCR	8	303	-	-	16/29/63/63	0/2/2/2
19	CLA	5	313	-	1/1/11/20	5/13/91/115	-
19	CLA	1	5015	39	1/1/12/20	6/19/97/115	-
19	CLA	A	807	-	1/1/12/20	9/21/99/115	-
19	CLA	3	5015	-	1/1/11/20	6/13/91/115	-
34	3PH	6	325	-	-	15/30/30/49	-
19	CLA	B	814	-	1/1/14/20	15/31/109/115	-
19	CLA	Z	312	23	1/1/15/20	17/37/115/115	-
19	CLA	A	837	-	1/1/12/20	7/21/99/115	-
33	SPH	7	321	-	-	12/21/21/21	-
19	CLA	B	827	-	1/1/14/20	19/31/109/115	-
24	LMT	7	323	-	-	4/21/61/61	0/2/2/2
32	CHL	Z	313	39	3/3/16/26	4/15/113/137	-
31	LUT	7	304	-	-	5/29/67/67	0/2/2/2
32	CHL	6	316	39	3/3/19/26	13/33/131/137	-
32	CHL	4	315	39	3/3/17/26	8/21/119/137	-
24	LMT	4	321	-	-	2/21/61/61	0/2/2/2
24	LMT	1	5002	-	-	4/21/61/61	0/2/2/2
19	CLA	6	309	17	1/1/14/20	7/31/109/115	-
31	LUT	5	303	-	-	9/29/67/67	0/2/2/2
19	CLA	6	322	-	1/1/11/20	6/15/93/115	-
24	LMT	A	855	-	-	3/21/61/61	0/2/2/2
19	CLA	4	313	-	1/1/13/20	12/25/103/115	-
19	CLA	A	827	-	1/1/15/20	23/37/115/115	-
19	CLA	B	810	-	1/1/12/20	10/22/100/115	-
19	CLA	Z	305	11	1/1/15/20	16/37/115/115	-
19	CLA	A	828	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMT	F	305	-	-	4/21/61/61	0/2/2/2
19	CLA	5	308	16	1/1/13/20	7/27/105/115	-
19	CLA	A	822	-	1/1/13/20	12/25/103/115	-
19	CLA	A	841	-	1/1/15/20	11/37/115/115	-
19	CLA	8	320	14	1/1/11/20	7/15/93/115	-
19	CLA	A	813	-	1/1/15/20	13/37/115/115	-
19	CLA	F	303	39	1/1/11/20	4/13/91/115	-
19	CLA	7	309	13	1/1/15/20	10/37/115/115	-
22	BCR	6	308	-	-	10/29/63/63	0/2/2/2
22	BCR	B	842	-	-	13/29/63/63	0/2/2/2
19	CLA	J	1901	9	1/1/10/20	6/10/88/115	-
19	CLA	1	5007	11	1/1/11/20	5/13/91/115	-
24	LMT	G	1604	-	-	1/21/61/61	0/2/2/2
19	CLA	A	811	19	1/1/15/20	12/37/115/115	-
22	BCR	A	850	-	-	15/29/63/63	0/2/2/2
19	CLA	A	819	-	1/1/15/20	13/37/115/115	-
19	CLA	K	204	10	1/1/11/20	9/18/96/115	-
19	CLA	A	804	19	1/1/13/20	13/25/103/115	-
19	CLA	6	314	23	1/1/13/20	9/25/103/115	-
19	CLA	B	850	6	1/1/15/20	22/37/115/115	-
19	CLA	3	5008	12	1/1/15/20	8/37/115/115	-
19	CLA	A	809	1	1/1/13/20	9/27/105/115	-
28	C7Z	1	5005	-	-	9/29/67/67	0/2/2/2
19	CLA	6	302	15	1/1/14/20	15/31/109/115	-
19	CLA	6	318	17	1/1/12/20	3/19/97/115	-
19	CLA	1	5006	11	1/1/15/20	16/37/115/115	-
19	CLA	A	817	-	1/1/14/20	13/31/109/115	-
22	BCR	3	5005	-	-	7/29/63/63	0/2/2/2
19	CLA	1	5010	-	1/1/13/20	7/25/103/115	-
38	ERG	8	325	-	-	11/13/71/71	0/4/4/4
22	BCR	A	849	-	-	15/29/63/63	0/2/2/2
19	CLA	7	317	13	1/1/12/20	8/19/97/115	-
29	LMG	J	1903	-	-	8/30/50/70	0/1/1/1
28	C7Z	J	1902	-	-	14/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	A	852	-	-	35/53/53/53	-
19	CLA	A	816	39	1/1/14/20	13/33/111/115	-
19	CLA	5	325	-	1/1/13/20	12/25/103/115	-
22	BCR	A	846	-	-	14/29/63/63	0/2/2/2
19	CLA	6	320	39	1/1/14/20	10/33/111/115	-
19	CLA	Z	314	11	1/1/11/20	7/15/93/115	-
19	CLA	7	319	13	1/1/13/20	17/29/107/115	-
24	LMT	Z	319	19	-	8/21/61/61	0/2/2/2
32	CHL	5	320	16	3/3/15/26	0/12/110/137	-
19	CLA	7	310	-	1/1/14/20	14/33/111/115	-
19	CLA	A	825	39	1/1/15/20	16/37/115/115	-
24	LMT	A	856	-	-	8/21/61/61	0/2/2/2
19	CLA	B	839	-	1/1/11/20	6/15/93/115	-
19	CLA	B	838	39	1/1/12/20	6/22/100/115	-
19	CLA	B	835	-	1/1/14/20	12/31/109/115	-
19	CLA	A	810	-	1/1/15/20	16/37/115/115	-
19	CLA	1	5018	11	1/1/12/20	5/21/99/115	-
24	LMT	Z	301	-	-	6/21/61/61	0/2/2/2
34	3PH	3	5022	-	-	20/40/40/49	-
19	CLA	B	825	39	1/1/15/20	14/37/115/115	-
19	CLA	5	311	39	1/1/12/20	10/19/97/115	-
19	CLA	B	807	2	1/1/15/20	24/37/115/115	-
19	CLA	B	822	-	1/1/13/20	15/30/108/115	-
29	LMG	7	301	-	-	5/24/44/70	0/1/1/1
32	CHL	8	317	39	3/3/17/26	3/21/119/137	-
19	CLA	A	815	-	1/1/15/20	6/37/115/115	-
19	CLA	7	318	39	1/1/10/20	4/10/88/115	-
19	CLA	B	808	-	1/1/15/20	18/37/115/115	-
19	CLA	A	818	-	1/1/14/20	15/31/109/115	-
27	RRX	5	302	-	-	7/29/65/65	0/2/2/2
19	CLA	5	309	16	1/1/15/20	11/37/115/115	-
19	CLA	3	5013	39	1/1/15/20	15/37/115/115	-
19	CLA	B	831	-	1/1/15/20	16/37/115/115	-
23	LHG	6	303	-	-	26/36/36/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	5	304	-	-	13/29/63/63	0/2/2/2
32	CHL	1	5009	11	3/3/19/26	14/33/131/137	-
19	CLA	A	820	-	1/1/14/20	11/31/109/115	-
19	CLA	3	5019	39	1/1/13/20	8/25/103/115	-
19	CLA	A	806	1	1/1/15/20	17/37/115/115	-
31	LUT	1	5004	-	-	4/29/67/67	0/2/2/2
19	CLA	8	318	14	1/1/11/20	3/15/93/115	-
19	CLA	A	829	-	1/1/15/20	12/37/115/115	-
19	CLA	1	5013	-	1/1/11/20	3/17/95/115	-
31	LUT	3	5003	-	-	6/29/67/67	0/2/2/2
20	PQN	B	841	-	-	10/23/43/43	0/2/2/2
22	BCR	A	858	-	-	12/29/63/63	0/2/2/2
22	BCR	K	206	-	-	10/29/63/63	0/2/2/2
19	CLA	B	821	-	1/1/15/20	16/37/115/115	-

The worst 5 of 2860 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	5003	LUT	C24-C25	23.05	1.61	1.33
31	Z	318	LUT	C24-C25	22.96	1.61	1.33
31	8	304	LUT	C24-C25	22.89	1.61	1.33
31	3	5003	LUT	C24-C25	22.58	1.61	1.33
31	6	305	LUT	C24-C25	22.44	1.61	1.33

The worst 5 of 4512 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Z	317	LUT	C35-C34-C33	-13.98	107.35	127.31
31	Z	317	LUT	C31-C30-C29	-13.44	108.13	127.31
22	3	5007	BCR	C11-C10-C9	-11.28	111.21	127.31
22	3	5007	BCR	C20-C21-C22	-10.51	112.31	127.31
19	B	831	CLA	C4A-NA-C1A	9.99	111.20	106.71

5 of 273 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	801	CL0	NC
18	A	801	CL0	NA
18	A	801	CL0	ND

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Mol	Chain	Res	Type	Atom
19	A	802	CLA	ND
19	A	803	CLA	ND

5 of 3534 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	802	CLA	C2-C1-O2A-CGA
19	A	802	CLA	CHA-CBD-CGD-O1D
19	A	803	CLA	C1A-C2A-CAA-CBA
19	A	803	CLA	CBA-CGA-O2A-C1
19	A	803	CLA	O1A-CGA-O2A-C1

There are no ring outliers.

311 monomers are involved in 2490 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	7	313	CLA	4	0
31	8	304	LUT	11	0
19	A	838	CLA	13	0
22	7	305	BCR	5	0
19	3	5018	CLA	14	0
19	B	804	CLA	11	0
31	8	305	LUT	5	0
19	A	805	CLA	13	0
31	Z	318	LUT	9	0
19	5	301	CLA	8	0
24	A	853	LMT	8	0
19	K	202	CLA	11	0
25	B	848	DGD	5	0
19	7	307	CLA	14	0
22	B	845	BCR	18	0
32	1	5017	CHL	12	0
19	Z	315	CLA	10	0
19	B	815	CLA	10	0
19	4	311	CLA	10	0
19	5	321	CLA	14	0
22	8	306	BCR	7	0
32	4	314	CHL	13	0
32	6	319	CHL	17	0
31	6	305	LUT	11	0
19	5	319	CLA	11	0
31	1	5003	LUT	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	823	CLA	22	0
23	A	851	LHG	7	0
24	4	302	LMT	5	0
19	6	323	CLA	14	0
34	5	324	3PH	3	0
19	6	312	CLA	13	0
32	Z	310	CHL	11	0
32	5	316	CHL	6	0
19	4	307	CLA	15	0
19	B	830	CLA	10	0
19	3	5010	CLA	10	0
19	A	835	CLA	16	0
19	6	311	CLA	10	0
27	4	303	RRX	6	0
23	3	5021	LHG	4	0
19	6	313	CLA	25	0
19	B	820	CLA	9	0
19	1	5011	CLA	9	0
32	Z	302	CHL	14	0
34	8	322	3PH	6	0
19	5	322	CLA	7	0
19	3	5020	CLA	7	0
38	6	326	ERG	24	0
19	K	205	CLA	9	0
22	A	847	BCR	13	0
19	Z	303	CLA	7	0
19	7	306	CLA	14	0
19	7	312	CLA	14	0
32	5	315	CHL	18	0
19	4	308	CLA	11	0
22	A	859	BCR	12	0
19	B	817	CLA	5	0
19	8	311	CLA	13	0
19	B	837	CLA	18	0
19	B	812	CLA	10	0
19	A	808	CLA	16	0
19	5	310	CLA	18	0
19	4	312	CLA	13	0
28	6	304	C7Z	4	0
18	A	801	CL0	12	0
32	6	315	CHL	15	0
19	B	828	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	8	319	CHL	5	0
19	B	802	CLA	12	0
19	1	5016	CLA	26	0
19	5	314	CLA	16	0
19	A	824	CLA	17	0
24	4	322	LMT	11	0
19	A	833	CLA	11	0
19	B	811	CLA	7	0
31	Z	317	LUT	13	0
27	F	304	RRX	9	0
22	5	305	BCR	6	0
19	B	824	CLA	15	0
22	3	5006	BCR	21	0
22	A	848	BCR	7	0
19	K	203	CLA	13	0
22	6	307	BCR	23	0
22	3	5007	BCR	8	0
19	3	5016	CLA	16	0
24	8	324	LMT	3	0
19	Z	306	CLA	2	0
19	6	301	CLA	18	0
32	8	315	CHL	13	0
19	Z	308	CLA	11	0
22	B	843	BCR	5	0
21	C	102	SF4	5	0
30	K	201	DAO	4	0
19	5	307	CLA	18	0
21	A	845	SF4	4	0
32	4	317	CHL	11	0
19	5	312	CLA	13	0
19	3	5011	CLA	7	0
19	B	832	CLA	19	0
19	8	313	CLA	12	0
19	A	857	CLA	13	0
33	3	5001	SPH	12	0
23	Z	316	LHG	6	0
24	8	323	LMT	5	0
32	4	319	CHL	5	0
19	Z	307	CLA	7	0
19	1	5012	CLA	13	0
19	B	819	CLA	17	0
19	5	317	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	G	1603	BCR	12	0
19	6	310	CLA	24	0
19	4	318	CLA	4	0
32	Z	309	CHL	16	0
19	8	307	CLA	19	0
19	1	5008	CLA	10	0
19	A	834	CLA	9	0
23	5	323	LHG	7	0
19	4	310	CLA	11	0
19	5	306	CLA	20	0
19	A	830	CLA	12	0
19	B	836	CLA	13	0
32	7	314	CHL	12	0
19	3	5012	CLA	20	0
19	4	316	CLA	10	0
19	B	818	CLA	7	0
19	7	311	CLA	11	0
23	6	324	LHG	13	0
19	A	802	CLA	14	0
22	B	847	BCR	8	0
19	8	312	CLA	17	0
19	A	812	CLA	14	0
22	3	5004	BCR	7	0
29	J	1904	LMG	12	0
19	A	839	CLA	19	0
31	3	5002	LUT	5	0
35	7	302	DGA	14	0
19	A	814	CLA	17	0
19	A	842	CLA	12	0
23	1	5019	LHG	10	0
19	B	840	CLA	16	0
19	3	5009	CLA	7	0
19	A	843	CLA	7	0
22	B	846	BCR	20	0
19	F	301	CLA	13	0
36	7	322	PLM	2	0
19	A	826	CLA	9	0
19	3	5014	CLA	11	0
19	7	316	CLA	5	0
19	A	840	CLA	10	0
32	3	5017	CHL	13	0
19	7	324	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	7	303	LUT	5	0
33	4	301	SPH	7	0
24	A	854	LMT	5	0
19	Z	311	CLA	12	0
22	F	302	BCR	9	0
19	B	801	CLA	16	0
22	B	844	BCR	11	0
19	A	832	CLA	13	0
37	8	302	SQD	11	0
19	B	806	CLA	8	0
19	A	831	CLA	1	0
19	B	833	CLA	14	0
19	7	308	CLA	14	0
23	7	320	LHG	3	0
19	8	308	CLA	8	0
23	4	320	LHG	14	0
19	B	803	CLA	14	0
19	G	1602	CLA	12	0
19	8	314	CLA	3	0
31	4	304	LUT	13	0
32	8	316	CHL	7	0
19	4	306	CLA	23	0
23	8	321	LHG	7	0
19	Z	304	CLA	4	0
32	6	317	CHL	7	0
19	A	836	CLA	14	0
19	B	826	CLA	17	0
20	A	844	PQN	4	0
19	B	834	CLA	13	0
32	6	321	CHL	9	0
19	B	816	CLA	12	0
31	6	306	LUT	5	0
19	A	823	CLA	18	0
32	1	5014	CHL	8	0
32	8	301	CHL	14	0
19	A	821	CLA	17	0
22	4	305	BCR	14	0
19	8	310	CLA	9	0
24	3	5023	LMT	7	0
19	G	1601	CLA	6	0
19	B	829	CLA	10	0
19	I	201	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	809	CLA	10	0
19	B	805	CLA	3	0
19	B	813	CLA	11	0
19	4	309	CLA	8	0
32	7	315	CHL	6	0
19	A	803	CLA	7	0
32	5	318	CHL	15	0
19	8	309	CLA	12	0
22	8	303	BCR	10	0
19	5	313	CLA	10	0
19	1	5015	CLA	5	0
19	A	807	CLA	9	0
19	3	5015	CLA	7	0
34	6	325	3PH	5	0
19	B	814	CLA	12	0
19	Z	312	CLA	9	0
19	A	837	CLA	7	0
33	7	321	SPH	7	0
19	B	827	CLA	9	0
24	7	323	LMT	2	0
32	Z	313	CHL	10	0
31	7	304	LUT	12	0
32	6	316	CHL	17	0
32	4	315	CHL	5	0
24	4	321	LMT	4	0
24	1	5002	LMT	9	0
19	6	309	CLA	13	0
31	5	303	LUT	10	0
19	6	322	CLA	8	0
24	A	855	LMT	1	0
19	4	313	CLA	11	0
19	A	827	CLA	19	0
19	B	810	CLA	6	0
19	Z	305	CLA	14	0
19	A	828	CLA	22	0
24	F	305	LMT	9	0
19	5	308	CLA	8	0
19	A	822	CLA	19	0
19	A	841	CLA	14	0
19	8	320	CLA	4	0
19	A	813	CLA	6	0
19	F	303	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	7	309	CLA	10	0
22	6	308	BCR	16	0
22	B	842	BCR	16	0
19	J	1901	CLA	4	0
19	1	5007	CLA	13	0
24	G	1604	LMT	11	0
19	A	811	CLA	13	0
22	A	850	BCR	11	0
19	A	819	CLA	15	0
19	K	204	CLA	8	0
19	A	804	CLA	9	0
19	6	314	CLA	16	0
19	B	850	CLA	29	0
19	3	5008	CLA	14	0
19	A	809	CLA	10	0
28	1	5005	C7Z	1	0
19	6	302	CLA	16	0
19	6	318	CLA	8	0
19	1	5006	CLA	6	0
19	A	817	CLA	10	0
22	3	5005	BCR	7	0
19	1	5010	CLA	13	0
38	8	325	ERG	14	0
22	A	849	BCR	17	0
19	7	317	CLA	9	0
29	J	1903	LMG	4	0
28	J	1902	C7Z	1	0
23	A	852	LHG	5	0
19	A	816	CLA	16	0
19	5	325	CLA	15	0
22	A	846	BCR	8	0
19	6	320	CLA	11	0
19	Z	314	CLA	7	0
19	7	319	CLA	7	0
24	Z	319	LMT	4	0
32	5	320	CHL	8	0
19	7	310	CLA	6	0
19	A	825	CLA	8	0
24	A	856	LMT	8	0
19	B	839	CLA	7	0
19	B	838	CLA	9	0
19	B	835	CLA	19	0

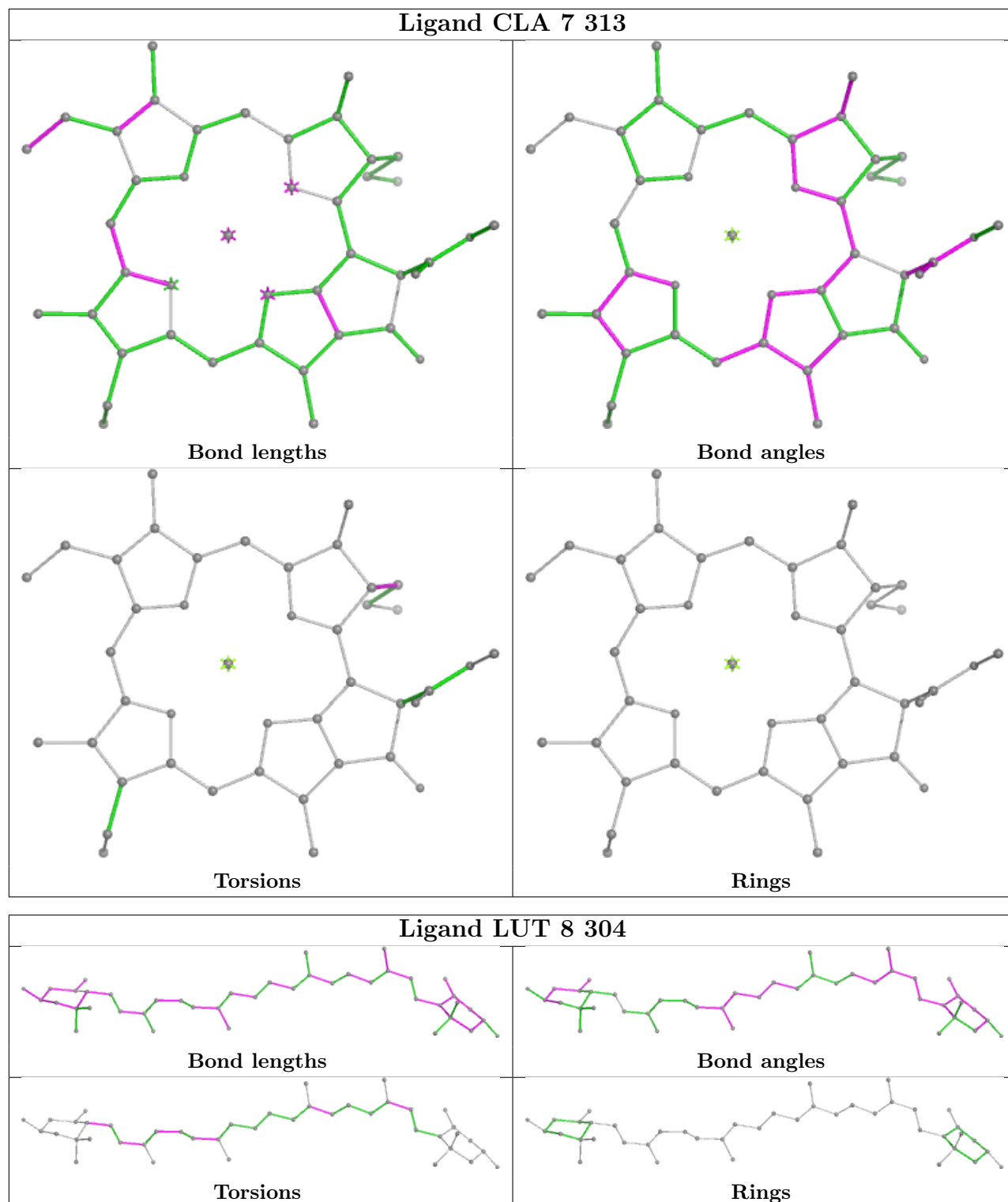
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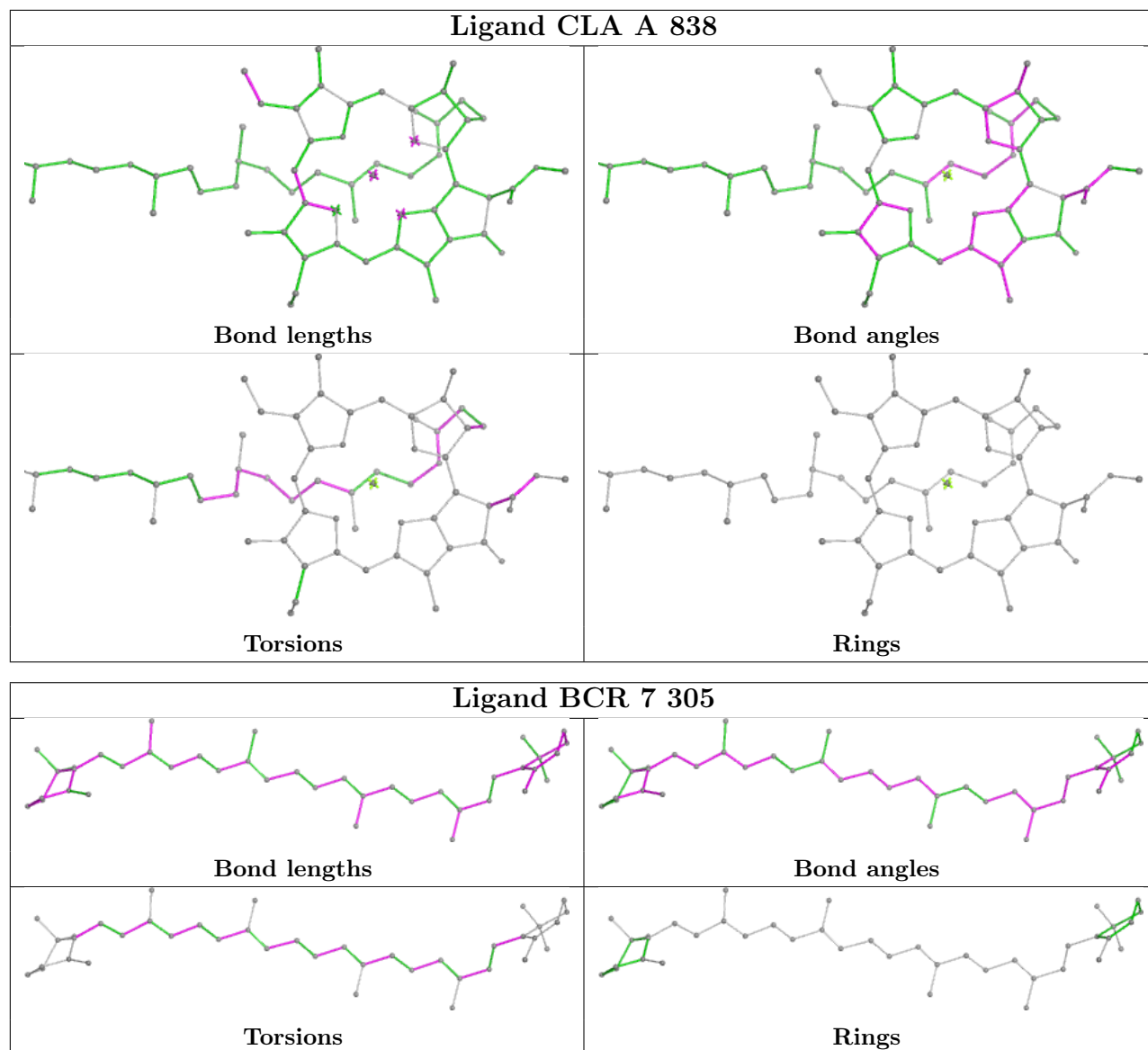
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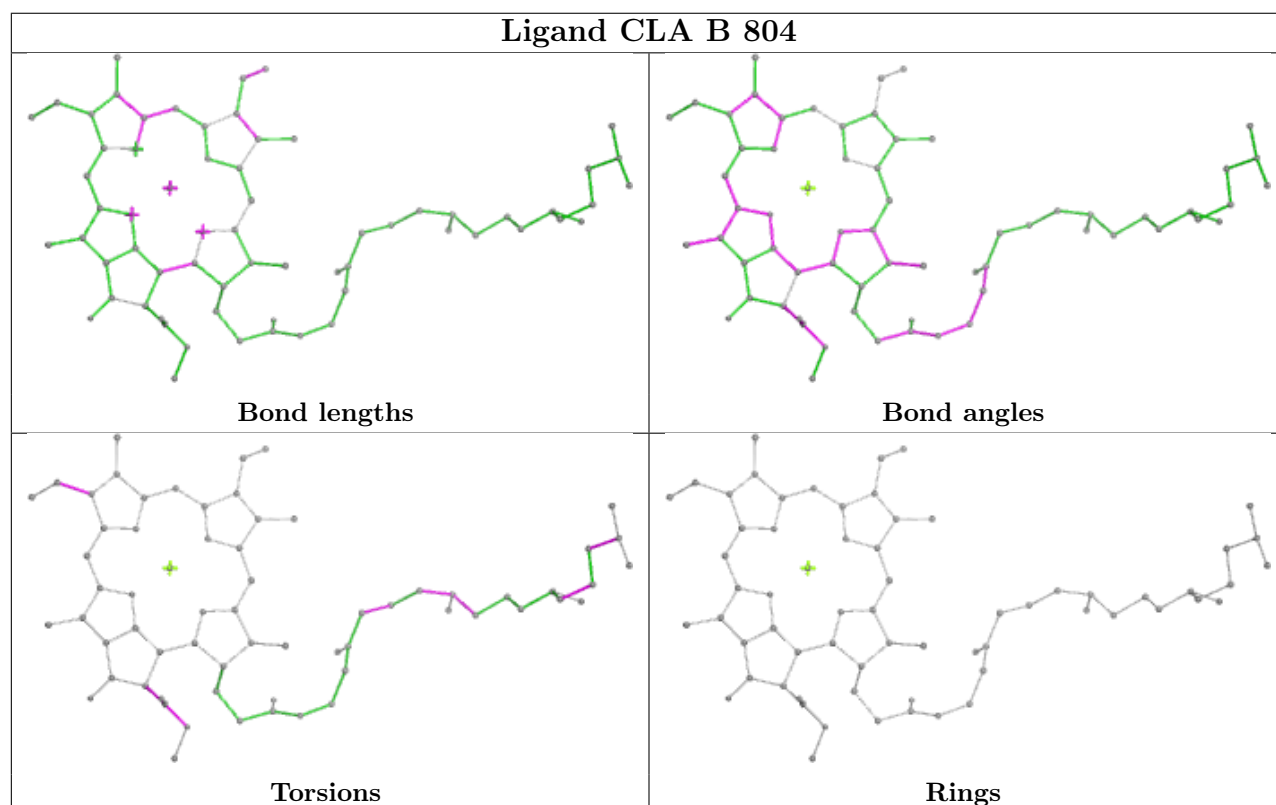
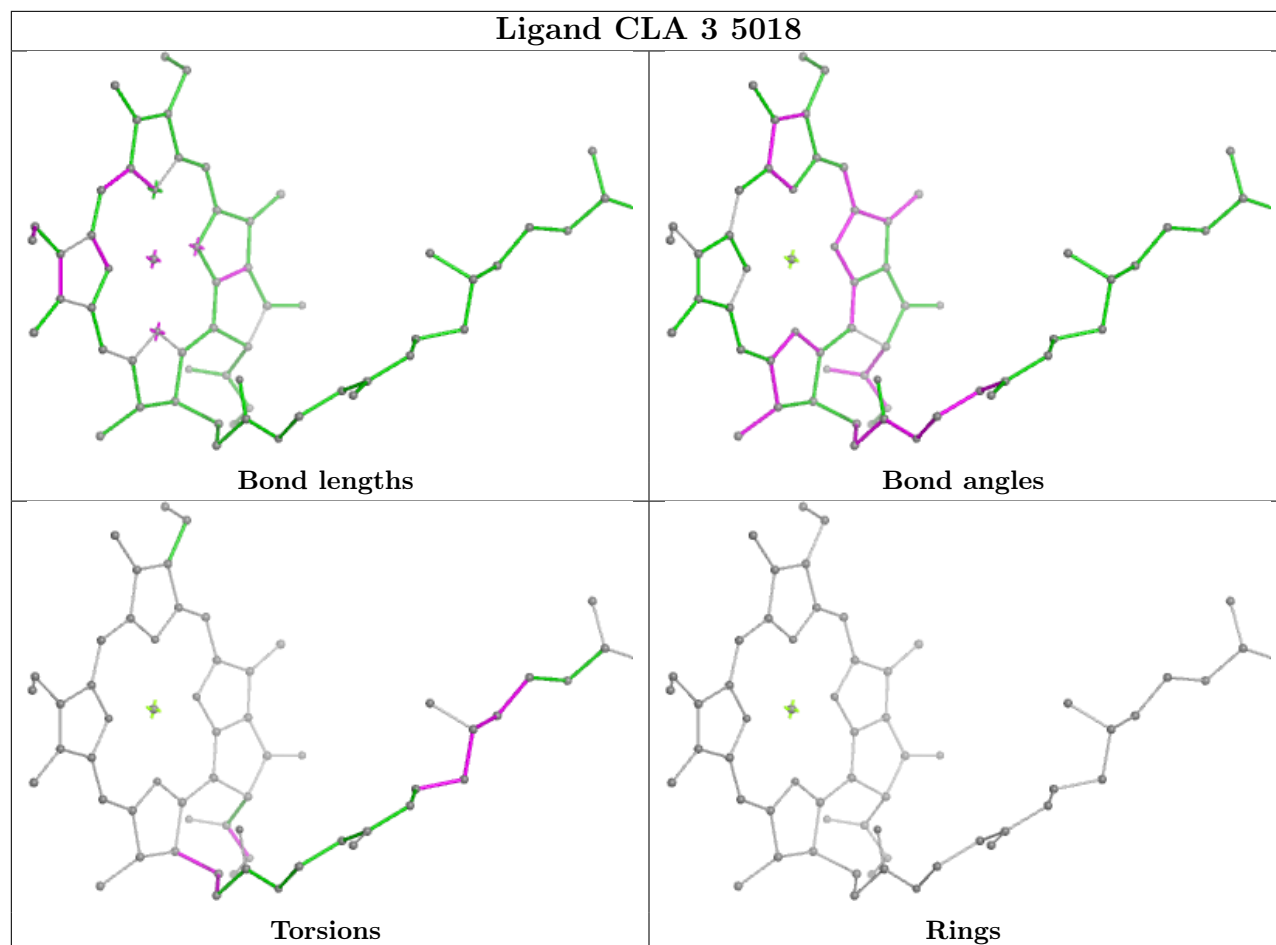
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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19	1	5018	CLA	4	0
24	Z	301	LMT	7	0
34	3	5022	3PH	4	0
19	B	825	CLA	19	0
19	5	311	CLA	12	0
19	B	807	CLA	5	0
19	B	822	CLA	16	0
29	7	301	LMG	1	0
32	8	317	CHL	7	0
19	A	815	CLA	20	0
19	7	318	CLA	4	0
19	B	808	CLA	14	0
19	A	818	CLA	17	0
27	5	302	RRX	11	0
19	5	309	CLA	14	0
19	3	5013	CLA	12	0
19	B	831	CLA	15	0
23	6	303	LHG	9	0
22	5	304	BCR	11	0
32	1	5009	CHL	5	0
19	A	820	CLA	10	0
19	3	5019	CLA	12	0
19	A	806	CLA	11	0
31	1	5004	LUT	8	0
19	8	318	CLA	13	0
19	A	829	CLA	12	0
19	1	5013	CLA	8	0
31	3	5003	LUT	9	0
20	B	841	PQN	5	0
22	A	858	BCR	6	0
22	K	206	BCR	12	0
19	B	821	CLA	20	0

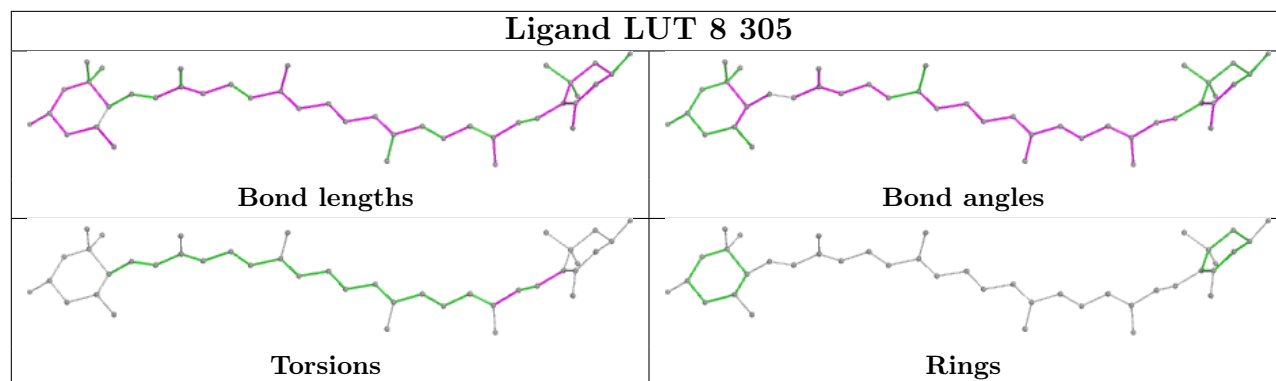
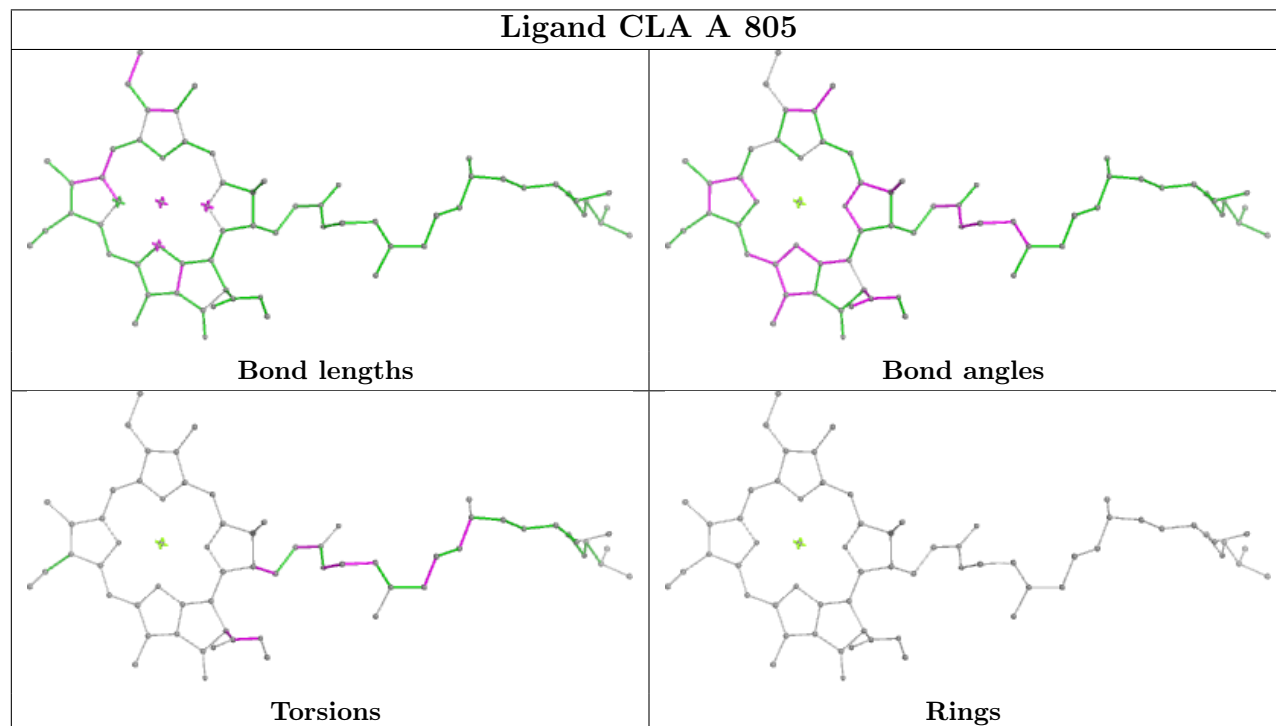
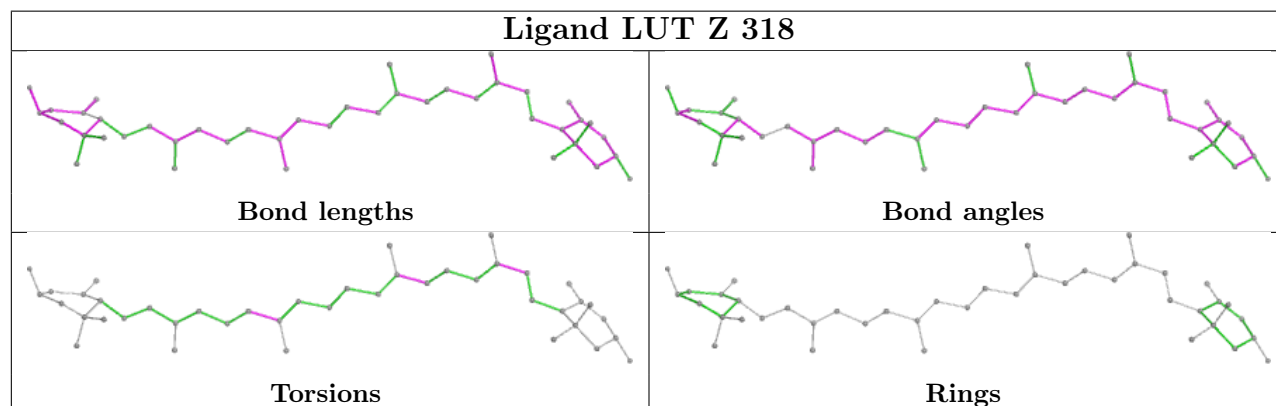
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

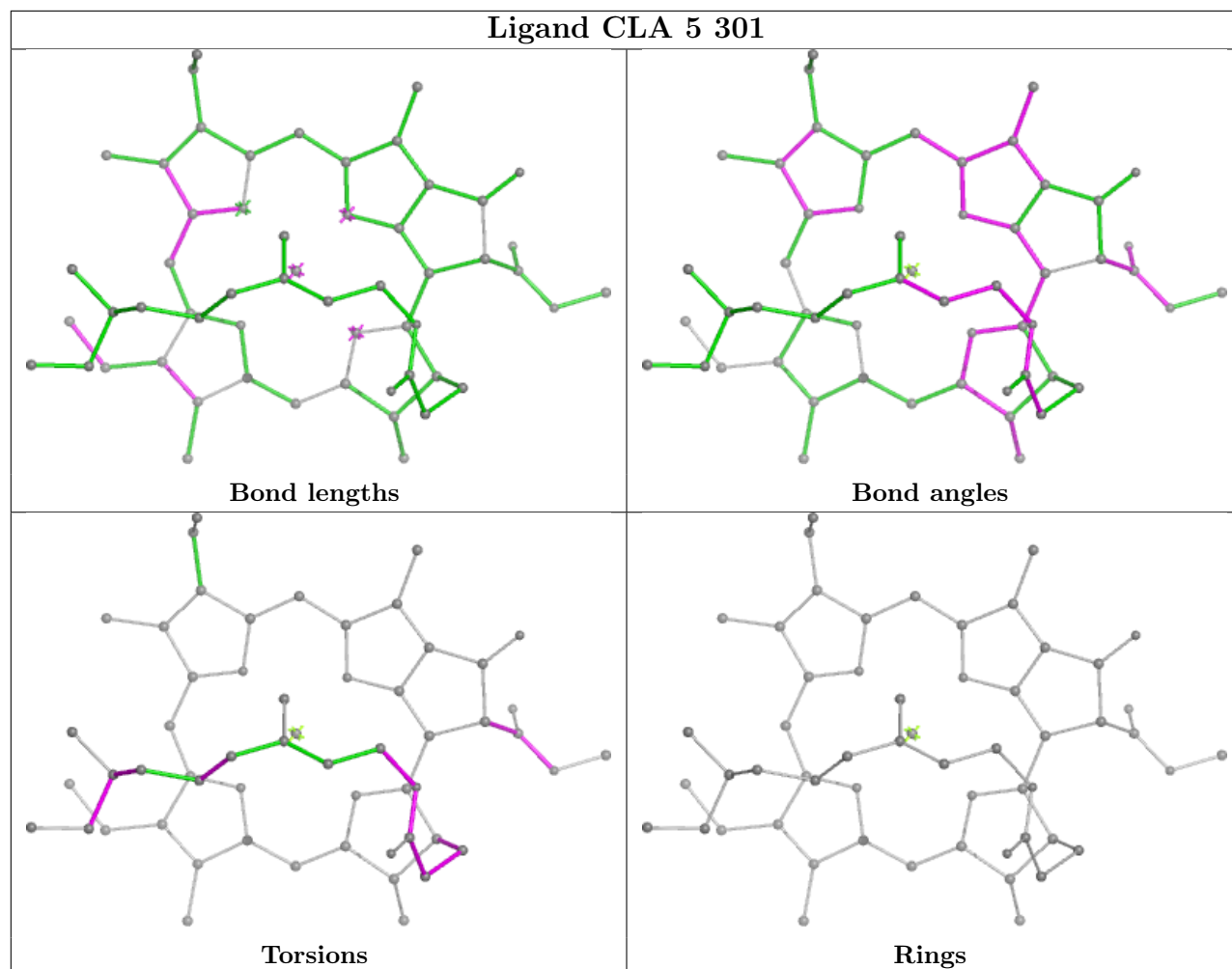




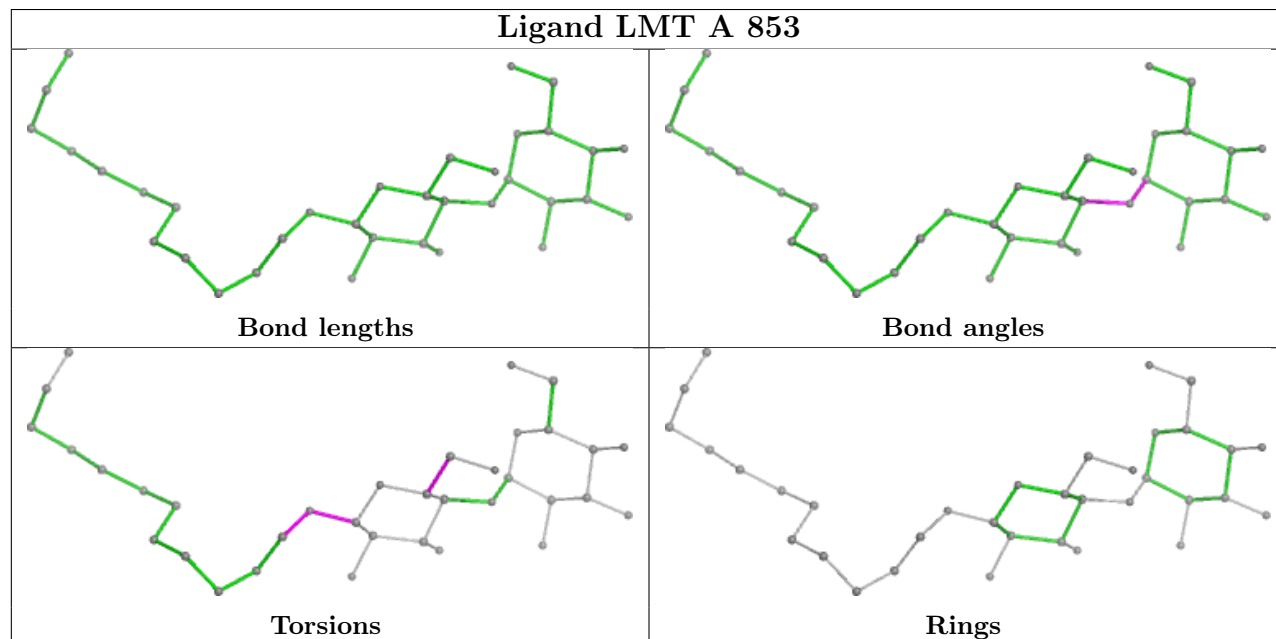


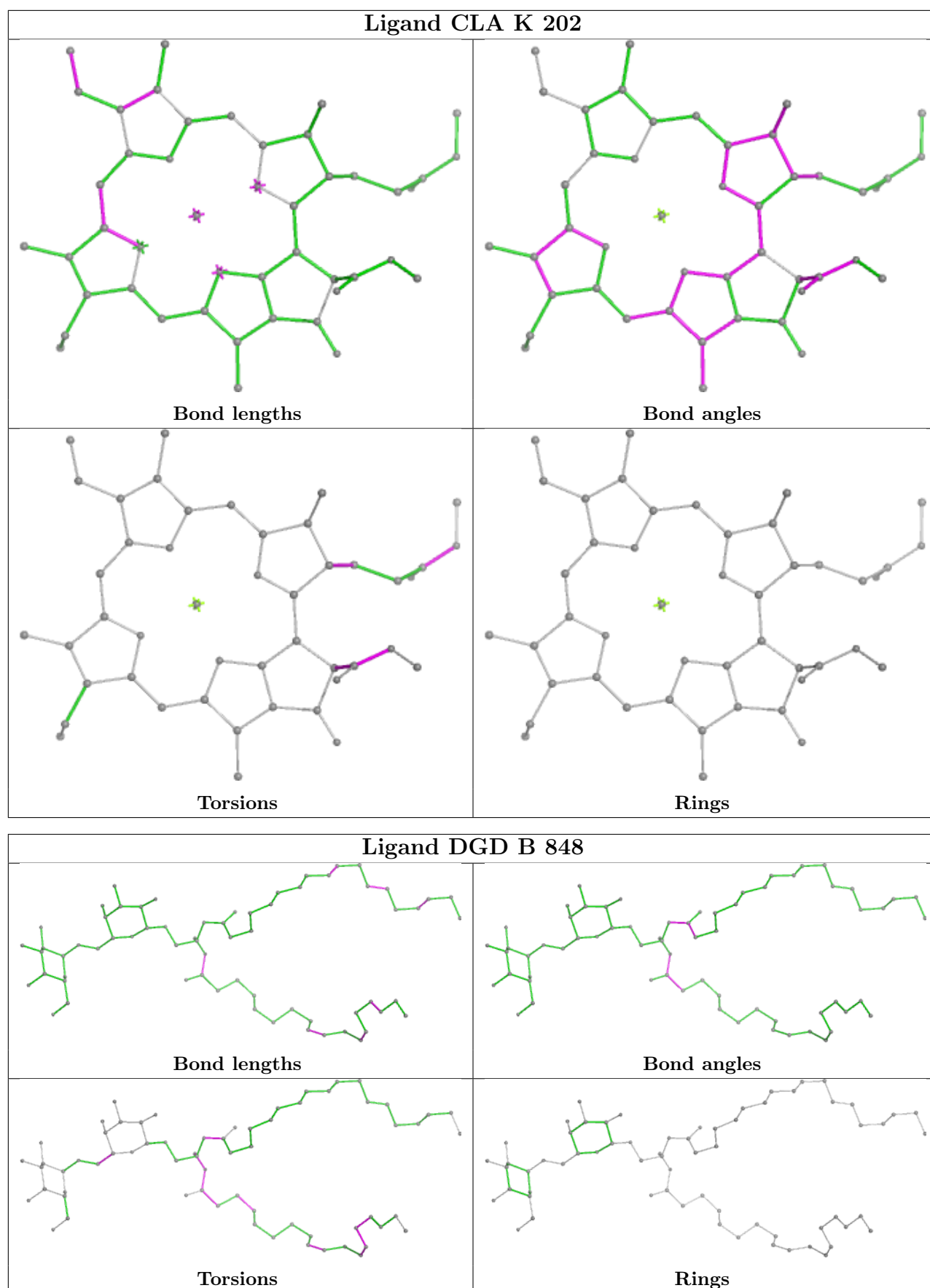
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Ligand CLA 5 301

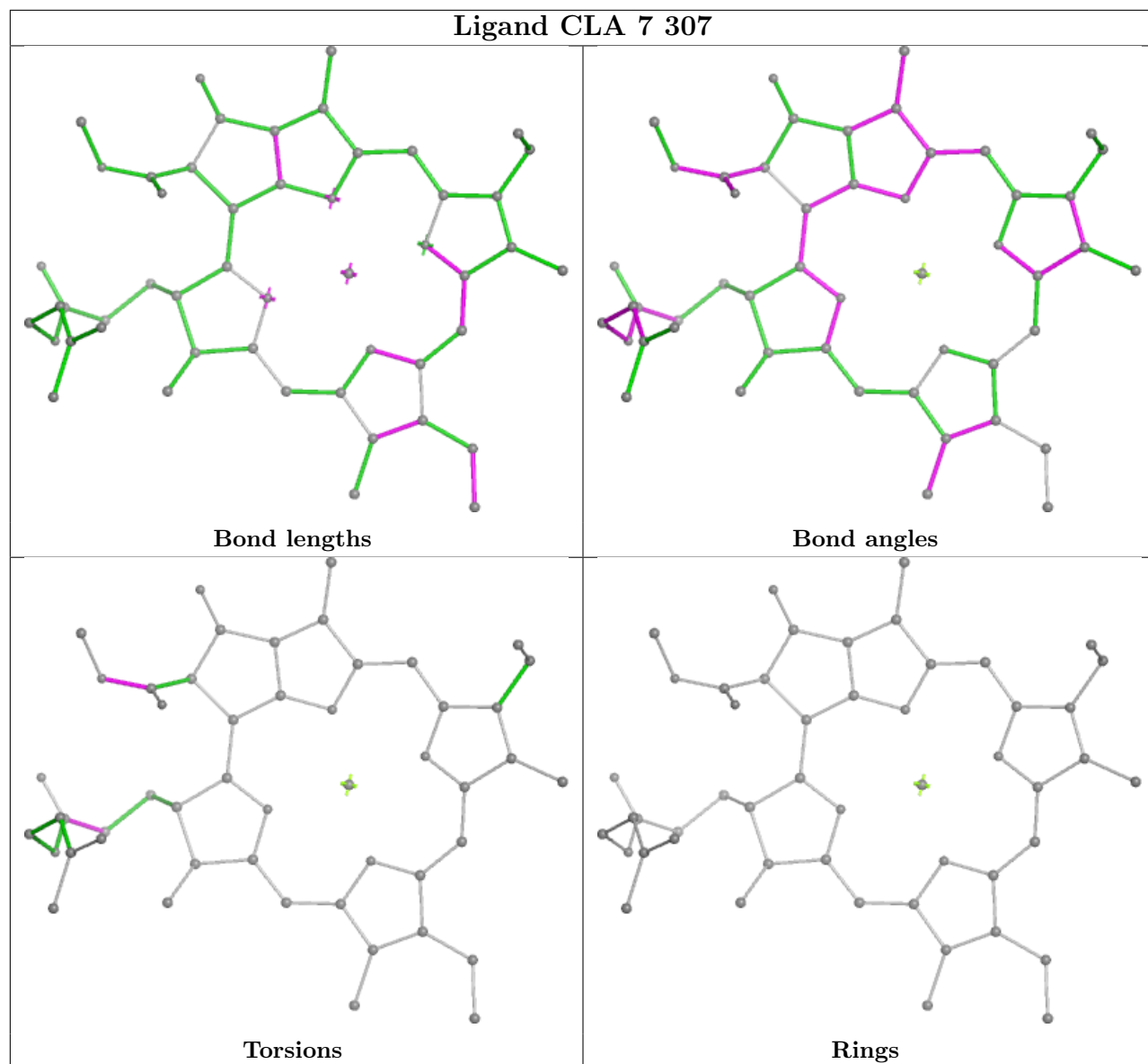


Ligand LMT A 853

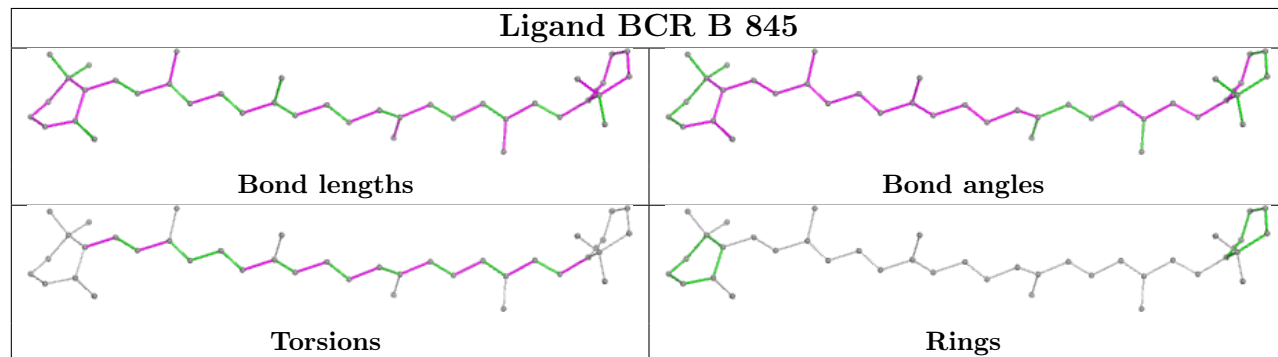


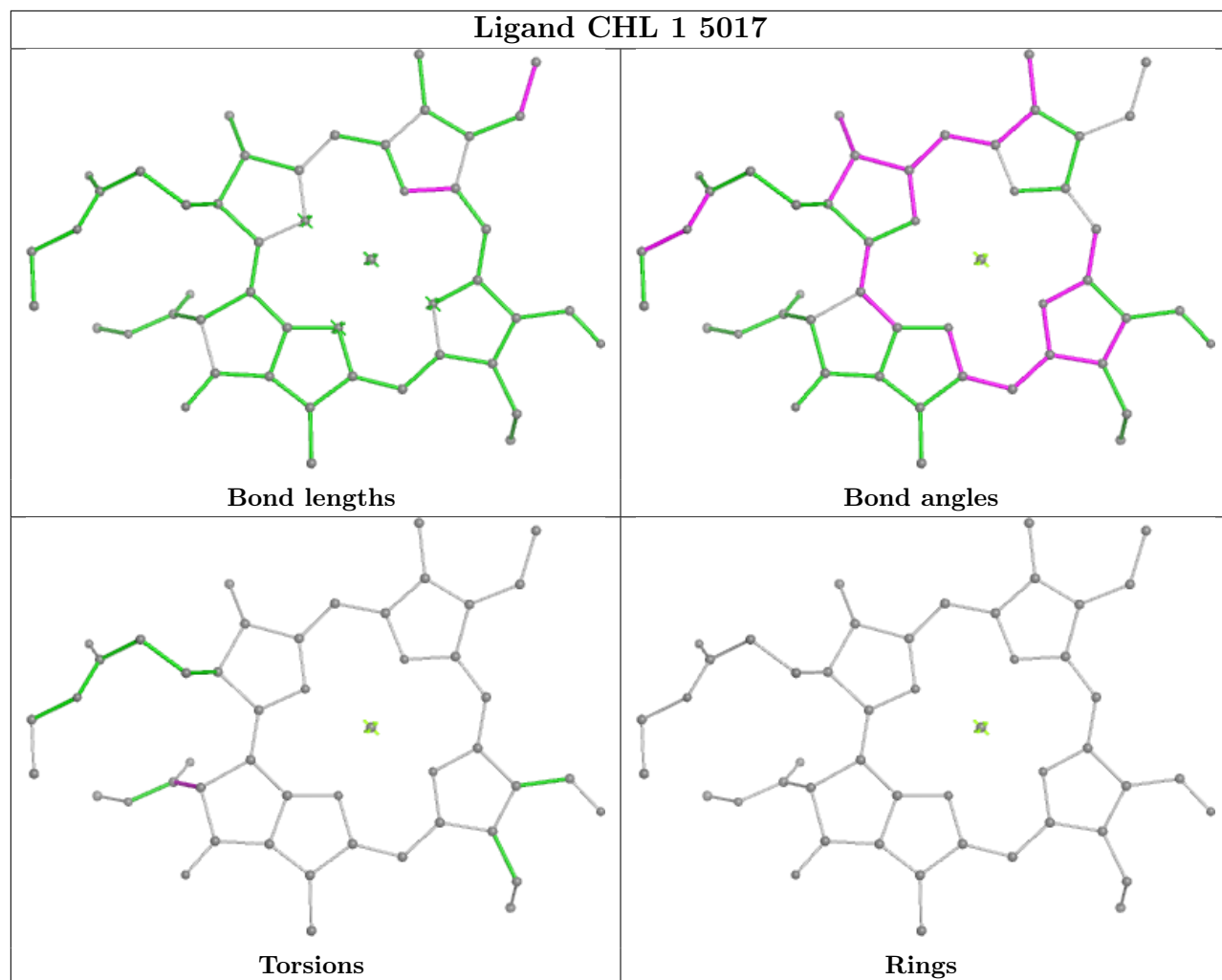


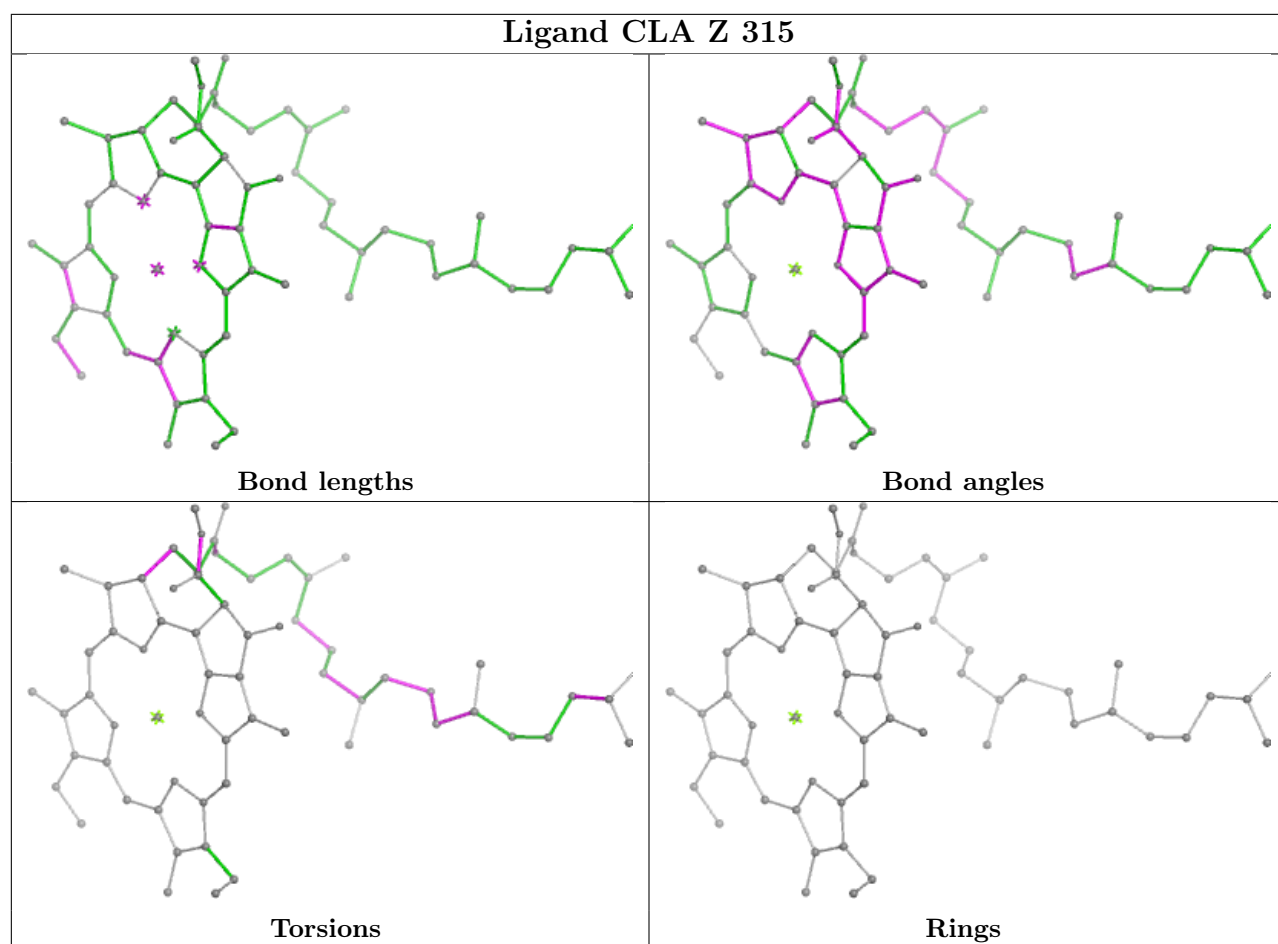
Ligand CLA 7 307



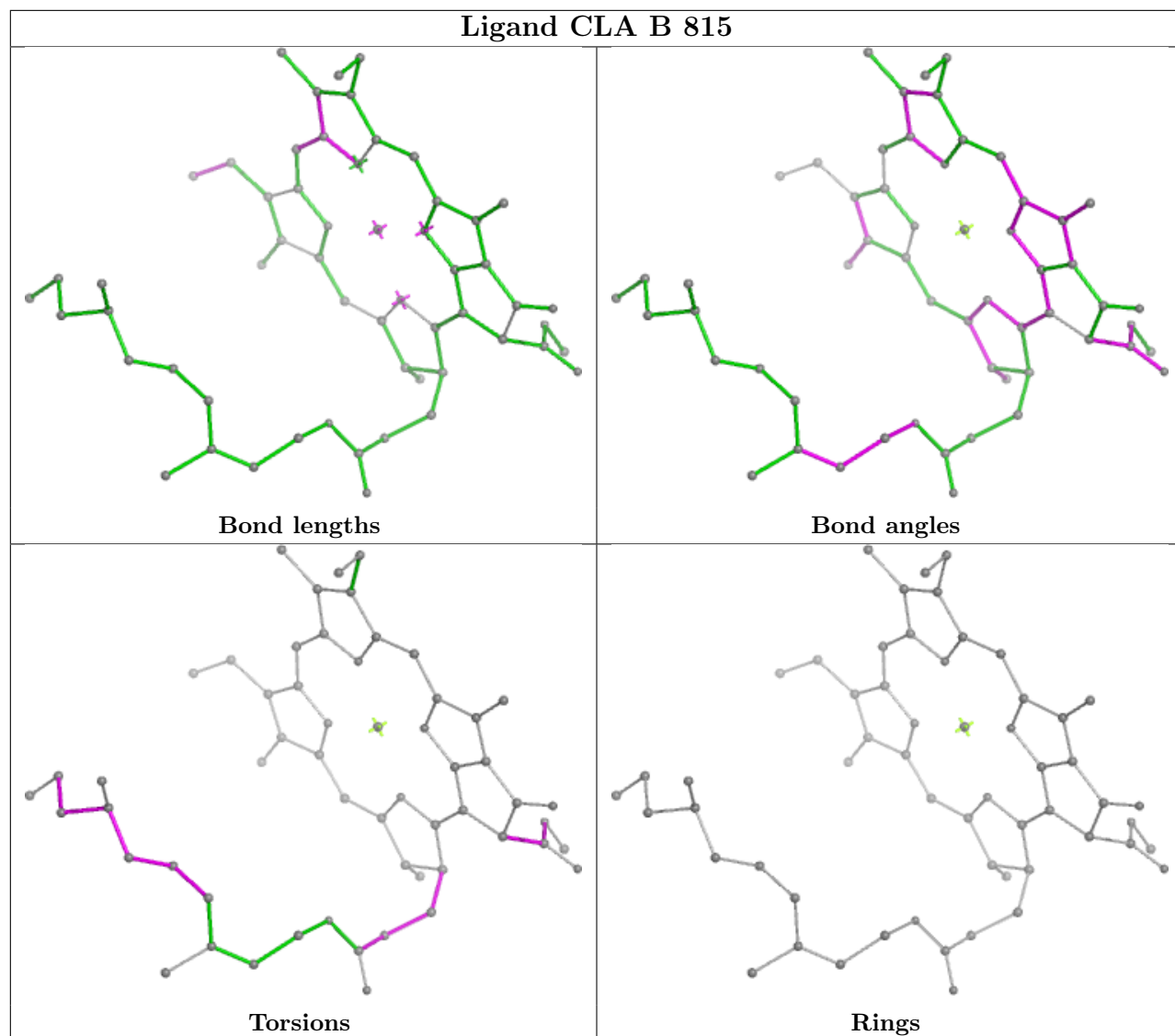
Ligand BCR B 845



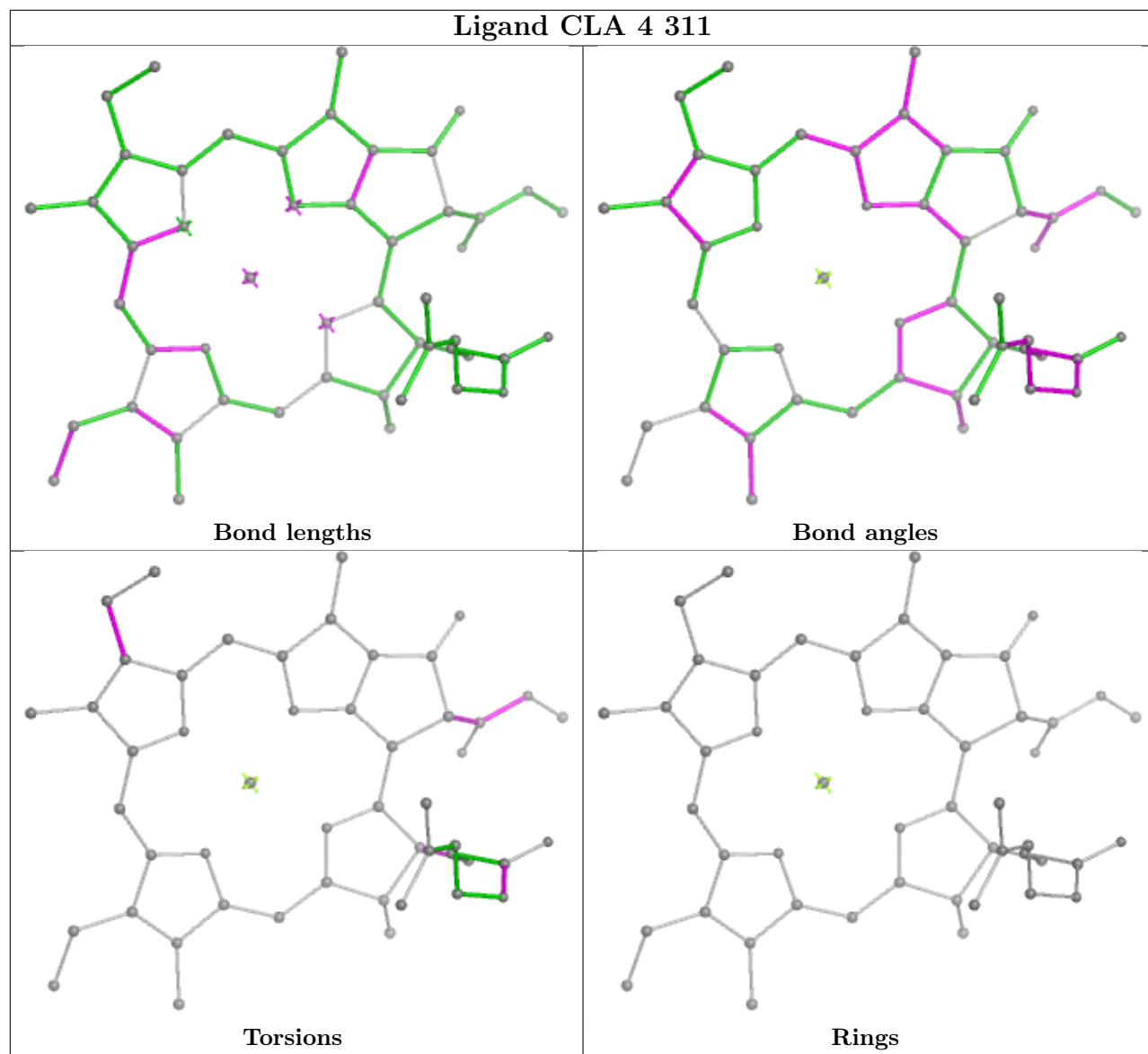


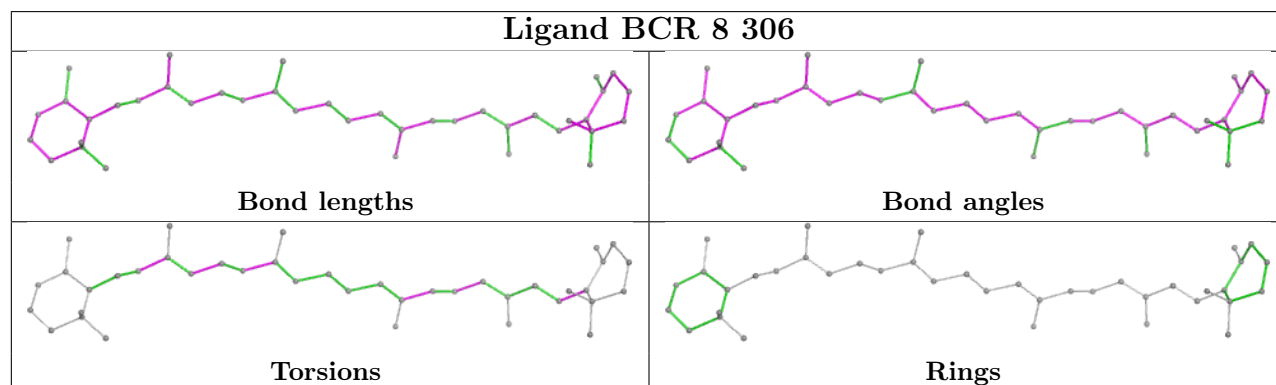
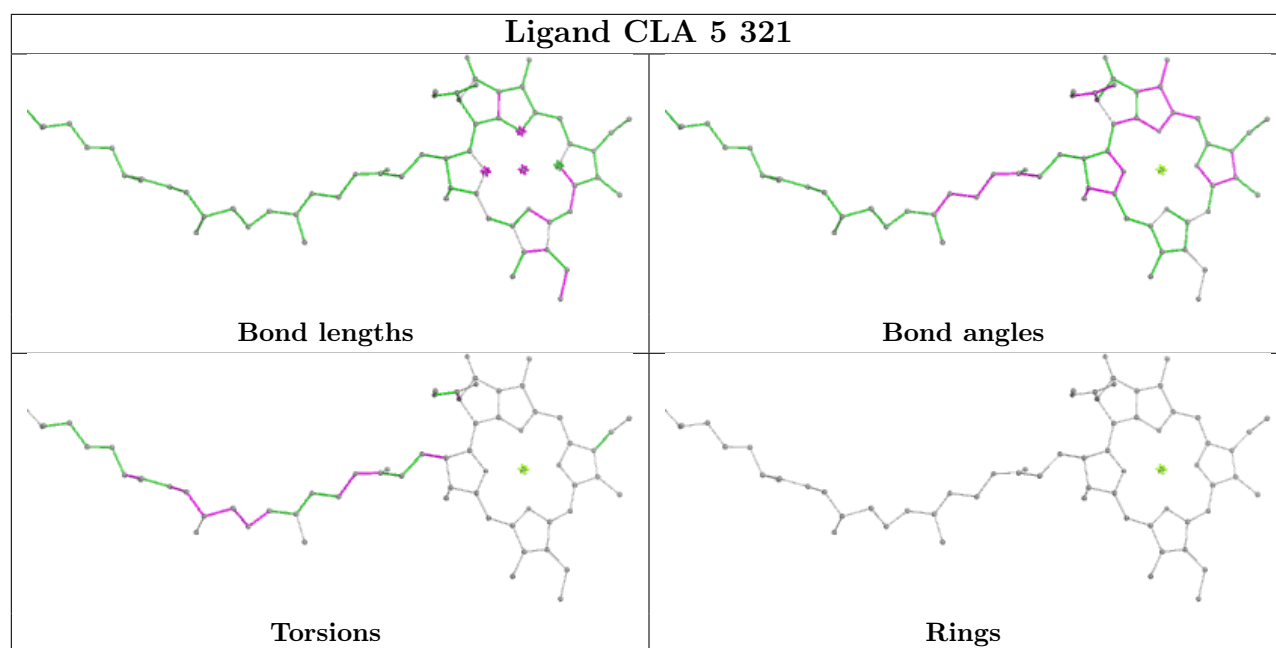


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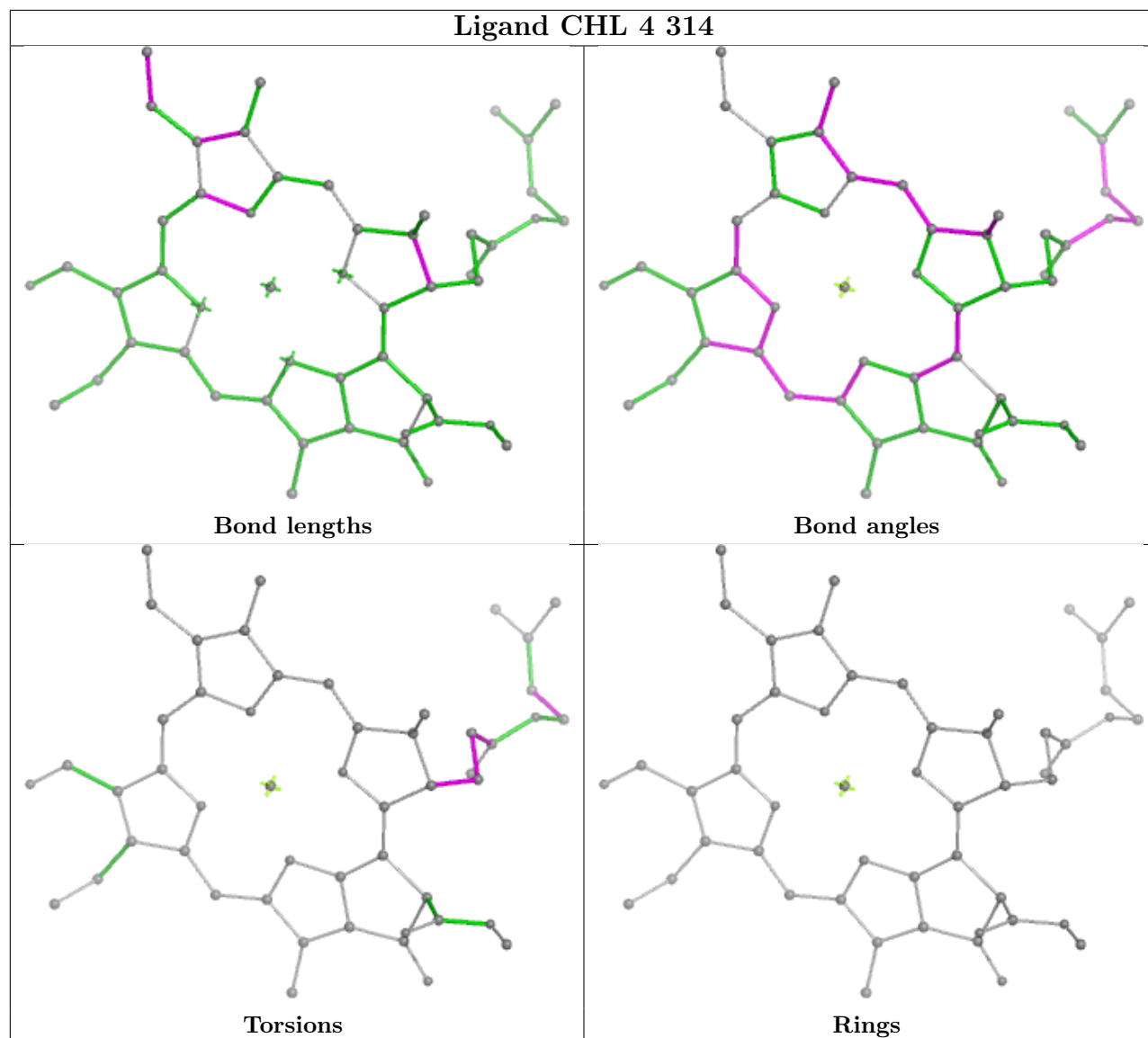


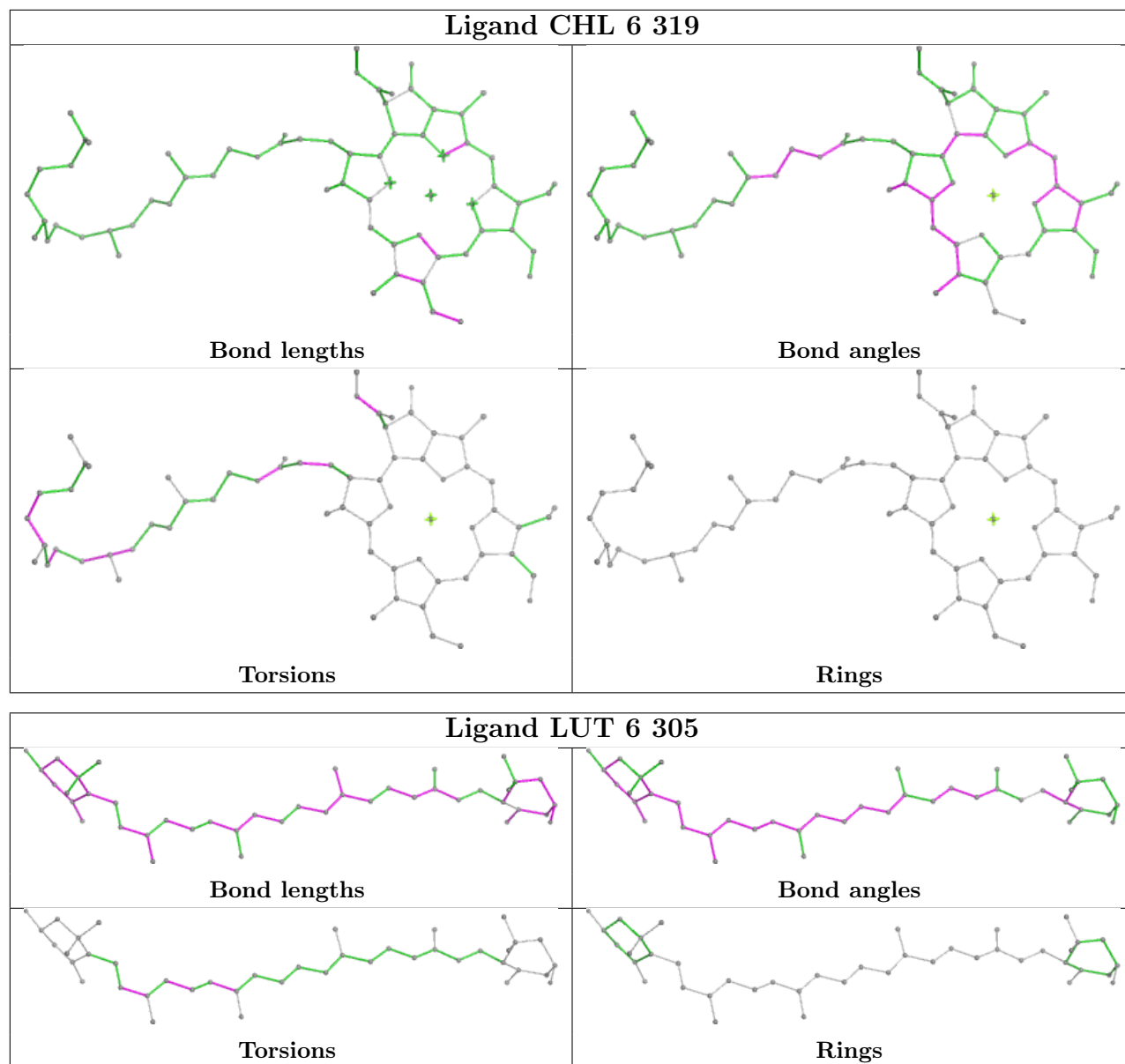
Ligand CLA 4 311



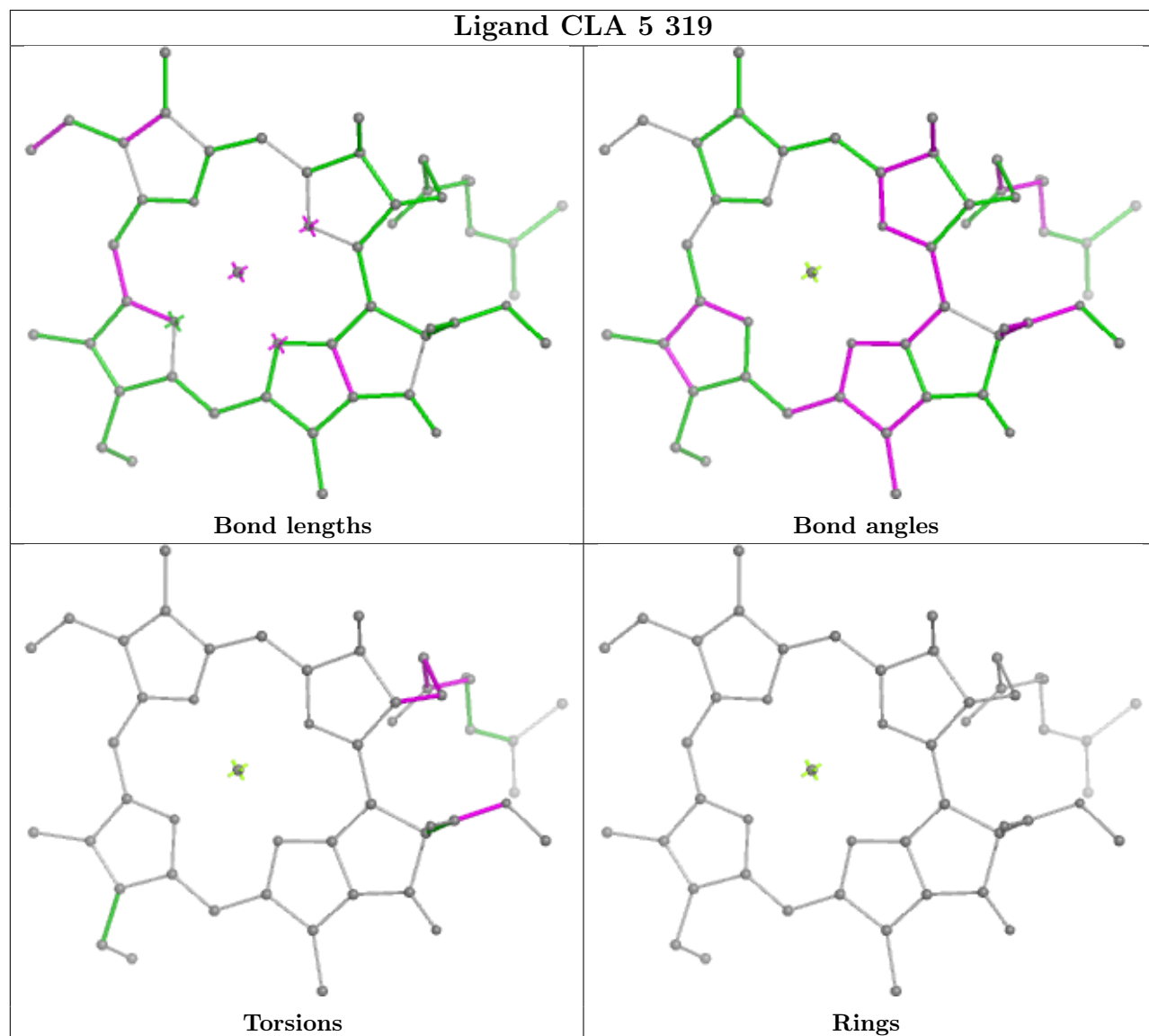


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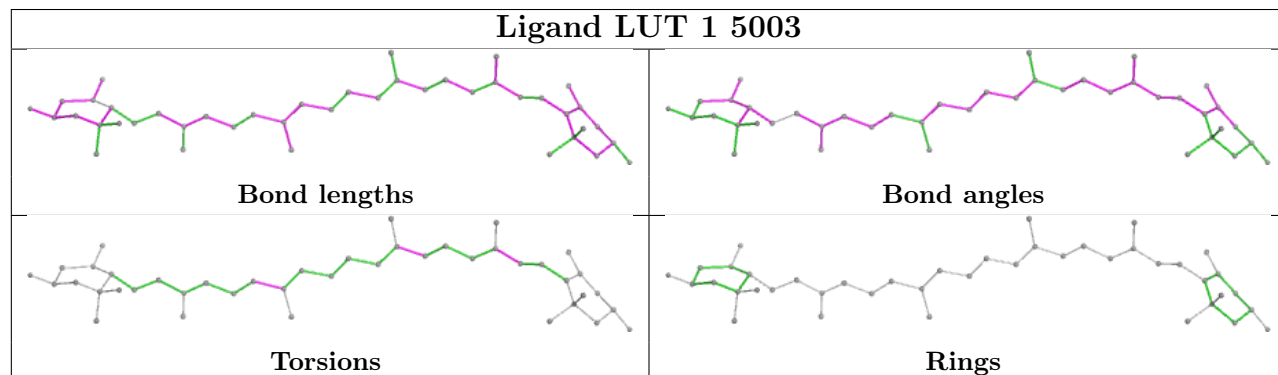




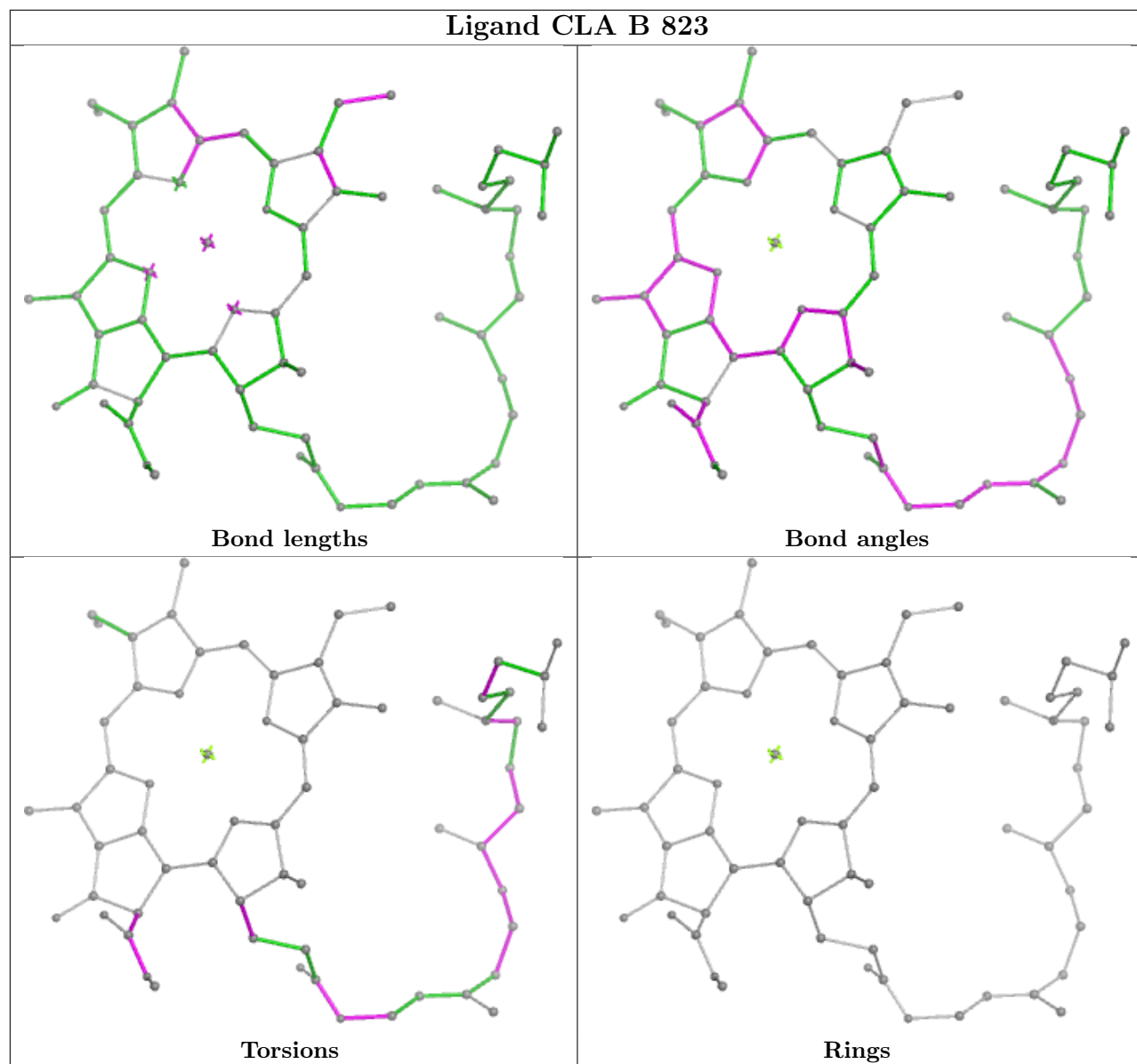
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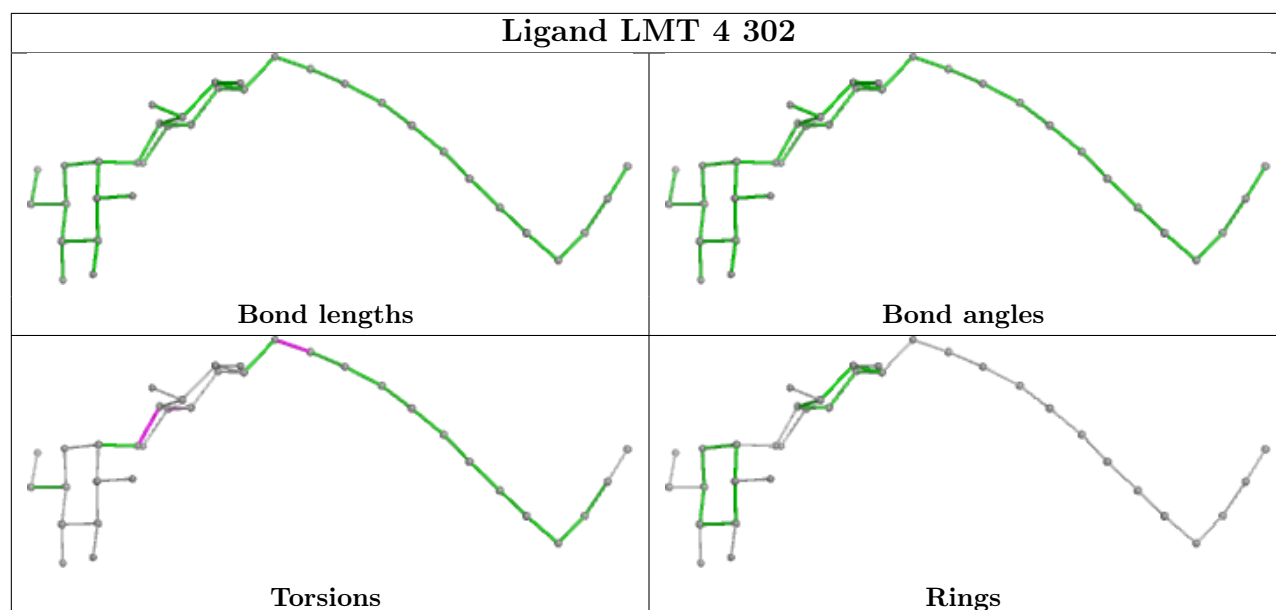
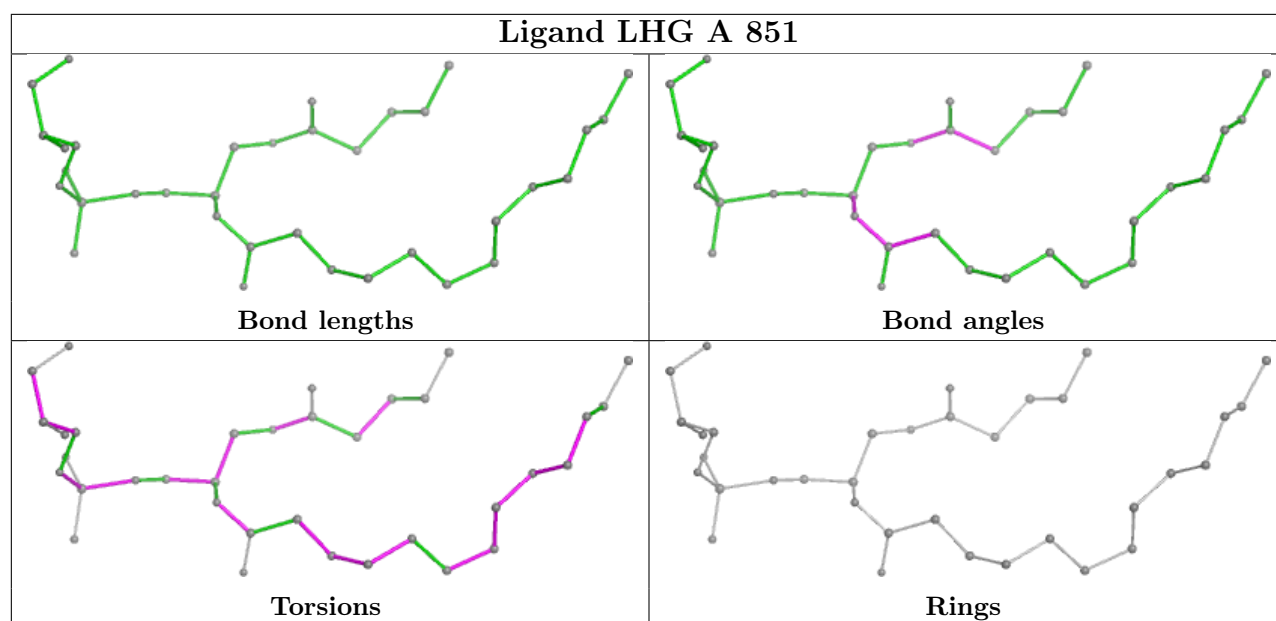


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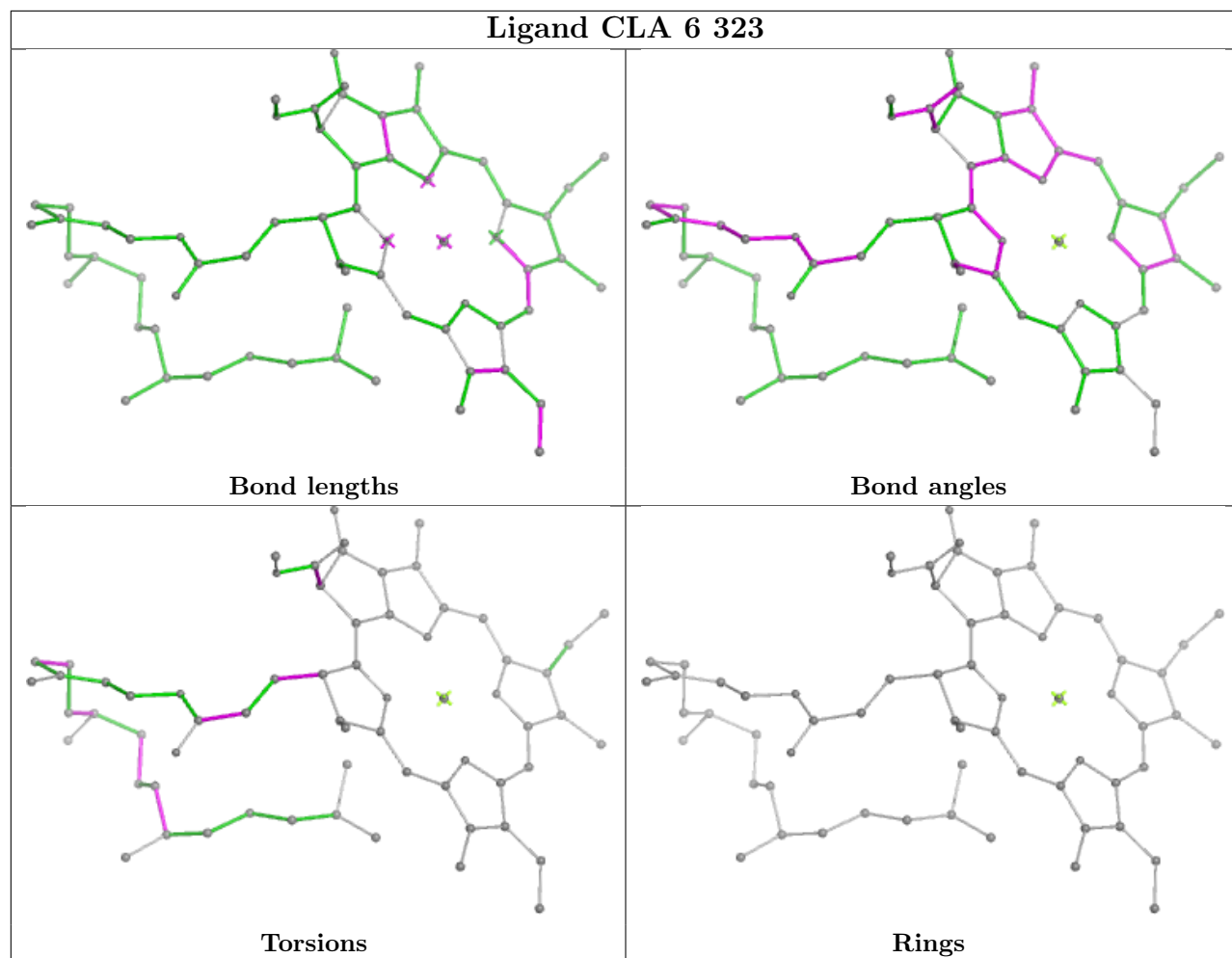


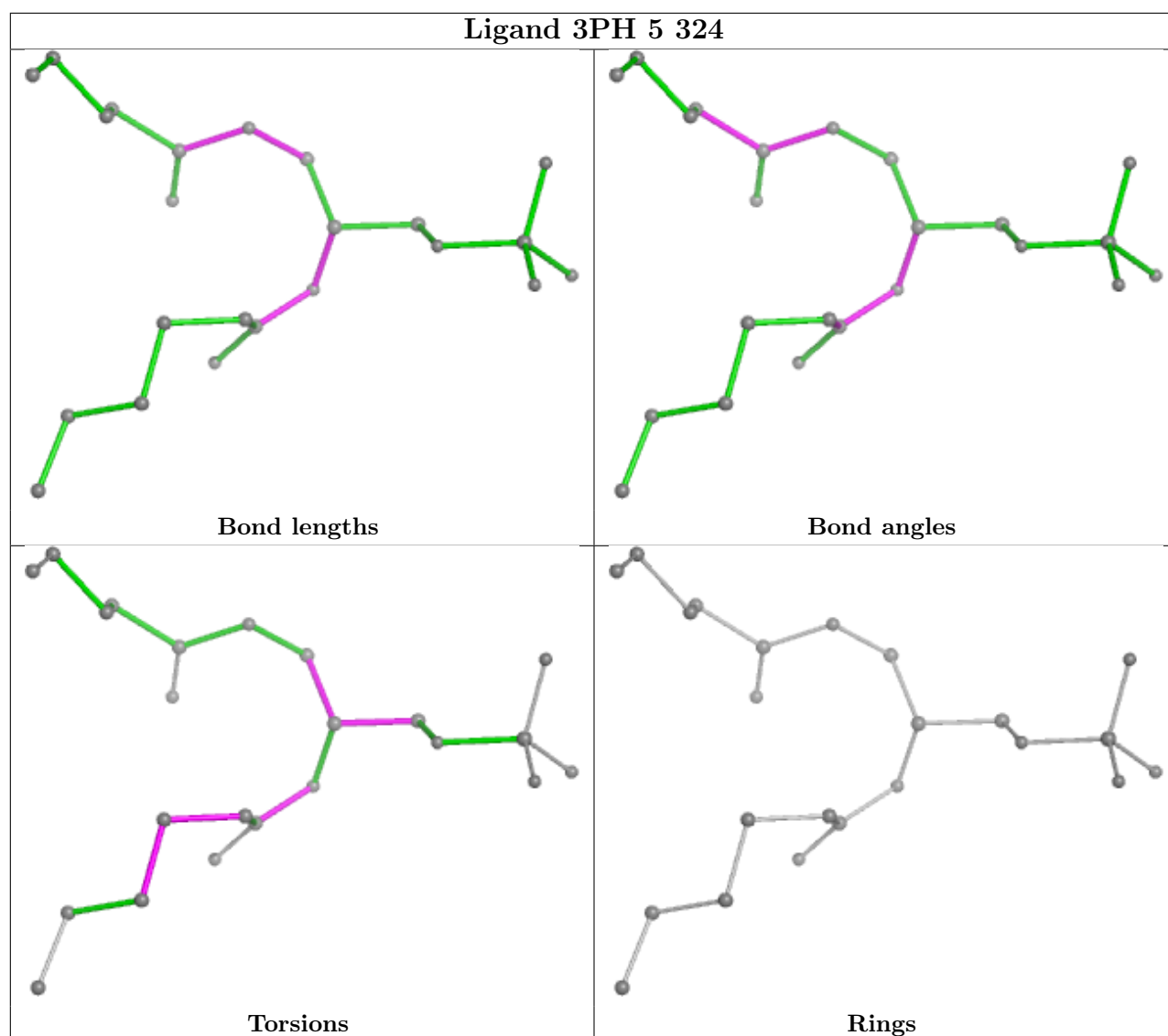
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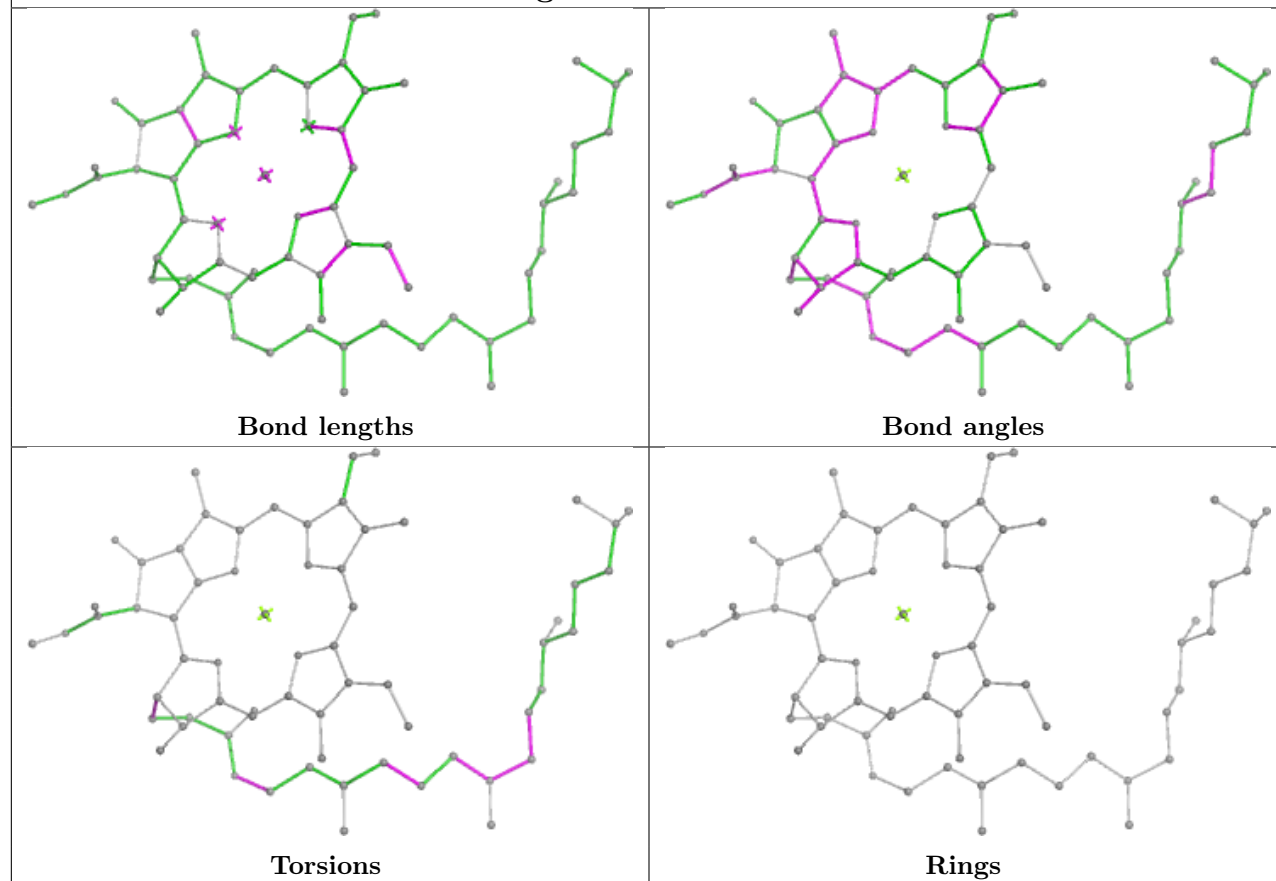


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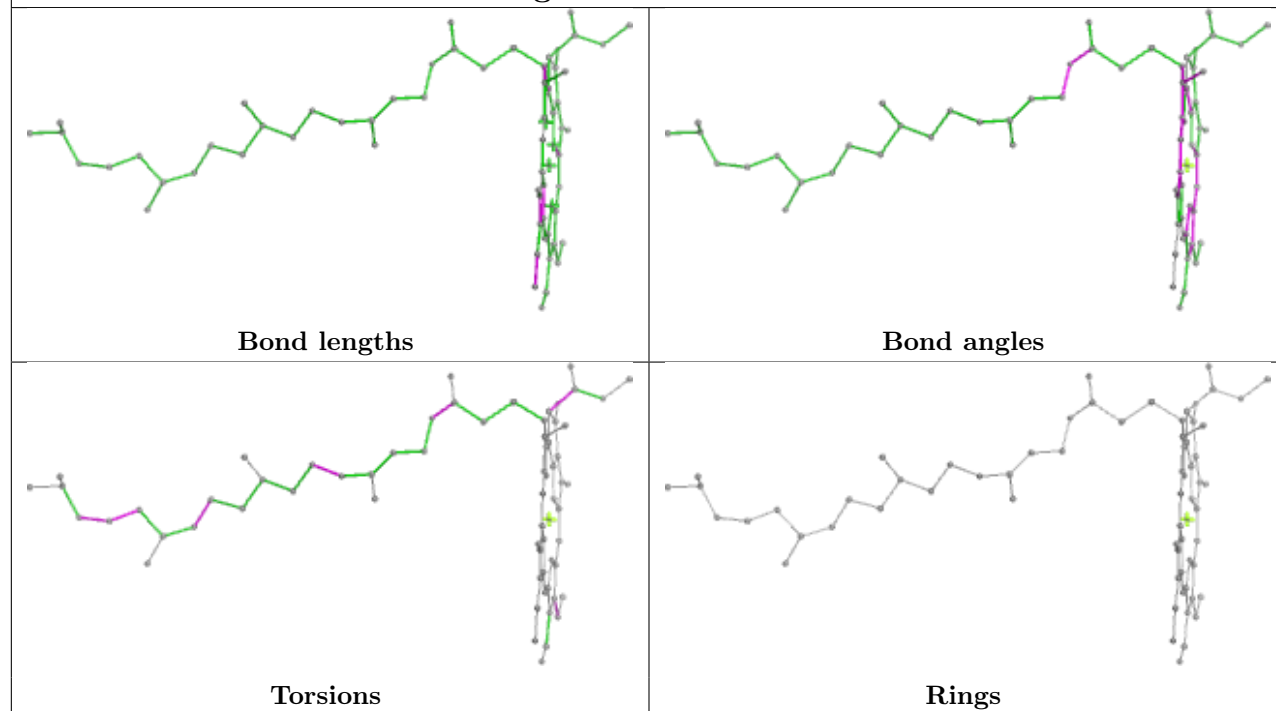




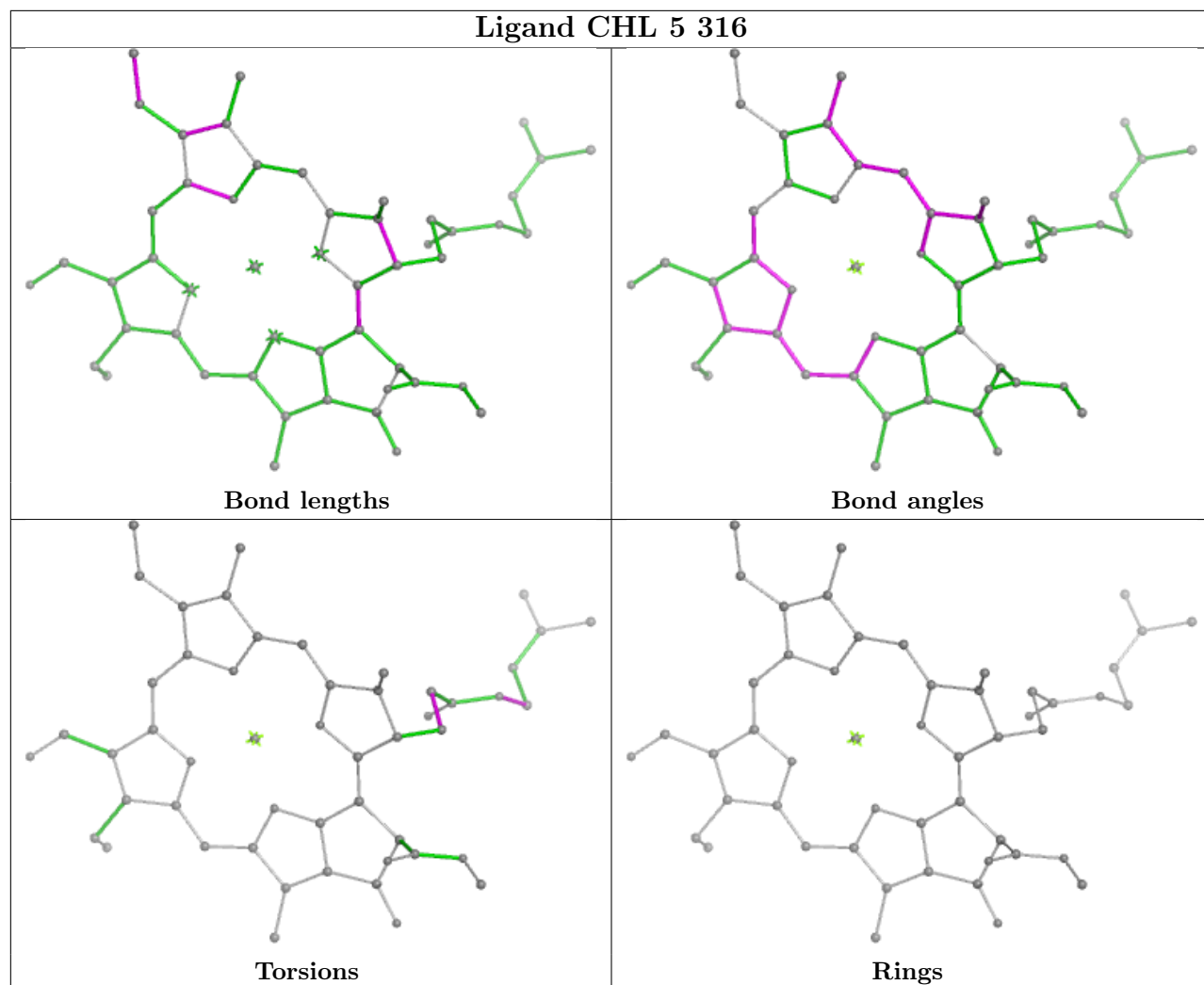
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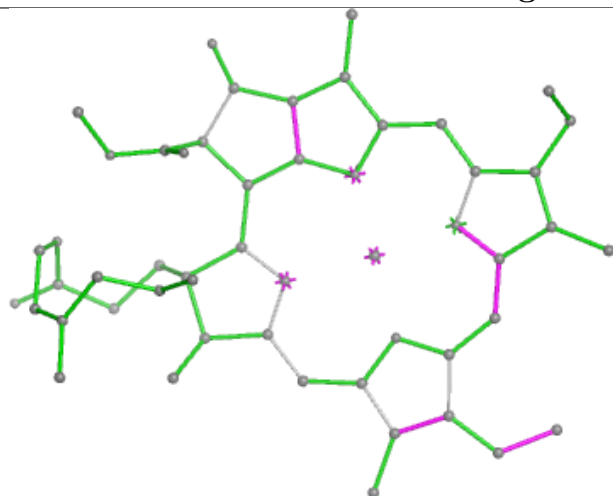
Ligand CHL Z 310



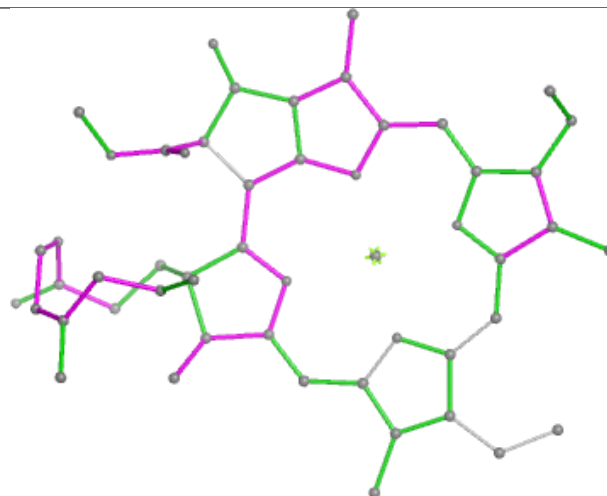
Ligand CHL 5 316



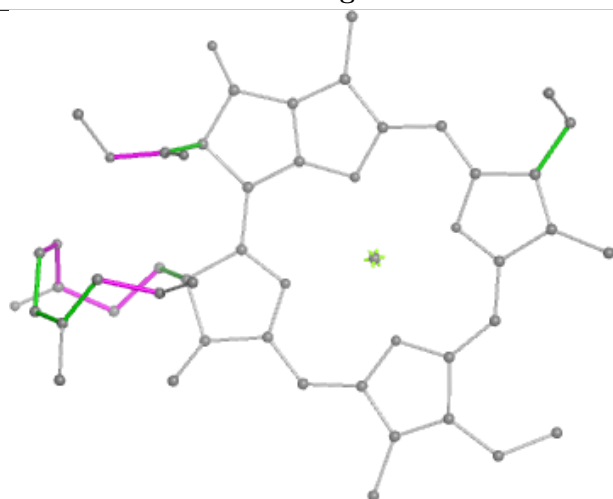
Ligand CLA 4 307



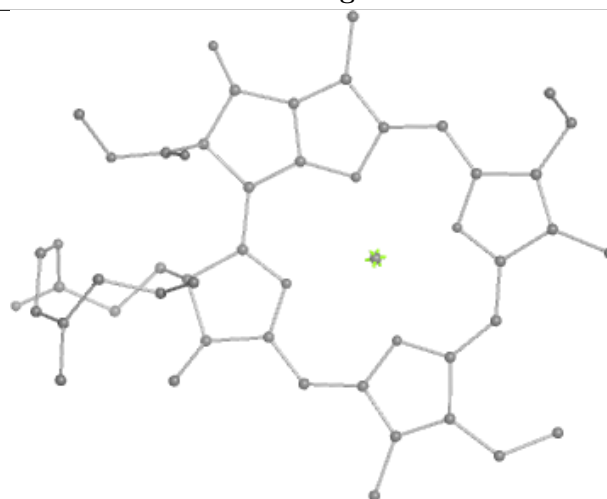
Bond lengths



Bond angles

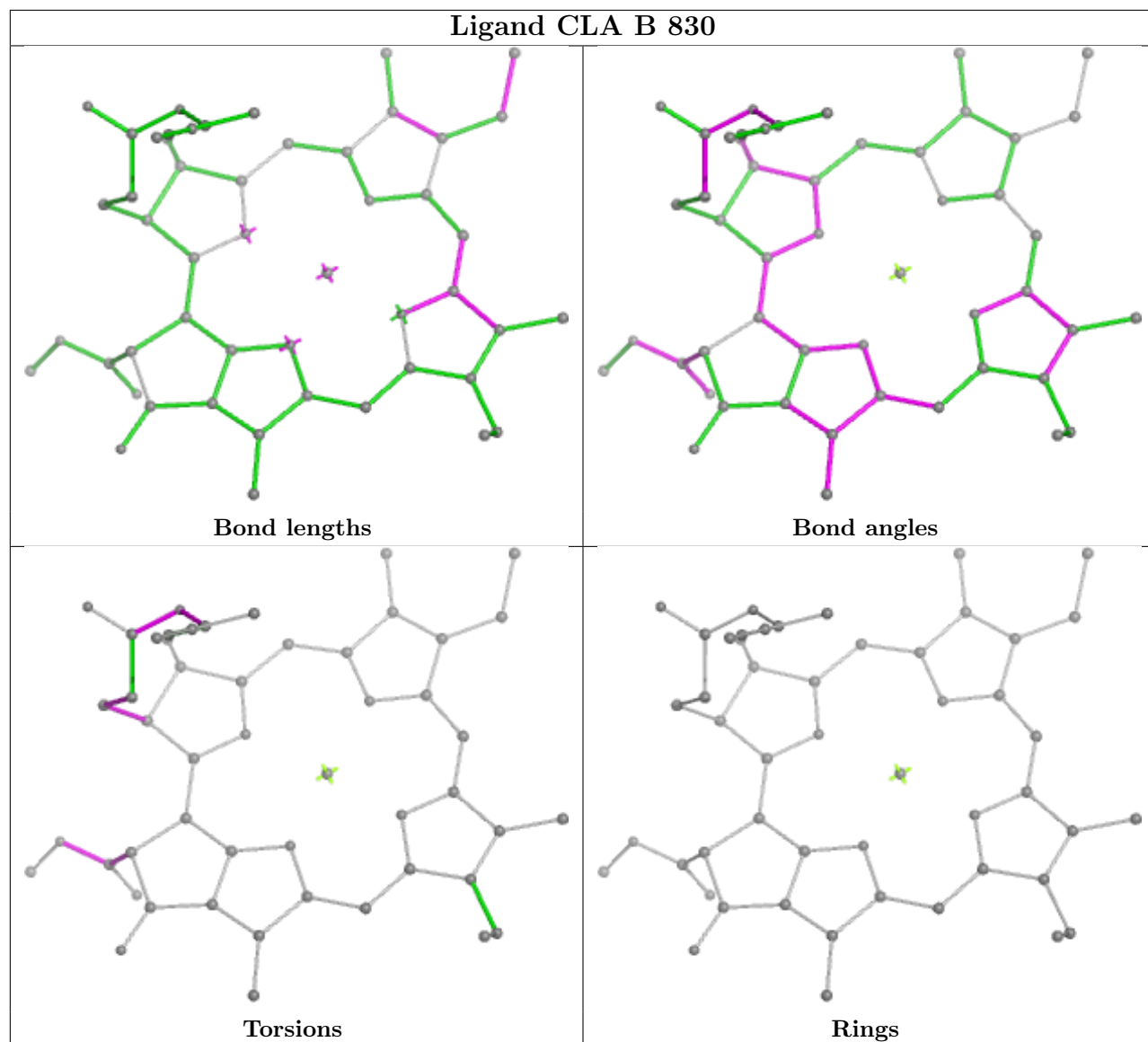


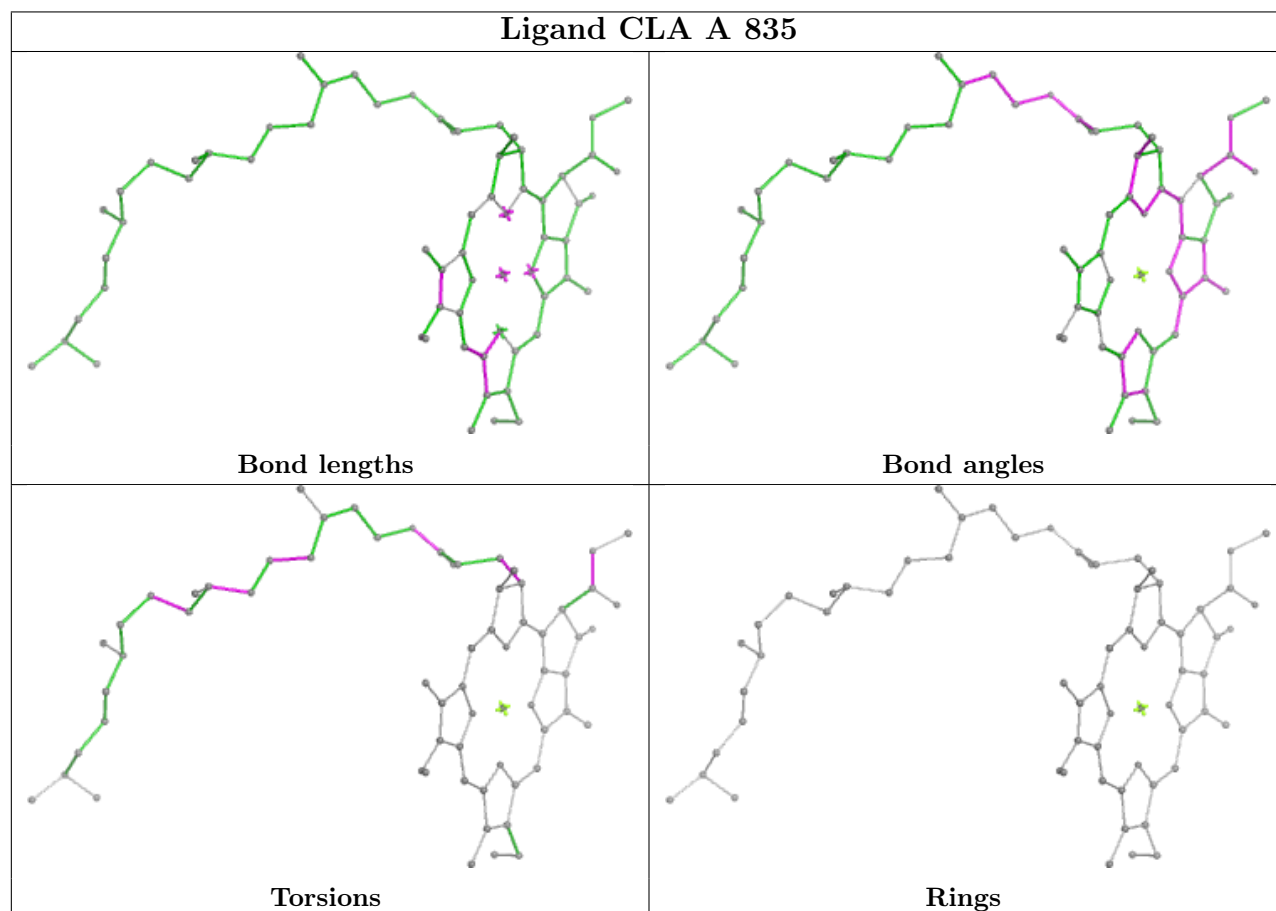
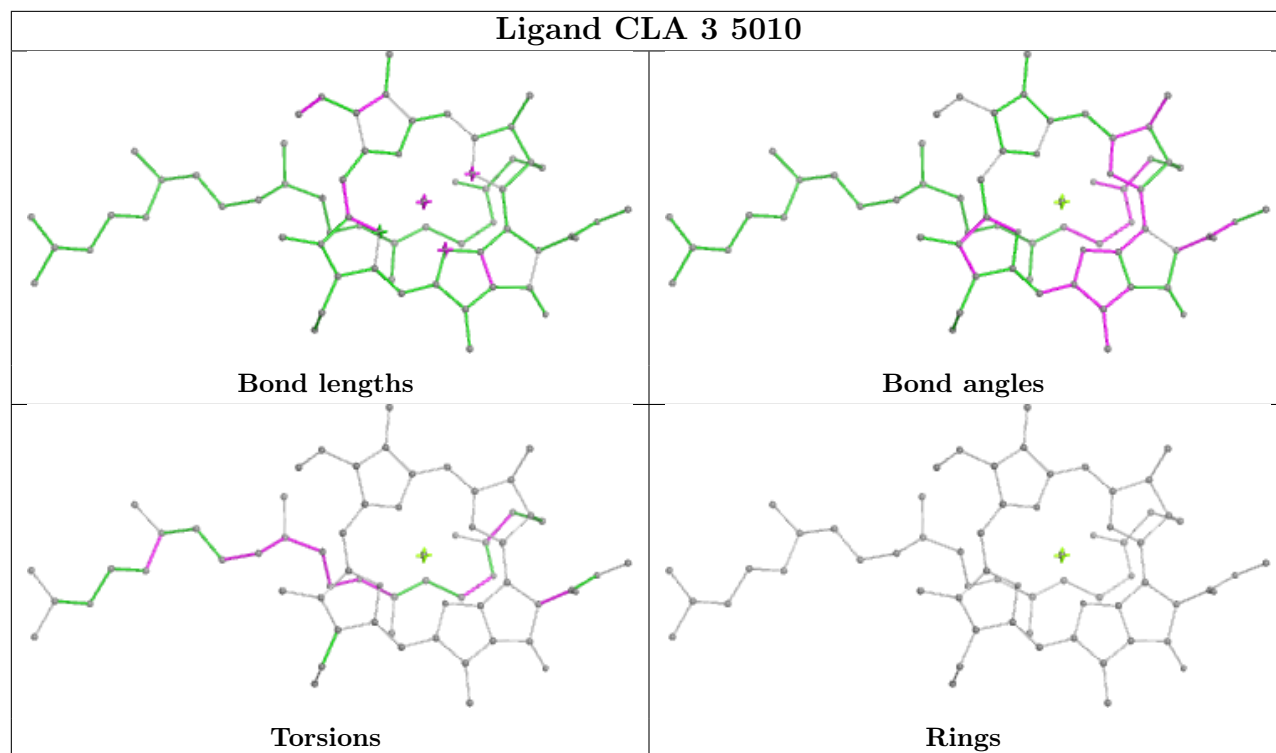
Torsions



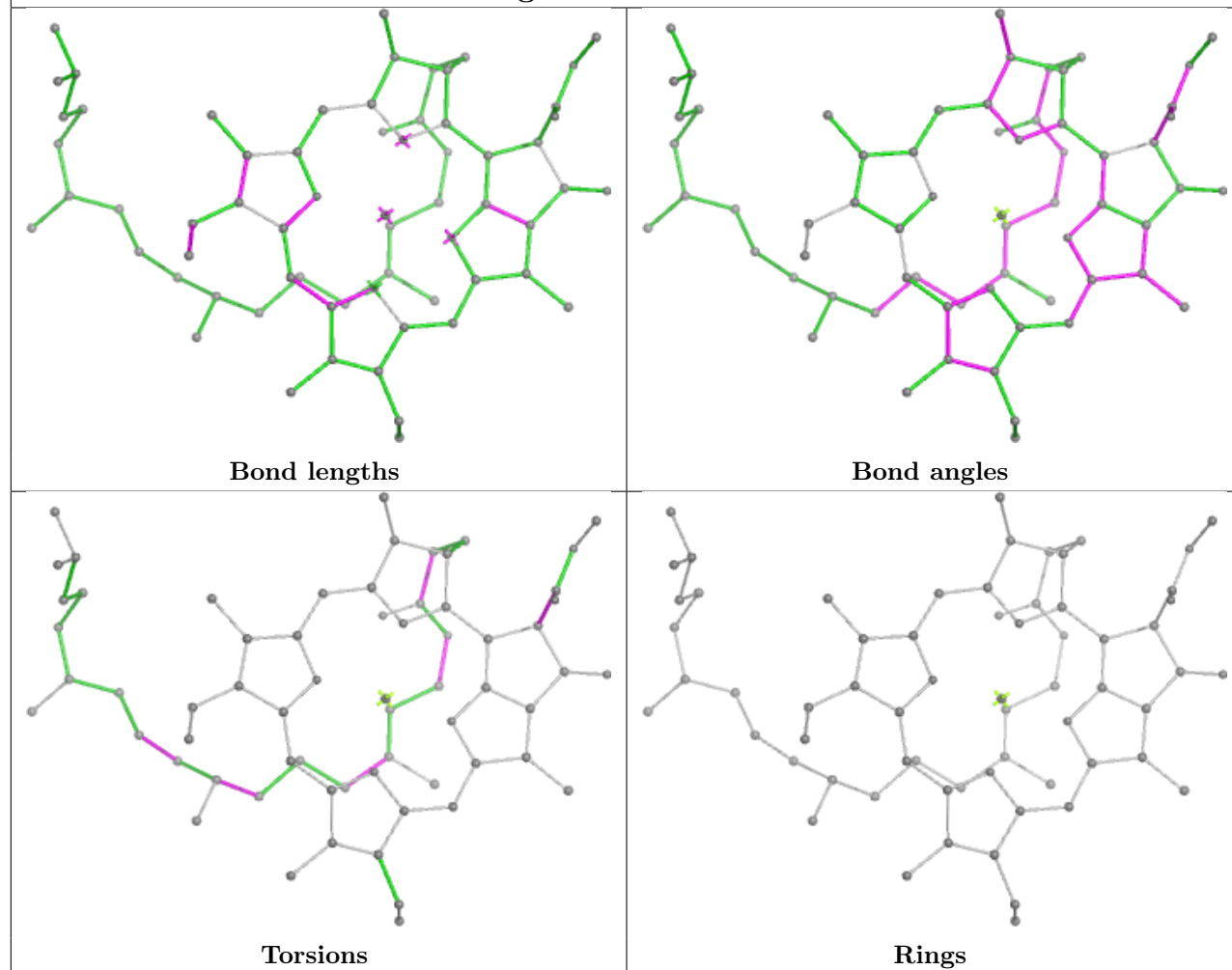
Rings

Ligand CLA B 830

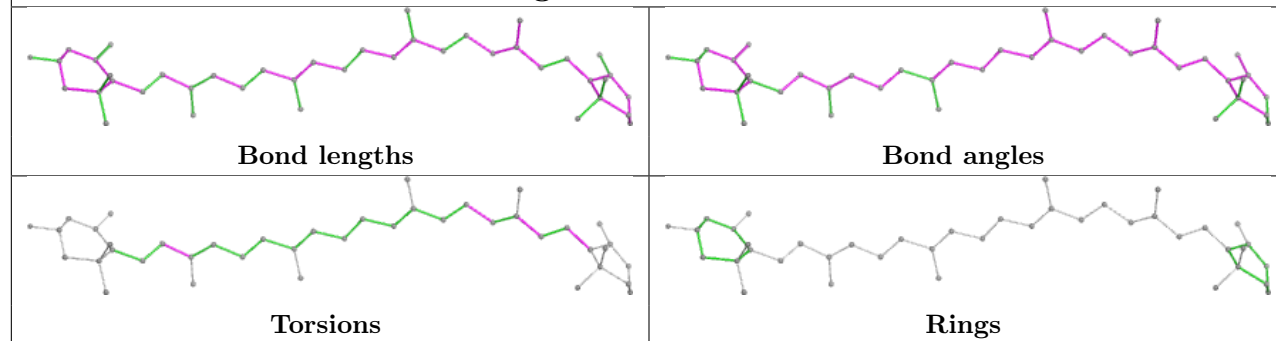


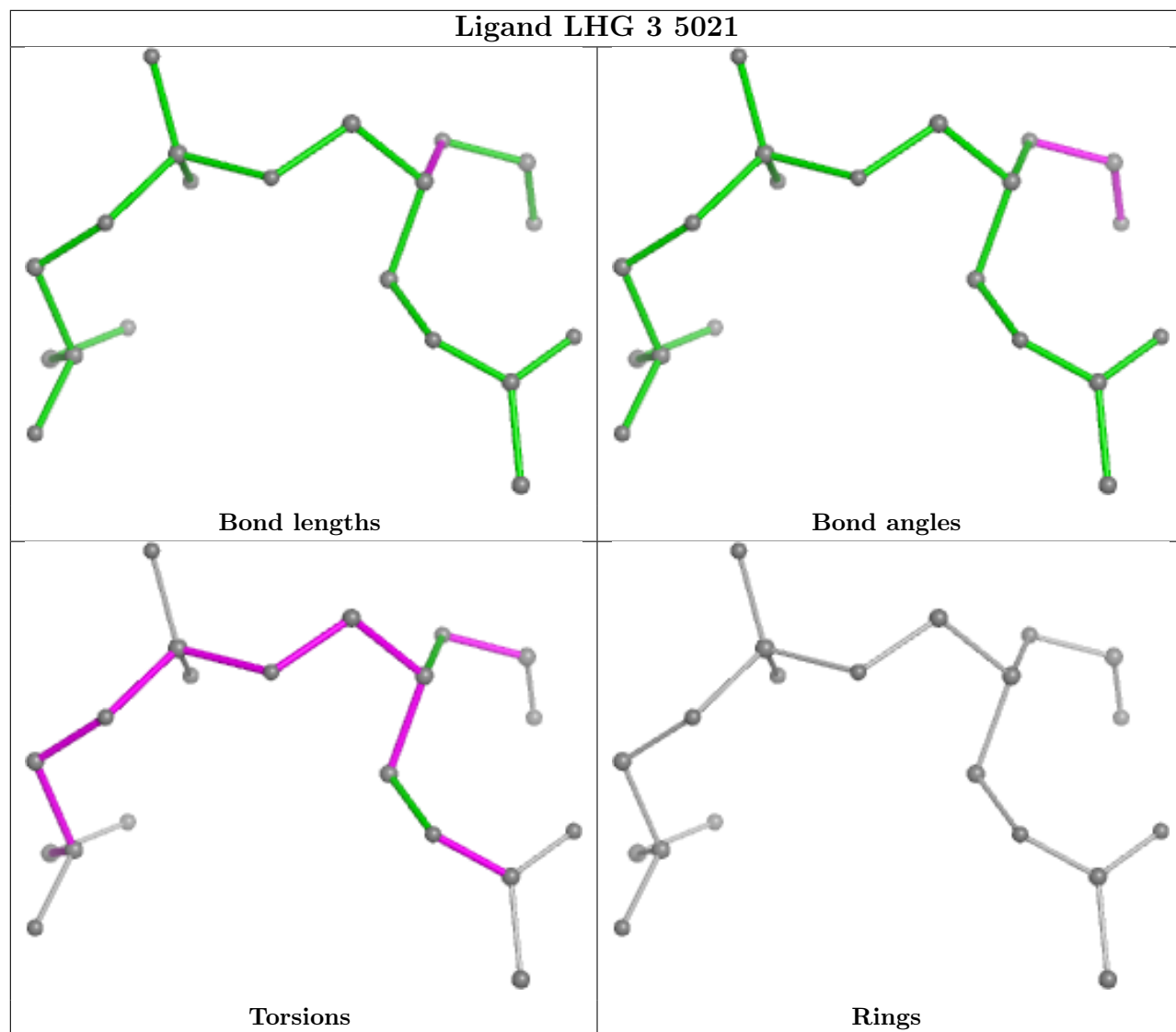


Ligand CLA 6 311

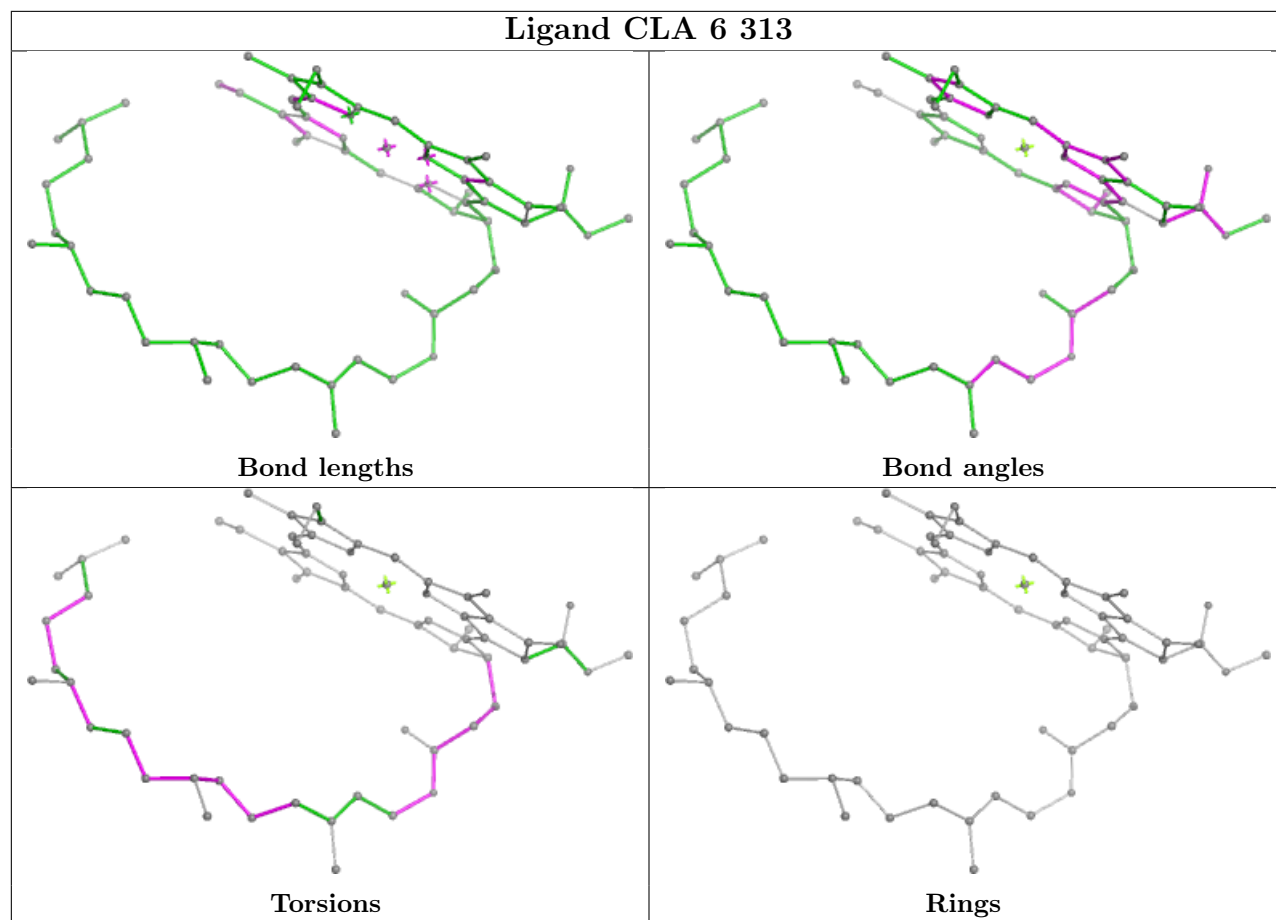


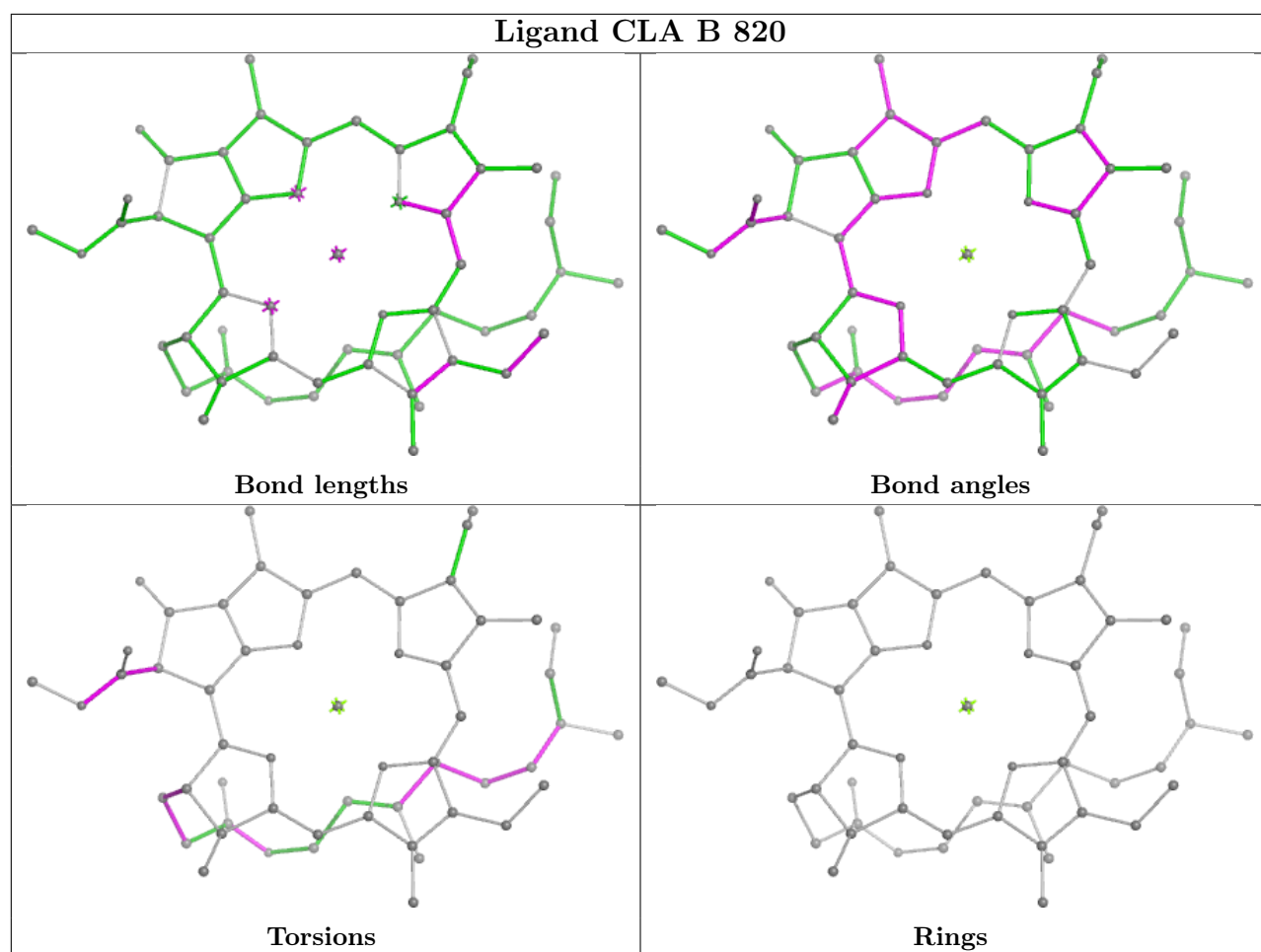
Ligand RRX 4 303

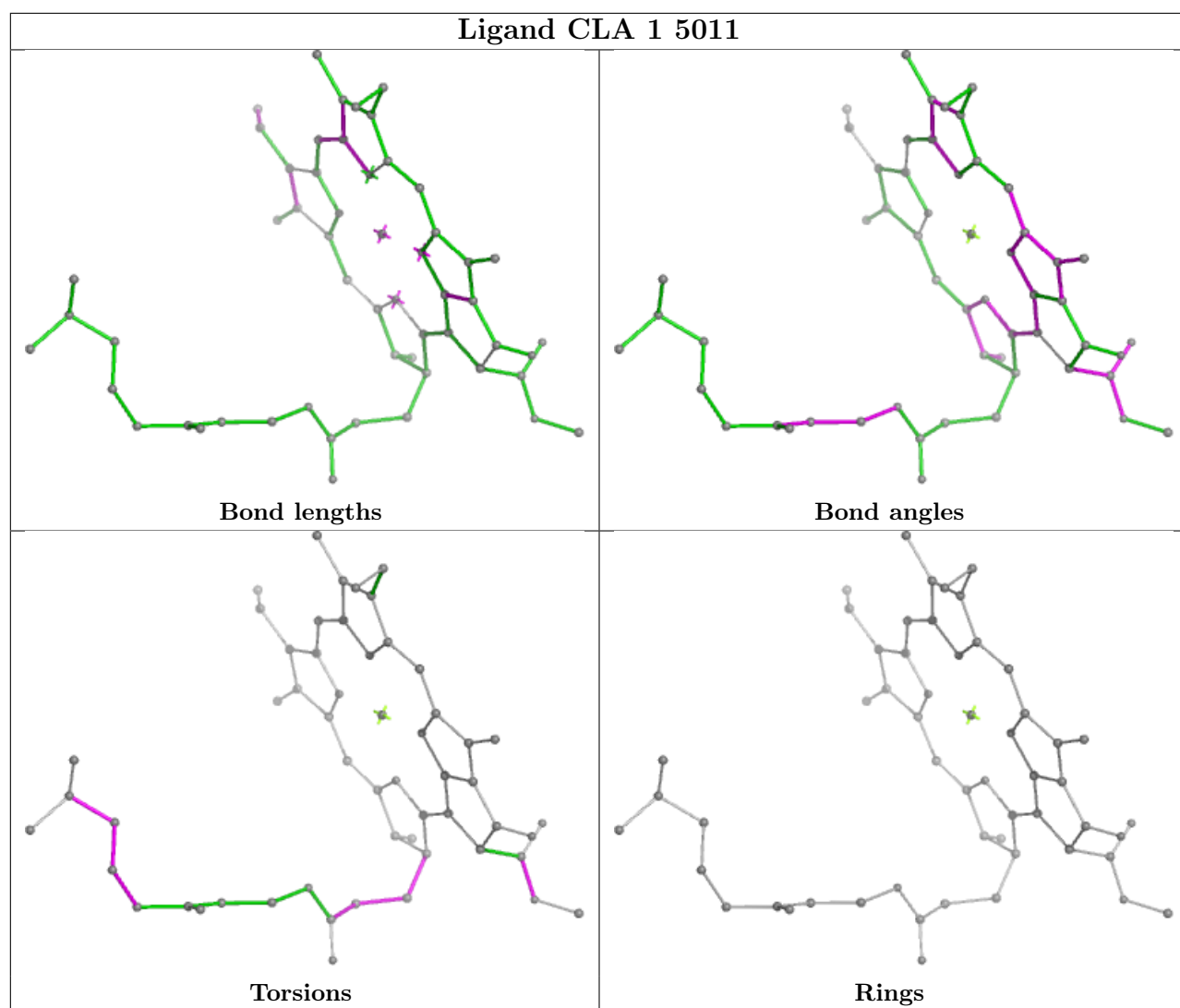




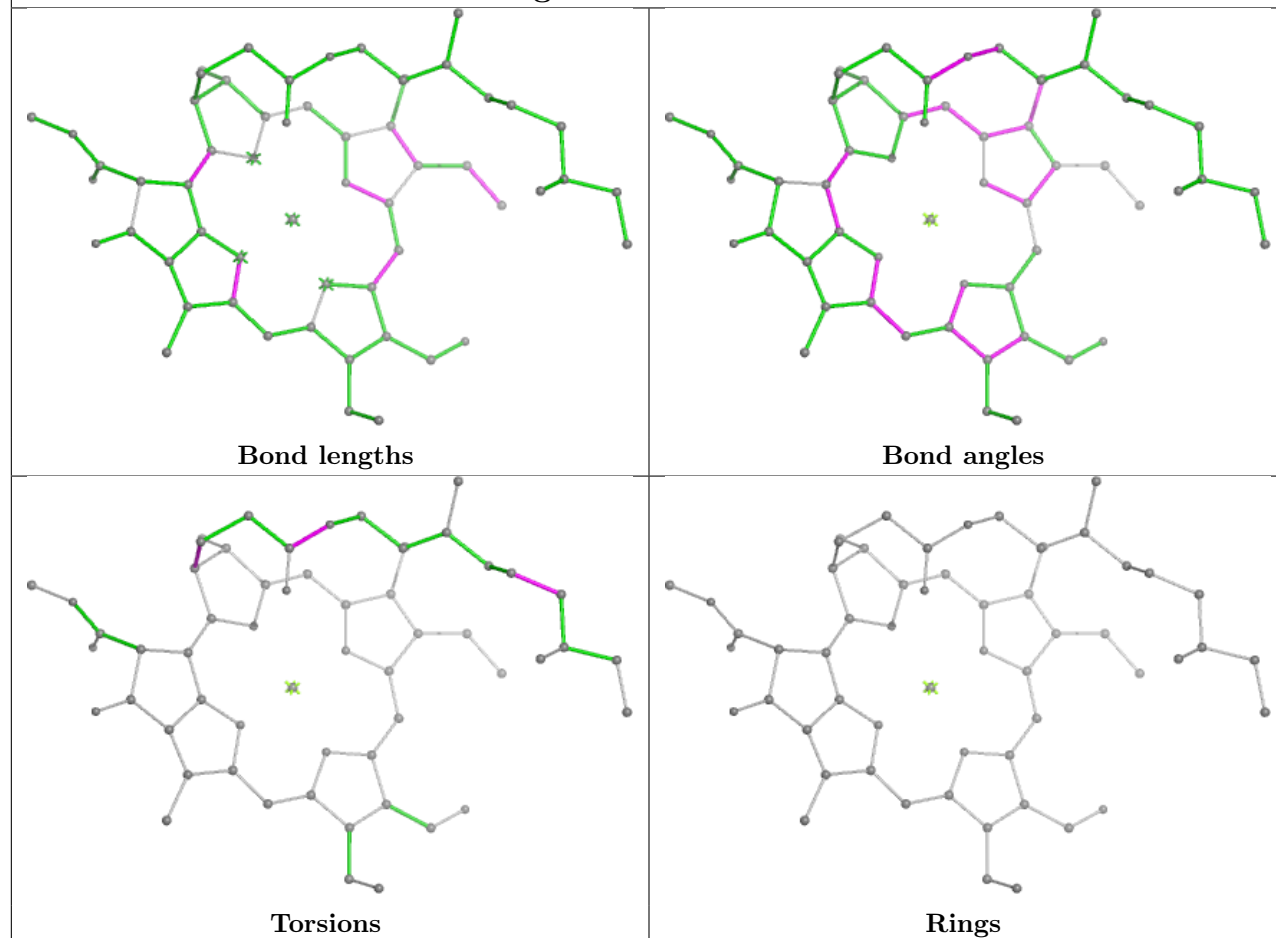
Ligand CLA 6 313



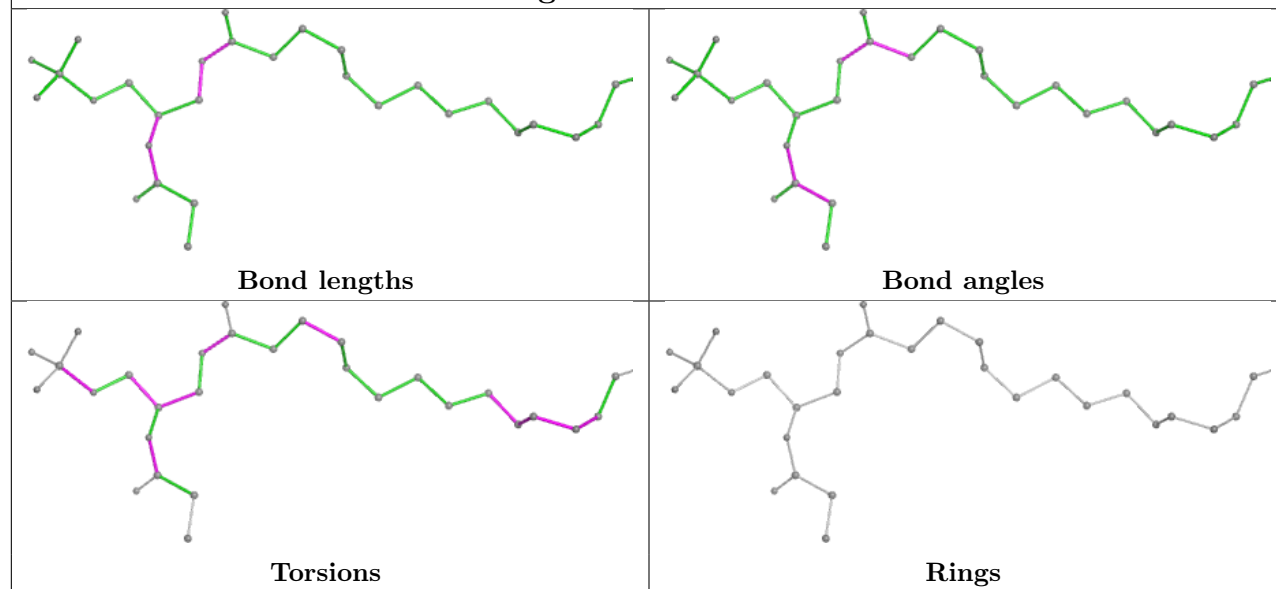




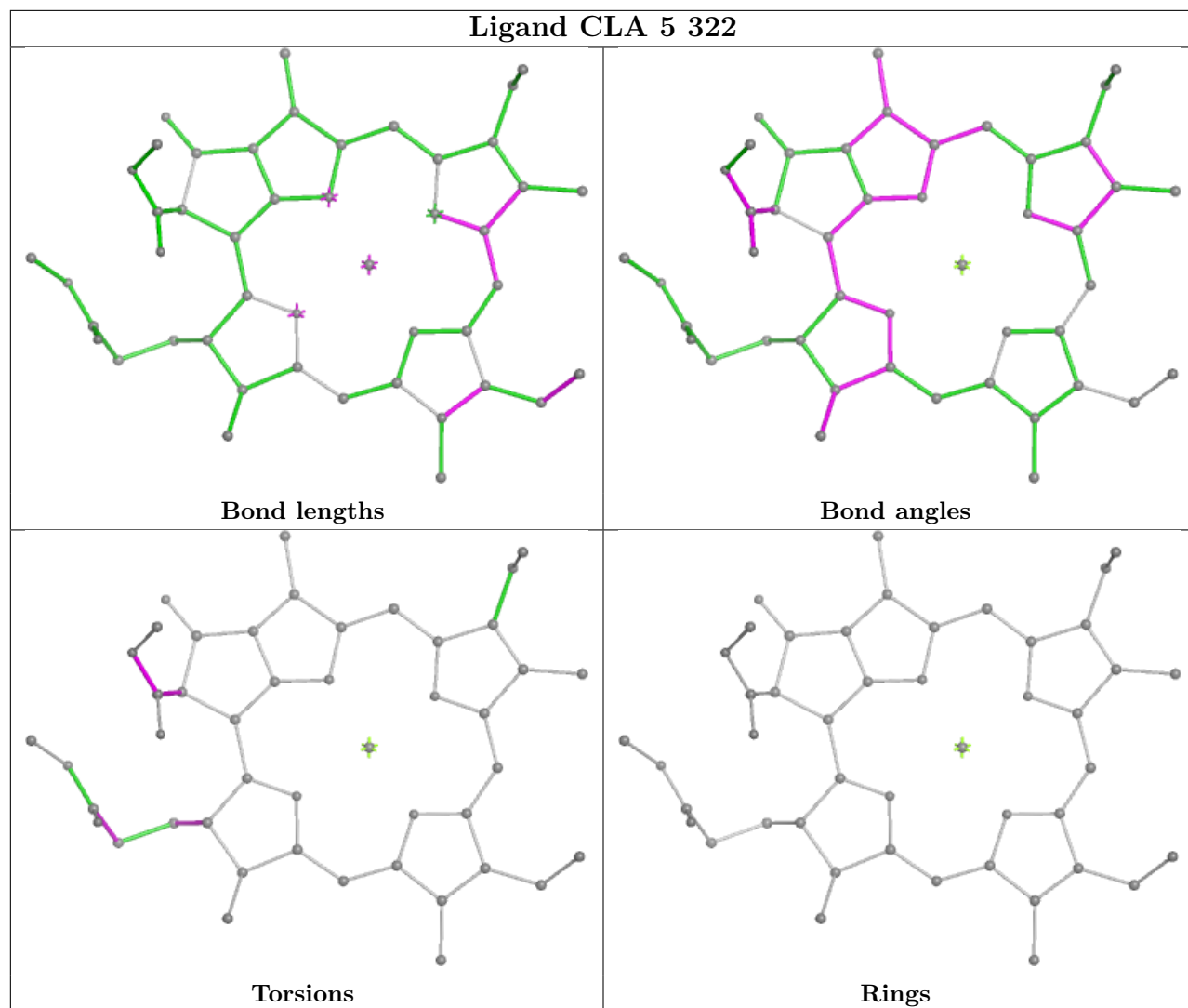
Ligand CHL Z 302

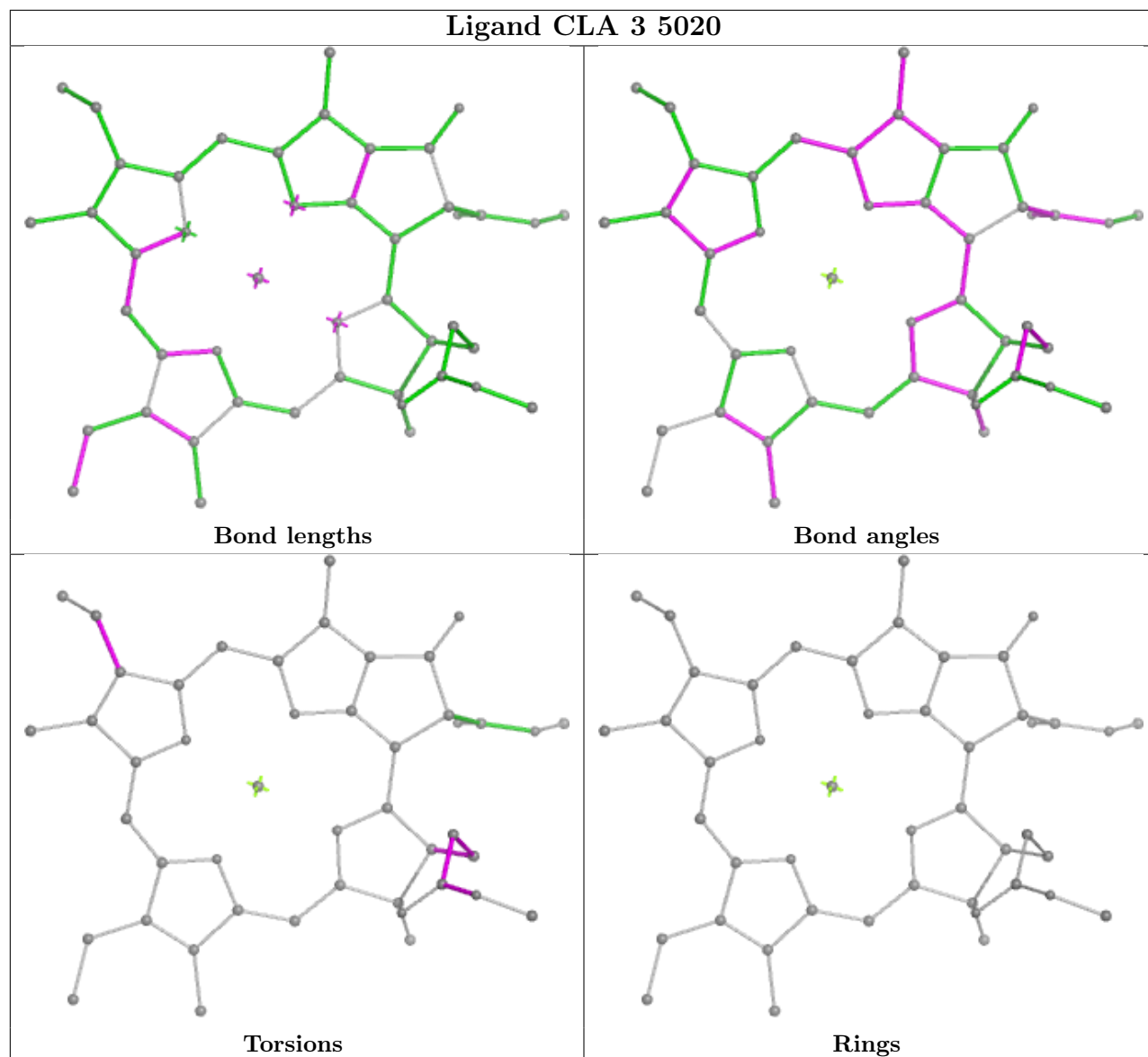


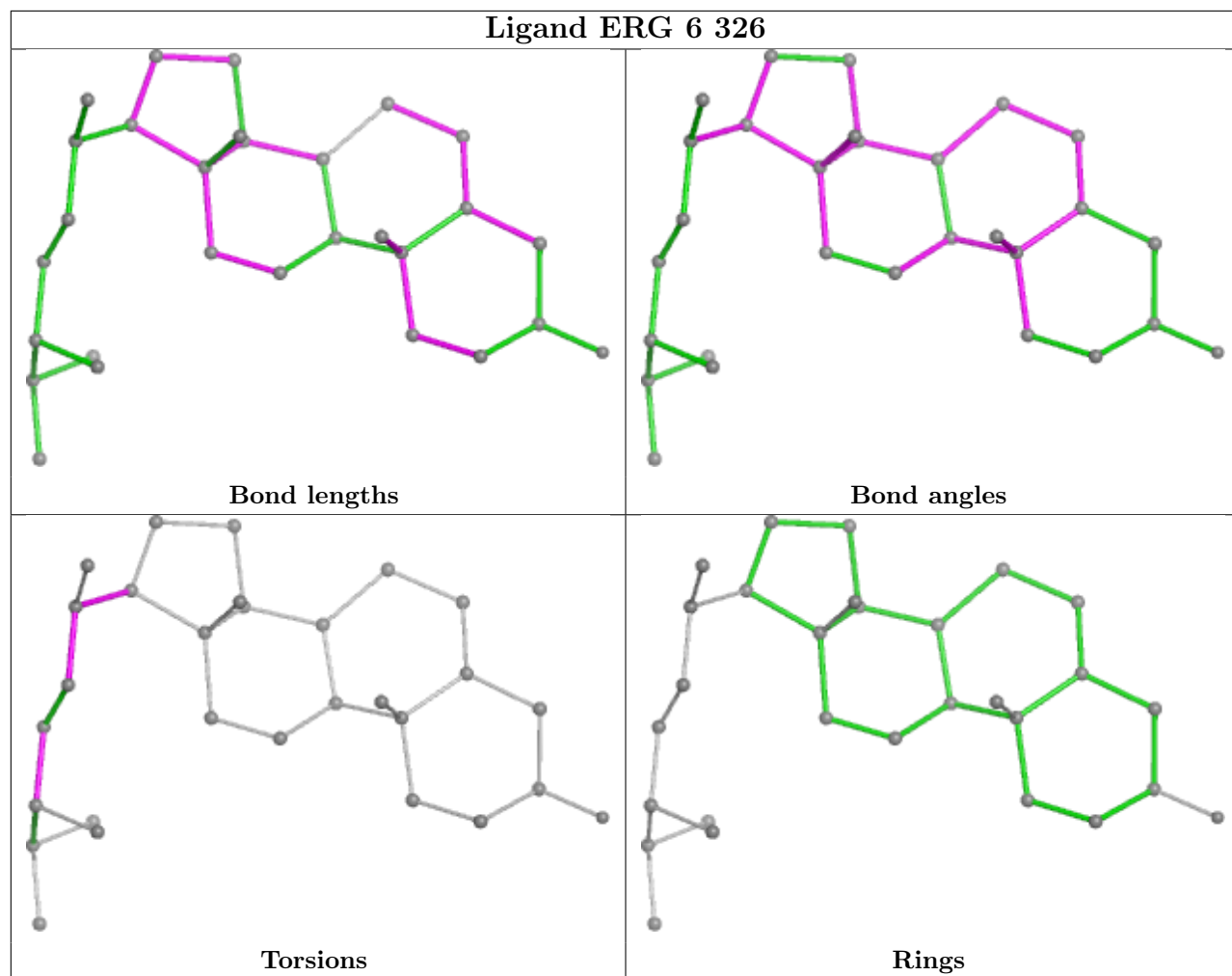
Ligand 3PH 8 322



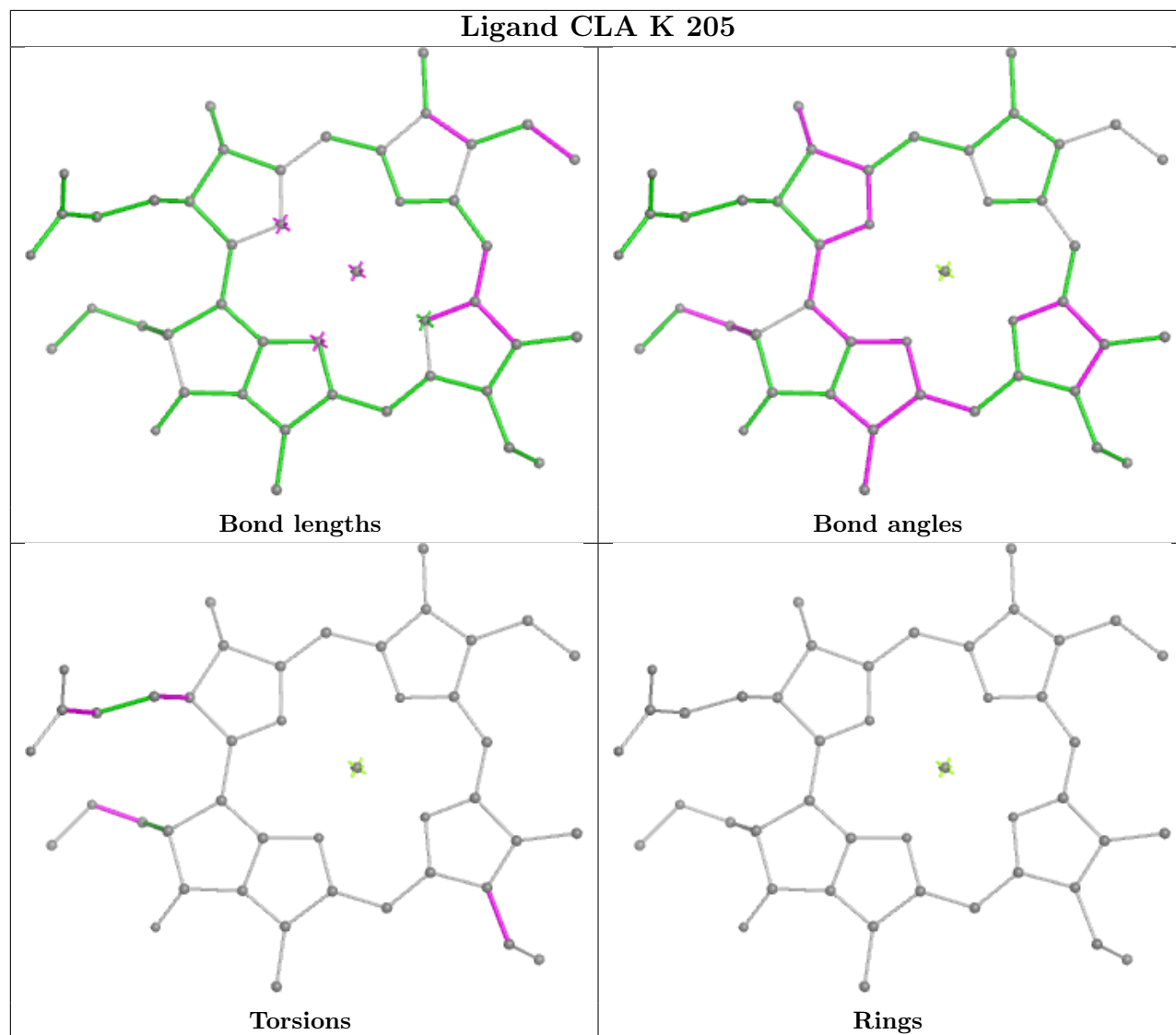
Ligand CLA 5 322



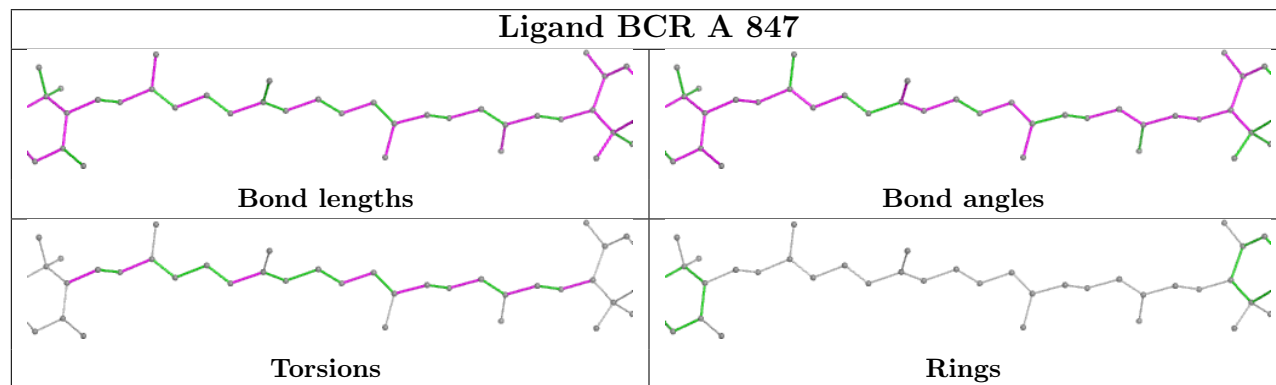




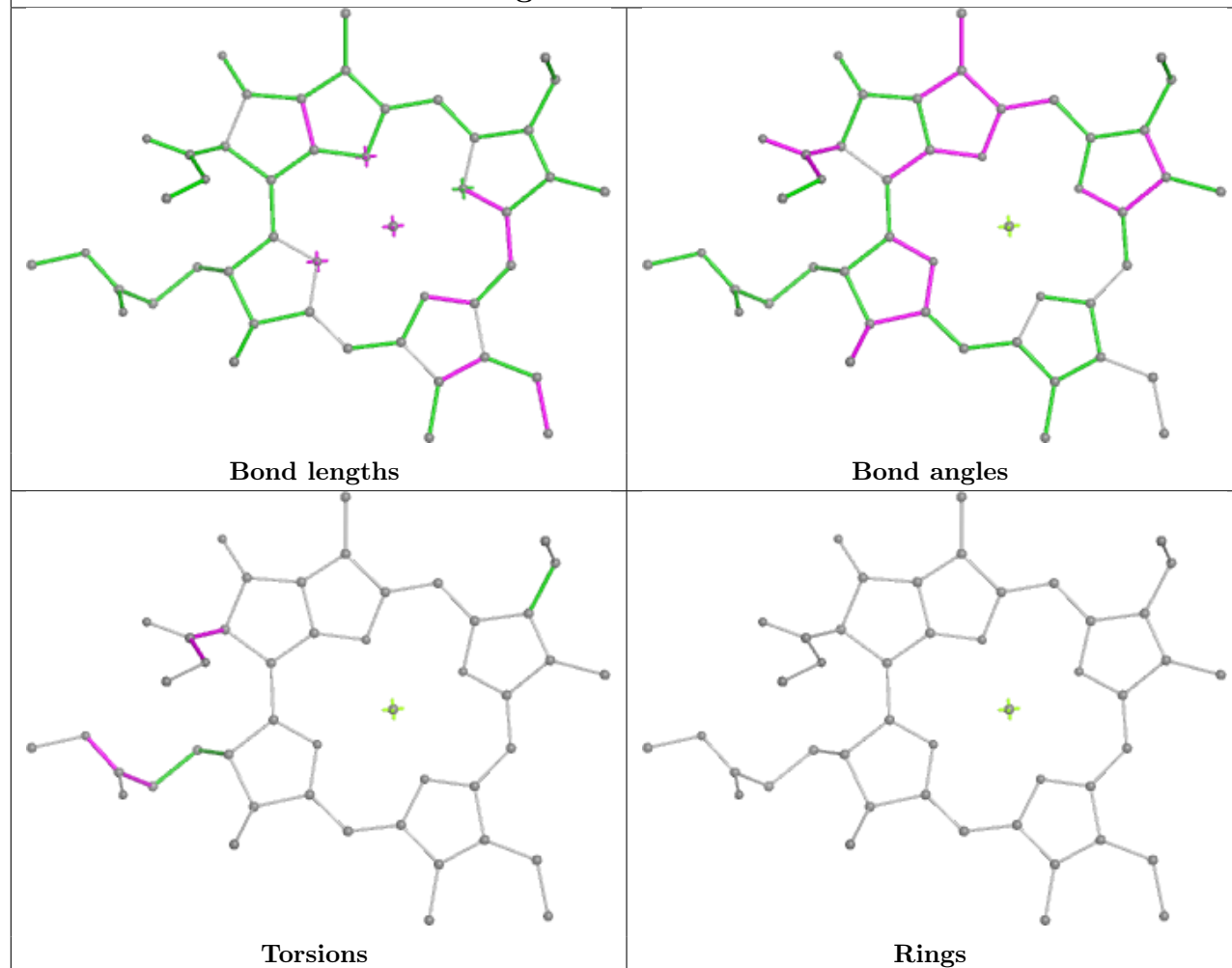
Ligand CLA K 205



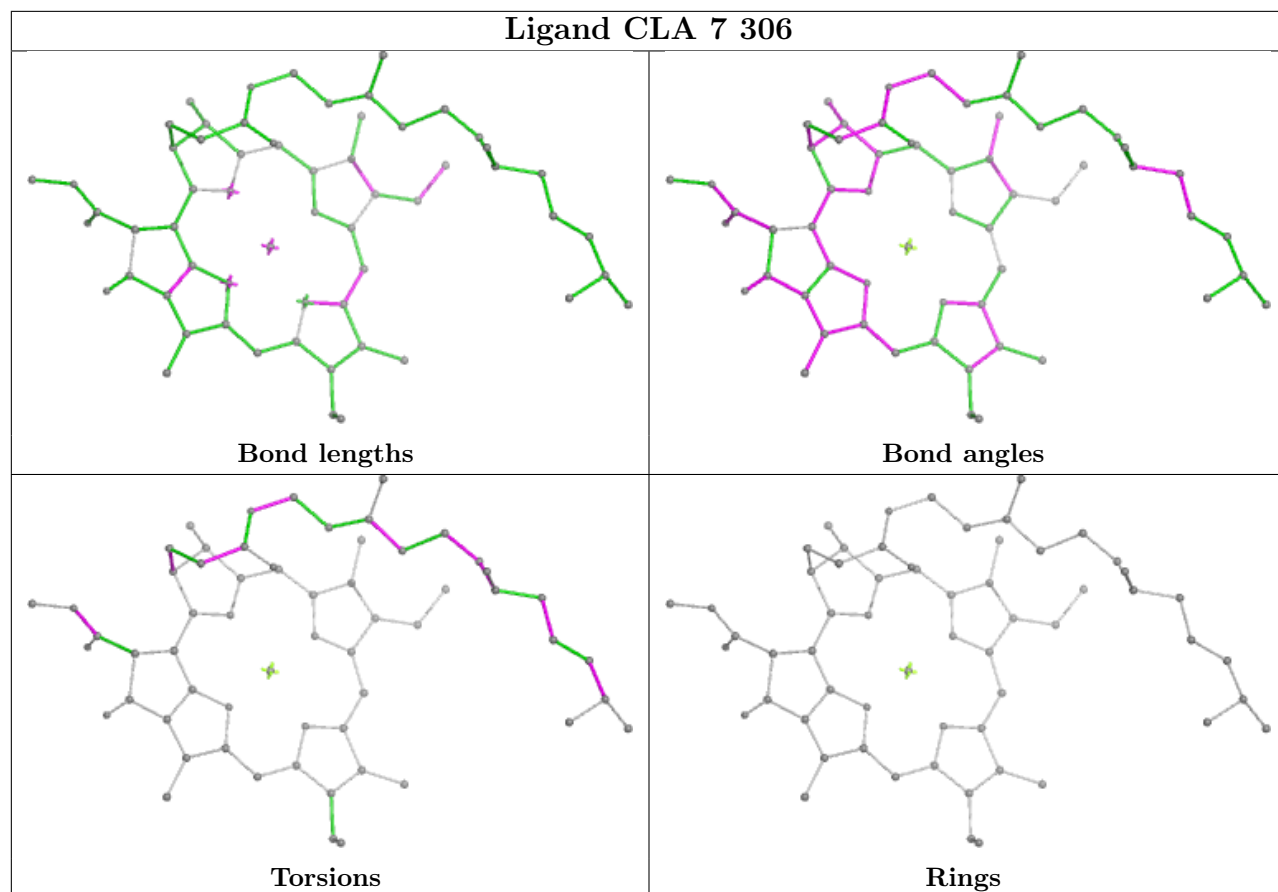
Ligand BCR A 847



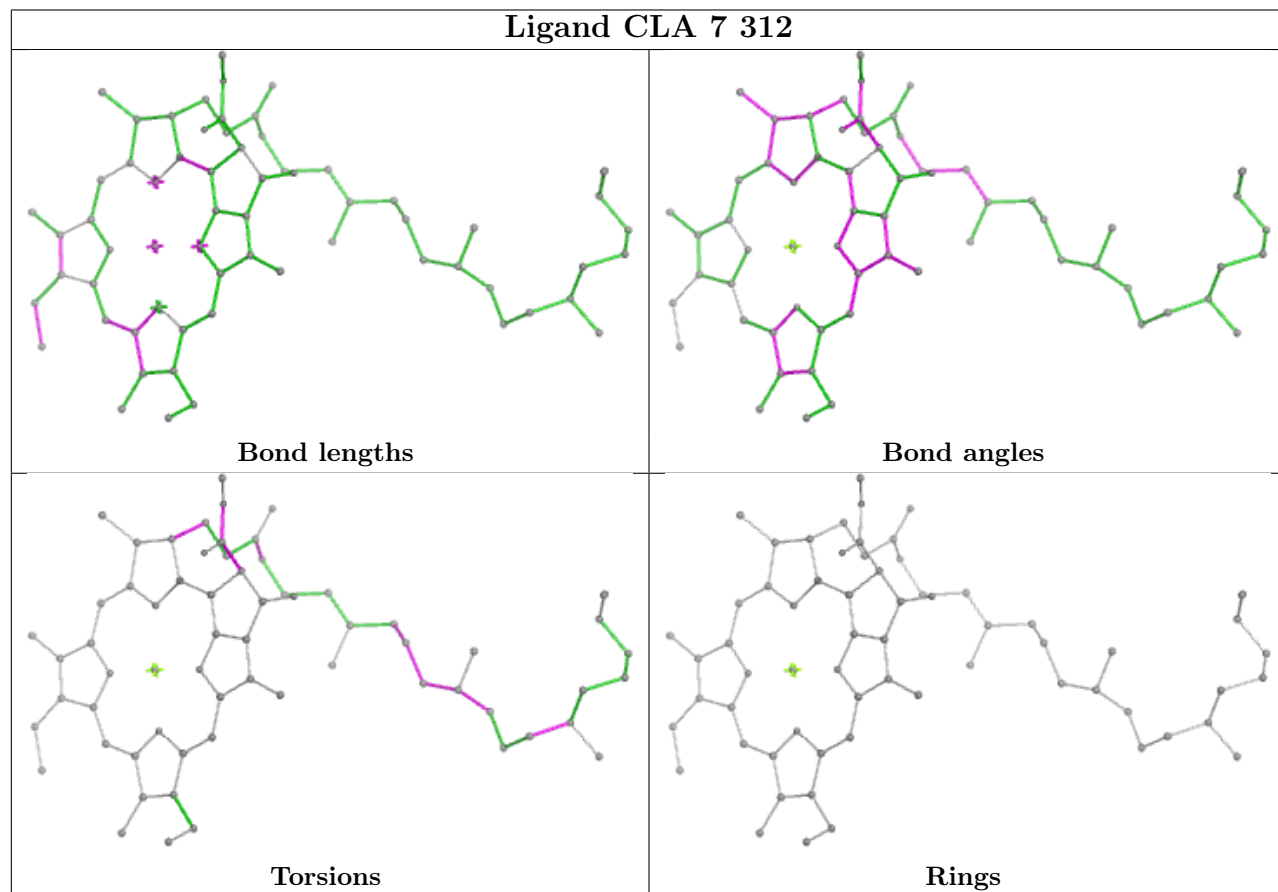
Ligand CLA Z 303

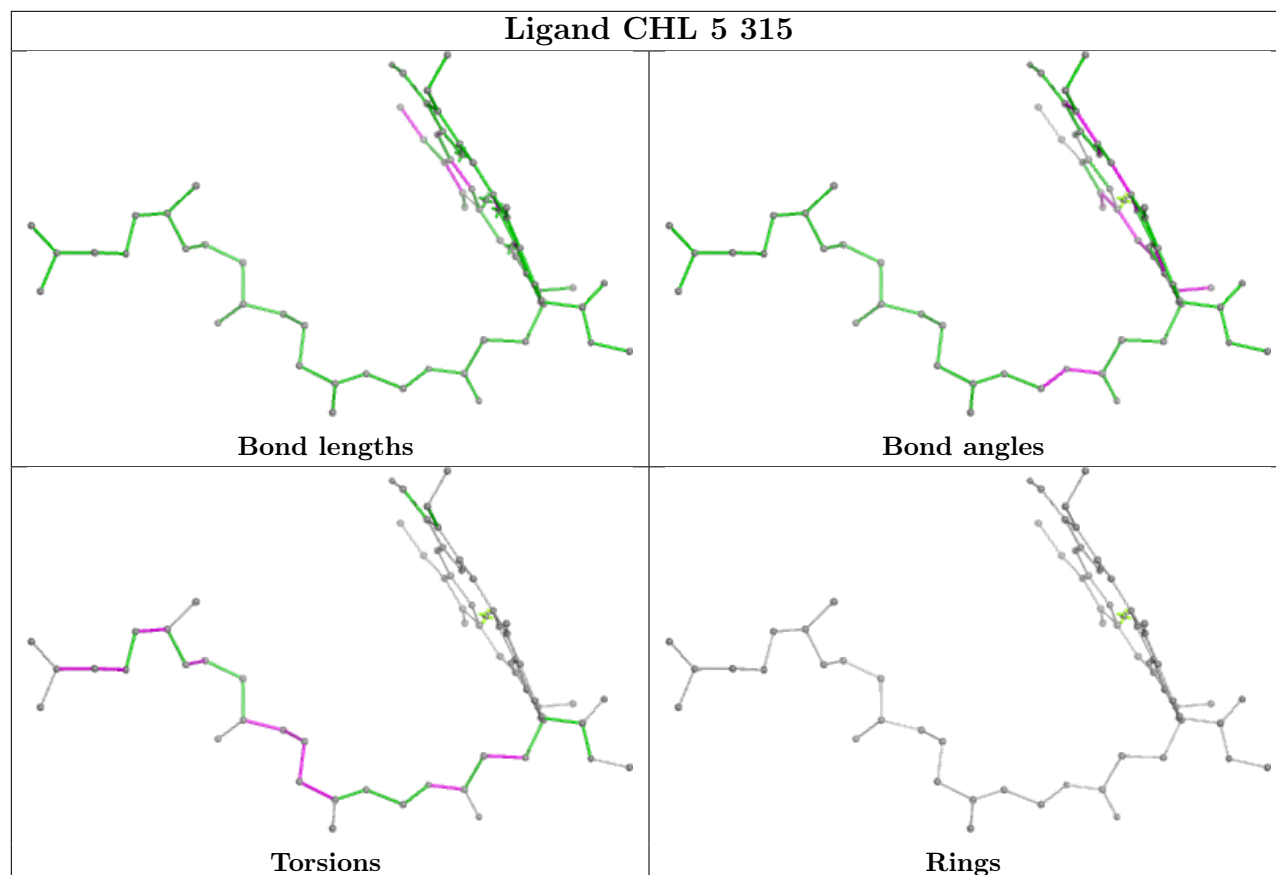


Ligand CLA 7 306

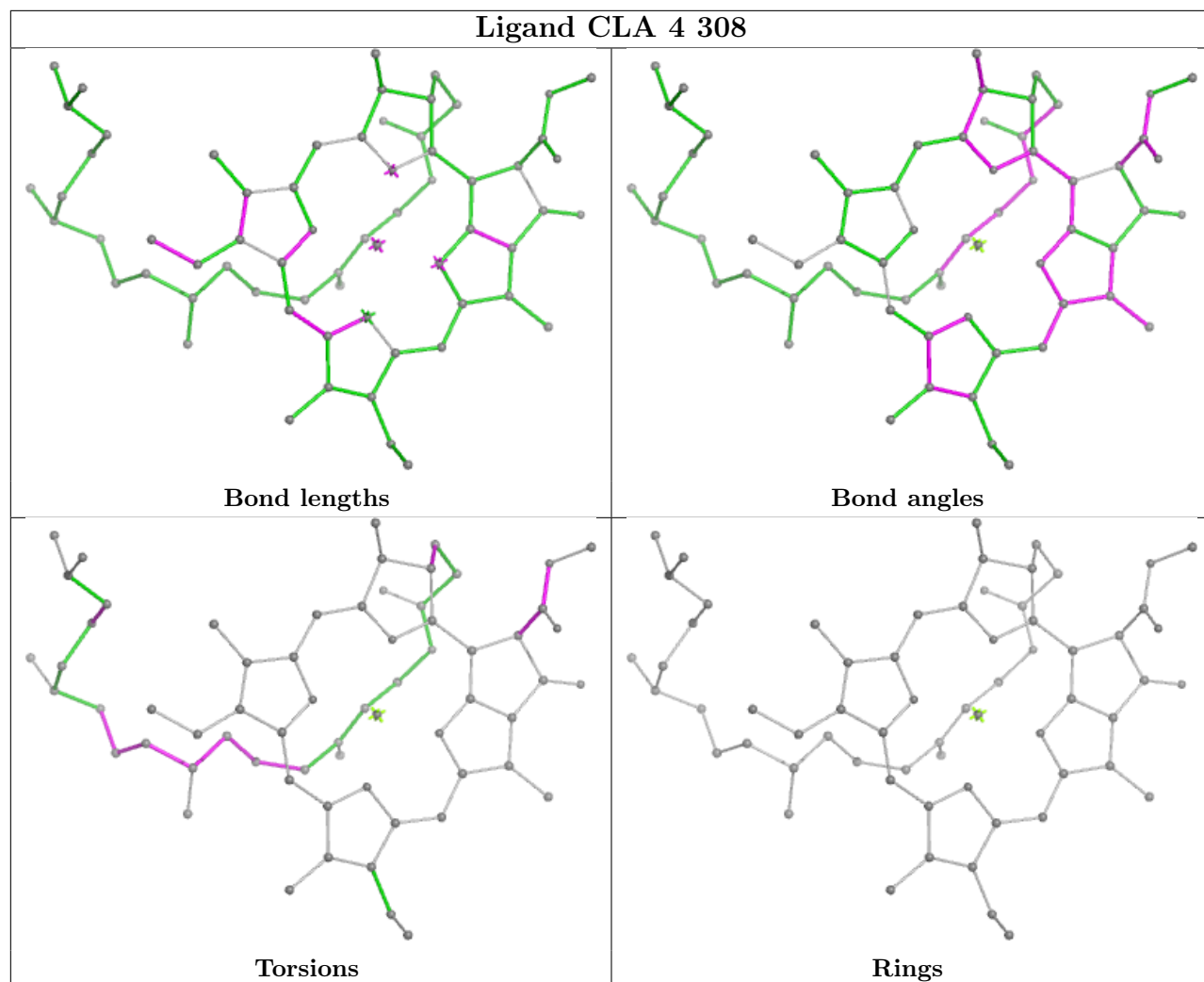


Ligand CLA 7 312

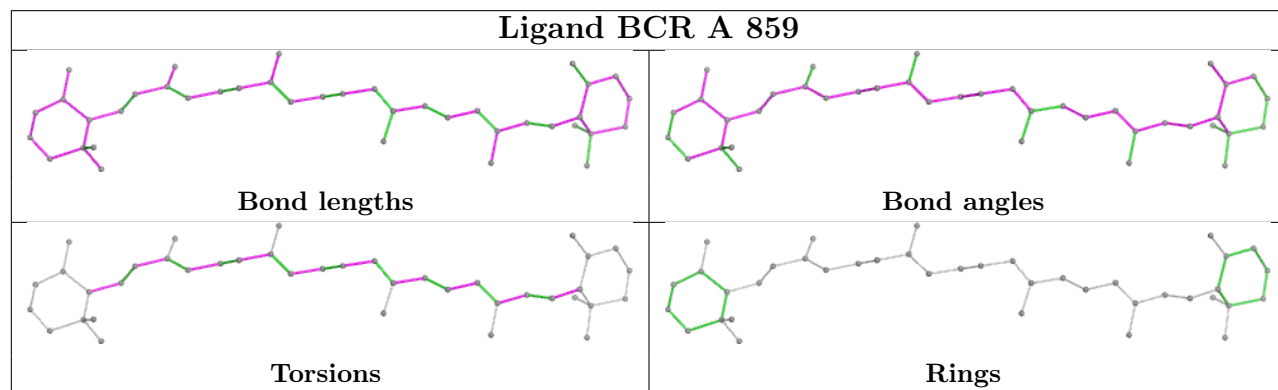


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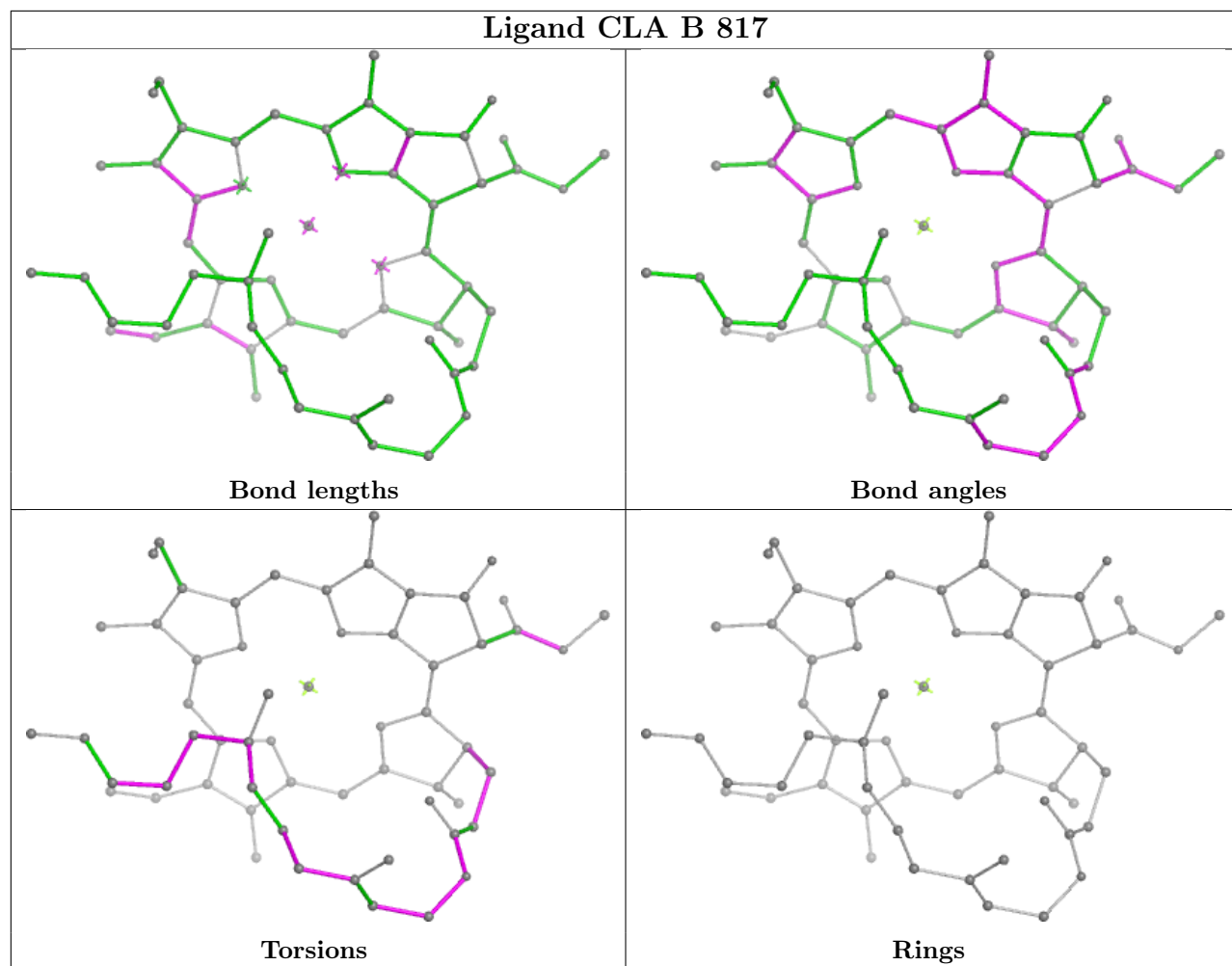
Ligand CLA 4 308



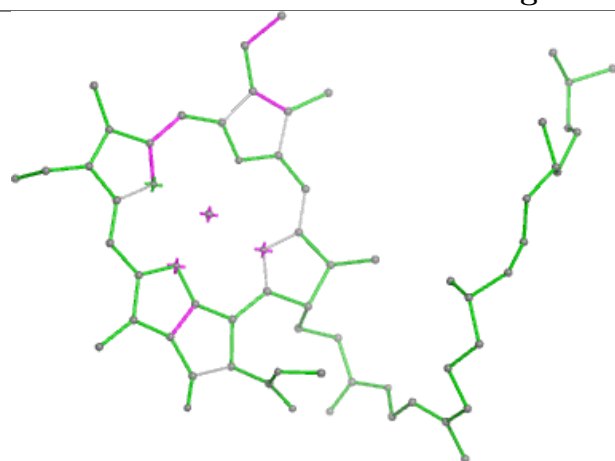
Ligand BCR A 859



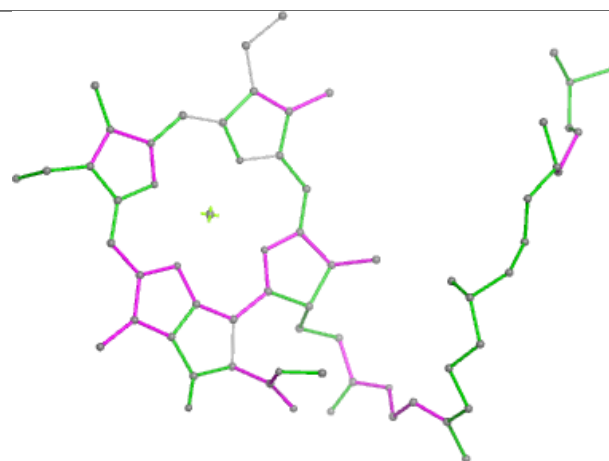
Ligand CLA B 817



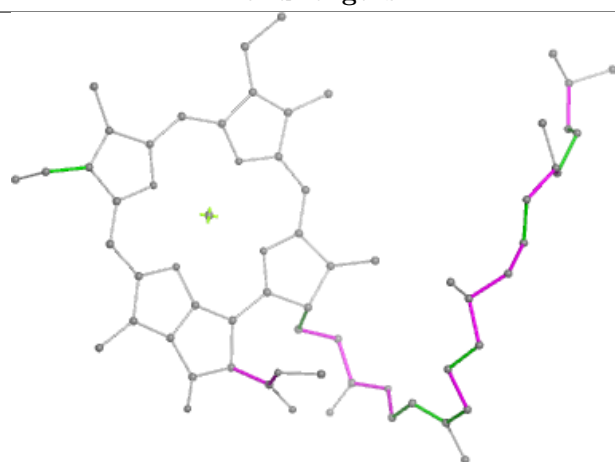
Ligand CLA 8 311



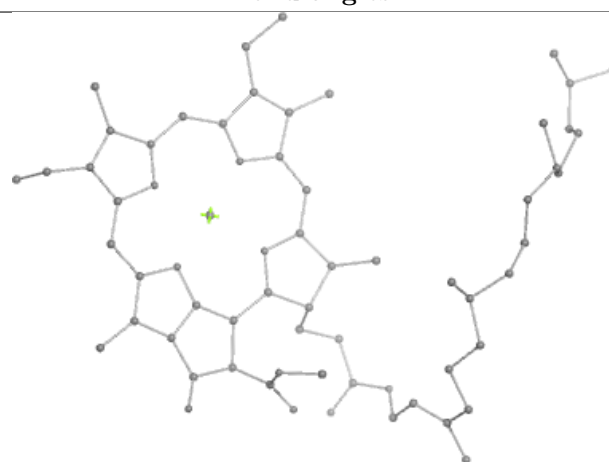
Bond lengths



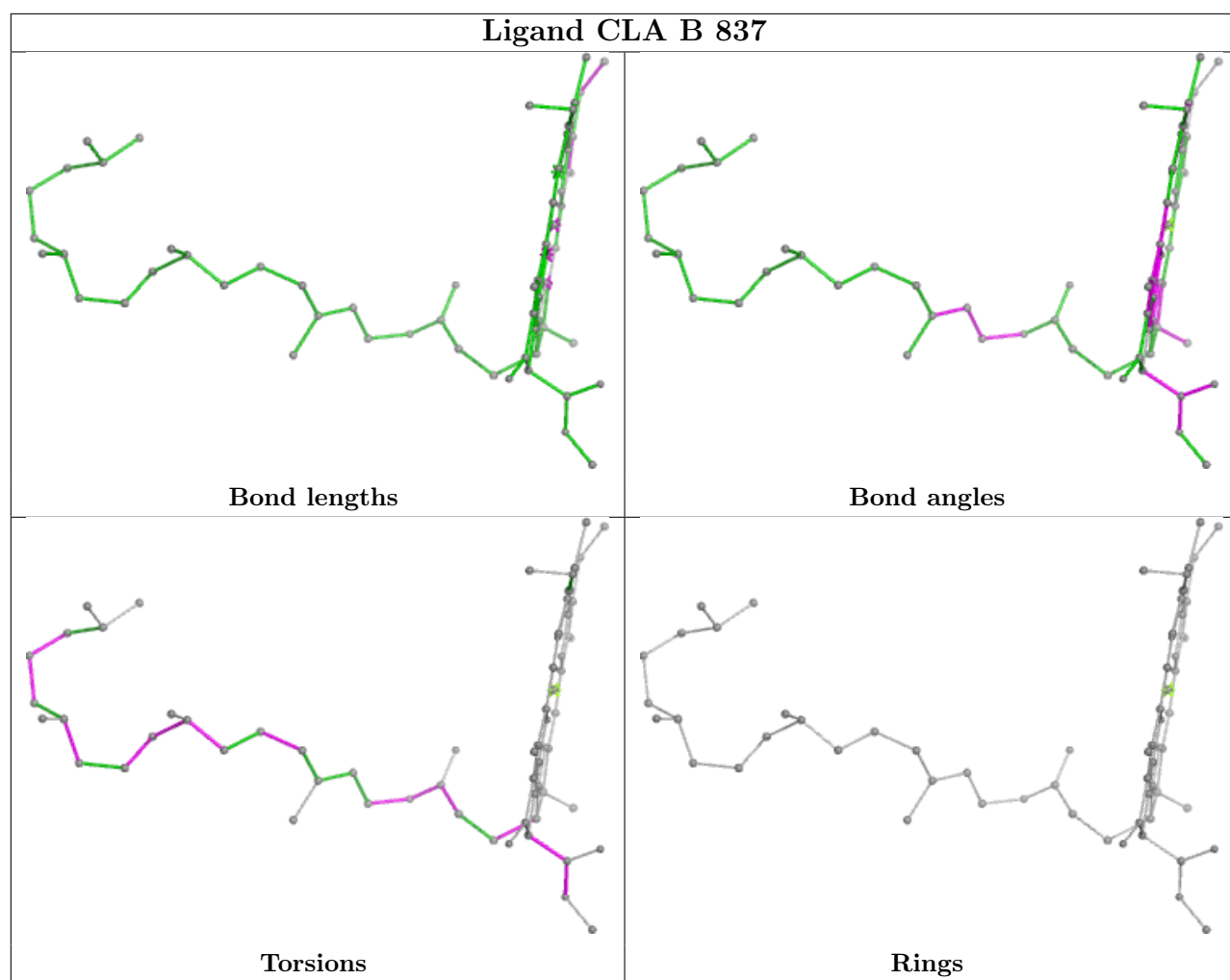
Bond angles

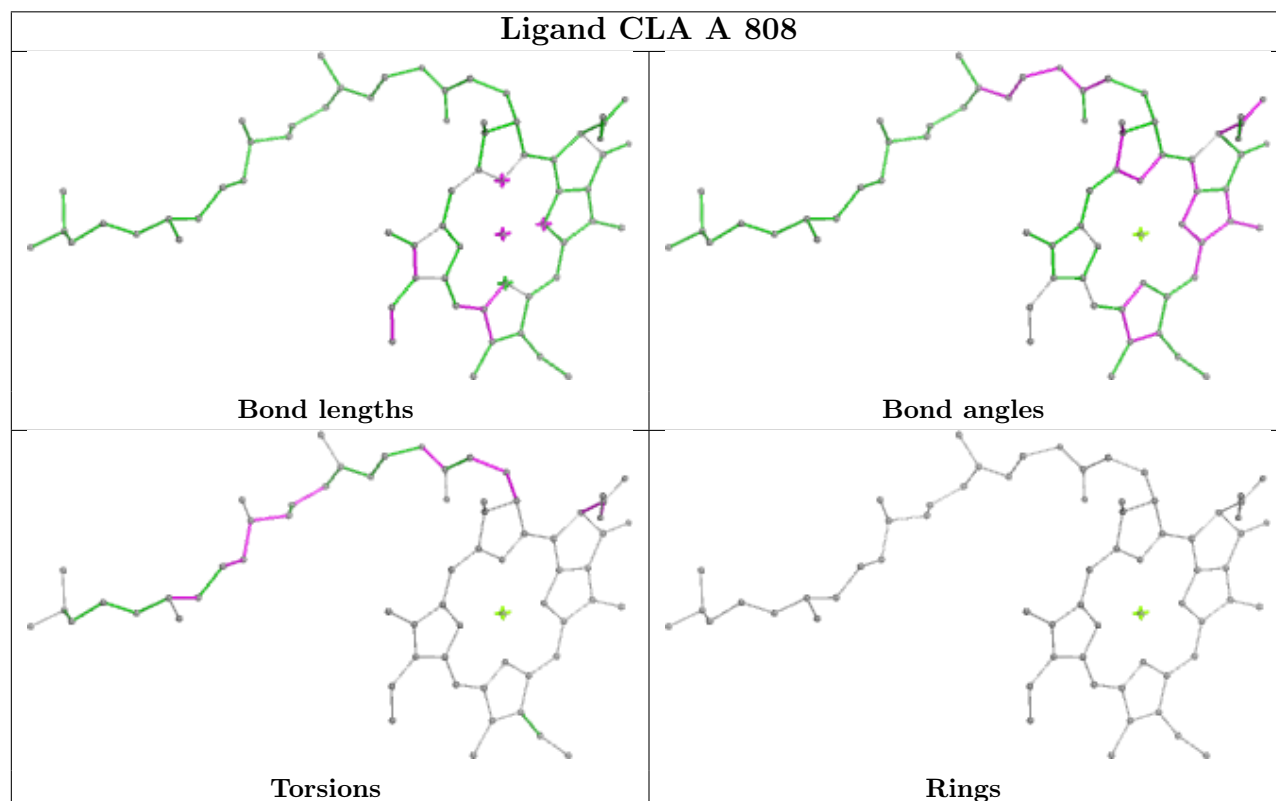
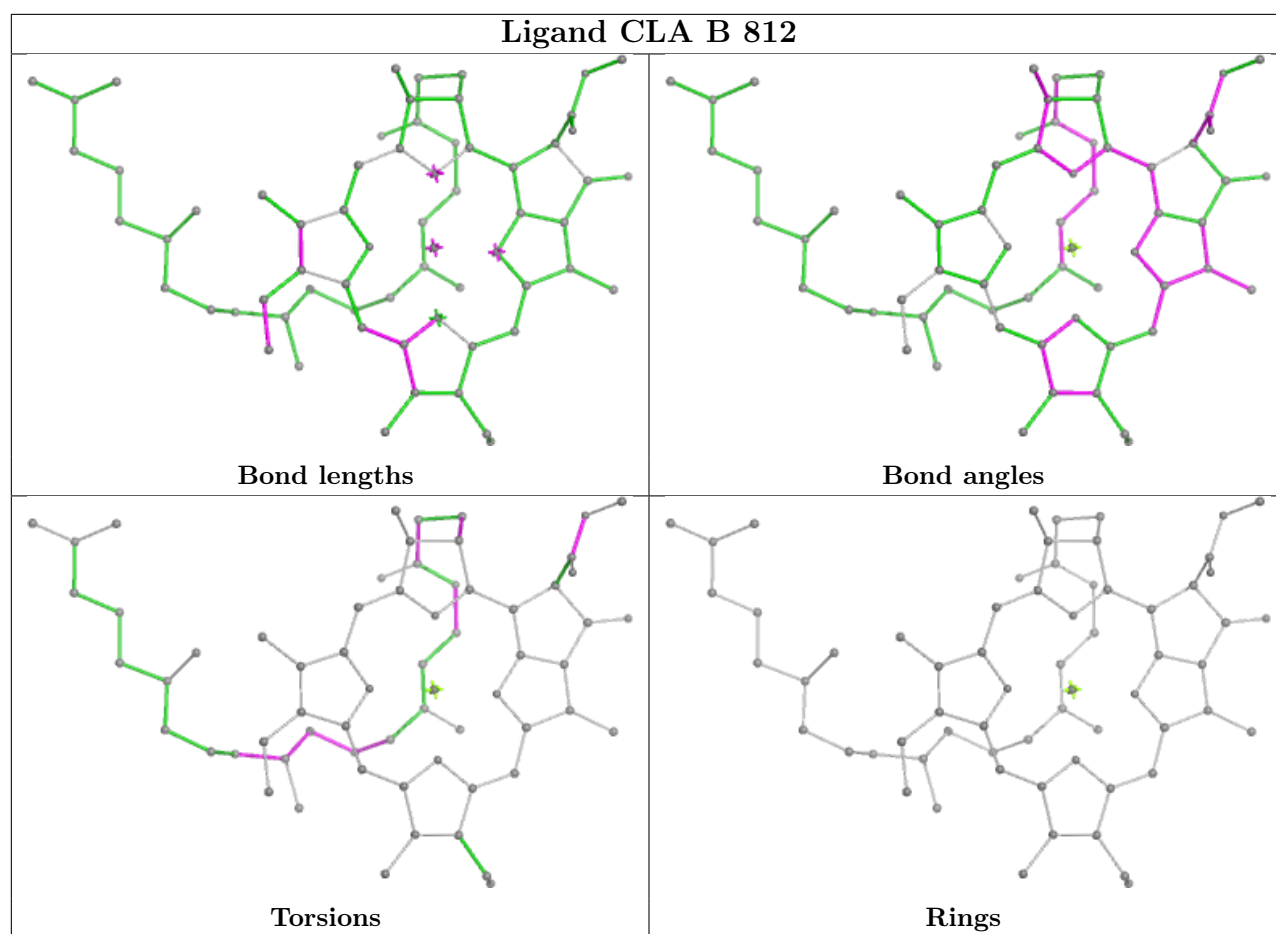


Torsions

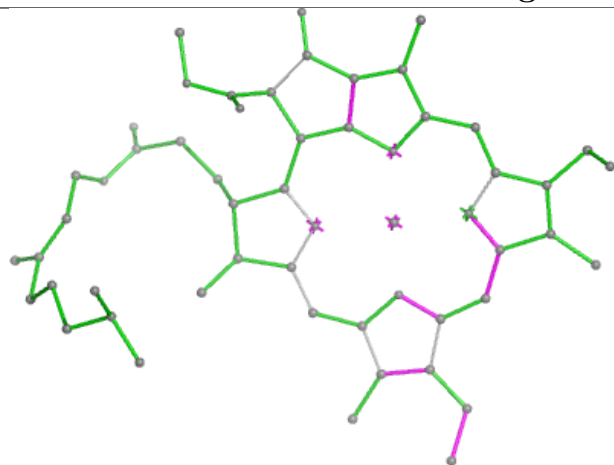


Rings

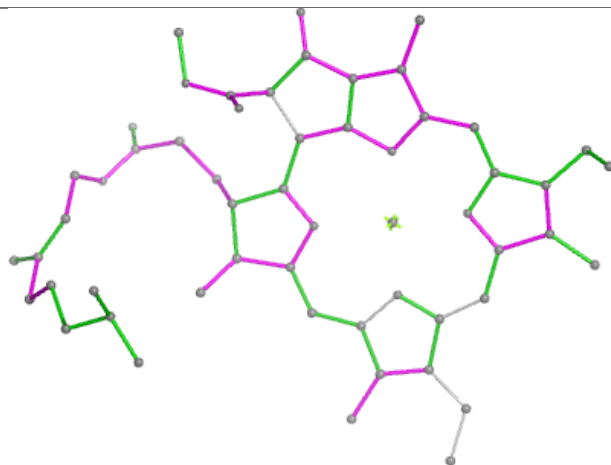




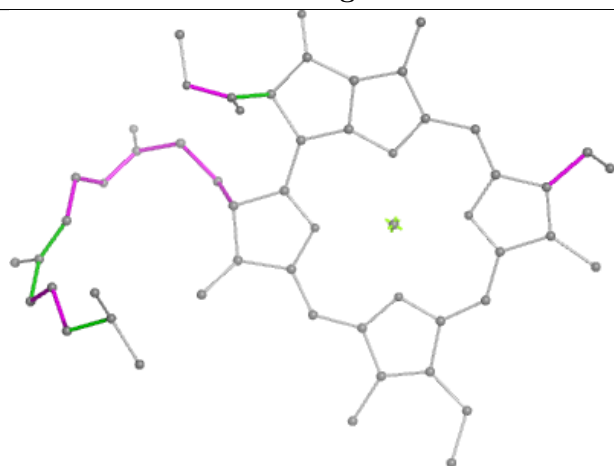
Ligand CLA 5 310



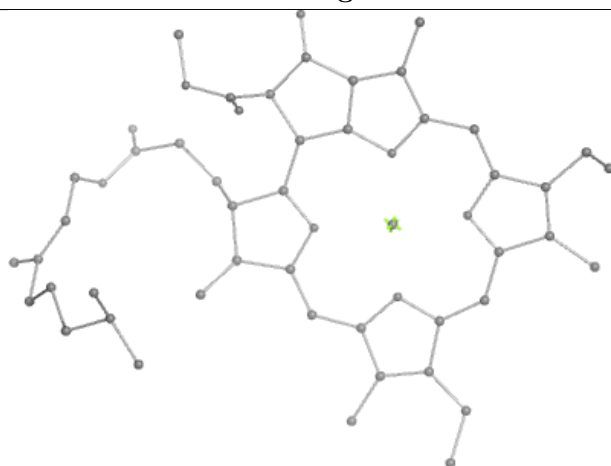
Bond lengths



Bond angles

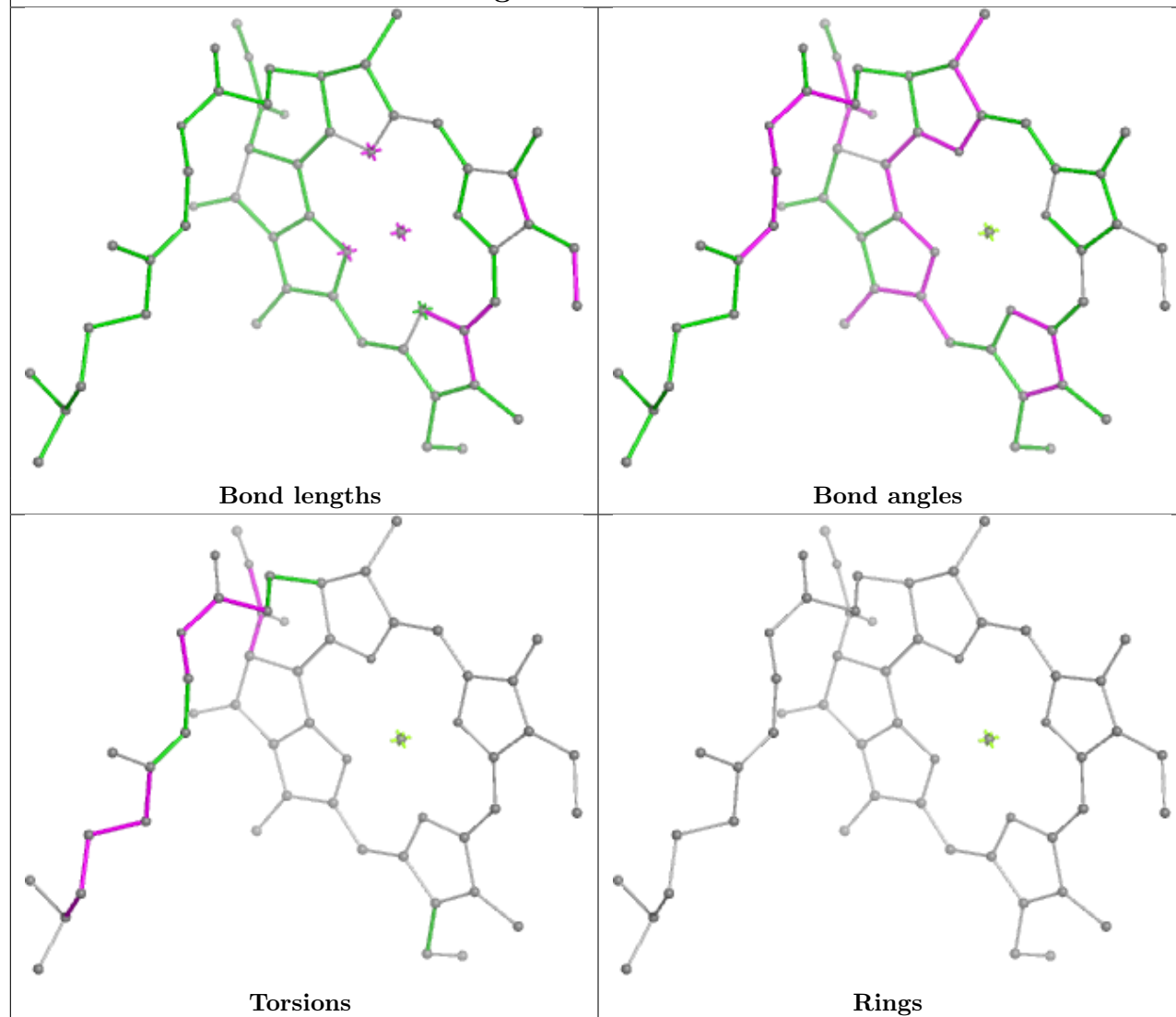


Torsions

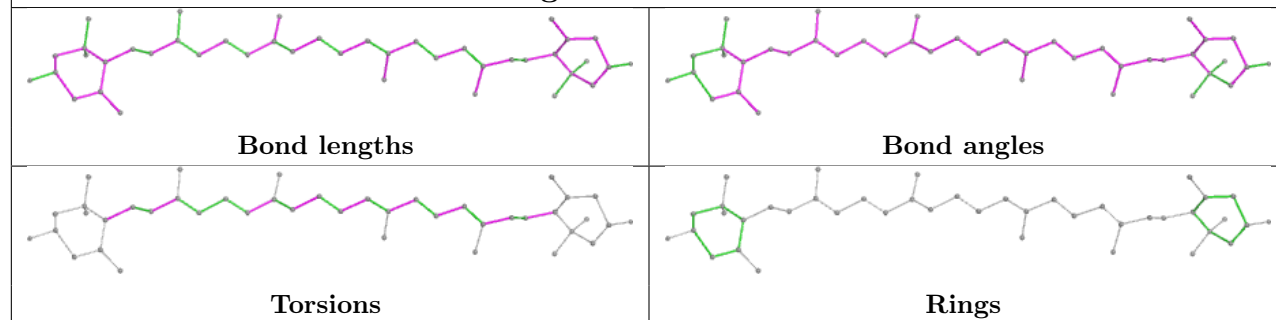


Rings

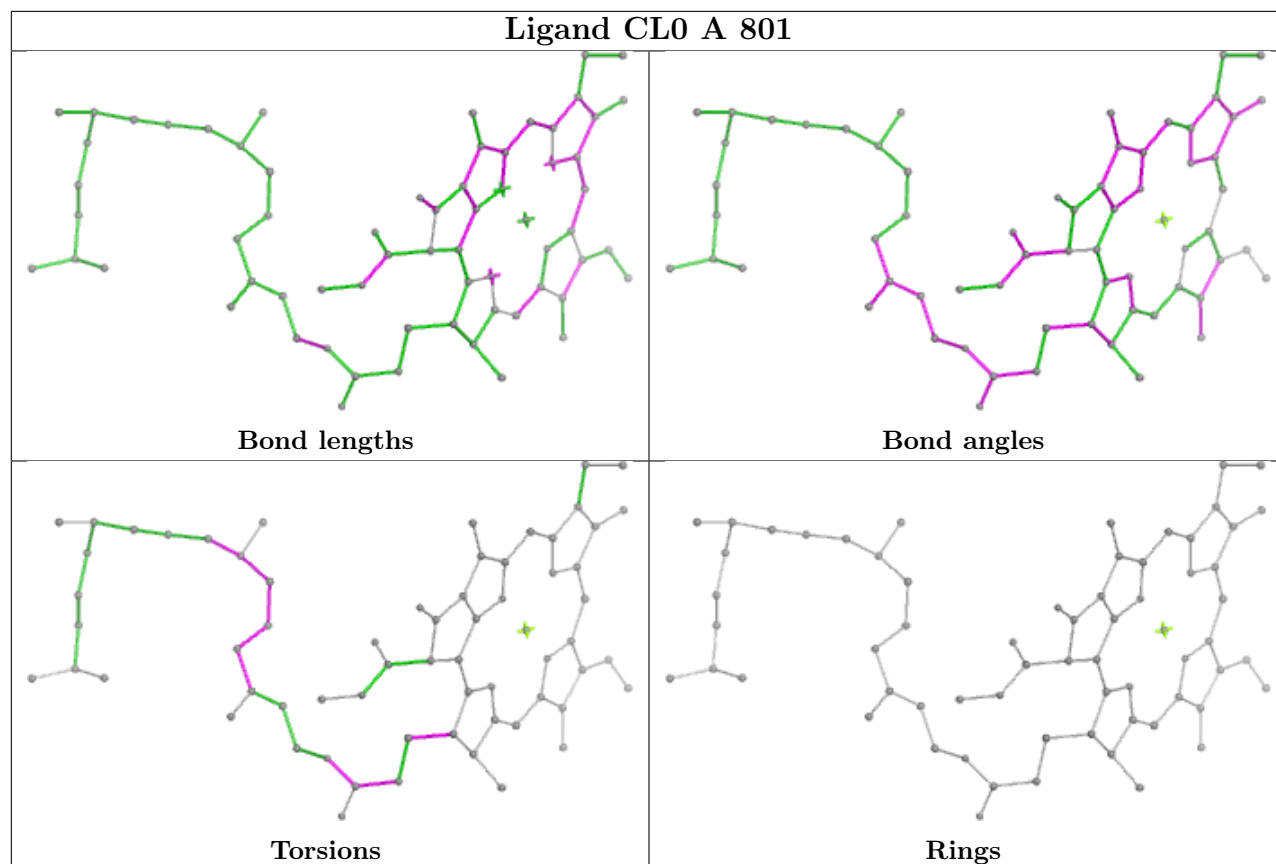
Ligand CLA 4 312



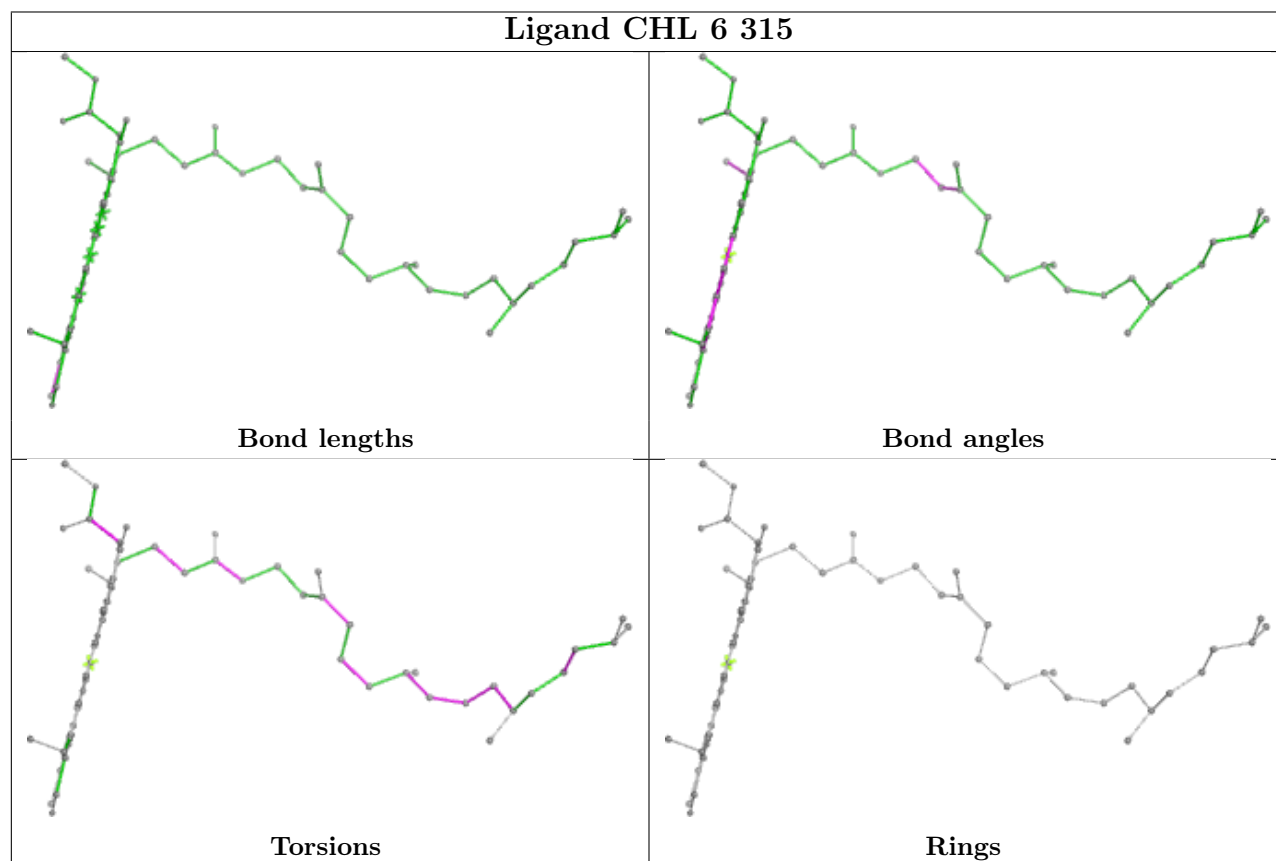
Ligand C7Z 6 304

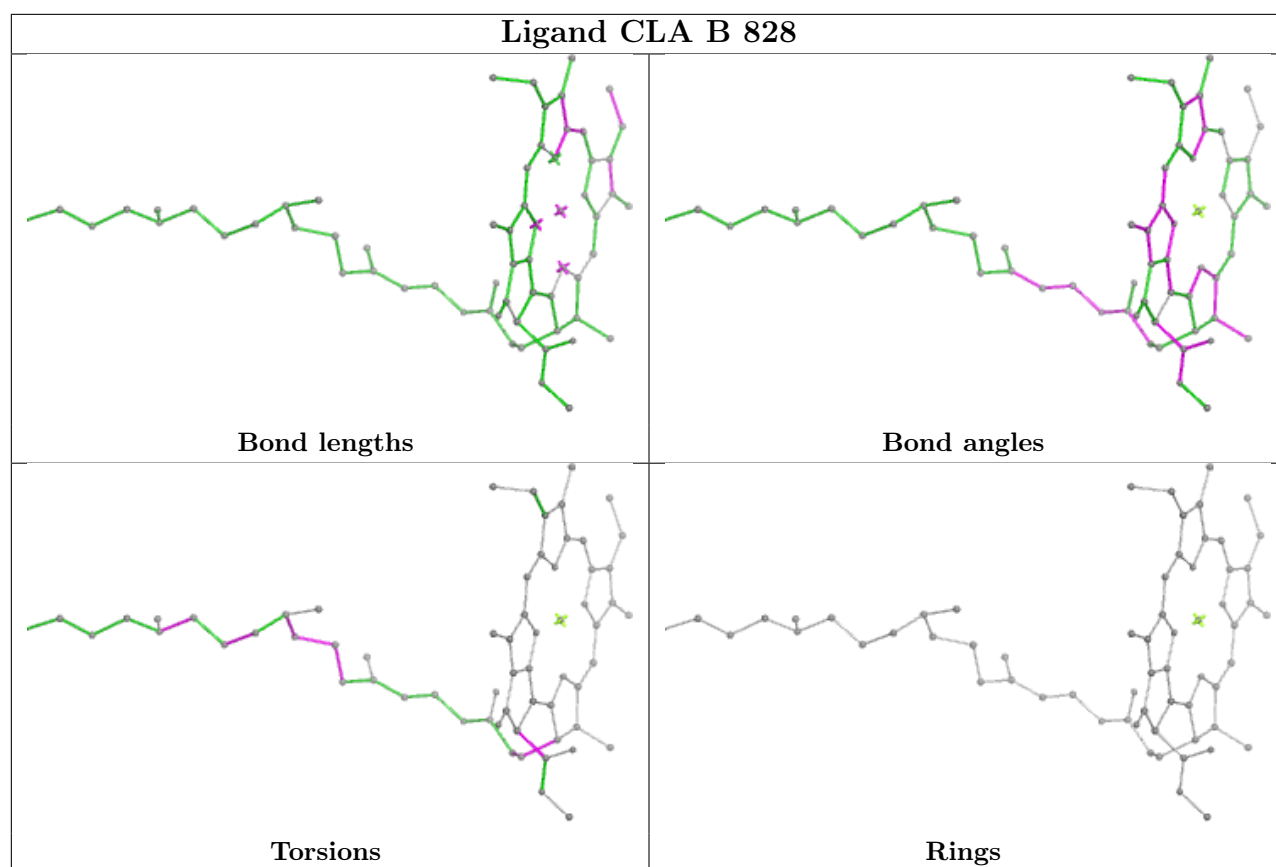


Ligand CL0 A 801

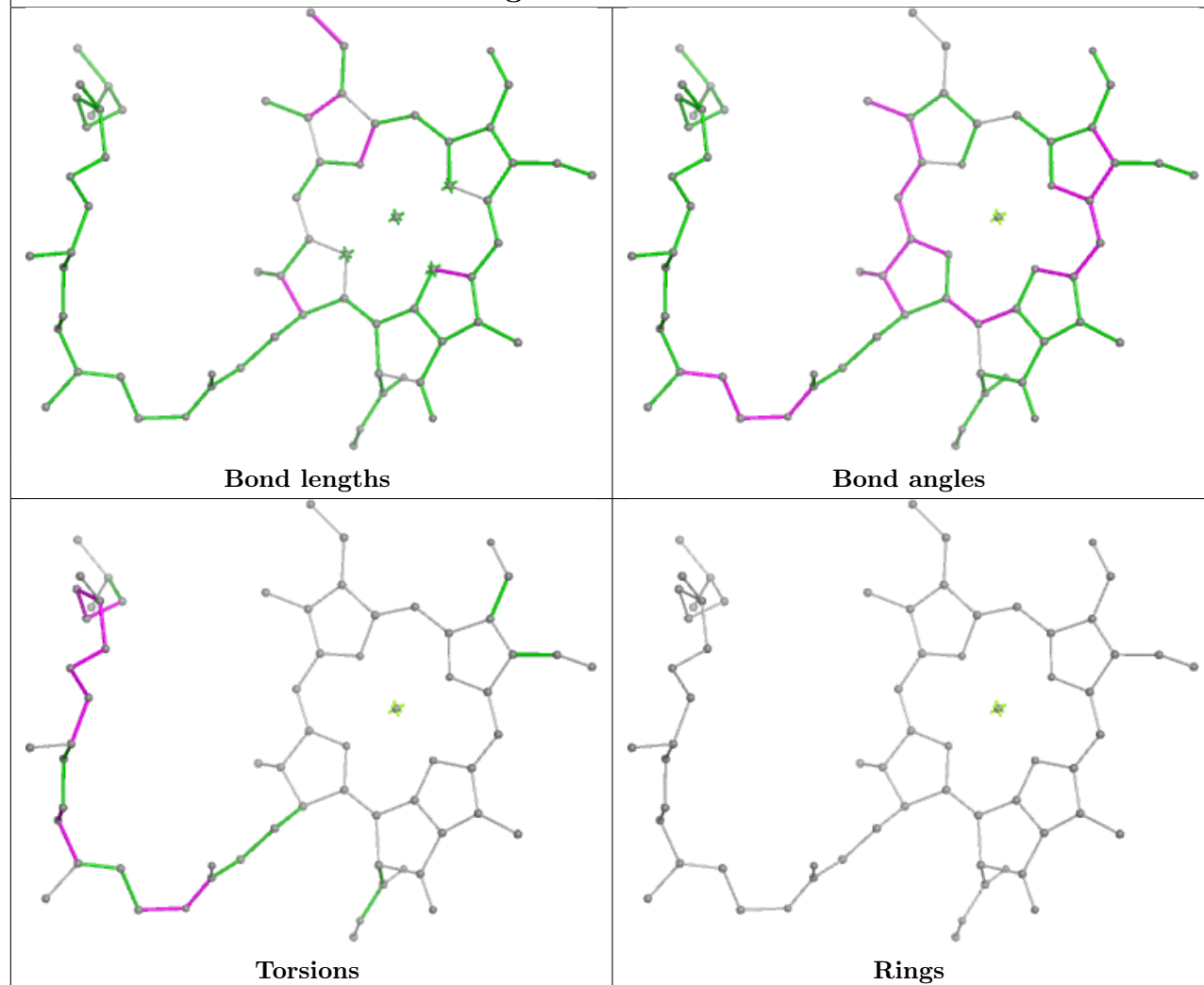


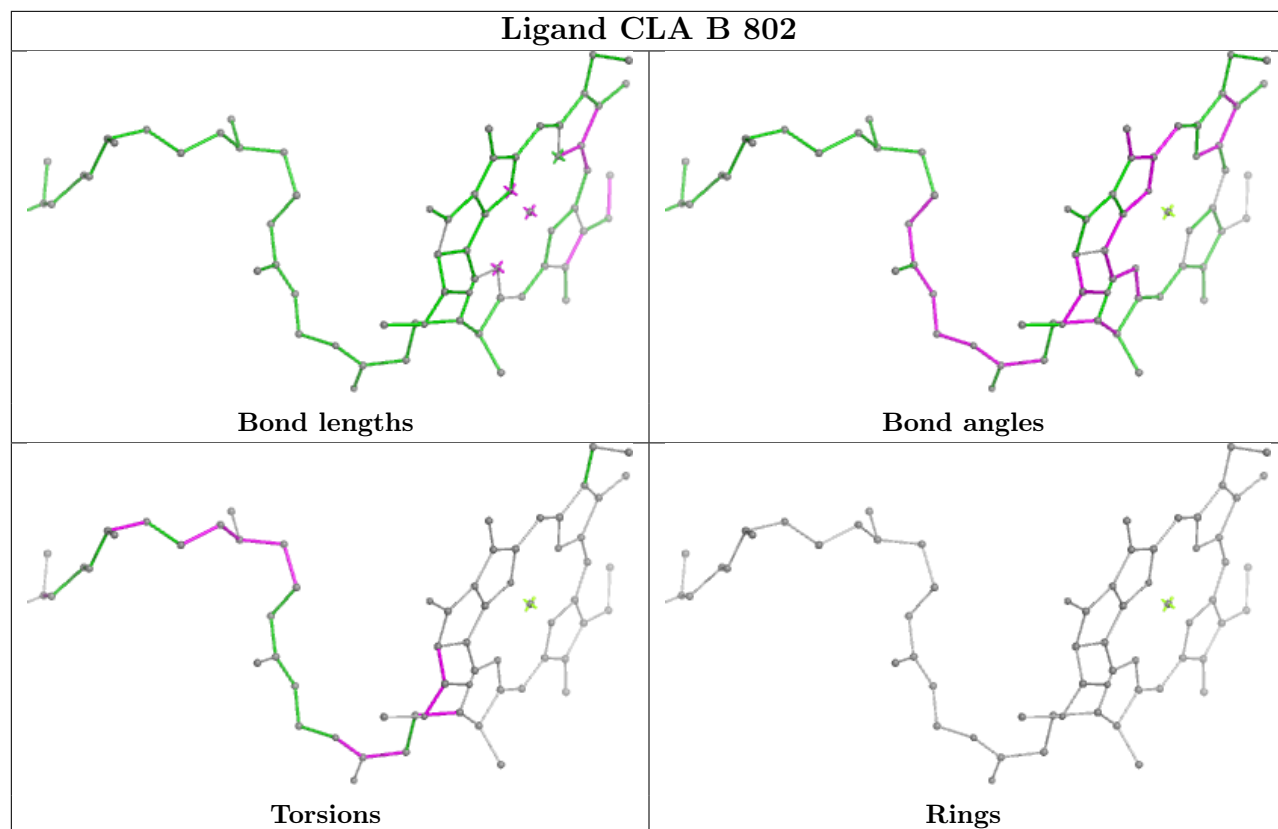
Ligand CHL 6 315

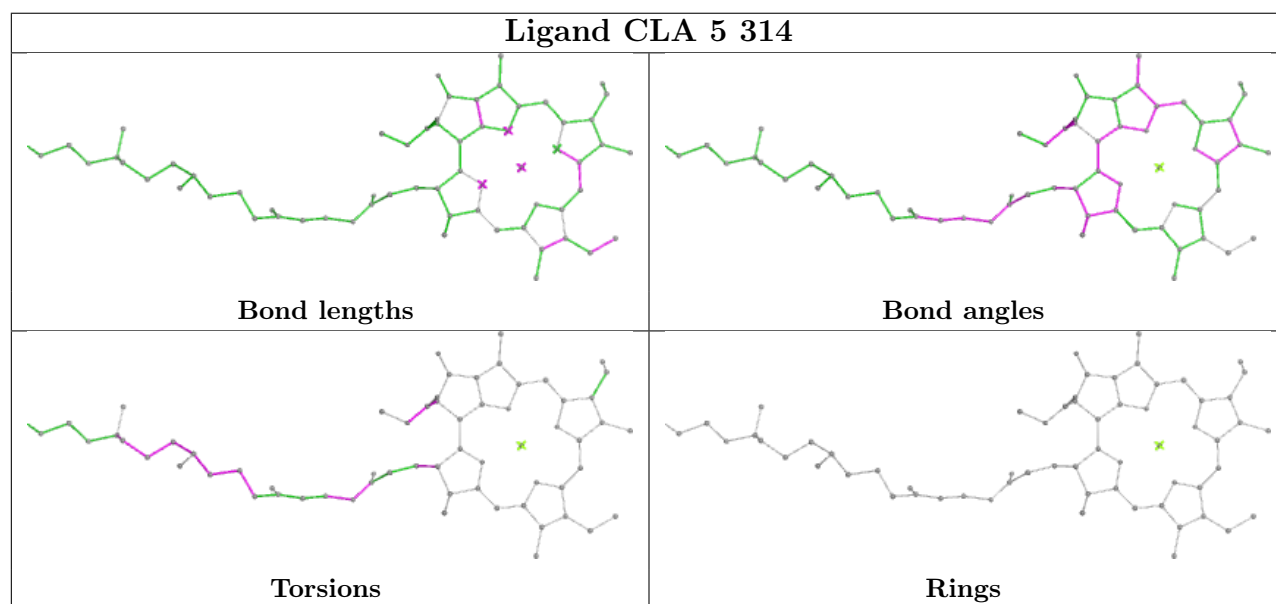
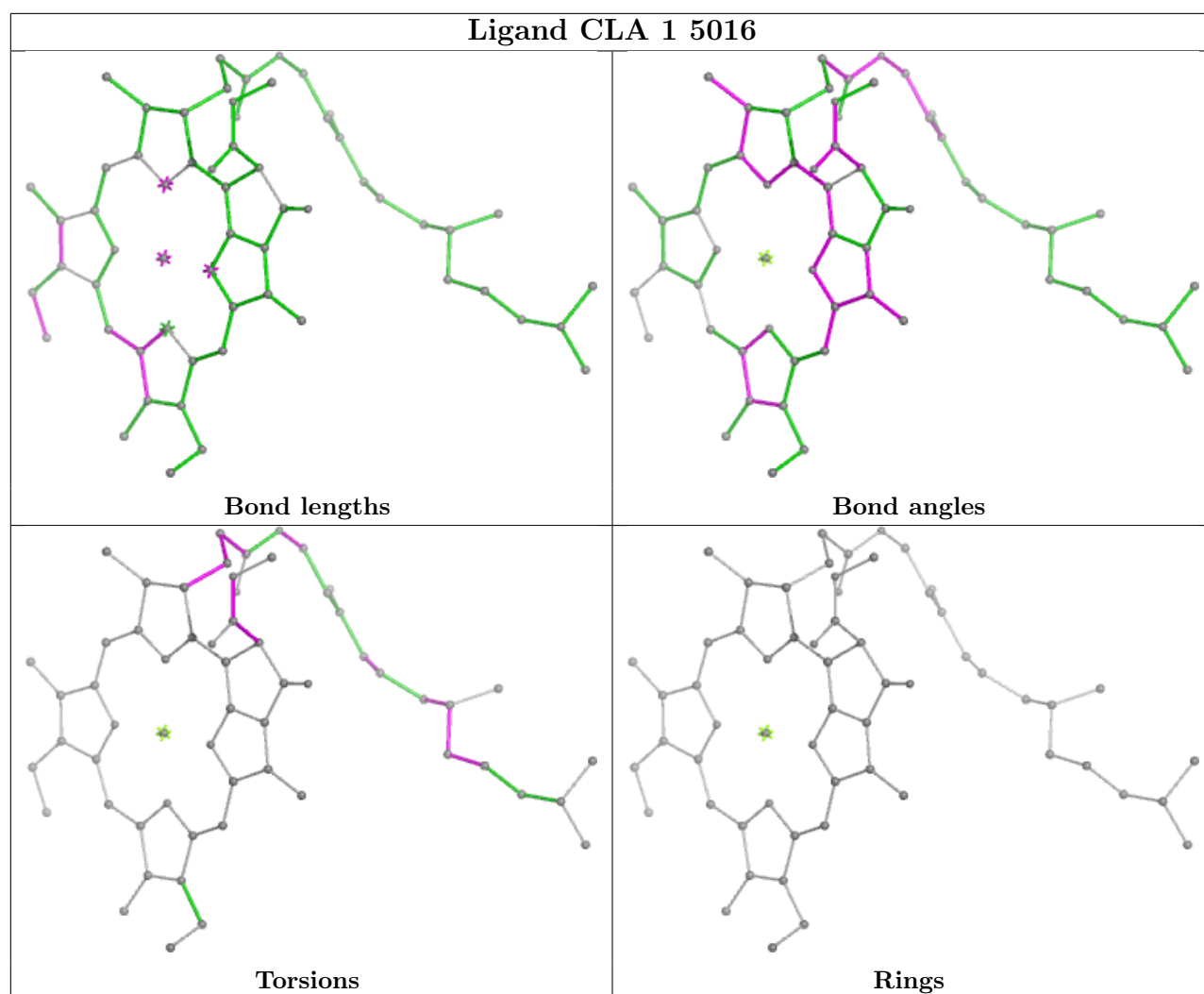




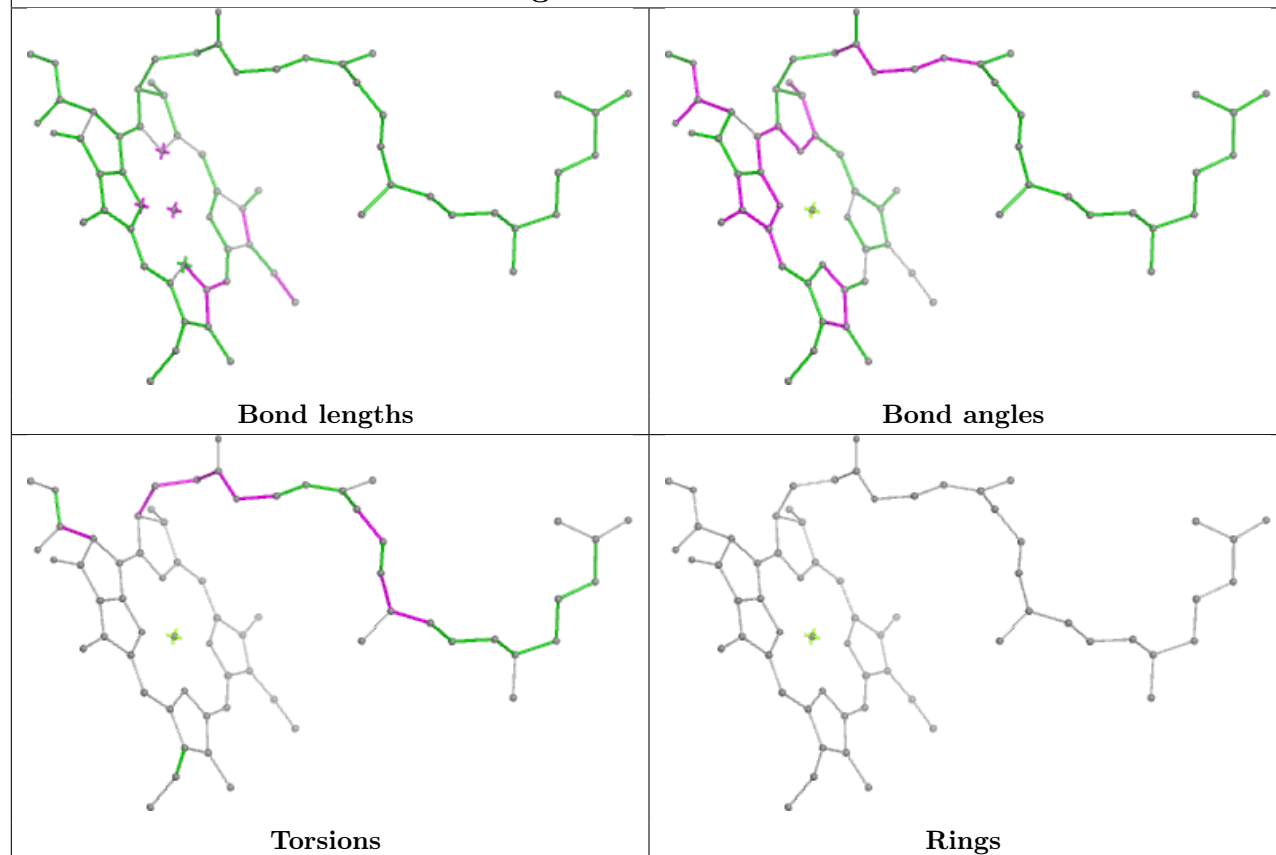
Ligand CHL 8 319



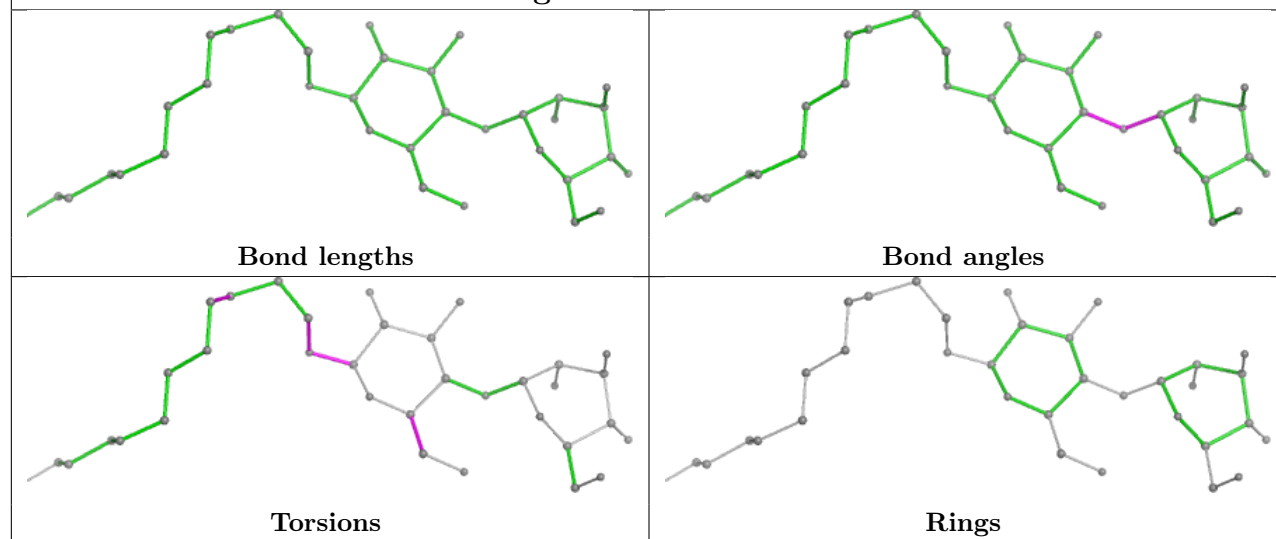


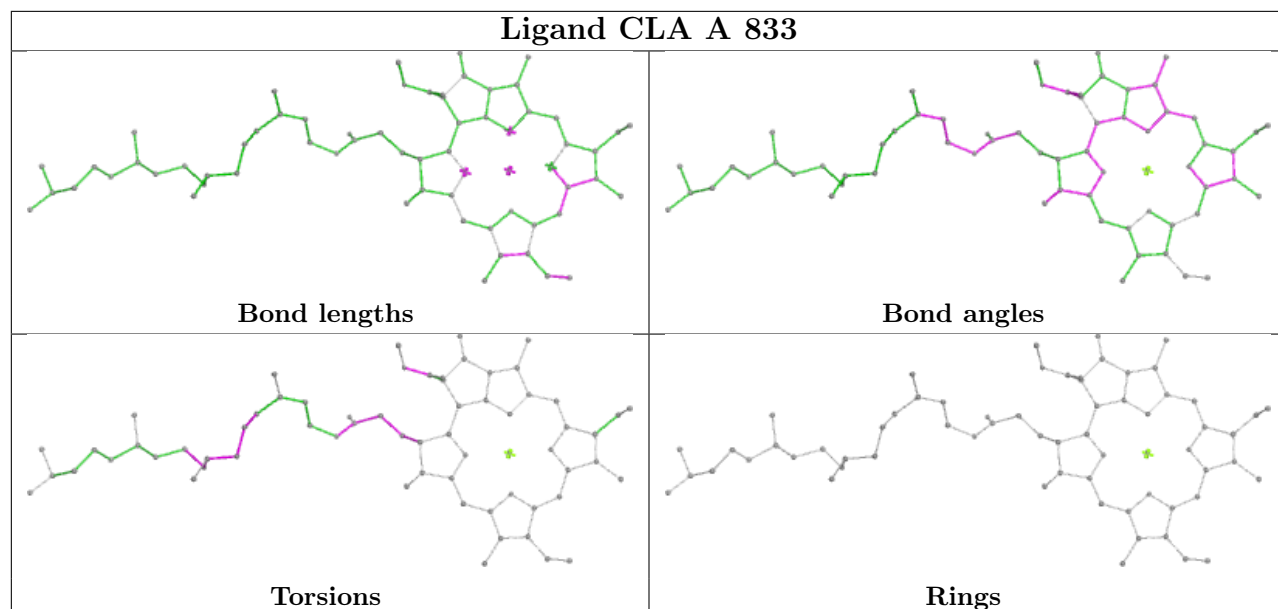
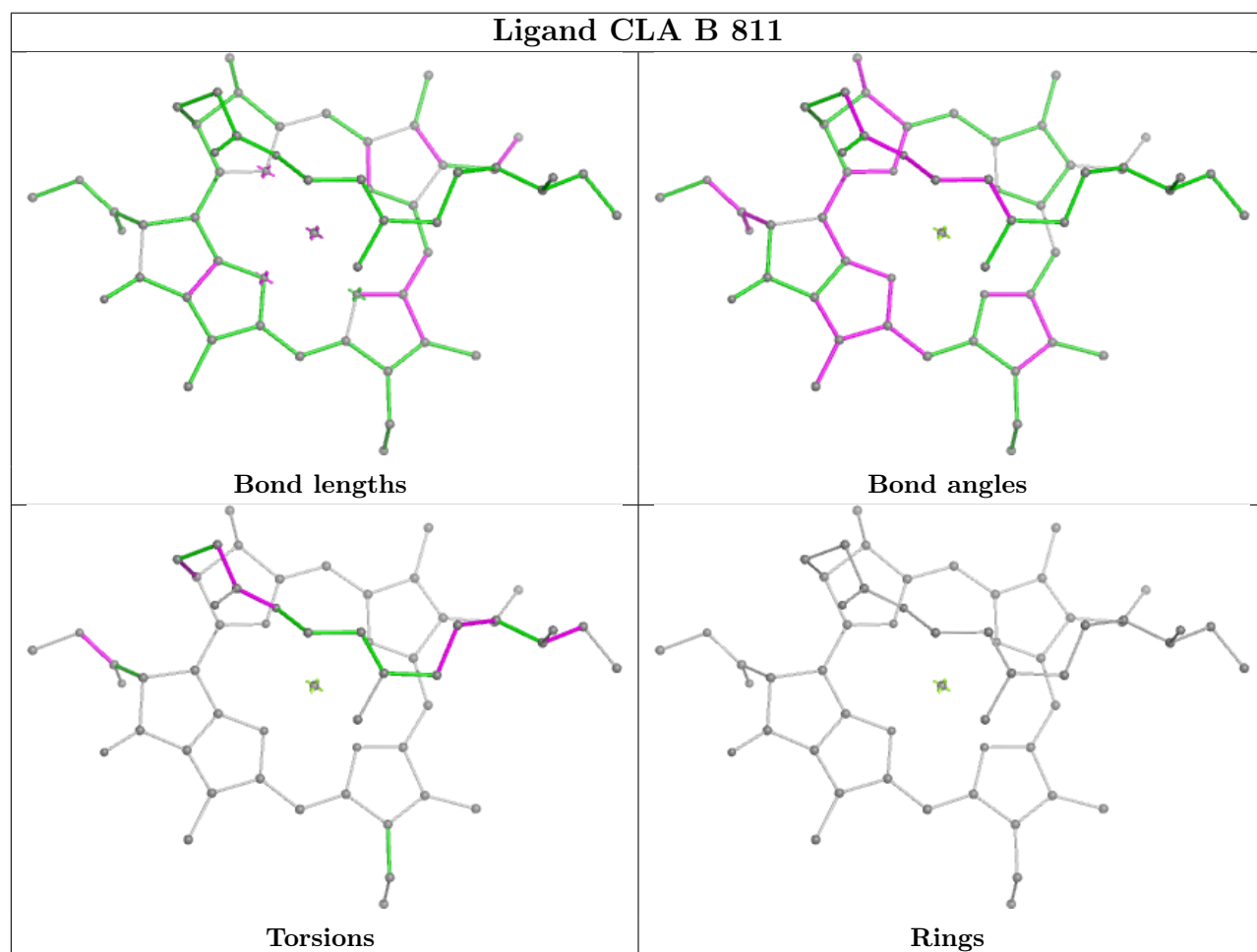


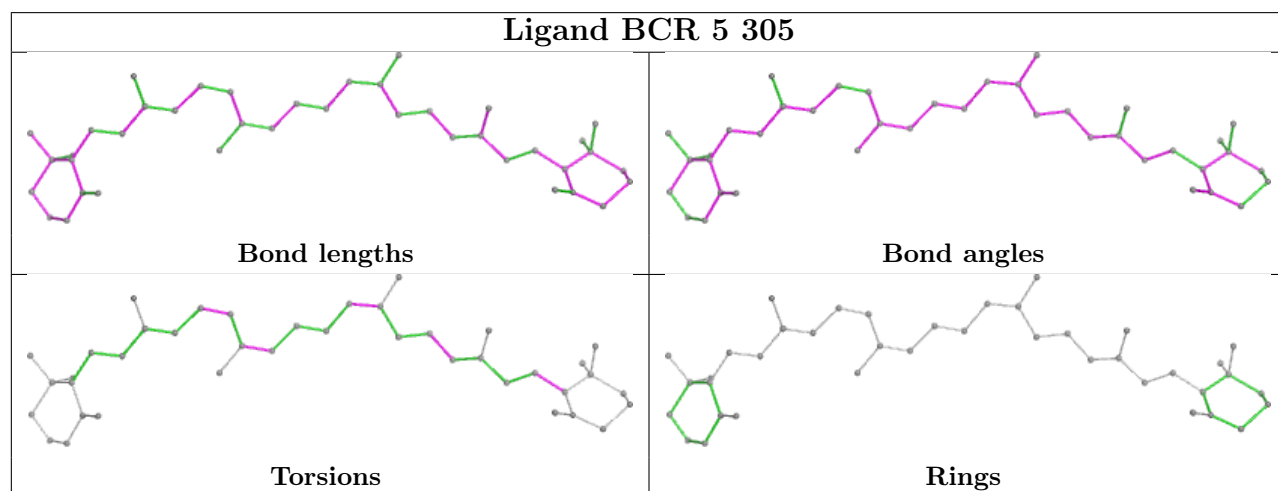
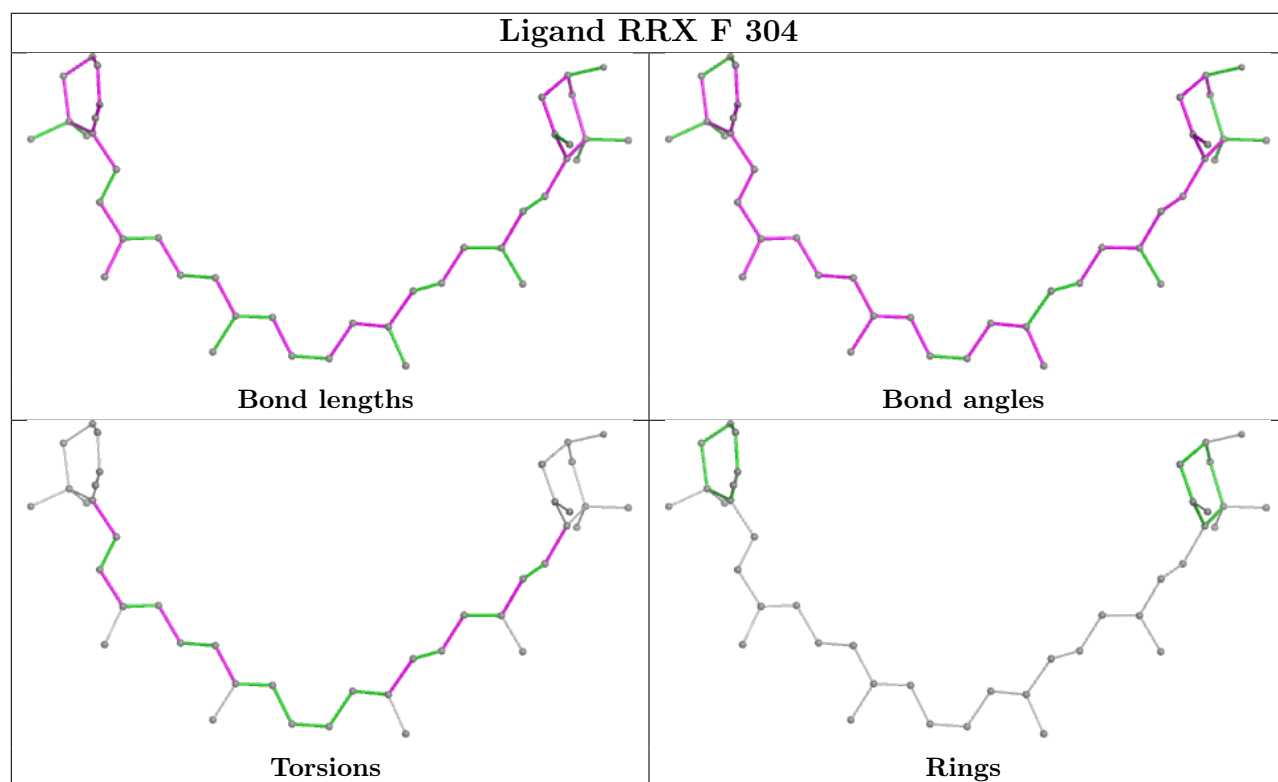
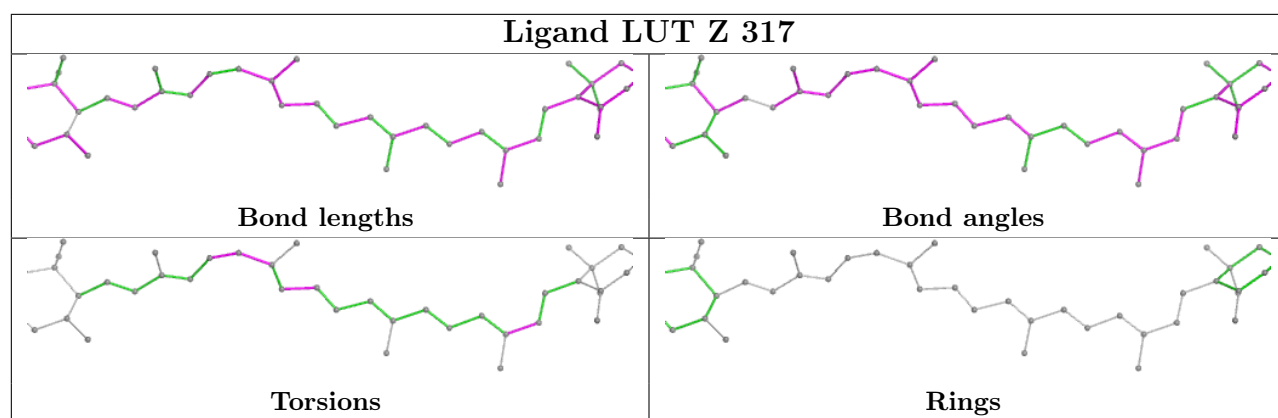
Ligand CLA A 824

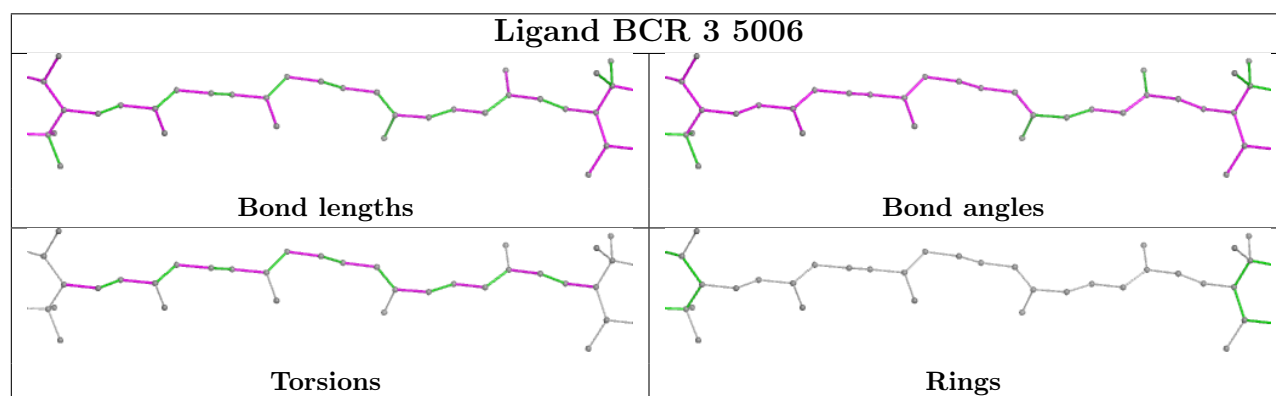
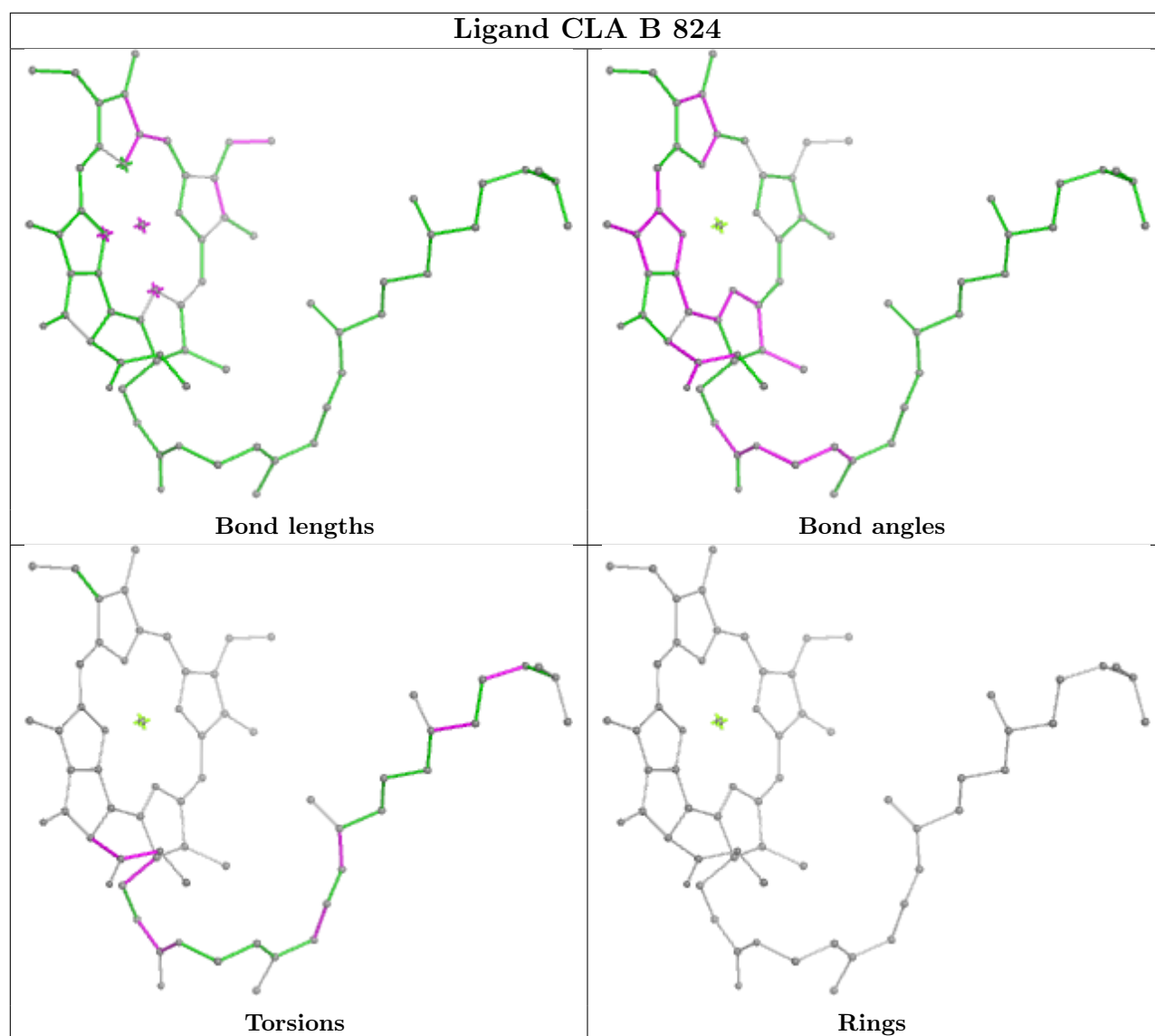


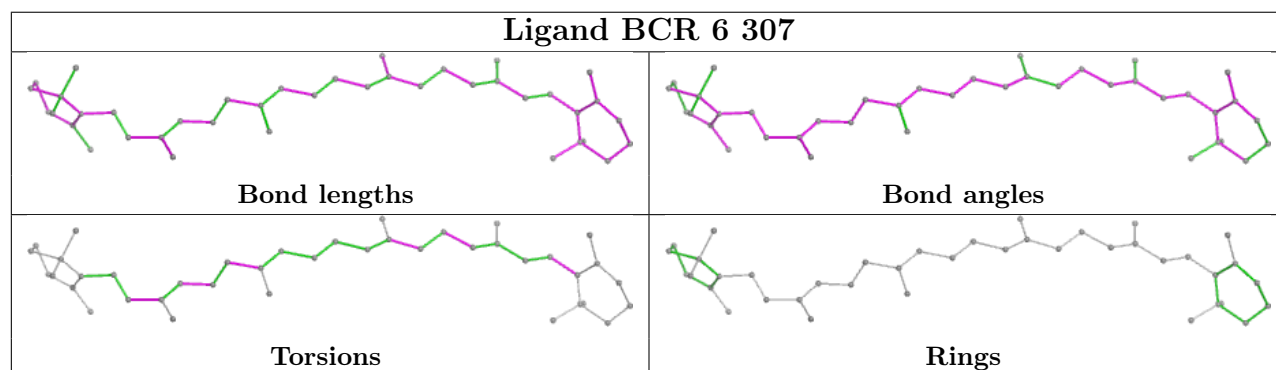
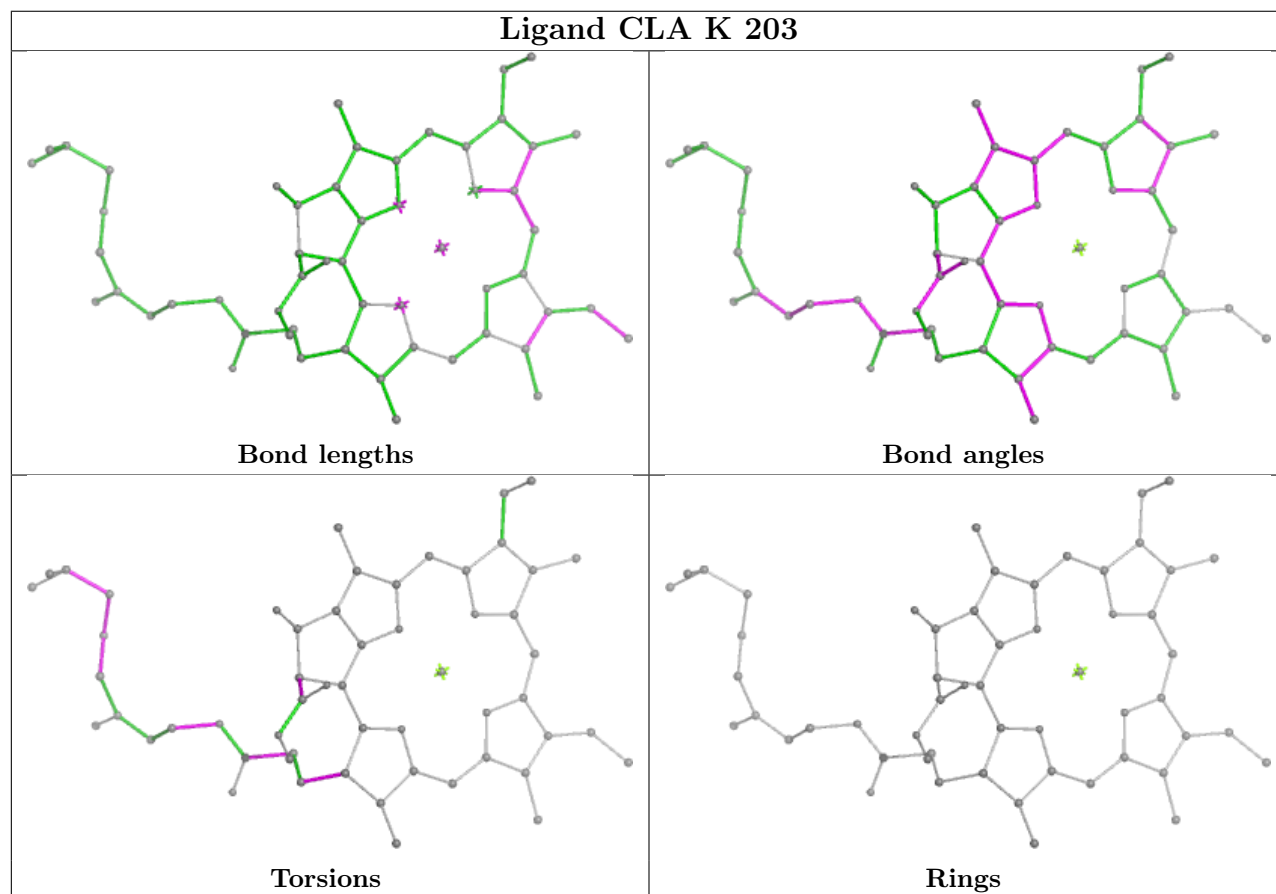
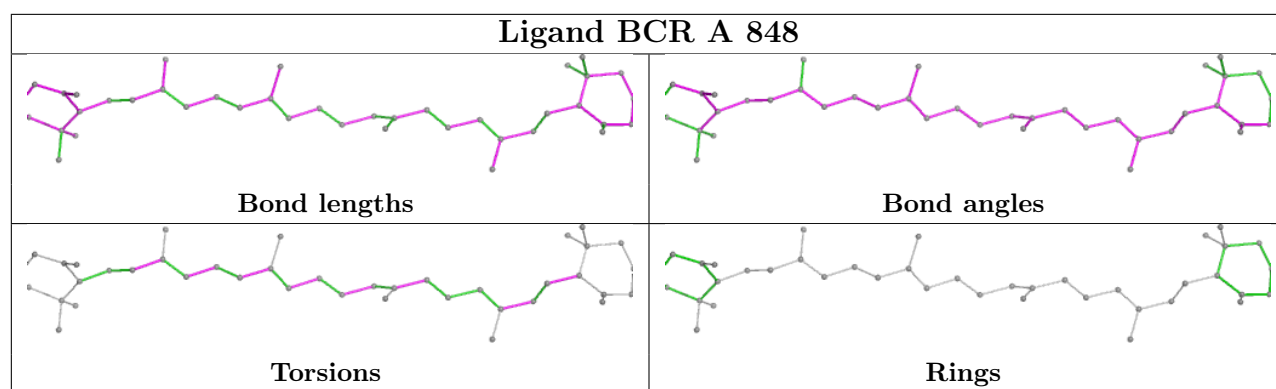
Ligand LMT 4 322

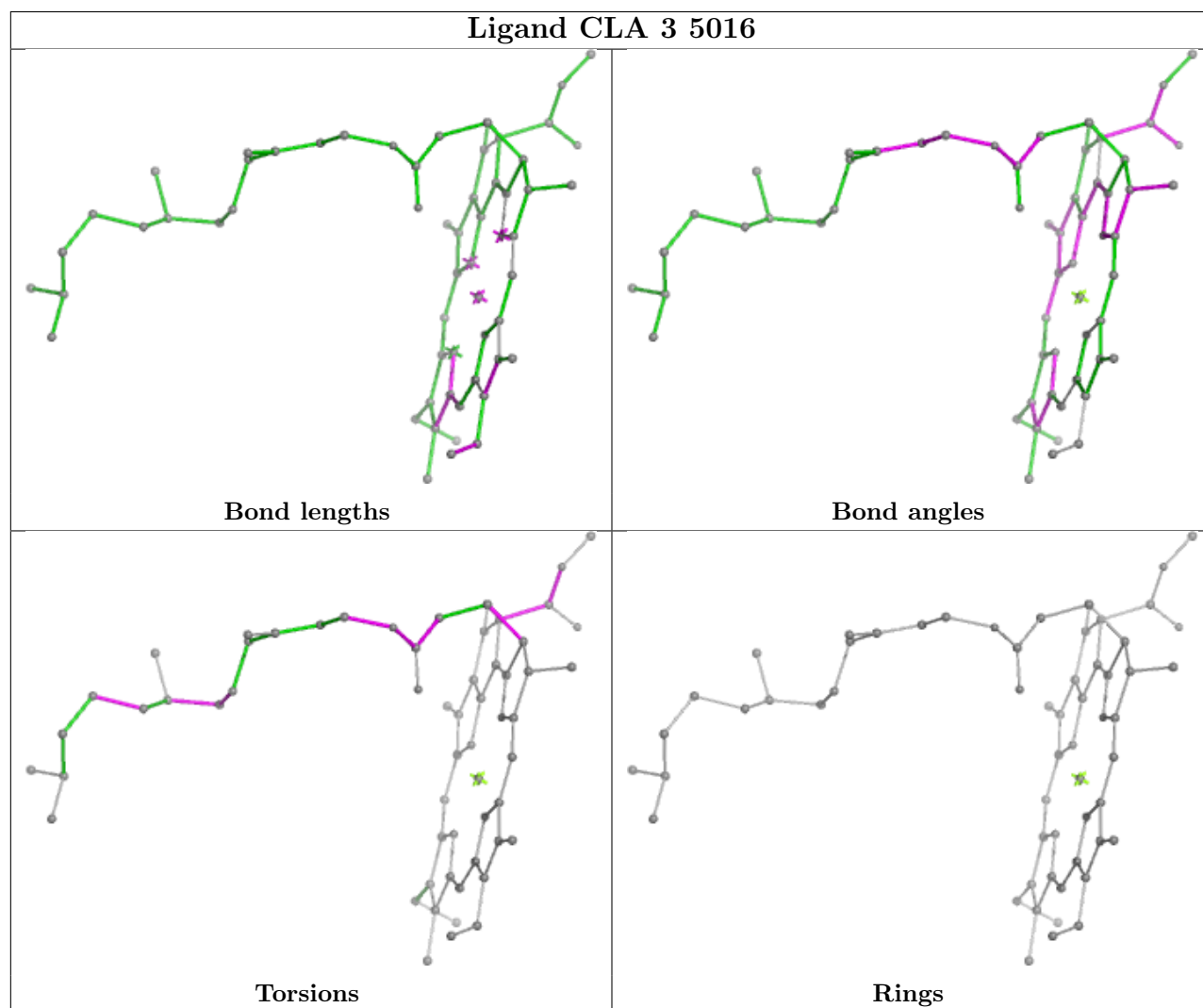
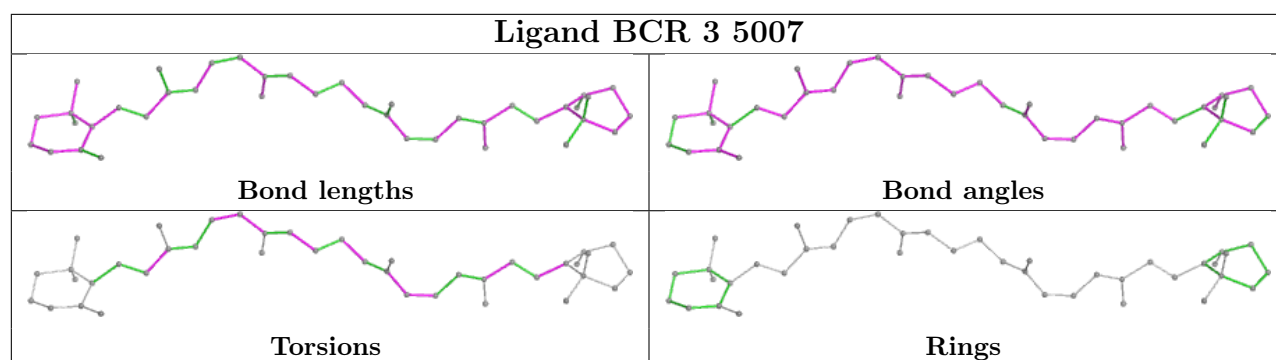


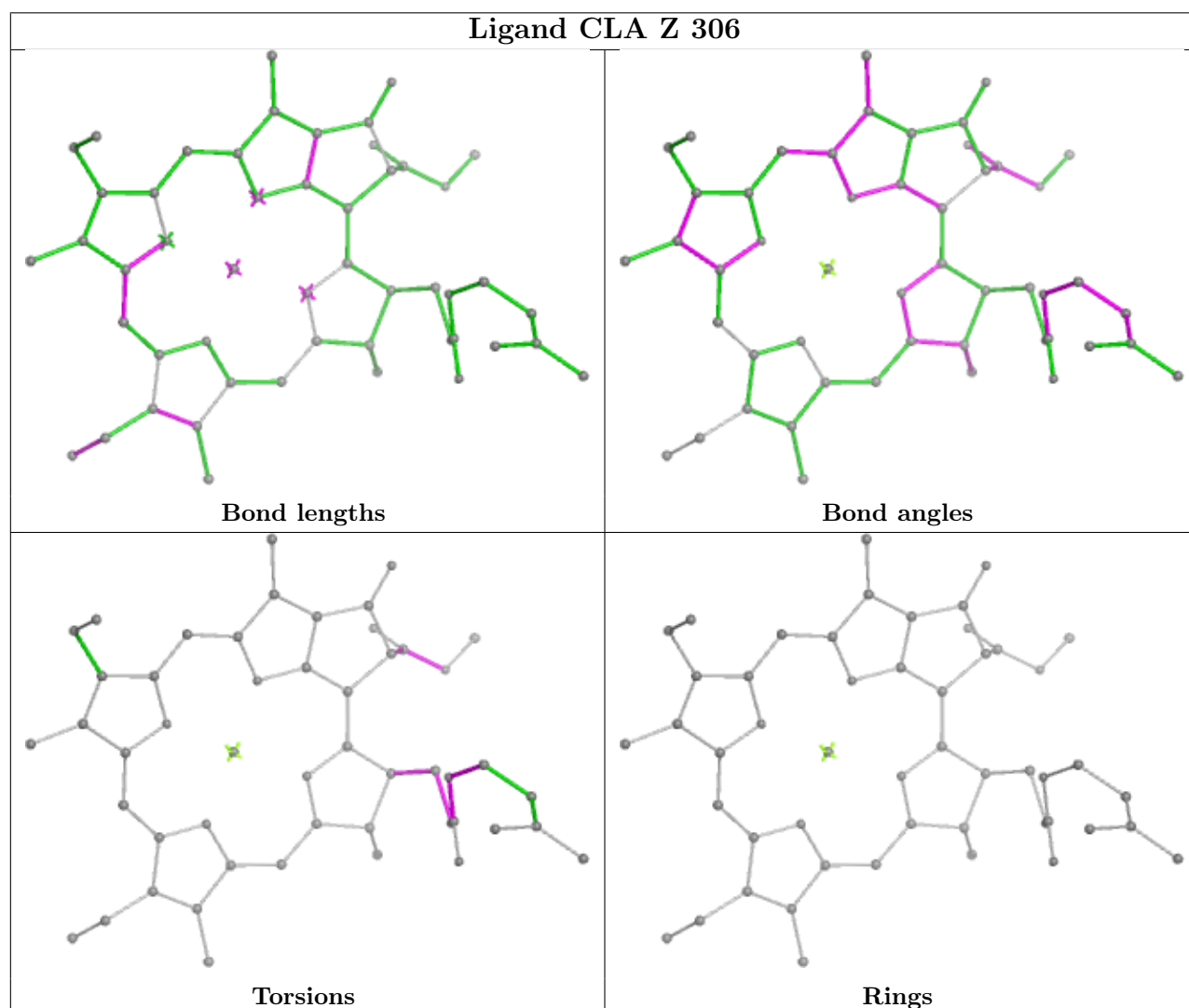
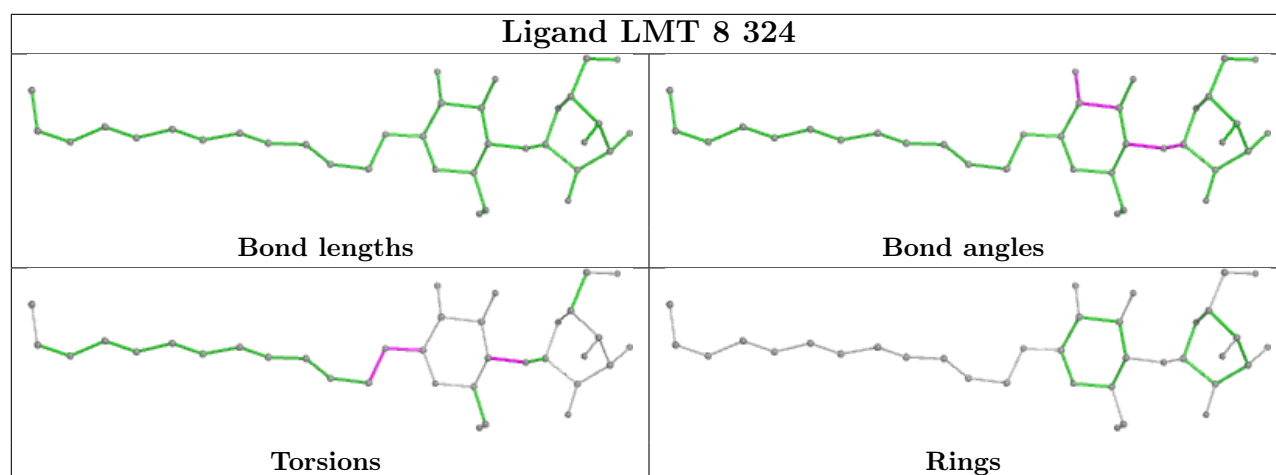
Ligand CLA A 833**Ligand CLA B 811**

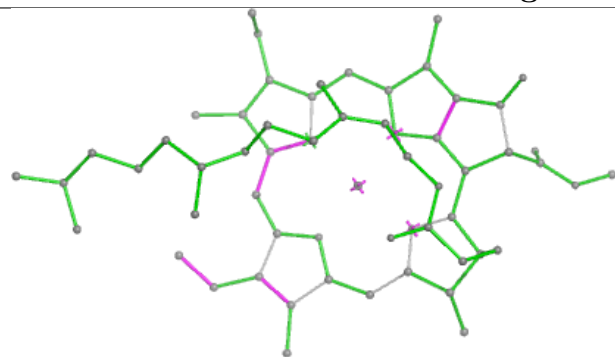
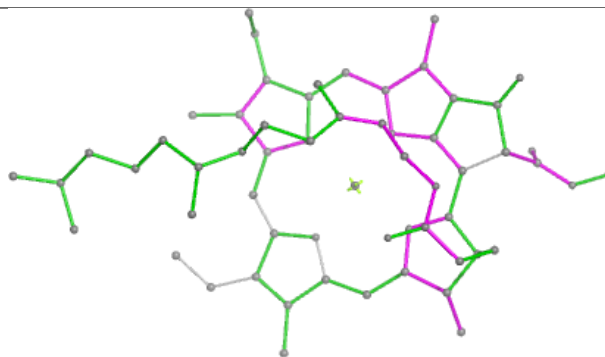
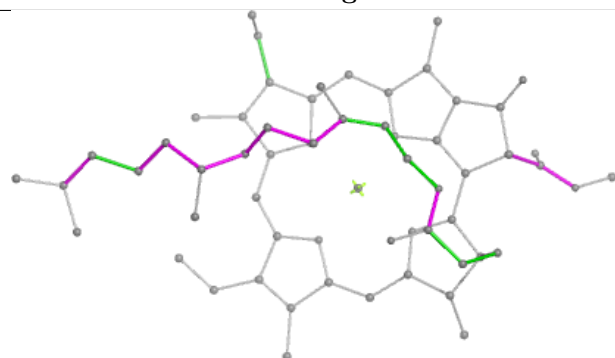
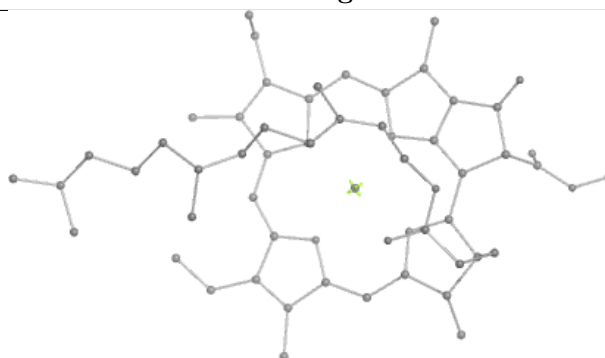


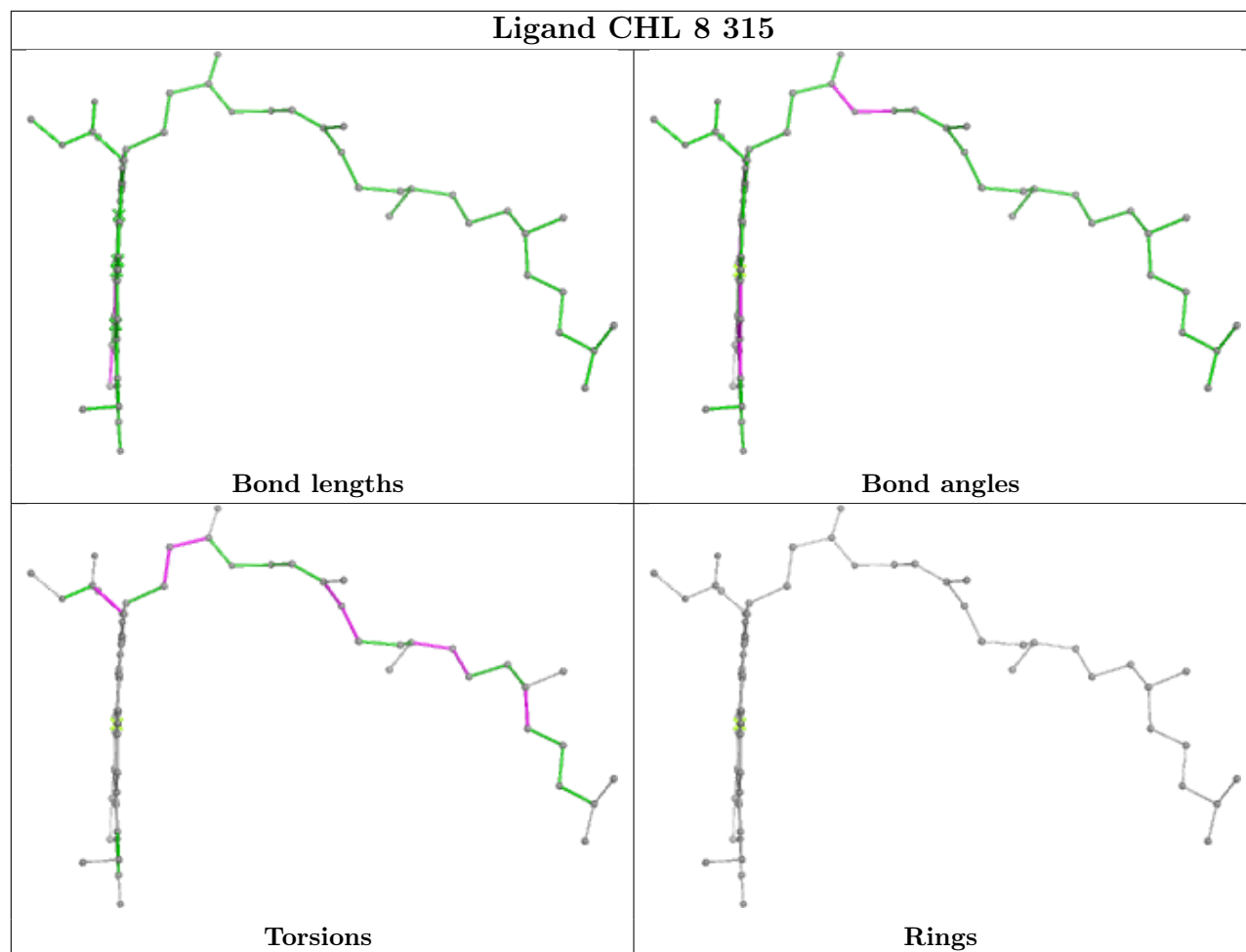


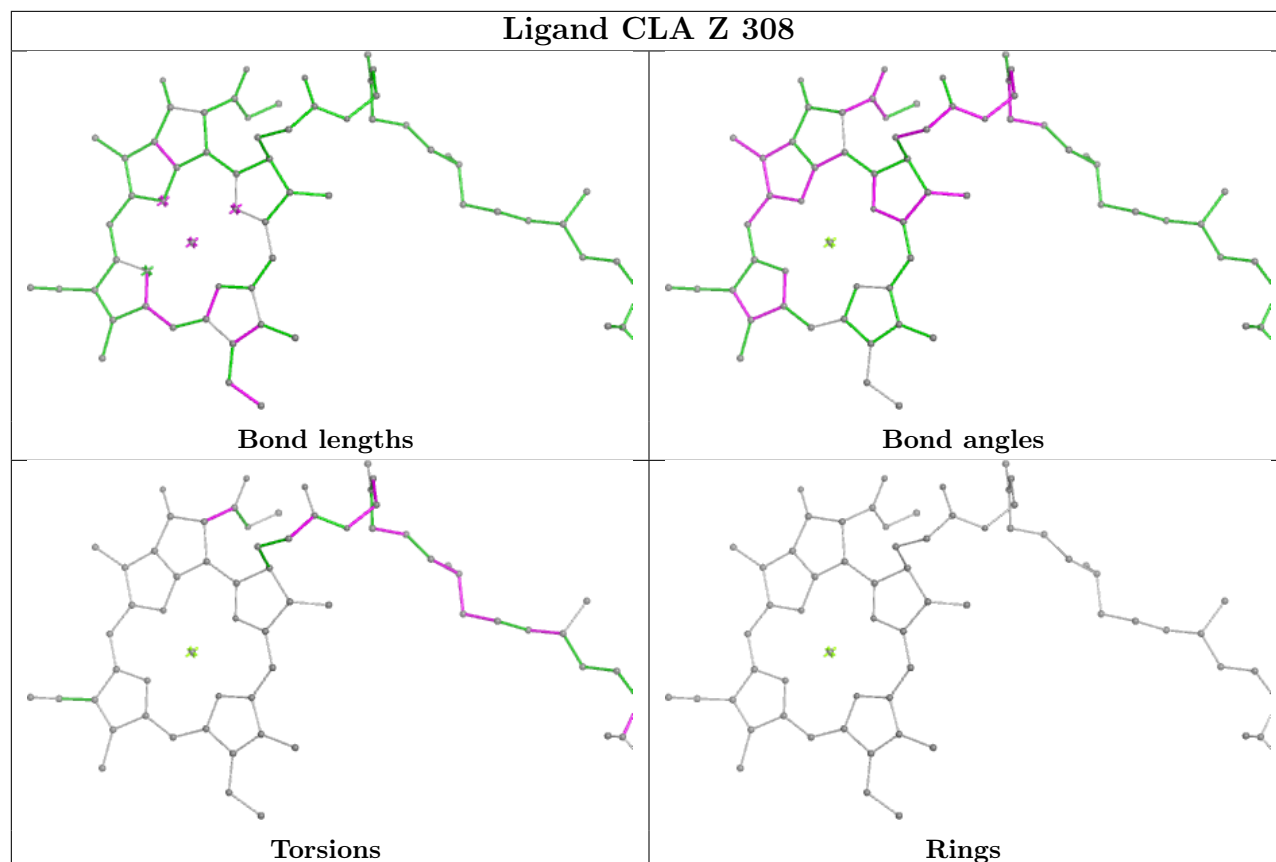
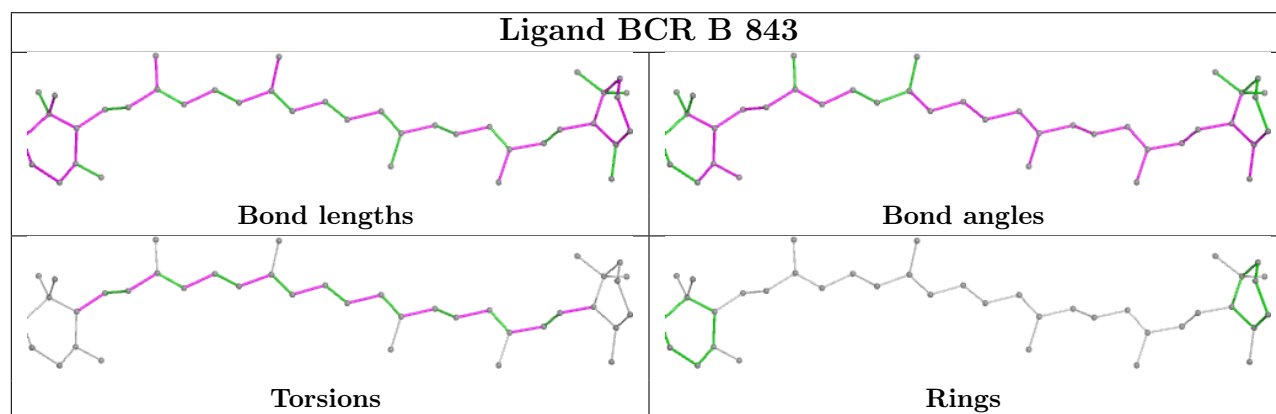




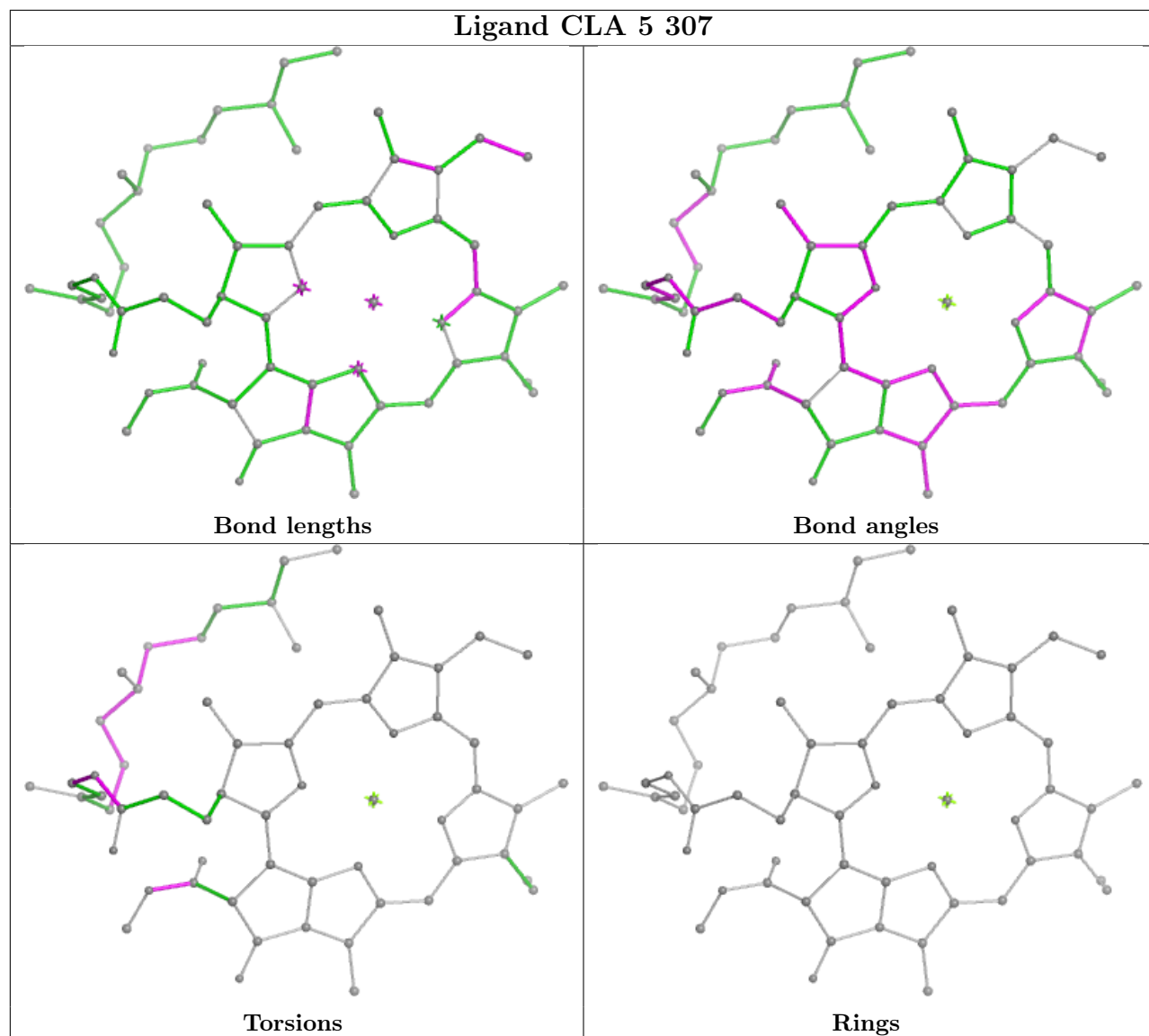


Ligand CLA 6 301**Bond lengths****Bond angles****Torsions****Rings**

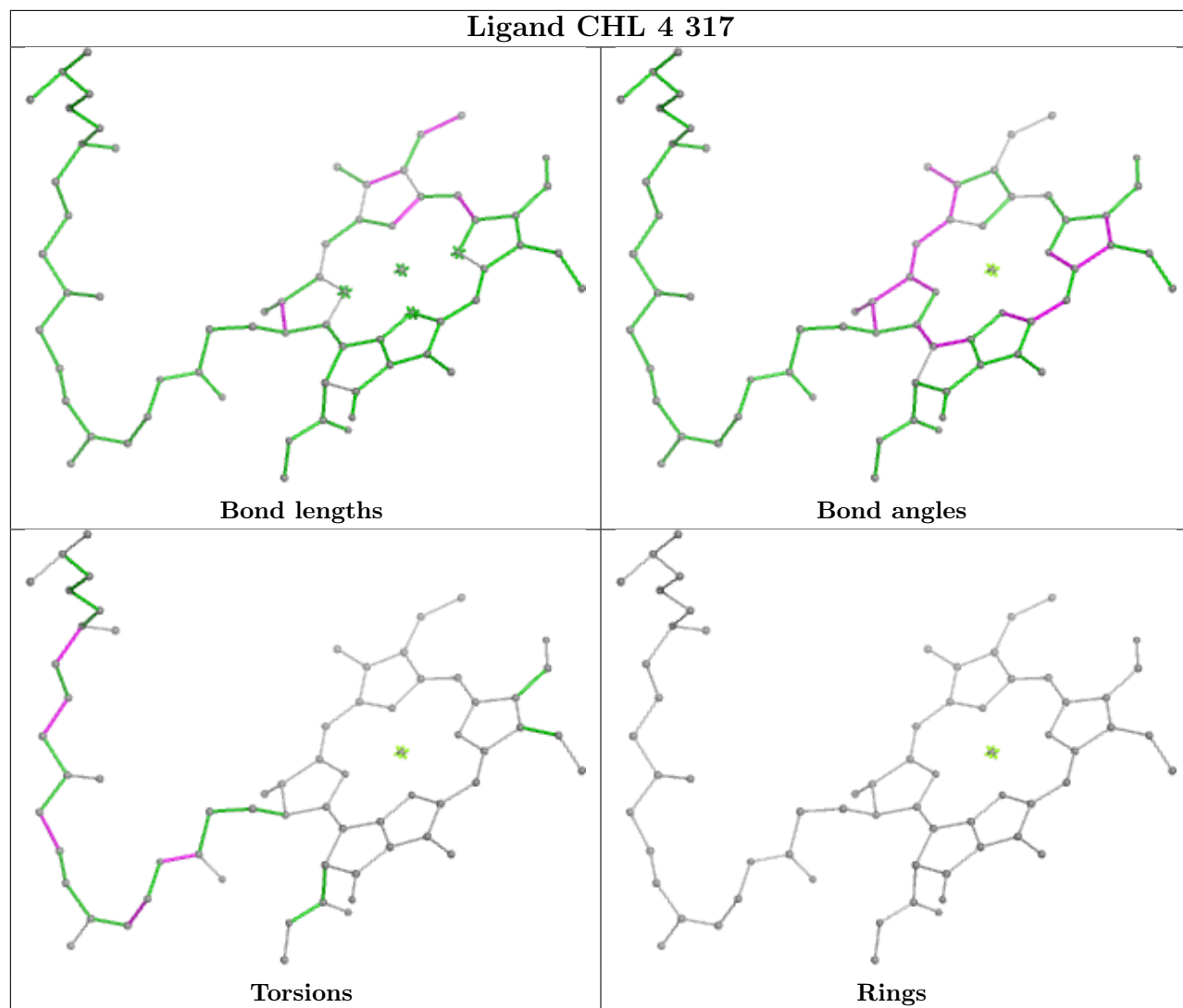


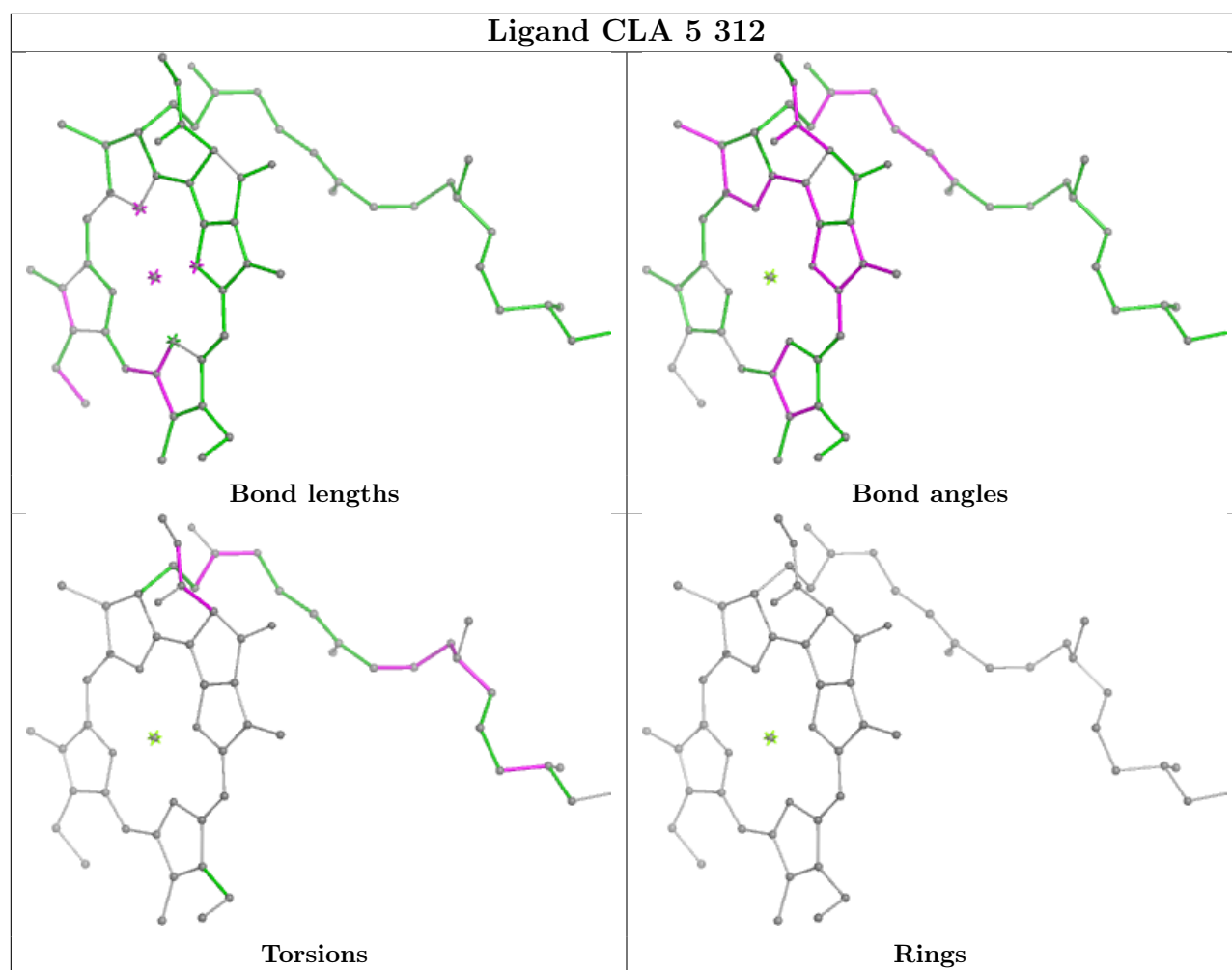
Ligand CLA Z 308**Ligand BCR B 843**

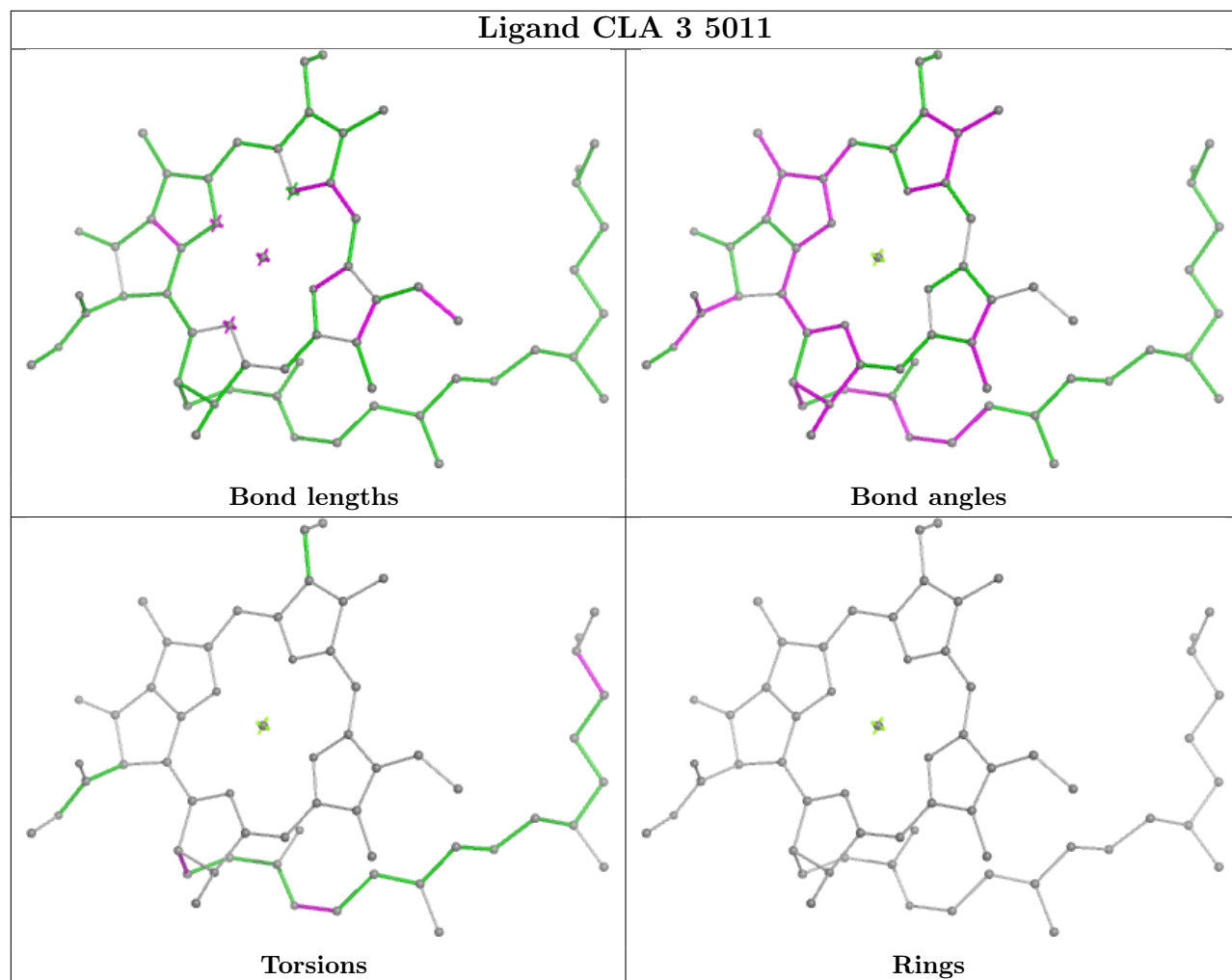
Ligand CLA 5 307

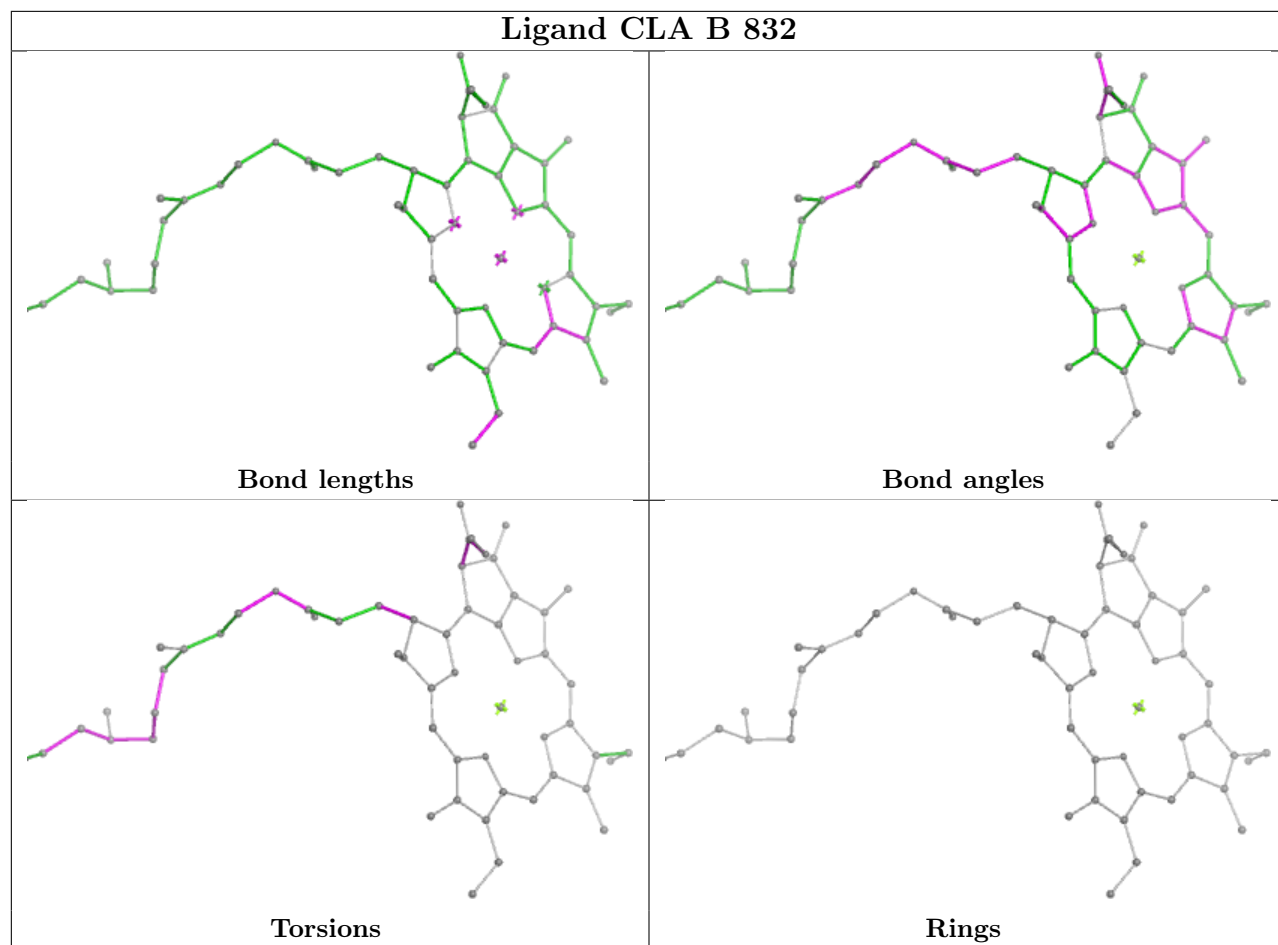


Ligand CHL 4 317

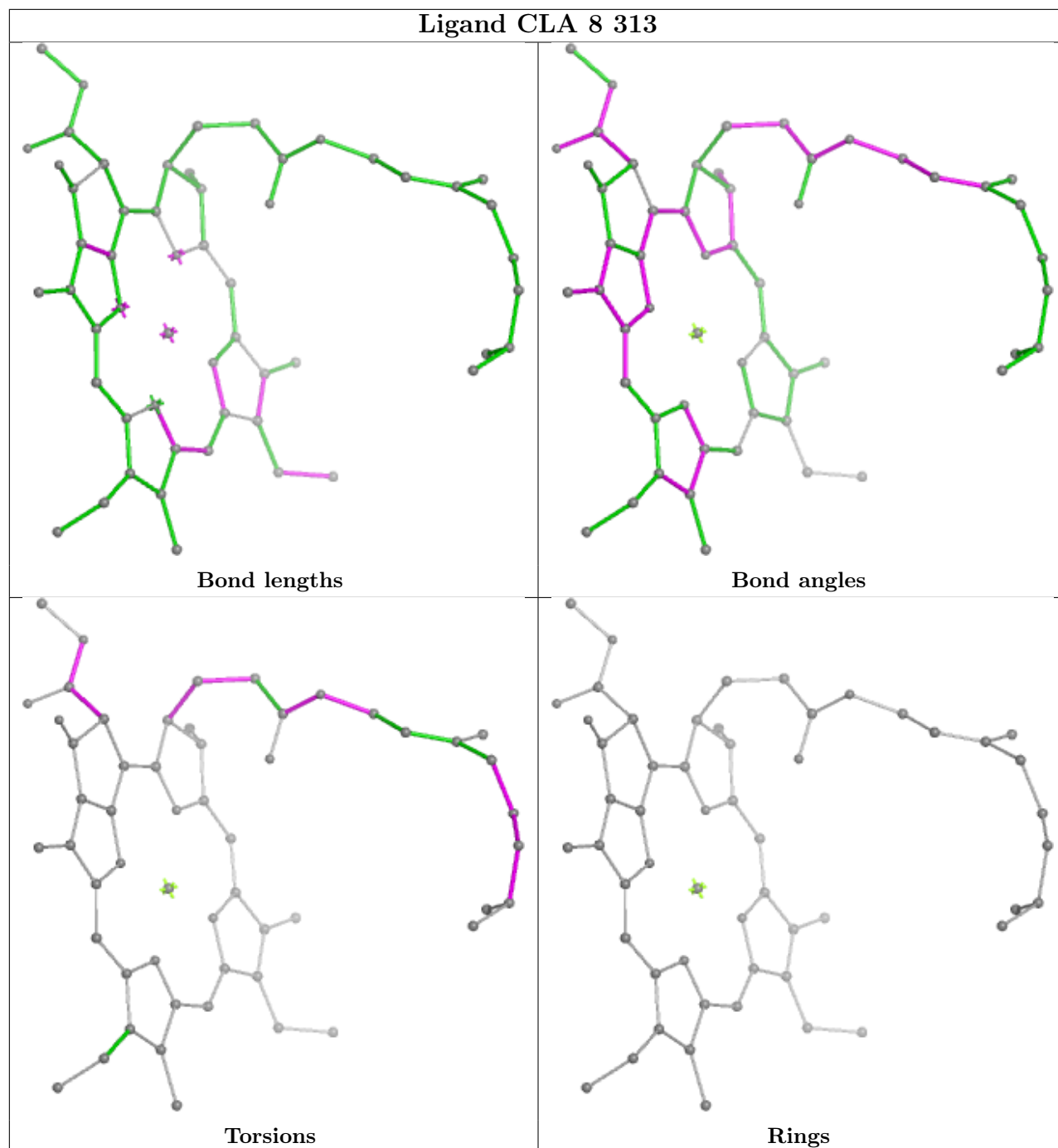




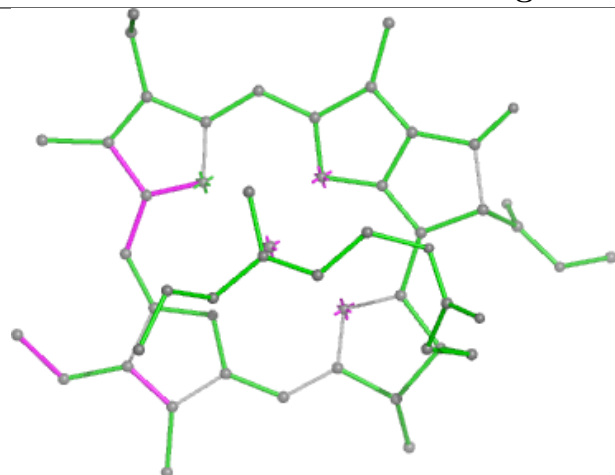




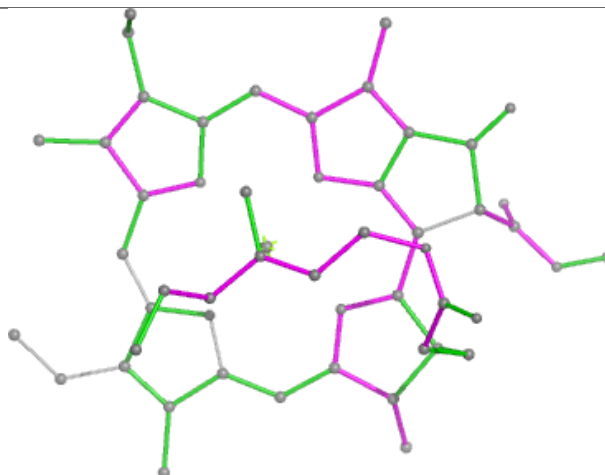
Ligand CLA 8 313



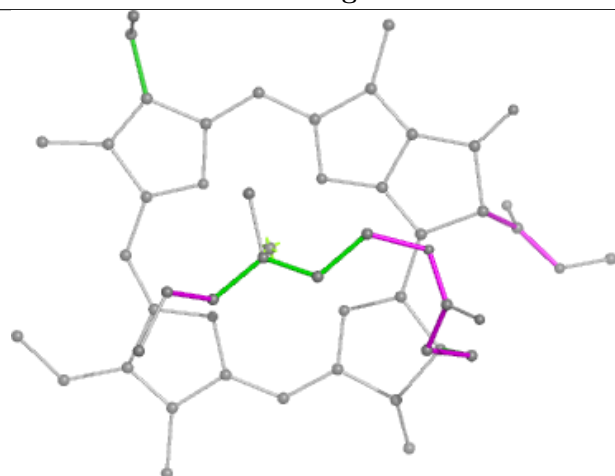
Ligand CLA A 857



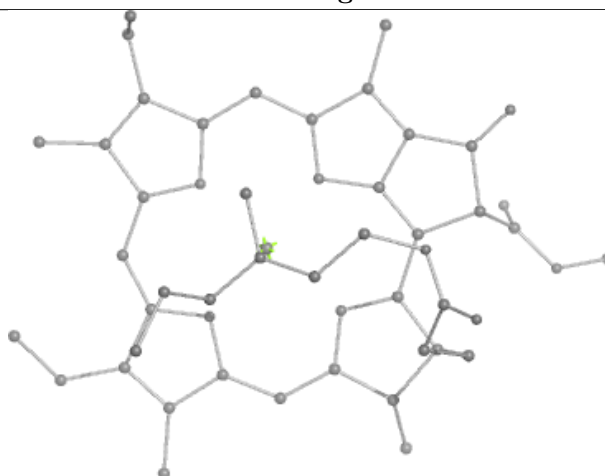
Bond lengths



Bond angles

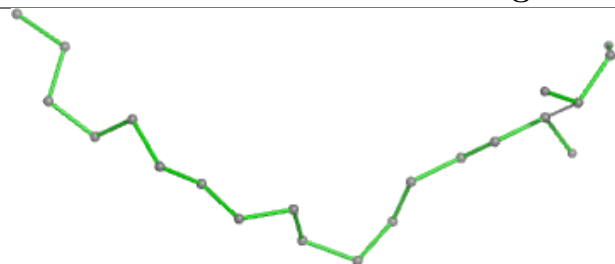


Torsions

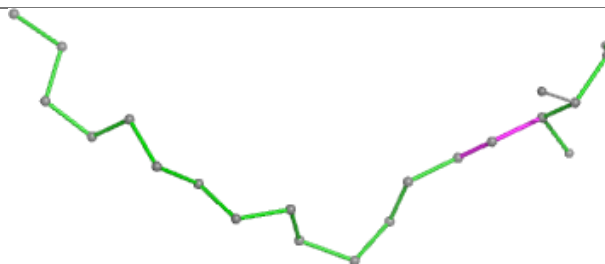


Rings

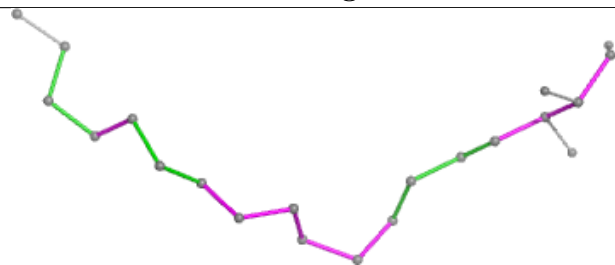
Ligand SPH 3 5001



Bond lengths



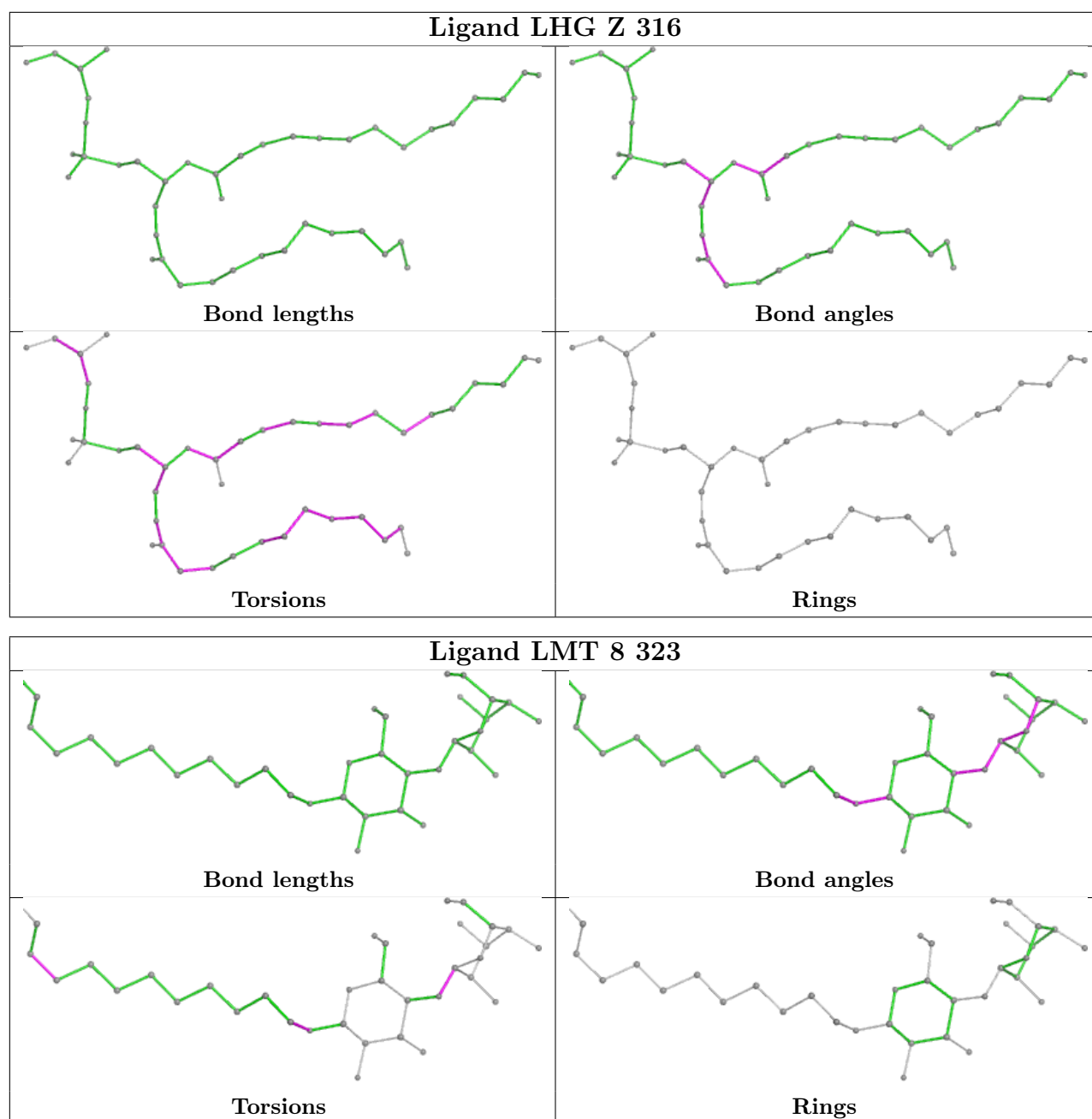
Bond angles



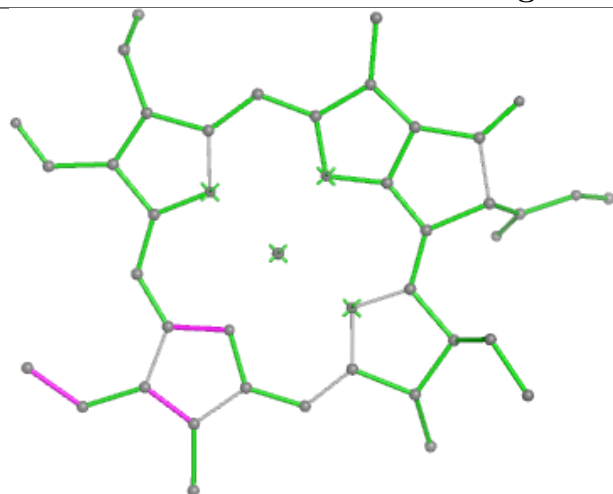
Torsions



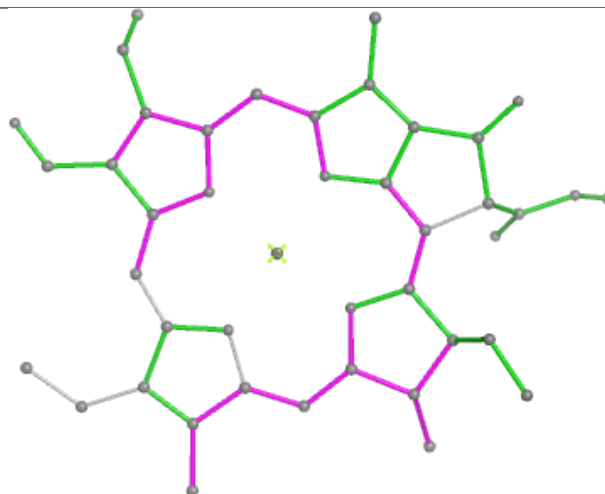
Rings



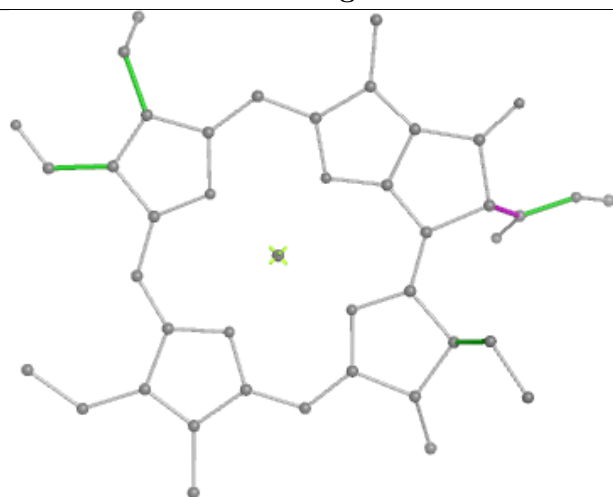
Ligand CHL 4 319



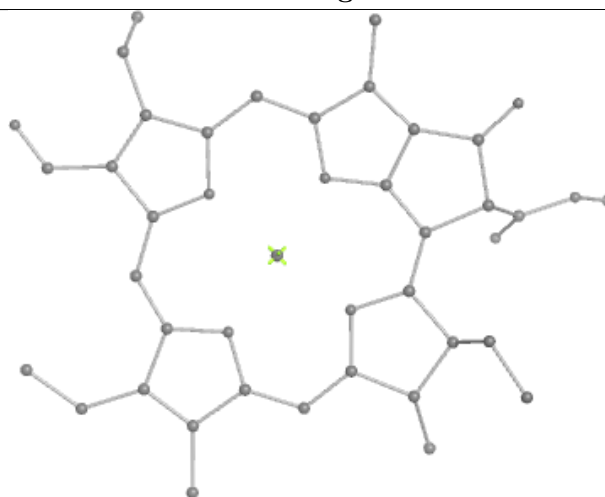
Bond lengths



Bond angles

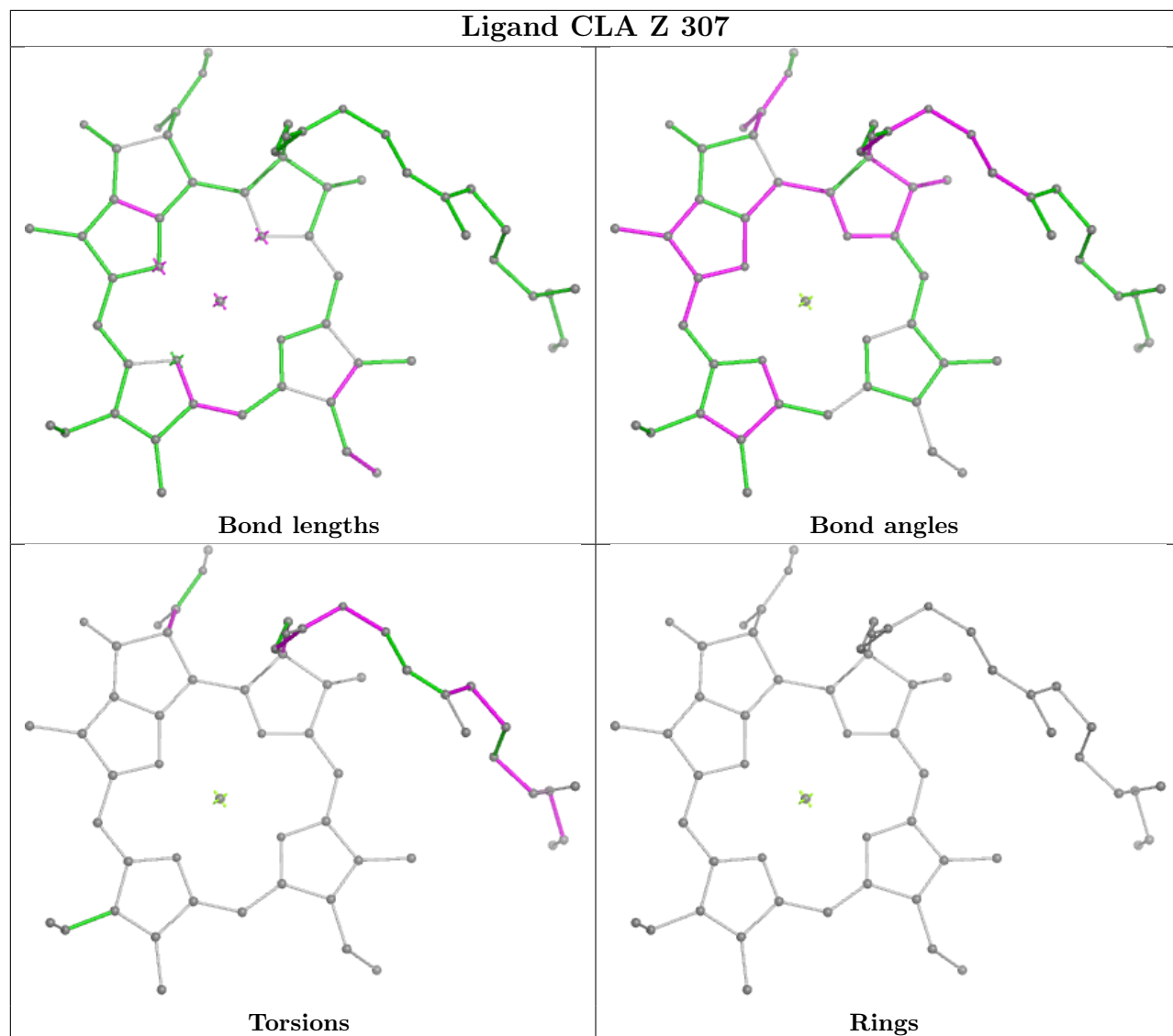


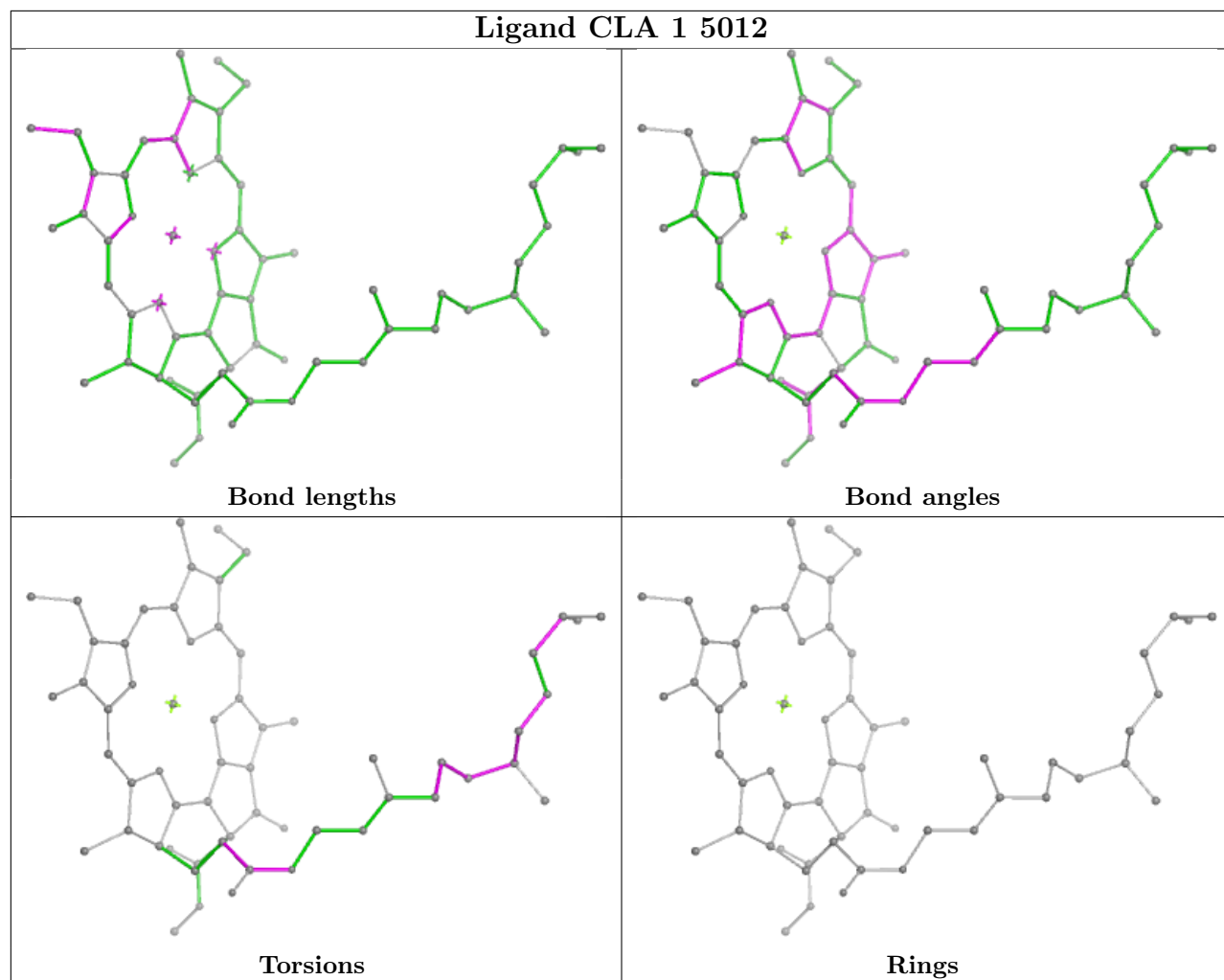
Torsions

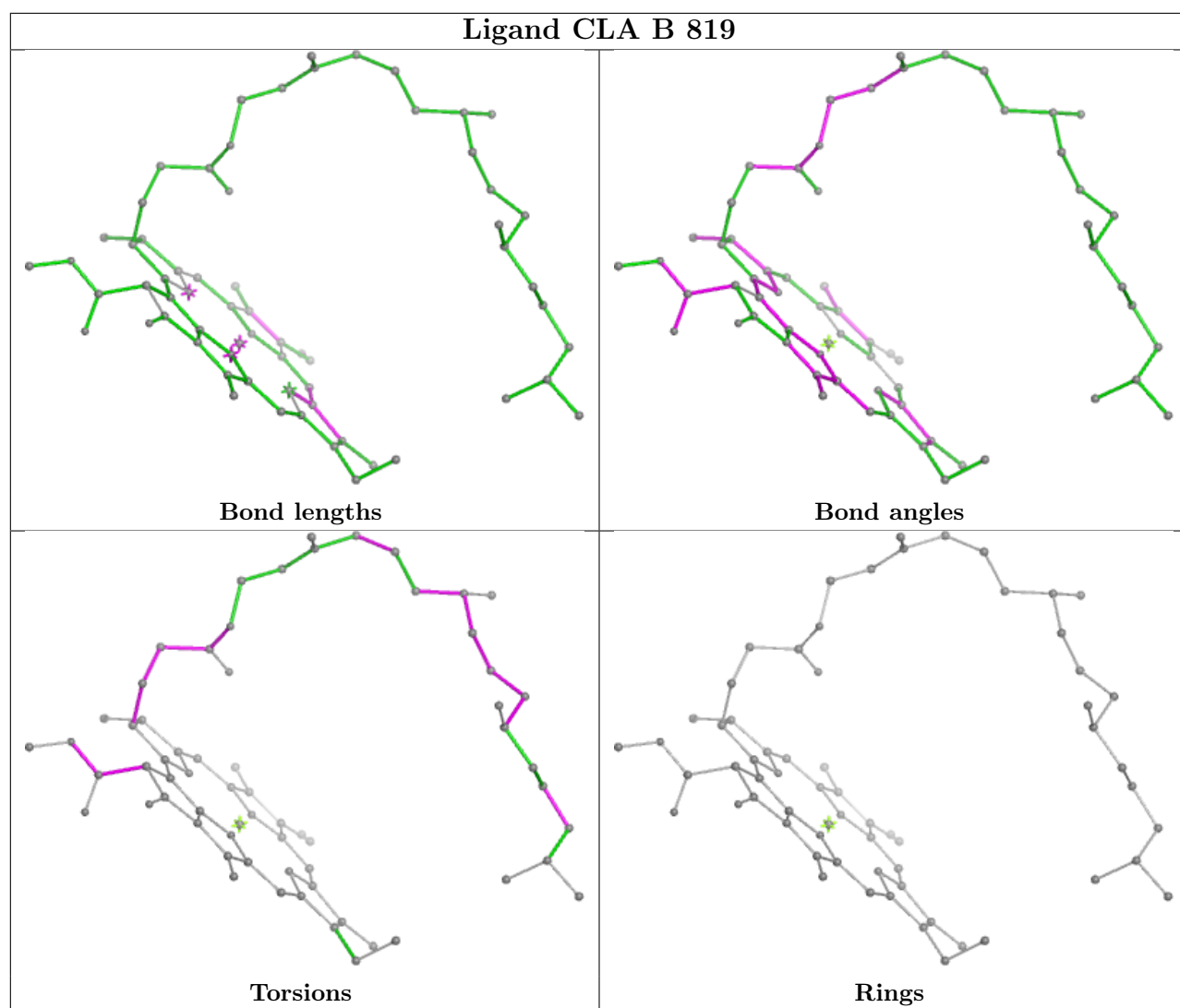


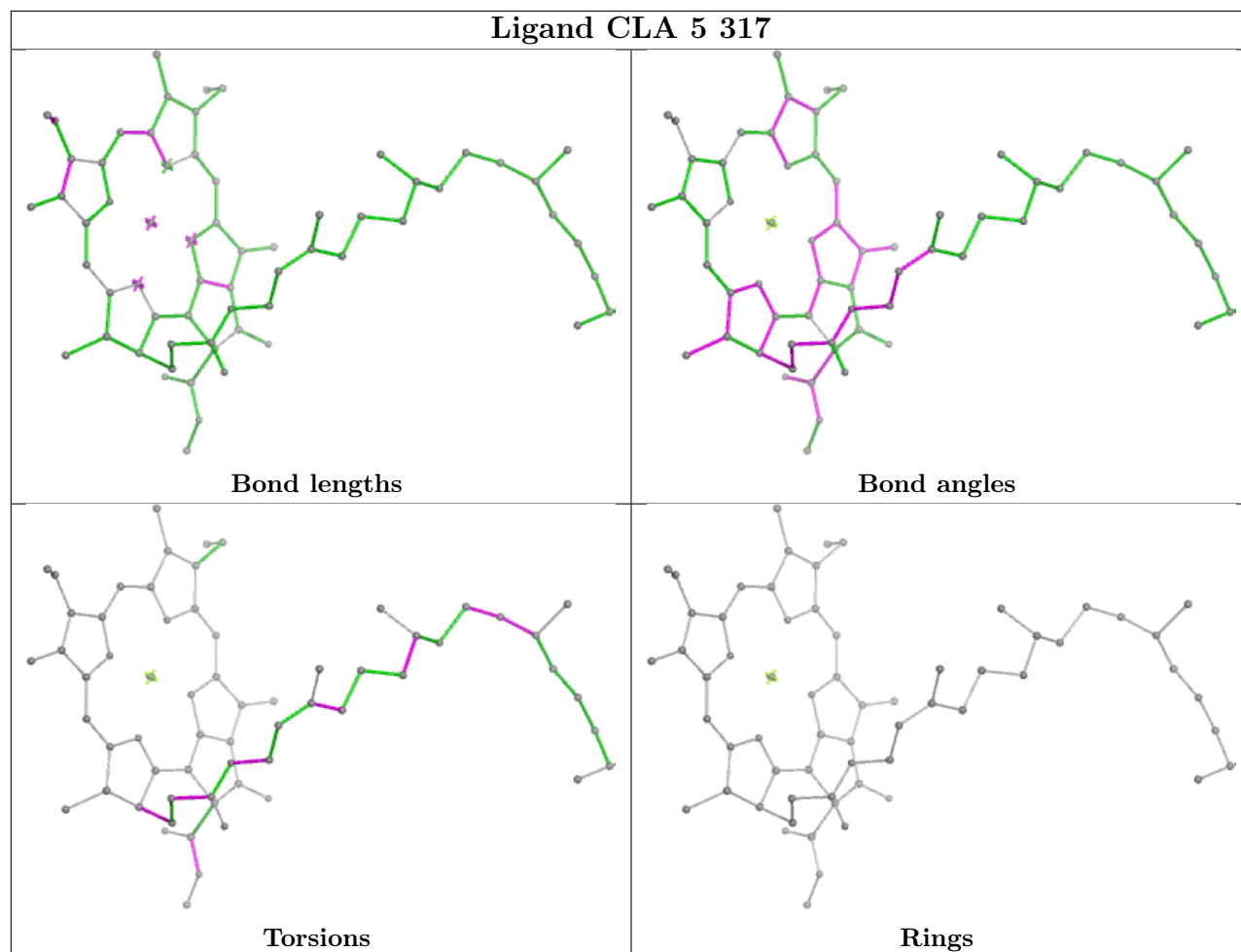
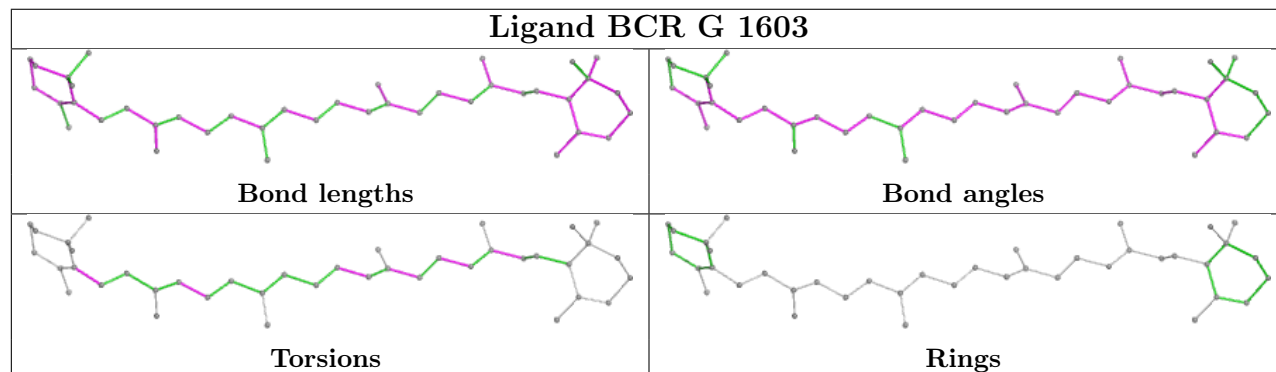
Rings

Ligand CLA Z 307

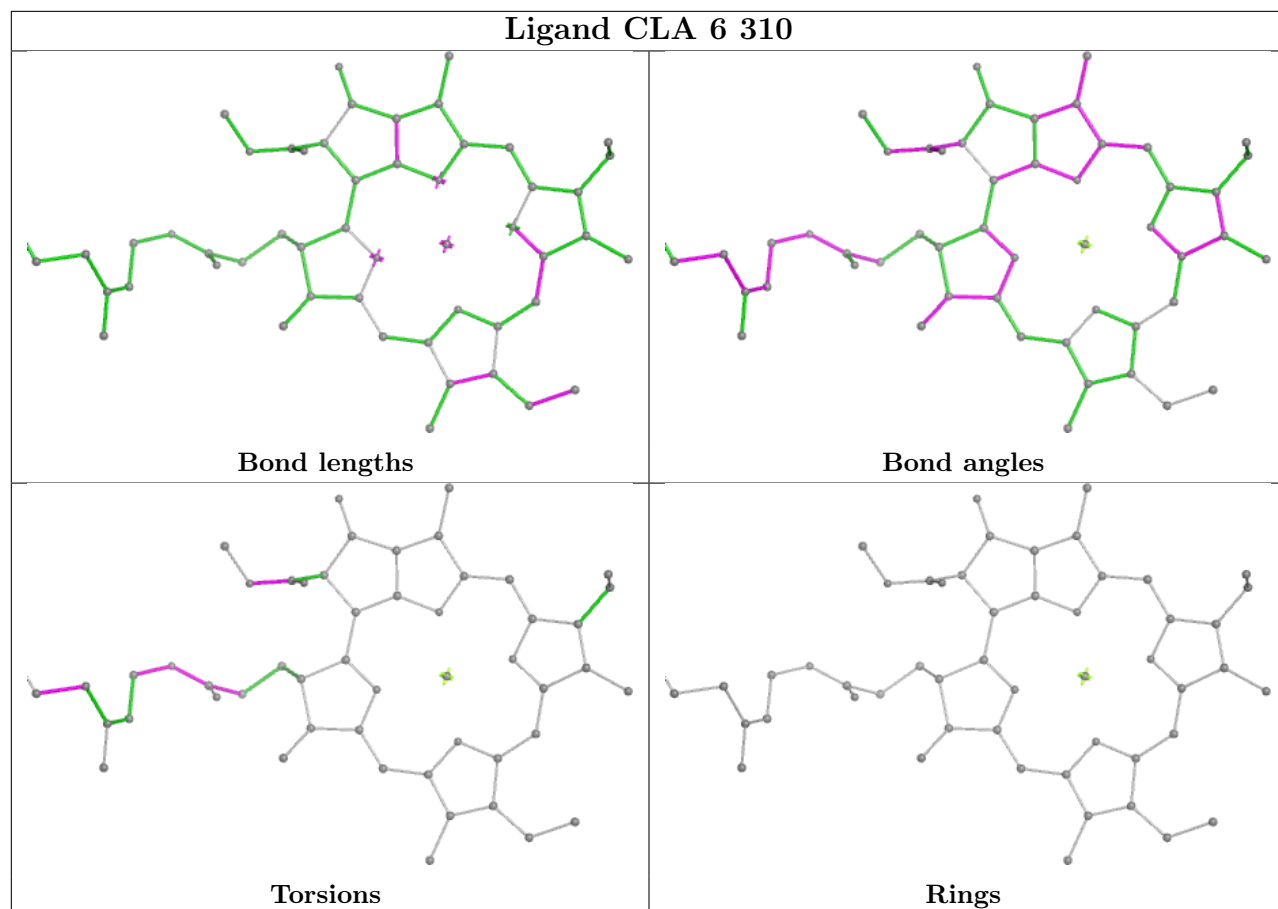




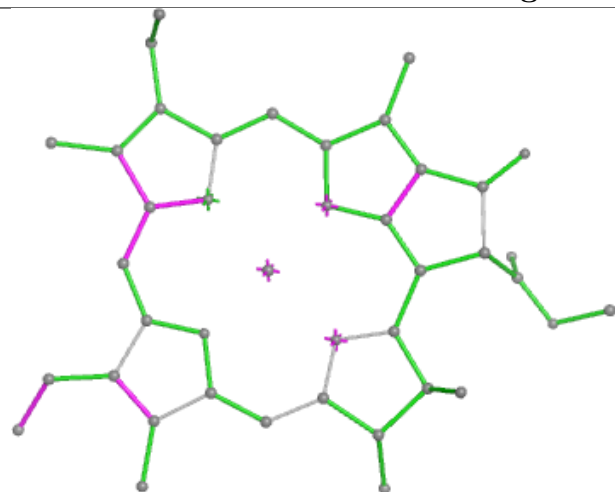


Ligand CLA 5 317**Ligand BCR G 1603**

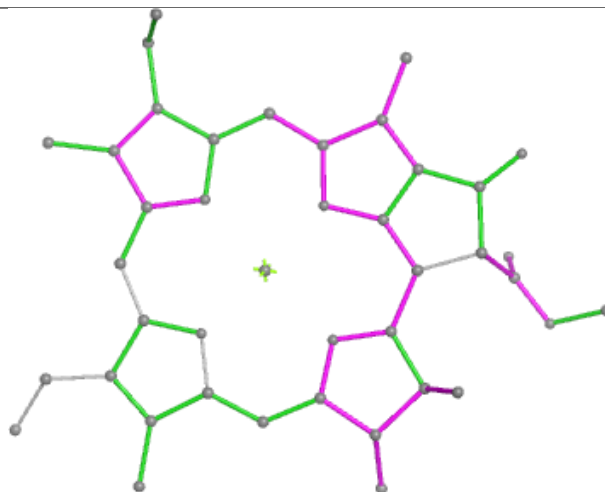
Ligand CLA 6 310



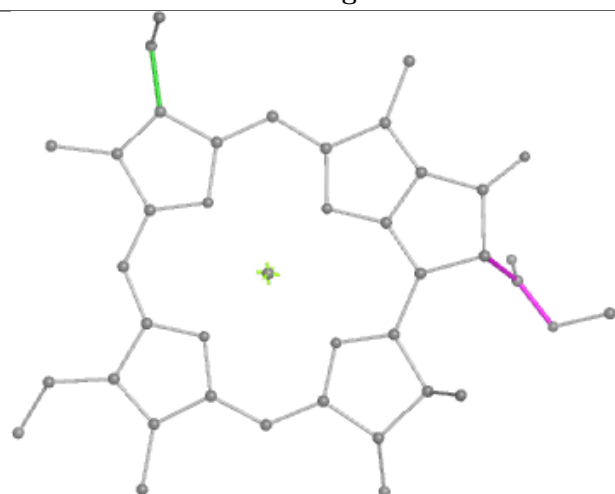
Ligand CLA 4 318



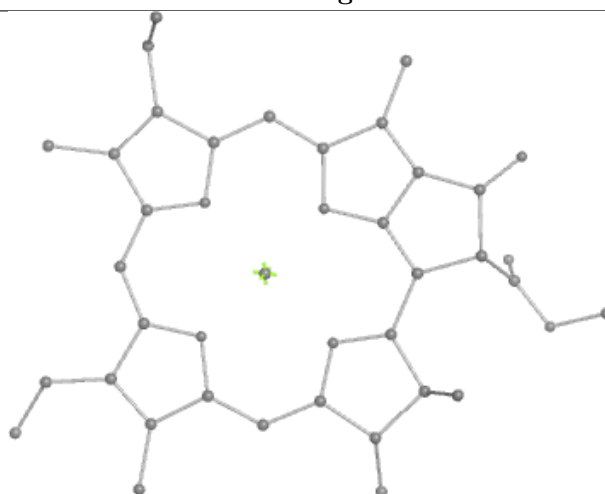
Bond lengths



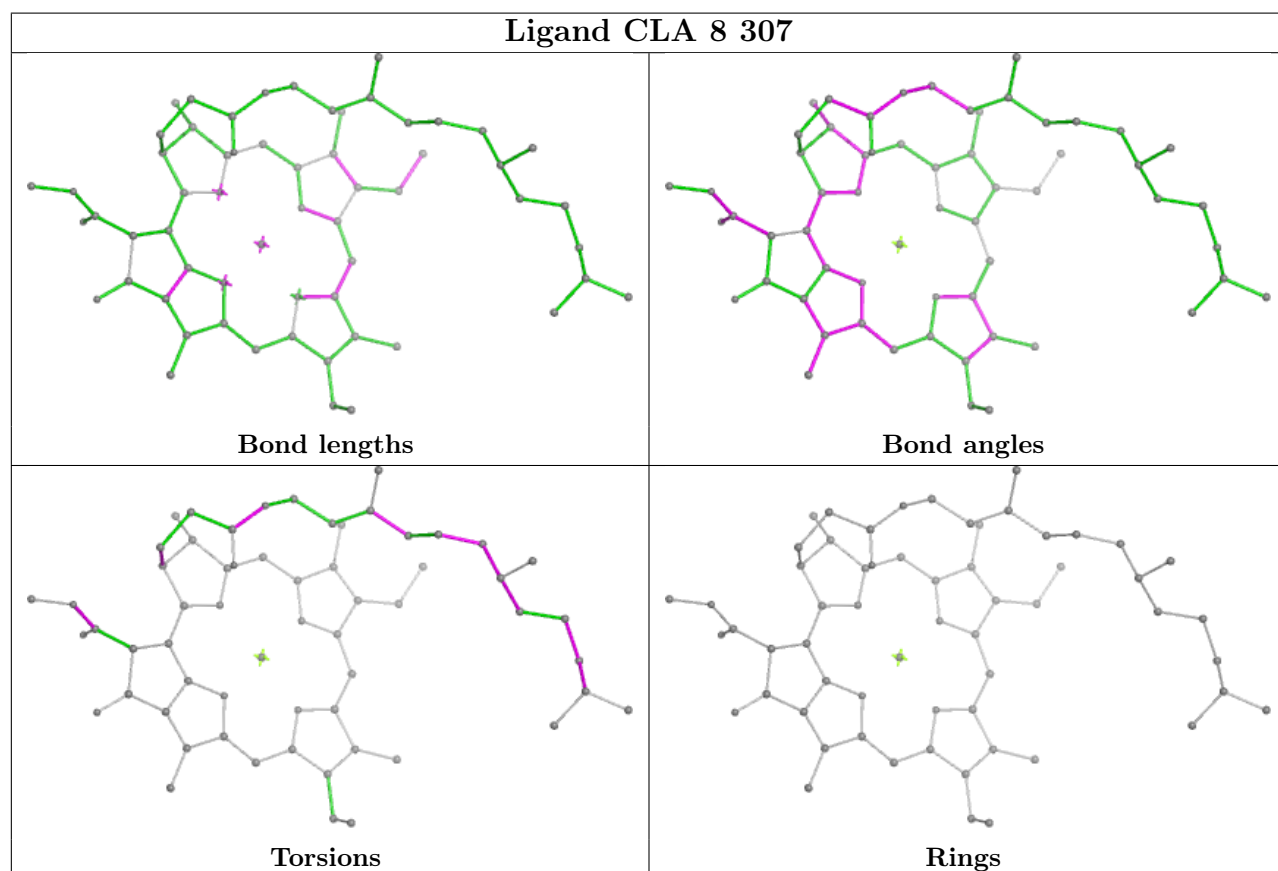
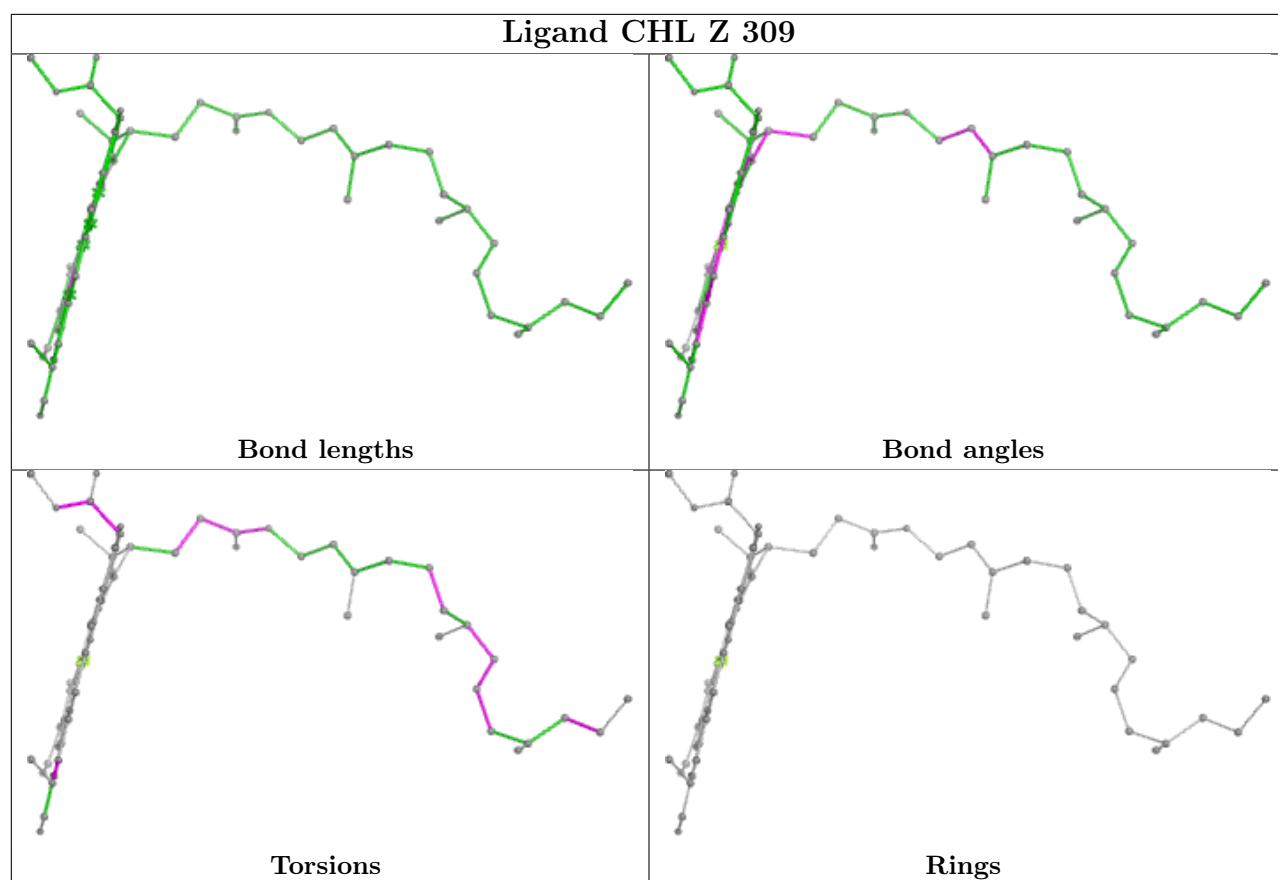
Bond angles

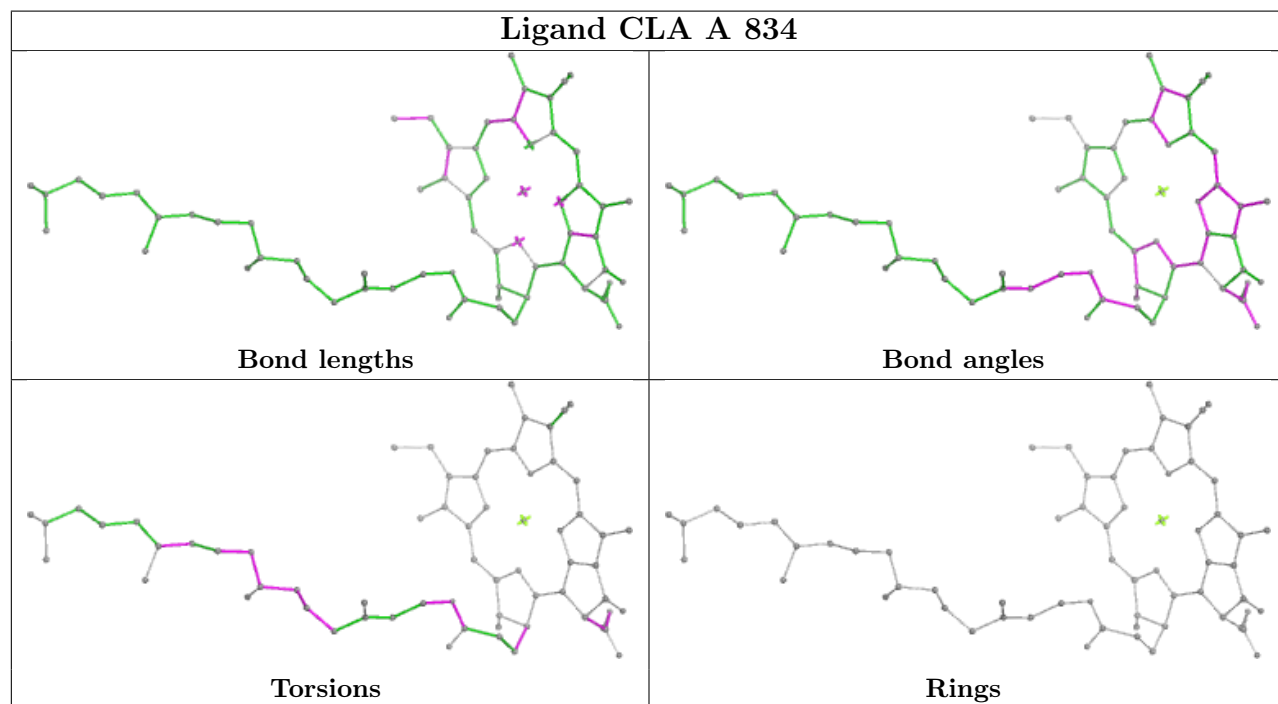
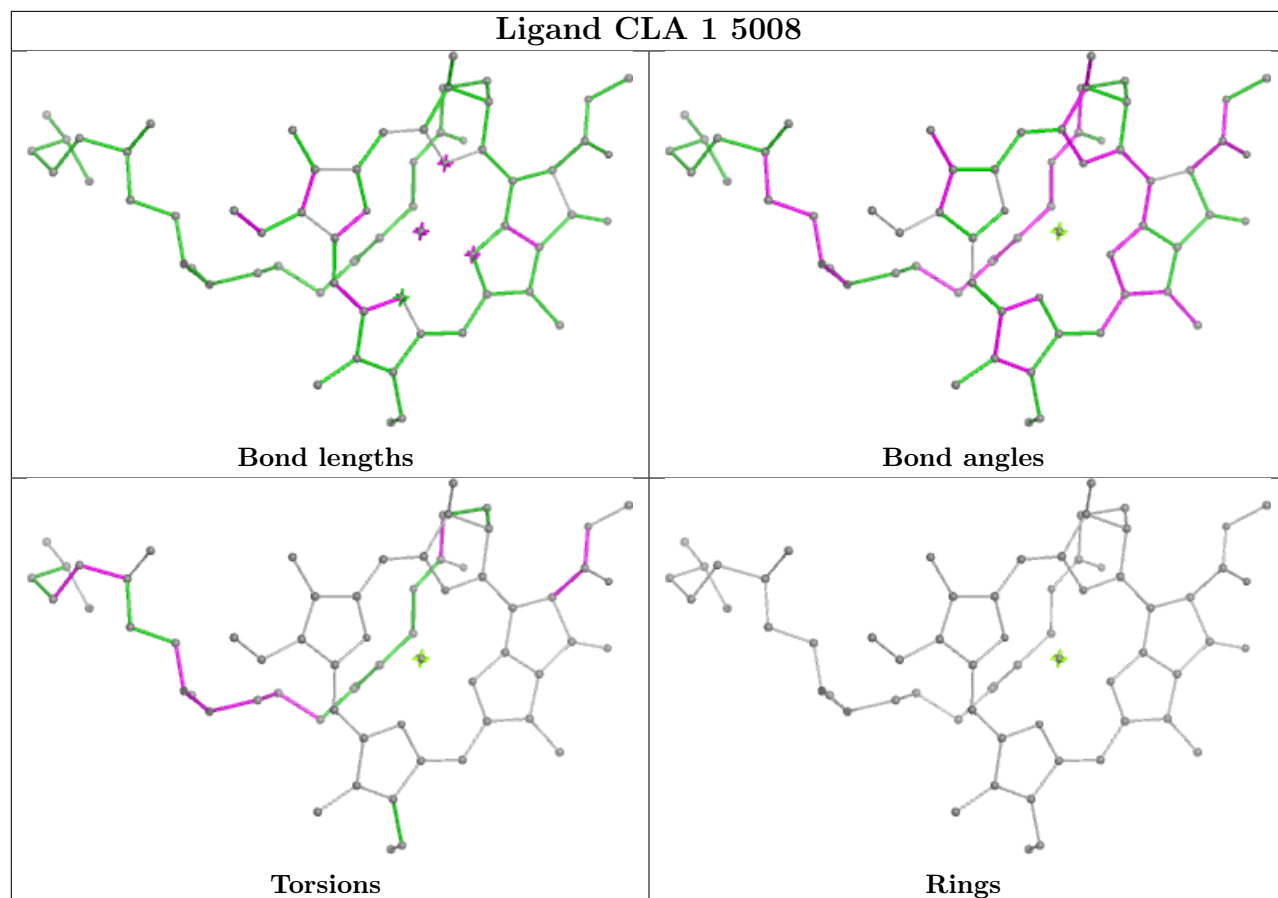


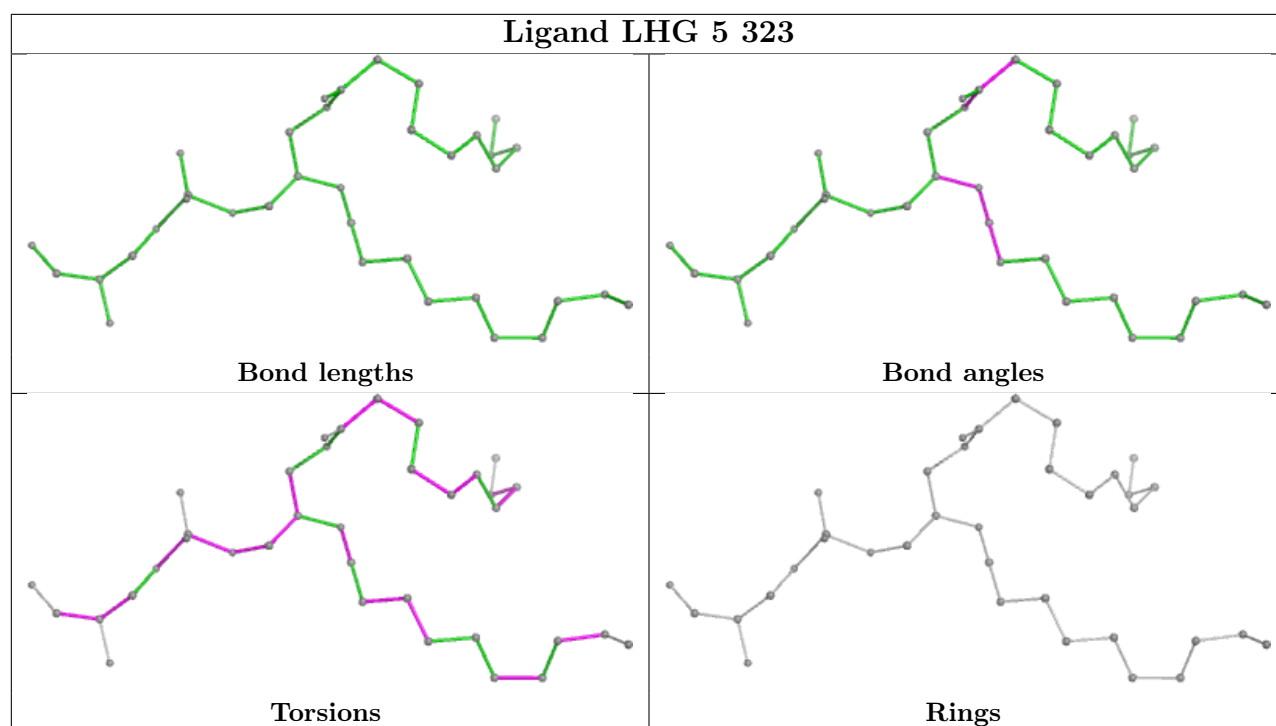
Torsions

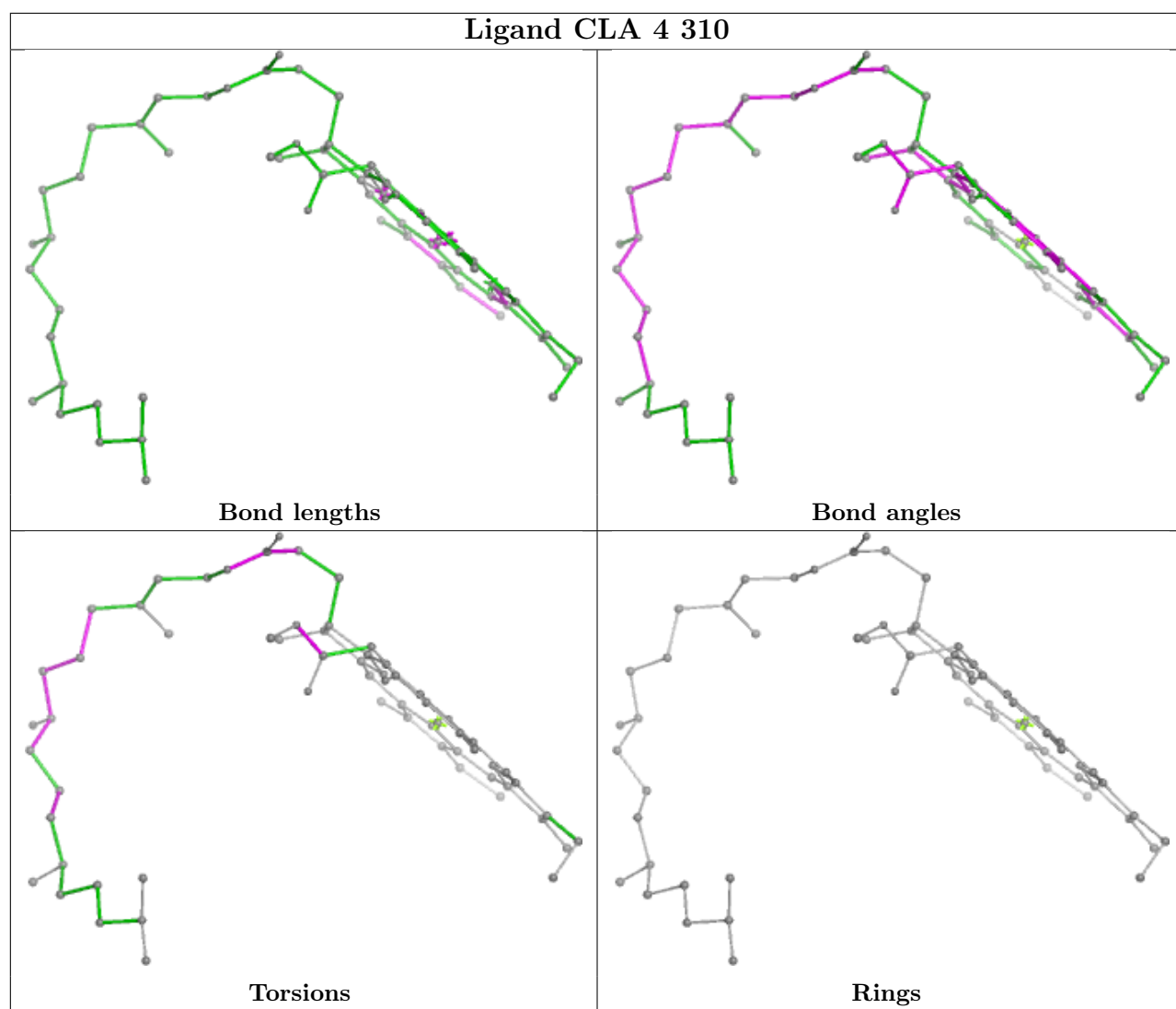


Rings

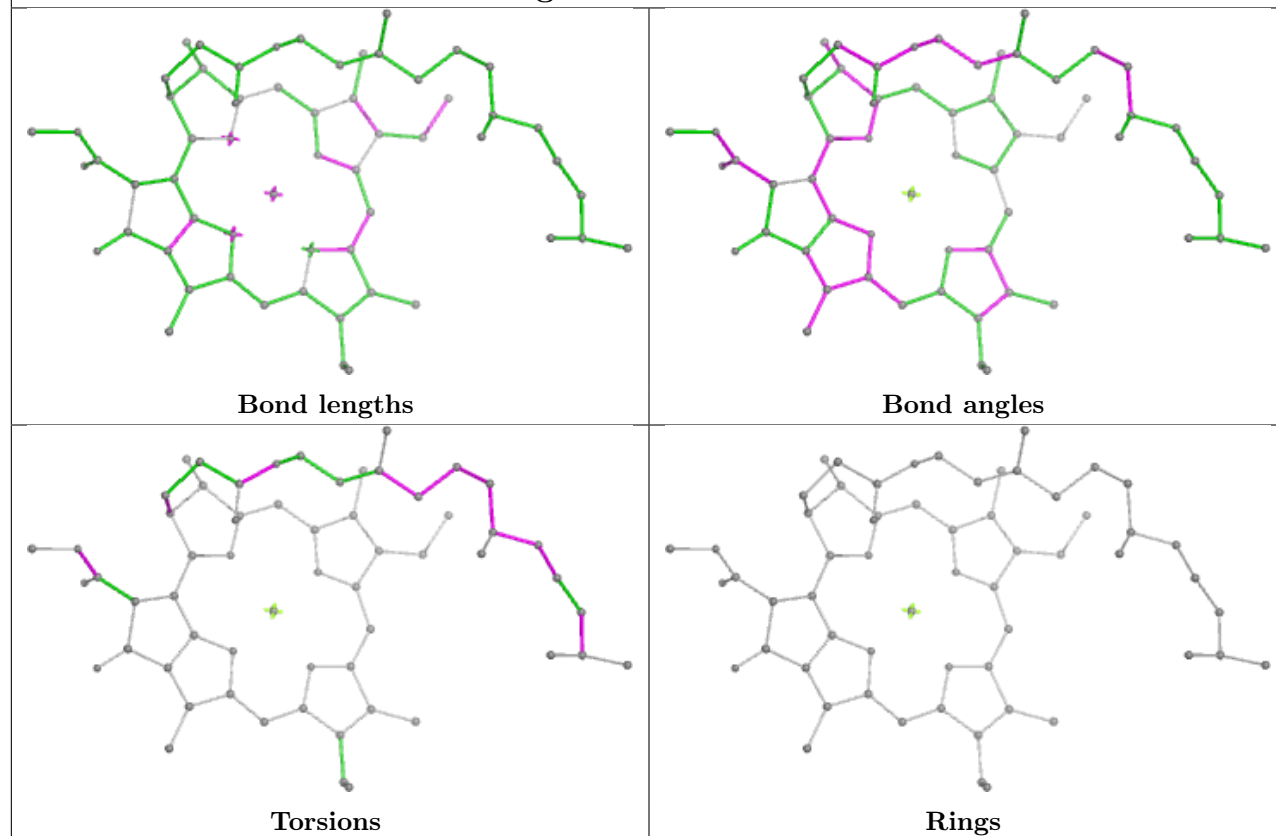




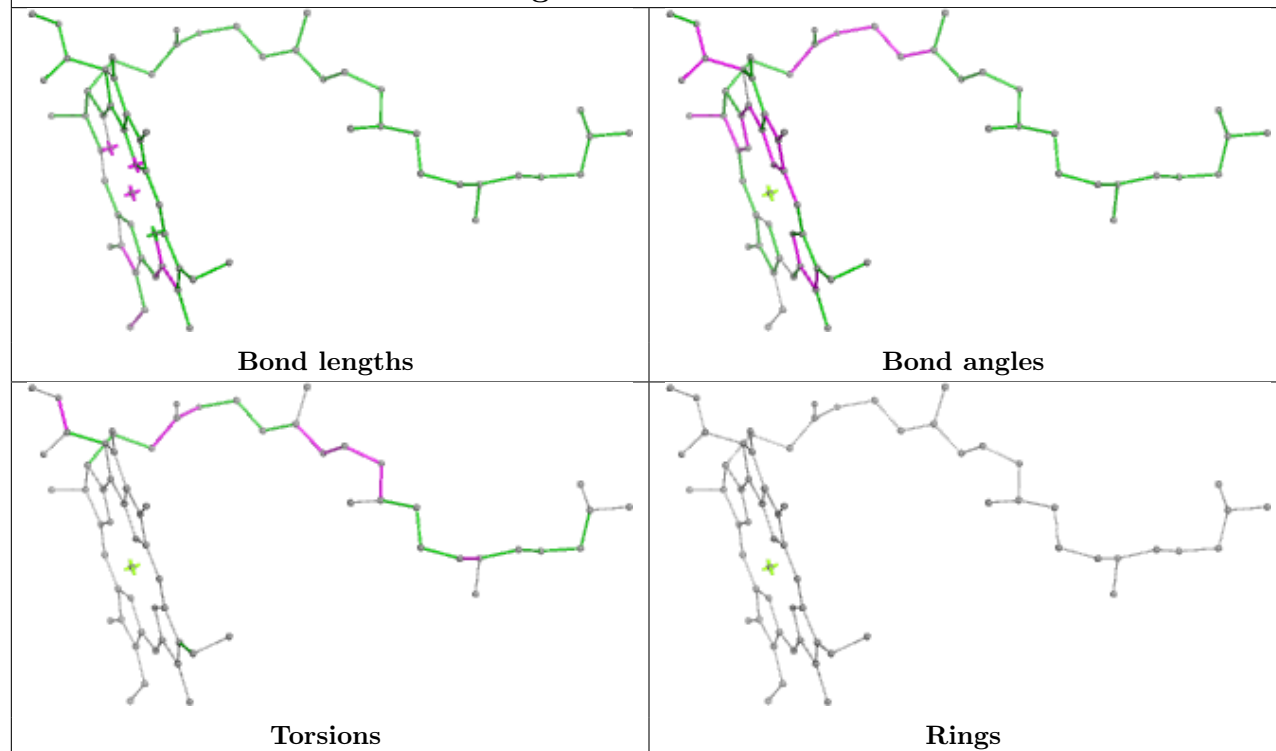


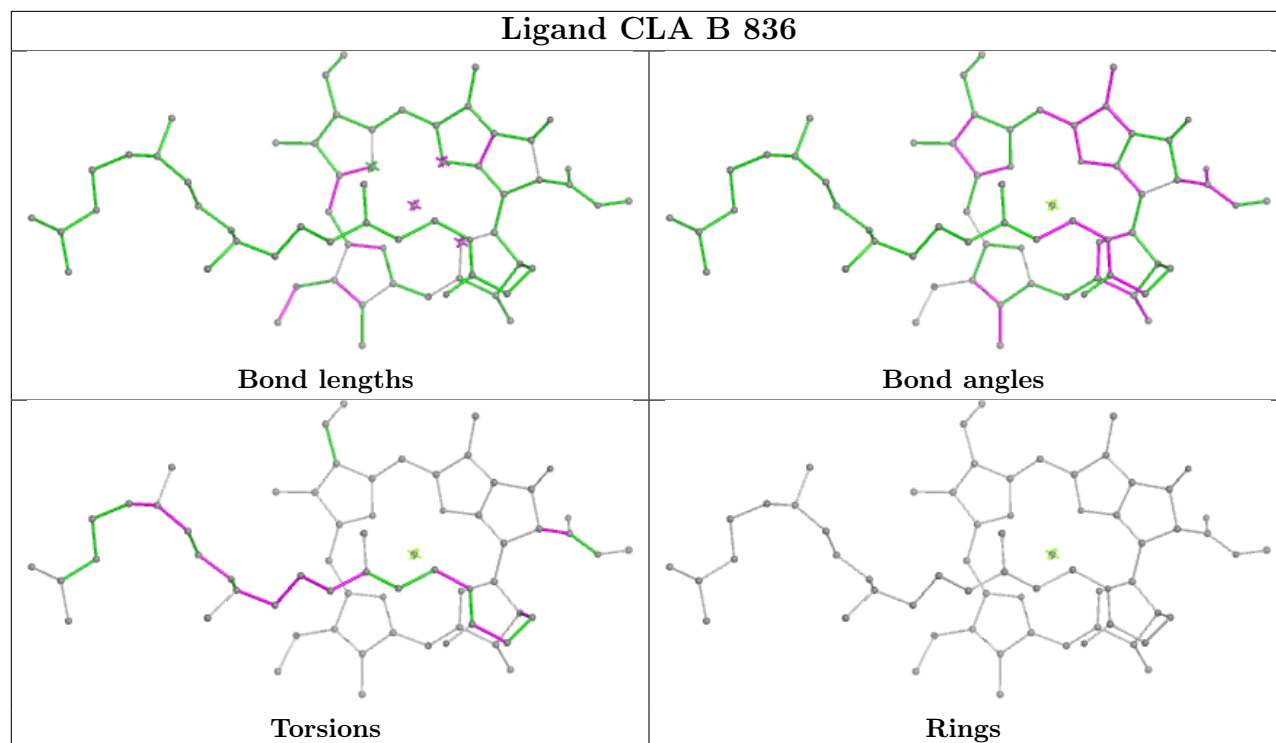
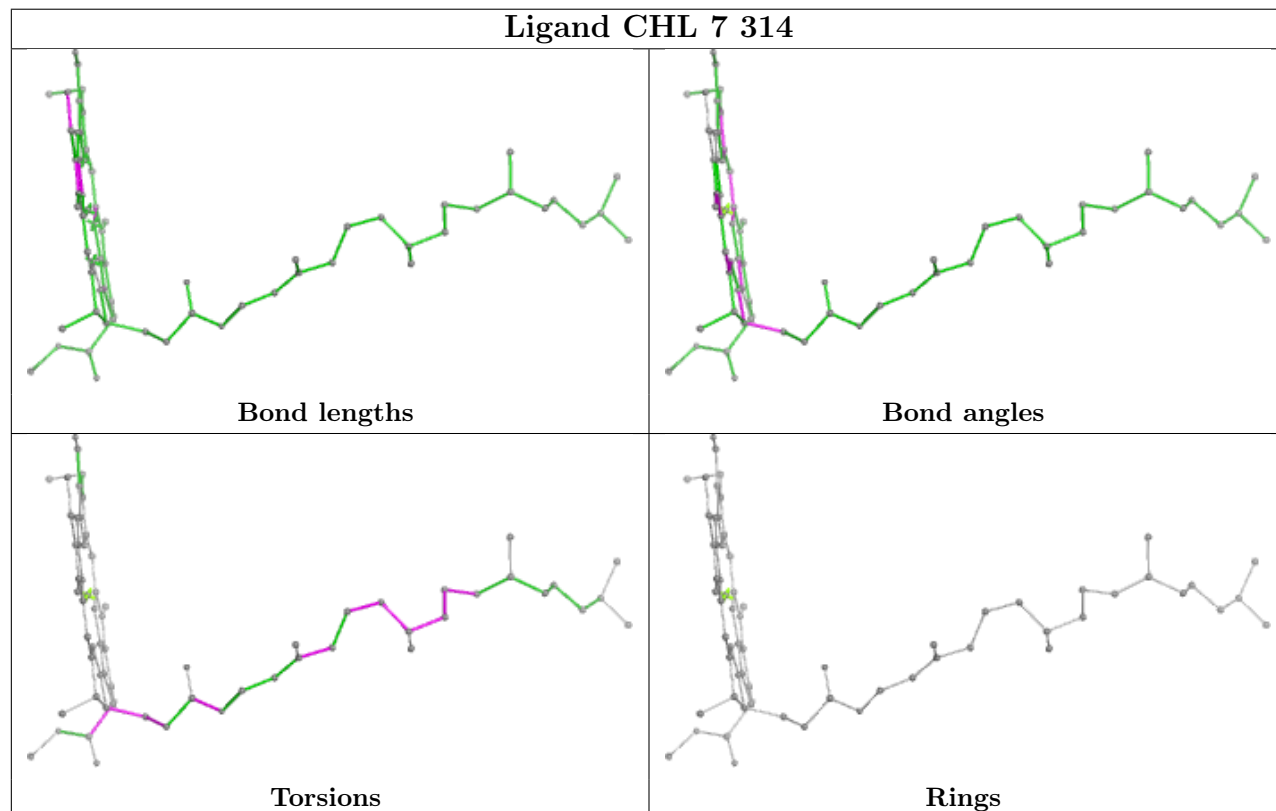


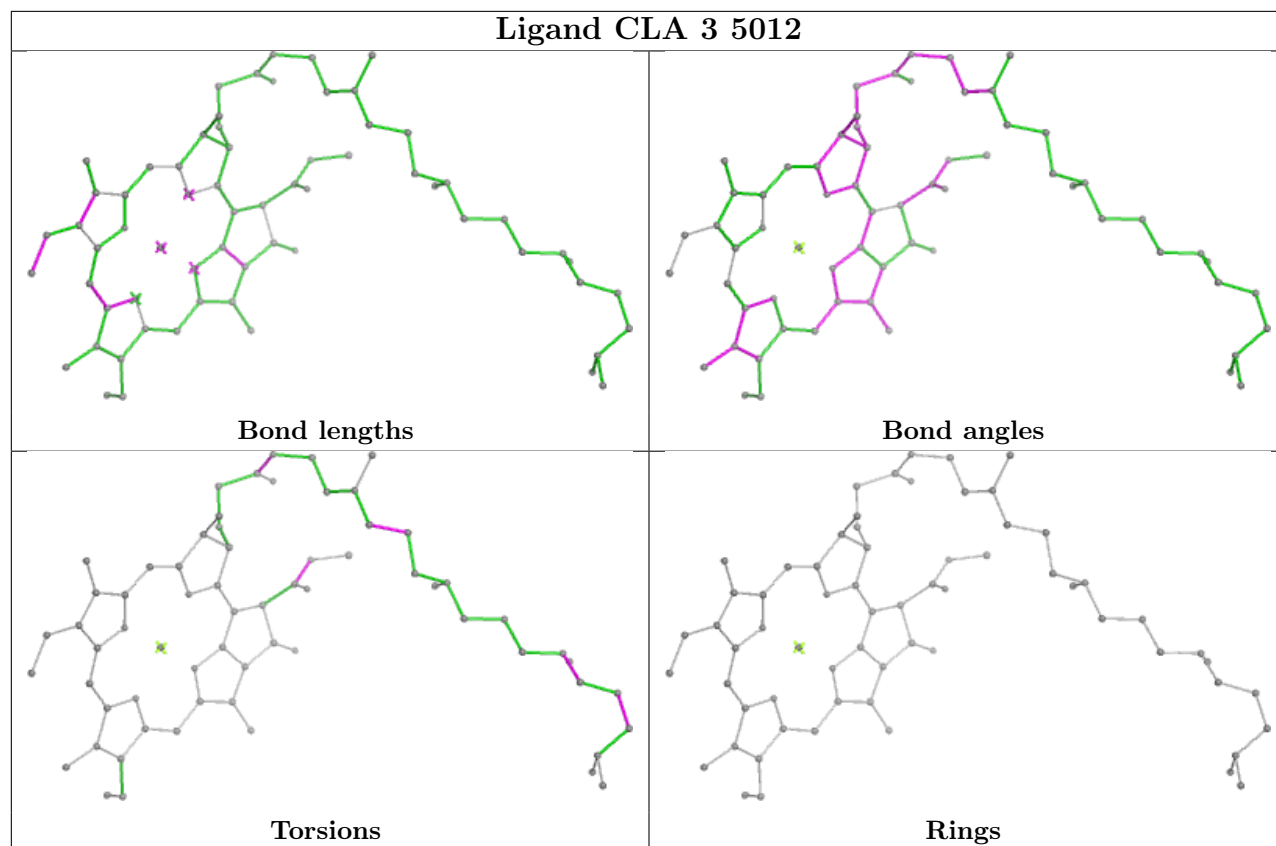
Ligand CLA 5 306



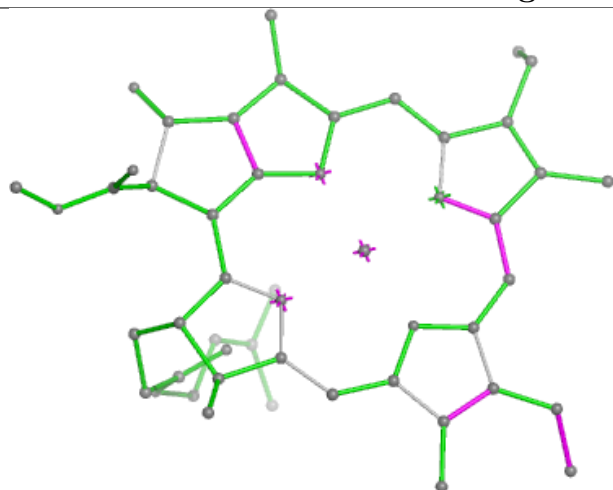
Ligand CLA A 830



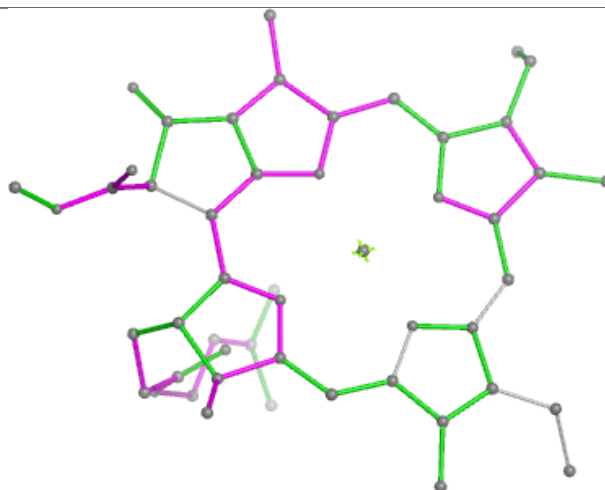
Ligand CLA B 836**Ligand CHL 7 314**



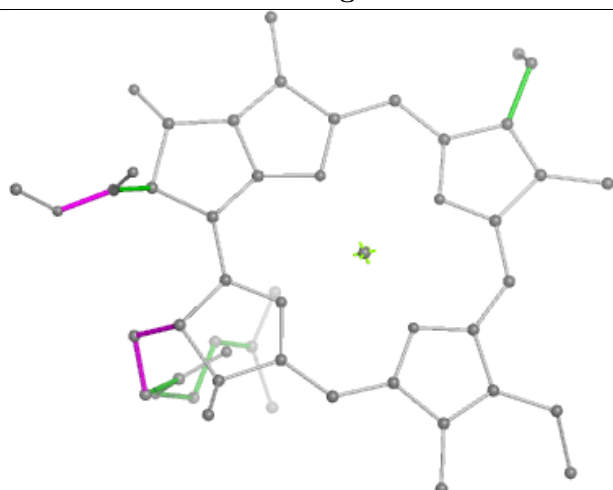
Ligand CLA 4 316



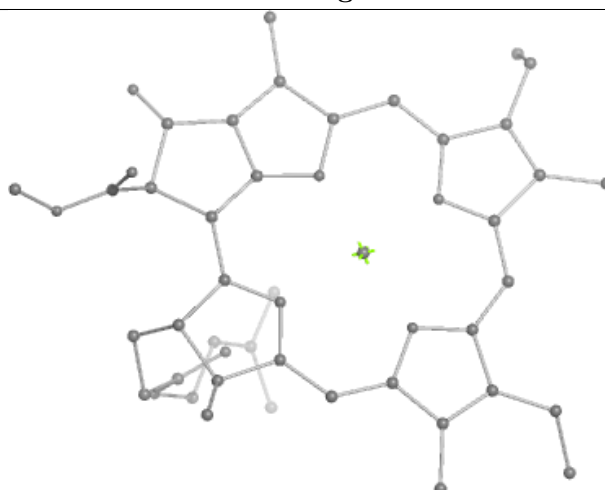
Bond lengths



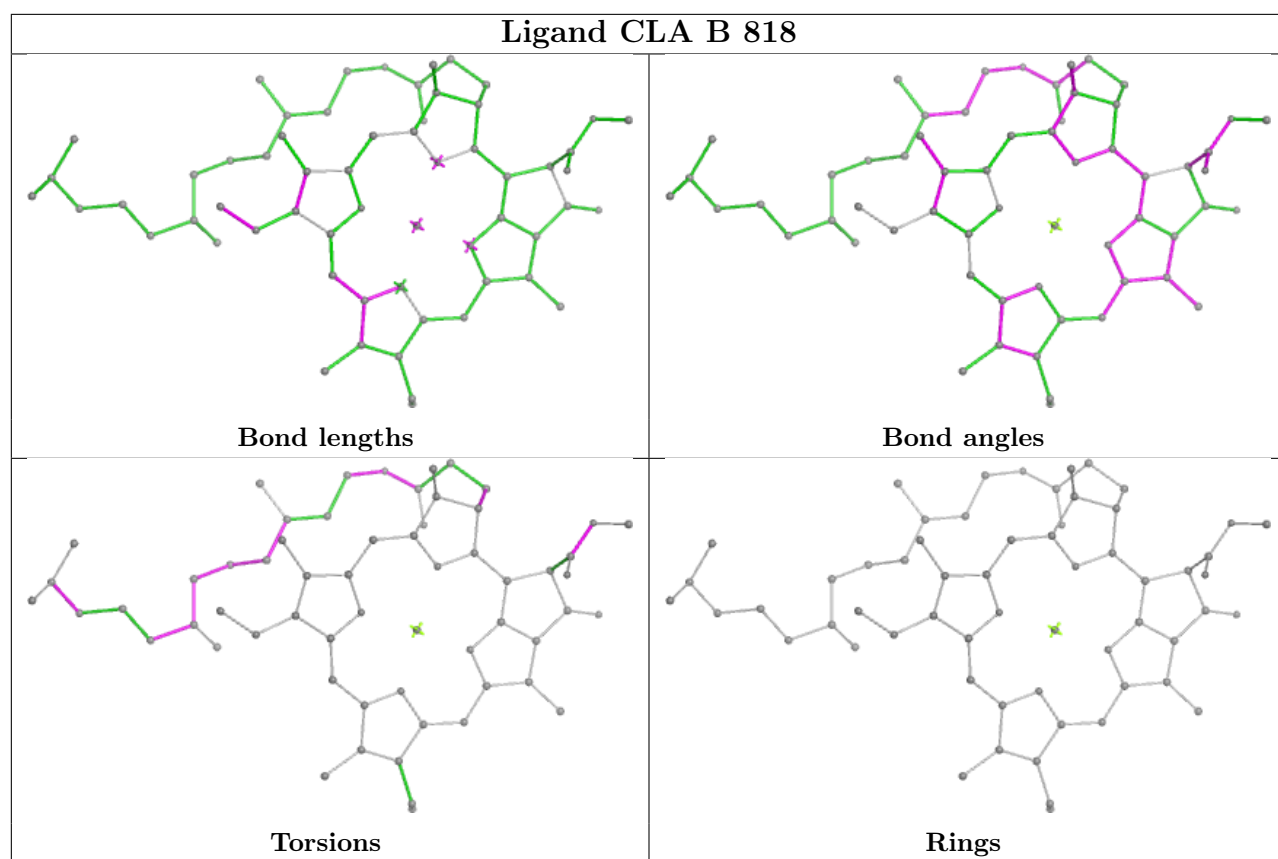
Bond angles

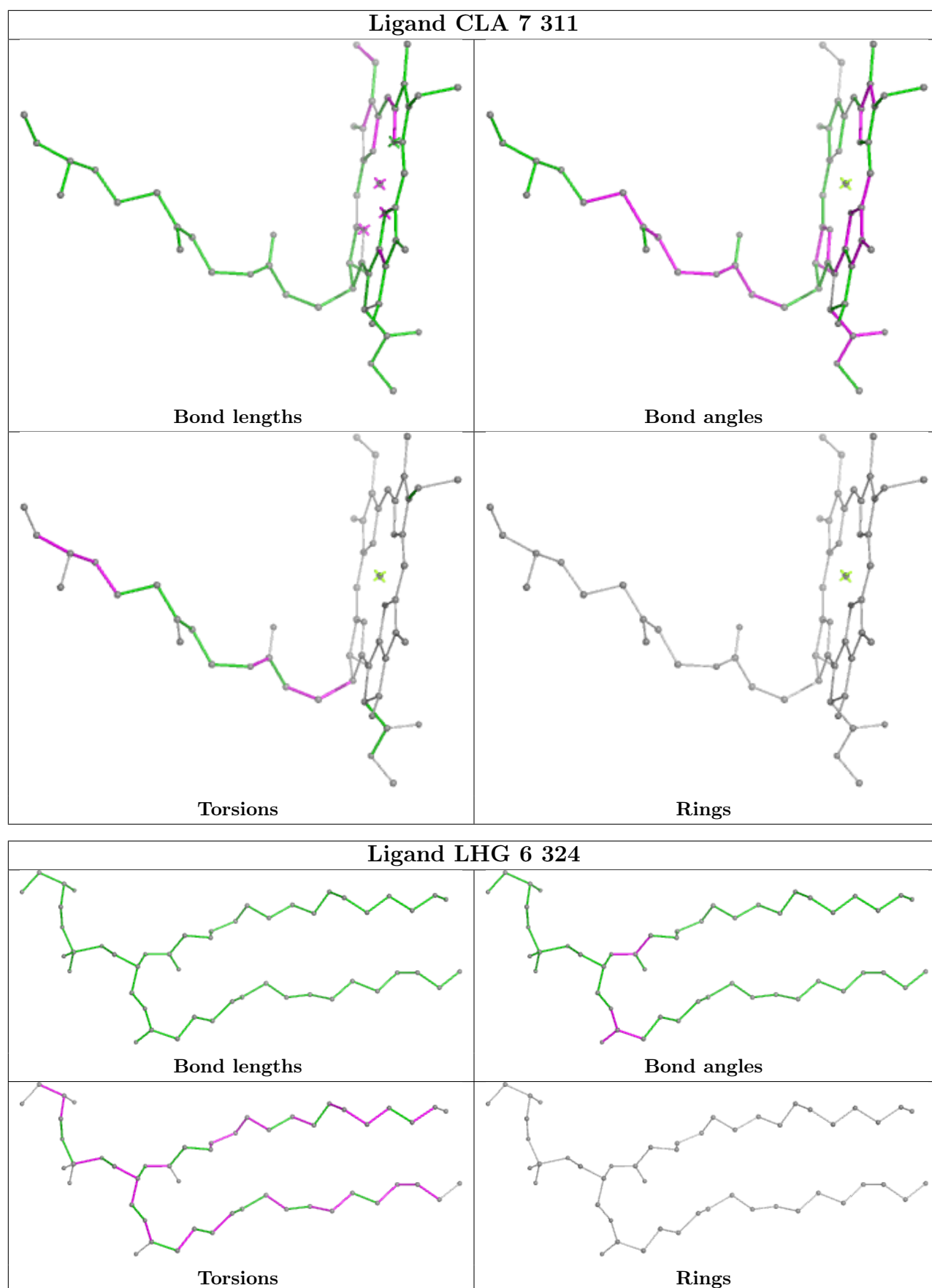


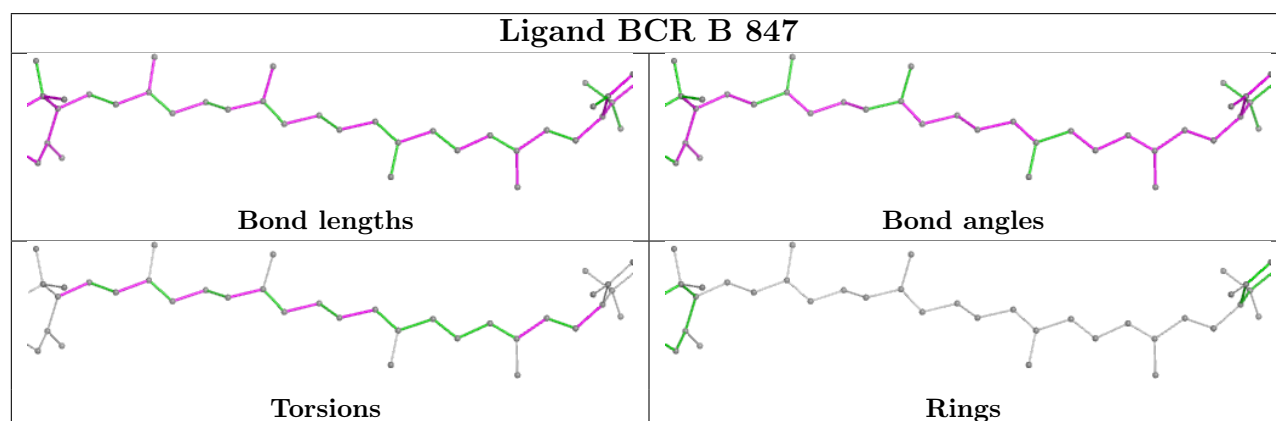
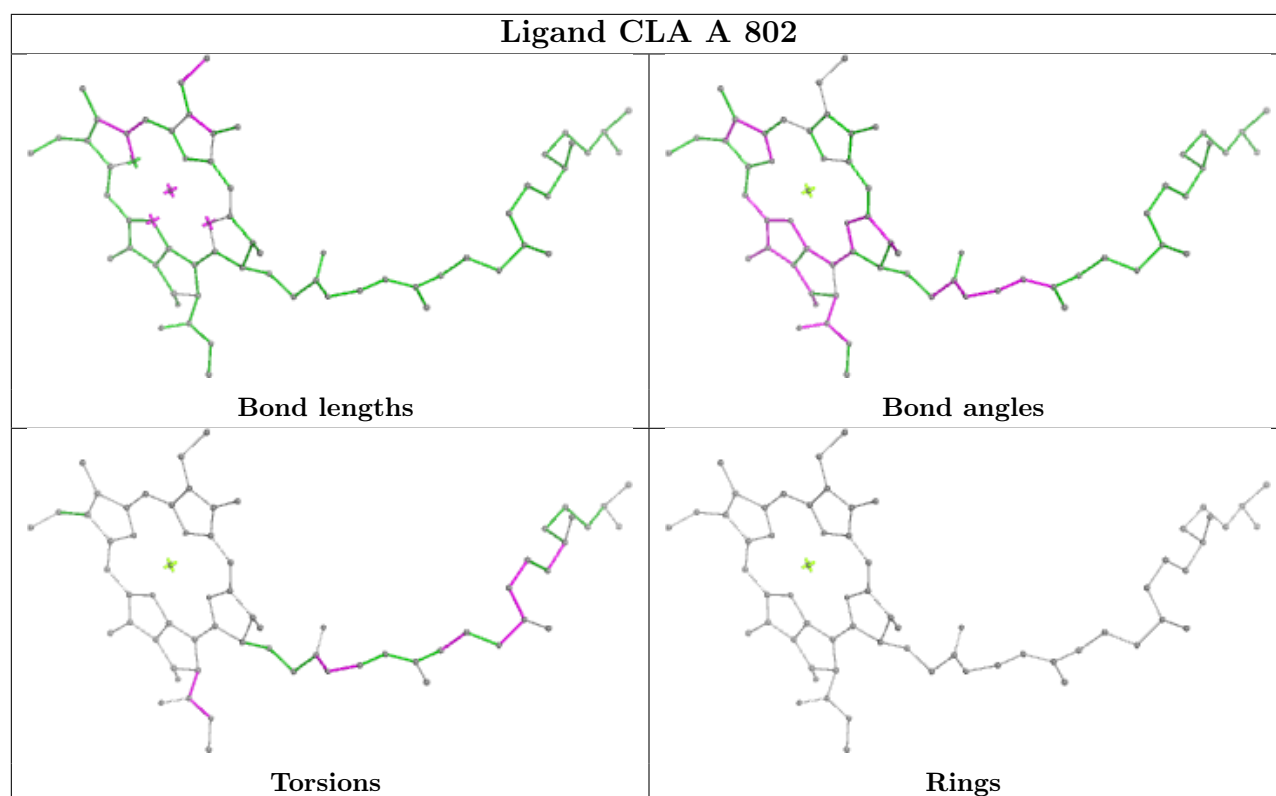
Torsions



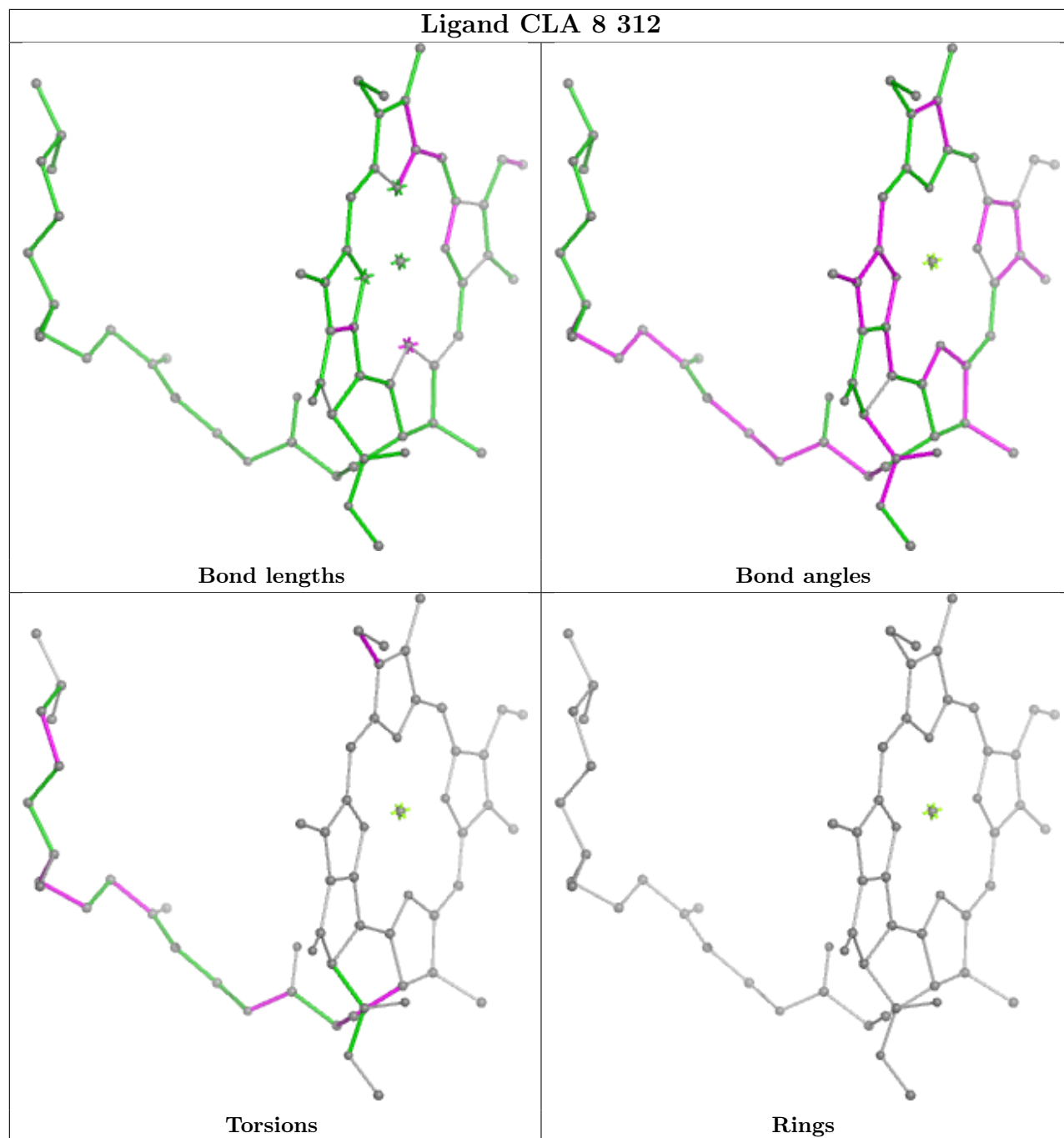
Rings

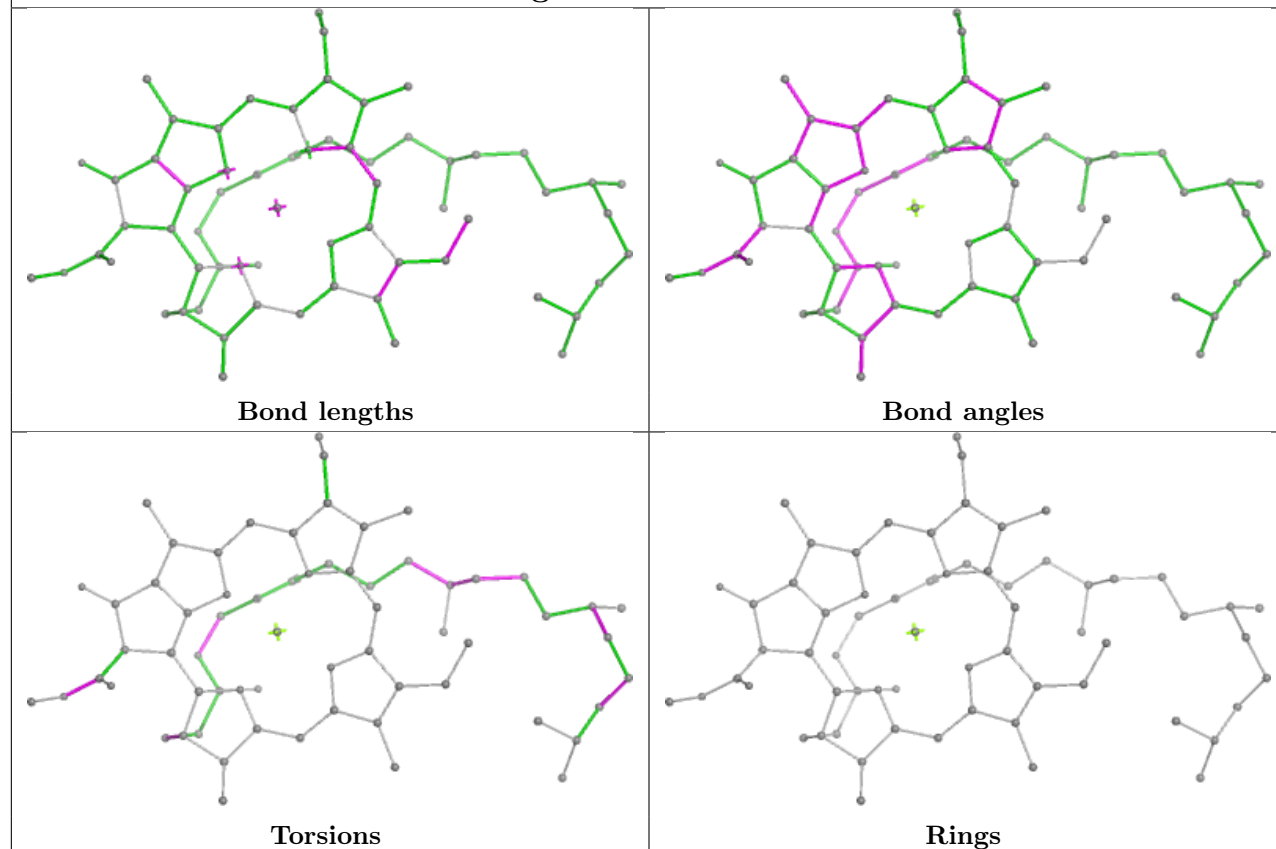
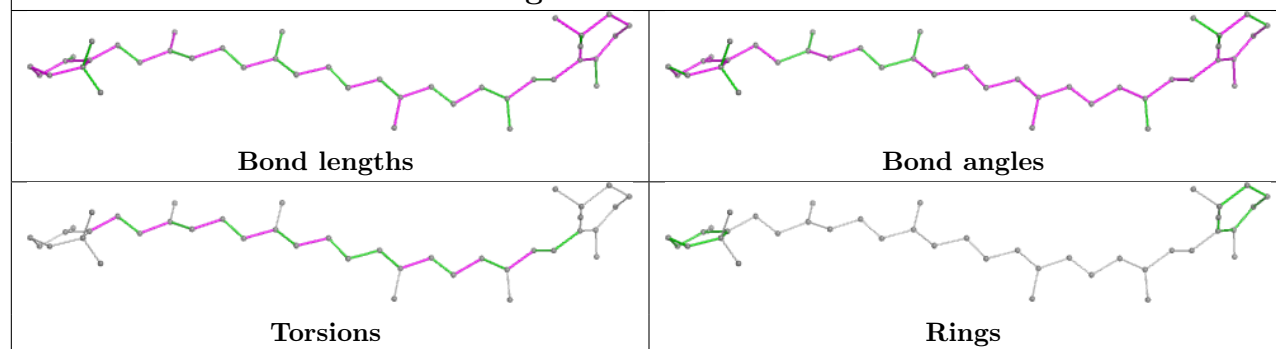


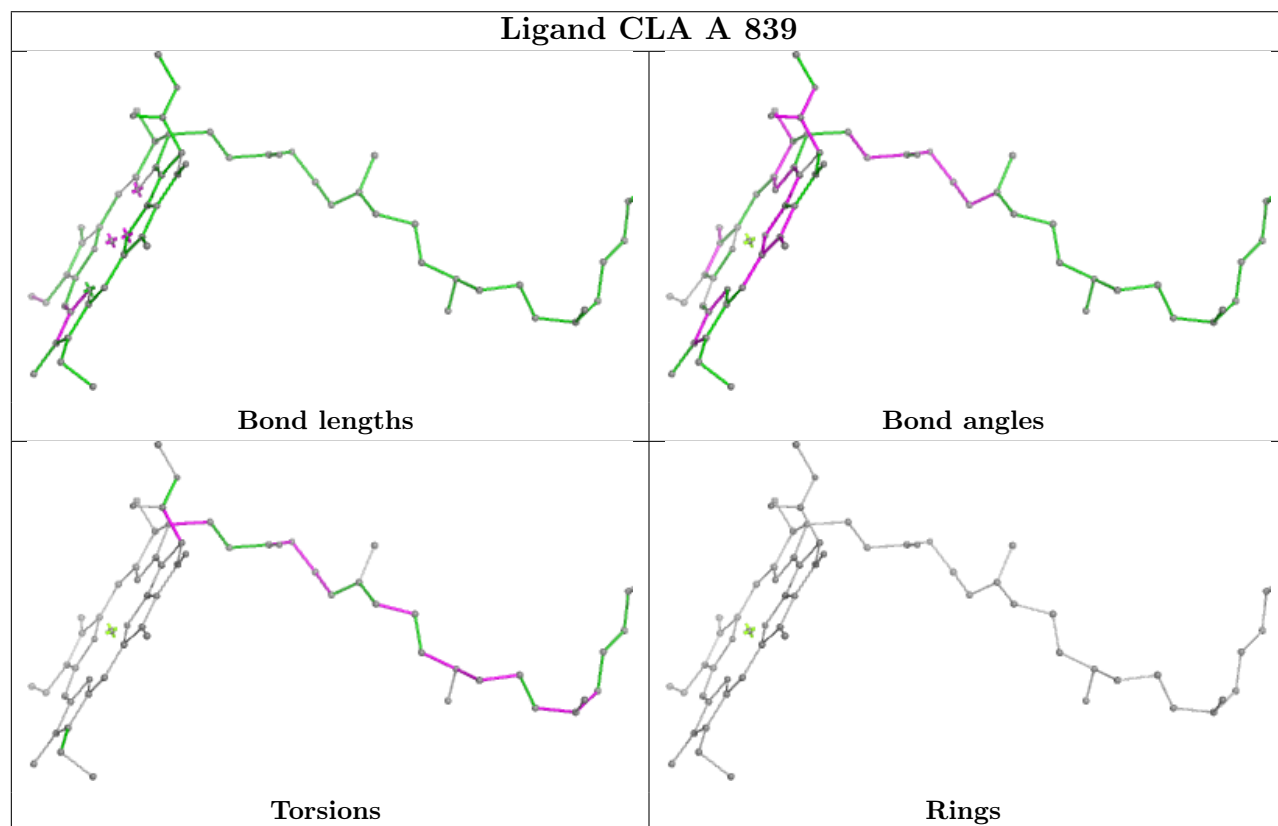
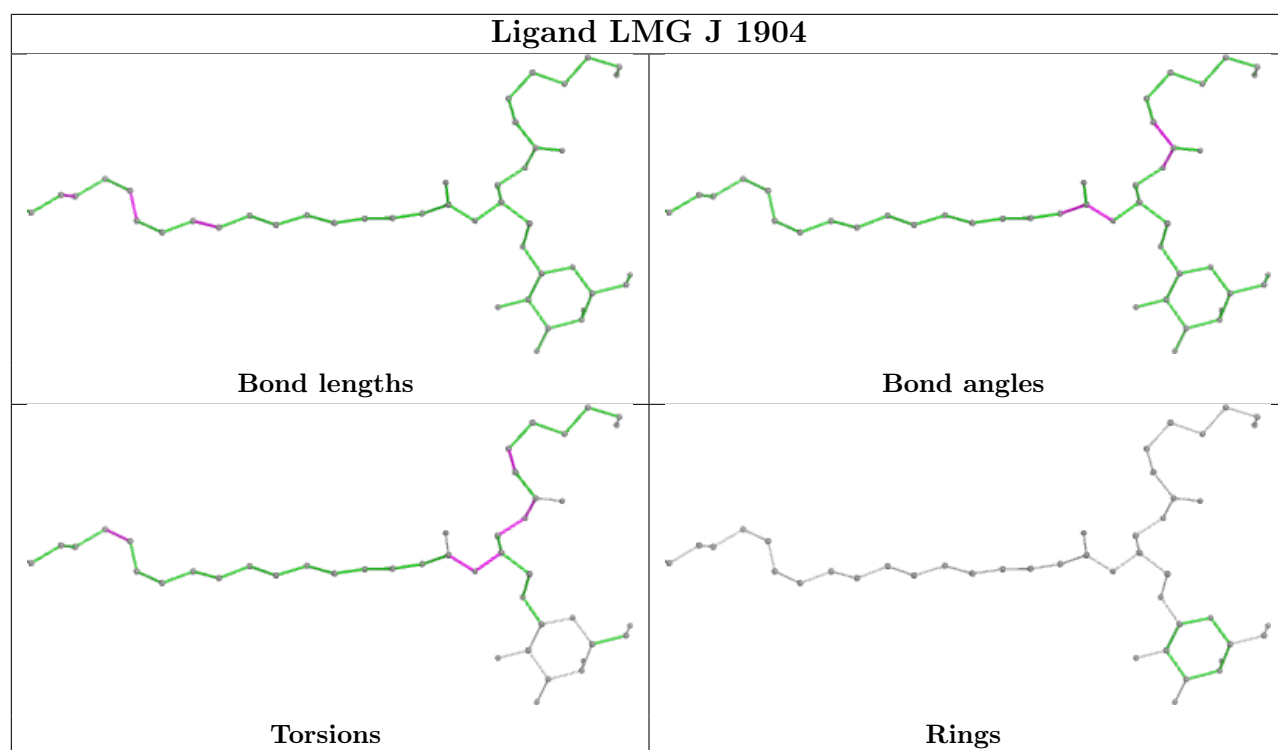


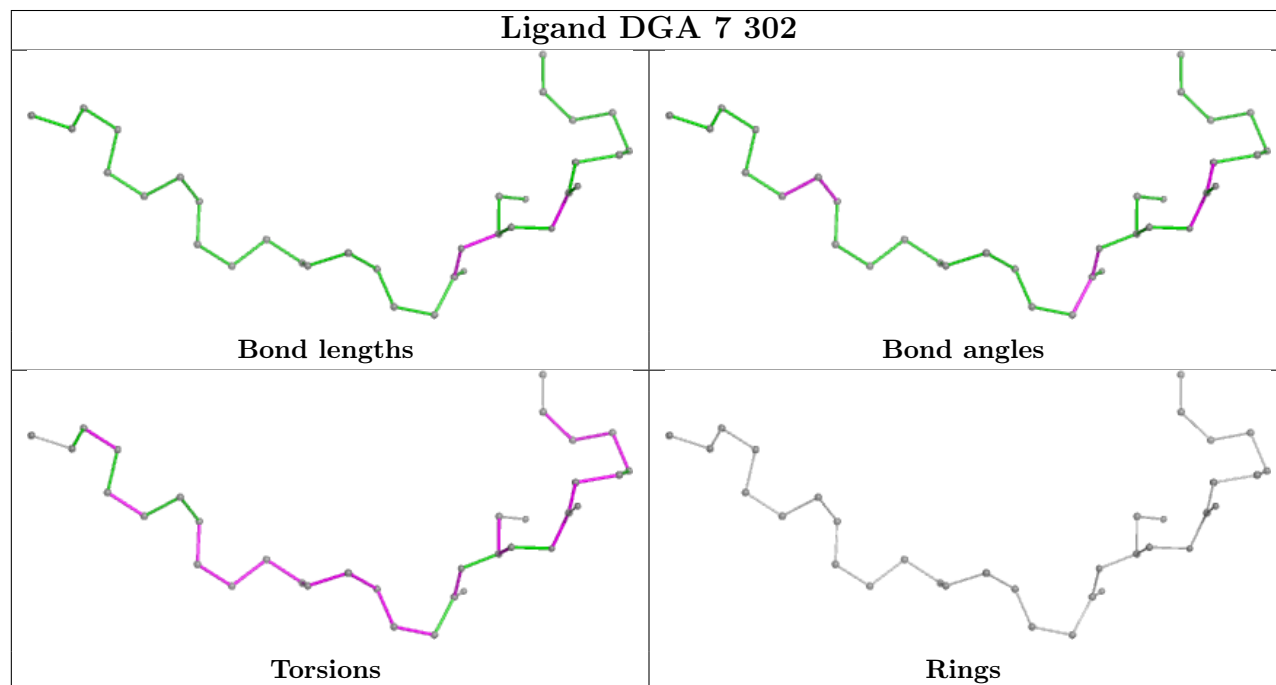
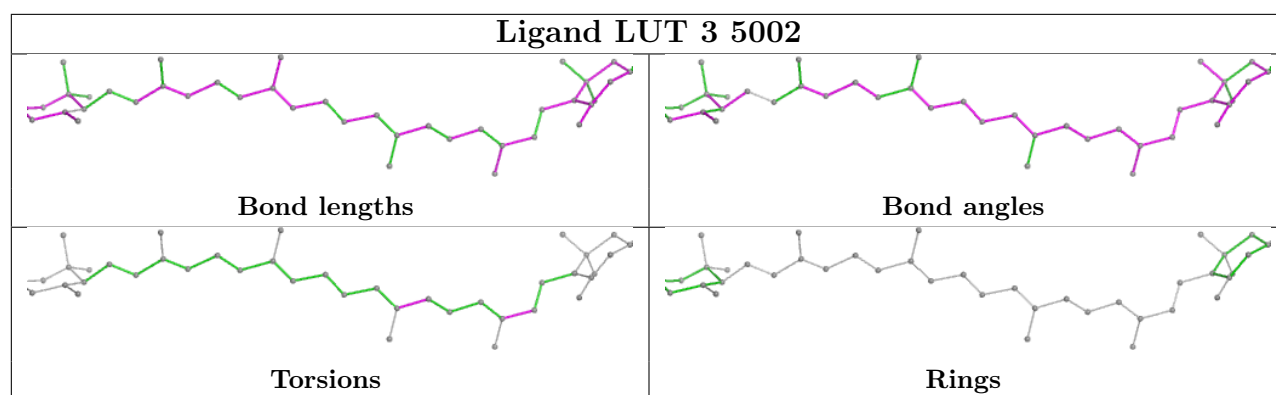


Ligand CLA 8 312

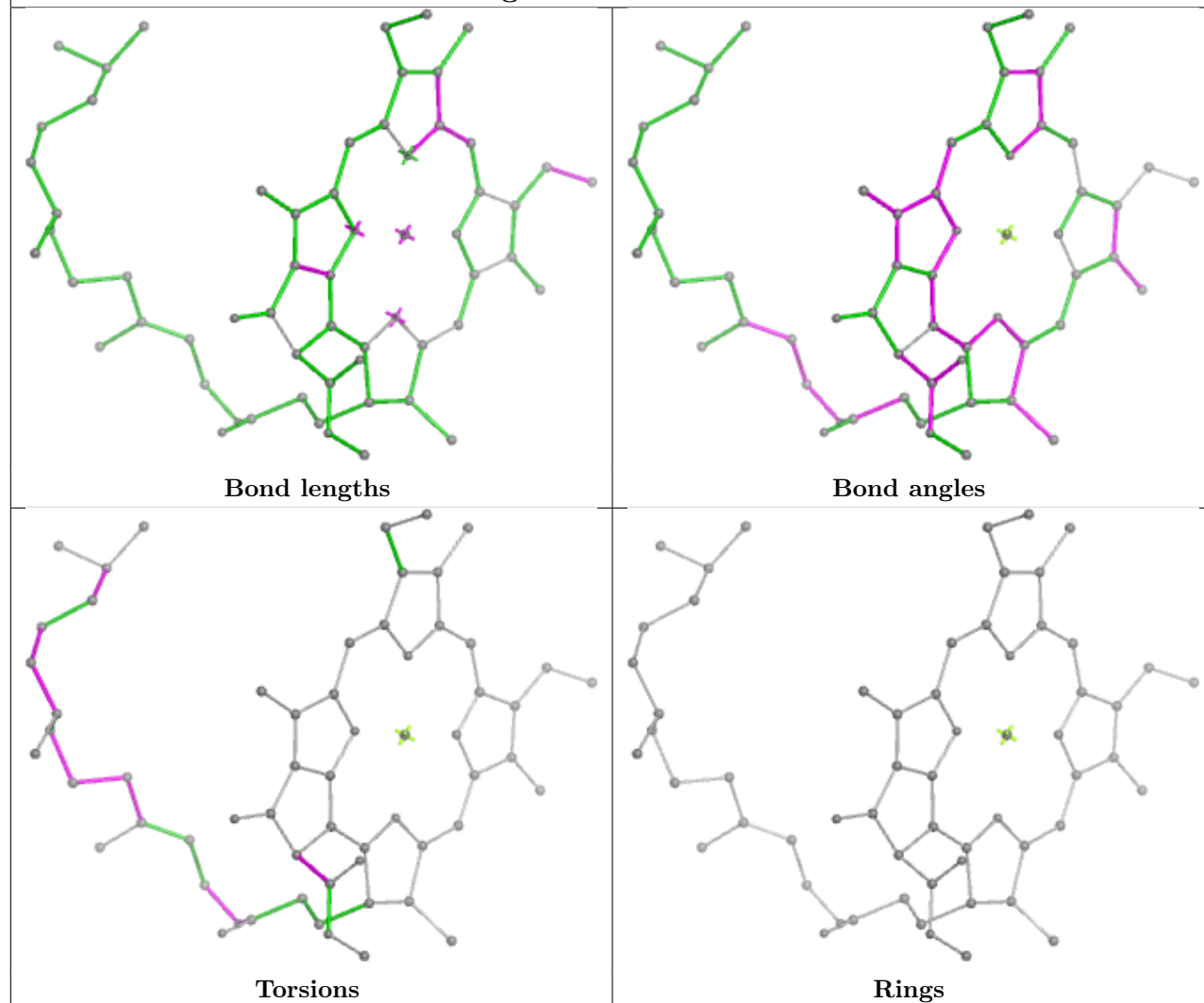


Ligand CLA A 812**Ligand BCR 3 5004**

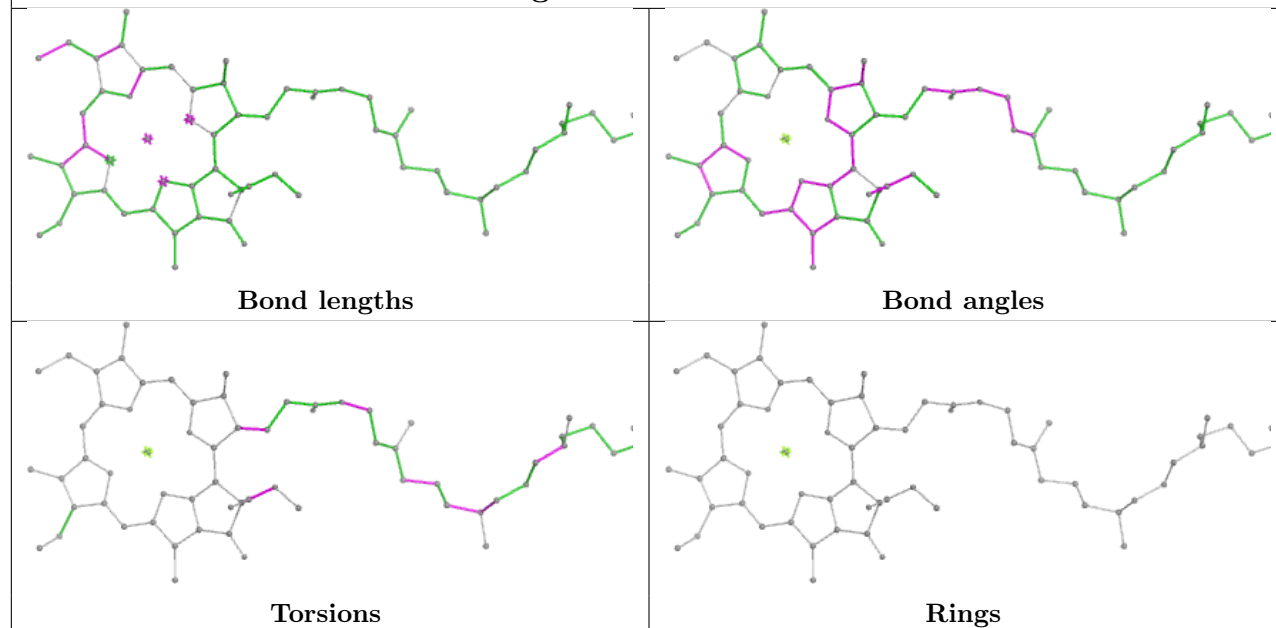


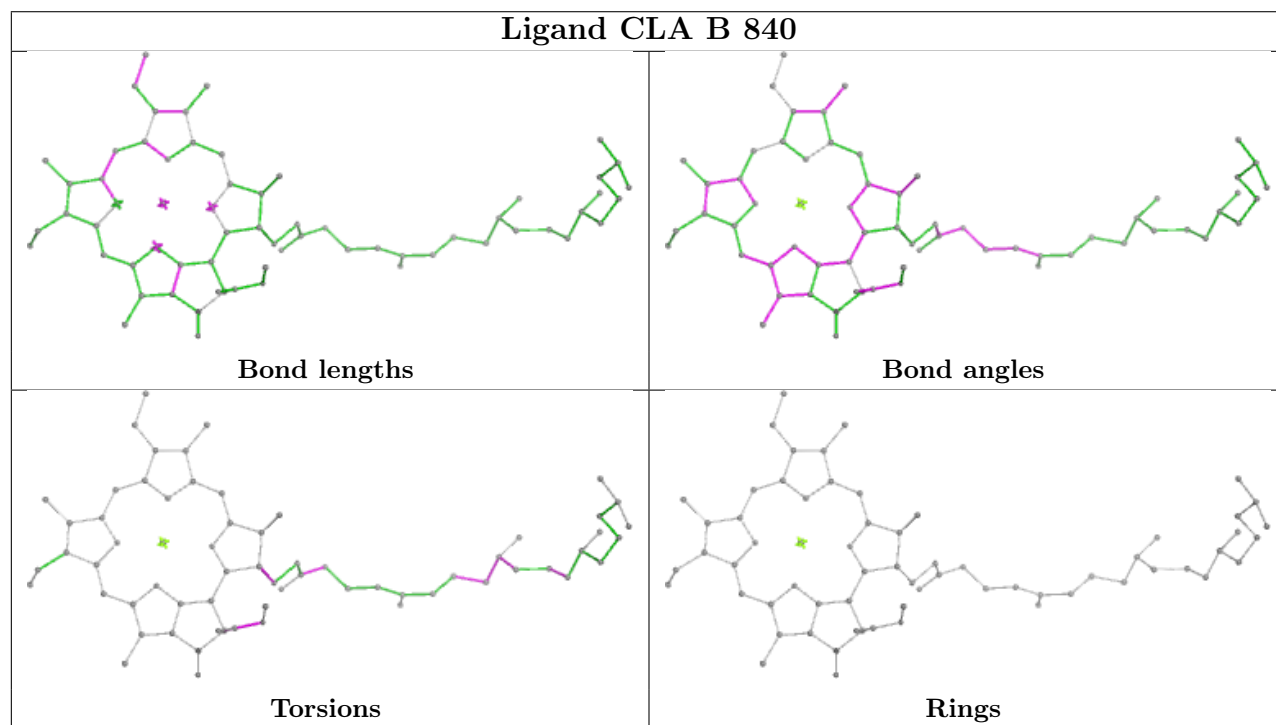
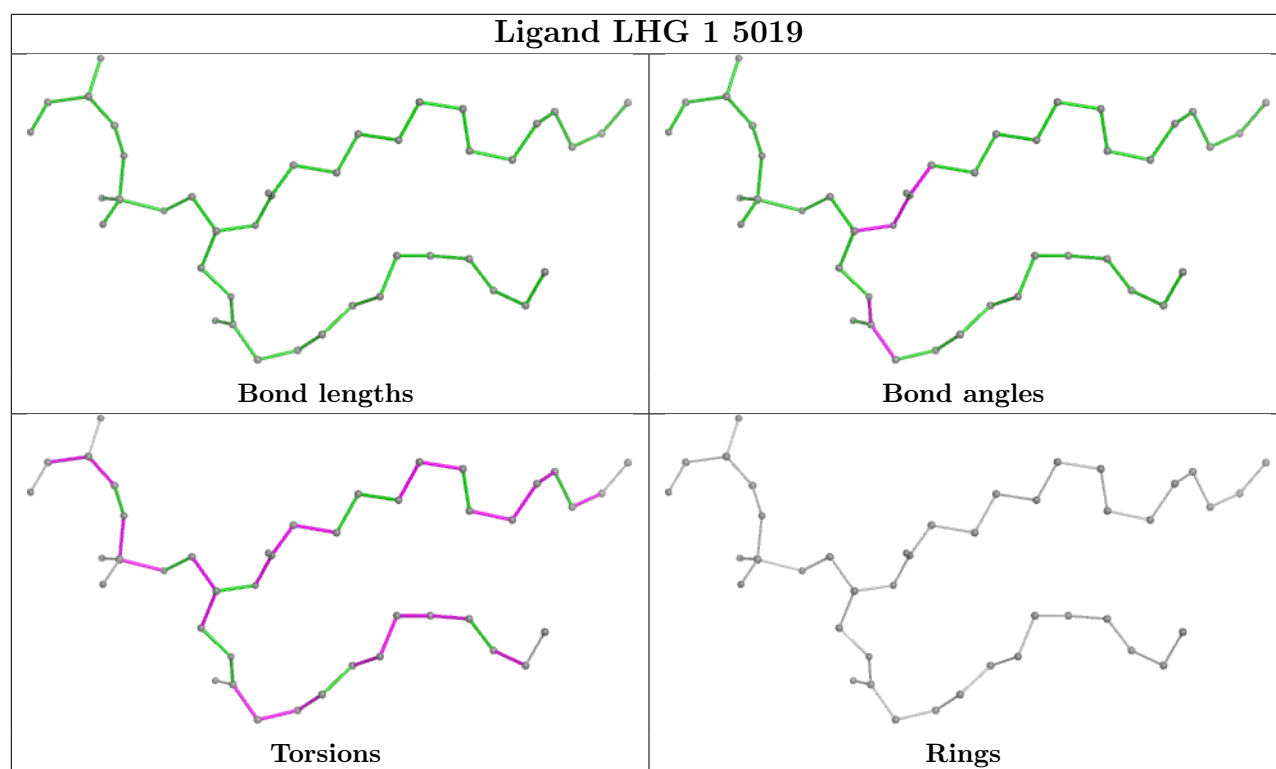


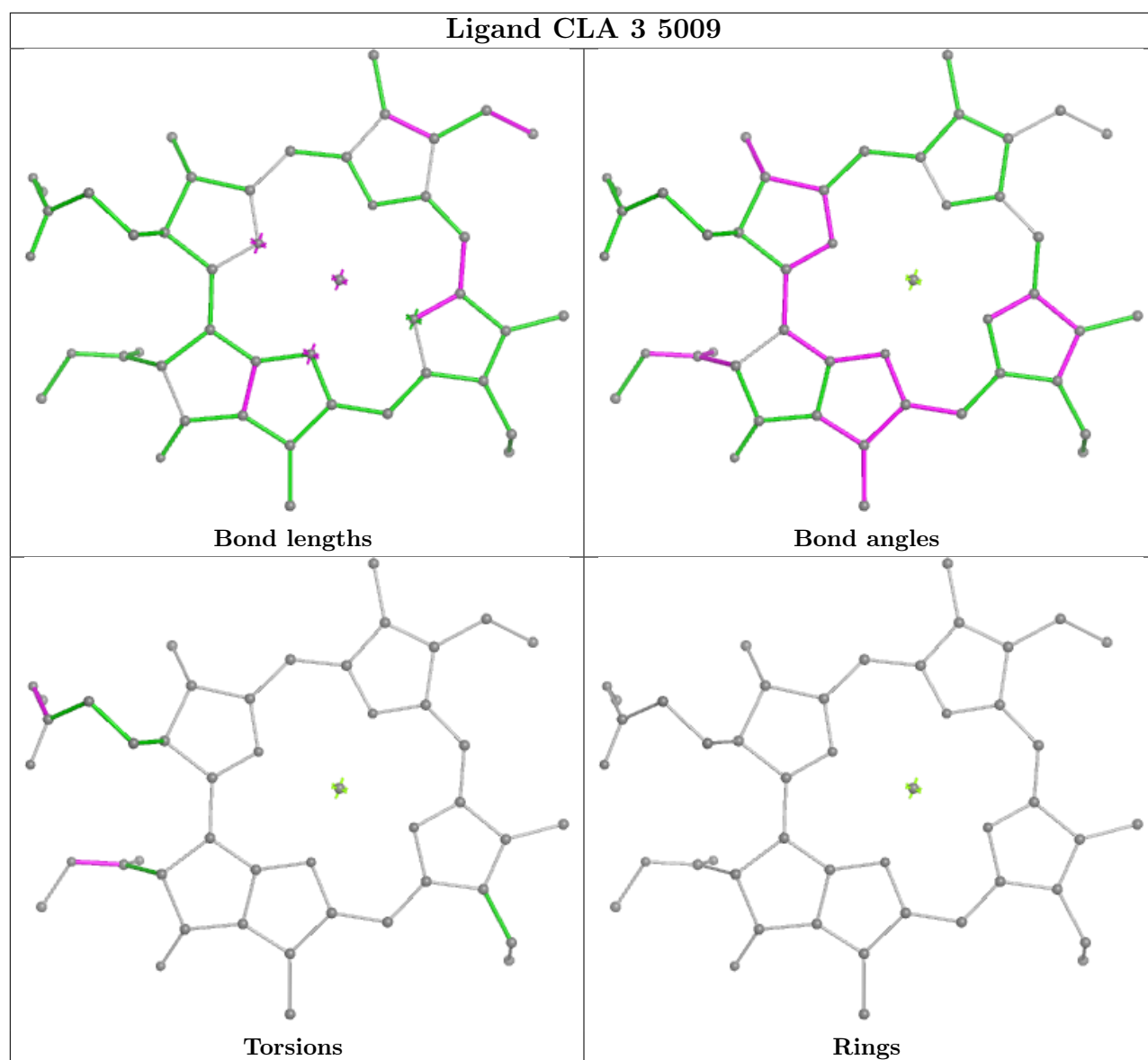
Ligand CLA A 814



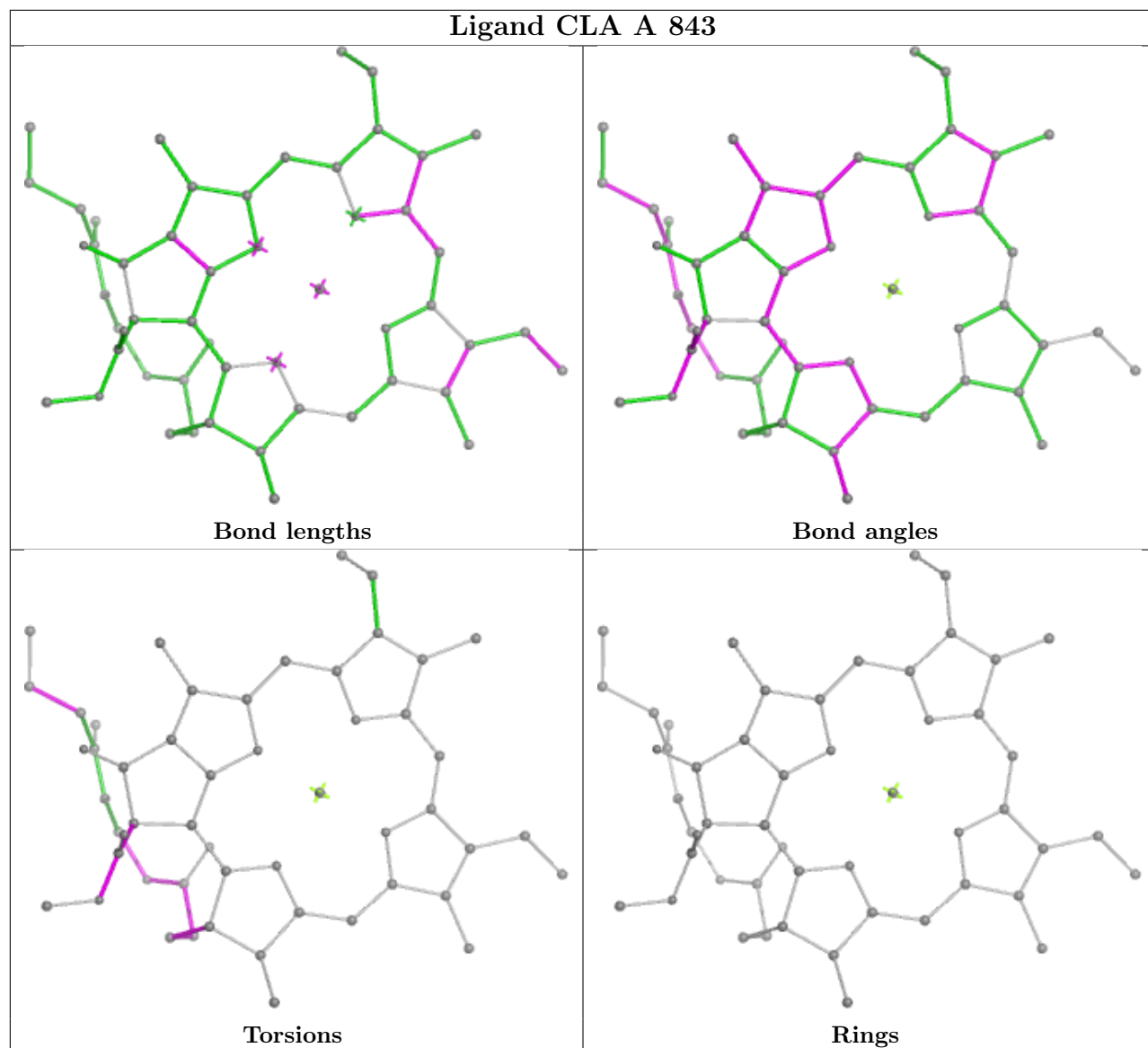
Ligand CLA A 842



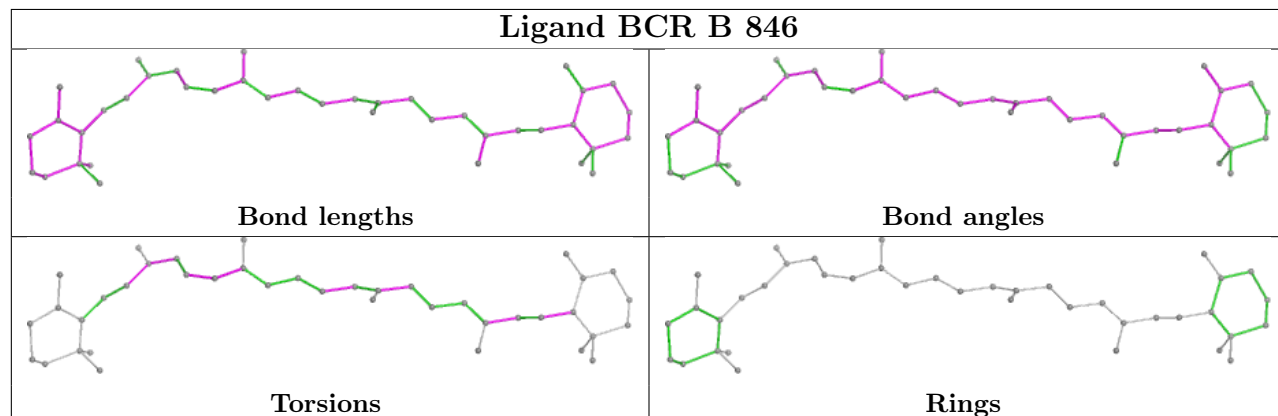


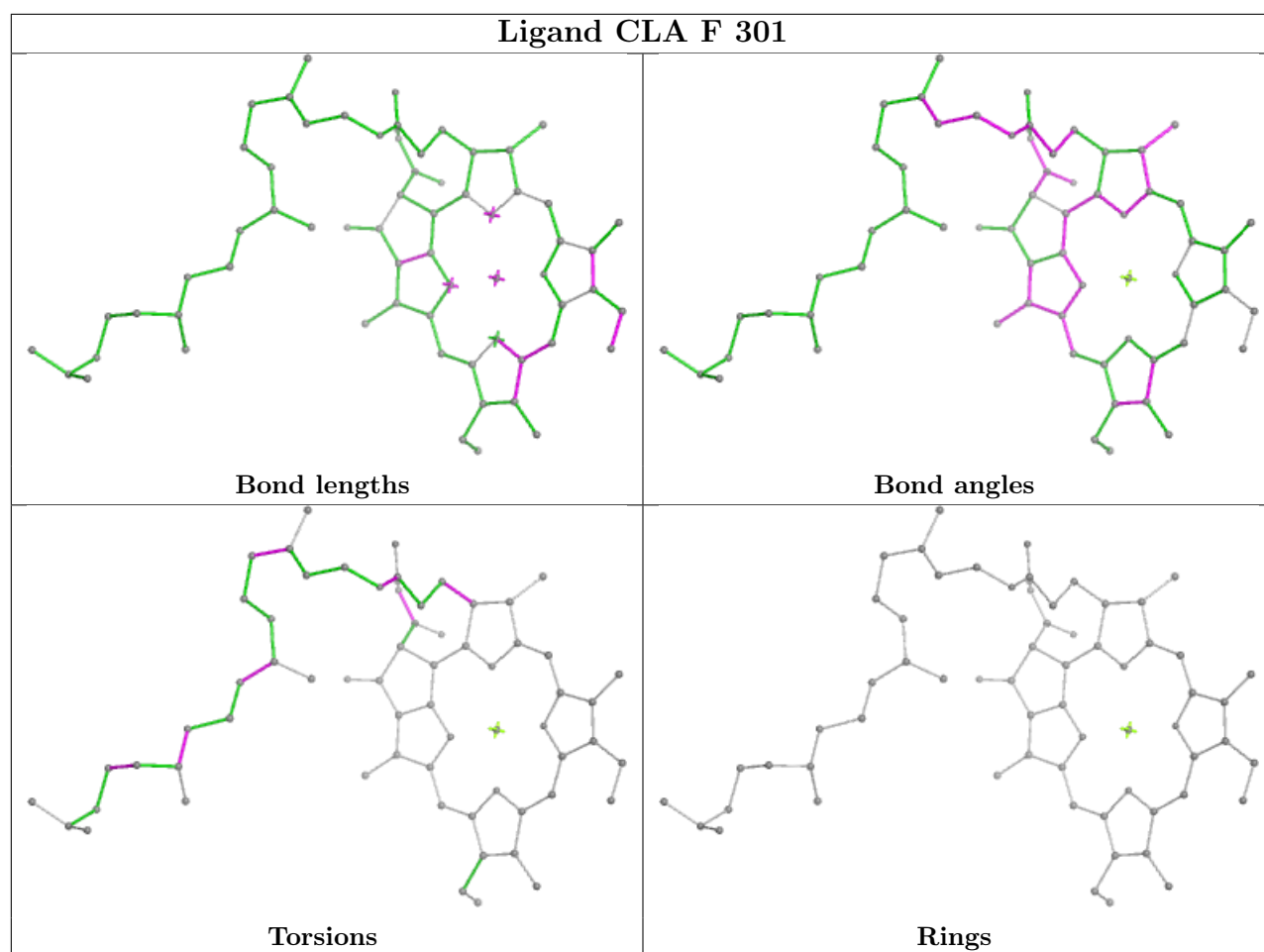


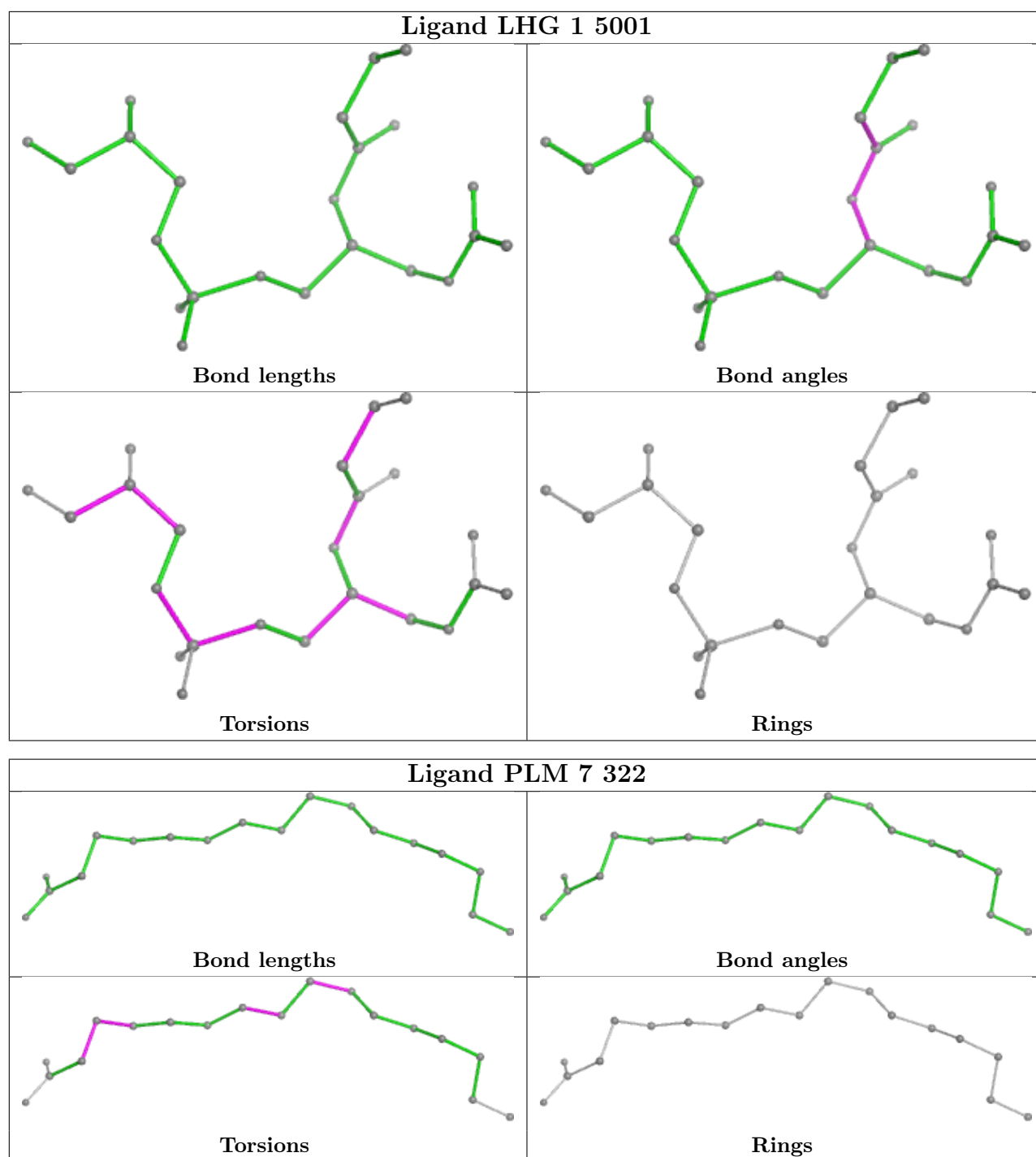
Ligand CLA A 843

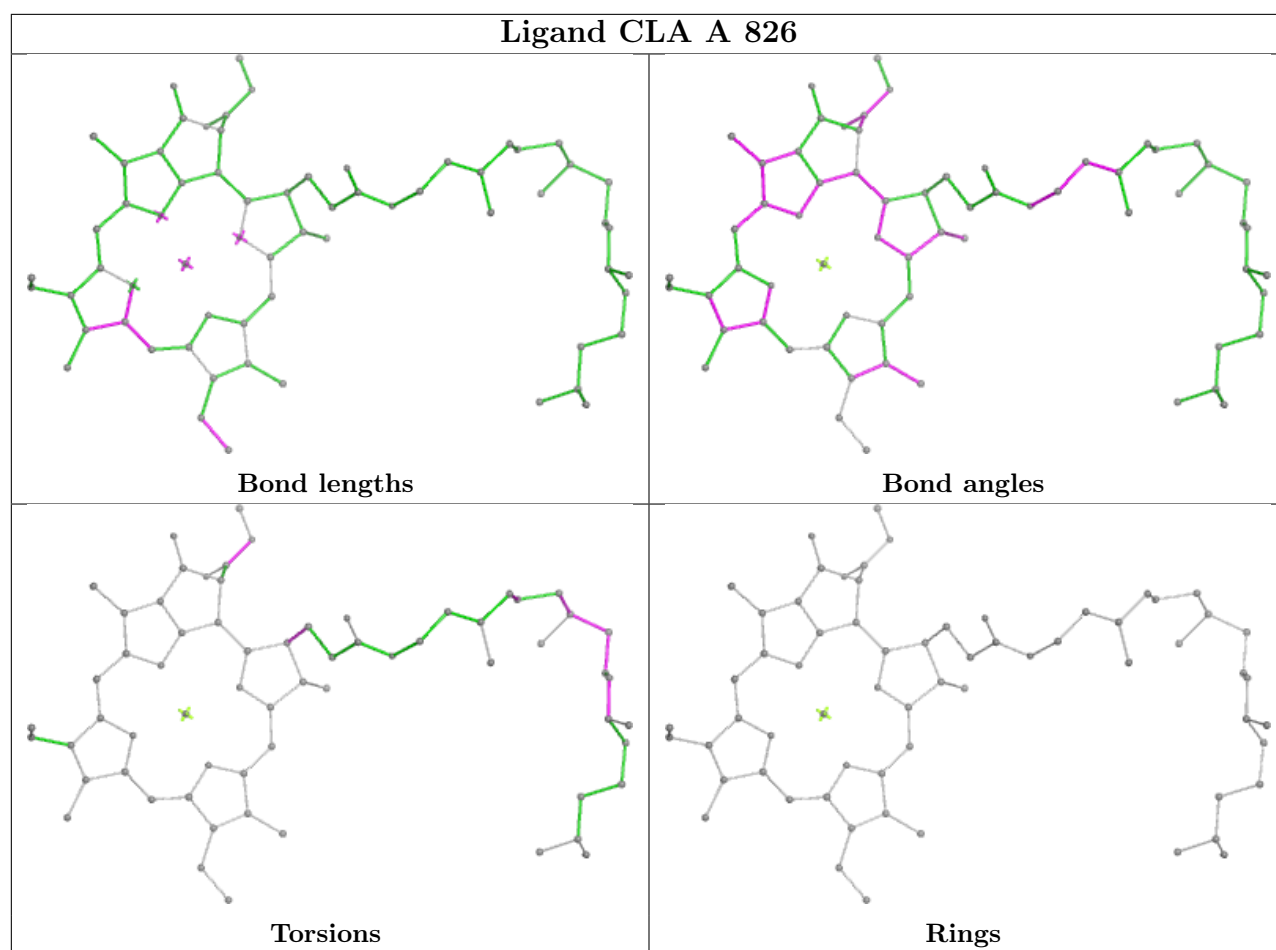


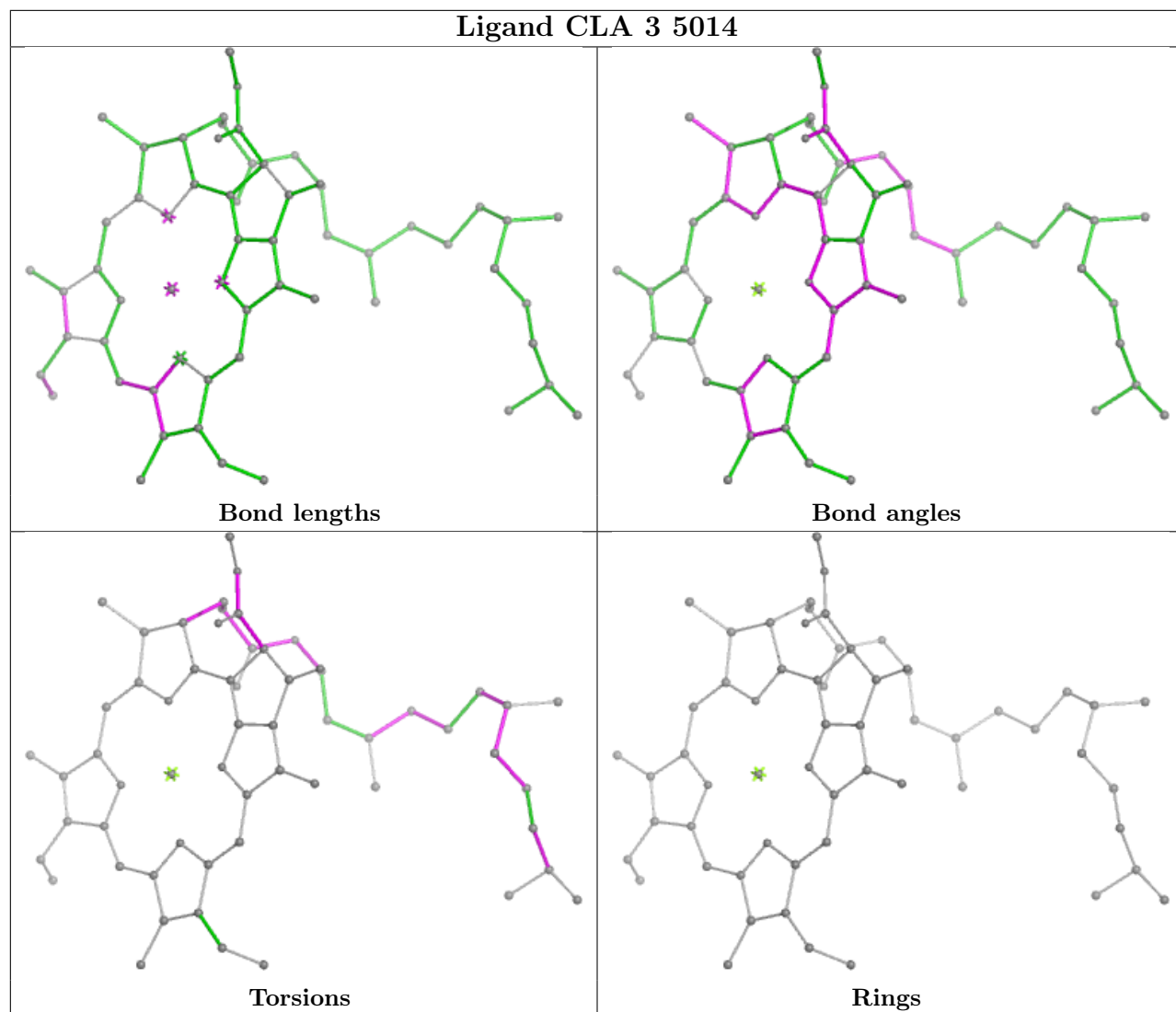
Ligand BCR B 846



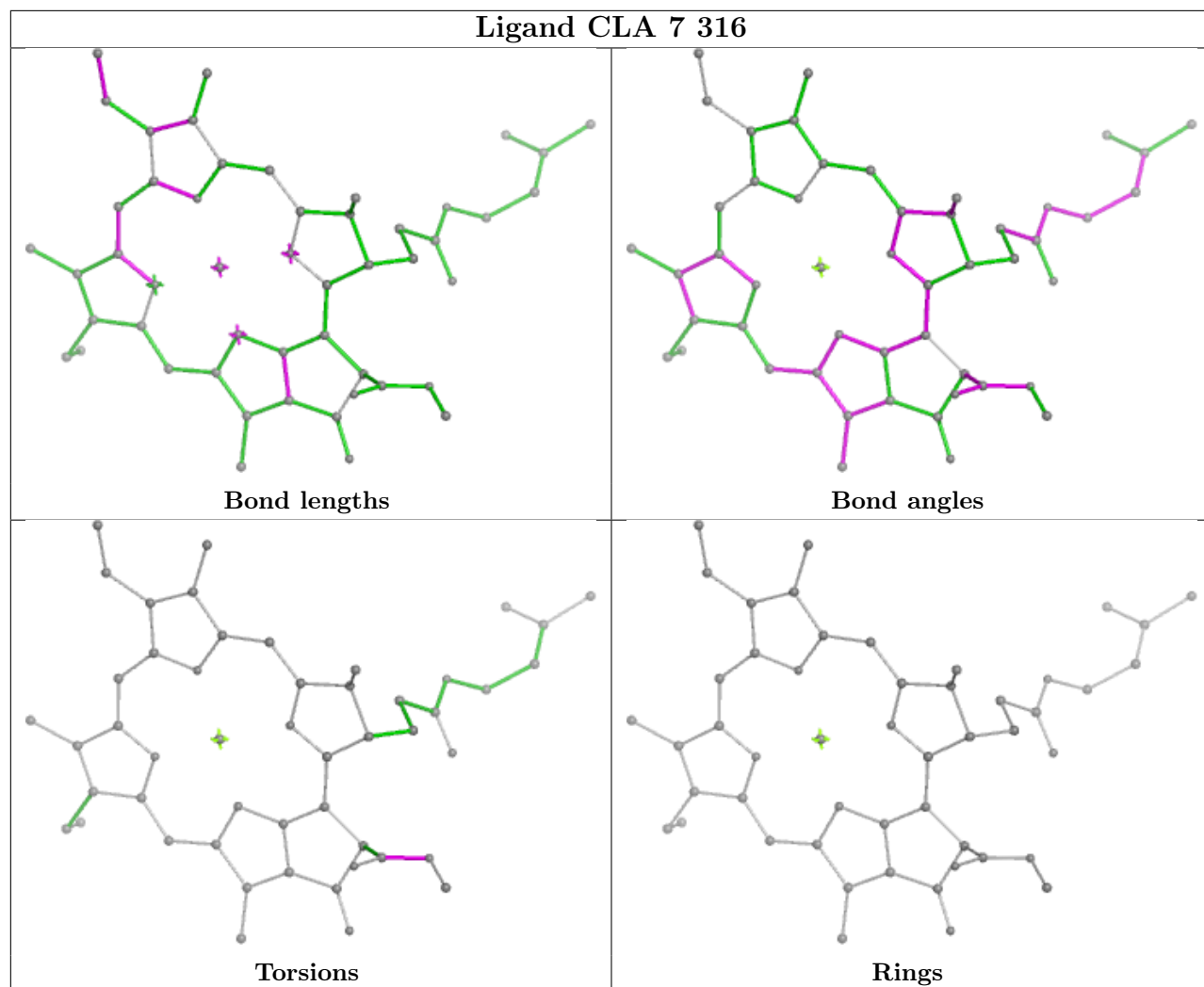


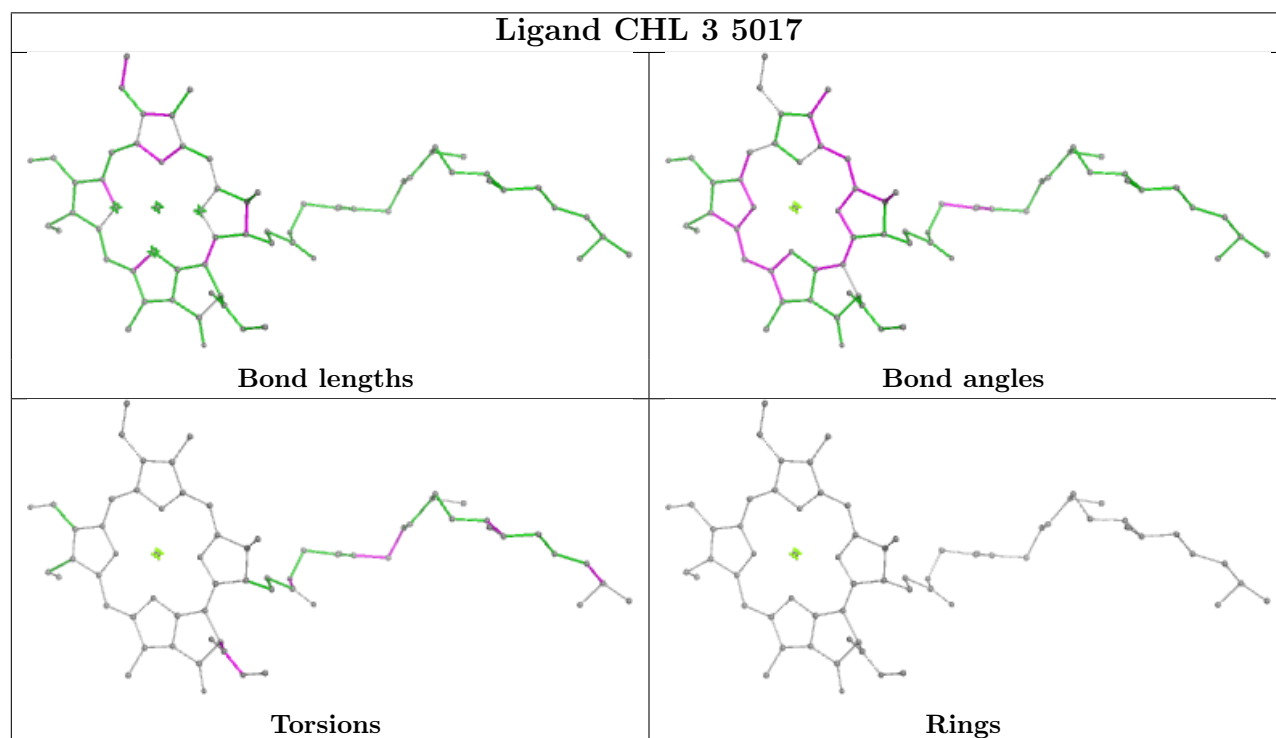
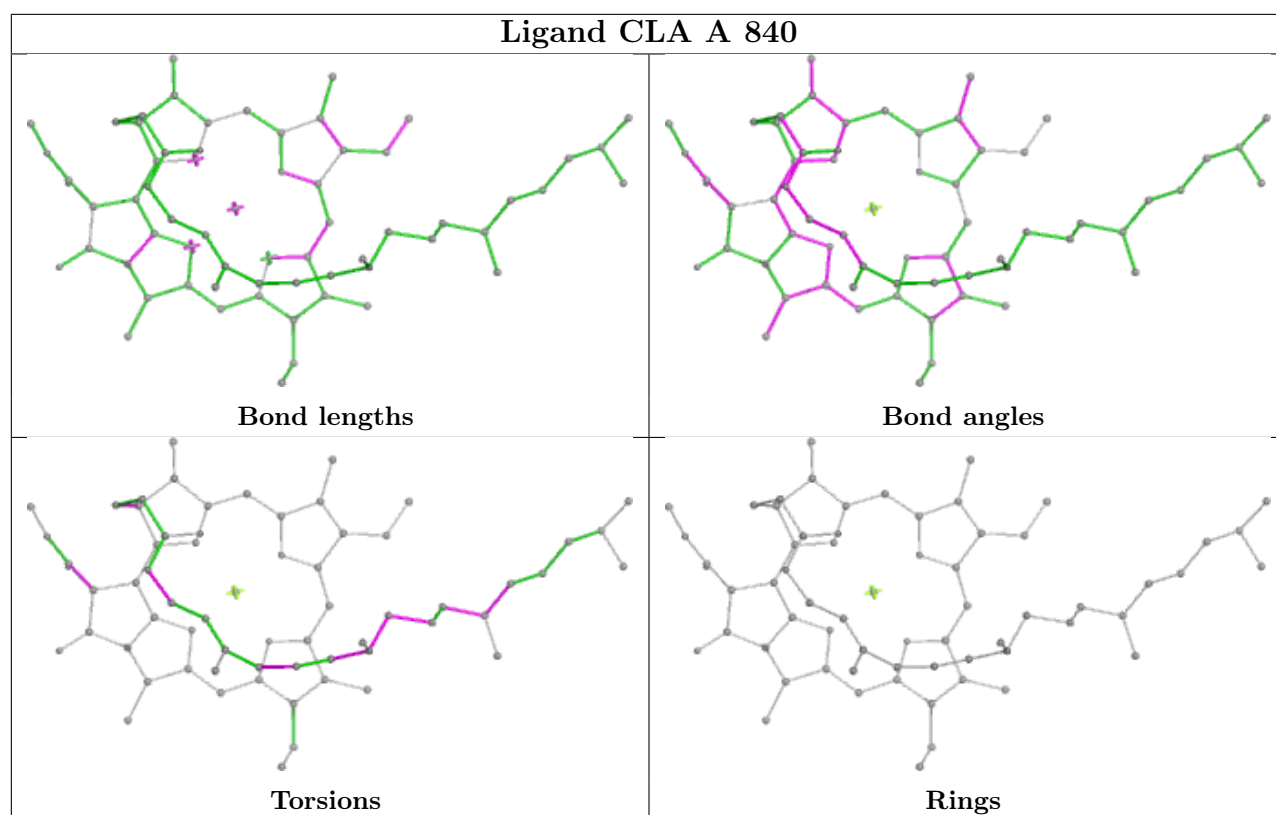




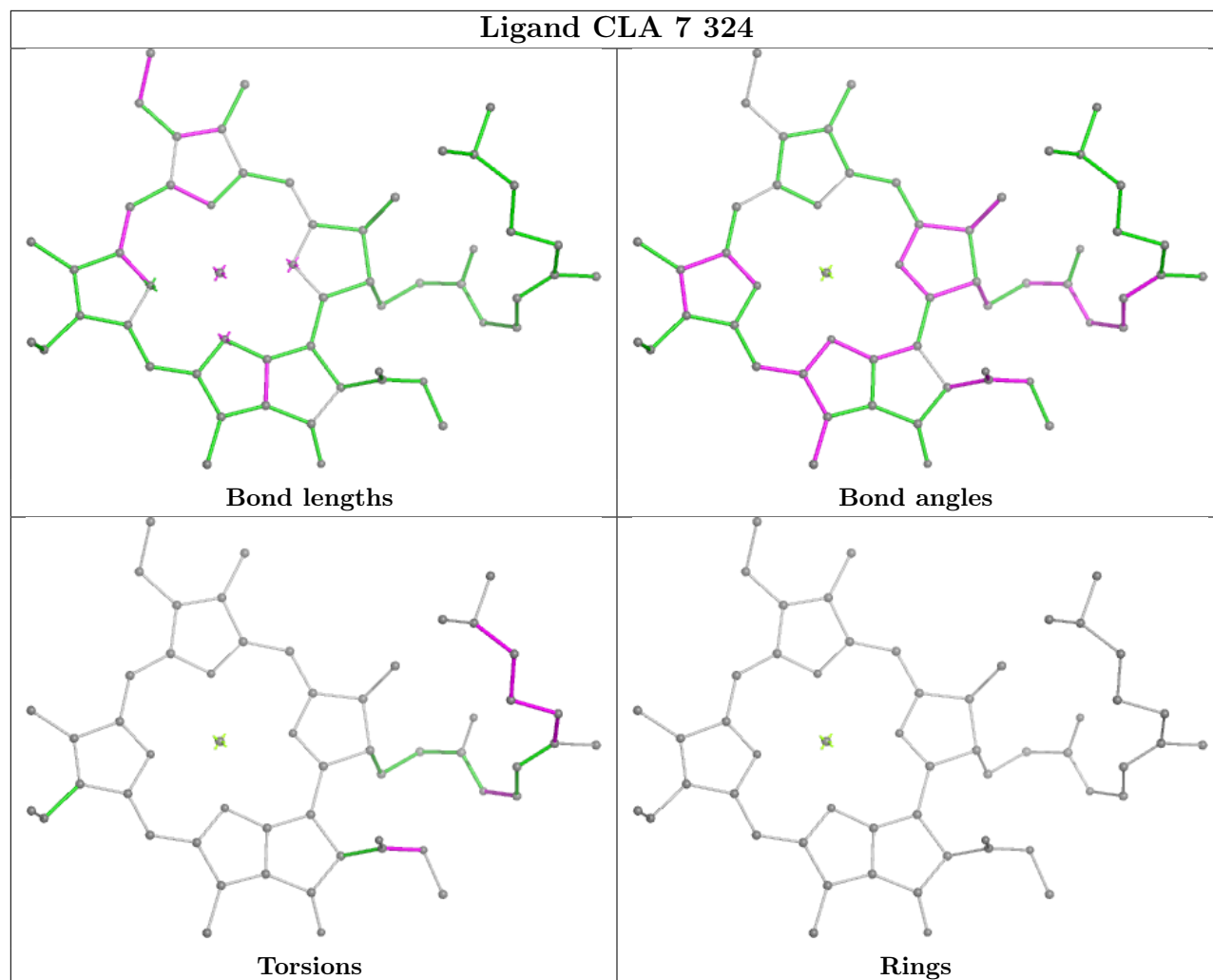


Ligand CLA 7 316

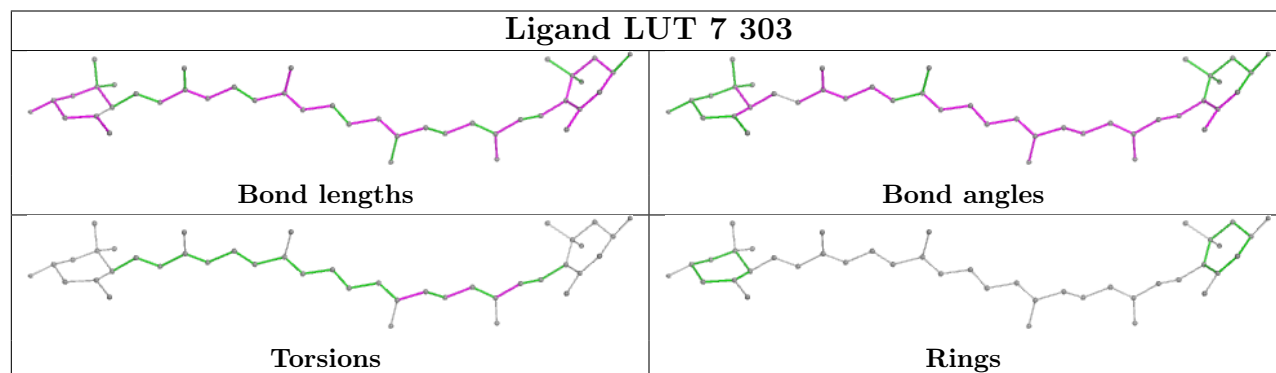


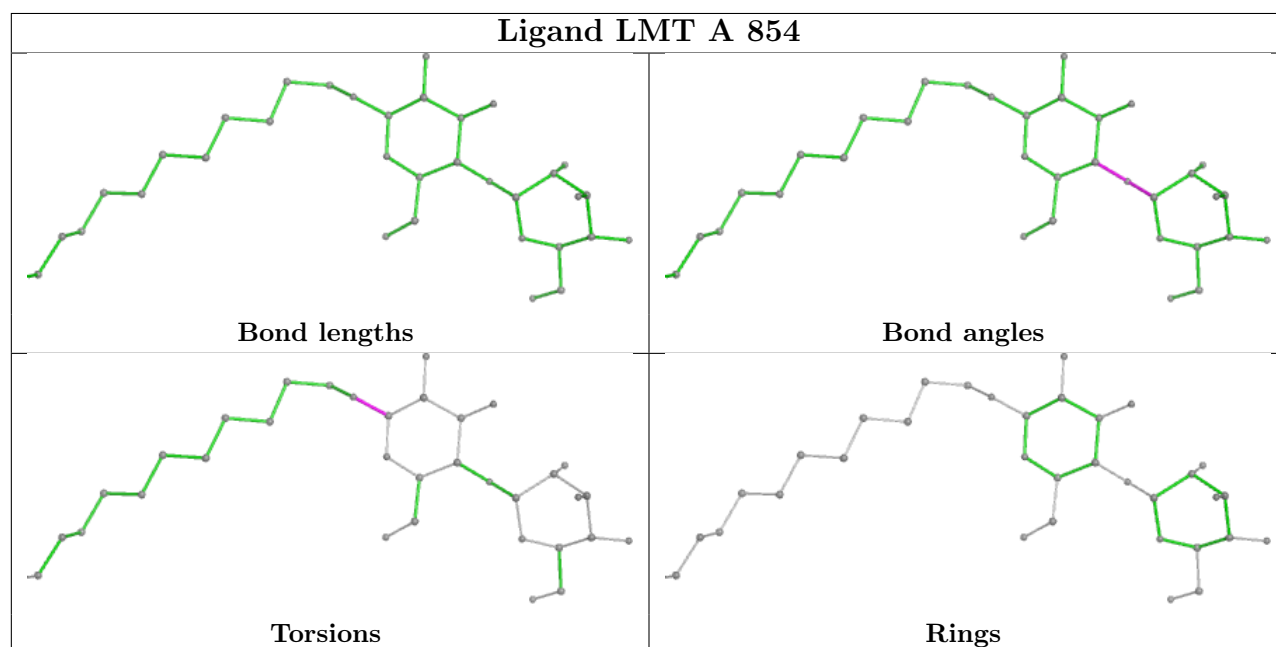
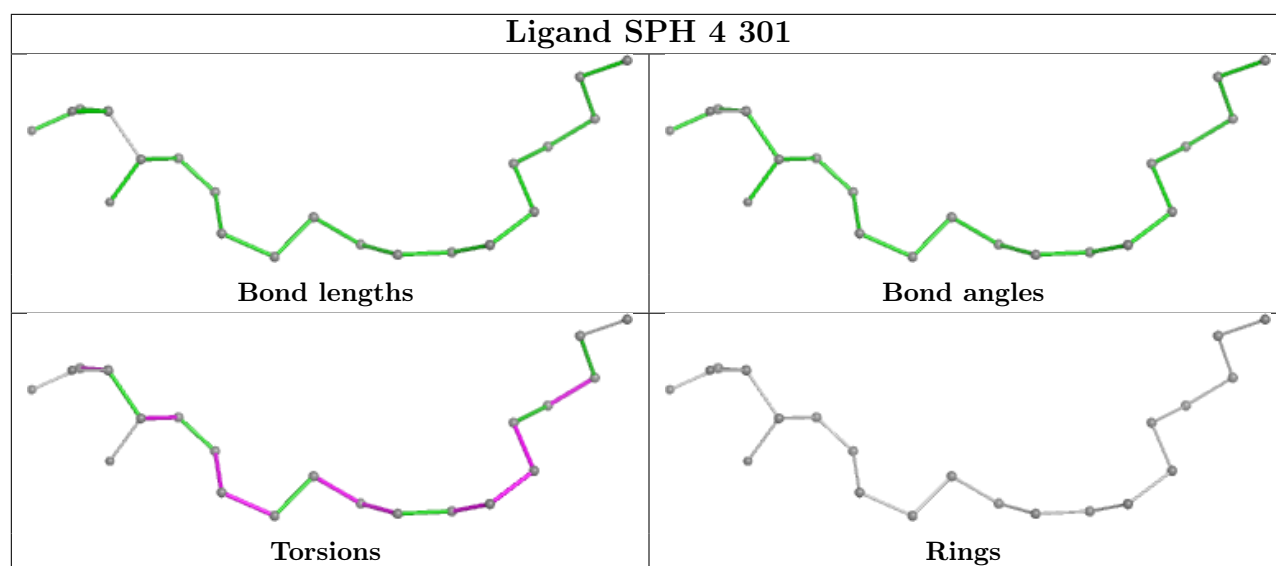


Ligand CLA 7 324

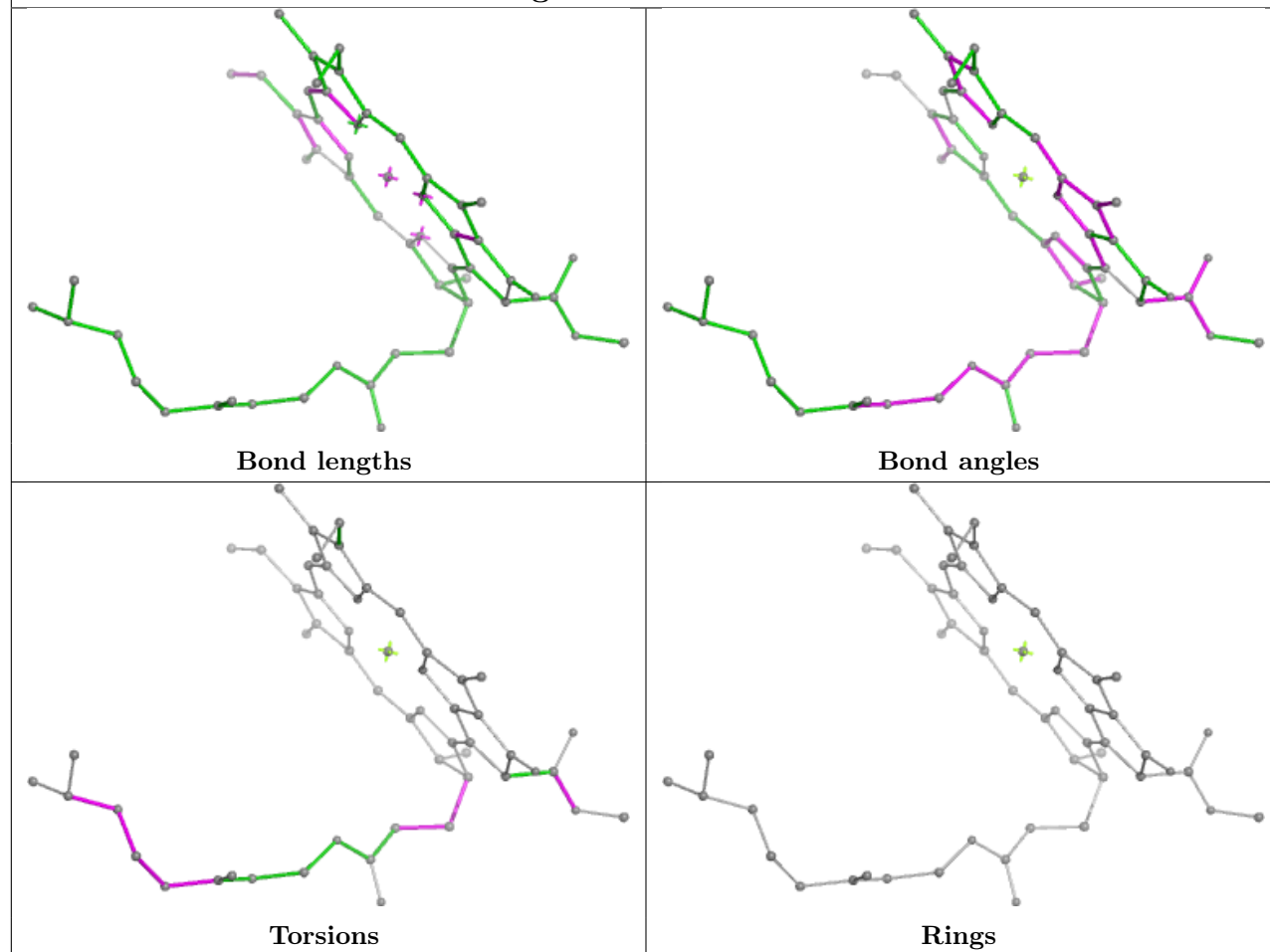


Ligand LUT 7 303

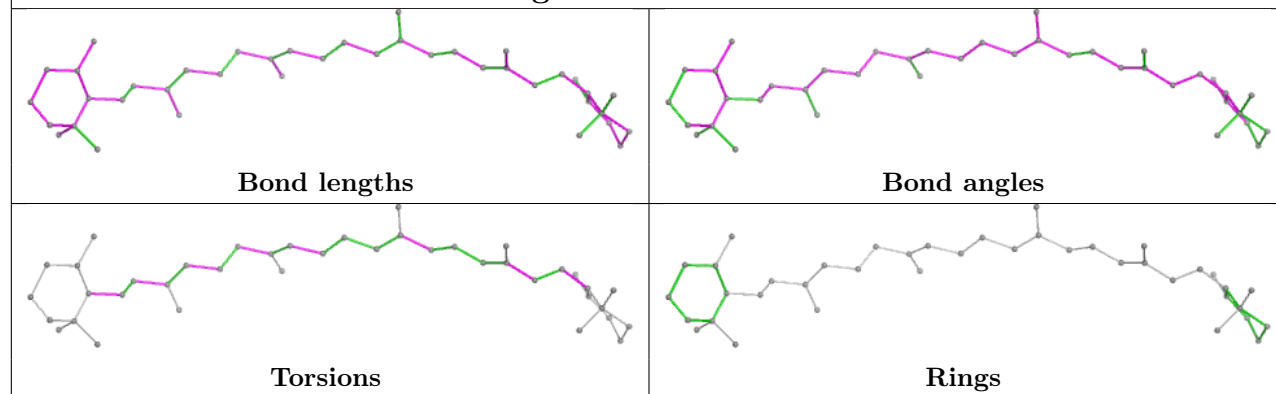


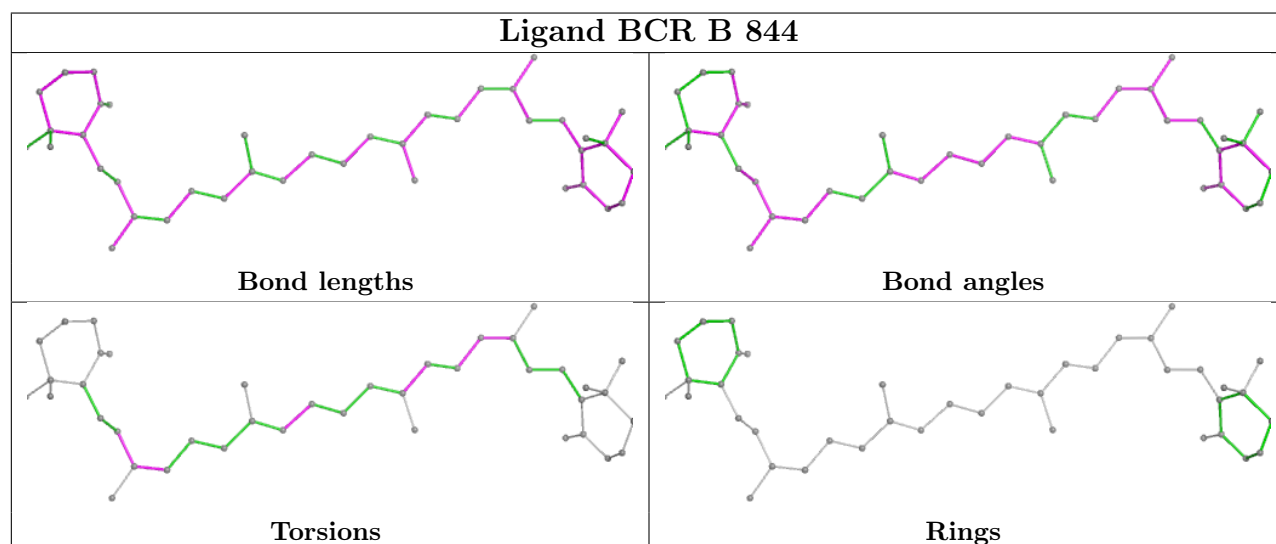
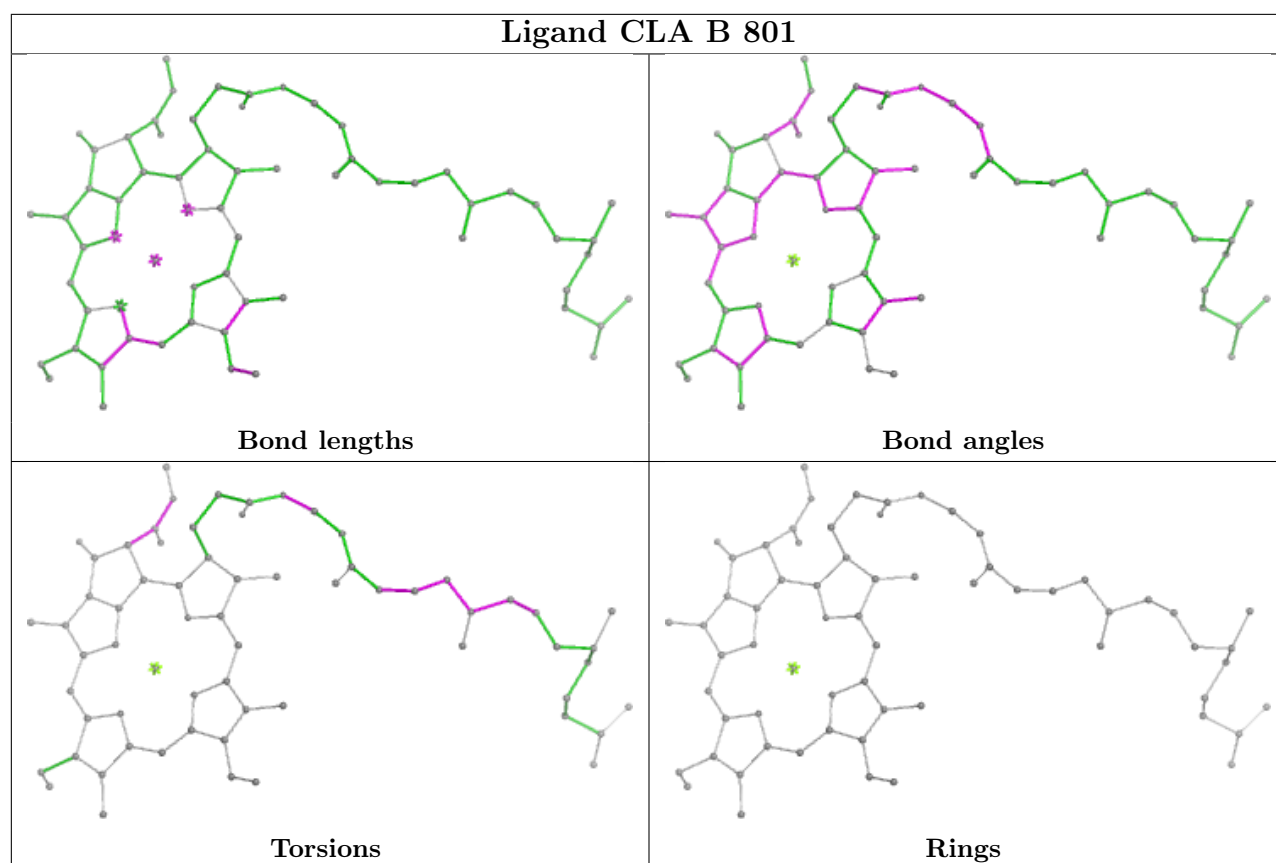


Ligand CLA Z 311

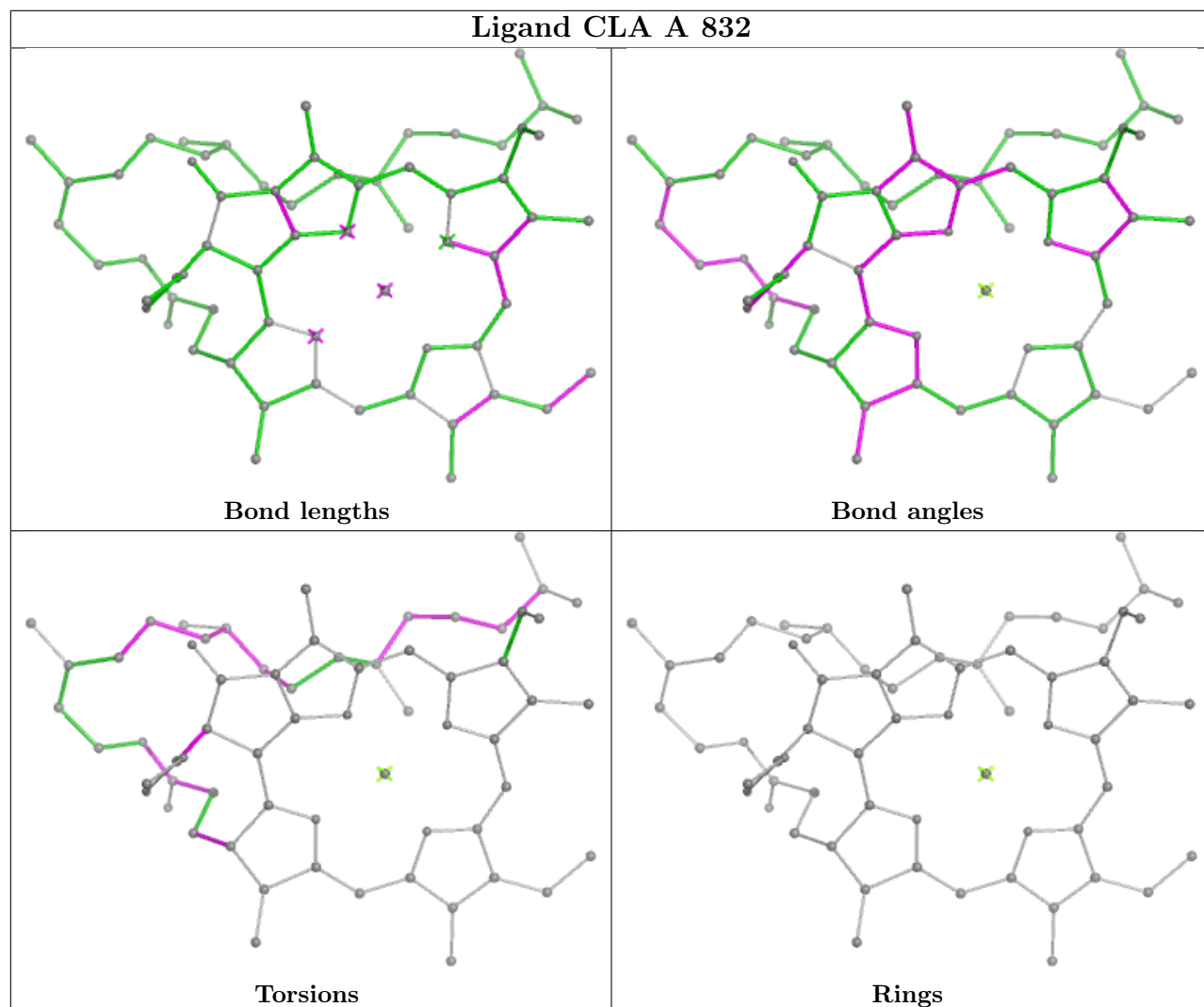


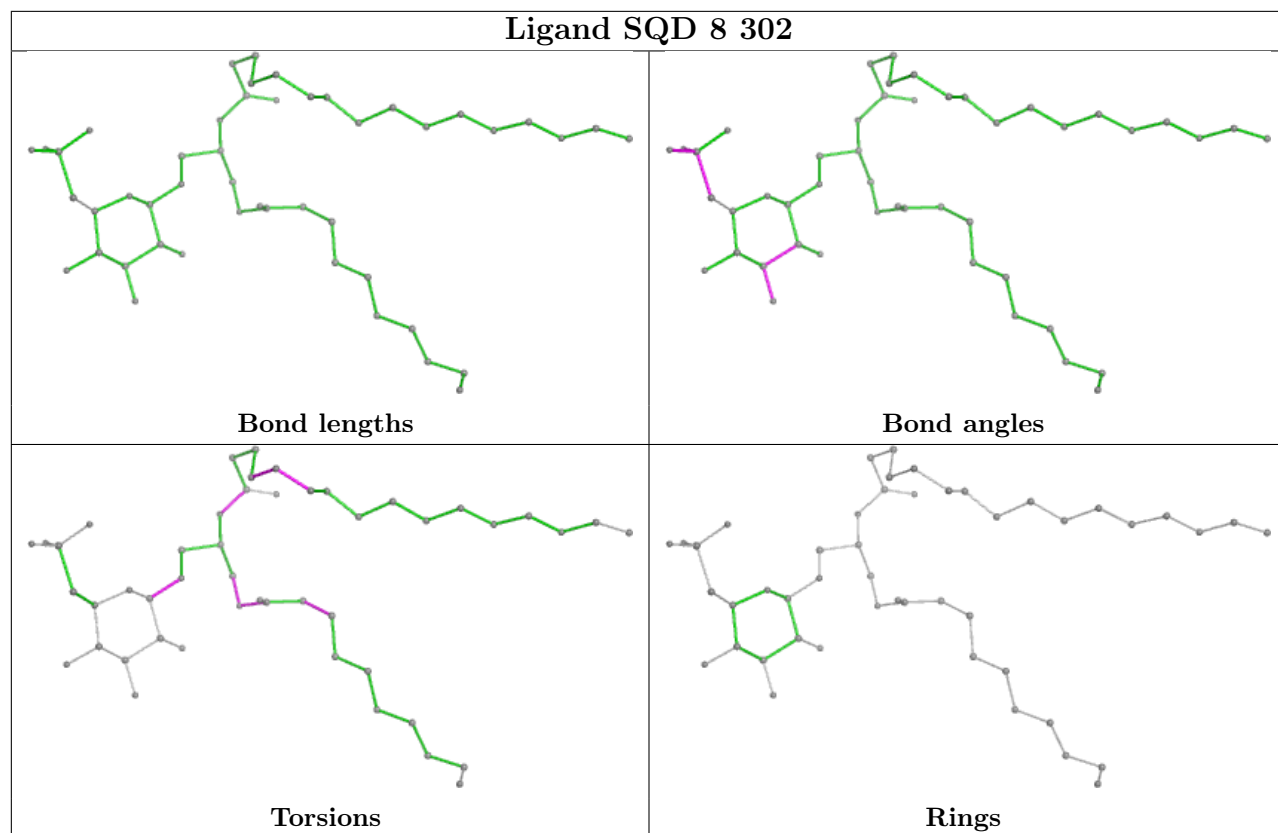
Ligand BCR F 302

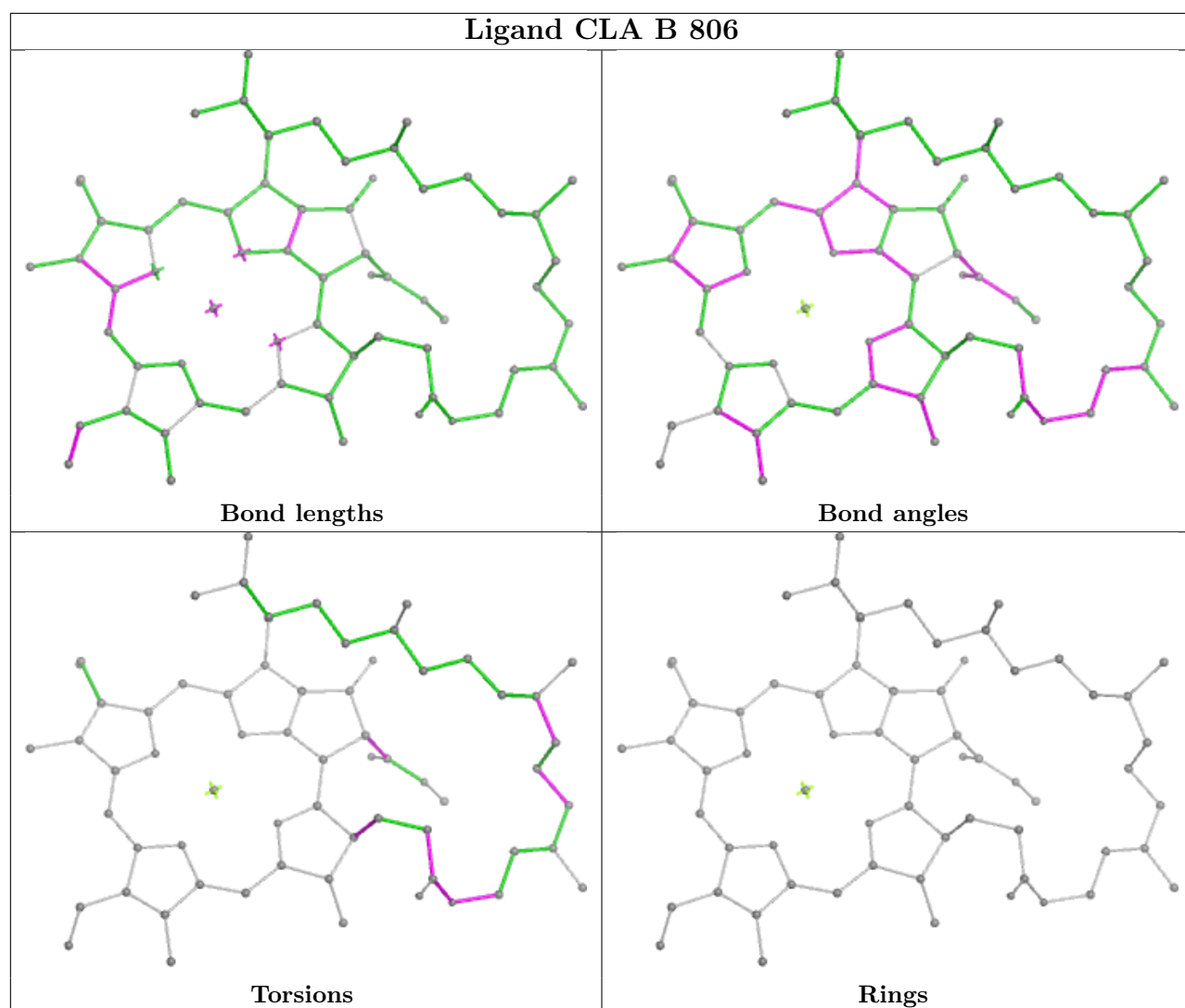




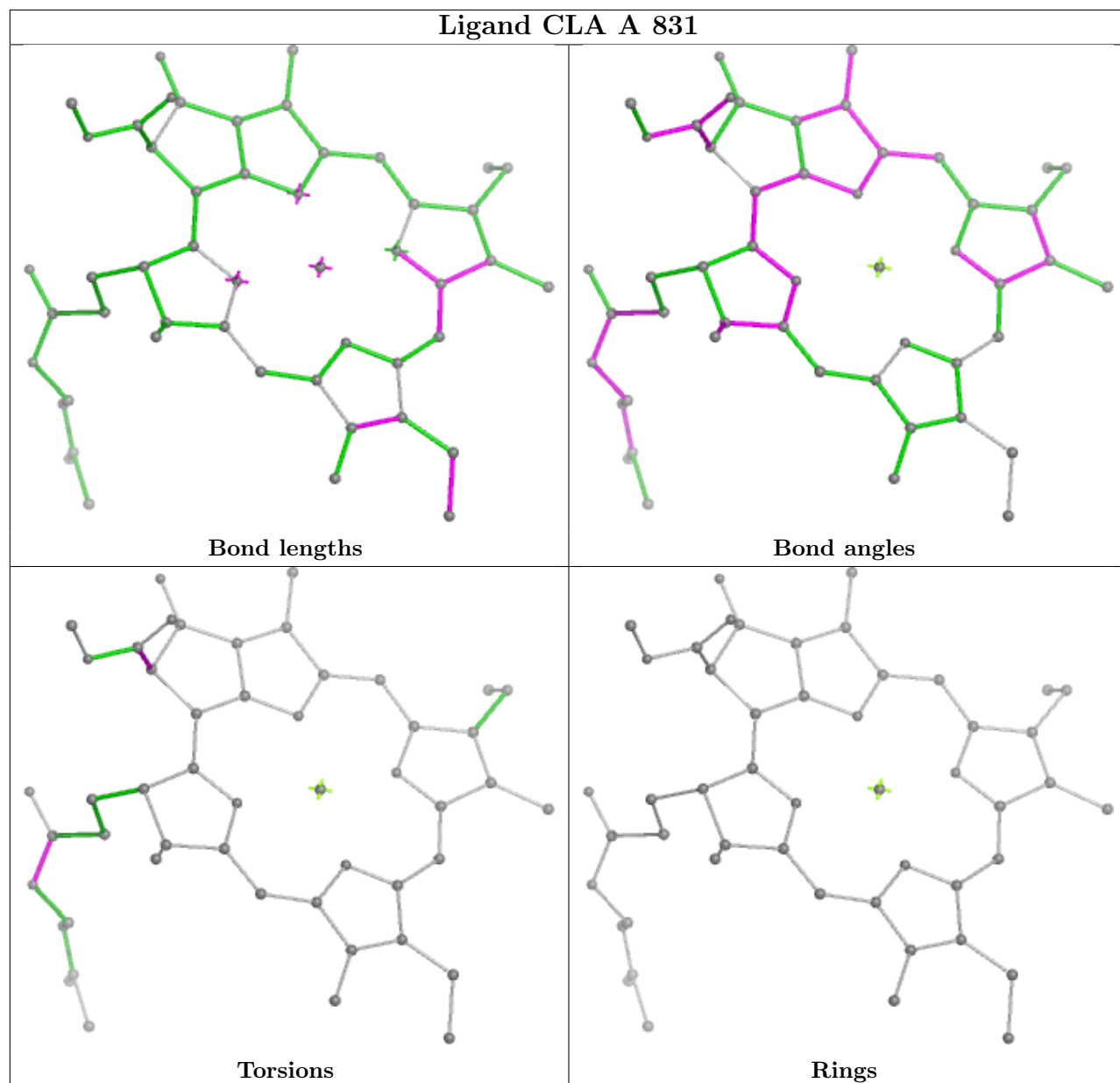
Ligand CLA A 832



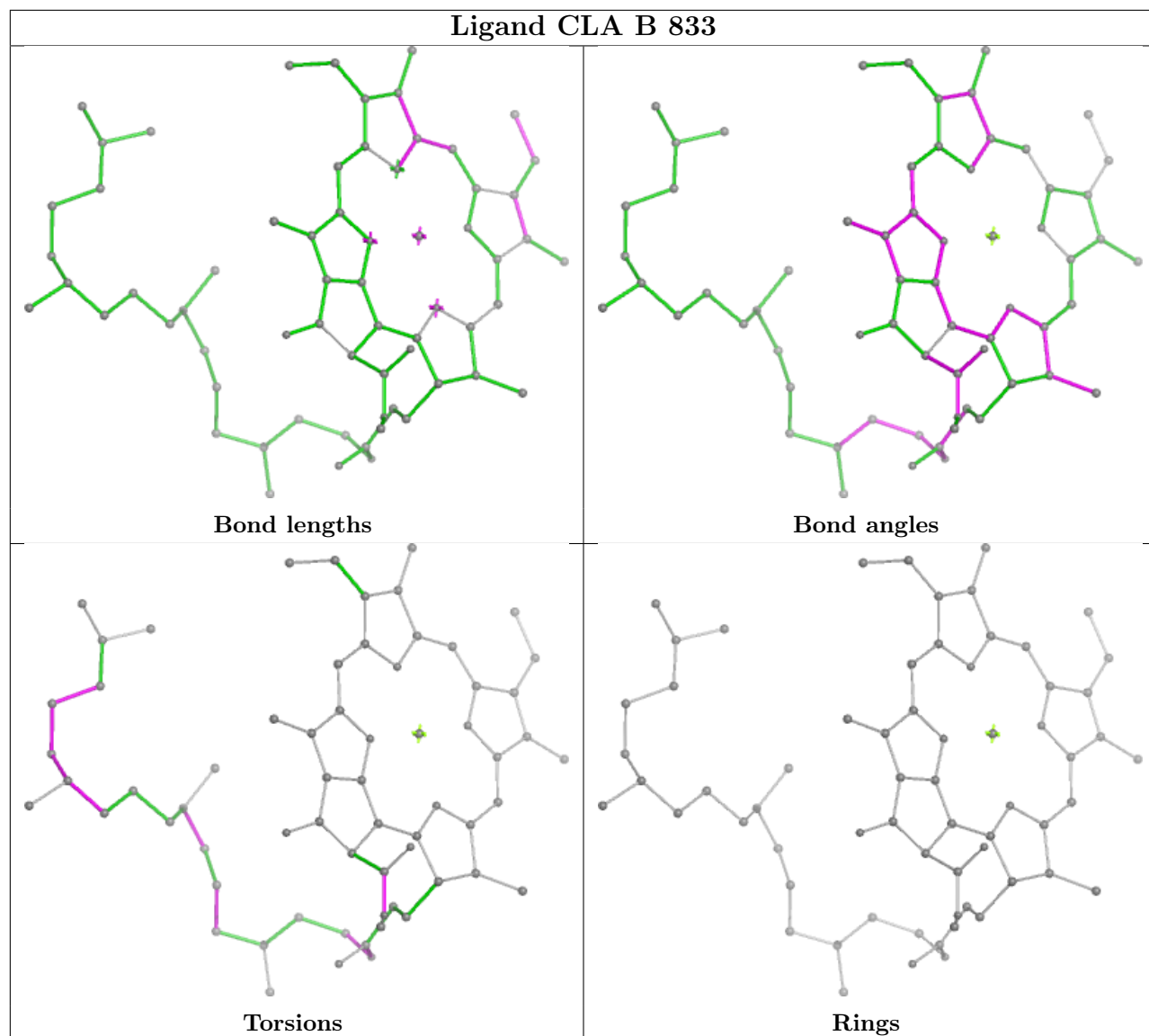




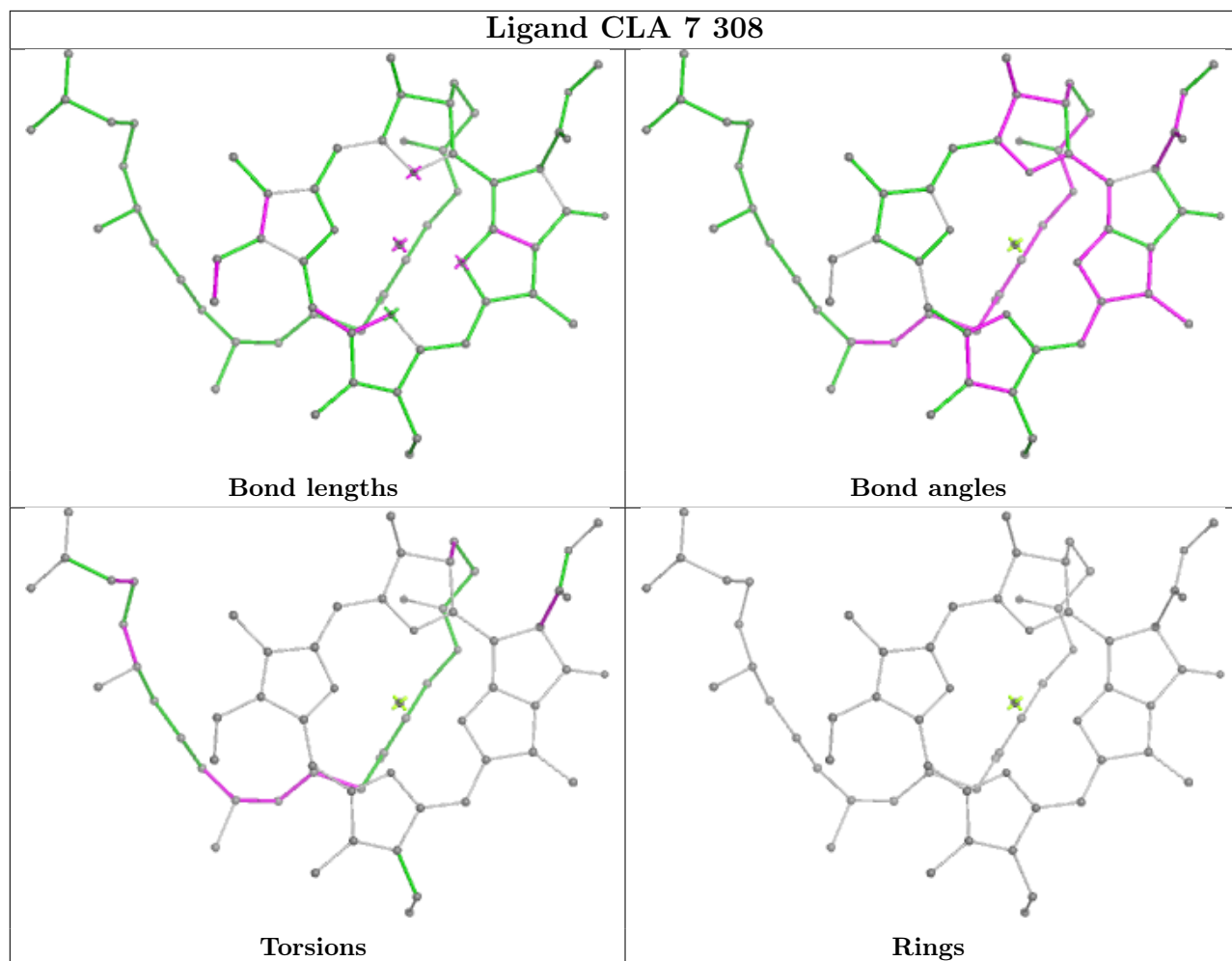
Ligand CLA A 831



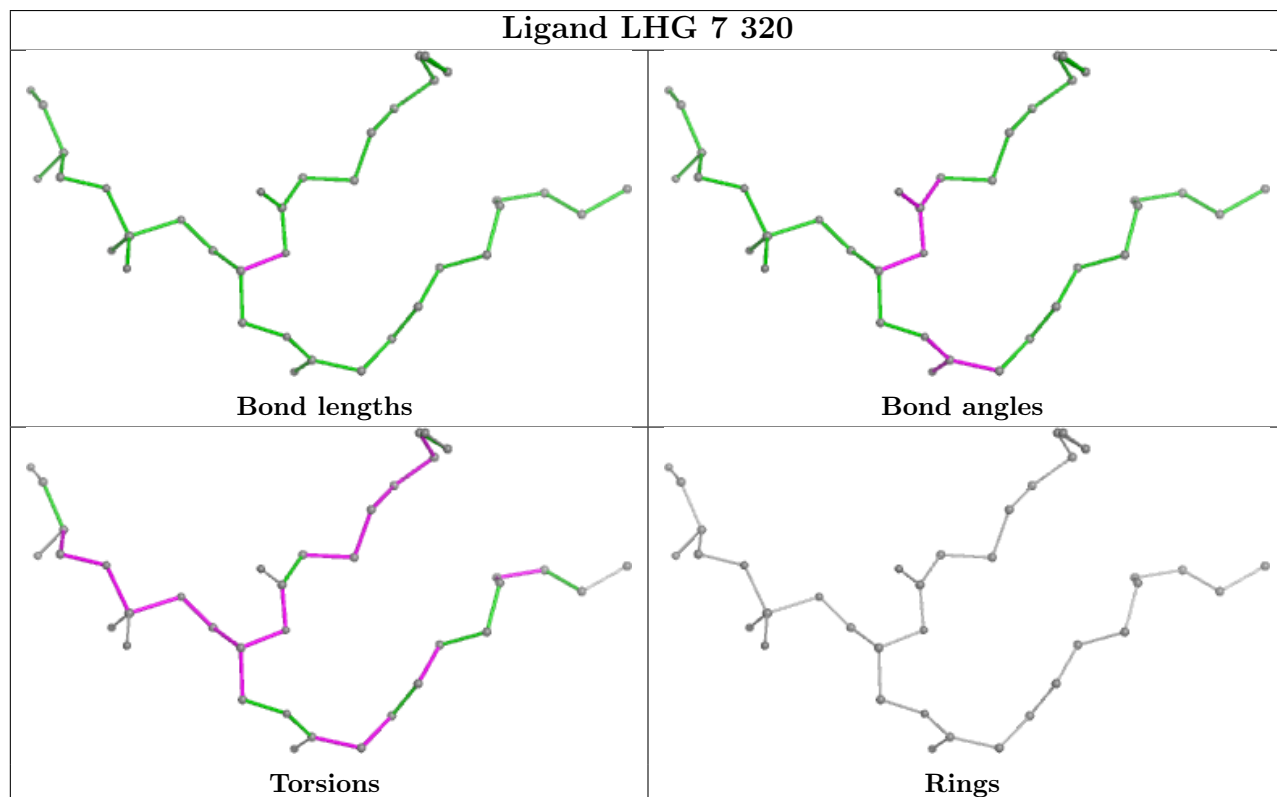
Ligand CLA B 833

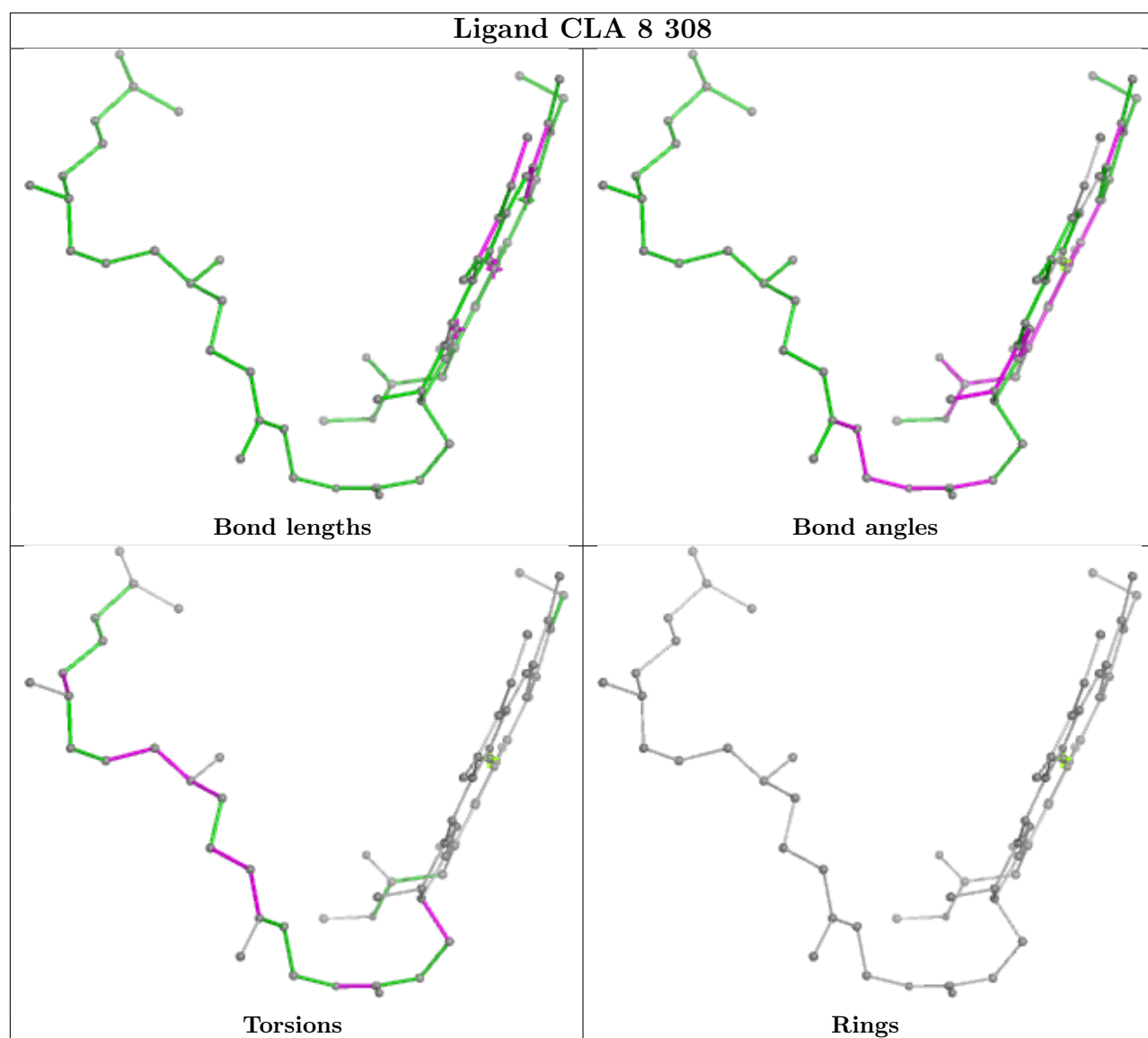


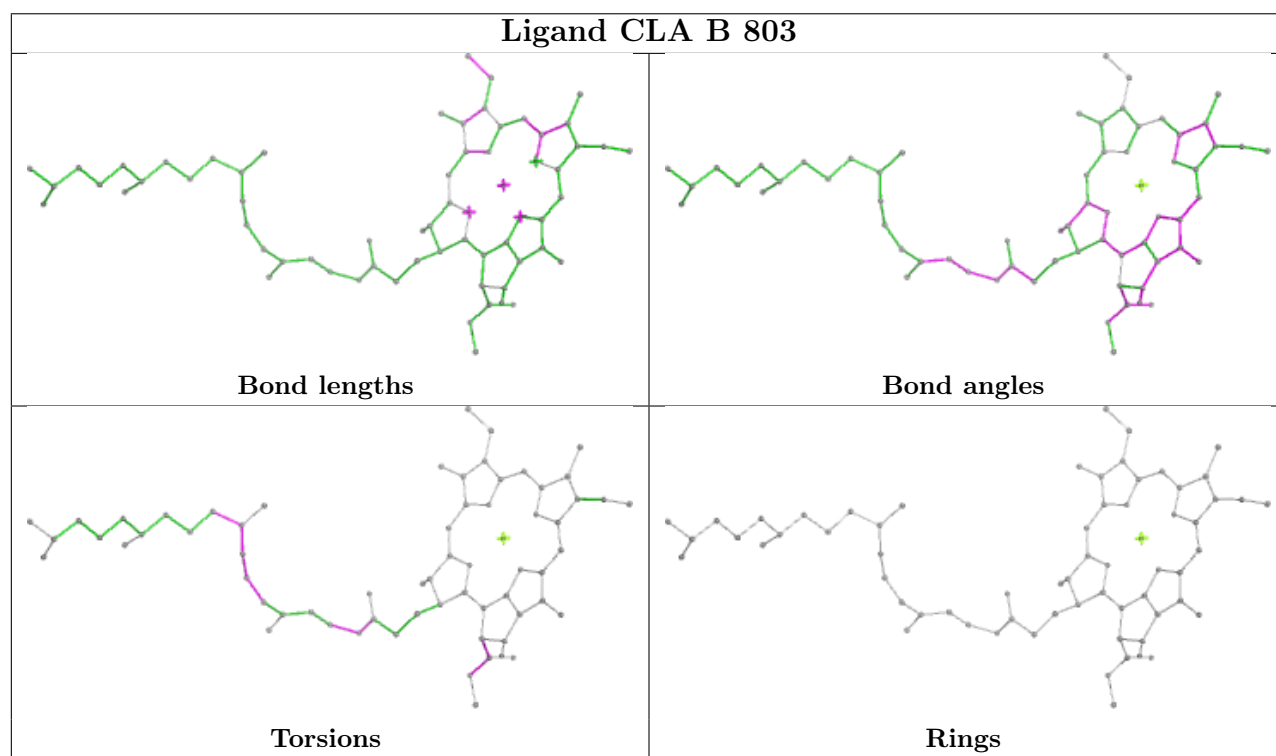
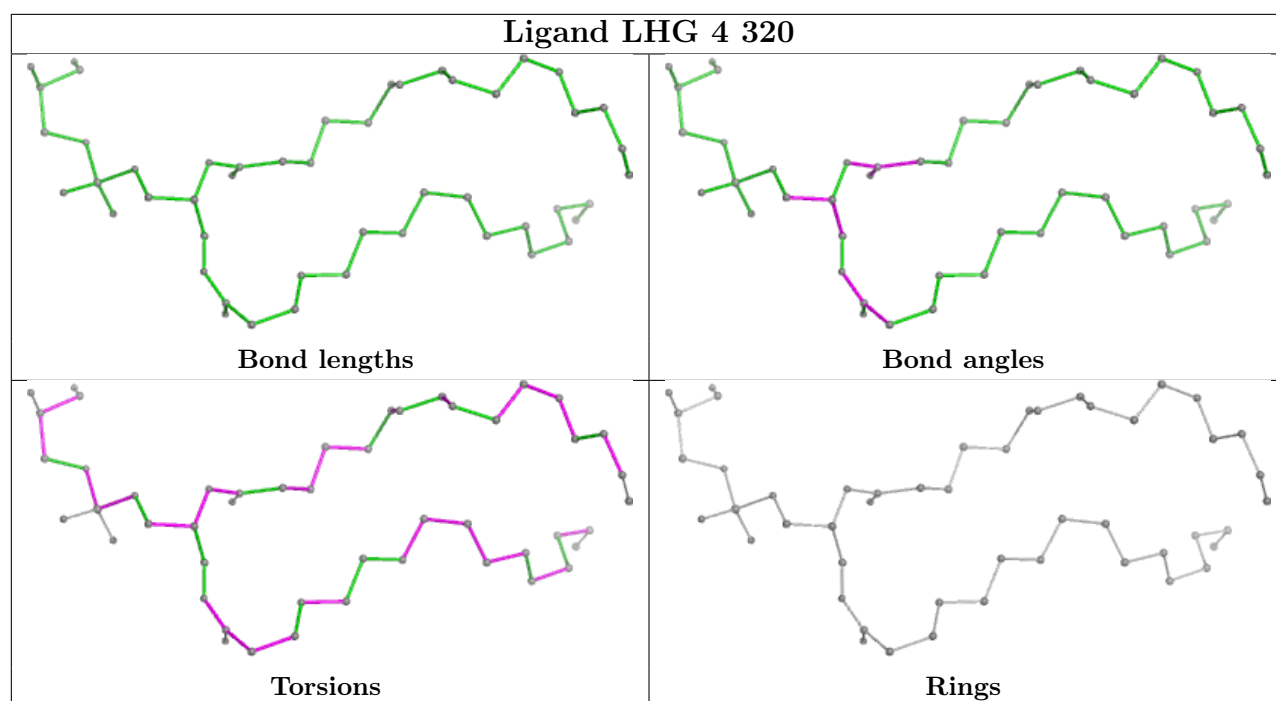
Ligand CLA 7 308



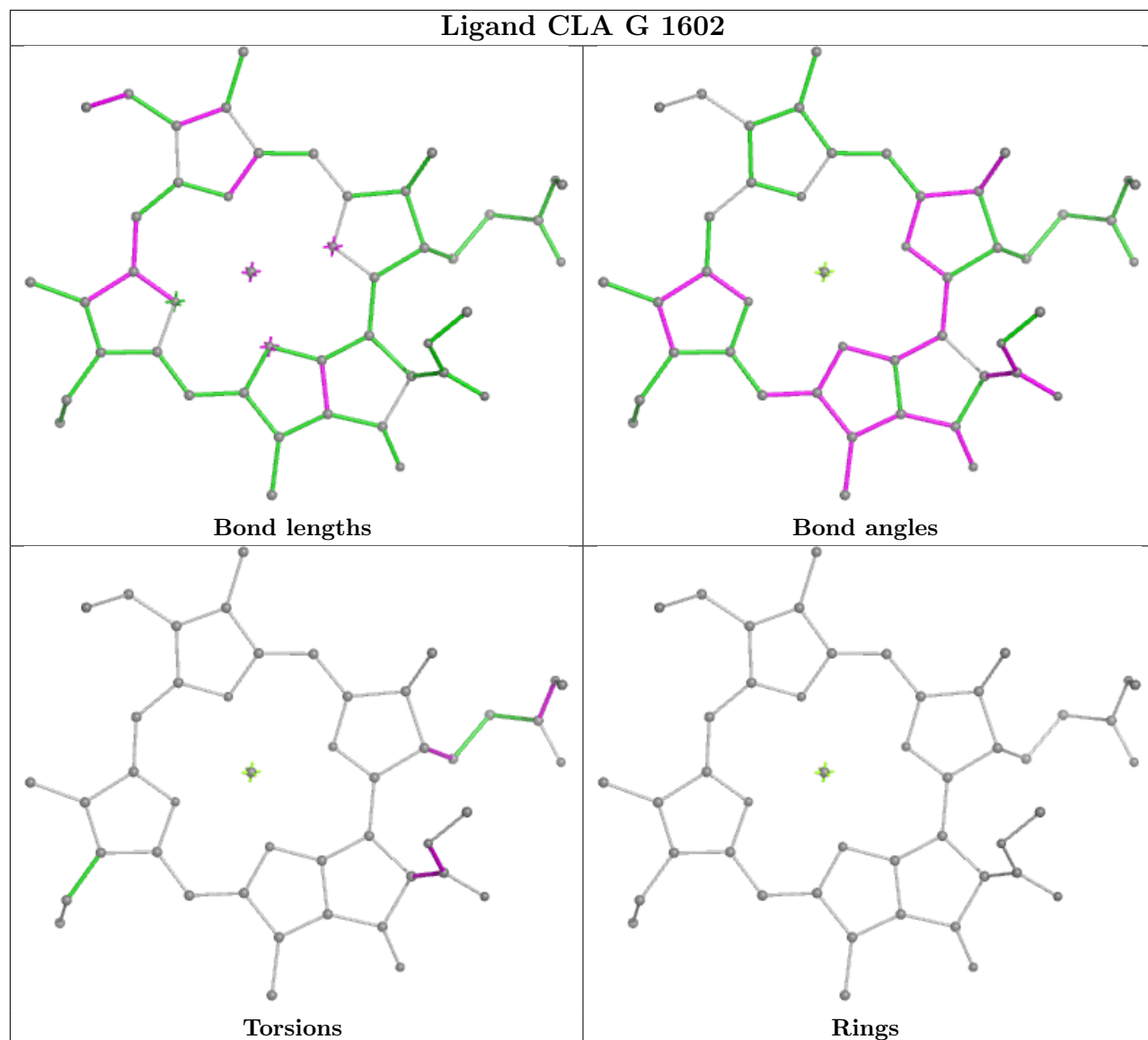
Ligand LHG 7 320



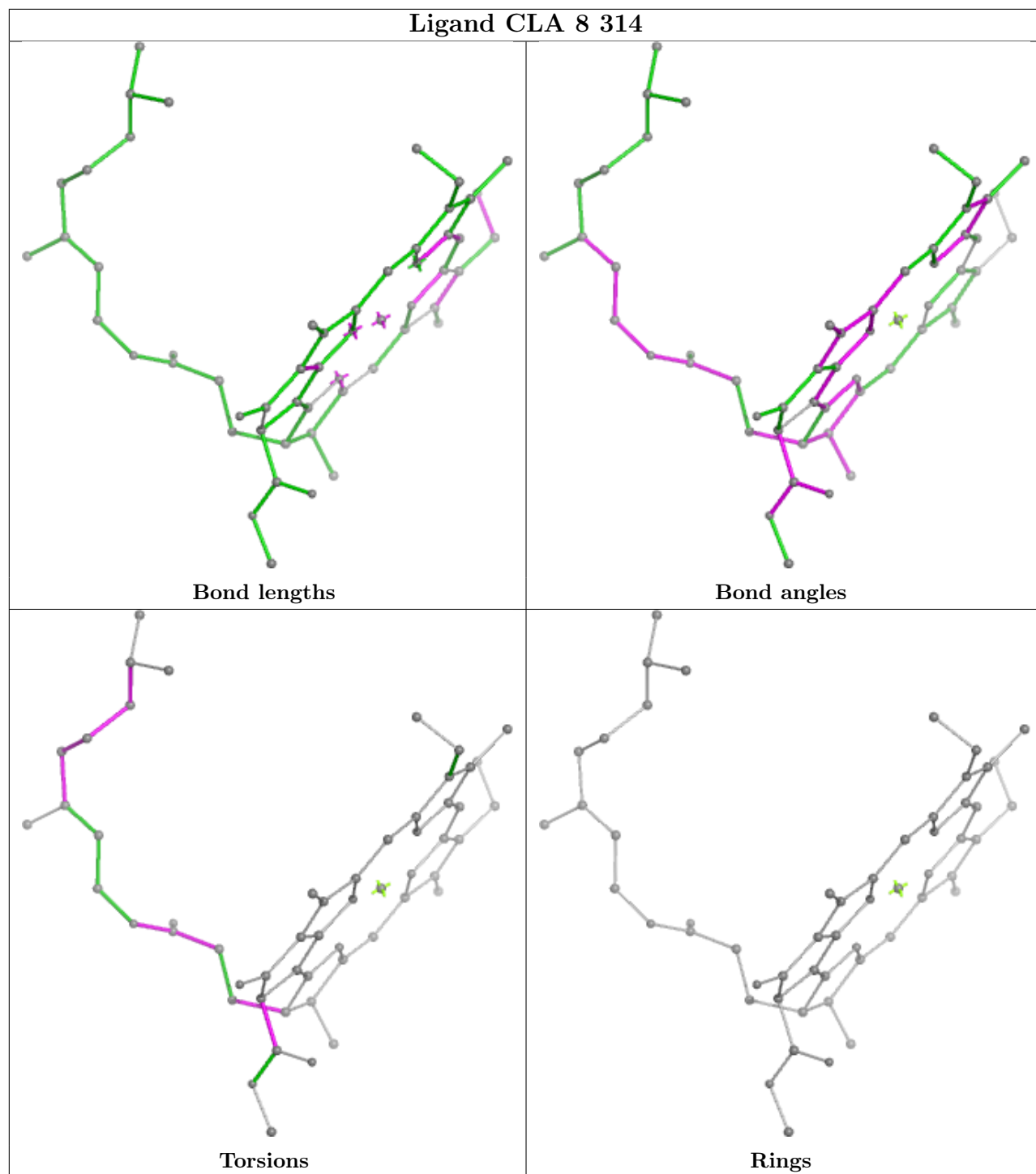


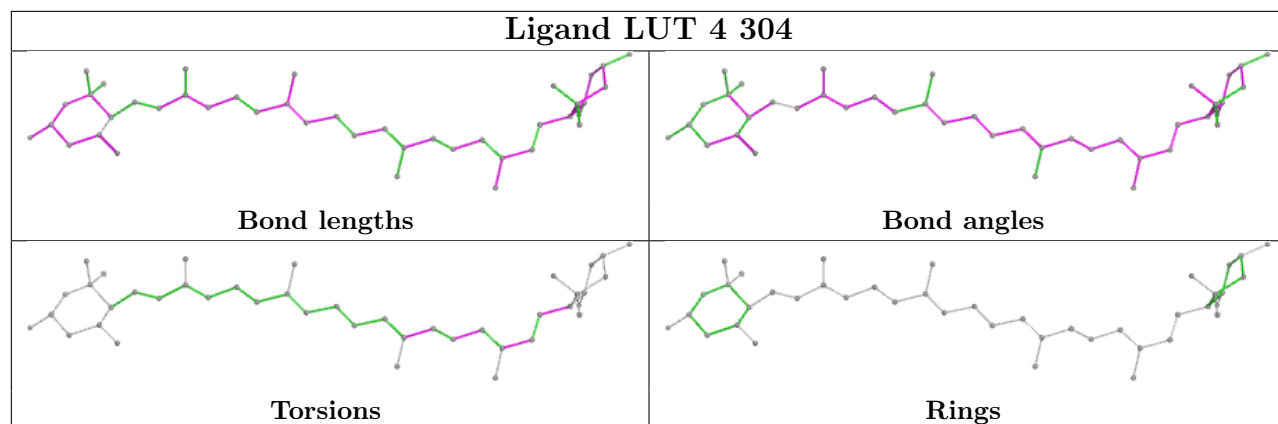
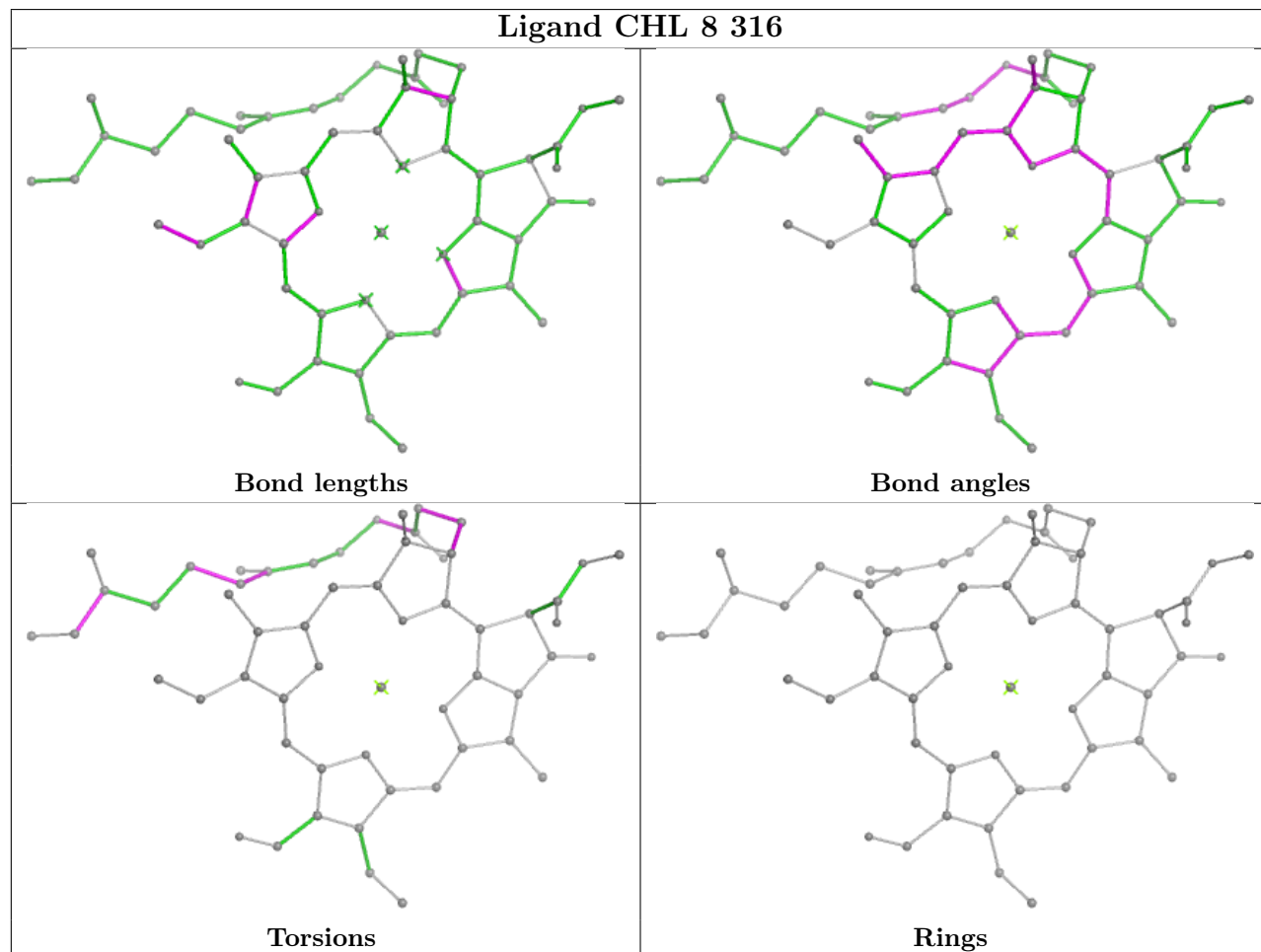


Ligand CLA G 1602

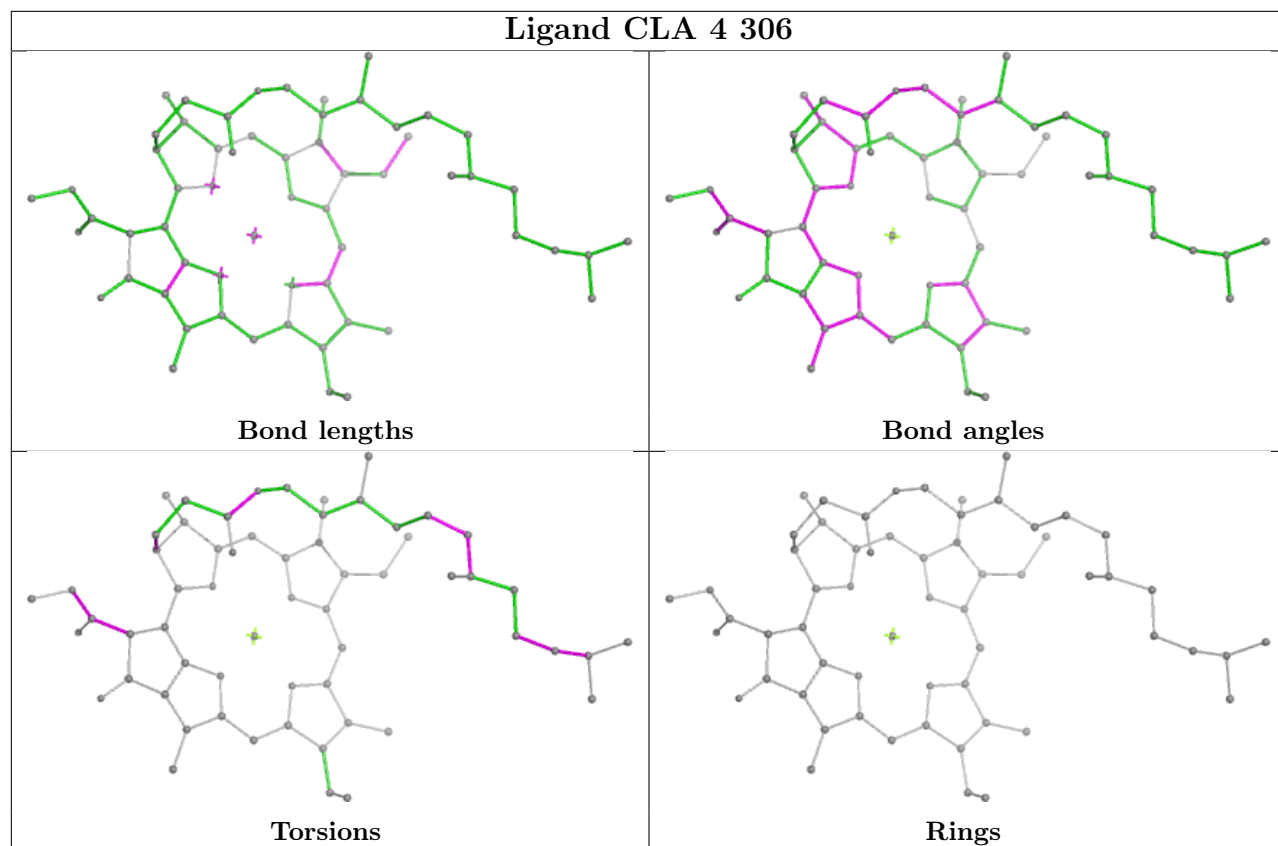


Ligand CLA 8 314

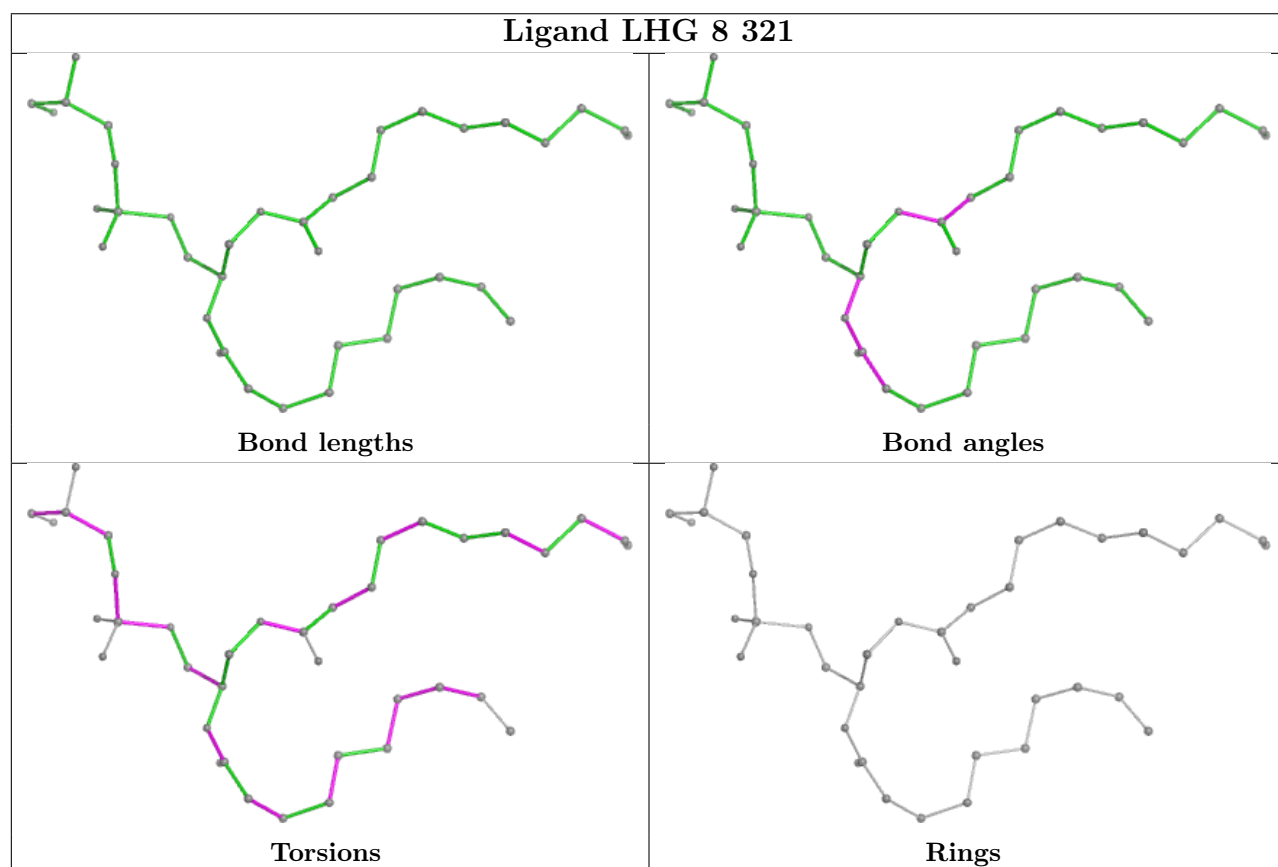


Ligand LUT 4 304**Ligand CHL 8 316**

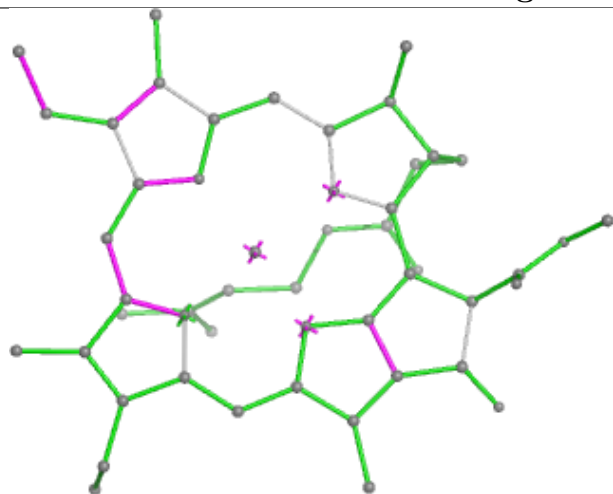
Ligand CLA 4 306



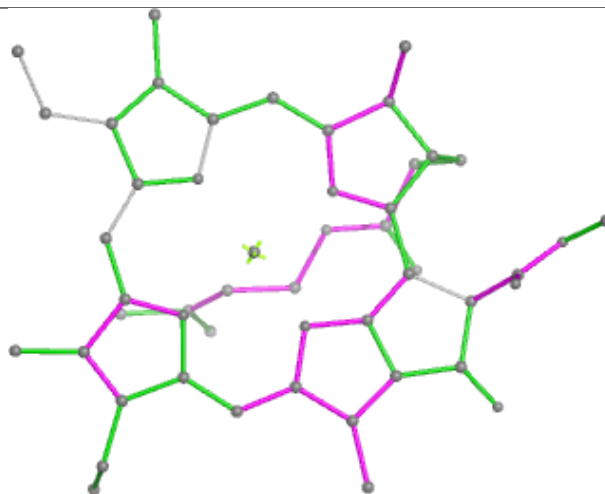
Ligand LHG 8 321



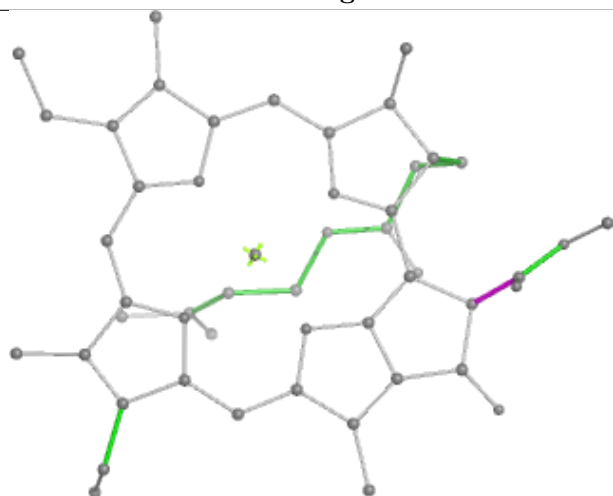
Ligand CLA Z 304



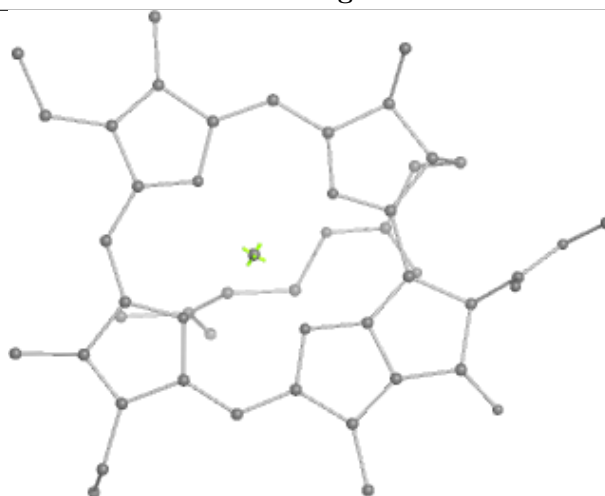
Bond lengths



Bond angles

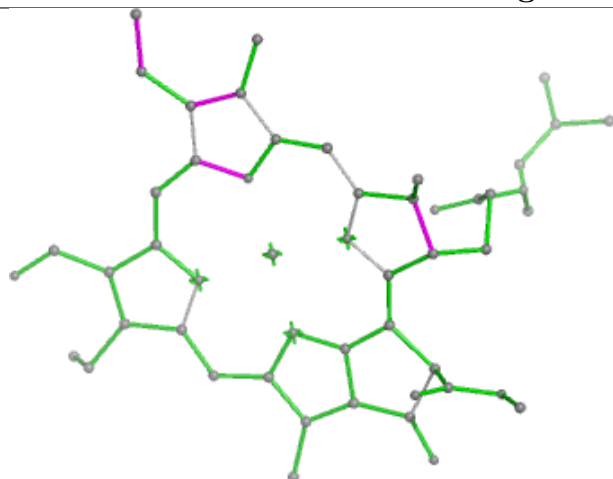


Torsions

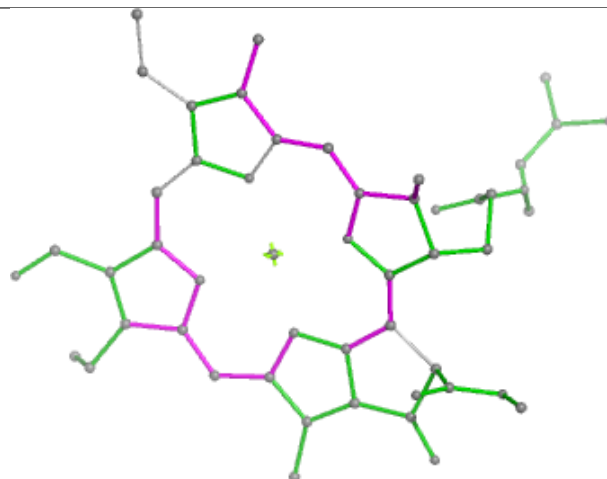


Rings

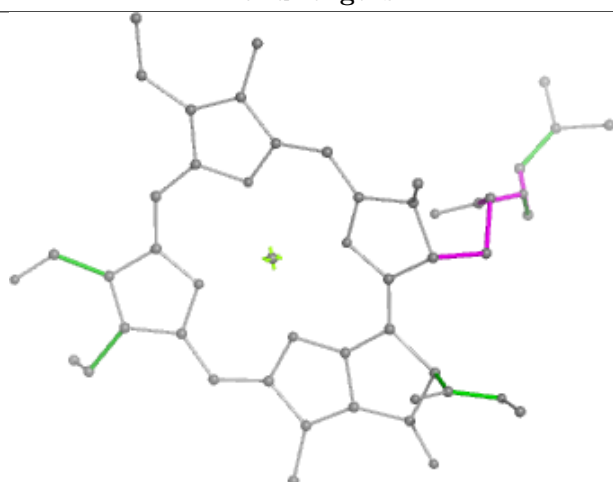
Ligand CHL 6 317



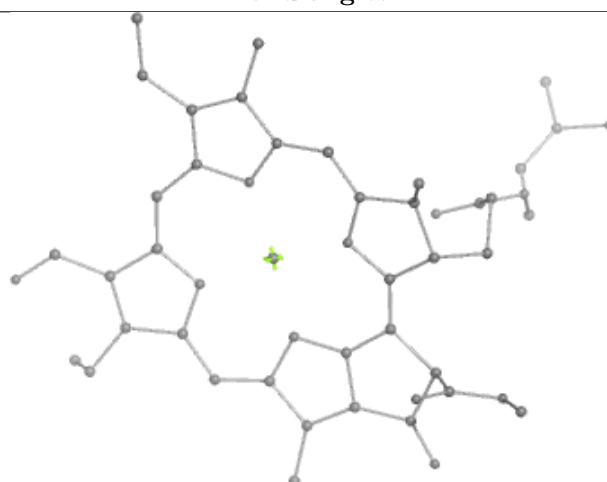
Bond lengths



Bond angles

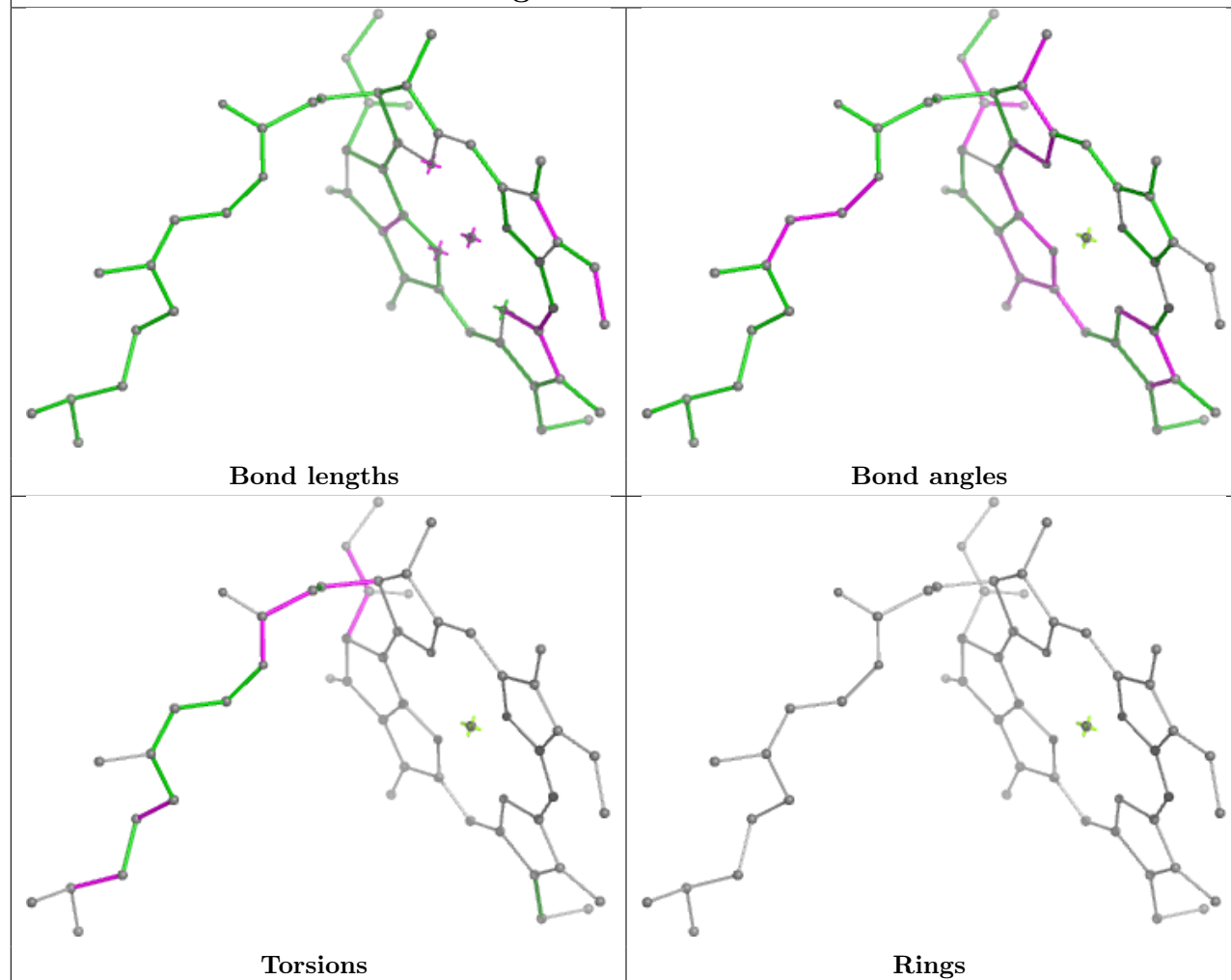


Torsions

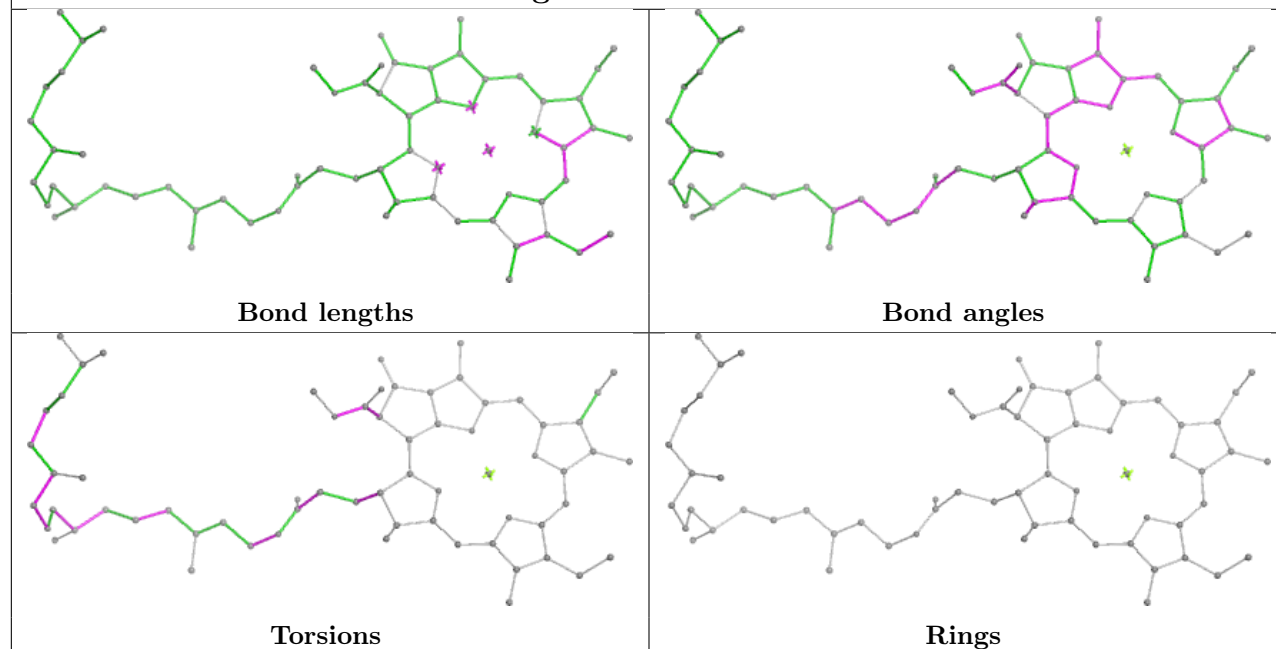


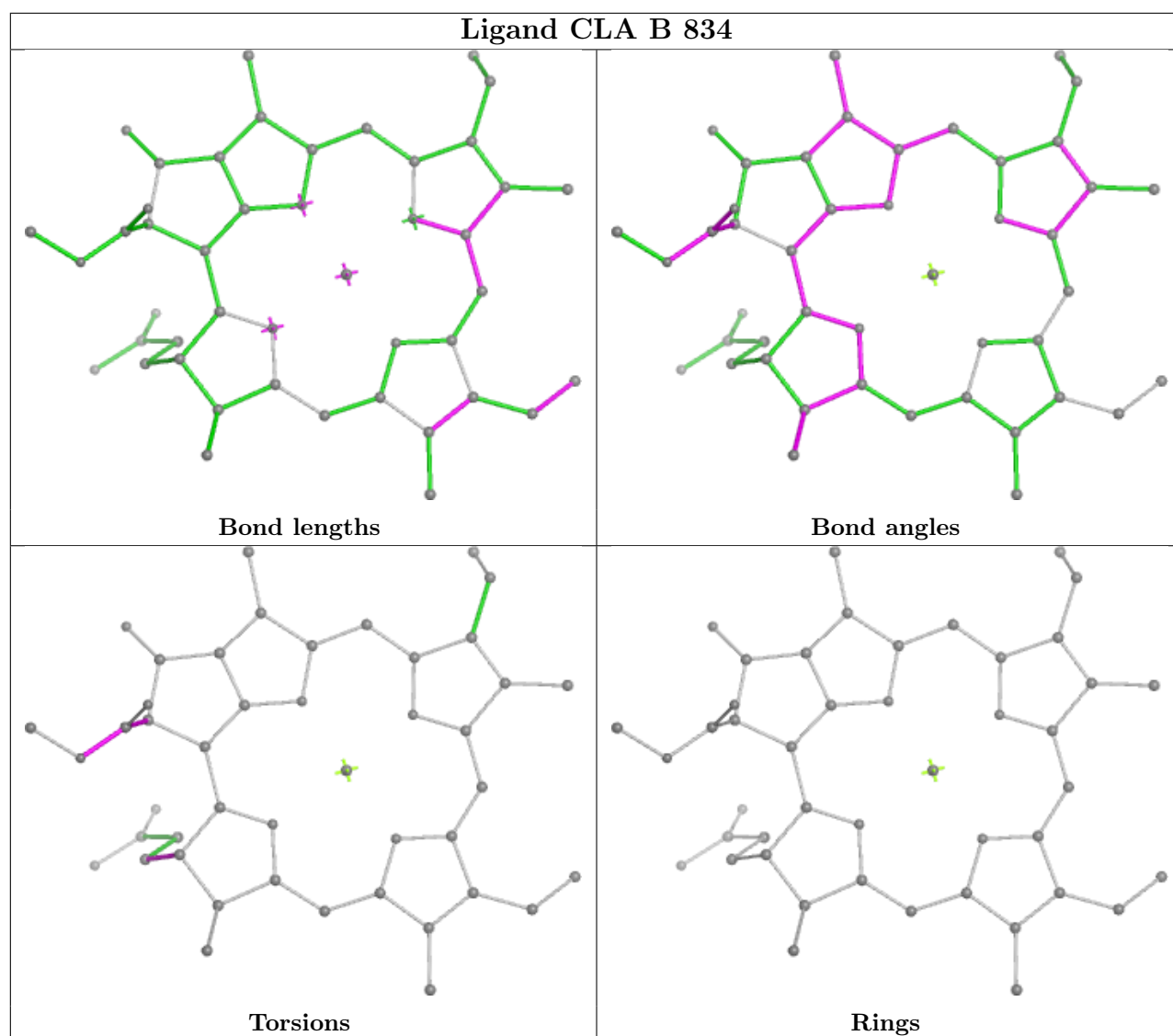
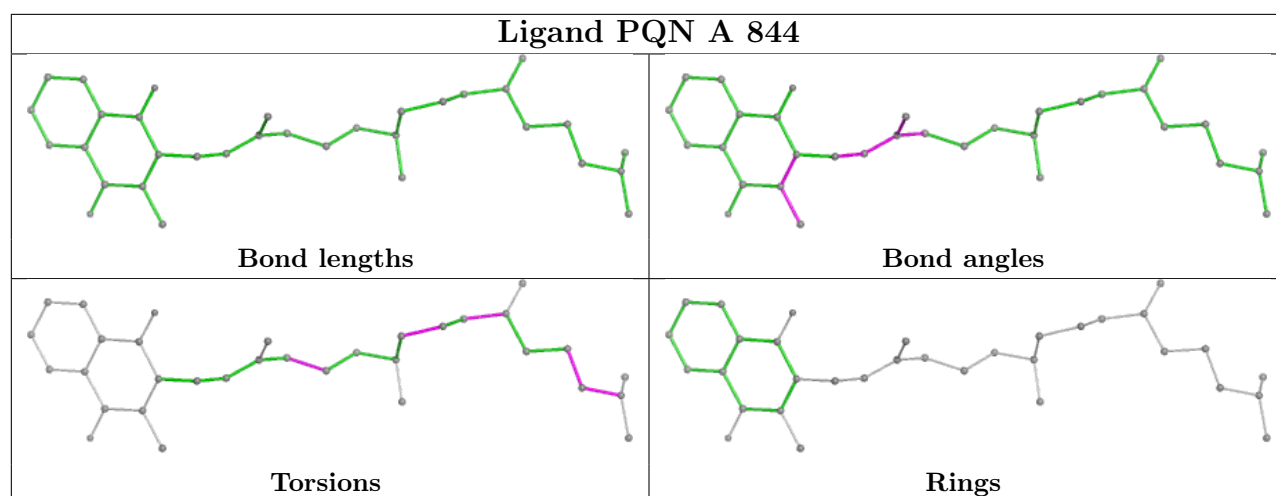
Rings

Ligand CLA A 836

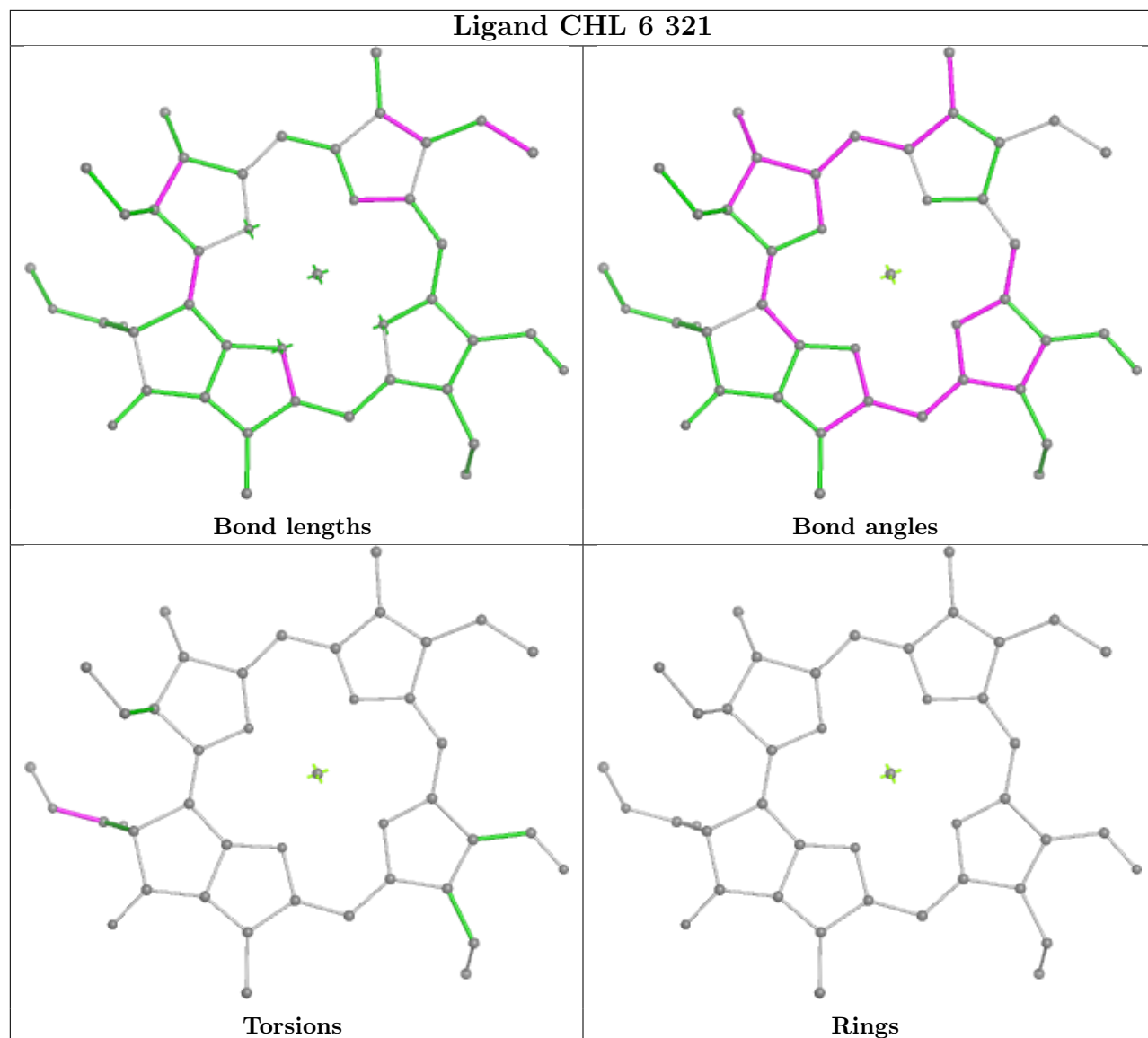


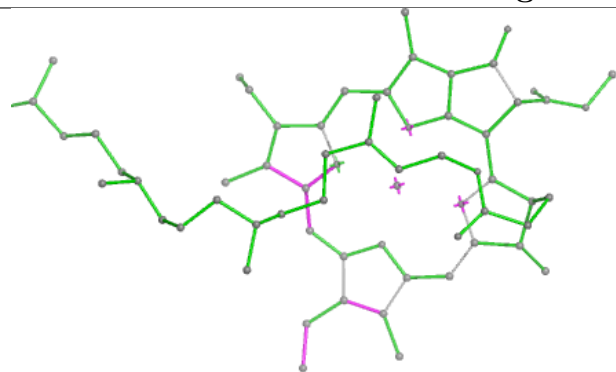
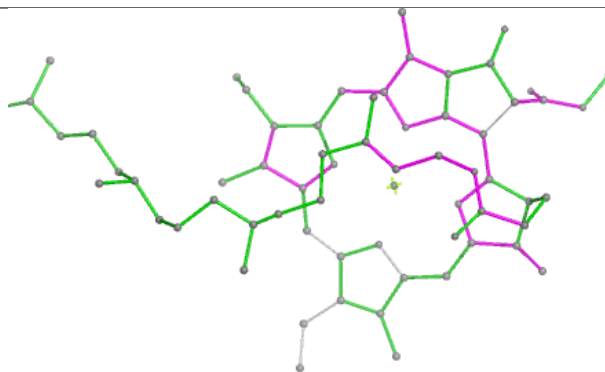
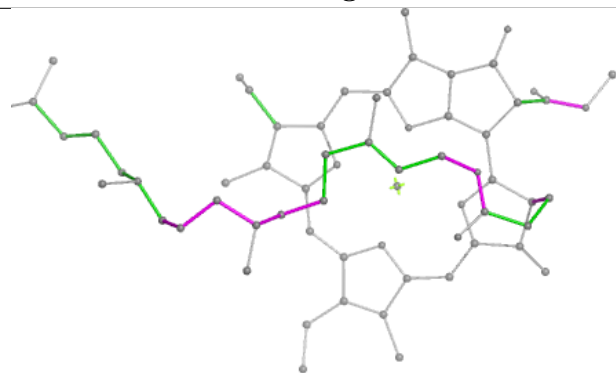
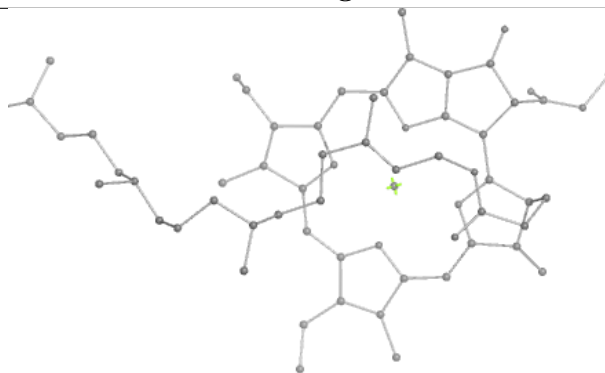
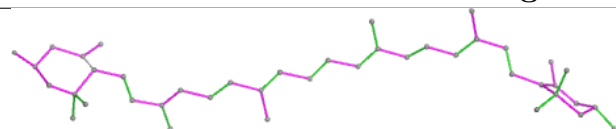
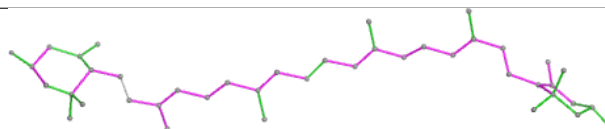
Ligand CLA B 826

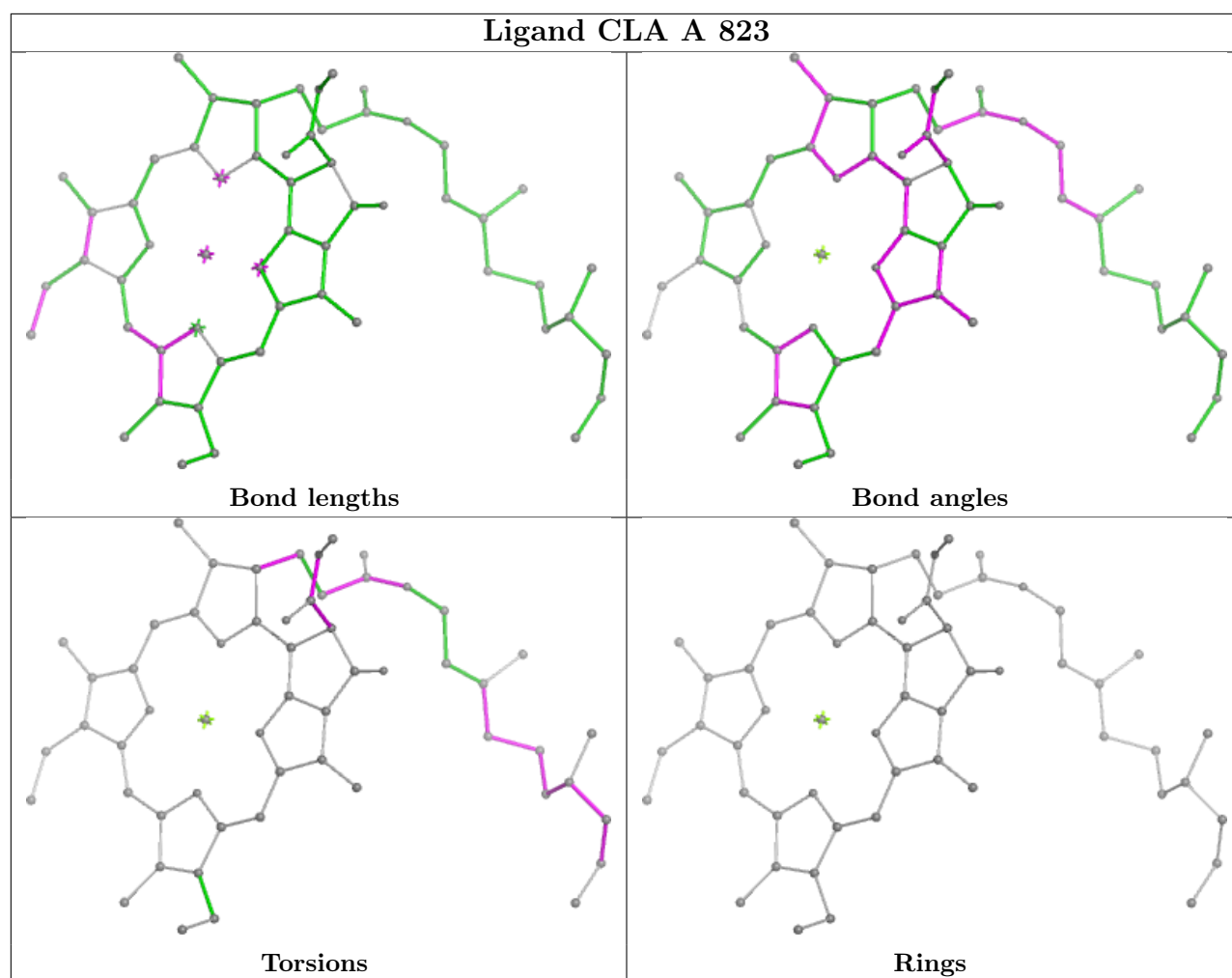


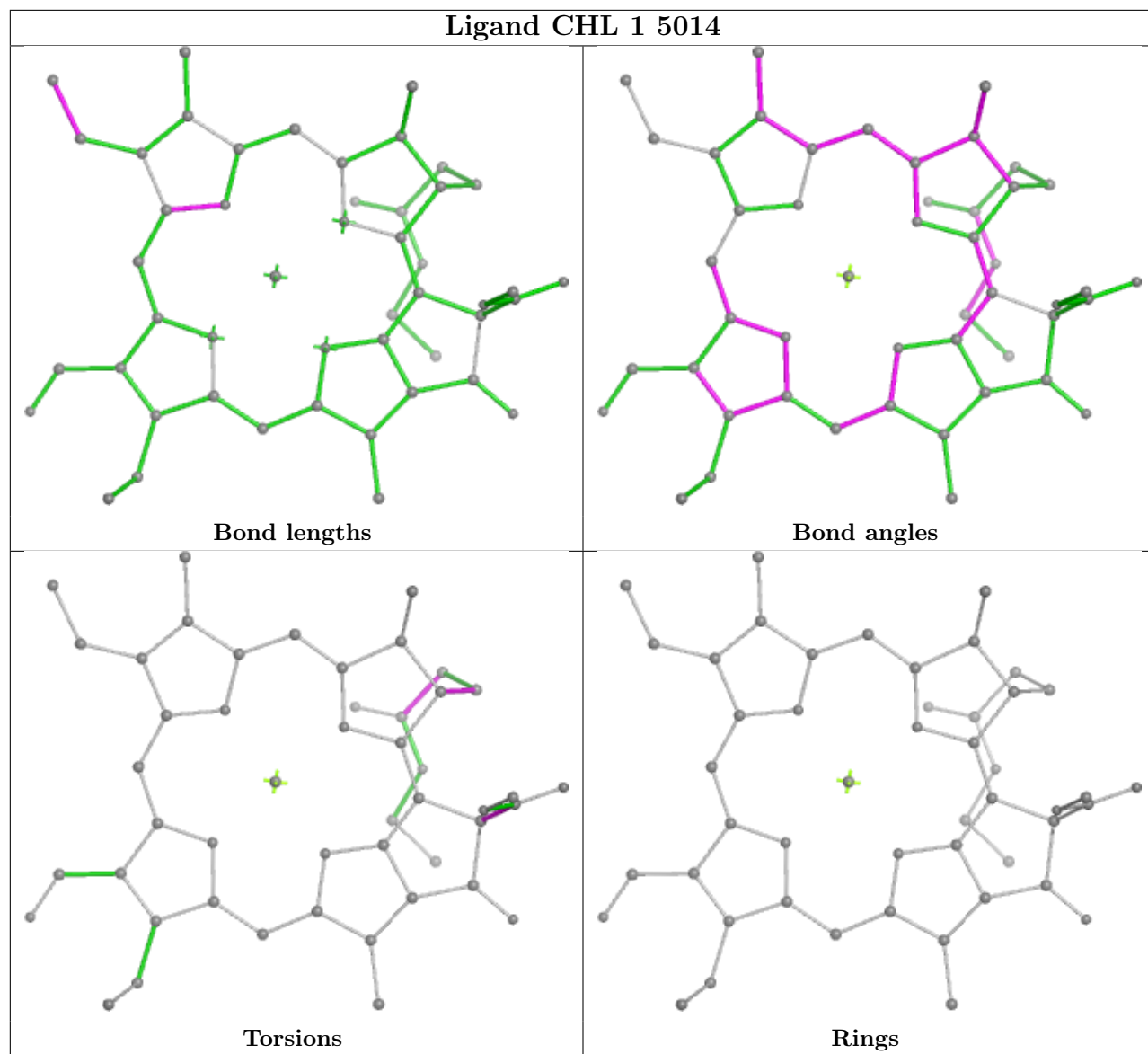


Ligand CHL 6 321

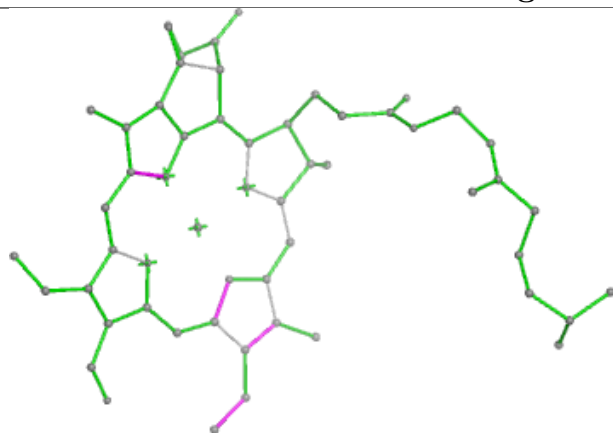


Ligand CLA B 816**Bond lengths****Bond angles****Torsions****Rings****Ligand LUT 6 306****Bond lengths****Bond angles****Torsions****Rings**

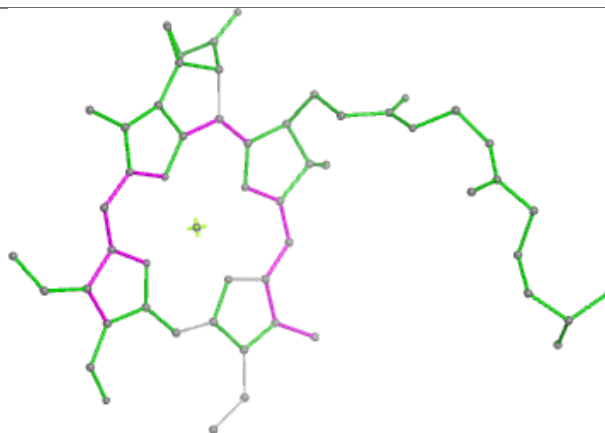




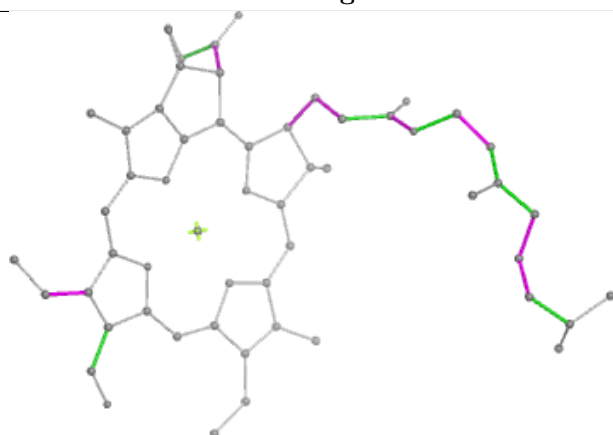
Ligand CHL 8 301



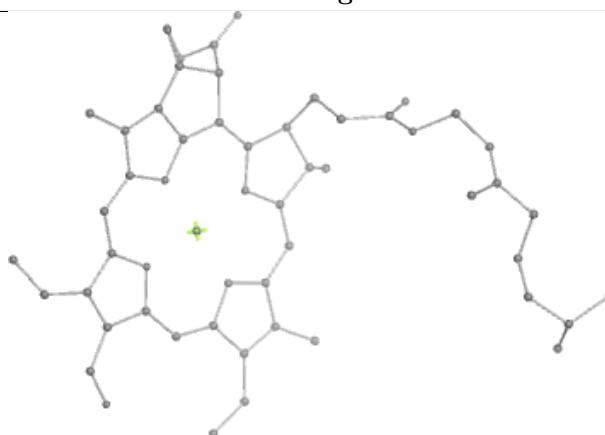
Bond lengths



Bond angles

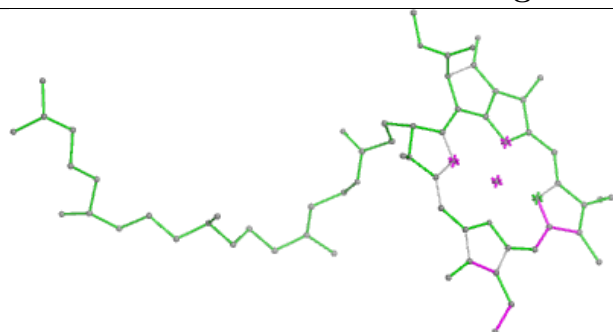


Torsions

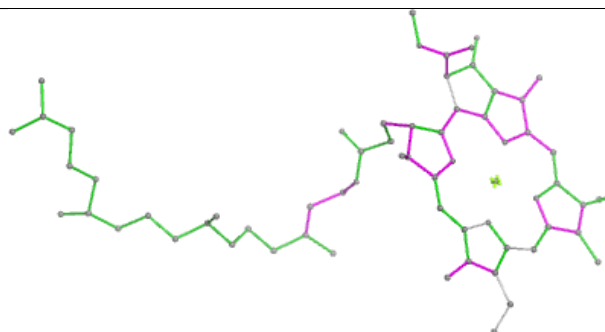


Rings

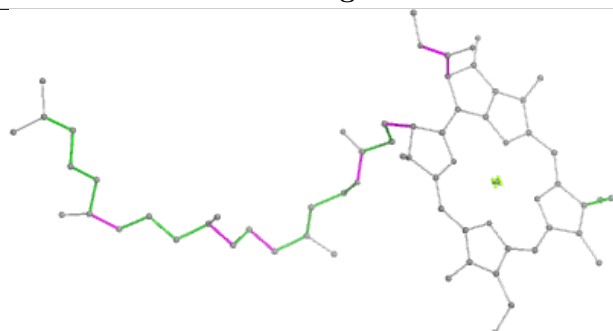
Ligand CLA A 821



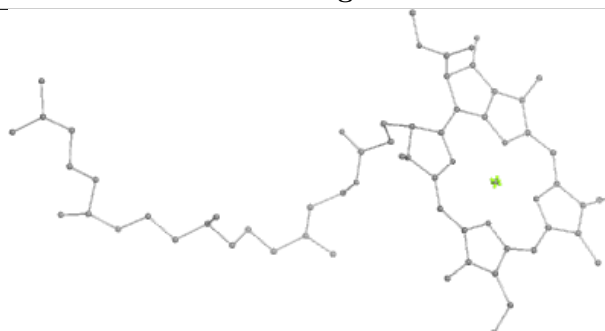
Bond lengths



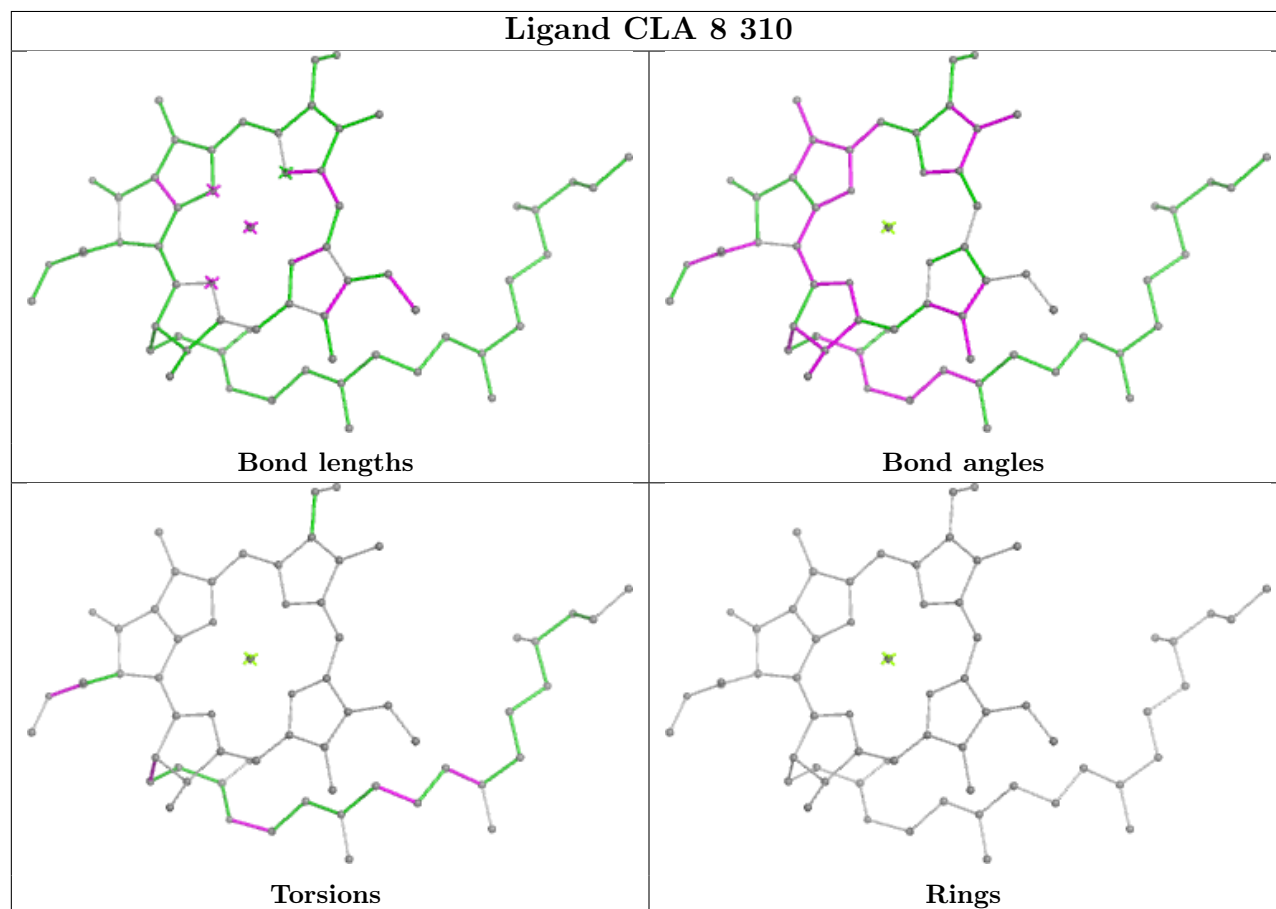
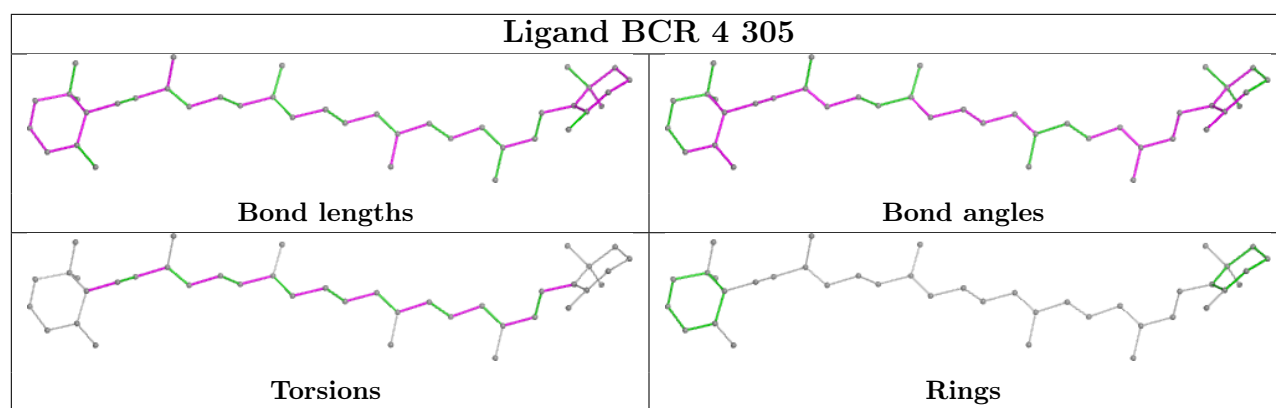
Bond angles

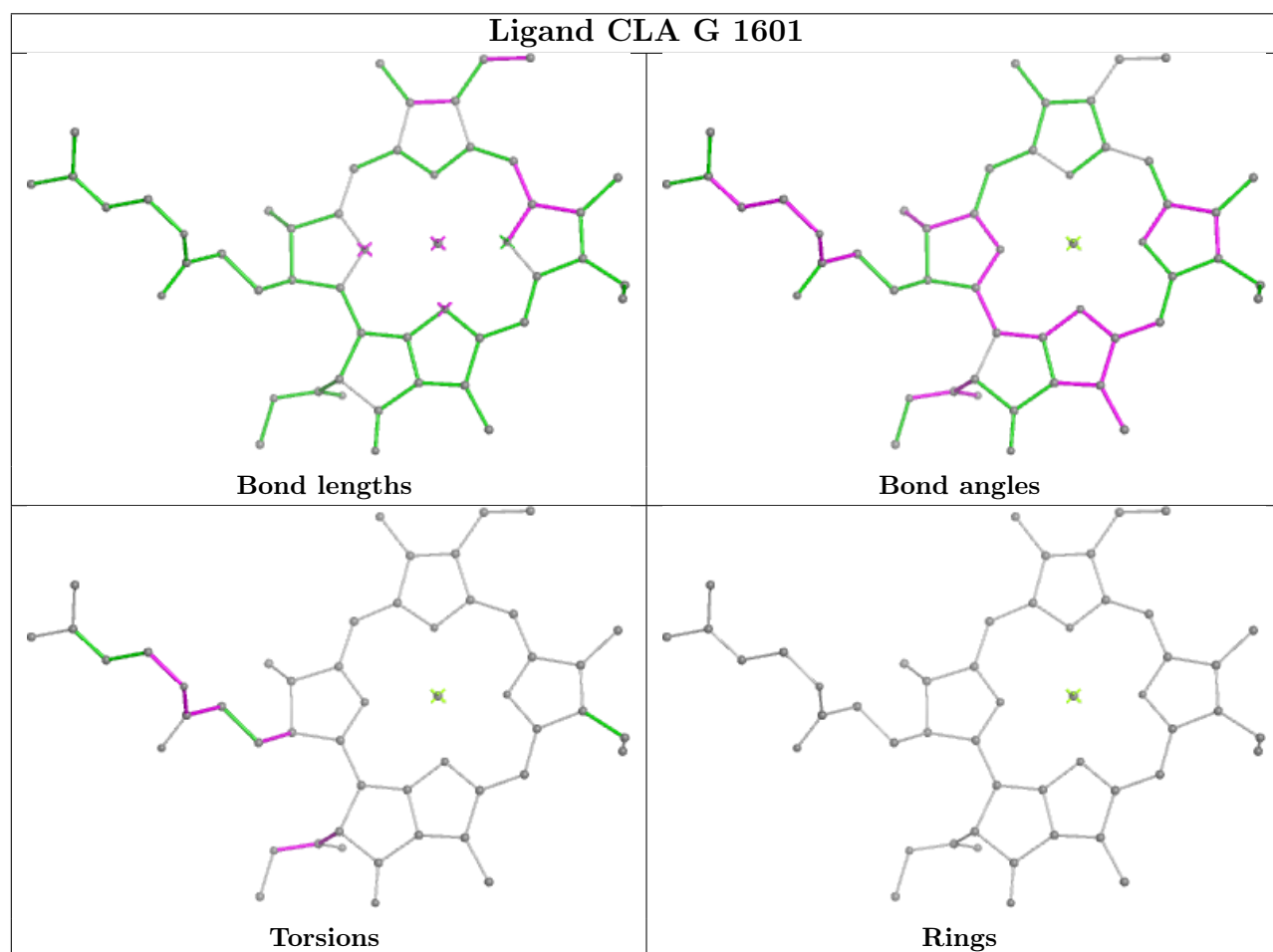
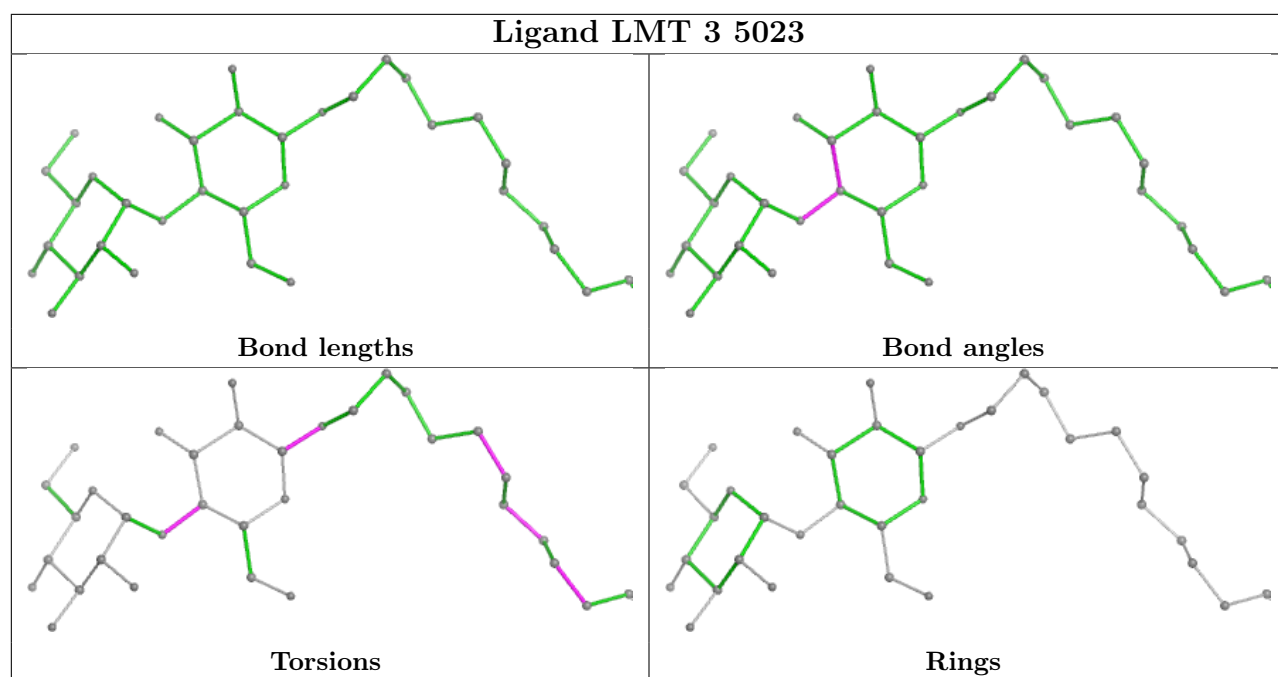


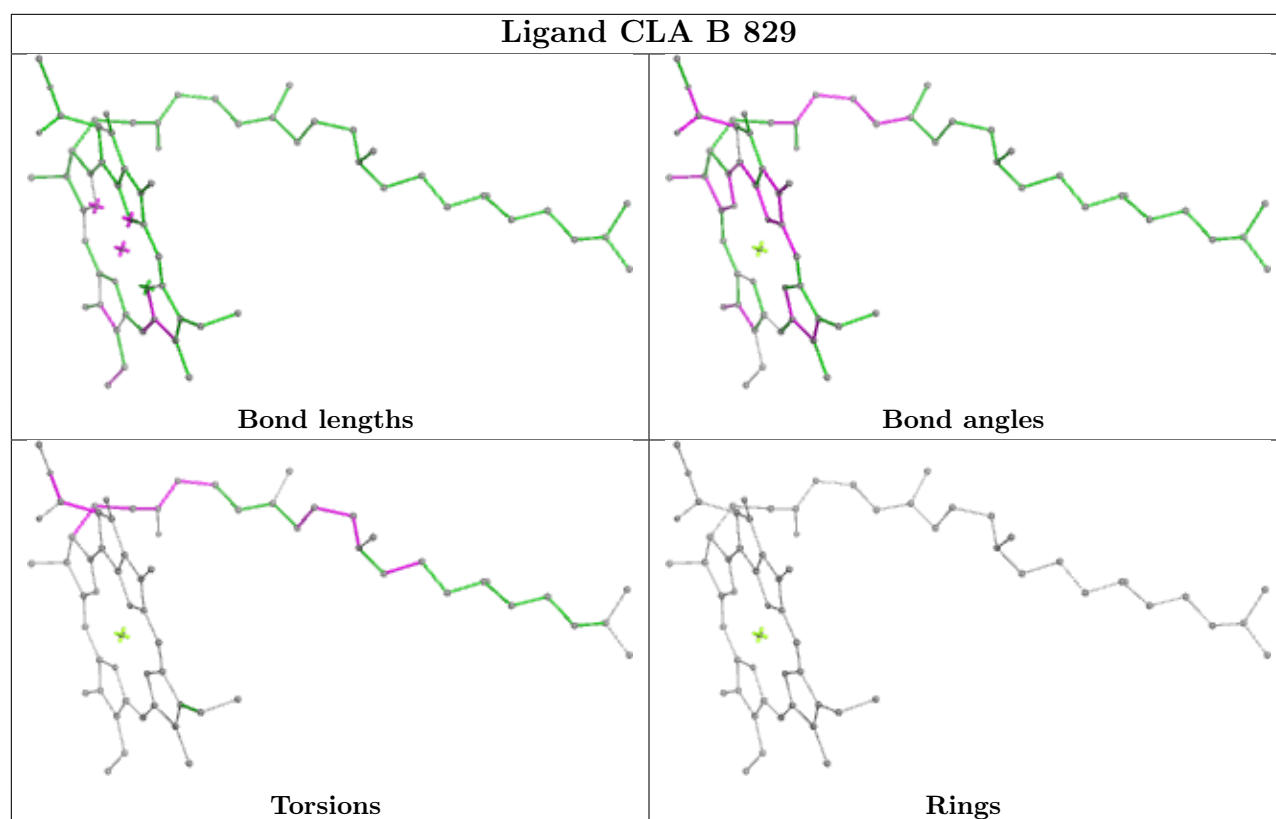
Torsions



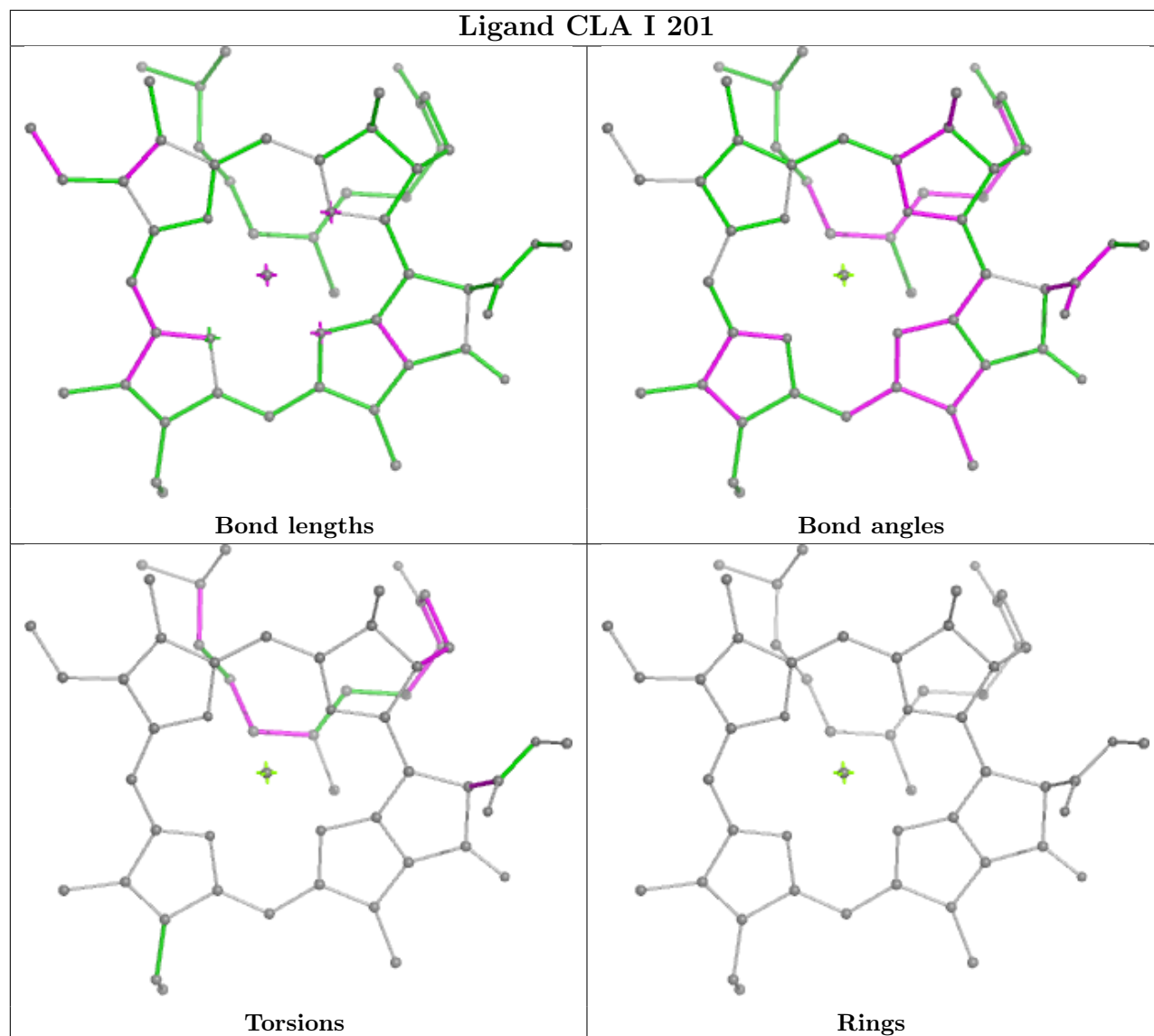
Rings



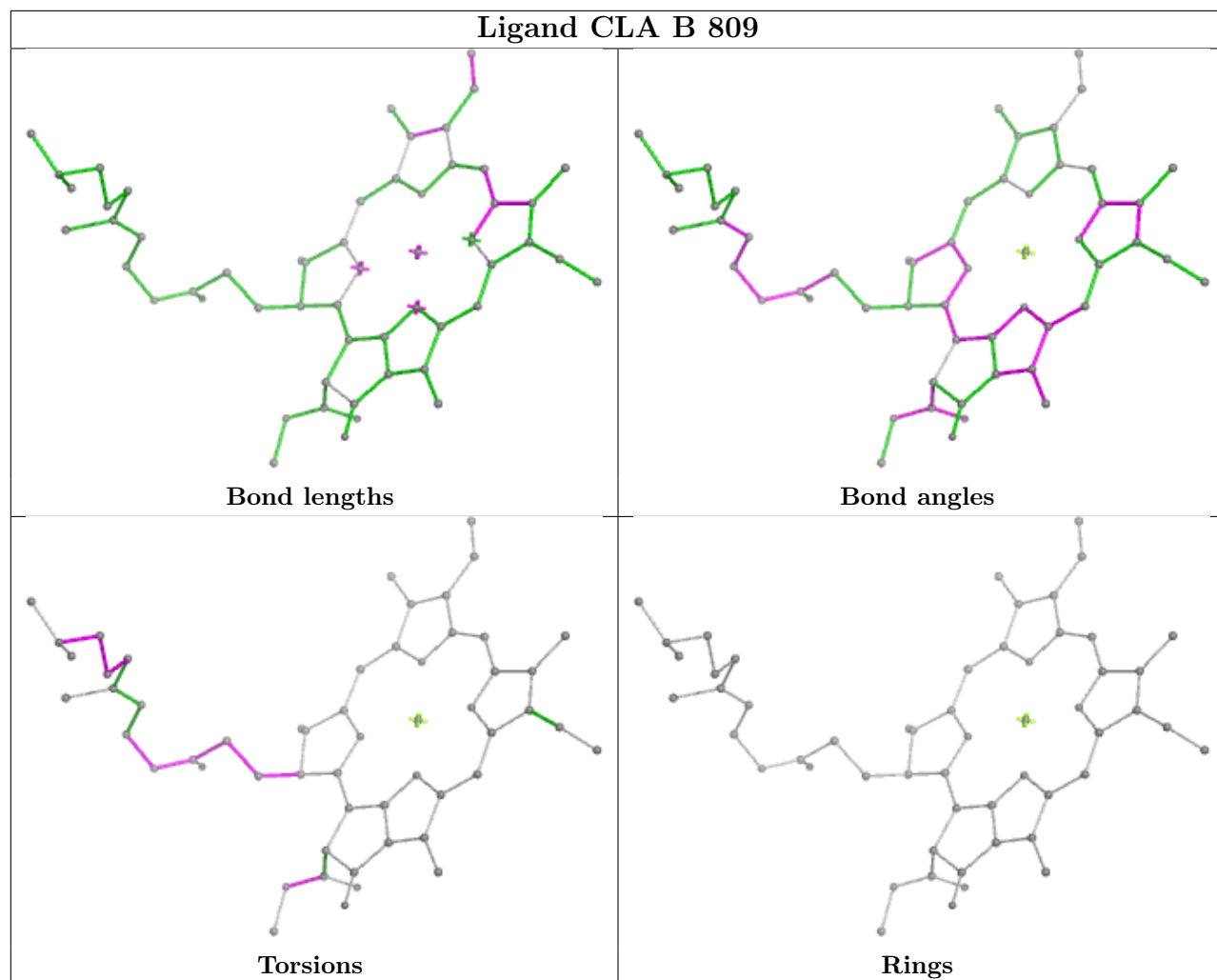




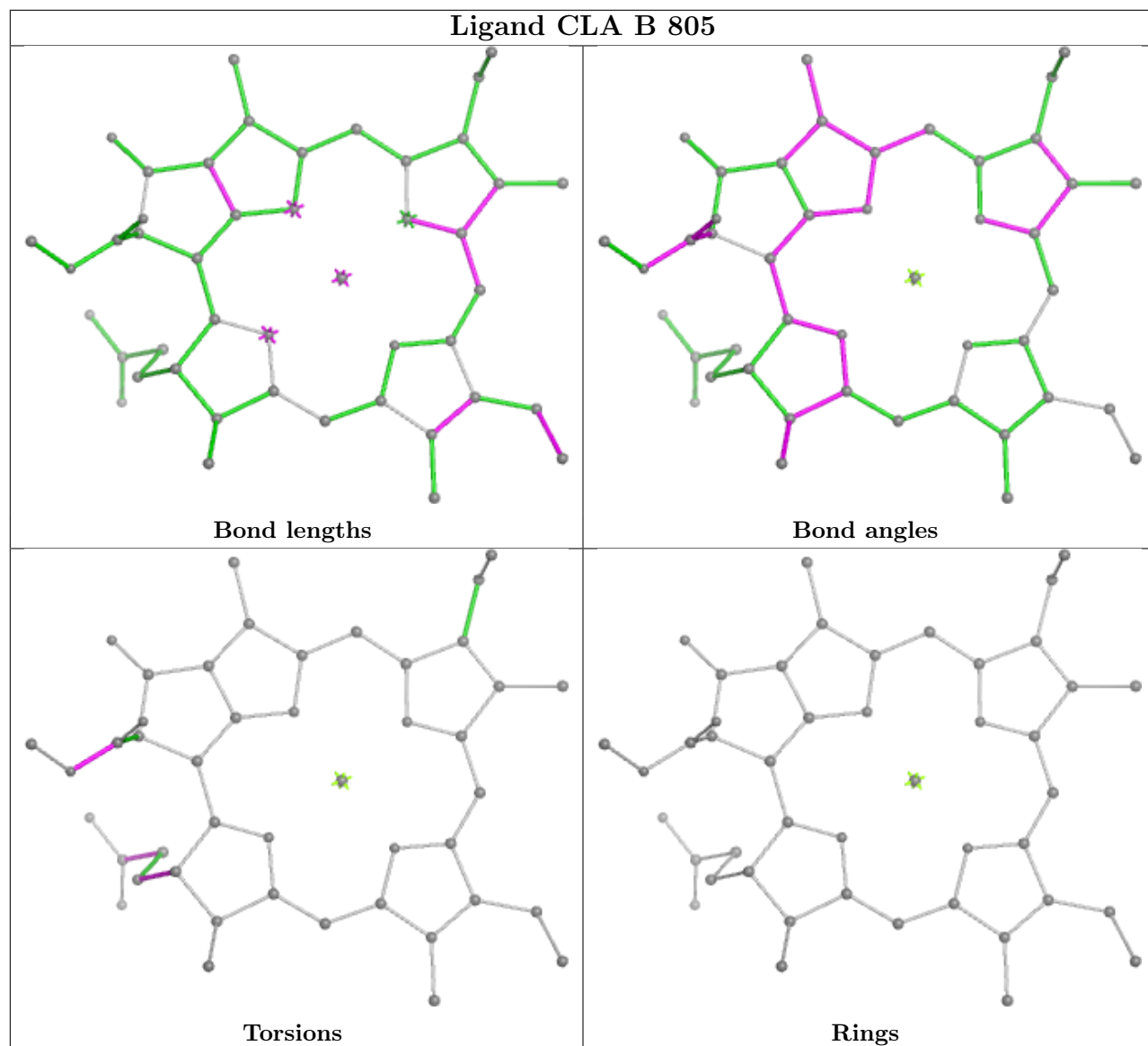
Ligand CLA I 201



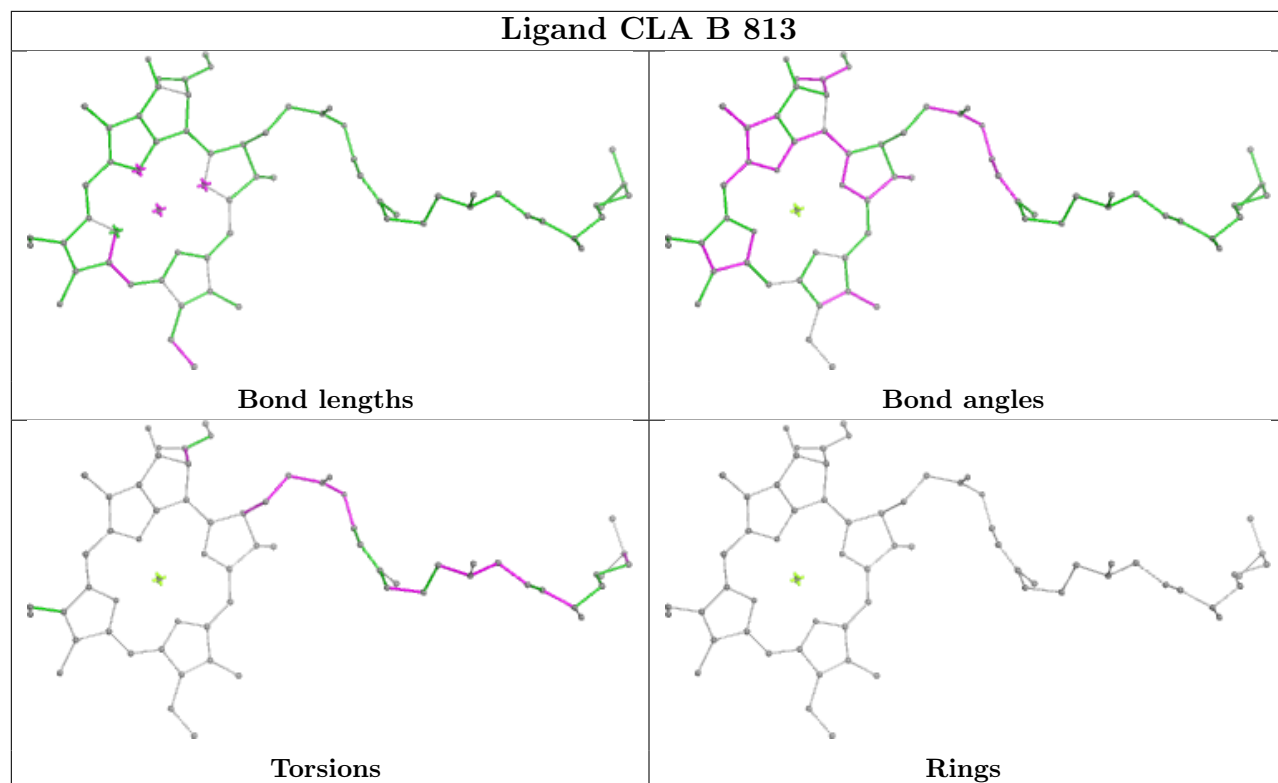
Ligand CLA B 809



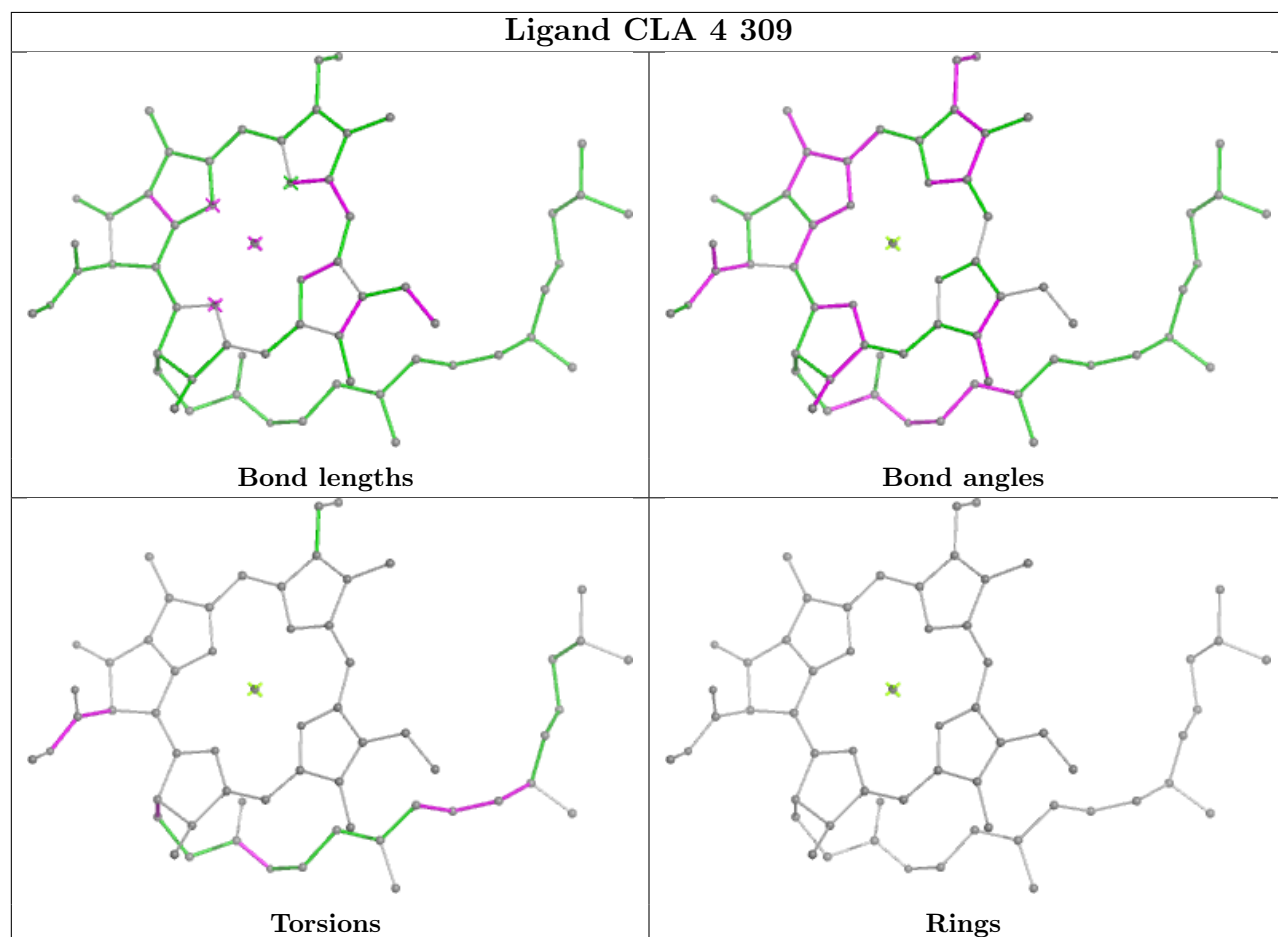
Ligand CLA B 805



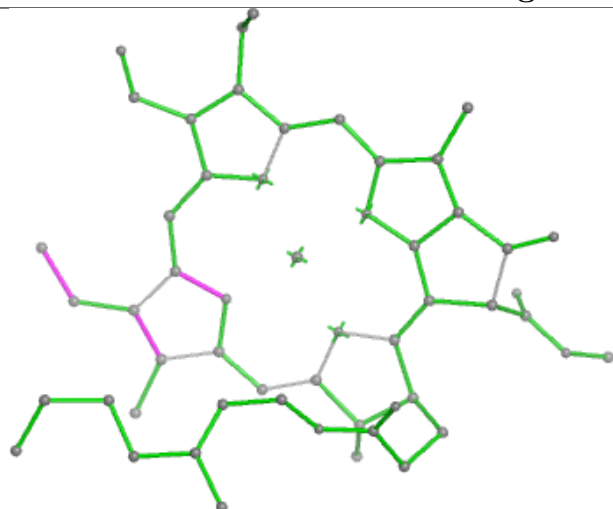
Ligand CLA B 813



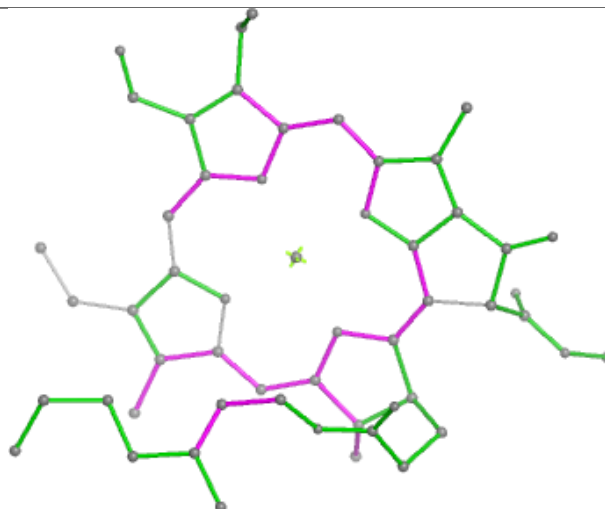
Ligand CLA 4 309



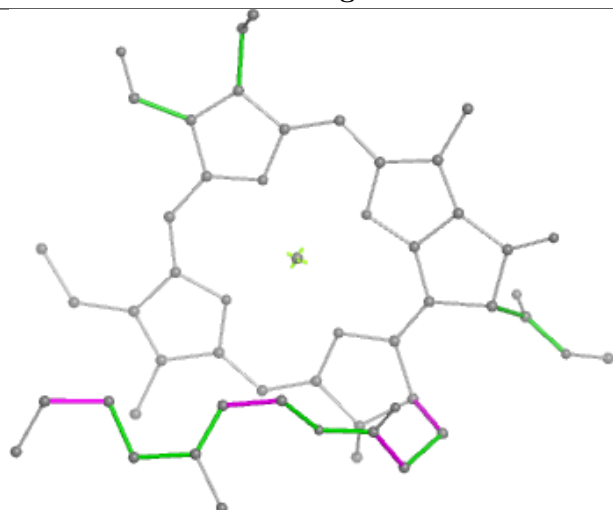
Ligand CHL 7 315



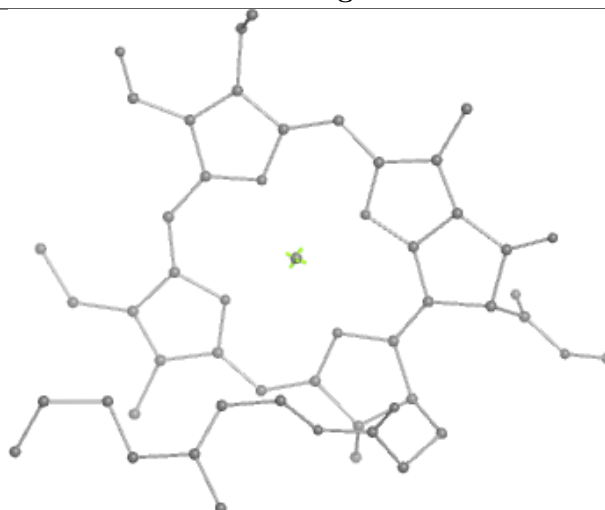
Bond lengths



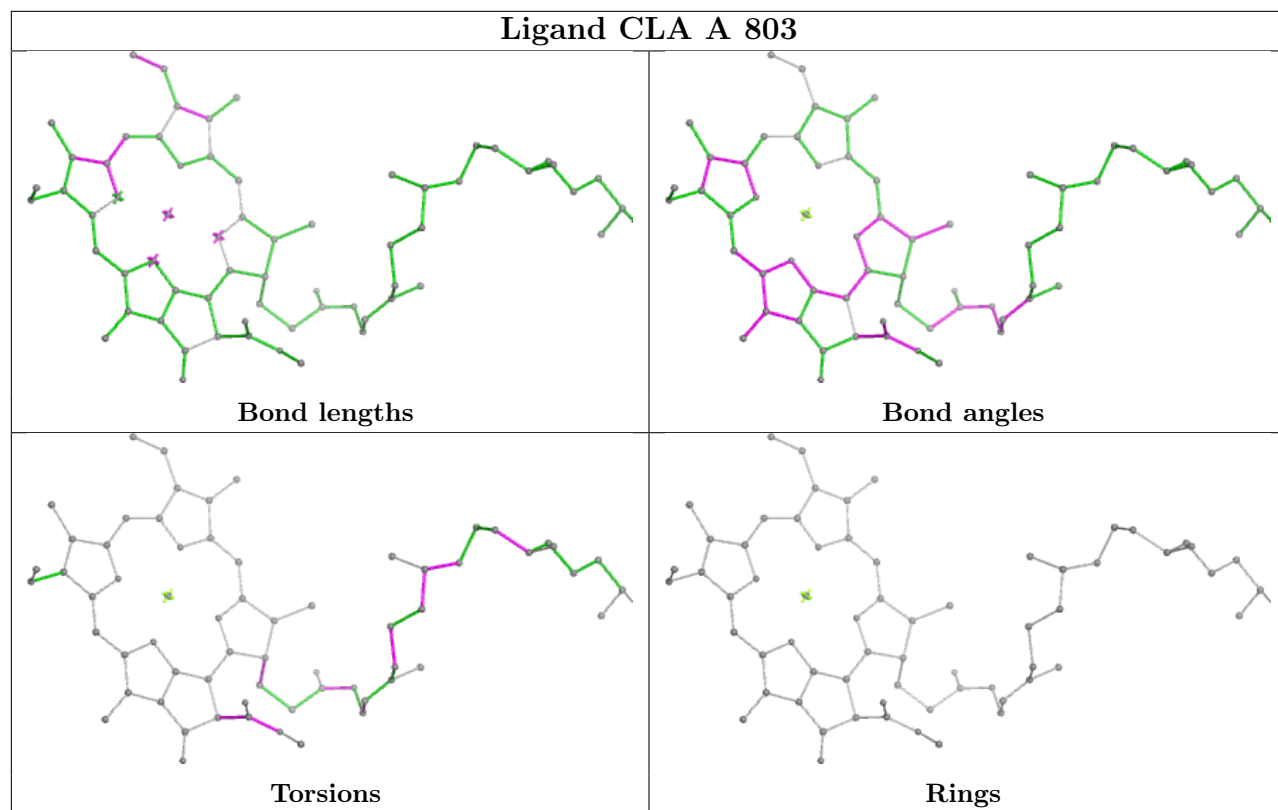
Bond angles



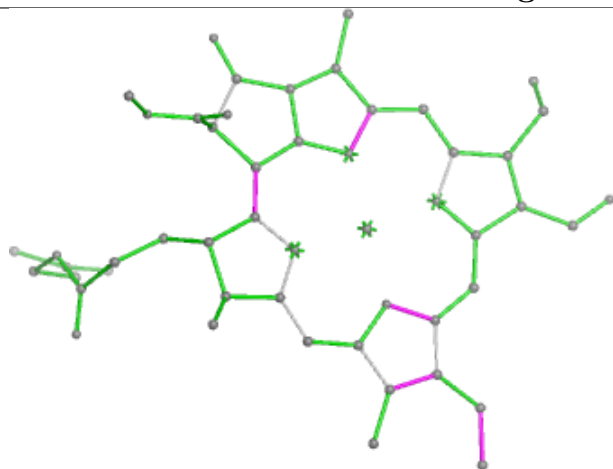
Torsions



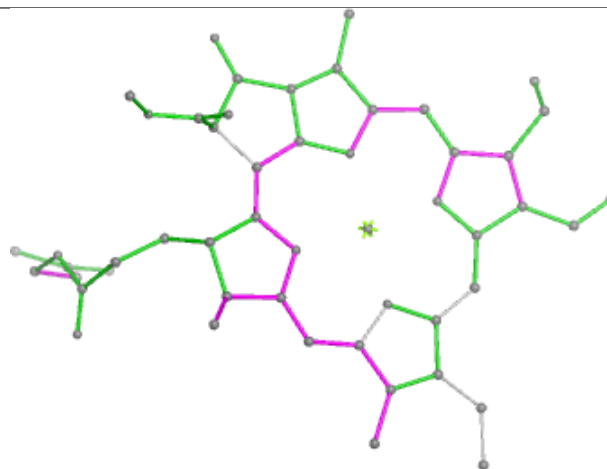
Rings



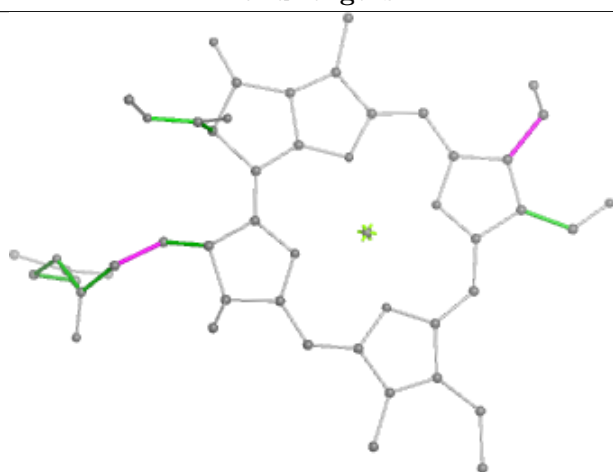
Ligand CHL 5 318



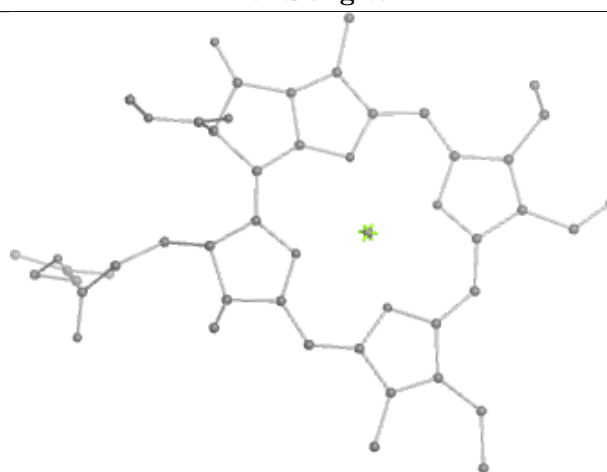
Bond lengths



Bond angles

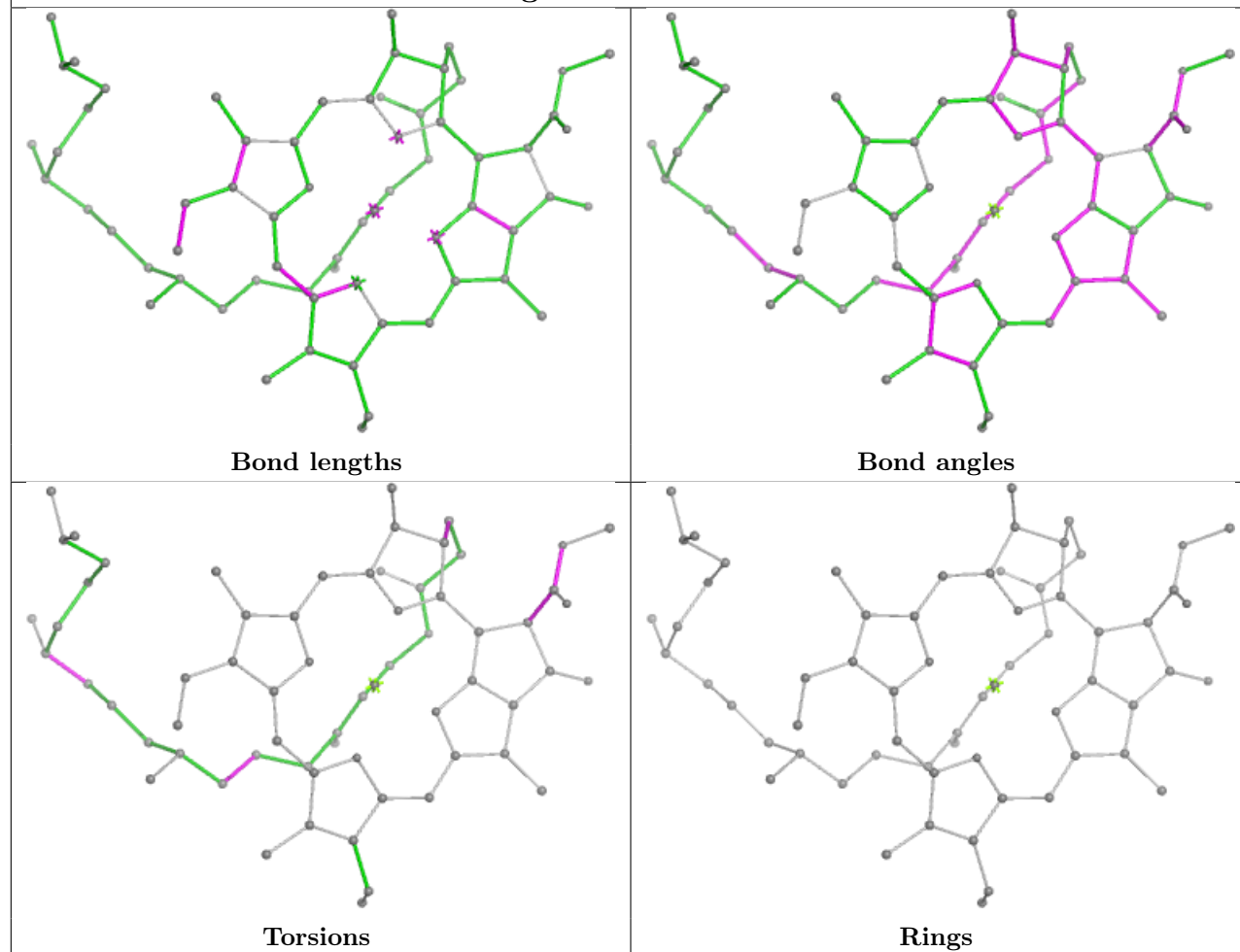


Torsions

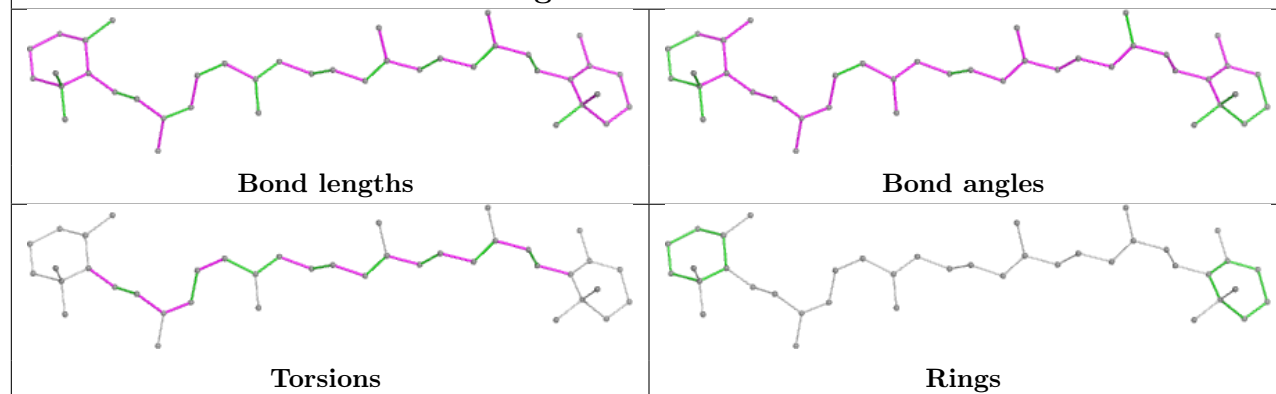


Rings

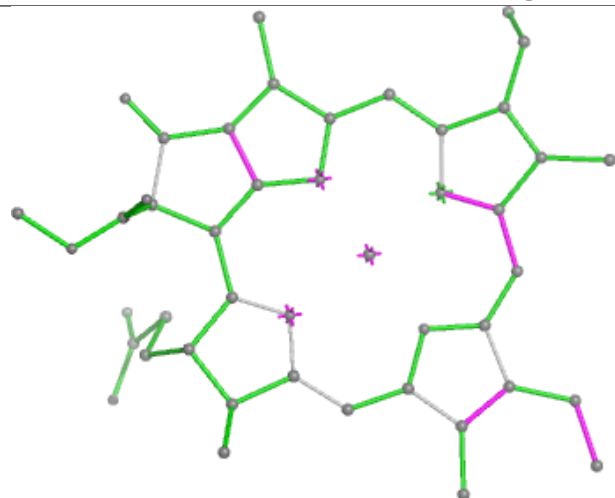
Ligand CLA 8 309



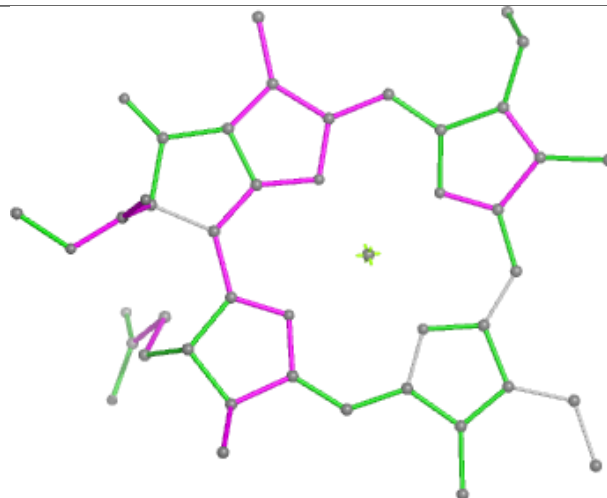
Ligand BCR 8 303



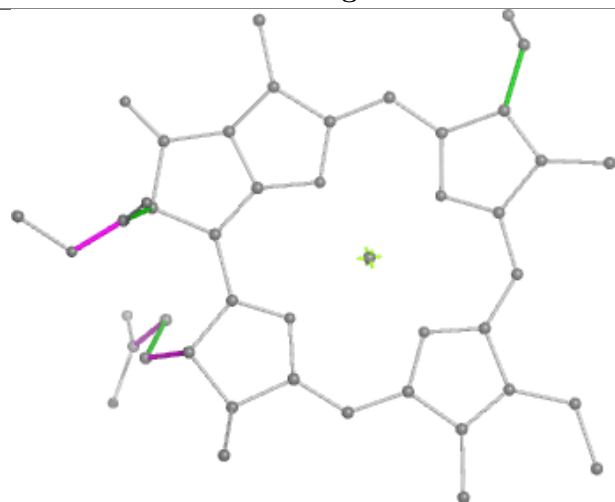
Ligand CLA 5 313



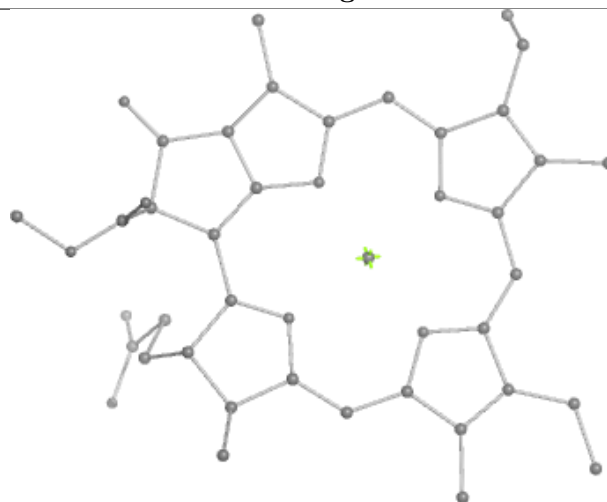
Bond lengths



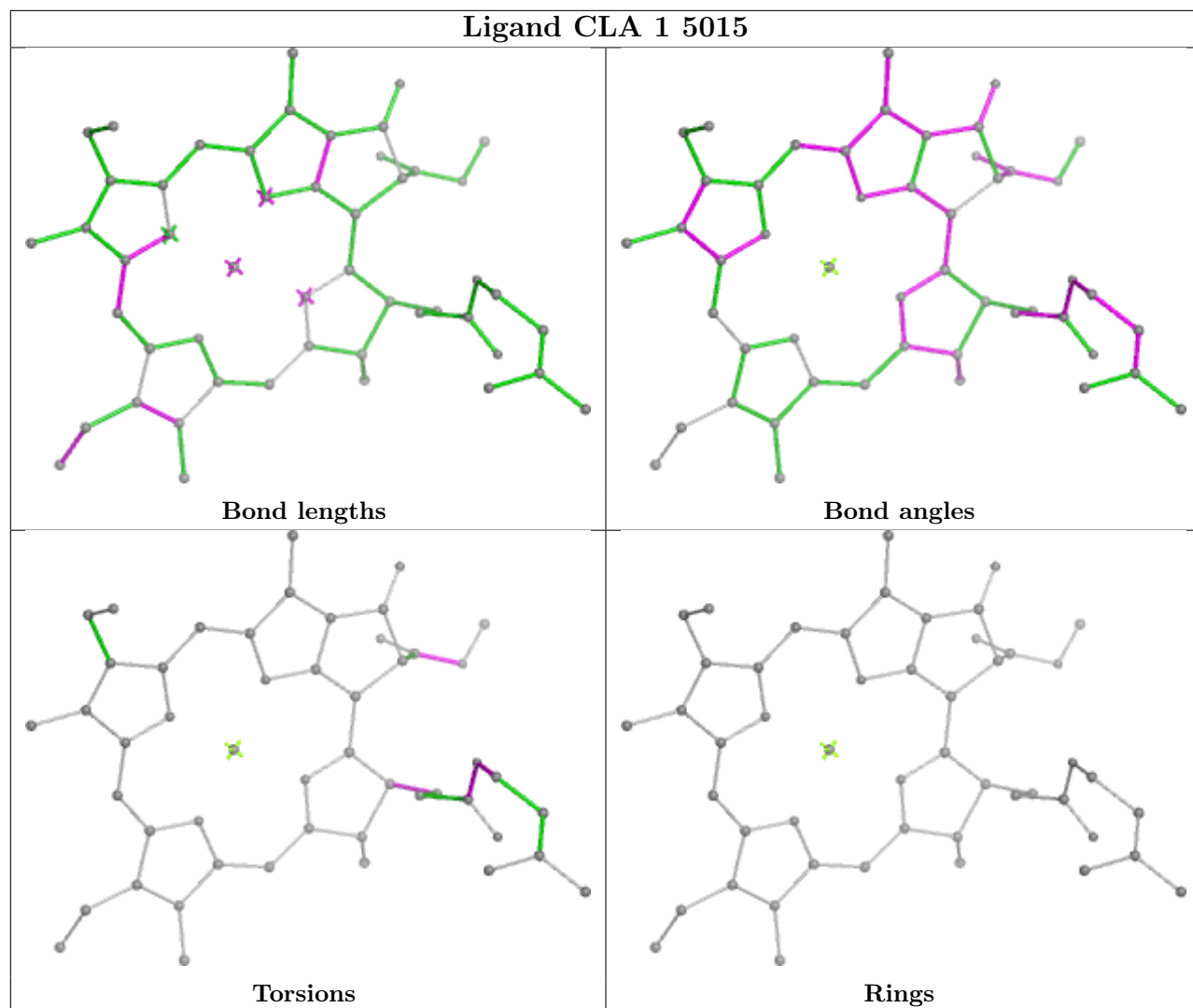
Bond angles



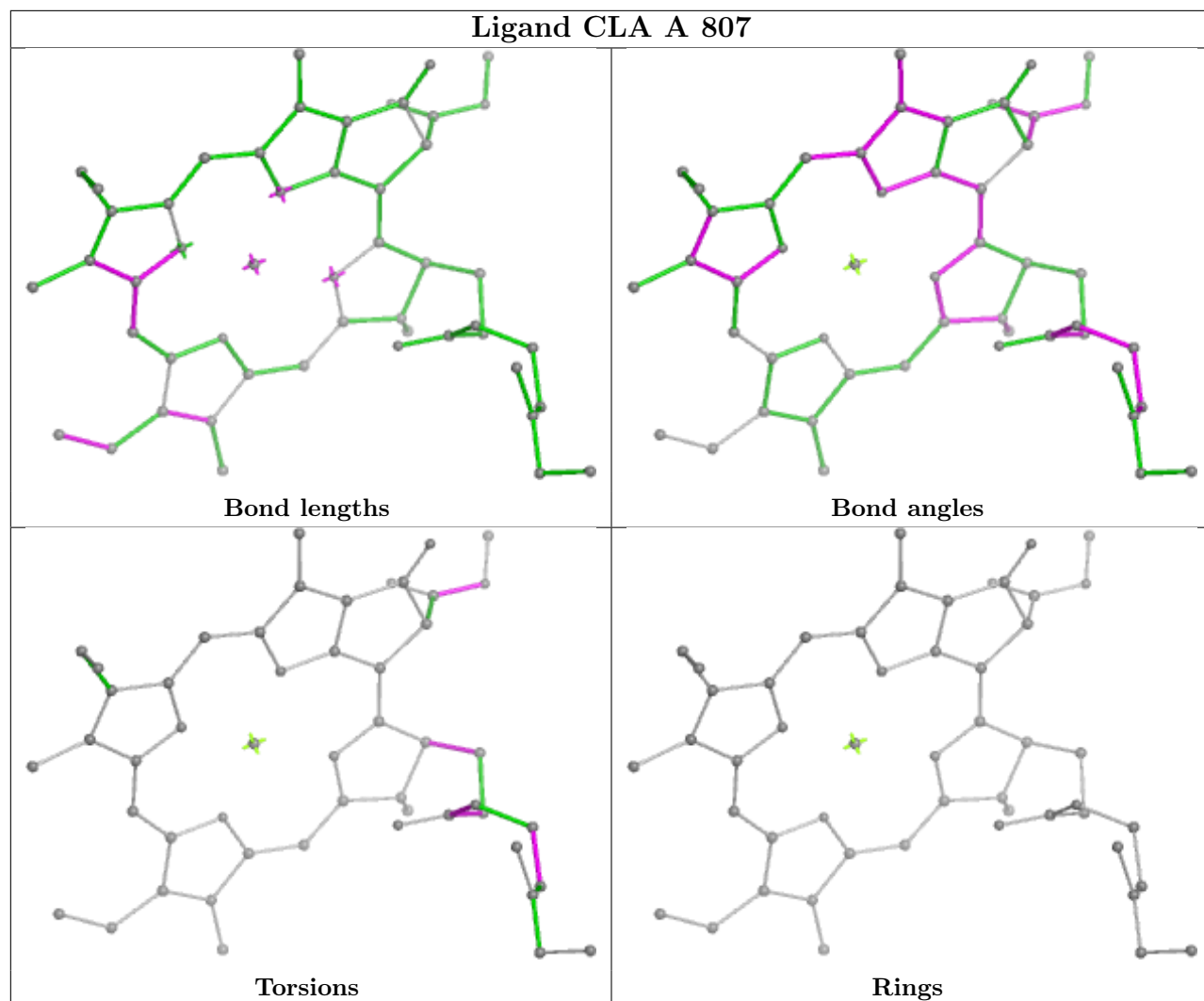
Torsions

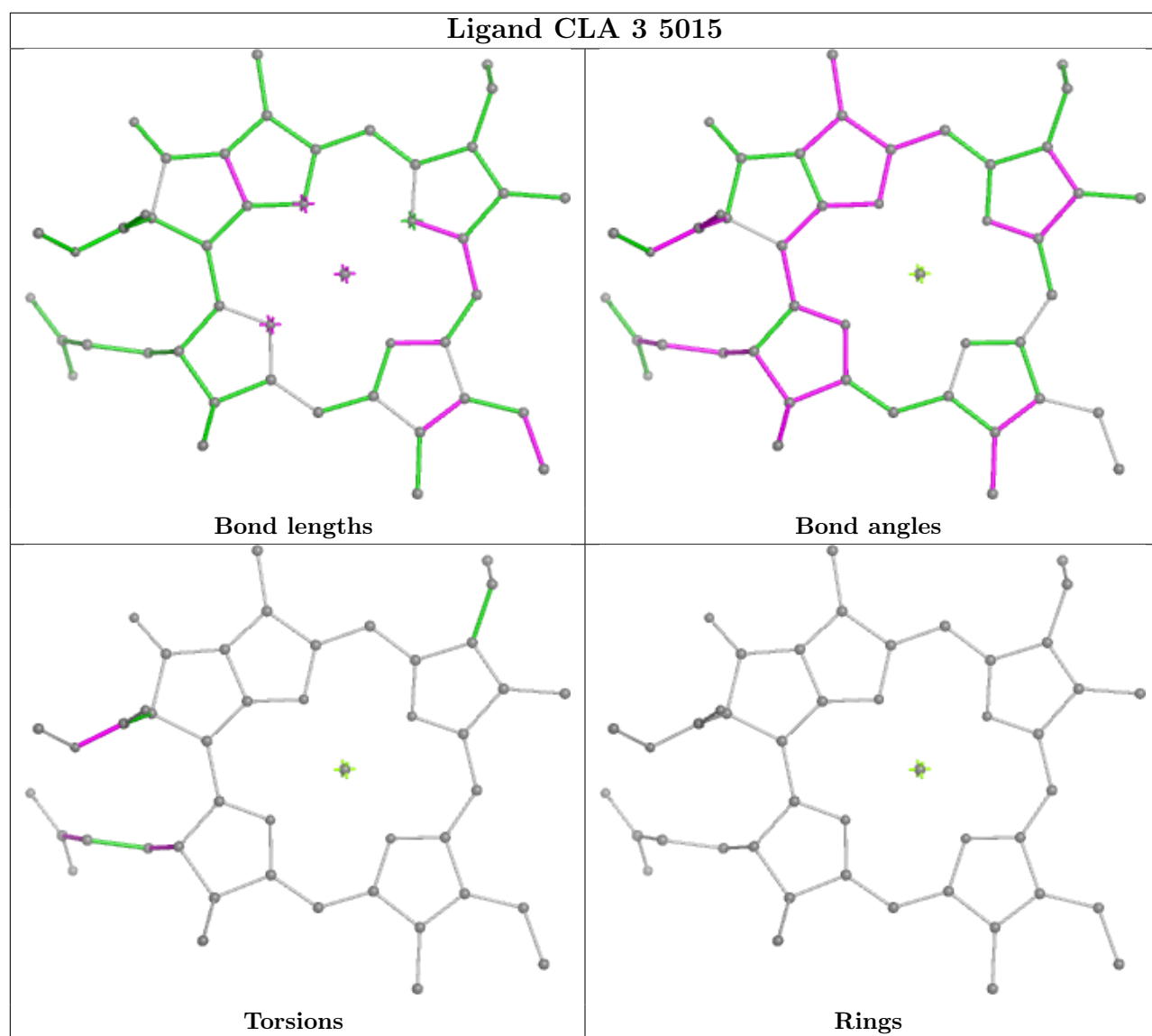


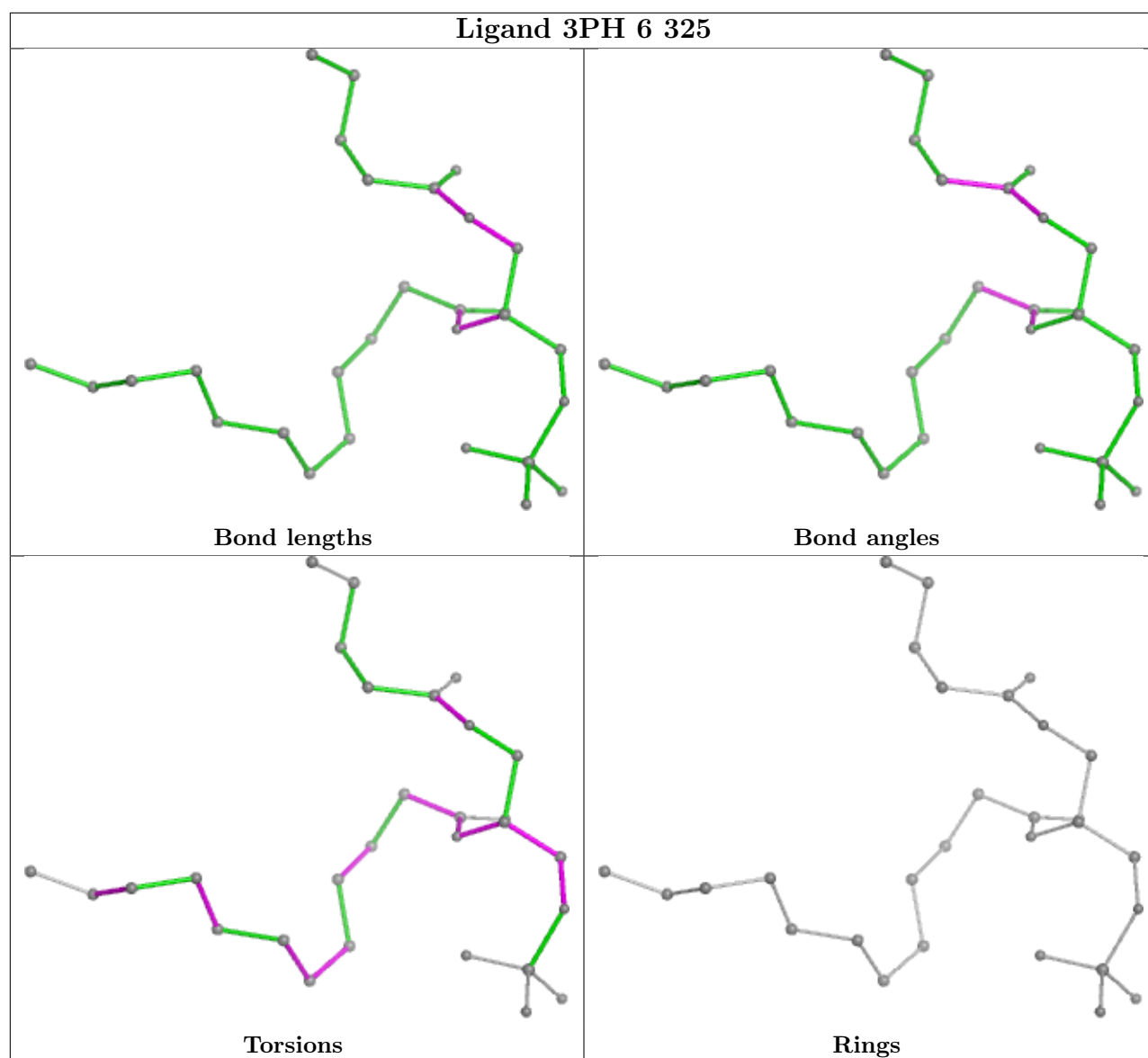
Rings

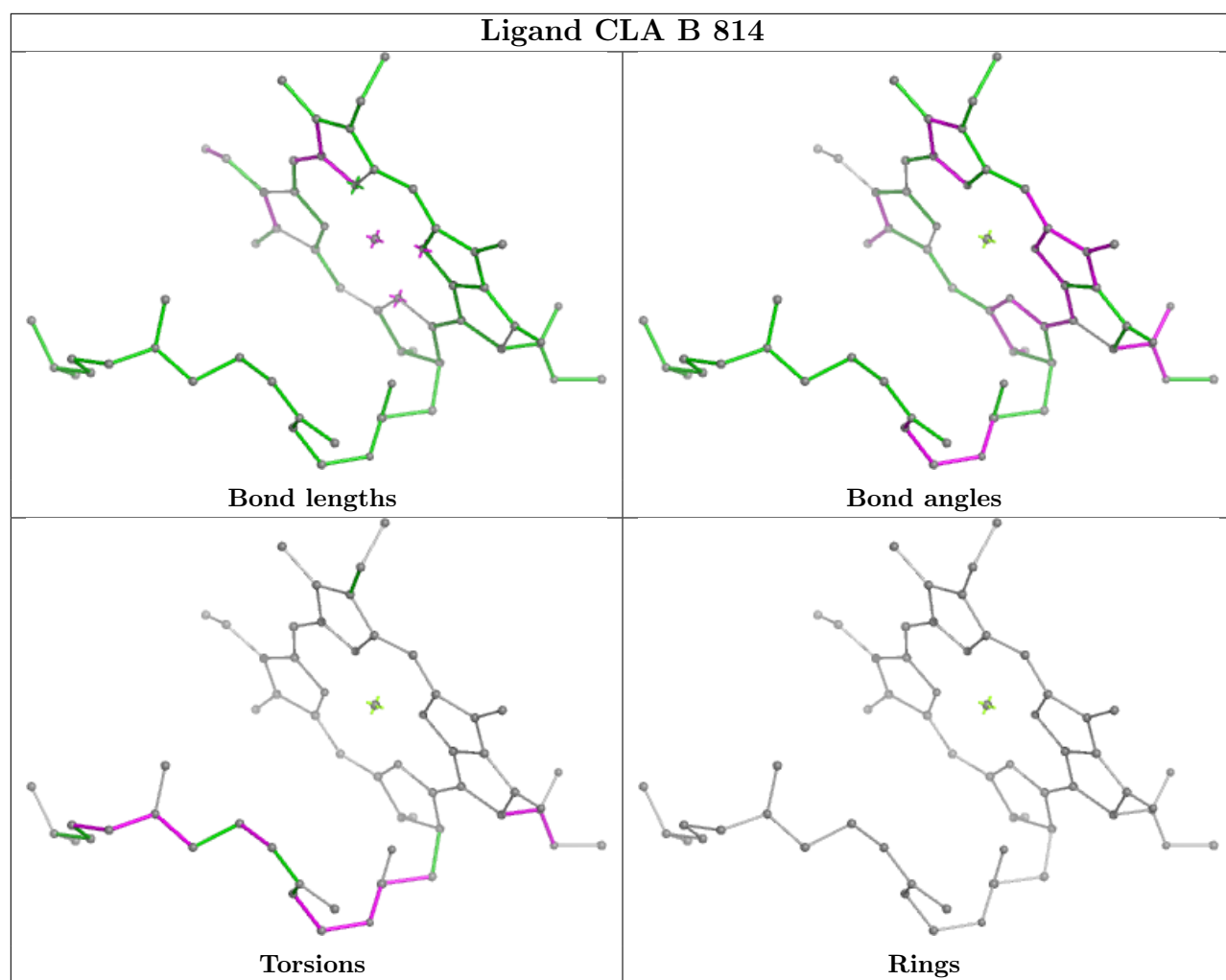


Ligand CLA A 807

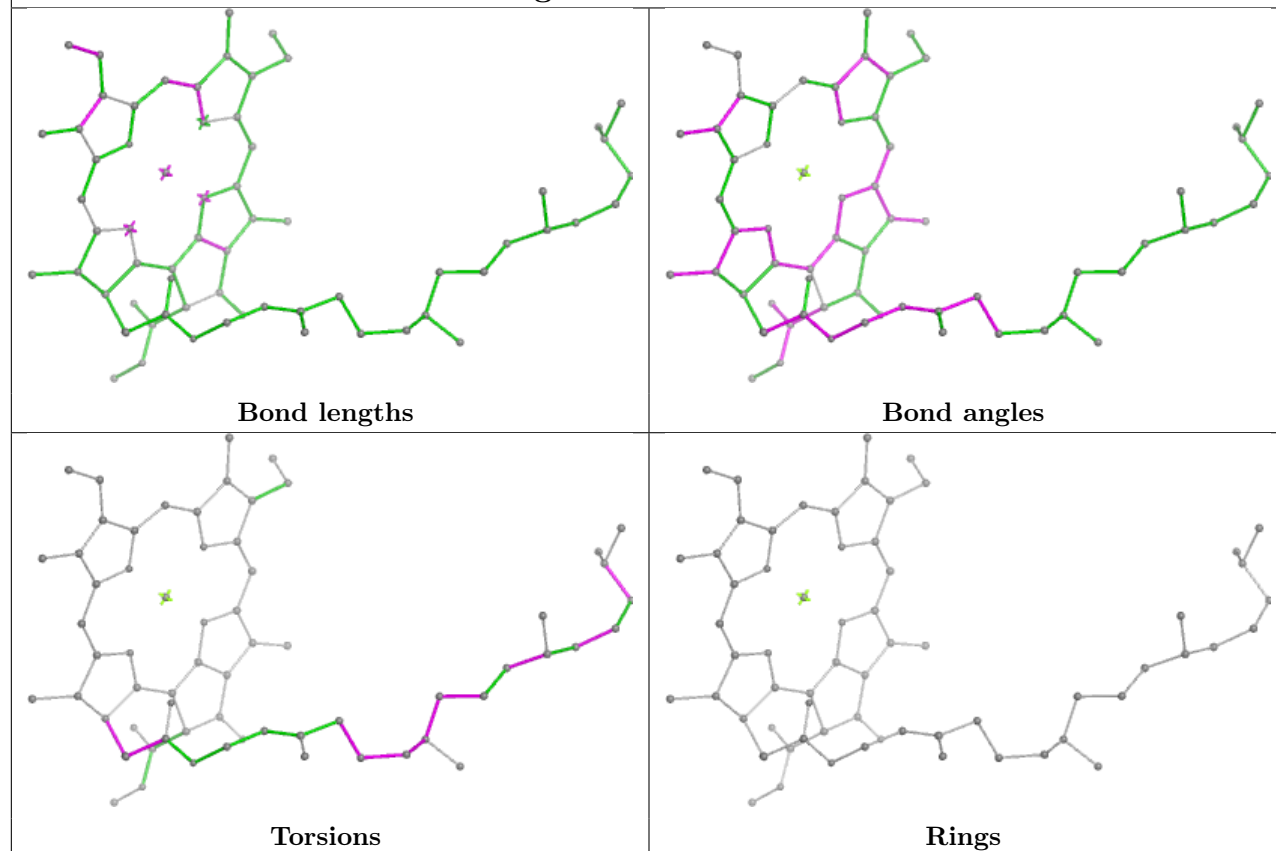




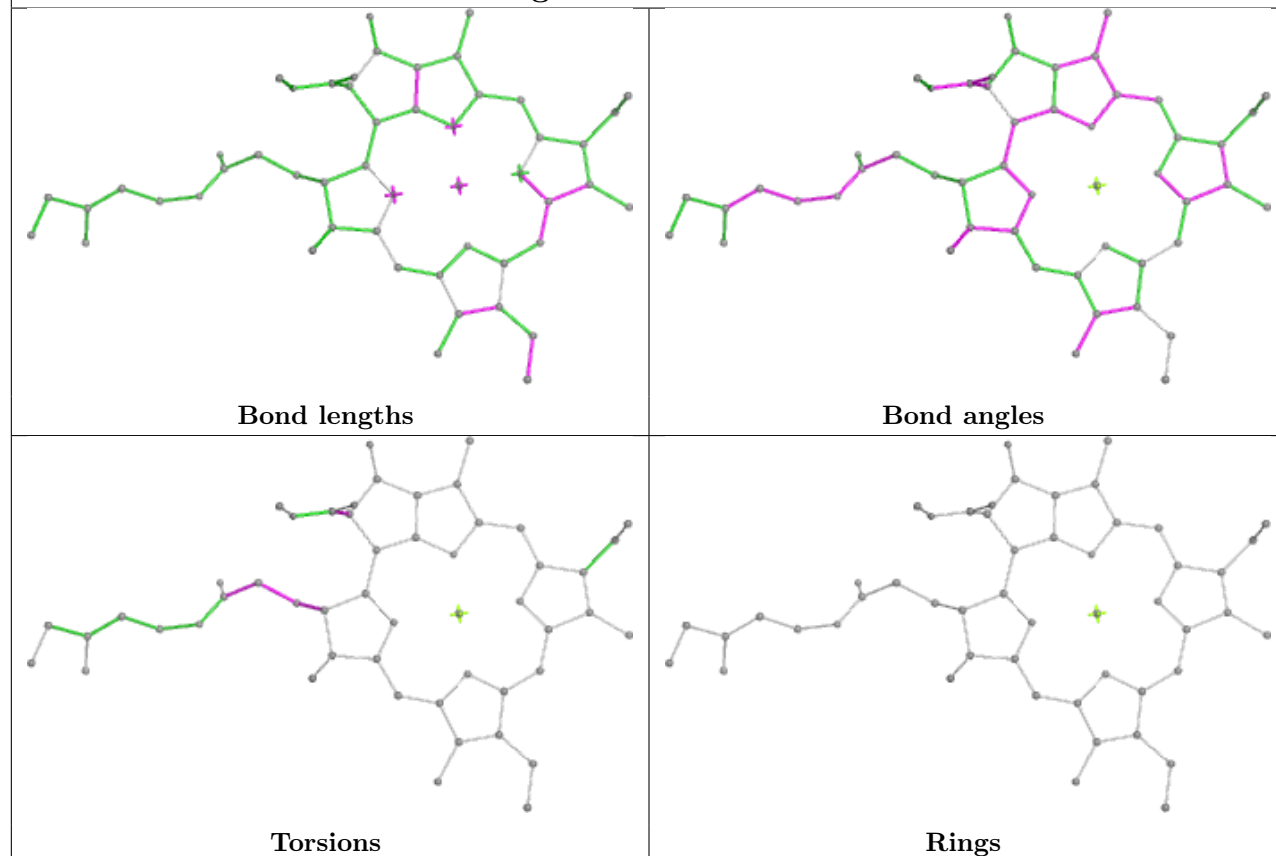


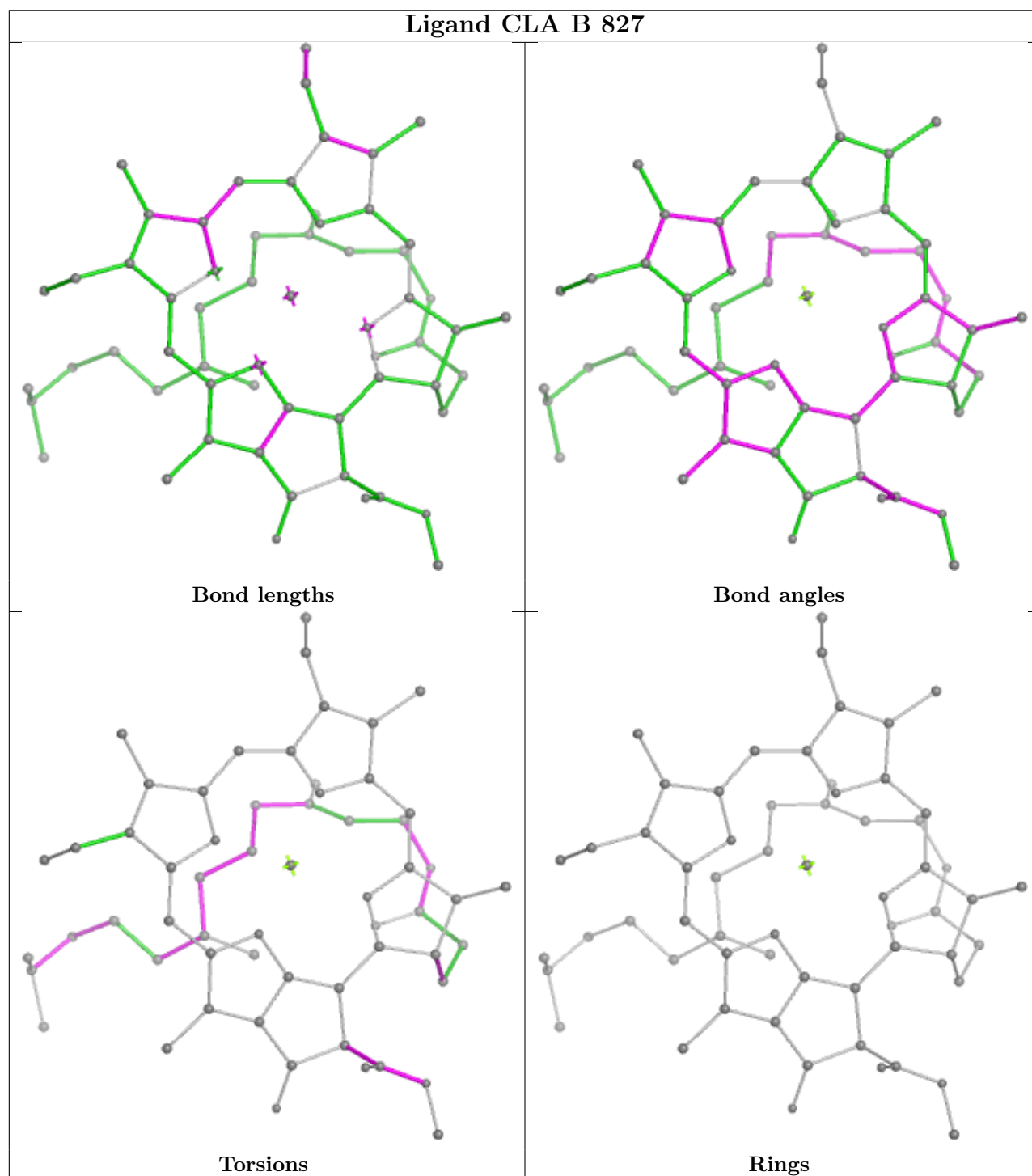
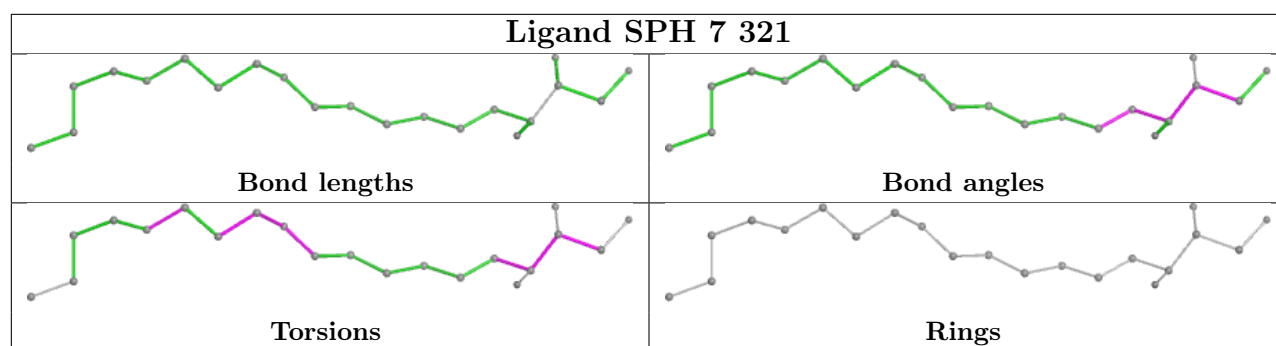


Ligand CLA Z 312

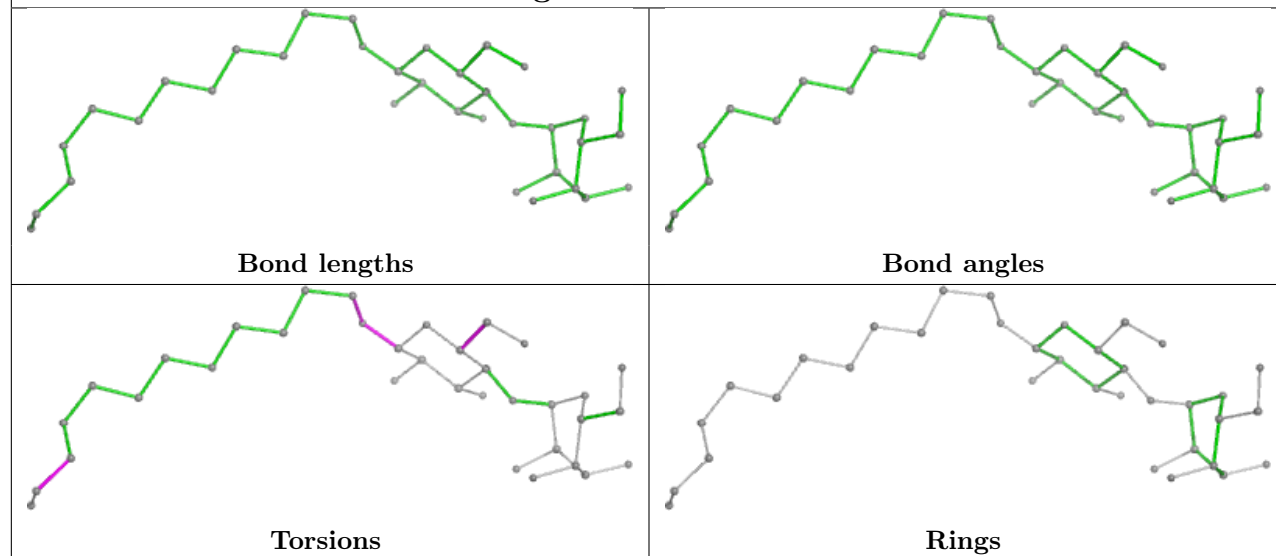


Ligand CLA A 837

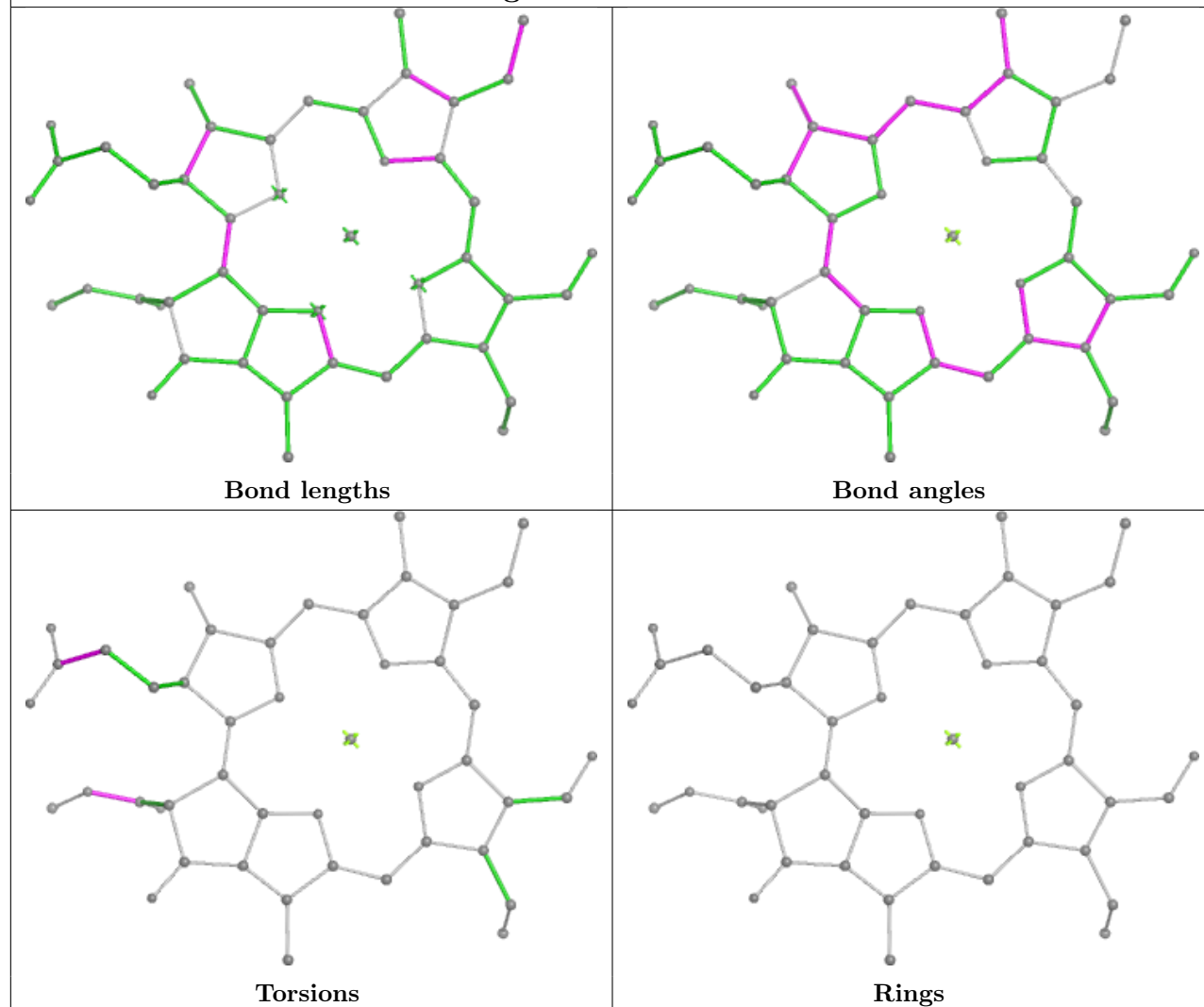


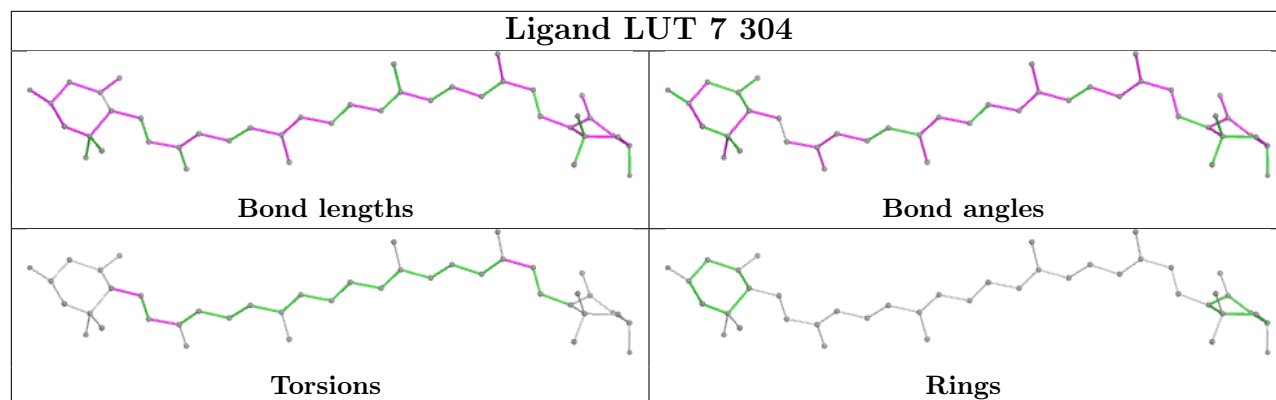
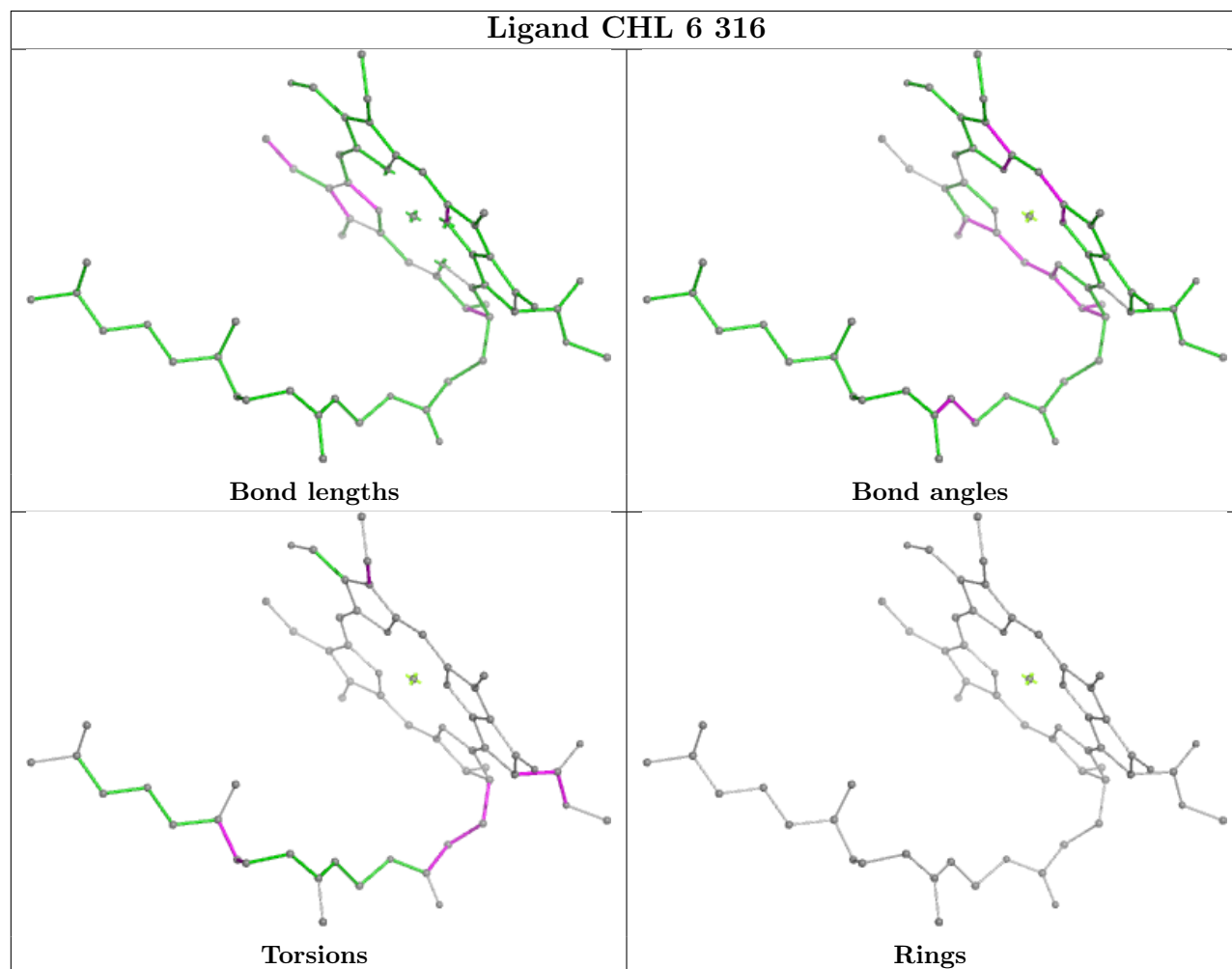


Ligand LMT 7 323

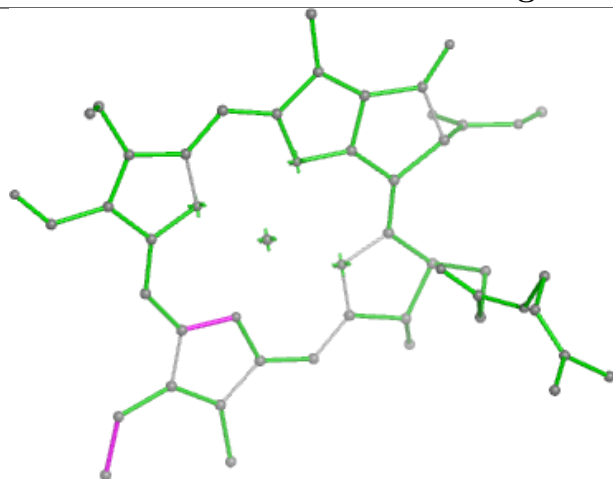


Ligand CHL Z 313

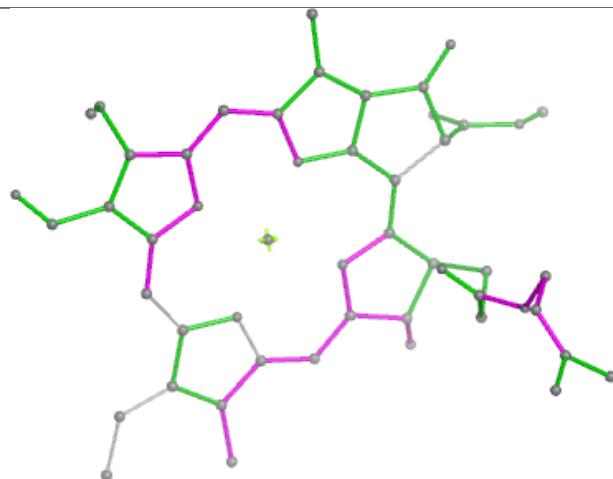


Ligand LUT 7 304**Ligand CHL 6 316**

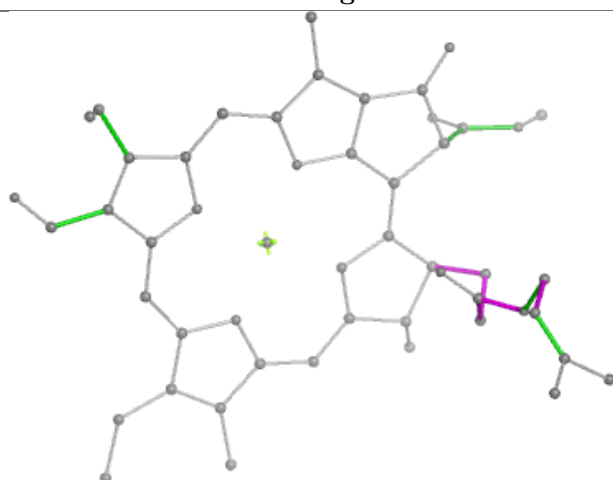
Ligand CHL 4 315



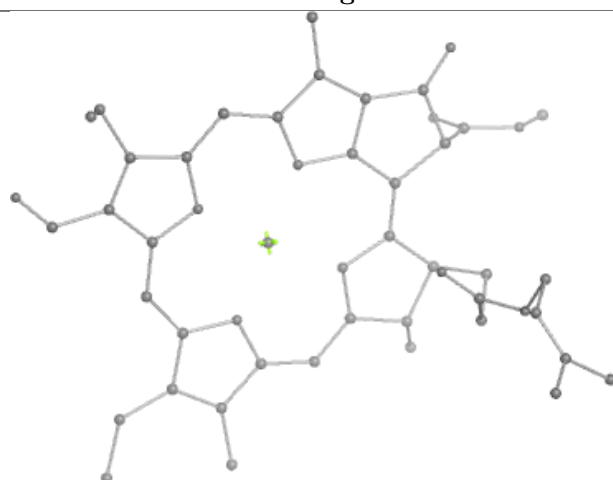
Bond lengths



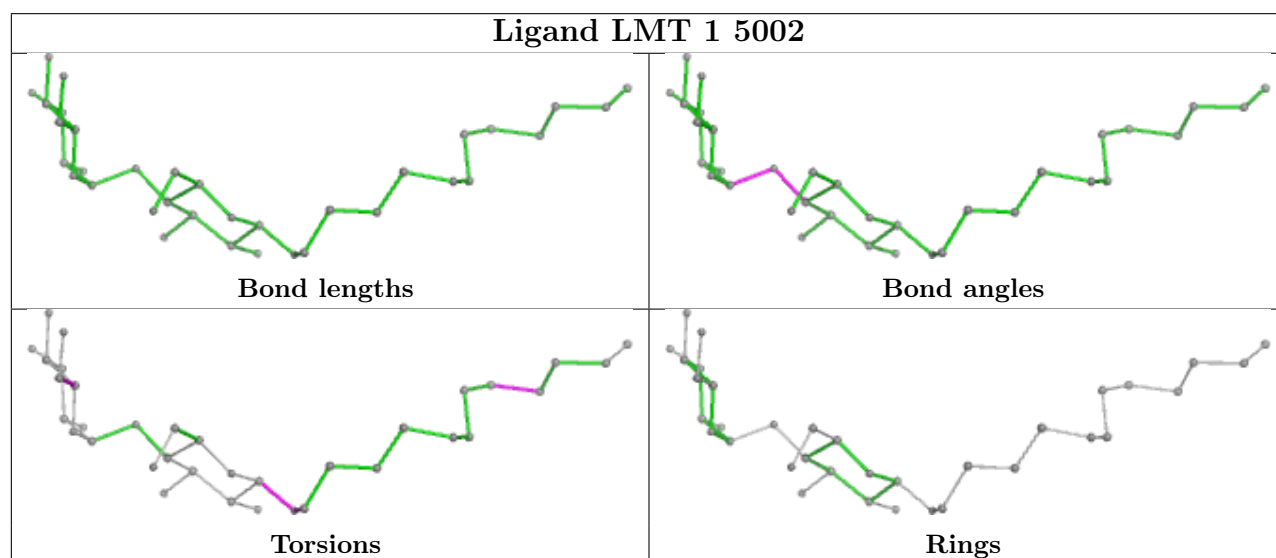
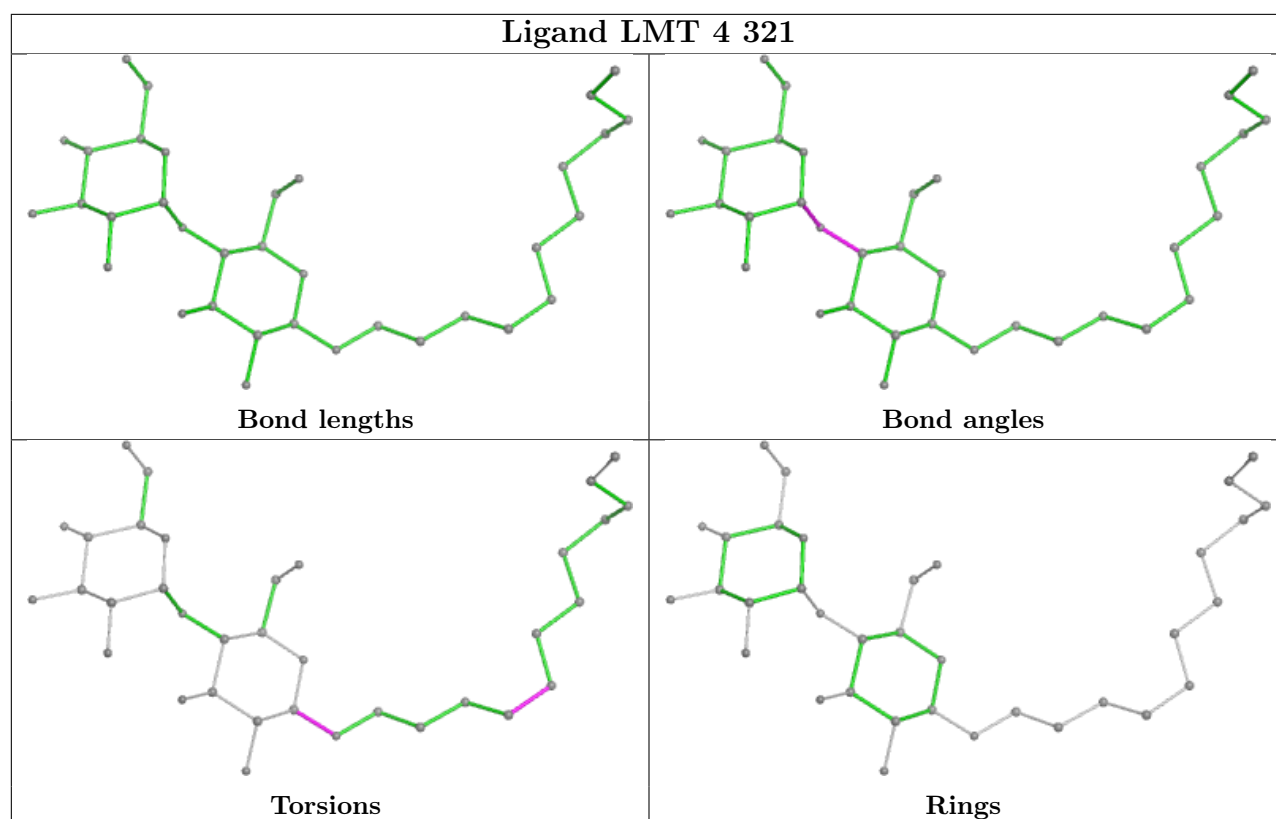
Bond angles



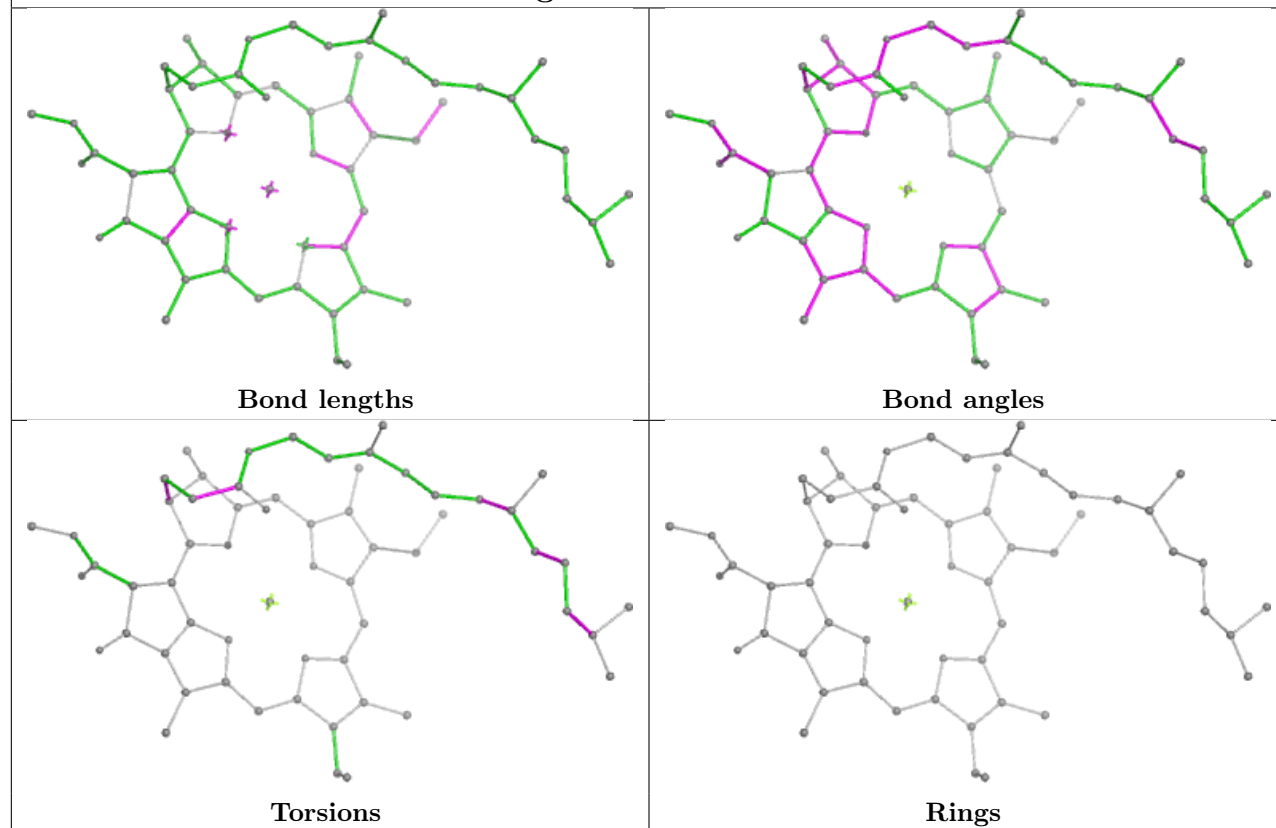
Torsions



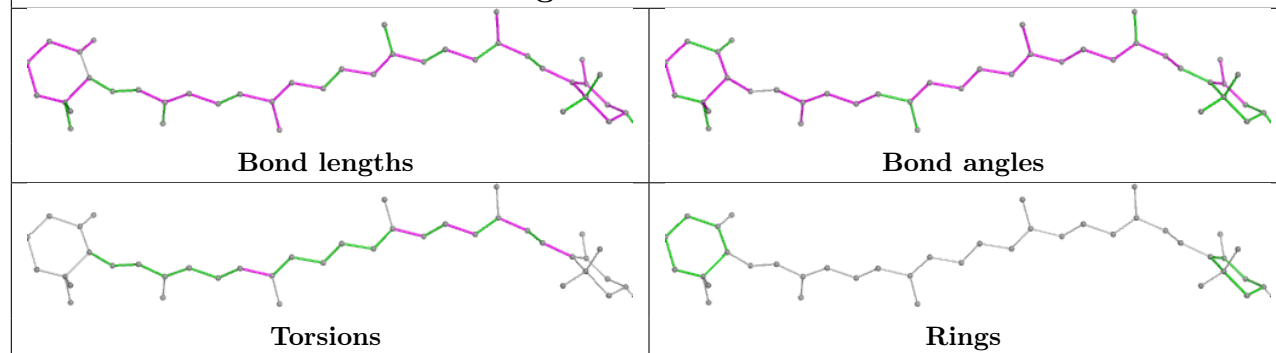
Rings



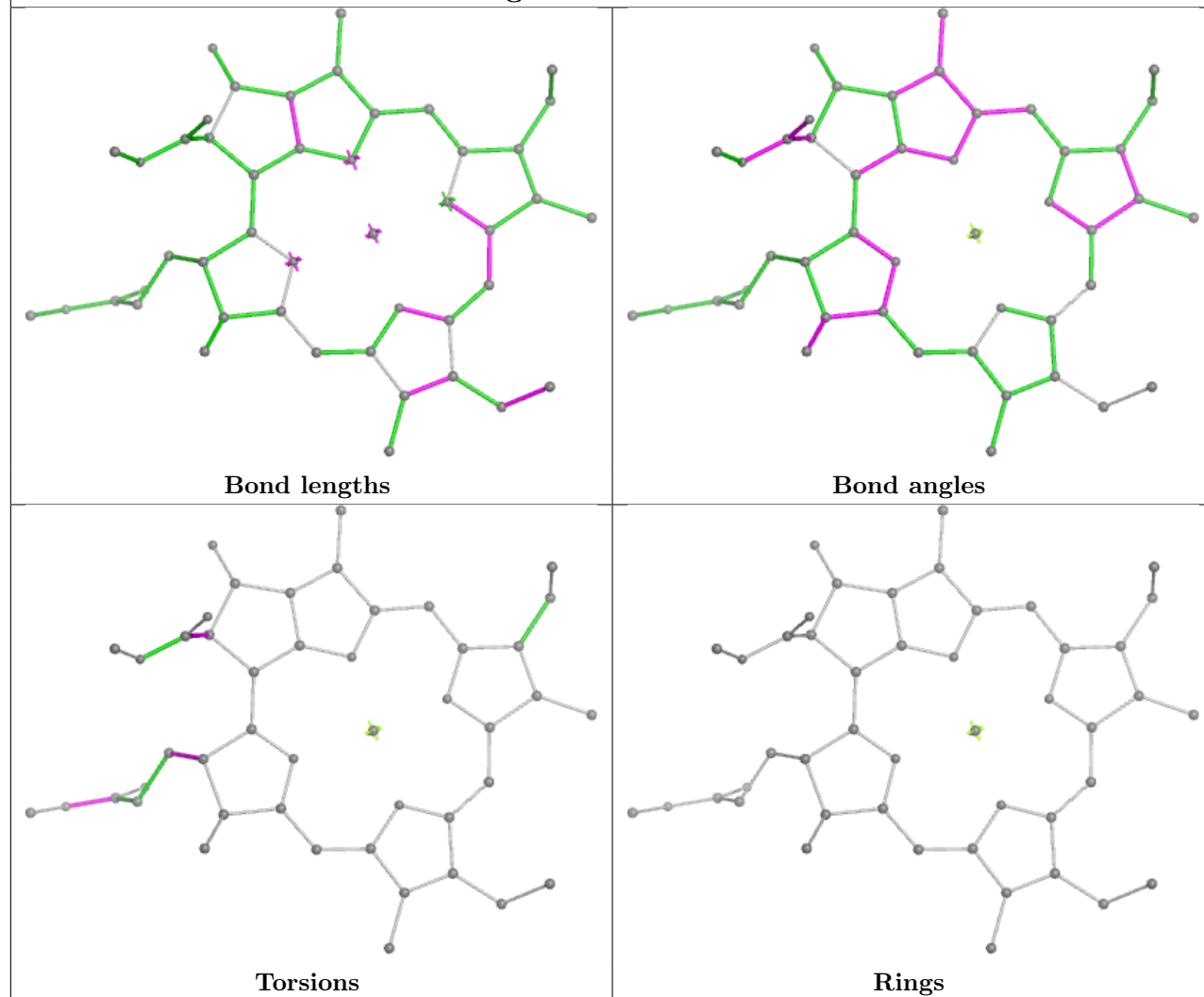
Ligand CLA 6 309



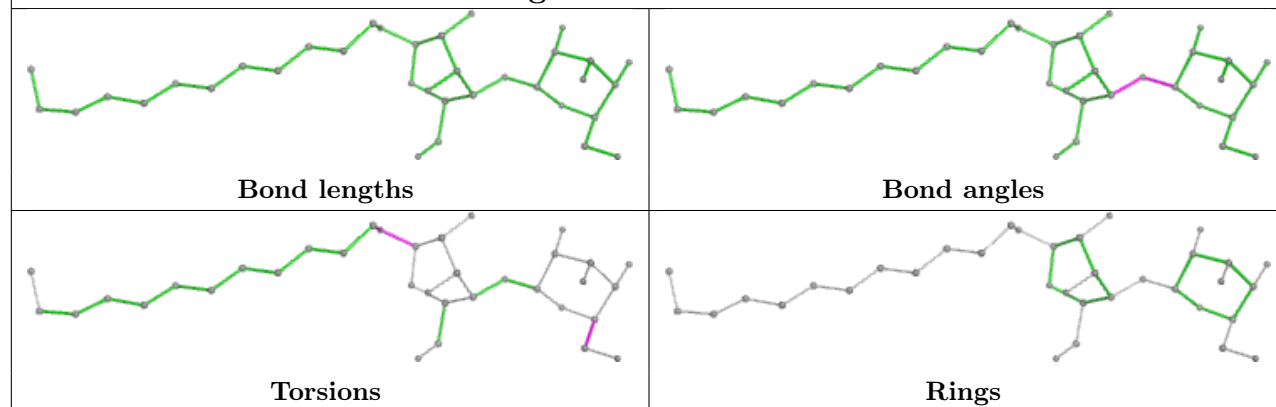
Ligand LUT 5 303

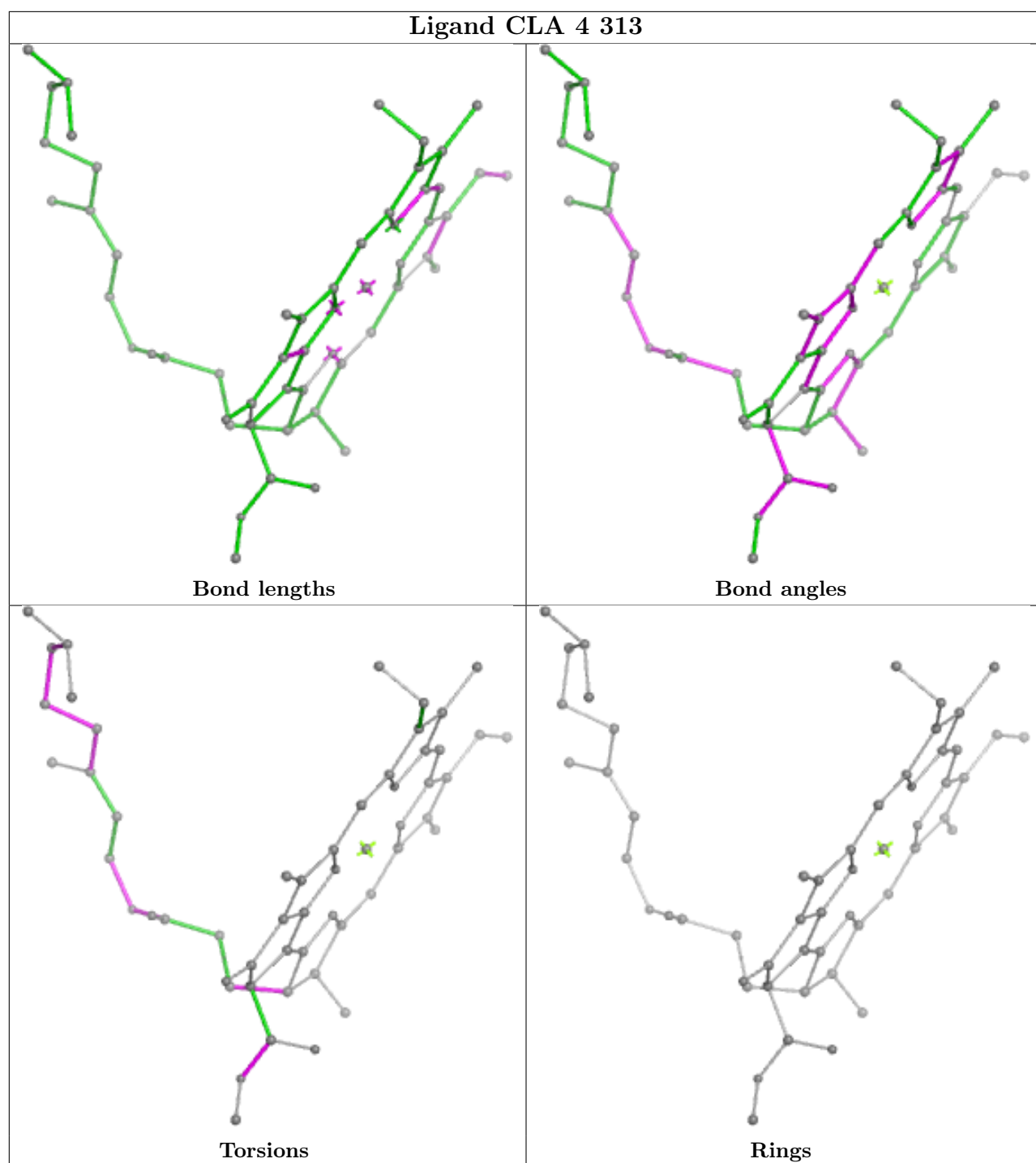


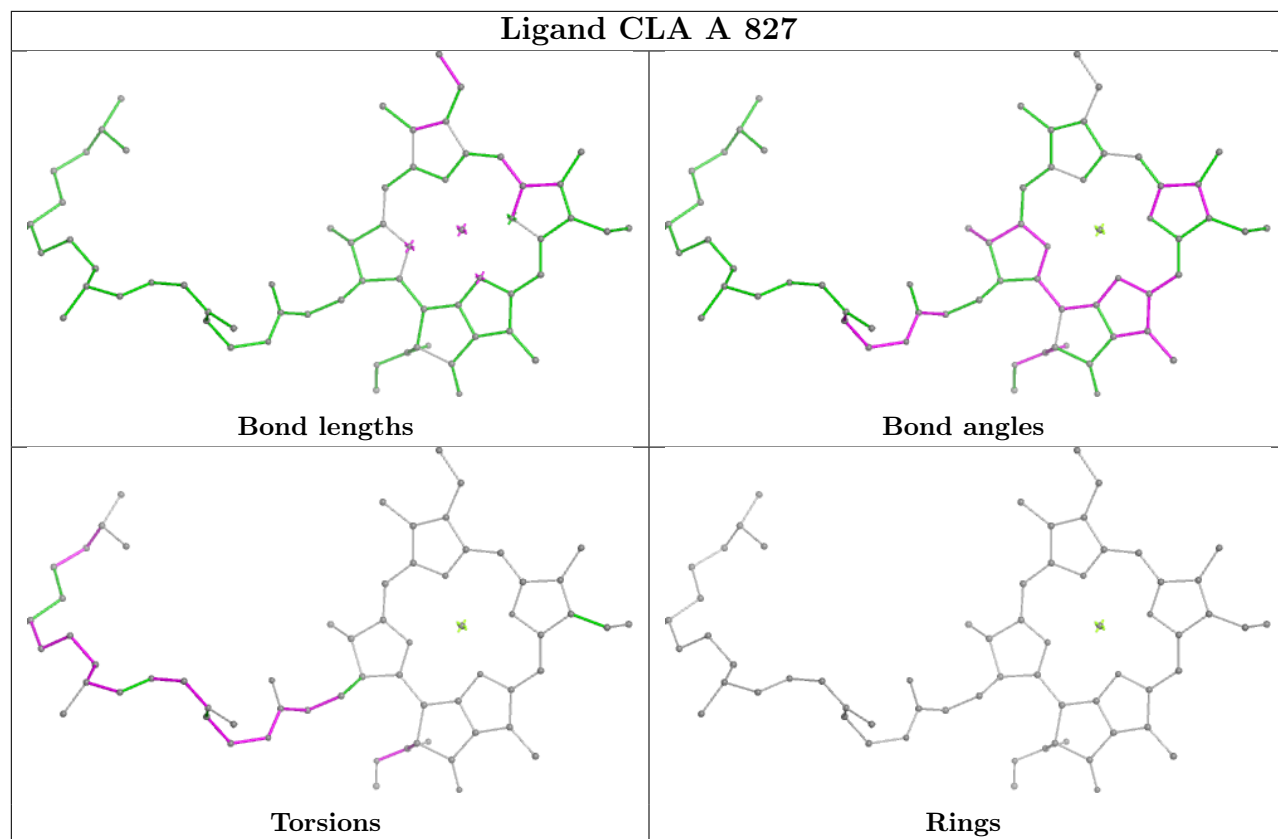
Ligand CLA 6 322



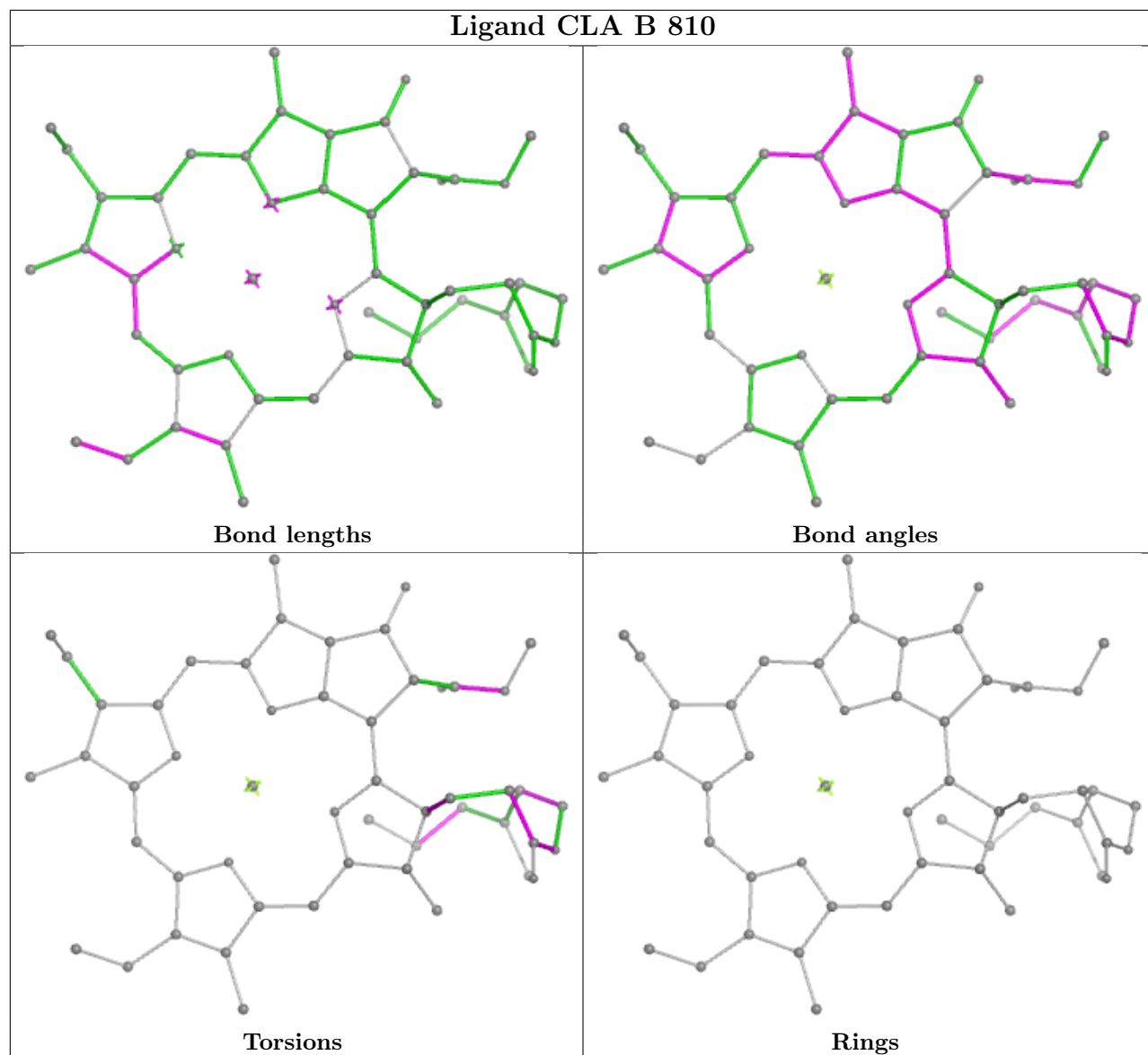
Ligand LMT A 855



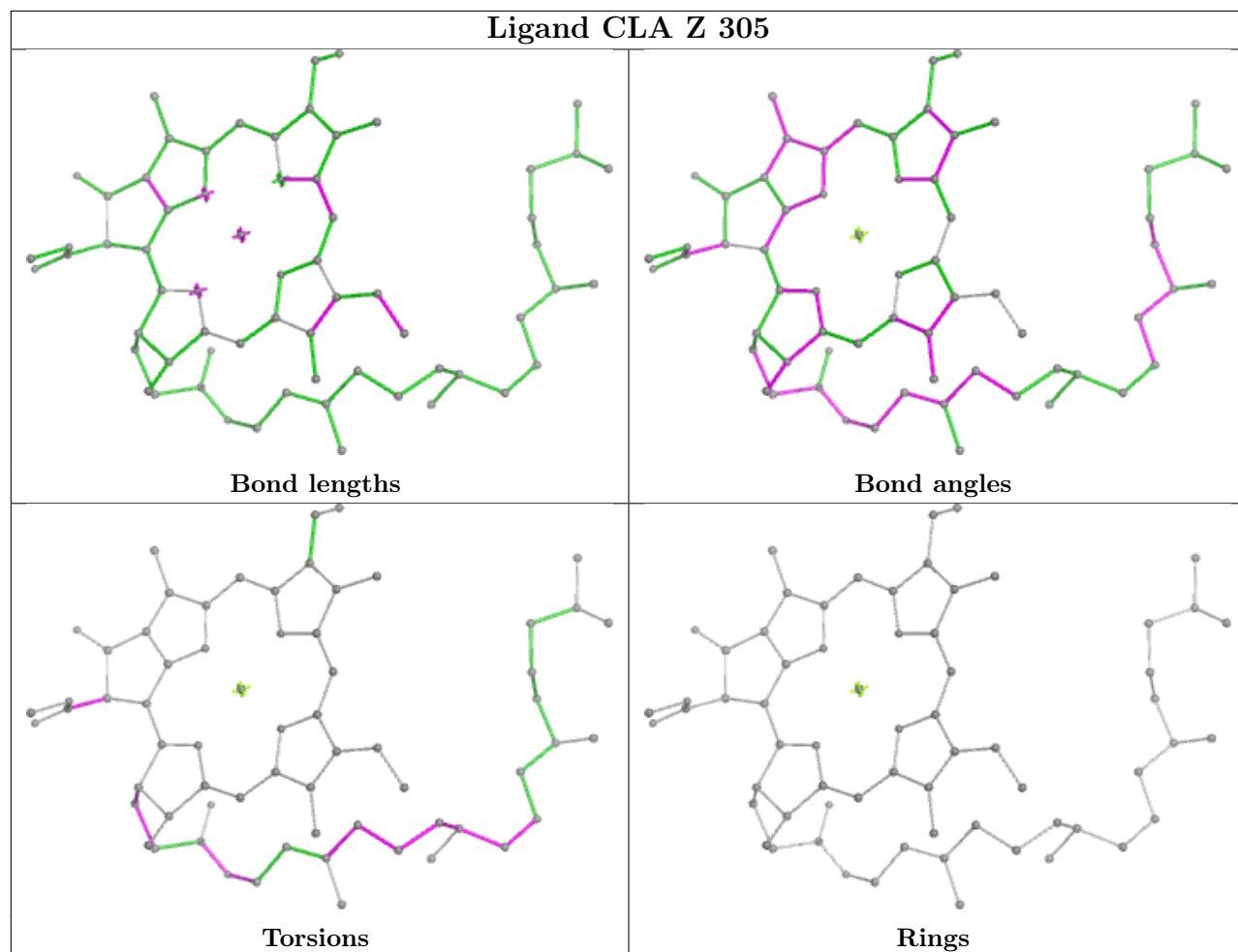


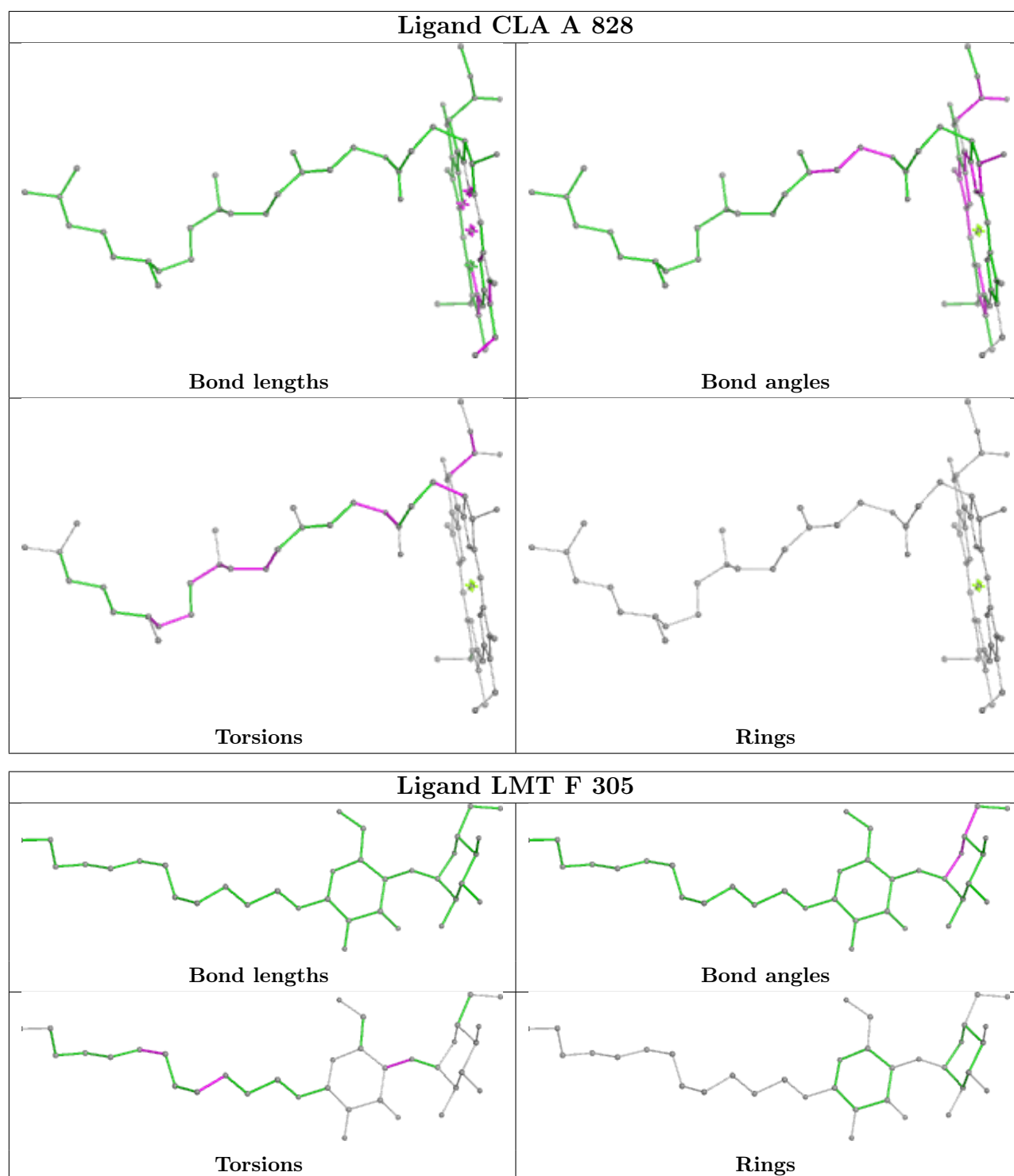


Ligand CLA B 810

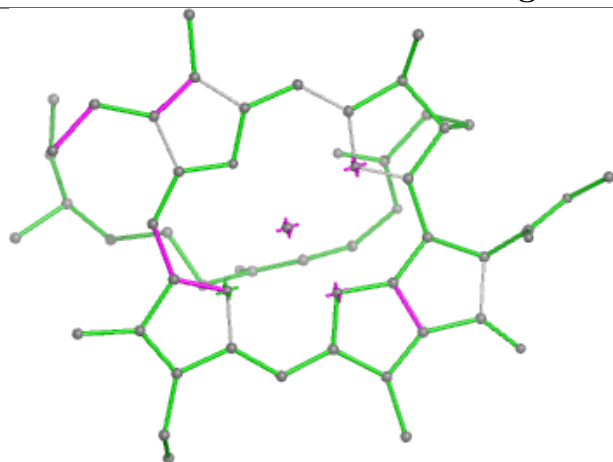


Ligand CLA Z 305

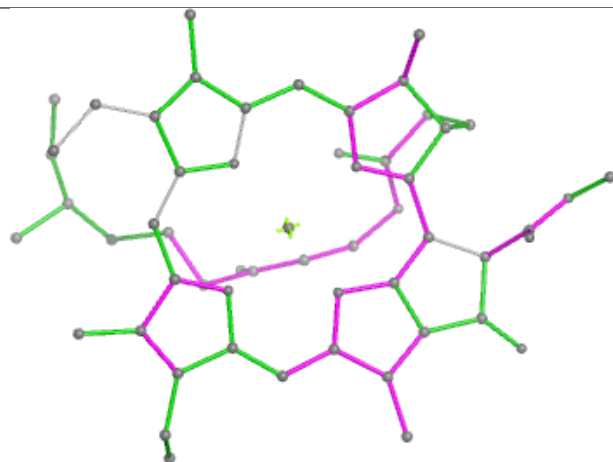




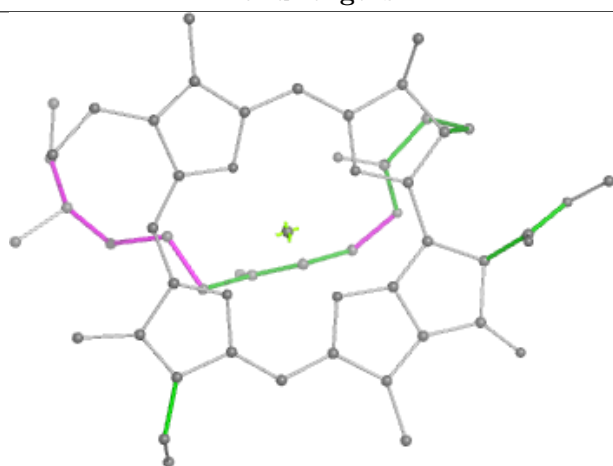
Ligand CLA 5 308



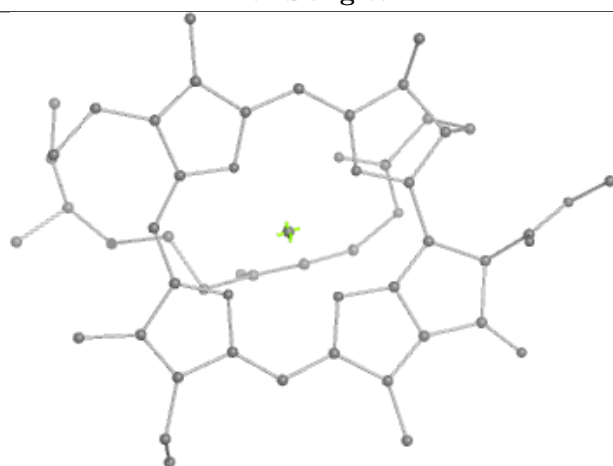
Bond lengths



Bond angles

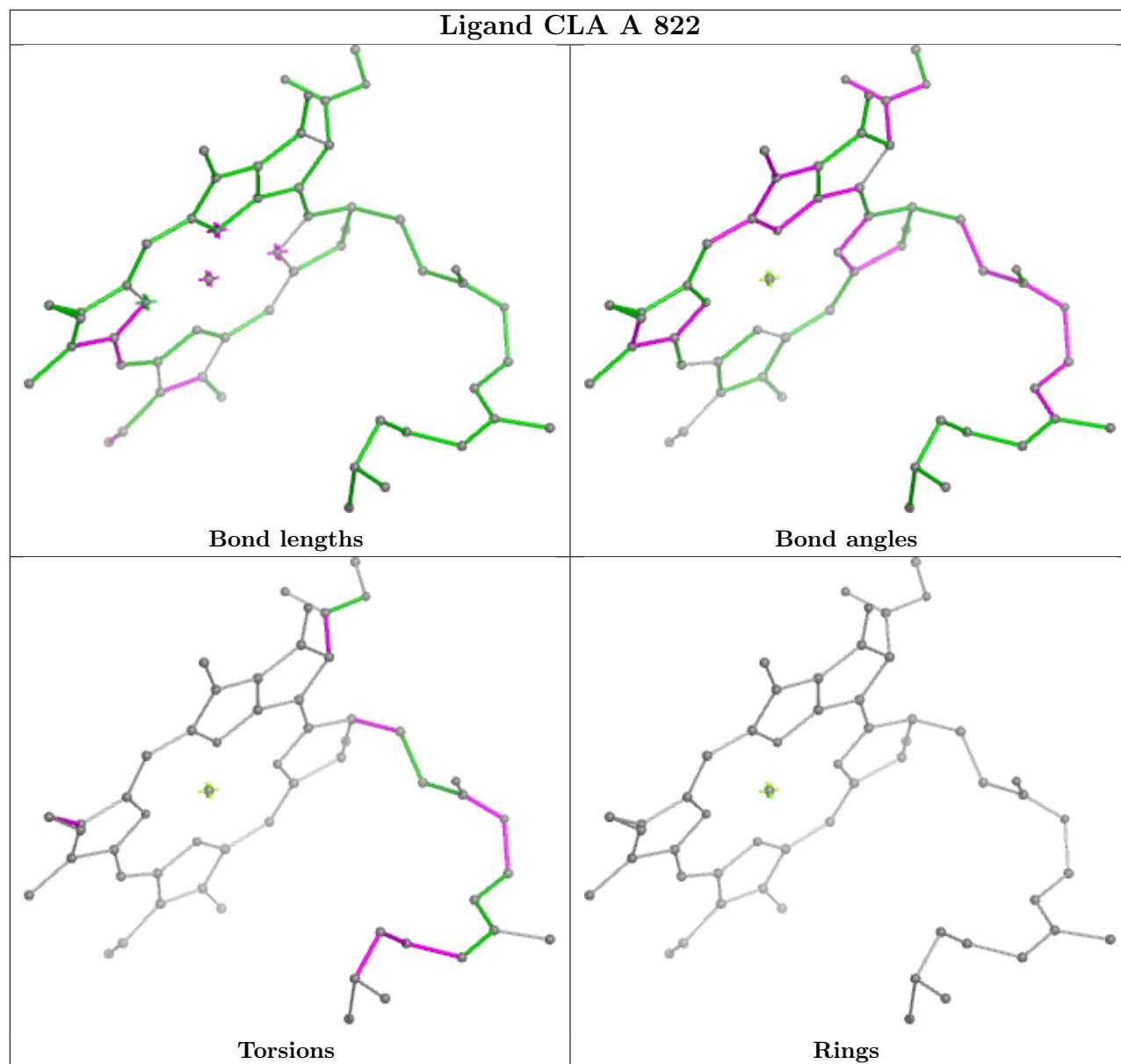


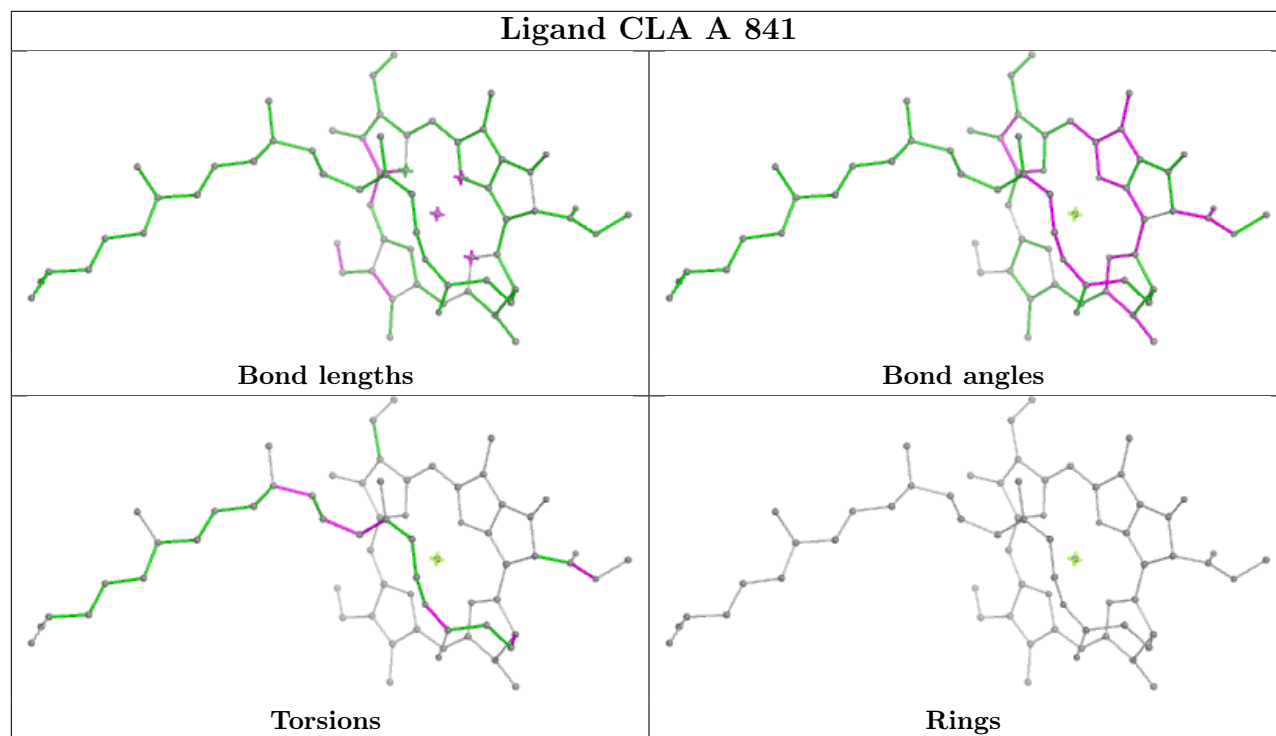
Torsions



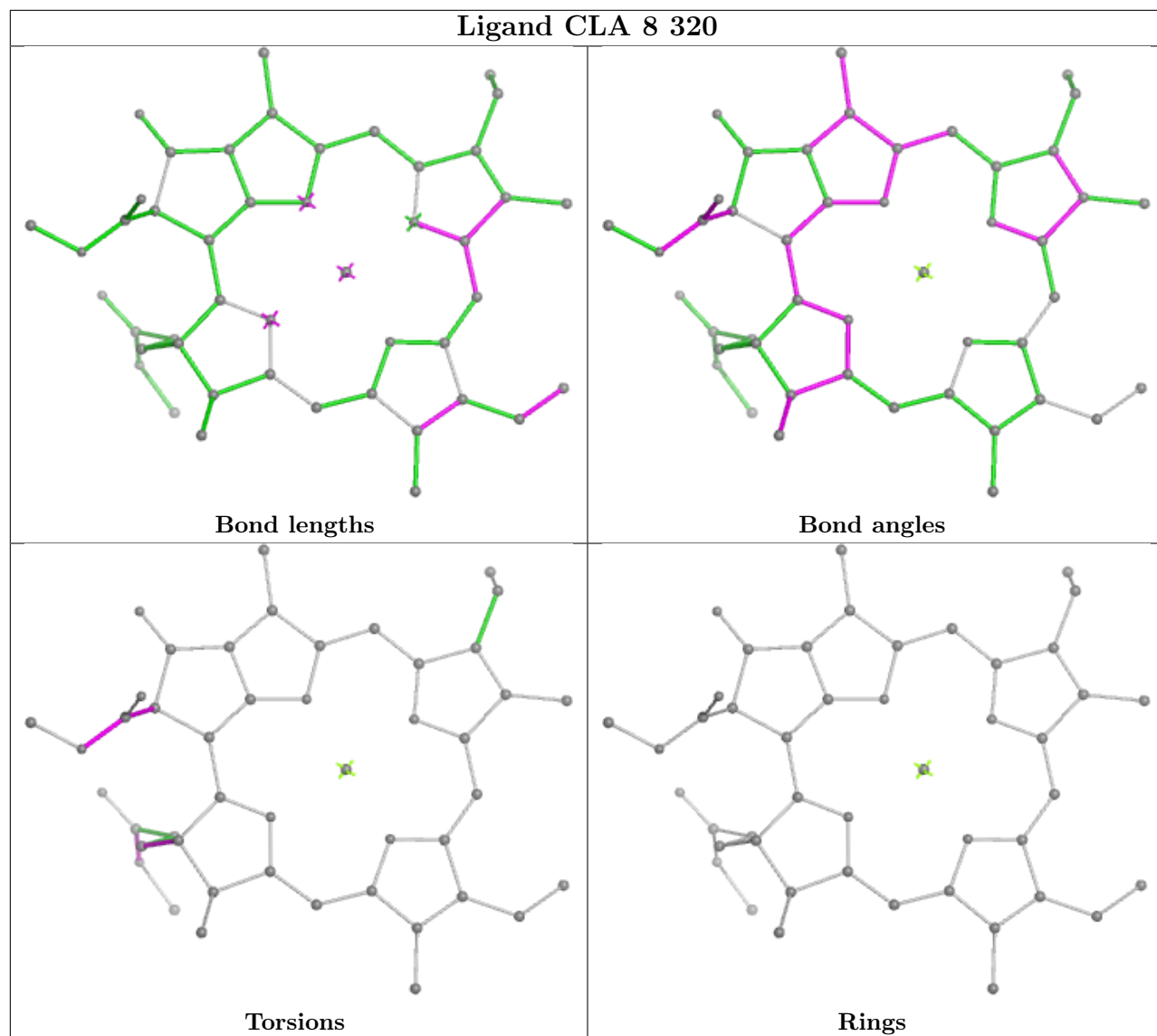
Rings

Ligand CLA A 822

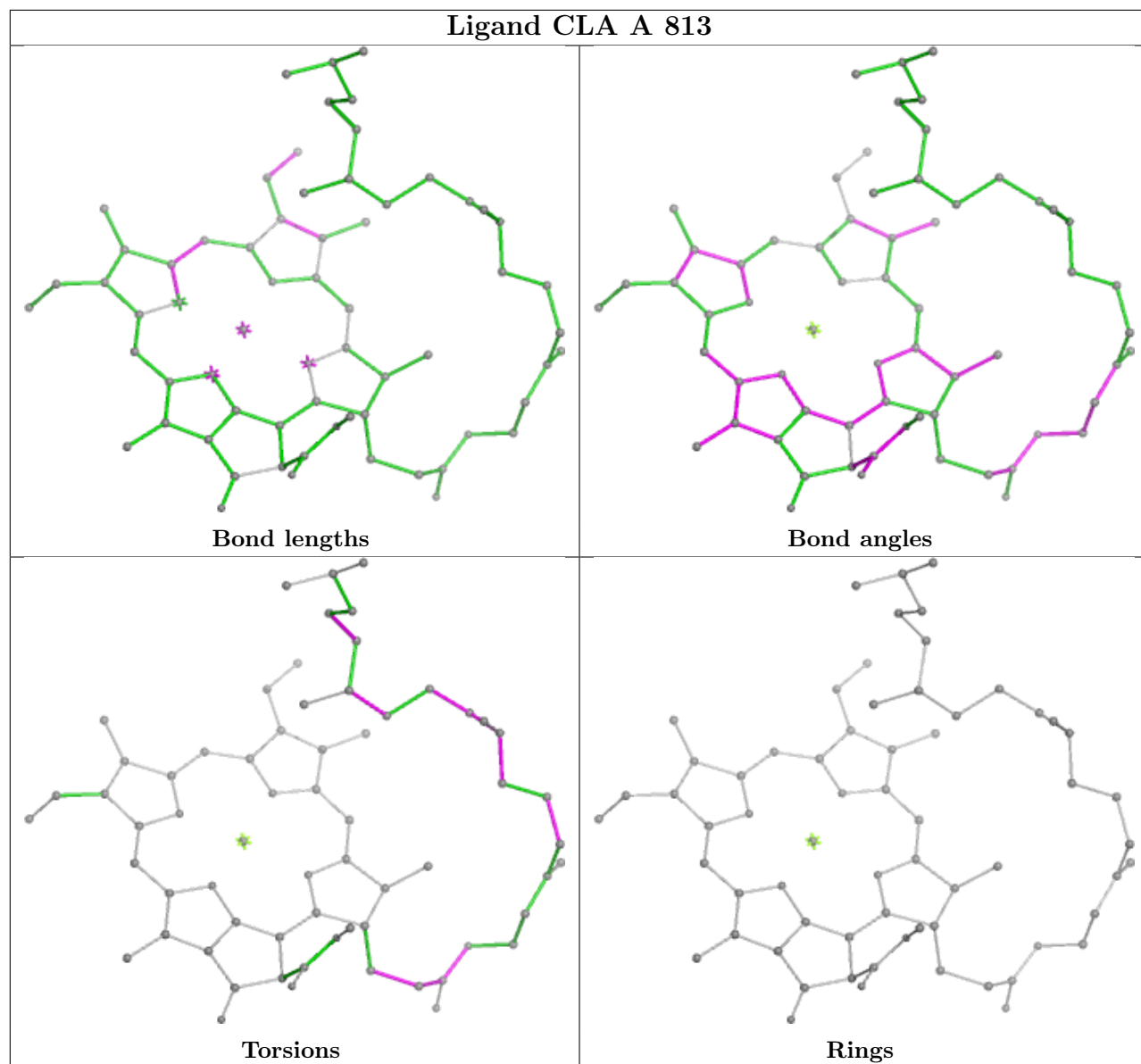




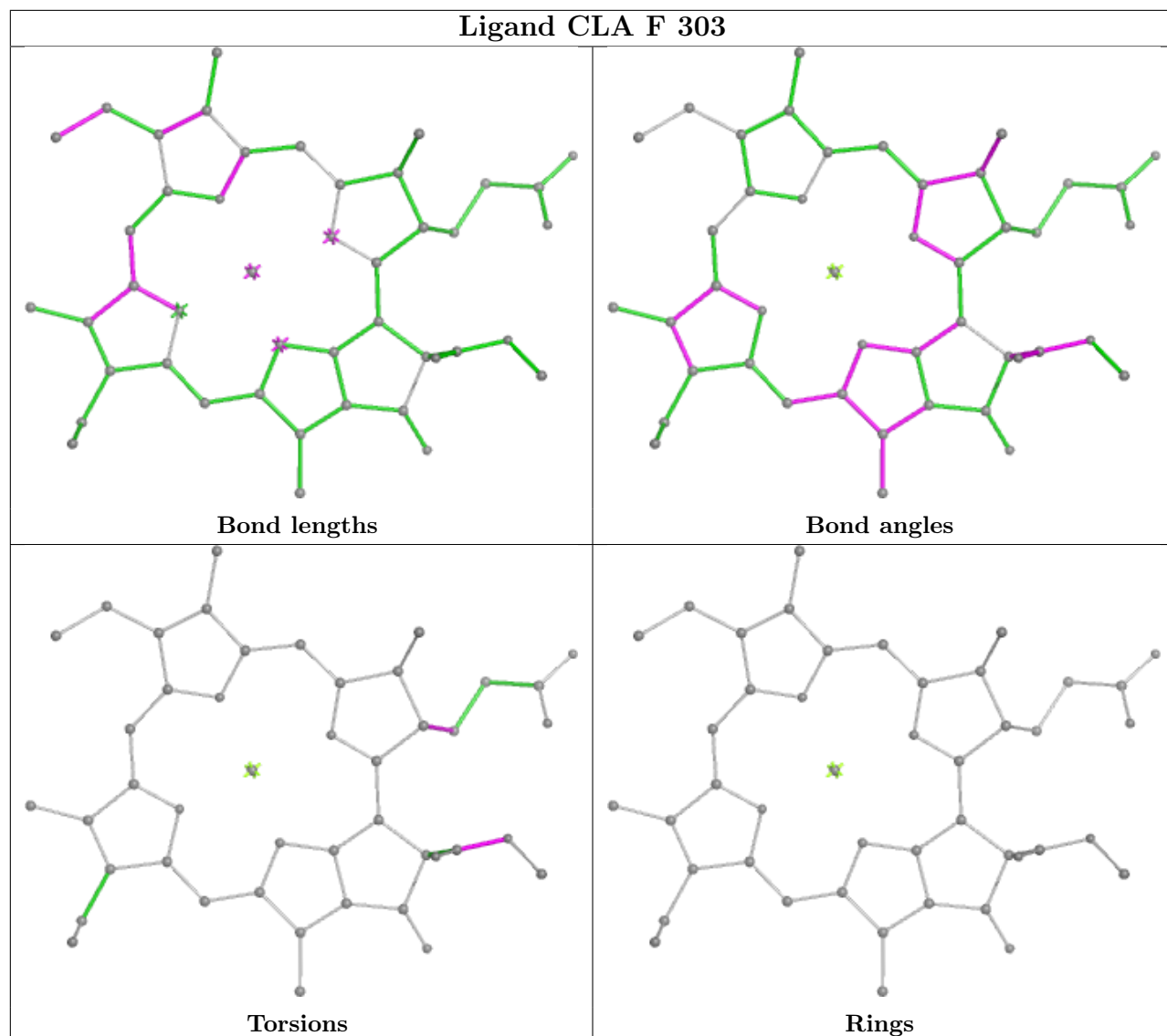
Ligand CLA 8 320

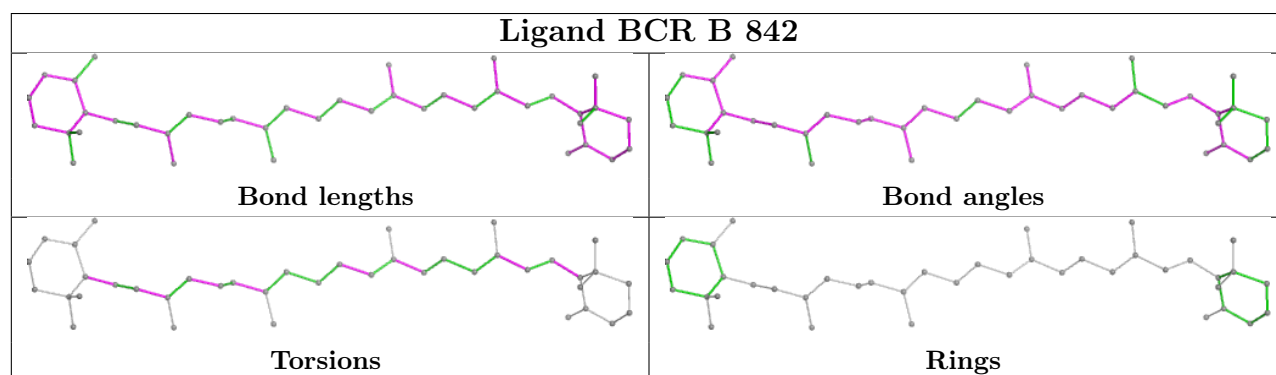
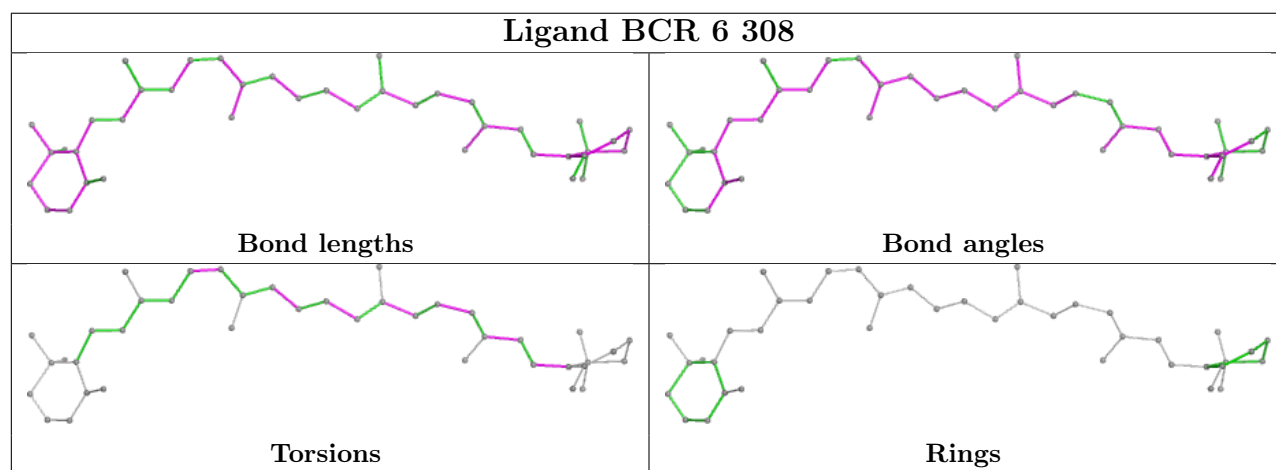
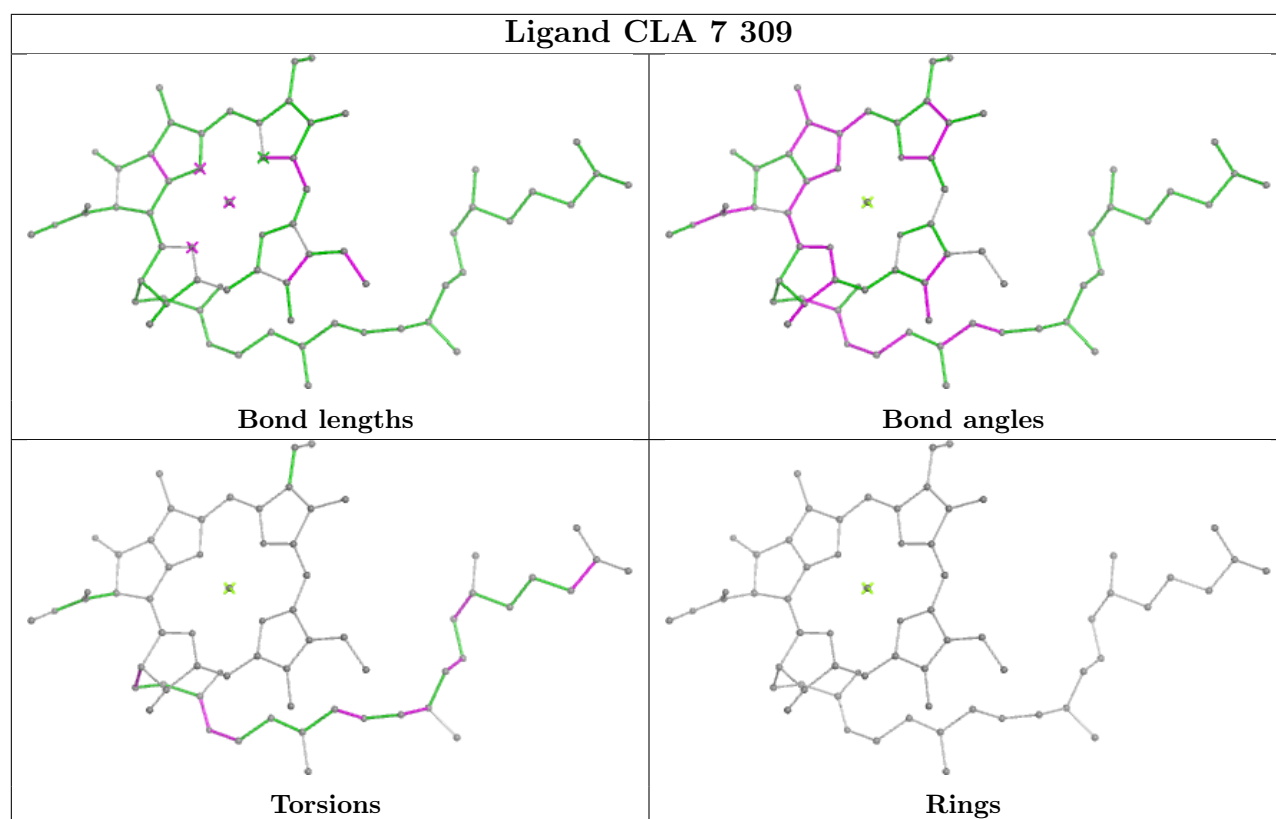


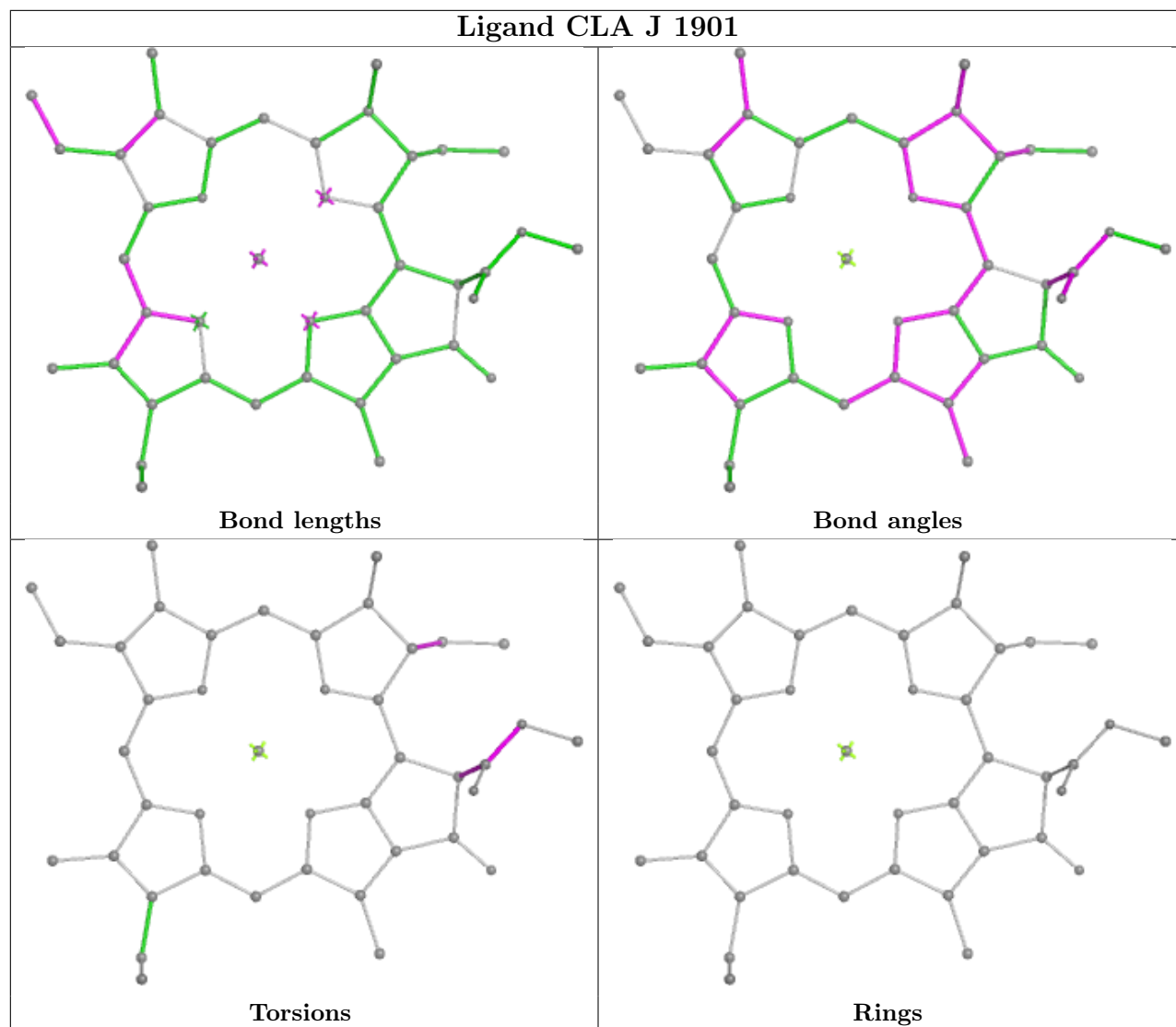
Ligand CLA A 813

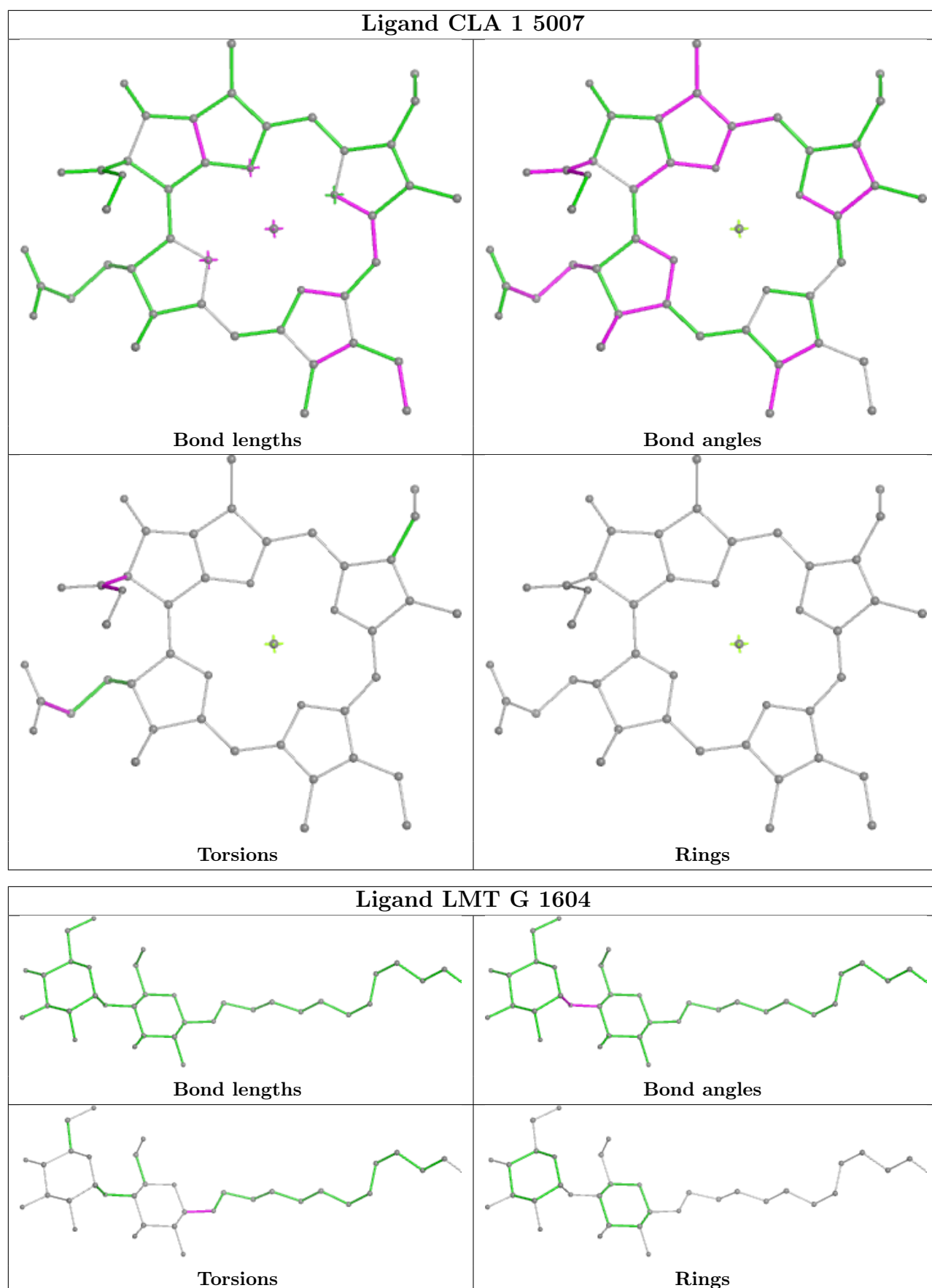


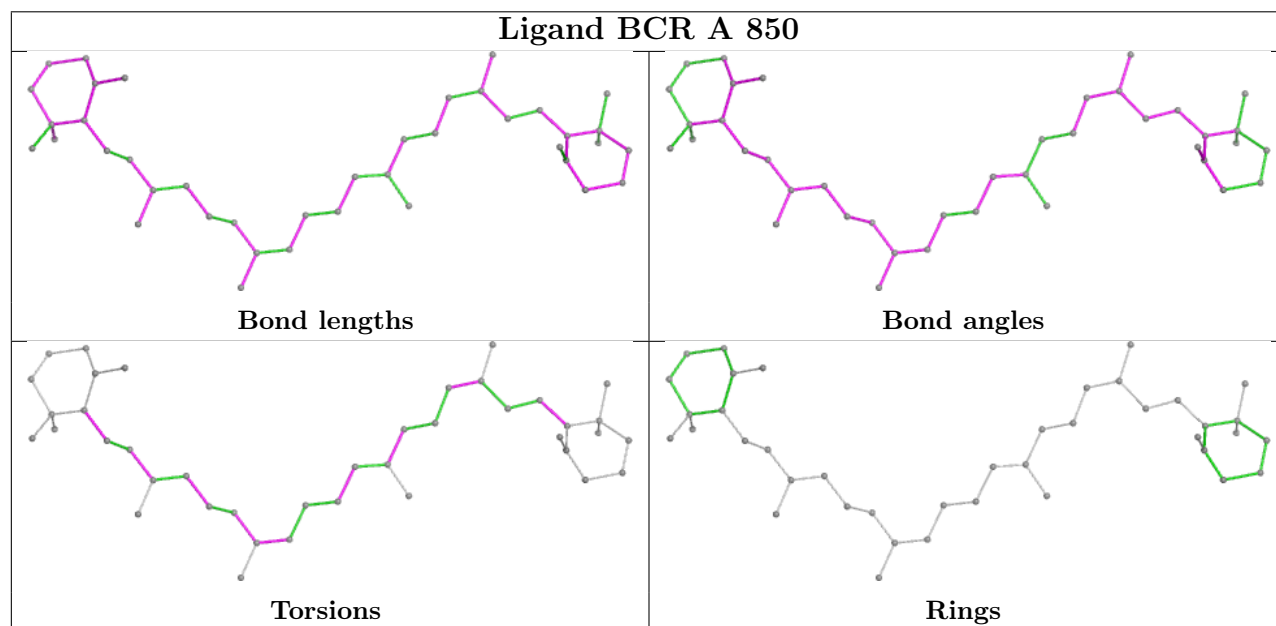
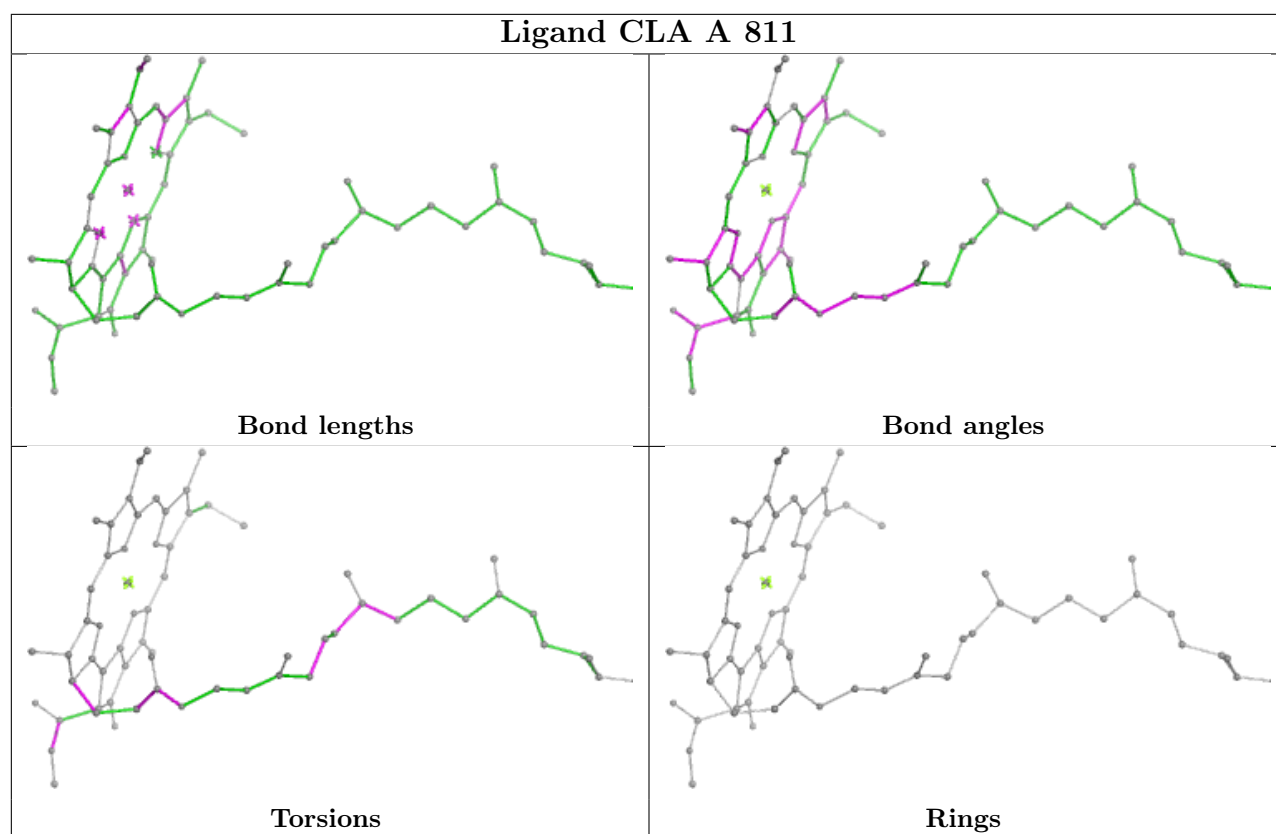
Ligand CLA F 303

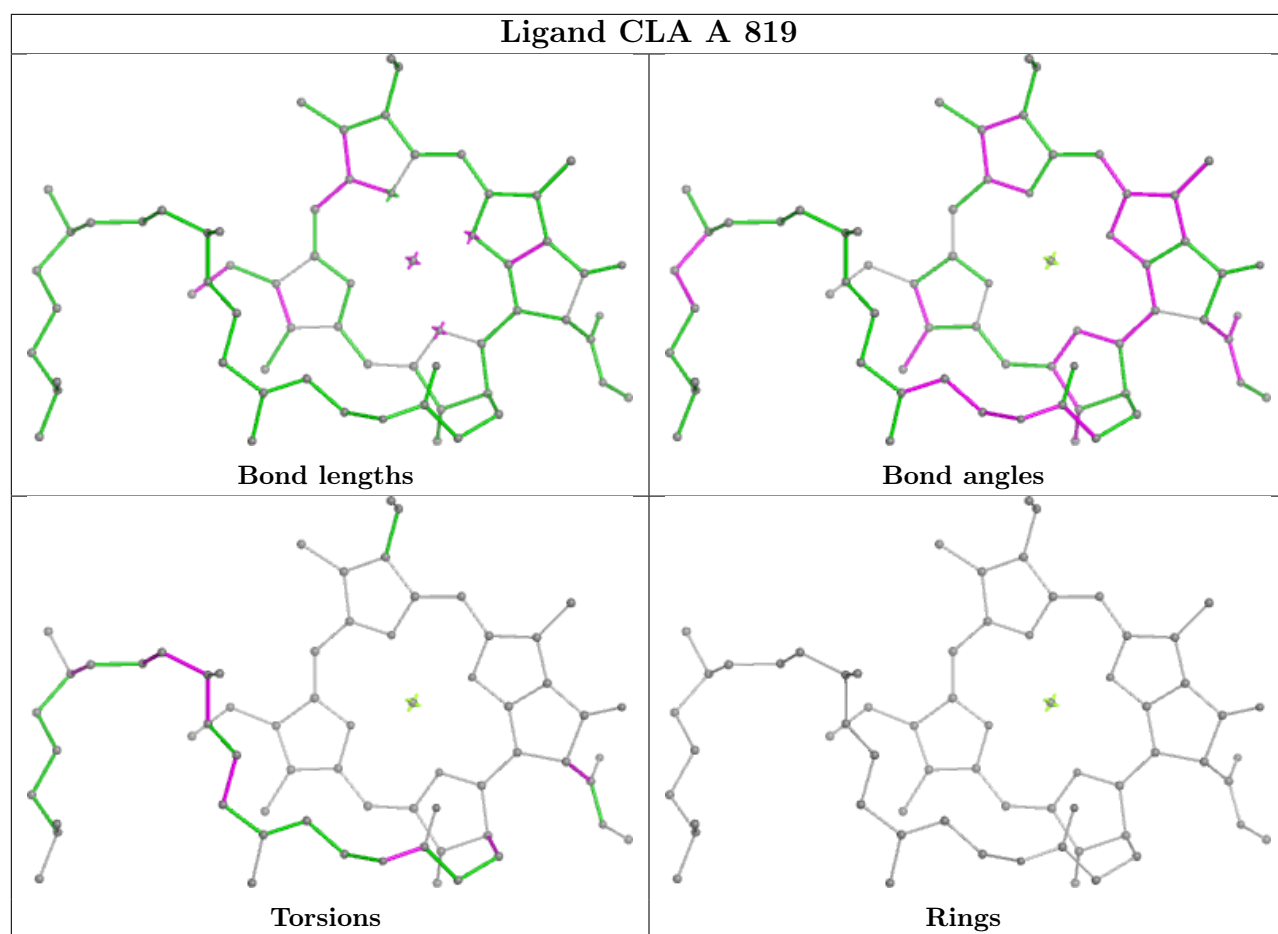


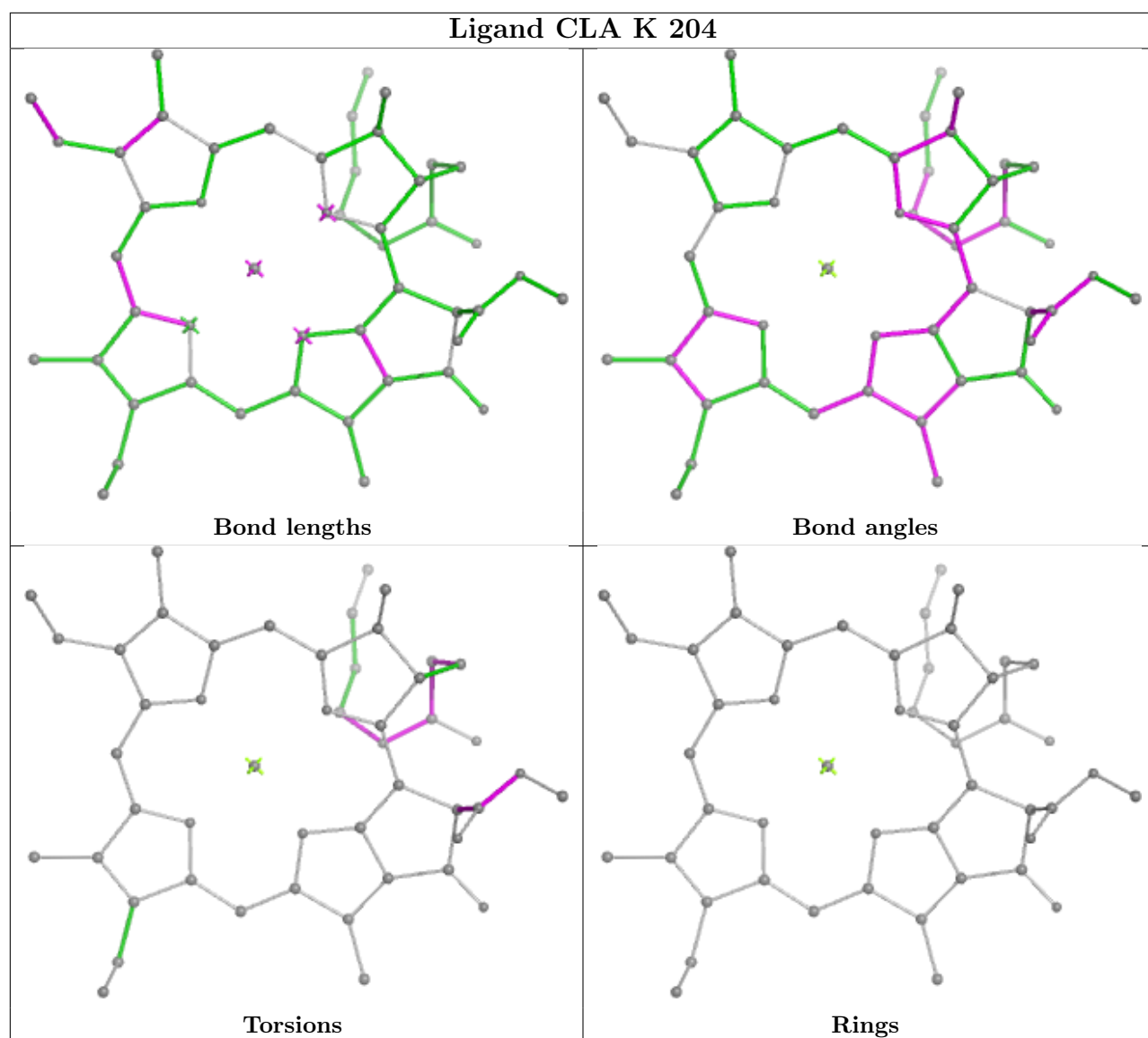


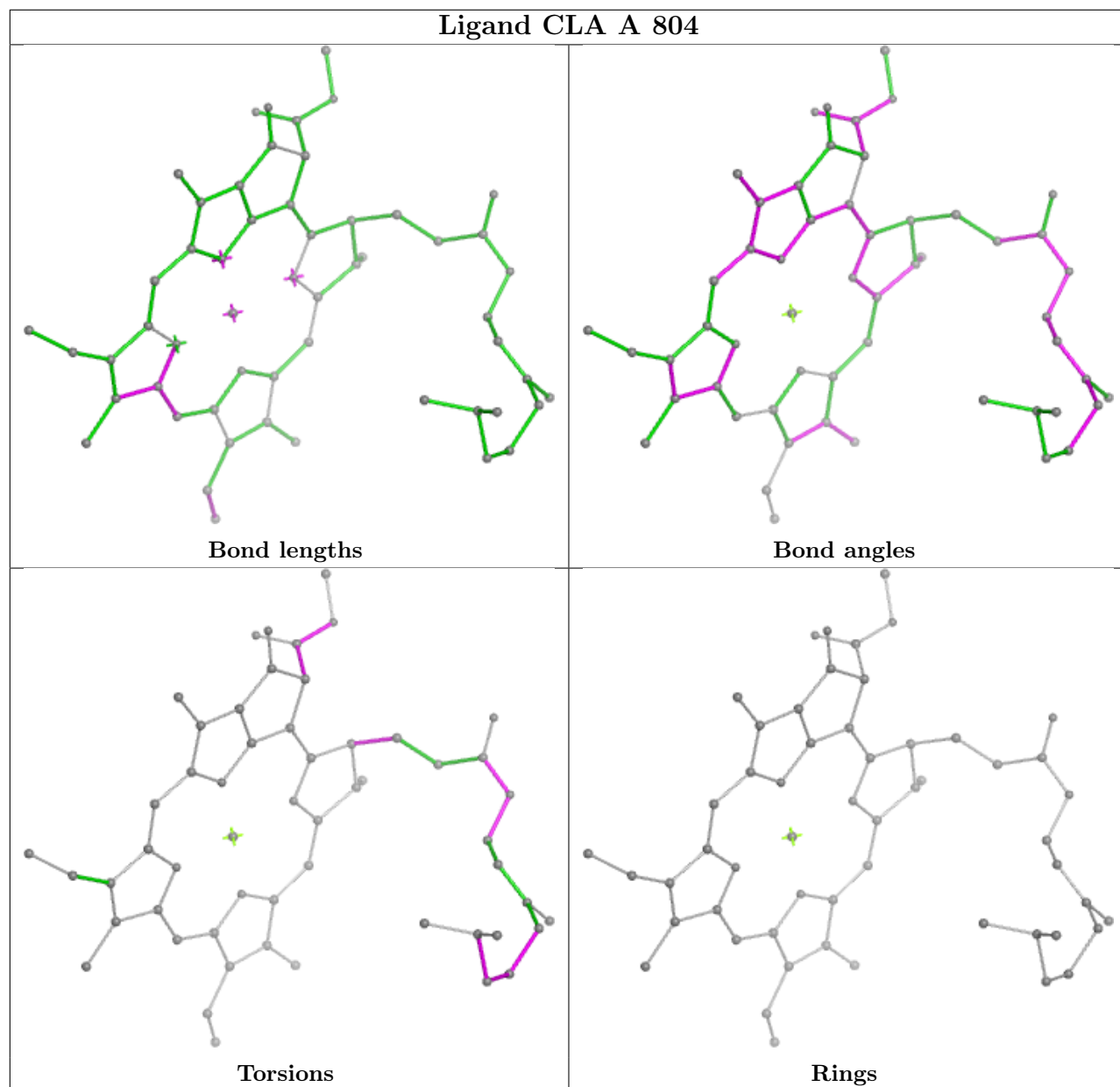




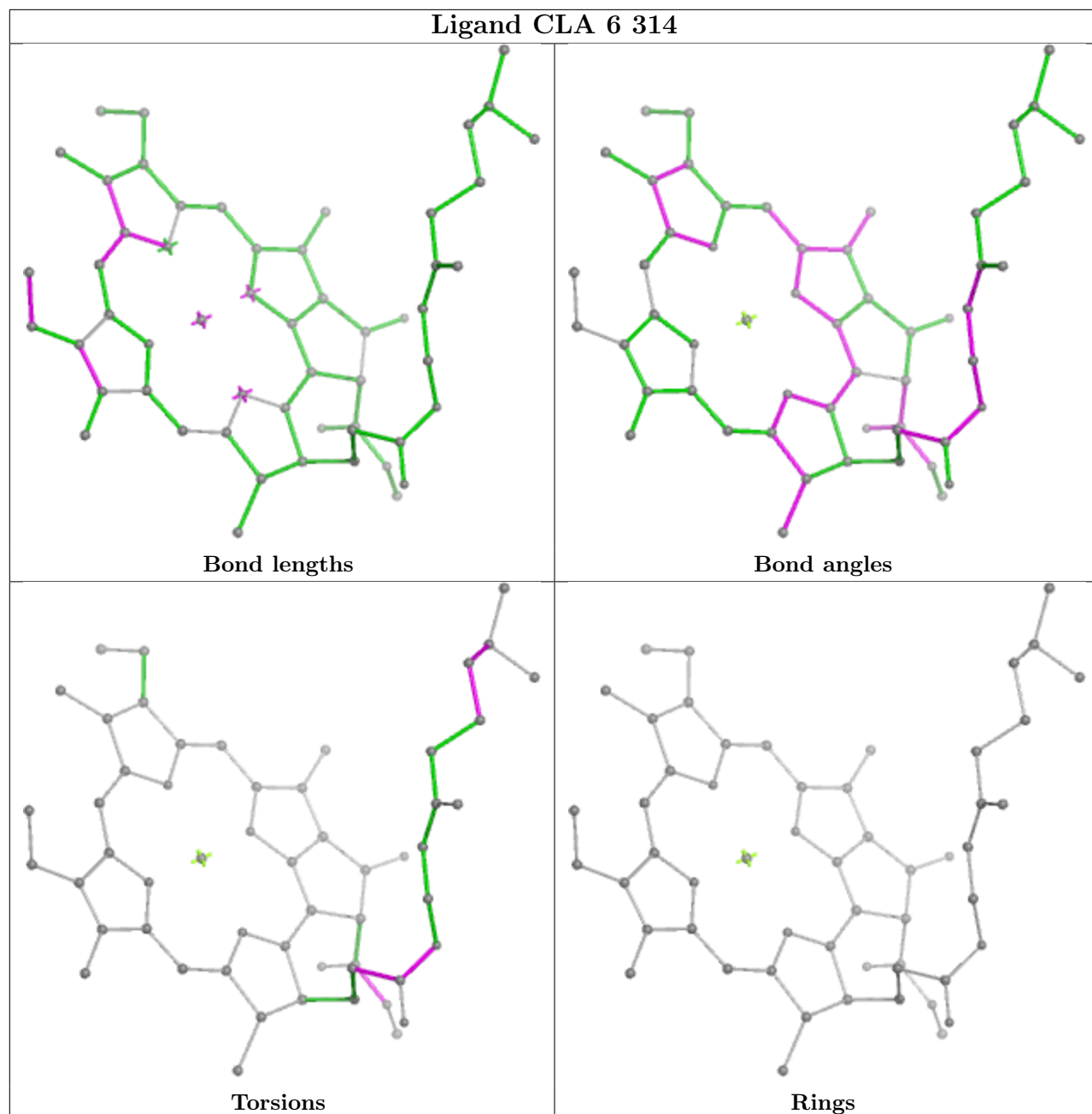




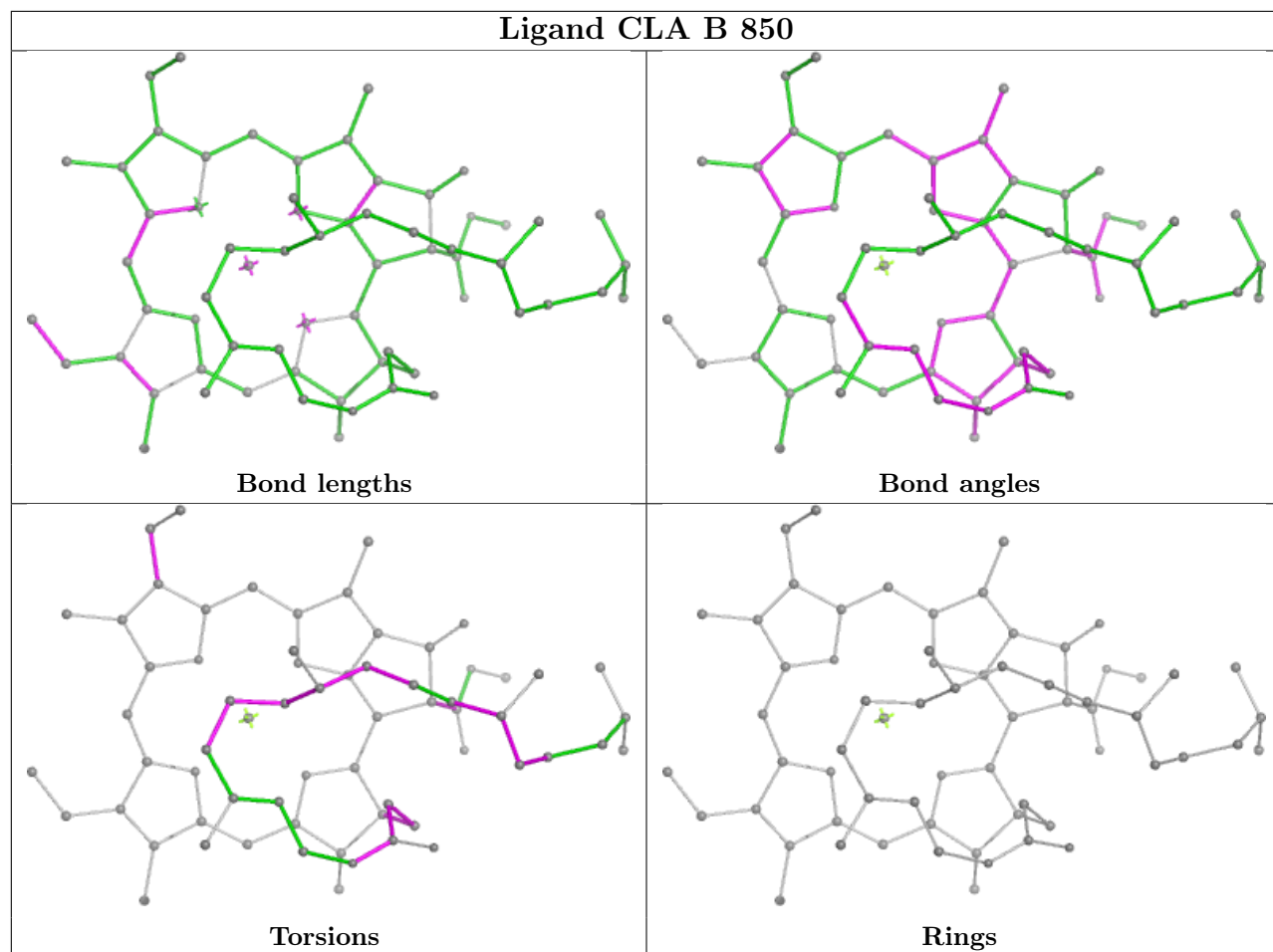


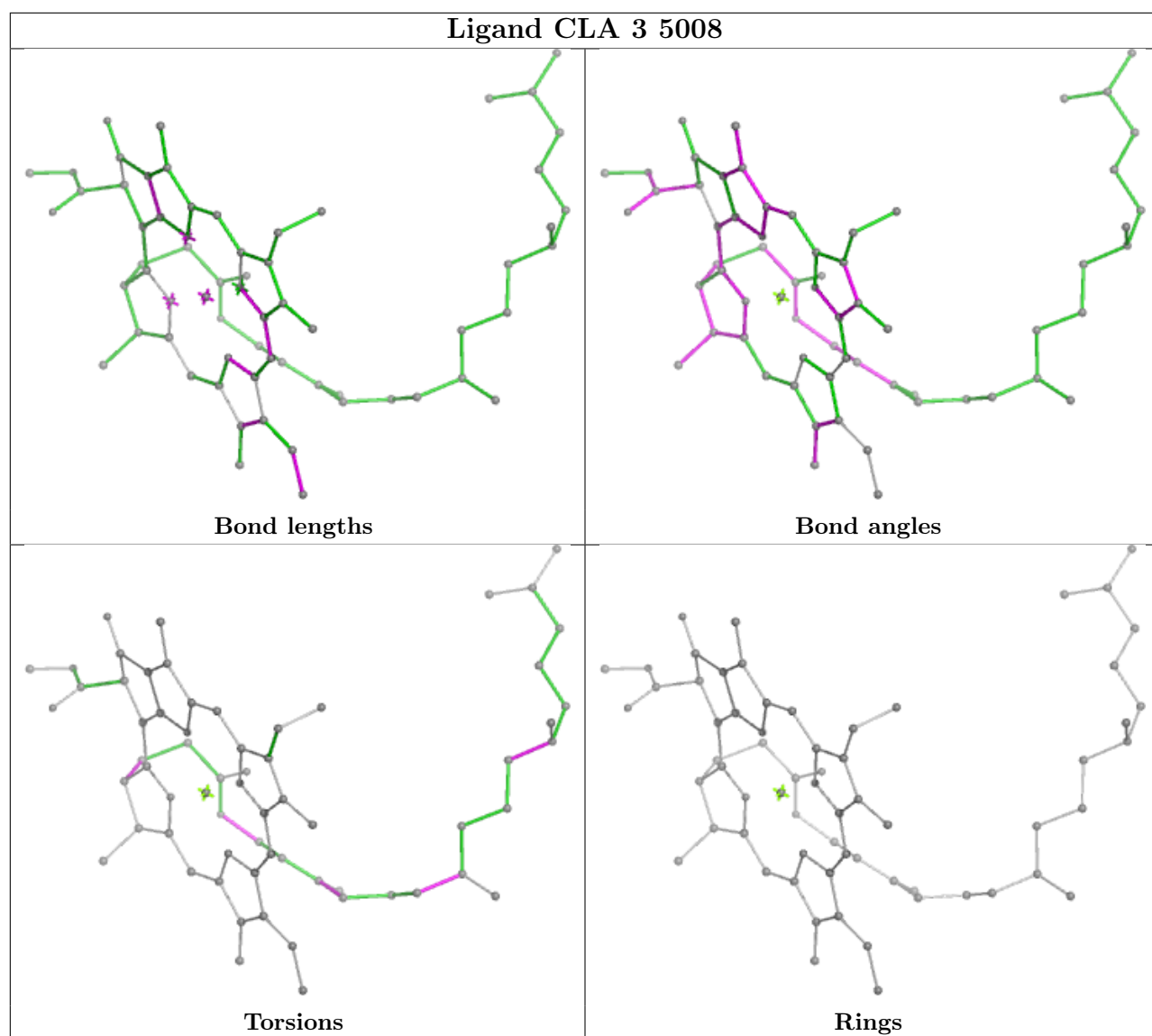


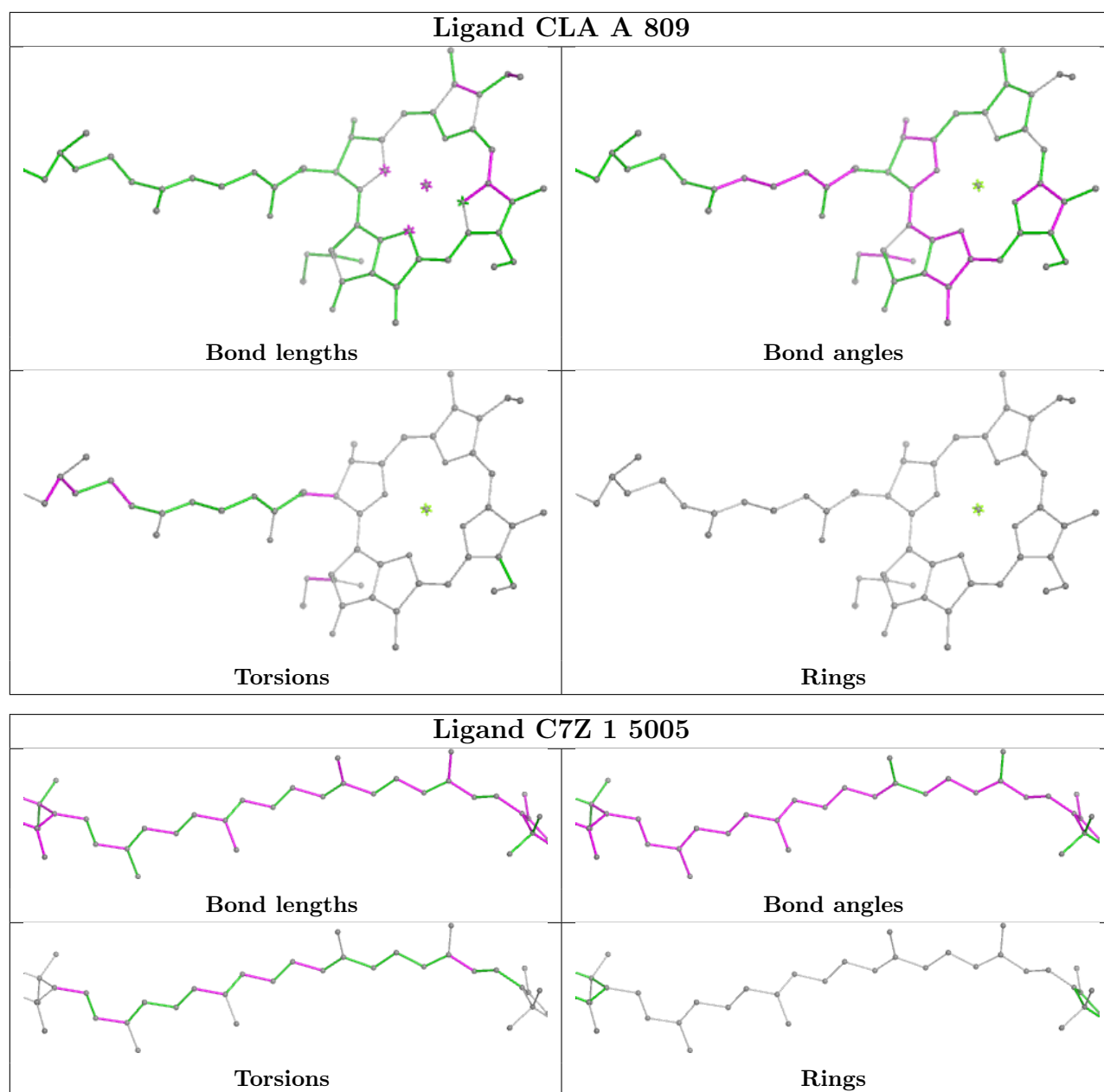
Ligand CLA 6 314



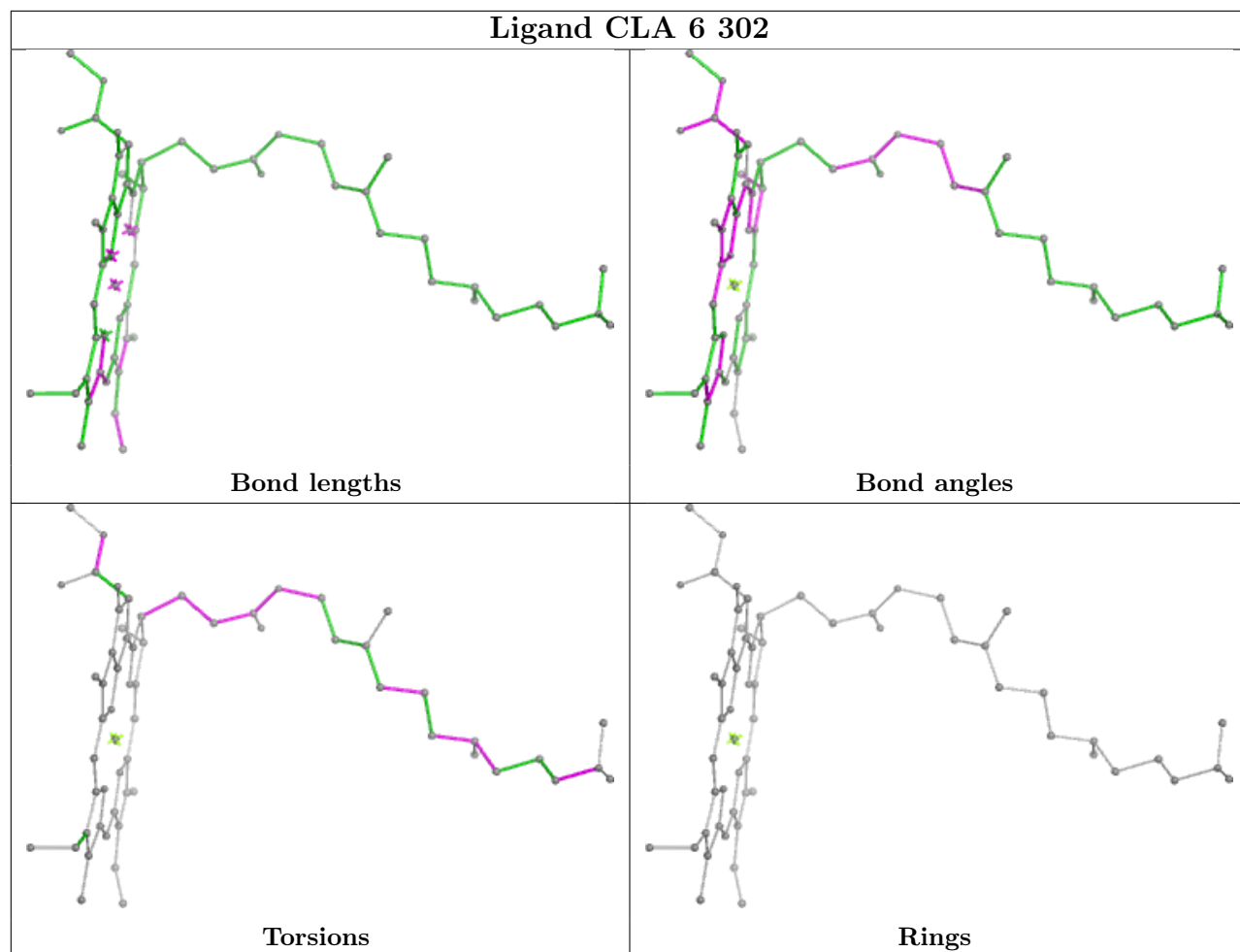
Ligand CLA B 850



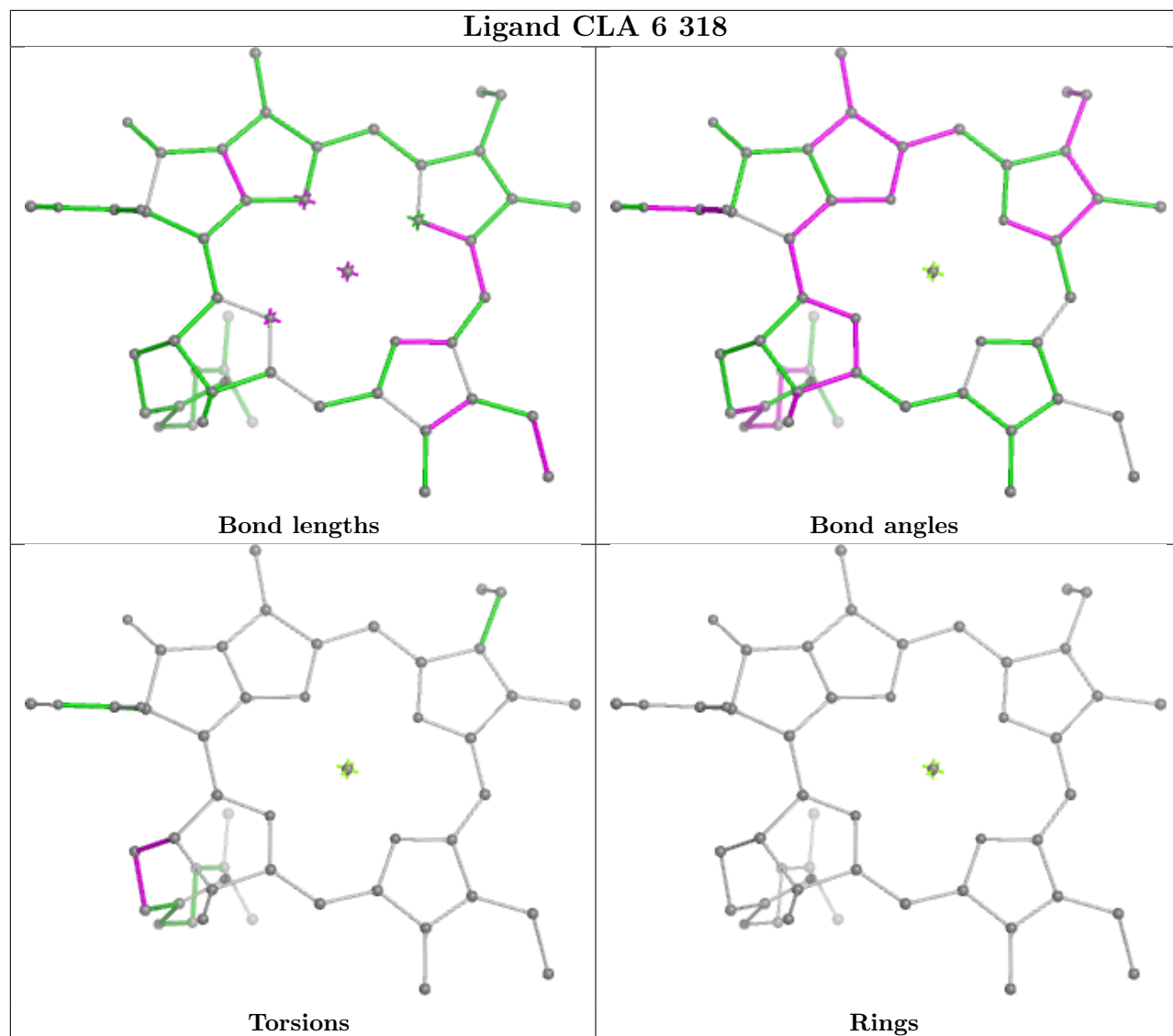


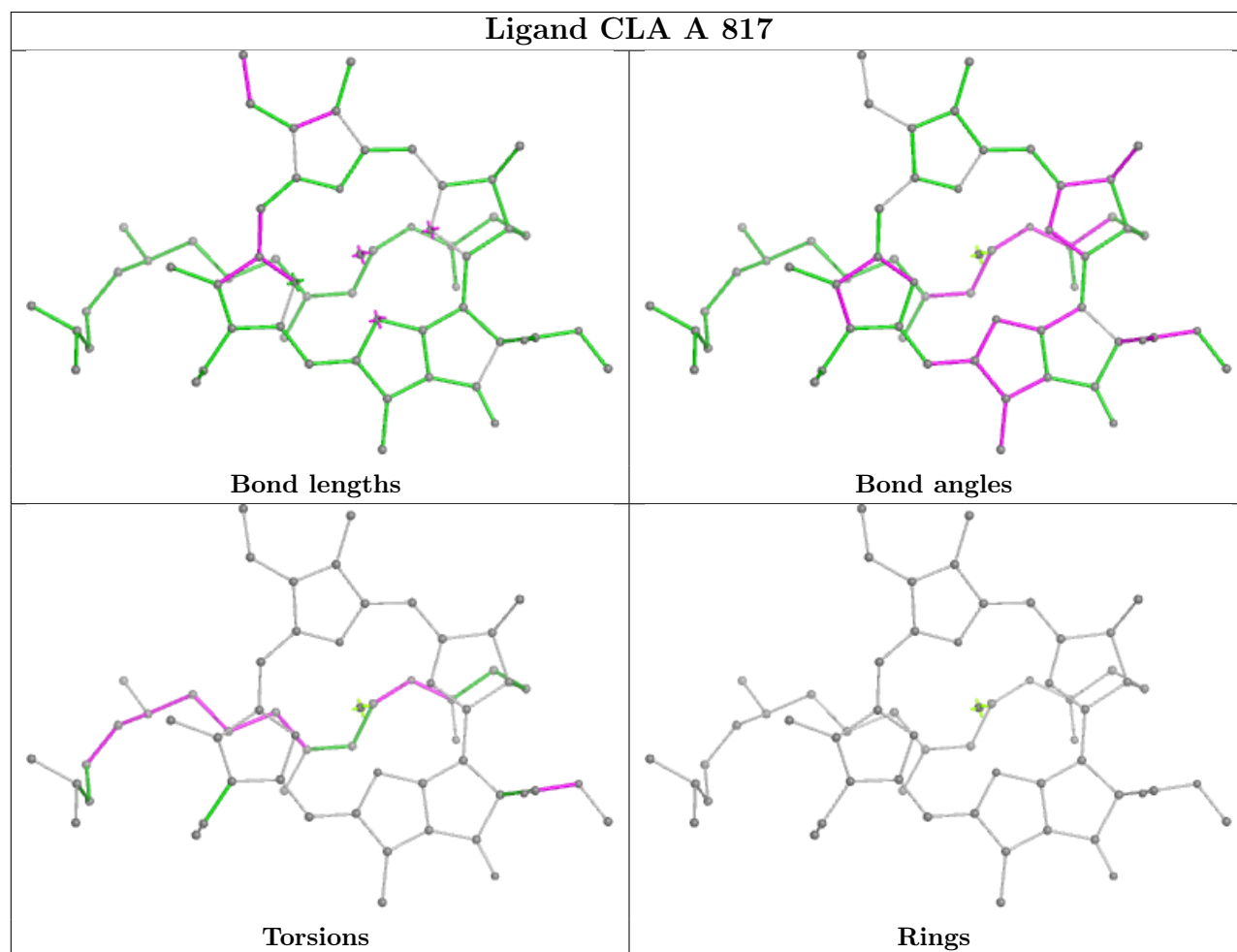
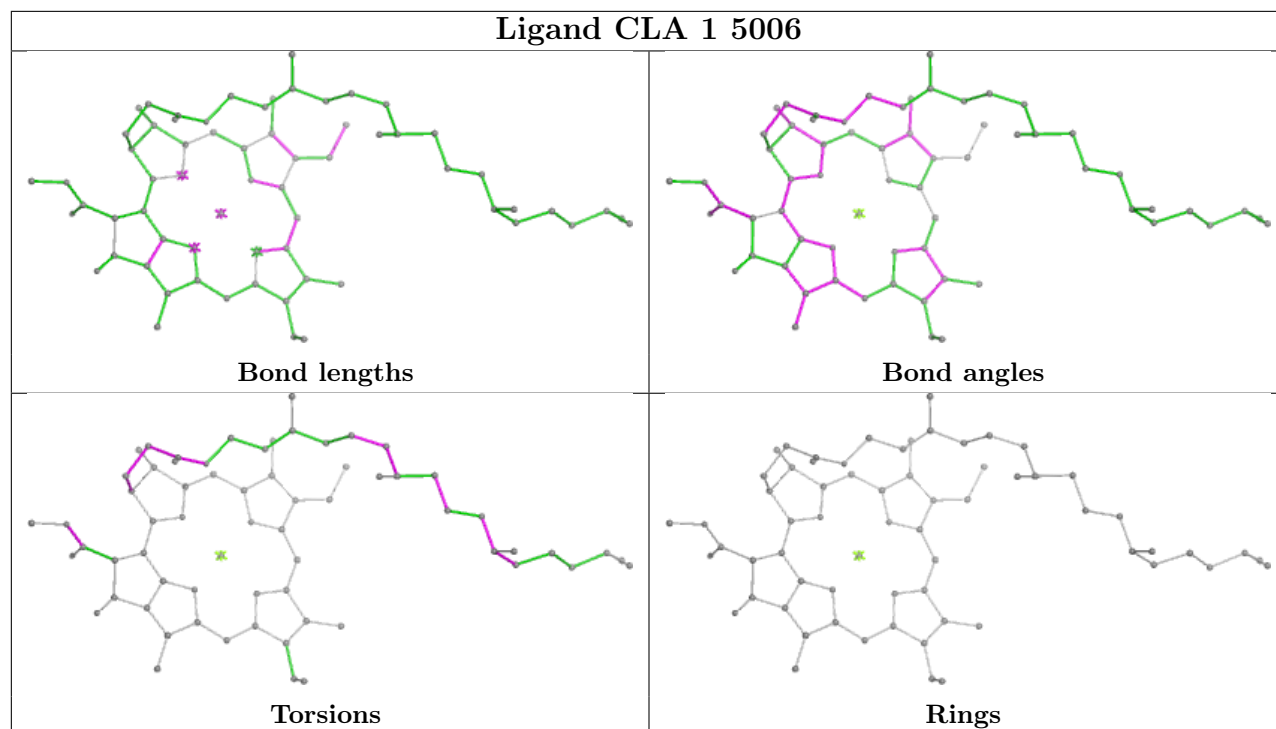


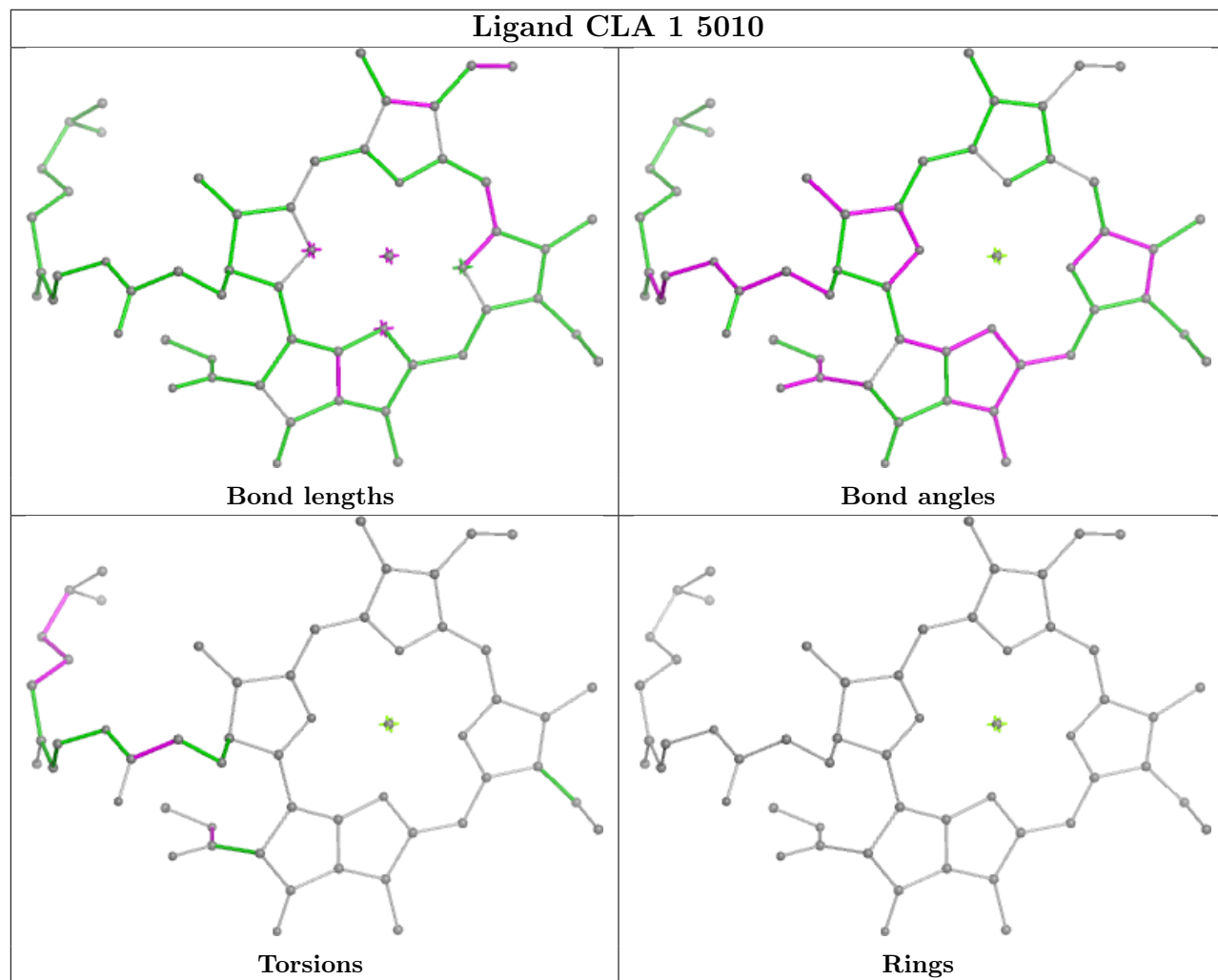
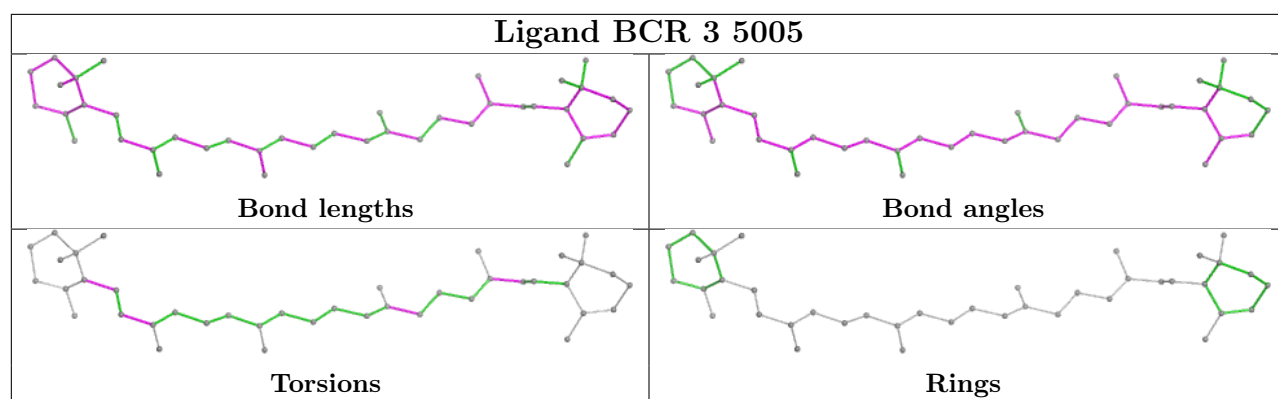
Ligand CLA 6 302

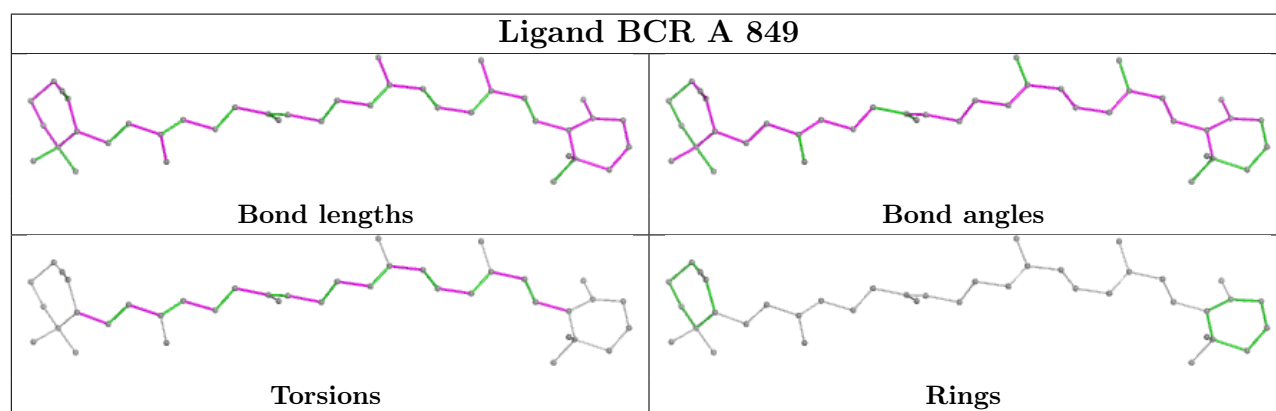
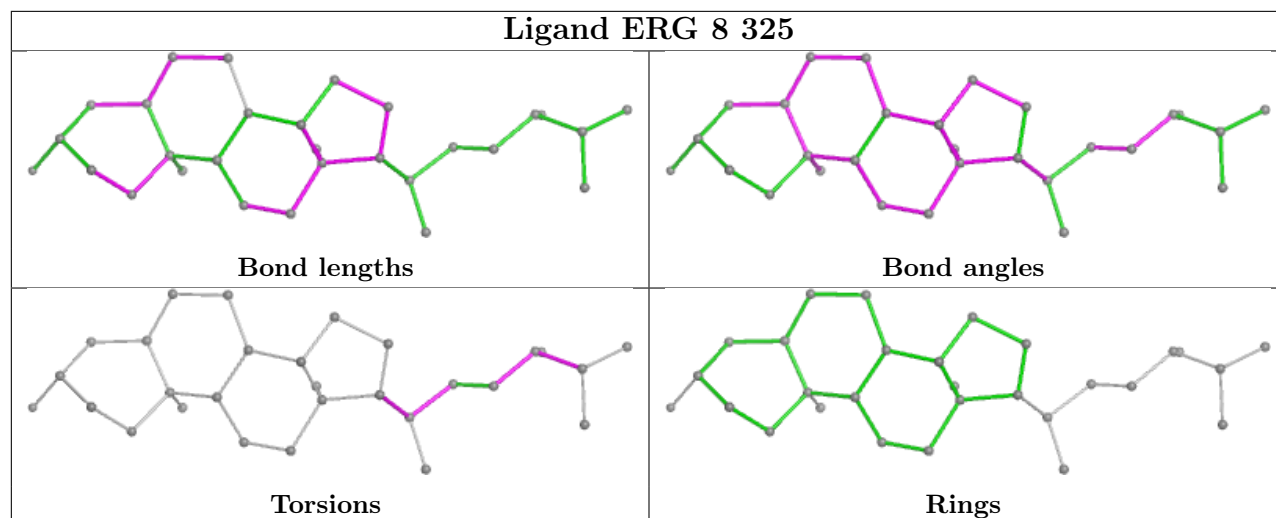


Ligand CLA 6 318

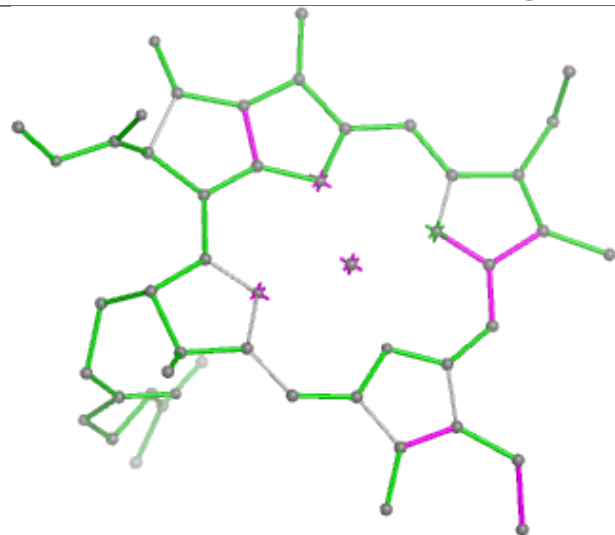




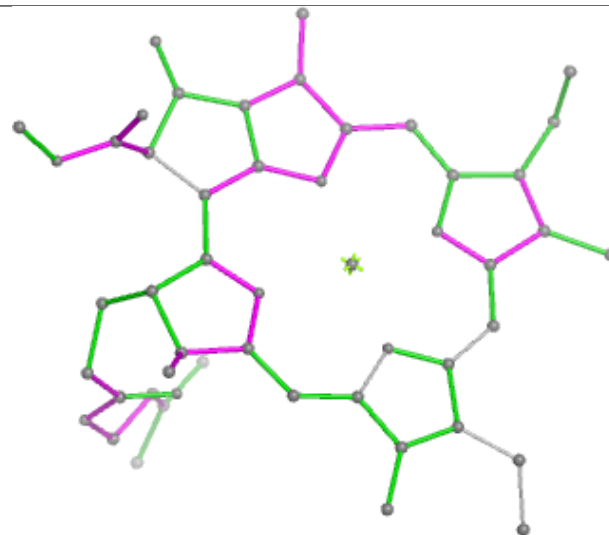




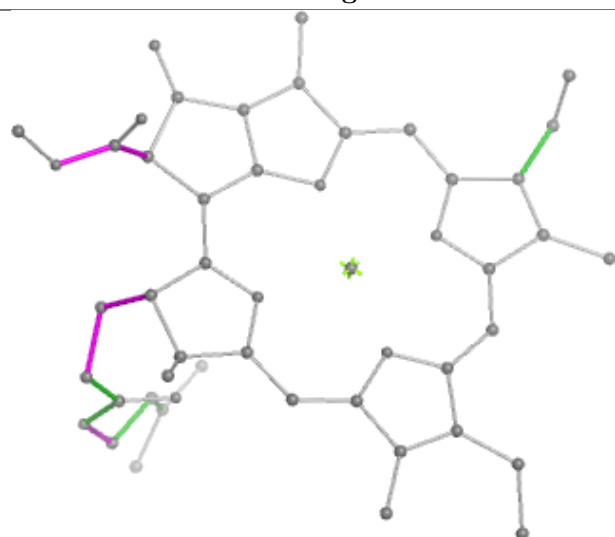
Ligand CLA 7 317



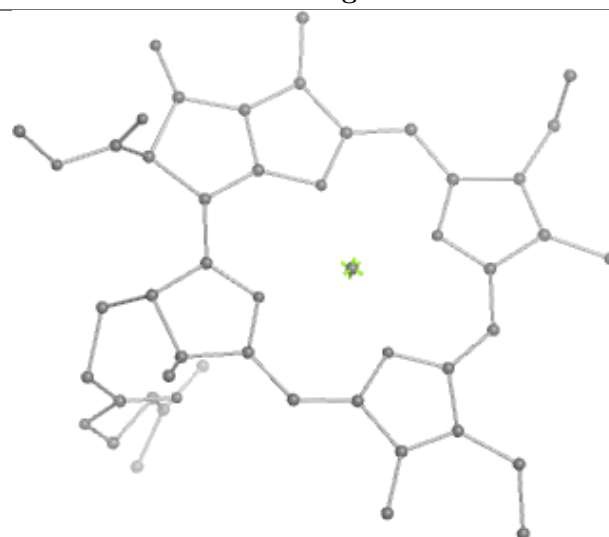
Bond lengths



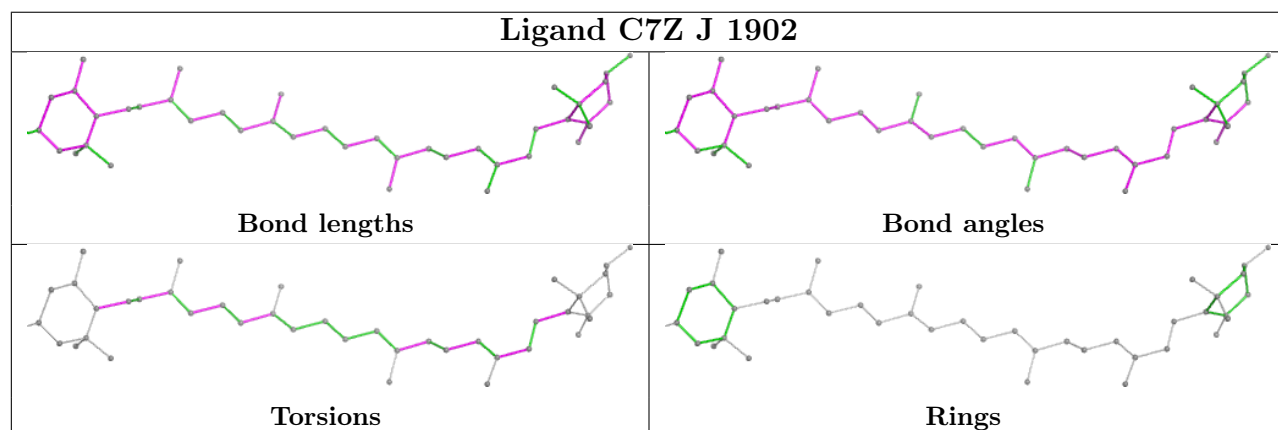
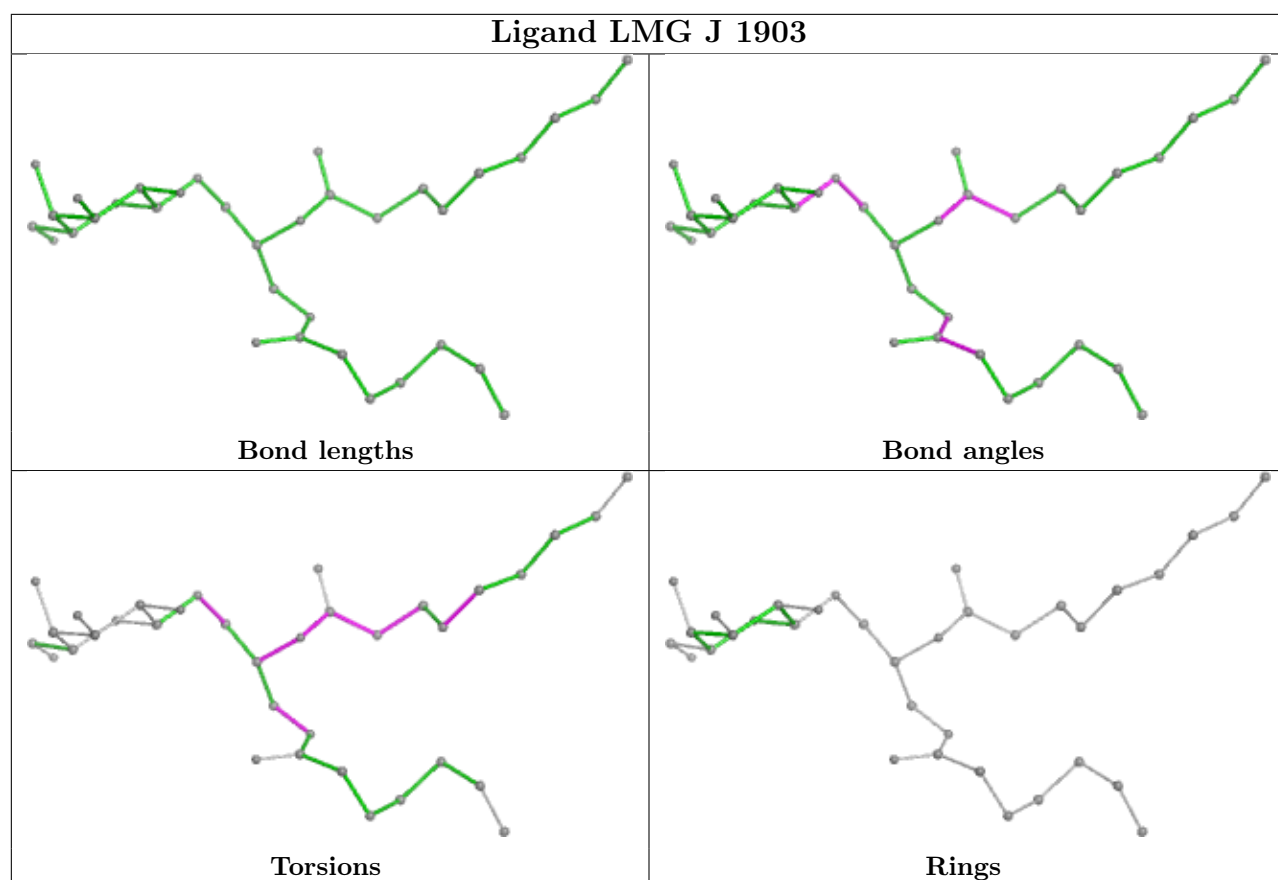
Bond angles

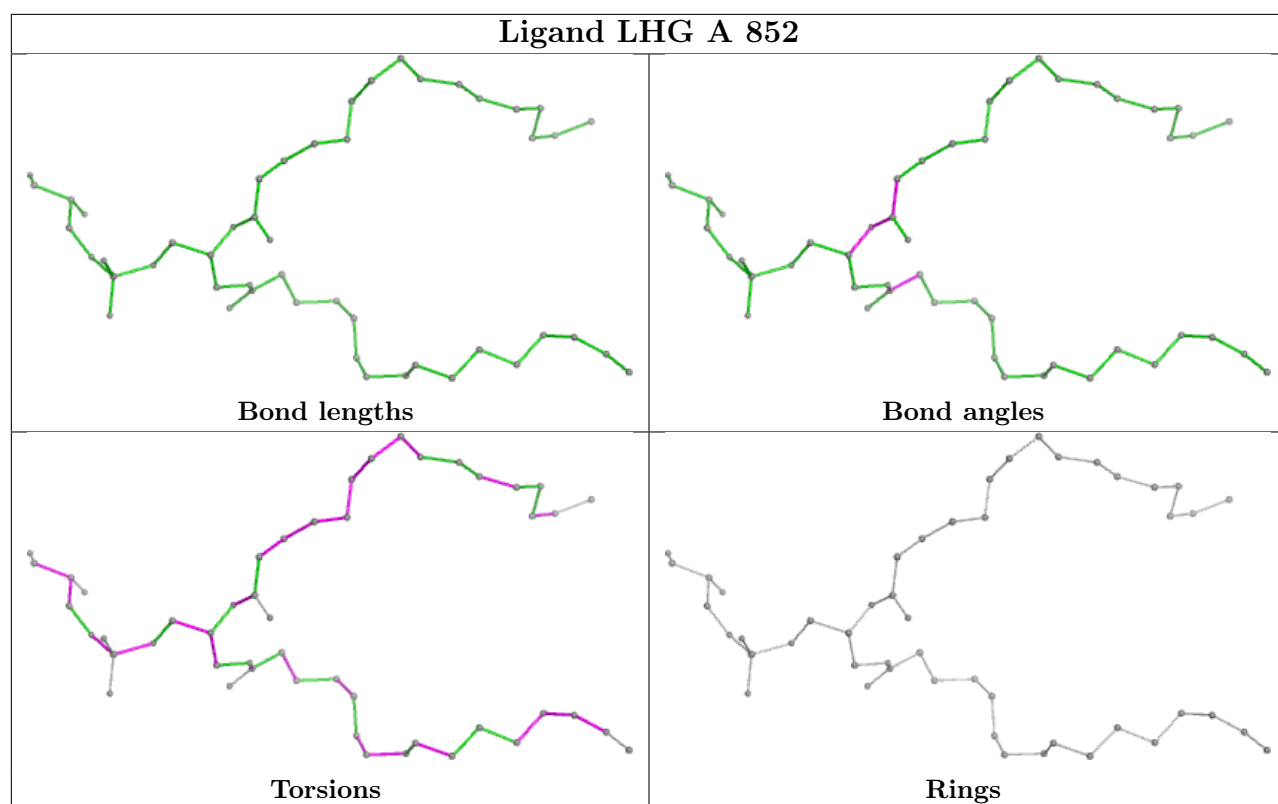


Torsions

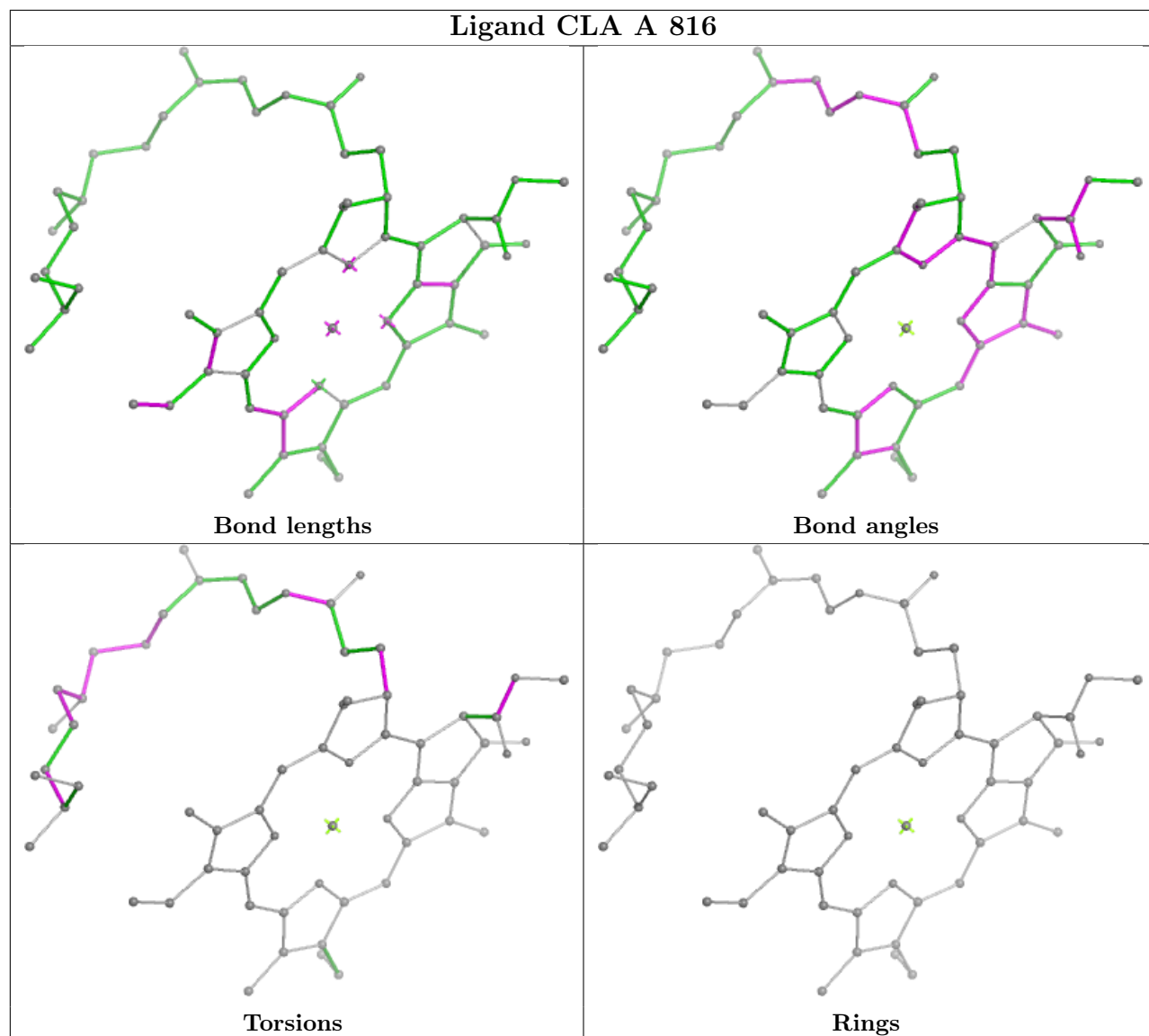


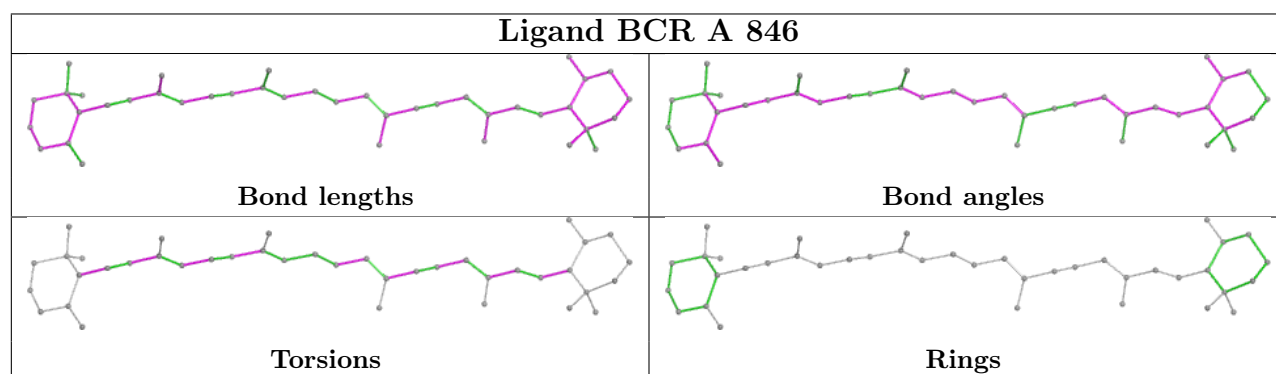
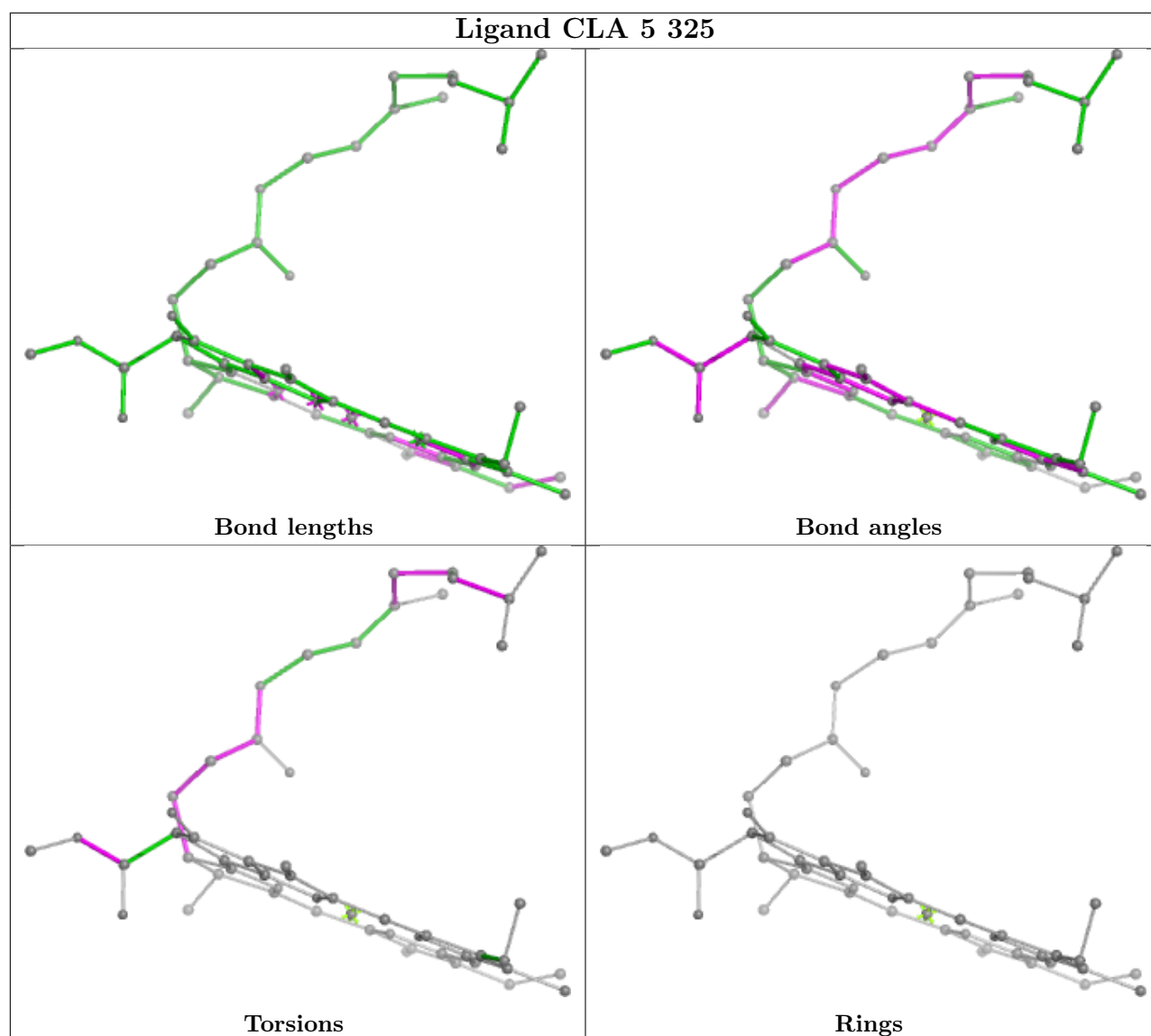
Rings

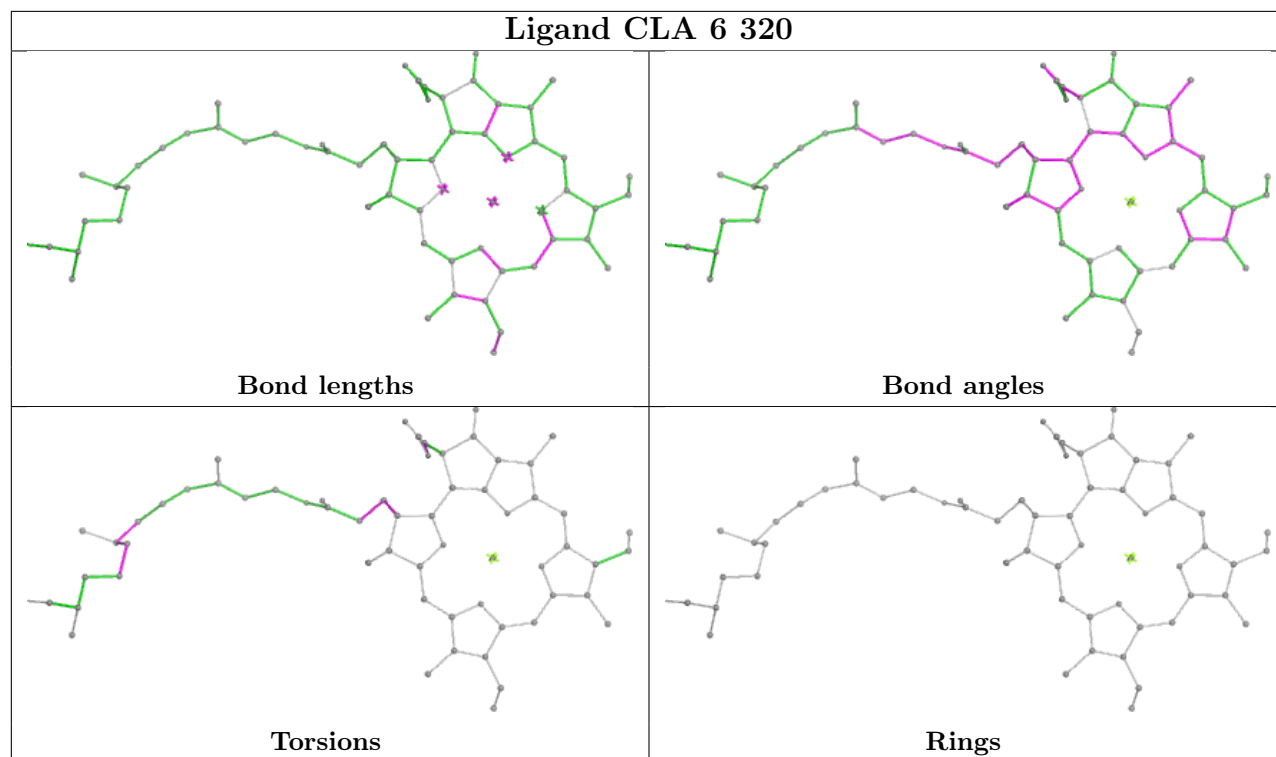




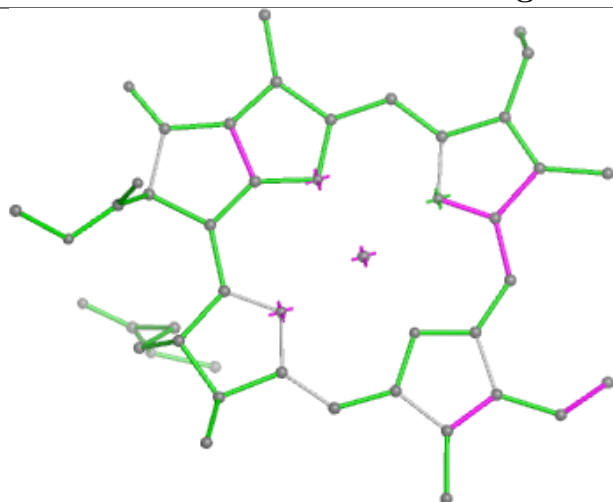
Ligand CLA A 816



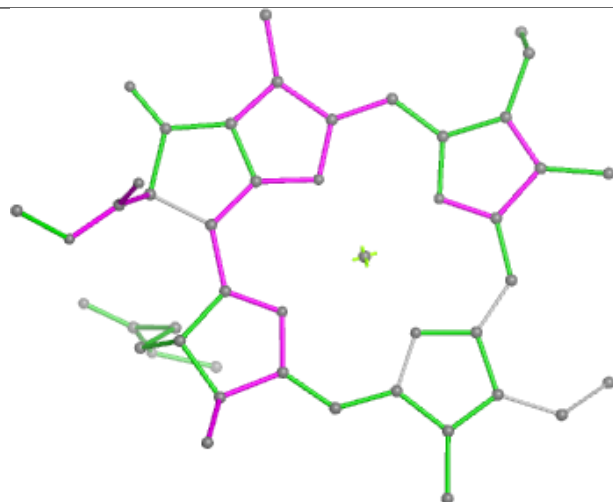




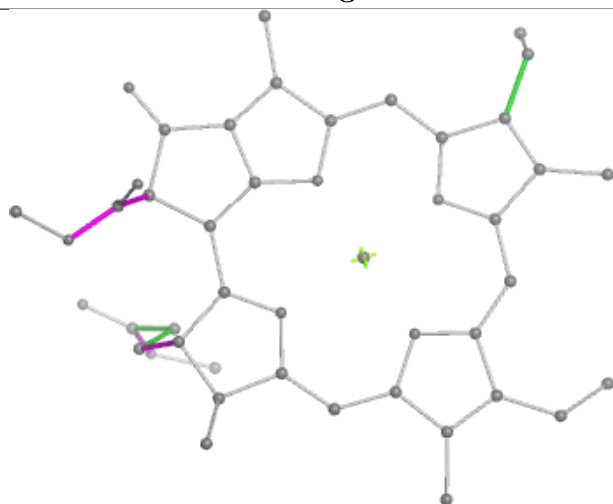
Ligand CLA Z 314



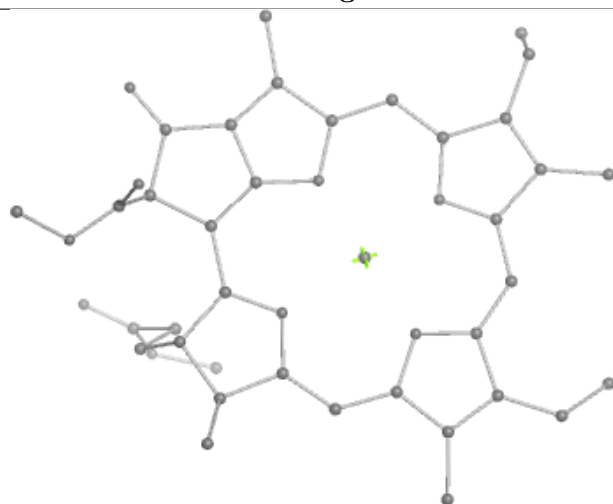
Bond lengths



Bond angles

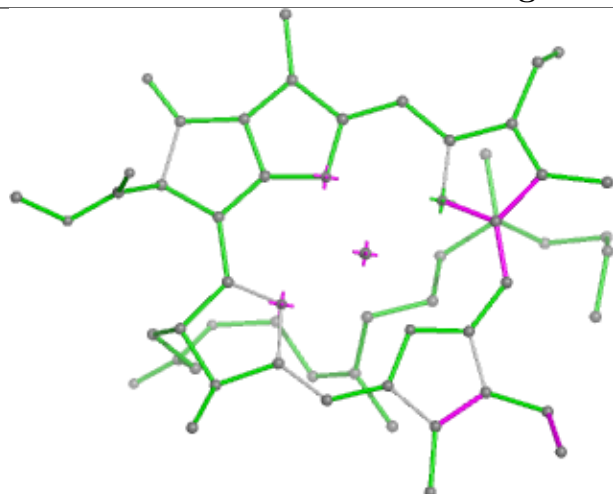


Torsions

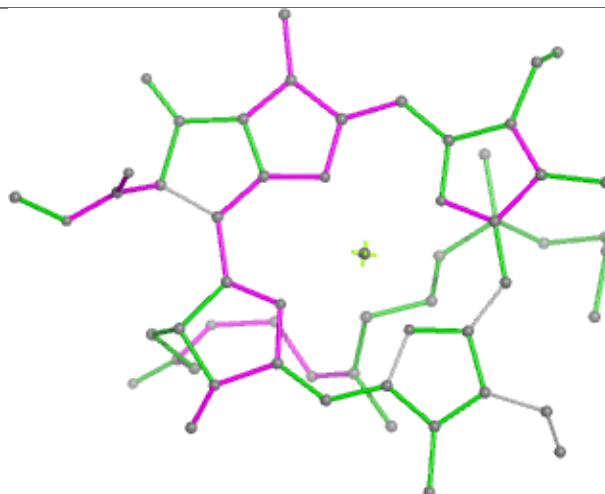


Rings

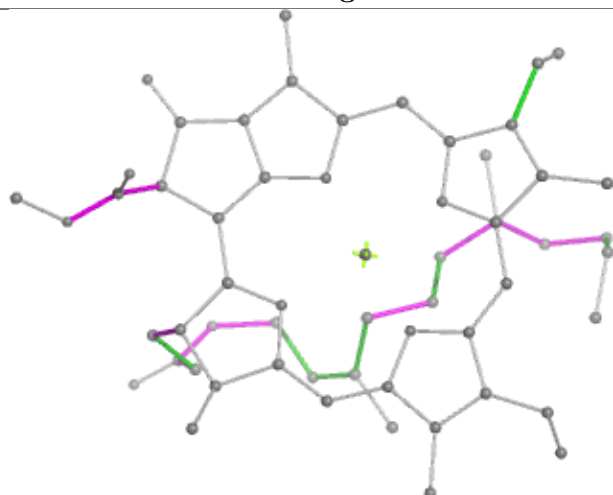
Ligand CLA 7 319



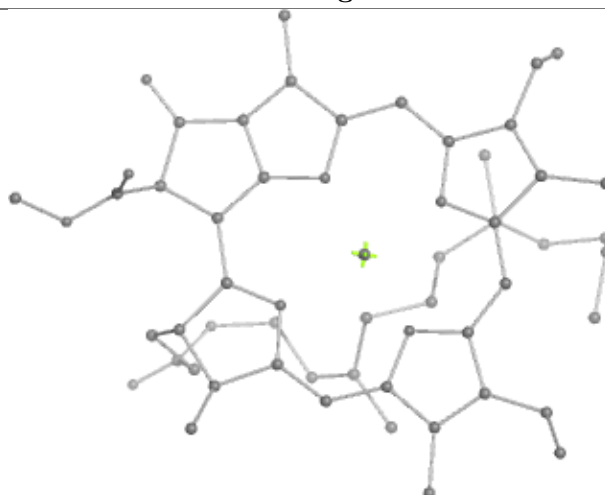
Bond lengths



Bond angles

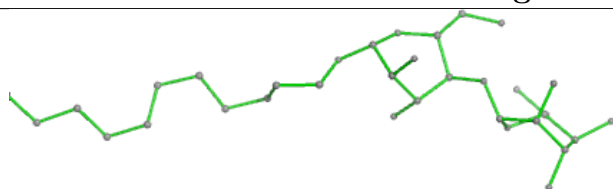


Torsions

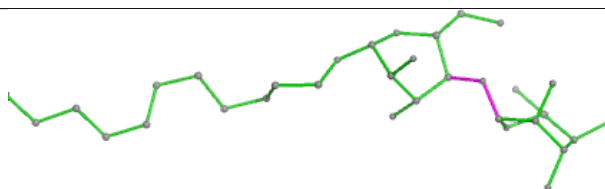


Rings

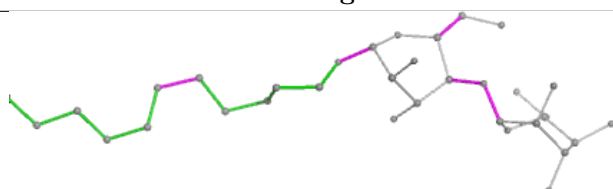
Ligand LMT Z 319



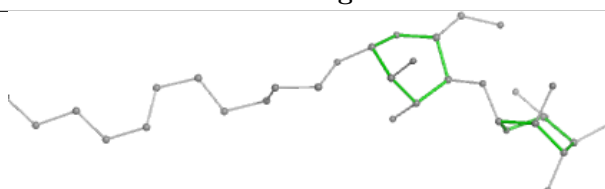
Bond lengths



Bond angles

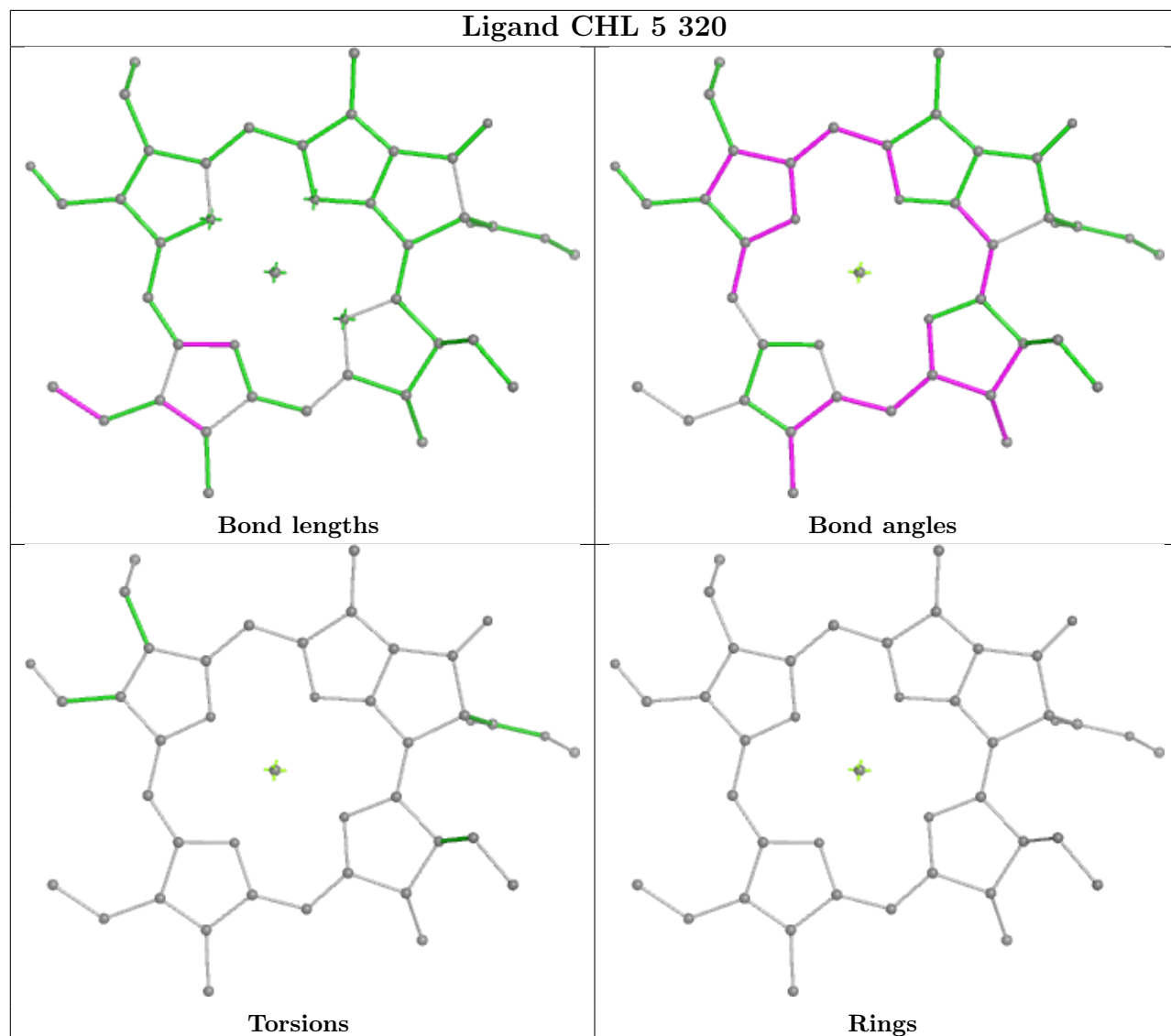


Torsions

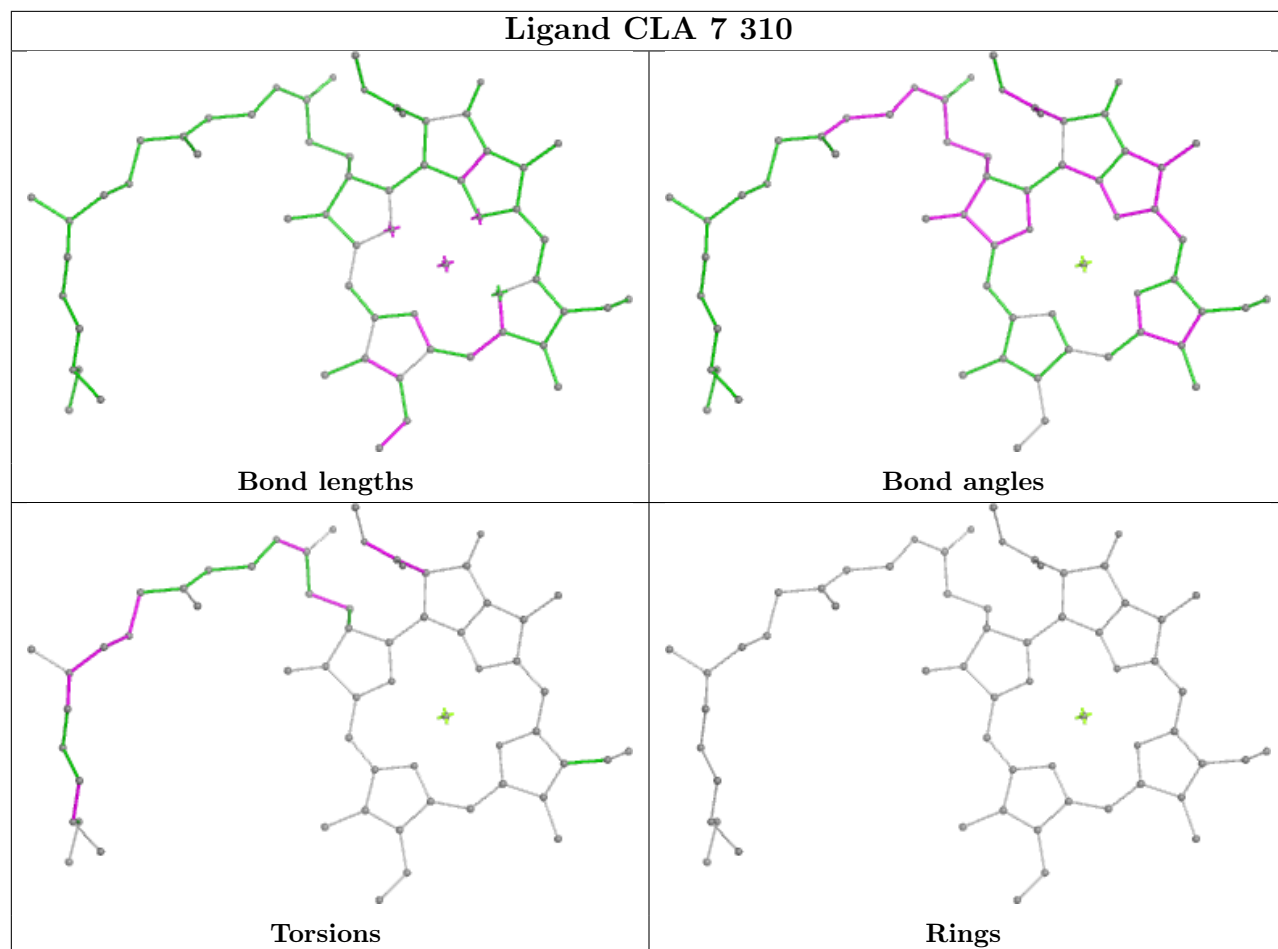


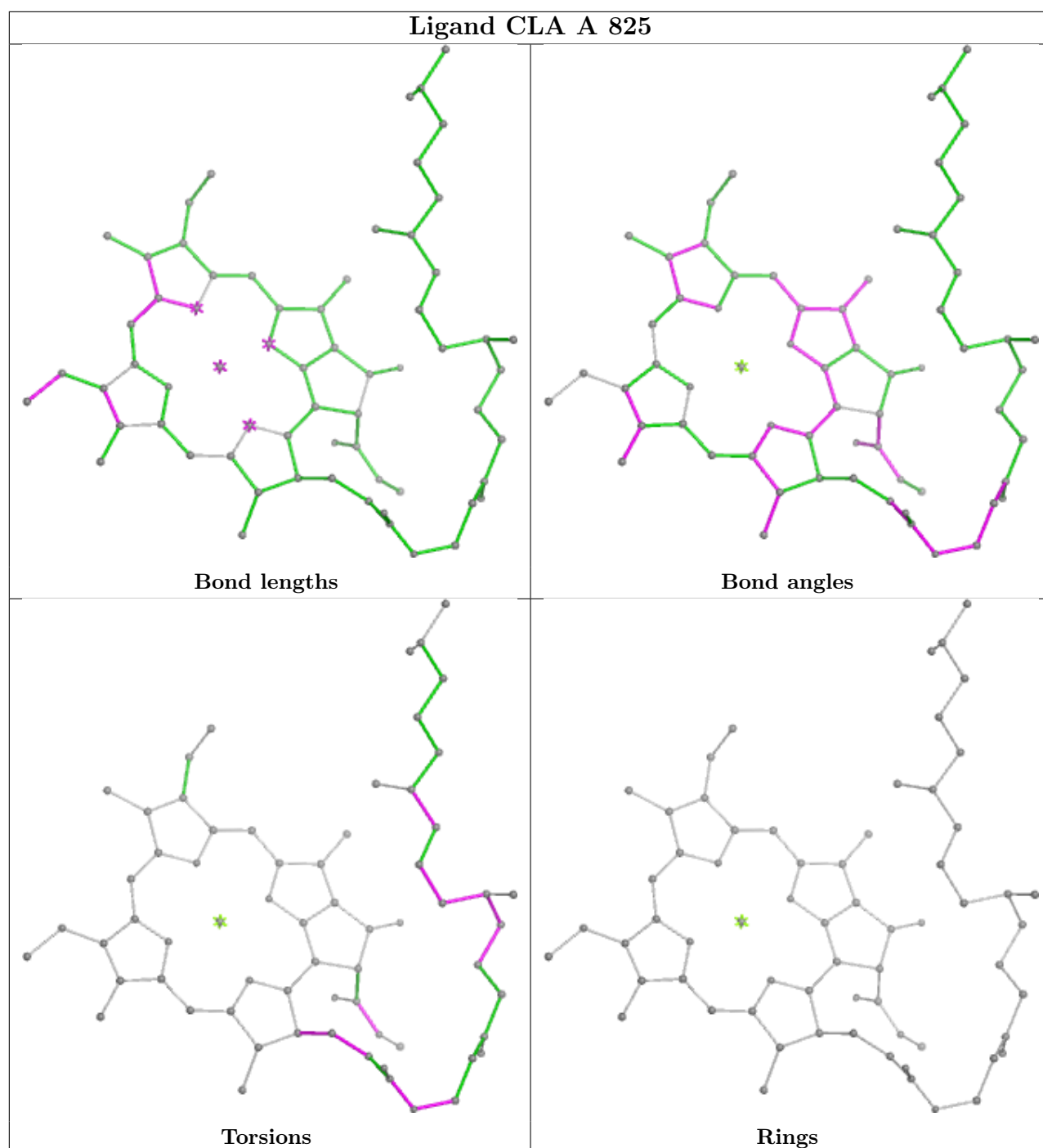
Rings

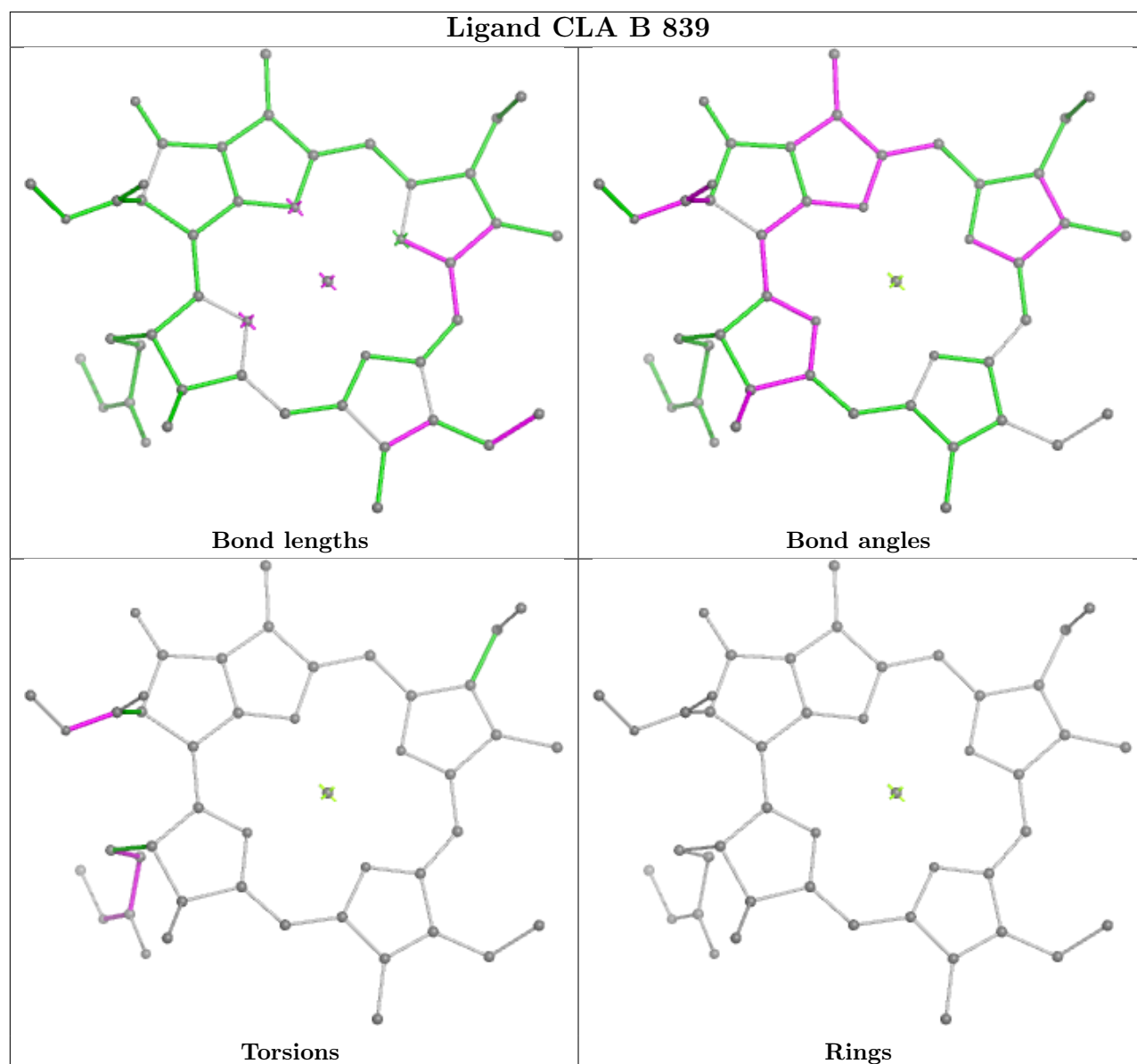
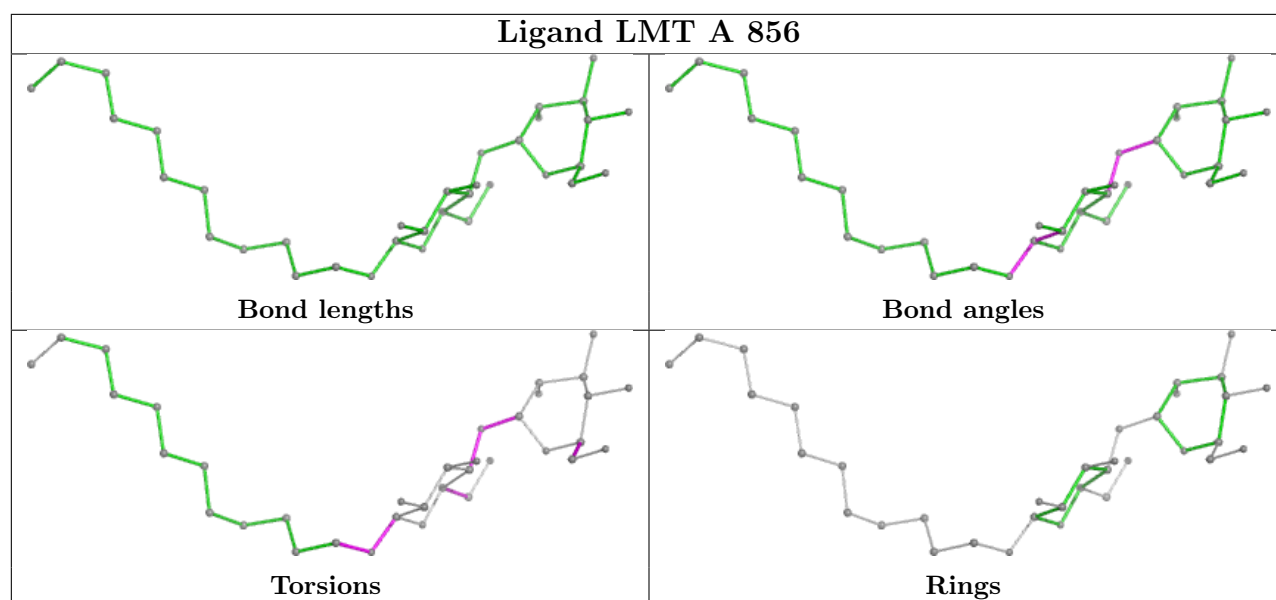
Ligand CHL 5 320

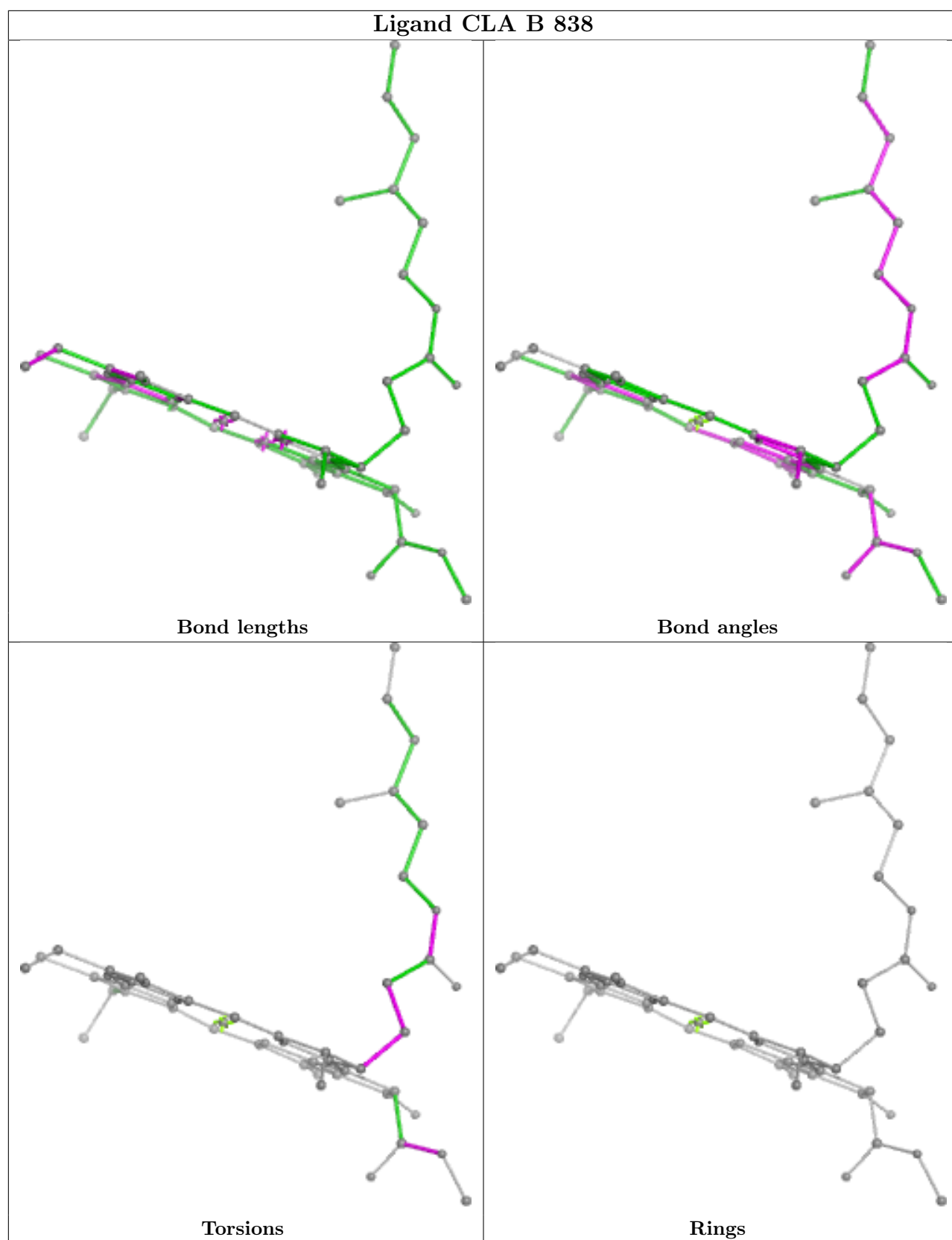


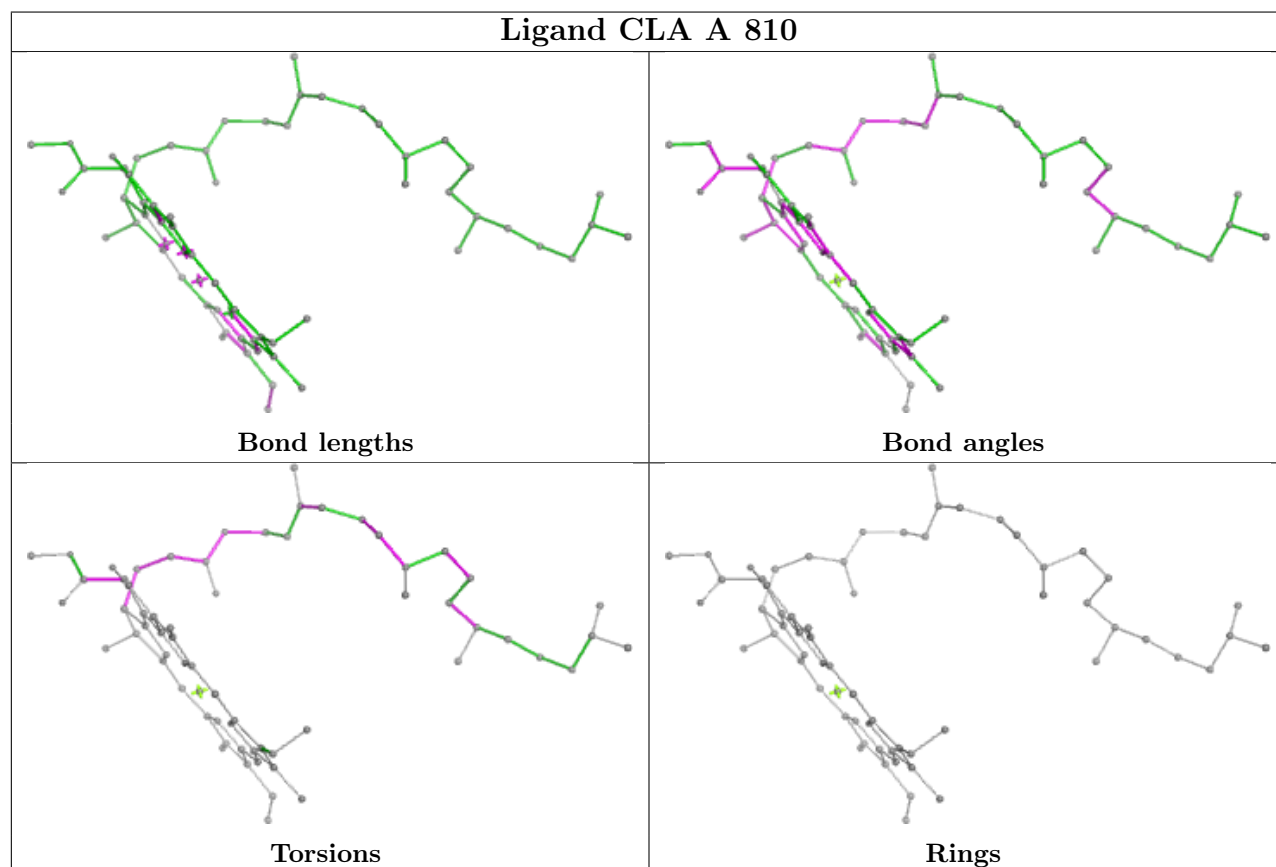
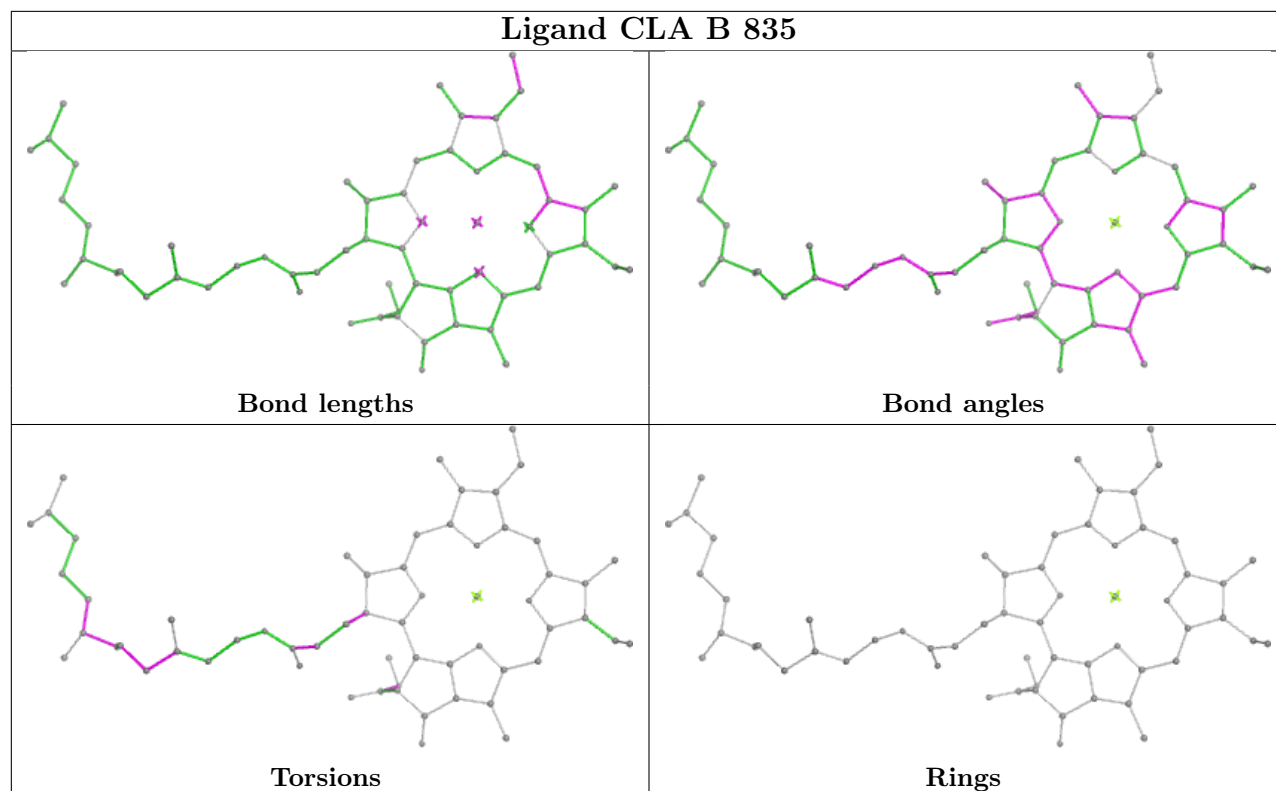
Ligand CLA 7 310

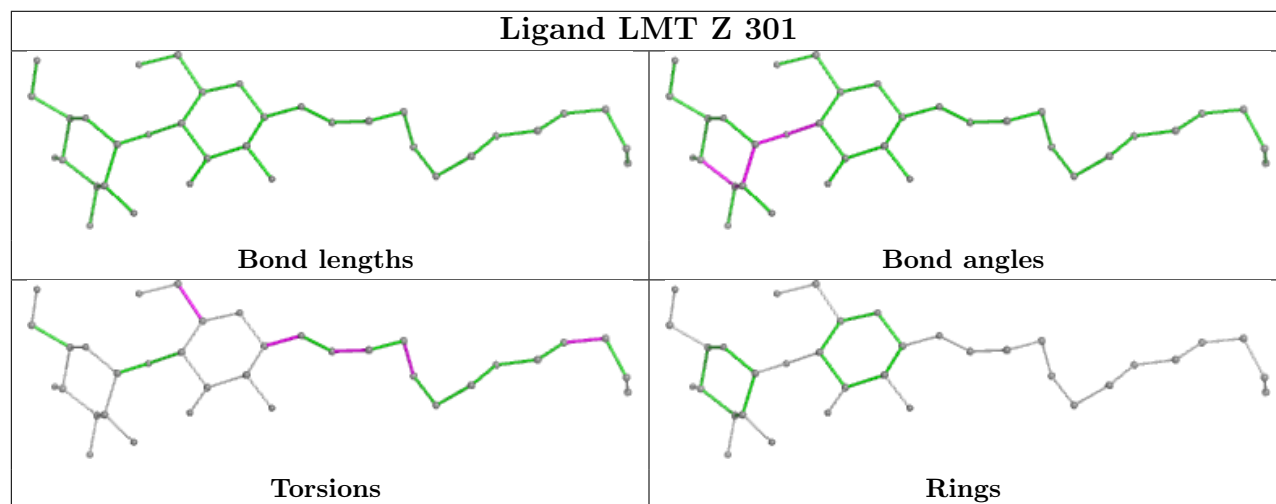
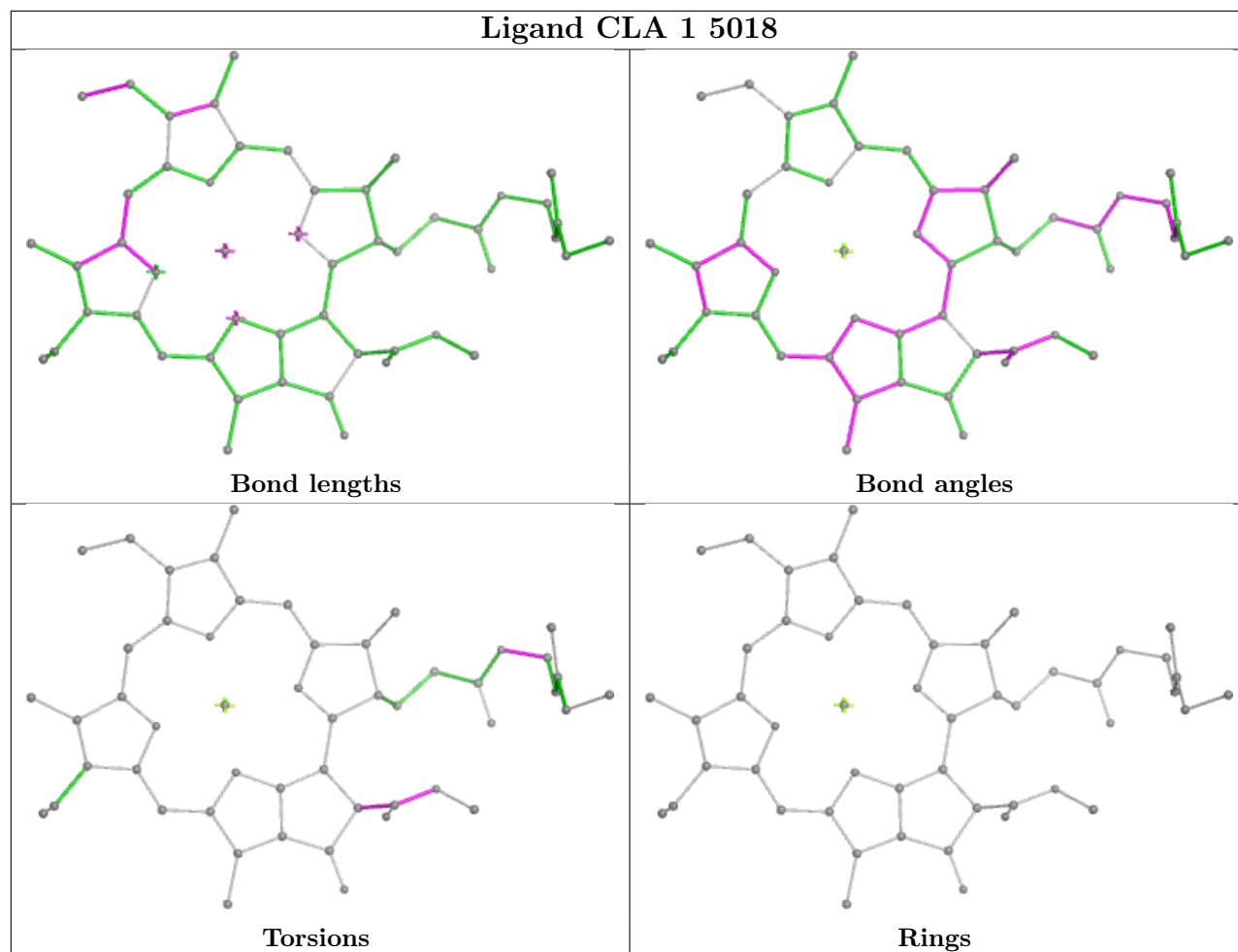


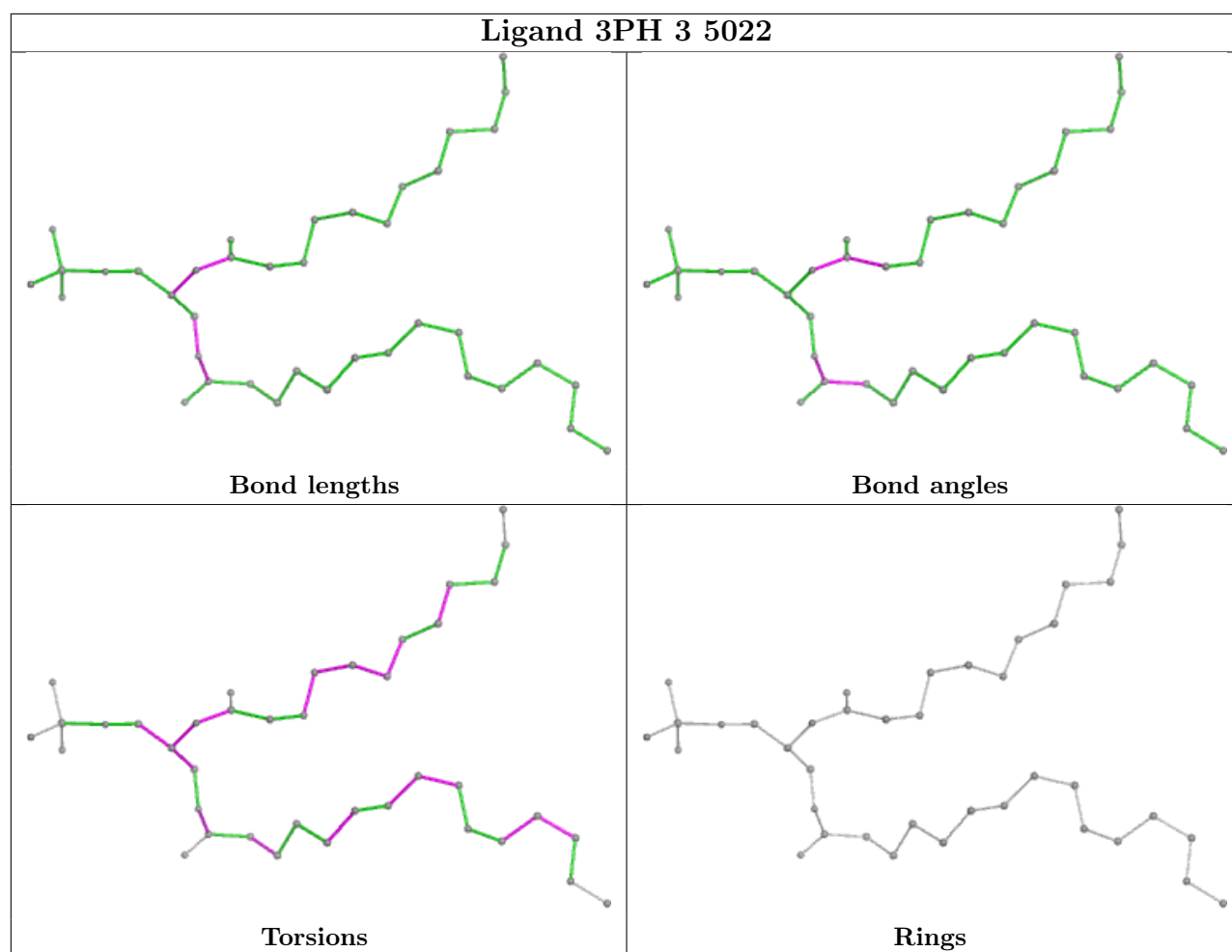


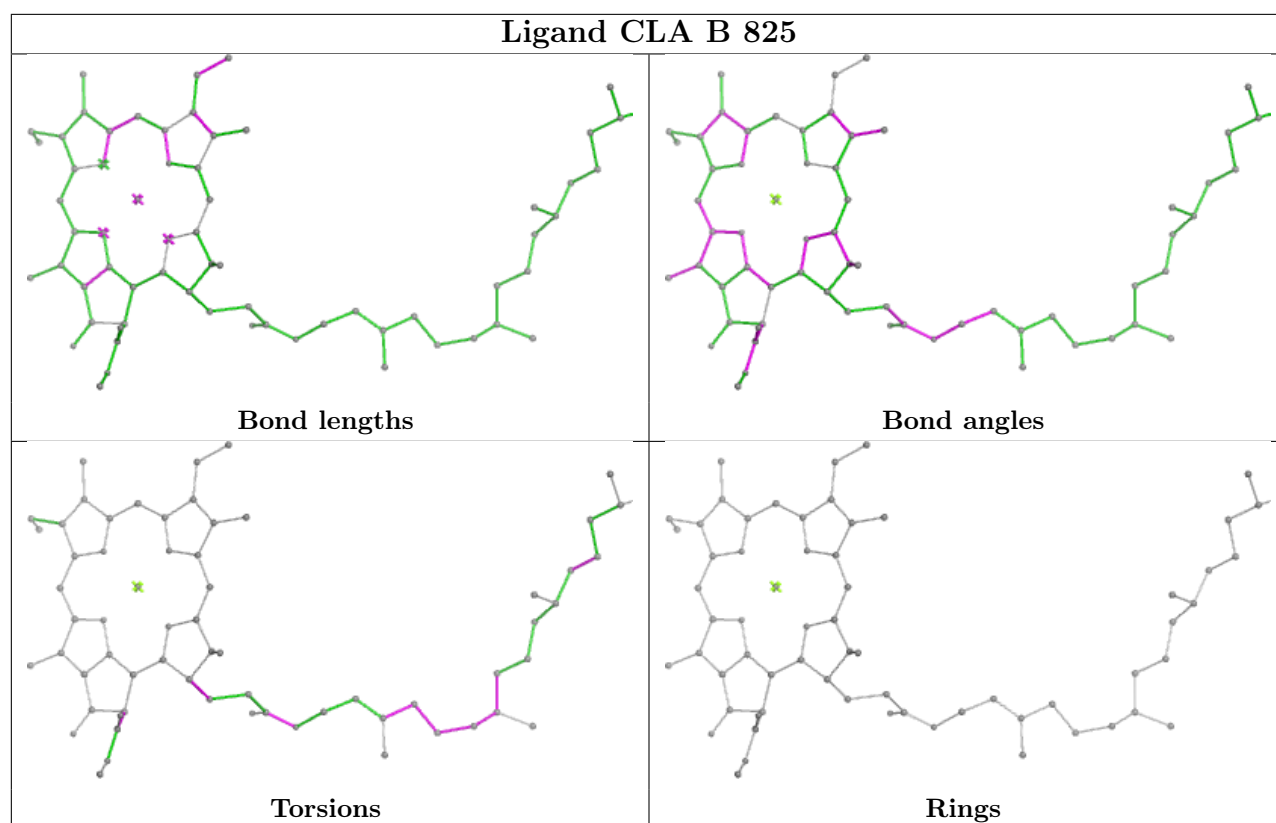




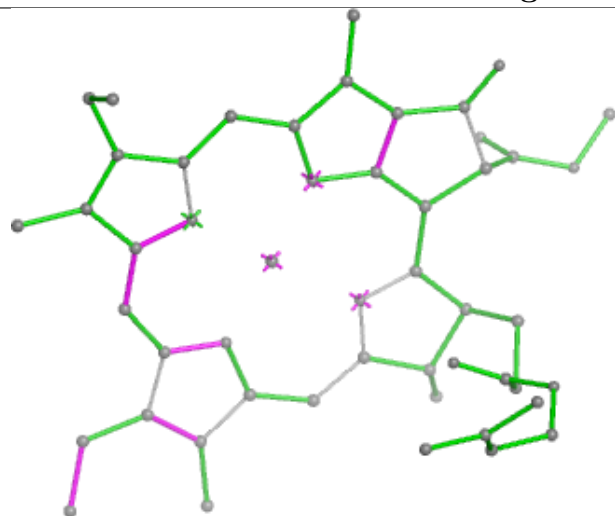




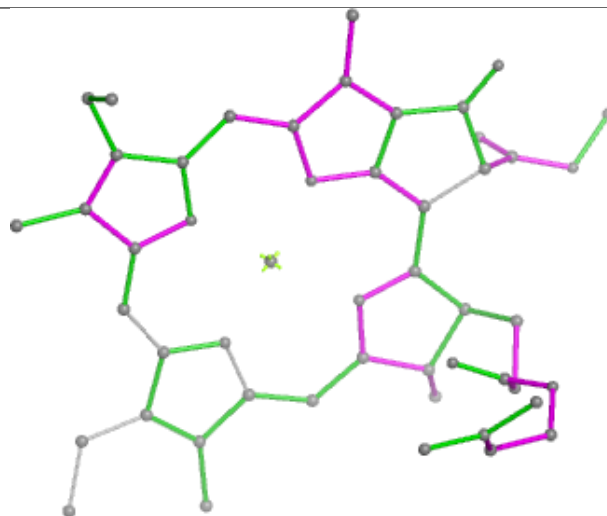




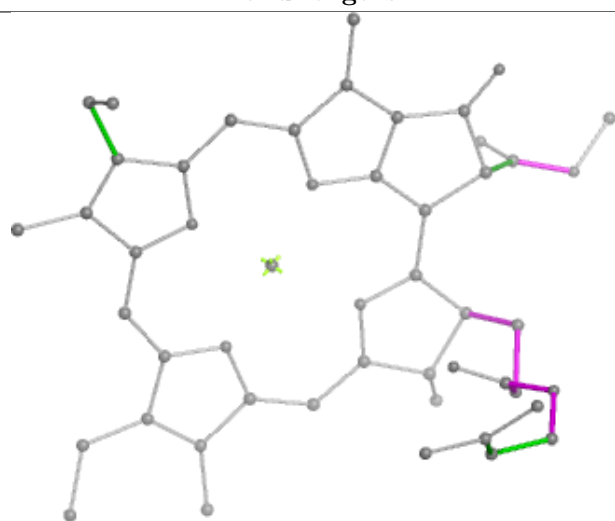
Ligand CLA 5 311



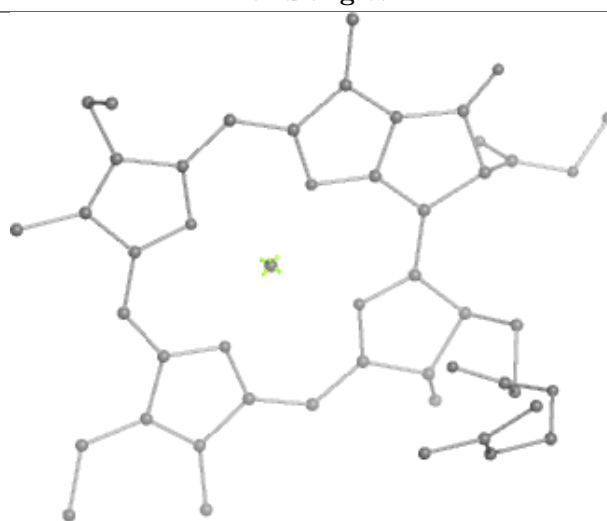
Bond lengths



Bond angles

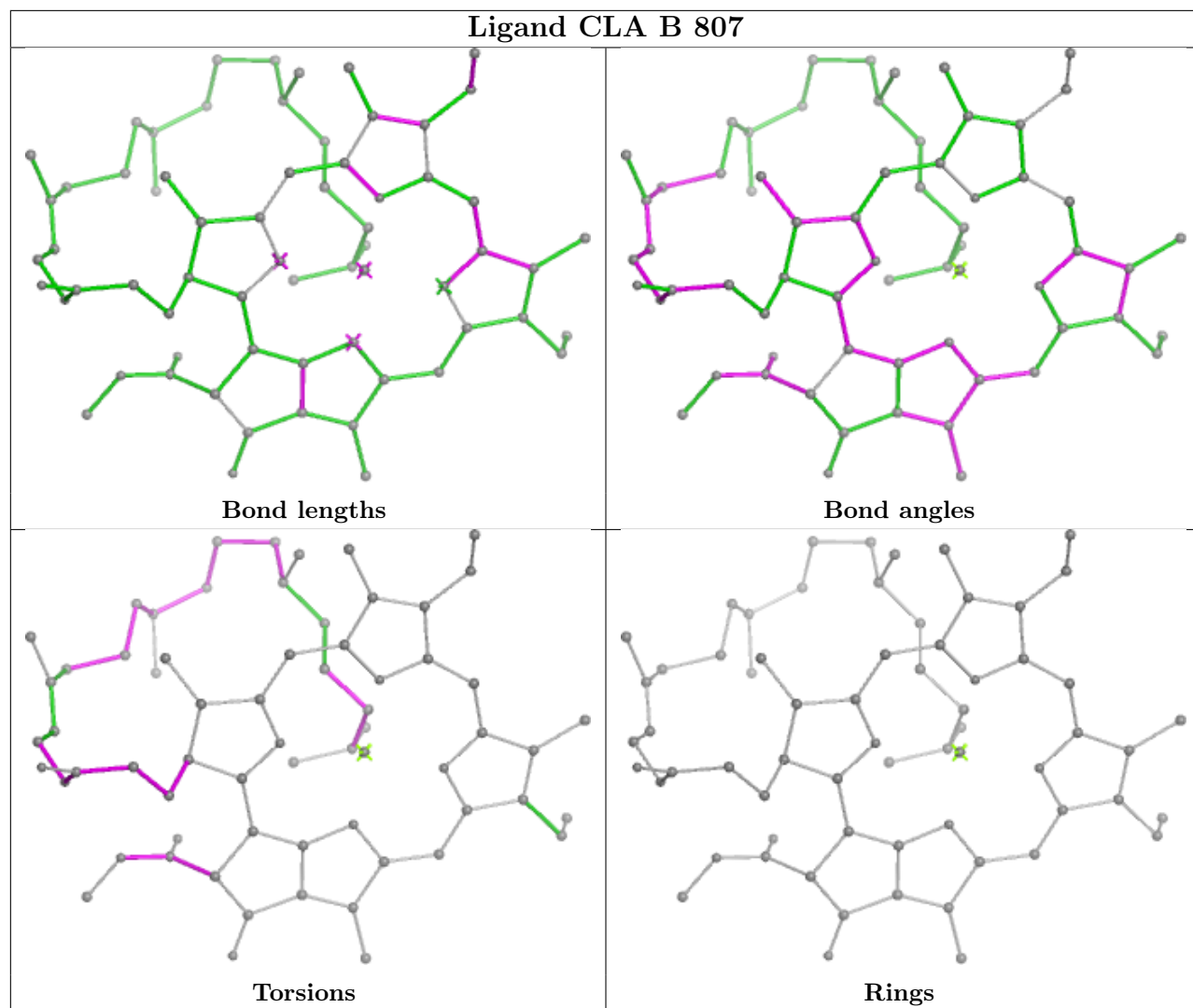


Torsions

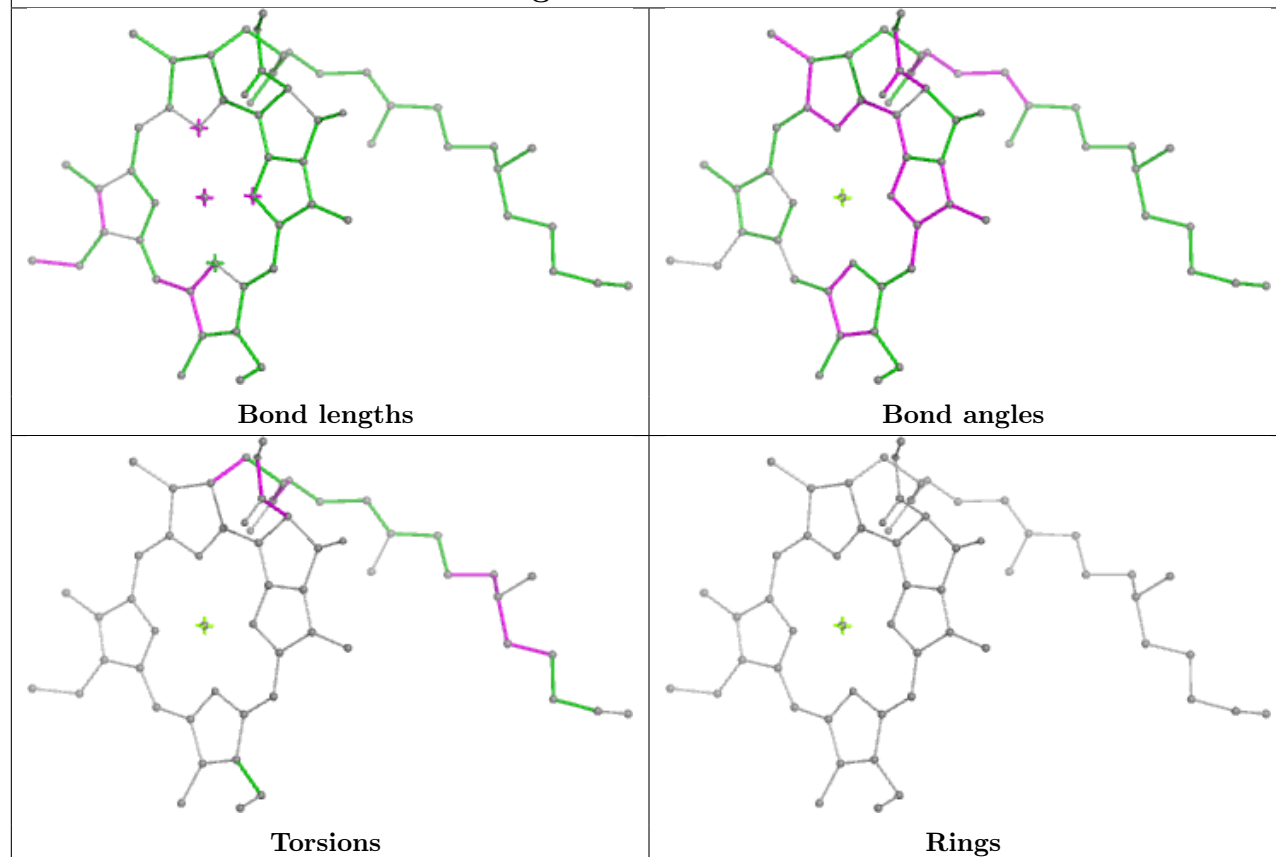


Rings

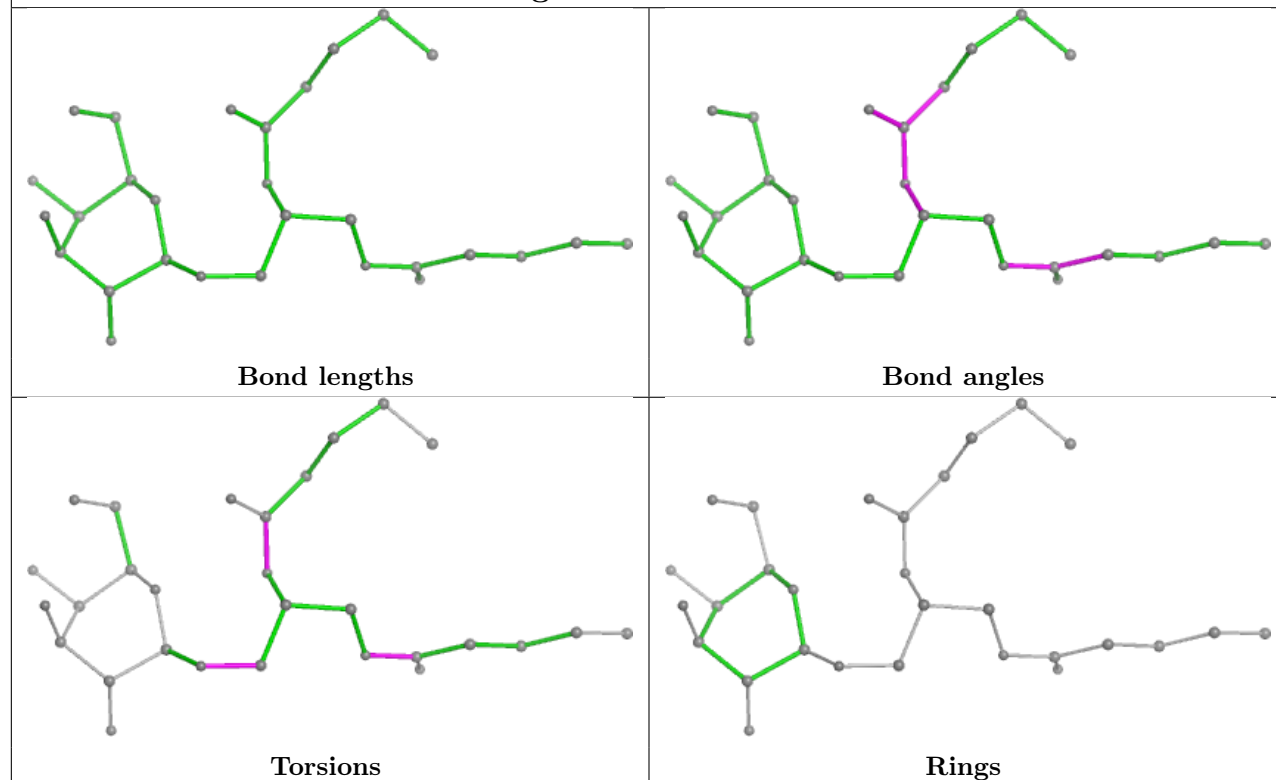
Ligand CLA B 807



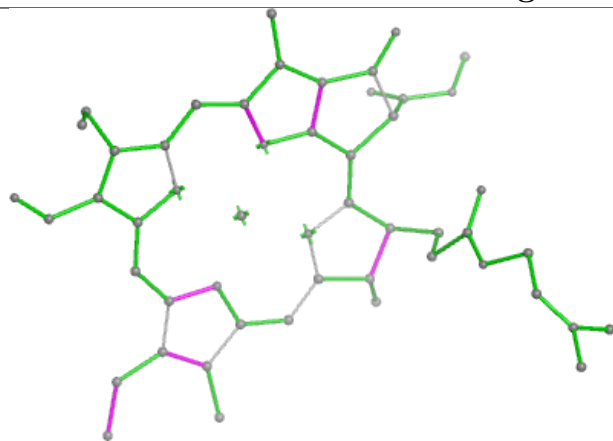
Ligand CLA B 822



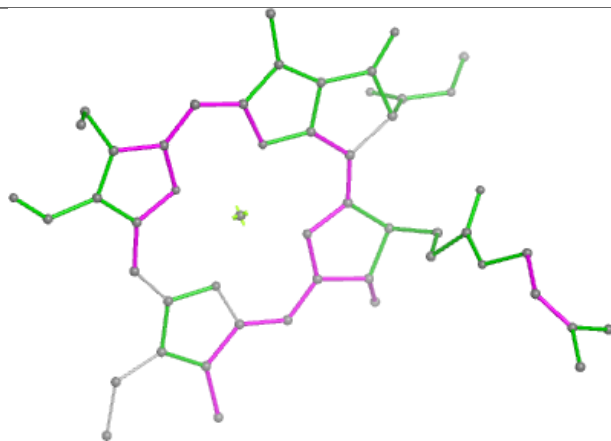
Ligand LMG 7 301



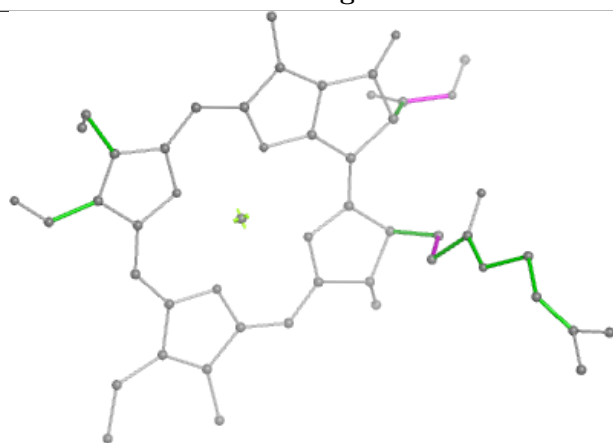
Ligand CHL 8 317



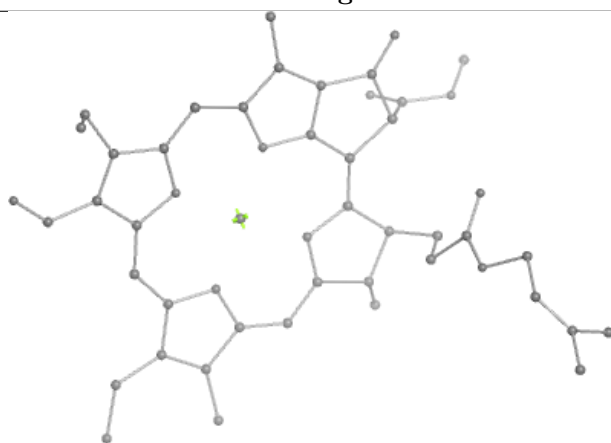
Bond lengths



Bond angles

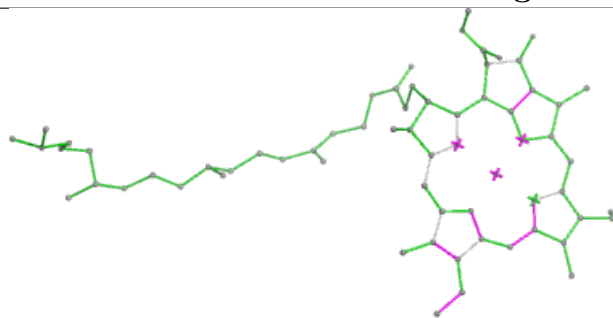


Torsions

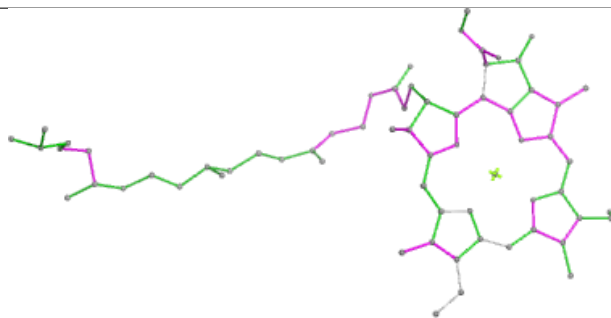


Rings

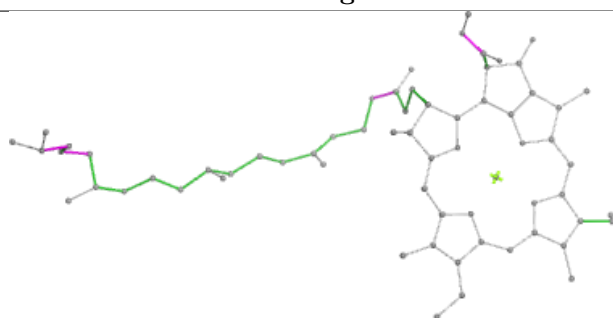
Ligand CLA A 815



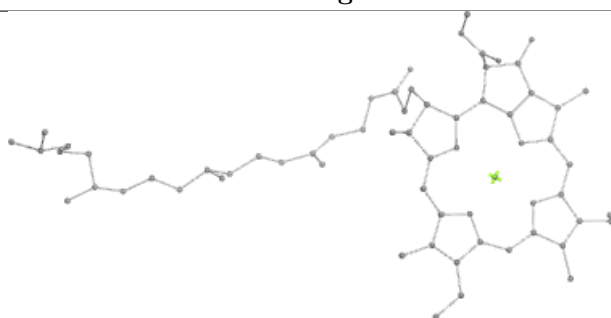
Bond lengths



Bond angles

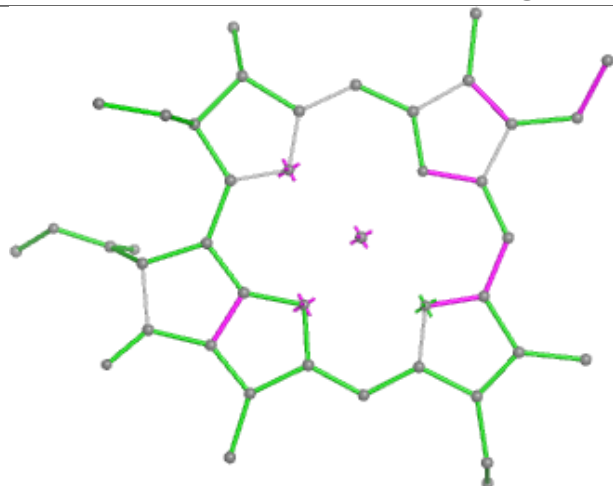


Torsions

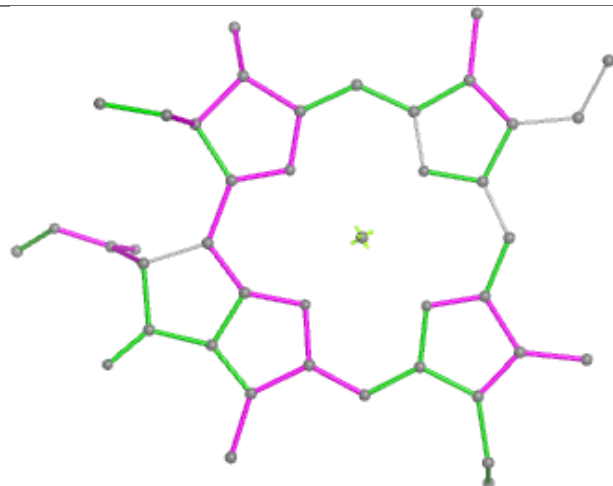


Rings

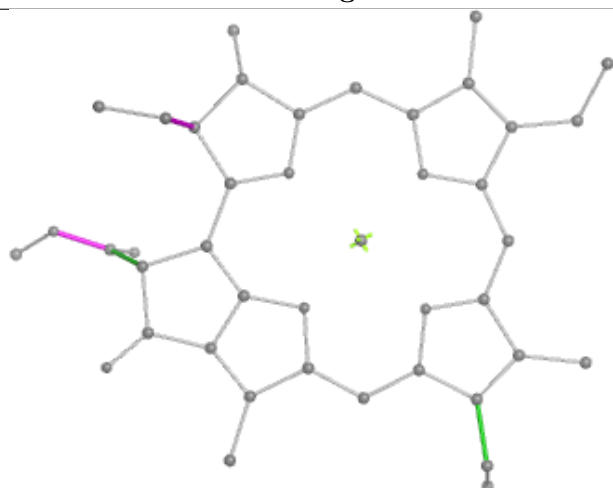
Ligand CLA 7 318



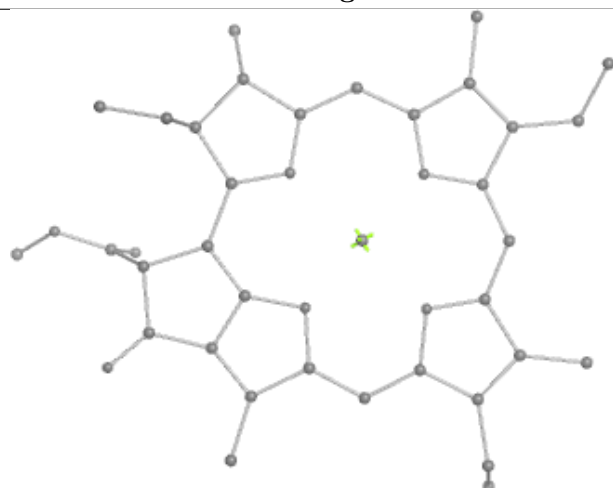
Bond lengths



Bond angles

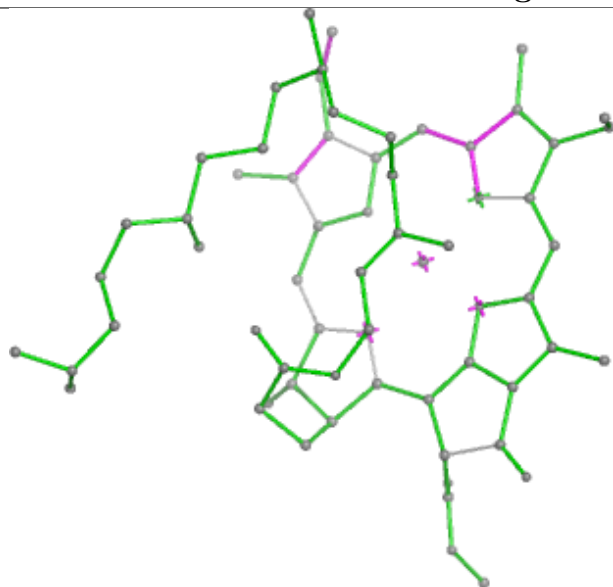


Torsions

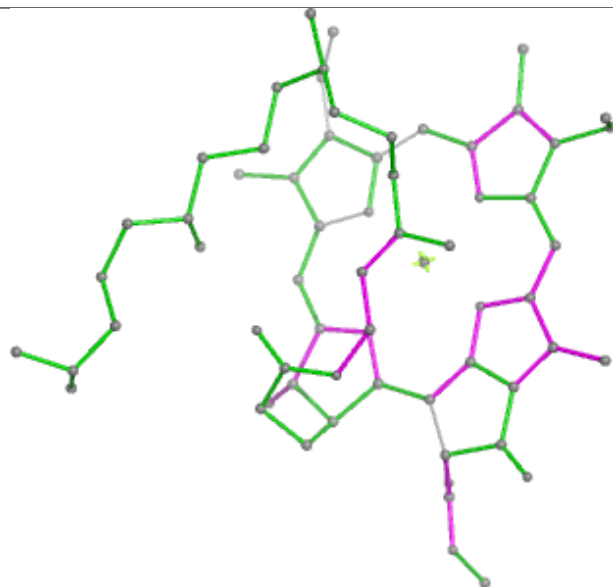


Rings

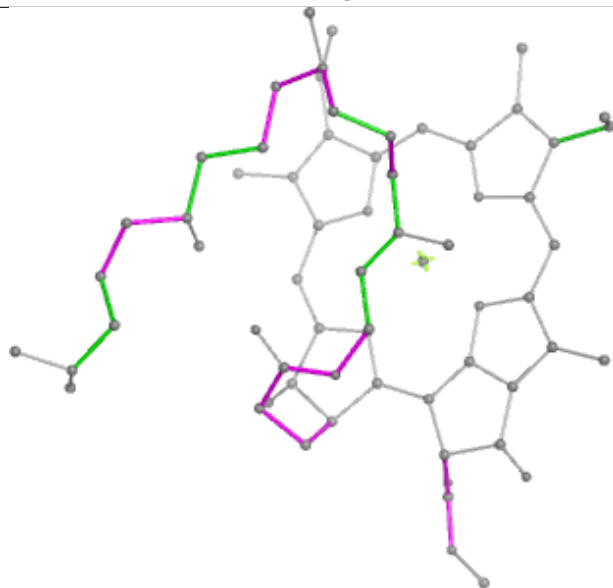
Ligand CLA B 808



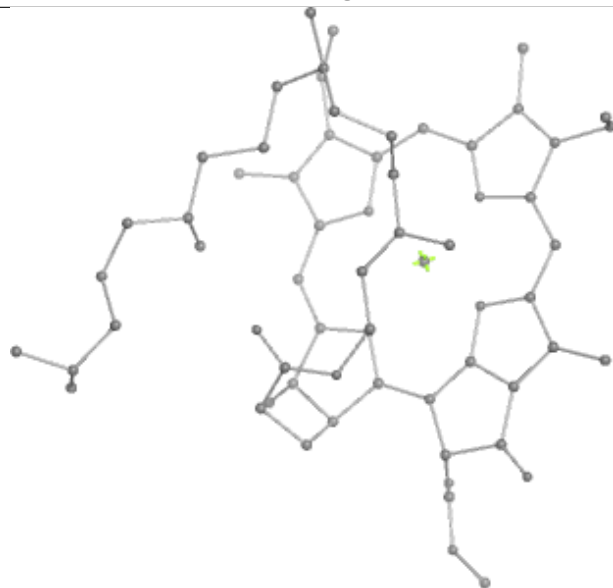
Bond lengths



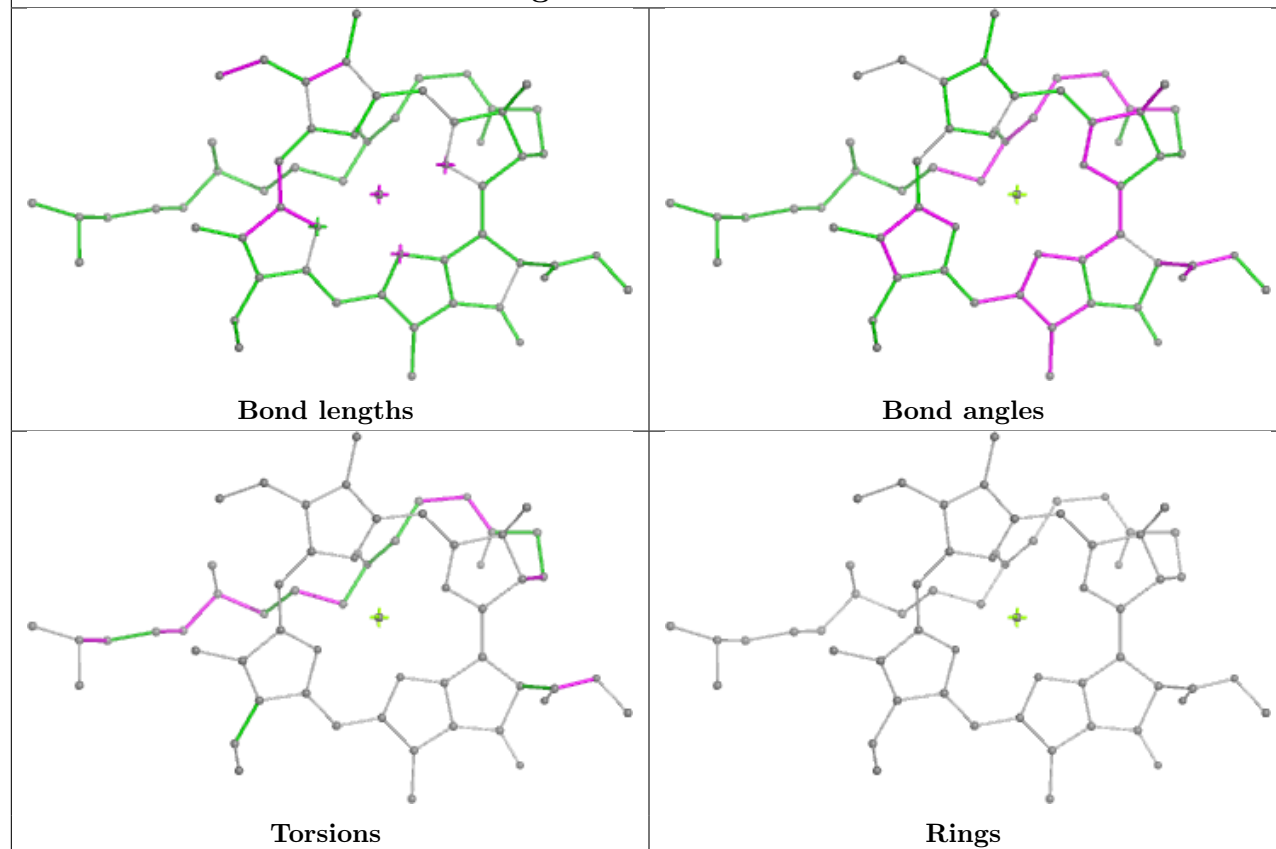
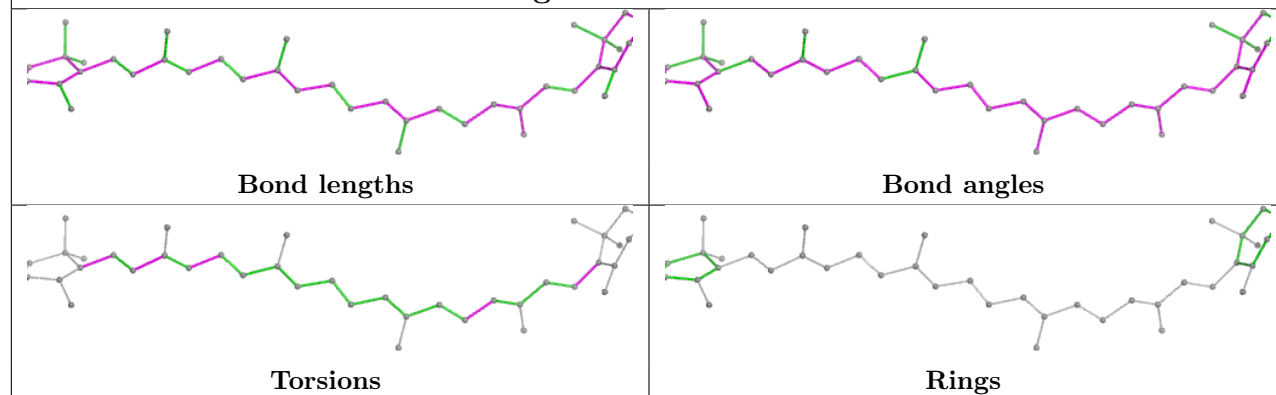
Bond angles



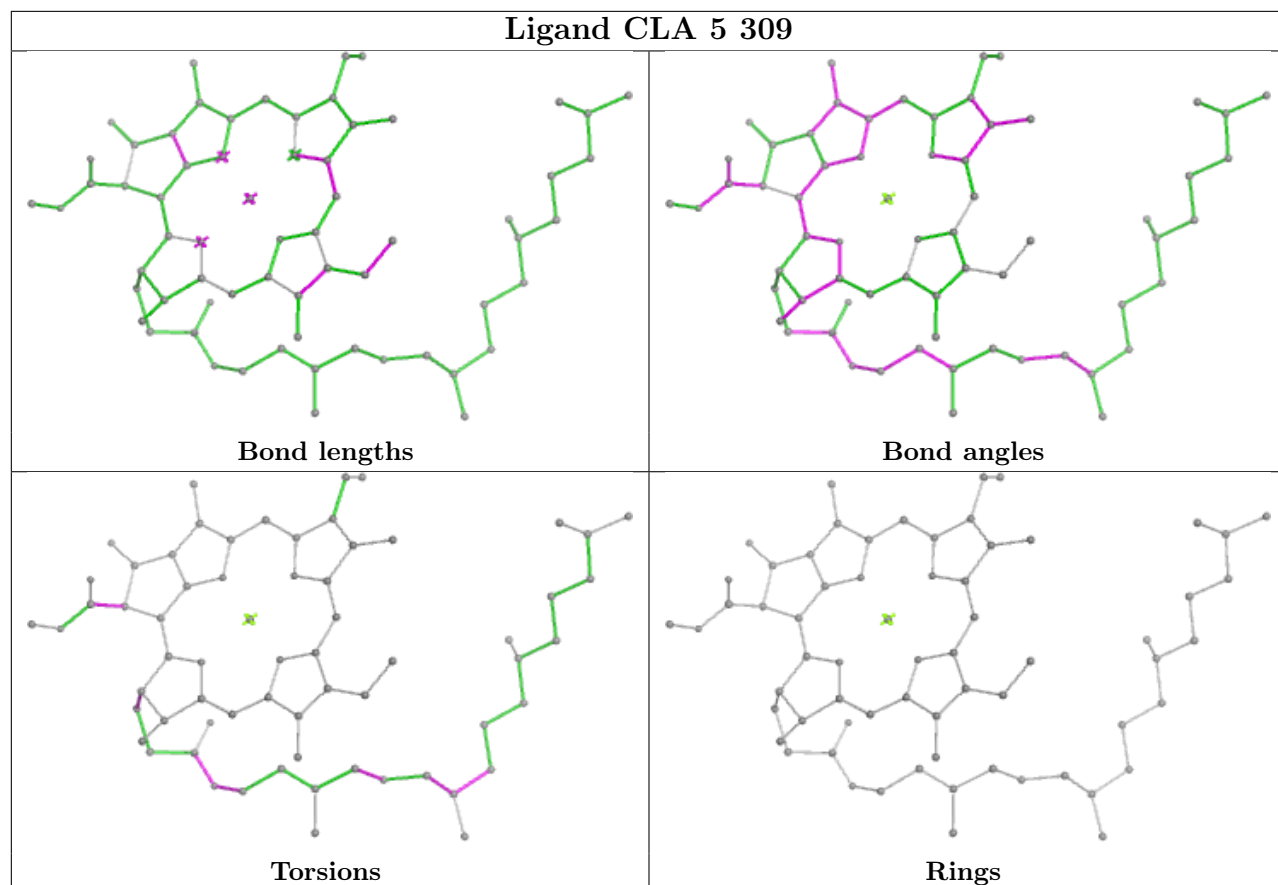
Torsions

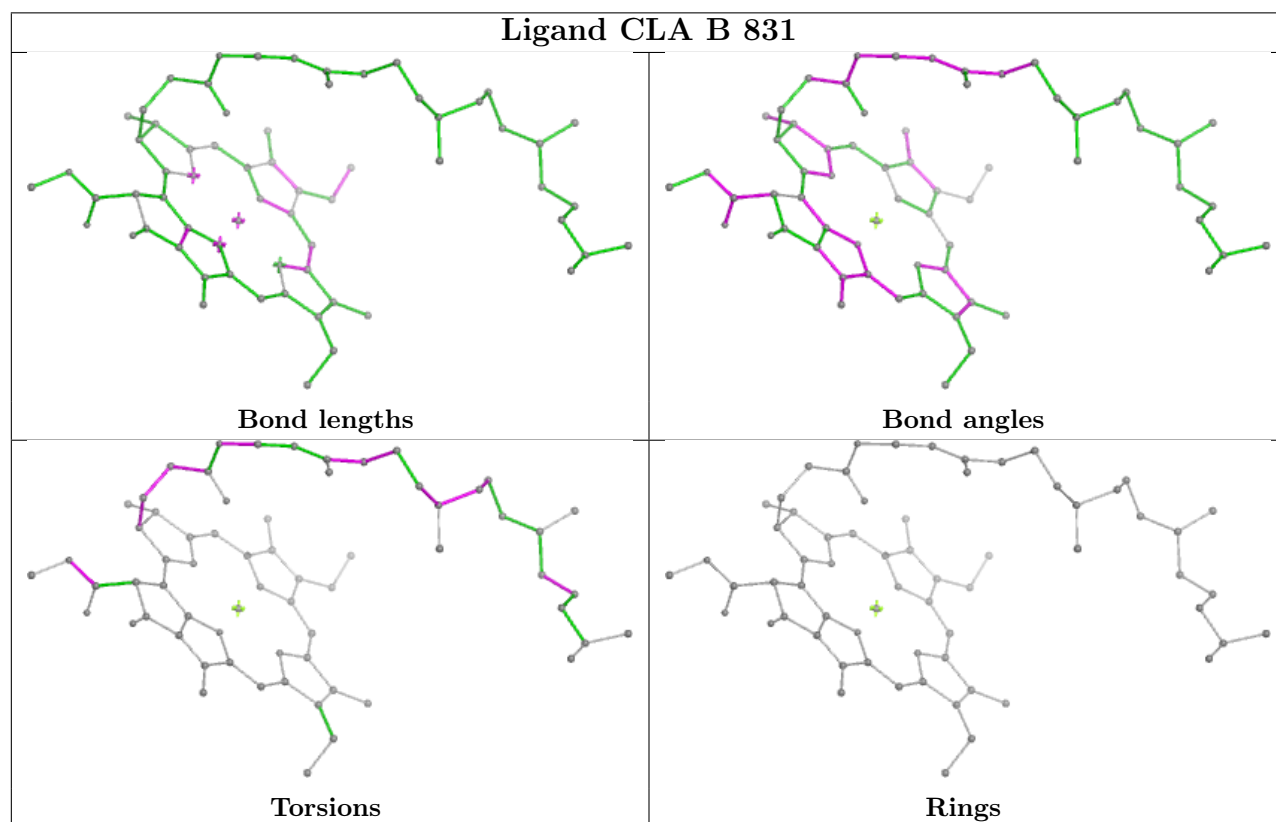
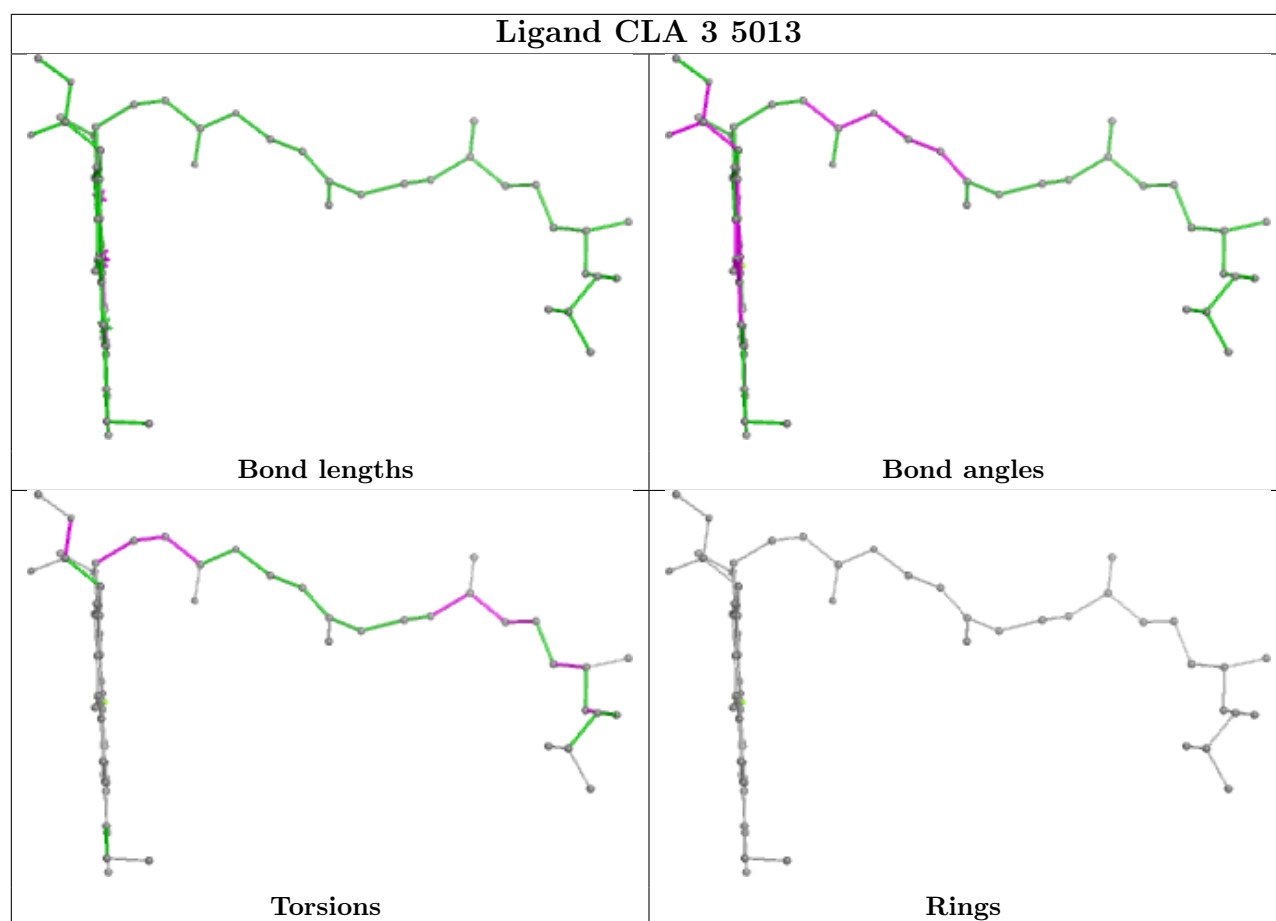


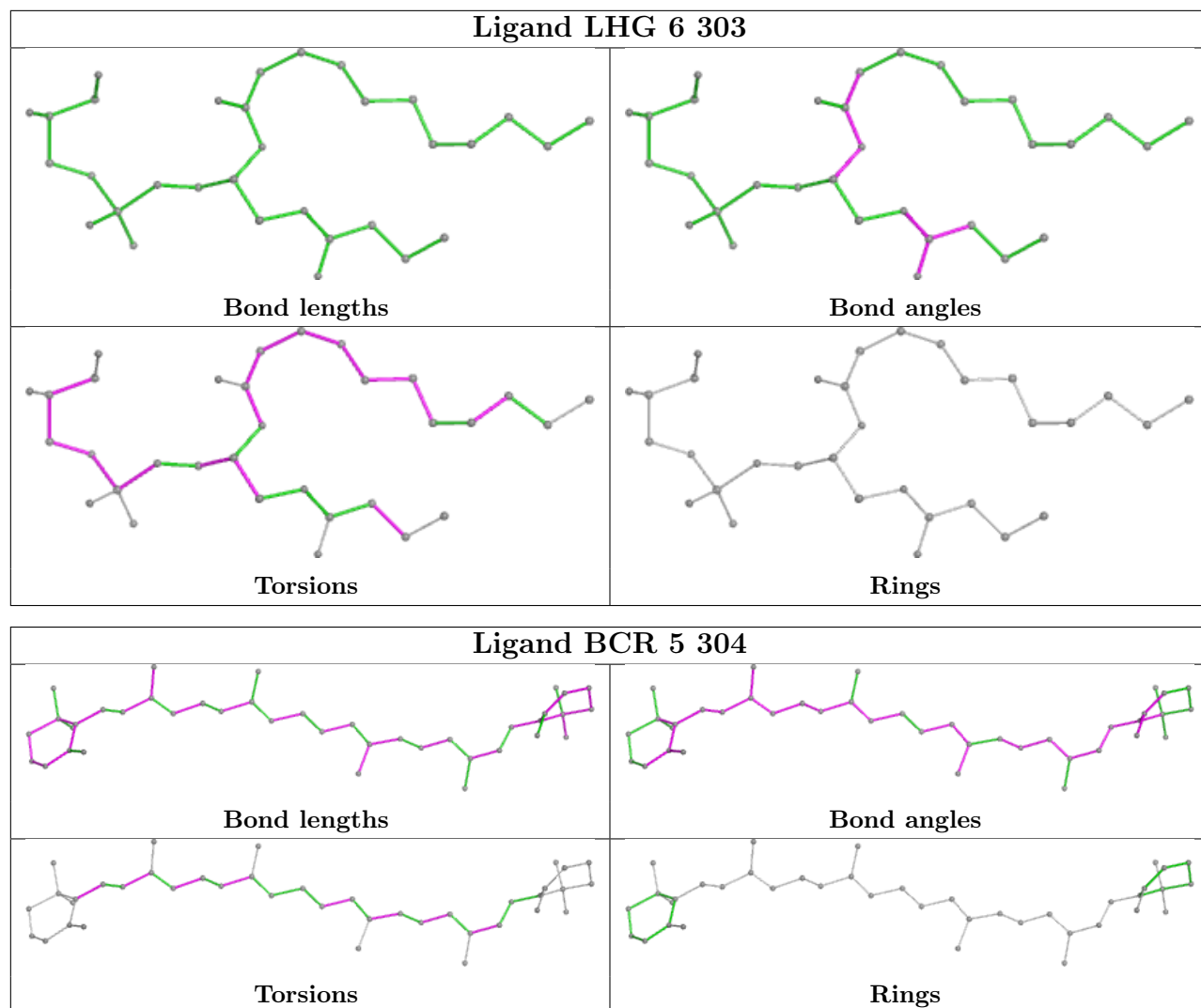
Rings

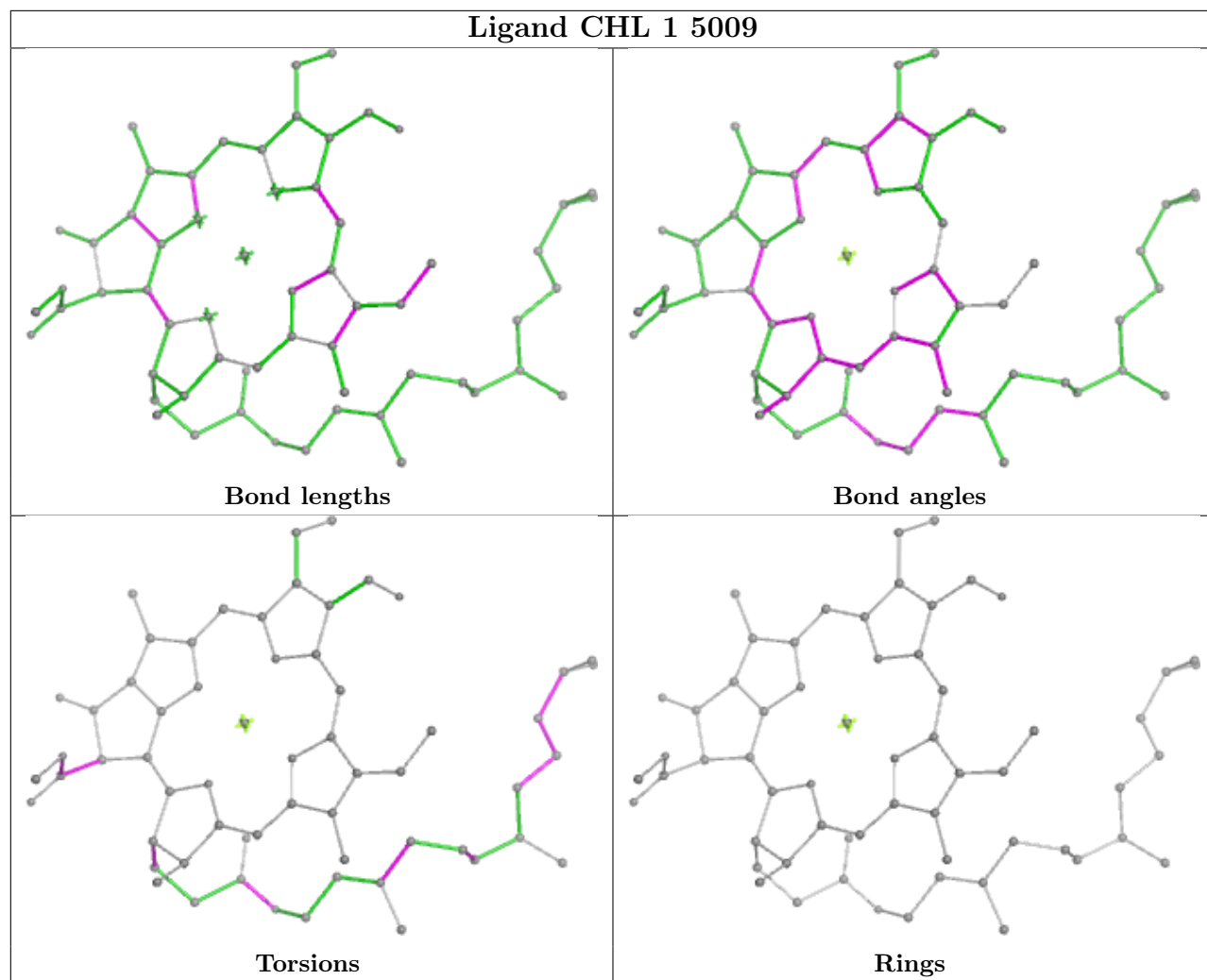
Ligand CLA A 818**Ligand RRX 5 302**

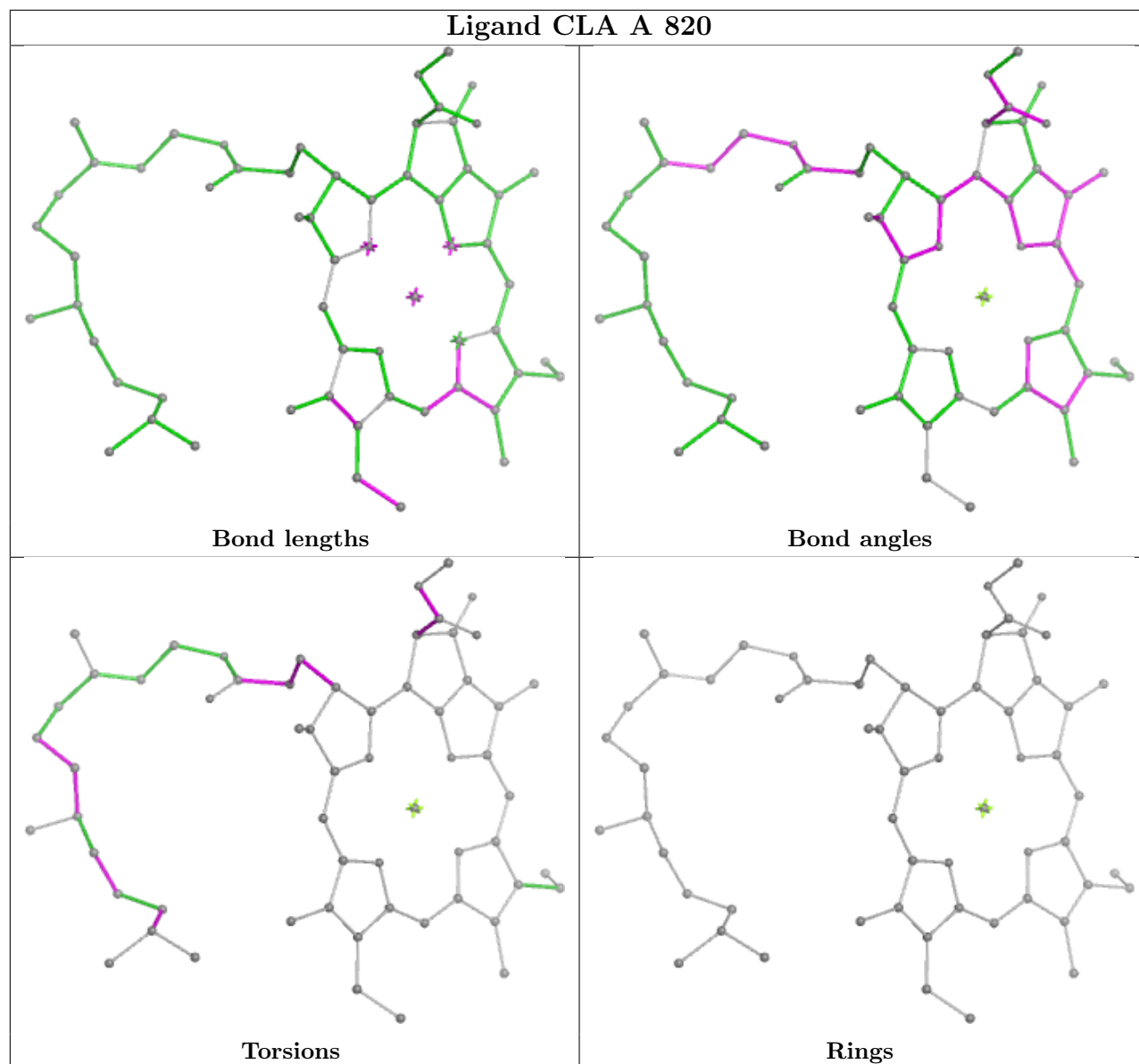
Ligand CLA 5 309

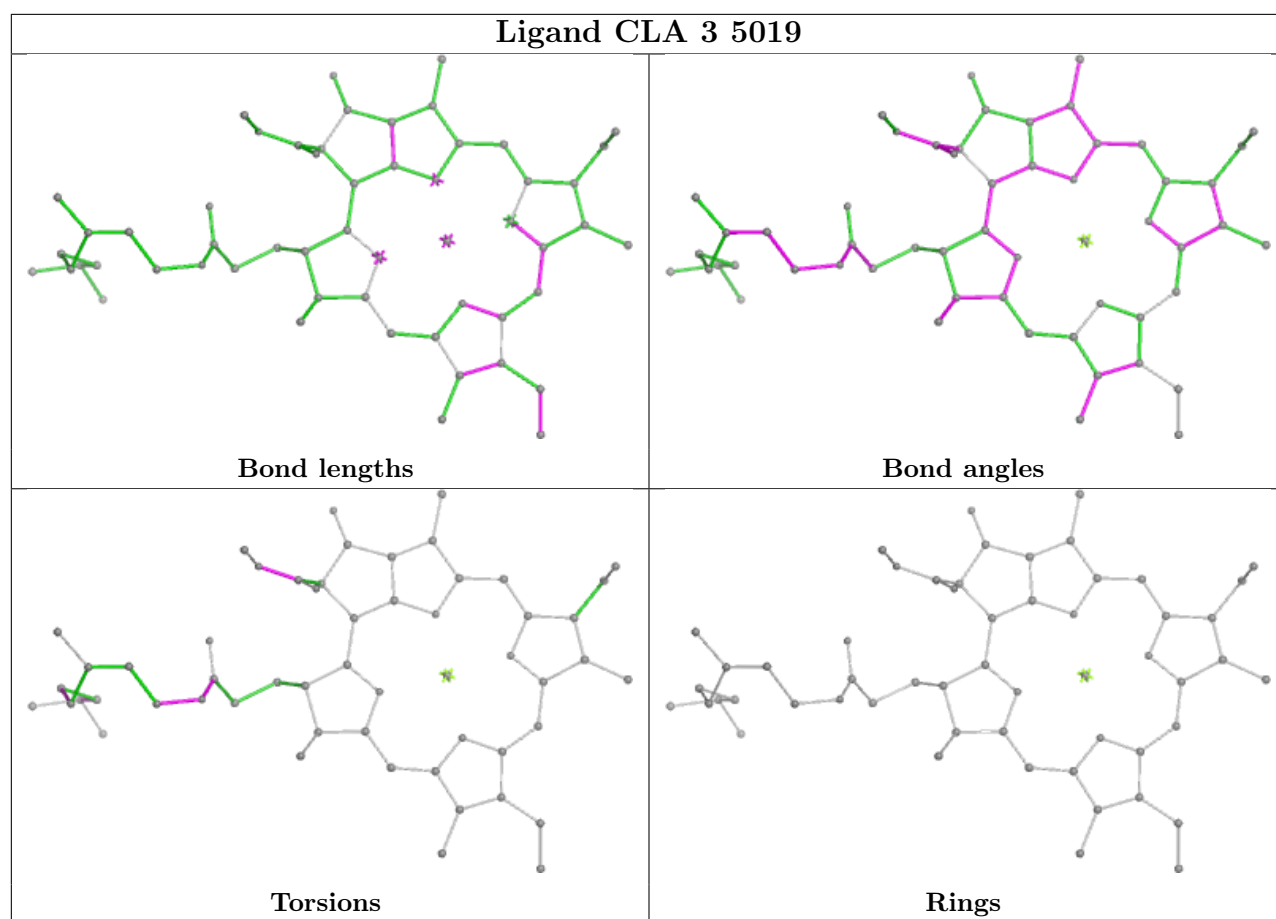




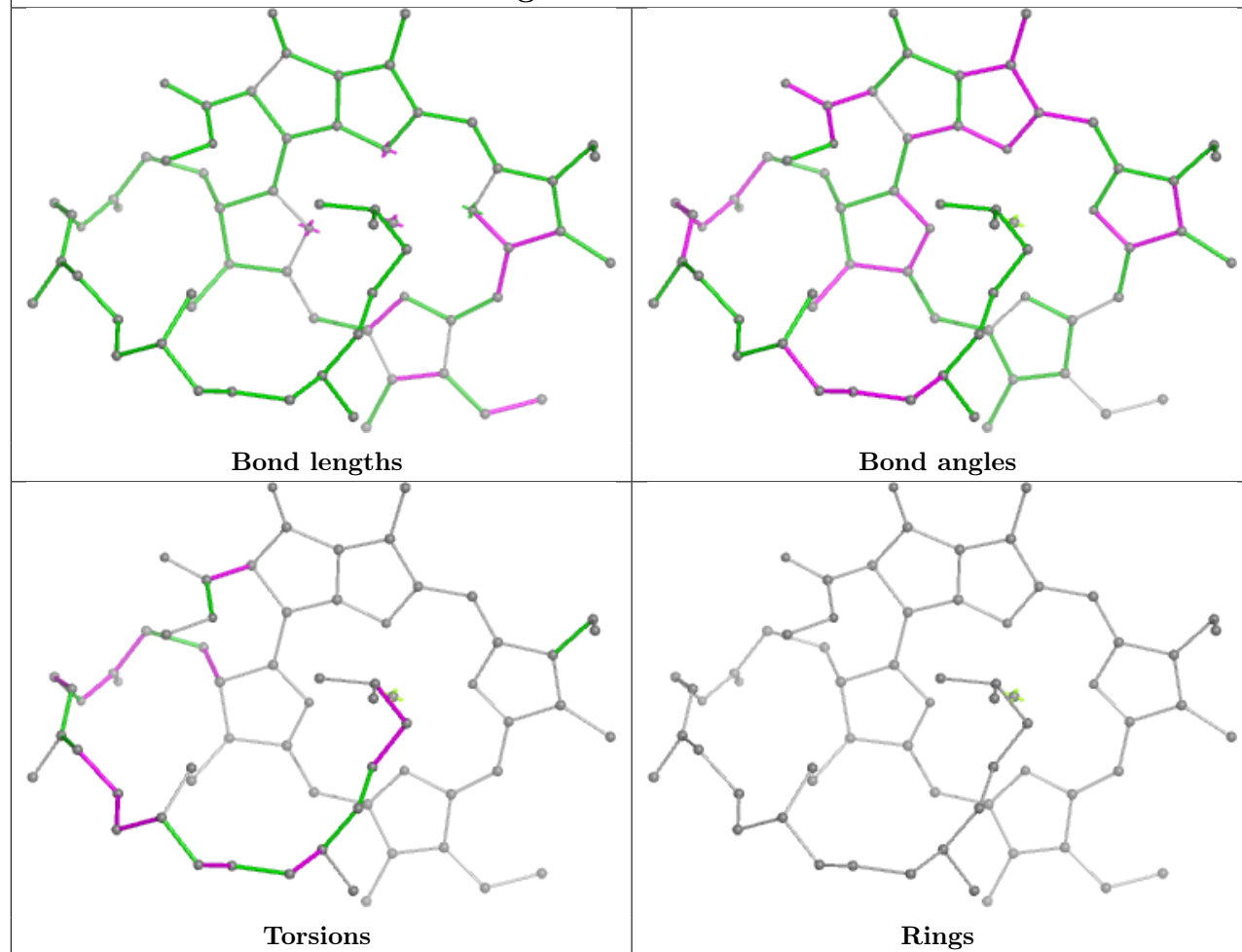




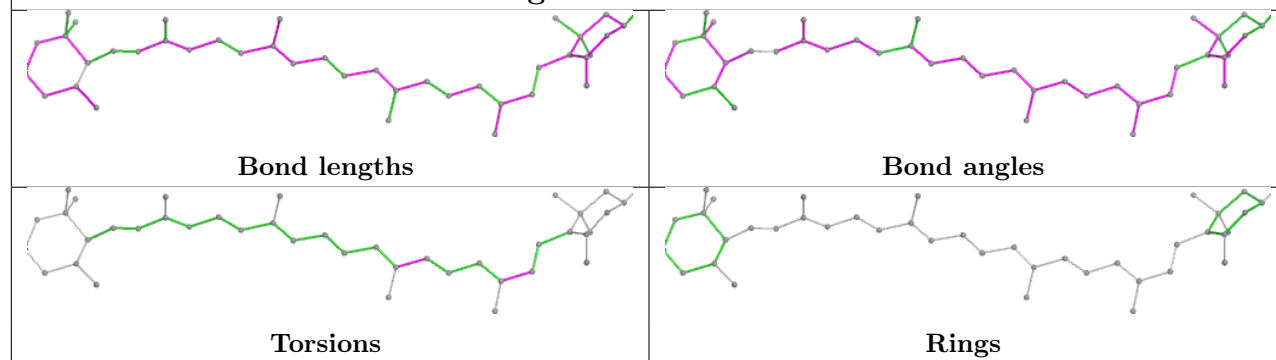




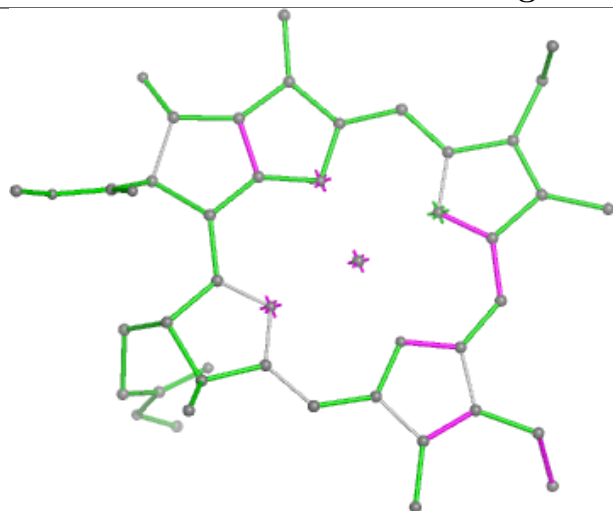
Ligand CLA A 806



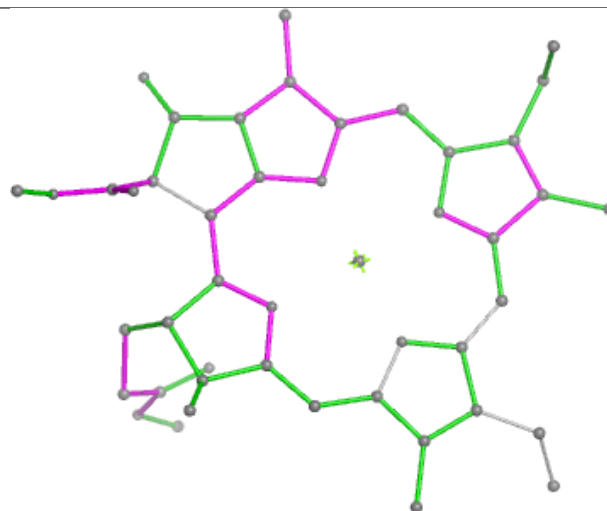
Ligand LUT 1 5004



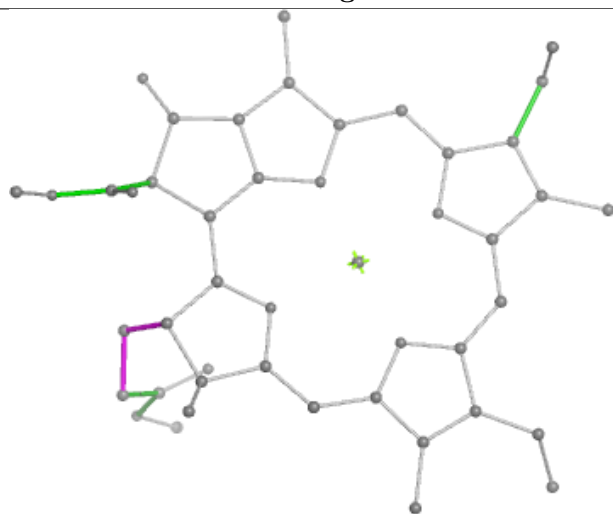
Ligand CLA 8 318



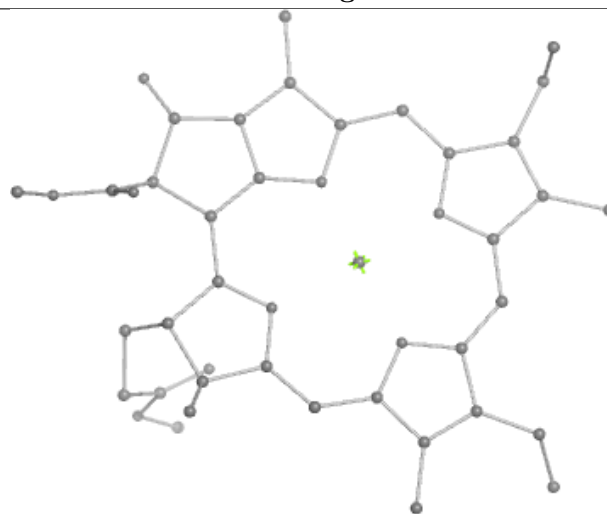
Bond lengths



Bond angles

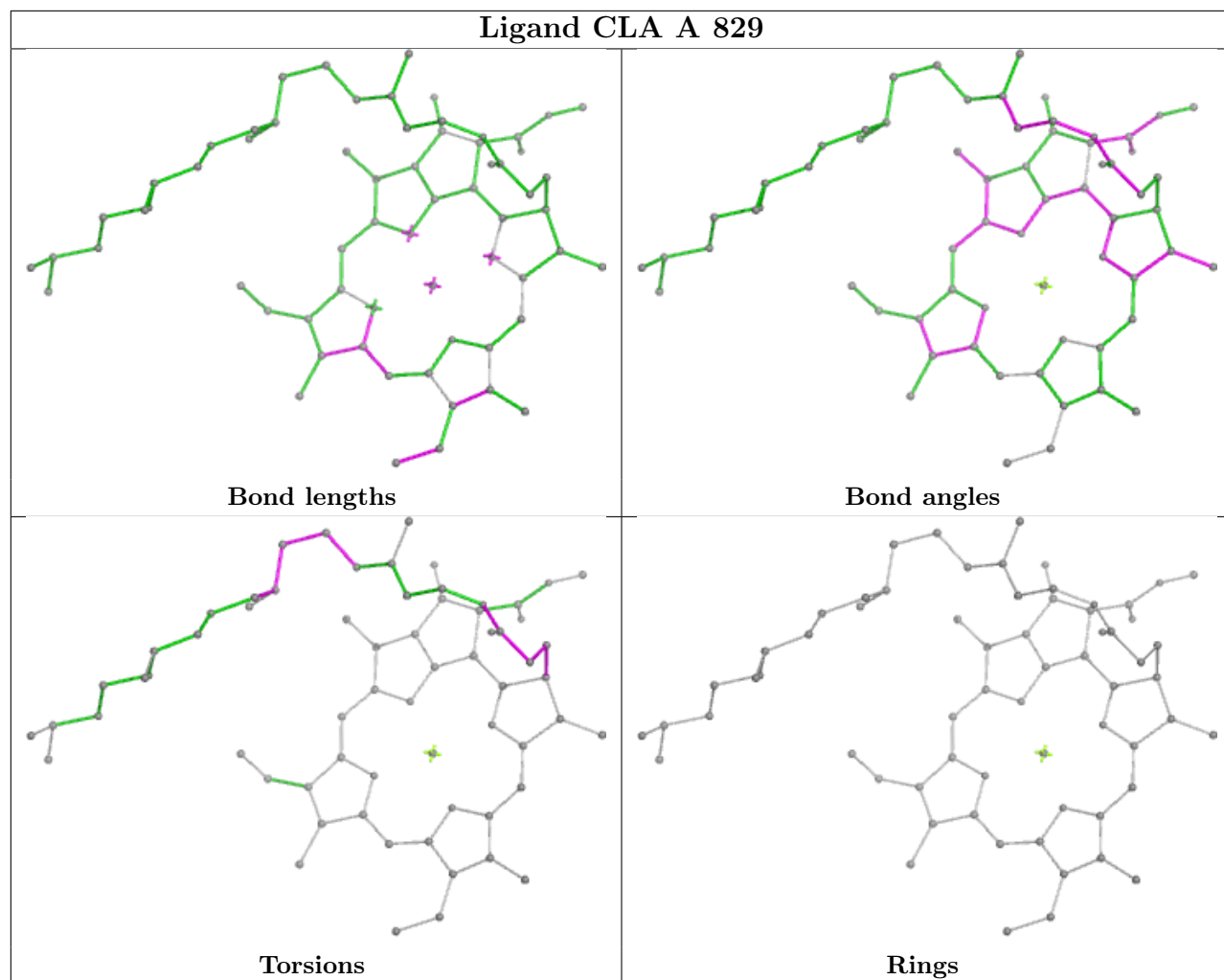


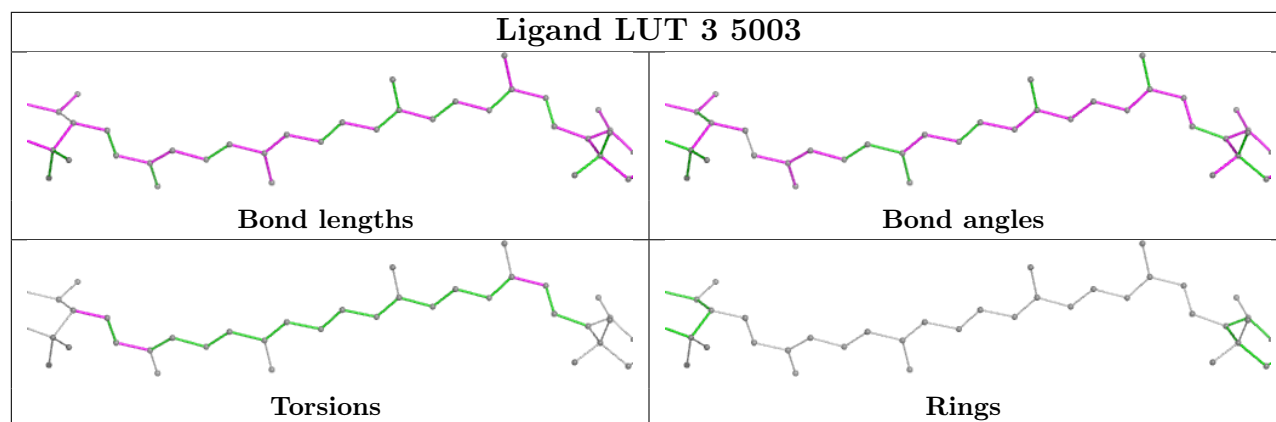
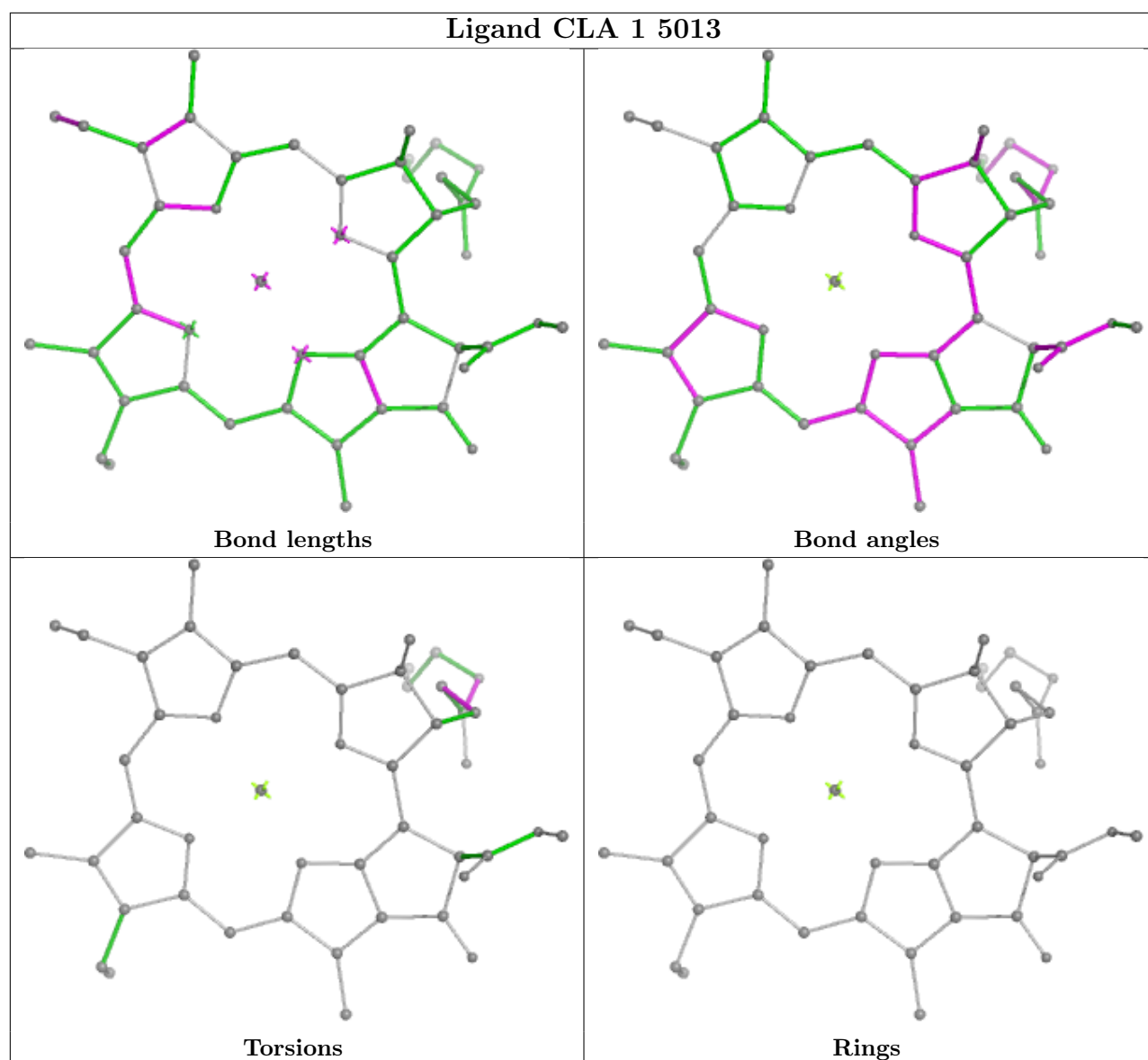
Torsions

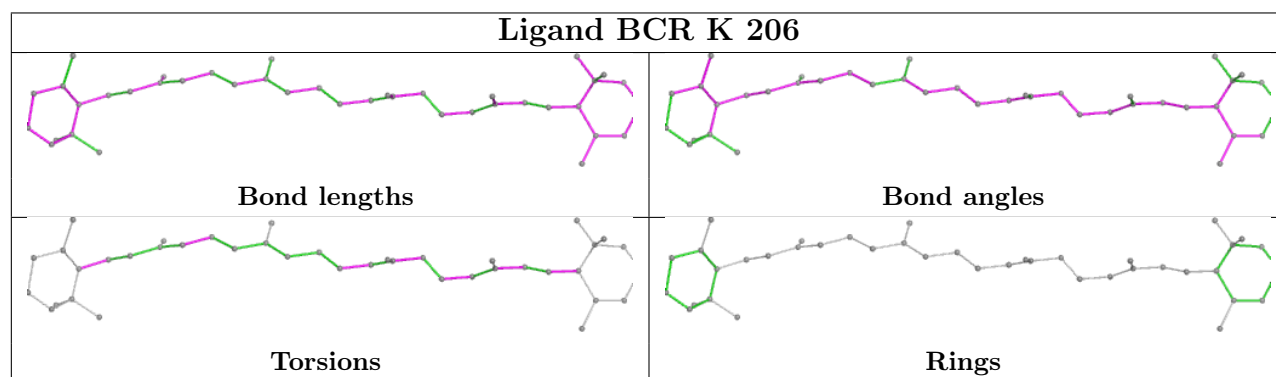
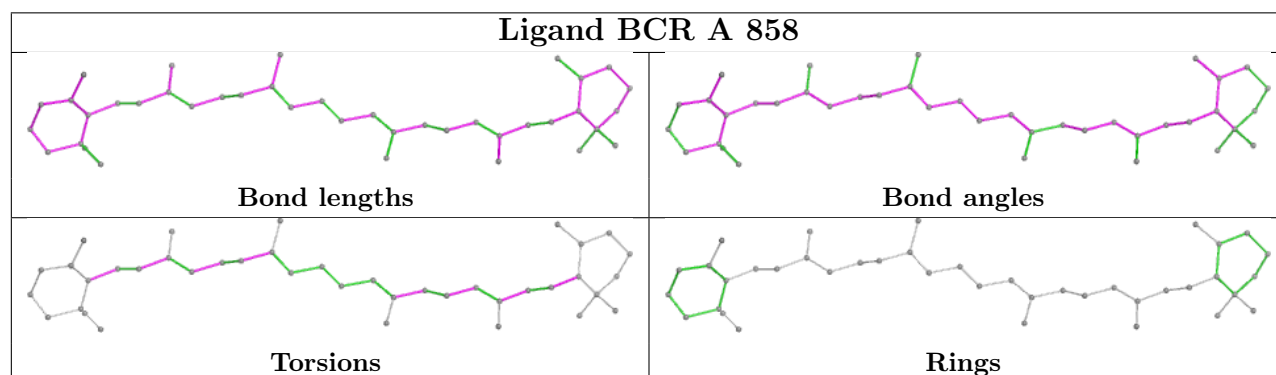
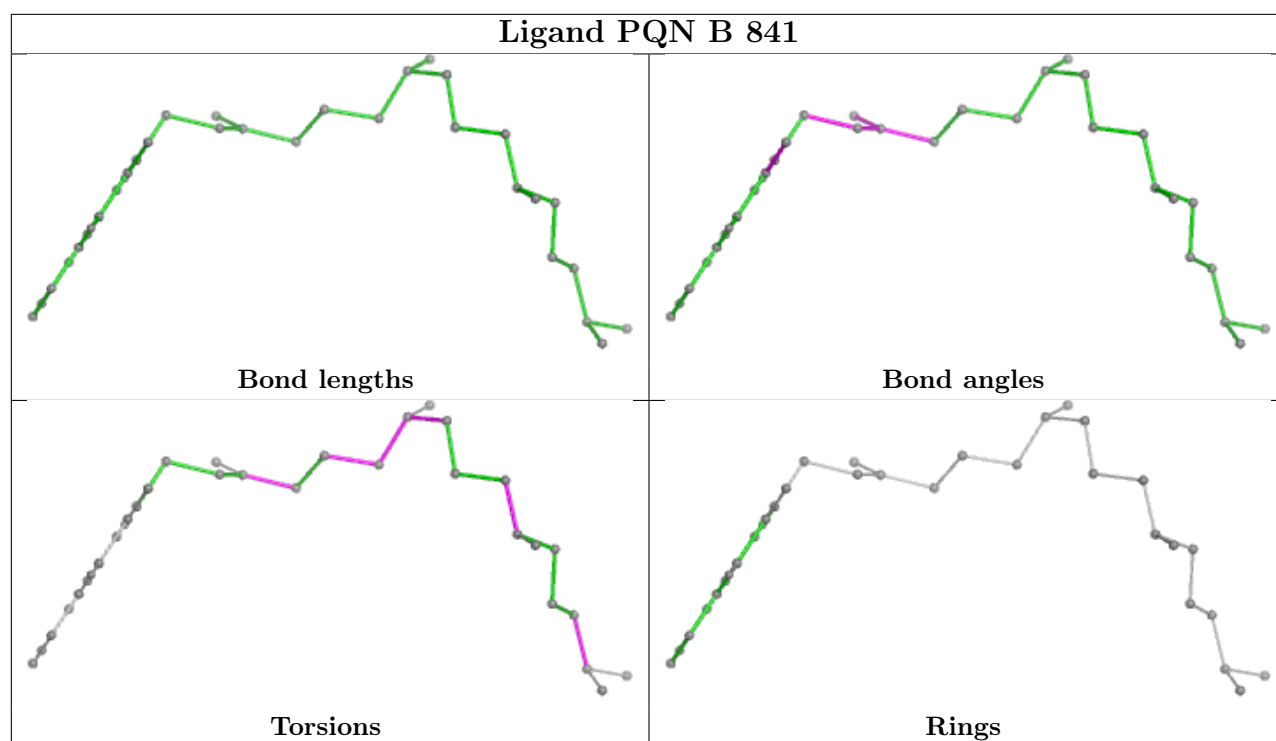


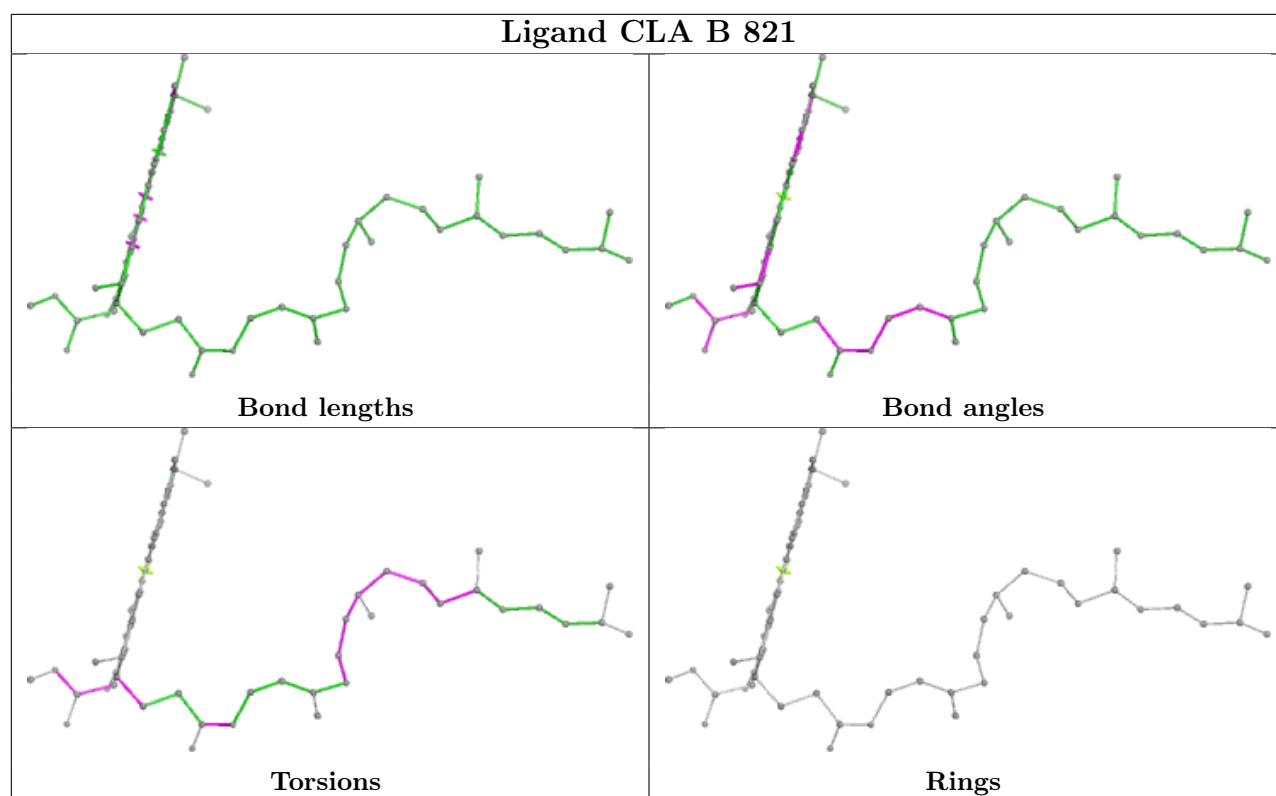
Rings

Ligand CLA A 829









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.

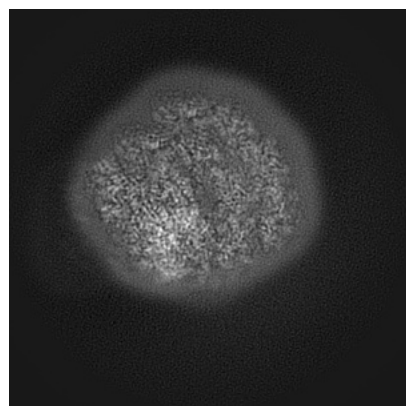
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14248. These allow visual inspection of the internal detail of the map and identification of artifacts.

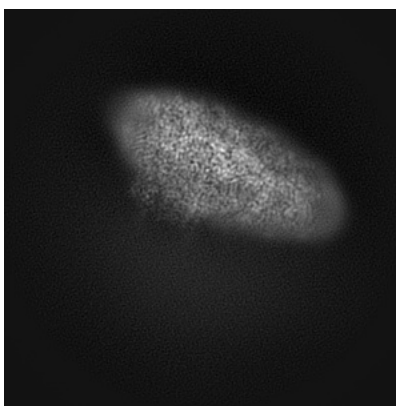
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

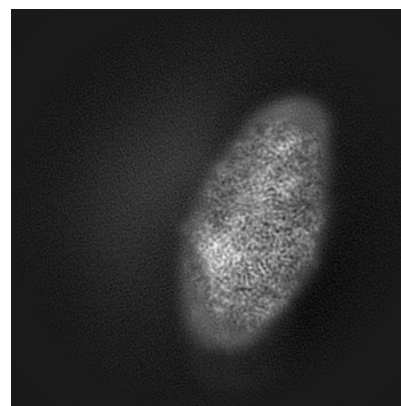
6.1.1 Primary map



X

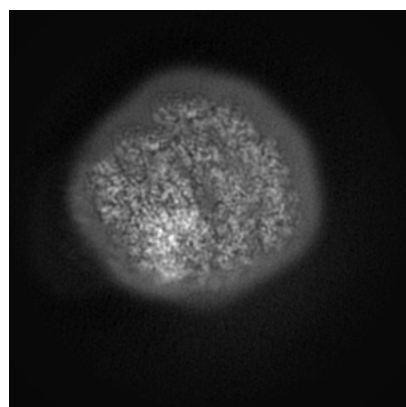


Y

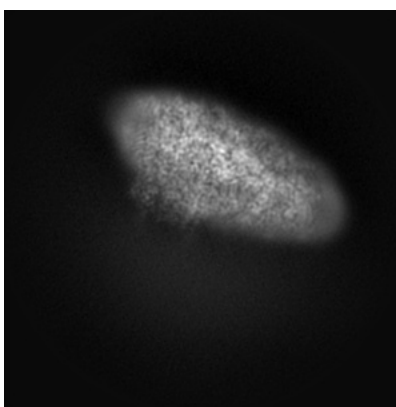


Z

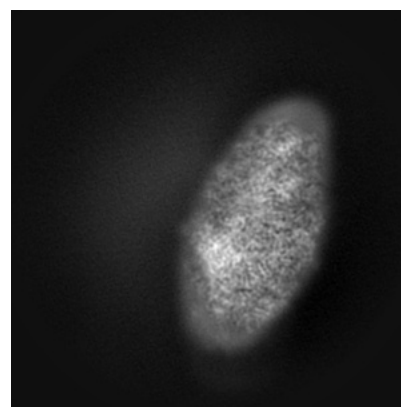
6.1.2 Raw map



X



Y

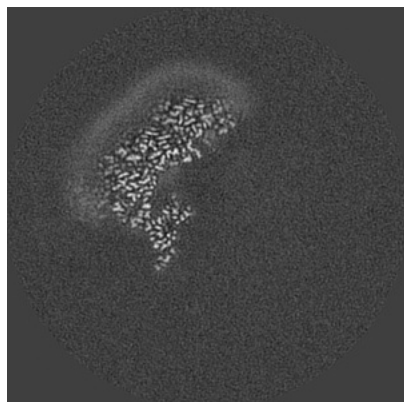


Z

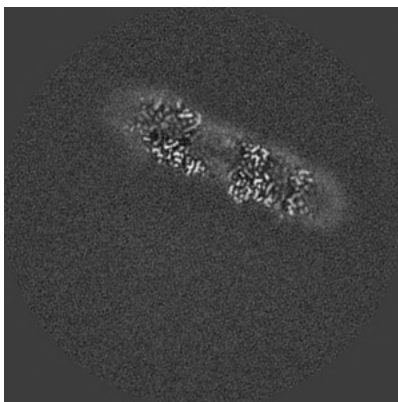
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

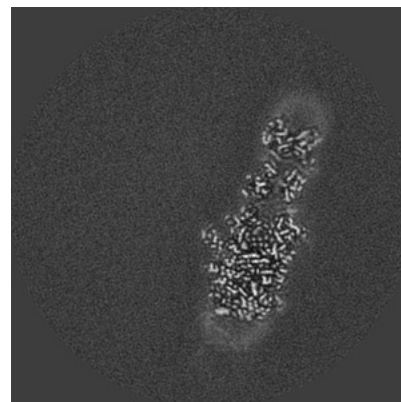
6.2.1 Primary map



X Index: 195

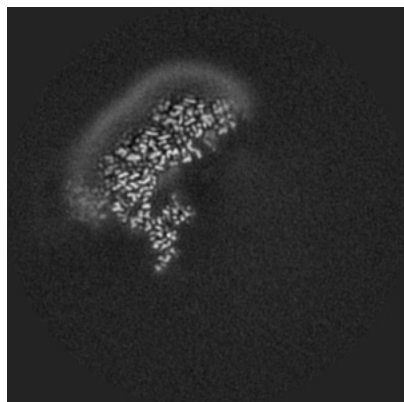


Y Index: 195

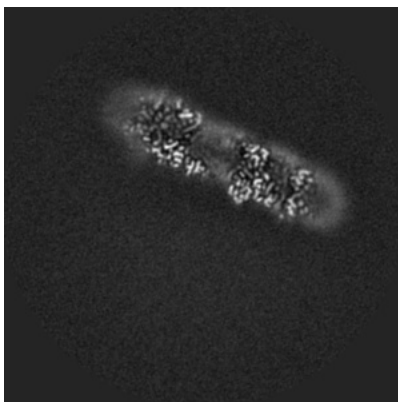


Z Index: 195

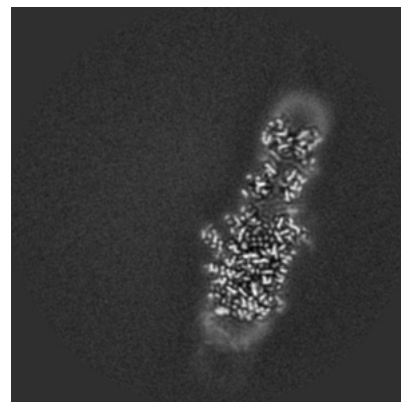
6.2.2 Raw map



X Index: 195



Y Index: 195

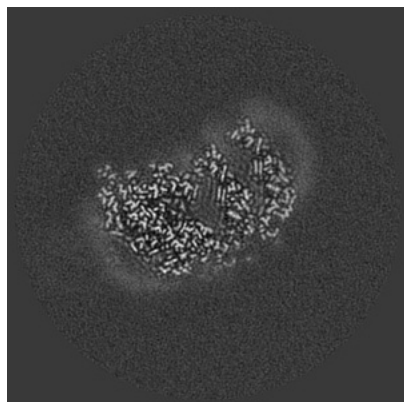


Z Index: 195

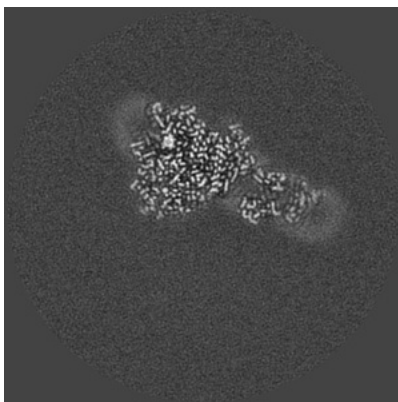
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

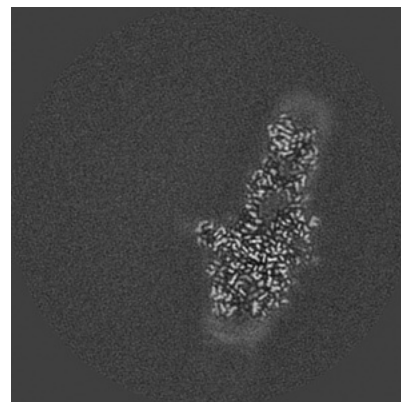
6.3.1 Primary map



X Index: 252

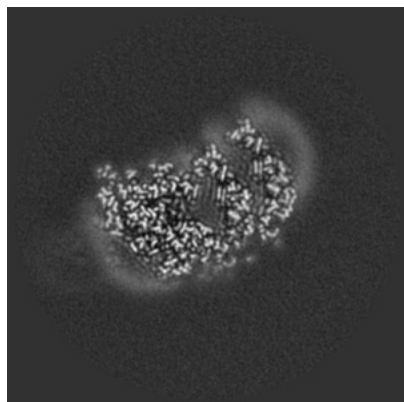


Y Index: 151

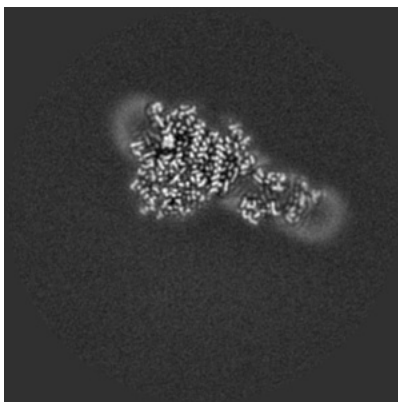


Z Index: 187

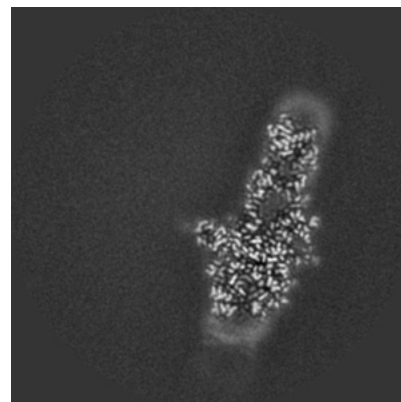
6.3.2 Raw map



X Index: 252



Y Index: 151

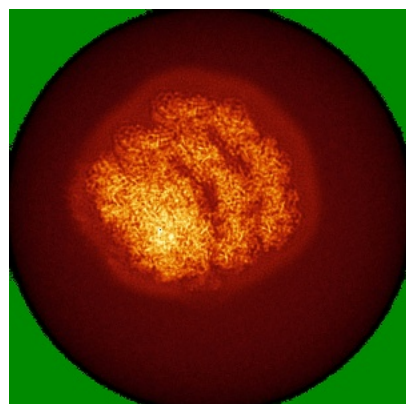


Z Index: 187

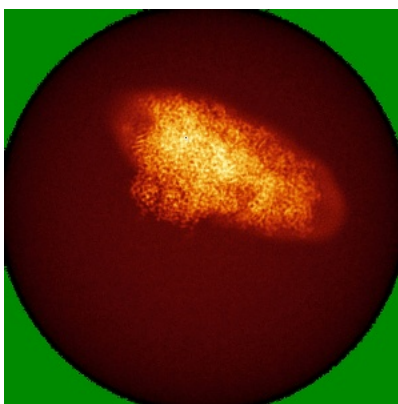
The images above show the largest variance slices of the map in three orthogonal directions.

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

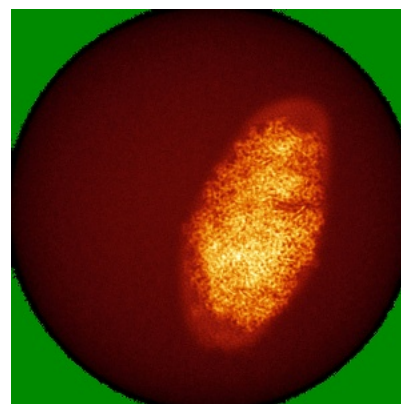
6.4.1 Primary map



X

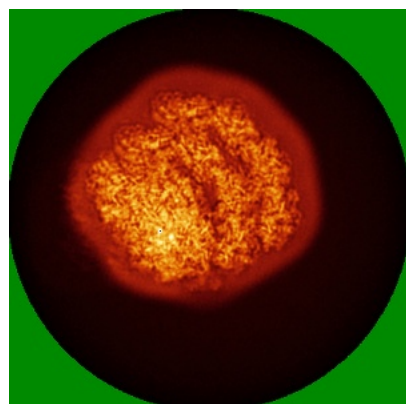


Y

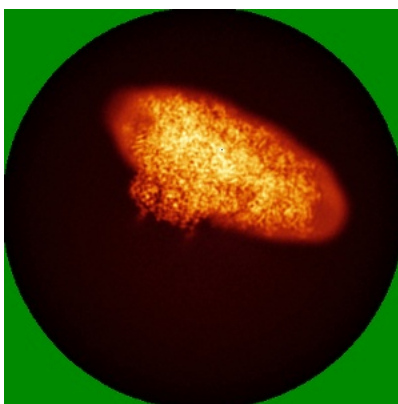


Z

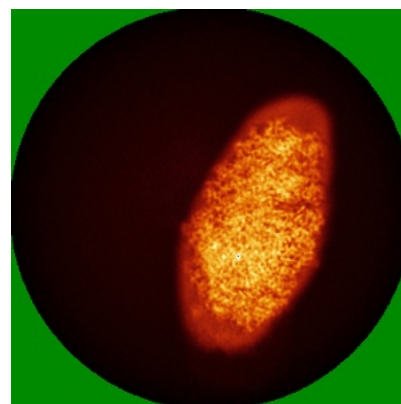
6.4.2 Raw map



X



Y

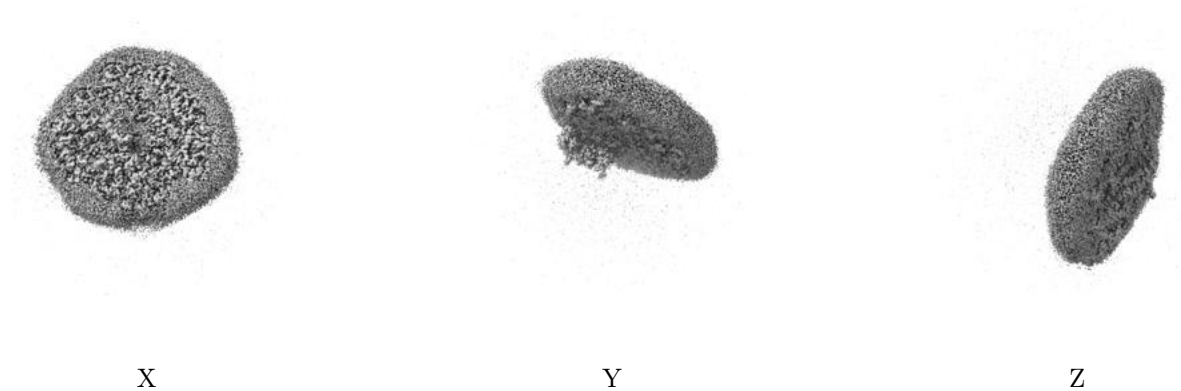


Z

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.

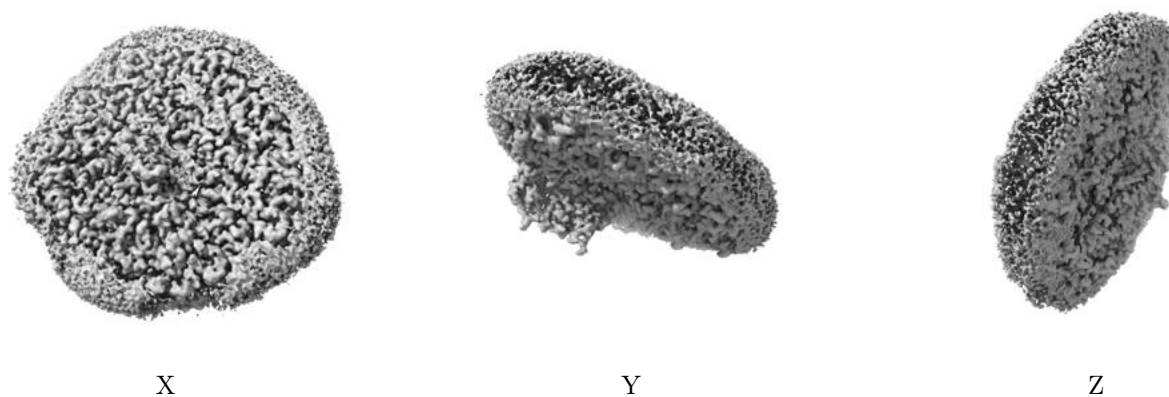
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

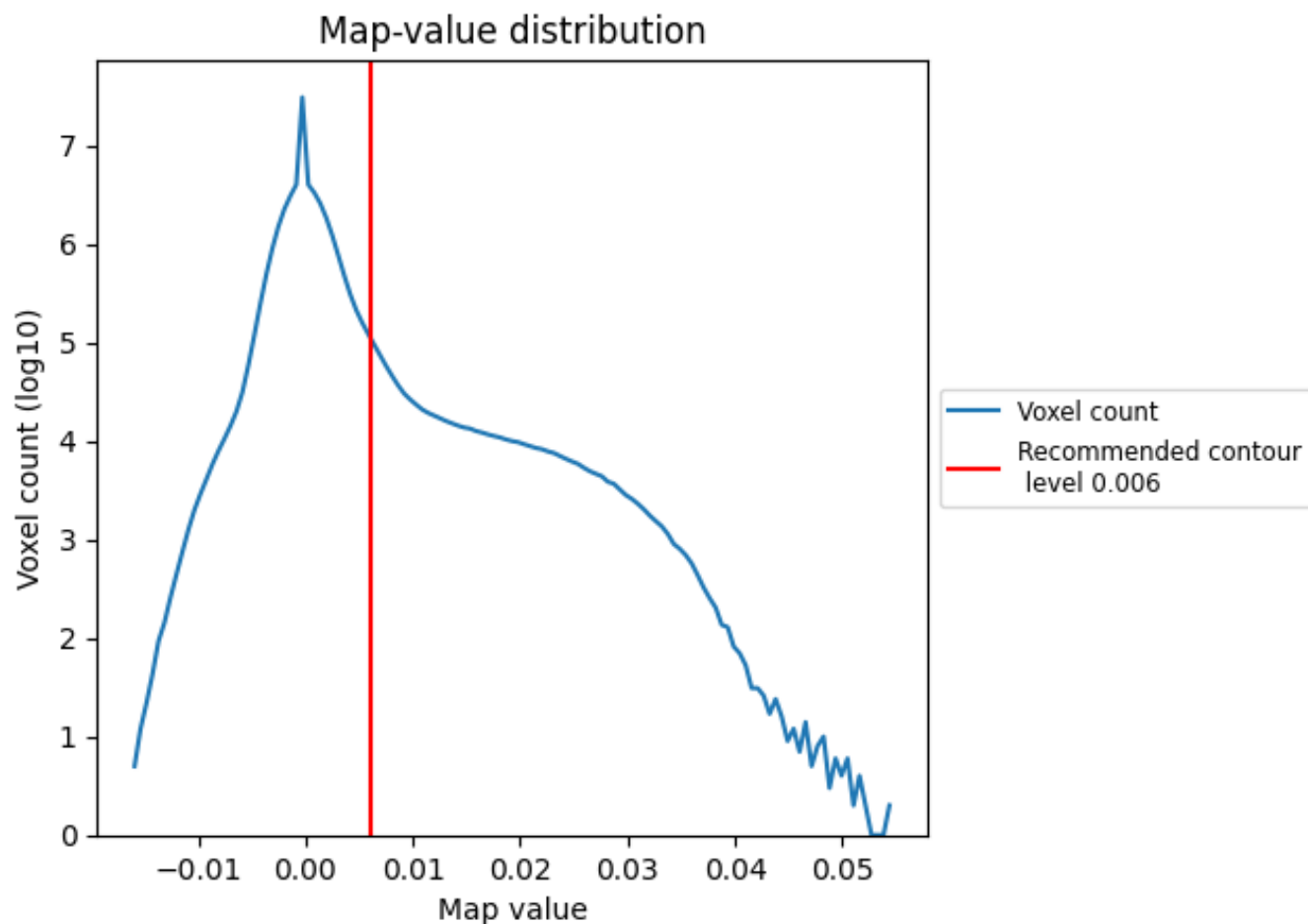
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

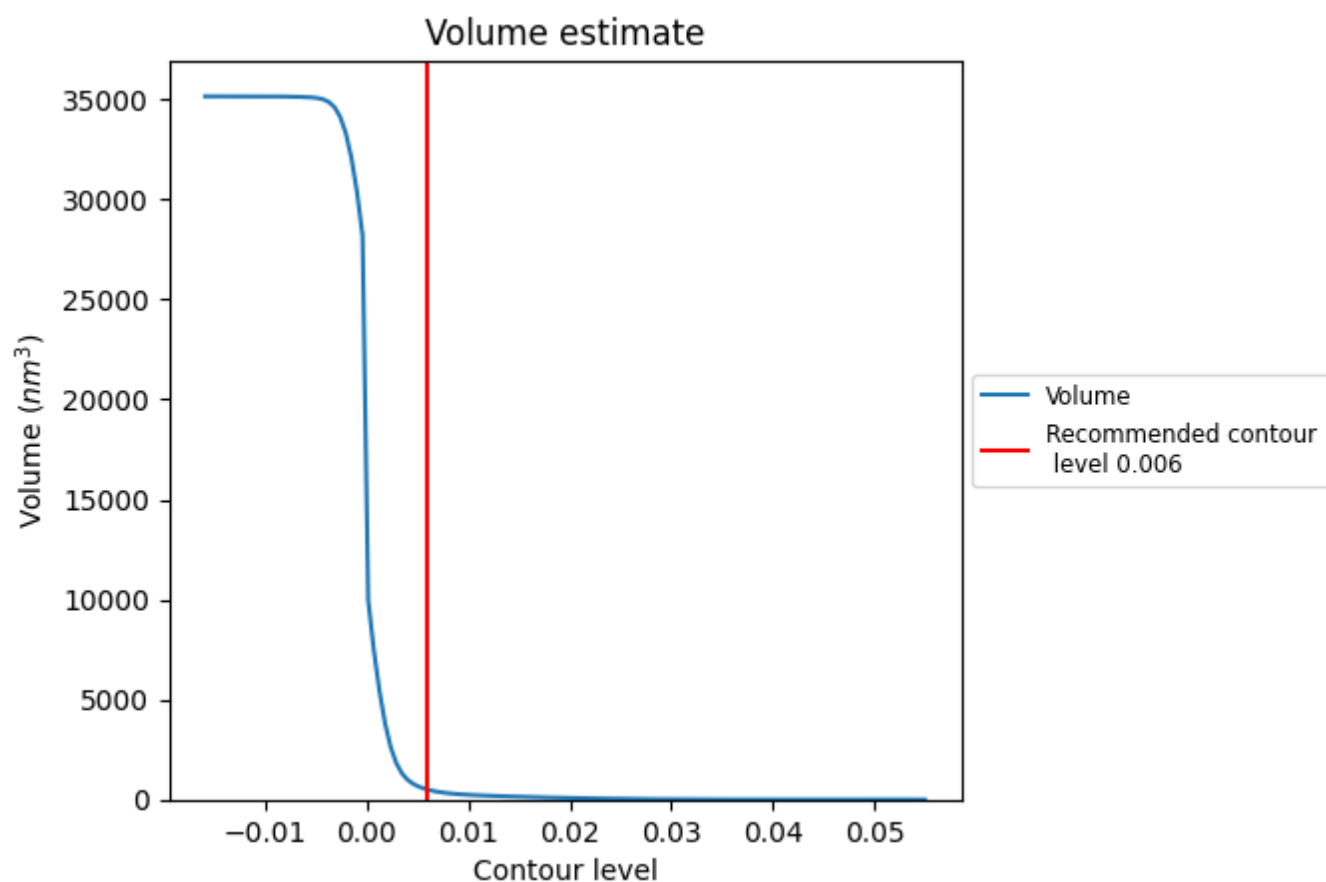
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

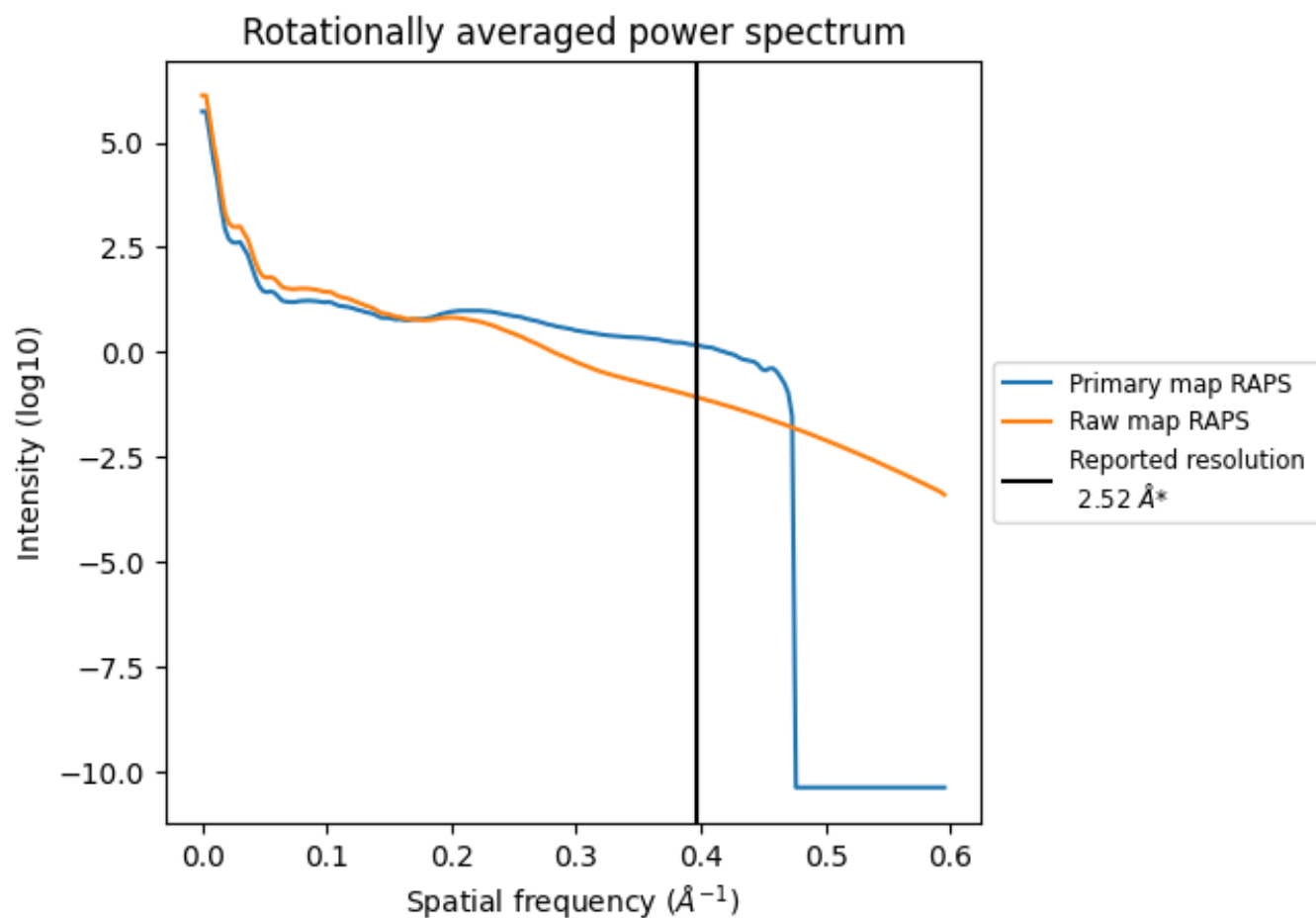
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 497 nm³; this corresponds to an approximate mass of 449 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 ⓘ

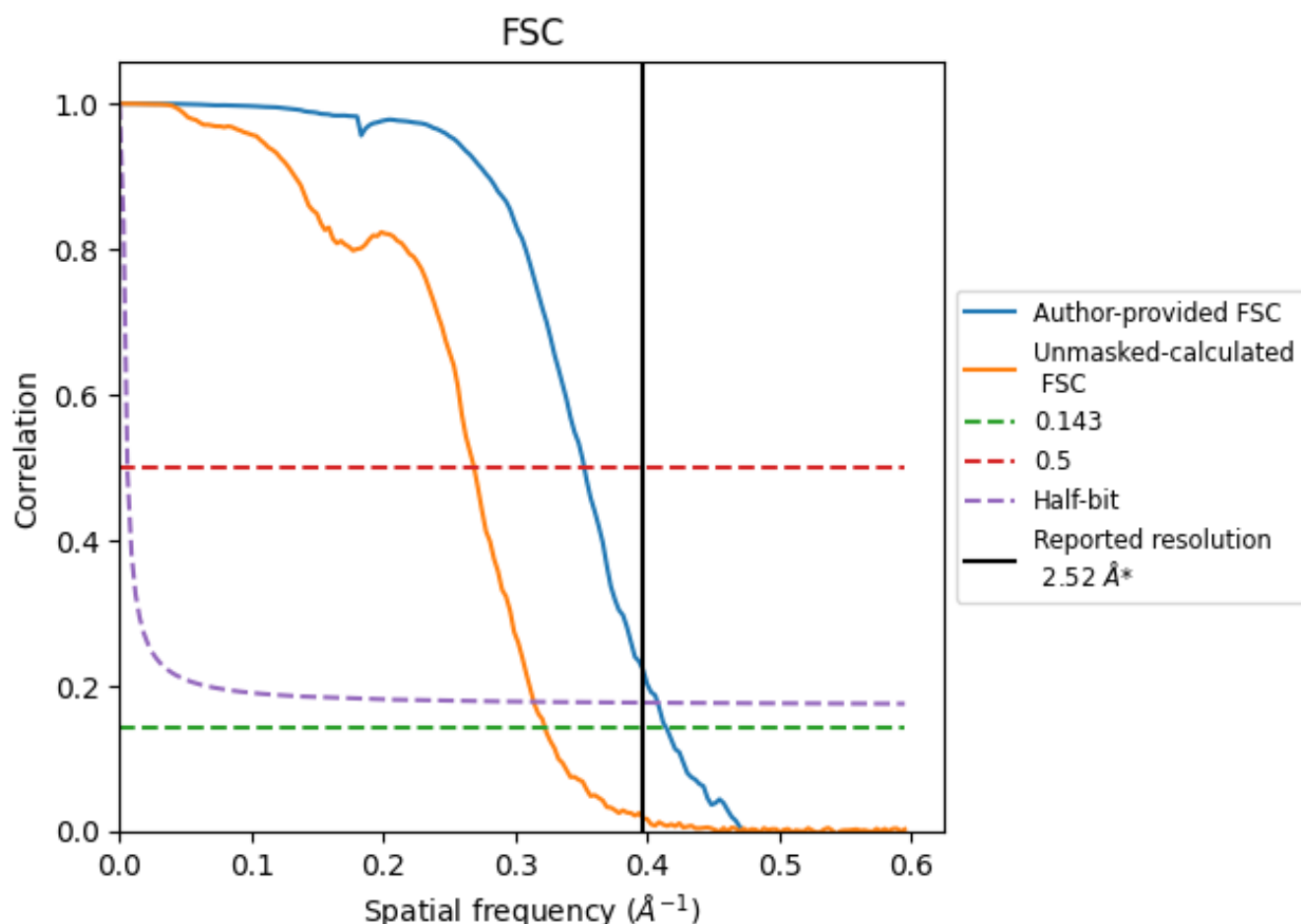


*Reported resolution corresponds to spatial frequency of 0.397 Å⁻¹

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 0.397 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	2.42	2.84	2.45
Unmasked-calculated*	3.10	3.72	3.18

*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 3.10 differs from the reported value 2.52 by more than 10 %

9 Map-model fit [i](#)

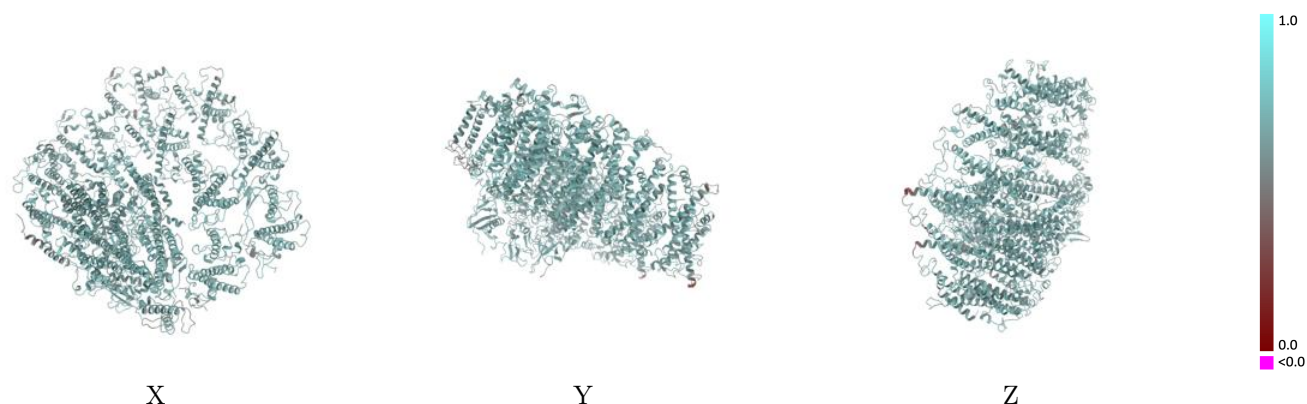
This section contains information regarding the fit between EMDB map EMD-14248 and PDB model 7R3K. Per-residue inclusion information can be found in section [3](#) on page [38](#).

9.1 Map-model overlay [i](#)



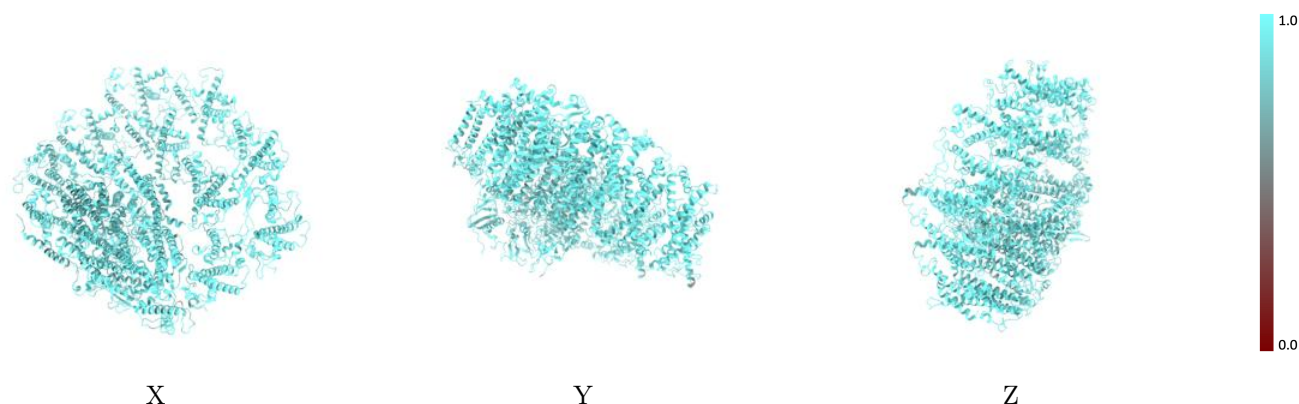
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



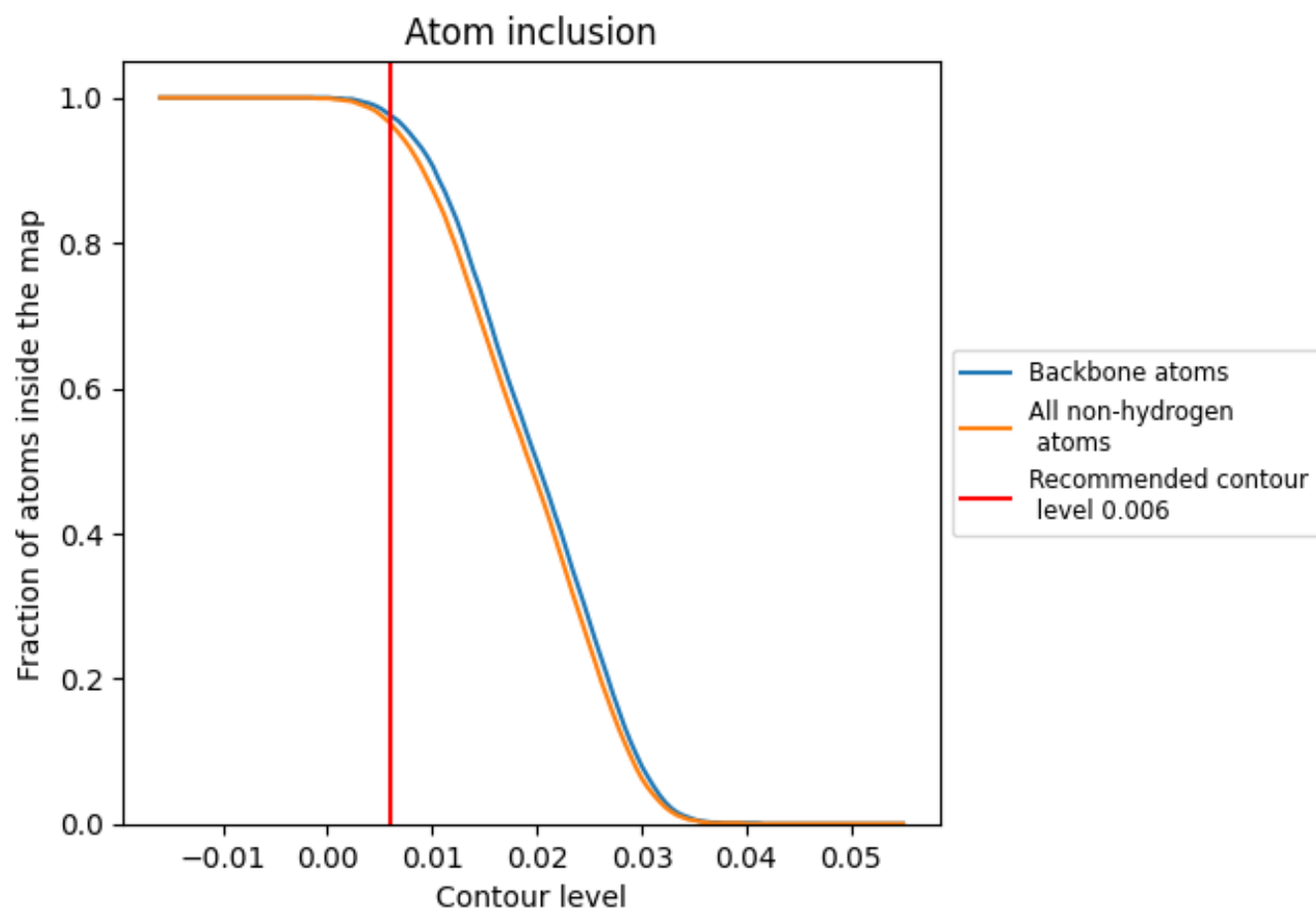
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9650	<div><div></div></div> 0.6330
1	<div><div></div></div> 0.9590	<div><div></div></div> 0.6210
3	<div><div></div></div> 0.9620	<div><div></div></div> 0.6300
4	<div><div></div></div> 0.9570	<div><div></div></div> 0.6120
5	<div><div></div></div> 0.9600	<div><div></div></div> 0.6220
6	<div><div></div></div> 0.9680	<div><div></div></div> 0.6260
7	<div><div></div></div> 0.9720	<div><div></div></div> 0.6480
8	<div><div></div></div> 0.9770	<div><div></div></div> 0.6500
A	<div><div></div></div> 0.9710	<div><div></div></div> 0.6480
B	<div><div></div></div> 0.9690	<div><div></div></div> 0.6450
C	<div><div></div></div> 0.9870	<div><div></div></div> 0.6580
D	<div><div></div></div> 0.9740	<div><div></div></div> 0.6410
E	<div><div></div></div> 0.9690	<div><div></div></div> 0.6340
F	<div><div></div></div> 0.9690	<div><div></div></div> 0.6490
G	<div><div></div></div> 0.9520	<div><div></div></div> 0.5770
I	<div><div></div></div> 0.8390	<div><div></div></div> 0.5170
J	<div><div></div></div> 0.9600	<div><div></div></div> 0.6270
K	<div><div></div></div> 0.8880	<div><div></div></div> 0.5350
Z	<div><div></div></div> 0.9510	<div><div></div></div> 0.6010

1.0

0.0

<0.0