



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 12:58 pm GMT

PDB ID : 8CMO
EMDB ID : EMD-16732
Title : Cryo-EM structure of the Photosystem I - LHCI supercomplex from Coelastrella sp.
Authors : Fadeeva, M.; Klaiman, D.; Nelson, N.
Deposited on : 2023-02-20
Resolution : 2.81 Å(reported)

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

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

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

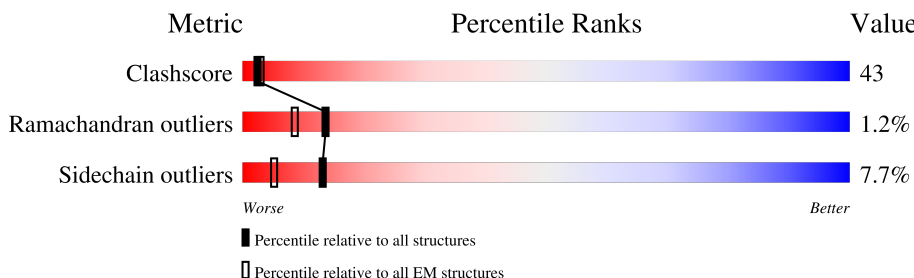
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.81 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.





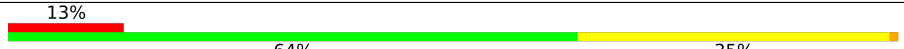
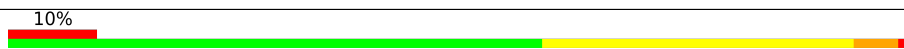

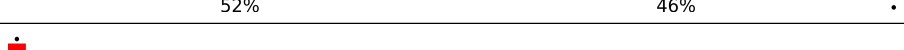


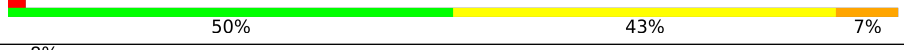


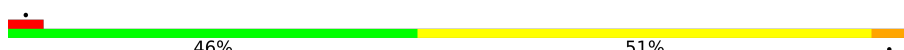

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	740	
2	B	732	
3	C	80	
4	D	142	
5	E	61	
6	F	165	
7	G	93	
8	I	41	

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Mol	Chain	Length	Quality of chain
9	J	40	
10	K	89	
11	L	123	
12	1	194	
12	Z	194	
13	3	218	
14	7	220	
15	8	214	
16	4	207	
17	5	226	
18	6	226	
19	9	184	
20	2	70	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL0	A	801	X	-	-	-
22	CLA	1	304	X	-	-	-
22	CLA	1	305	X	-	-	-
22	CLA	1	306	X	-	-	-
22	CLA	1	307	X	-	X	-
22	CLA	1	308	X	-	X	-
22	CLA	1	309	X	-	-	-
22	CLA	1	310	X	-	-	-
22	CLA	1	311	X	-	-	-
22	CLA	1	313	X	-	-	-
22	CLA	1	314	X	-	-	-
22	CLA	1	315	X	-	-	-
22	CLA	1	316	X	-	-	-
22	CLA	2	301	X	-	-	-
22	CLA	2	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	2	304	X	-	-	-
22	CLA	3	308	X	-	-	-
22	CLA	3	309	X	-	-	-
22	CLA	3	310	X	-	-	-
22	CLA	3	311	X	-	-	-
22	CLA	3	312	X	-	X	-
22	CLA	3	313	X	-	X	-
22	CLA	3	314	X	-	-	-
22	CLA	3	315	X	-	-	-
22	CLA	3	316	X	-	-	-
22	CLA	3	318	X	-	-	-
22	CLA	3	319	X	-	-	-
22	CLA	3	320	X	-	-	-
22	CLA	3	322	X	-	-	-
22	CLA	4	805	X	-	-	-
22	CLA	4	806	X	-	-	-
22	CLA	4	807	X	-	-	-
22	CLA	4	808	X	-	-	-
22	CLA	4	809	X	-	-	-
22	CLA	4	810	X	-	-	-
22	CLA	4	811	X	-	-	-
22	CLA	4	812	X	-	-	-
22	CLA	4	815	X	-	-	-
22	CLA	4	817	X	-	-	-
22	CLA	4	818	X	-	-	-
22	CLA	5	301	X	-	-	-
22	CLA	5	307	X	-	X	-
22	CLA	5	308	X	-	X	-
22	CLA	5	309	X	-	-	-
22	CLA	5	310	X	-	-	-
22	CLA	5	311	X	-	-	-
22	CLA	5	312	X	-	-	-
22	CLA	5	313	X	-	-	-
22	CLA	5	314	X	-	-	-
22	CLA	5	315	X	-	-	-
22	CLA	5	318	X	-	X	-
22	CLA	5	319	X	-	-	-
22	CLA	5	320	X	-	-	-
22	CLA	5	322	X	-	-	-
22	CLA	5	323	X	-	-	-
22	CLA	5	326	X	-	-	-
22	CLA	6	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	6	302	X	-	-	-
22	CLA	6	307	X	-	X	-
22	CLA	6	308	X	-	-	-
22	CLA	6	309	X	-	X	-
22	CLA	6	310	X	-	-	-
22	CLA	6	311	X	-	-	-
22	CLA	6	312	X	-	-	-
22	CLA	6	313	X	-	-	-
22	CLA	6	314	X	-	-	-
22	CLA	6	317	X	-	-	-
22	CLA	6	319	X	-	-	-
22	CLA	6	321	X	-	-	-
22	CLA	6	322	X	-	X	-
22	CLA	7	304	X	-	-	-
22	CLA	7	305	X	-	-	-
22	CLA	7	306	X	-	-	-
22	CLA	7	307	X	-	X	-
22	CLA	7	308	X	-	-	-
22	CLA	7	309	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-
22	CLA	7	314	X	-	-	-
22	CLA	7	315	X	-	-	-
22	CLA	7	316	X	-	-	-
22	CLA	7	317	X	-	-	-
22	CLA	7	322	X	-	-	-
22	CLA	7	323	X	-	-	-
22	CLA	7	324	X	-	-	-
22	CLA	8	305	X	-	X	-
22	CLA	8	306	X	-	-	-
22	CLA	8	307	X	-	-	-
22	CLA	8	308	X	-	-	-
22	CLA	8	309	X	-	-	-
22	CLA	8	310	X	-	-	-
22	CLA	8	311	X	-	-	-
22	CLA	8	313	X	-	-	-
22	CLA	8	314	X	-	-	-
22	CLA	8	316	X	-	-	-
22	CLA	9	303	X	-	-	-
22	CLA	9	304	X	-	-	-
22	CLA	9	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	9	306	X	-	-	-
22	CLA	9	307	X	-	-	-
22	CLA	9	308	X	-	-	-
22	CLA	9	309	X	-	-	-
22	CLA	9	310	X	-	-	-
22	CLA	9	311	X	-	-	-
22	CLA	9	313	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	X	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	X	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	X	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	X	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	X	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	X	-
22	CLA	A	822	X	-	X	-
22	CLA	A	823	X	-	X	-
22	CLA	A	824	X	-	-	-
22	CLA	A	825	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	A	855	X	-	-	-
22	CLA	B	801	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	X	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	X	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	X	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	X	-
22	CLA	B	825	X	-	X	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	X	-
22	CLA	B	828	X	-	X	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	840	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	B	842	X	-	X	-
22	CLA	F	301	X	-	-	-
22	CLA	F	302	X	-	-	-
22	CLA	F	304	X	-	X	-
22	CLA	F	305	X	-	-	-
22	CLA	G	201	X	-	-	-
22	CLA	G	202	X	-	-	-
22	CLA	J	103	X	-	-	-
22	CLA	K	202	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	K	204	X	-	-	-
22	CLA	K	205	X	-	-	-
22	CLA	L	201	X	-	-	-
22	CLA	L	202	X	-	-	-
22	CLA	L	203	X	-	-	-
22	CLA	Z	303	X	-	X	-
22	CLA	Z	304	X	-	-	-
22	CLA	Z	305	X	-	-	-
22	CLA	Z	306	X	-	-	-
22	CLA	Z	307	X	-	-	-
22	CLA	Z	308	X	-	-	-
22	CLA	Z	309	X	-	X	-
22	CLA	Z	310	X	-	-	-
22	CLA	Z	313	X	-	X	-
22	CLA	Z	314	X	-	-	-
22	CLA	Z	315	X	-	-	-
22	CLA	Z	316	X	-	-	-
24	BCR	3	304	-	X	-	-
24	BCR	3	307	-	X	-	-
24	BCR	4	804	-	-	X	-
24	BCR	5	304	-	-	X	-
24	BCR	6	306	-	X	-	-
24	BCR	A	844	-	-	X	-
24	BCR	A	845	-	X	-	-
24	BCR	A	856	-	X	X	-
24	BCR	B	846	-	X	-	-
24	BCR	B	847	-	-	X	-
24	BCR	B	848	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	BCR	B	853	-	X	X	-
29	SF4	B	802	-	-	X	-
29	SF4	C	101	-	-	X	-
29	SF4	C	102	-	-	X	-
31	DGD	3	301	-	-	X	-
37	DAO	K	201	-	-	X	-
38	LUT	Z	301	-	-	X	-
39	CHL	1	312	X	-	-	-
39	CHL	2	303	X	-	-	-
39	CHL	3	317	X	-	-	-
39	CHL	4	813	X	-	-	-
39	CHL	4	814	X	-	-	-
39	CHL	4	816	X	-	-	-
39	CHL	4	819	X	-	-	-
39	CHL	5	316	X	-	-	-
39	CHL	5	317	X	-	-	-
39	CHL	5	321	X	-	-	-
39	CHL	6	315	X	-	X	-
39	CHL	6	316	X	-	-	-
39	CHL	6	318	X	-	-	-
39	CHL	6	320	X	-	-	-
39	CHL	7	313	X	-	-	-
39	CHL	8	301	X	-	-	-
39	CHL	8	312	X	-	-	-
39	CHL	8	315	X	-	X	-
39	CHL	9	312	X	-	X	-
39	CHL	9	314	X	-	-	-
39	CHL	Z	311	X	-	-	-
39	CHL	Z	312	X	-	-	-

2 Entry composition [i](#)

There are 44 unique types of molecules in this entry. The entry contains 50057 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	740	Total	C	N	O	S	0	0
			5819	3806	991	1000	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	0	0
			5800	3804	973	1005	18		

- Molecule 3 is a protein called Photosystem I subunit VII PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			603	370	105	116	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	142	Total	C	N	O	S	0	0
			1129	724	196	204	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	61	Total	C	N	O	0	0
			484	309	83	92		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1265	813	219	230	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	93	Total	C	N	O	S	0	0
			690	440	116	131	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	41	Total	C	N	O	S	0	0
			308	210	44	53	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	40	Total	C	N	O	S	0	0
			319	217	47	54	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	89	Total	C	N	O	S	0	0
			617	390	110	115	2		

- Molecule 11 is a protein called Photosystem I reaction centre subunit XI PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			897	580	148	165	4		

- Molecule 12 is a protein called Light-harvesting protein of photosystem I Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	194	Total	C	N	O	S	0	0
			1457	936	248	265	8		
12	Z	194	Total	C	N	O	S	0	0
			1457	936	248	265	8		

- Molecule 13 is a protein called Light-harvesting protein of photosystem I Lhca3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	218	Total	C	N	O	S	0	0
			1695	1107	272	309	7		

- Molecule 14 is a protein called Light-harvesting protein of photosystem I Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	220	Total	C	N	O	S	0	0
			1705	1102	283	313	7		

- Molecule 15 is a protein called Light-harvesting protein of photosystem I Lhca8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	8	214	Total	C	N	O	S	0	0
			1602	1032	269	291	10		

- Molecule 16 is a protein called Light-harvesting protein of photosystem I Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	207	Total	C	N	O	S	0	0
			1598	1036	272	284	6		

- Molecule 17 is a protein called Light-harvesting protein of photosystem I Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	226	Total	C	N	O	S	0	0
			1764	1136	302	318	8		

- Molecule 18 is a protein called Light-harvesting protein of photosystem I Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	226	Total	C	N	O	S	0	0
			1762	1162	289	303	8		

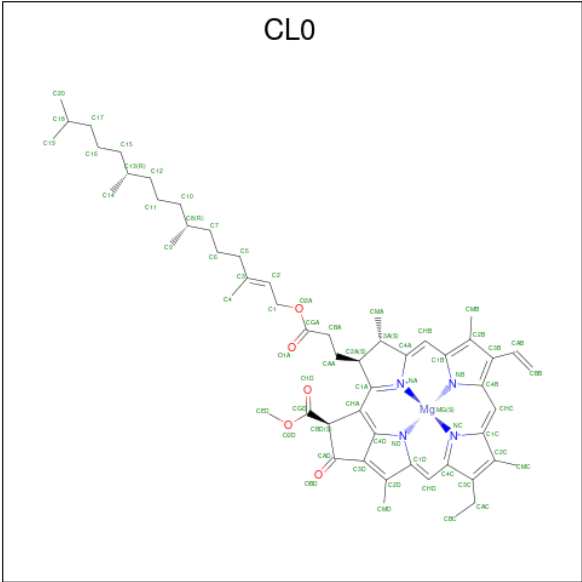
- Molecule 19 is a protein called Light-harvesting protein of photosystem I Lhca9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	9	184	Total	C	N	O	S	0	0
			1416	914	239	254	9		

- Molecule 20 is a protein called Light-harvesting protein of photosystem I Lhca2 partial.

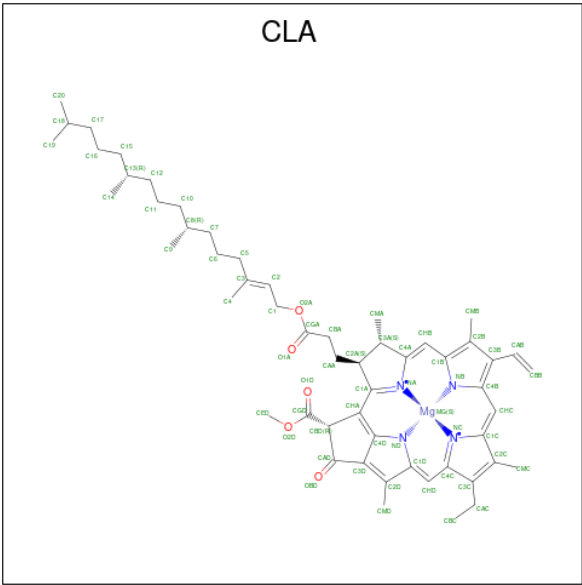
Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	70	Total	C	N	O	S	0	0
			525	336	90	94	5		

- Molecule 21 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	K	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Z	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	Z	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Z	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	7	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	7	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	8	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	4	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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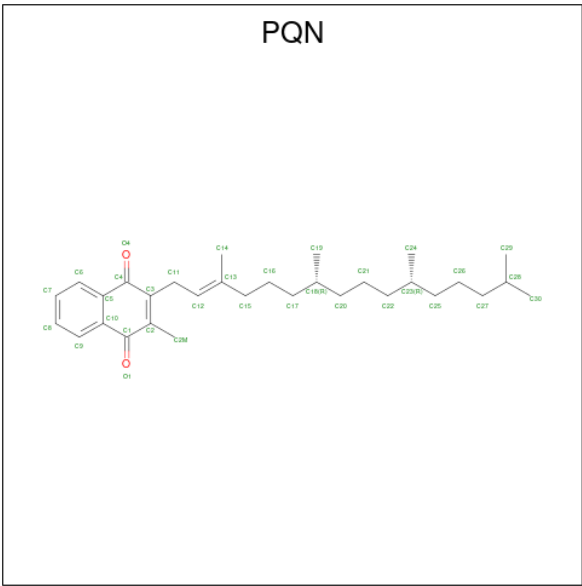
Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0

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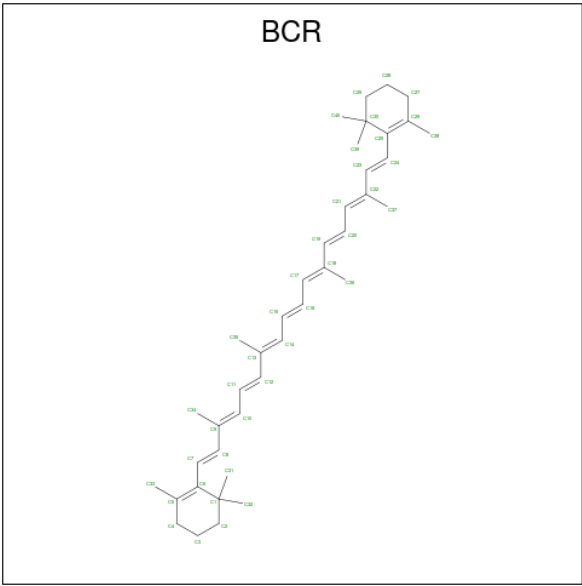
Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

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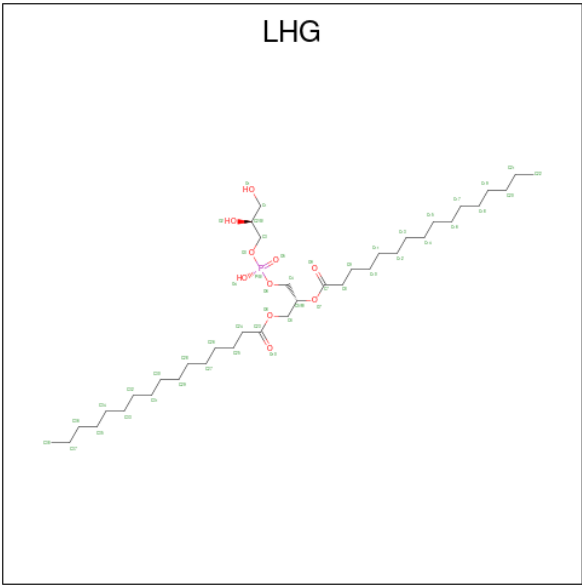
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
24	3	1	Total C 40 40	0
24	7	1	Total C 40 40	0
24	8	1	Total C 40 40	0
24	4	1	Total C 40 40	0
24	5	1	Total C 40 40	0
24	5	1	Total C 40 40	0
24	6	1	Total C 40 40	0
24	6	1	Total C 40 40	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C O P 35 24 10 1	0
25	A	1	Total C O P 49 38 10 1	0
25	B	1	Total C O P 33 22 10 1	0

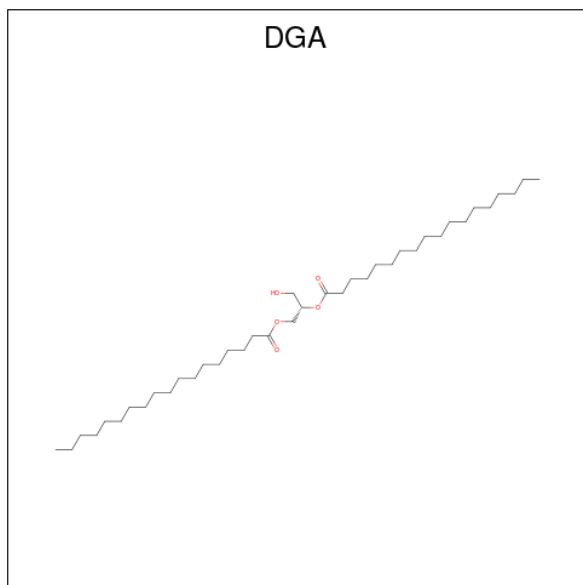
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Mol	Chain	Residues	Atoms				AltConf
25	B	1	Total 23	C 12	O 10	P 1	0
25	B	1	Total 20	C 9	O 10	P 1	0
25	1	1	Total 43	C 32	O 10	P 1	0
25	Z	1	Total 43	C 32	O 10	P 1	0
25	3	1	Total 20	C 9	O 10	P 1	0
25	7	1	Total 37	C 26	O 10	P 1	0
25	8	1	Total 38	C 27	O 10	P 1	0
25	4	1	Total 49	C 38	O 10	P 1	0
25	4	1	Total 32	C 21	O 10	P 1	0
25	5	1	Total 37	C 26	O 10	P 1	0
25	6	1	Total 49	C 38	O 10	P 1	0
25	9	1	Total 33	C 22	O 10	P 1	0

- # NKP

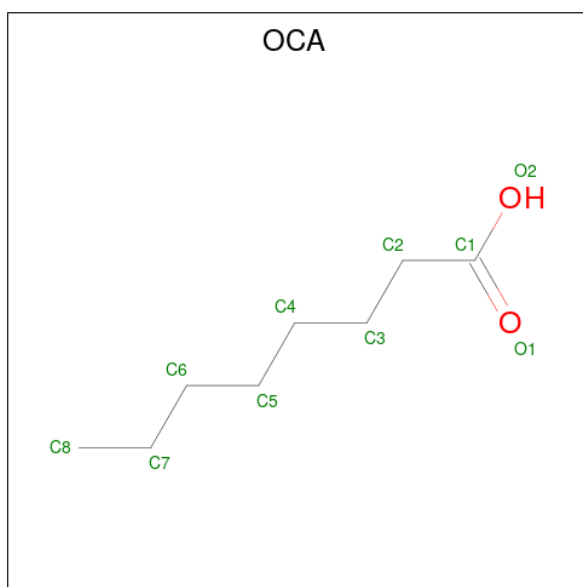
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			23	15	7	1	
26	8	1	Total	C	O	P	0
			29	21	7	1	

- Molecule 27 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



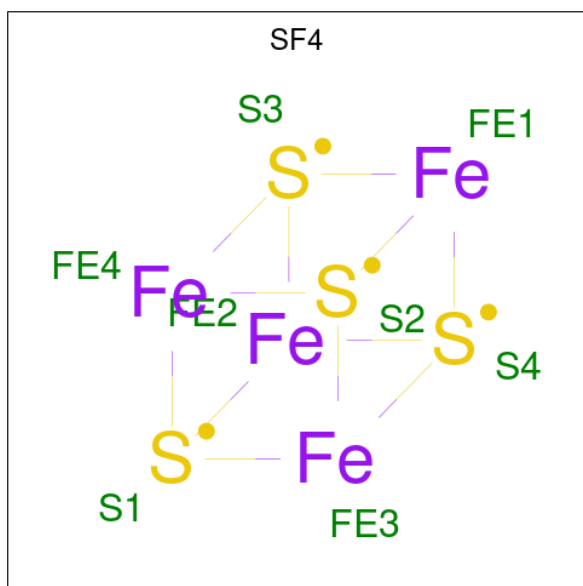
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O		0
			40	35	5		

- Molecule 28 is OCTANOIC ACID (CAPRYLIC ACID) (three-letter code: OCA) (formula: $C_8H_{16}O_2$).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			10	8	2	

- Molecule 29 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

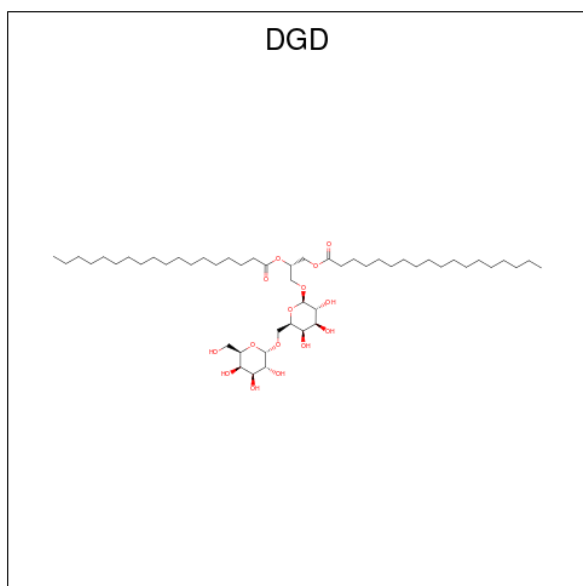


Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is CALCIUM ION (three-letter code: CA) (formula: Ca).

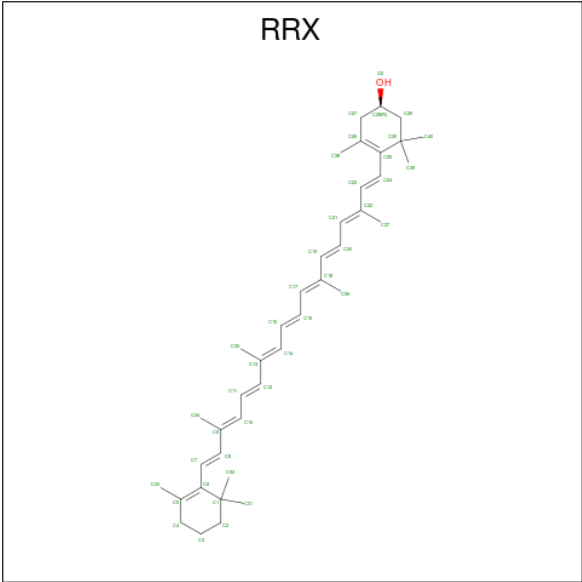
Mol	Chain	Residues	Atoms		AltConf
30	B	1	Total	Ca	0
			1	1	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



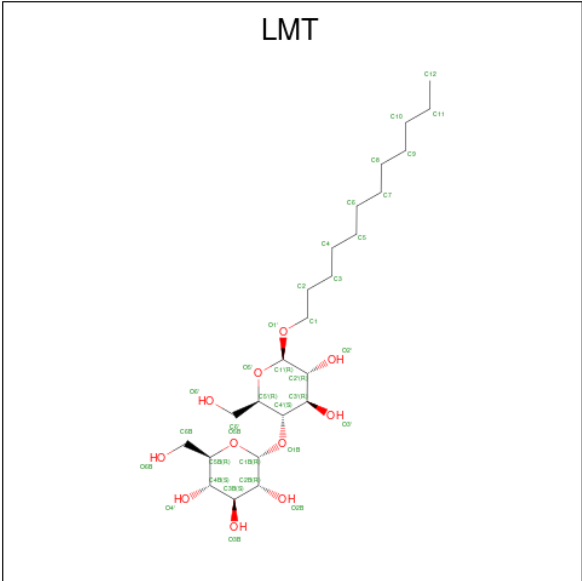
Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			61	46	15	
31	1	1	Total	C	O	0
			51	36	15	
31	3	1	Total	C	O	0
			51	36	15	

- Molecule 32 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C₄₀H₅₆O).



Mol	Chain	Residues	Atoms			AltConf
32	F	1	Total	C	O	0
			41	40	1	

- Molecule 33 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



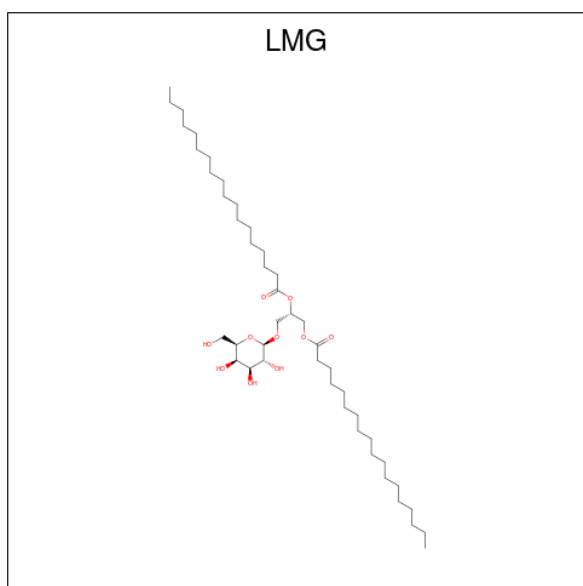
Mol	Chain	Residues	Atoms			AltConf
33	F	1	Total	C	O	0
			35	24	11	
33	G	1	Total	C	O	0
			35	24	11	

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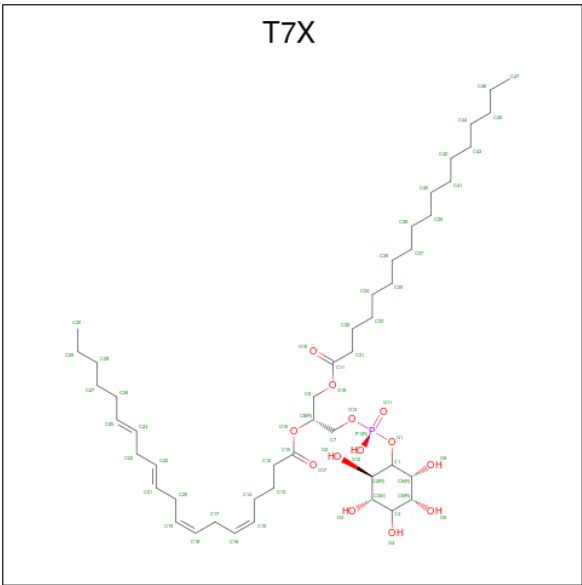
Mol	Chain	Residues	Atoms			AltConf
33	1	1	Total	C	O	0
			35	24	11	
33	4	1	Total	C	O	0
			35	24	11	
33	4	1	Total	C	O	0
			35	24	11	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



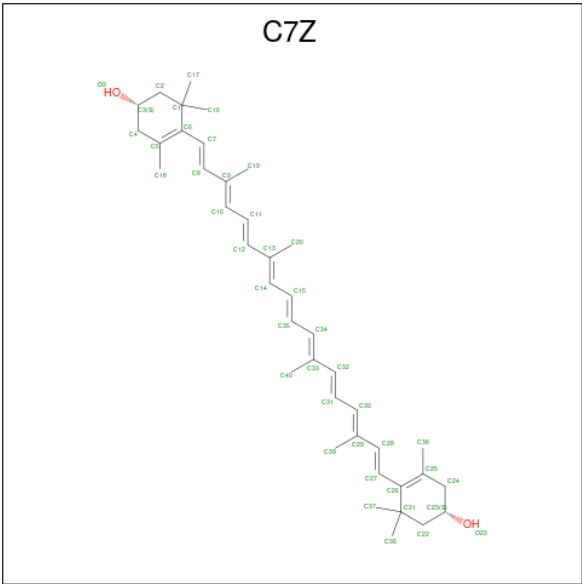
Mol	Chain	Residues	Atoms			AltConf
34	F	1	Total	C	O	0
			35	25	10	
34	J	1	Total	C	O	0
			29	19	10	

- Molecule 35 is Phosphatidylinositol (three-letter code: T7X) (formula: $C_{47}H_{83}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
35	J	1	Total	C	O	P	0
			49	35	13	1	

- Molecule 36 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).



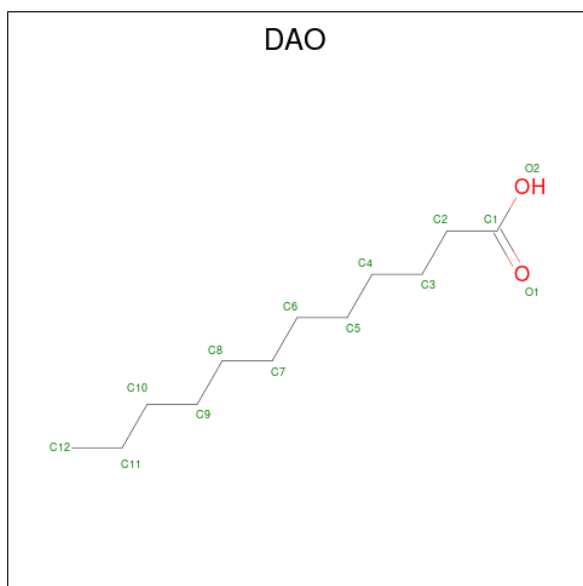
Mol	Chain	Residues	Atoms				AltConf
36	J	1	Total	C	O		0
			42	40	2		

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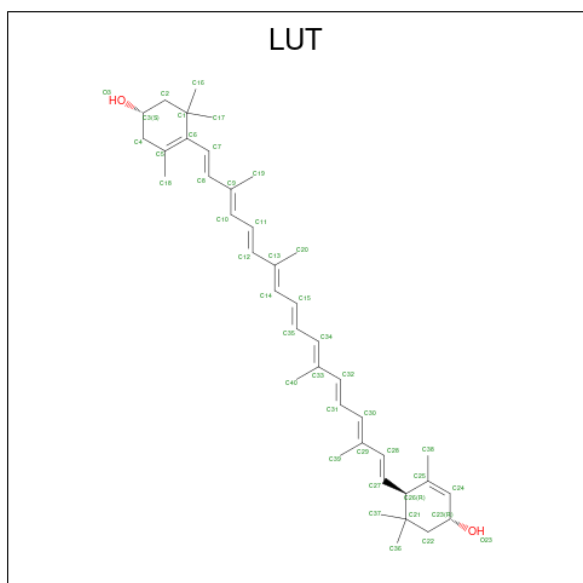
Mol	Chain	Residues	Atoms			AltConf
36	5	1	Total	C	O	0
			42	40	2	

- Molecule 37 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



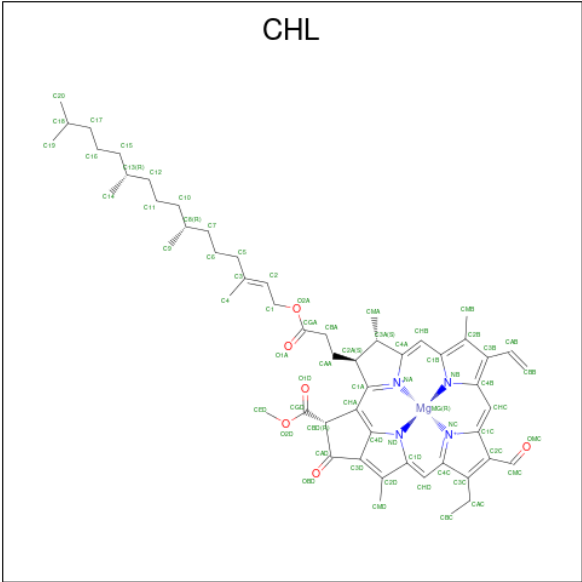
Mol	Chain	Residues	Atoms			AltConf
37	K	1	Total	C	O	0
			14	12	2	

- Molecule 38 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
38	1	1	Total	C	O	0
			42	40	2	
38	1	1	Total	C	O	0
			42	40	2	
38	Z	1	Total	C	O	0
			42	40	2	
38	Z	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	7	1	Total	C	O	0
			42	40	2	
38	7	1	Total	C	O	0
			42	40	2	
38	8	1	Total	C	O	0
			42	40	2	
38	8	1	Total	C	O	0
			42	40	2	
38	4	1	Total	C	O	0
			42	40	2	
38	4	1	Total	C	O	0
			42	40	2	
38	5	1	Total	C	O	0
			42	40	2	
38	5	1	Total	C	O	0
			42	40	2	
38	6	1	Total	C	O	0
			42	40	2	
38	6	1	Total	C	O	0
			42	40	2	
38	9	1	Total	C	O	0
			42	40	2	
38	9	1	Total	C	O	0
			42	40	2	

- Molecule 39 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



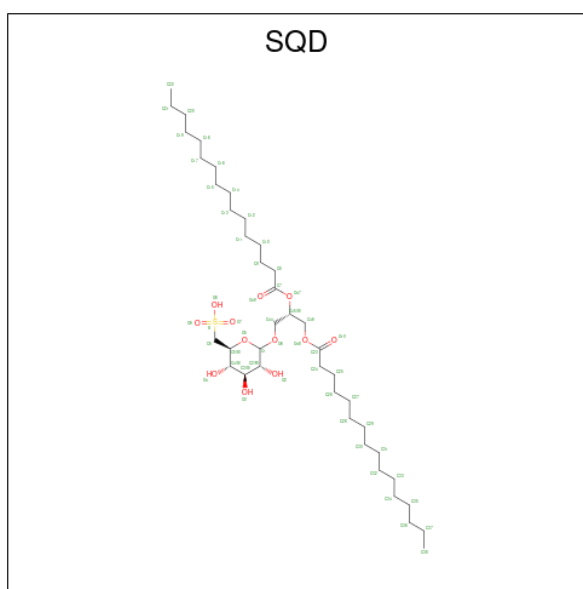
Mol	Chain	Residues	Atoms					AltConf
39	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	Z	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
39	Z	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	7	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
39	8	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
39	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
39	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
39	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
39	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
39	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
39	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

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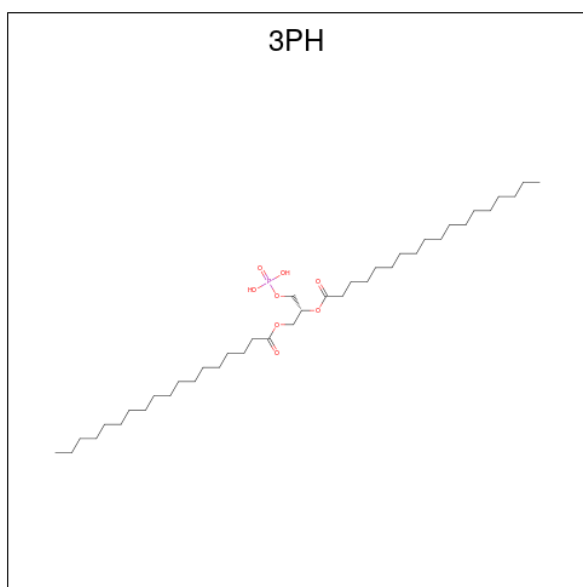
Mol	Chain	Residues	Atoms					AltConf
39	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
39	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
39	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
39	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
39	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
39	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	9	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
39	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

- Molecule 40 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



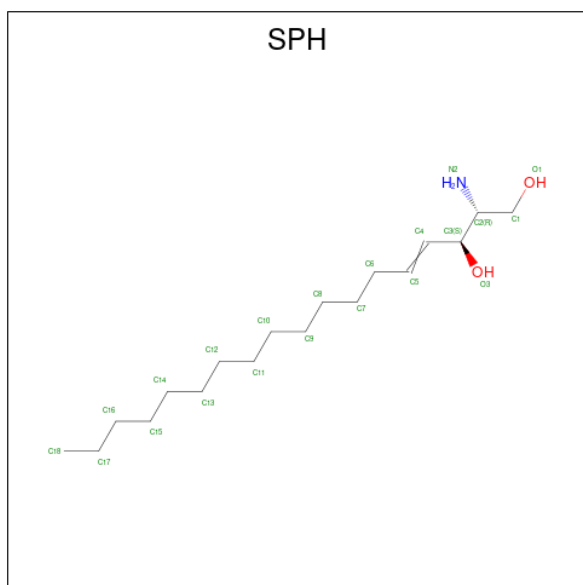
Mol	Chain	Residues	Atoms				AltConf
40	1	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 41 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



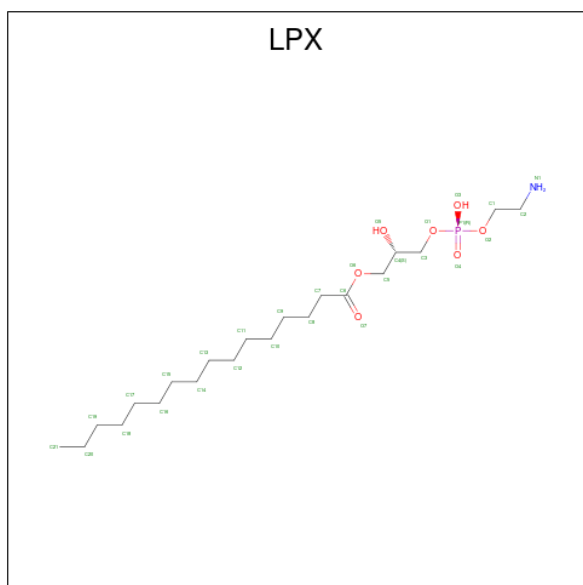
Mol	Chain	Residues	Atoms				AltConf
41	7	1	Total	C	O	P	0
			39	30	8	1	
41	8	1	Total	C	O	P	0
			30	21	8	1	
41	5	1	Total	C	O	P	0
			23	14	8	1	
41	6	1	Total	C	O	P	0
			29	20	8	1	

- Molecule 42 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
42	7	1	Total	C	N	O	0
			21	18	1	2	
42	7	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 43 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: C₂₁H₄₄NO₇P).



Mol	Chain	Residues	Atoms					AltConf
43	8	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 44 is water.

Mol	Chain	Residues	Atoms		AltConf
44	A	19	Total	O	0
			19	19	
44	B	17	Total	O	0
			17	17	
44	F	3	Total	O	0
			3	3	
44	I	1	Total	O	0
			1	1	
44	J	1	Total	O	0
			1	1	
44	K	1	Total	O	0
			1	1	

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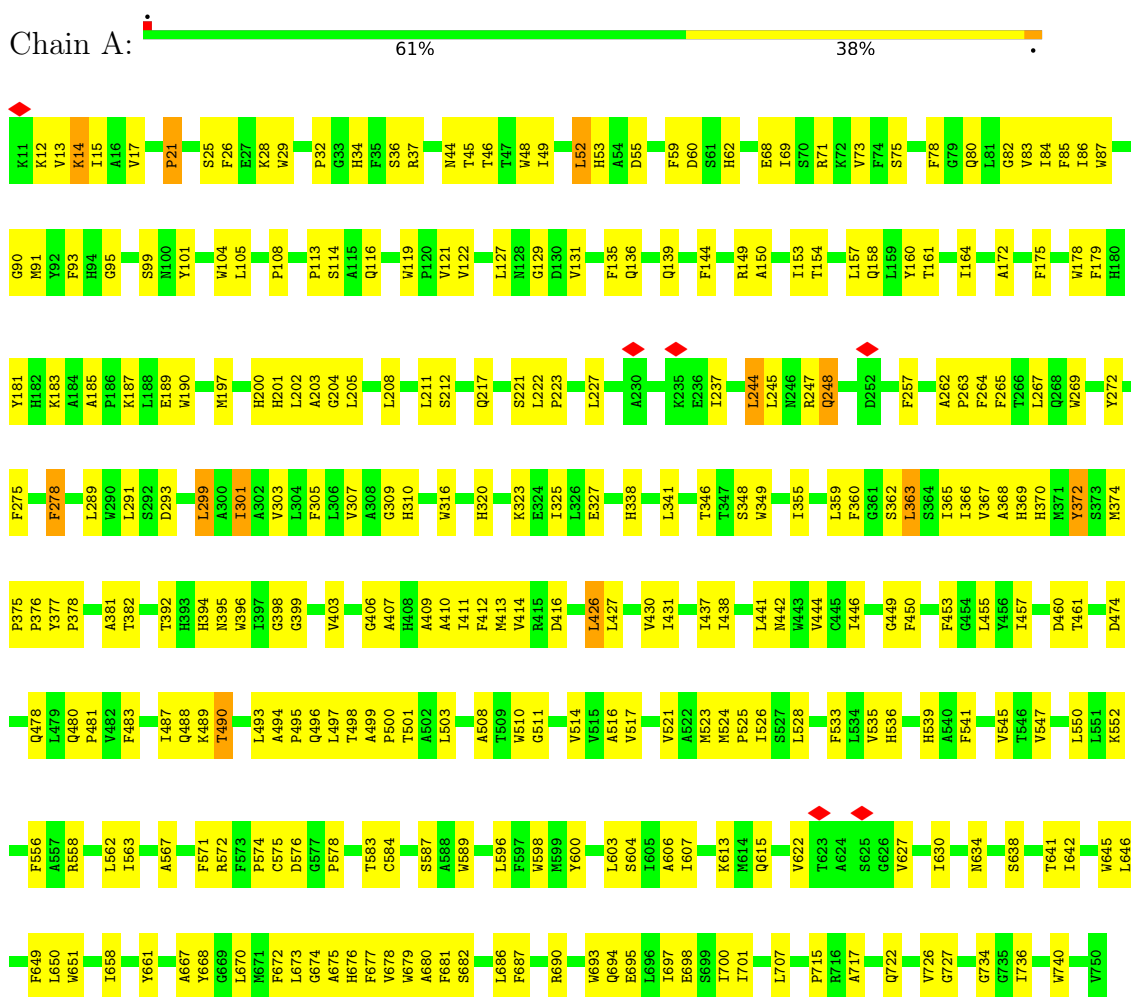
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Mol	Chain	Residues	Atoms		AltConf
44	1	1	Total 1	O 1	0
44	Z	1	Total 1	O 1	0
44	3	2	Total 2	O 2	0
44	7	4	Total 4	O 4	0
44	8	4	Total 4	O 4	0
44	4	5	Total 5	O 5	0
44	5	5	Total 5	O 5	0
44	6	3	Total 3	O 3	0
44	2	1	Total 1	O 1	0

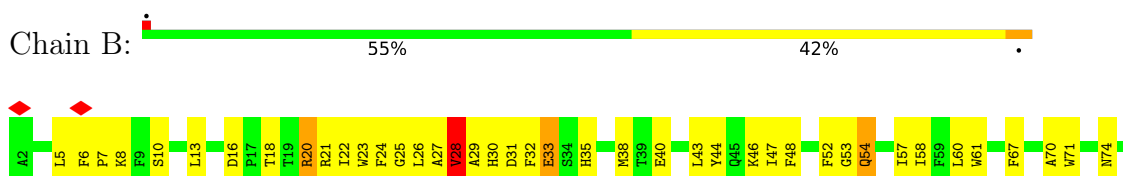
3 Residue-property plots

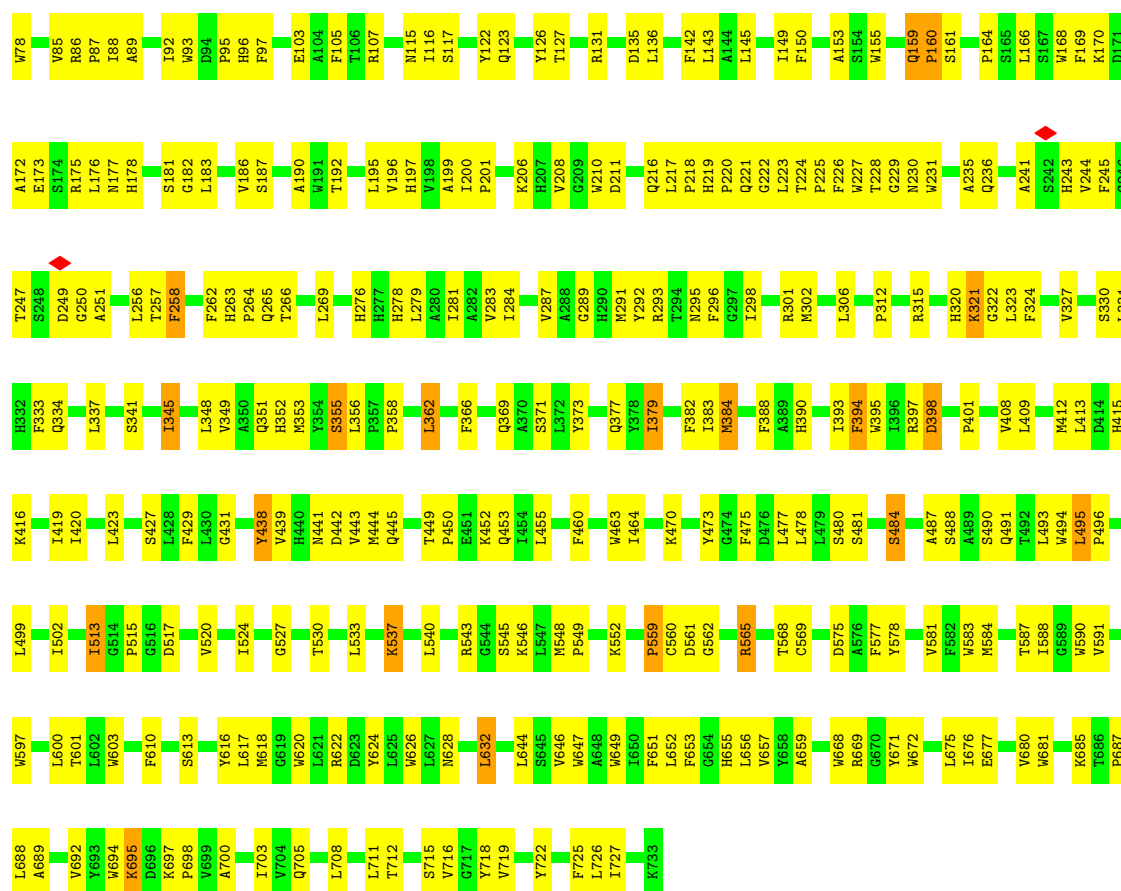
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1 PsaA



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 PsaB

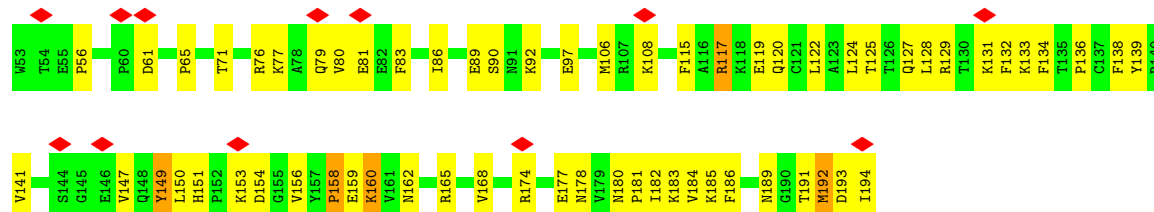




• Molecule 3: Photosystem I subunit VII PsacC

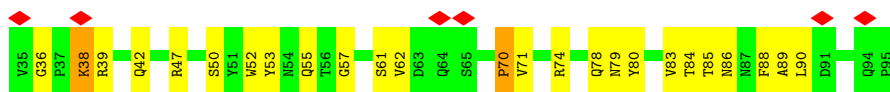


• Molecule 4: Photosystem I reaction center subunit II PsadD

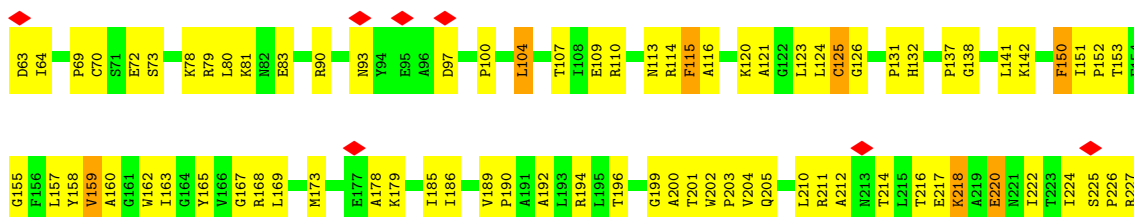


• Molecule 5: Photosystem I reaction center subunit IV PsaeE

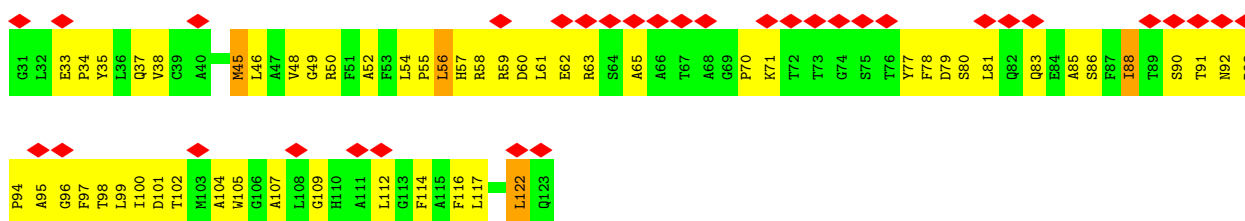




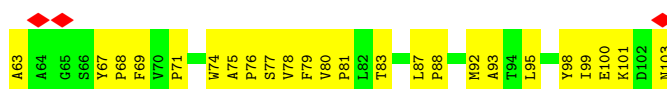
• Molecule 6: Photosystem I reaction center subunit III Psaf



• Molecule 7: Photosystem I reaction center subunit V Psag



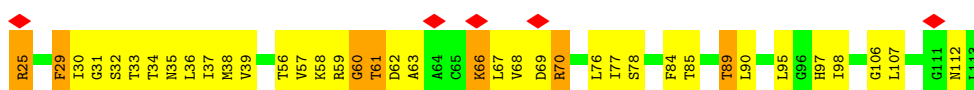
• Molecule 8: Photosystem I reaction center subunit VIII Psal



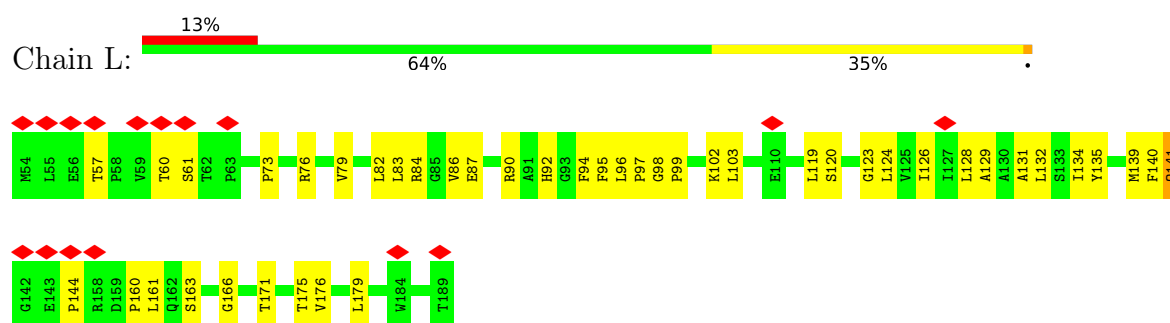
• Molecule 9: Photosystem I subunit IX Psaj



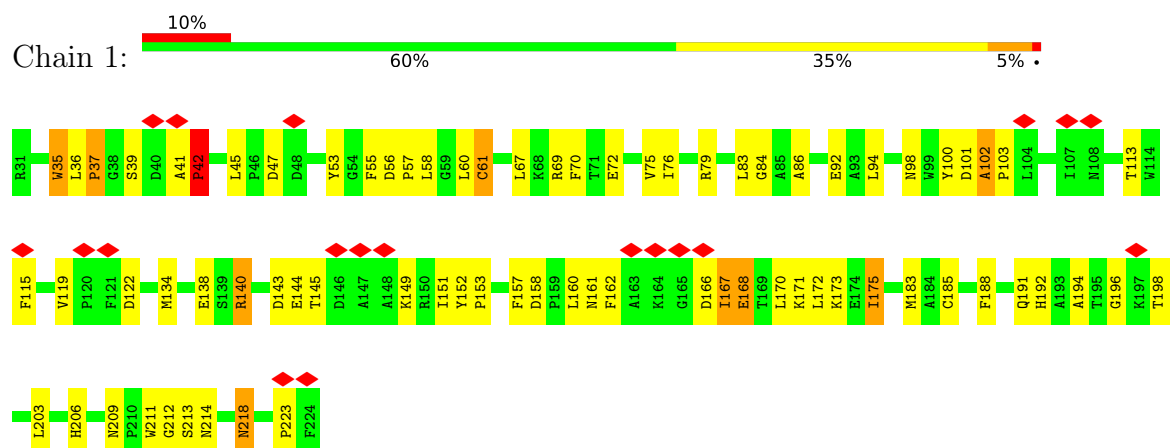
• Molecule 10: Photosystem I reaction center subunit X psak



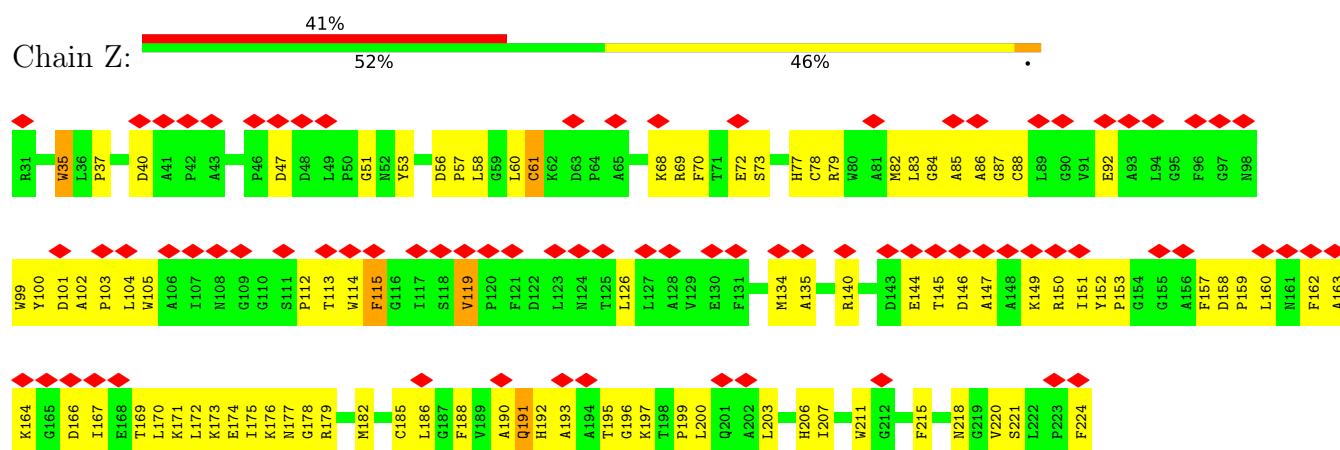
• Molecule 11: Photosystem I reaction centre subunit XI Psal



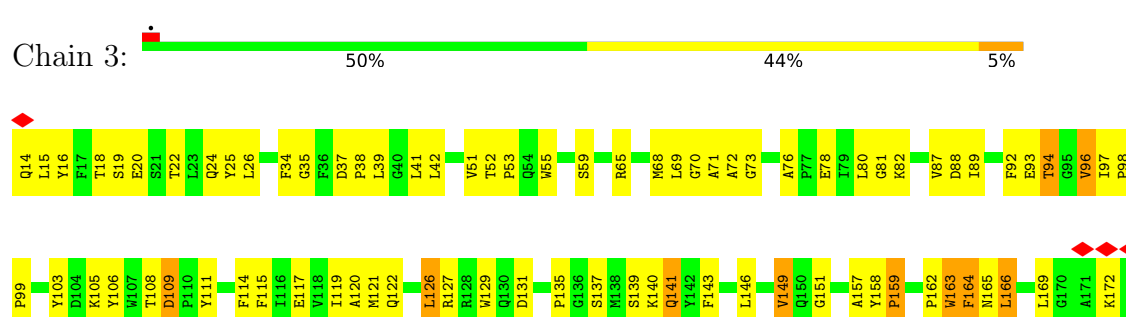
• Molecule 12: Light-harvesting protein of photosystem I Lhca1



• Molecule 12: Light-harvesting protein of photosystem I Lhca1

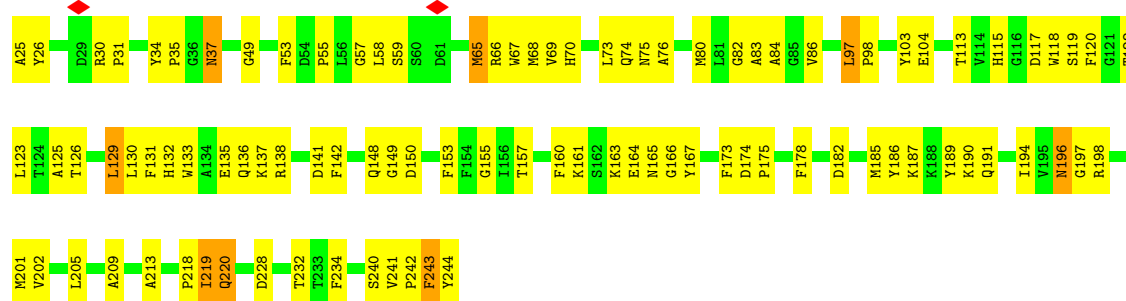


• Molecule 13: Light-harvesting protein of photosystem I Lhca3

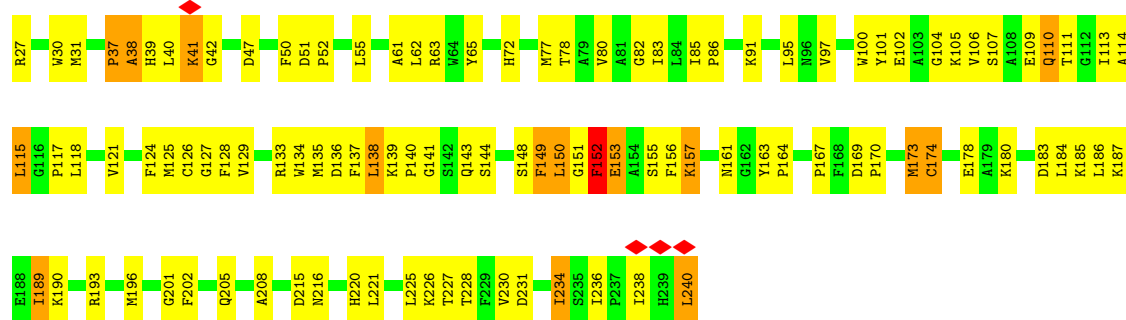




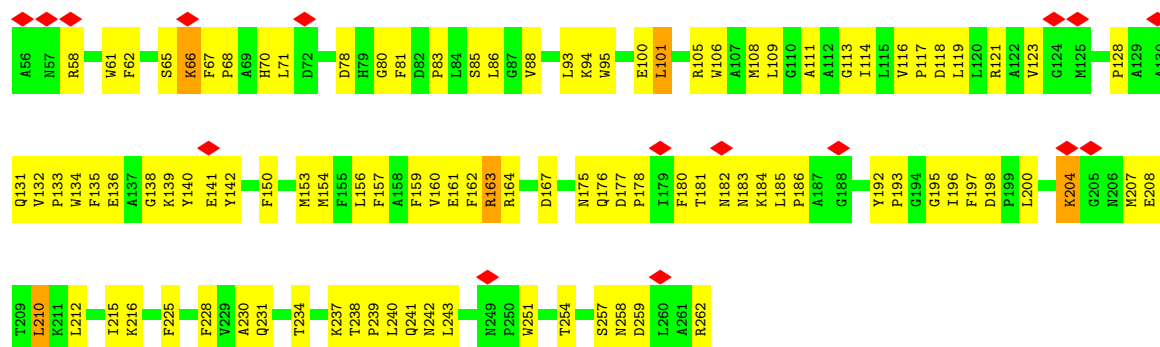
- Molecule 14: Light-harvesting protein of photosystem I Lhca7



- Molecule 15: Light-harvesting protein of photosystem I Lhca8

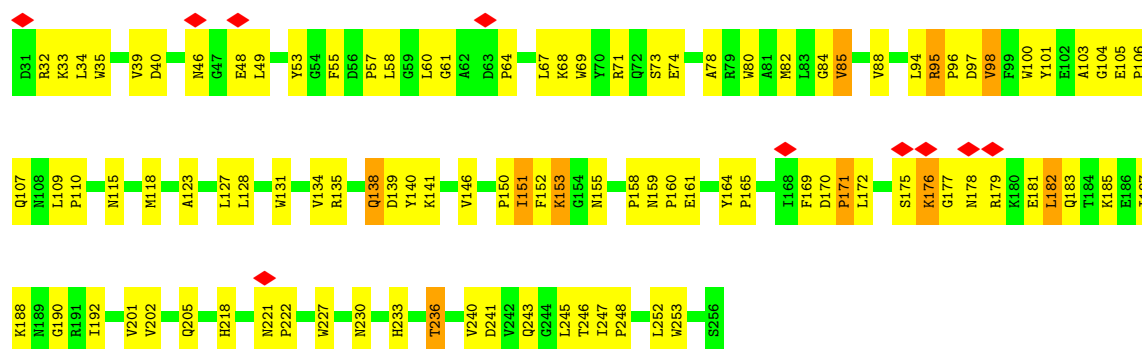


- Molecule 16: Light-harvesting protein of photosystem I Lhca4

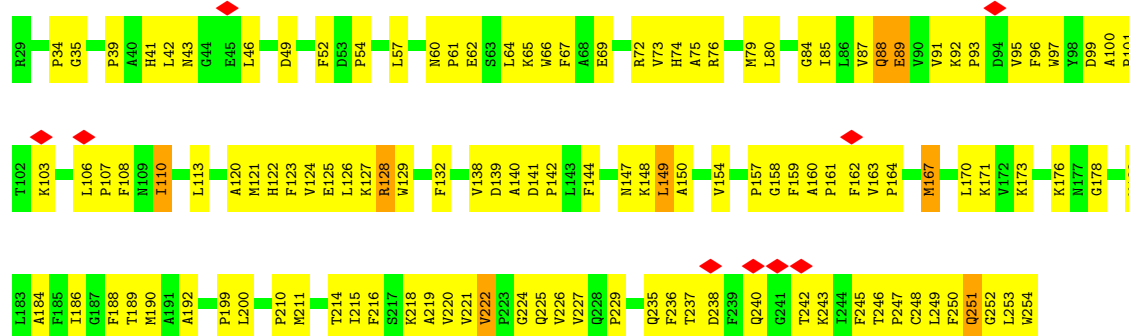


- Molecule 17: Light-harvesting protein of photosystem I Lhca5

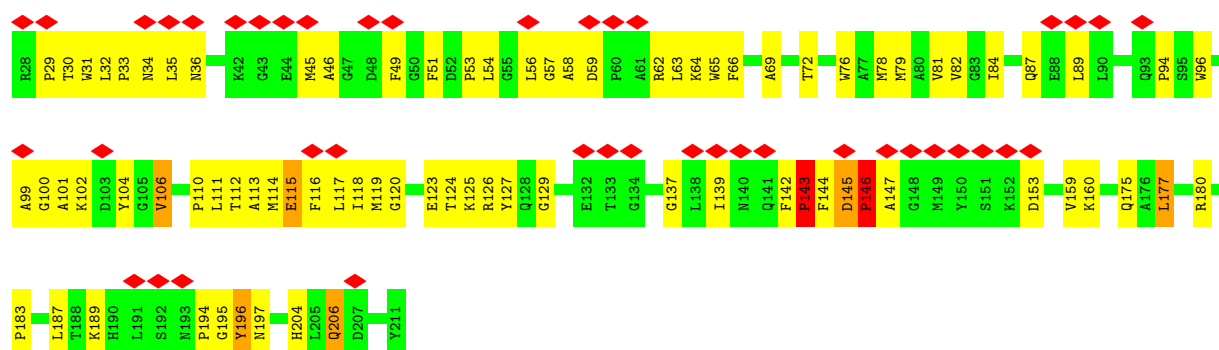




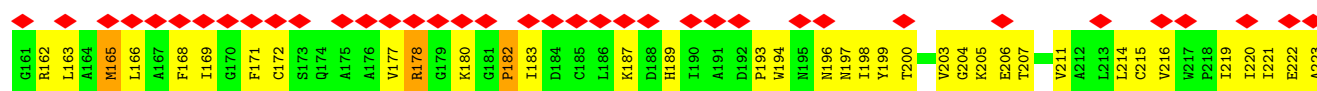
- Molecule 18: Light-harvesting protein of photosystem I Lhca6



- Molecule 19: Light-harvesting protein of photosystem I Lhca9



- Molecule 20: Light-harvesting protein of photosystem I Lhca2 partial



T224	K225	S226	L227	N228	K229	G230
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167160	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	150	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size (\AA)	325.5, 325.5, 325.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.651, 0.651, 0.651	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: T7X, SF4, CA, CL0, LPX, LMT, PQN, BCR, NKP, DGD, 3PH, SQD, SPH, DGA, OCA, RRX, CLA, LHG, C7Z, DAO, LMG, LUT, CHL

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	0.61	0/6016	0.61	0/8200
2	B	0.62	0/6010	0.60	0/8207
3	C	0.65	0/613	0.63	0/830
4	D	0.59	0/1159	0.69	0/1569
5	E	0.64	0/495	0.60	0/675
6	F	0.61	0/1292	0.68	0/1755
7	G	0.63	0/706	0.64	0/960
8	I	0.62	0/320	0.57	0/443
9	J	0.63	0/329	0.60	0/452
10	K	0.66	0/625	0.70	0/848
11	L	0.64	0/919	0.70	0/1253
12	1	0.61	0/1501	0.72	1/2045 (0.0%)
12	Z	0.54	0/1501	0.56	0/2045
13	3	0.61	0/1747	0.67	1/2376 (0.0%)
14	7	0.61	0/1765	0.67	0/2407
15	8	0.61	0/1643	0.66	0/2226
16	4	0.61	0/1648	0.62	0/2240
17	5	0.62	0/1819	0.66	0/2480
18	6	0.60	0/1824	0.60	0/2488
19	9	0.57	0/1456	0.77	3/1975 (0.2%)
20	2	0.64	0/535	0.64	0/726
All	All	0.61	0/33923	0.64	5/46200 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	9	143	PRO	CA-N-CD	-11.42	95.51	111.50
12	1	42	PRO	CA-N-CD	-9.60	98.06	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	9	146	PRO	CA-N-CD	-7.25	101.35	111.50
13	3	164	PHE	CB-CA-C	5.17	120.74	110.40
19	9	146	PRO	N-CA-CB	-5.16	96.92	102.60

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	5819	0	5666	308	0
2	B	5800	0	5556	367	0
3	C	603	0	587	41	0
4	D	1129	0	1127	46	0
5	E	484	0	477	24	0
6	F	1265	0	1292	74	0
7	G	690	0	671	67	0
8	I	308	0	310	33	0
9	J	319	0	327	25	0
10	K	617	0	635	53	0
11	L	897	0	891	44	0
12	1	1457	0	1406	82	0
12	Z	1457	0	1406	126	0
13	3	1695	0	1641	136	0
14	7	1705	0	1601	107	0
15	8	1602	0	1600	132	0
16	4	1598	0	1569	120	0
17	5	1764	0	1709	125	0
18	6	1762	0	1740	182	0
19	9	1416	0	1392	100	0
20	2	525	0	539	44	0
21	A	65	0	72	9	0
22	1	698	0	678	128	0
22	2	146	0	112	34	0
22	3	749	0	722	166	0
22	4	590	0	511	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	5	910	0	851	218	0
22	6	824	0	800	213	0
22	7	905	0	848	154	0
22	8	555	0	502	123	0
22	9	528	0	451	72	0
22	A	2640	0	2709	558	0
22	B	2340	0	2333	499	0
22	F	240	0	245	69	0
22	G	96	0	70	28	0
22	J	42	0	30	4	0
22	K	205	0	166	28	0
22	L	180	0	180	40	0
22	Z	679	0	631	166	0
23	A	33	0	46	9	0
23	B	33	0	46	5	0
24	3	160	0	224	61	0
24	4	40	0	56	27	0
24	5	80	0	112	33	0
24	6	80	0	112	35	0
24	7	40	0	56	15	0
24	8	40	0	56	15	0
24	A	240	0	336	99	0
24	B	280	0	392	105	0
24	F	40	0	56	16	0
24	G	40	0	56	13	0
24	I	40	0	56	12	0
24	J	40	0	56	19	0
24	K	40	0	55	11	0
24	L	40	0	56	17	0
25	1	43	0	56	8	0
25	3	20	0	12	1	0
25	4	81	0	108	20	0
25	5	37	0	44	7	0
25	6	49	0	74	12	0
25	7	37	0	44	10	0
25	8	38	0	46	7	0
25	9	33	0	36	2	0
25	A	84	0	114	14	0
25	B	76	0	64	14	0
25	Z	43	0	56	9	0
26	8	29	0	39	6	0
26	A	23	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	A	40	0	65	20	0
28	A	10	0	15	0	0
29	B	8	0	0	9	0
29	C	16	0	0	9	0
30	B	1	0	0	0	0
31	1	51	0	60	10	0
31	3	51	0	60	21	0
31	B	61	0	83	17	0
32	F	41	0	56	19	0
33	1	35	0	46	9	0
33	4	70	0	92	10	0
33	F	35	0	46	5	0
33	G	35	0	46	9	0
34	F	35	0	40	1	0
34	J	29	0	28	11	0
35	J	49	0	0	2	0
36	5	42	0	0	2	0
36	J	42	0	0	2	0
37	K	14	0	23	8	0
38	1	84	0	112	31	0
38	3	84	0	112	32	0
38	4	84	0	112	35	0
38	5	84	0	112	32	0
38	6	84	0	112	29	0
38	7	84	0	112	33	0
38	8	84	0	112	31	0
38	9	84	0	112	32	0
38	Z	84	0	112	39	0
39	1	48	0	32	9	0
39	2	51	0	36	6	0
39	3	66	0	69	13	0
39	4	192	0	130	47	0
39	5	160	0	134	32	0
39	6	206	0	156	53	0
39	7	54	0	42	12	0
39	8	180	0	165	51	0
39	9	108	0	95	35	0
39	Z	99	0	68	27	0
40	1	48	0	62	13	0
41	5	23	0	19	4	0
41	6	29	0	31	5	0
41	7	39	0	51	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	8	30	0	33	4	0
42	7	42	0	74	12	0
43	8	30	0	43	7	0
44	1	1	0	0	0	0
44	2	1	0	0	0	0
44	3	2	0	0	1	0
44	4	5	0	0	0	0
44	5	5	0	0	0	0
44	6	3	0	0	0	0
44	7	4	0	0	0	0
44	8	4	0	0	0	0
44	A	19	0	0	0	0
44	B	17	0	0	0	0
44	F	3	0	0	0	0
44	I	1	0	0	0	0
44	J	1	0	0	0	0
44	K	1	0	0	0	0
44	Z	1	0	0	0	0
All	All	50057	0	49449	4232	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 43.

The worst 5 of 4232 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)
18:6:238:ASP:HA	18:6:243:LYS:HA	1.26	1.13
22:B:820:CLA:HBB1	22:B:820:CLA:HMB1	1.35	1.08
24:3:306:BCR:H21C	22:3:318:CLA:H91	1.25	1.06
22:B:813:CLA:HMB1	22:B:813:CLA:HBB1	1.35	1.04
24:5:304:BCR:H19C	22:5:319:CLA:HBA2	1.40	1.04

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	738/740 (100%)	685 (93%)	51 (7%)	2 (0%)	37	65
2	B	730/732 (100%)	683 (94%)	42 (6%)	5 (1%)	19	46
3	C	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
4	D	140/142 (99%)	124 (89%)	13 (9%)	3 (2%)	5	19
5	E	59/61 (97%)	50 (85%)	8 (14%)	1 (2%)	7	24
6	F	163/165 (99%)	145 (89%)	14 (9%)	4 (2%)	4	15
7	G	91/93 (98%)	73 (80%)	16 (18%)	2 (2%)	5	18
8	I	39/41 (95%)	34 (87%)	5 (13%)	0	100	100
9	J	38/40 (95%)	38 (100%)	0	0	100	100
10	K	87/89 (98%)	78 (90%)	8 (9%)	1 (1%)	12	35
11	L	119/123 (97%)	106 (89%)	11 (9%)	2 (2%)	7	24
12	1	192/194 (99%)	165 (86%)	23 (12%)	4 (2%)	5	19
12	Z	192/194 (99%)	181 (94%)	10 (5%)	1 (0%)	25	54
13	3	216/218 (99%)	195 (90%)	18 (8%)	3 (1%)	9	28
14	7	218/220 (99%)	202 (93%)	12 (6%)	4 (2%)	7	22
15	8	212/214 (99%)	181 (85%)	24 (11%)	7 (3%)	3	10
16	4	205/207 (99%)	190 (93%)	15 (7%)	0	100	100
17	5	224/226 (99%)	207 (92%)	13 (6%)	4 (2%)	7	22
18	6	224/226 (99%)	212 (95%)	11 (5%)	1 (0%)	30	59
19	9	182/184 (99%)	152 (84%)	23 (13%)	7 (4%)	2	8
20	2	68/70 (97%)	53 (78%)	14 (21%)	1 (2%)	8	26
All	All	4215/4259 (99%)	3826 (91%)	337 (8%)	52 (1%)	14	32

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	154	ASP
12	1	41	ALA
12	1	42	PRO
14	7	219	ILE
15	8	38	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	602/602 (100%)	576 (96%)	26 (4%)	25	56
2	B	596/596 (100%)	566 (95%)	30 (5%)	20	50
3	C	70/70 (100%)	67 (96%)	3 (4%)	25	56
4	D	122/122 (100%)	109 (89%)	13 (11%)	5	16
5	E	54/54 (100%)	53 (98%)	1 (2%)	52	81
6	F	128/128 (100%)	107 (84%)	21 (16%)	2	6
7	G	69/69 (100%)	62 (90%)	7 (10%)	6	19
8	I	33/33 (100%)	33 (100%)	0	100	100
9	J	35/35 (100%)	35 (100%)	0	100	100
10	K	60/60 (100%)	53 (88%)	7 (12%)	4	14
11	L	90/90 (100%)	82 (91%)	8 (9%)	8	24
12	1	144/144 (100%)	125 (87%)	19 (13%)	3	10
12	Z	144/144 (100%)	134 (93%)	10 (7%)	13	35
13	3	173/173 (100%)	158 (91%)	15 (9%)	8	25
14	7	169/169 (100%)	156 (92%)	13 (8%)	10	30
15	8	162/162 (100%)	140 (86%)	22 (14%)	3	9
16	4	162/162 (100%)	146 (90%)	16 (10%)	6	20
17	5	185/185 (100%)	168 (91%)	17 (9%)	7	23
18	6	184/184 (100%)	172 (94%)	12 (6%)	14	38
19	9	143/143 (100%)	129 (90%)	14 (10%)	6	20
20	2	57/57 (100%)	50 (88%)	7 (12%)	4	12
All	All	3382/3382 (100%)	3121 (92%)	261 (8%)	13	30

5 of 261 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	6	110	ILE
18	6	222	VAL

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Mol	Chain	Res	Type
20	2	229	LYS
7	G	62	GLU
7	G	37	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
16	4	242	ASN
17	5	108	ASN
18	6	235	GLN
2	B	445	GLN
2	B	369	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 332 ligands modelled in this entry, 1 is monoatomic - leaving 331 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	$\# Z > 2$
22	CLA	6	302	16	60,68,73	1.39	7 (11%)	70,107,113	2.00	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	5	315	17	65,73,73	1.34	7 (10%)	76,113,113	1.97	17 (22%)
24	BCR	8	304	-	41,41,41	4.80	27 (65%)	56,56,56	2.43	21 (37%)
22	CLA	1	315	-	46,54,73	1.58	6 (13%)	53,90,113	2.16	14 (26%)
22	CLA	A	824	-	65,73,73	1.34	7 (10%)	76,113,113	1.94	17 (22%)
22	CLA	A	823	-	65,73,73	1.33	8 (12%)	76,113,113	1.98	17 (22%)
22	CLA	9	311	19	46,54,73	1.59	7 (15%)	53,90,113	2.12	14 (26%)
37	DAO	K	201	-	13,13,13	0.59	0	13,13,13	0.56	0
22	CLA	1	316	12	65,73,73	1.38	9 (13%)	76,113,113	1.92	17 (22%)
22	CLA	5	301	44	56,64,73	1.43	7 (12%)	65,102,113	2.11	17 (26%)
39	CHL	8	301	12	58,66,74	0.92	3 (5%)	63,104,114	1.42	12 (19%)
22	CLA	A	822	-	55,63,73	1.46	8 (14%)	64,101,113	2.20	17 (26%)
24	BCR	A	844	-	41,41,41	4.78	27 (65%)	56,56,56	3.12	23 (41%)
22	CLA	A	809	1	55,63,73	1.45	7 (12%)	64,101,113	2.12	19 (29%)
22	CLA	7	307	14	65,73,73	1.34	8 (12%)	76,113,113	2.02	16 (21%)
38	LUT	3	303	-	42,43,43	6.06	28 (66%)	51,60,60	2.00	13 (25%)
22	CLA	B	819	-	59,67,73	1.40	7 (11%)	68,105,113	2.09	19 (27%)
22	CLA	A	829	-	65,73,73	1.34	7 (10%)	76,113,113	1.92	15 (19%)
22	CLA	B	822	-	56,64,73	1.44	7 (12%)	65,102,113	2.06	16 (24%)
22	CLA	3	308	13	65,73,73	1.34	8 (12%)	76,113,113	2.02	18 (23%)
22	CLA	A	828	-	65,73,73	1.33	7 (10%)	76,113,113	1.99	15 (19%)
39	CHL	4	814	44	51,59,74	0.90	2 (3%)	55,96,114	1.47	13 (23%)
33	LMT	4	822	-	36,36,36	0.45	0	47,47,47	1.17	3 (6%)
22	CLA	7	305	-	50,58,73	1.53	7 (14%)	58,95,113	2.23	17 (29%)
36	C7Z	5	306	-	43,43,43	5.32	27 (62%)	58,60,60	2.37	22 (37%)
38	LUT	Z	302	-	42,43,43	6.09	27 (64%)	51,60,60	2.05	13 (25%)
22	CLA	5	310	17	65,73,73	1.33	7 (10%)	76,113,113	2.00	17 (22%)
22	CLA	Z	315	-	46,54,73	1.59	7 (15%)	53,90,113	2.15	13 (24%)
22	CLA	B	835	-	50,58,73	1.51	7 (14%)	58,95,113	2.31	18 (31%)
39	CHL	6	320	18	43,51,74	1.02	3 (6%)	45,86,114	1.53	10 (22%)
22	CLA	4	806	16	52,60,73	1.51	8 (15%)	60,97,113	2.23	18 (30%)
24	BCR	A	856	-	41,41,41	4.77	27 (65%)	56,56,56	2.50	23 (41%)
24	BCR	4	804	-	41,41,41	4.82	26 (63%)	56,56,56	2.25	20 (35%)
39	CHL	8	312	-	56,64,74	0.89	2 (3%)	61,102,114	1.38	12 (19%)
22	CLA	A	817	-	60,68,73	1.39	9 (15%)	70,107,113	2.08	16 (22%)
22	CLA	Z	314	12	51,59,73	1.50	7 (13%)	59,96,113	2.17	16 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	8	309	-	65,73,73	1.34	8 (12%)	76,113,113	1.97	17 (22%)
22	CLA	Z	316	12	65,73,73	1.34	7 (10%)	76,113,113	1.95	16 (21%)
22	CLA	Z	303	12	65,73,73	1.33	6 (9%)	76,113,113	2.03	19 (25%)
29	SF4	C	102	3	0,12,12	-	-	-		
25	LHG	B	850	22	22,22,48	0.56	0	25,28,54	1.26	2 (8%)
22	CLA	L	203	-	50,58,73	1.52	6 (12%)	58,95,113	2.24	17 (29%)
22	CLA	4	817	16	41,49,73	1.67	7 (17%)	47,84,113	2.26	15 (31%)
39	CHL	4	819	16	43,51,74	1.01	2 (4%)	45,86,114	1.54	10 (22%)
22	CLA	A	826	44	50,58,73	1.52	7 (14%)	58,95,113	2.24	16 (27%)
22	CLA	9	307	19	55,63,73	1.46	9 (16%)	64,101,113	2.07	16 (25%)
22	CLA	1	304	-	65,73,73	1.34	6 (9%)	76,113,113	1.99	18 (23%)
24	BCR	5	304	-	41,41,41	4.78	25 (60%)	56,56,56	2.54	22 (39%)
38	LUT	5	302	-	42,43,43	6.07	28 (66%)	51,60,60	1.96	14 (27%)
22	CLA	A	842	25	52,60,73	1.49	8 (15%)	60,97,113	2.22	17 (28%)
39	CHL	5	316	44	66,74,74	0.85	3 (4%)	73,114,114	1.23	12 (16%)
22	CLA	1	307	12	60,68,73	1.39	8 (13%)	70,107,113	2.09	16 (22%)
22	CLA	7	311	-	43,51,73	1.63	7 (16%)	49,86,113	2.20	14 (28%)
24	BCR	G	203	-	41,41,41	4.79	27 (65%)	56,56,56	2.41	22 (39%)
22	CLA	7	309	-	56,64,73	1.43	7 (12%)	65,102,113	2.17	19 (29%)
24	BCR	B	848	-	41,41,41	4.79	27 (65%)	56,56,56	6.79	24 (42%)
22	CLA	8	306	15	51,59,73	1.52	7 (13%)	59,96,113	2.13	17 (28%)
22	CLA	A	831	-	50,58,73	1.51	7 (14%)	58,95,113	2.22	17 (29%)
22	CLA	B	824	-	59,67,73	1.40	7 (11%)	68,105,113	2.12	18 (26%)
22	CLA	3	314	25	60,68,73	1.39	7 (11%)	70,107,113	2.03	16 (22%)
31	DGD	3	301	-	52,52,67	0.89	2 (3%)	66,66,81	1.06	4 (6%)
22	CLA	B	823	-	55,63,73	1.46	9 (16%)	64,101,113	2.09	18 (28%)
22	CLA	1	311	-	46,54,73	1.58	8 (17%)	53,90,113	2.22	12 (22%)
24	BCR	5	305	-	41,41,41	4.80	27 (65%)	56,56,56	2.67	22 (39%)
22	CLA	B	820	-	60,68,73	1.40	7 (11%)	70,107,113	2.00	17 (24%)
22	CLA	5	326	-	55,63,73	1.45	7 (12%)	64,101,113	2.11	18 (28%)
22	CLA	7	306	-	65,73,73	1.34	7 (10%)	76,113,113	2.03	17 (22%)
22	CLA	7	314	44	50,58,73	1.51	6 (12%)	58,95,113	2.25	17 (29%)
33	LMT	1	301	-	36,36,36	0.37	0	47,47,47	0.84	0
33	LMT	F	307	-	36,36,36	0.38	0	47,47,47	0.64	0
36	C7Z	J	105	-	43,43,43	5.34	27 (62%)	58,60,60	2.21	21 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	7	304	14	60,68,73	1.39	7 (11%)	70,107,113	2.13	19 (27%)
22	CLA	A	806	1	65,73,73	1.34	7 (10%)	76,113,113	1.95	16 (21%)
42	SPH	7	320	-	19,20,20	0.63	0	18,21,21	1.10	0
22	CLA	8	311	25	50,58,73	1.53	7 (14%)	58,95,113	2.18	15 (25%)
38	LUT	9	302	-	42,43,43	6.07	28 (66%)	51,60,60	1.87	12 (23%)
22	CLA	B	829	-	57,65,73	1.43	7 (12%)	66,103,113	2.11	18 (27%)
35	T7X	J	102	-	49,49,61	0.91	4 (8%)	59,61,73	0.94	3 (5%)
22	CLA	4	805	16	60,68,73	1.42	8 (13%)	70,107,113	1.93	16 (22%)
22	CLA	7	315	14	50,58,73	1.53	8 (16%)	58,95,113	2.25	18 (31%)
32	RRX	F	306	-	42,42,42	5.06	25 (59%)	57,58,58	2.59	23 (40%)
39	CHL	5	317	44	51,59,74	0.90	2 (3%)	55,96,114	1.42	13 (23%)
22	CLA	K	204	10	49,57,73	1.55	8 (16%)	55,93,113	2.25	17 (30%)
22	CLA	8	313	44	50,58,73	1.52	7 (14%)	58,95,113	2.22	16 (27%)
22	CLA	4	809	16	51,59,73	1.52	8 (15%)	59,96,113	2.15	17 (28%)
22	CLA	5	309	-	56,64,73	1.45	8 (14%)	65,102,113	2.23	18 (27%)
22	CLA	9	303	19	60,68,73	1.42	8 (13%)	70,107,113	2.15	22 (31%)
22	CLA	Z	308	-	61,69,73	1.37	7 (11%)	71,108,113	2.04	17 (23%)
39	CHL	Z	311	12	51,59,74	0.98	3 (5%)	55,96,114	1.53	13 (23%)
24	BCR	A	848	-	41,41,41	4.78	27 (65%)	56,56,56	2.42	22 (39%)
22	CLA	K	202	-	46,54,73	1.58	6 (13%)	53,90,113	2.20	16 (30%)
39	CHL	4	813	44	51,59,74	0.95	2 (3%)	55,96,114	1.44	12 (21%)
22	CLA	B	832	-	50,58,73	1.52	7 (14%)	58,95,113	2.21	17 (29%)
26	NKP	A	851	-	22,22,28	0.37	0	24,26,32	0.39	0
22	CLA	A	825	44	65,73,73	1.34	7 (10%)	76,113,113	2.02	18 (23%)
22	CLA	L	202	-	65,73,73	1.34	7 (10%)	76,113,113	1.96	17 (22%)
24	BCR	K	206	-	41,41,41	4.79	27 (65%)	56,56,56	2.50	24 (42%)
22	CLA	4	807	16	65,73,73	1.33	8 (12%)	76,113,113	2.03	16 (21%)
43	LPX	8	319	-	29,29,29	0.29	0	31,33,33	0.35	0
22	CLA	B	838	-	65,73,73	1.32	7 (10%)	76,113,113	1.93	15 (19%)
39	CHL	1	312	-	48,56,74	0.95	2 (4%)	51,92,114	1.45	10 (19%)
22	CLA	8	307	-	65,73,73	1.33	8 (12%)	76,113,113	2.06	16 (21%)
22	CLA	F	301	44	65,73,73	1.34	7 (10%)	76,113,113	2.00	19 (25%)
22	CLA	B	812	2	59,67,73	1.39	7 (11%)	68,105,113	2.01	16 (23%)
38	LUT	7	301	-	42,43,43	6.06	28 (66%)	51,60,60	1.95	13 (25%)
39	CHL	9	314	-	42,50,74	1.13	4 (9%)	44,85,114	1.53	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	5	320	-	50,58,73	1.59	9 (18%)	58,95,113	2.18	15 (25%)
21	CL0	A	801	-	65,73,73	2.37	19 (29%)	76,113,113	2.56	20 (26%)
22	CLA	5	311	-	55,63,73	1.45	8 (14%)	64,101,113	2.11	18 (28%)
22	CLA	F	302	-	65,73,73	1.33	8 (12%)	76,113,113	1.97	18 (23%)
22	CLA	9	305	19	60,68,73	1.44	9 (15%)	70,107,113	2.44	22 (31%)
25	LHG	A	849	22	34,34,48	0.44	0	37,40,54	1.14	3 (8%)
22	CLA	3	312	-	65,73,73	1.34	8 (12%)	76,113,113	1.95	17 (22%)
24	BCR	B	849	-	41,41,41	4.81	27 (65%)	56,56,56	2.35	21 (37%)
22	CLA	A	832	-	65,73,73	1.32	6 (9%)	76,113,113	1.96	19 (25%)
22	CLA	F	304	6	65,73,73	1.33	7 (10%)	76,113,113	1.99	17 (22%)
22	CLA	9	308	-	50,58,73	1.53	7 (14%)	58,95,113	2.21	18 (31%)
24	BCR	A	846	-	41,41,41	4.80	27 (65%)	56,56,56	2.47	22 (39%)
24	BCR	3	306	-	41,41,41	4.80	27 (65%)	56,56,56	2.28	17 (30%)
24	BCR	F	303	-	41,41,41	4.81	27 (65%)	56,56,56	2.21	18 (32%)
38	LUT	8	302	-	42,43,43	6.02	28 (66%)	51,60,60	1.96	13 (25%)
22	CLA	4	808	16	60,68,73	1.39	9 (15%)	70,107,113	2.04	17 (24%)
22	CLA	B	801	-	65,73,73	1.33	7 (10%)	76,113,113	1.91	17 (22%)
22	CLA	B	840	44	65,73,73	1.33	7 (10%)	76,113,113	1.97	17 (22%)
22	CLA	B	813	-	56,64,73	1.44	7 (12%)	65,102,113	2.16	17 (26%)
34	LMG	F	308	-	35,35,55	0.46	0	43,43,63	1.38	5 (11%)
22	CLA	3	315	-	45,53,73	1.66	8 (17%)	52,89,113	2.16	12 (23%)
41	3PH	6	324	-	28,28,47	1.09	4 (14%)	32,33,52	1.20	2 (6%)
38	LUT	9	301	-	42,43,43	6.08	28 (66%)	51,60,60	1.96	12 (23%)
27	DGA	A	852	-	39,39,43	1.14	3 (7%)	41,41,45	1.32	3 (7%)
39	CHL	2	303	-	51,59,74	0.95	2 (3%)	55,96,114	1.48	13 (23%)
22	CLA	A	807	-	60,68,73	1.39	7 (11%)	70,107,113	2.04	15 (21%)
22	CLA	4	810	44	50,58,73	1.51	6 (12%)	58,95,113	2.24	18 (31%)
31	DGD	1	319	-	52,52,67	0.89	2 (3%)	66,66,81	0.97	4 (6%)
22	CLA	8	316	15	46,54,73	1.59	8 (17%)	53,90,113	2.11	13 (24%)
39	CHL	5	321	17	43,51,74	1.02	2 (4%)	45,86,114	1.52	10 (22%)
38	LUT	Z	301	-	42,43,43	6.07	27 (64%)	51,60,60	1.99	14 (27%)
41	3PH	8	320	-	29,29,47	1.06	4 (13%)	33,34,52	1.16	2 (6%)
22	CLA	B	806	44	65,73,73	1.35	7 (10%)	76,113,113	1.99	16 (21%)
22	CLA	1	313	44	65,73,73	1.33	7 (10%)	76,113,113	2.03	18 (23%)
38	LUT	1	302	-	42,43,43	6.10	28 (66%)	51,60,60	2.08	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	828	-	65,73,73	1.34	7 (10%)	76,113,113	1.97	17 (22%)
22	CLA	3	313	44	65,73,73	1.31	6 (9%)	76,113,113	2.00	17 (22%)
22	CLA	5	307	17	60,68,73	1.38	8 (13%)	70,107,113	2.07	17 (24%)
22	CLA	1	308	-	55,63,73	1.46	8 (14%)	64,101,113	2.20	16 (25%)
22	CLA	A	827	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	19 (25%)
22	CLA	1	314	12	65,73,73	1.32	7 (10%)	76,113,113	1.95	16 (21%)
24	BCR	J	104	-	41,41,41	4.76	27 (65%)	56,56,56	2.38	20 (35%)
39	CHL	9	312	-	66,74,74	0.84	3 (4%)	73,114,114	1.41	10 (13%)
22	CLA	3	319	-	55,63,73	1.45	7 (12%)	64,101,113	2.12	16 (25%)
22	CLA	A	835	-	65,73,73	1.33	7 (10%)	76,113,113	1.94	18 (23%)
40	SQD	1	318	-	47,48,54	0.83	0	56,59,65	0.96	3 (5%)
22	CLA	1	310	25	60,68,73	1.38	8 (13%)	70,107,113	2.04	16 (22%)
22	CLA	1	305	12	45,53,73	1.61	8 (17%)	52,89,113	2.15	16 (30%)
22	CLA	3	310	13	65,73,73	1.34	8 (12%)	76,113,113	2.06	20 (26%)
31	DGD	B	852	-	62,62,67	1.12	6 (9%)	76,76,81	0.96	3 (3%)
24	BCR	B	844	-	41,41,41	4.79	26 (63%)	56,56,56	2.77	24 (42%)
24	BCR	7	303	-	41,41,41	4.78	27 (65%)	56,56,56	2.39	21 (37%)
22	CLA	A	815	-	65,73,73	1.32	6 (9%)	76,113,113	2.00	17 (22%)
22	CLA	1	306	-	65,73,73	1.34	7 (10%)	76,113,113	2.01	17 (22%)
25	LHG	B	851	-	19,19,48	0.87	1 (5%)	20,24,54	1.36	1 (5%)
22	CLA	8	305	15	60,68,73	1.39	6 (10%)	70,107,113	2.09	17 (24%)
22	CLA	A	839	-	51,59,73	1.51	8 (15%)	59,96,113	2.22	17 (28%)
24	BCR	B	846	-	41,41,41	4.79	27 (65%)	56,56,56	2.40	22 (39%)
22	CLA	7	316	44	42,50,73	1.64	7 (16%)	48,85,113	2.24	16 (33%)
23	PQN	B	843	-	34,34,34	0.37	0	42,45,45	1.13	3 (7%)
22	CLA	A	820	-	60,68,73	1.40	7 (11%)	70,107,113	2.00	17 (24%)
24	BCR	3	304	-	41,41,41	4.82	27 (65%)	56,56,56	3.07	28 (50%)
24	BCR	6	306	-	41,41,41	4.77	27 (65%)	56,56,56	2.79	23 (41%)
22	CLA	A	855	44	65,73,73	1.34	7 (10%)	76,113,113	1.95	16 (21%)
39	CHL	6	318	-	56,64,74	0.91	2 (3%)	61,102,114	1.40	12 (19%)
22	CLA	6	307	18	60,68,73	1.39	8 (13%)	70,107,113	2.06	17 (24%)
22	CLA	K	205	10	55,63,73	1.54	10 (18%)	64,101,113	2.21	15 (23%)
38	LUT	4	803	-	42,43,43	6.06	28 (66%)	51,60,60	2.15	13 (25%)
25	LHG	1	317	22	42,42,48	0.45	0	45,48,54	1.18	3 (6%)
41	3PH	7	319	-	38,38,47	0.94	4 (10%)	42,43,52	1.13	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	Z	304	12	45,53,73	1.61	7 (15%)	52,89,113	2.07	12 (23%)
22	CLA	A	841	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	17 (22%)
22	CLA	Z	305	-	56,64,73	1.43	7 (12%)	65,102,113	2.09	15 (23%)
22	CLA	L	201	-	65,73,73	1.33	7 (10%)	76,113,113	2.00	17 (22%)
22	CLA	B	842	25	65,73,73	1.33	7 (10%)	76,113,113	1.98	16 (21%)
34	LMG	J	101	-	29,29,55	0.53	0	37,37,63	1.12	3 (8%)
22	CLA	B	830	-	65,73,73	1.34	7 (10%)	76,113,113	1.94	16 (21%)
23	PQN	A	843	-	34,34,34	0.37	0	42,45,45	1.20	6 (14%)
22	CLA	B	831	-	58,66,73	1.41	8 (13%)	67,104,113	2.12	17 (25%)
22	CLA	2	301	-	55,63,73	1.45	8 (14%)	64,101,113	2.14	15 (23%)
38	LUT	1	303	-	42,43,43	6.07	28 (66%)	51,60,60	2.06	12 (23%)
22	CLA	5	322	-	65,73,73	1.33	7 (10%)	76,113,113	1.97	17 (22%)
22	CLA	A	830	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	16 (21%)
39	CHL	6	316	-	51,59,74	0.96	3 (5%)	55,96,114	1.49	12 (21%)
22	CLA	8	314	15	46,54,73	1.57	7 (15%)	53,90,113	2.09	13 (24%)
22	CLA	3	309	13	46,54,73	1.58	8 (17%)	53,90,113	2.13	15 (28%)
38	LUT	6	303	-	42,43,43	6.11	27 (64%)	51,60,60	1.92	16 (31%)
22	CLA	B	811	-	65,73,73	1.34	7 (10%)	76,113,113	2.01	18 (23%)
22	CLA	5	318	17	65,73,73	1.32	7 (10%)	76,113,113	1.95	17 (22%)
38	LUT	8	303	-	42,43,43	6.07	28 (66%)	51,60,60	1.97	14 (27%)
22	CLA	A	836	-	55,63,73	1.44	8 (14%)	64,101,113	2.11	19 (29%)
22	CLA	A	805	-	65,73,73	1.33	9 (13%)	76,113,113	1.98	17 (22%)
22	CLA	B	837	-	51,59,73	1.51	7 (13%)	59,96,113	2.24	18 (30%)
22	CLA	4	812	-	55,63,73	1.46	7 (12%)	64,101,113	2.12	17 (26%)
22	CLA	2	304	44	46,54,73	1.58	7 (15%)	53,90,113	2.12	13 (24%)
22	CLA	7	308	14	61,69,73	1.39	8 (13%)	71,108,113	2.04	18 (25%)
24	BCR	I	4001	-	41,41,41	4.78	27 (65%)	56,56,56	2.58	19 (33%)
22	CLA	B	818	-	65,73,73	1.33	8 (12%)	76,113,113	1.96	17 (22%)
22	CLA	6	313	25	55,63,73	1.47	7 (12%)	64,101,113	2.08	16 (25%)
33	LMT	G	204	-	36,36,36	0.39	0	47,47,47	0.74	2 (4%)
25	LHG	B	803	-	32,32,48	0.46	0	35,38,54	1.18	3 (8%)
22	CLA	A	812	-	65,73,73	1.33	8 (12%)	76,113,113	1.97	17 (22%)
22	CLA	A	818	-	60,68,73	1.38	7 (11%)	70,107,113	2.12	17 (24%)
22	CLA	6	319	44	61,69,73	1.38	7 (11%)	71,108,113	2.06	17 (23%)
22	CLA	6	314	18	65,73,73	1.34	7 (10%)	76,113,113	1.95	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	6	309	44	65,73,73	1.34	8 (12%)	76,113,113	2.07	19 (25%)
22	CLA	5	312	44	50,58,73	1.52	7 (14%)	58,95,113	2.19	16 (27%)
25	LHG	6	323	22	48,48,48	0.38	0	51,54,54	1.09	3 (5%)
39	CHL	Z	312	-	48,56,74	0.96	2 (4%)	51,92,114	1.43	11 (21%)
39	CHL	4	816	44	47,55,74	0.99	3 (6%)	50,91,114	1.44	8 (16%)
22	CLA	7	323	15	65,73,73	1.33	7 (10%)	76,113,113	2.01	18 (23%)
29	SF4	B	802	-	0,12,12	-	-	-		
22	CLA	2	302	-	45,53,73	1.60	7 (15%)	52,89,113	2.19	15 (28%)
22	CLA	A	834	-	65,73,73	1.34	7 (10%)	76,113,113	1.96	17 (22%)
22	CLA	Z	307	-	55,63,73	1.46	7 (12%)	64,101,113	2.18	17 (26%)
22	CLA	6	310	18	65,73,73	1.34	9 (13%)	76,113,113	1.94	18 (23%)
22	CLA	9	313	19	50,58,73	1.52	7 (14%)	58,95,113	2.23	17 (29%)
22	CLA	J	103	9	42,50,73	1.65	7 (16%)	48,85,113	2.22	15 (31%)
22	CLA	3	311	13	60,68,73	1.39	7 (11%)	70,107,113	2.05	19 (27%)
22	CLA	A	811	22	65,73,73	1.33	8 (12%)	76,113,113	1.93	17 (22%)
24	BCR	3	307	-	41,41,41	4.78	27 (65%)	56,56,56	3.25	27 (48%)
38	LUT	4	802	-	42,43,43	6.08	28 (66%)	51,60,60	2.02	12 (23%)
22	CLA	B	808	-	65,73,73	1.33	6 (9%)	76,113,113	1.98	18 (23%)
22	CLA	5	319	44	55,63,73	1.45	7 (12%)	64,101,113	2.12	17 (26%)
25	LHG	4	821	-	31,31,48	0.48	0	34,37,54	1.19	3 (8%)
22	CLA	7	317	-	58,66,73	1.41	7 (12%)	67,104,113	2.06	16 (23%)
22	CLA	5	308	17	61,69,73	1.37	8 (13%)	71,108,113	2.05	18 (25%)
26	NKP	8	318	-	28,28,28	0.33	0	31,32,32	0.34	0
22	CLA	4	811	25	55,63,73	1.46	7 (12%)	64,101,113	2.14	17 (26%)
24	BCR	A	845	-	41,41,41	4.77	27 (65%)	56,56,56	2.50	24 (42%)
22	CLA	B	807	-	45,53,73	1.59	7 (15%)	52,89,113	2.13	14 (26%)
25	LHG	3	321	22	19,19,48	1.07	1 (5%)	20,24,54	1.53	1 (5%)
22	CLA	A	854	-	65,73,73	1.33	7 (10%)	76,113,113	1.94	17 (22%)
22	CLA	G	201	-	50,58,73	1.53	6 (12%)	58,95,113	2.25	18 (31%)
22	CLA	B	827	44	65,73,73	1.33	7 (10%)	76,113,113	2.02	17 (22%)
25	LHG	A	850	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
22	CLA	G	202	7	46,54,73	1.58	7 (15%)	53,90,113	2.16	15 (28%)
22	CLA	6	321	-	46,54,73	1.58	7 (15%)	53,90,113	2.15	13 (24%)
22	CLA	B	815	-	65,73,73	1.34	6 (9%)	76,113,113	2.05	18 (23%)
41	3PH	5	325	-	22,22,47	1.22	4 (18%)	26,27,52	1.28	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	LUT	5	303	-	42,43,43	6.11	28 (66%)	51,60,60	2.00	14 (27%)
22	CLA	A	808	1	65,73,73	1.33	7 (10%)	76,113,113	2.00	17 (22%)
22	CLA	A	840	-	65,73,73	1.33	8 (12%)	76,113,113	1.99	17 (22%)
22	CLA	B	836	-	45,53,73	1.58	7 (15%)	52,89,113	2.16	16 (30%)
22	CLA	F	305	-	45,53,73	1.59	8 (17%)	52,89,113	2.12	13 (25%)
22	CLA	B	833	-	65,73,73	1.32	6 (9%)	76,113,113	1.97	17 (22%)
22	CLA	B	839	-	52,60,73	1.49	8 (15%)	60,97,113	2.22	18 (30%)
22	CLA	6	308	18	52,60,73	1.47	6 (11%)	60,97,113	2.27	20 (33%)
39	CHL	7	313	44	54,62,74	0.92	3 (5%)	58,99,114	1.36	12 (20%)
22	CLA	A	833	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	18 (23%)
22	CLA	B	821	44	65,73,73	1.34	7 (10%)	76,113,113	1.96	16 (21%)
22	CLA	Z	313	44	65,73,73	1.34	7 (10%)	76,113,113	1.98	18 (23%)
22	CLA	5	314	-	45,53,73	1.60	7 (15%)	52,89,113	2.13	13 (25%)
22	CLA	B	816	-	60,68,73	1.38	7 (11%)	70,107,113	2.04	17 (24%)
22	CLA	1	309	-	61,69,73	1.37	8 (13%)	71,108,113	2.07	16 (22%)
25	LHG	9	315	22	32,32,48	0.48	0	35,38,54	1.05	3 (8%)
38	LUT	6	304	-	42,43,43	6.08	28 (66%)	51,60,60	2.05	13 (25%)
33	LMT	4	801	-	36,36,36	0.36	0	47,47,47	0.72	1 (2%)
22	CLA	A	816	44	56,64,73	1.44	8 (14%)	65,102,113	2.18	19 (29%)
22	CLA	Z	309	25	60,68,73	1.39	7 (11%)	70,107,113	2.03	16 (22%)
22	CLA	K	203	44	55,63,73	1.45	7 (12%)	64,101,113	2.15	17 (26%)
22	CLA	6	317	18	50,58,73	1.52	6 (12%)	58,95,113	2.24	16 (27%)
22	CLA	B	826	44	65,73,73	1.34	7 (10%)	76,113,113	2.00	18 (23%)
22	CLA	B	825	-	65,73,73	1.33	6 (9%)	76,113,113	1.98	18 (23%)
24	BCR	B	845	-	41,41,41	4.78	27 (65%)	56,56,56	2.39	20 (35%)
22	CLA	7	322	-	55,63,73	1.44	6 (10%)	64,101,113	2.11	18 (28%)
22	CLA	A	810	-	65,73,73	1.33	8 (12%)	76,113,113	1.98	17 (22%)
22	CLA	4	815	16	50,58,73	1.51	6 (12%)	58,95,113	2.24	15 (25%)
25	LHG	5	324	22	36,36,48	0.44	0	39,42,54	1.12	3 (7%)
22	CLA	3	318	13	60,68,73	1.38	7 (11%)	70,107,113	2.06	18 (25%)
29	SF4	C	101	3	0,12,12	-	-	-	-	-
24	BCR	L	204	-	41,41,41	4.78	27 (65%)	56,56,56	2.34	18 (32%)
42	SPH	7	321	-	19,20,20	0.65	1 (5%)	18,21,21	1.15	0
22	CLA	4	818	44	51,59,73	1.52	7 (13%)	59,96,113	2.26	19 (32%)
22	CLA	3	320	13	46,54,73	1.60	8 (17%)	53,90,113	2.21	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	6	315	44	56,64,74	0.87	2 (3%)	61,102,114	1.36	12 (19%)
22	CLA	7	324	-	60,68,73	1.39	7 (11%)	70,107,113	2.07	19 (27%)
22	CLA	B	814	-	60,68,73	1.39	7 (11%)	70,107,113	2.04	15 (21%)
22	CLA	6	311	-	55,63,73	1.45	7 (12%)	64,101,113	2.08	17 (26%)
22	CLA	5	323	44	46,54,73	1.57	7 (15%)	53,90,113	2.20	14 (26%)
22	CLA	6	312	-	65,73,73	1.34	8 (12%)	76,113,113	2.00	18 (23%)
22	CLA	Z	310	-	50,58,73	1.53	8 (16%)	58,95,113	2.17	17 (29%)
39	CHL	3	317	-	66,74,74	0.84	3 (4%)	73,114,114	1.29	9 (12%)
22	CLA	7	310	25	65,73,73	1.34	7 (10%)	76,113,113	1.96	15 (19%)
22	CLA	A	819	-	65,73,73	1.33	7 (10%)	76,113,113	1.95	17 (22%)
24	BCR	A	847	-	41,41,41	4.80	27 (65%)	56,56,56	2.38	20 (35%)
22	CLA	9	309	25	55,63,73	1.45	7 (12%)	64,101,113	2.17	13 (20%)
25	LHG	8	317	22	37,37,48	0.43	0	40,43,54	1.03	2 (5%)
39	CHL	8	315	44	66,74,74	0.81	2 (3%)	73,114,114	1.29	11 (15%)
28	OCA	A	853	-	9,9,9	0.70	0	9,9,9	0.70	0
38	LUT	3	302	-	42,43,43	6.05	28 (66%)	51,60,60	2.02	13 (25%)
22	CLA	8	308	15	62,70,73	1.36	7 (11%)	72,109,113	2.03	17 (23%)
24	BCR	3	305	-	41,41,41	4.78	27 (65%)	56,56,56	2.19	19 (33%)
22	CLA	A	813	-	65,73,73	1.34	6 (9%)	76,113,113	2.01	18 (23%)
22	CLA	B	805	-	65,73,73	1.33	7 (10%)	76,113,113	1.97	18 (23%)
22	CLA	7	312	-	60,68,73	1.39	7 (11%)	70,107,113	2.03	17 (24%)
24	BCR	6	305	-	41,41,41	4.79	26 (63%)	56,56,56	2.49	21 (37%)
38	LUT	7	302	-	42,43,43	6.08	28 (66%)	51,60,60	2.06	15 (29%)
22	CLA	3	316	13	52,60,73	1.49	7 (13%)	60,97,113	2.16	17 (28%)
22	CLA	B	809	2	65,73,73	1.33	8 (12%)	76,113,113	1.97	16 (21%)
24	BCR	B	847	-	41,41,41	4.78	27 (65%)	56,56,56	2.46	21 (37%)
22	CLA	B	841	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	17 (22%)
22	CLA	6	322	18	65,73,73	1.33	7 (10%)	76,113,113	2.02	18 (23%)
22	CLA	6	301	44	60,68,73	1.40	8 (13%)	70,107,113	2.06	18 (25%)
22	CLA	B	834	-	58,66,73	1.41	7 (12%)	67,104,113	2.10	17 (25%)
22	CLA	A	837	-	51,59,73	1.52	7 (13%)	59,96,113	2.18	16 (27%)
22	CLA	A	814	-	60,68,73	1.38	6 (10%)	70,107,113	2.10	19 (27%)
25	LHG	Z	317	22	42,42,48	0.41	0	45,48,54	1.08	3 (6%)
22	CLA	A	838	-	65,73,73	1.33	7 (10%)	76,113,113	2.02	17 (22%)
22	CLA	9	304	-	45,53,73	1.60	7 (15%)	52,89,113	2.14	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	B	853	-	41,41,41	4.83	27 (65%)	56,56,56	2.40	22 (39%)
25	LHG	7	318	22	36,36,48	0.43	0	39,42,54	1.14	3 (7%)
22	CLA	A	804	22	45,53,73	1.59	7 (15%)	52,89,113	2.16	15 (28%)
22	CLA	B	810	-	56,64,73	1.43	6 (10%)	65,102,113	2.18	20 (30%)
22	CLA	Z	306	12	60,68,73	1.39	8 (13%)	70,107,113	2.04	17 (24%)
22	CLA	9	310	-	45,53,73	1.59	8 (17%)	52,89,113	2.21	14 (26%)
22	CLA	B	817	-	57,65,73	1.42	7 (12%)	66,103,113	2.09	16 (24%)
22	CLA	3	322	14	65,73,73	1.34	8 (12%)	76,113,113	1.94	16 (21%)
22	CLA	A	802	44	65,73,73	1.34	7 (10%)	76,113,113	2.03	17 (22%)
22	CLA	A	803	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	17 (22%)
22	CLA	9	306	19	62,70,73	1.37	7 (11%)	72,109,113	2.10	19 (26%)
22	CLA	8	310	44	60,68,73	1.39	7 (11%)	70,107,113	2.09	17 (24%)
25	LHG	4	820	22	48,48,48	0.42	0	51,54,54	1.04	4 (7%)
22	CLA	5	313	25	61,69,73	1.39	8 (13%)	71,108,113	2.06	17 (23%)
22	CLA	A	821	44	65,73,73	1.33	7 (10%)	76,113,113	1.96	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
22	CLA	6	302	16	1/1/14/20	17/31/109/115	-
22	CLA	5	315	17	1/1/15/20	14/37/115/115	-
24	BCR	8	304	-	-	12/29/63/63	0/2/2/2
22	CLA	1	315	-	1/1/11/20	7/15/93/115	-
22	CLA	A	824	-	1/1/15/20	17/37/115/115	-
22	CLA	A	823	-	1/1/15/20	15/37/115/115	-
22	CLA	9	311	19	1/1/11/20	5/15/93/115	-
37	DAO	K	201	-	-	1/11/11/11	-
22	CLA	1	316	12	1/1/15/20	20/37/115/115	-
22	CLA	5	301	44	1/1/13/20	13/27/105/115	-
39	CHL	8	301	12	3/3/18/26	5/30/128/137	-
22	CLA	A	822	-	1/1/13/20	12/25/103/115	-
24	BCR	A	844	-	-	13/29/63/63	0/2/2/2
22	CLA	A	809	1	1/1/13/20	7/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	7	307	14	1/1/15/20	14/37/115/115	-
38	LUT	3	303	-	-	7/29/67/67	0/2/2/2
22	CLA	B	819	-	1/1/13/20	15/30/108/115	-
22	CLA	A	829	-	1/1/15/20	11/37/115/115	-
22	CLA	B	822	-	1/1/13/20	17/27/105/115	-
22	CLA	3	308	13	1/1/15/20	18/37/115/115	-
22	CLA	A	828	-	1/1/15/20	21/37/115/115	-
39	CHL	4	814	44	3/3/17/26	10/21/119/137	-
33	LMT	4	822	-	-	6/21/61/61	0/2/2/2
22	CLA	7	305	-	1/1/12/20	4/19/97/115	-
36	C7Z	5	306	-	-	13/29/67/67	0/2/2/2
38	LUT	Z	302	-	-	7/29/67/67	0/2/2/2
22	CLA	5	310	17	1/1/15/20	13/37/115/115	-
22	CLA	Z	315	-	1/1/11/20	8/15/93/115	-
22	CLA	B	835	-	1/1/12/20	8/19/97/115	-
39	CHL	6	320	18	3/3/15/26	0/12/110/137	-
22	CLA	4	806	16	1/1/12/20	10/22/100/115	-
24	BCR	A	856	-	-	16/29/63/63	0/2/2/2
24	BCR	4	804	-	-	14/29/63/63	0/2/2/2
39	CHL	8	312	-	3/3/18/26	9/27/125/137	-
22	CLA	A	817	-	1/1/14/20	13/31/109/115	-
22	CLA	Z	314	12	1/1/12/20	9/21/99/115	-
22	CLA	8	309	-	1/1/15/20	17/37/115/115	-
22	CLA	Z	316	12	1/1/15/20	21/37/115/115	-
22	CLA	Z	303	12	1/1/15/20	16/37/115/115	-
29	SF4	C	102	3	-	-	0/6/5/5
25	LHG	B	850	22	-	16/26/26/53	-
22	CLA	L	203	-	1/1/12/20	7/19/97/115	-
22	CLA	4	817	16	1/1/10/20	2/8/86/115	-
39	CHL	4	819	16	3/3/15/26	0/12/110/137	-
22	CLA	A	826	44	1/1/12/20	6/19/97/115	-
22	CLA	9	307	19	1/1/13/20	10/25/103/115	-
22	CLA	1	304	-	1/1/15/20	13/37/115/115	-
24	BCR	5	304	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LUT	5	302	-	-	9/29/67/67	0/2/2/2
22	CLA	A	842	25	1/1/12/20	12/22/100/115	-
39	CHL	5	316	44	3/3/20/26	12/39/137/137	-
22	CLA	1	307	12	1/1/14/20	18/31/109/115	-
22	CLA	7	311	-	1/1/10/20	5/11/89/115	-
24	BCR	G	203	-	-	15/29/63/63	0/2/2/2
22	CLA	7	309	-	1/1/13/20	14/27/105/115	-
24	BCR	B	848	-	-	16/29/63/63	0/2/2/2
22	CLA	8	306	15	1/1/12/20	9/21/99/115	-
22	CLA	A	831	-	1/1/12/20	10/19/97/115	-
22	CLA	B	824	-	1/1/13/20	19/30/108/115	-
22	CLA	3	314	25	1/1/14/20	19/31/109/115	-
31	DGD	3	301	-	-	12/40/80/95	0/2/2/2
22	CLA	B	823	-	1/1/13/20	13/25/103/115	-
22	CLA	1	311	-	1/1/11/20	6/15/93/115	-
24	BCR	5	305	-	-	13/29/63/63	0/2/2/2
22	CLA	B	820	-	1/1/14/20	18/31/109/115	-
22	CLA	5	326	-	1/1/13/20	8/25/103/115	-
22	CLA	7	306	-	1/1/15/20	16/37/115/115	-
22	CLA	7	314	44	1/1/12/20	7/19/97/115	-
33	LMT	1	301	-	-	4/21/61/61	0/2/2/2
33	LMT	F	307	-	-	8/21/61/61	0/2/2/2
36	C7Z	J	105	-	-	13/29/67/67	0/2/2/2
22	CLA	7	304	14	1/1/14/20	13/31/109/115	-
22	CLA	A	806	1	1/1/15/20	16/37/115/115	-
42	SPH	7	320	-	-	11/21/21/21	-
22	CLA	8	311	25	1/1/12/20	10/19/97/115	-
38	LUT	9	302	-	-	4/29/67/67	0/2/2/2
22	CLA	B	829	-	1/1/13/20	15/28/106/115	-
35	T7X	J	102	-	-	17/44/68/80	0/1/1/1
22	CLA	4	805	16	1/1/14/20	13/31/109/115	-
22	CLA	7	315	14	1/1/12/20	8/19/97/115	-
32	RRX	F	306	-	-	15/29/65/65	0/2/2/2
39	CHL	5	317	44	3/3/17/26	6/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	K	204	10	1/1/11/20	10/18/96/115	-
22	CLA	8	313	44	1/1/12/20	7/19/97/115	-
22	CLA	4	809	16	1/1/12/20	5/21/99/115	-
22	CLA	5	309	-	1/1/13/20	17/27/105/115	-
22	CLA	9	303	19	1/1/14/20	11/31/109/115	-
22	CLA	Z	308	-	1/1/14/20	14/33/111/115	-
39	CHL	Z	311	12	3/3/17/26	10/21/119/137	-
24	BCR	A	848	-	-	15/29/63/63	0/2/2/2
22	CLA	K	202	-	1/1/11/20	10/15/93/115	-
39	CHL	4	813	44	3/3/17/26	6/21/119/137	-
22	CLA	B	832	-	1/1/12/20	6/19/97/115	-
26	NKP	A	851	-	-	9/22/22/28	-
22	CLA	A	825	44	1/1/15/20	16/37/115/115	-
22	CLA	L	202	-	1/1/15/20	21/37/115/115	-
24	BCR	K	206	-	-	13/29/63/63	0/2/2/2
22	CLA	4	807	16	1/1/15/20	12/37/115/115	-
43	LPX	8	319	-	-	6/31/31/31	-
22	CLA	B	838	-	1/1/15/20	15/37/115/115	-
39	CHL	1	312	-	3/3/16/26	3/18/116/137	-
22	CLA	8	307	-	1/1/15/20	12/37/115/115	-
22	CLA	F	301	44	1/1/15/20	13/37/115/115	-
22	CLA	B	812	2	2/2/14/20	15/27/105/115	-
38	LUT	7	301	-	-	9/29/67/67	0/2/2/2
39	CHL	9	314	-	3/3/15/26	0/10/108/137	-
22	CLA	5	320	-	1/1/12/20	9/19/97/115	-
21	CL0	A	801	-	3/3/20/25	13/37/135/135	-
22	CLA	5	311	-	1/1/13/20	11/25/103/115	-
22	CLA	F	302	-	1/1/15/20	17/37/115/115	-
22	CLA	9	305	19	1/1/14/20	18/31/109/115	-
25	LHG	A	849	22	-	27/39/39/53	-
22	CLA	3	312	-	1/1/15/20	12/37/115/115	-
24	BCR	B	849	-	-	13/29/63/63	0/2/2/2
22	CLA	A	832	-	1/1/15/20	17/37/115/115	-
22	CLA	F	304	6	1/1/15/20	23/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	9	308	-	1/1/12/20	8/19/97/115	-
24	BCR	A	846	-	-	13/29/63/63	0/2/2/2
24	BCR	3	306	-	-	13/29/63/63	0/2/2/2
24	BCR	F	303	-	-	15/29/63/63	0/2/2/2
38	LUT	8	302	-	-	8/29/67/67	0/2/2/2
22	CLA	4	808	16	1/1/14/20	16/31/109/115	-
22	CLA	B	801	-	1/1/15/20	15/37/115/115	-
22	CLA	B	840	44	1/1/15/20	9/37/115/115	-
22	CLA	B	813	-	1/1/13/20	14/27/105/115	-
34	LMG	F	308	-	-	16/30/50/70	0/1/1/1
22	CLA	3	315	-	1/1/11/20	6/13/91/115	-
41	3PH	6	324	-	-	11/30/30/49	-
38	LUT	9	301	-	-	5/29/67/67	0/2/2/2
27	DGA	A	852	-	-	23/41/41/45	-
39	CHL	2	303	-	3/3/17/26	7/21/119/137	-
22	CLA	A	807	-	1/1/14/20	17/31/109/115	-
22	CLA	4	810	44	1/1/12/20	8/19/97/115	-
31	DGD	1	319	-	-	14/40/80/95	0/2/2/2
22	CLA	8	316	15	1/1/11/20	11/15/93/115	-
39	CHL	5	321	17	3/3/15/26	3/12/110/137	-
38	LUT	Z	301	-	-	7/29/67/67	0/2/2/2
41	3PH	8	320	-	-	13/31/31/49	-
22	CLA	B	806	44	1/1/15/20	12/37/115/115	-
22	CLA	1	313	44	1/1/15/20	12/37/115/115	-
38	LUT	1	302	-	-	9/29/67/67	0/2/2/2
22	CLA	B	828	-	1/1/15/20	18/37/115/115	-
22	CLA	3	313	44	1/1/15/20	17/37/115/115	-
22	CLA	5	307	17	1/1/14/20	14/31/109/115	-
22	CLA	1	308	-	1/1/13/20	13/25/103/115	-
22	CLA	A	827	-	1/1/15/20	17/37/115/115	-
22	CLA	1	314	12	1/1/15/20	13/37/115/115	-
24	BCR	J	104	-	-	14/29/63/63	0/2/2/2
39	CHL	9	312	-	3/3/20/26	16/39/137/137	-
22	CLA	3	319	-	1/1/13/20	9/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	835	-	1/1/15/20	13/37/115/115	-
40	SQD	1	318	-	-	12/43/63/69	0/1/1/1
22	CLA	1	310	25	1/1/14/20	17/31/109/115	-
22	CLA	1	305	12	1/1/11/20	6/13/91/115	-
22	CLA	3	310	13	1/1/15/20	14/37/115/115	-
31	DGD	B	852	-	-	11/50/90/95	0/2/2/2
24	BCR	B	844	-	-	12/29/63/63	0/2/2/2
24	BCR	7	303	-	-	16/29/63/63	0/2/2/2
22	CLA	A	815	-	1/1/15/20	16/37/115/115	-
22	CLA	1	306	-	1/1/15/20	18/37/115/115	-
25	LHG	B	851	-	-	15/22/22/53	-
22	CLA	8	305	15	1/1/14/20	14/31/109/115	-
22	CLA	A	839	-	1/1/12/20	10/21/99/115	-
24	BCR	B	846	-	-	17/29/63/63	0/2/2/2
22	CLA	7	316	44	1/1/10/20	6/10/88/115	-
23	PQN	B	843	-	-	9/23/43/43	0/2/2/2
22	CLA	A	820	-	1/1/14/20	21/31/109/115	-
24	BCR	3	304	-	-	10/29/63/63	0/2/2/2
24	BCR	6	306	-	-	16/29/63/63	0/2/2/2
22	CLA	A	855	44	1/1/15/20	18/37/115/115	-
39	CHL	6	318	-	3/3/18/26	8/27/125/137	-
22	CLA	6	307	18	1/1/14/20	12/31/109/115	-
22	CLA	K	205	10	1/1/13/20	15/25/103/115	-
38	LUT	4	803	-	-	8/29/67/67	0/2/2/2
25	LHG	1	317	22	-	22/47/47/53	-
41	3PH	7	319	-	-	17/40/40/49	-
22	CLA	Z	304	12	1/1/11/20	6/13/91/115	-
22	CLA	A	841	-	1/1/15/20	10/37/115/115	-
22	CLA	Z	305	-	1/1/13/20	12/27/105/115	-
22	CLA	L	201	-	1/1/15/20	17/37/115/115	-
22	CLA	B	842	25	1/1/15/20	17/37/115/115	-
34	LMG	J	101	-	-	7/24/44/70	0/1/1/1
22	CLA	B	830	-	1/1/15/20	13/37/115/115	-
23	PQN	A	843	-	-	8/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	831	-	1/1/13/20	17/29/107/115	-
22	CLA	2	301	-	1/1/13/20	11/25/103/115	-
38	LUT	1	303	-	-	8/29/67/67	0/2/2/2
22	CLA	5	322	-	1/1/15/20	11/37/115/115	-
22	CLA	A	830	-	1/1/15/20	14/37/115/115	-
39	CHL	6	316	-	3/3/17/26	9/21/119/137	-
22	CLA	8	314	15	1/1/11/20	10/15/93/115	-
22	CLA	3	309	13	1/1/11/20	6/15/93/115	-
38	LUT	6	303	-	-	9/29/67/67	0/2/2/2
22	CLA	B	811	-	1/1/15/20	15/37/115/115	-
22	CLA	5	318	17	1/1/15/20	14/37/115/115	-
38	LUT	8	303	-	-	3/29/67/67	0/2/2/2
22	CLA	A	836	-	1/1/13/20	12/25/103/115	-
22	CLA	A	805	-	1/1/15/20	19/37/115/115	-
22	CLA	B	837	-	1/1/12/20	9/21/99/115	-
22	CLA	4	812	-	1/1/13/20	8/25/103/115	-
22	CLA	2	304	44	1/1/11/20	9/15/93/115	-
22	CLA	7	308	14	1/1/14/20	16/33/111/115	-
24	BCR	I	4001	-	-	14/29/63/63	0/2/2/2
22	CLA	B	818	-	1/1/15/20	15/37/115/115	-
22	CLA	6	313	25	1/1/13/20	8/25/103/115	-
33	LMT	G	204	-	-	6/21/61/61	0/2/2/2
25	LHG	B	803	-	-	22/37/37/53	-
22	CLA	A	812	-	1/1/15/20	16/37/115/115	-
22	CLA	A	818	-	1/1/14/20	15/31/109/115	-
22	CLA	6	319	44	1/1/14/20	17/33/111/115	-
22	CLA	6	314	18	1/1/15/20	15/37/115/115	-
22	CLA	6	309	44	1/1/15/20	17/37/115/115	-
22	CLA	5	312	44	1/1/12/20	6/19/97/115	-
25	LHG	6	323	22	-	38/53/53/53	-
39	CHL	Z	312	-	3/3/16/26	9/18/116/137	-
39	CHL	4	816	44	3/3/16/26	6/17/115/137	-
22	CLA	7	323	15	1/1/15/20	19/37/115/115	-
29	SF4	B	802	-	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	2	302	-	1/1/11/20	8/13/91/115	-
22	CLA	A	834	-	1/1/15/20	15/37/115/115	-
22	CLA	Z	307	-	1/1/13/20	10/25/103/115	-
22	CLA	6	310	18	1/1/15/20	16/37/115/115	-
22	CLA	9	313	19	1/1/12/20	6/19/97/115	-
22	CLA	J	103	9	1/1/10/20	5/10/88/115	-
22	CLA	3	311	13	1/1/14/20	13/31/109/115	-
22	CLA	A	811	22	1/1/15/20	20/37/115/115	-
24	BCR	3	307	-	-	13/29/63/63	0/2/2/2
38	LUT	4	802	-	-	10/29/67/67	0/2/2/2
22	CLA	B	808	-	1/1/15/20	15/37/115/115	-
22	CLA	5	319	44	1/1/13/20	11/25/103/115	-
25	LHG	4	821	-	-	16/36/36/53	-
22	CLA	7	317	-	1/1/13/20	15/29/107/115	-
22	CLA	5	308	17	1/1/14/20	17/33/111/115	-
26	NKP	8	318	-	-	7/28/28/28	-
22	CLA	4	811	25	1/1/13/20	9/25/103/115	-
24	BCR	A	845	-	-	14/29/63/63	0/2/2/2
22	CLA	B	807	-	1/1/11/20	8/13/91/115	-
25	LHG	3	321	22	-	11/22/22/53	-
22	CLA	A	854	-	1/1/15/20	13/37/115/115	-
22	CLA	G	201	-	1/1/12/20	10/19/97/115	-
22	CLA	B	827	44	1/1/15/20	14/37/115/115	-
25	LHG	A	850	-	-	29/53/53/53	-
22	CLA	G	202	7	1/1/11/20	8/15/93/115	-
22	CLA	6	321	-	1/1/11/20	6/15/93/115	-
22	CLA	B	815	-	1/1/15/20	13/37/115/115	-
41	3PH	5	325	-	-	5/24/24/49	-
38	LUT	5	303	-	-	6/29/67/67	0/2/2/2
22	CLA	A	808	1	1/1/15/20	19/37/115/115	-
22	CLA	A	840	-	1/1/15/20	18/37/115/115	-
22	CLA	B	836	-	1/1/11/20	6/13/91/115	-
22	CLA	F	305	-	1/1/11/20	6/13/91/115	-
22	CLA	B	833	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	839	-	1/1/12/20	11/22/100/115	-
22	CLA	6	308	18	1/1/12/20	7/22/100/115	-
39	CHL	7	313	44	3/3/17/26	7/25/123/137	-
22	CLA	A	833	-	1/1/15/20	14/37/115/115	-
22	CLA	B	821	44	1/1/15/20	18/37/115/115	-
22	CLA	Z	313	44	1/1/15/20	13/37/115/115	-
22	CLA	5	314	-	1/1/11/20	6/13/91/115	-
22	CLA	B	816	-	1/1/14/20	13/31/109/115	-
22	CLA	1	309	-	1/1/14/20	13/33/111/115	-
25	LHG	9	315	22	-	20/37/37/53	-
38	LUT	6	304	-	-	6/29/67/67	0/2/2/2
33	LMT	4	801	-	-	1/21/61/61	0/2/2/2
22	CLA	A	816	44	1/1/13/20	14/27/105/115	-
22	CLA	Z	309	25	1/1/14/20	16/31/109/115	-
22	CLA	K	203	44	1/1/13/20	9/25/103/115	-
22	CLA	6	317	18	1/1/12/20	10/19/97/115	-
22	CLA	B	826	44	1/1/15/20	17/37/115/115	-
22	CLA	B	825	-	1/1/15/20	19/37/115/115	-
24	BCR	B	845	-	-	16/29/63/63	0/2/2/2
22	CLA	7	322	-	1/1/13/20	9/25/103/115	-
22	CLA	A	810	-	1/1/15/20	17/37/115/115	-
22	CLA	4	815	16	1/1/12/20	8/19/97/115	-
25	LHG	5	324	22	-	24/41/41/53	-
22	CLA	3	318	13	1/1/14/20	11/31/109/115	-
29	SF4	C	101	3	-	-	0/6/5/5
24	BCR	L	204	-	-	13/29/63/63	0/2/2/2
42	SPH	7	321	-	-	11/21/21/21	-
22	CLA	4	818	44	1/1/12/20	10/21/99/115	-
22	CLA	3	320	13	1/1/11/20	5/15/93/115	-
39	CHL	6	315	44	3/3/18/26	11/27/125/137	-
22	CLA	7	324	-	1/1/14/20	23/31/109/115	-
22	CLA	B	814	-	1/1/14/20	19/31/109/115	-
22	CLA	6	311	-	1/1/13/20	12/25/103/115	-
22	CLA	5	323	44	1/1/11/20	7/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	312	-	1/1/15/20	15/37/115/115	-
22	CLA	Z	310	-	1/1/12/20	10/19/97/115	-
39	CHL	3	317	-	3/3/20/26	12/39/137/137	-
22	CLA	7	310	25	1/1/15/20	15/37/115/115	-
22	CLA	A	819	-	1/1/15/20	12/37/115/115	-
24	BCR	A	847	-	-	16/29/63/63	0/2/2/2
22	CLA	9	309	25	1/1/13/20	7/25/103/115	-
25	LHG	8	317	22	-	27/42/42/53	-
39	CHL	8	315	44	3/3/20/26	12/39/137/137	-
28	OCA	A	853	-	-	3/7/7/7	-
38	LUT	3	302	-	-	4/29/67/67	0/2/2/2
22	CLA	8	308	15	1/1/14/20	15/34/112/115	-
24	BCR	3	305	-	-	14/29/63/63	0/2/2/2
22	CLA	A	813	-	1/1/15/20	14/37/115/115	-
22	CLA	B	805	-	1/1/15/20	16/37/115/115	-
22	CLA	7	312	-	1/1/14/20	18/31/109/115	-
24	BCR	6	305	-	-	13/29/63/63	0/2/2/2
38	LUT	7	302	-	-	5/29/67/67	0/2/2/2
22	CLA	3	316	13	1/1/12/20	8/22/100/115	-
22	CLA	B	809	2	1/1/15/20	19/37/115/115	-
24	BCR	B	847	-	-	11/29/63/63	0/2/2/2
22	CLA	B	841	-	1/1/15/20	11/37/115/115	-
22	CLA	6	322	18	1/1/15/20	15/37/115/115	-
22	CLA	6	301	44	1/1/14/20	18/31/109/115	-
22	CLA	B	834	-	1/1/13/20	15/29/107/115	-
22	CLA	A	837	-	1/1/12/20	10/21/99/115	-
22	CLA	A	814	-	1/1/14/20	19/31/109/115	-
25	LHG	Z	317	22	-	27/47/47/53	-
22	CLA	A	838	-	1/1/15/20	15/37/115/115	-
22	CLA	9	304	-	1/1/11/20	4/13/91/115	-
24	BCR	B	853	-	-	17/29/63/63	0/2/2/2
25	LHG	7	318	22	-	25/41/41/53	-
22	CLA	A	804	22	1/1/11/20	6/13/91/115	-
22	CLA	B	810	-	1/1/13/20	11/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Z	306	12	1/1/14/20	20/31/109/115	-
22	CLA	9	310	-	1/1/11/20	4/13/91/115	-
22	CLA	B	817	-	1/1/13/20	18/28/106/115	-
22	CLA	3	322	14	1/1/15/20	14/37/115/115	-
22	CLA	A	802	44	1/1/15/20	17/37/115/115	-
22	CLA	A	803	-	1/1/15/20	12/37/115/115	-
22	CLA	9	306	19	1/1/14/20	14/34/112/115	-
22	CLA	8	310	44	1/1/14/20	15/31/109/115	-
25	LHG	4	820	22	-	30/53/53/53	-
22	CLA	5	313	25	1/1/14/20	12/33/111/115	-
22	CLA	A	821	44	1/1/15/20	12/37/115/115	-

The worst 5 of 3038 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	6	303	LUT	C24-C25	23.39	1.62	1.33
38	5	303	LUT	C24-C25	23.37	1.62	1.33
38	1	302	LUT	C24-C25	23.34	1.62	1.33
38	7	302	LUT	C24-C25	23.27	1.62	1.33
38	Z	302	LUT	C24-C25	23.26	1.62	1.33

The worst 5 of 4873 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	848	BCR	C37-C22-C21	-29.76	81.23	122.92
24	B	848	BCR	C23-C22-C21	28.06	162.01	118.94
24	B	848	BCR	C37-C22-C23	-23.62	80.87	118.08
24	3	304	BCR	C11-C10-C9	-11.56	110.82	127.31
22	K	205	CLA	C4A-NA-C1A	11.24	111.76	106.71

5 of 283 chirality outliers are listed below:

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

5 of 4072 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	802	CLA	C1A-C2A-CAA-CBA
22	A	802	CLA	C2-C1-O2A-CGA
22	A	803	CLA	C1A-C2A-CAA-CBA
22	A	803	CLA	CBA-CGA-O2A-C1
22	A	803	CLA	O1A-CGA-O2A-C1

There are no ring outliers.

328 monomers are involved in 3221 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	302	CLA	17	0
22	5	315	CLA	20	0
24	8	304	BCR	15	0
22	1	315	CLA	4	0
22	A	824	CLA	15	0
22	A	823	CLA	25	0
22	9	311	CLA	5	0
37	K	201	DAO	8	0
22	1	316	CLA	5	0
22	5	301	CLA	14	0
39	8	301	CHL	13	0
22	A	822	CLA	24	0
24	A	844	BCR	30	0
22	A	809	CLA	15	0
22	7	307	CLA	23	0
38	3	303	LUT	20	0
22	B	819	CLA	18	0
22	A	829	CLA	16	0
22	B	822	CLA	11	0
22	3	308	CLA	18	0
22	A	828	CLA	17	0
39	4	814	CHL	8	0
33	4	822	LMT	2	0
22	7	305	CLA	8	0
36	5	306	C7Z	2	0
38	Z	302	LUT	14	0
22	5	310	CLA	17	0
22	Z	315	CLA	11	0
22	B	835	CLA	11	0
39	6	320	CHL	13	0
22	4	806	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	856	BCR	25	0
24	4	804	BCR	27	0
39	8	312	CHL	16	0
22	A	817	CLA	14	0
22	Z	314	CLA	9	0
22	8	309	CLA	15	0
22	Z	316	CLA	15	0
22	Z	303	CLA	32	0
29	C	102	SF4	5	0
25	B	850	LHG	4	0
22	L	203	CLA	5	0
22	4	817	CLA	4	0
39	4	819	CHL	10	0
22	A	826	CLA	9	0
22	9	307	CLA	11	0
22	1	304	CLA	17	0
24	5	304	BCR	22	0
38	5	302	LUT	14	0
22	A	842	CLA	5	0
39	5	316	CHL	16	0
22	1	307	CLA	22	0
22	7	311	CLA	2	0
24	G	203	BCR	13	0
22	7	309	CLA	11	0
24	B	848	BCR	15	0
22	8	306	CLA	15	0
22	A	831	CLA	4	0
22	B	824	CLA	22	0
22	3	314	CLA	14	0
31	3	301	DGD	21	0
22	B	823	CLA	16	0
24	5	305	BCR	11	0
22	B	820	CLA	12	0
22	5	326	CLA	20	0
22	7	306	CLA	13	0
22	7	314	CLA	5	0
33	1	301	LMT	9	0
33	F	307	LMT	5	0
36	J	105	C7Z	2	0
22	7	304	CLA	13	0
22	A	806	CLA	12	0
42	7	320	SPH	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	8	311	CLA	16	0
38	9	302	LUT	15	0
22	B	829	CLA	13	0
35	J	102	T7X	2	0
22	4	805	CLA	18	0
22	7	315	CLA	11	0
32	F	306	RRX	19	0
39	5	317	CHL	10	0
22	K	204	CLA	5	0
22	8	313	CLA	12	0
22	4	809	CLA	10	0
22	5	309	CLA	13	0
22	9	303	CLA	7	0
22	Z	308	CLA	14	0
39	Z	311	CHL	13	0
24	A	848	BCR	8	0
22	K	202	CLA	8	0
39	4	813	CHL	14	0
22	B	832	CLA	10	0
26	A	851	NKP	3	0
22	A	825	CLA	20	0
22	L	202	CLA	19	0
24	K	206	BCR	11	0
22	4	807	CLA	12	0
43	8	319	LPX	7	0
22	B	838	CLA	16	0
39	1	312	CHL	9	0
22	8	307	CLA	19	0
22	F	301	CLA	11	0
22	B	812	CLA	15	0
38	7	301	LUT	16	0
39	9	314	CHL	13	0
22	5	320	CLA	12	0
21	A	801	CL0	9	0
22	5	311	CLA	20	0
22	F	302	CLA	19	0
22	9	305	CLA	7	0
25	A	849	LHG	5	0
22	3	312	CLA	25	0
24	B	849	BCR	9	0
22	A	832	CLA	13	0
22	F	304	CLA	30	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	9	308	CLA	8	0
24	A	846	BCR	10	0
24	3	306	BCR	14	0
24	F	303	BCR	16	0
38	8	302	LUT	18	0
22	4	808	CLA	20	0
22	B	801	CLA	15	0
22	B	840	CLA	16	0
22	B	813	CLA	9	0
34	F	308	LMG	1	0
22	3	315	CLA	11	0
41	6	324	3PH	5	0
38	9	301	LUT	17	0
27	A	852	DGA	20	0
39	2	303	CHL	6	0
22	A	807	CLA	20	0
22	4	810	CLA	17	0
31	1	319	DGD	10	0
22	8	316	CLA	3	0
39	5	321	CHL	6	0
38	Z	301	LUT	25	0
41	8	320	3PH	4	0
22	B	806	CLA	22	0
22	1	313	CLA	16	0
38	1	302	LUT	11	0
22	B	828	CLA	26	0
22	3	313	CLA	26	0
22	5	307	CLA	24	0
22	1	308	CLA	23	0
22	A	827	CLA	20	0
22	1	314	CLA	19	0
24	J	104	BCR	19	0
39	9	312	CHL	24	0
22	3	319	CLA	4	0
22	A	835	CLA	20	0
40	1	318	SQD	13	0
22	1	310	CLA	11	0
22	1	305	CLA	12	0
22	3	310	CLA	7	0
31	B	852	DGD	17	0
24	B	844	BCR	20	0
24	7	303	BCR	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	815	CLA	20	0
22	1	306	CLA	8	0
25	B	851	LHG	2	0
22	8	305	CLA	24	0
22	A	839	CLA	9	0
24	B	846	BCR	12	0
22	7	316	CLA	12	0
23	B	843	PQN	5	0
22	A	820	CLA	8	0
24	3	304	BCR	15	0
24	6	306	BCR	16	0
22	A	855	CLA	16	0
39	6	318	CHL	14	0
22	6	307	CLA	22	0
22	K	205	CLA	4	0
38	4	803	LUT	20	0
25	1	317	LHG	8	0
41	7	319	3PH	12	0
22	Z	304	CLA	18	0
22	A	841	CLA	17	0
22	Z	305	CLA	17	0
22	L	201	CLA	16	0
22	B	842	CLA	27	0
34	J	101	LMG	11	0
22	B	830	CLA	15	0
23	A	843	PQN	9	0
22	B	831	CLA	9	0
22	2	301	CLA	19	0
38	1	303	LUT	20	0
22	5	322	CLA	13	0
22	A	830	CLA	14	0
39	6	316	CHL	10	0
22	8	314	CLA	6	0
22	3	309	CLA	10	0
38	6	303	LUT	12	0
22	B	811	CLA	26	0
22	5	318	CLA	22	0
38	8	303	LUT	13	0
22	A	836	CLA	15	0
22	A	805	CLA	22	0
22	B	837	CLA	2	0
22	4	812	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	2	304	CLA	9	0
22	7	308	CLA	13	0
24	I	4001	BCR	12	0
22	B	818	CLA	13	0
22	6	313	CLA	7	0
33	G	204	LMT	9	0
25	B	803	LHG	8	0
22	A	812	CLA	24	0
22	A	818	CLA	15	0
22	6	319	CLA	12	0
22	6	314	CLA	20	0
22	6	309	CLA	22	0
22	5	312	CLA	12	0
25	6	323	LHG	12	0
39	Z	312	CHL	14	0
39	4	816	CHL	20	0
22	7	323	CLA	17	0
29	B	802	SF4	9	0
22	2	302	CLA	7	0
22	A	834	CLA	13	0
22	Z	307	CLA	13	0
22	6	310	CLA	20	0
22	9	313	CLA	19	0
22	J	103	CLA	4	0
22	3	311	CLA	13	0
22	A	811	CLA	19	0
24	3	307	BCR	19	0
38	4	802	LUT	15	0
22	B	808	CLA	13	0
22	5	319	CLA	16	0
25	4	821	LHG	4	0
22	7	317	CLA	6	0
22	5	308	CLA	21	0
26	8	318	NKP	6	0
22	4	811	CLA	7	0
24	A	845	BCR	20	0
22	B	807	CLA	9	0
25	3	321	LHG	1	0
22	A	854	CLA	10	0
22	G	201	CLA	13	0
22	B	827	CLA	24	0
25	A	850	LHG	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	G	202	CLA	15	0
22	6	321	CLA	9	0
22	B	815	CLA	23	0
41	5	325	3PH	4	0
38	5	303	LUT	18	0
22	A	808	CLA	12	0
22	A	840	CLA	16	0
22	B	836	CLA	7	0
22	F	305	CLA	9	0
22	B	833	CLA	11	0
22	B	839	CLA	13	0
22	6	308	CLA	17	0
39	7	313	CHL	12	0
22	A	833	CLA	17	0
22	B	821	CLA	15	0
22	Z	313	CLA	24	0
22	5	314	CLA	8	0
22	B	816	CLA	14	0
22	1	309	CLA	10	0
25	9	315	LHG	2	0
38	6	304	LUT	17	0
33	4	801	LMT	8	0
22	A	816	CLA	22	0
22	Z	309	CLA	21	0
22	K	203	CLA	11	0
22	6	317	CLA	14	0
22	B	826	CLA	18	0
22	B	825	CLA	26	0
24	B	845	BCR	9	0
22	7	322	CLA	18	0
22	A	810	CLA	22	0
22	4	815	CLA	16	0
25	5	324	LHG	7	0
22	3	318	CLA	20	0
29	C	101	SF4	4	0
24	L	204	BCR	17	0
42	7	321	SPH	8	0
22	4	818	CLA	9	0
22	3	320	CLA	9	0
39	6	315	CHL	22	0
22	7	324	CLA	7	0
22	B	814	CLA	16	0

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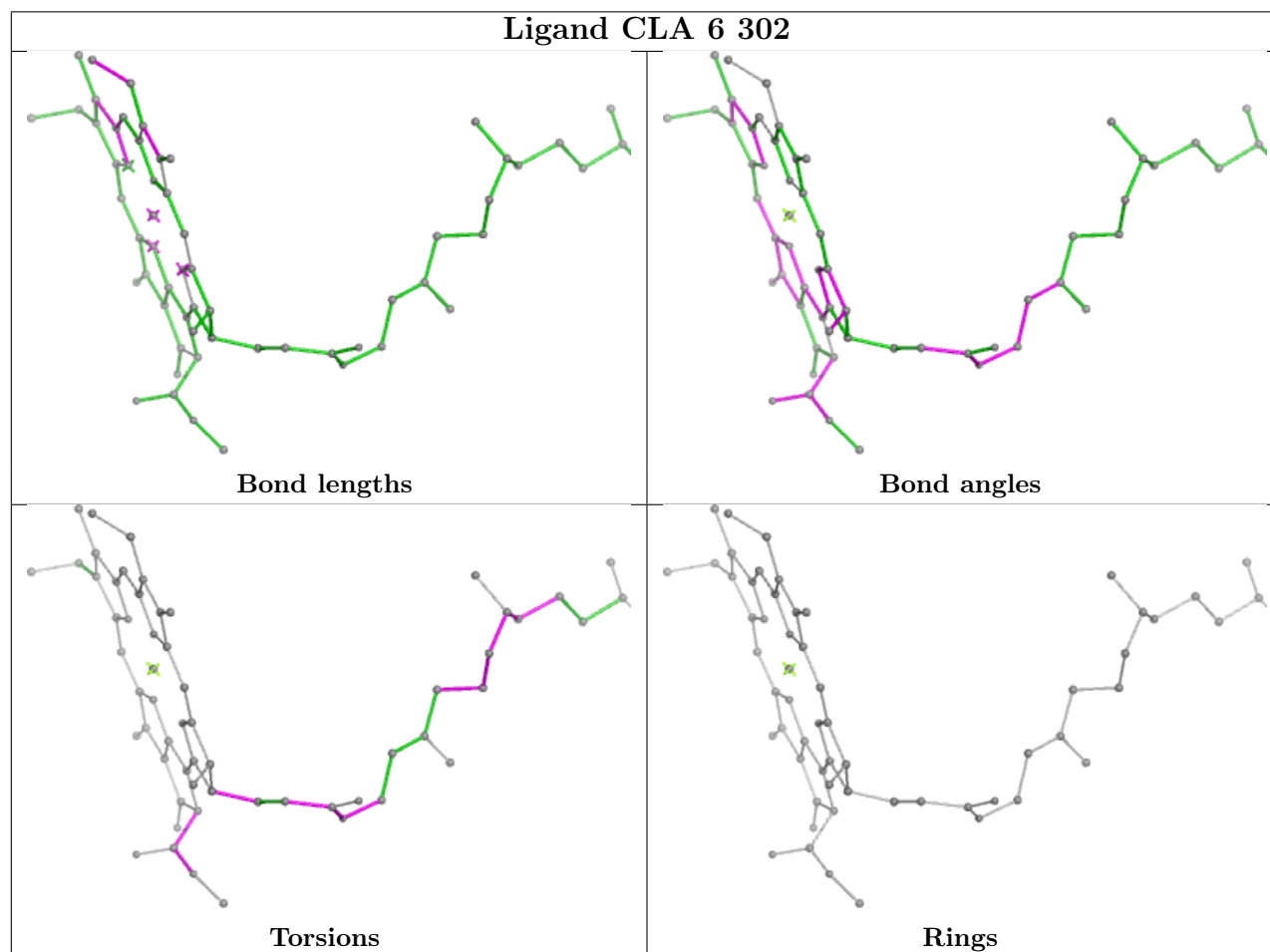
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	311	CLA	12	0
22	5	323	CLA	10	0
22	6	312	CLA	18	0
22	Z	310	CLA	3	0
39	3	317	CHL	13	0
22	7	310	CLA	15	0
22	A	819	CLA	12	0
24	A	847	BCR	14	0
25	8	317	LHG	7	0
39	8	315	CHL	24	0
38	3	302	LUT	12	0
22	8	308	CLA	15	0
24	3	305	BCR	15	0
22	A	813	CLA	19	0
22	B	805	CLA	12	0
22	7	312	CLA	6	0
24	6	305	BCR	19	0
38	7	302	LUT	17	0
22	3	316	CLA	10	0
22	B	809	CLA	13	0
24	B	847	BCR	21	0
22	B	841	CLA	15	0
22	6	322	CLA	21	0
22	6	301	CLA	20	0
22	B	834	CLA	14	0
22	A	837	CLA	9	0
22	A	814	CLA	22	0
25	Z	317	LHG	9	0
22	A	838	CLA	9	0
22	9	304	CLA	2	0
24	B	853	BCR	21	0
25	7	318	LHG	10	0
22	A	804	CLA	14	0
22	B	810	CLA	17	0
22	Z	306	CLA	19	0
22	9	310	CLA	1	0
22	B	817	CLA	18	0
22	3	322	CLA	20	0
22	A	802	CLA	14	0
22	A	803	CLA	8	0
22	9	306	CLA	16	0
22	8	310	CLA	13	0

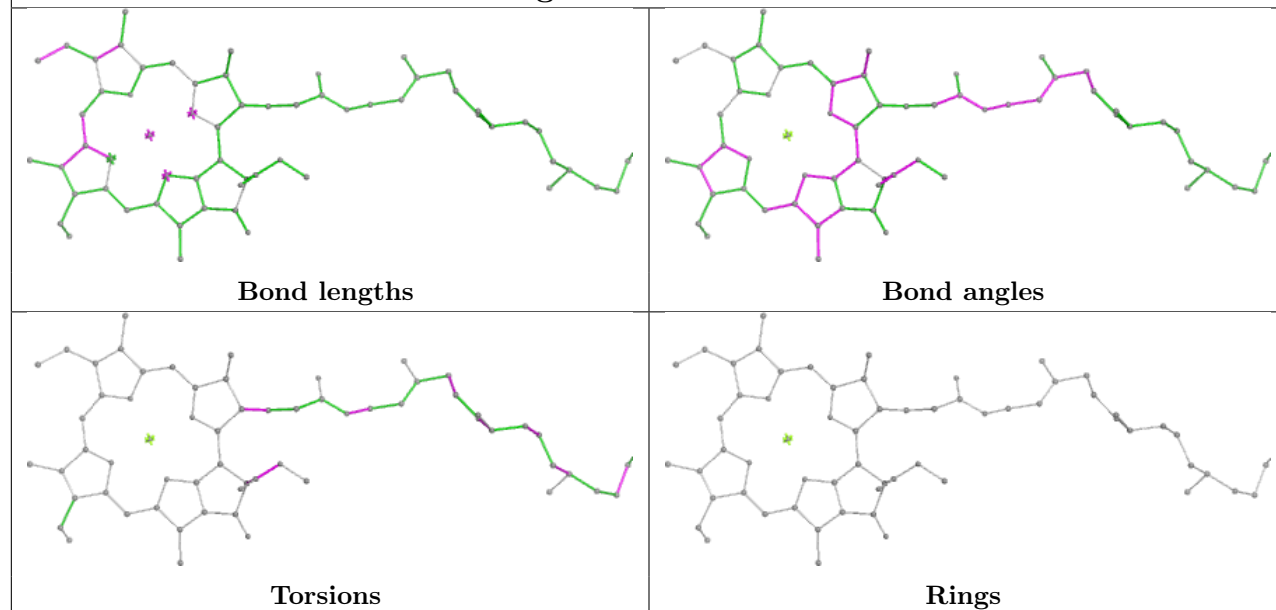
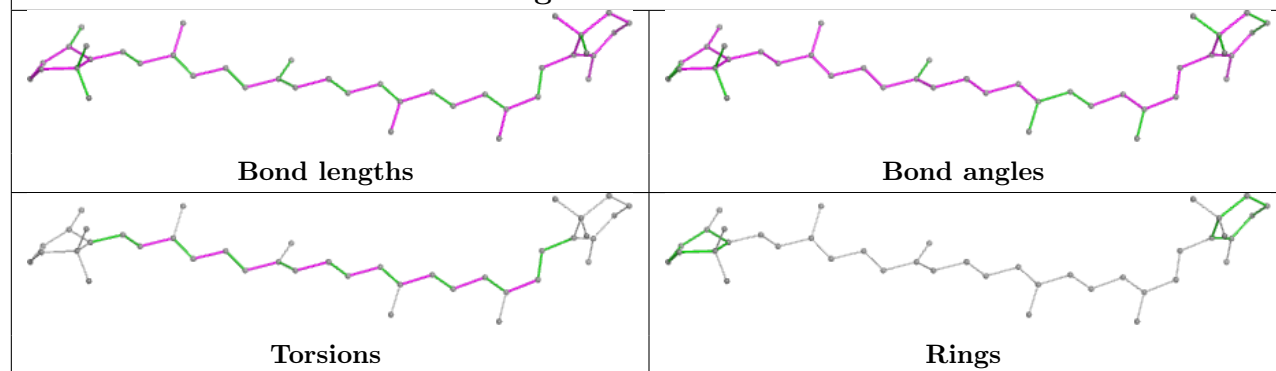
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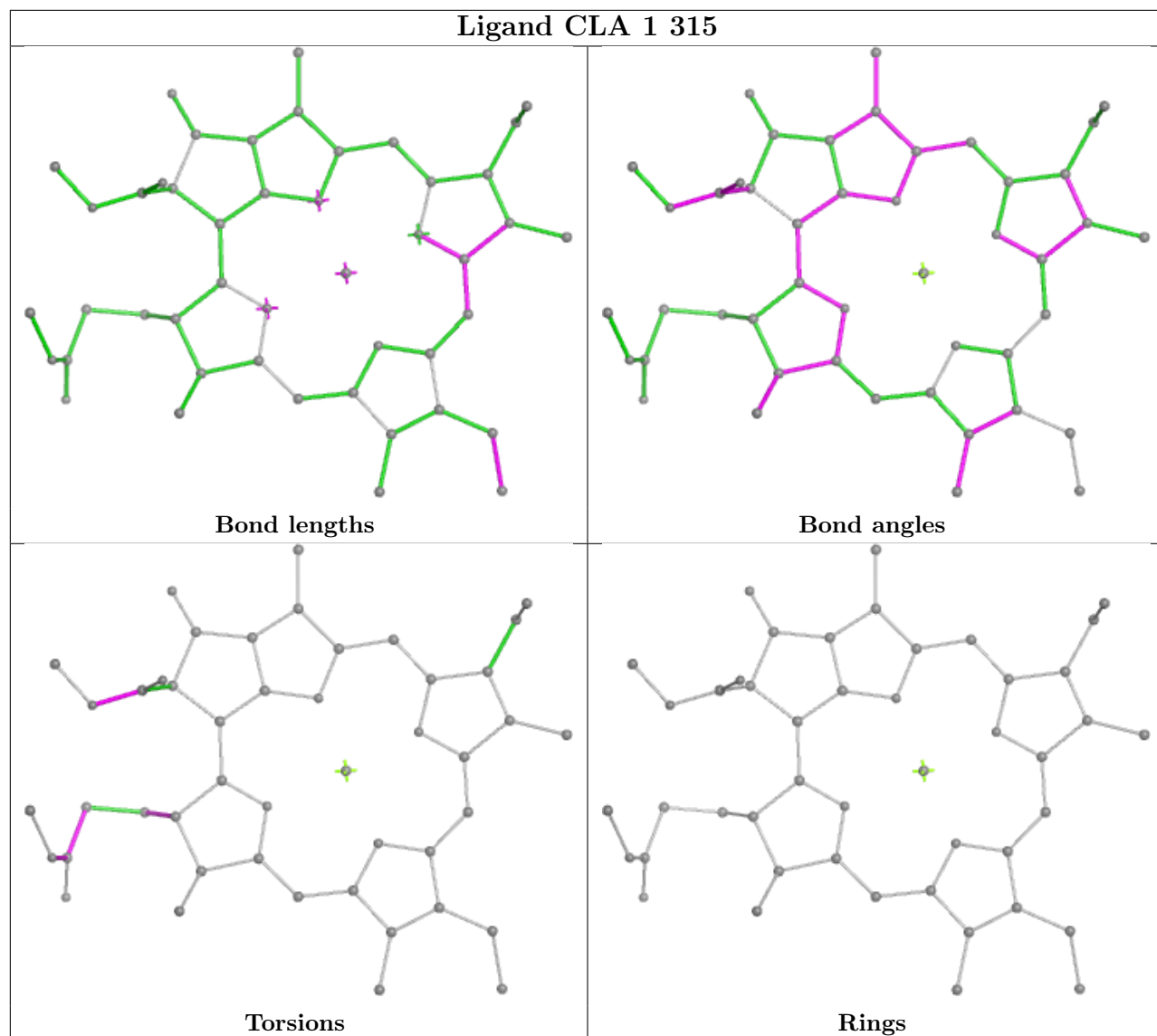
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	4	820	LHG	16	0
22	5	313	CLA	13	0
22	A	821	CLA	25	0

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

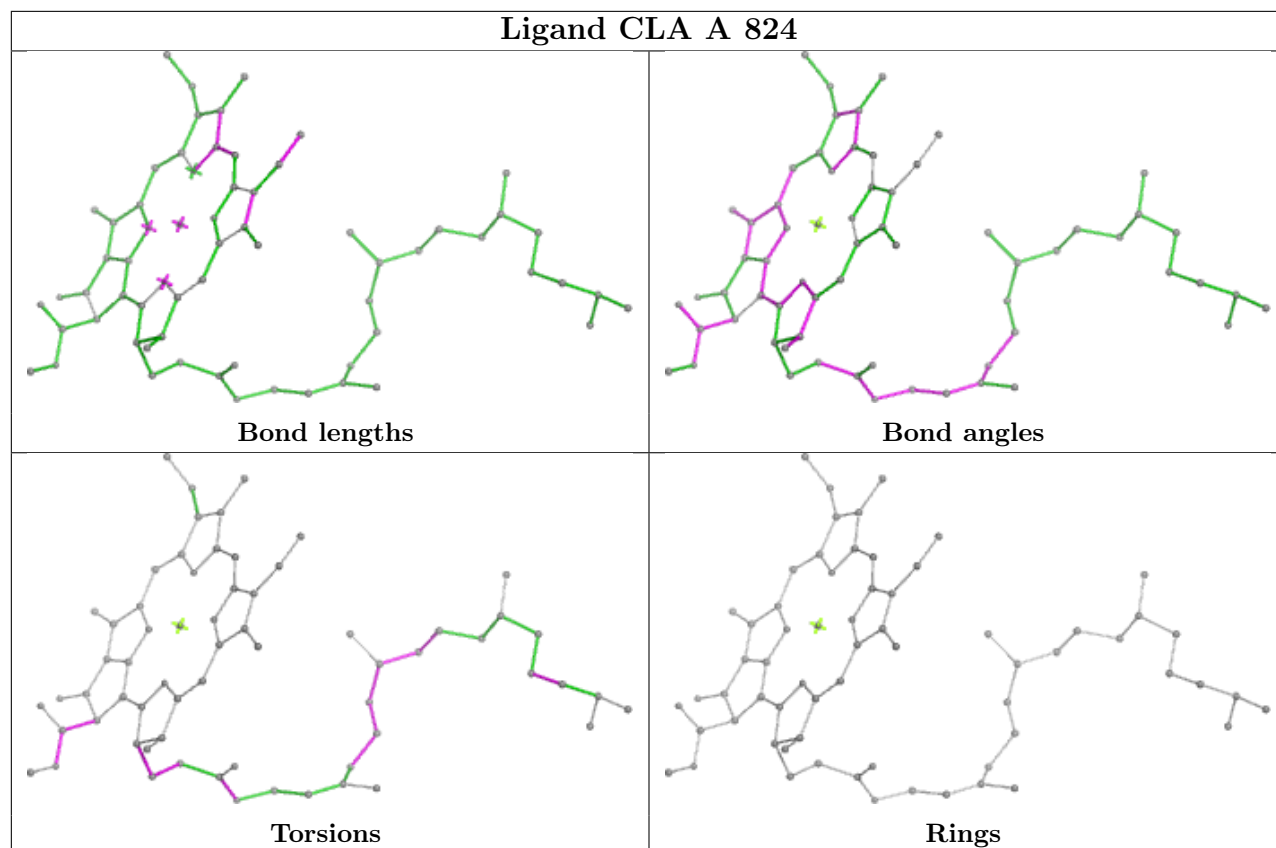


Ligand CLA 5 315**Ligand BCR 8 304**

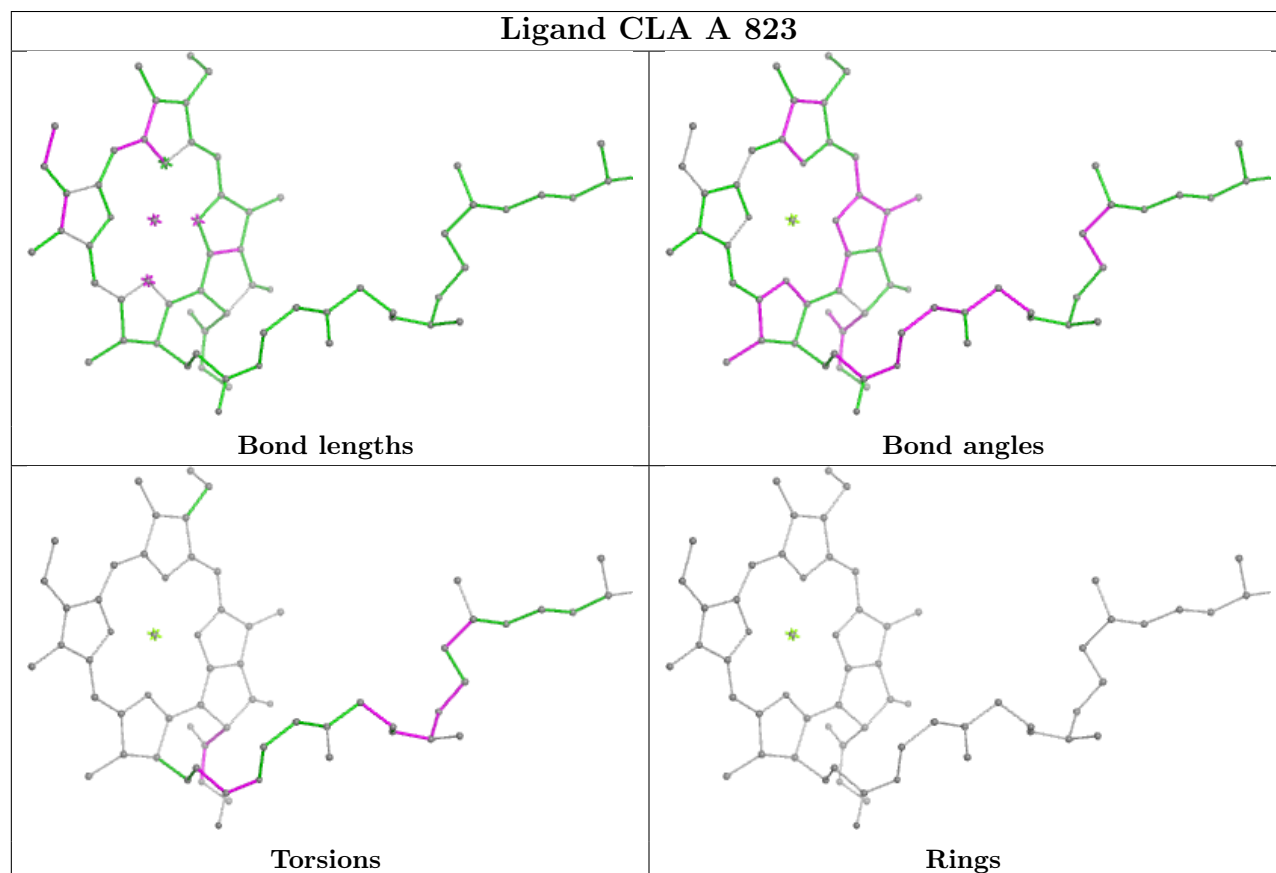
Ligand CLA 1 315



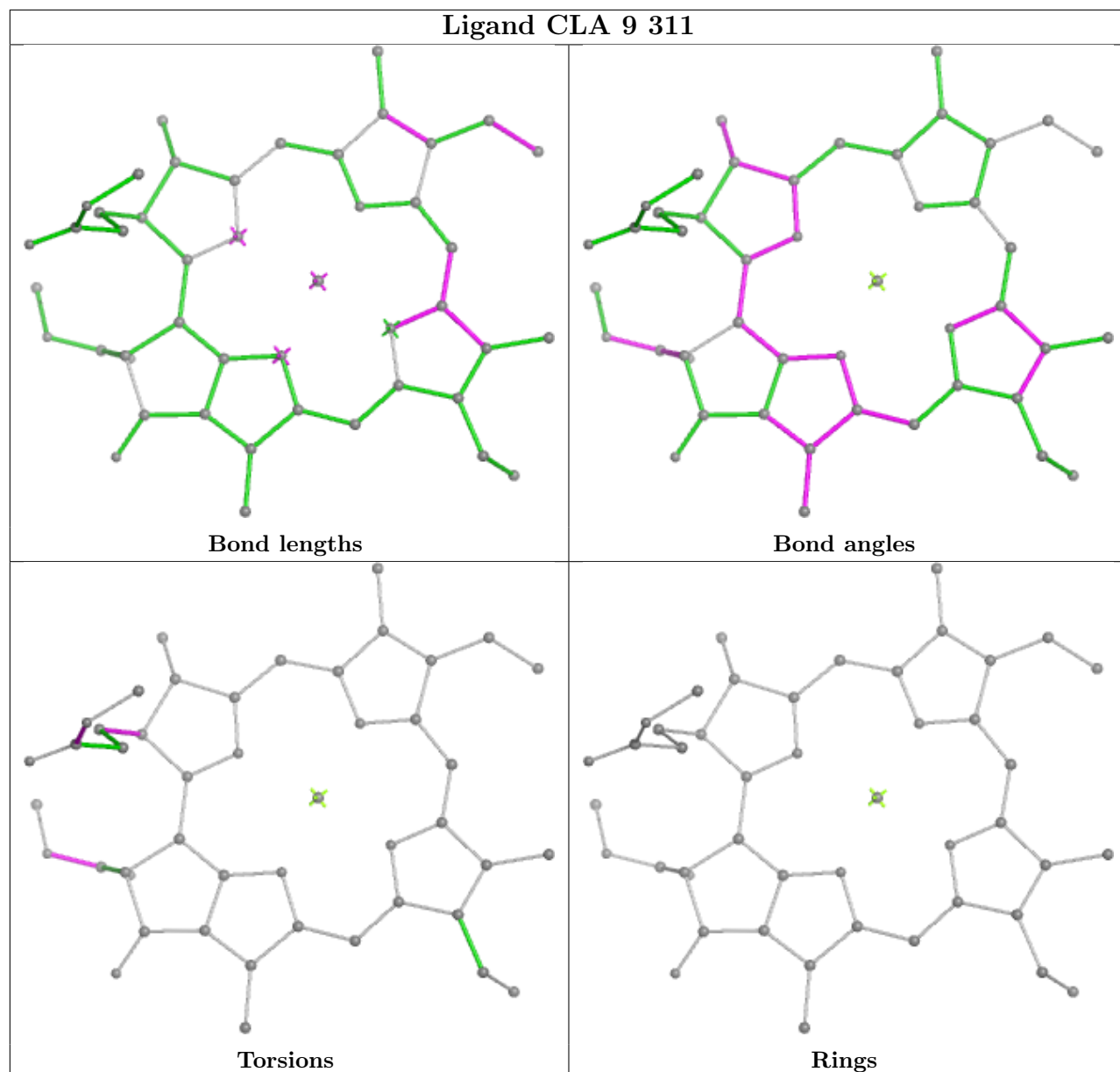
Ligand CLA A 824



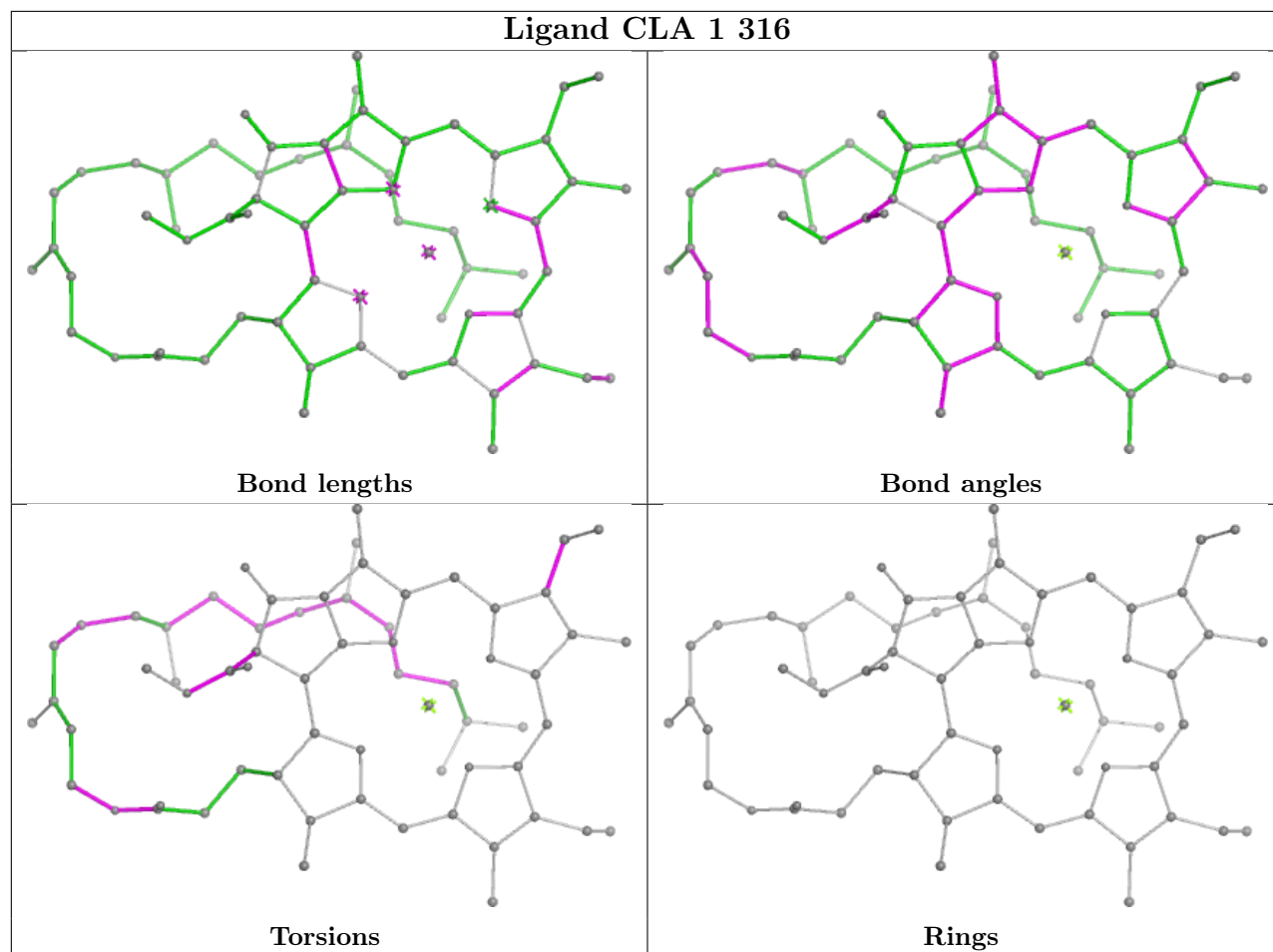
Ligand CLA A 823



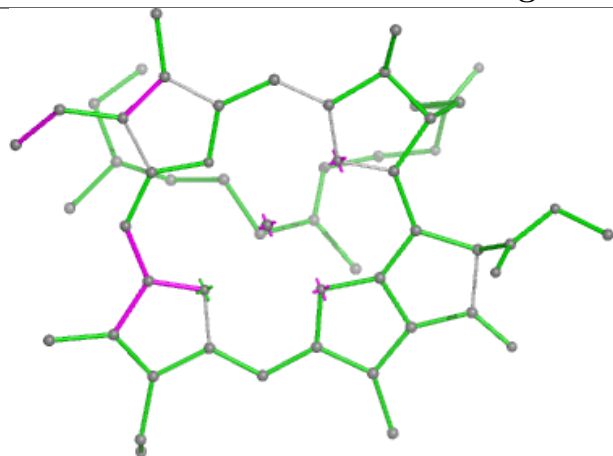
Ligand CLA 9 311



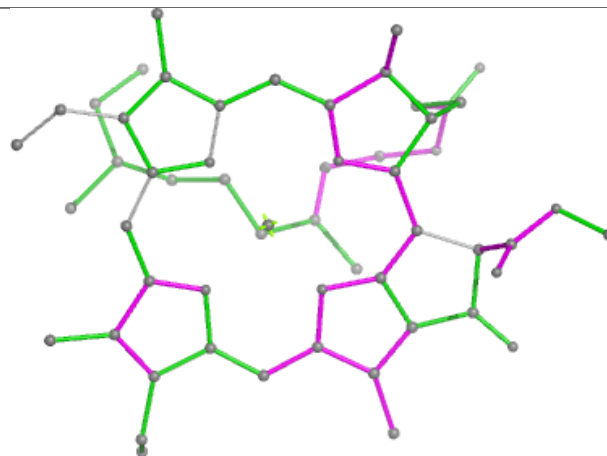
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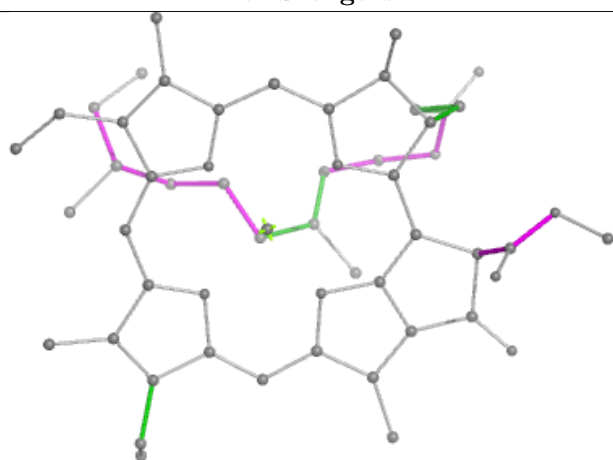
Ligand CLA 5 301



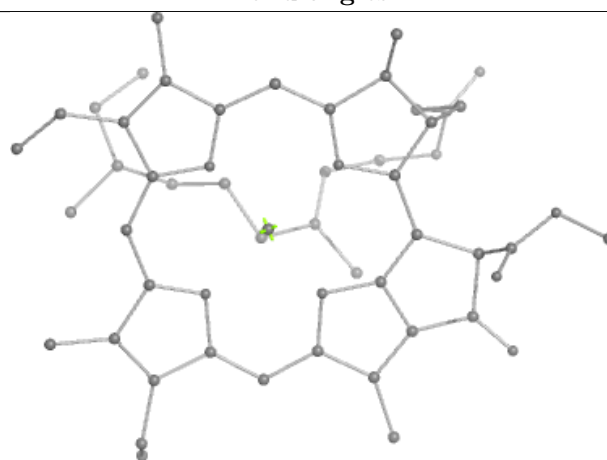
Bond lengths



Bond angles

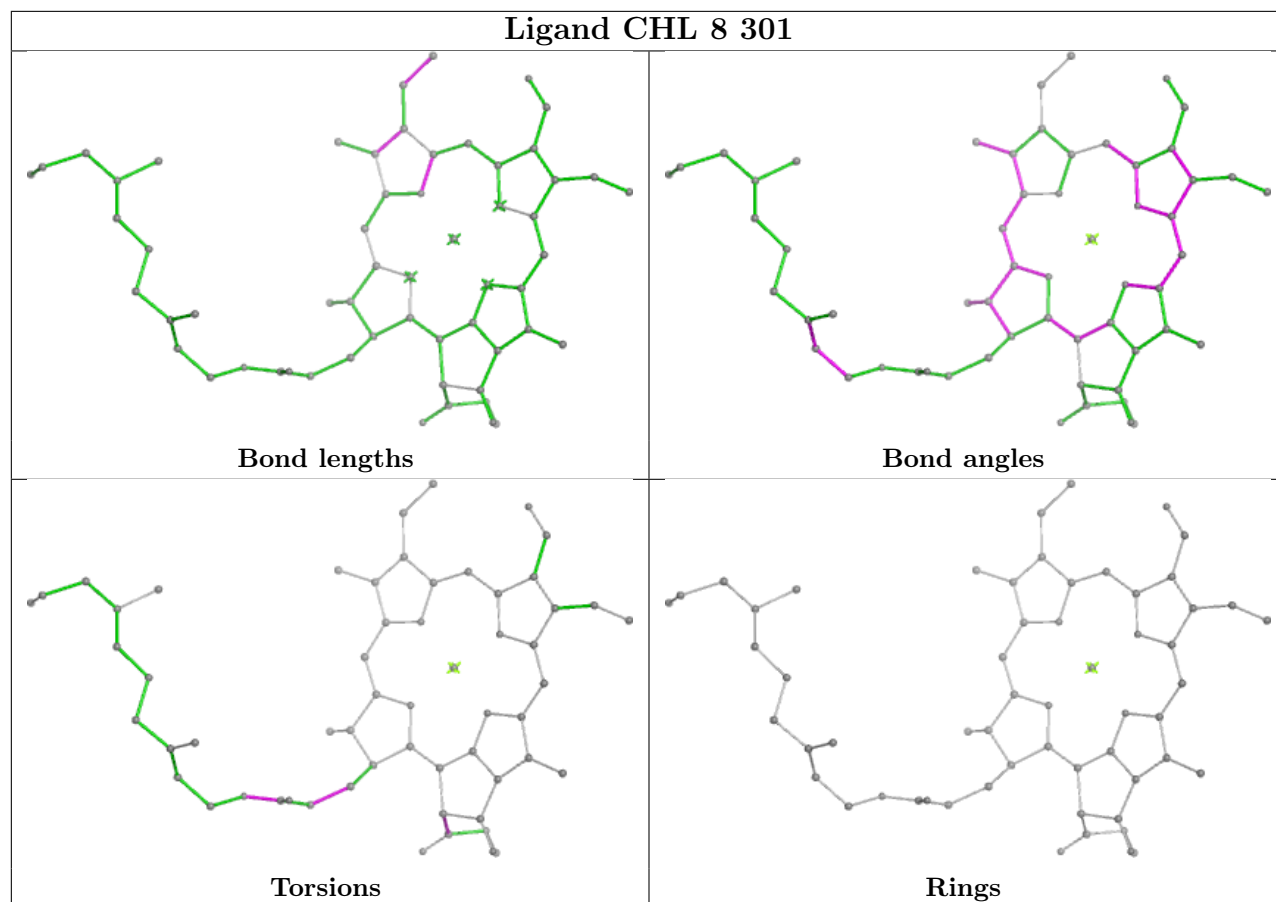


Torsions

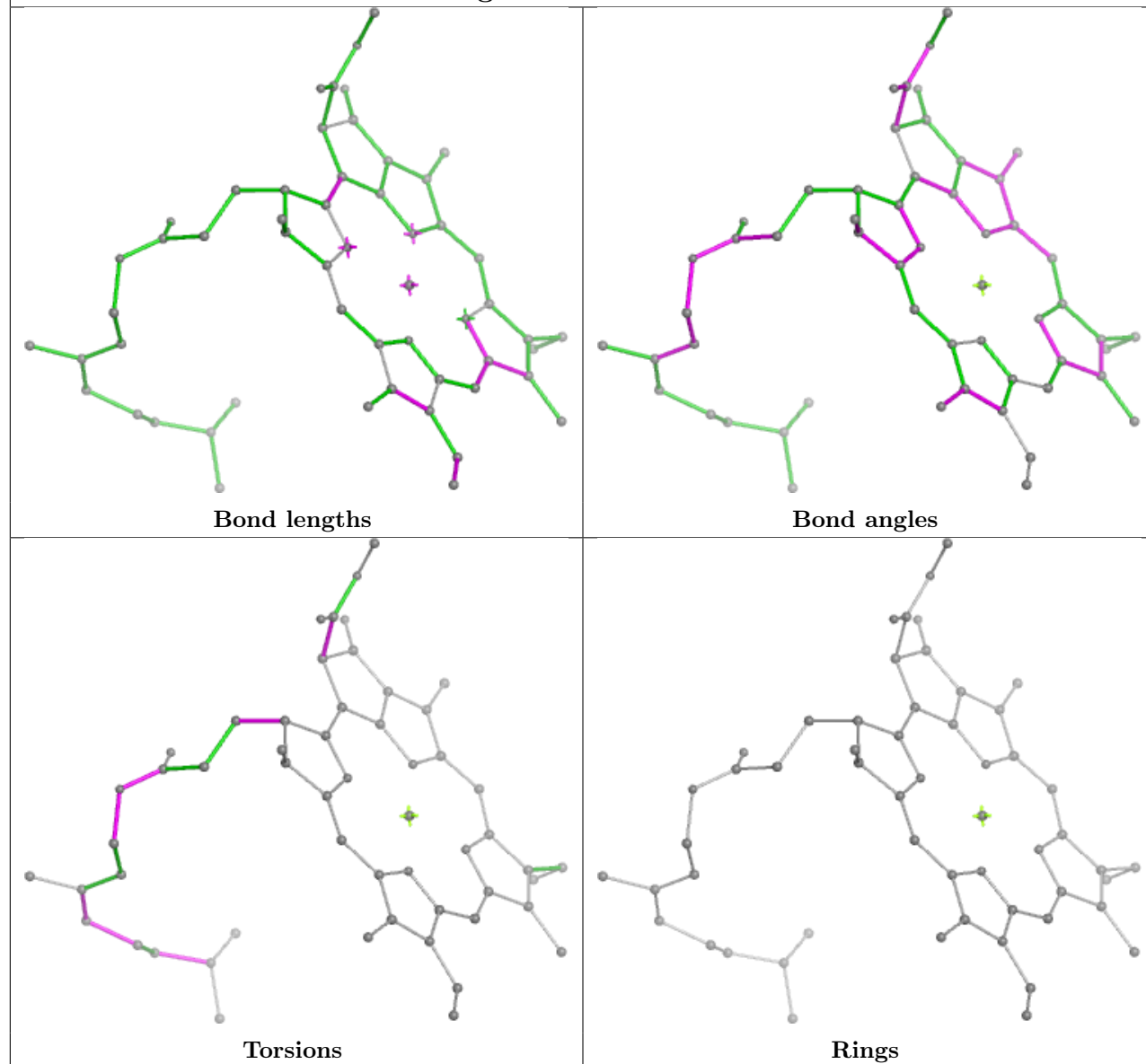


Rings

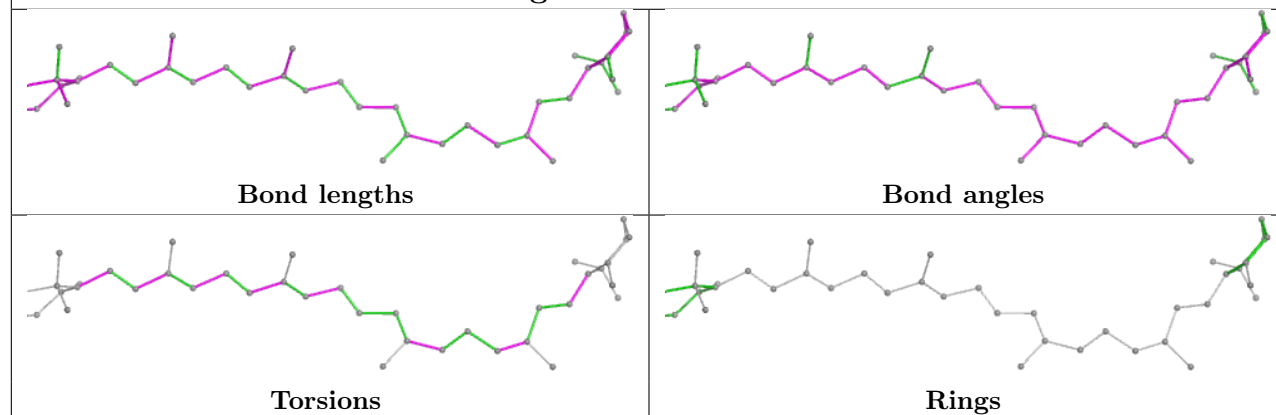
Ligand CHL 8 301



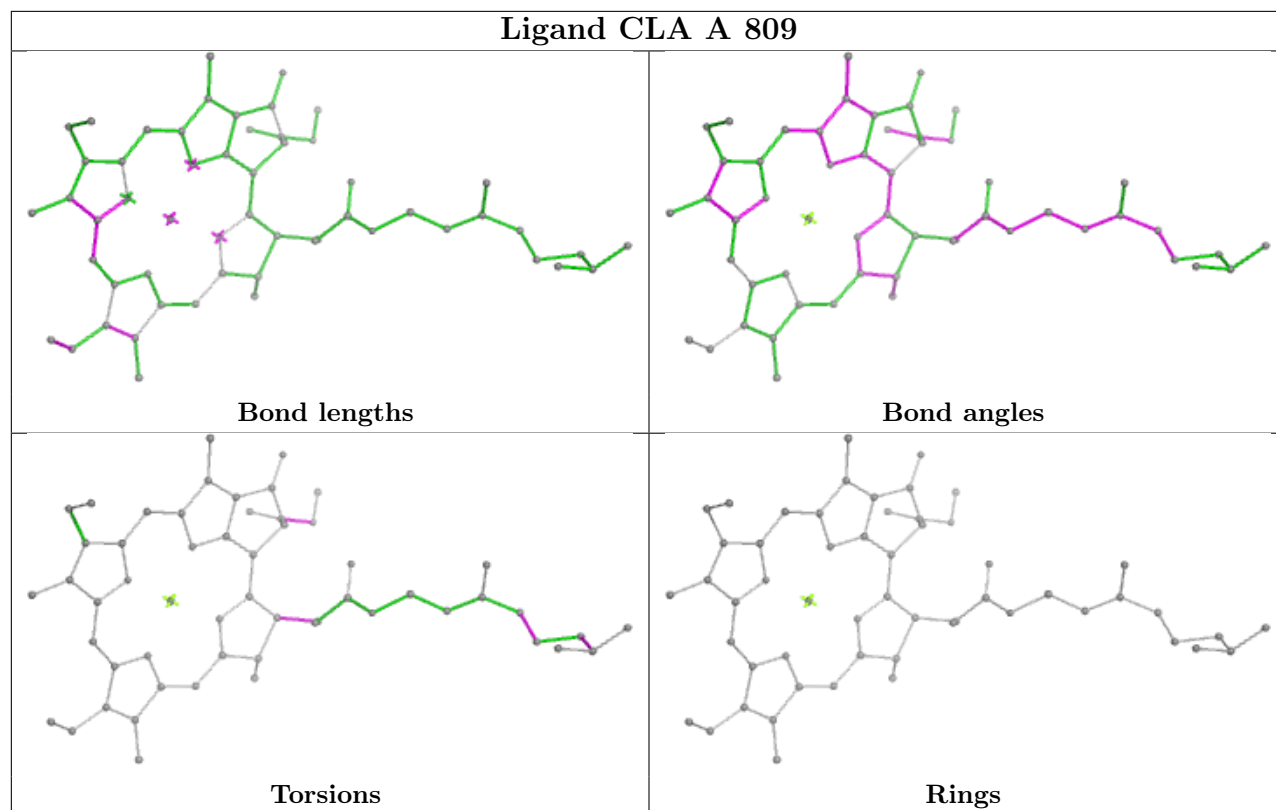
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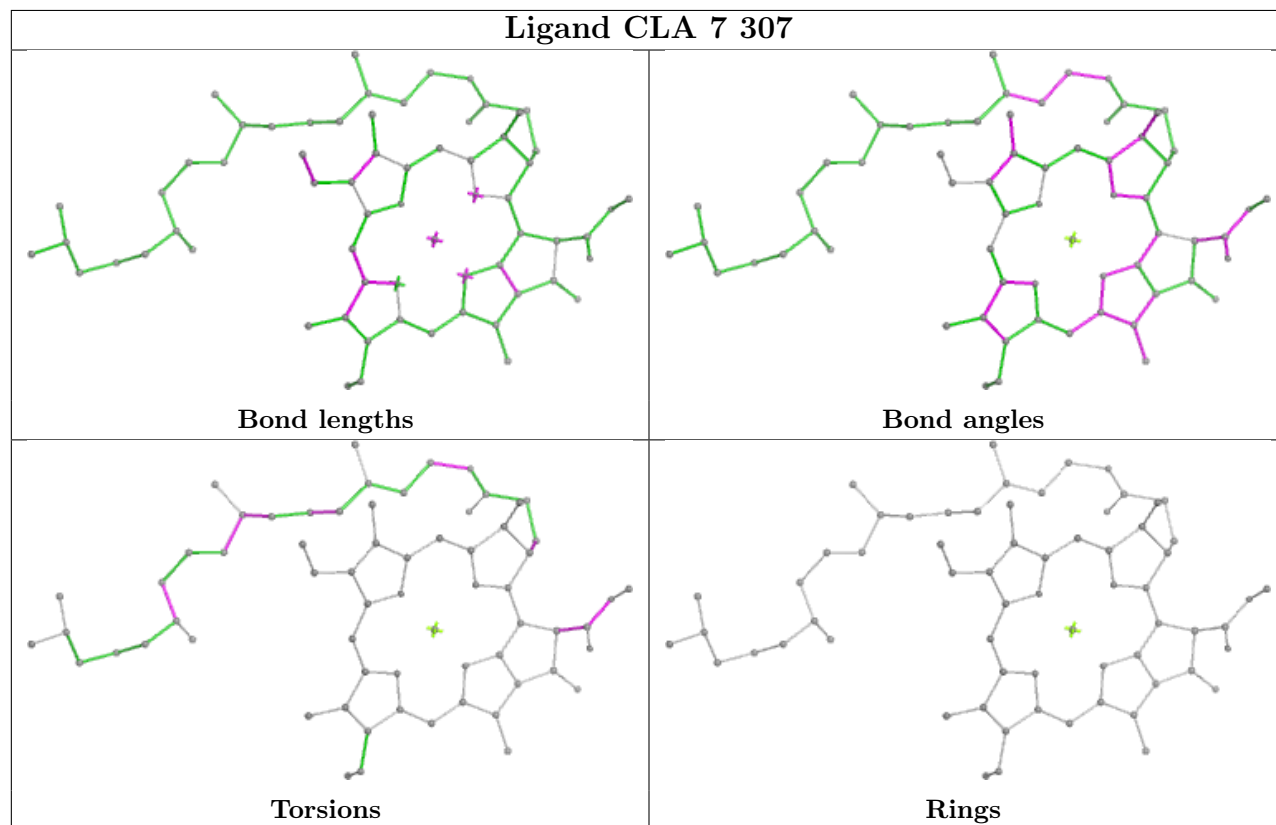
Ligand BCR A 844

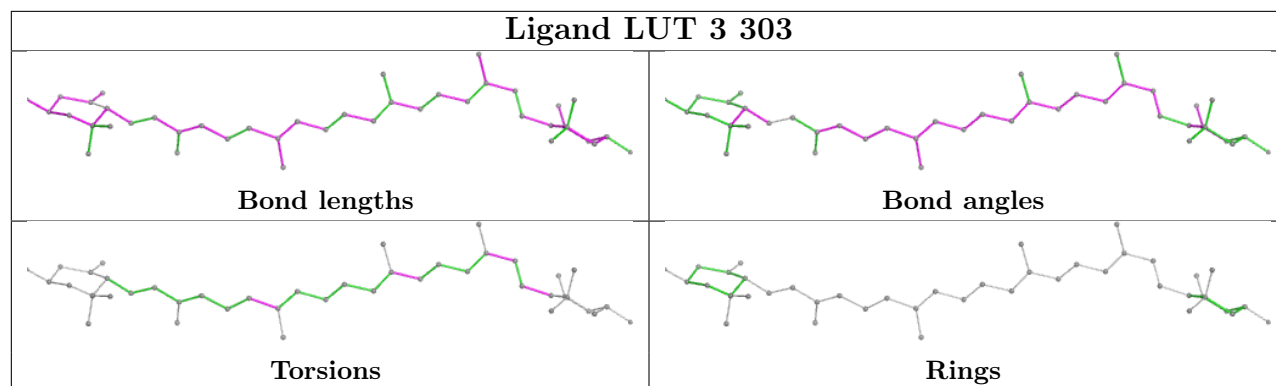
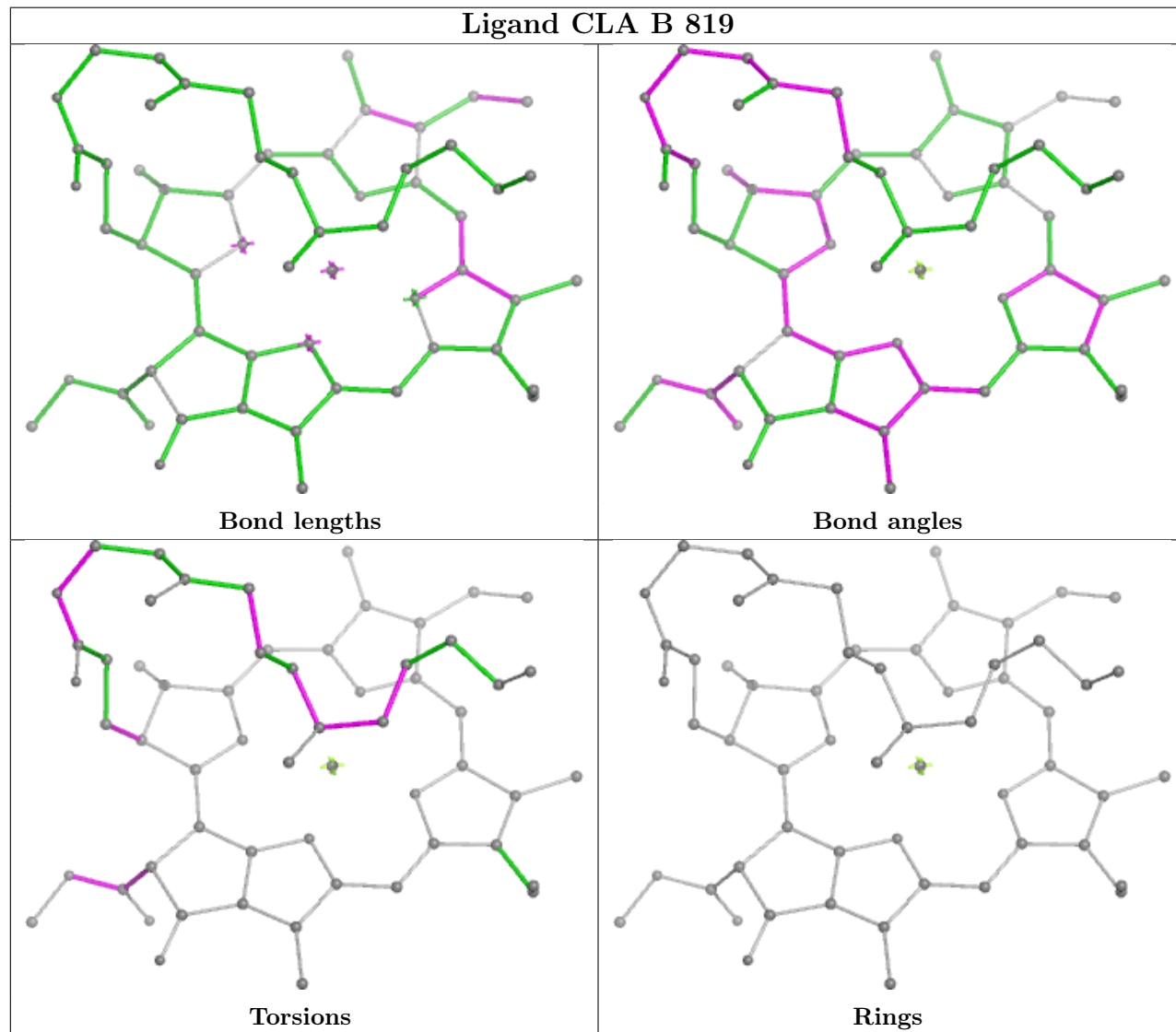


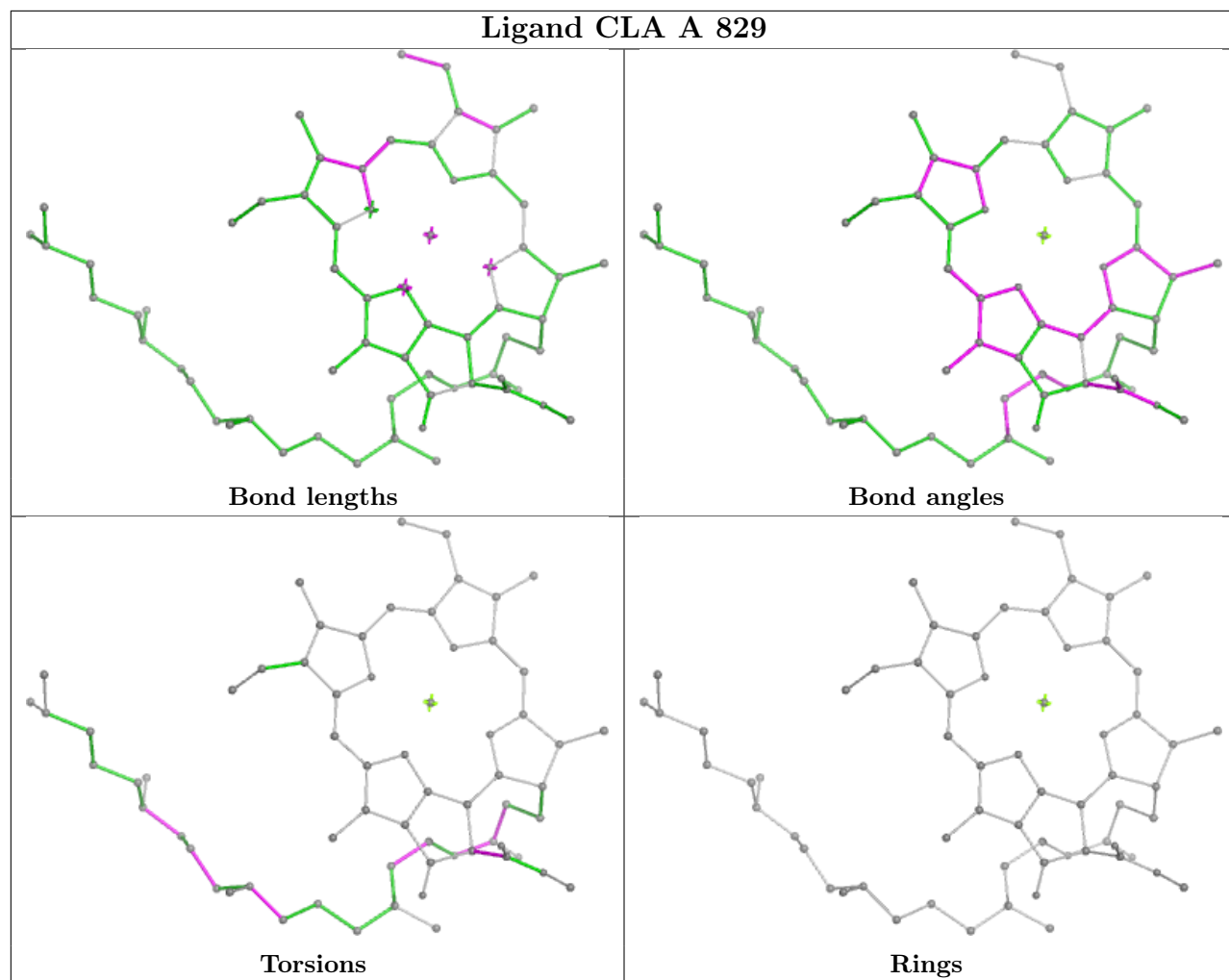
Ligand CLA A 809



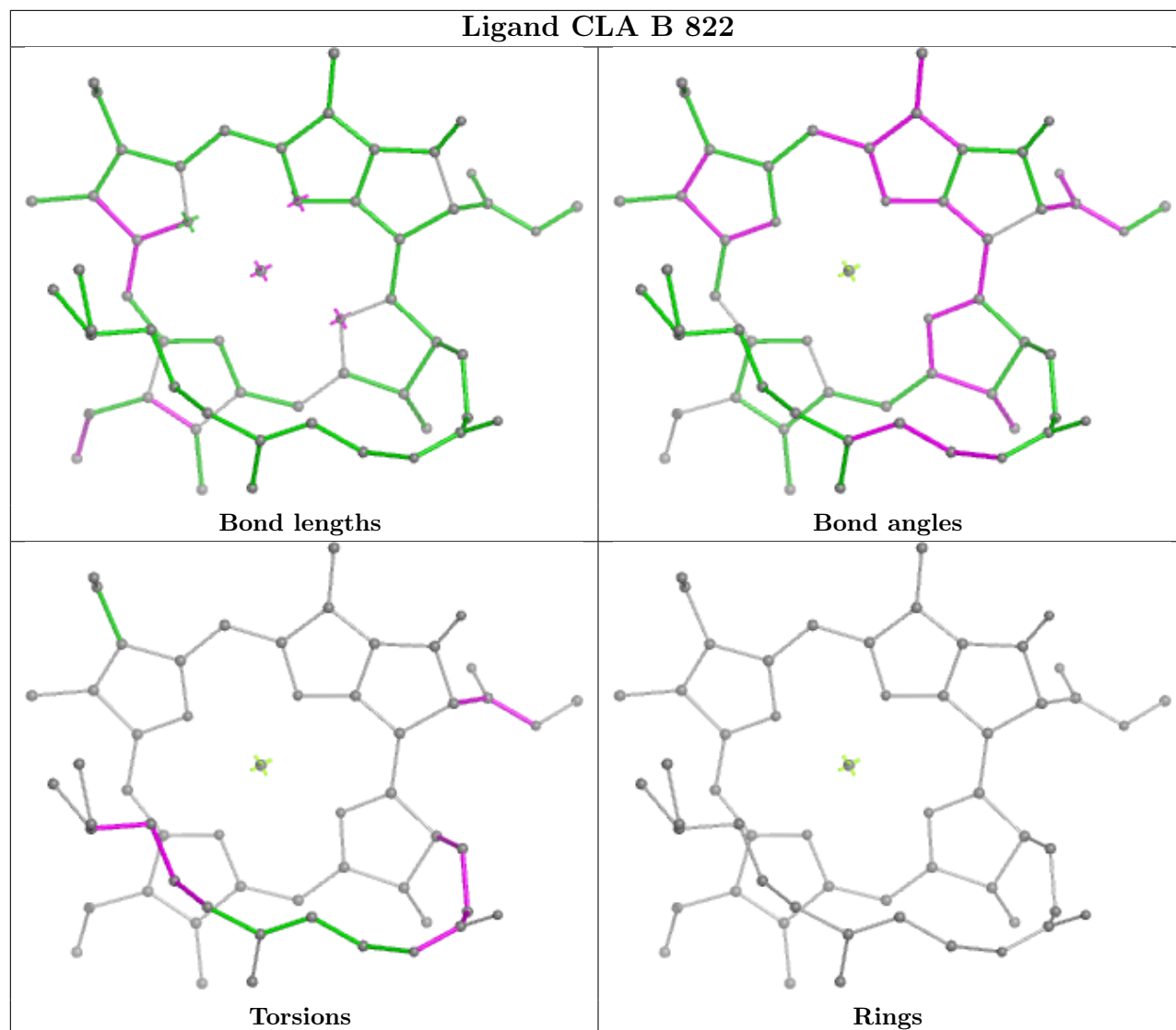
Ligand CLA 7 307



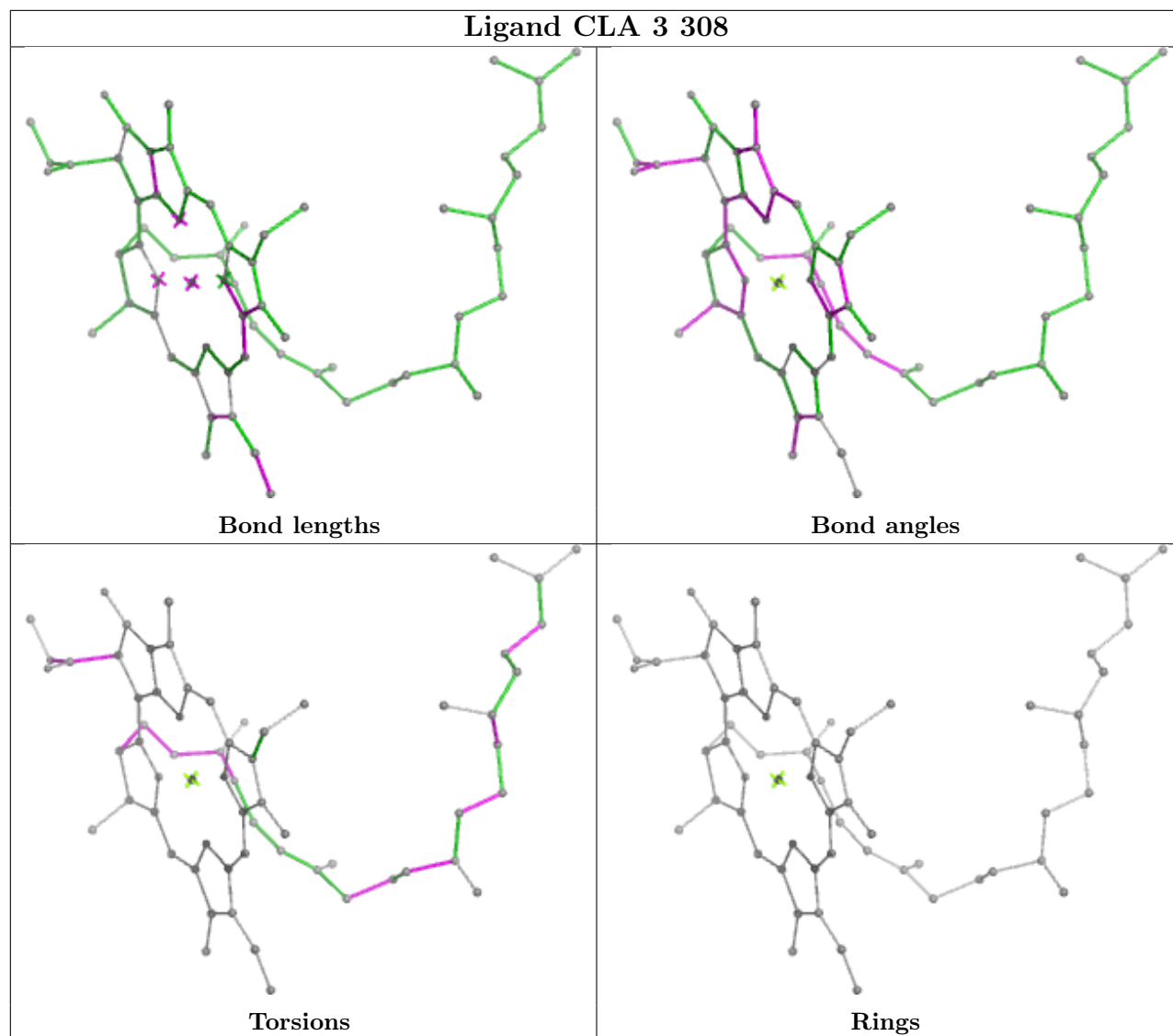
Ligand LUT 3 303**Ligand CLA B 819**

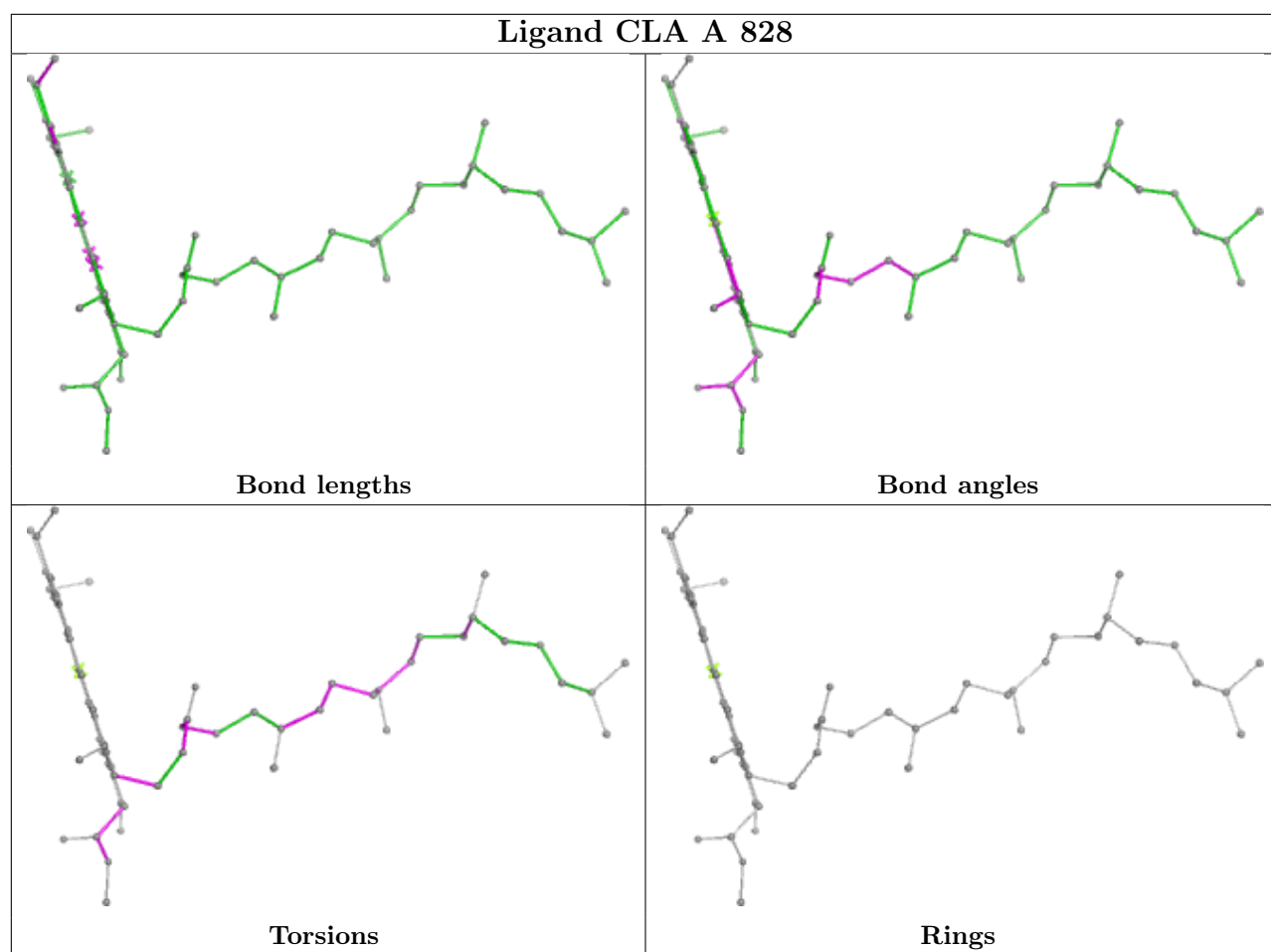


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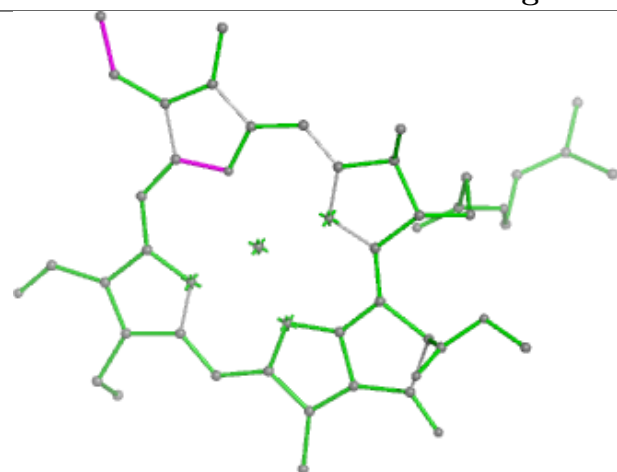


Ligand CLA 3 308

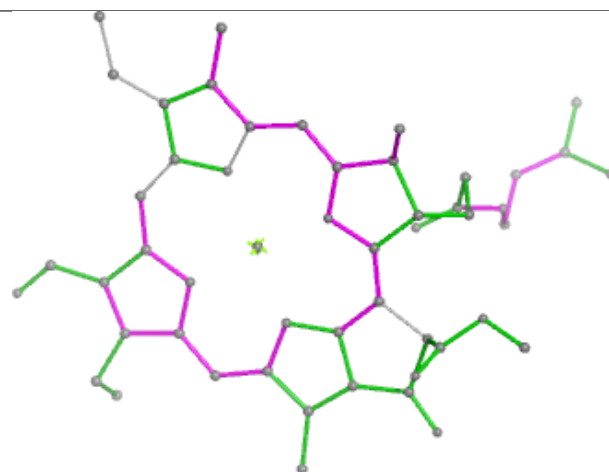




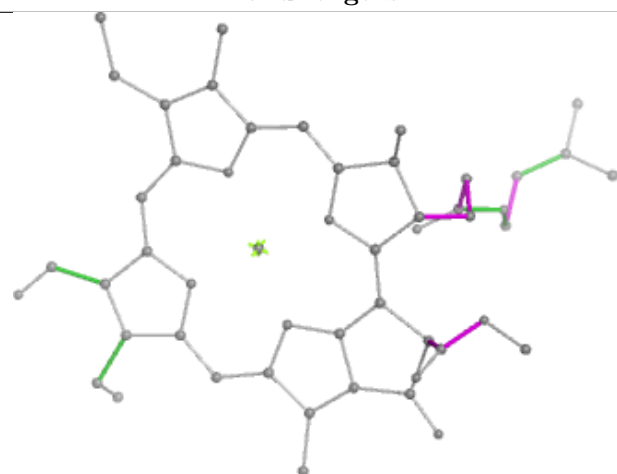
Ligand CHL 4 814



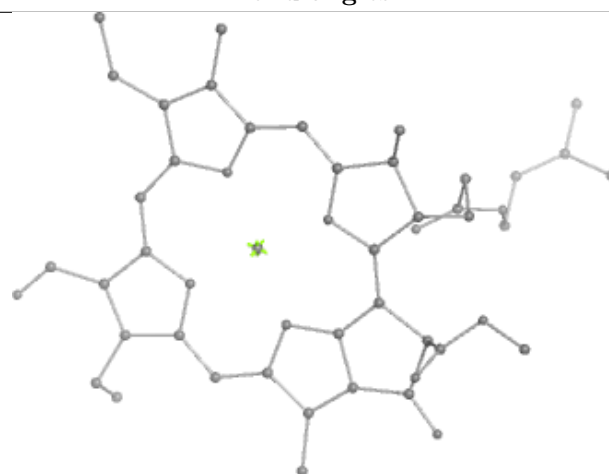
Bond lengths



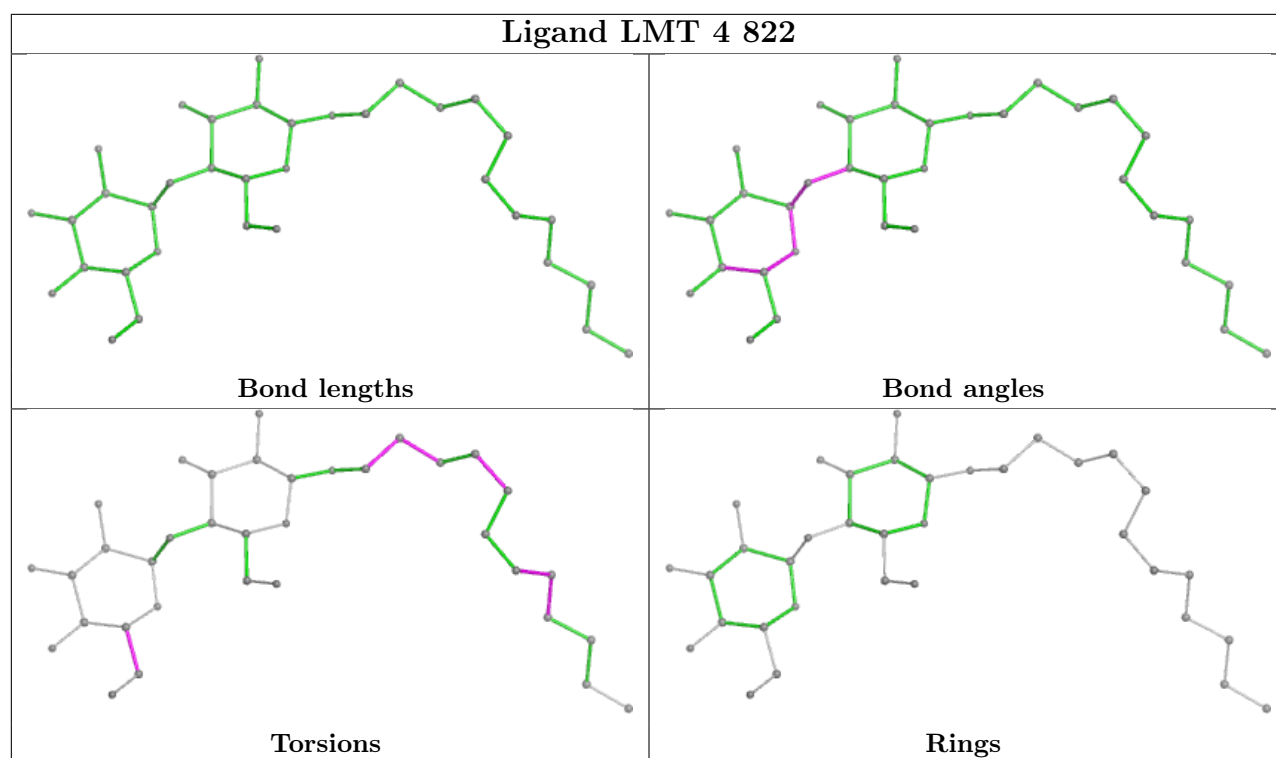
Bond angles



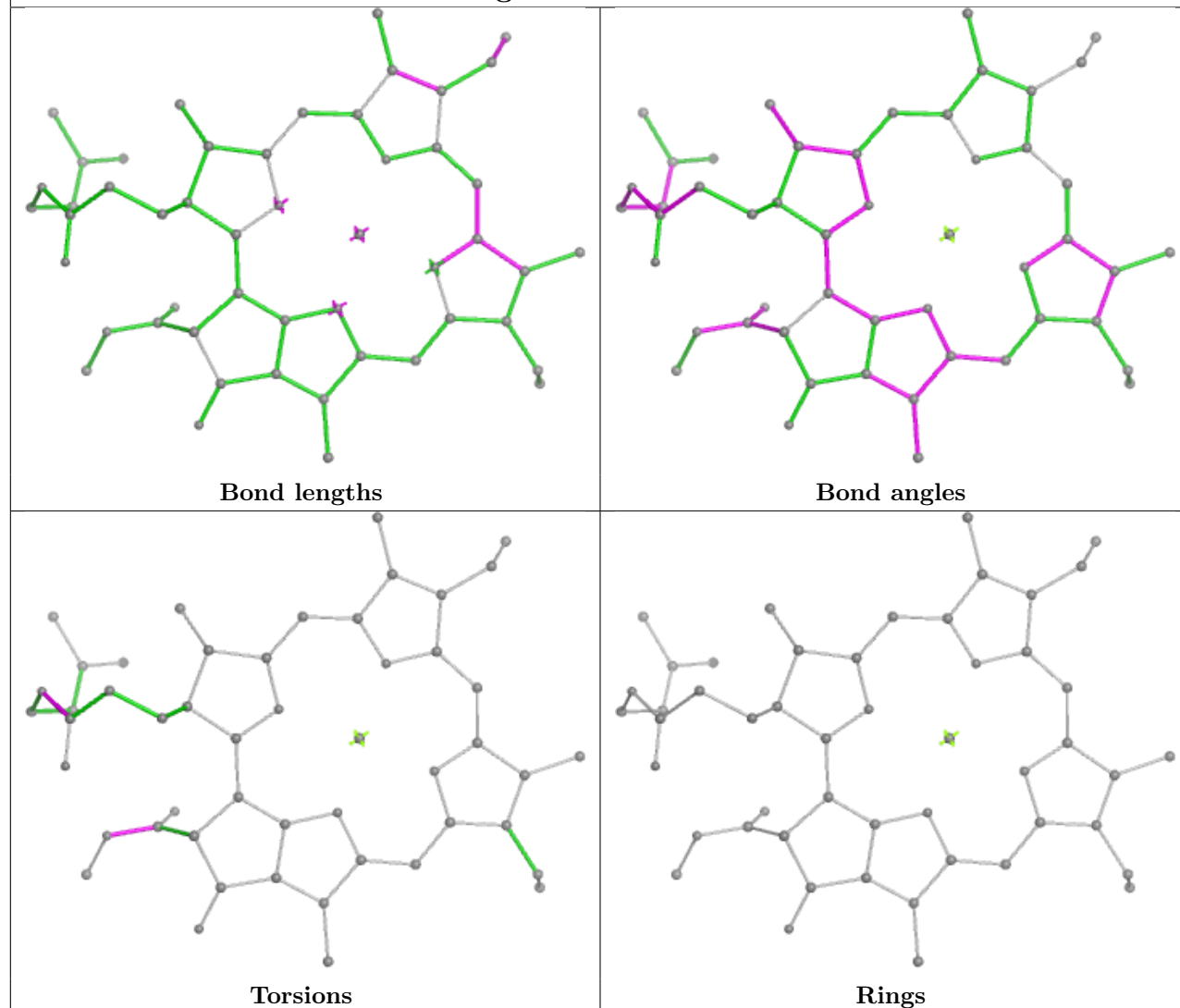
Torsions



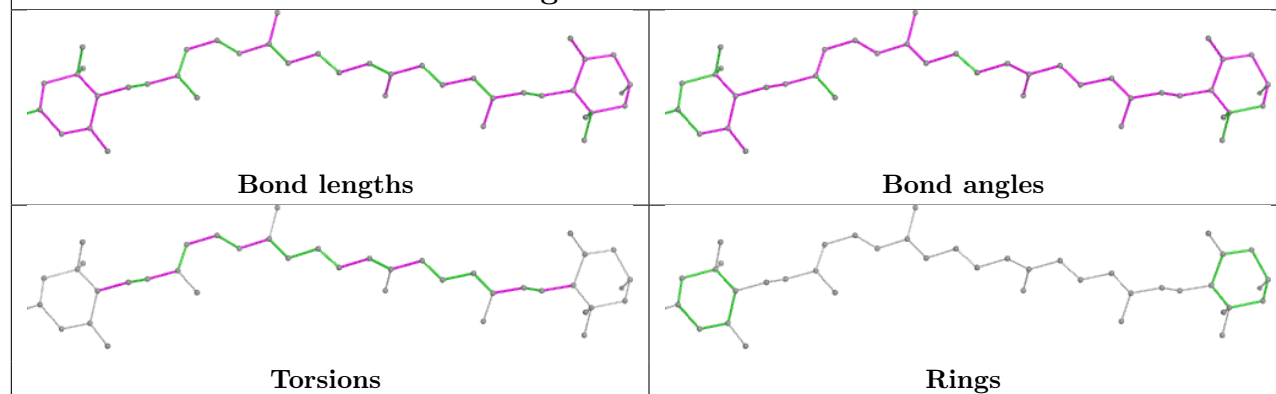
Rings

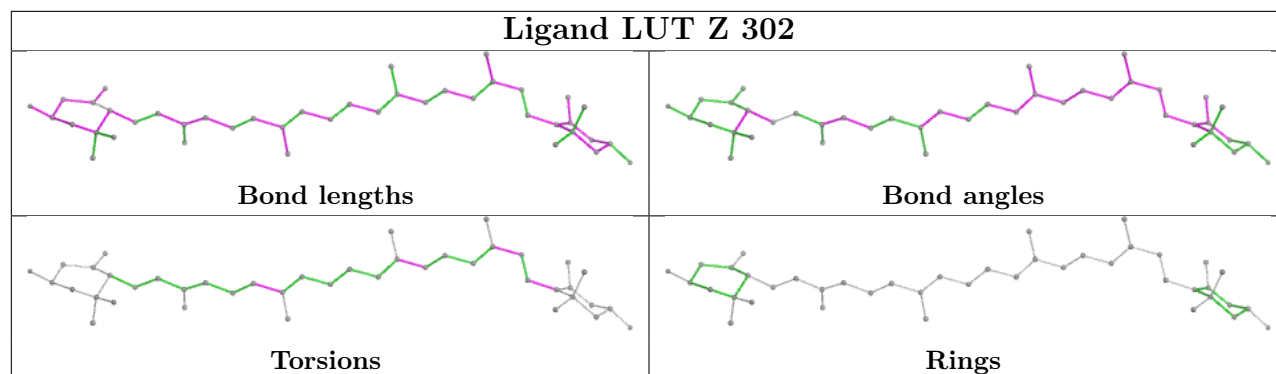
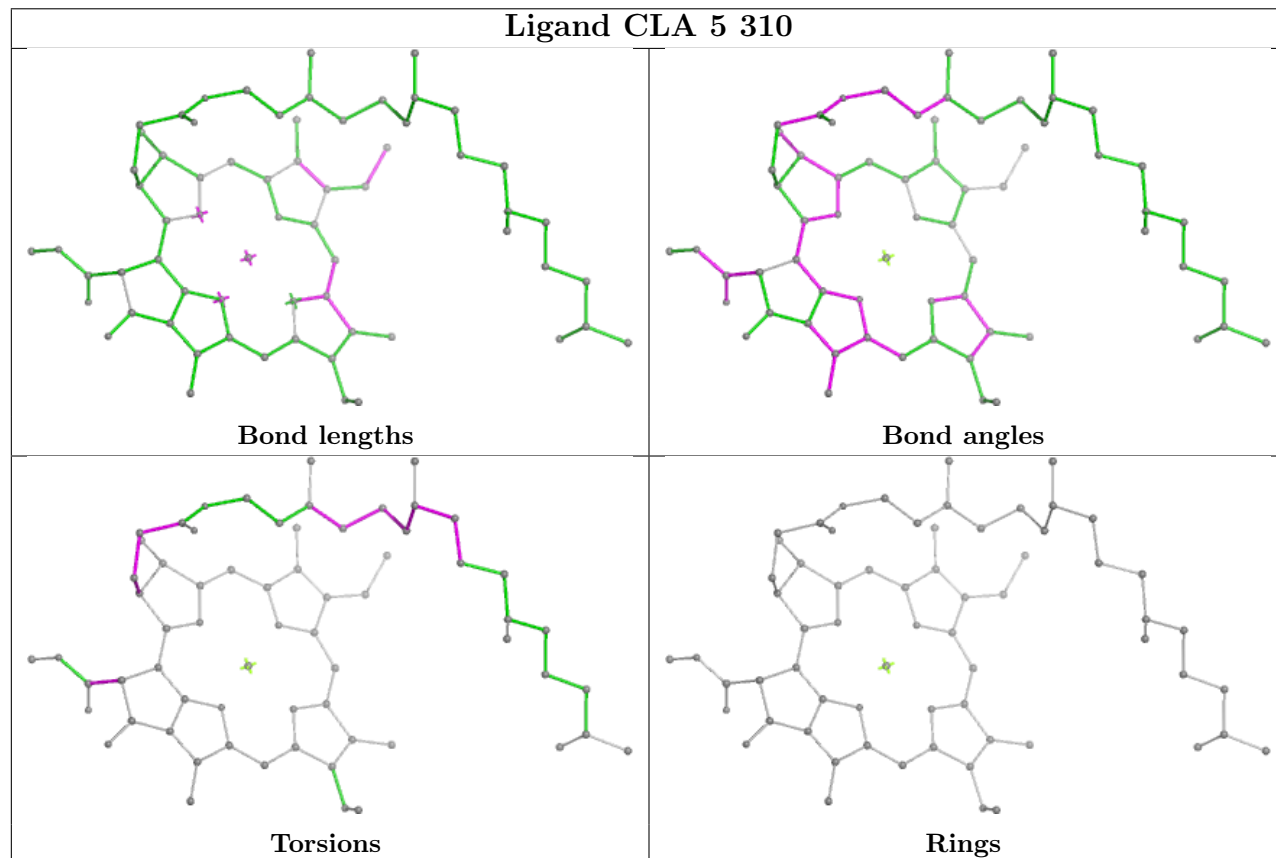


Ligand CLA 7 305

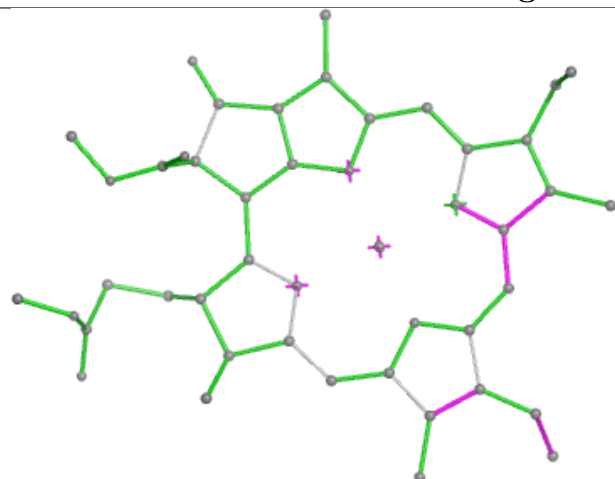


Ligand C7Z 5 306

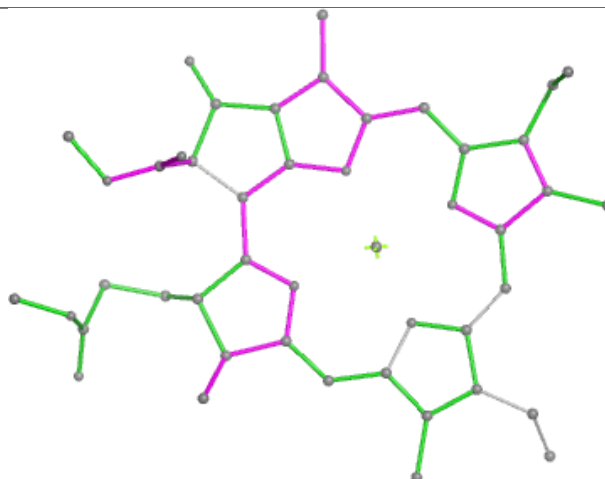


Ligand LUT Z 302**Ligand CLA 5 310**

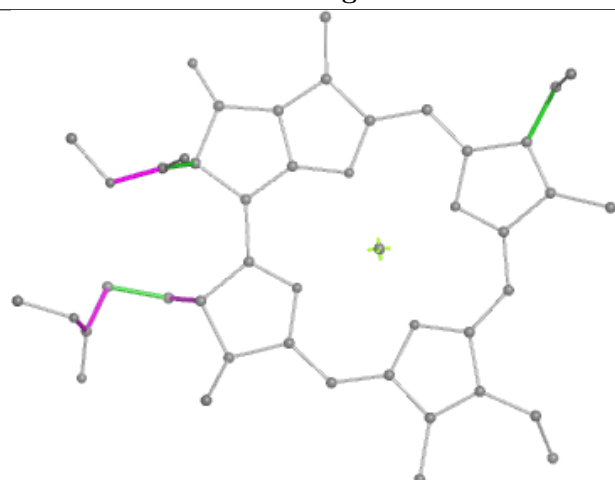
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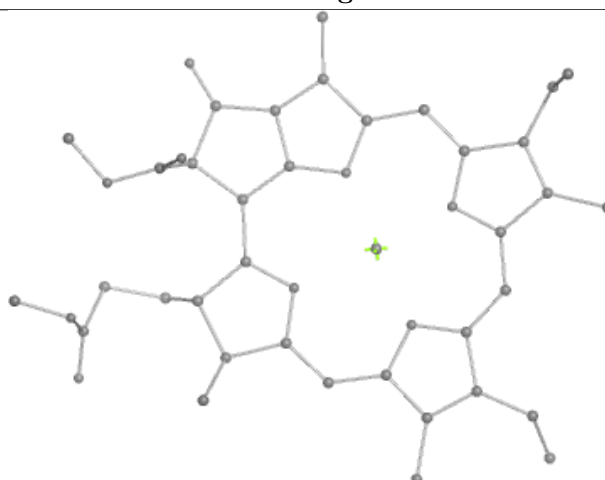
Bond lengths



Bond angles

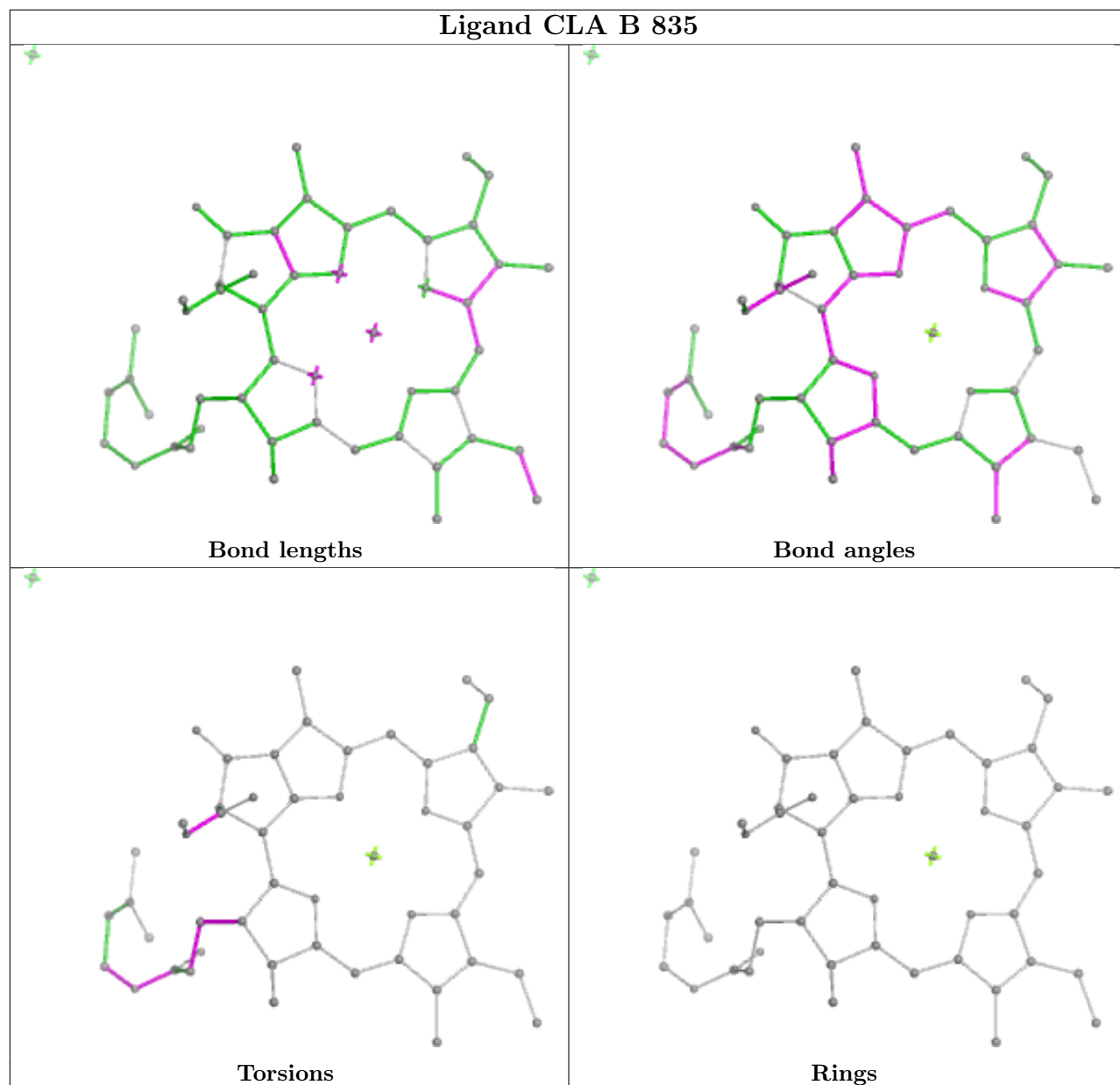


Torsions

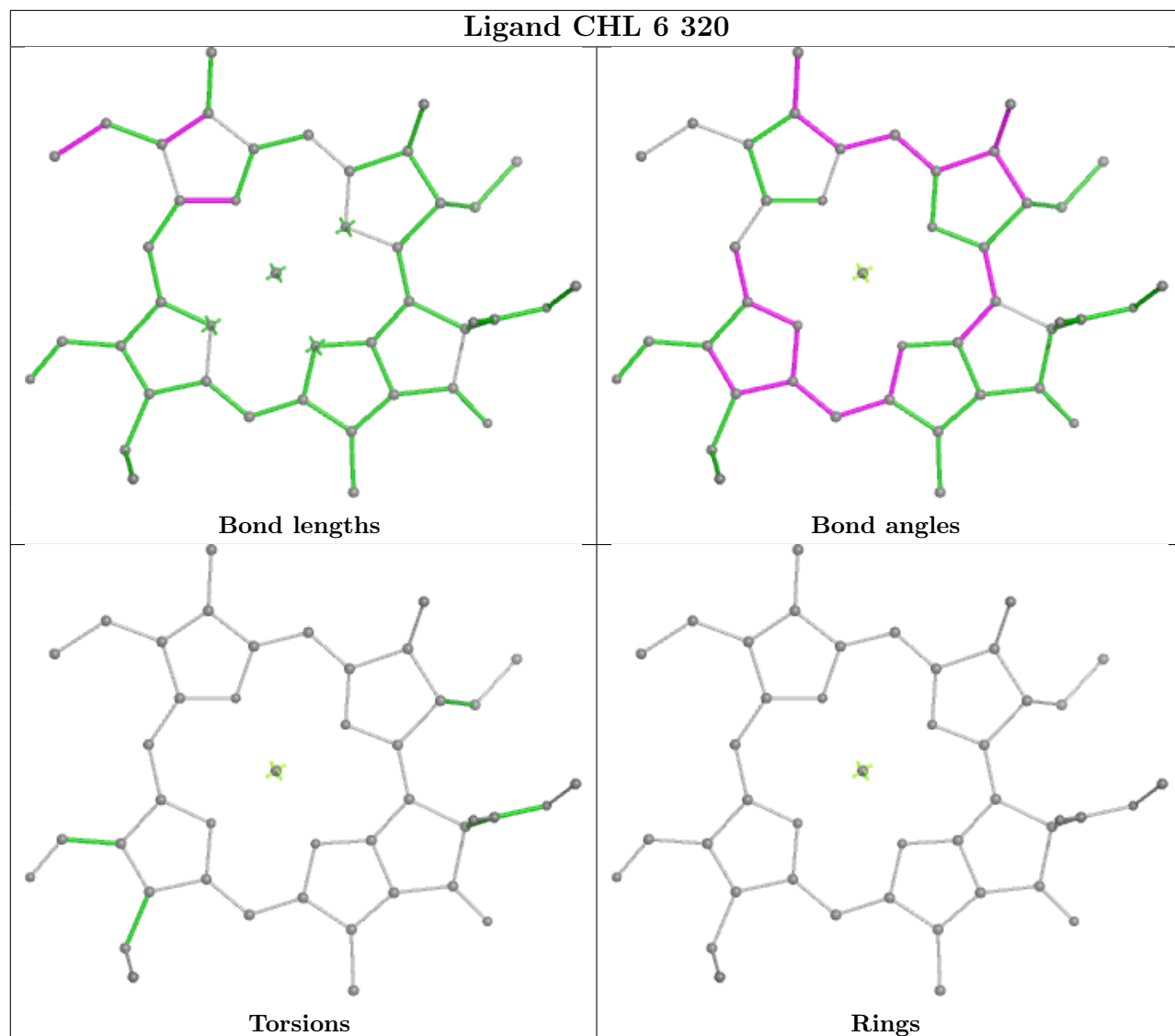


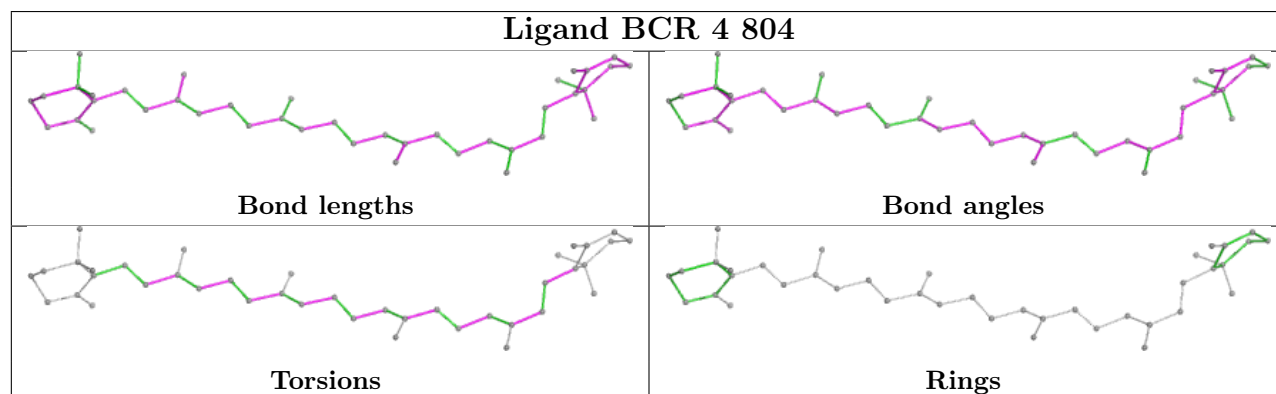
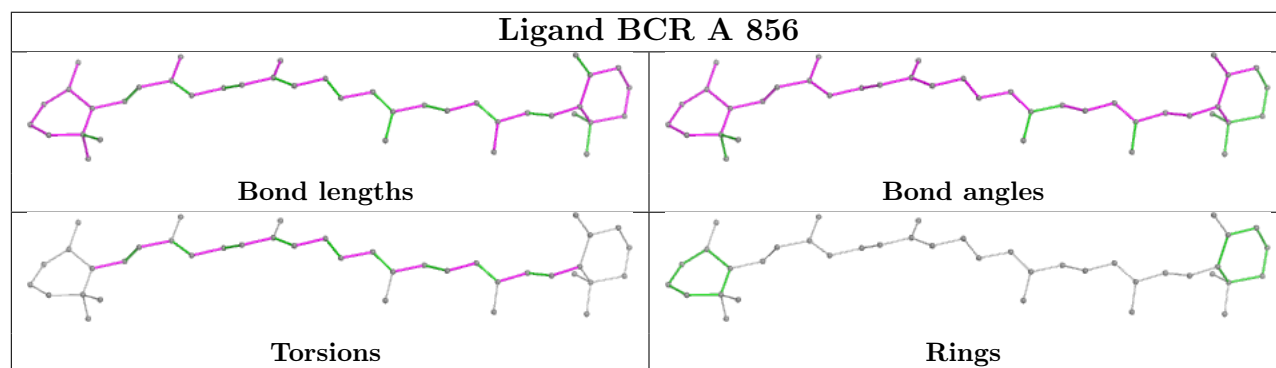
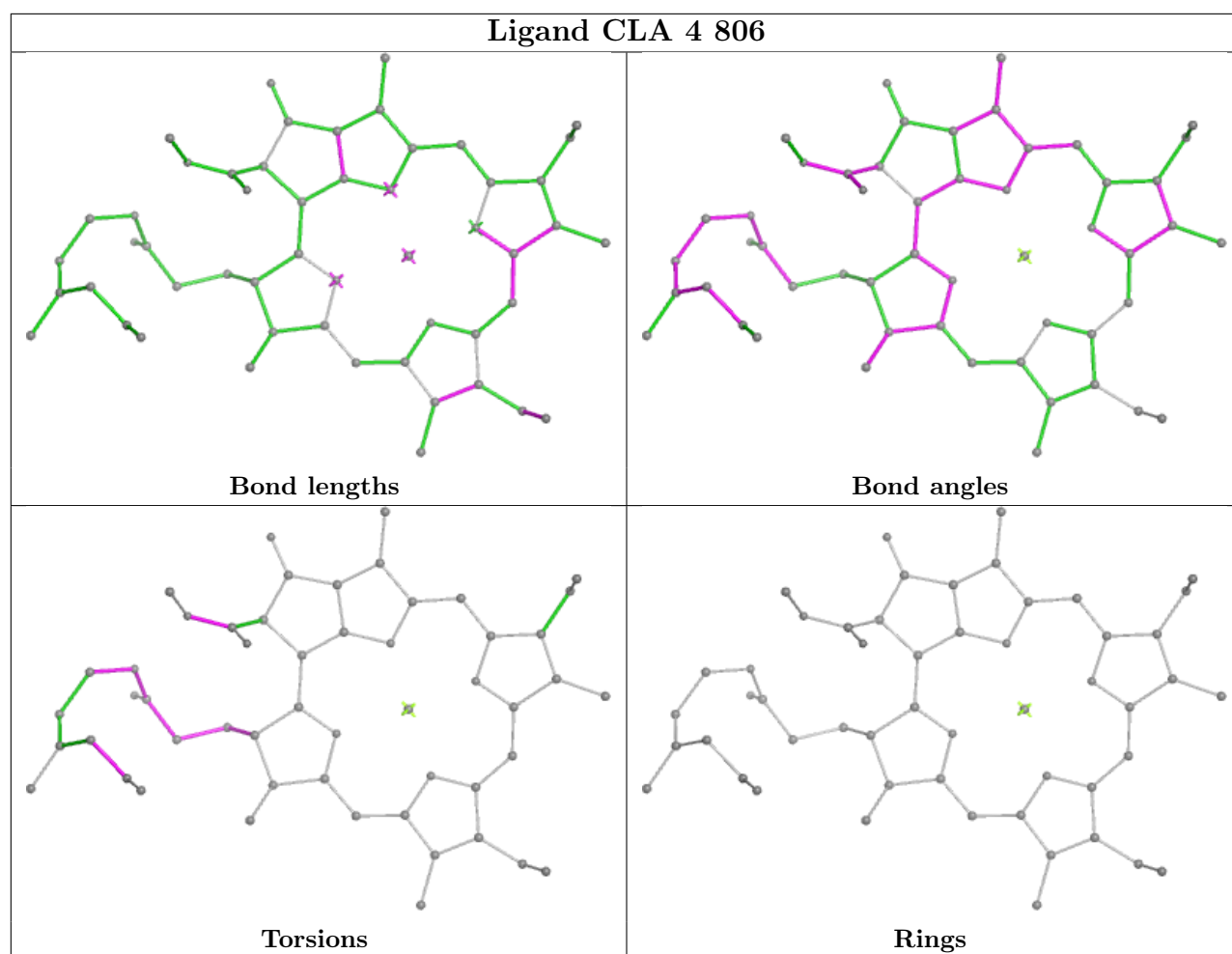
Rings

Ligand CLA B 835

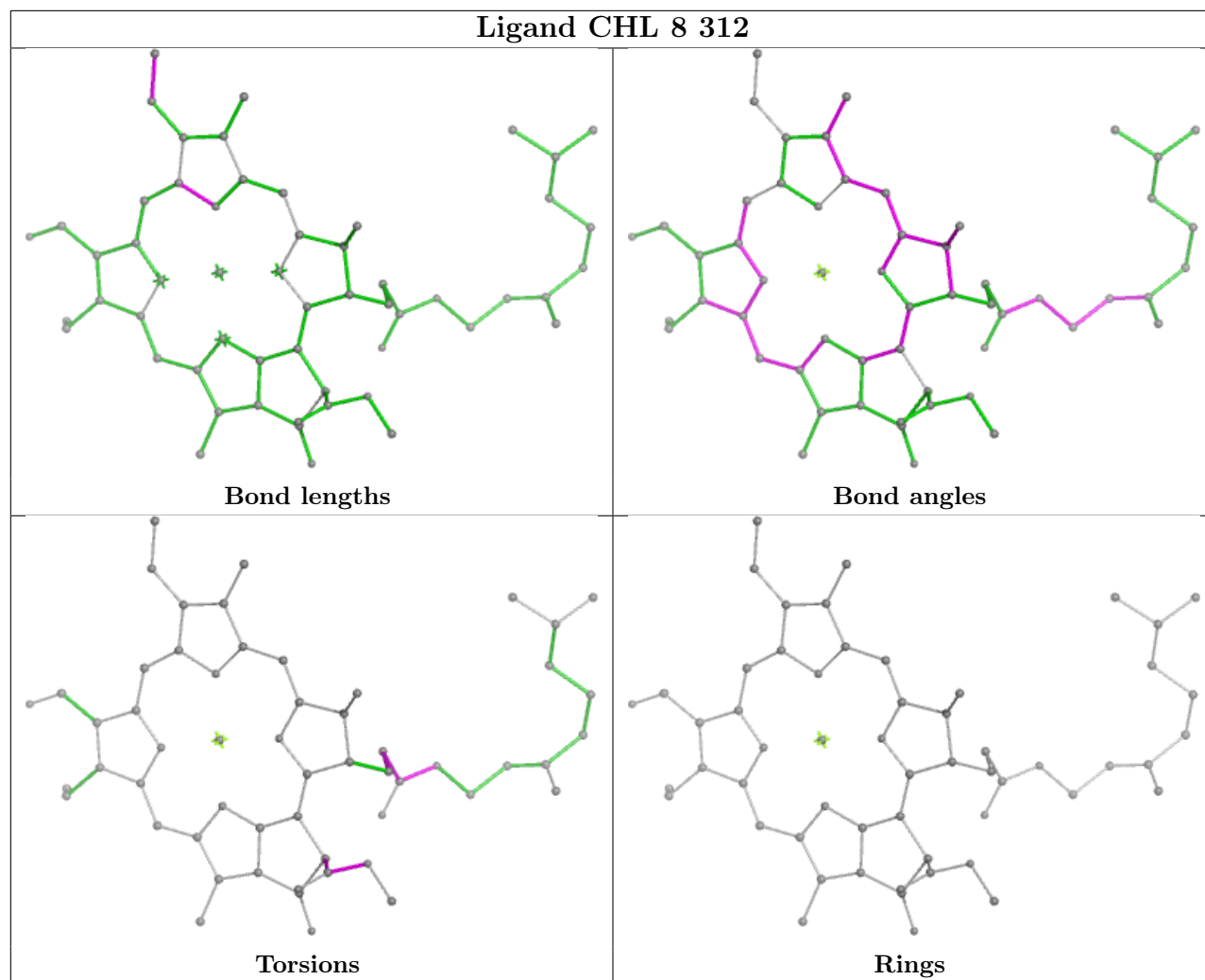


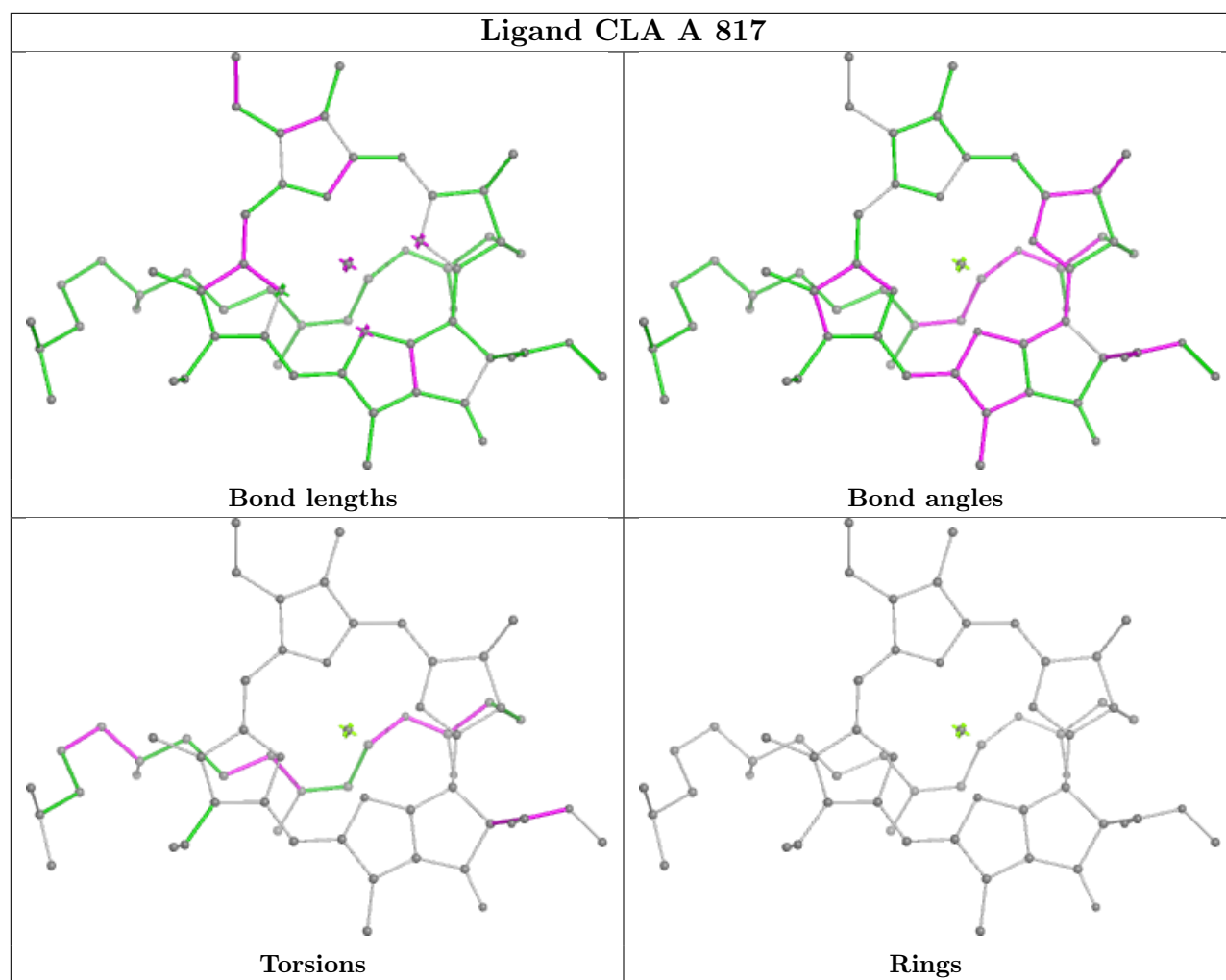
Ligand CHL 6 320



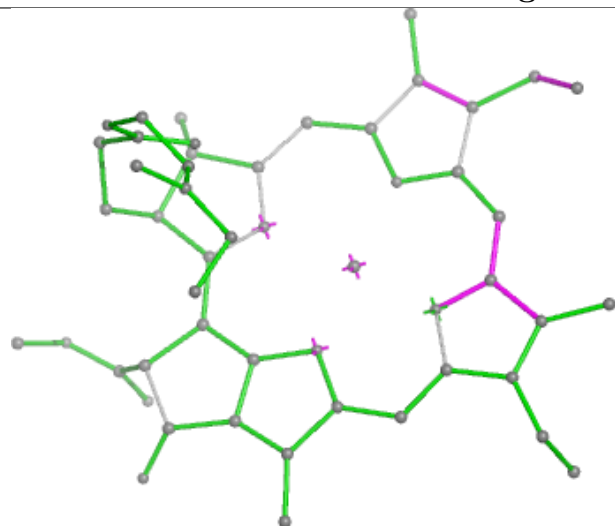


Ligand CHL 8 312

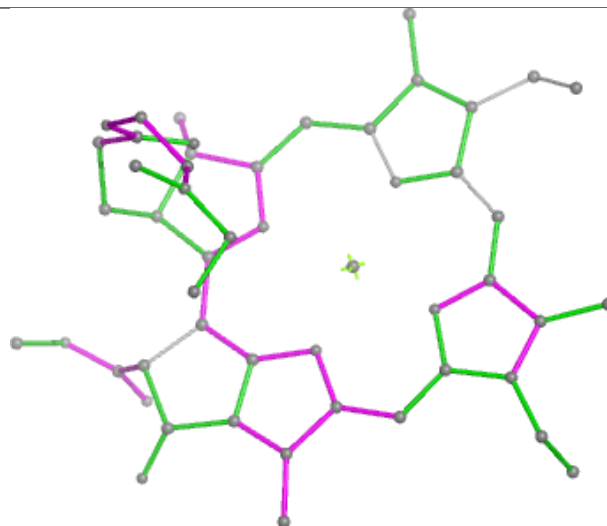




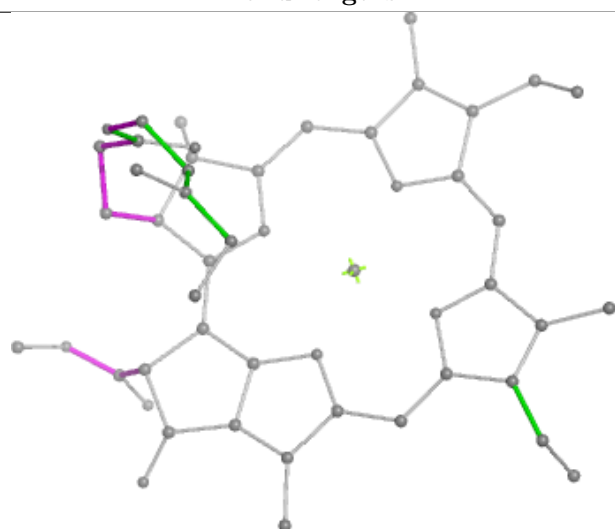
Ligand CLA Z 314



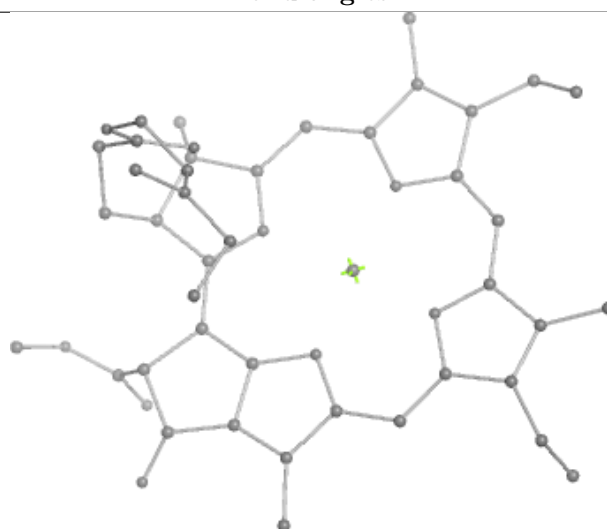
Bond lengths



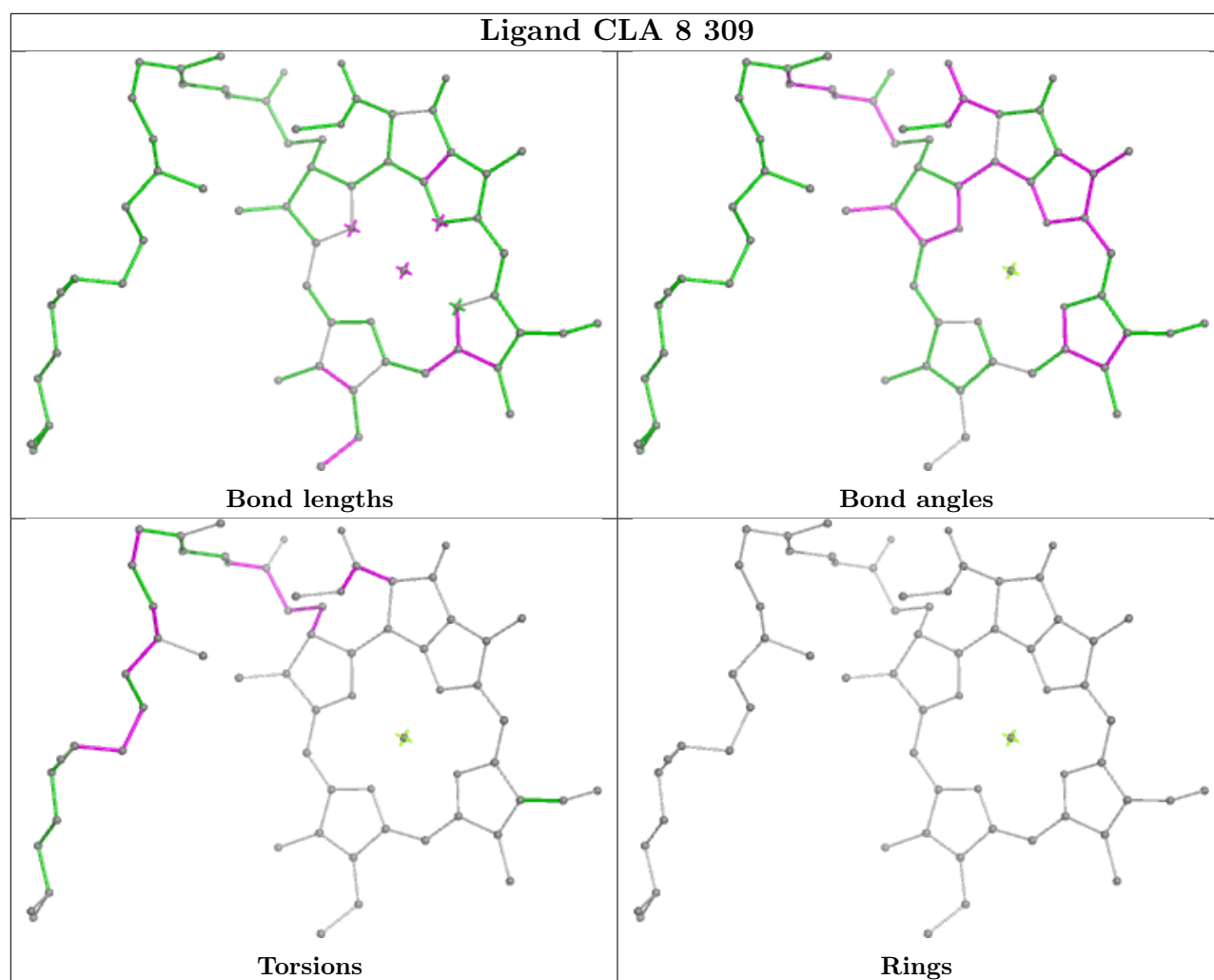
Bond angles



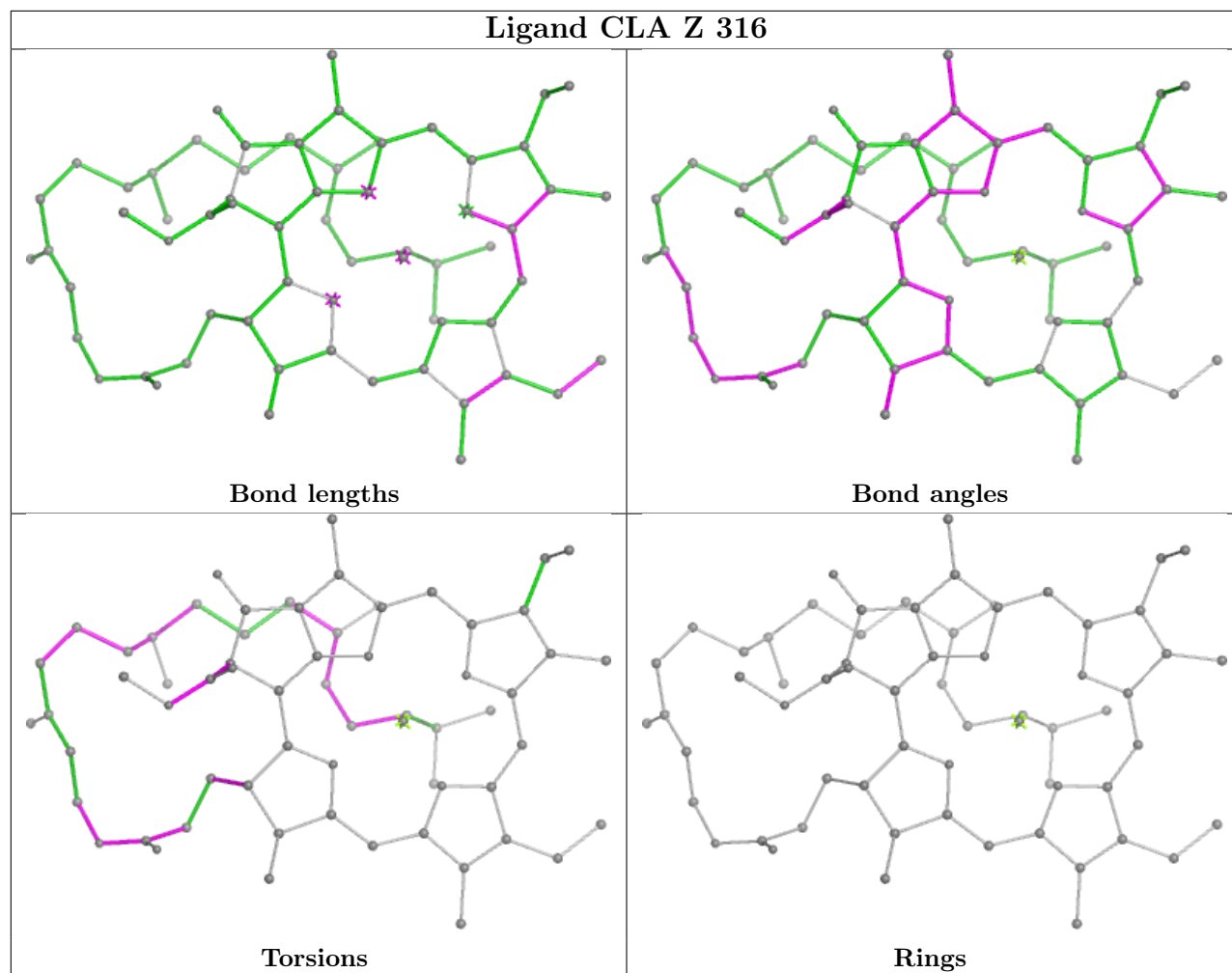
Torsions



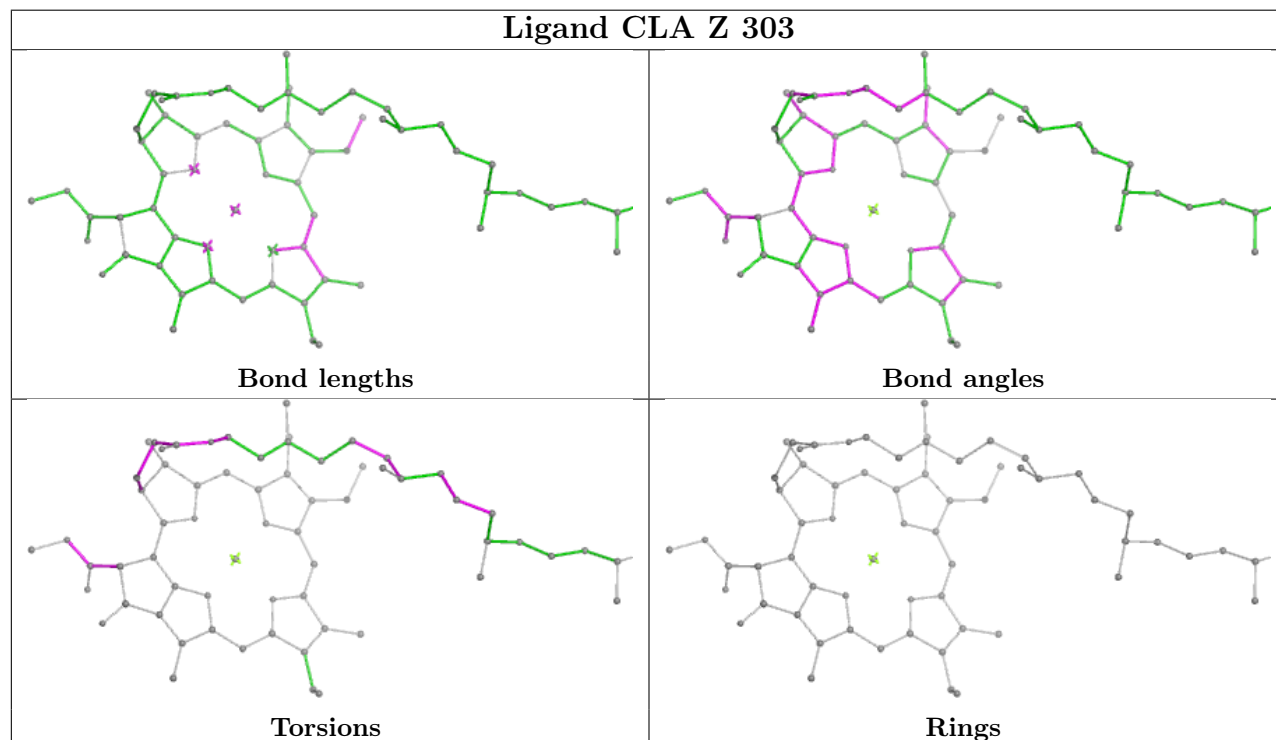
Rings

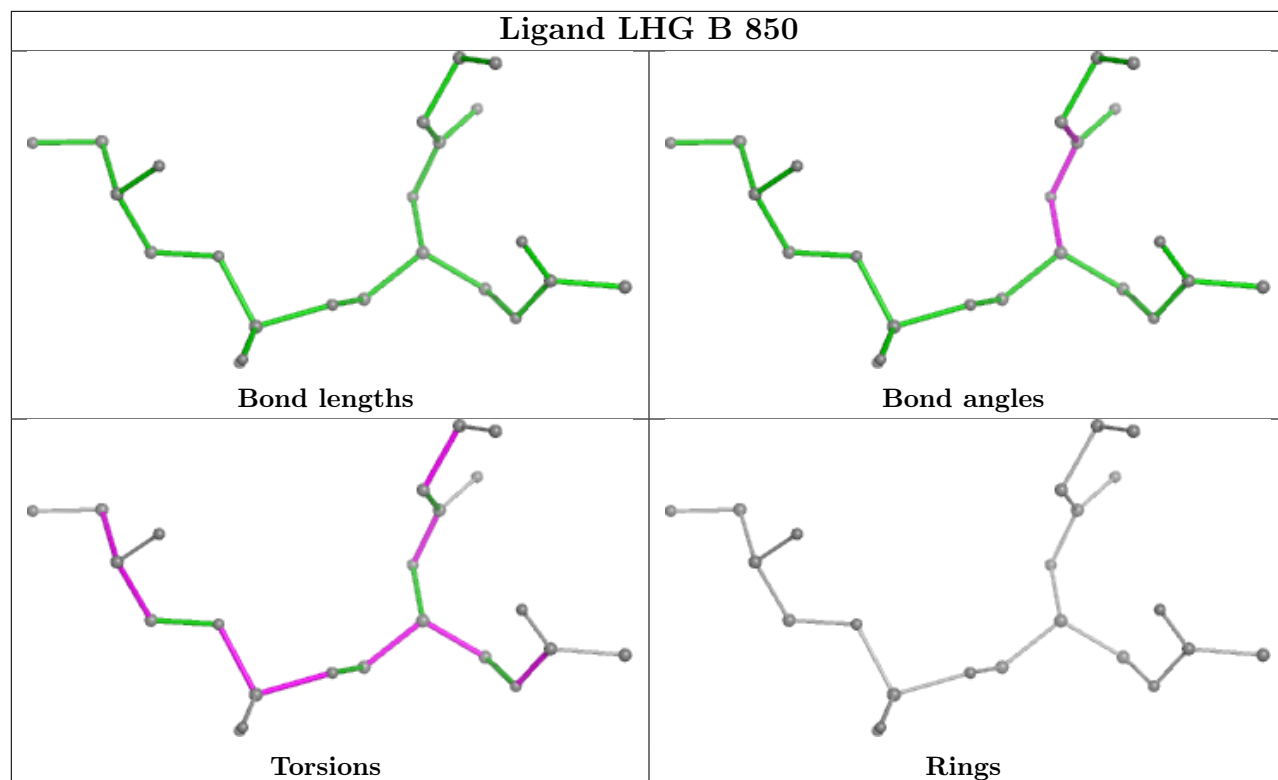


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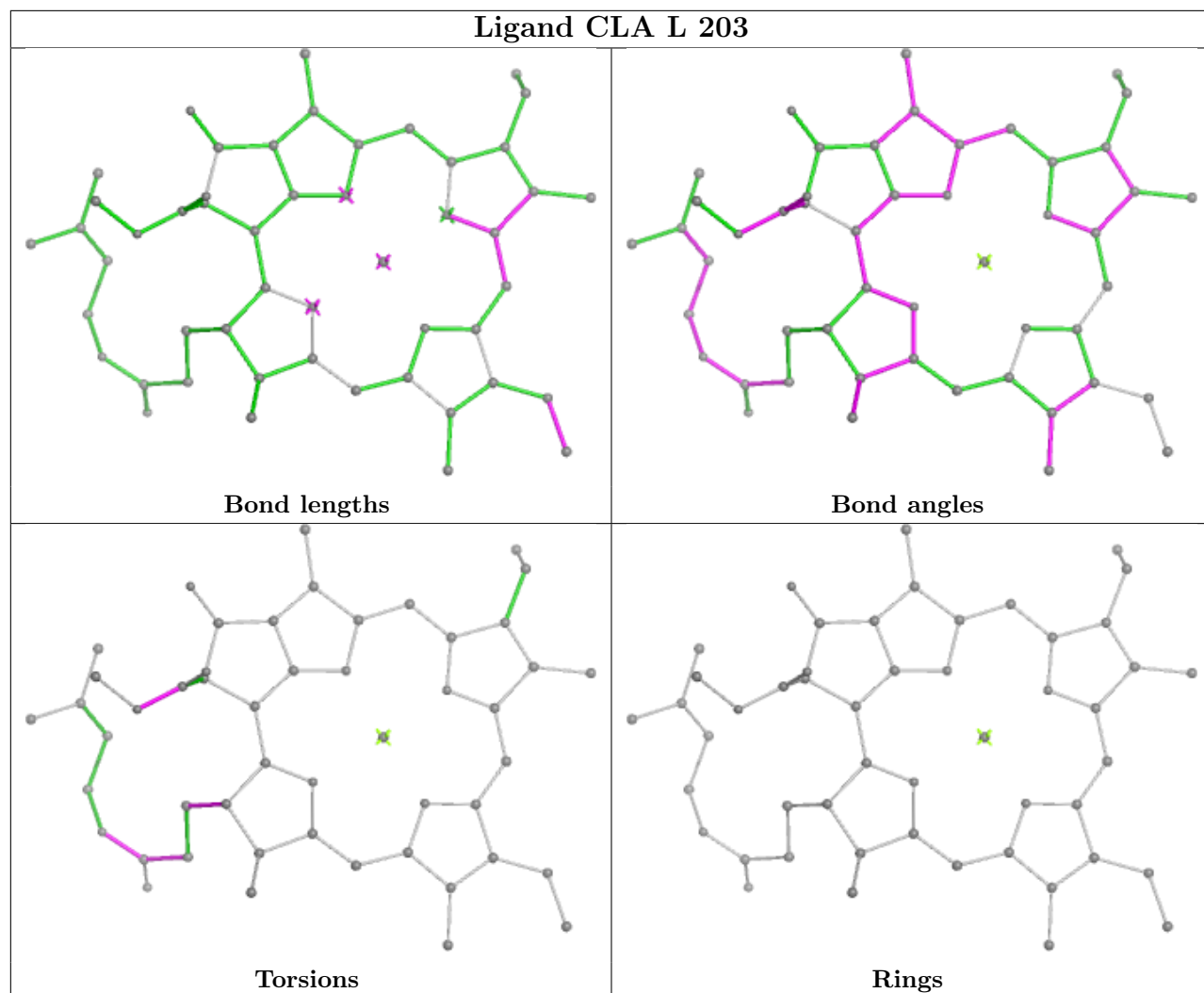


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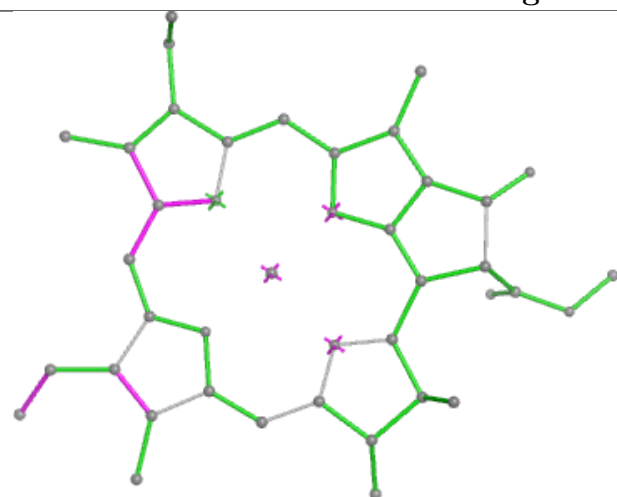




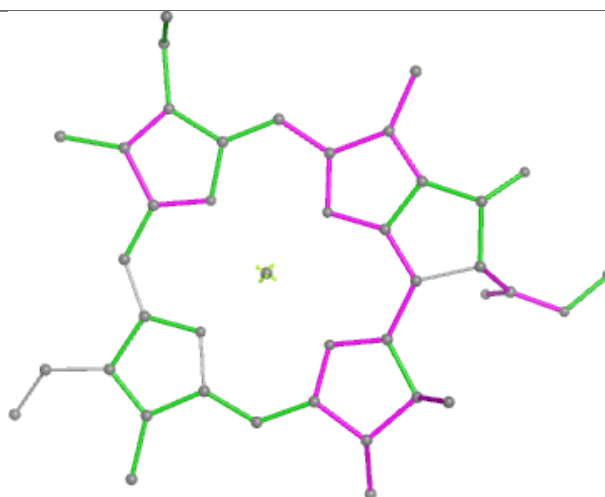
Ligand CLA L 203



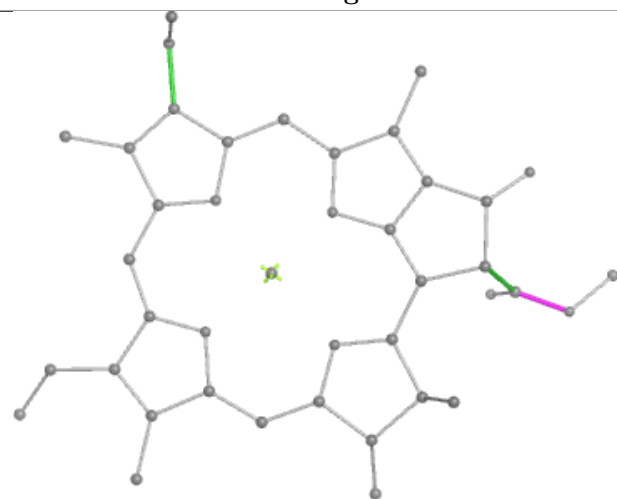
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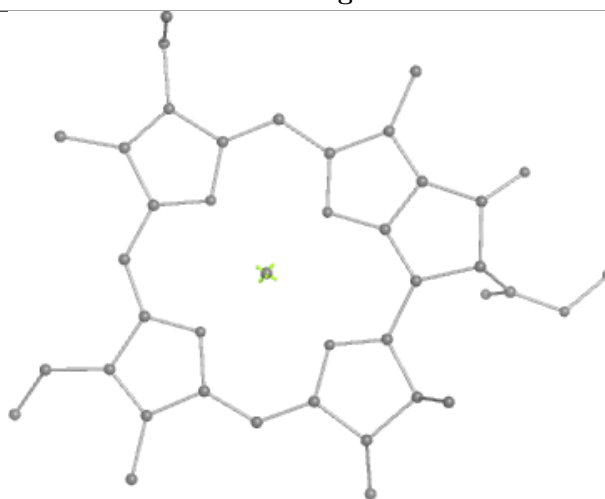
Bond lengths



Bond angles

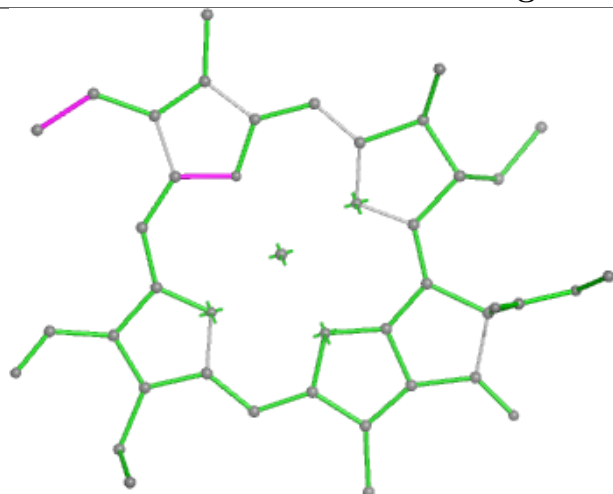


Torsions

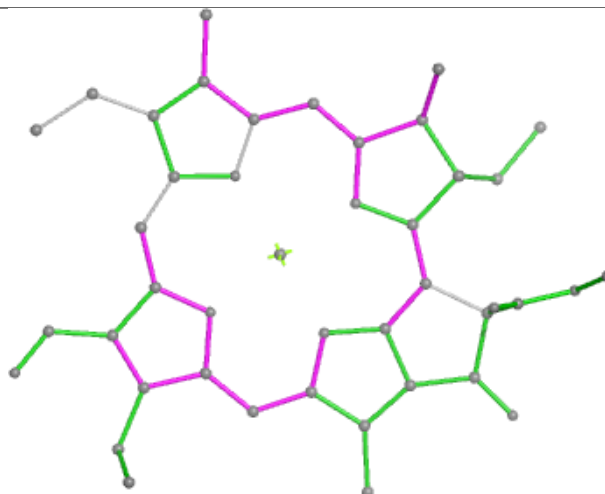


Rings

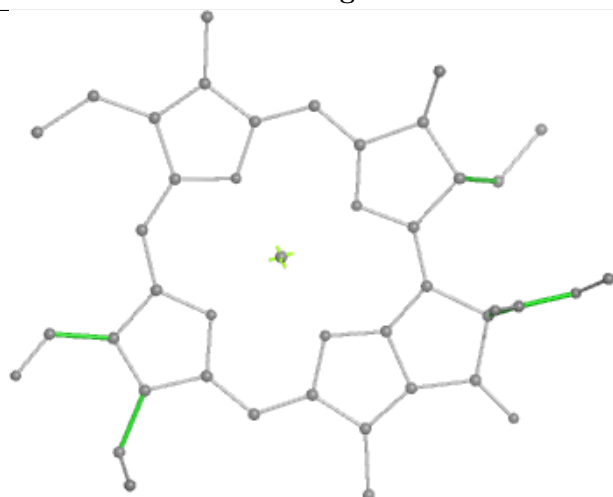
Ligand CHL 4 819



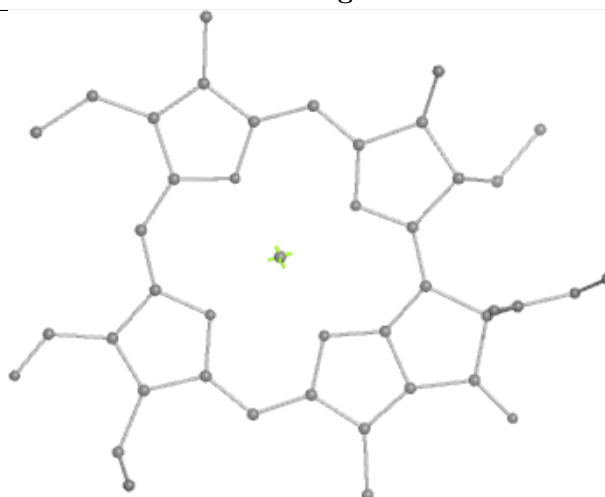
Bond lengths



Bond angles

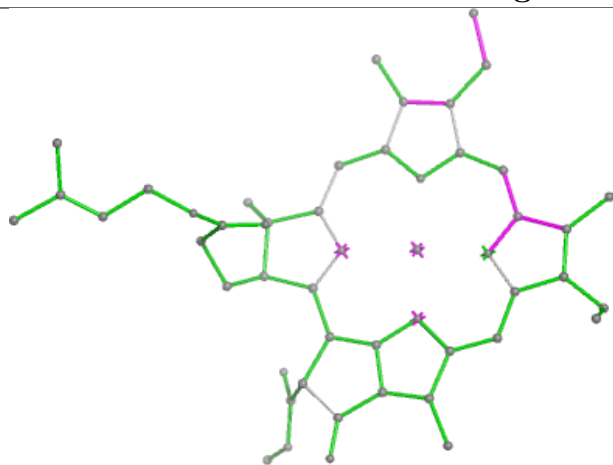


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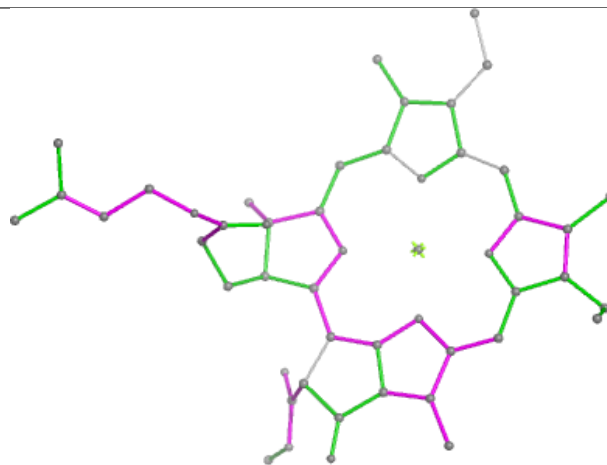


Rings

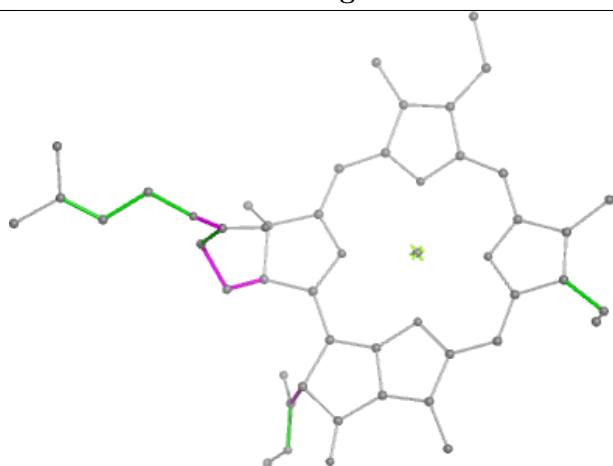
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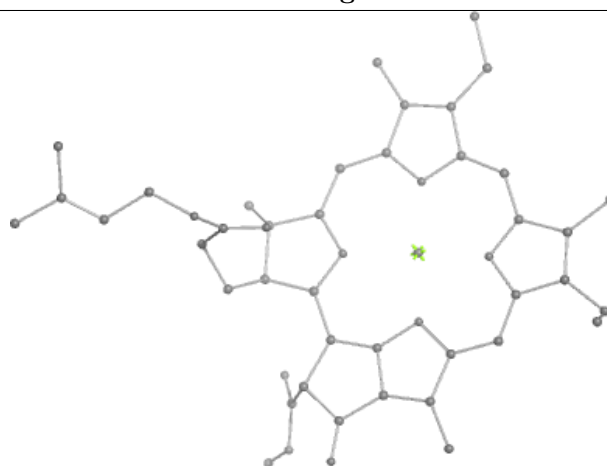
Bond lengths



Bond angles

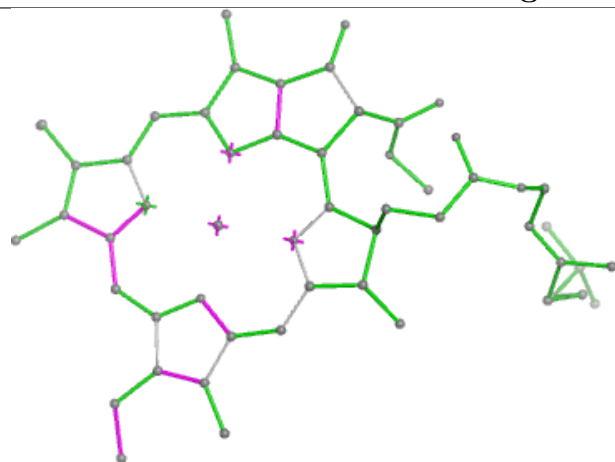


Torsions

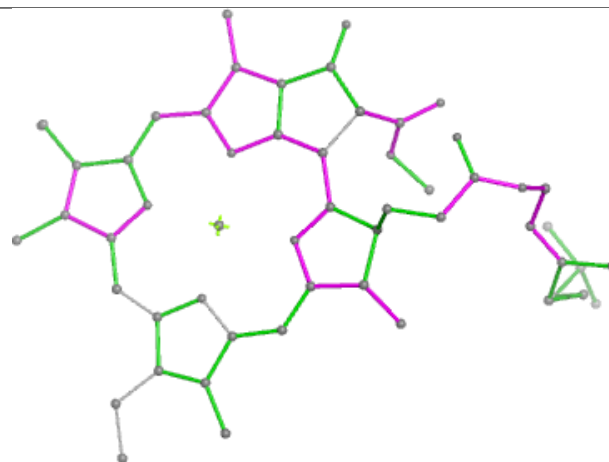


Rings

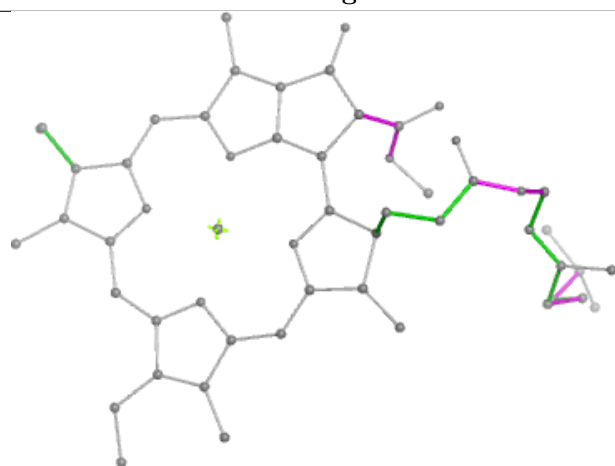
Ligand CLA 9 307



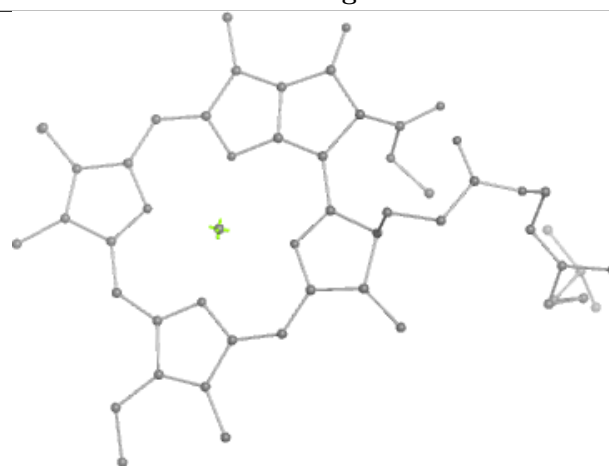
Bond lengths



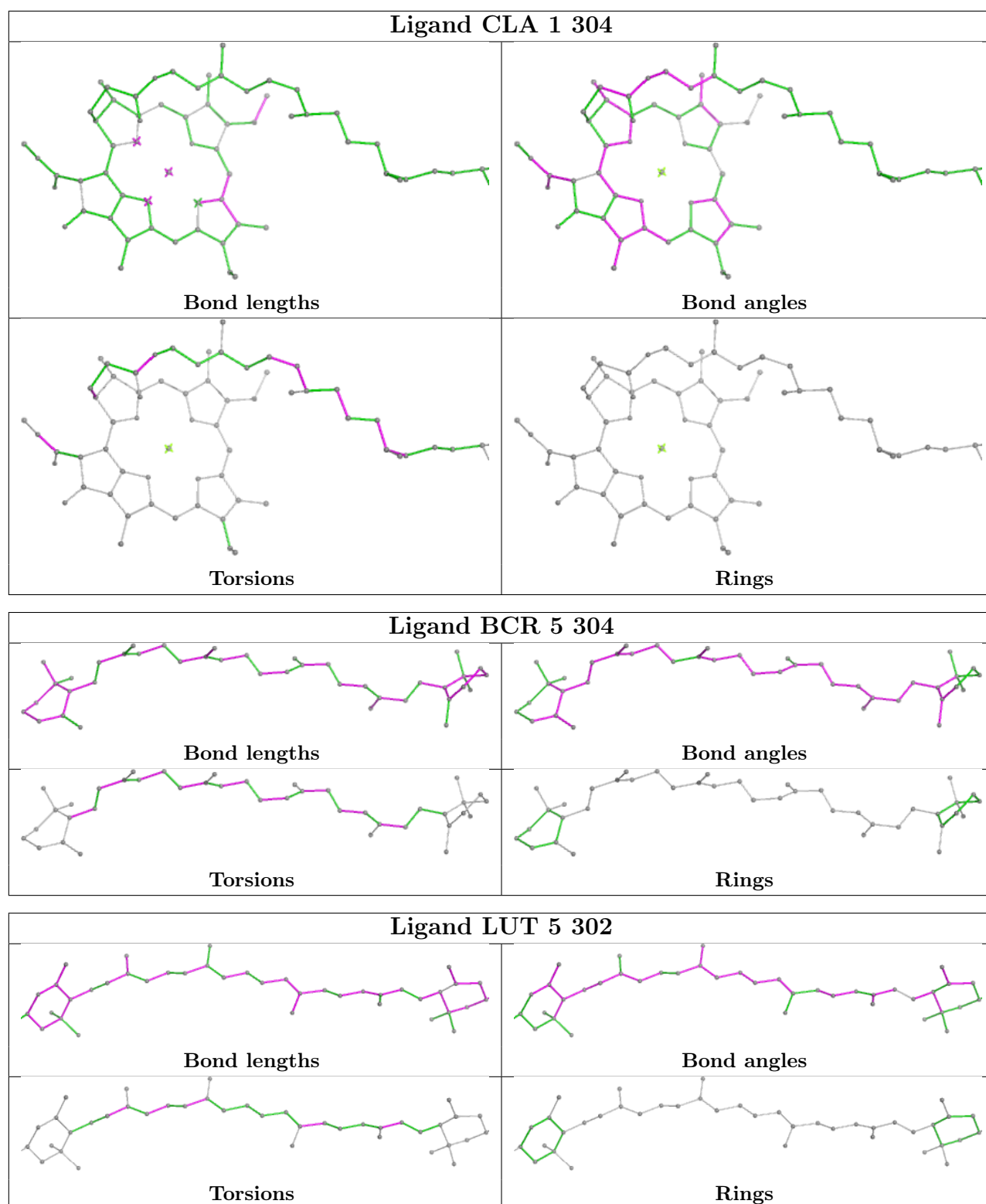
Bond angles



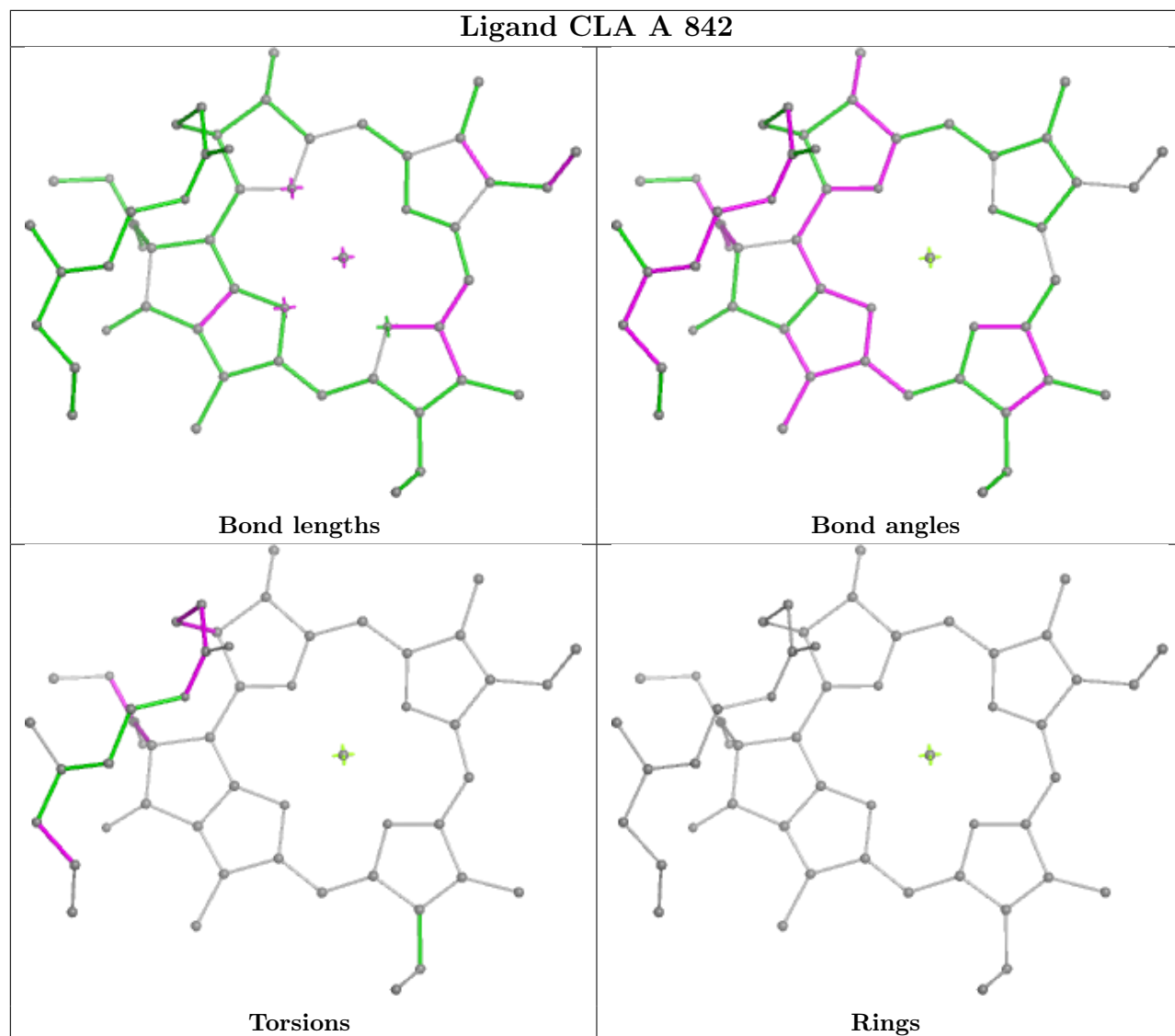
Torsions

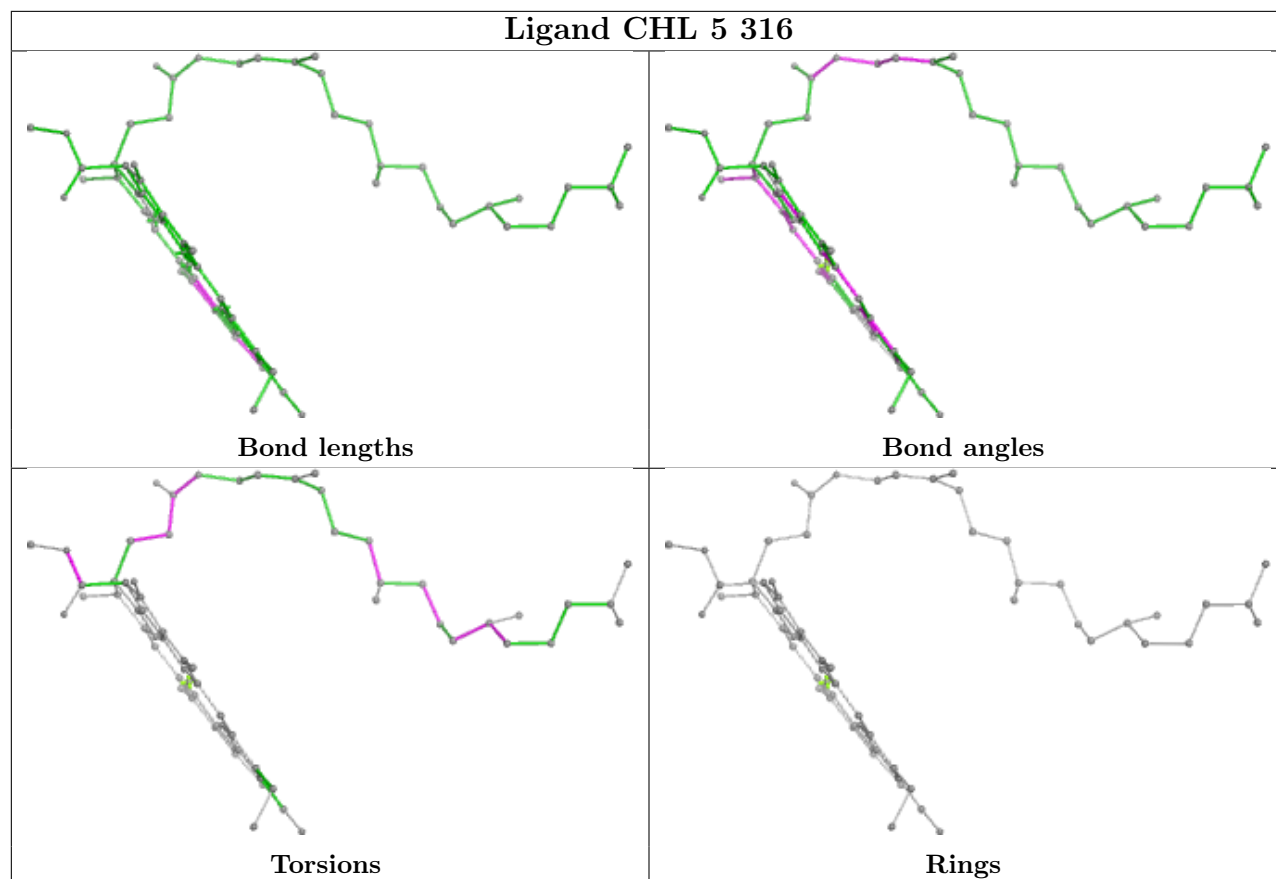


Rings

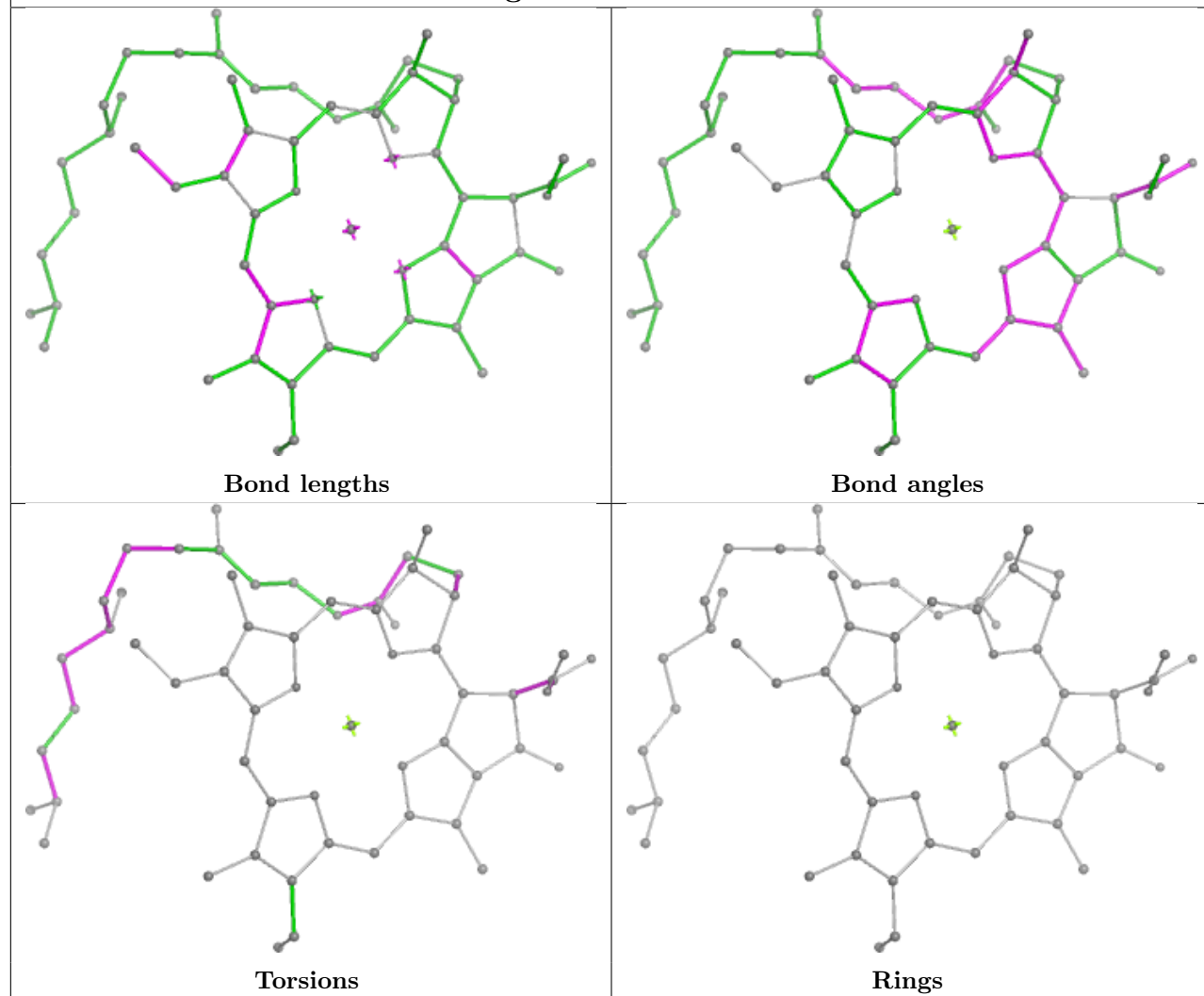


Ligand CLA A 842

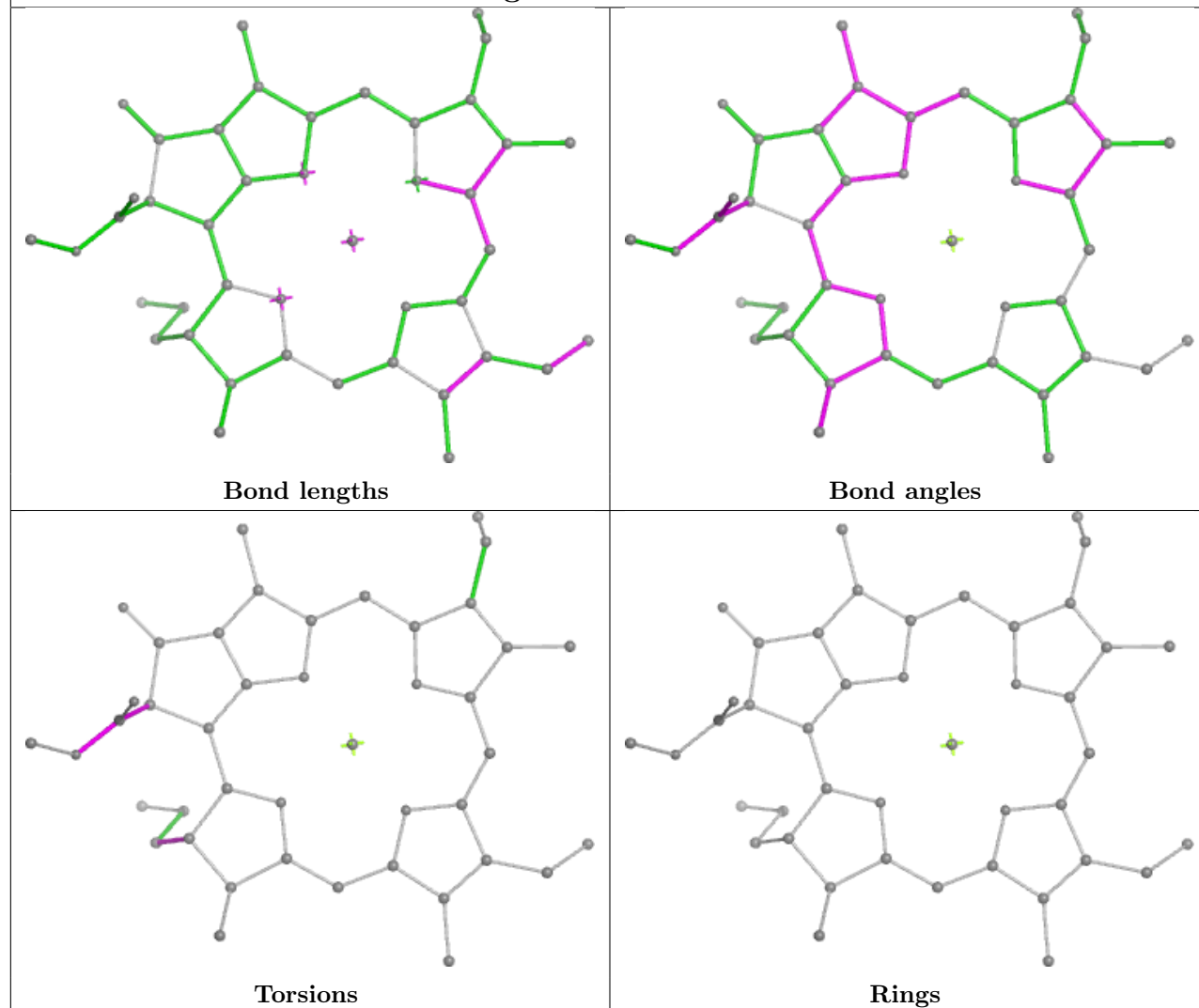




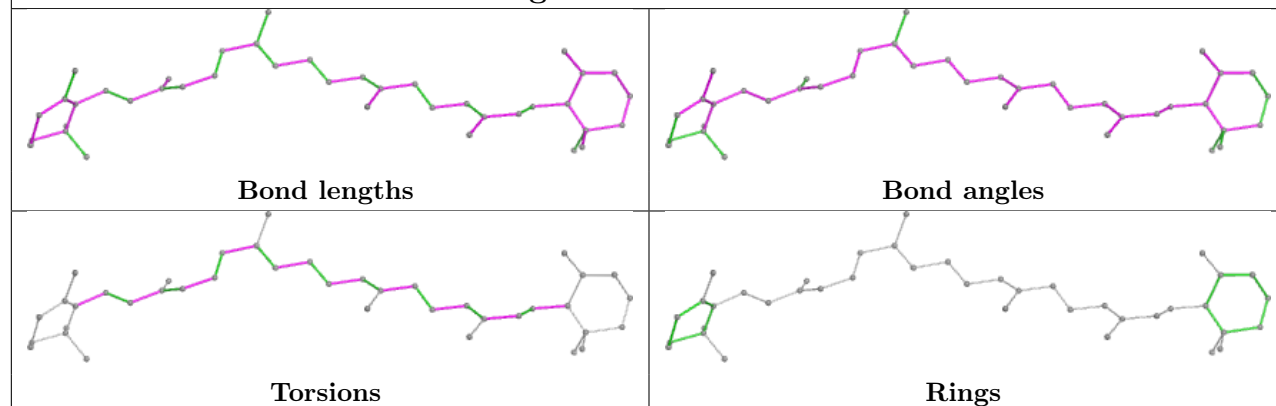
Ligand CLA 1 307

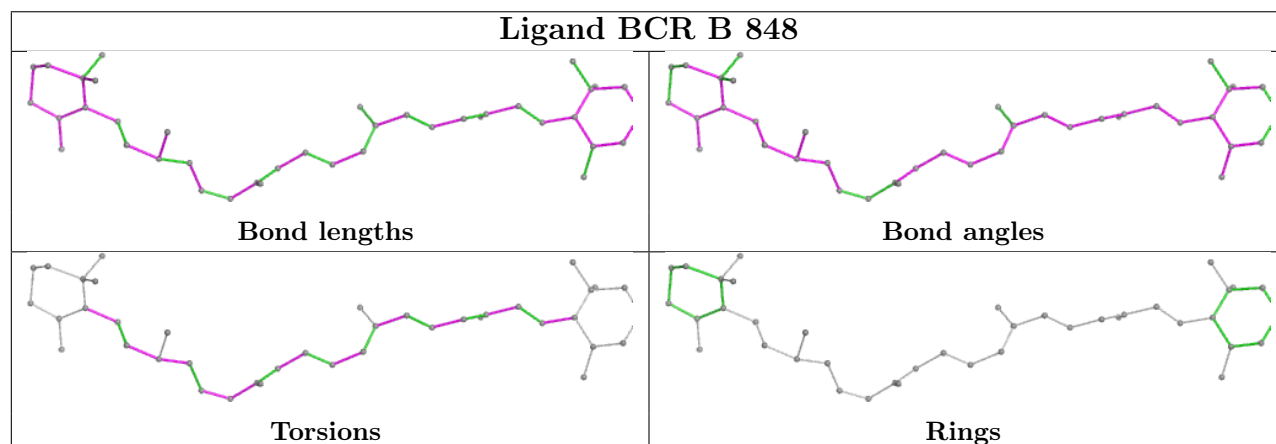
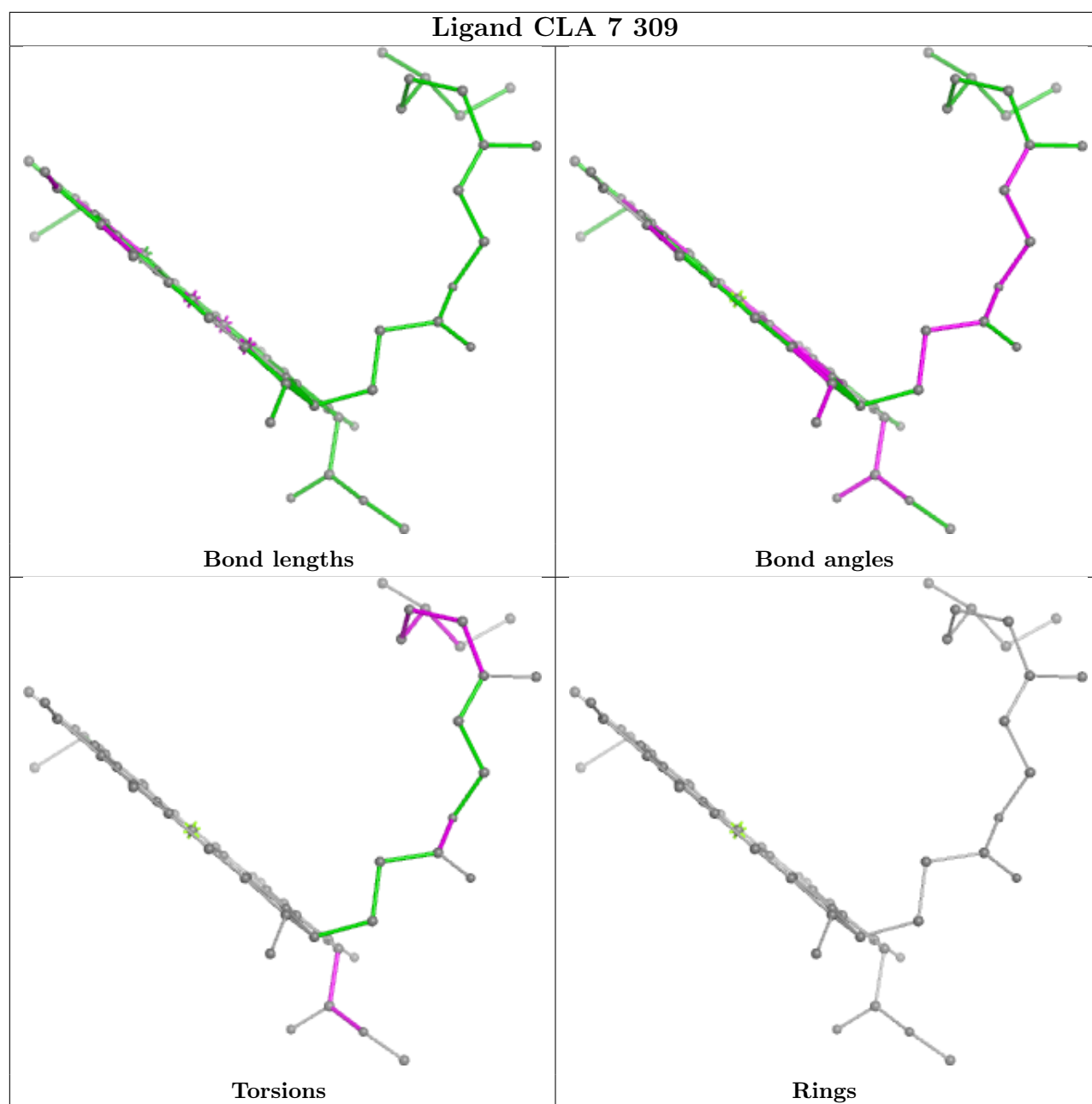


Ligand CLA 7 311

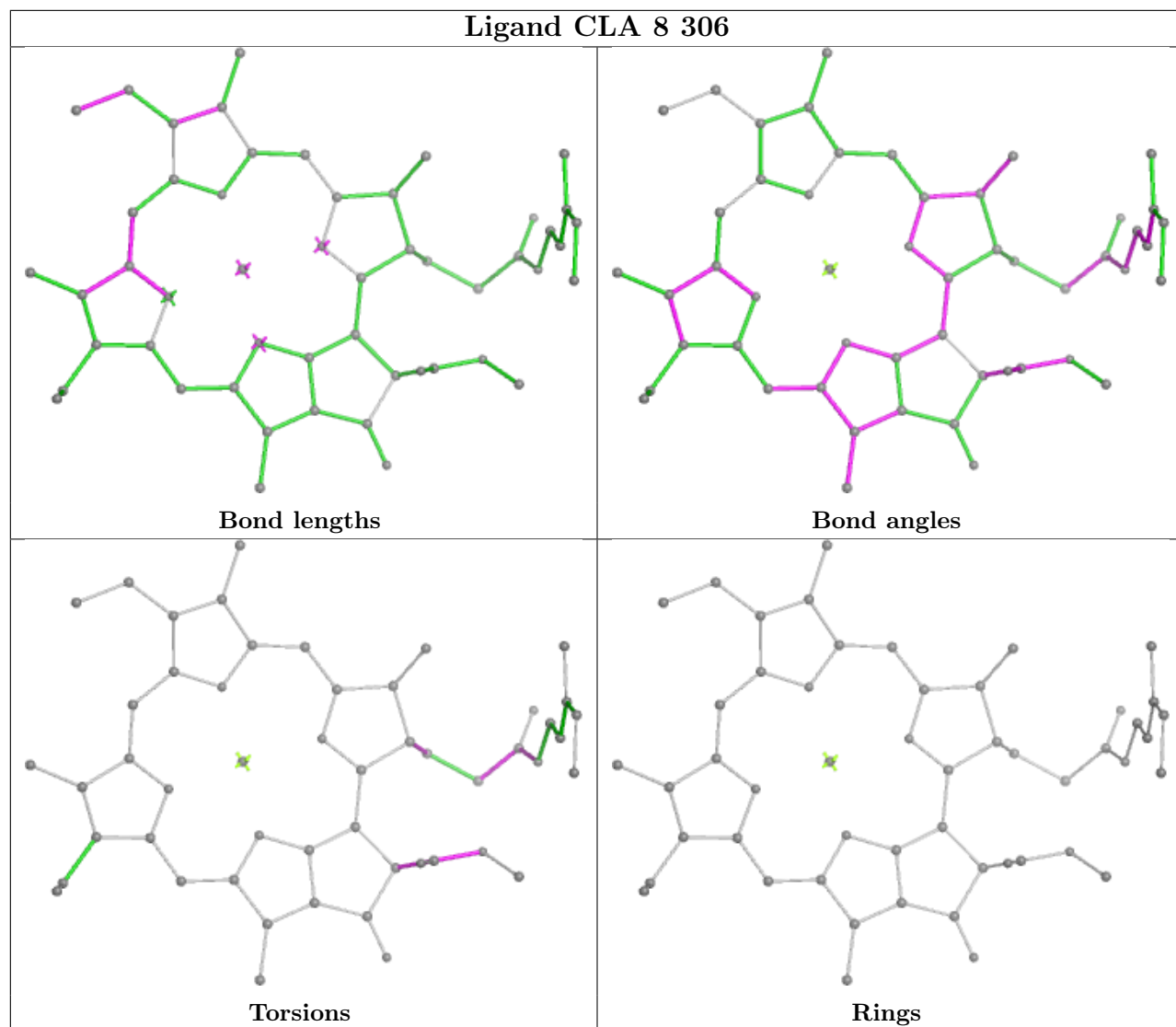


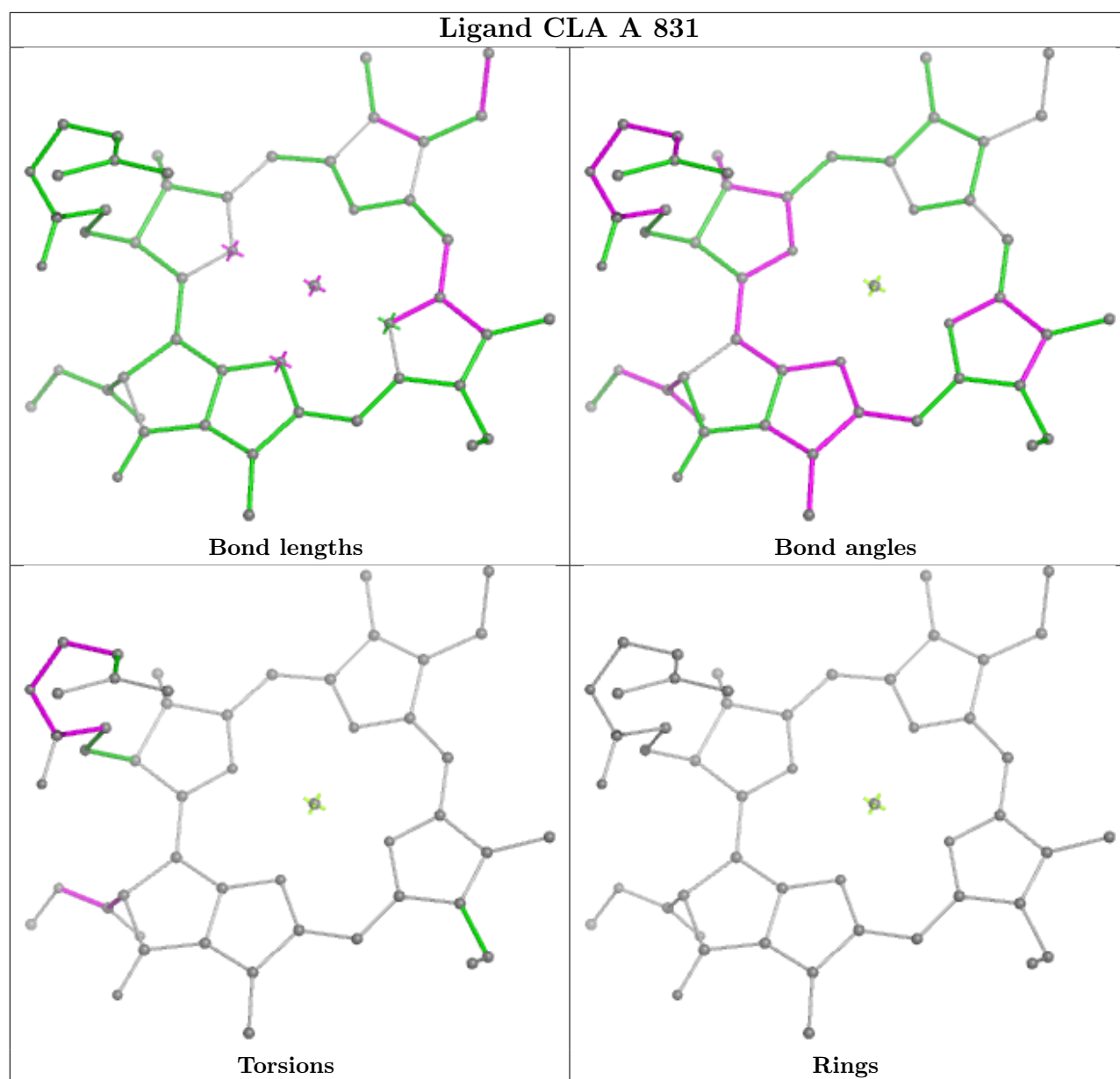
Ligand BCR G 203

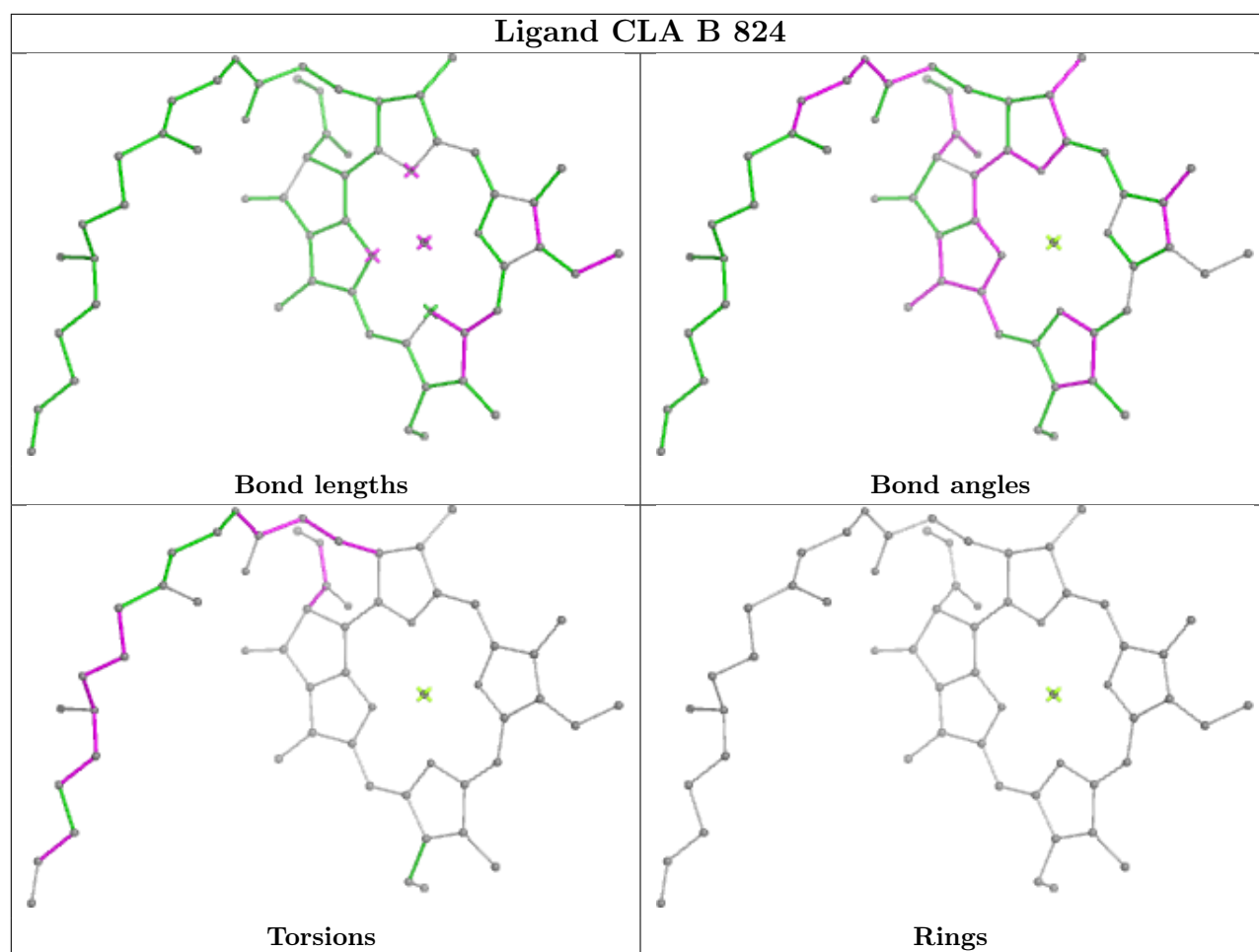




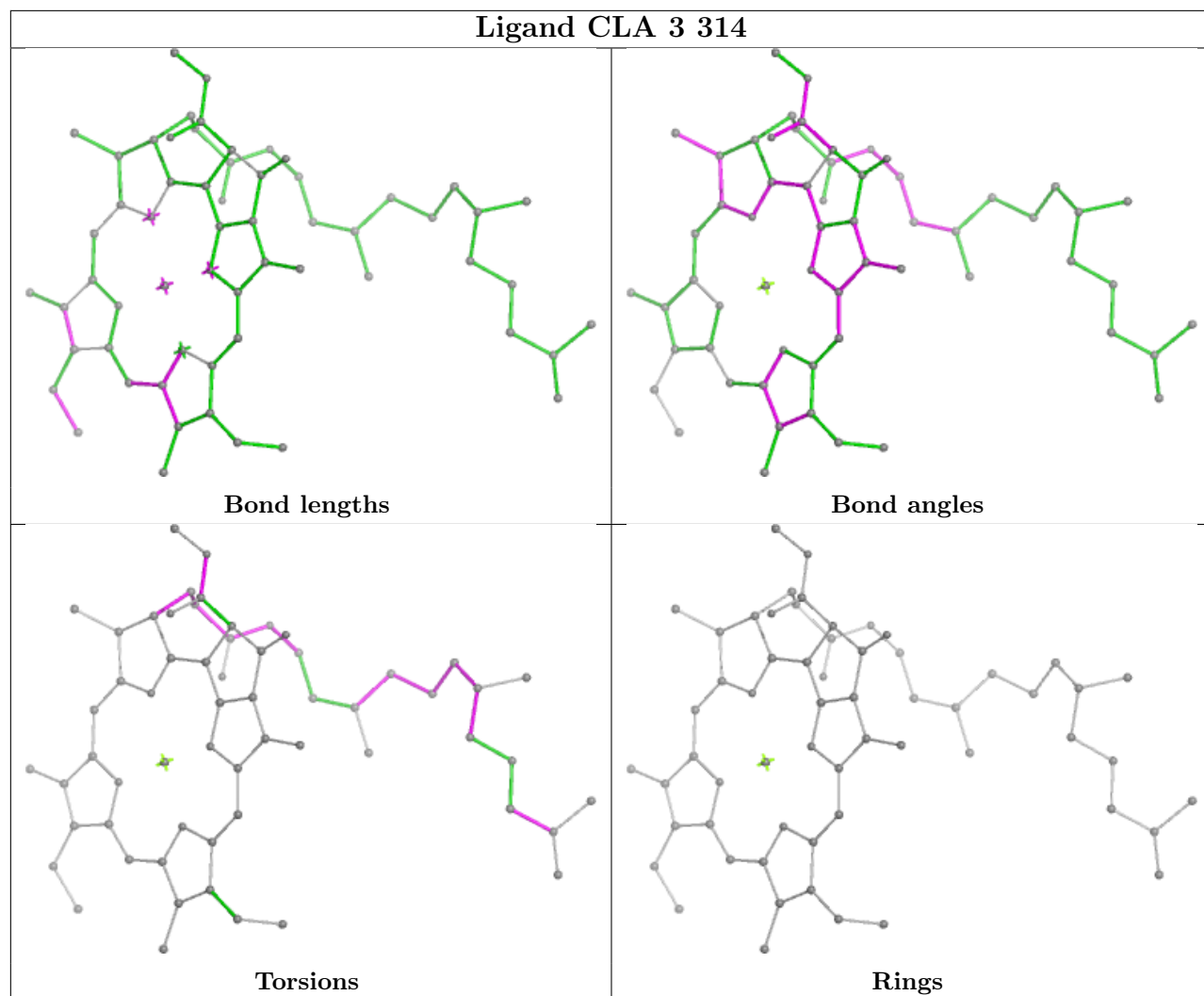
Ligand CLA 8 306

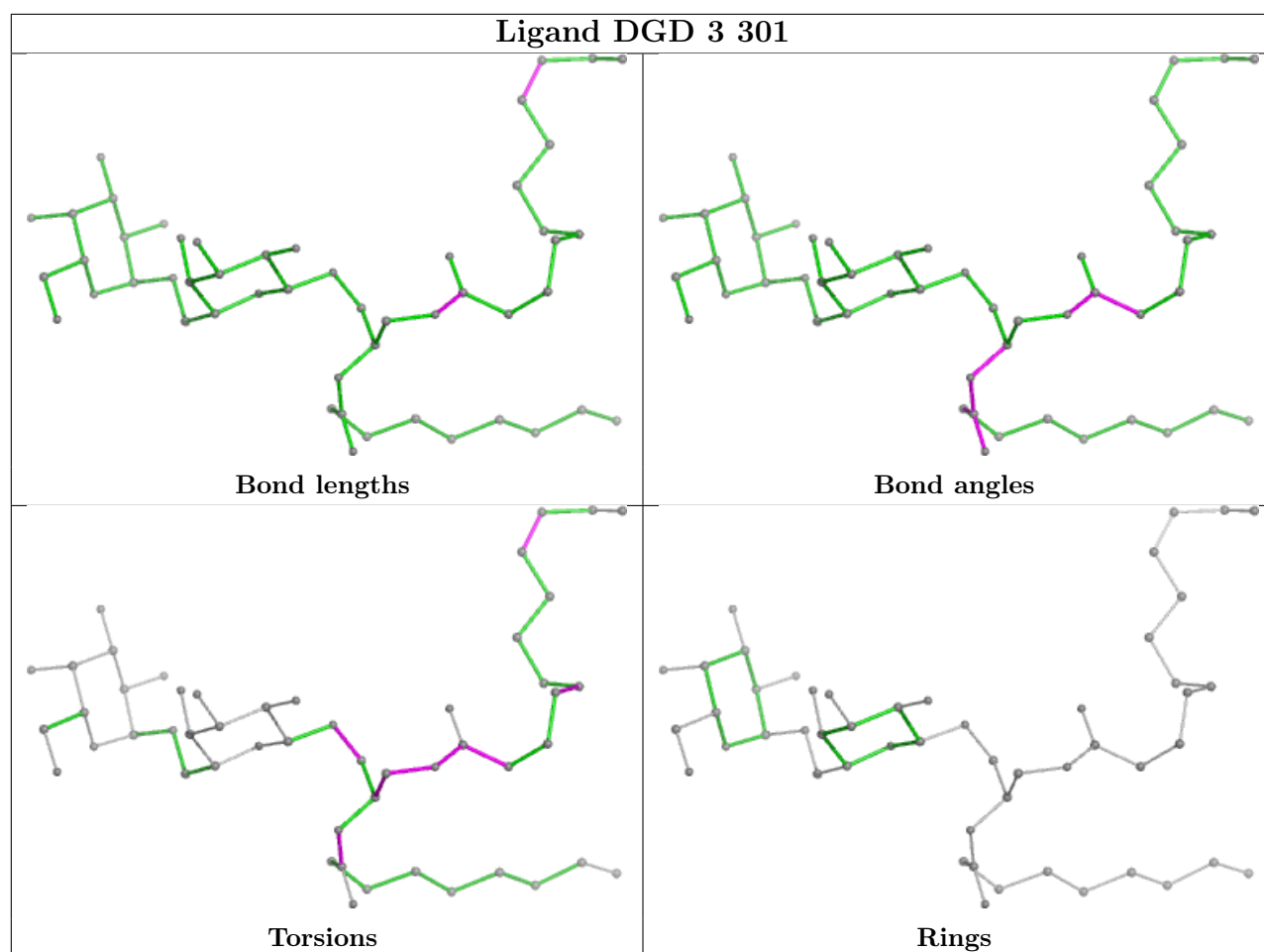




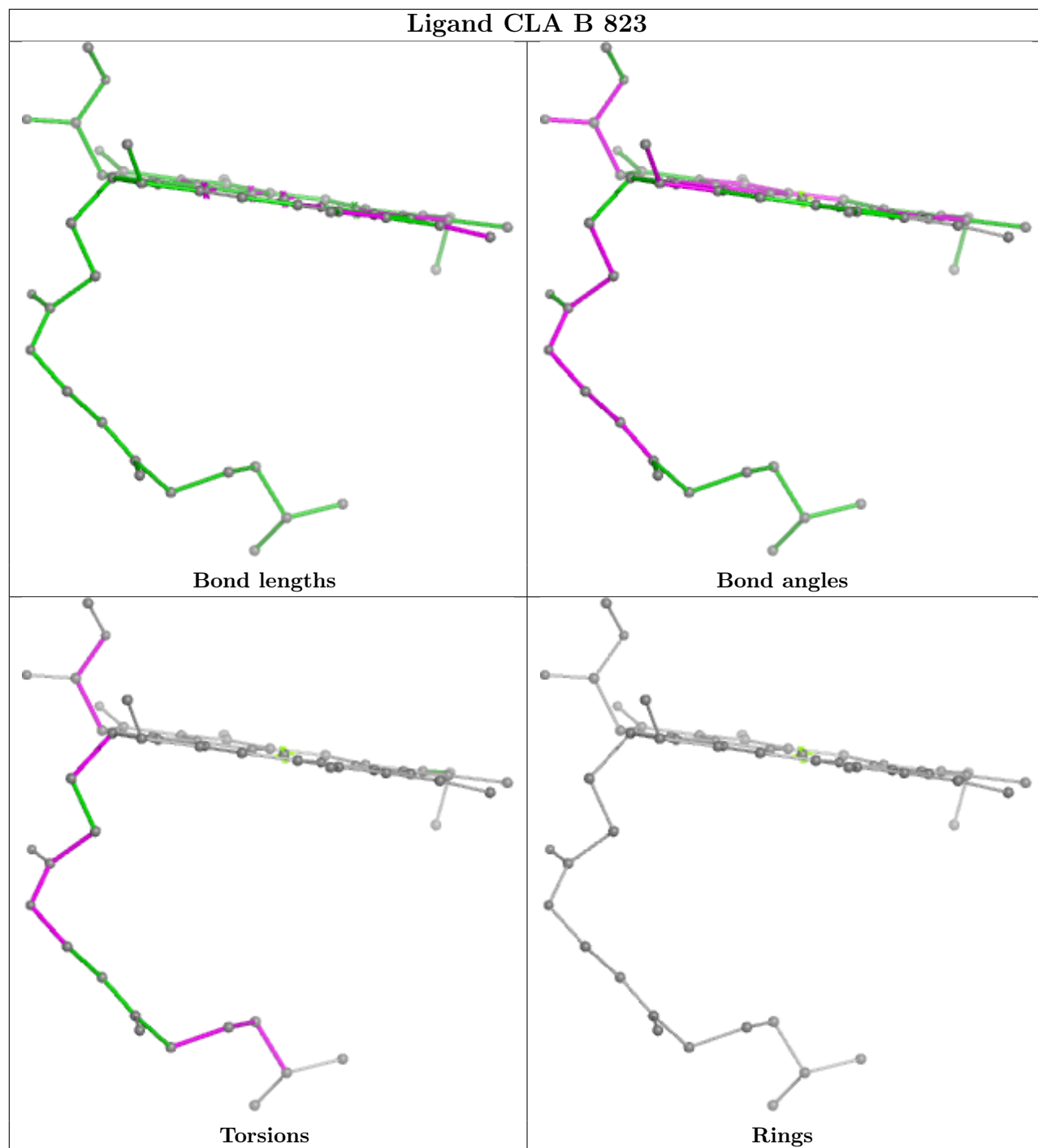


Ligand CLA 3 314

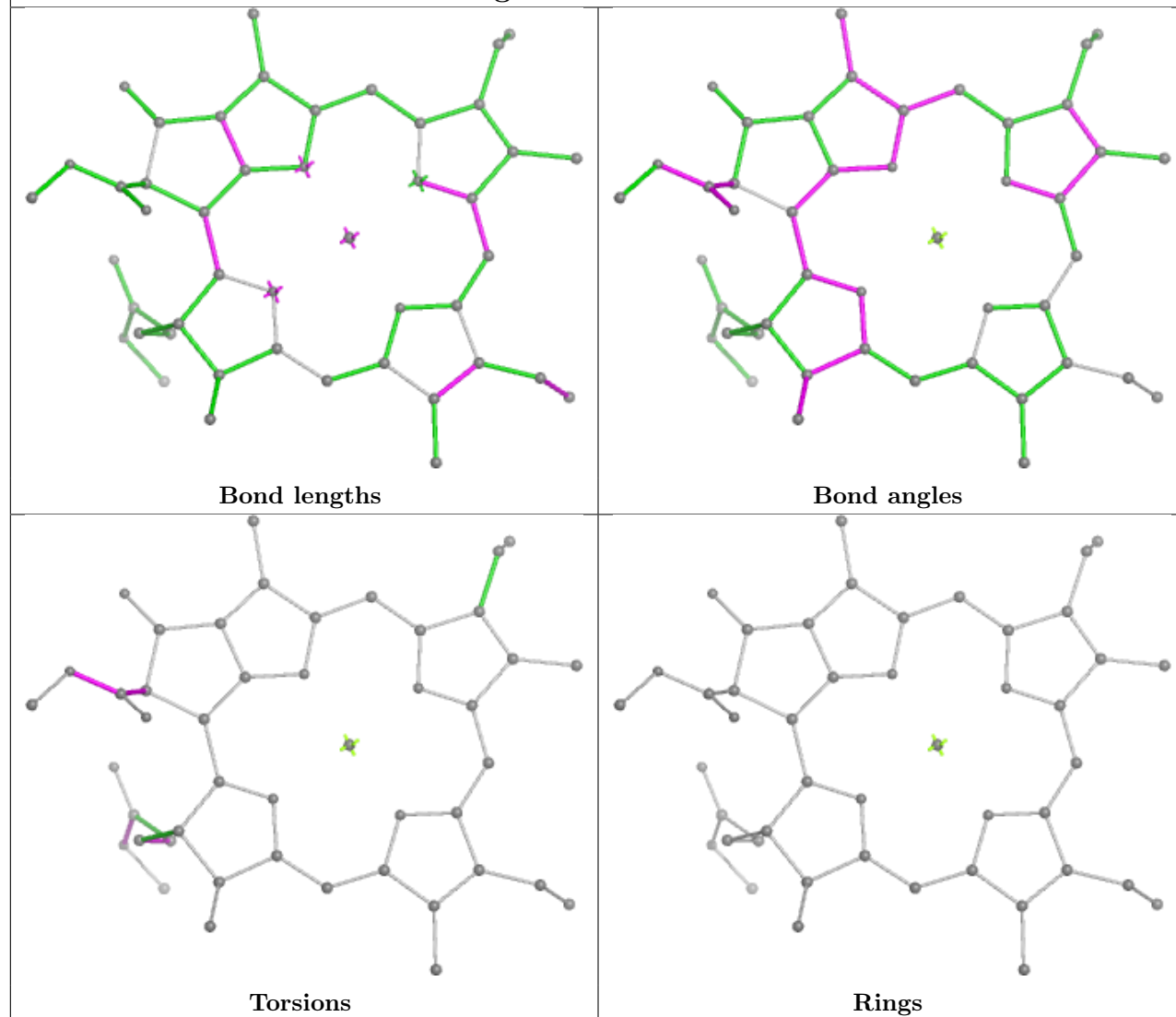




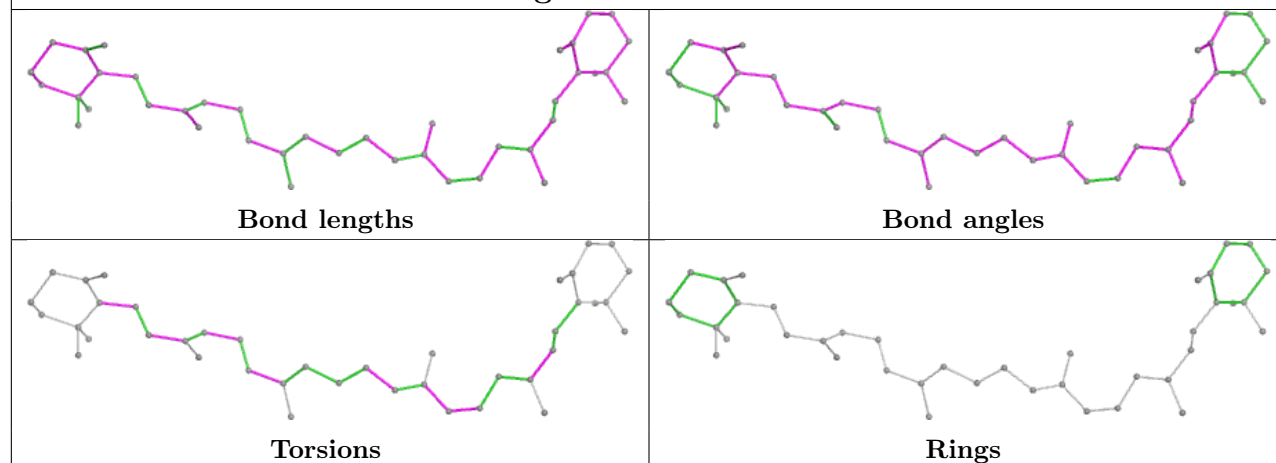
Ligand CLA B 823

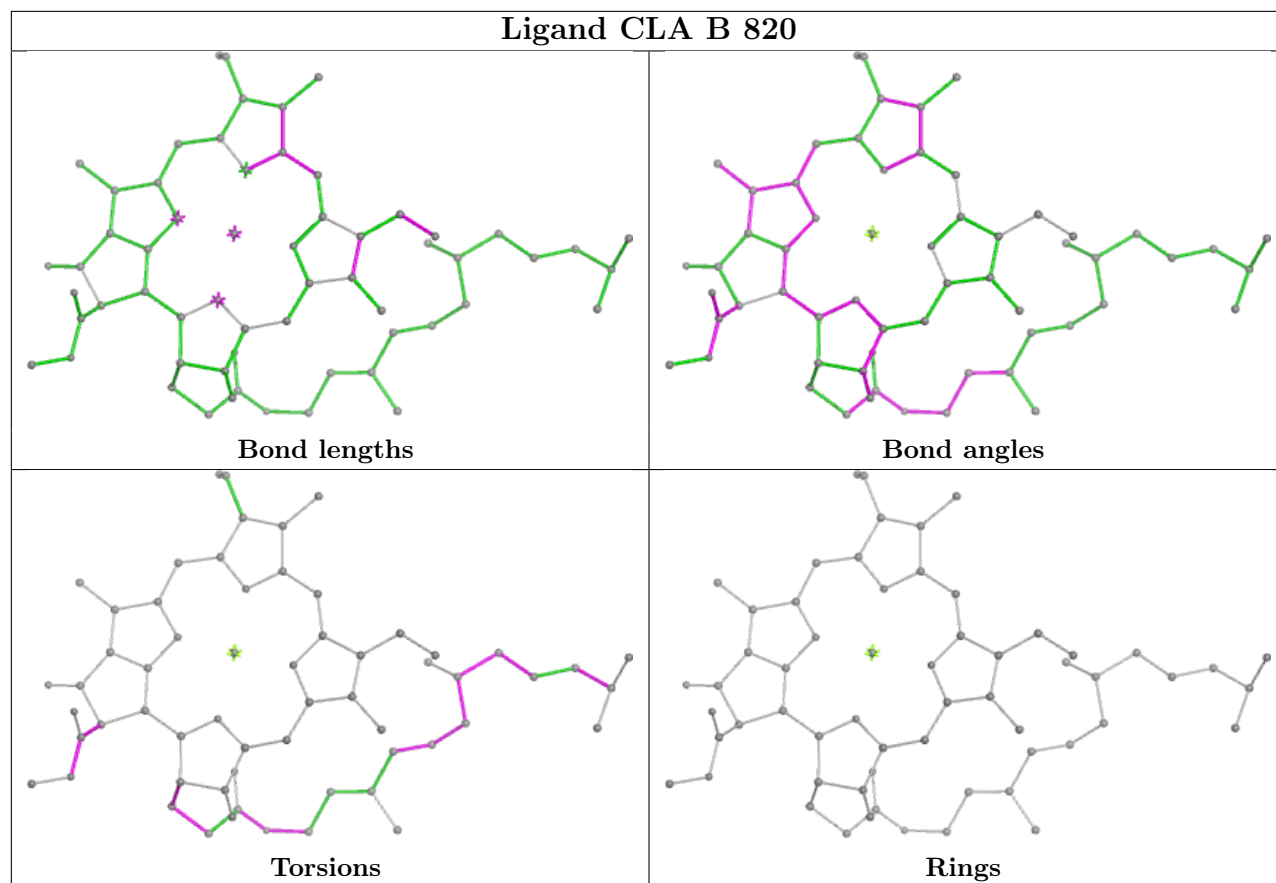


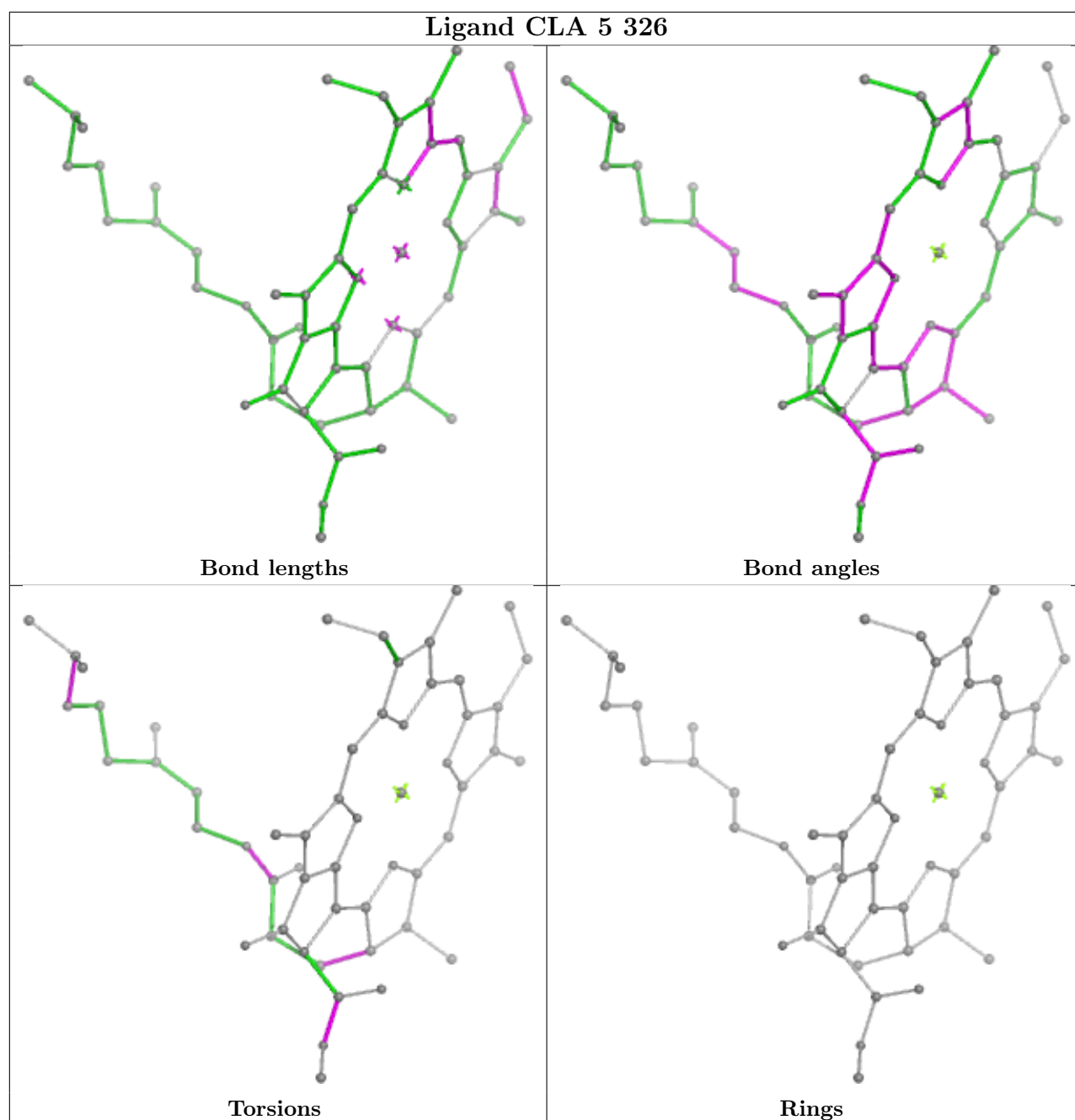
Ligand CLA 1 311



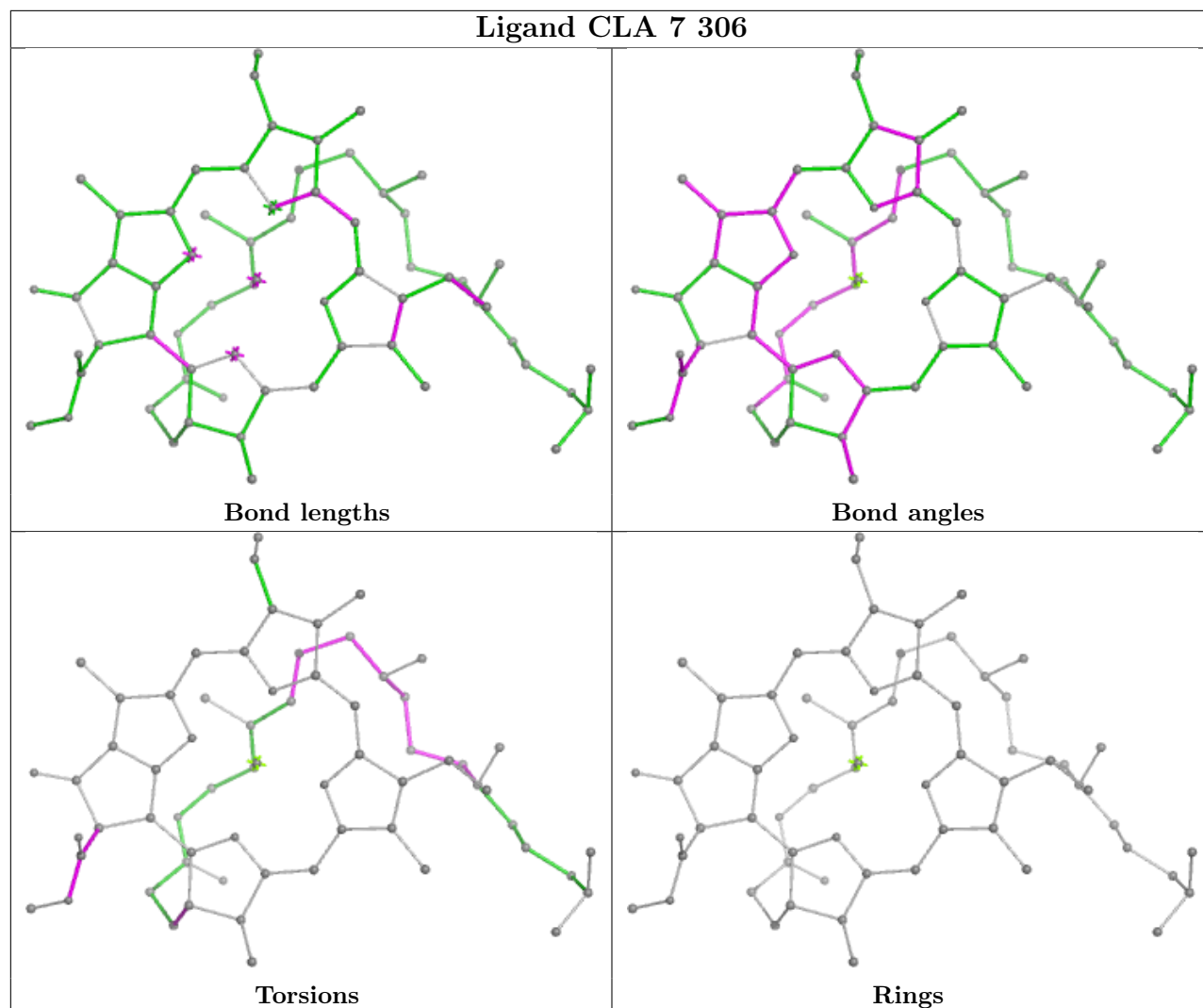
Ligand BCR 5 305



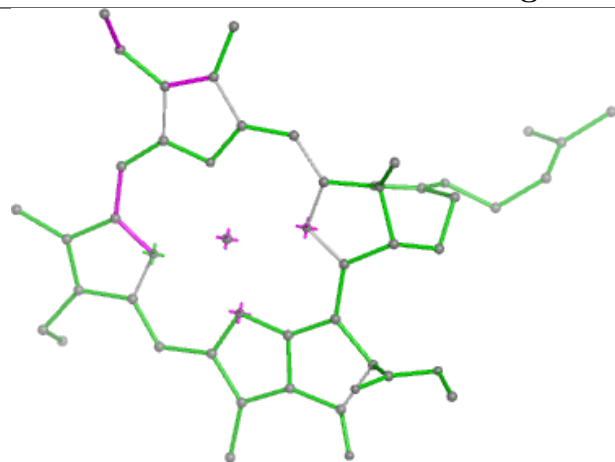




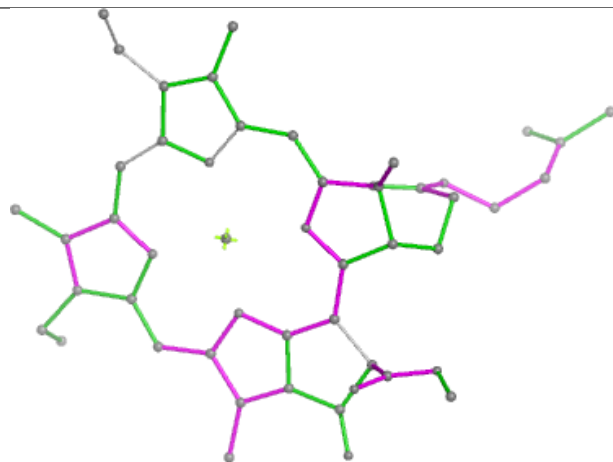
Ligand CLA 7 306



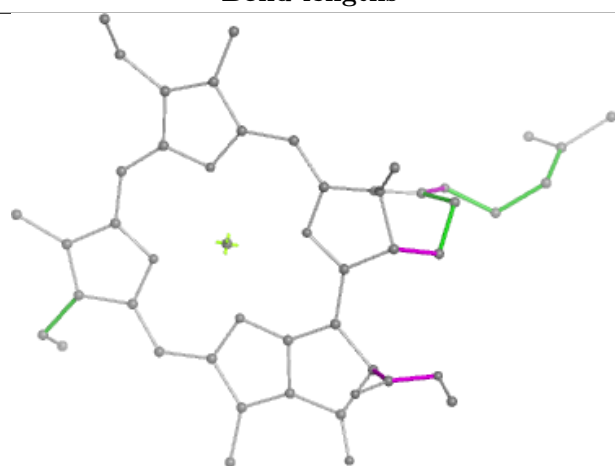
Ligand CLA 7 314



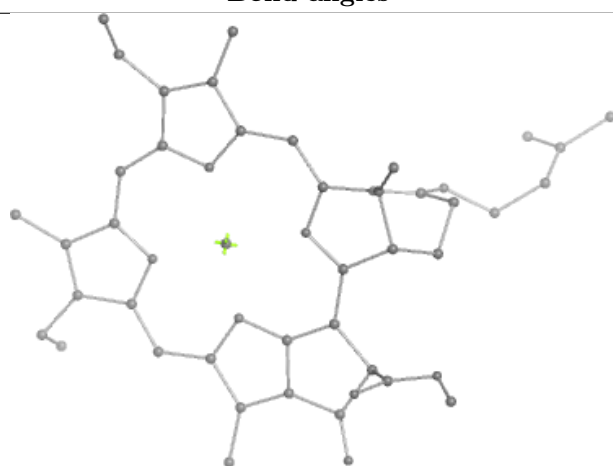
Bond lengths



Bond angles

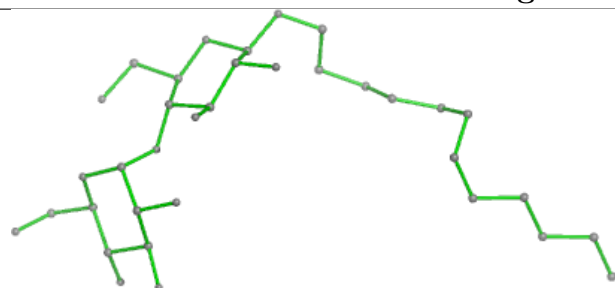


Torsions

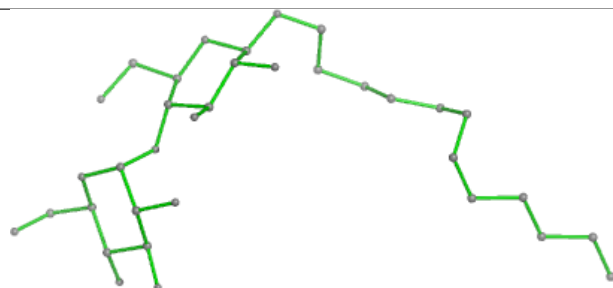


Rings

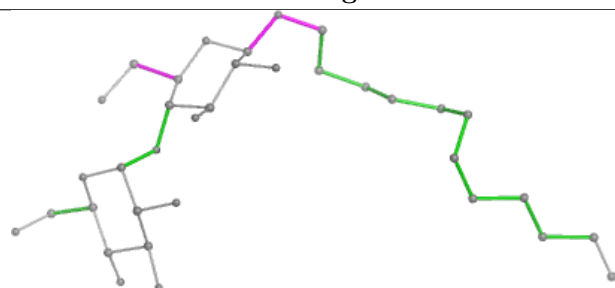
Ligand LMT 1 301



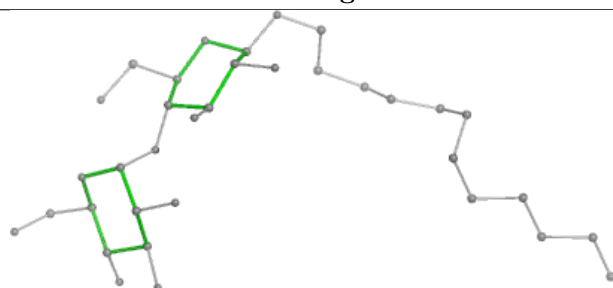
Bond lengths



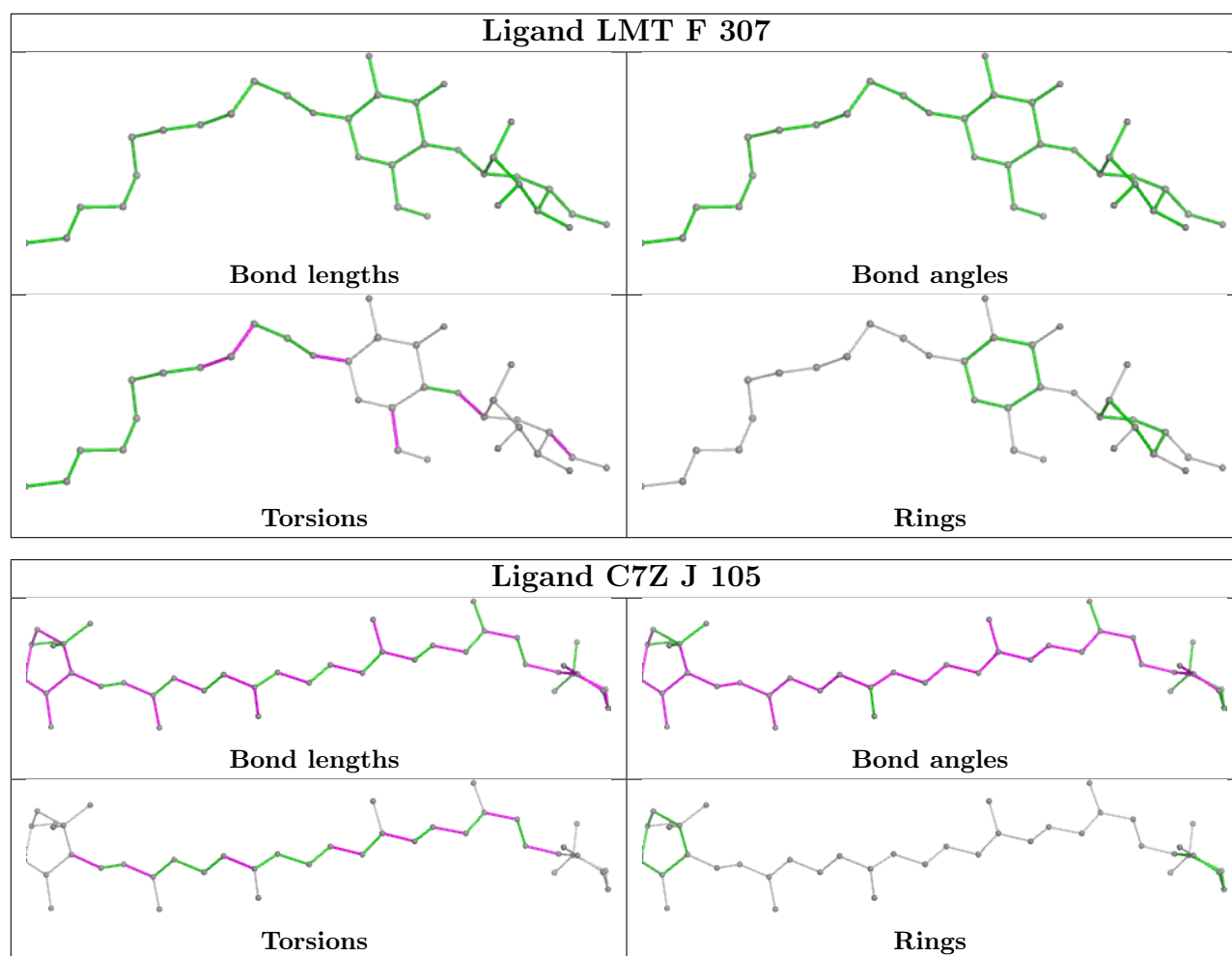
Bond angles



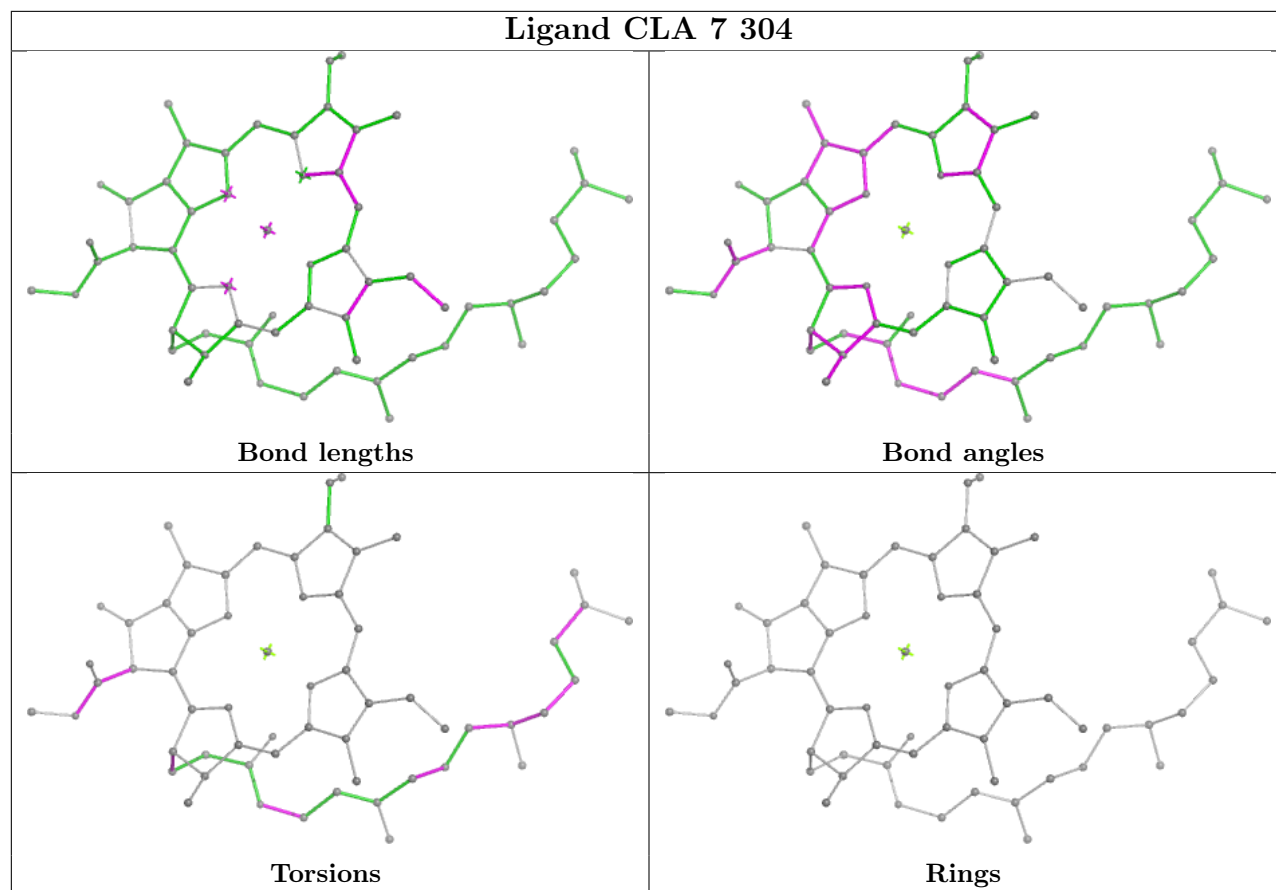
Torsions



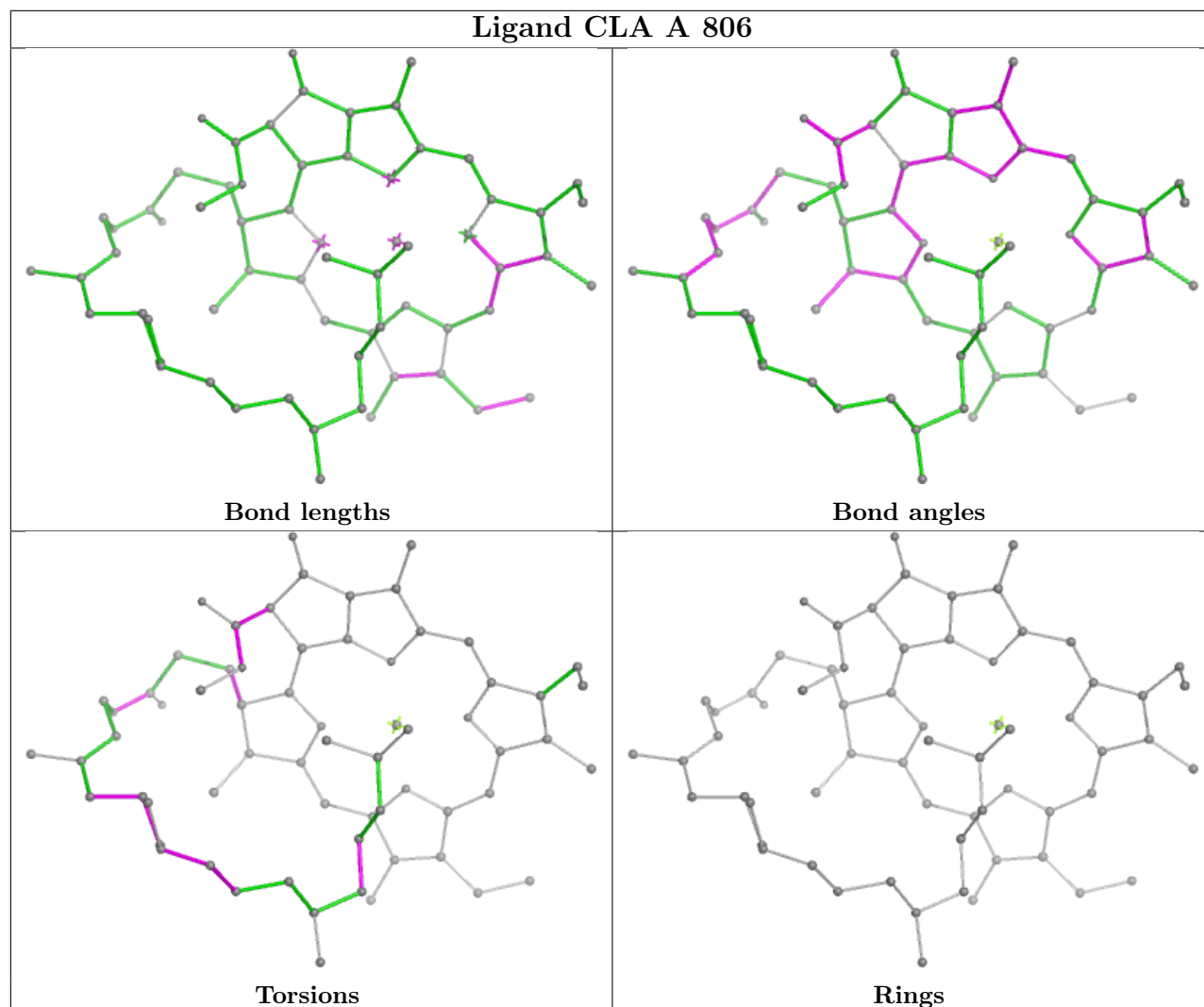
Rings



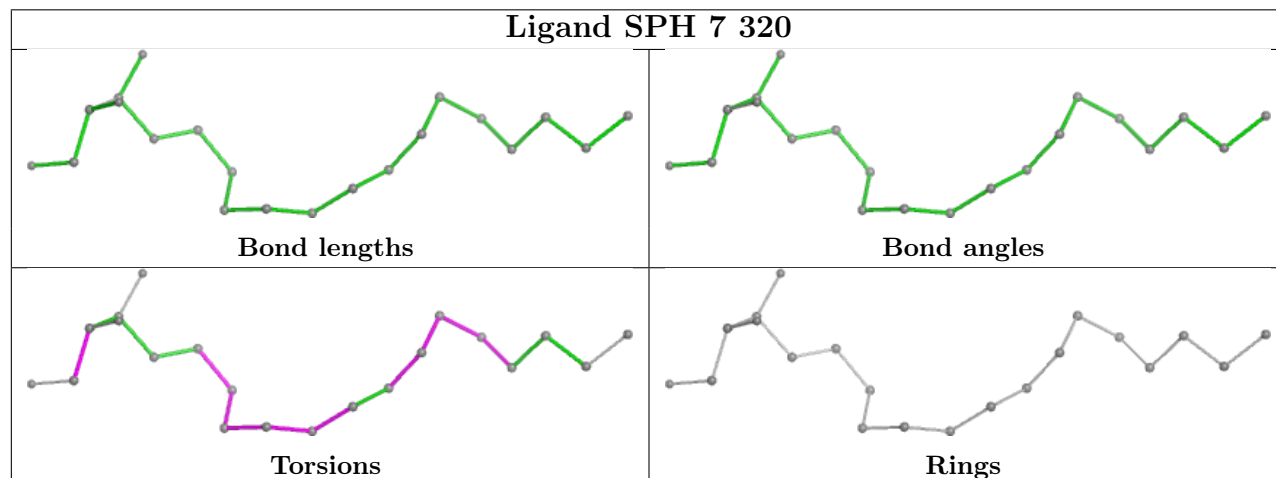
Ligand CLA 7 304



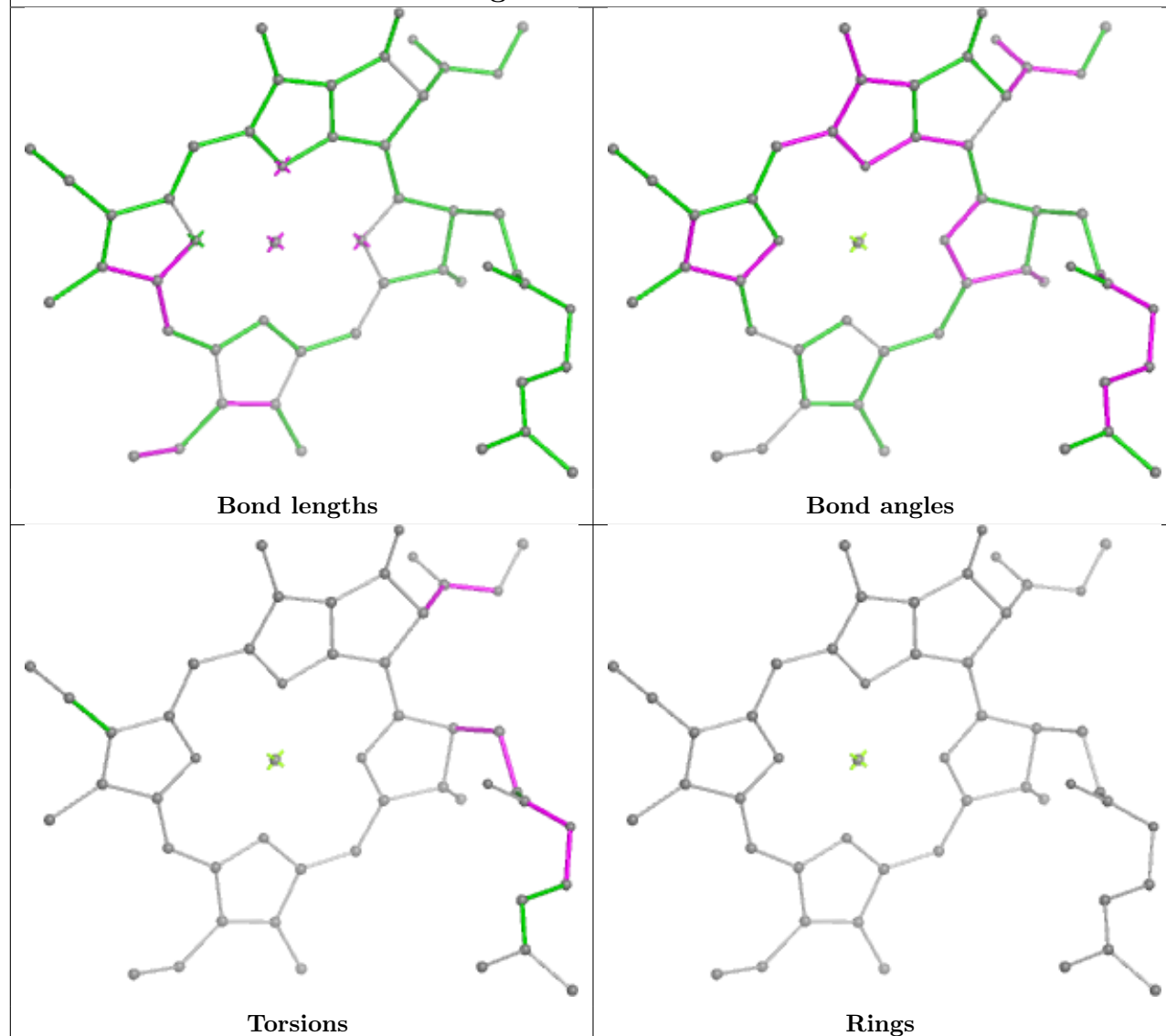
Ligand CLA A 806



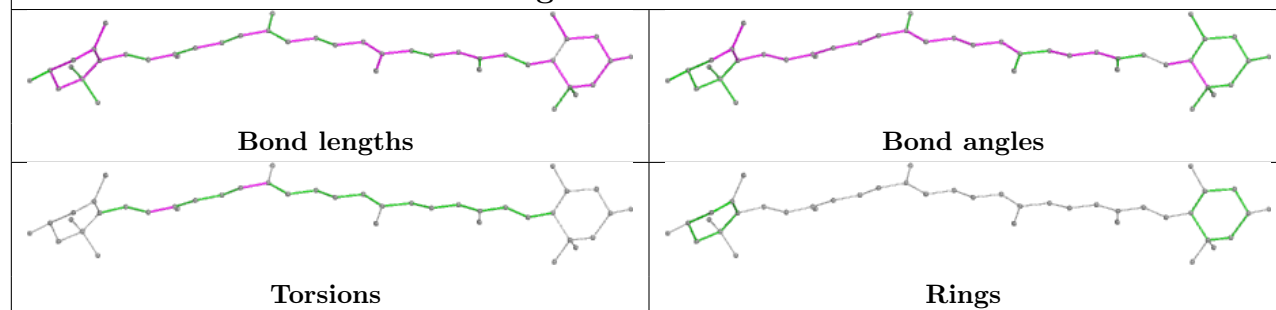
Ligand SPH 7 320



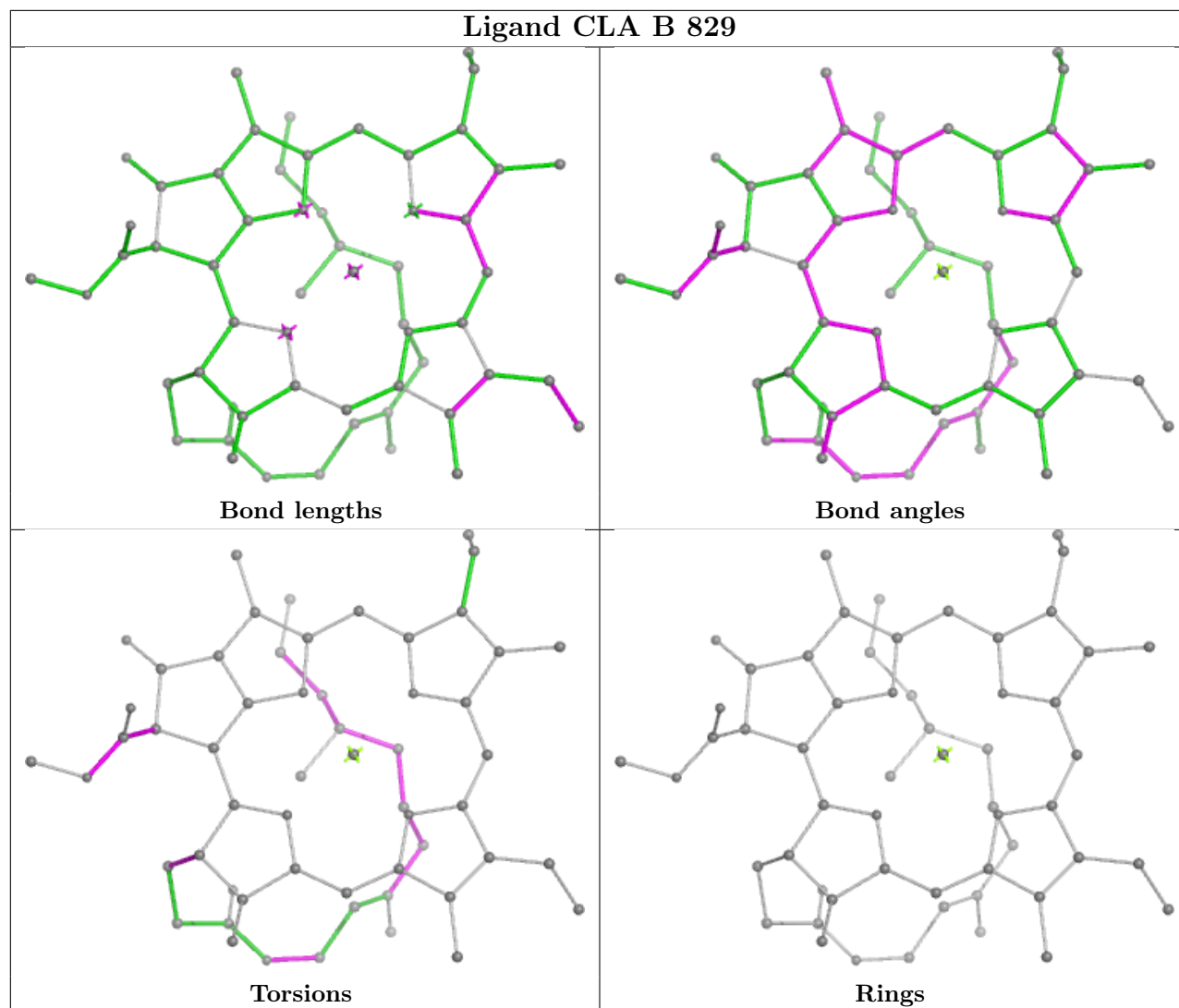
Ligand CLA 8 311



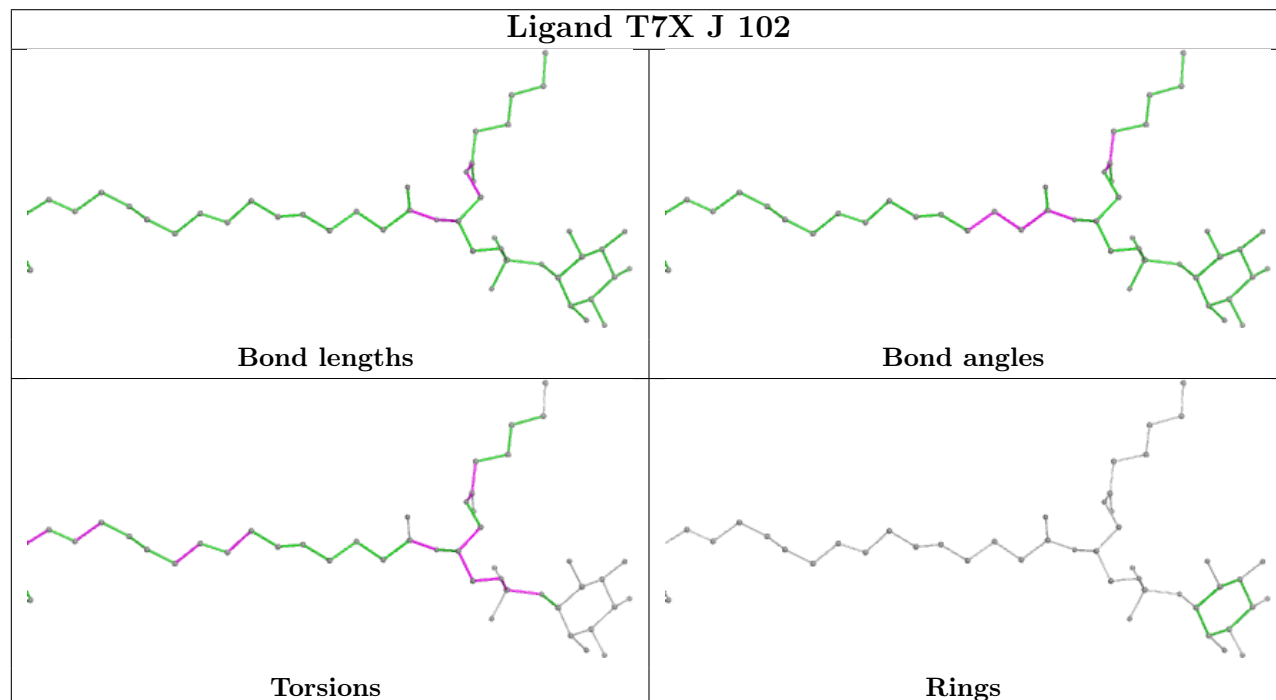
Ligand LUT 9 302

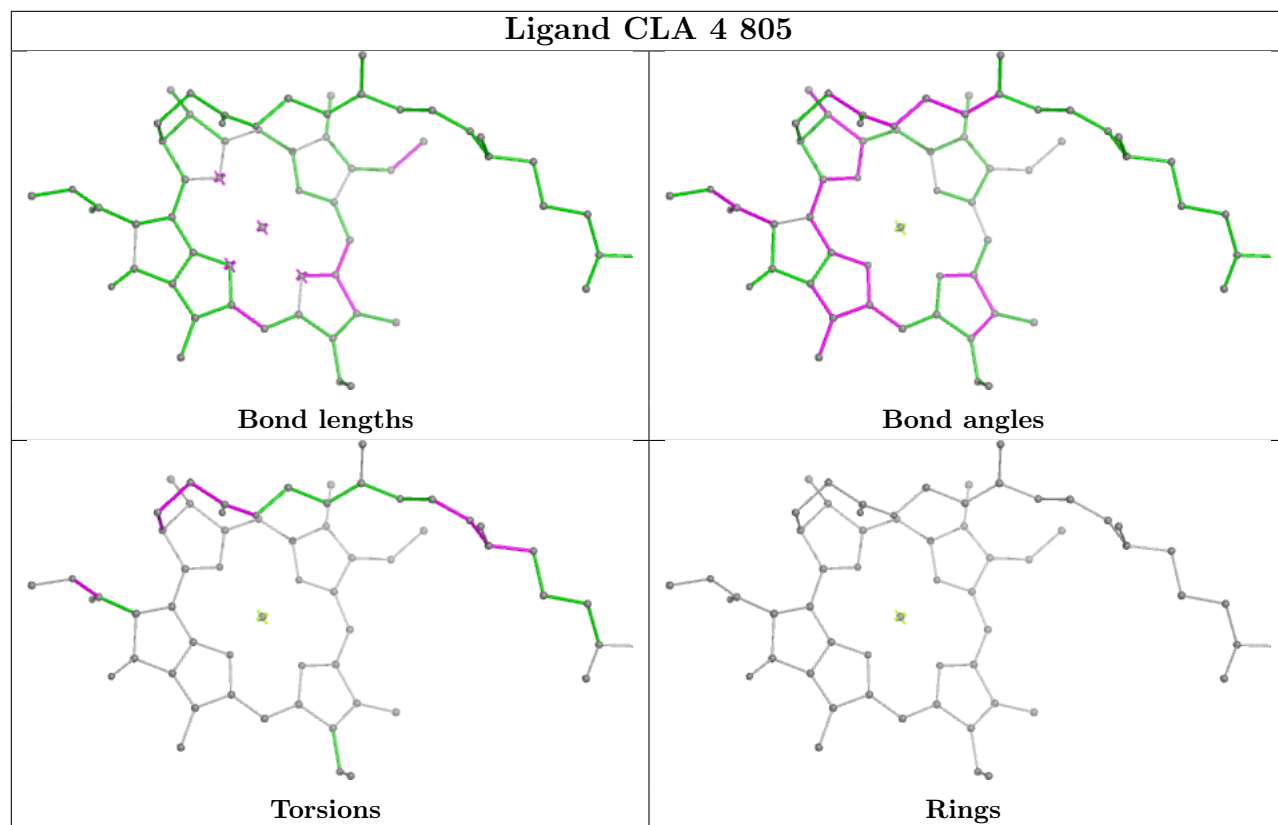


Ligand CLA B 829

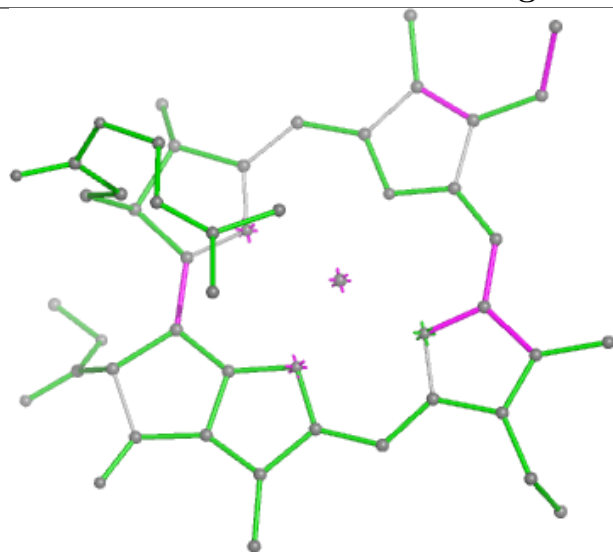


Ligand T7X J 102

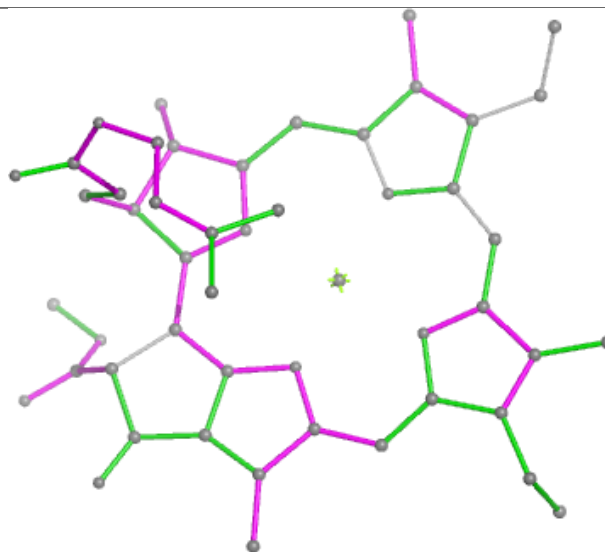




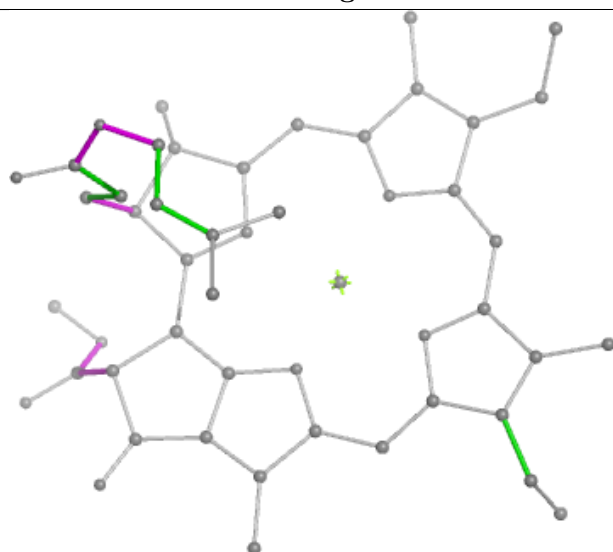
Ligand CLA 7 315



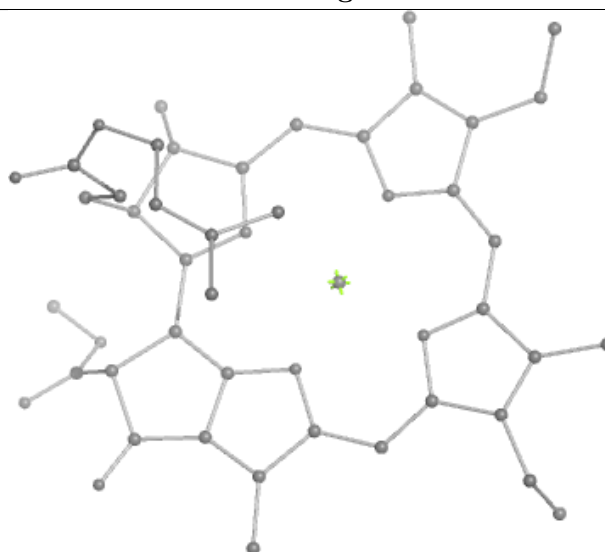
Bond lengths



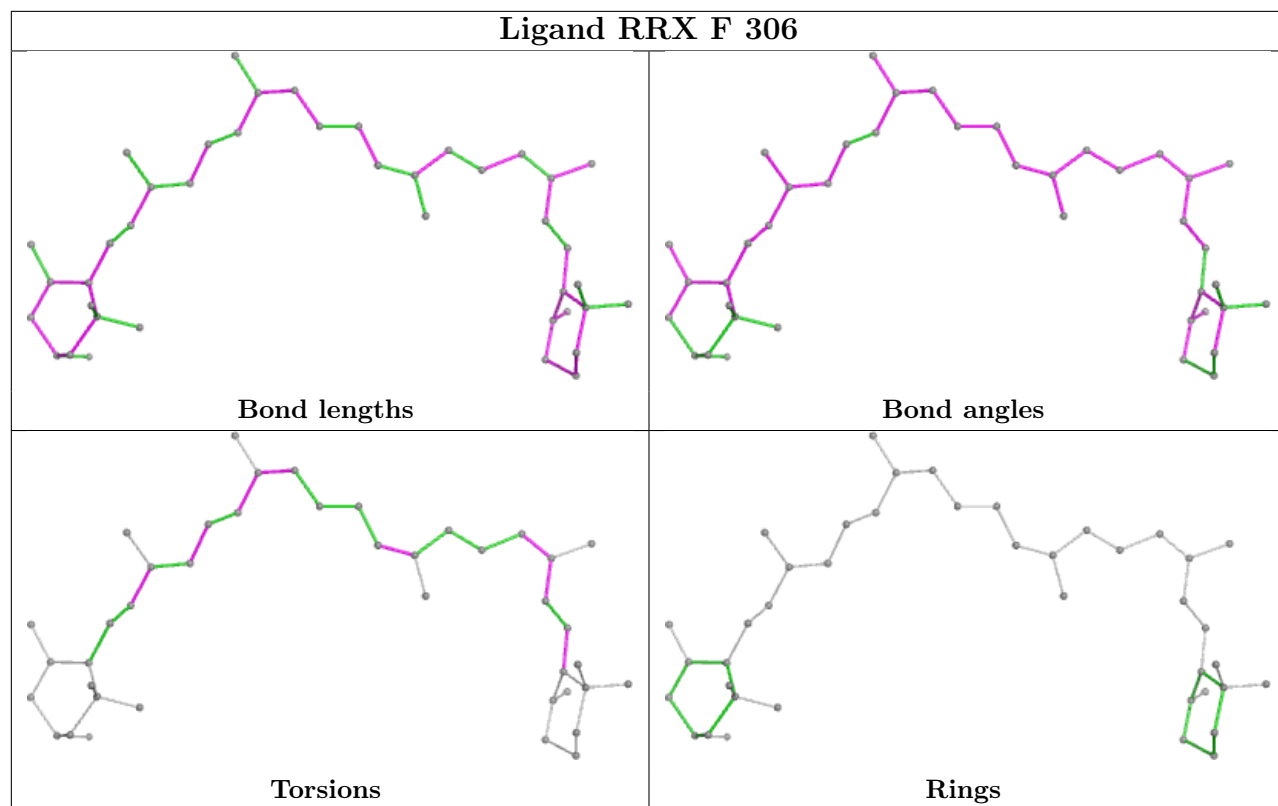
Bond angles



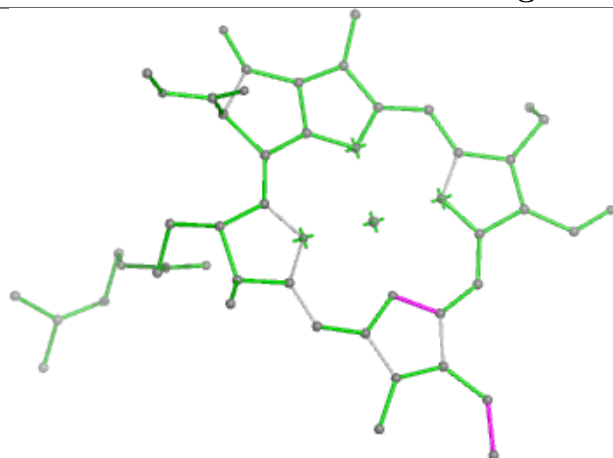
Torsions



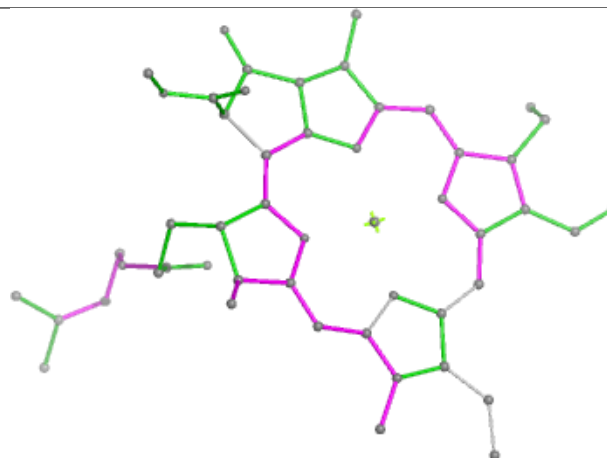
Rings



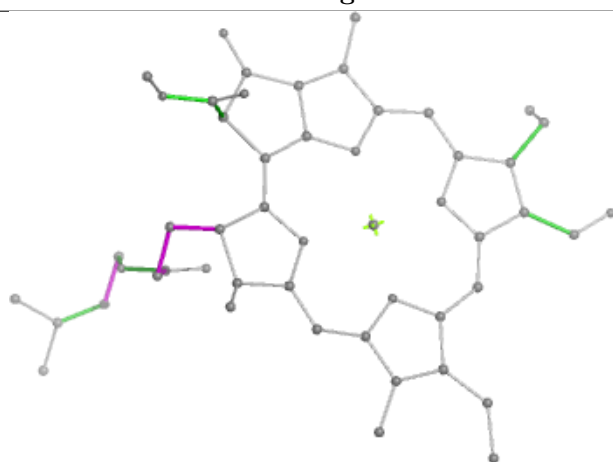
Ligand CHL 5 317



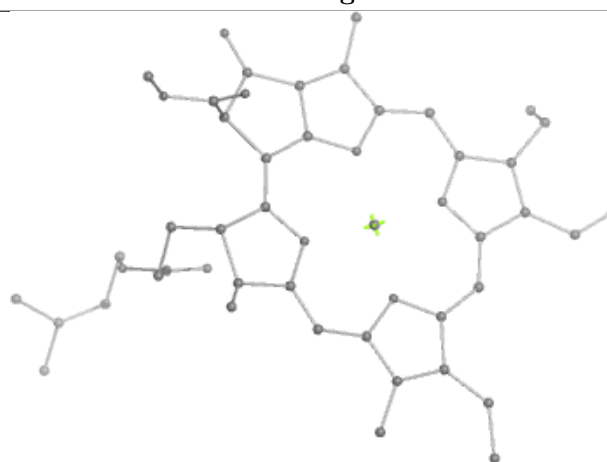
Bond lengths



Bond angles

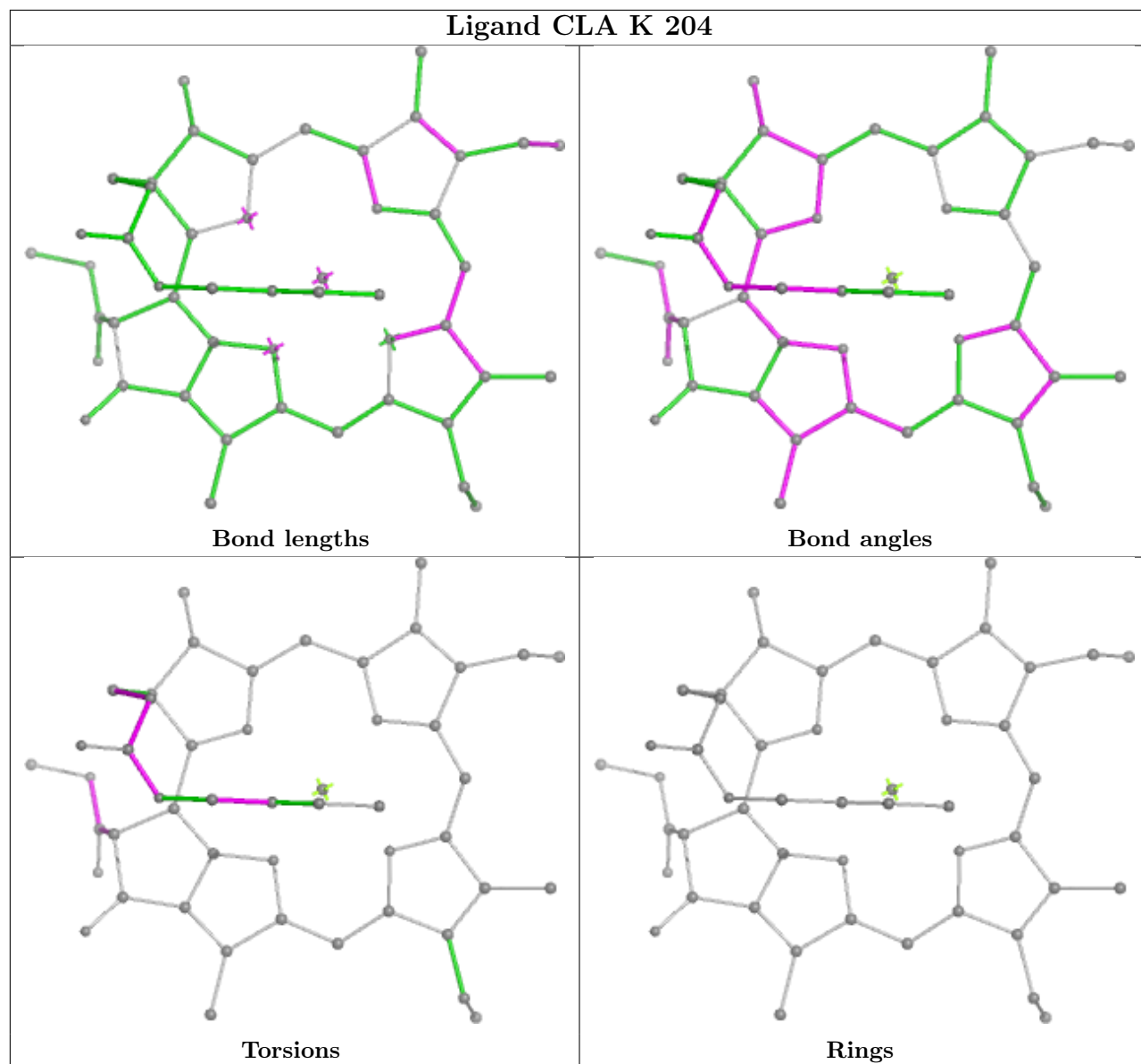


Torsions

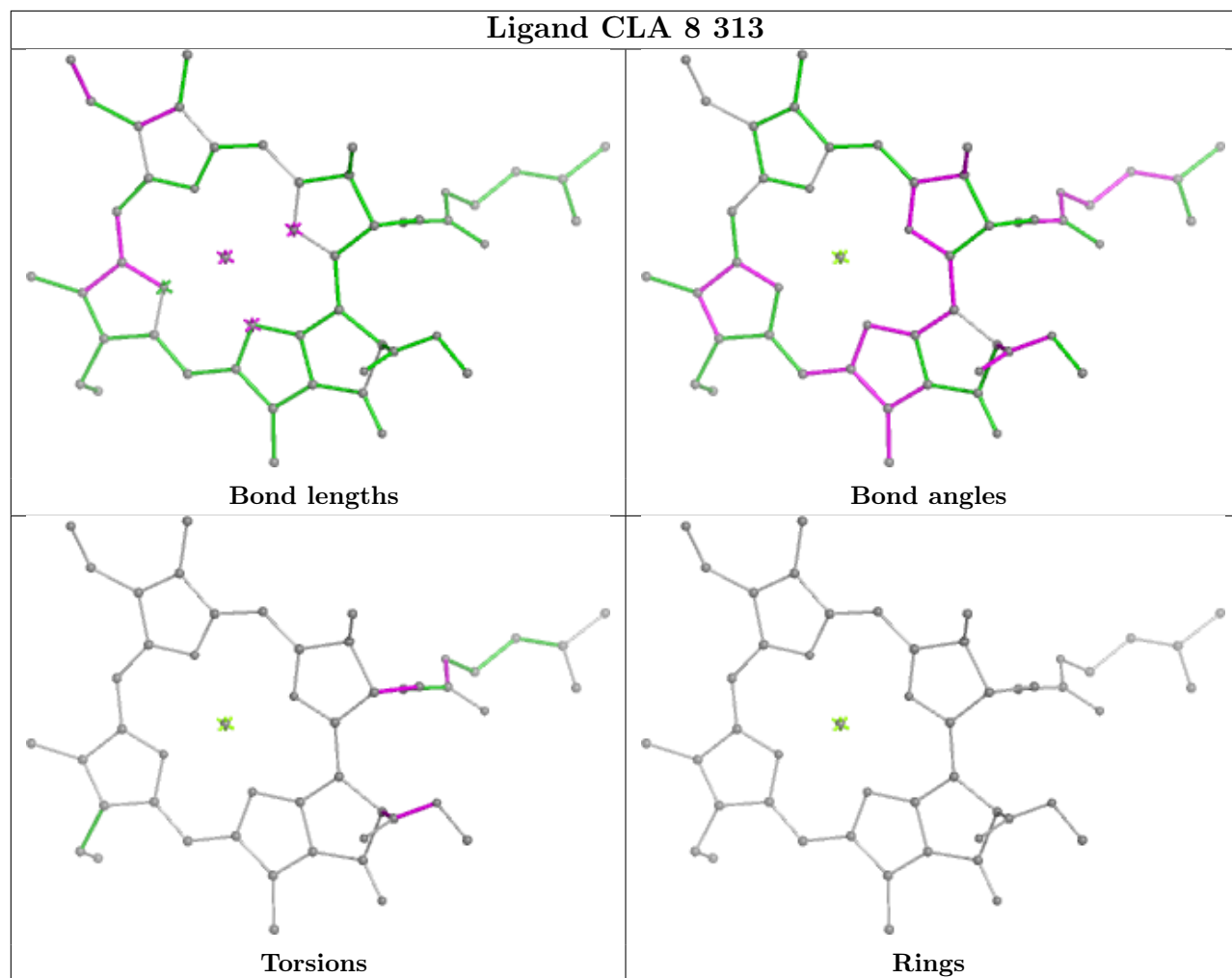


Rings

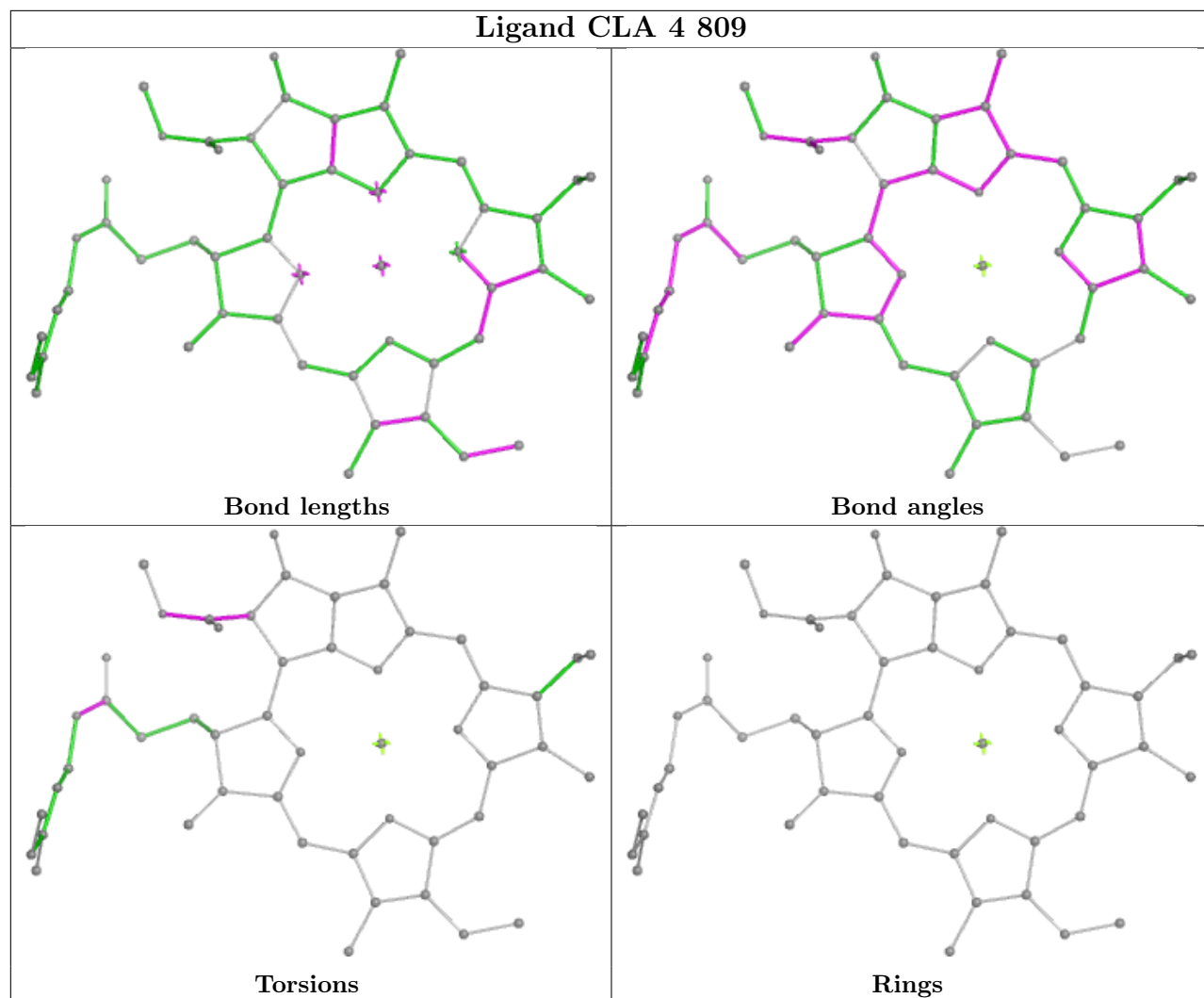
Ligand CLA K 204



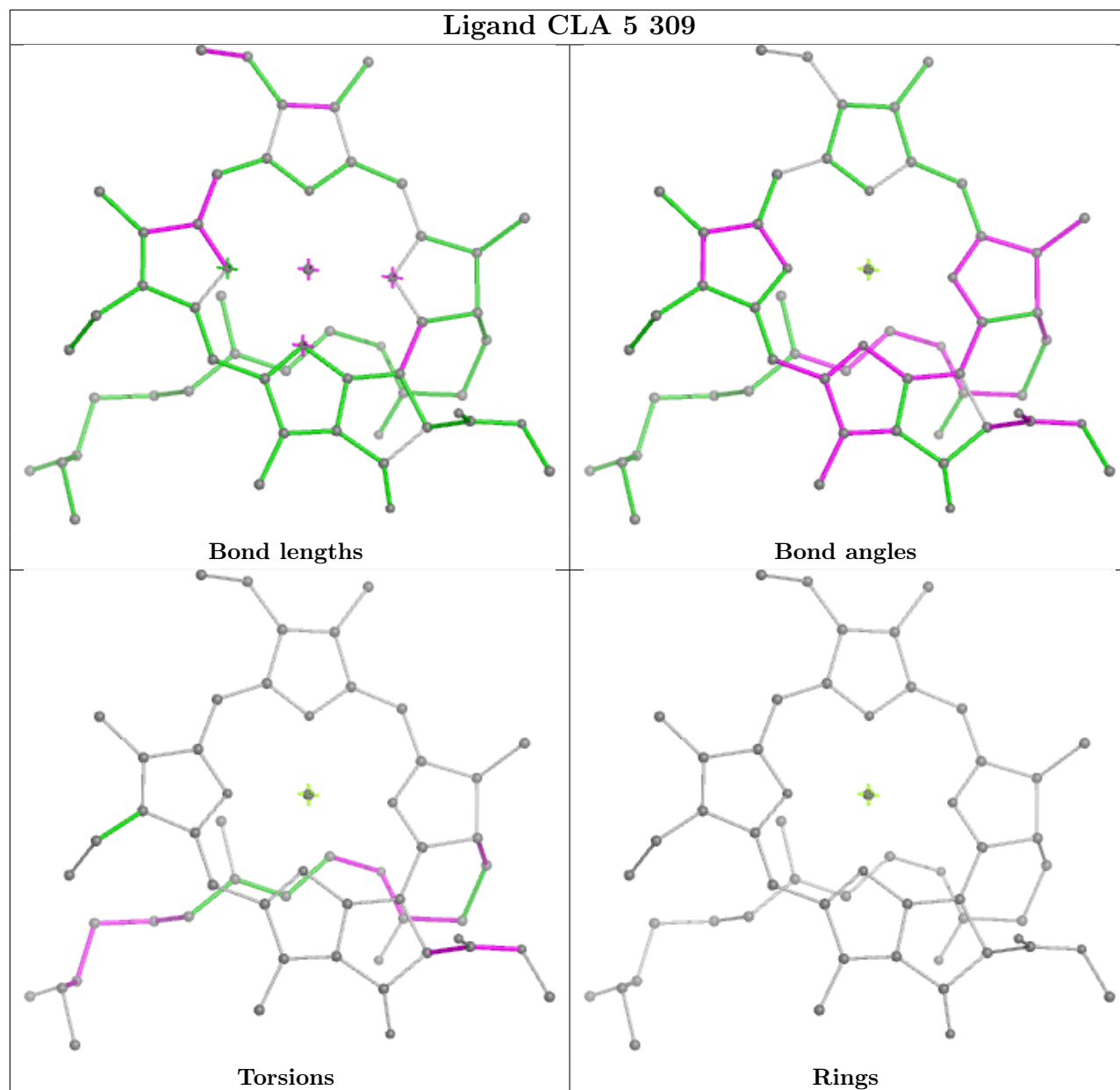
Ligand CLA 8 313

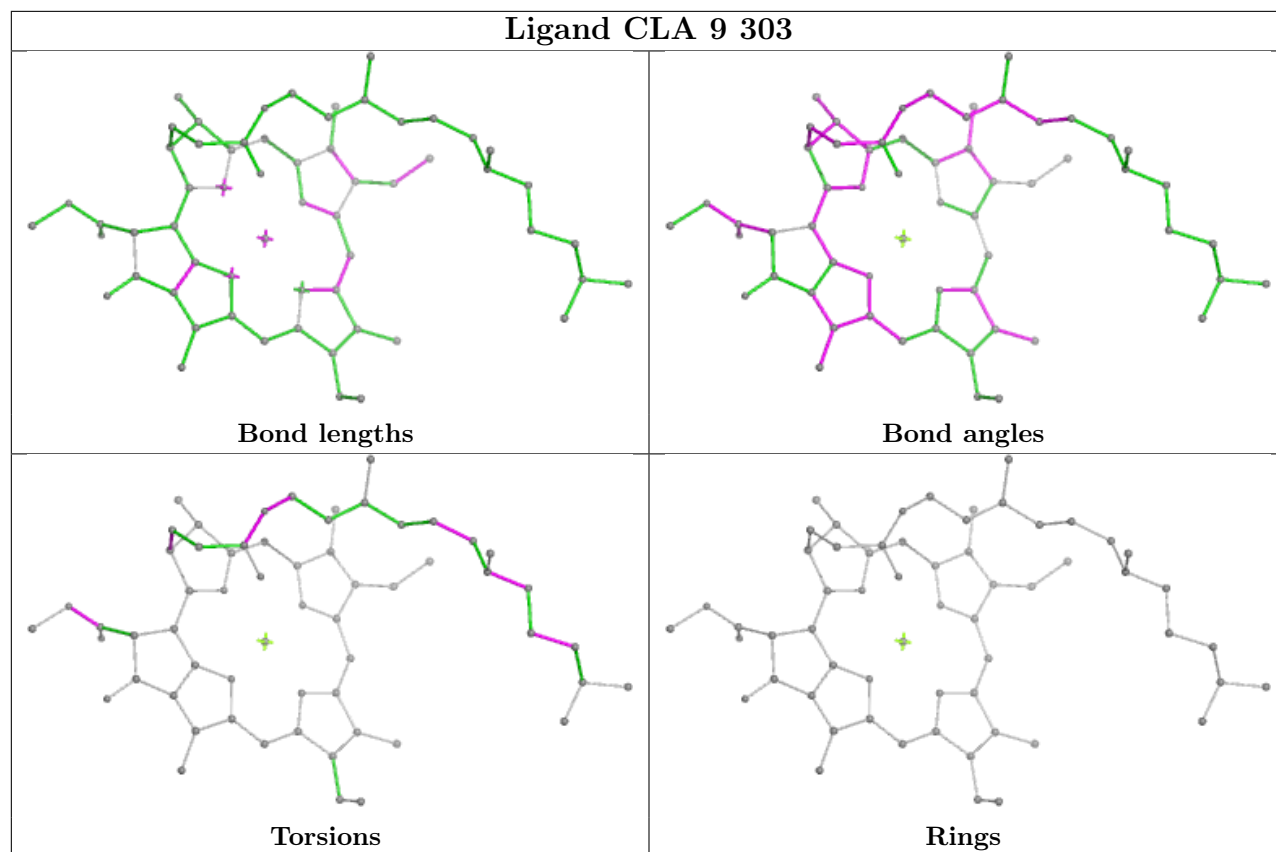
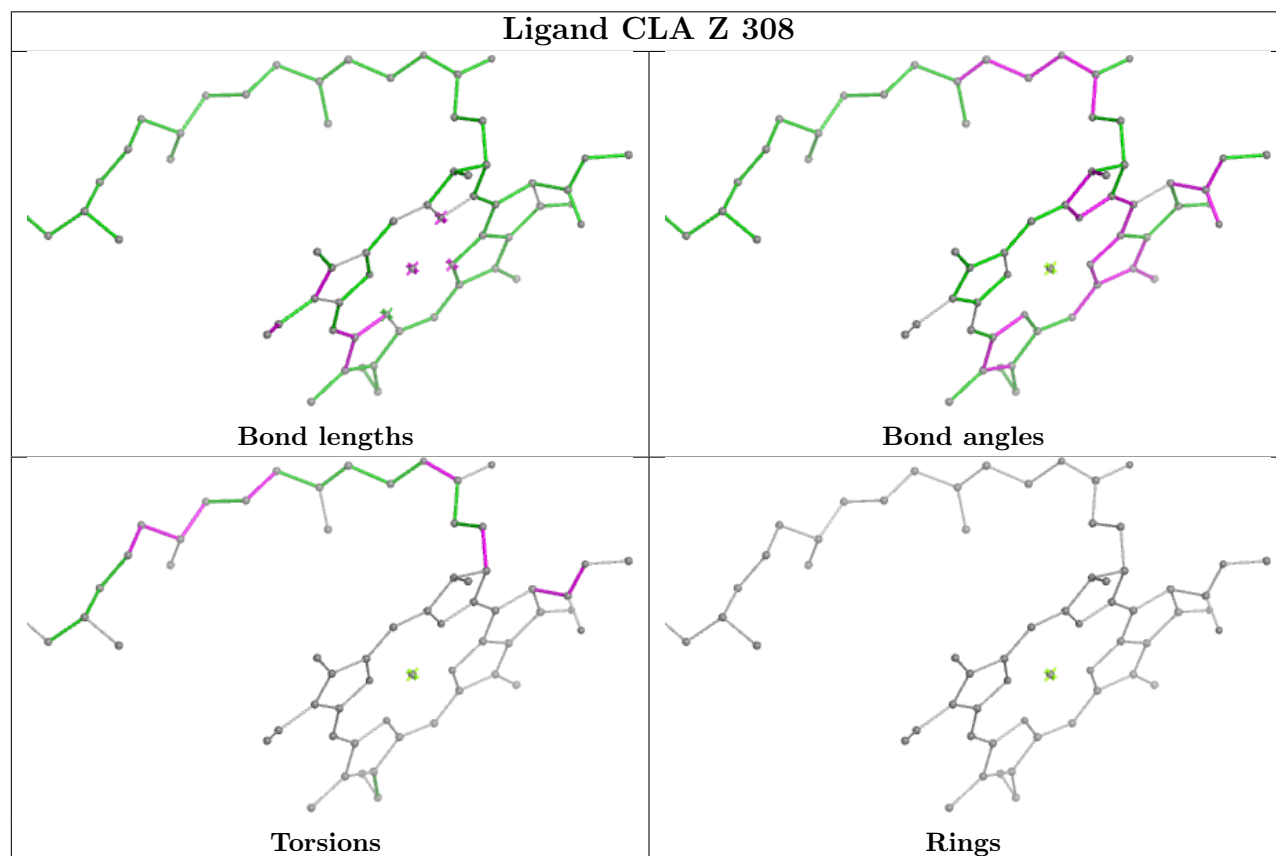


Ligand CLA 4 809

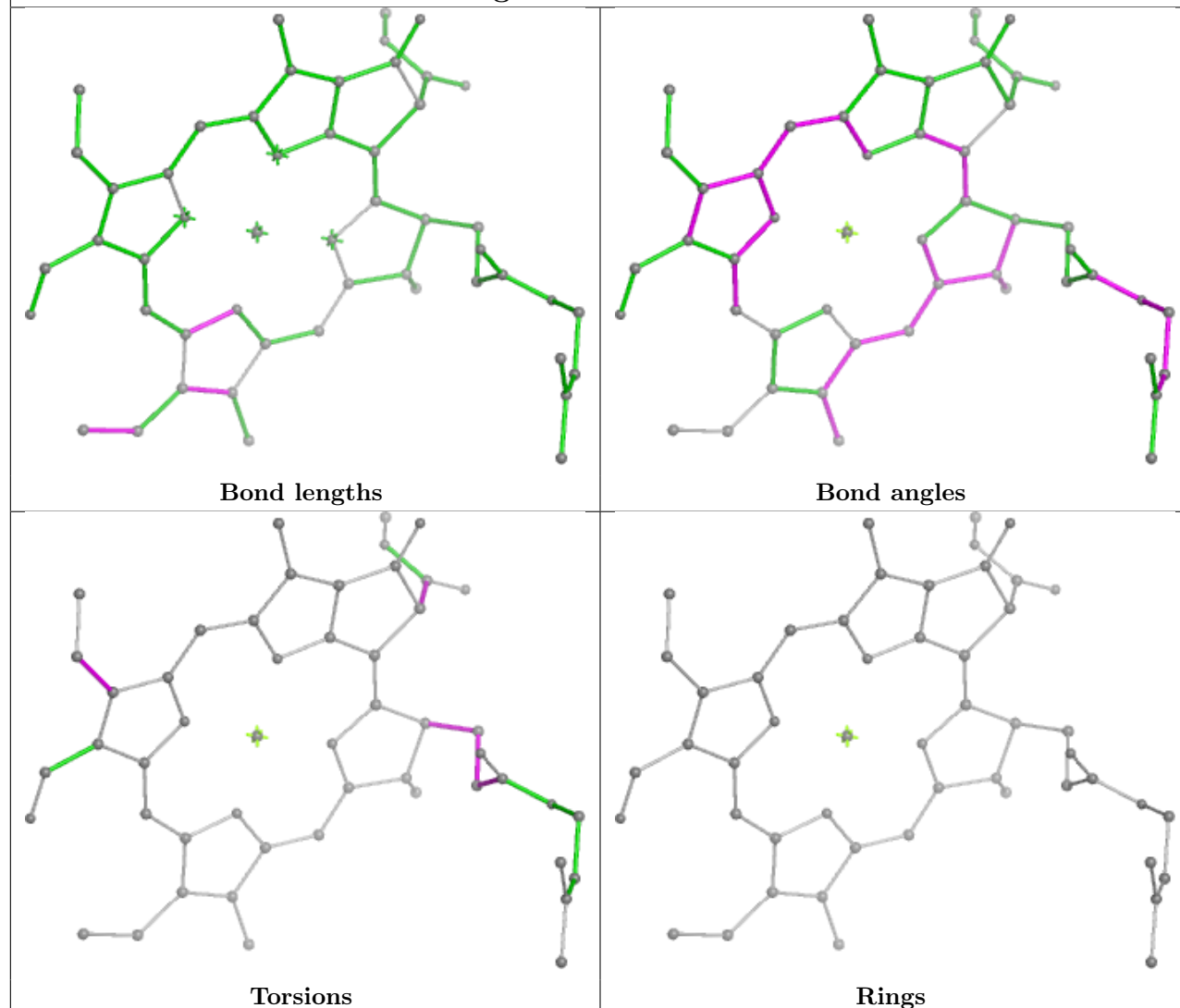


Ligand CLA 5 309

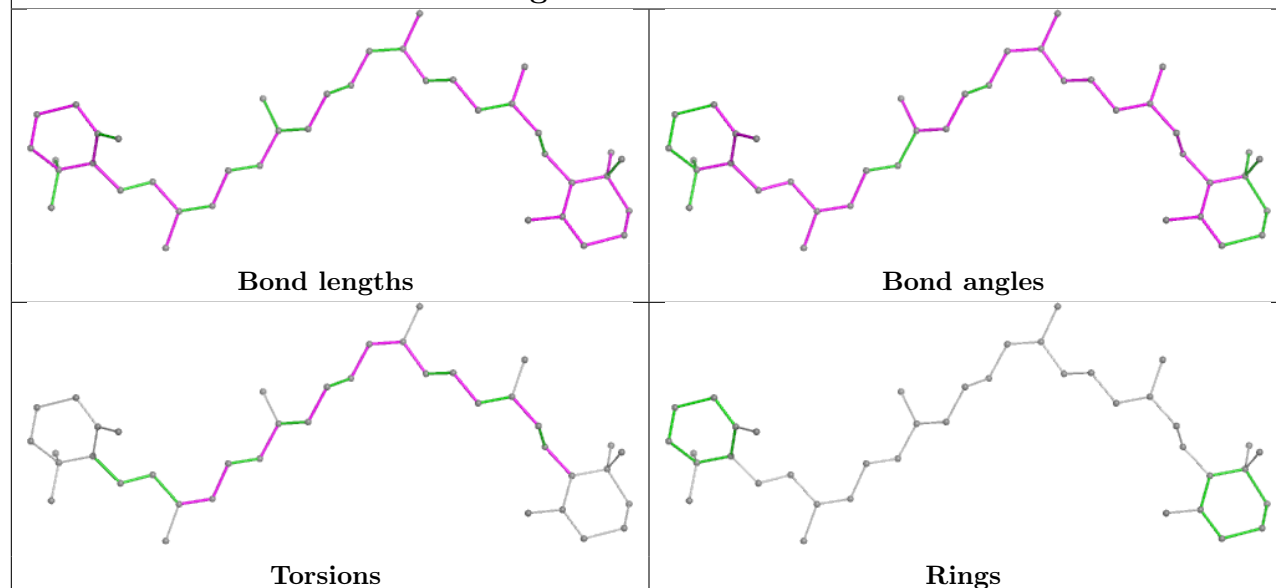


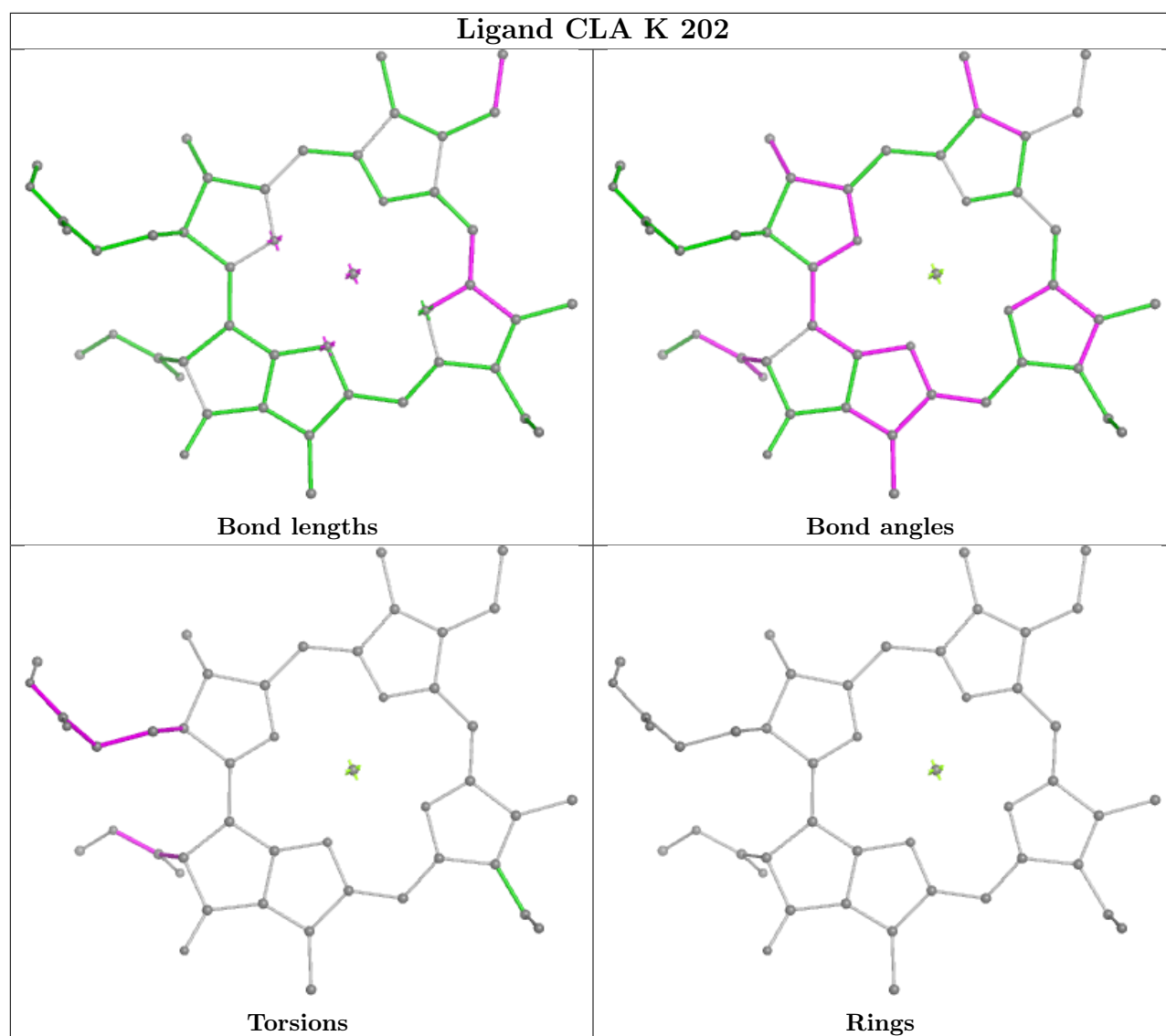
Ligand CLA 9 303**Ligand CLA Z 308**

Ligand CHL Z 311

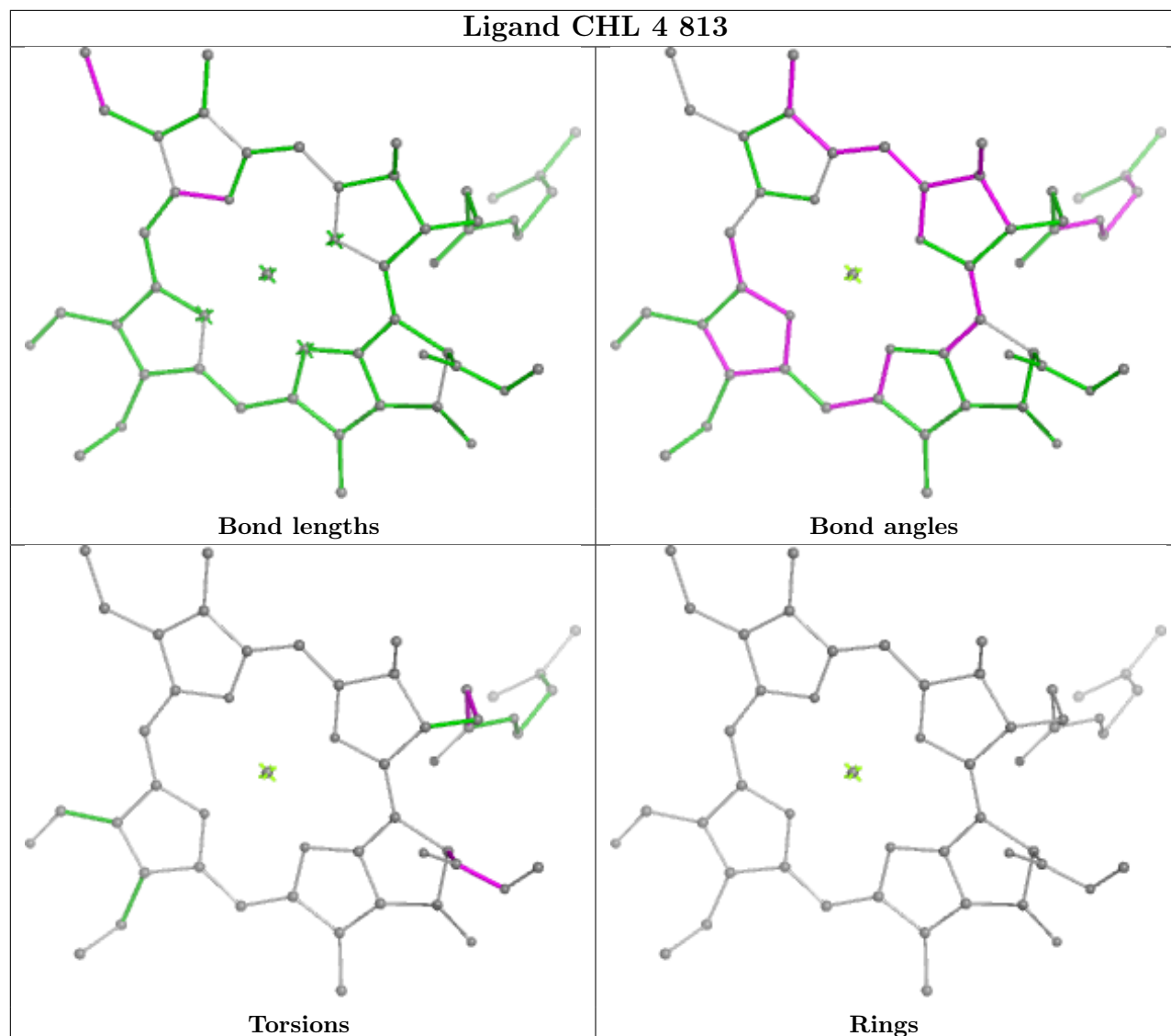


Ligand BCR A 848

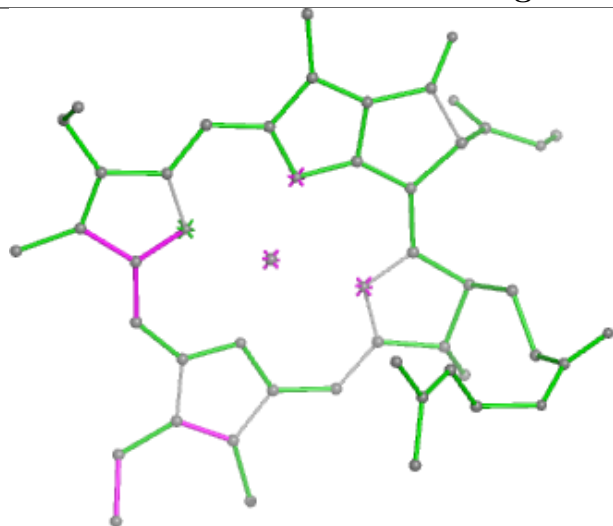




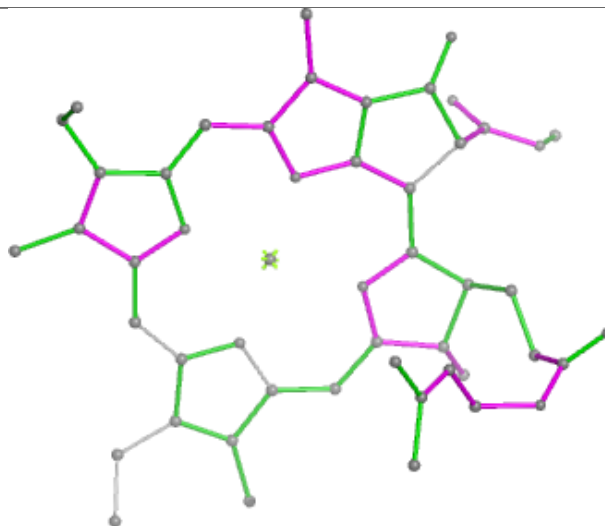
Ligand CHL 4 813



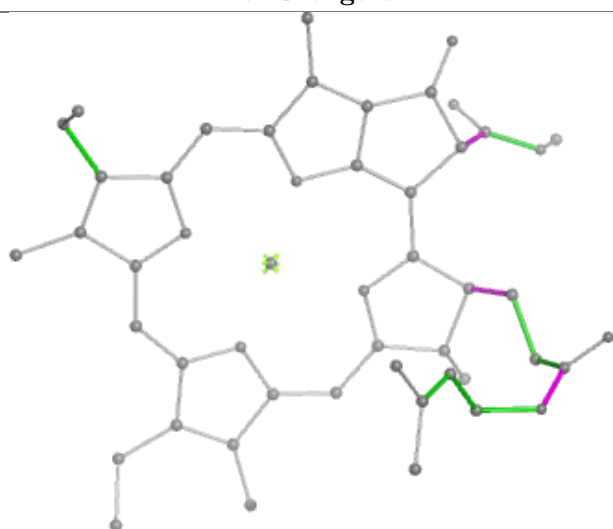
Ligand CLA B 832



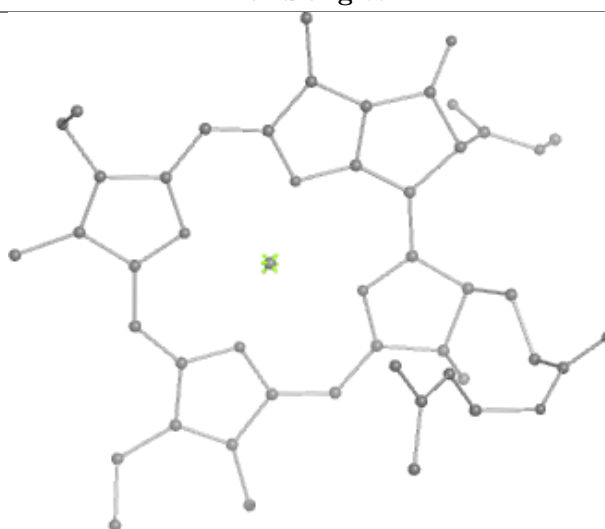
Bond lengths



Bond angles

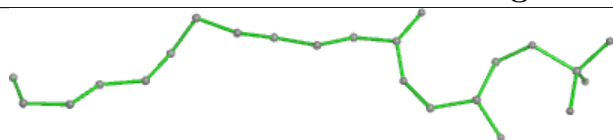


Torsions

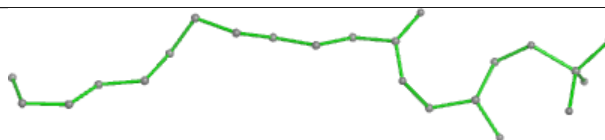


Rings

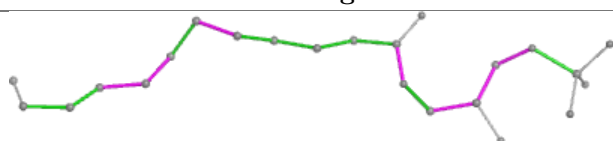
Ligand NKP A 851



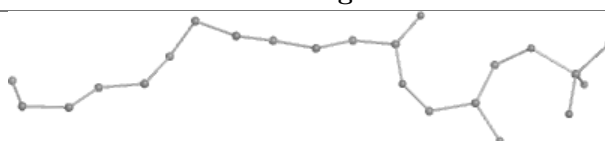
Bond lengths



Bond angles

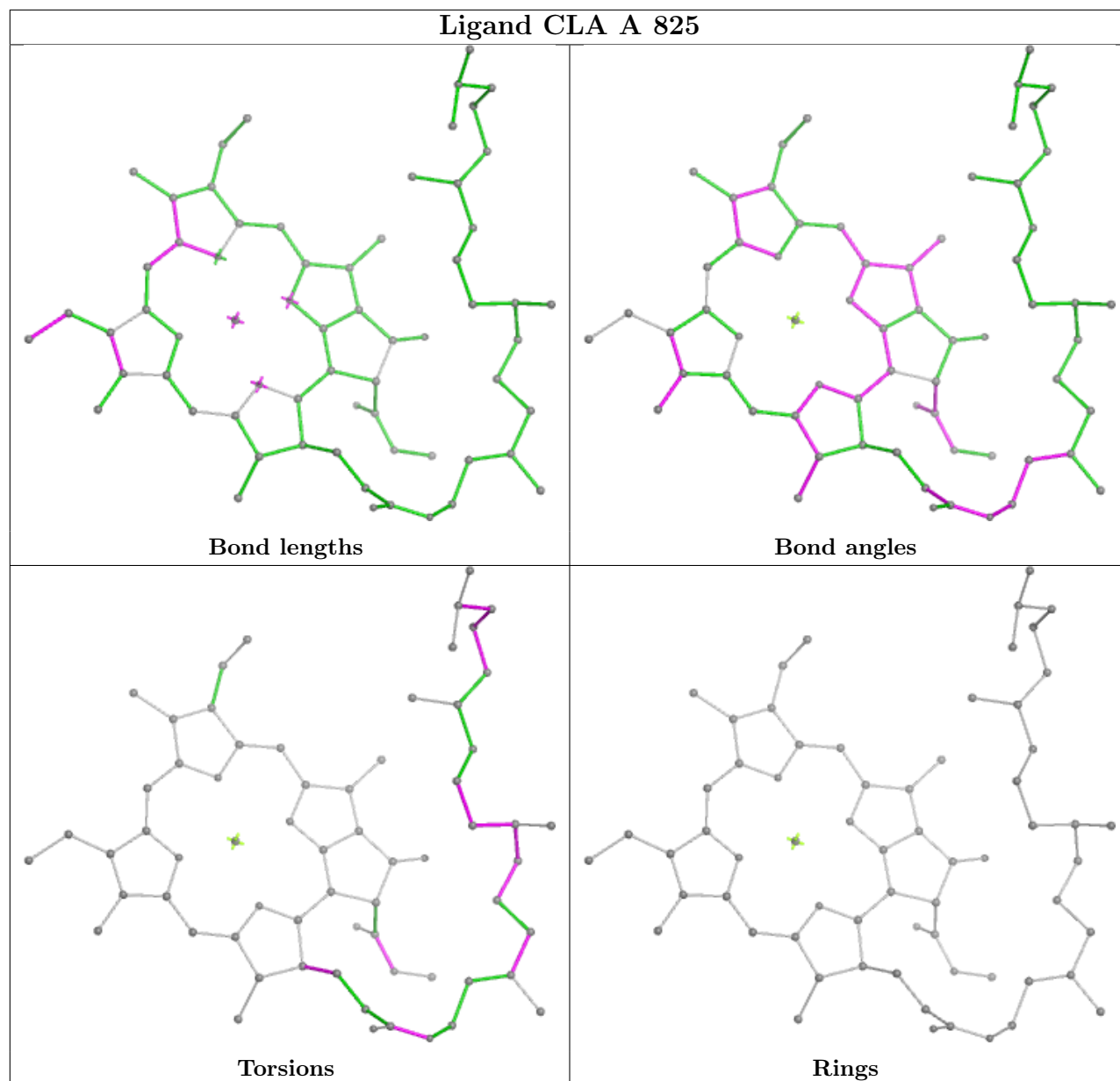


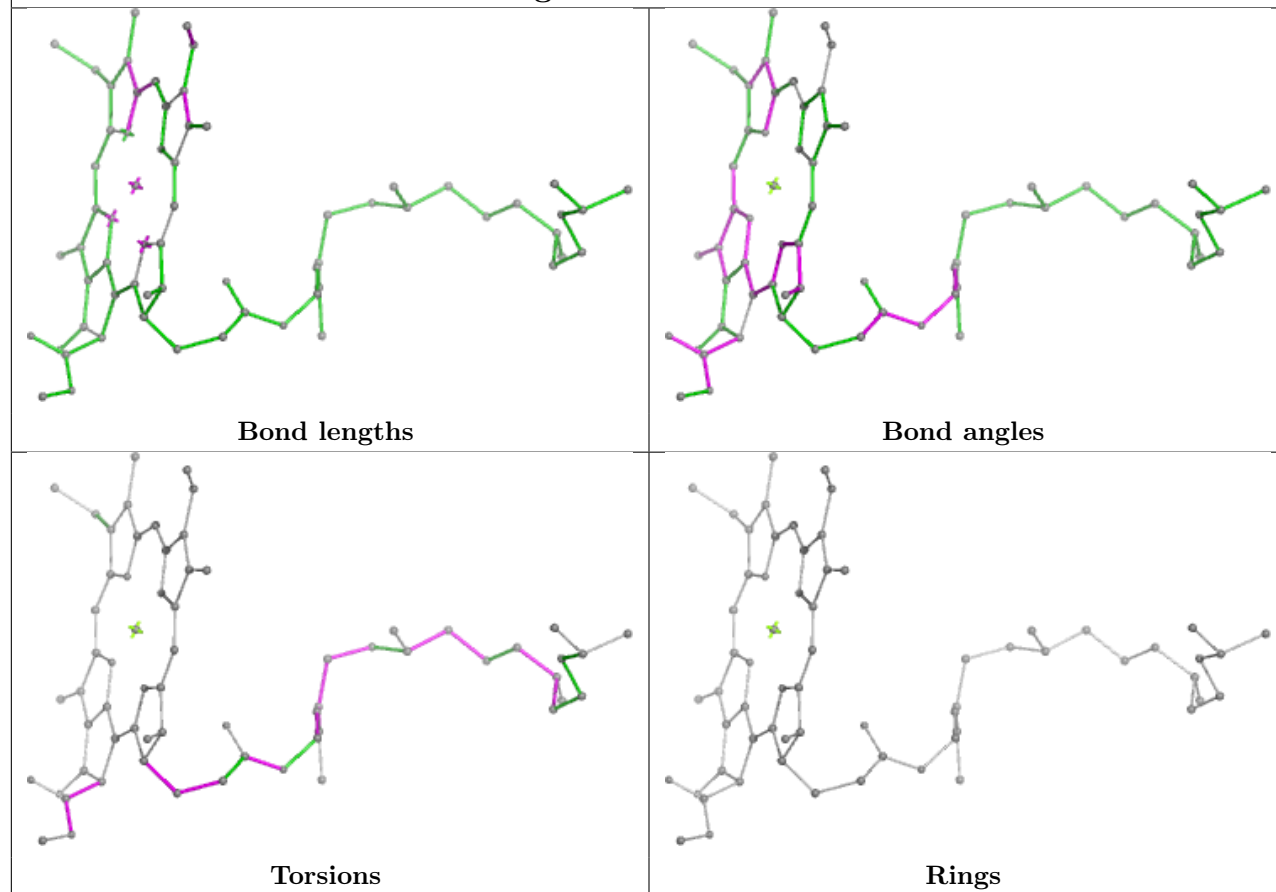
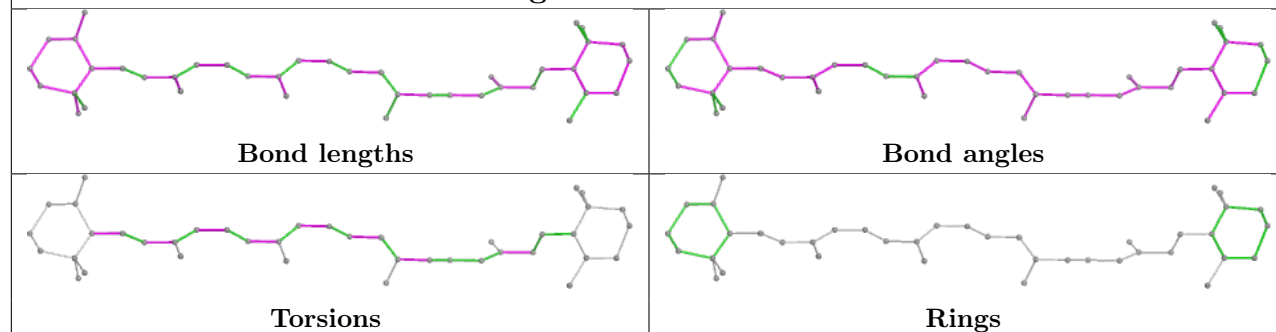
Torsions



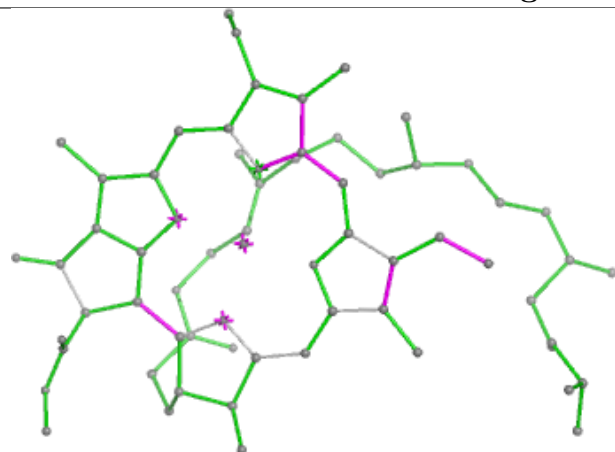
Rings

Ligand CLA A 825

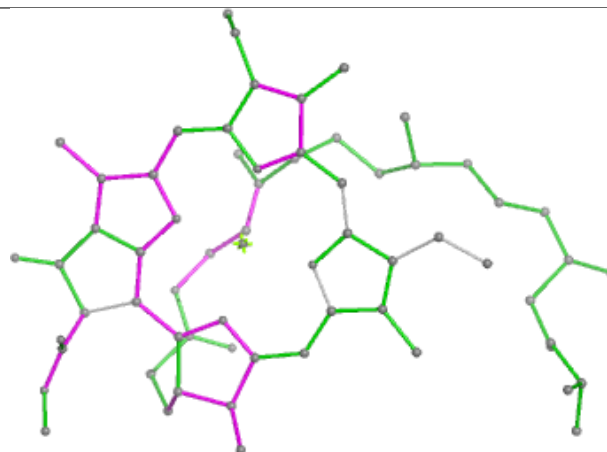


Ligand CLA L 202**Ligand BCR K 206**

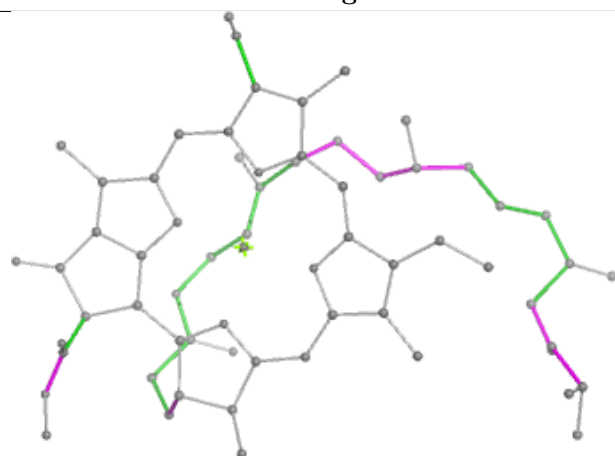
Ligand CLA 4 807



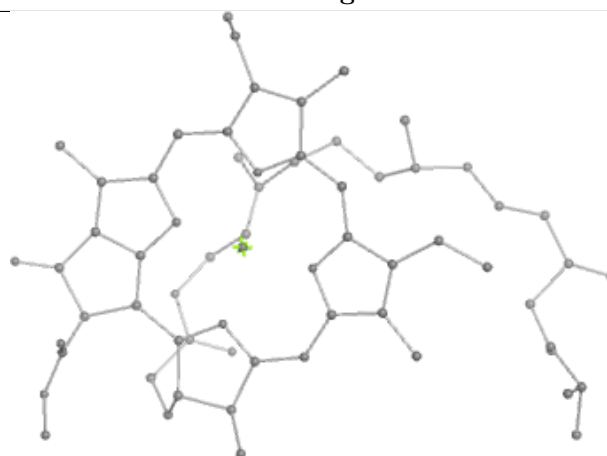
Bond lengths



Bond angles

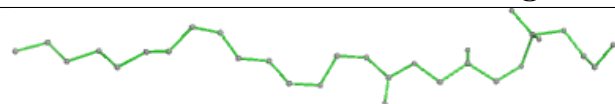


Torsions

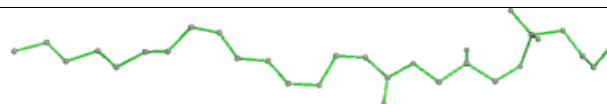


Rings

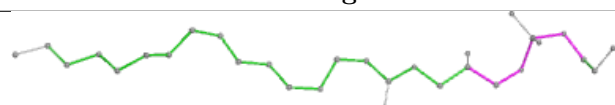
Ligand LPX 8 319



Bond lengths



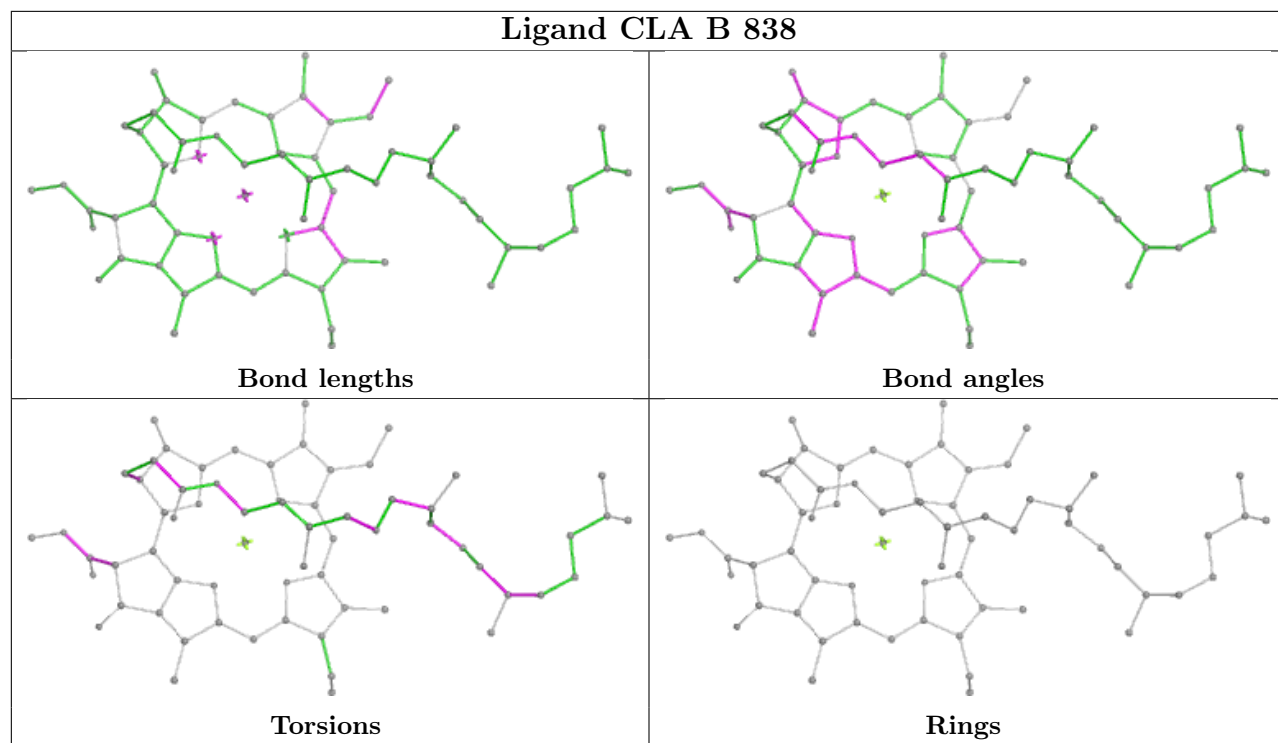
Bond angles



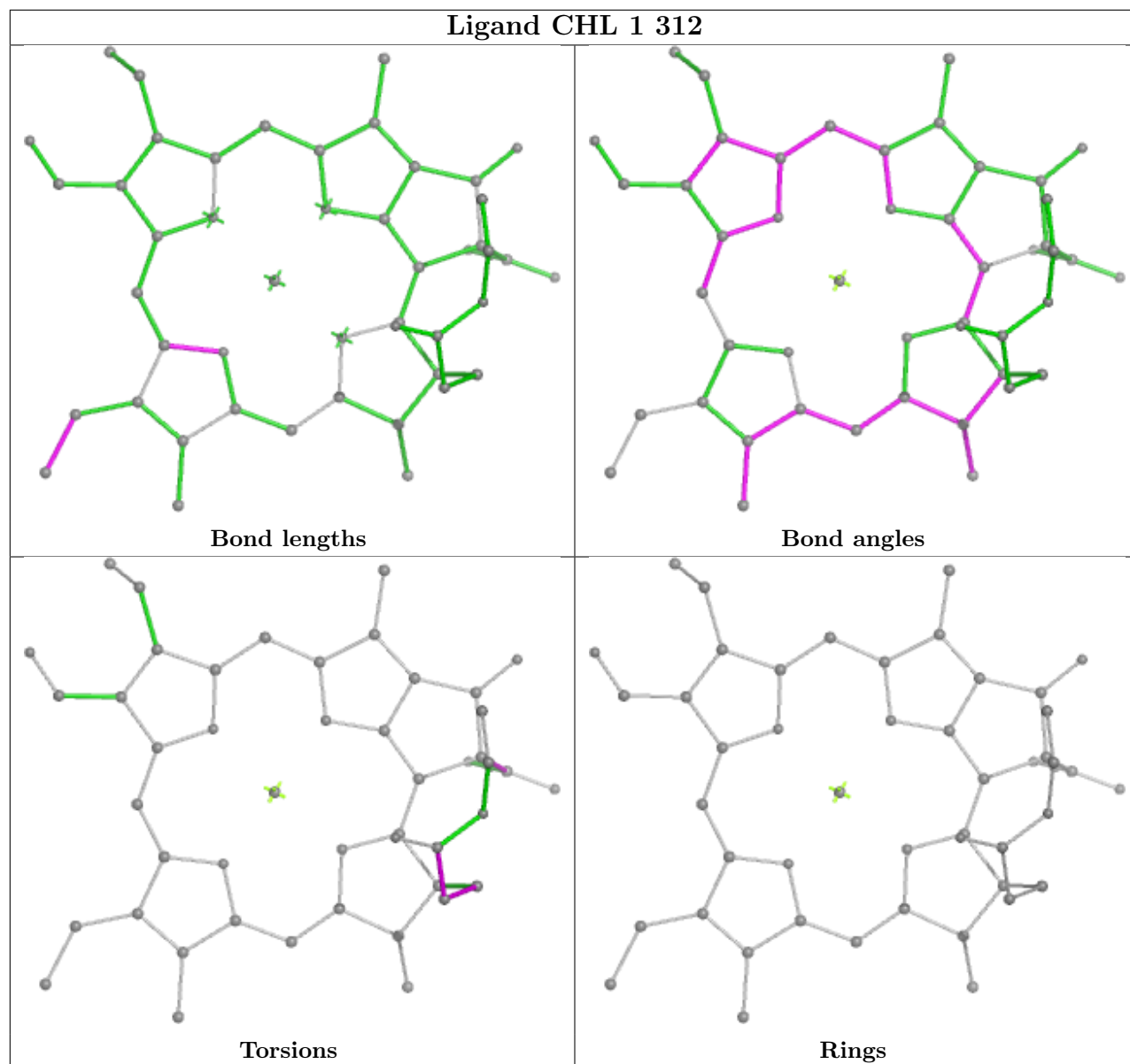
Torsions



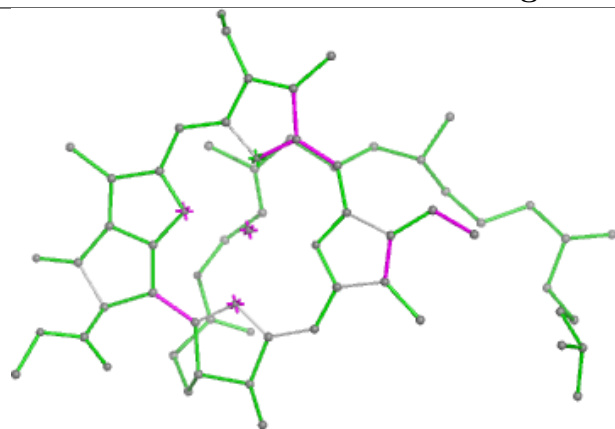
Rings



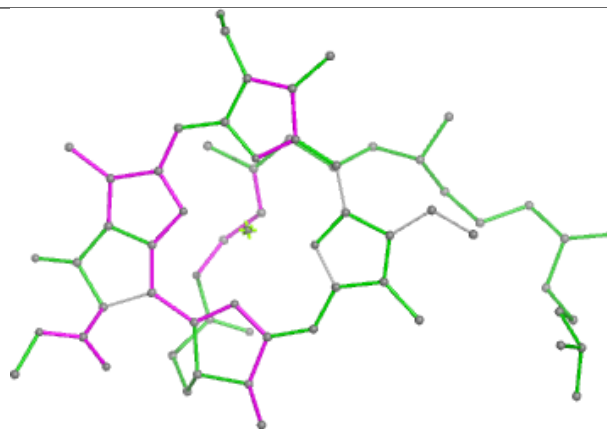
Ligand CHL 1 312



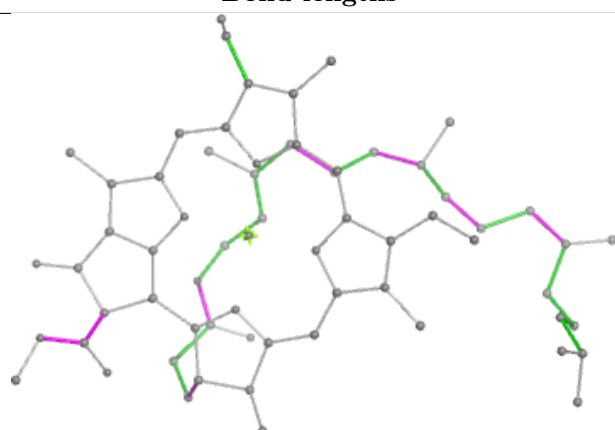
Ligand CLA 8 307



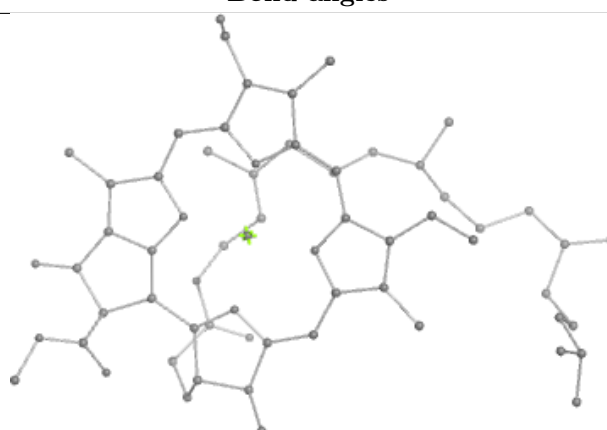
Bond lengths



Bond angles

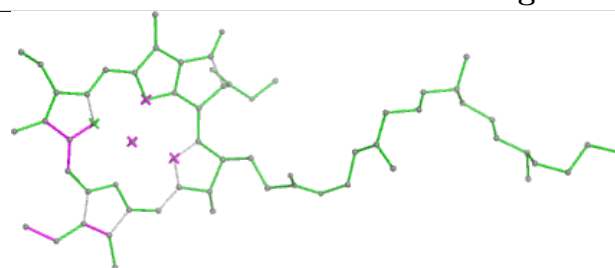


Torsions

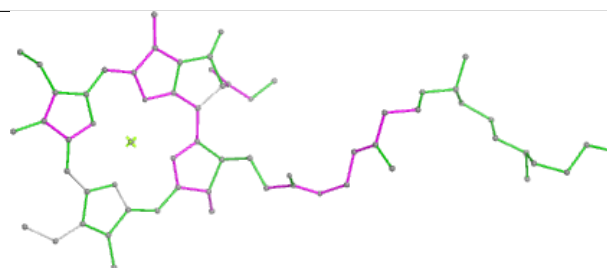


Rings

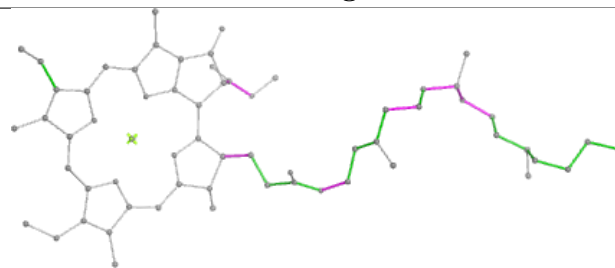
Ligand CLA F 301



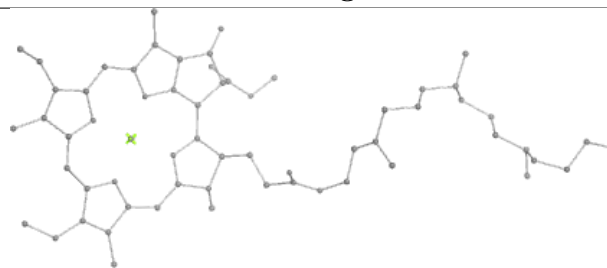
Bond lengths



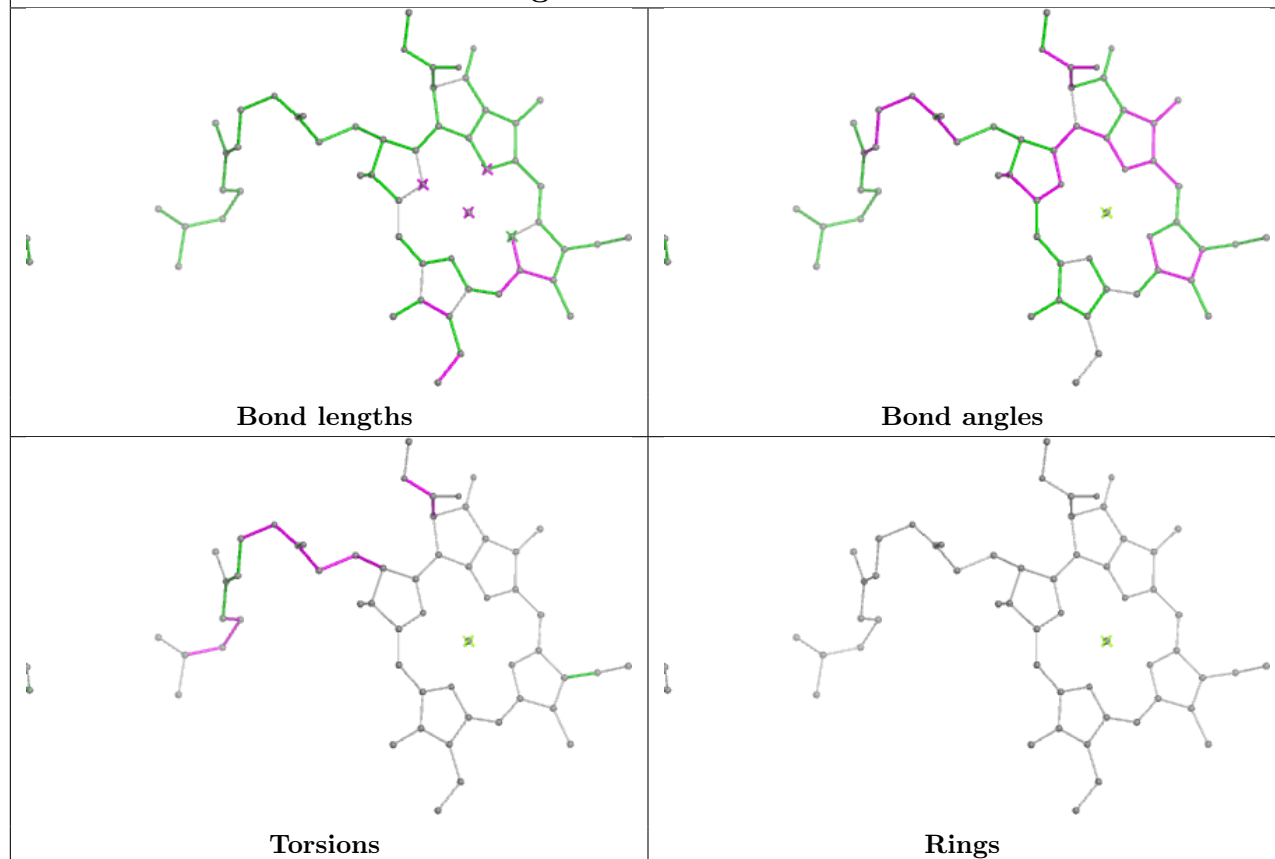
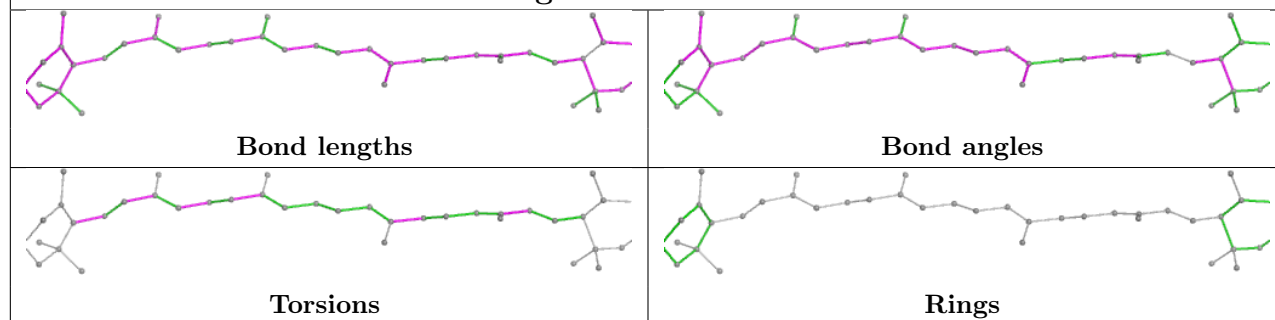
Bond angles



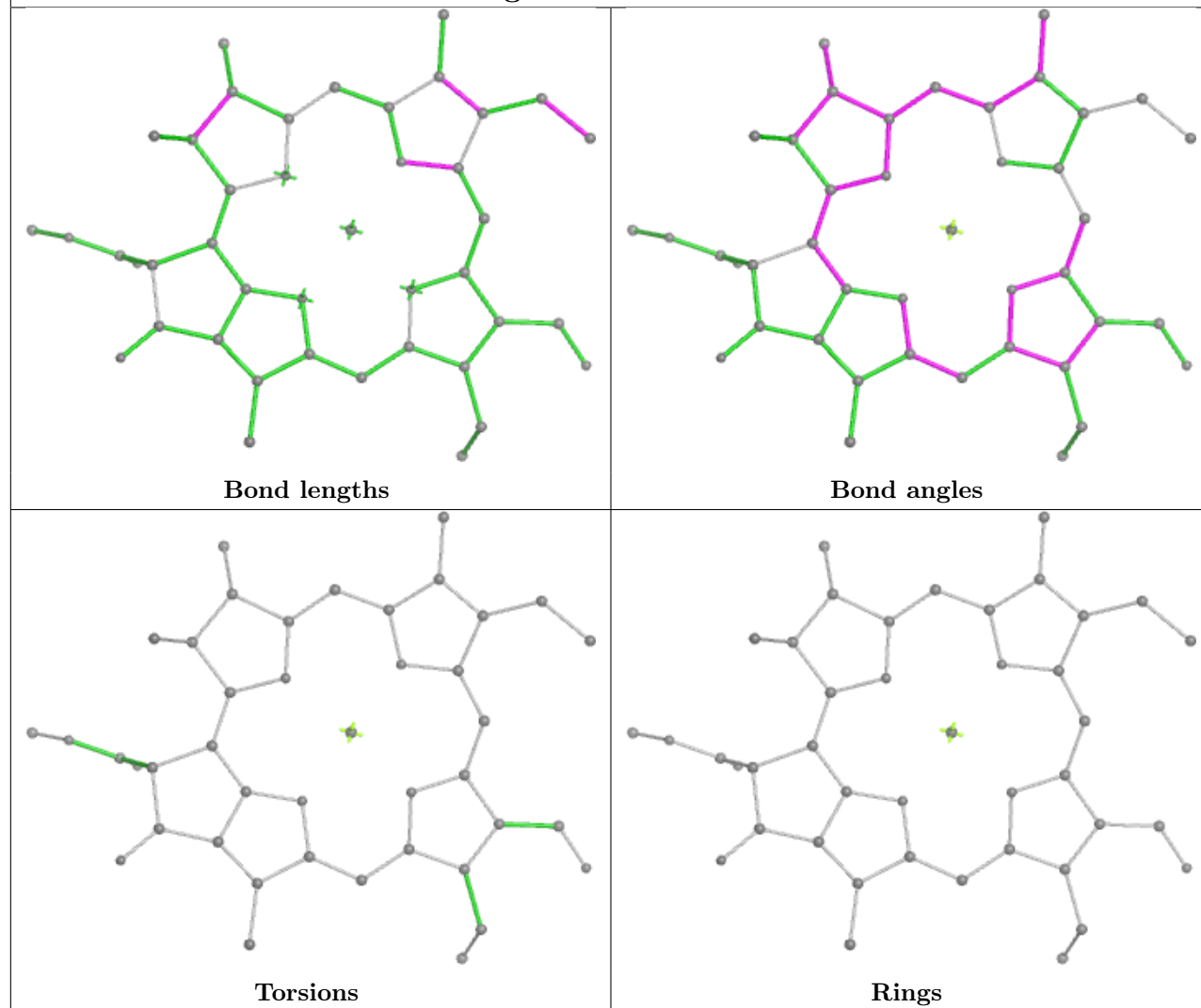
Torsions



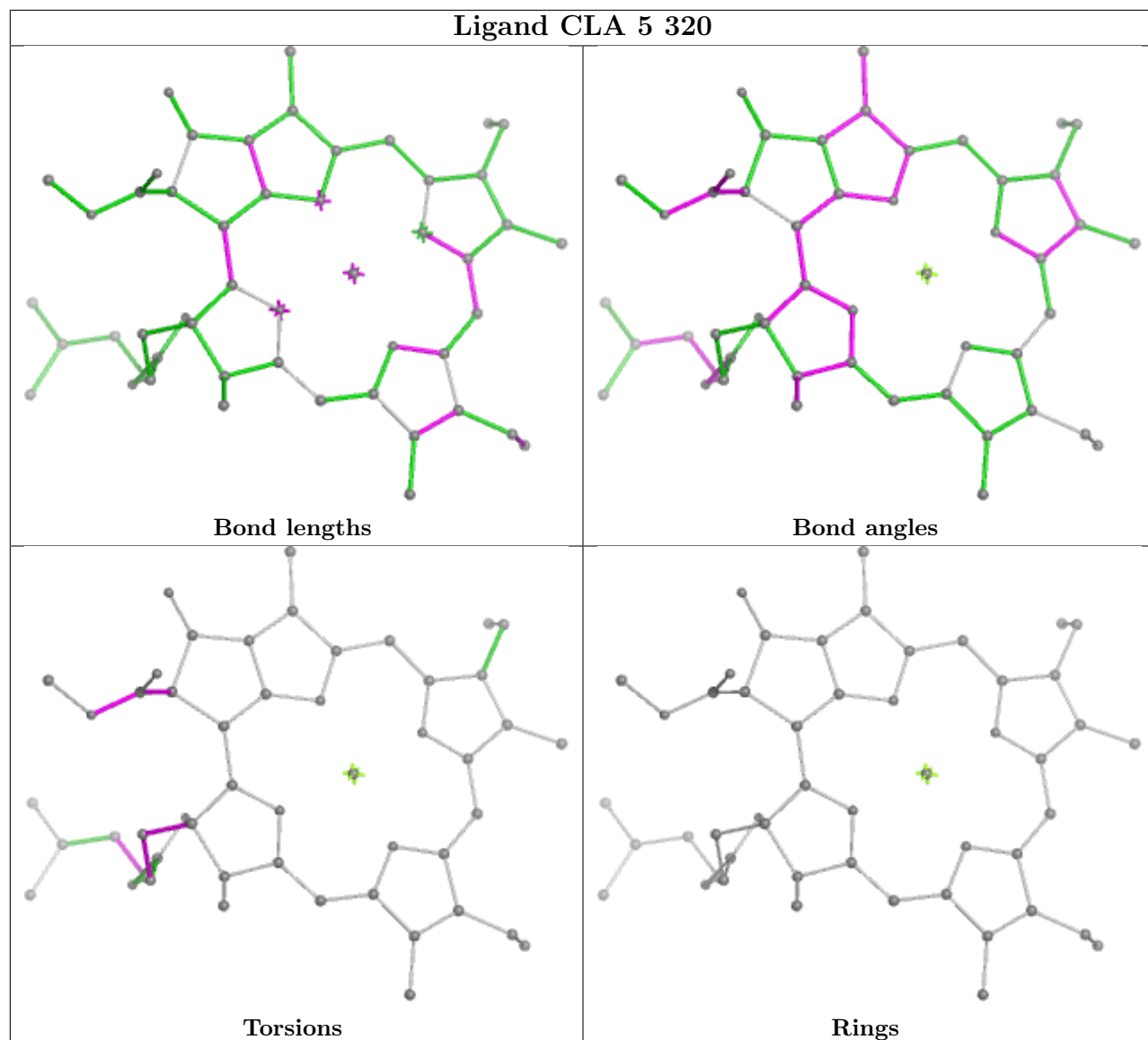
Rings

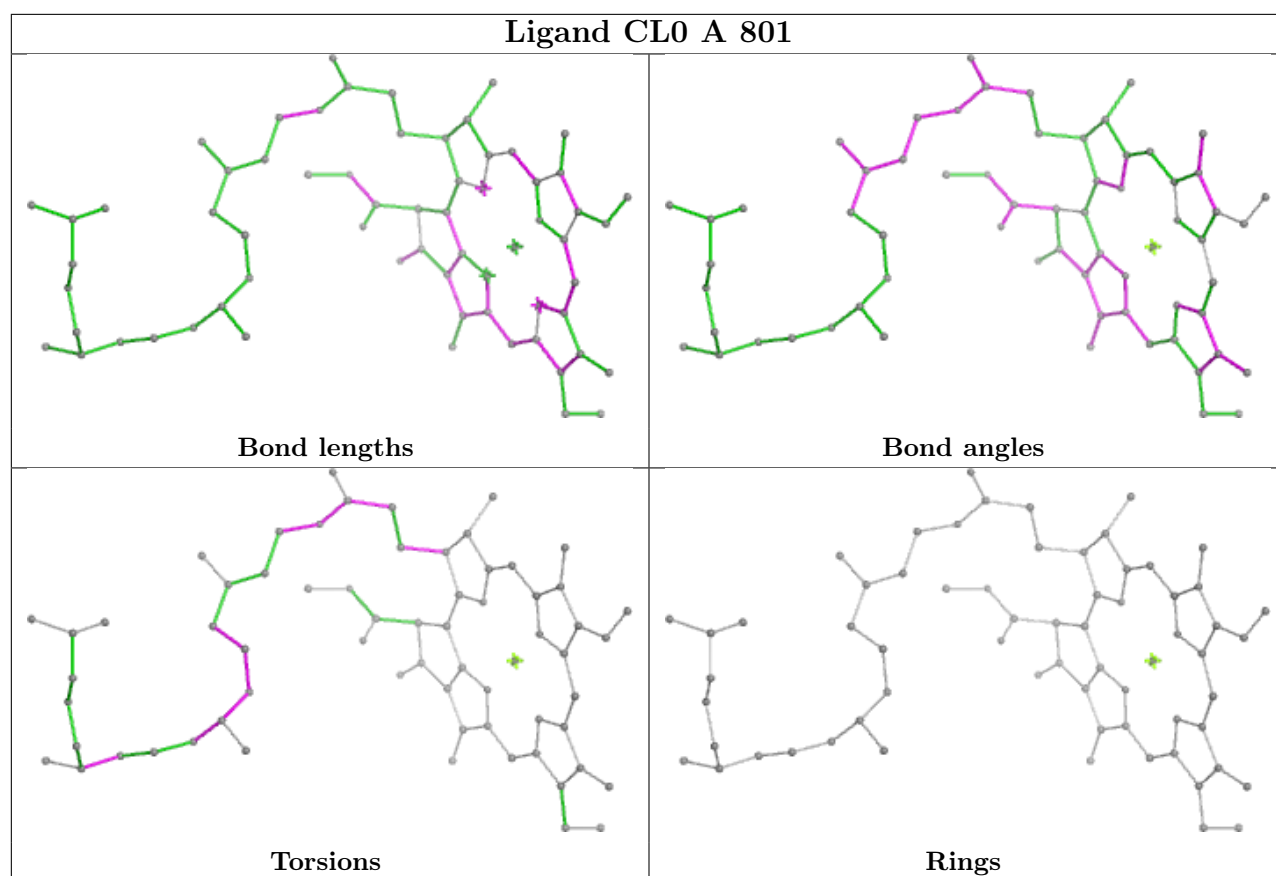
Ligand CLA B 812**Ligand LUT 7 301**

Ligand CHL 9 314

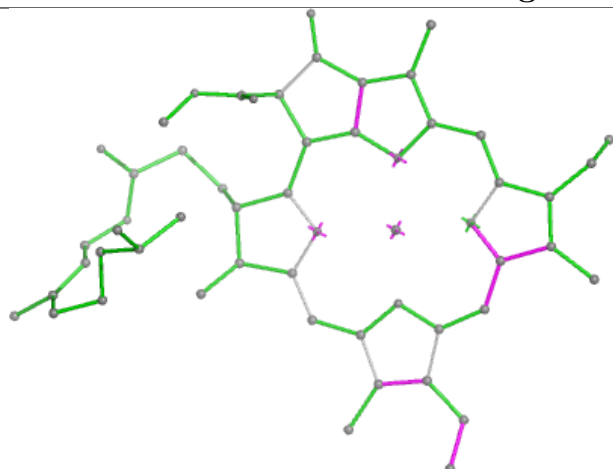


Ligand CLA 5 320

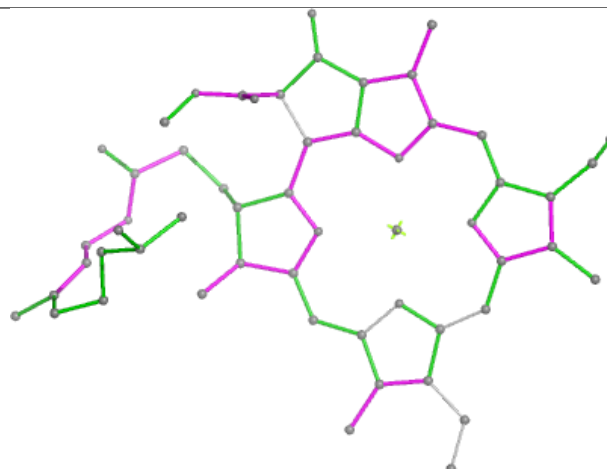




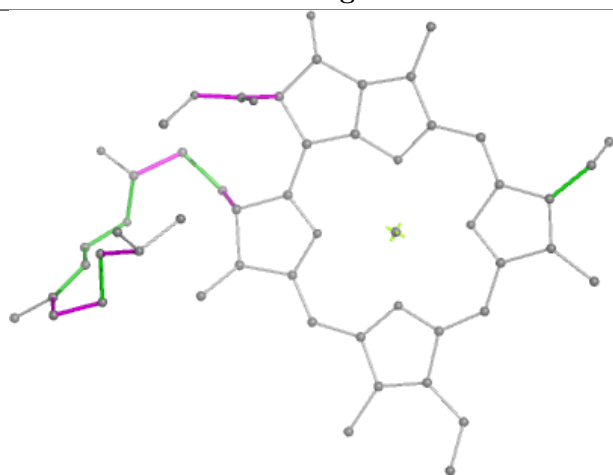
Ligand CLA 5 311



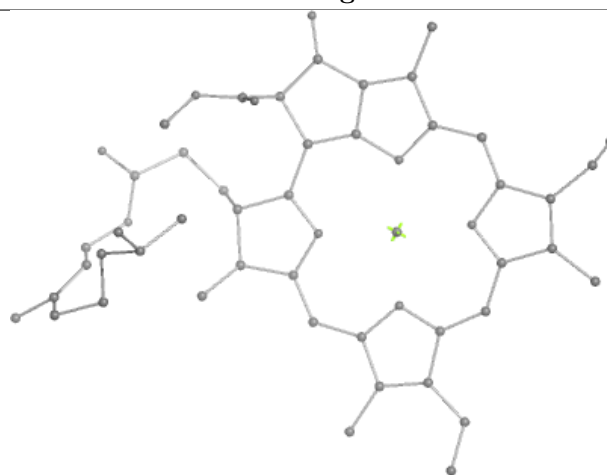
Bond lengths



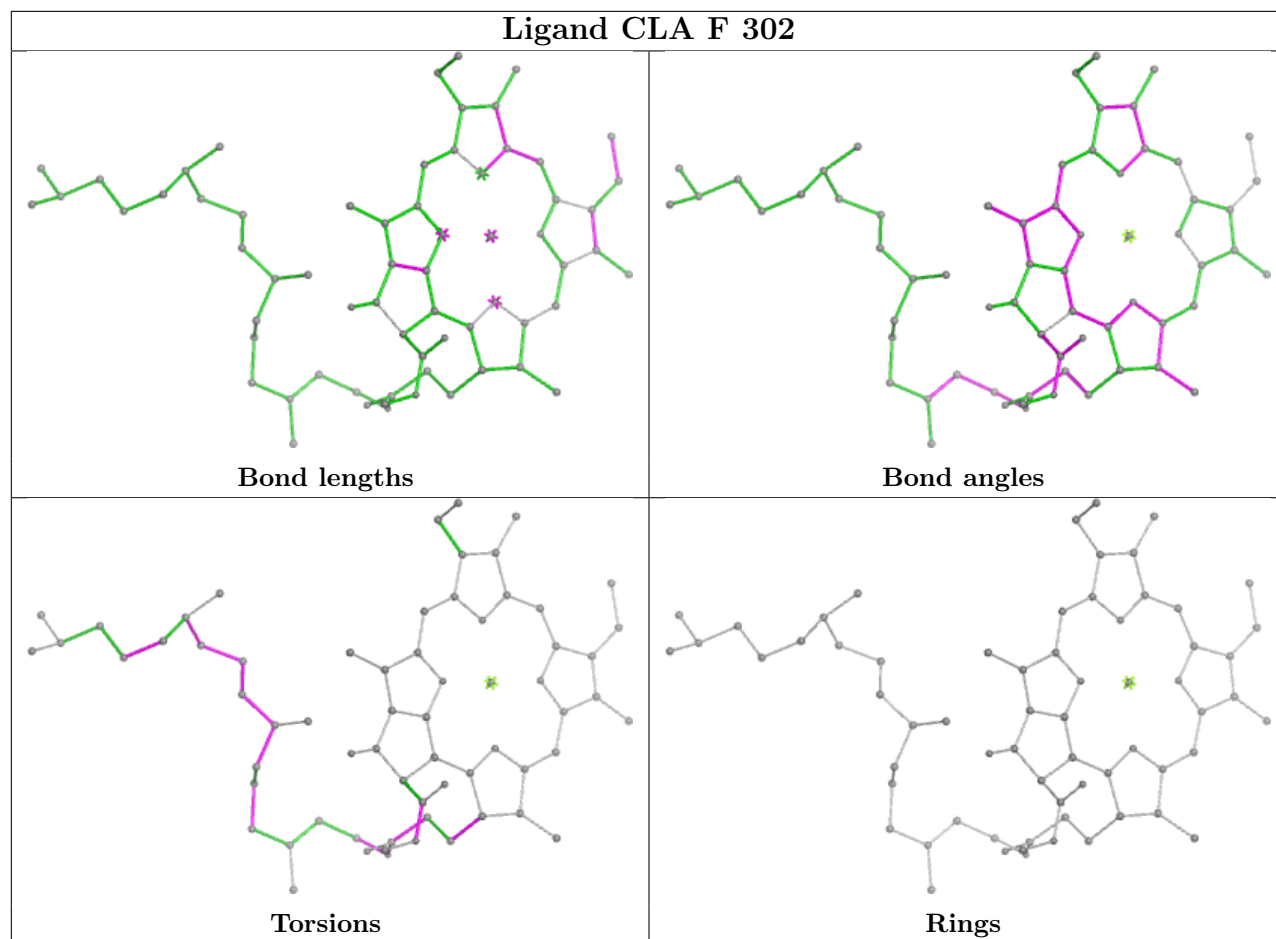
Bond angles



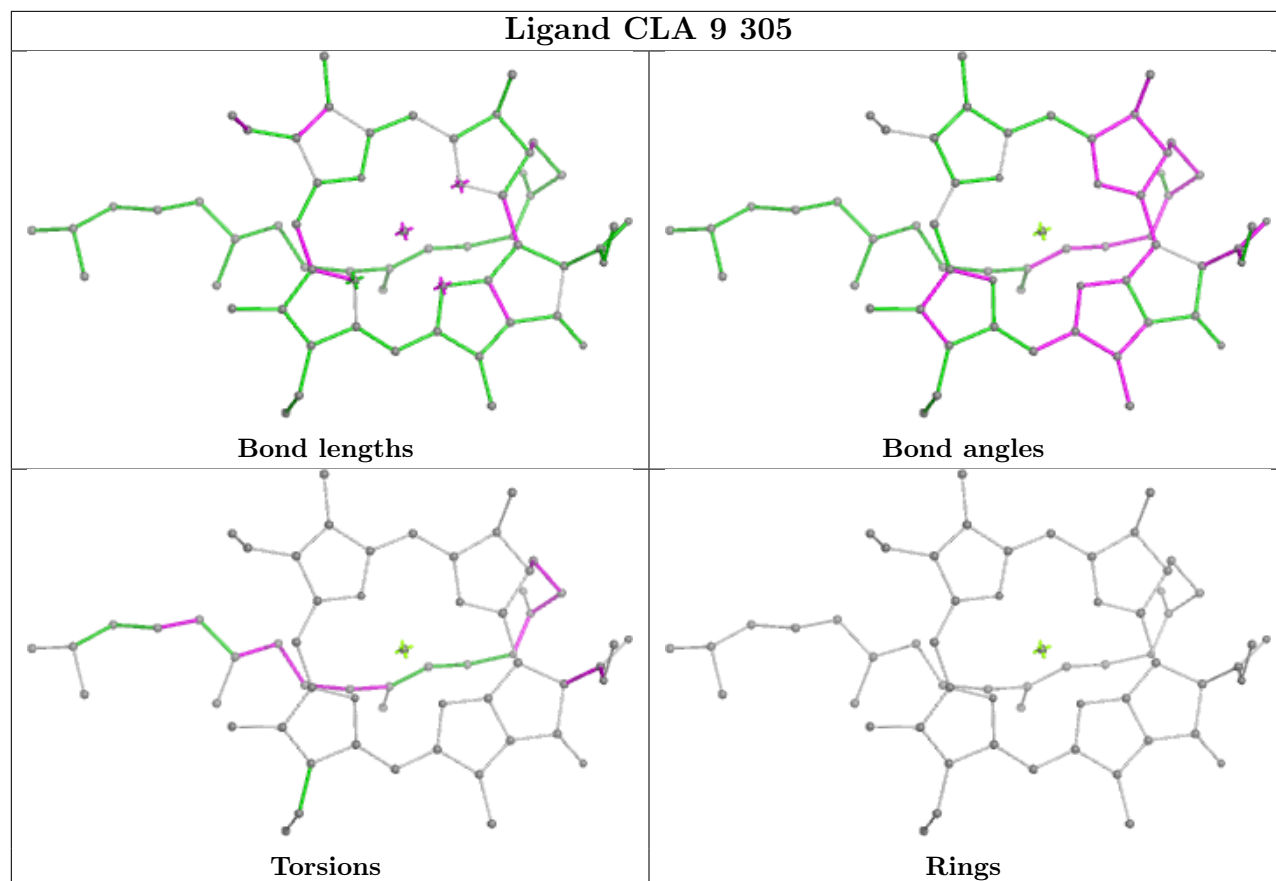
Torsions



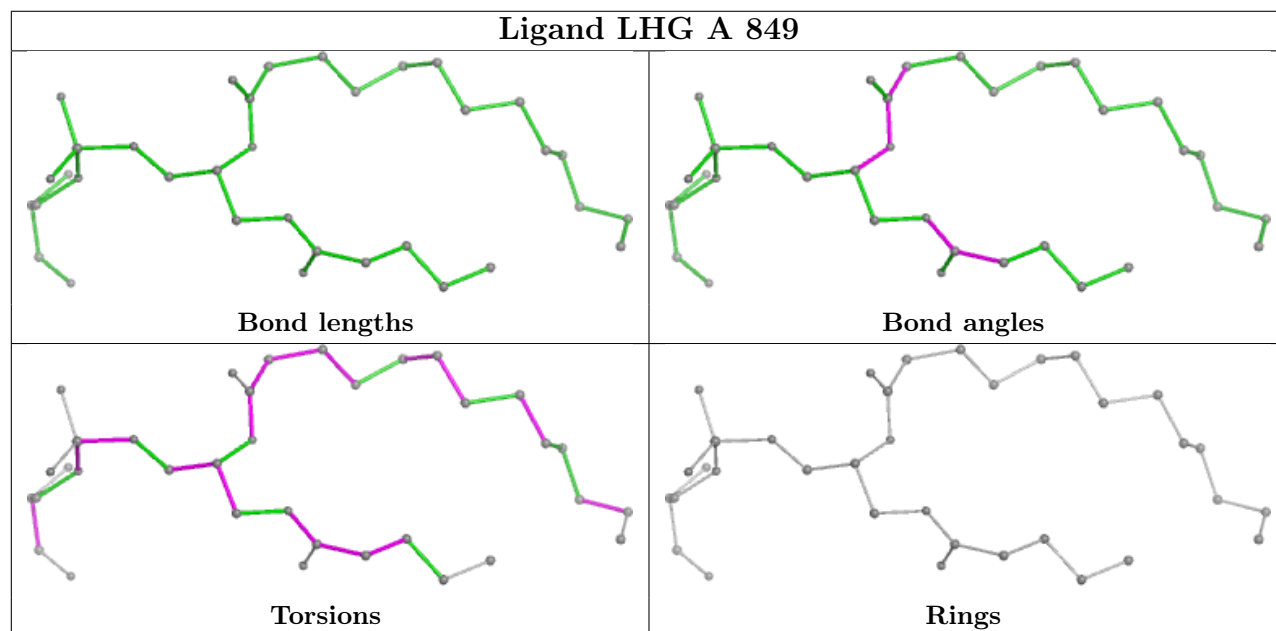
Rings

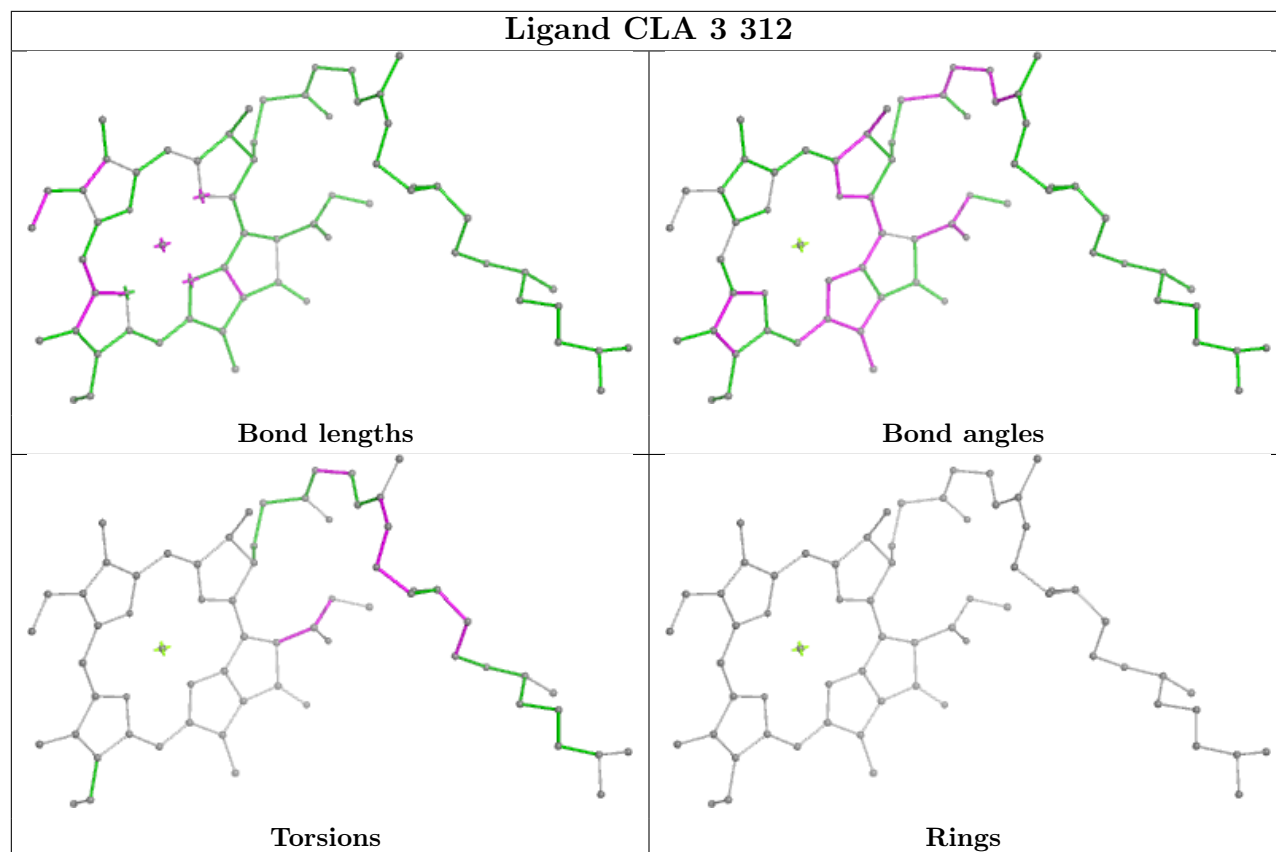
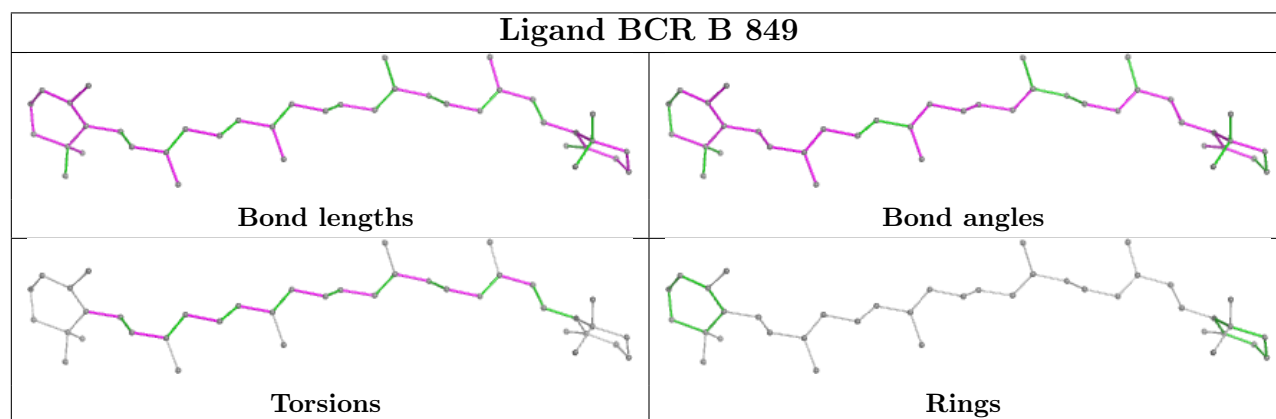
Ligand CLA F 302

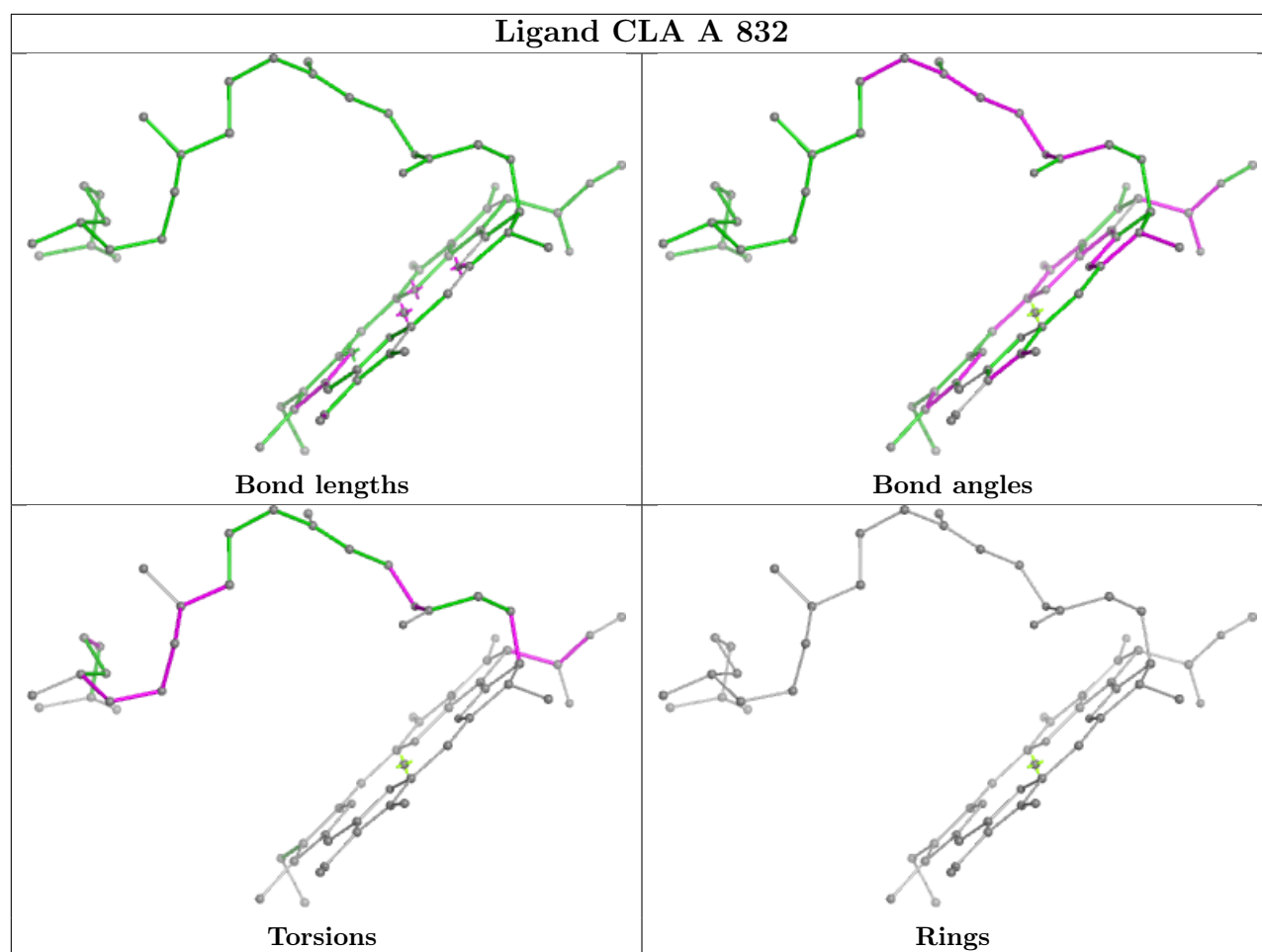
Ligand CLA 9 305

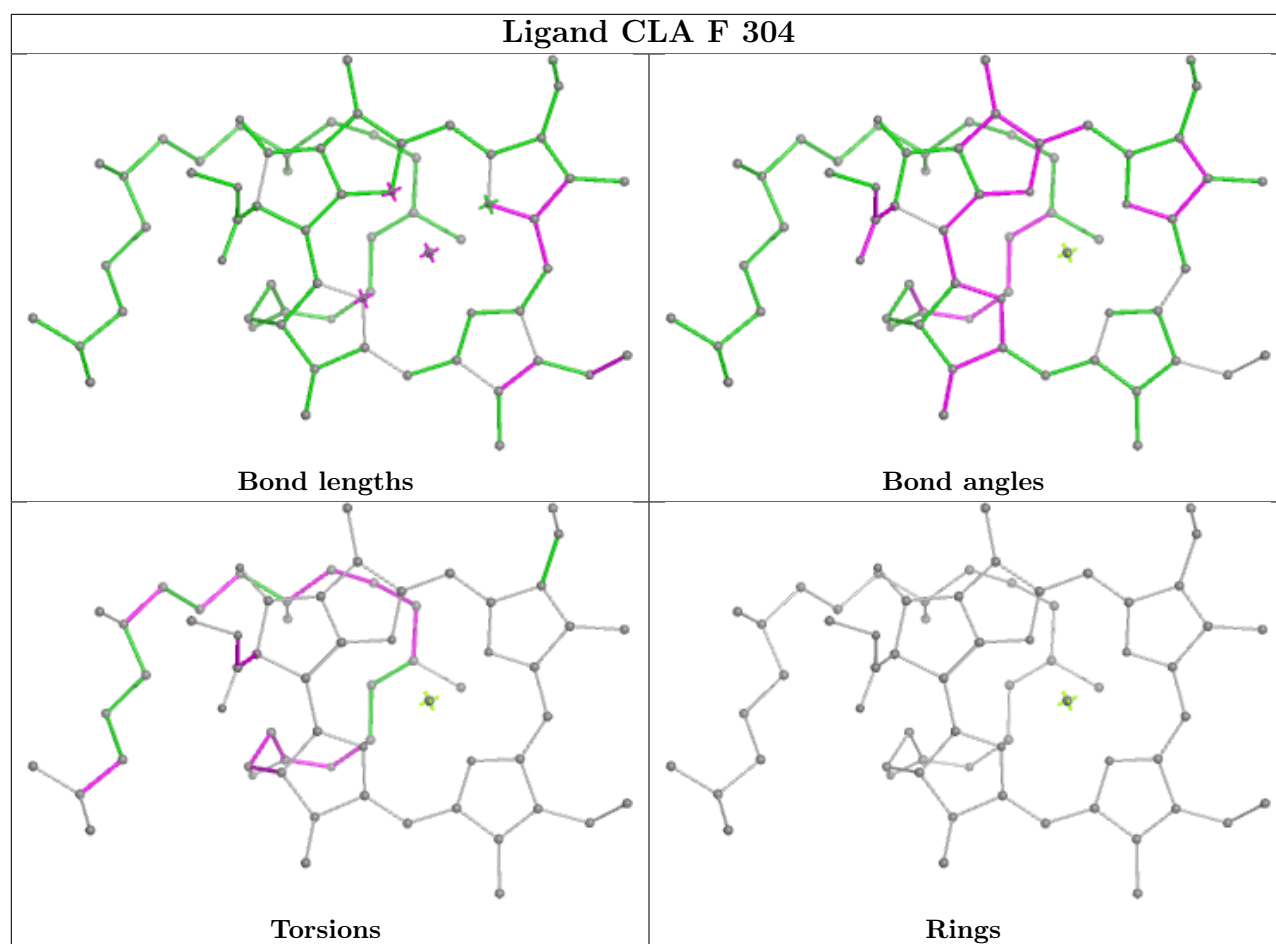


Ligand LHG A 849

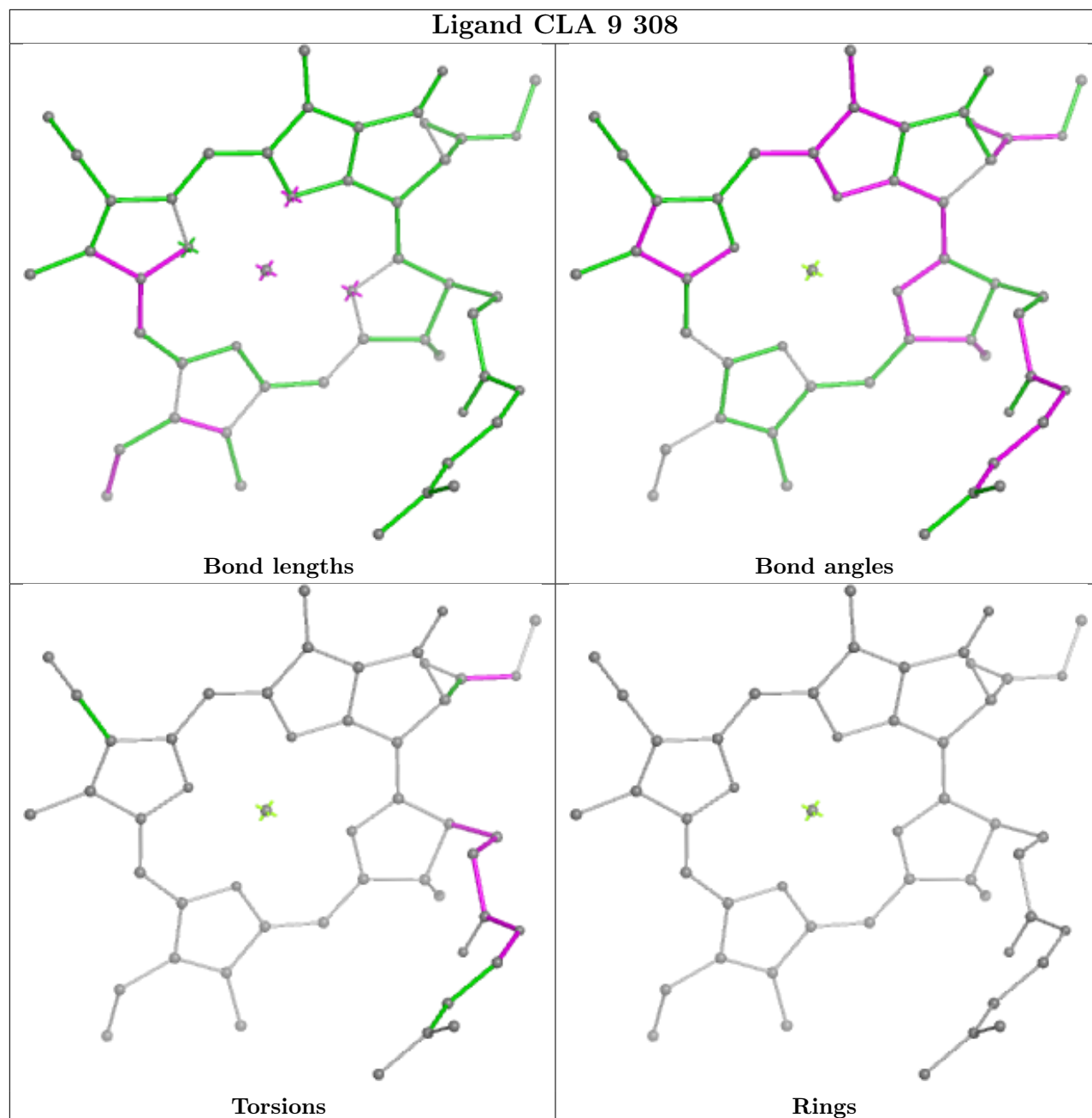


Ligand CLA 3 312**Ligand BCR B 849**

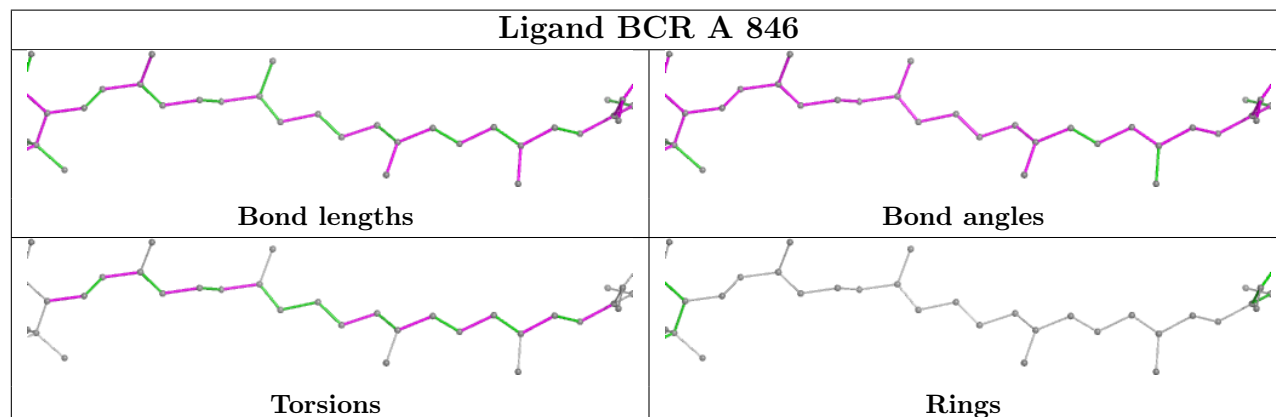


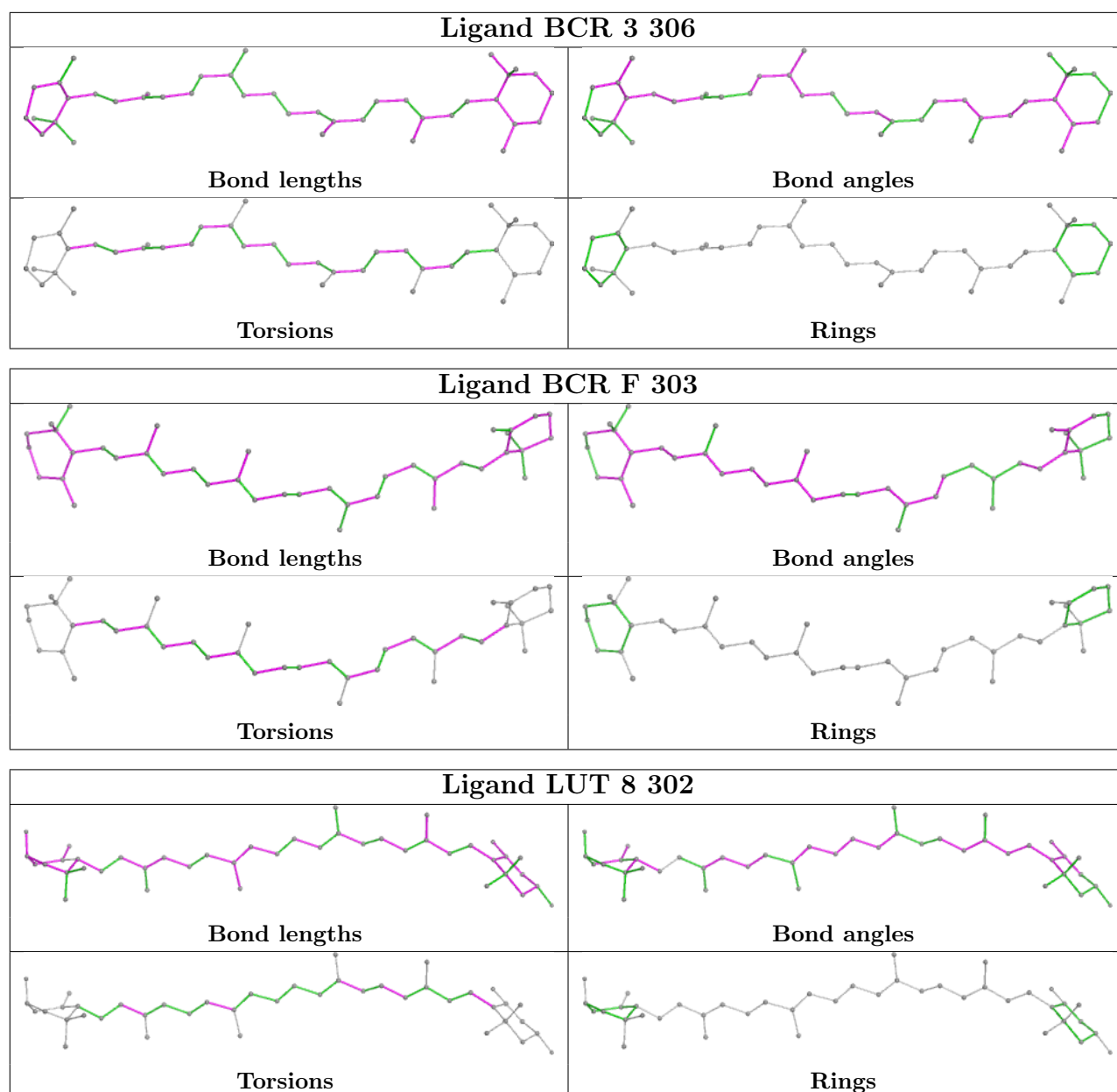


Ligand CLA 9 308

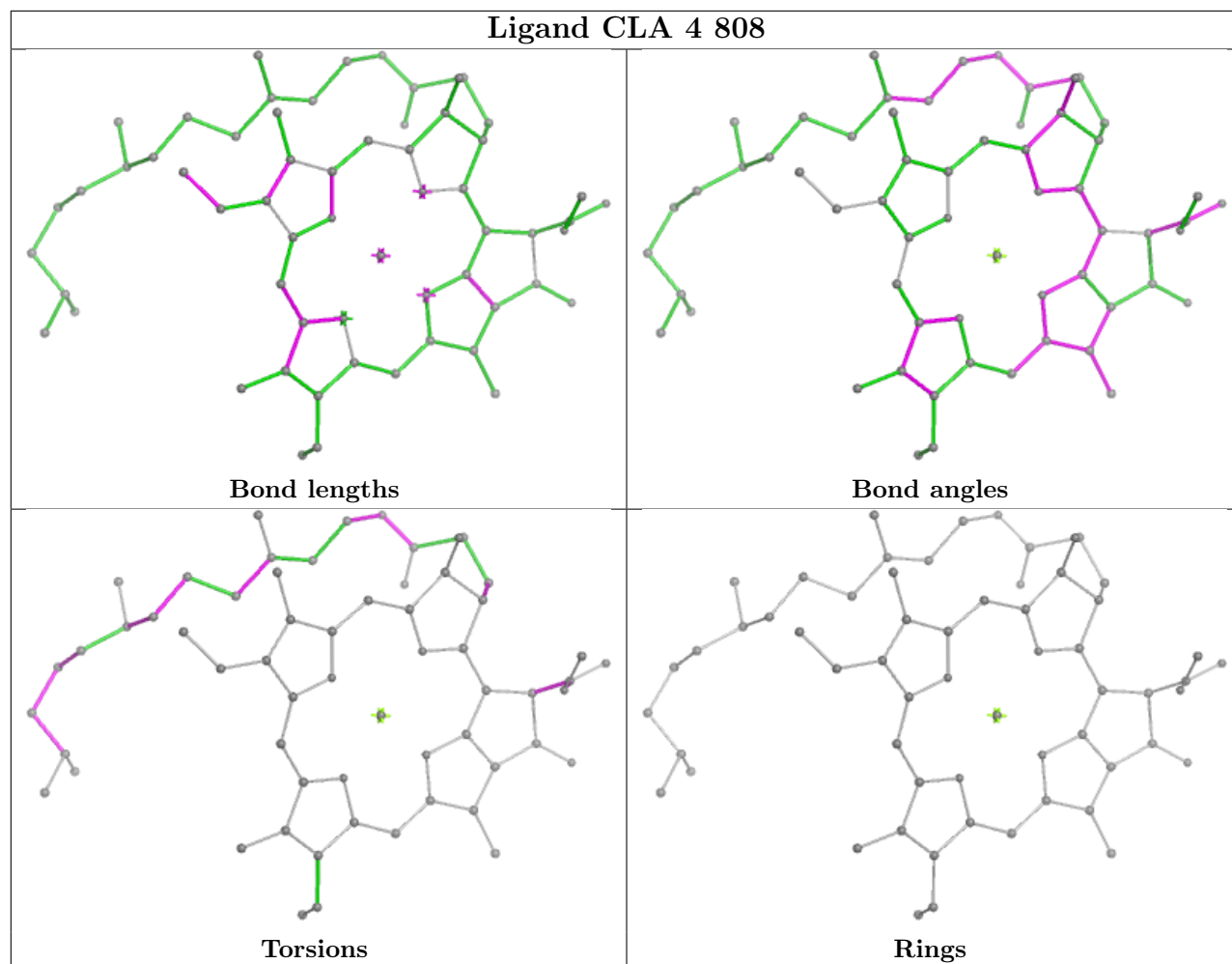


Ligand BCR A 846

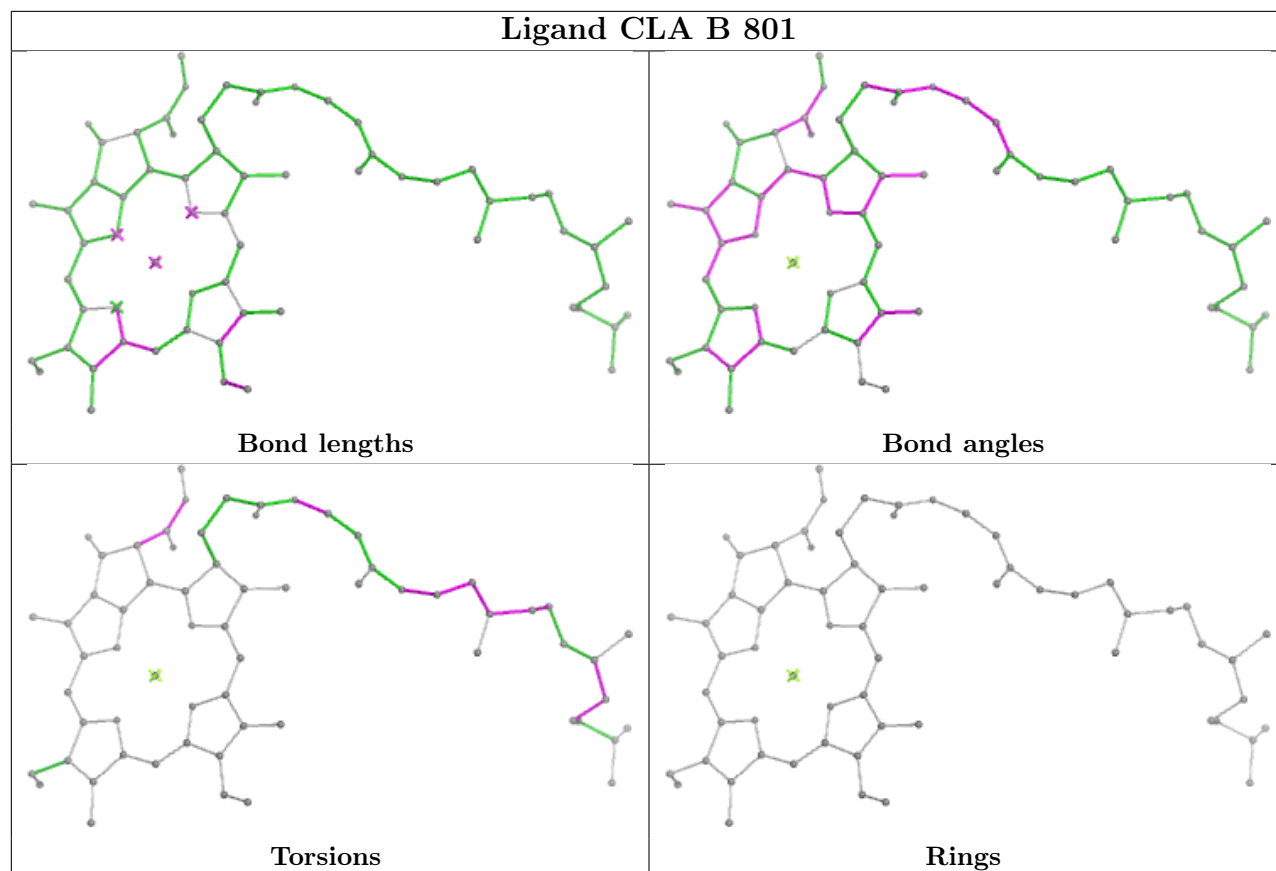




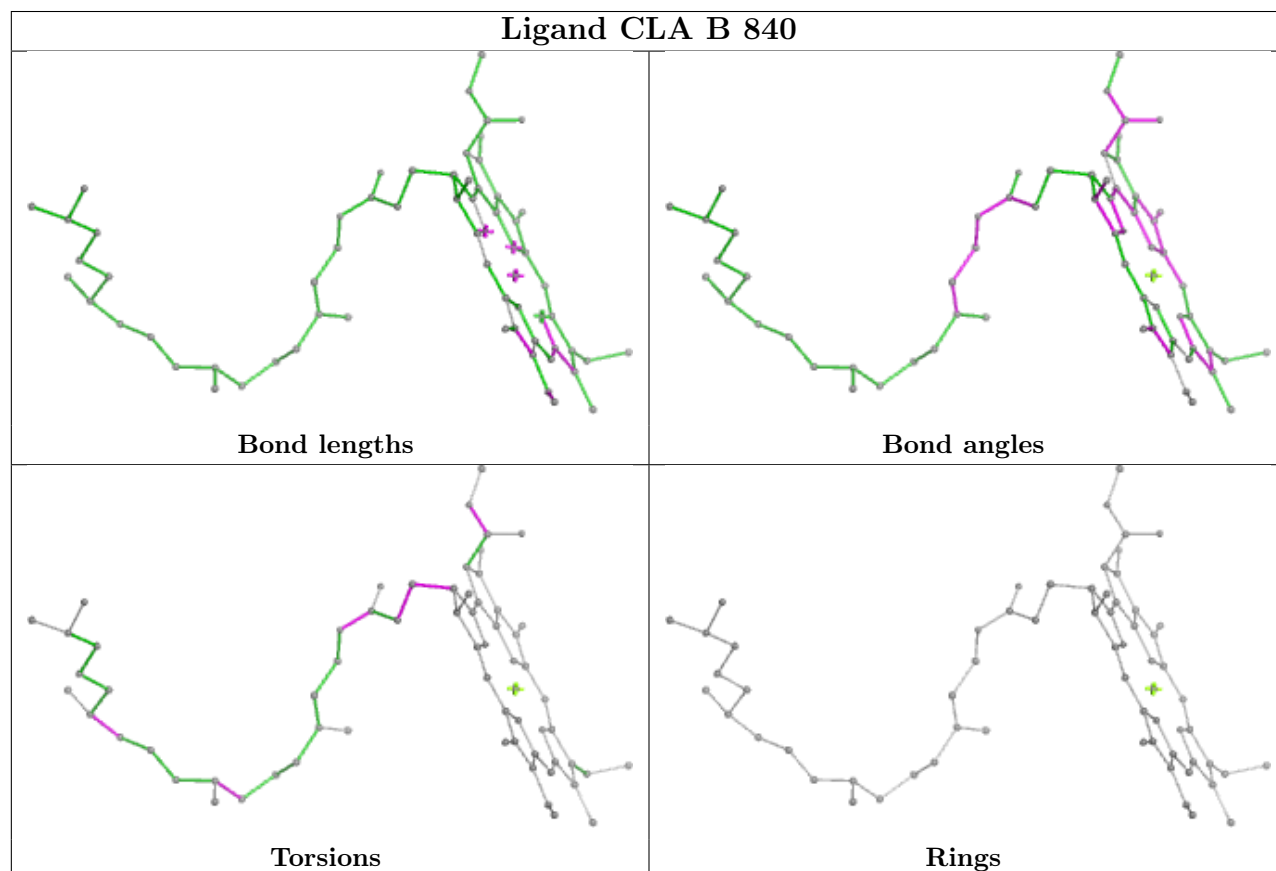
Ligand CLA 4 808



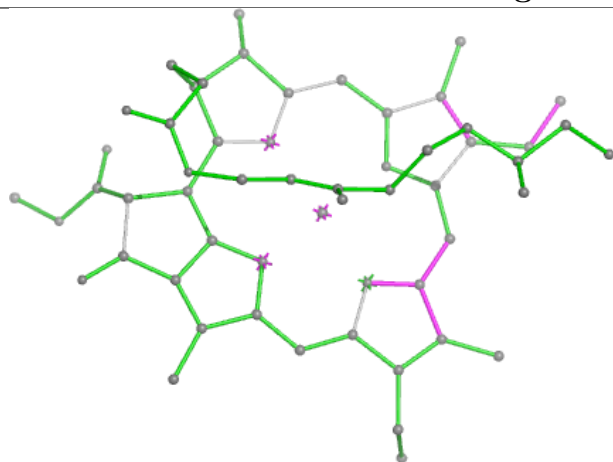
Ligand CLA B 801



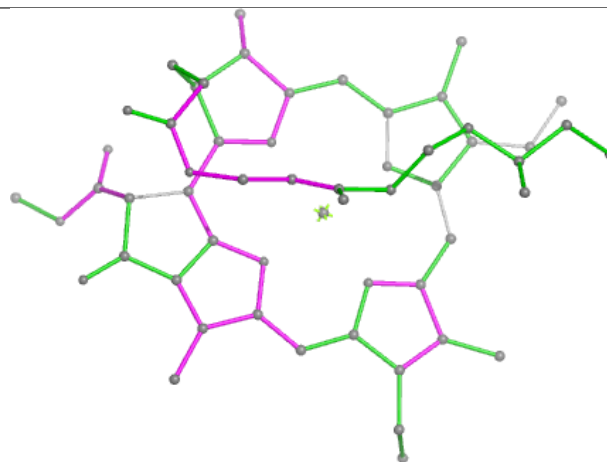
Ligand CLA B 840



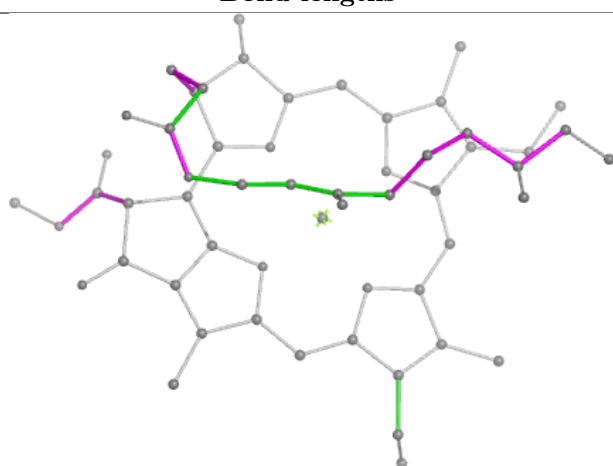
Ligand CLA B 813



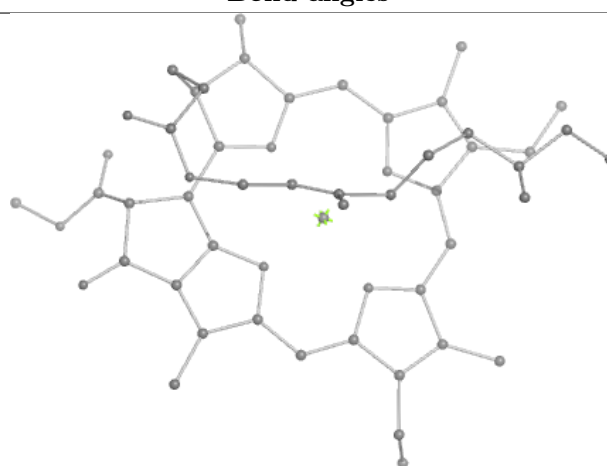
Bond lengths



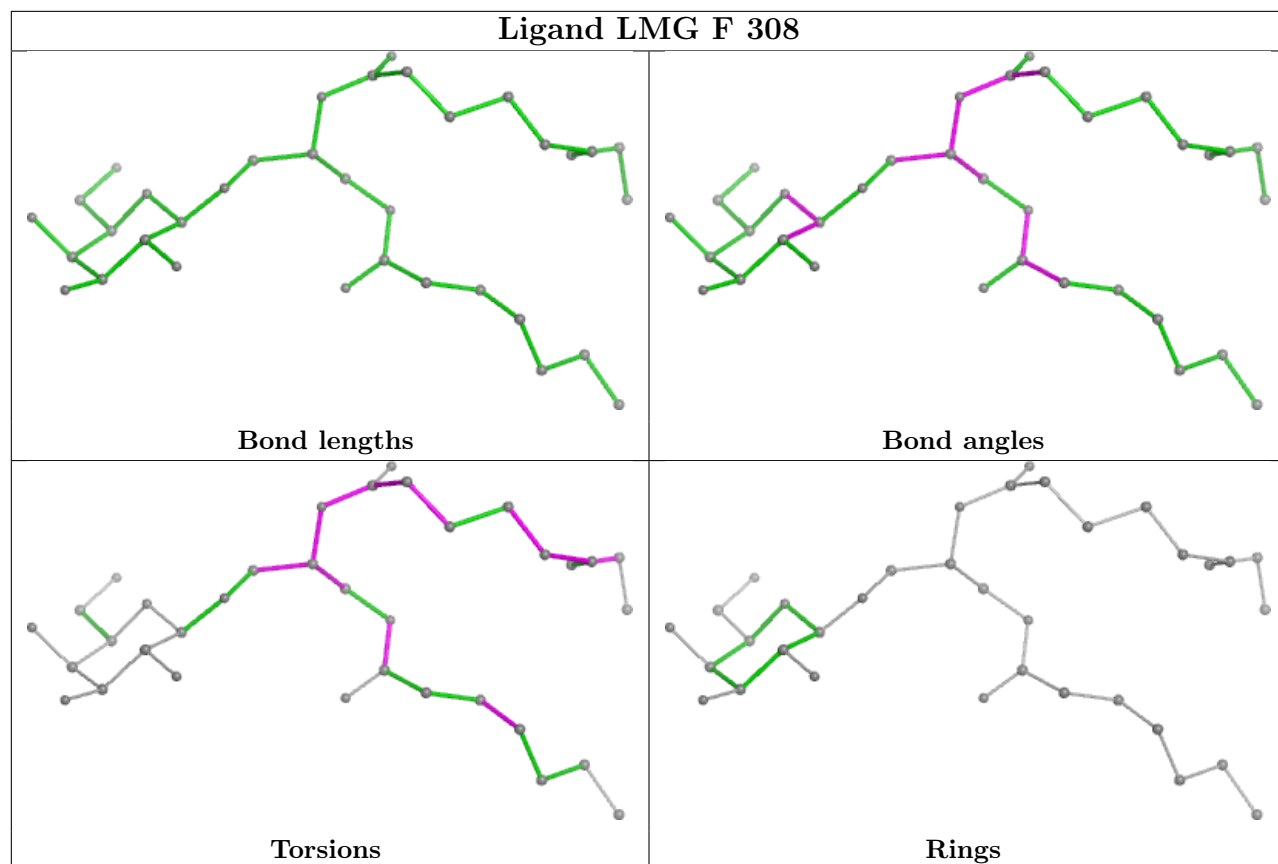
Bond angles



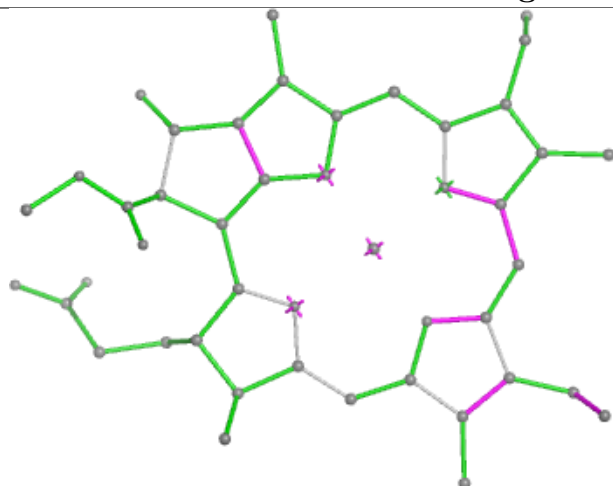
Torsions



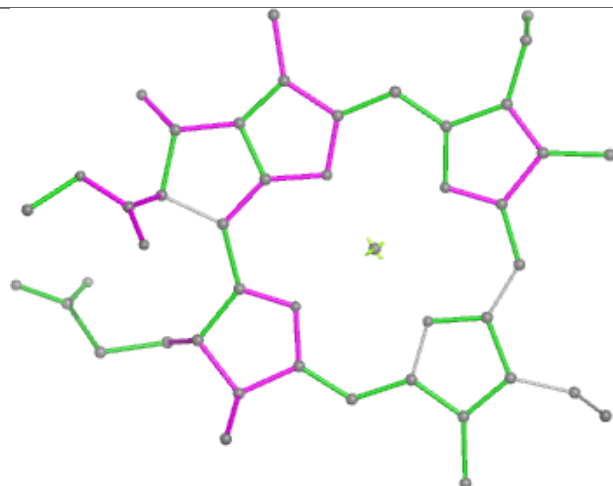
Rings



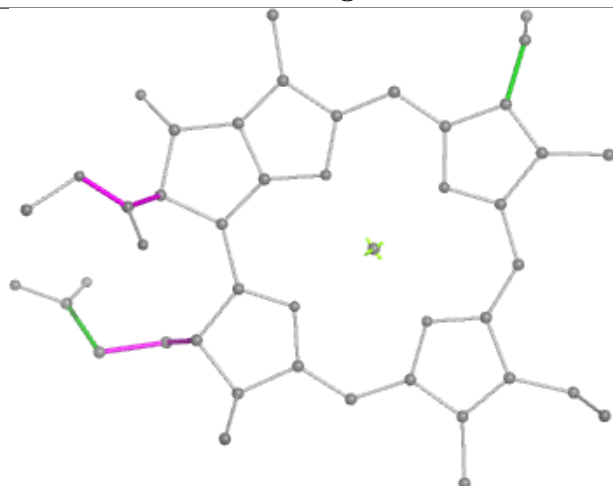
Ligand CLA 3 315



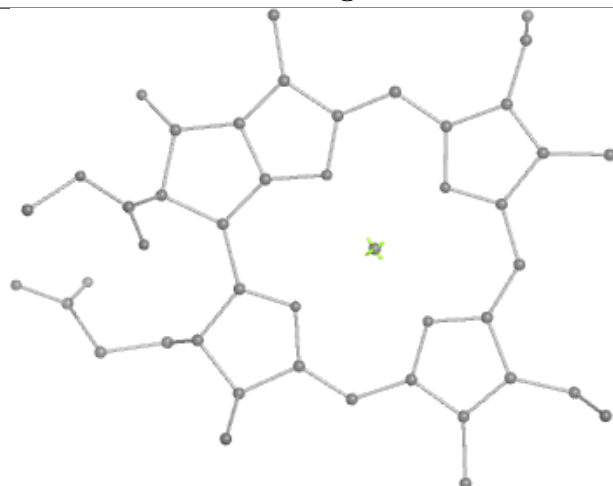
Bond lengths



Bond angles

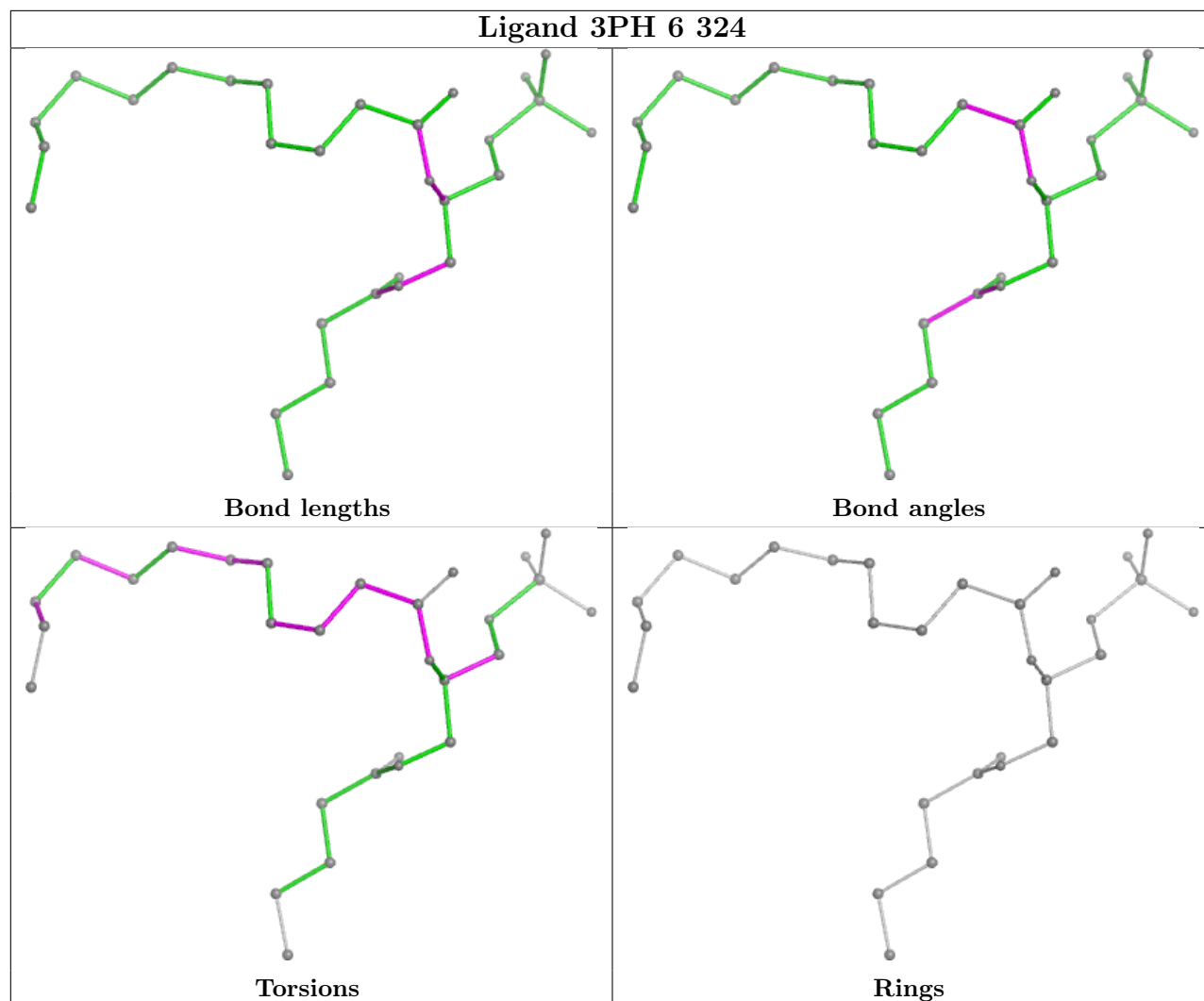


Torsions

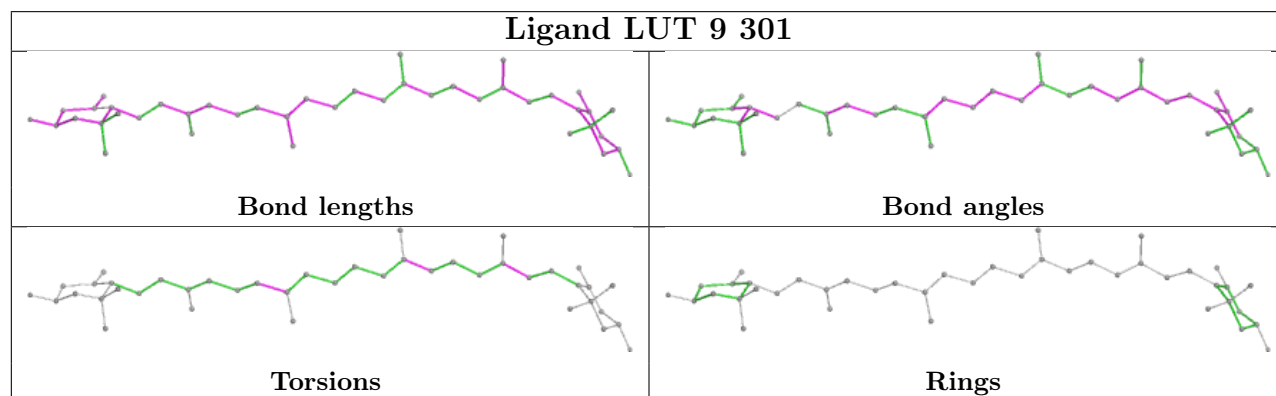


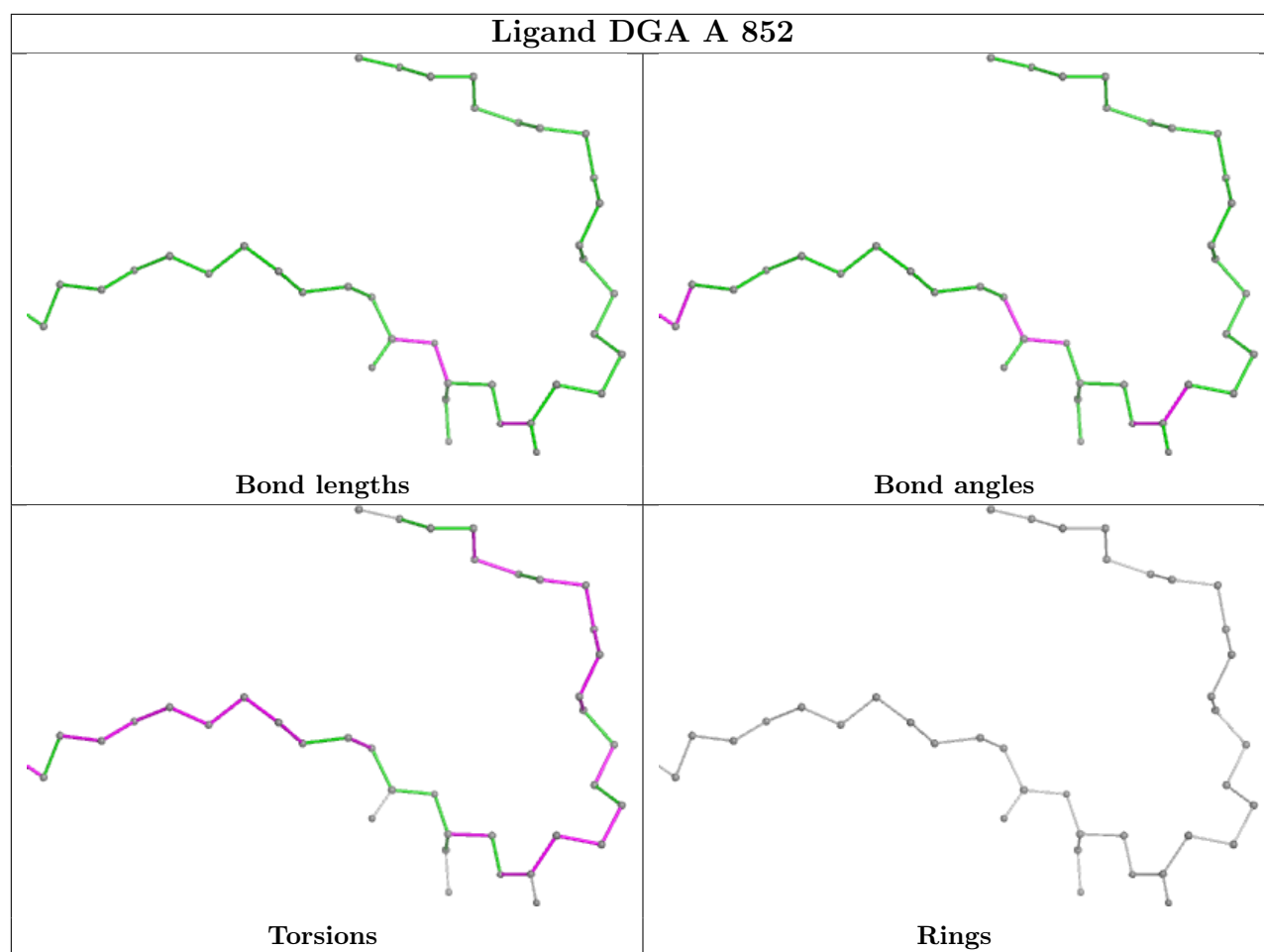
Rings

Ligand 3PH 6 324

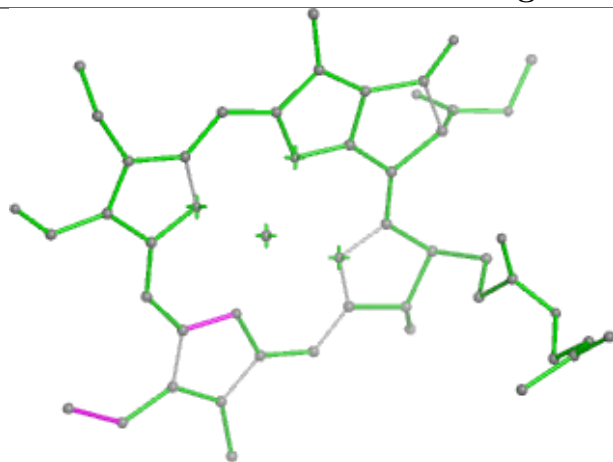


Ligand LUT 9 301

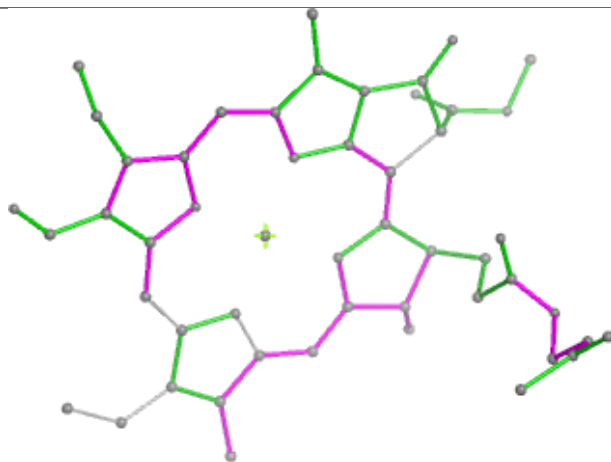




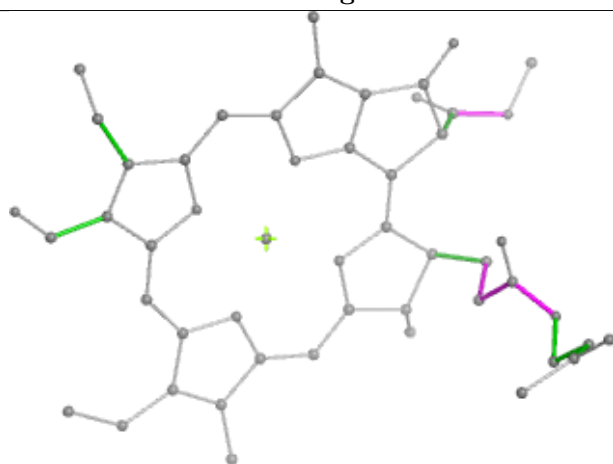
Ligand CHL 2 303



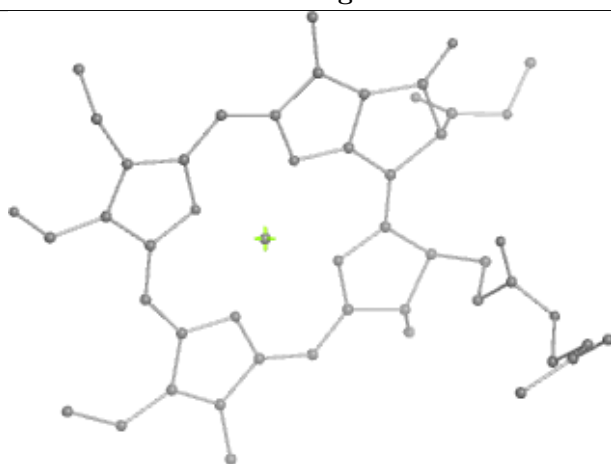
Bond lengths



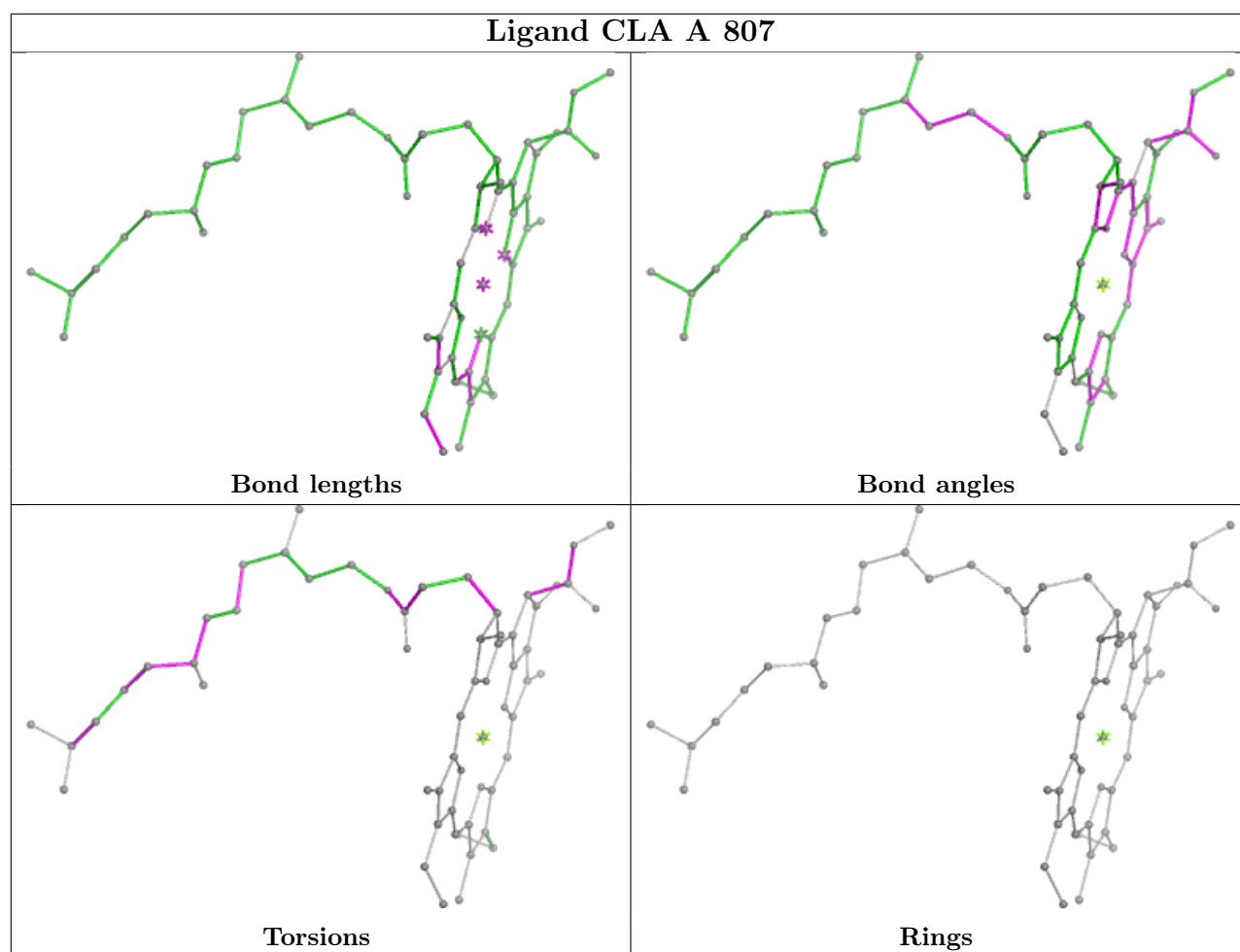
Bond angles



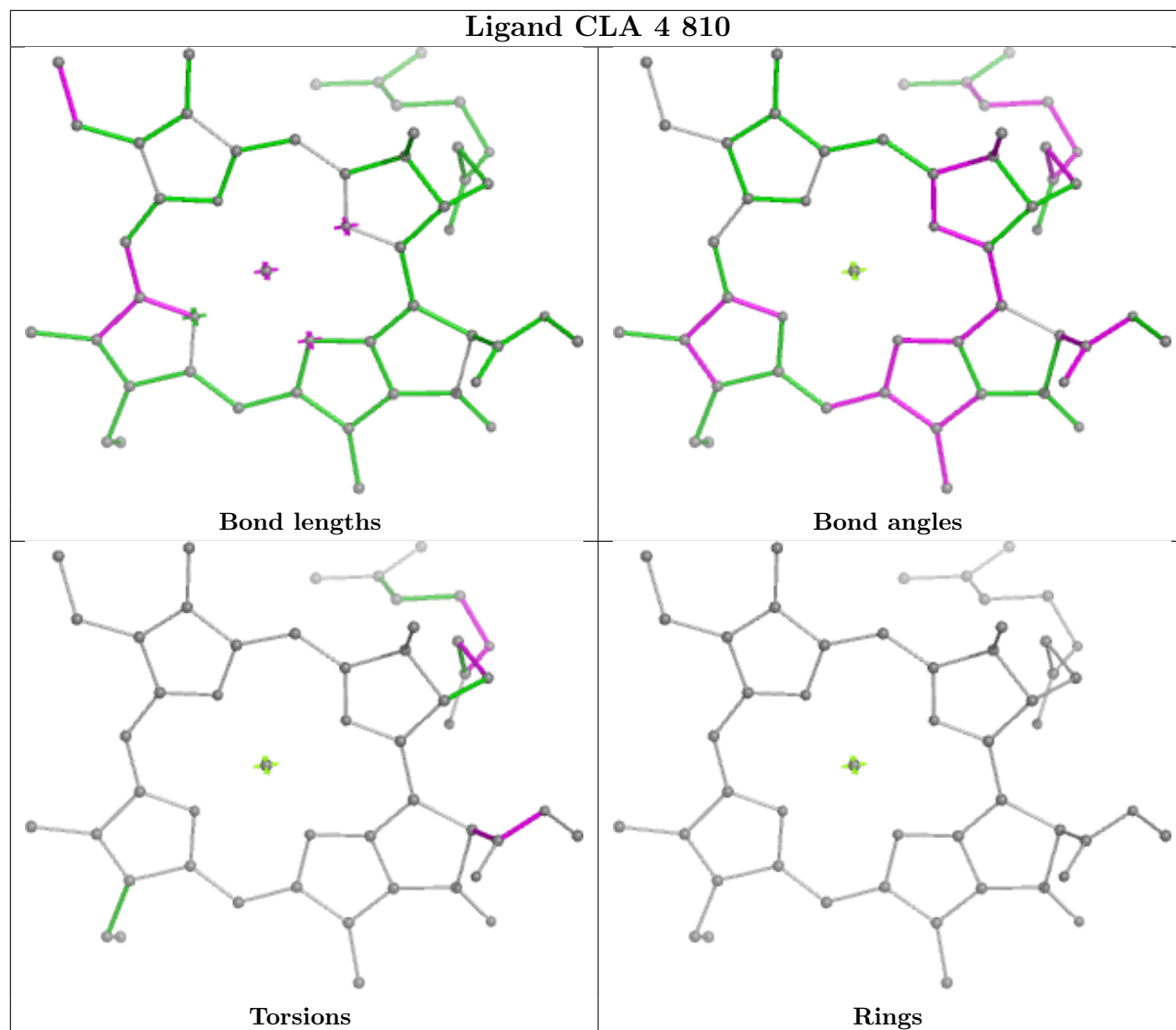
Torsions

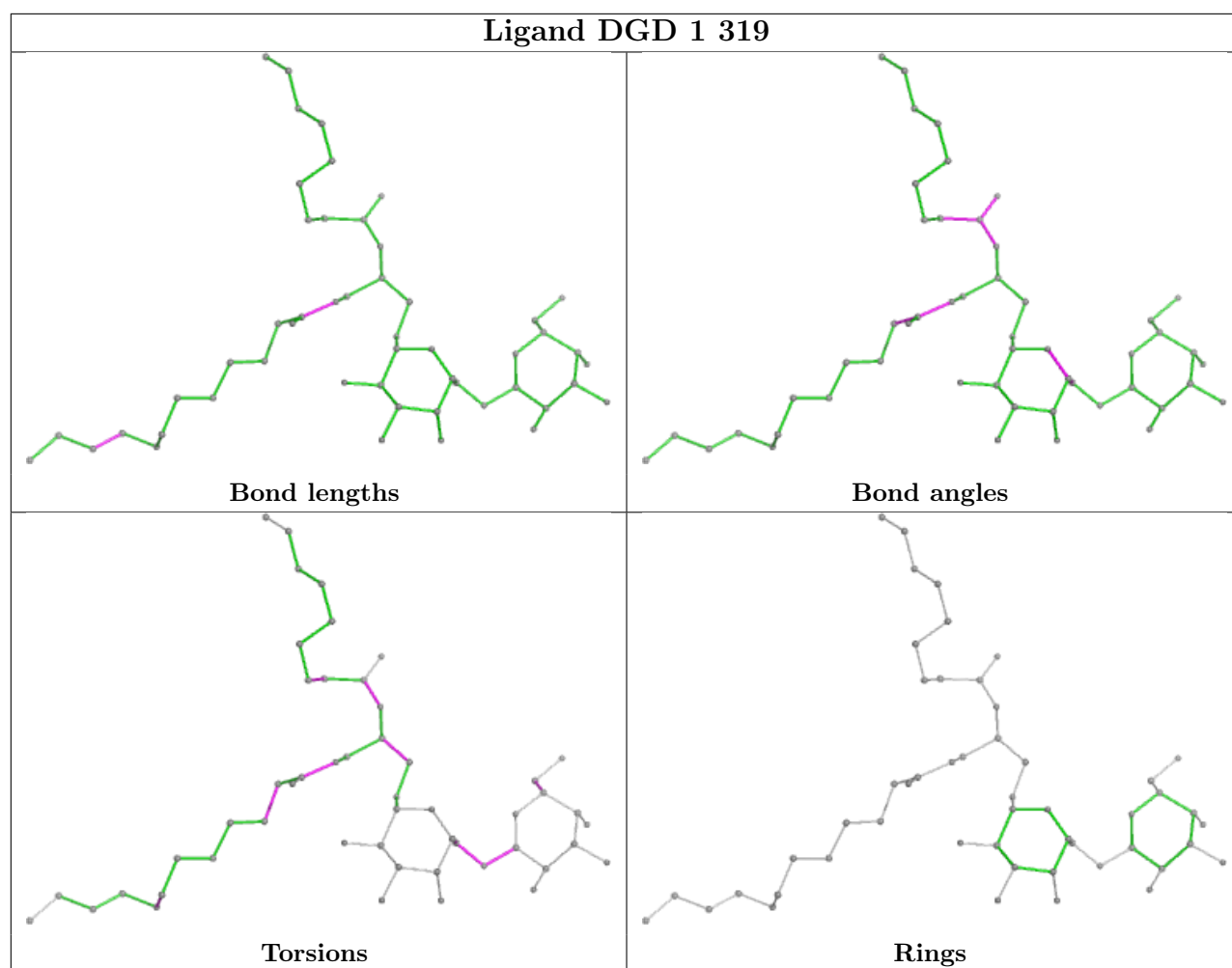


Rings

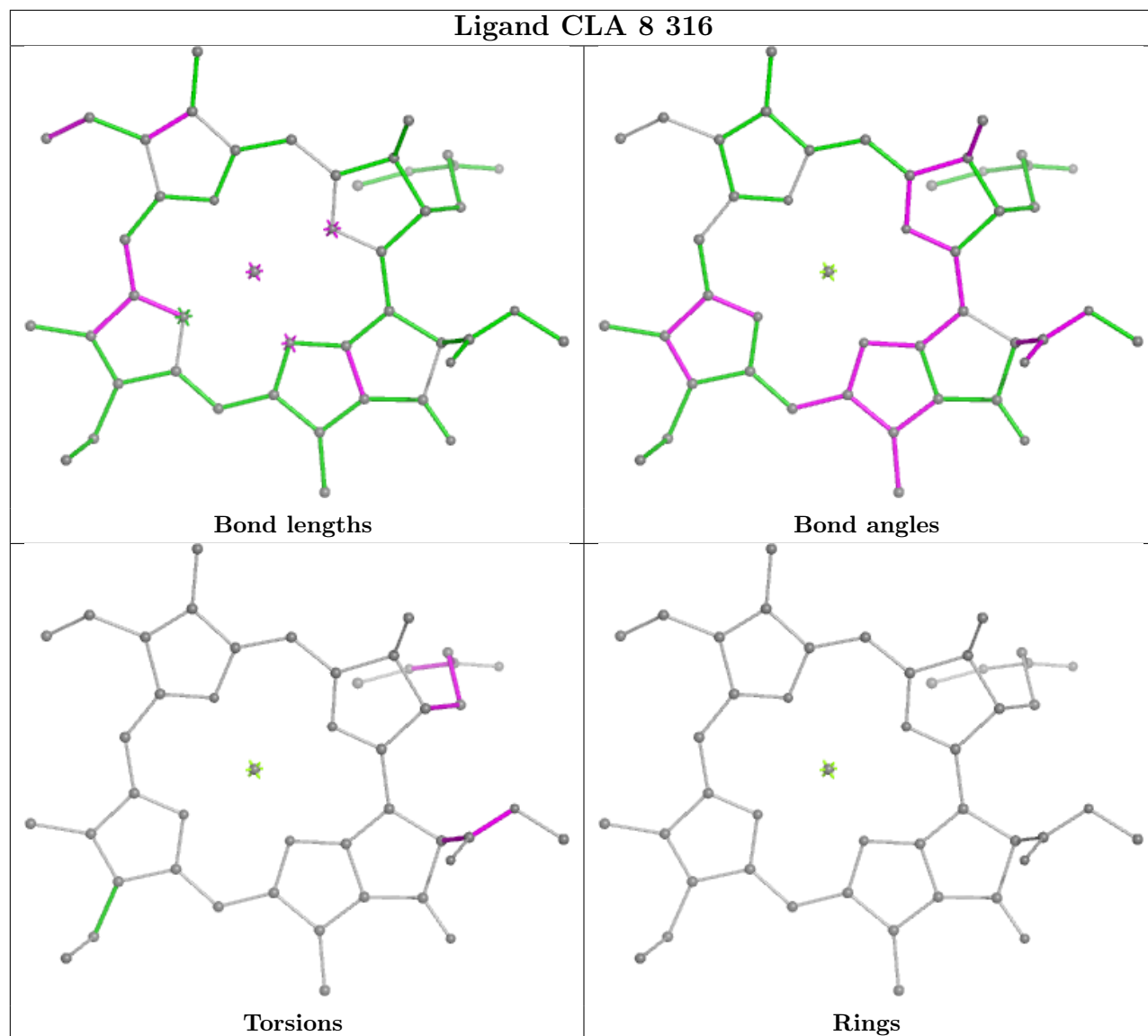


Ligand CLA 4 810

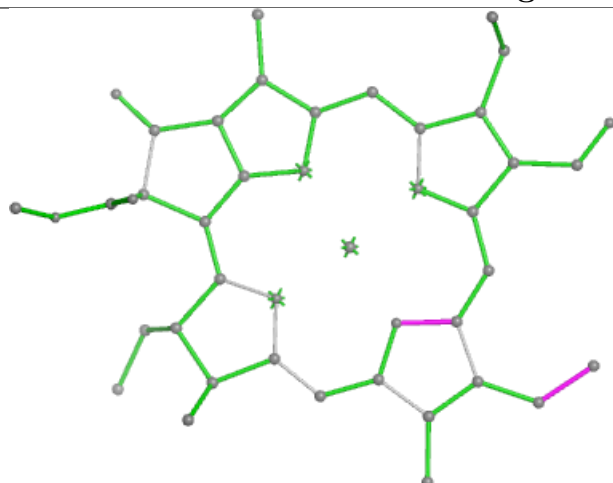




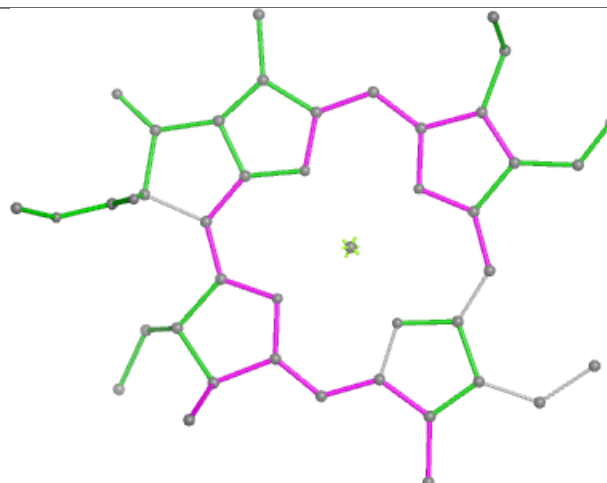
Ligand CLA 8 316



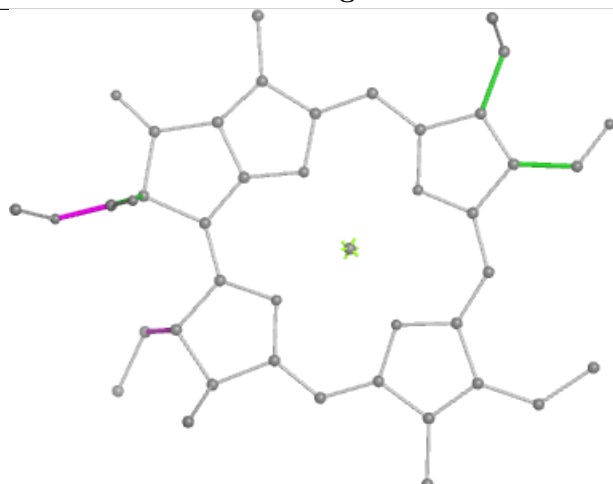
Ligand CHL 5 321



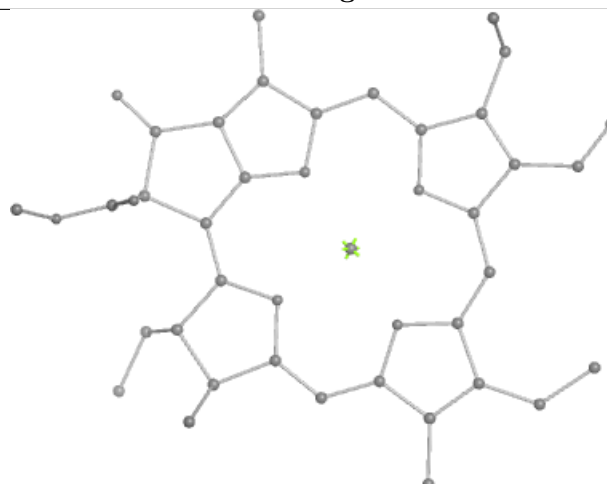
Bond lengths



Bond angles

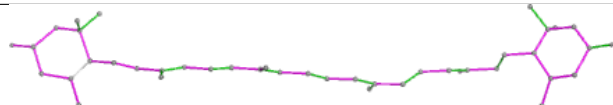


Torsions



Rings

Ligand LUT Z 301



Bond lengths



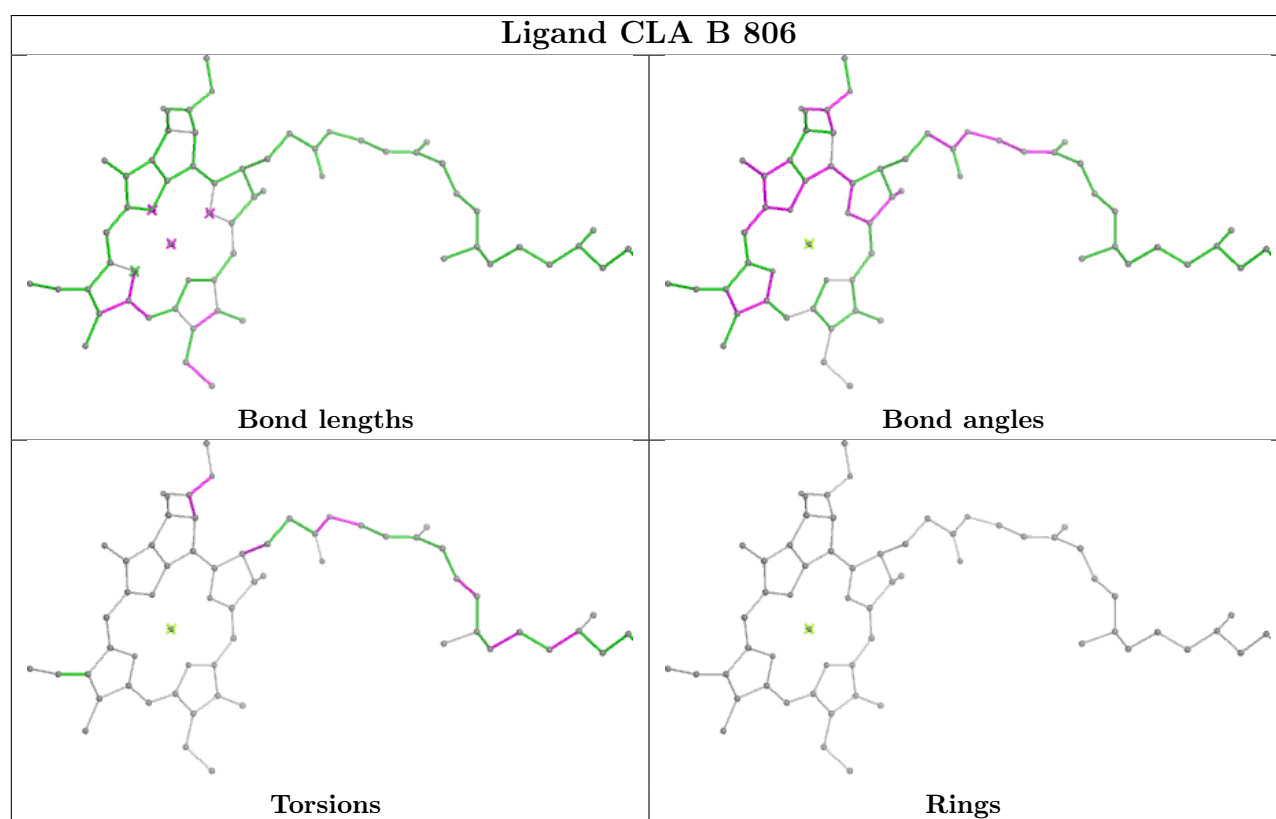
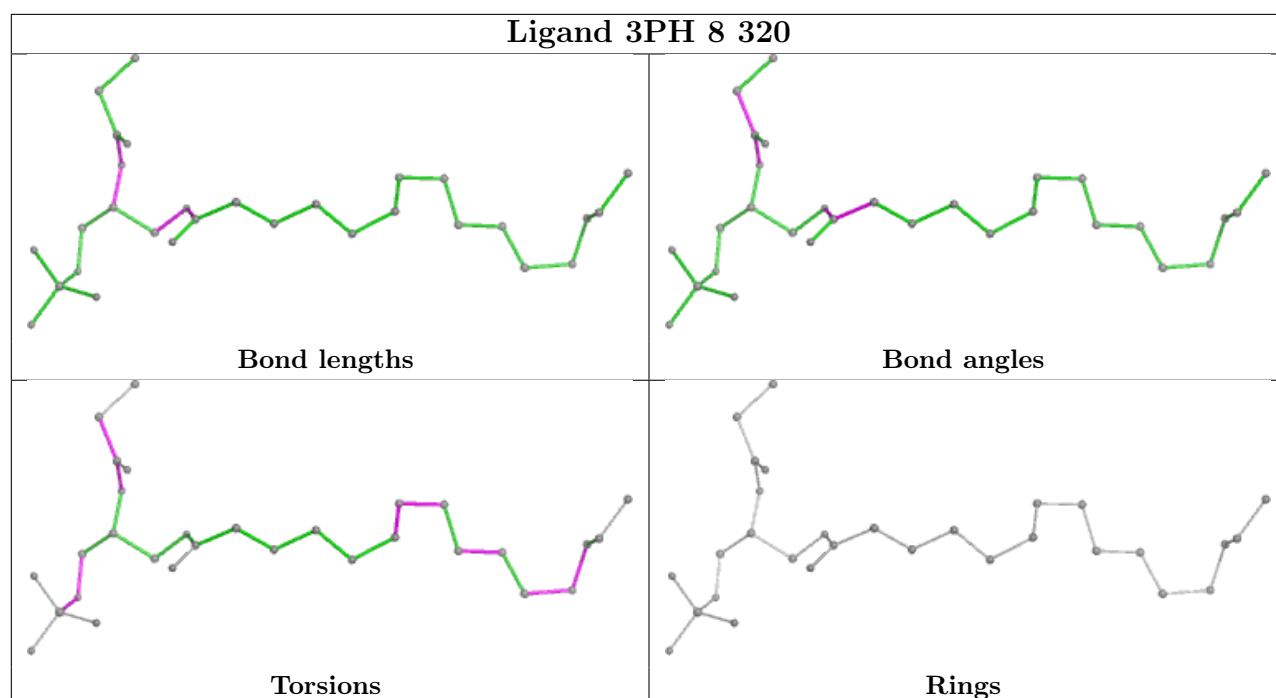
Bond angles

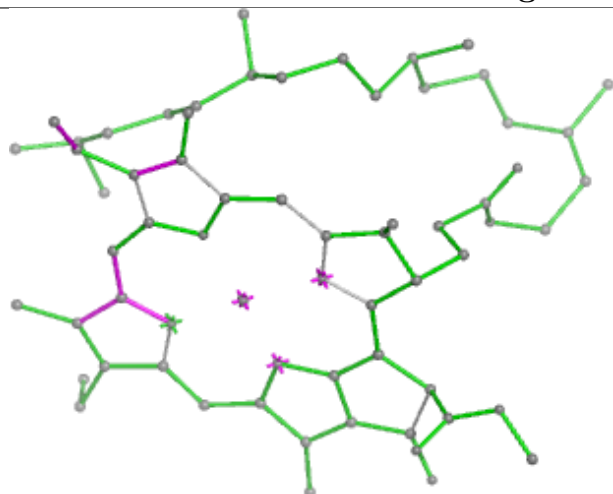
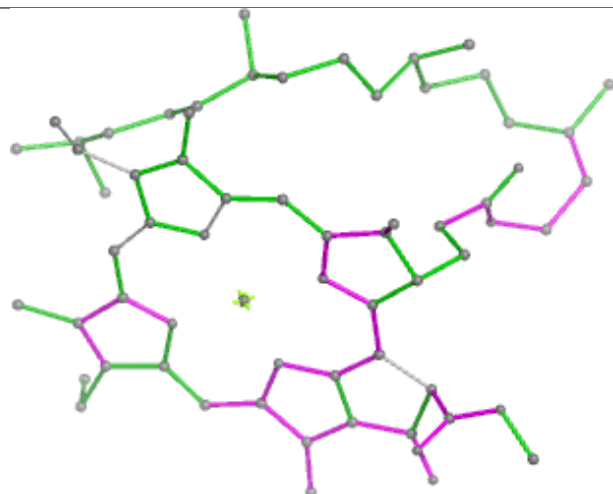
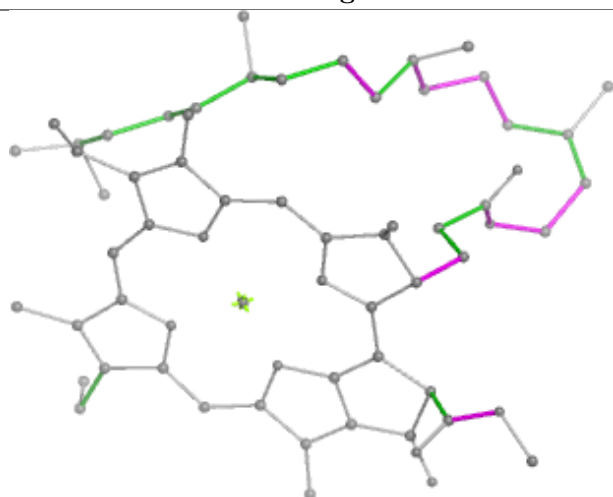
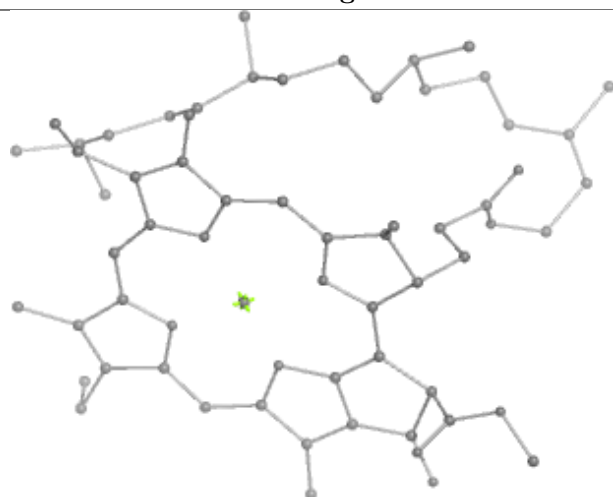
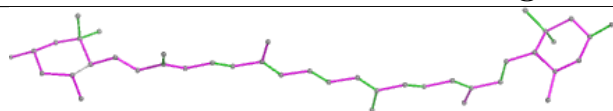
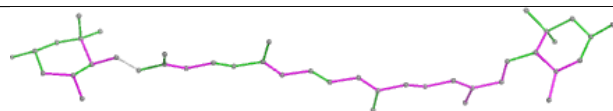


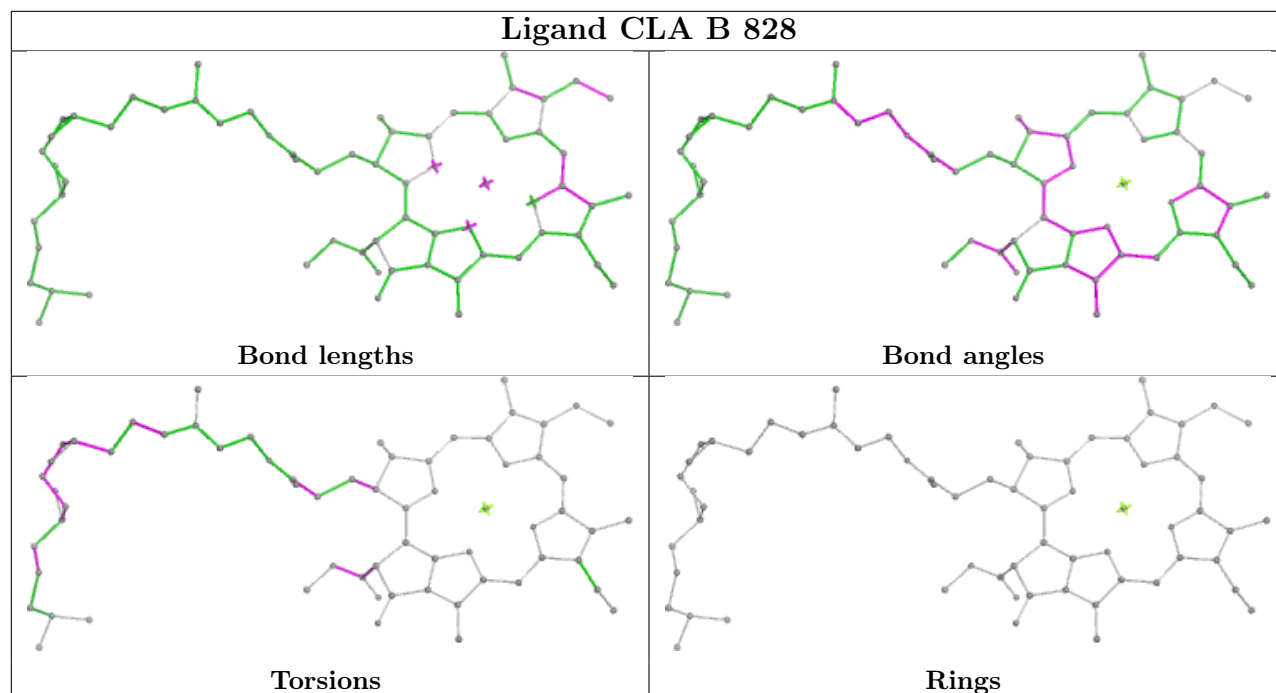
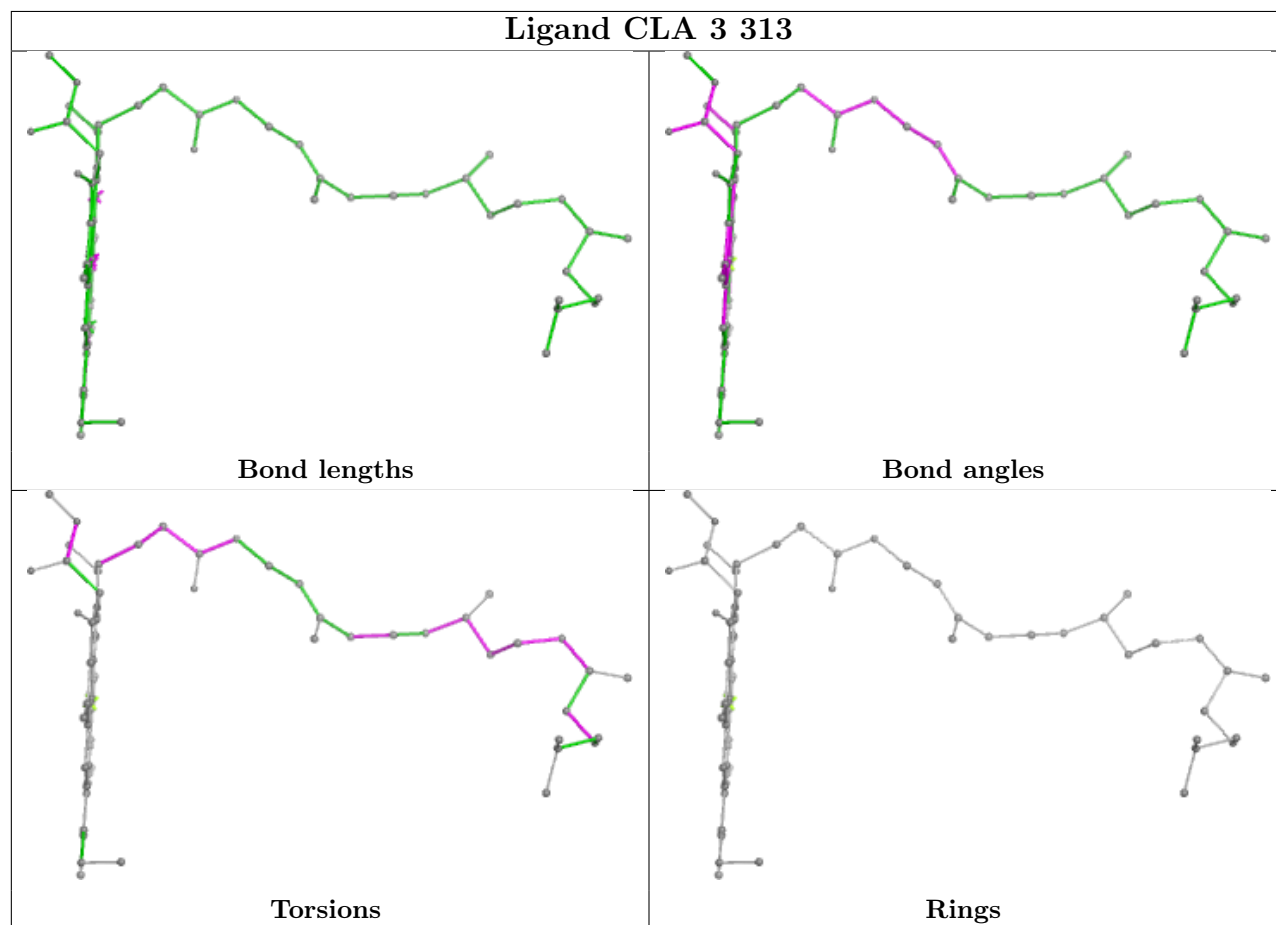
Torsions



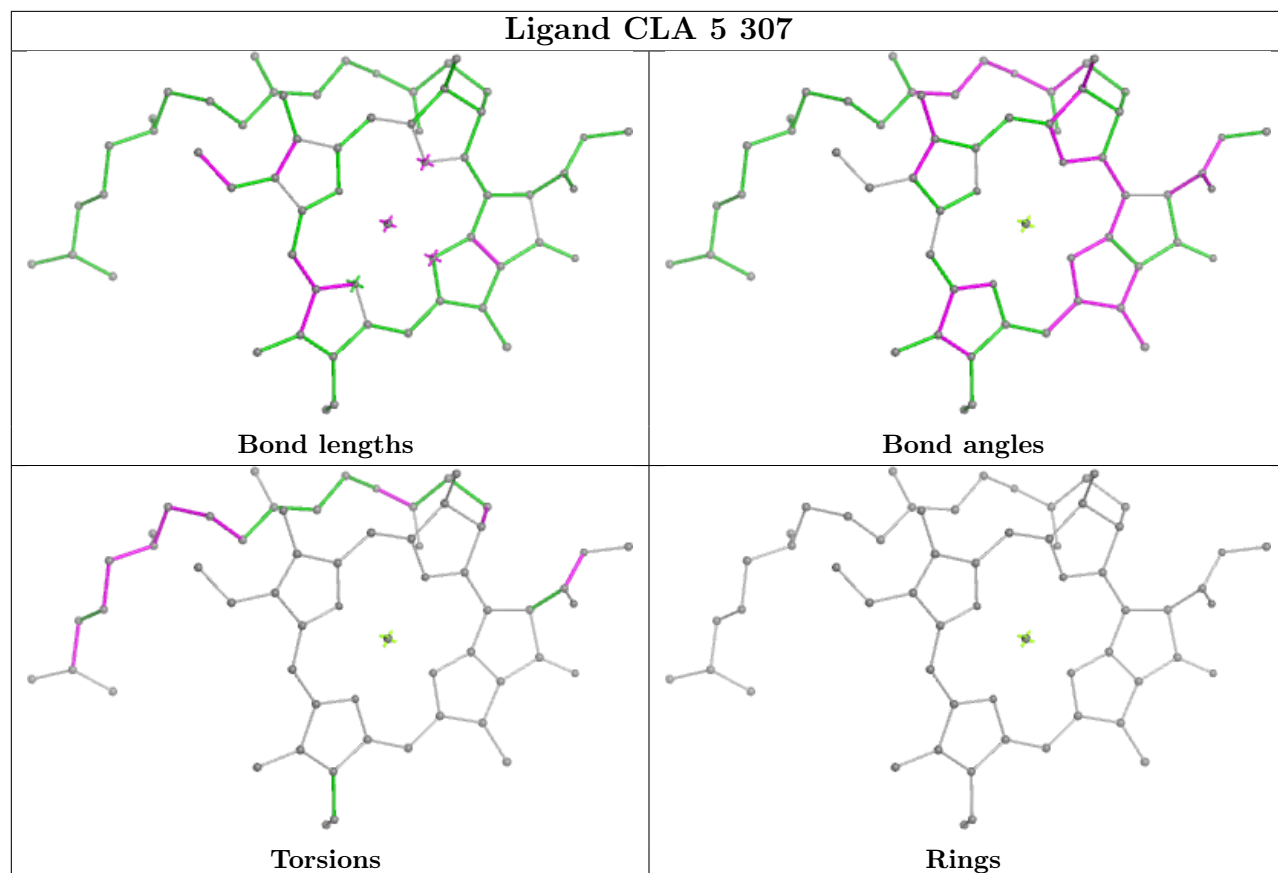
Rings



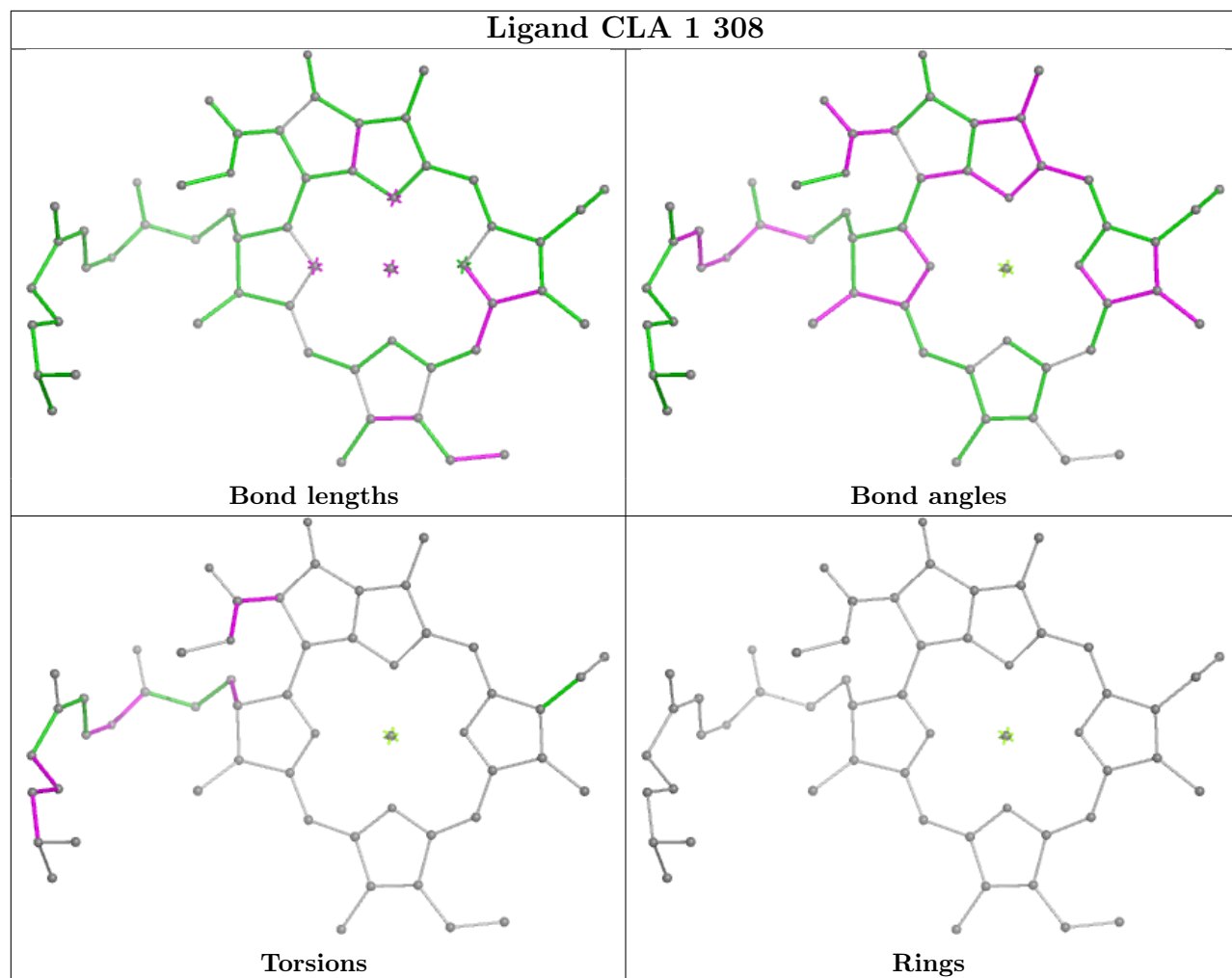
Ligand CLA 1 313**Bond lengths****Bond angles****Torsions****Rings****Ligand LUT 1 302****Bond lengths****Bond angles****Torsions****Rings**

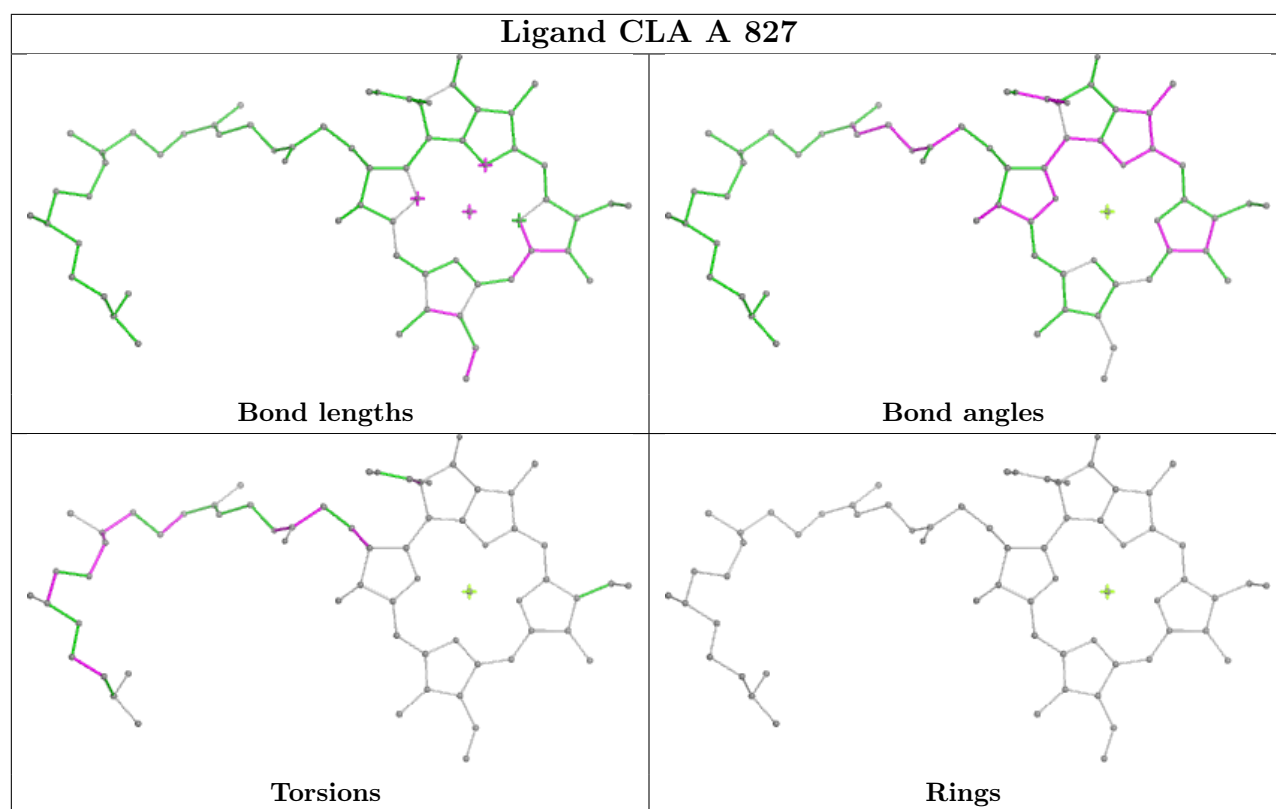
Ligand CLA B 828**Ligand CLA 3 313**

Ligand CLA 5 307

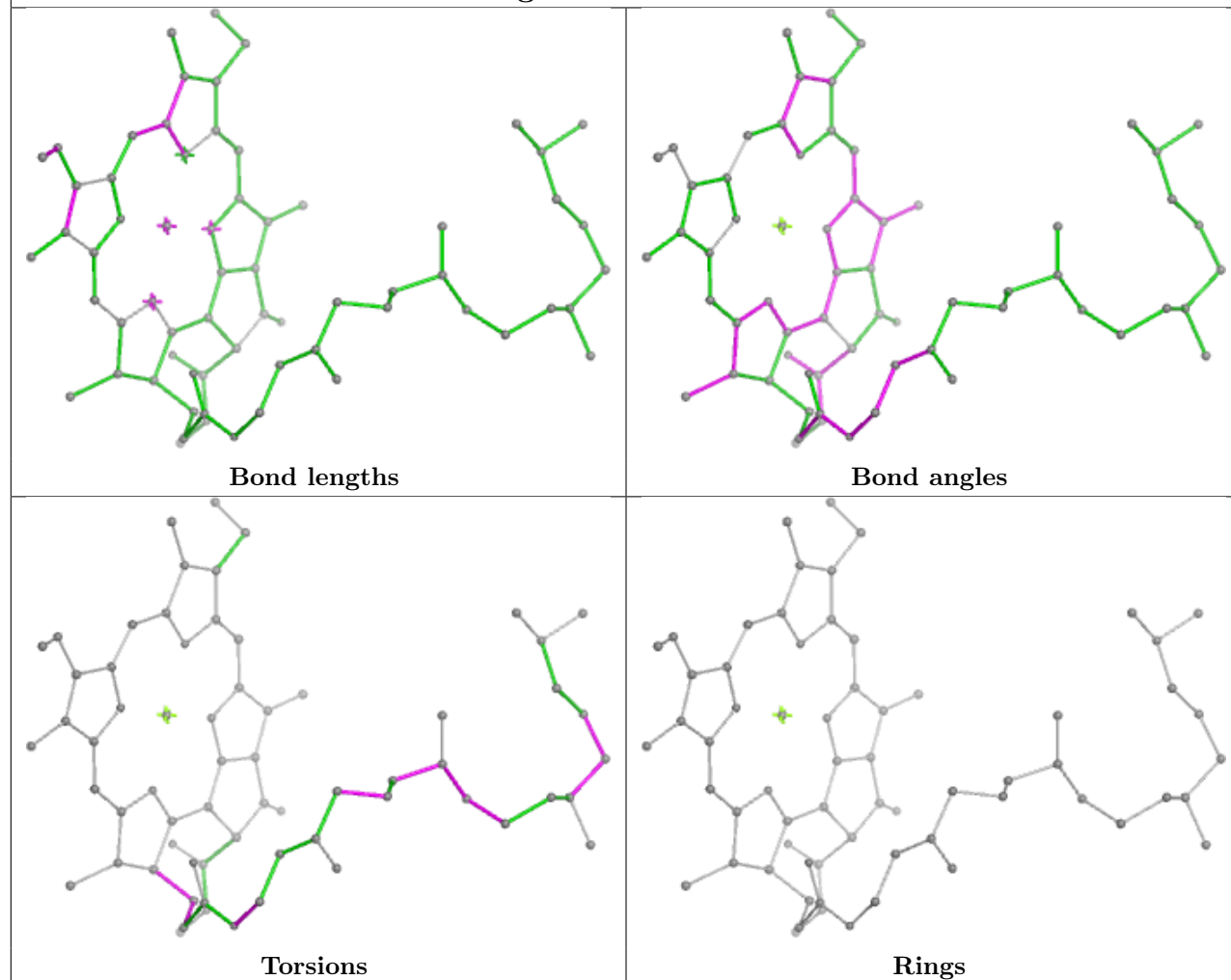


Ligand CLA 1 308

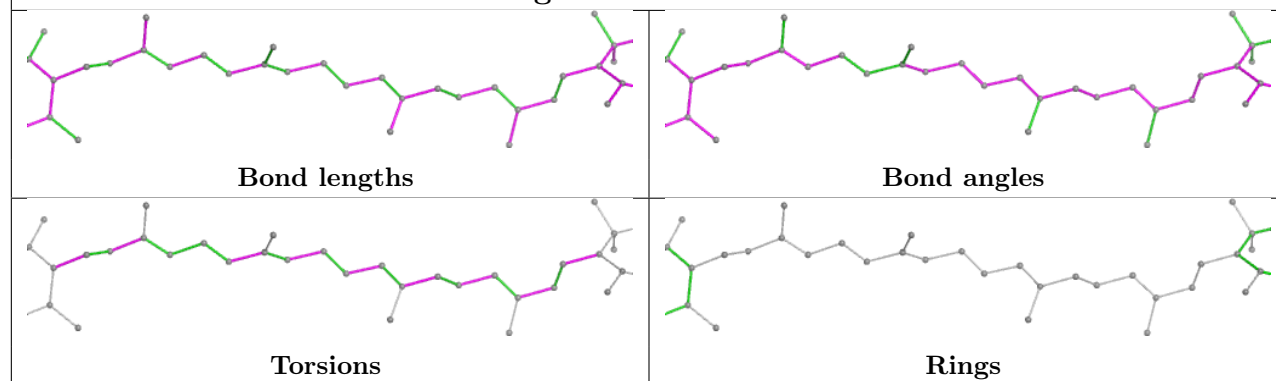




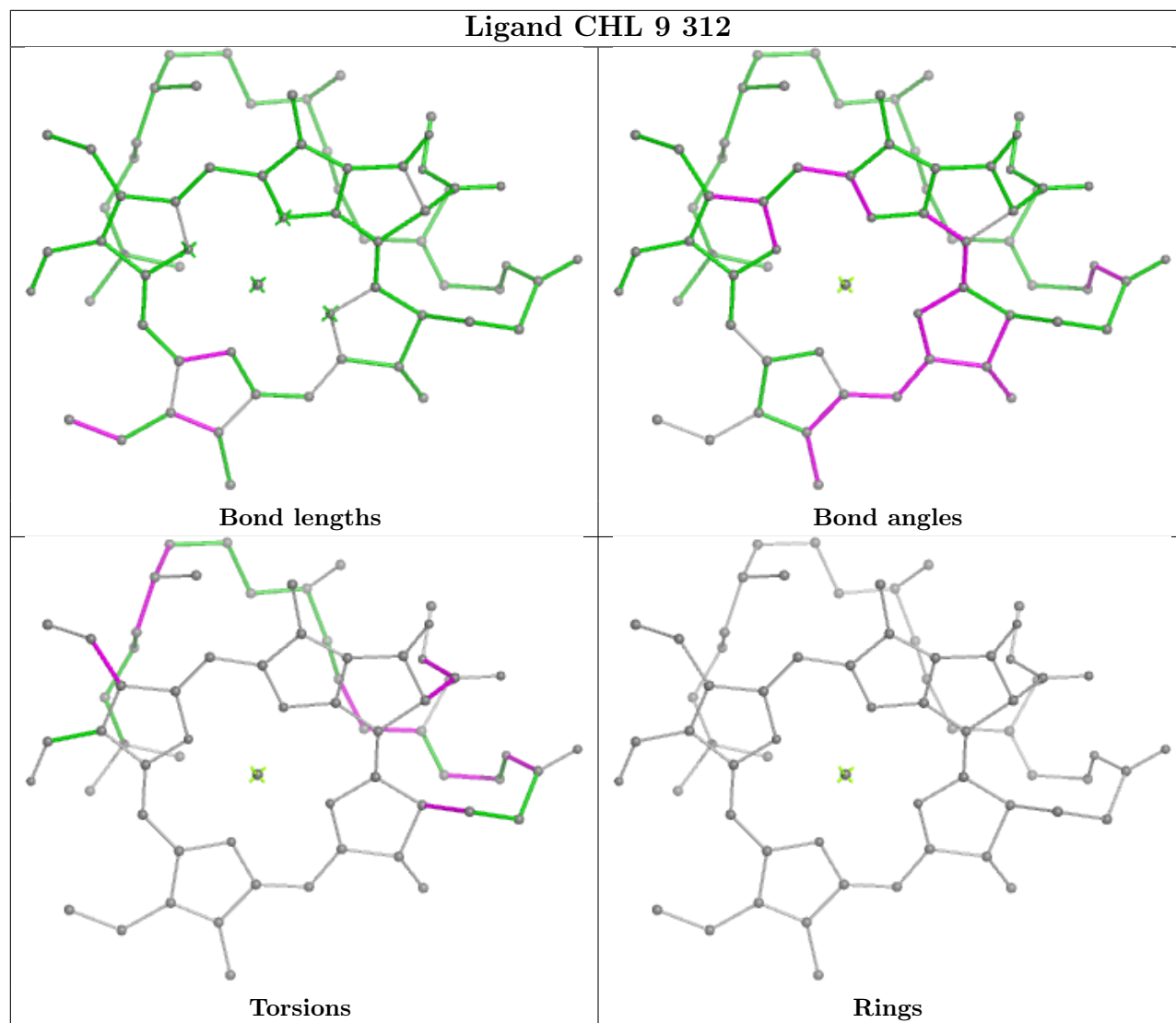
Ligand CLA 1 314

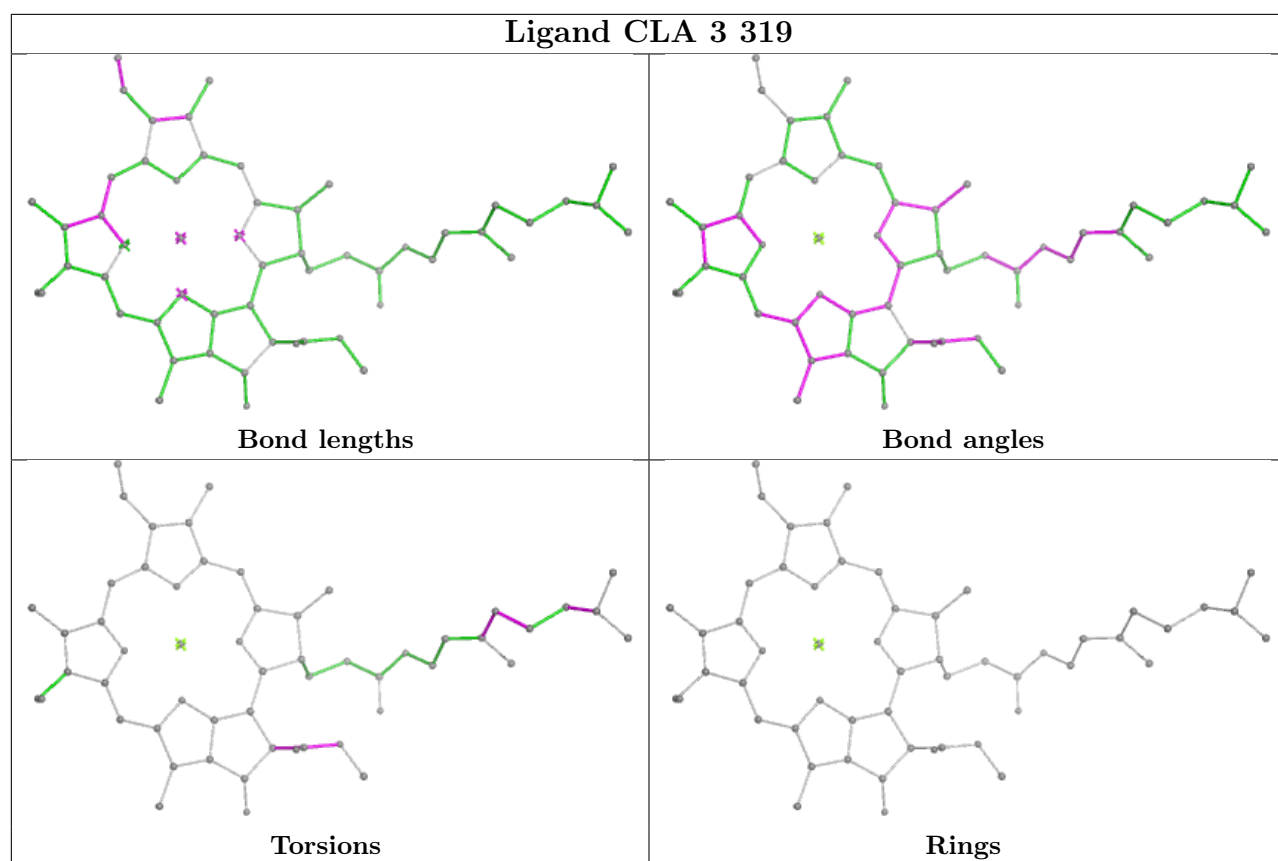


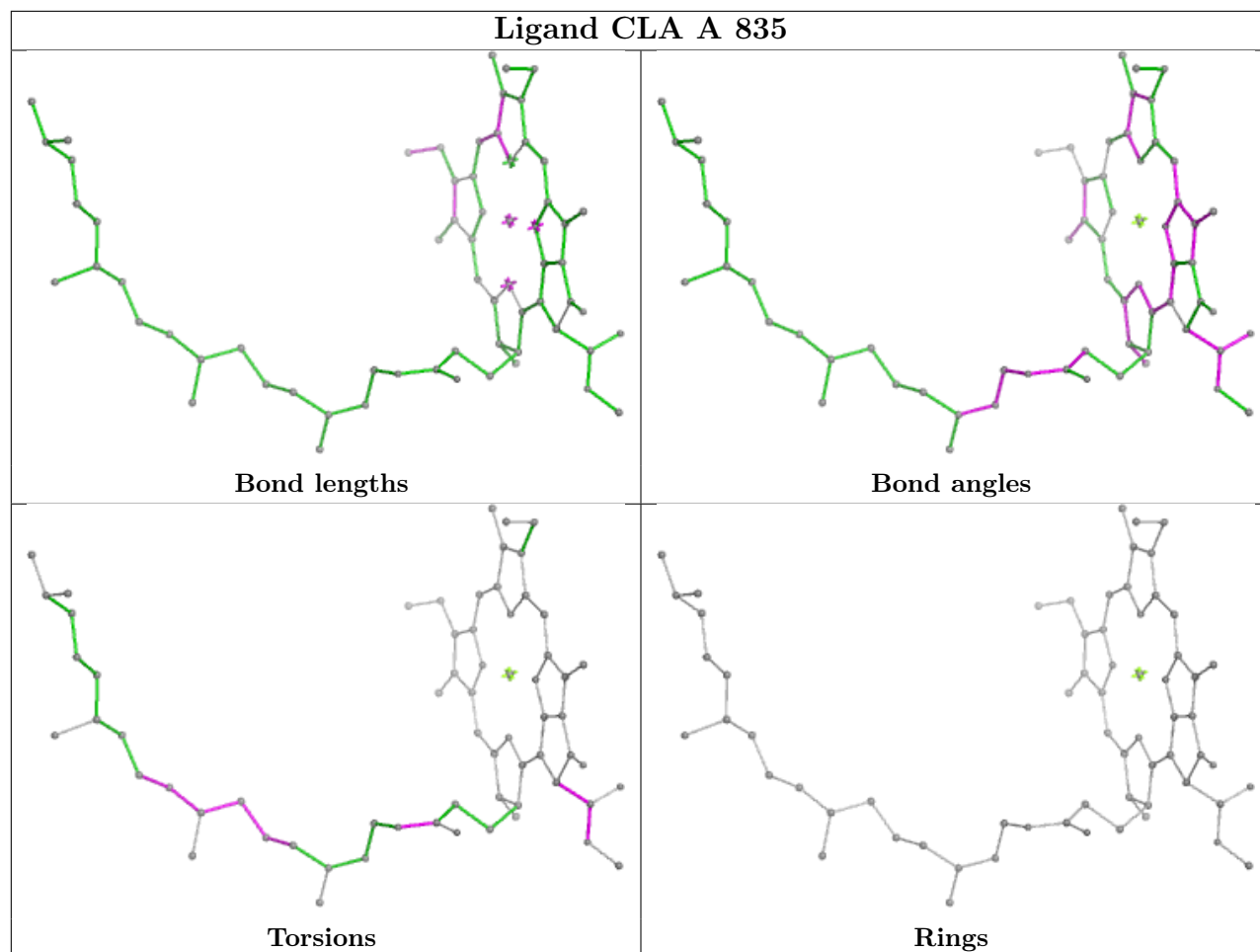
Ligand BCR J 104

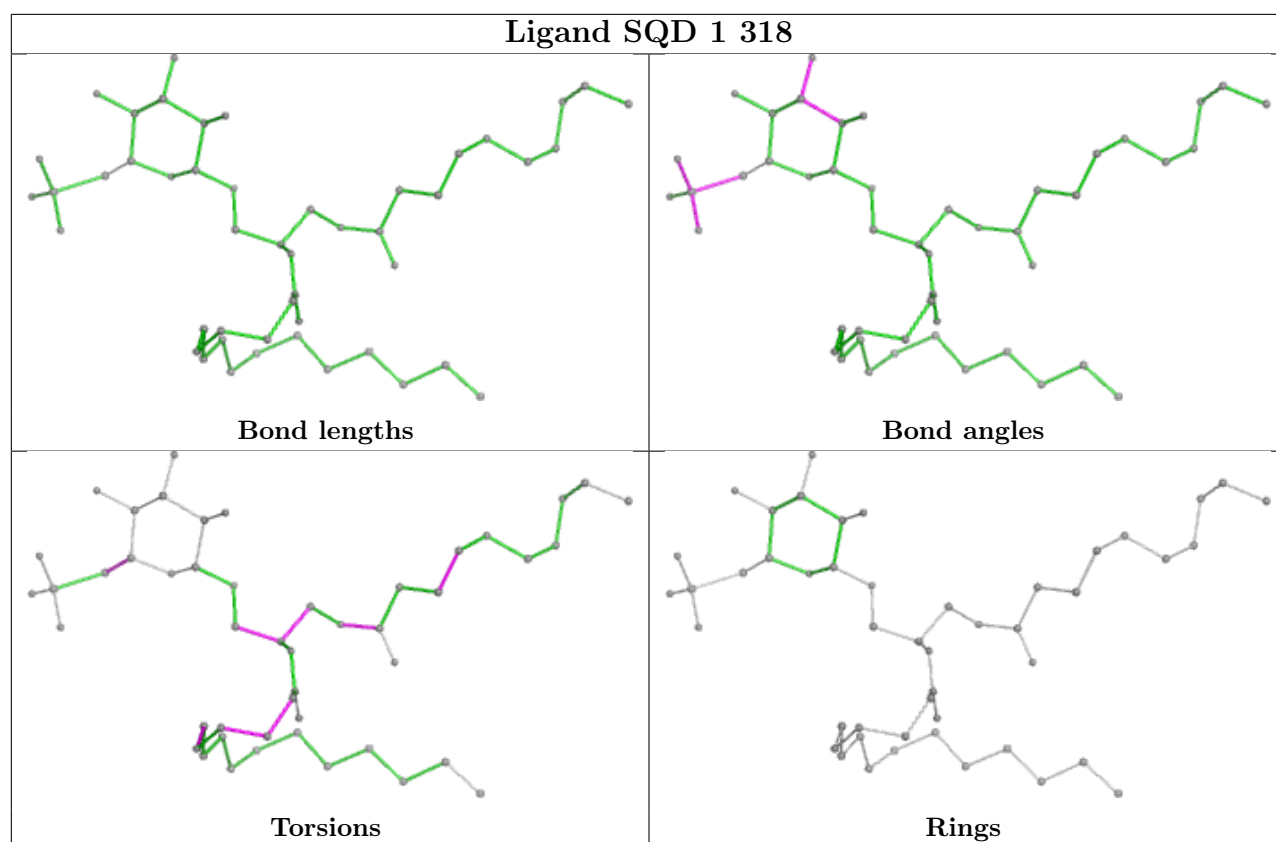


Ligand CHL 9 312

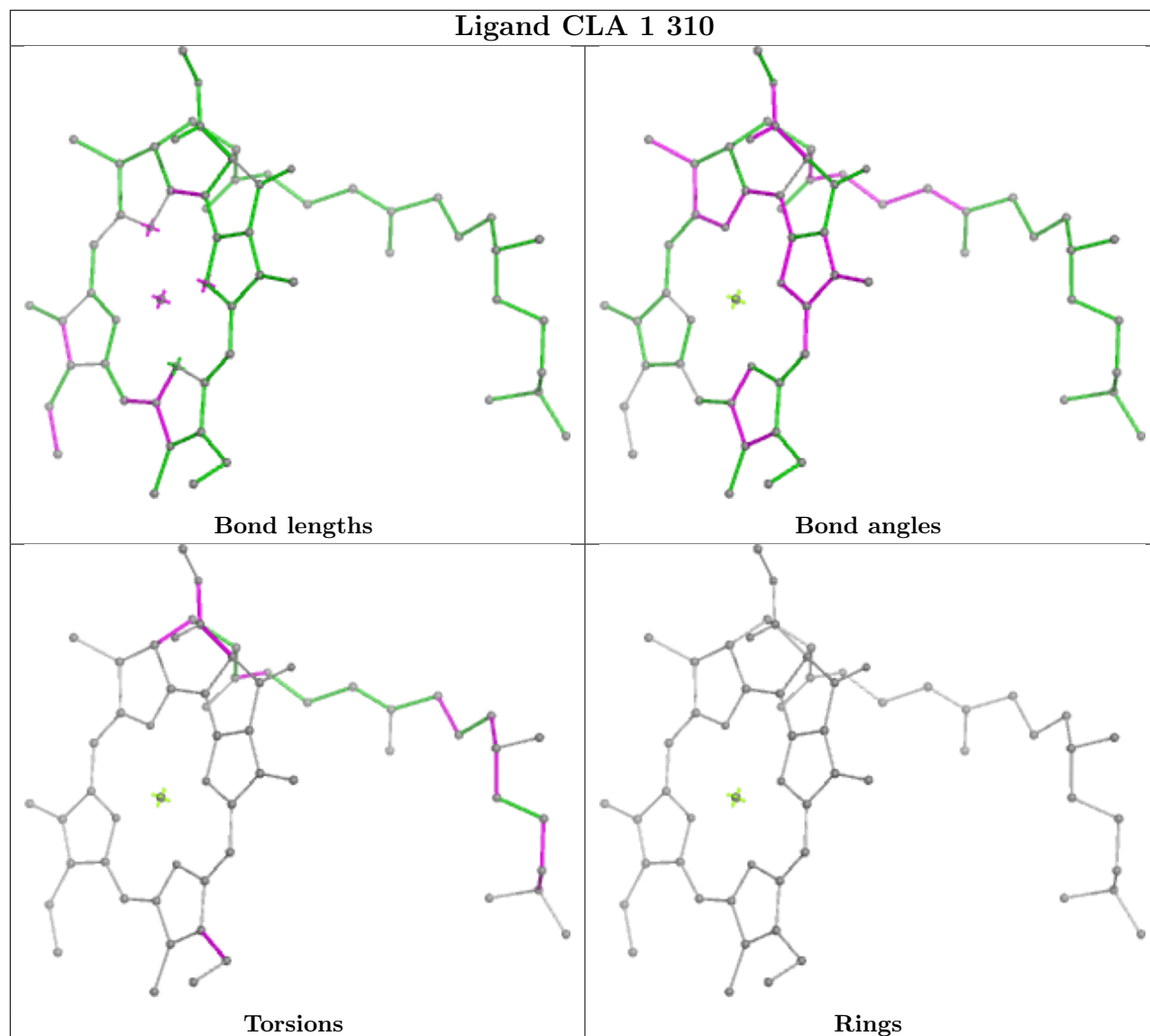




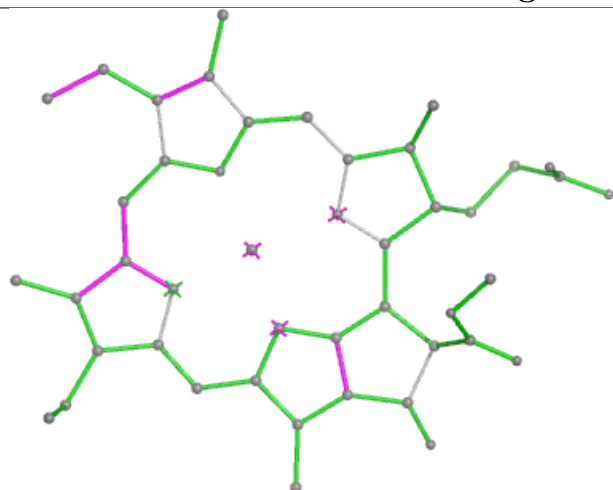




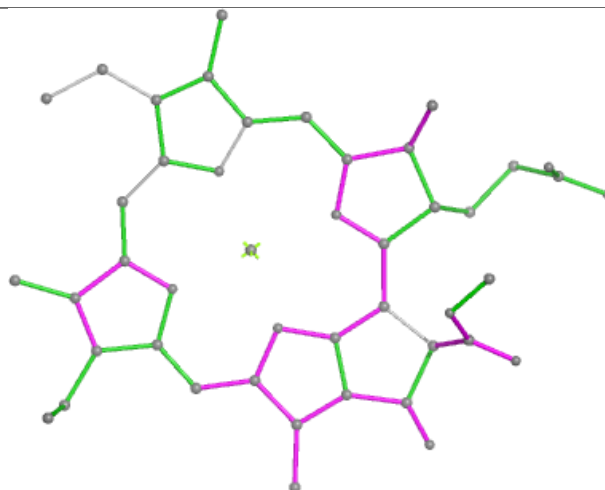
Ligand CLA 1 310



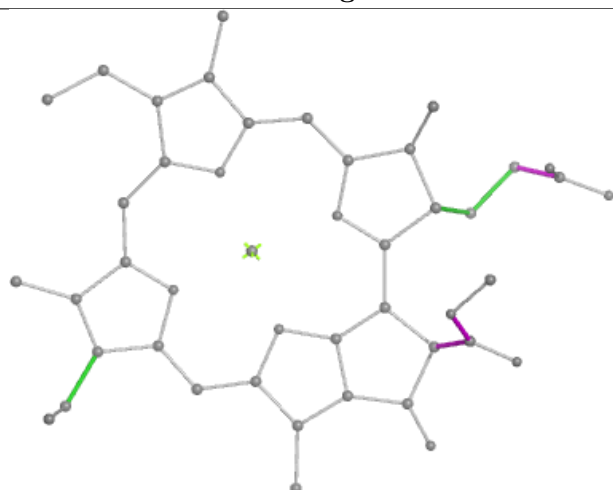
Ligand CLA 1 305



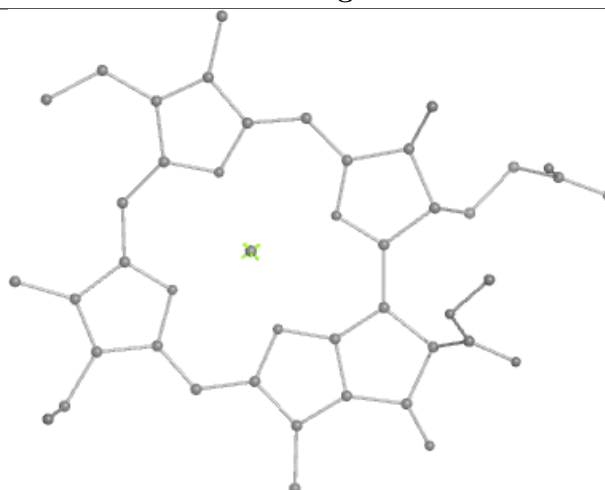
Bond lengths



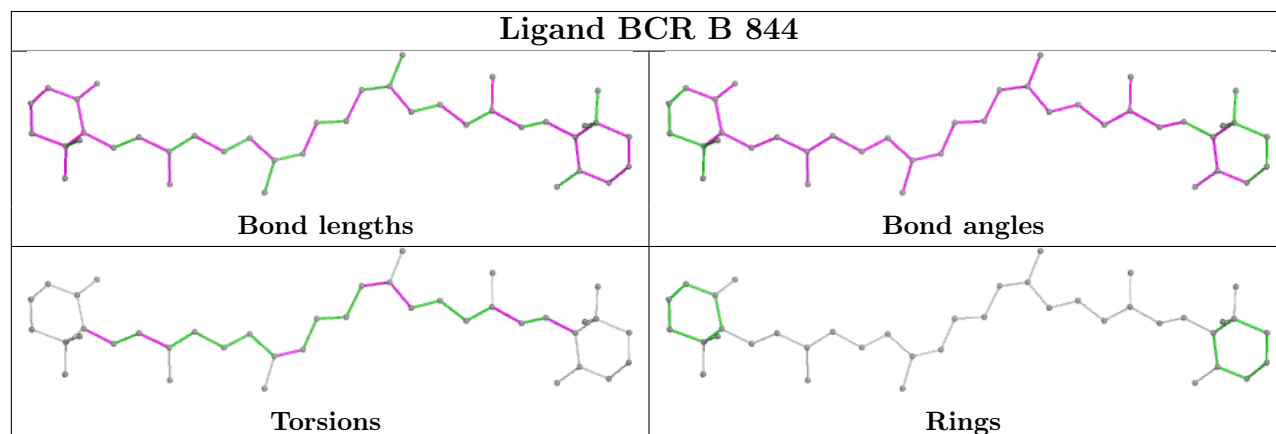
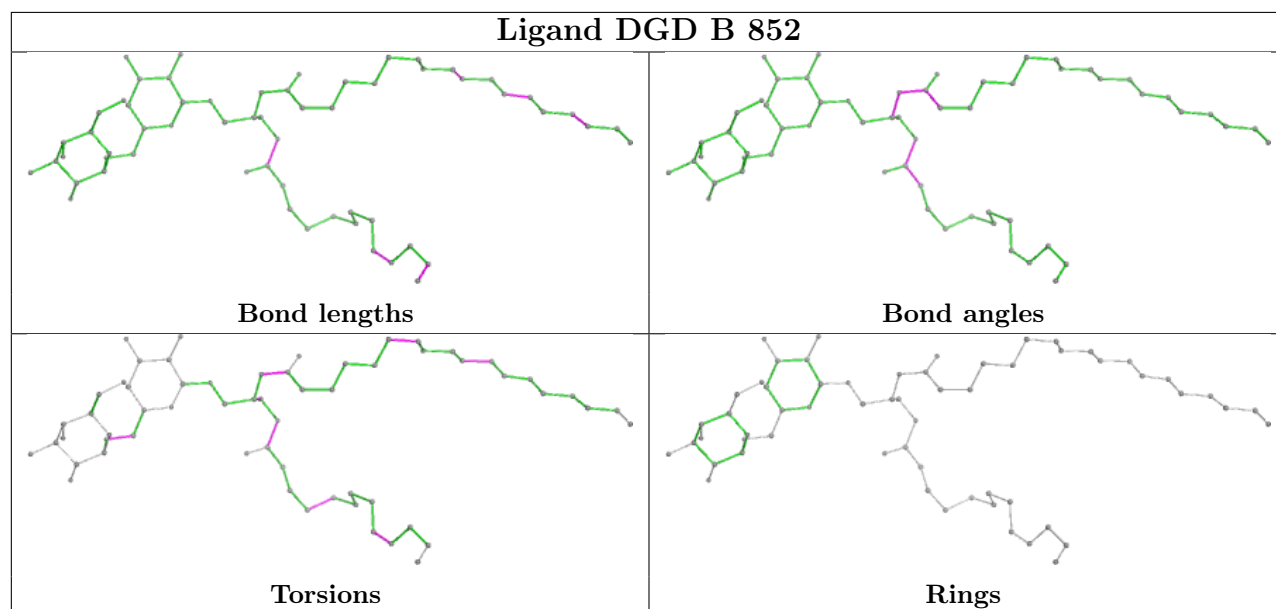
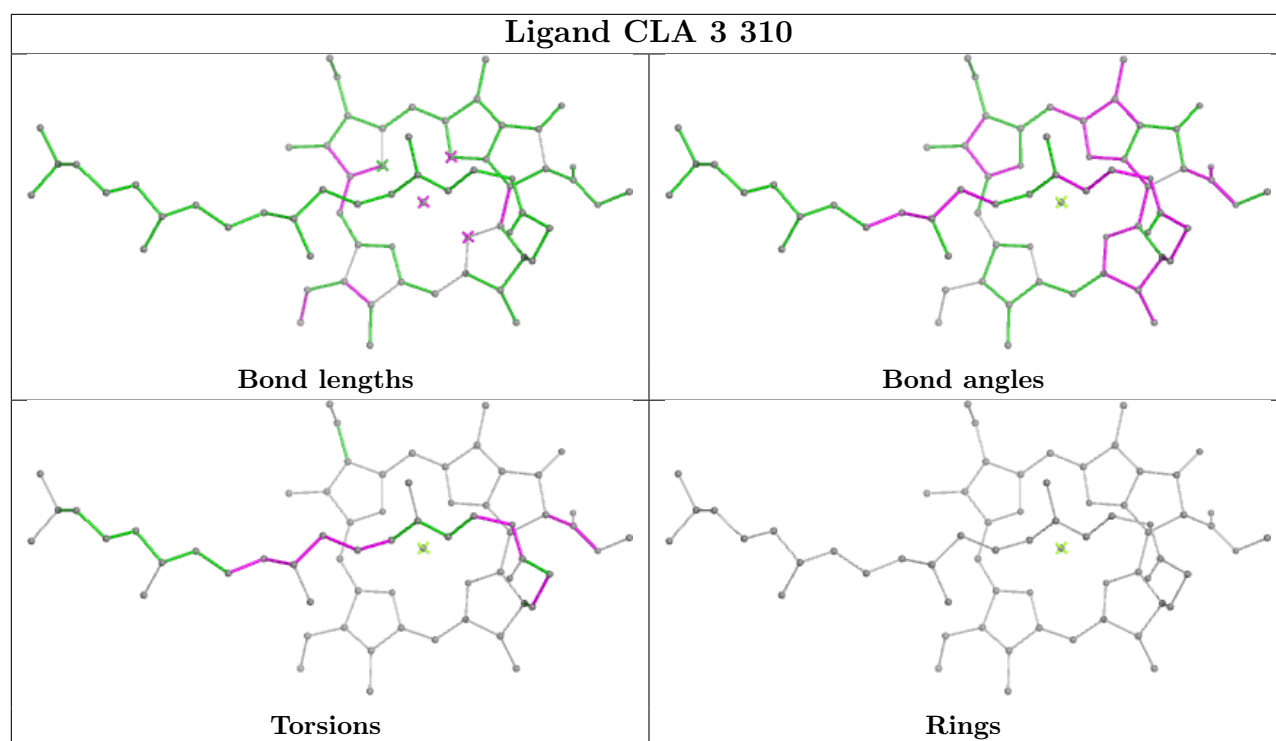
Bond angles

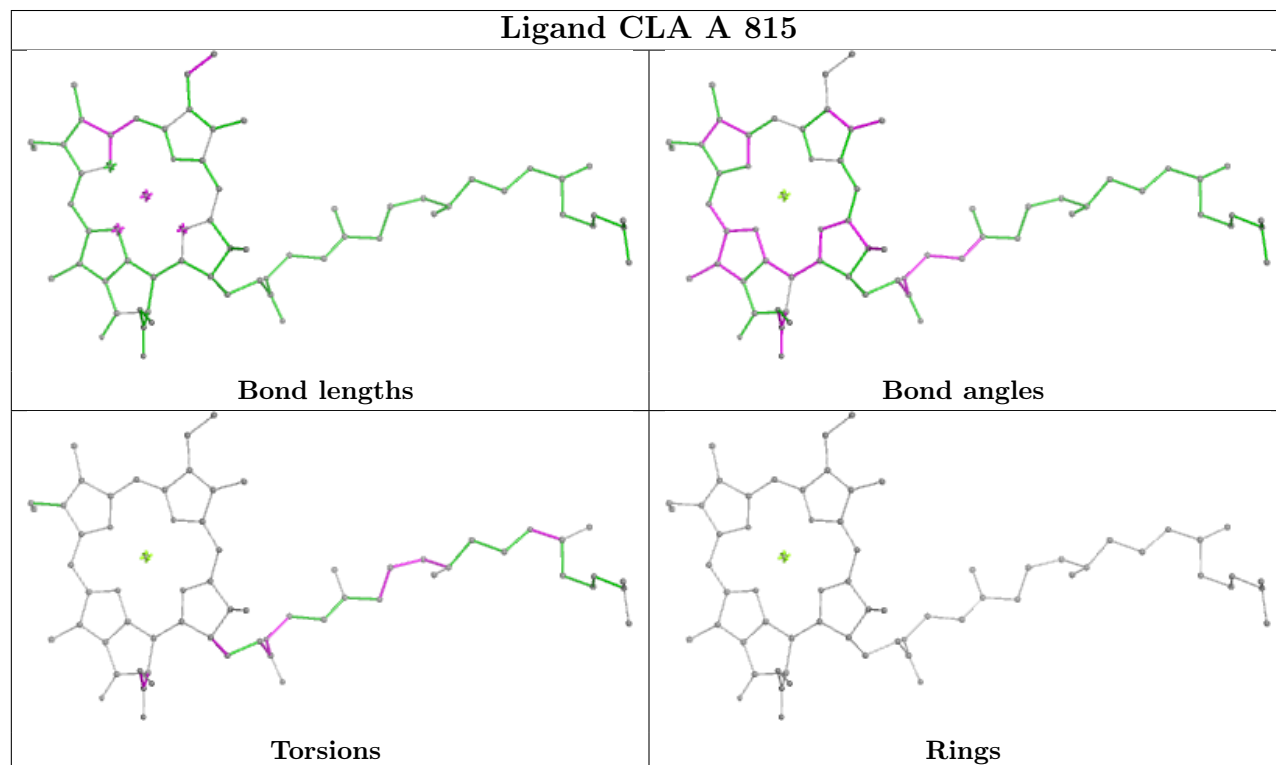
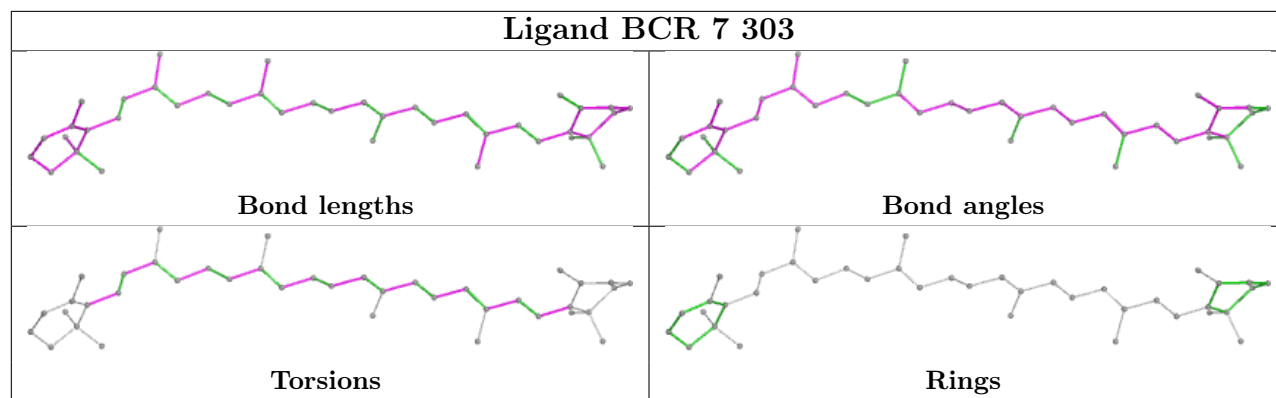


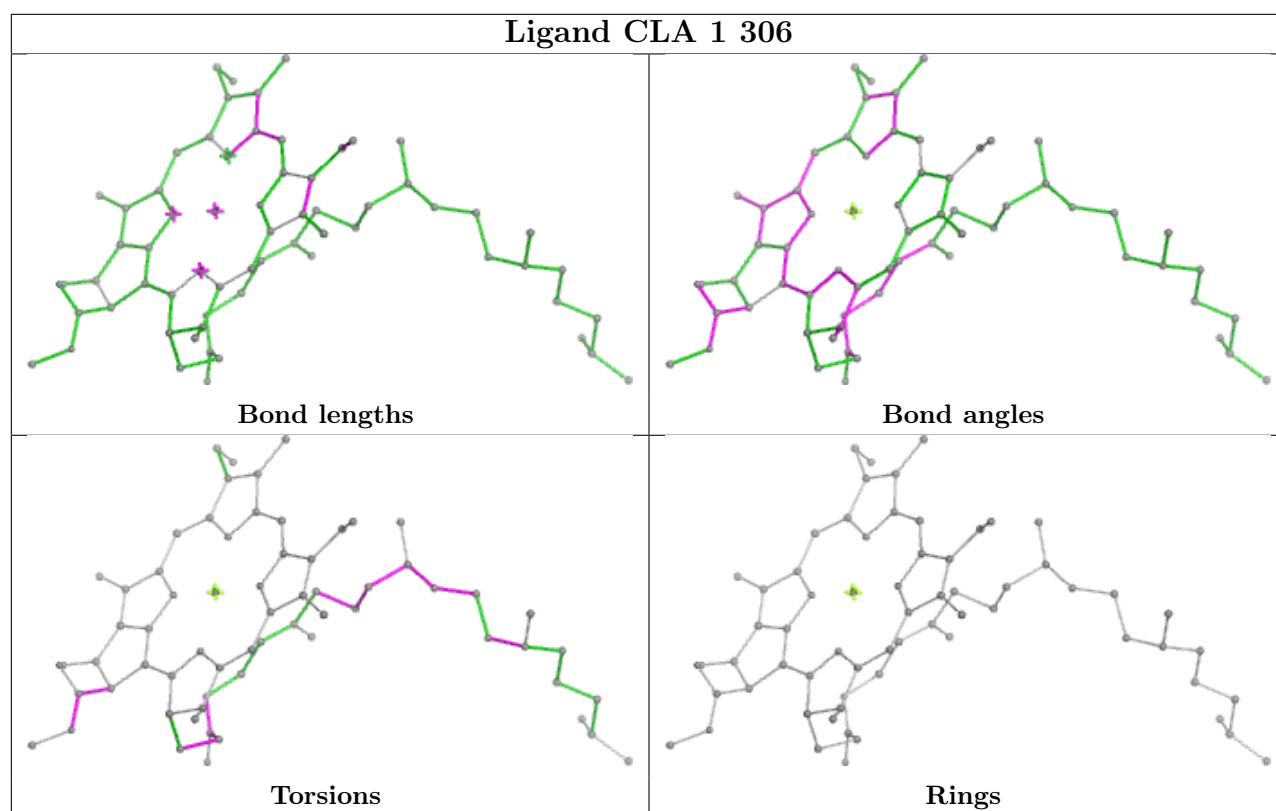
Torsions

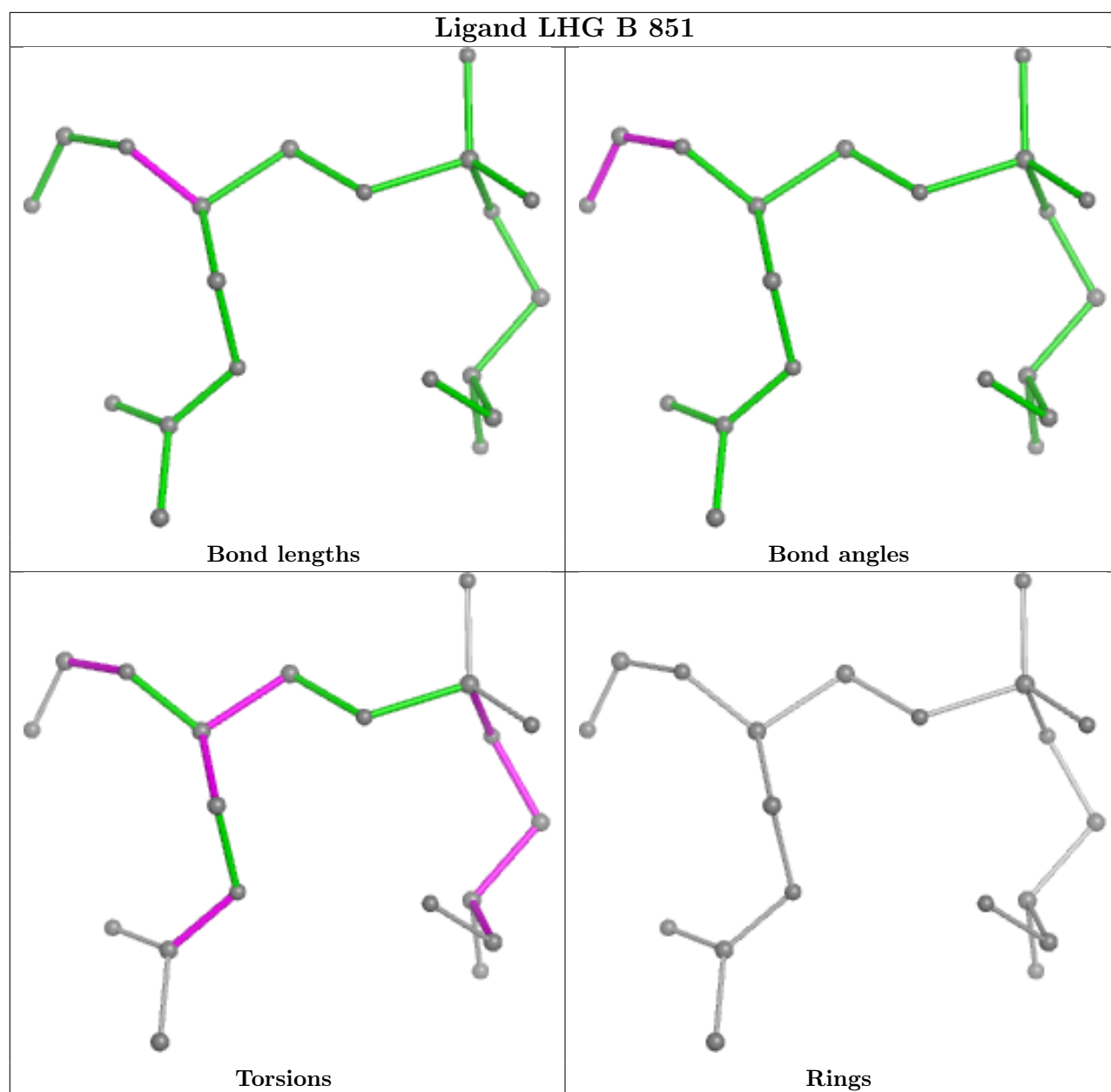


Rings

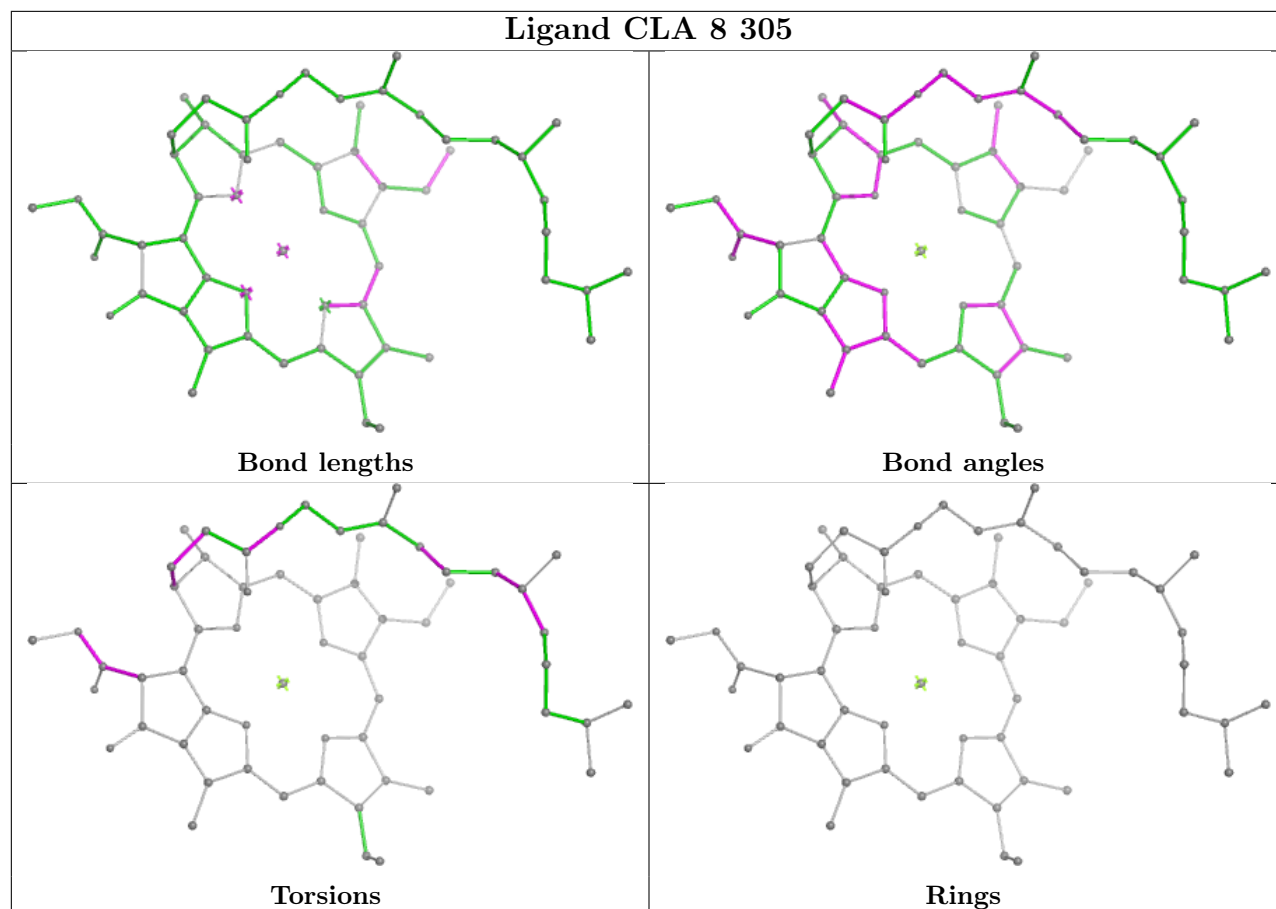




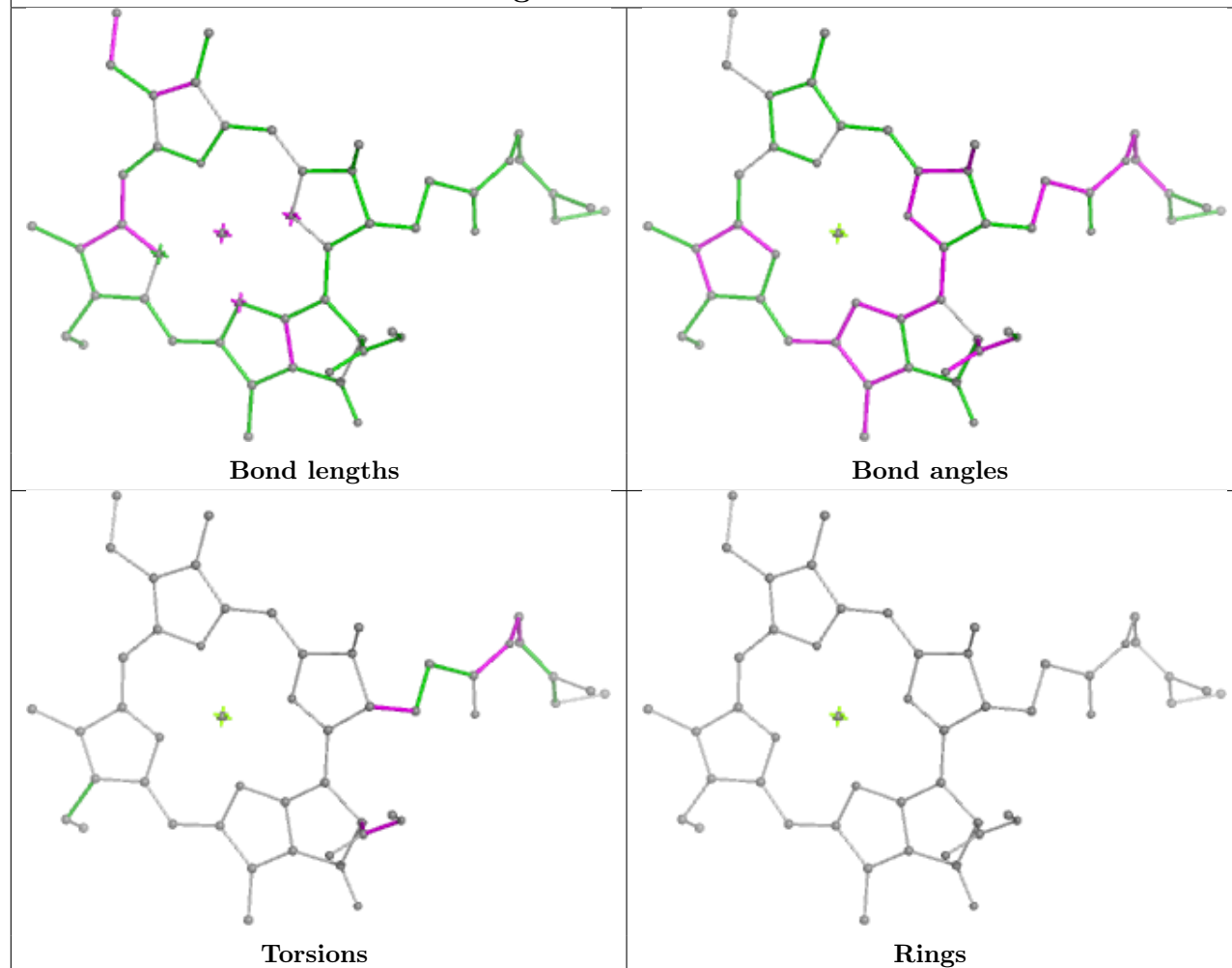




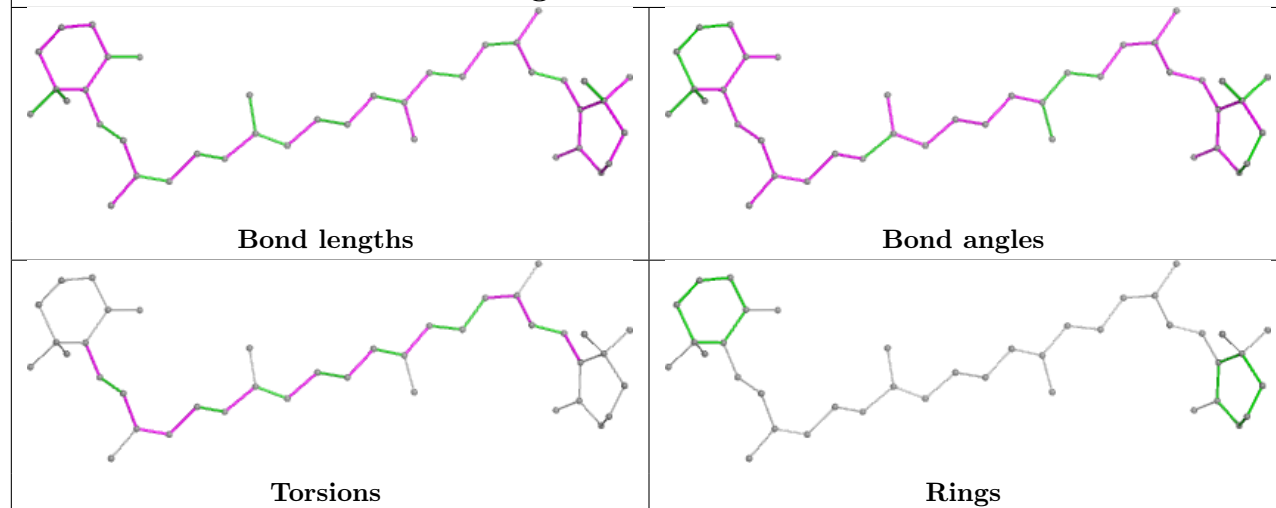
Ligand CLA 8 305



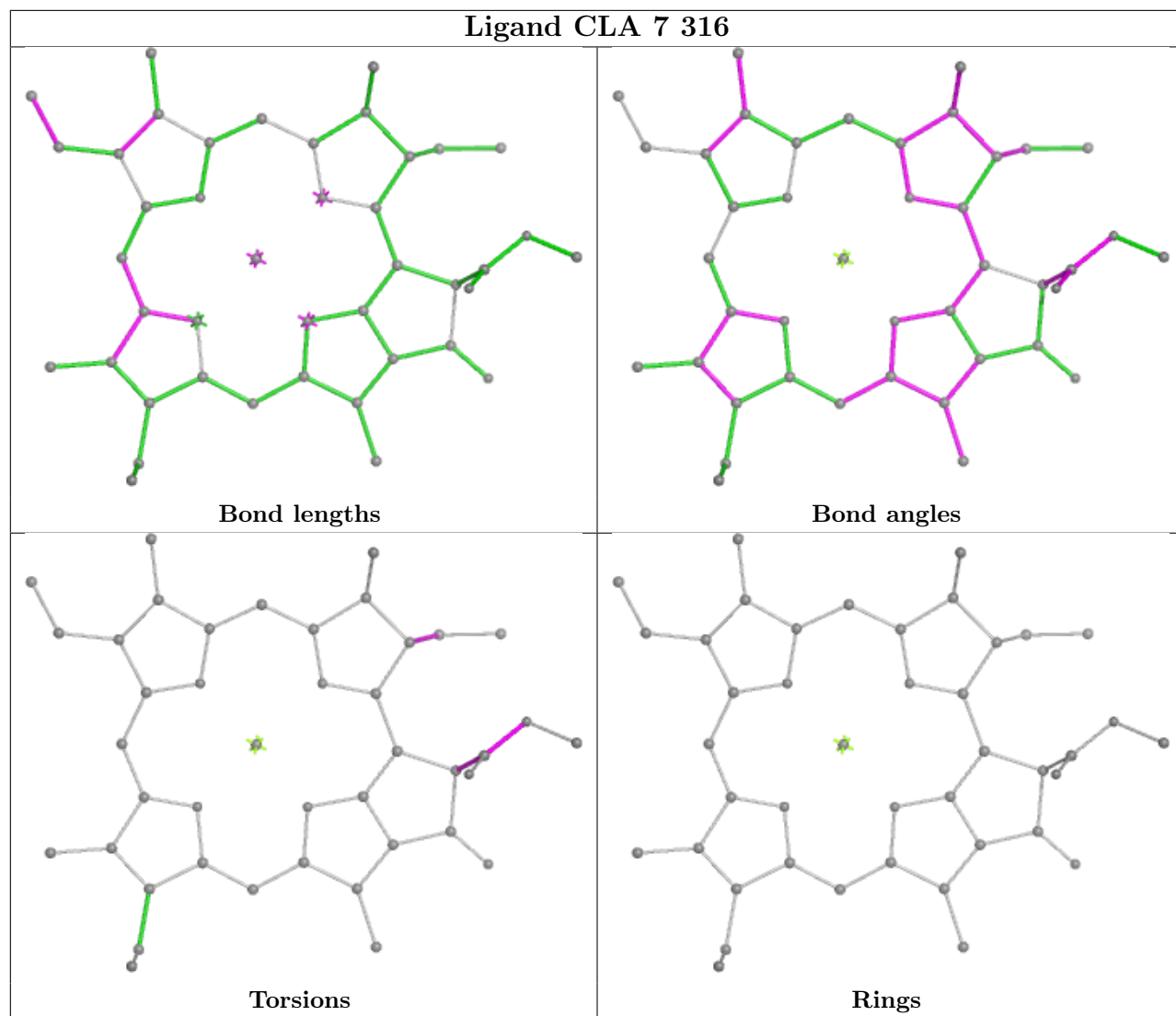
Ligand CLA A 839

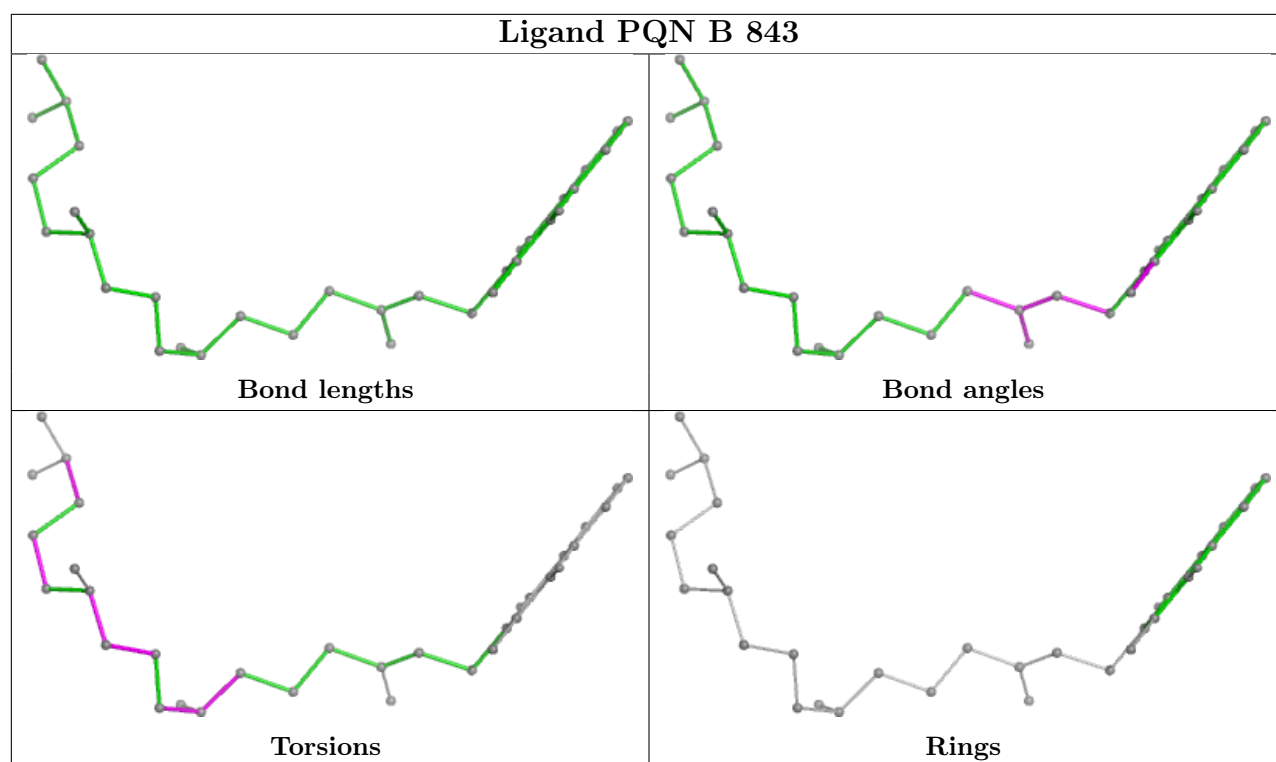


Ligand BCR B 846

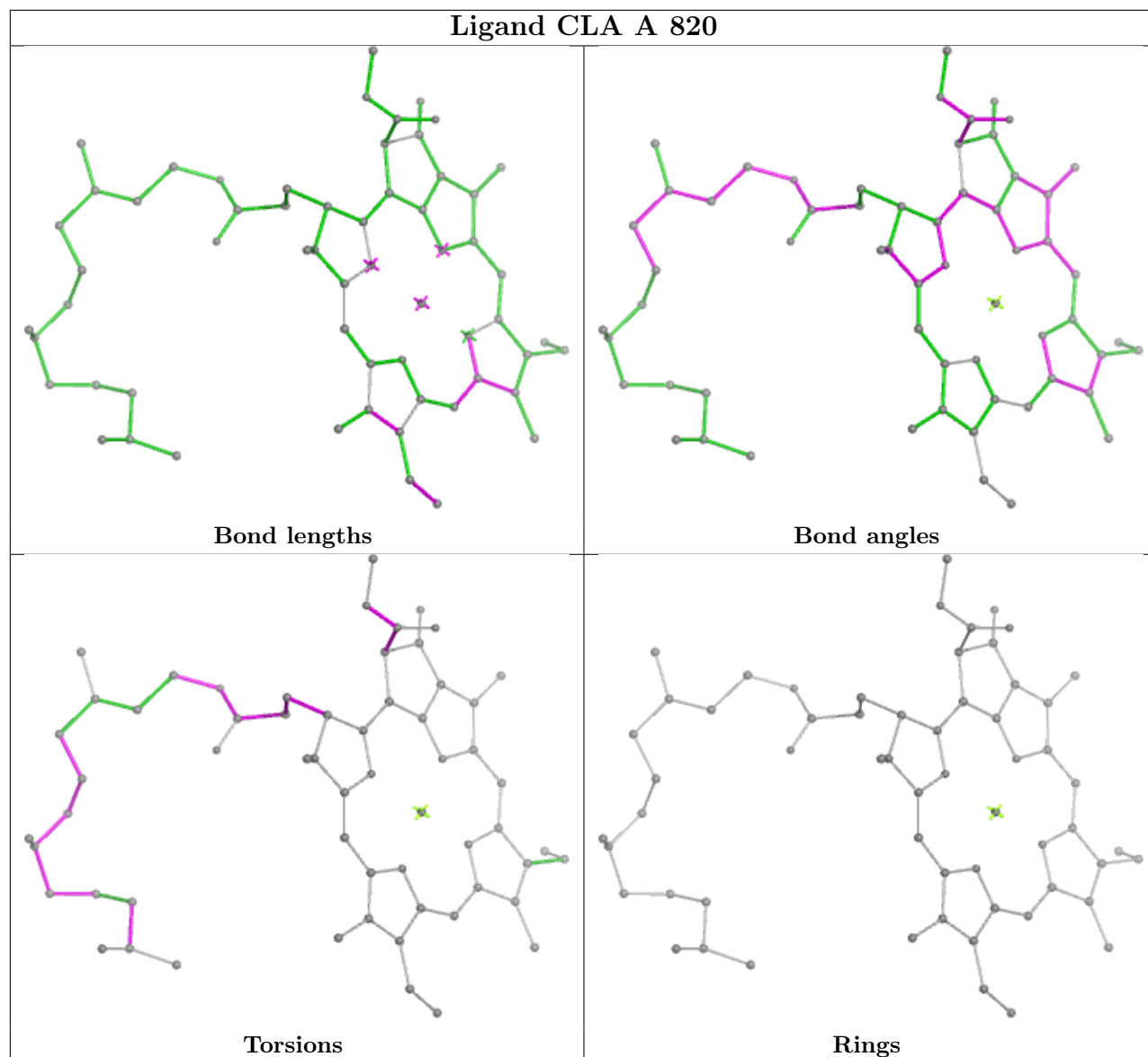


Ligand CLA 7 316

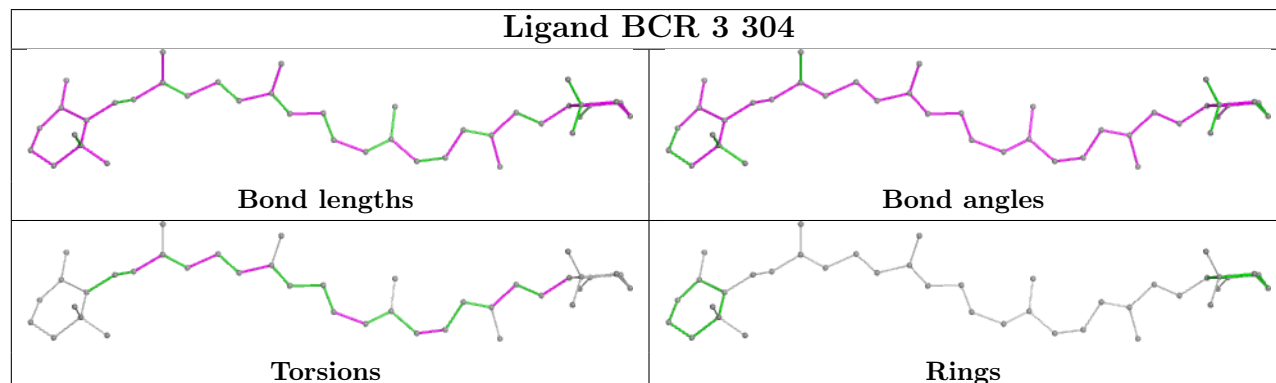


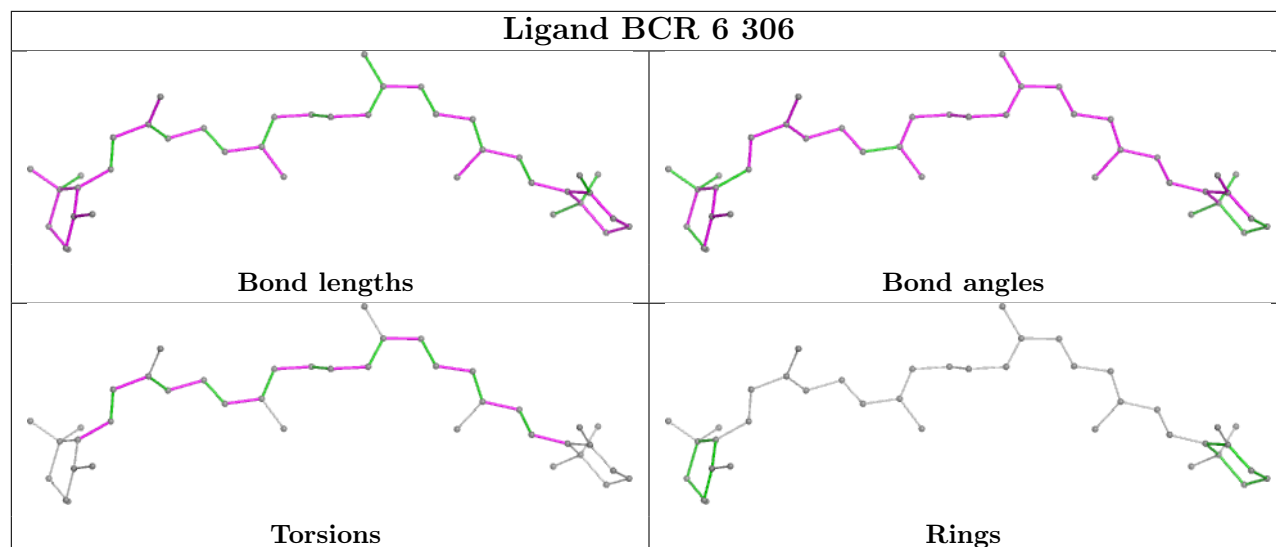
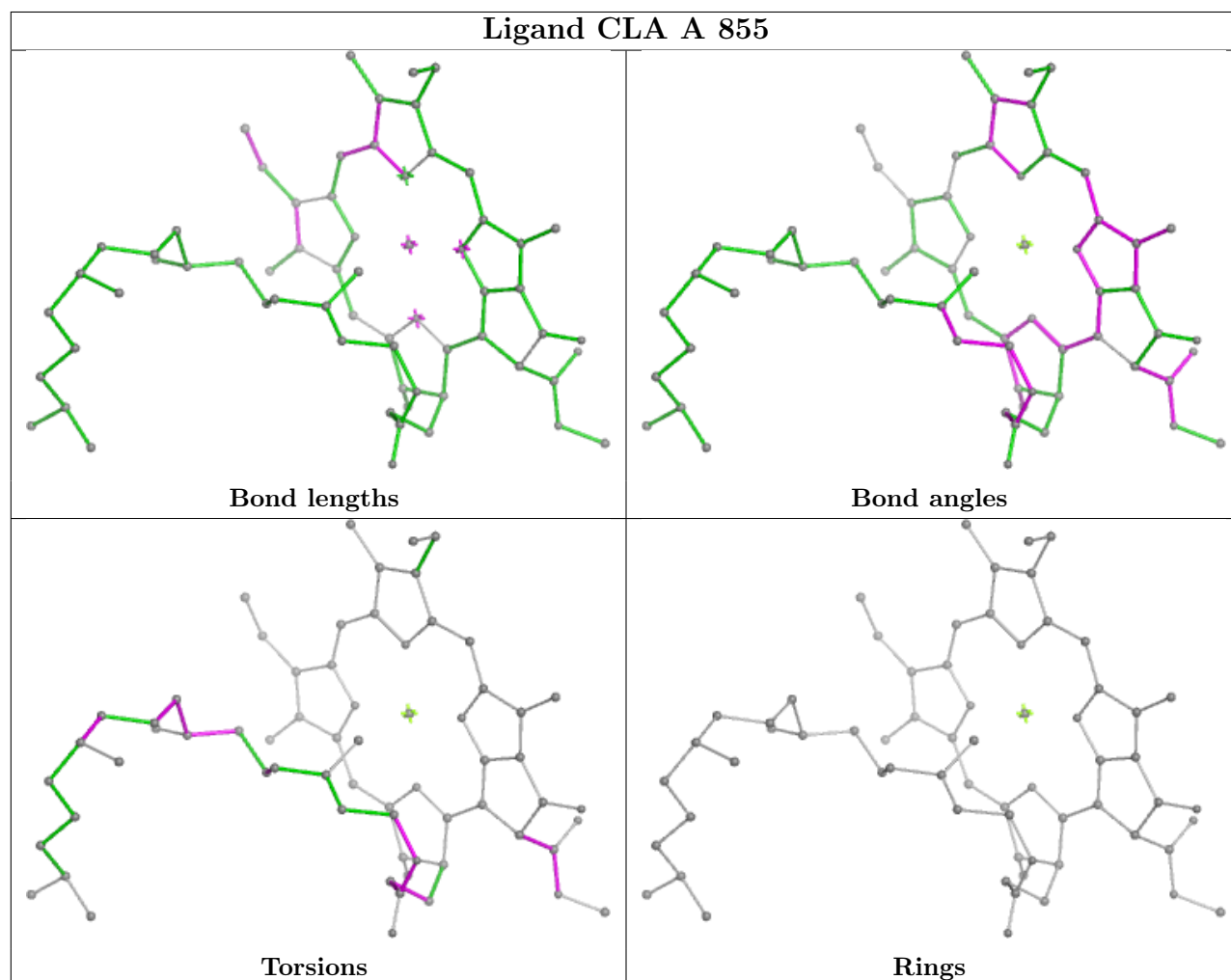


Ligand CLA A 820

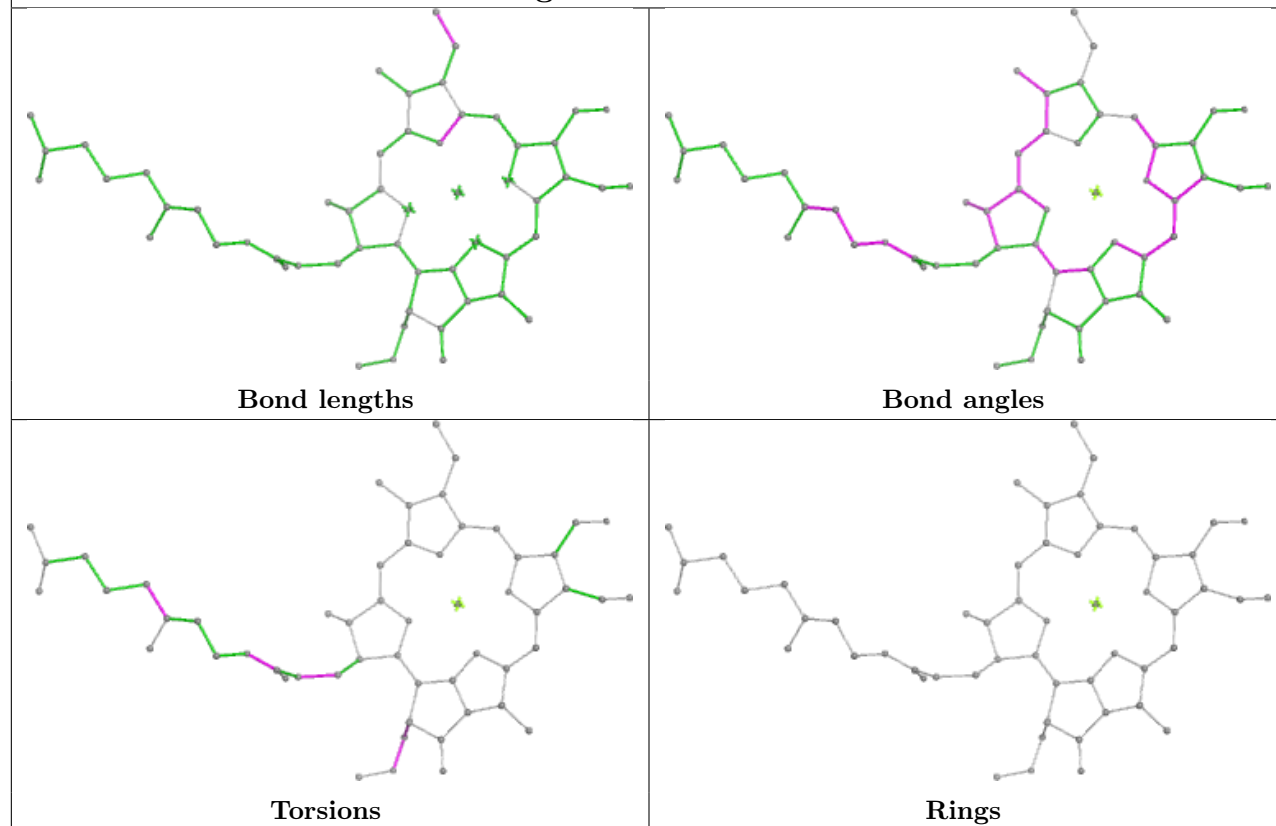


Ligand BCR 3 304

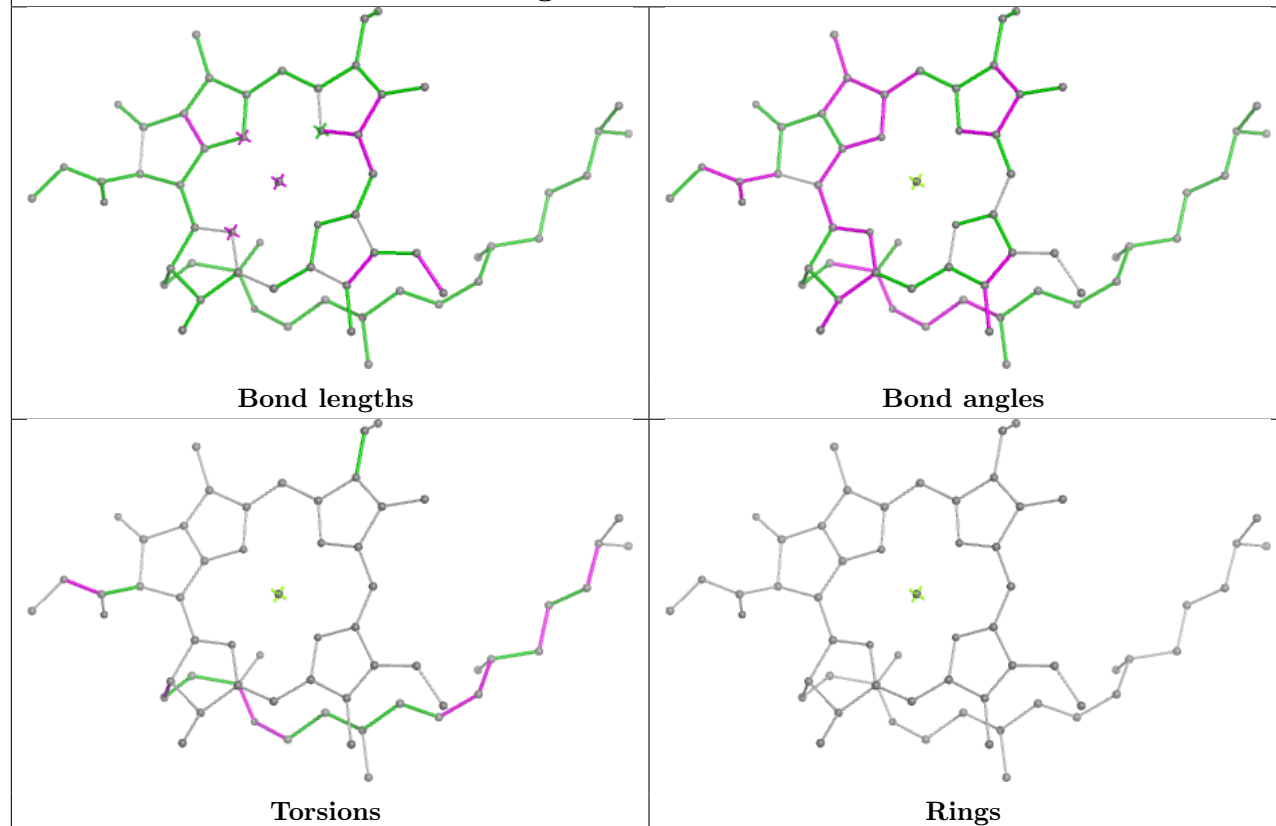


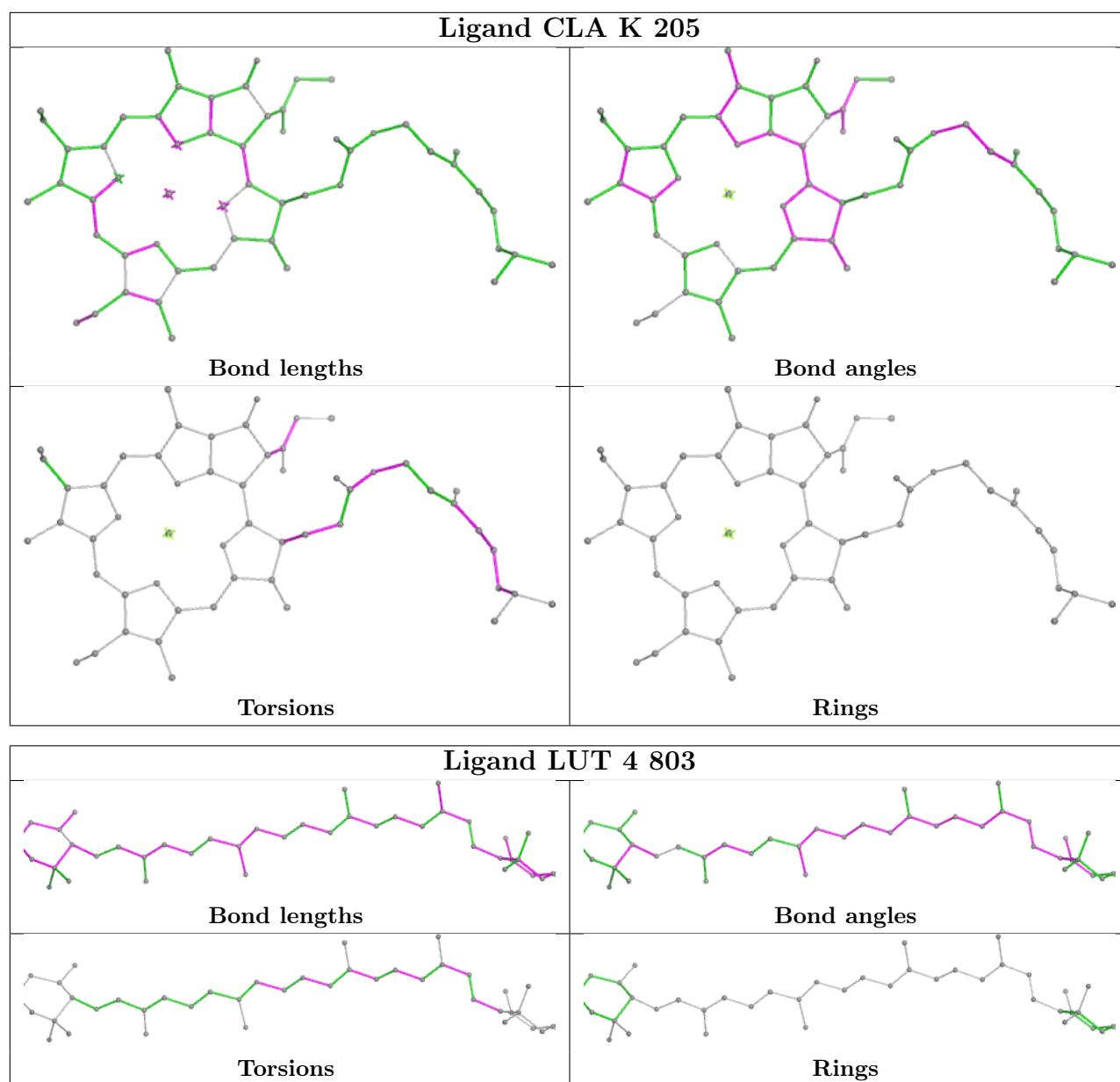
Ligand BCR 6 306**Ligand CLA A 855**

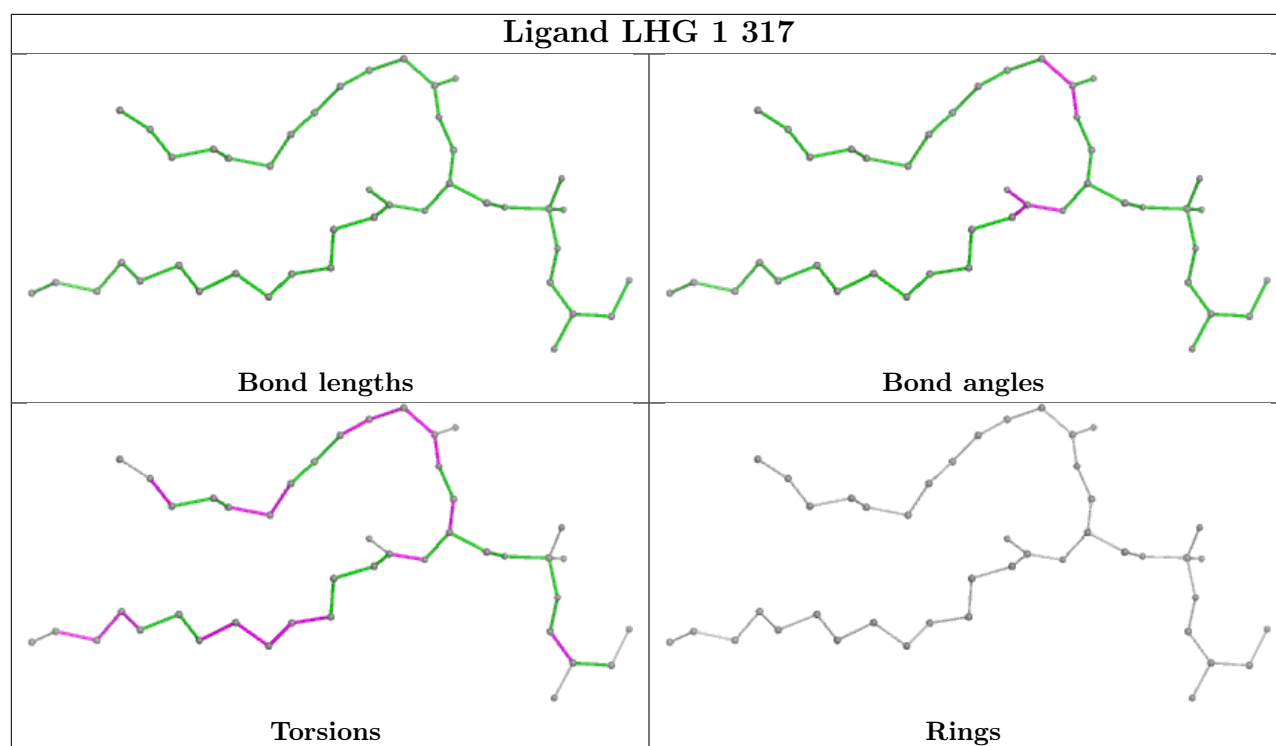
Ligand CHL 6 318

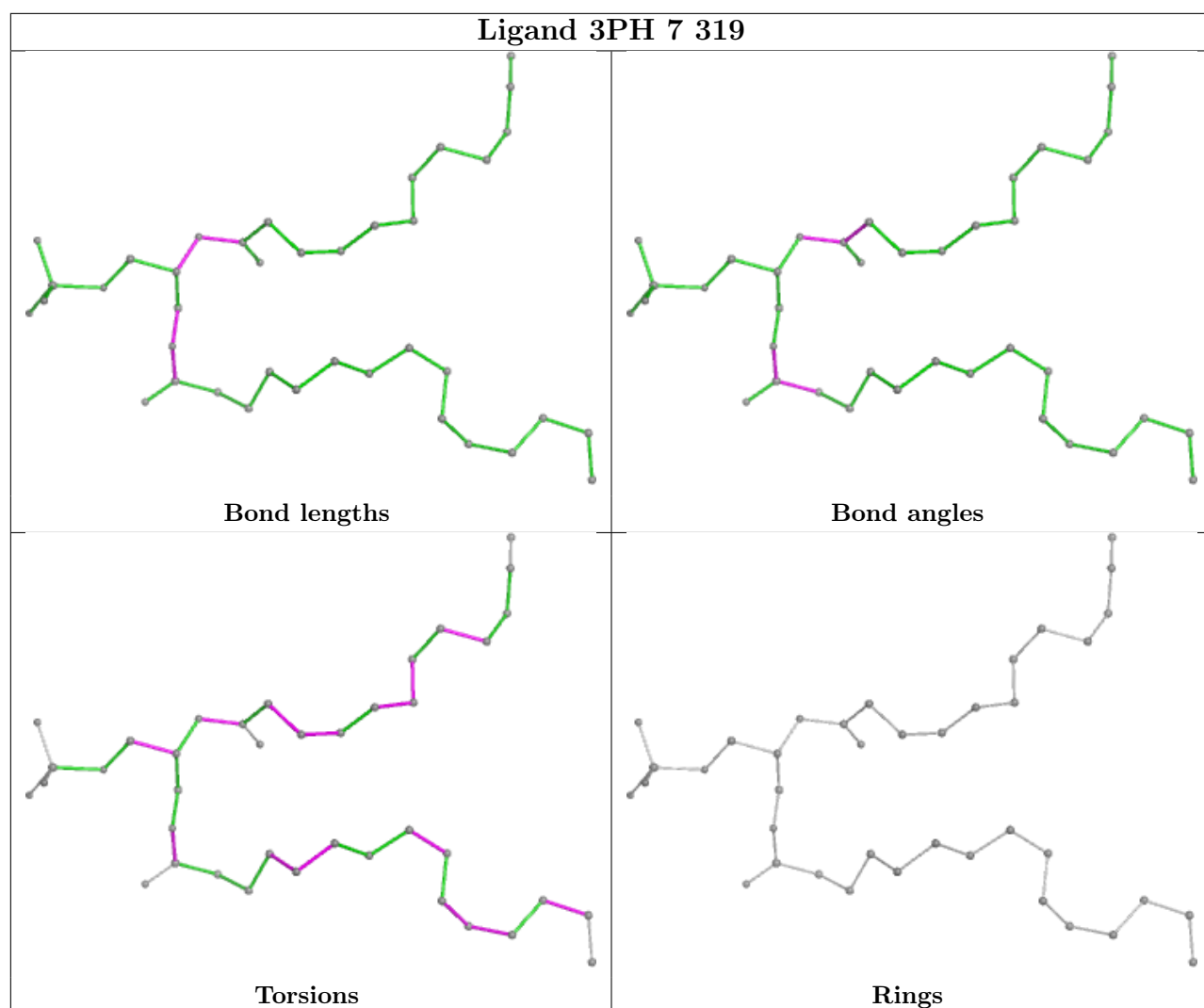


Ligand CLA 6 307

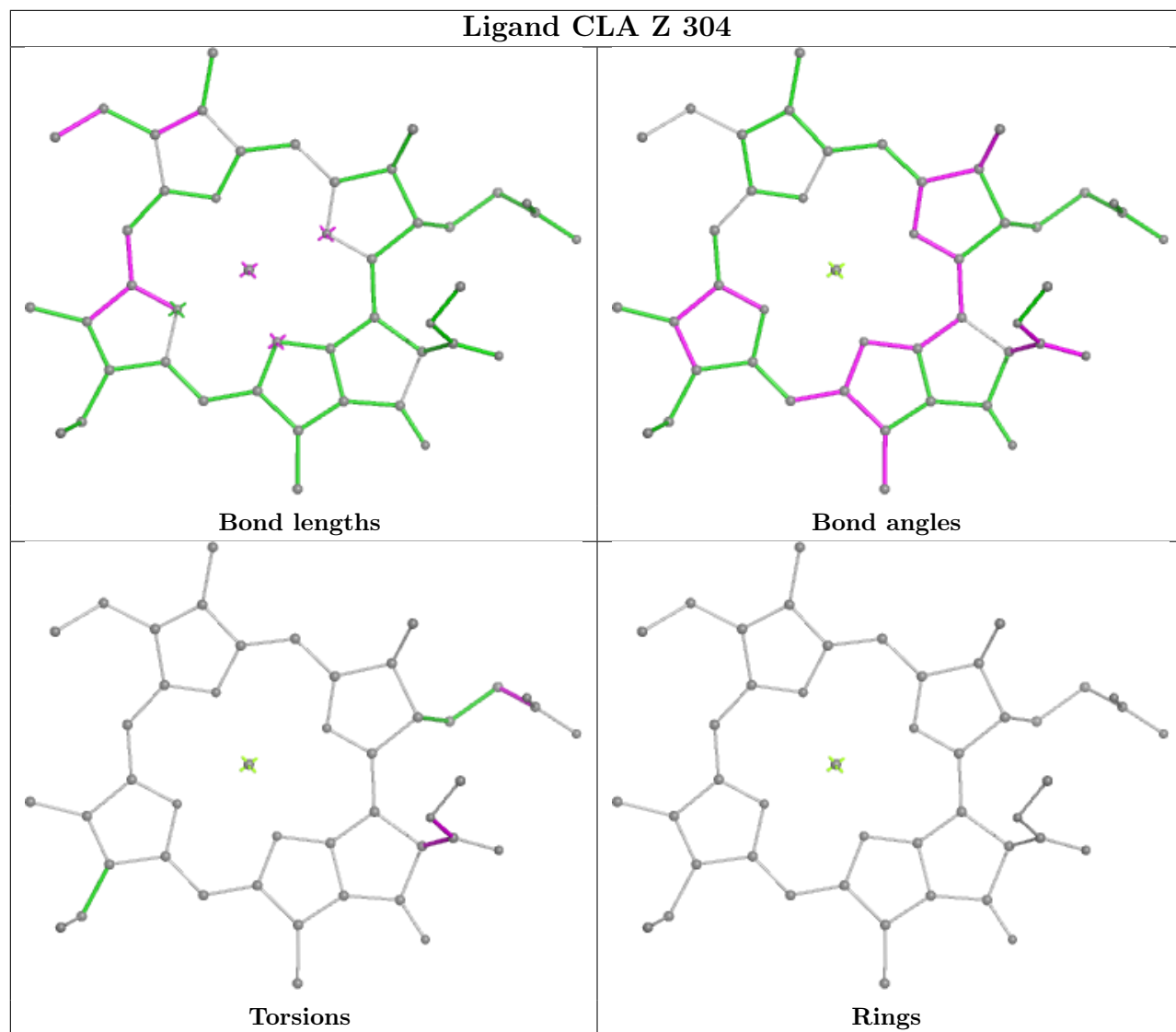




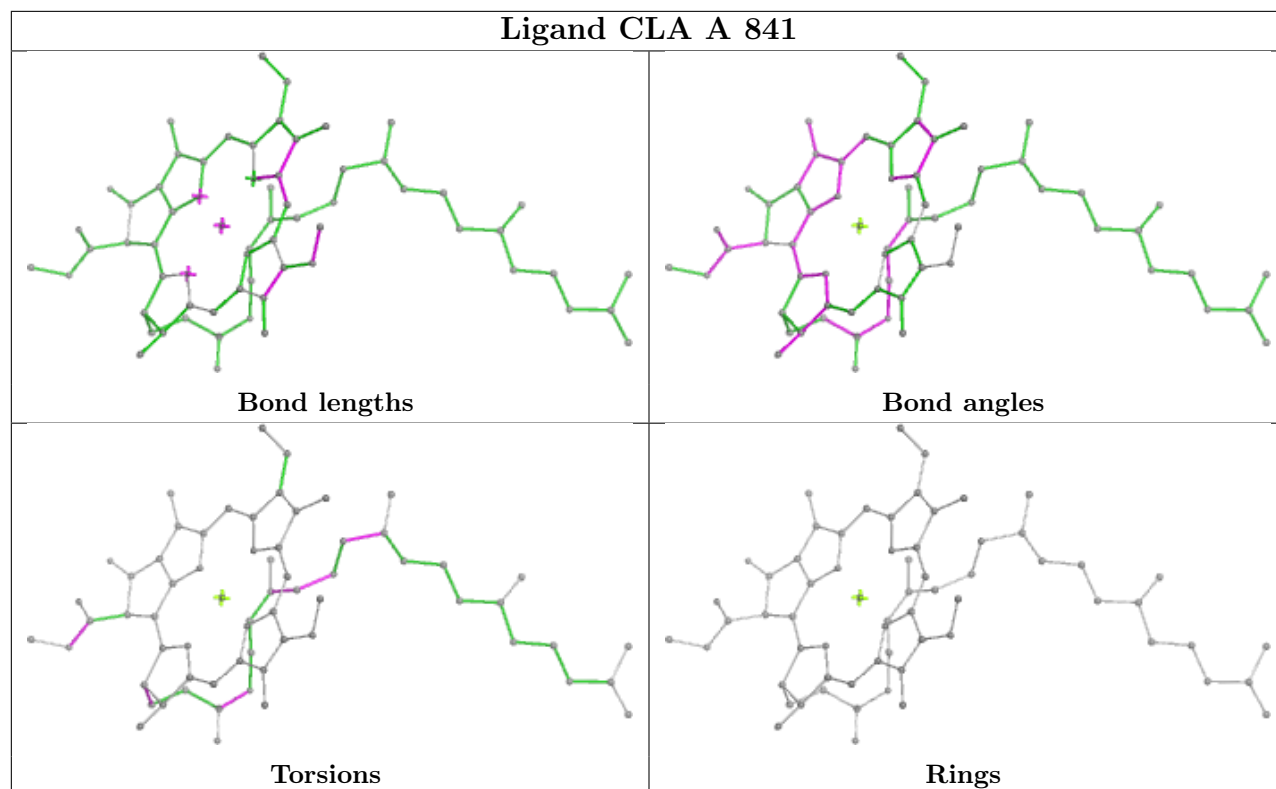




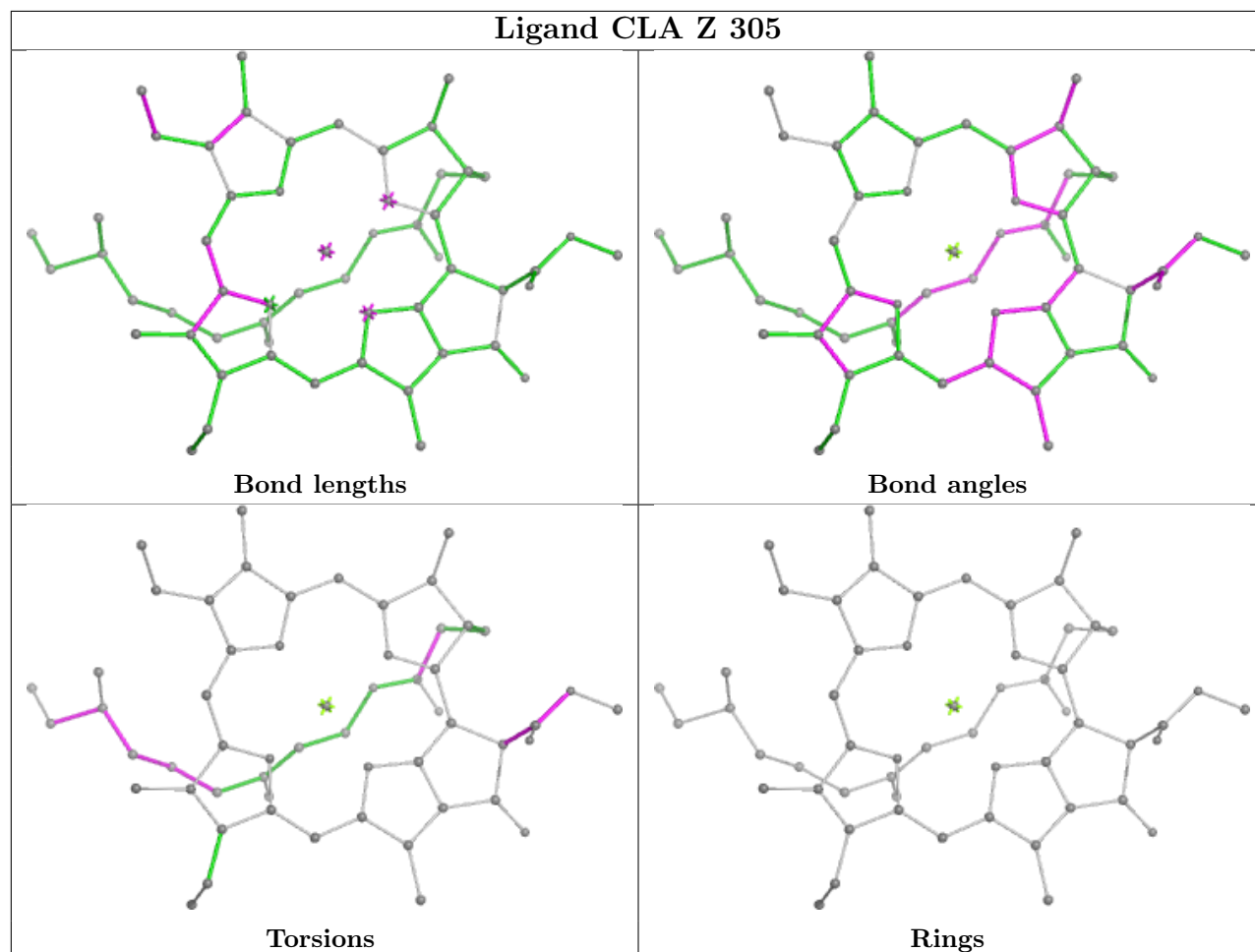
Ligand CLA Z 304

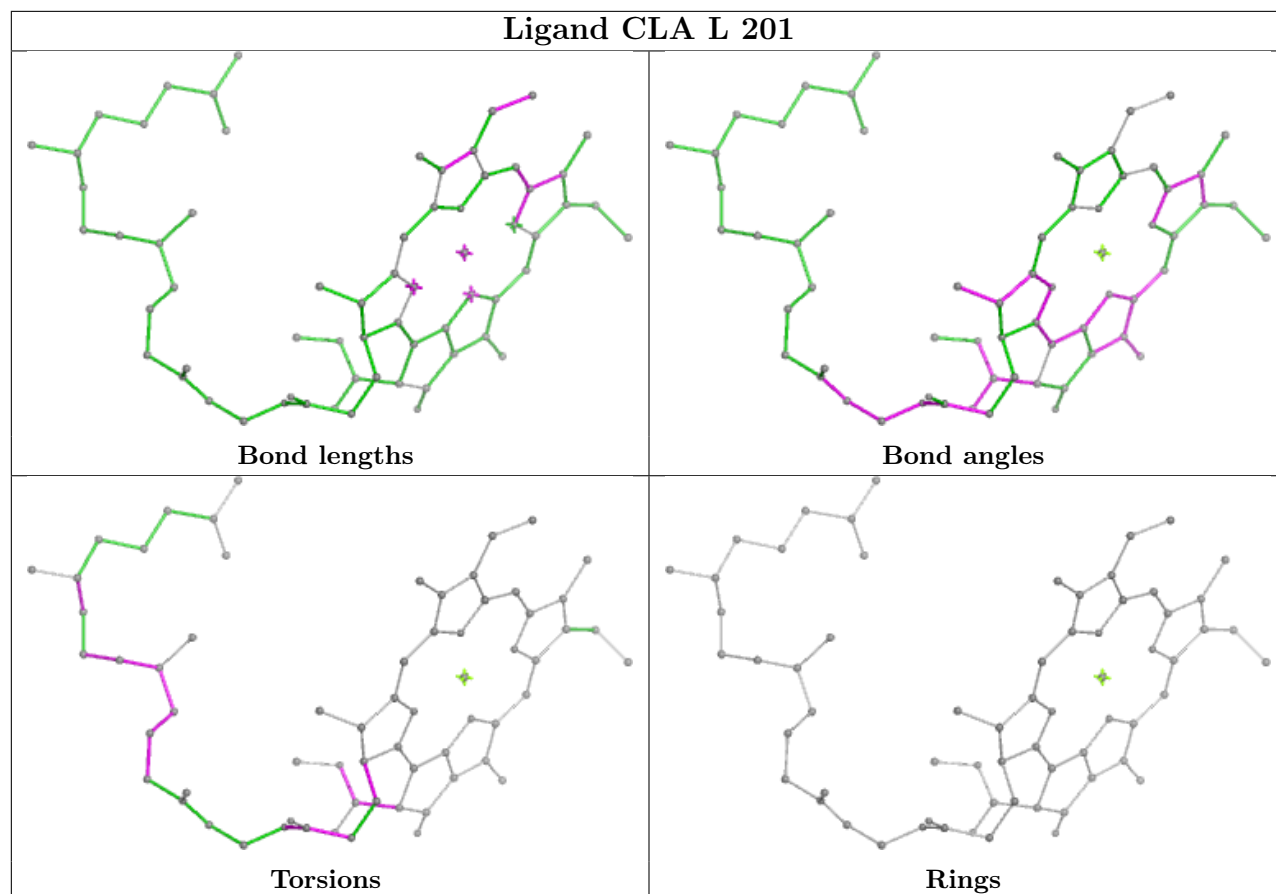
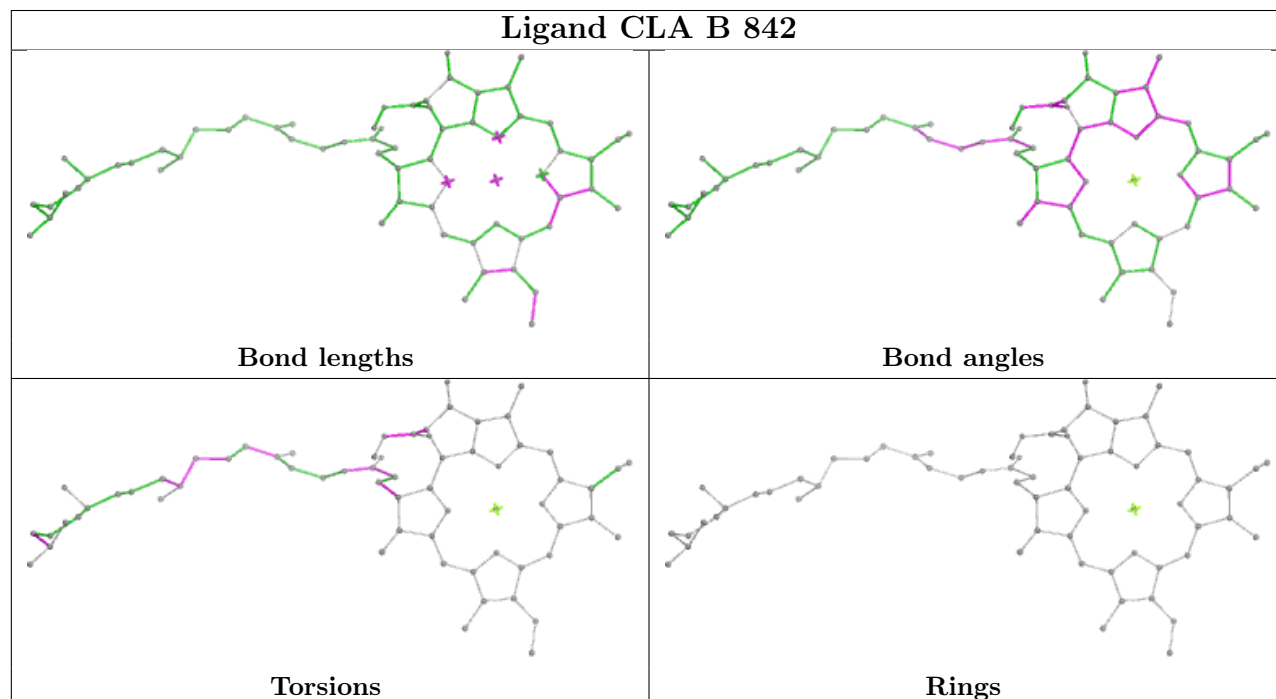


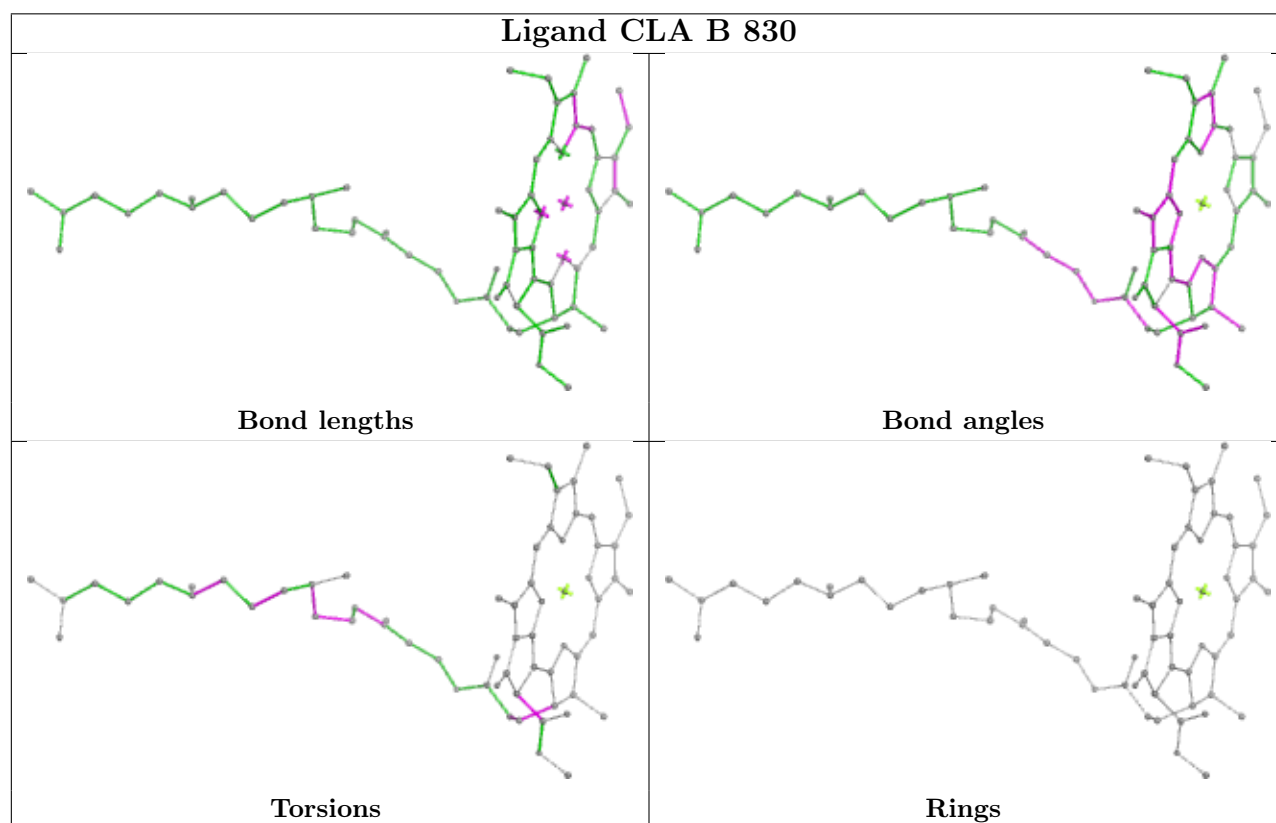
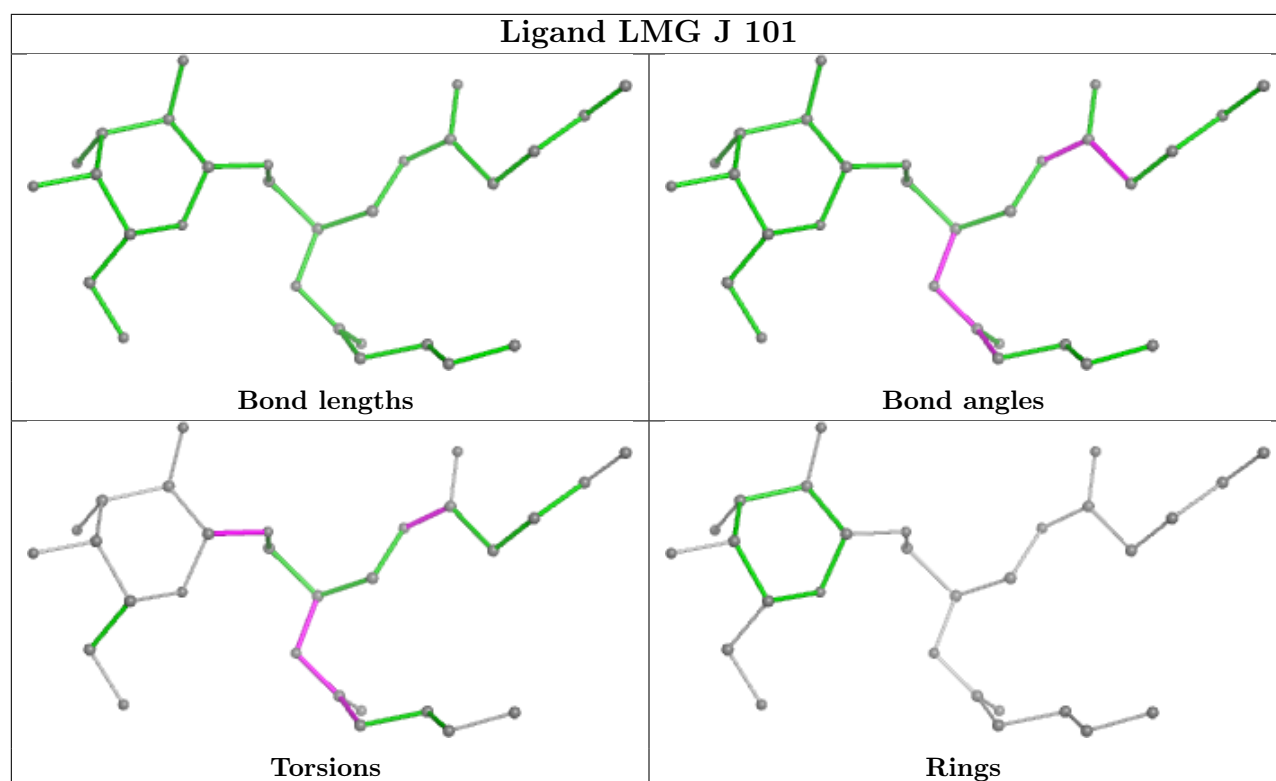
Ligand CLA A 841

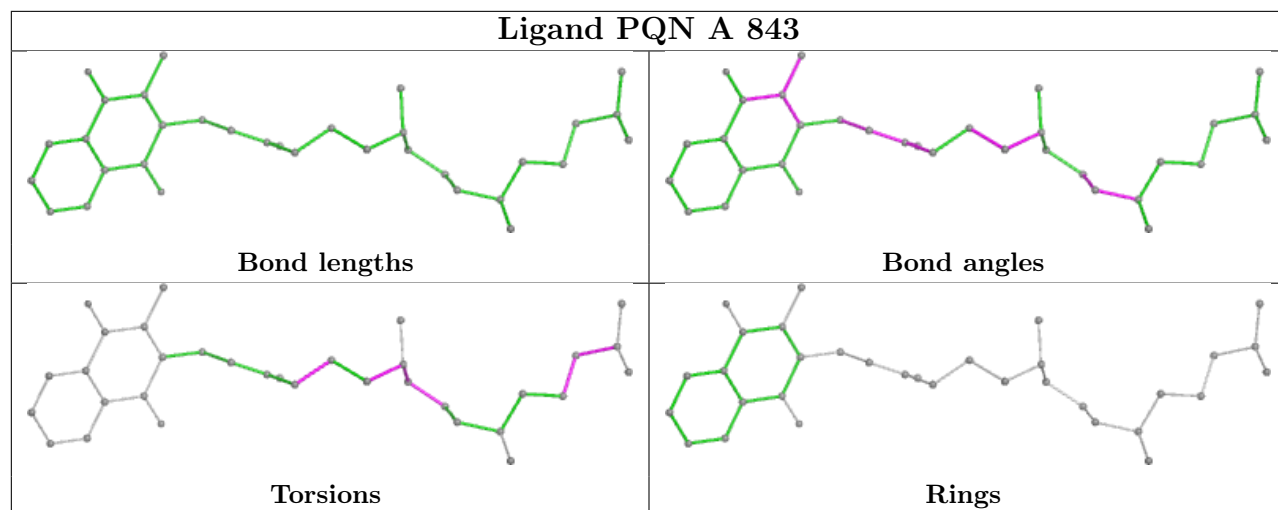


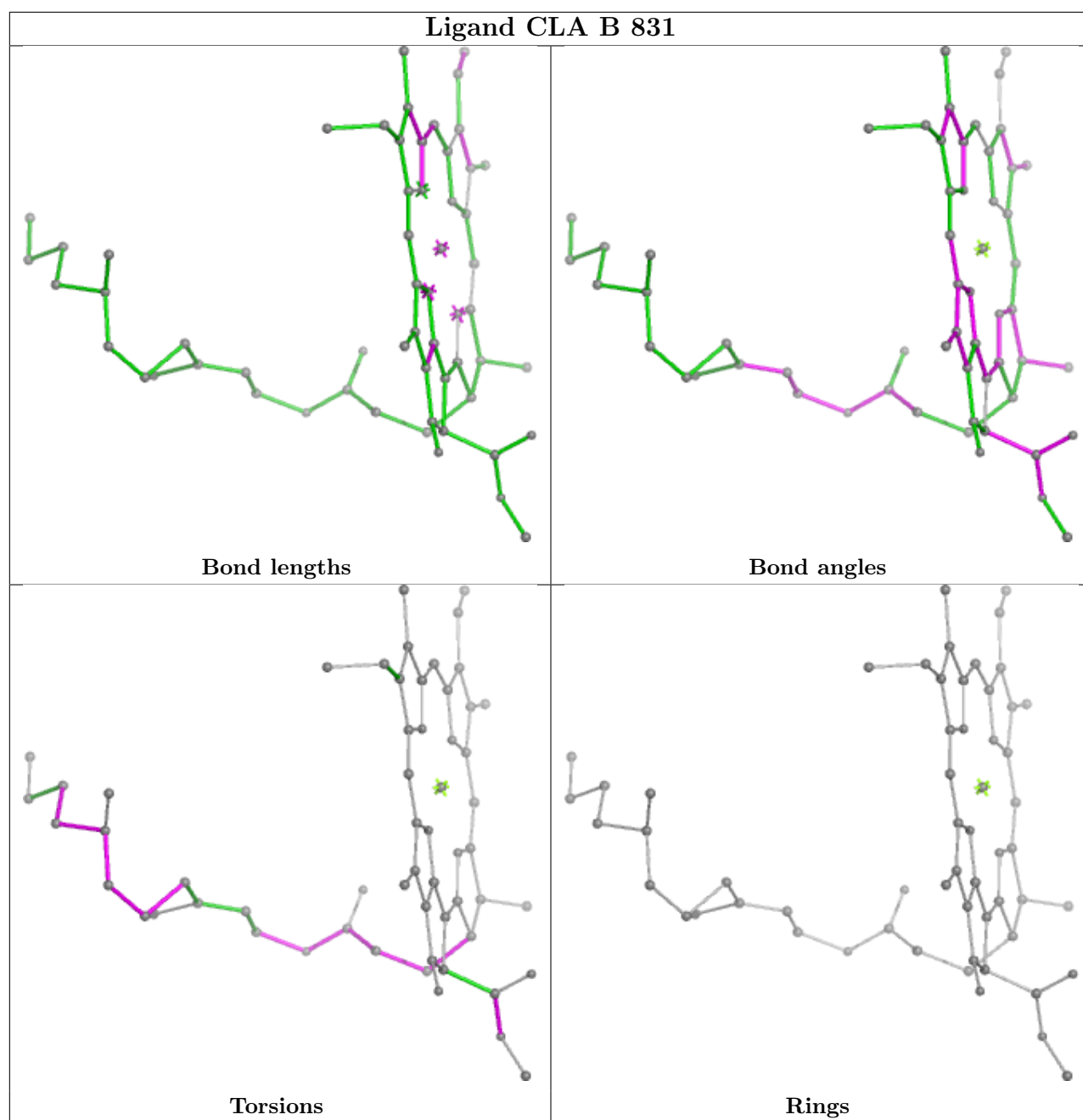
Ligand CLA Z 305



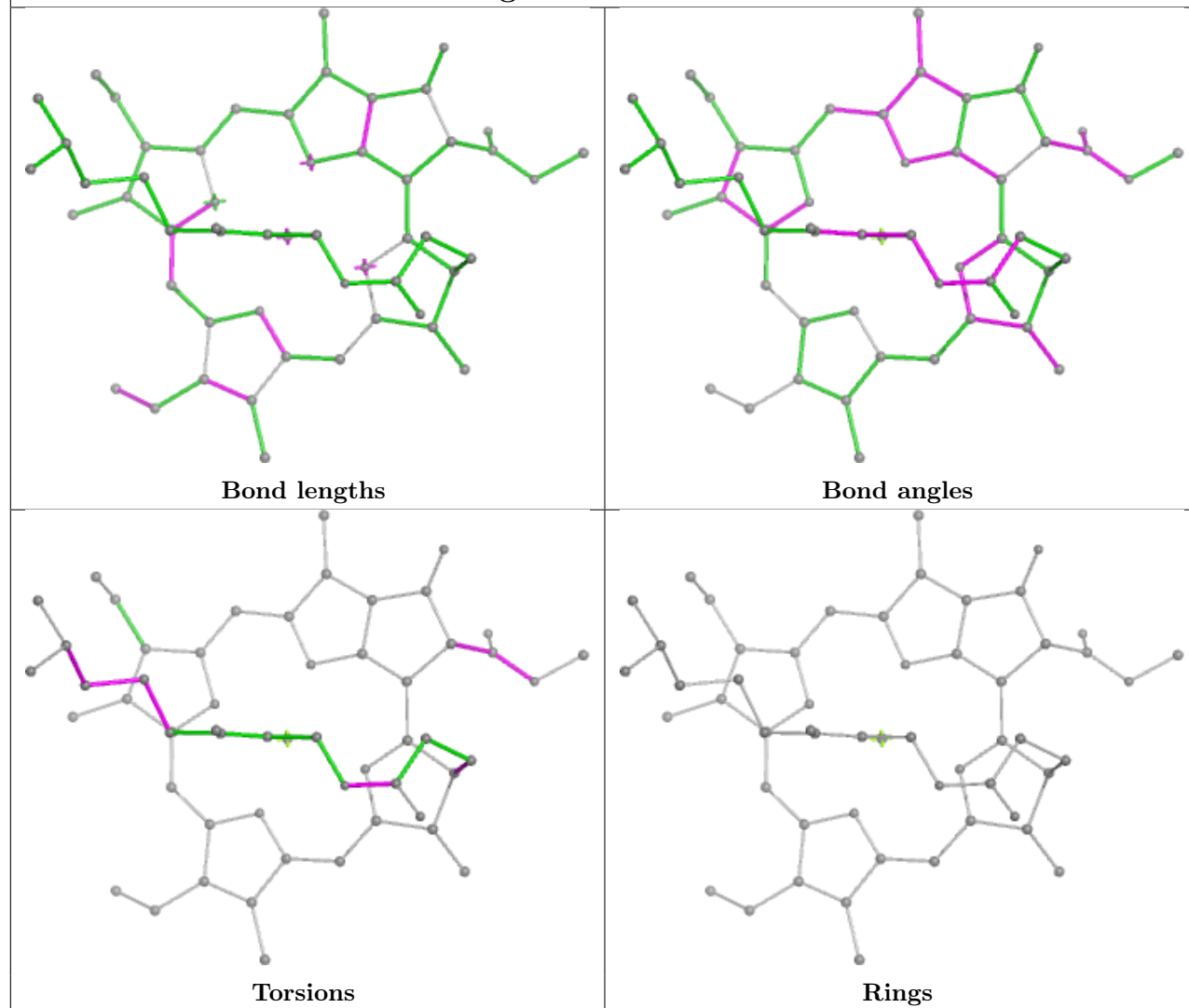
Ligand CLA L 201**Ligand CLA B 842**



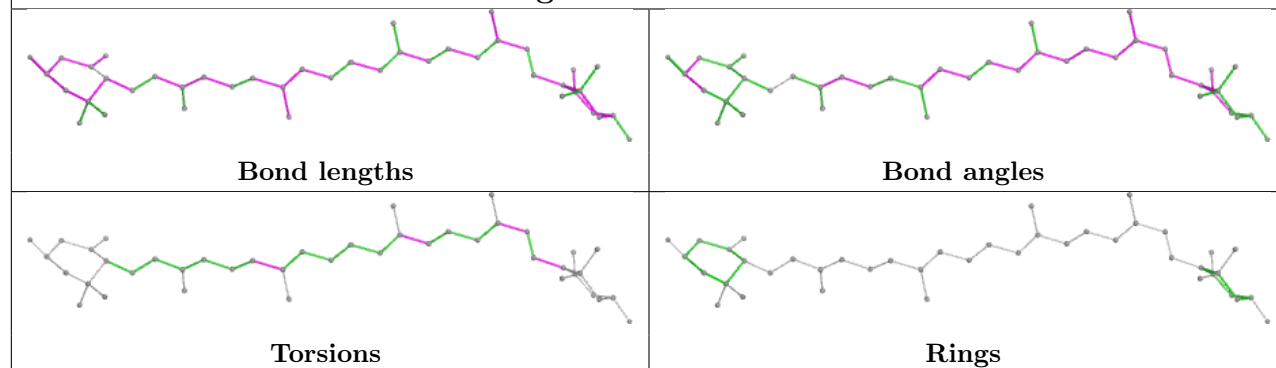


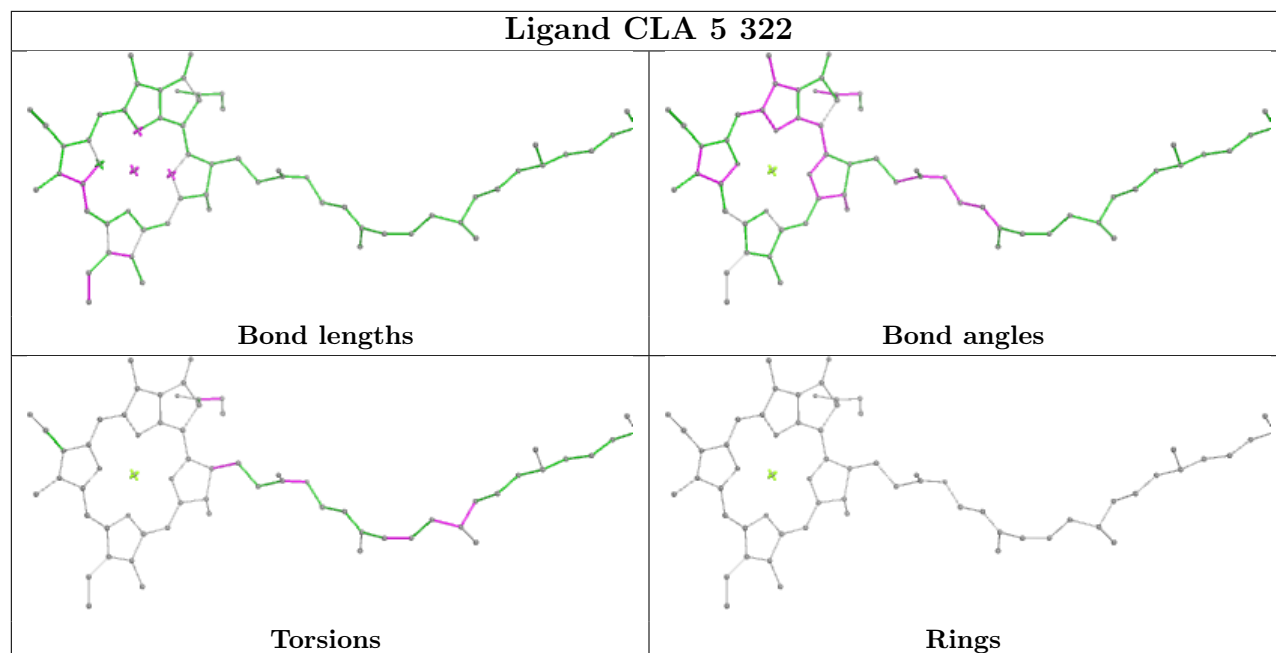
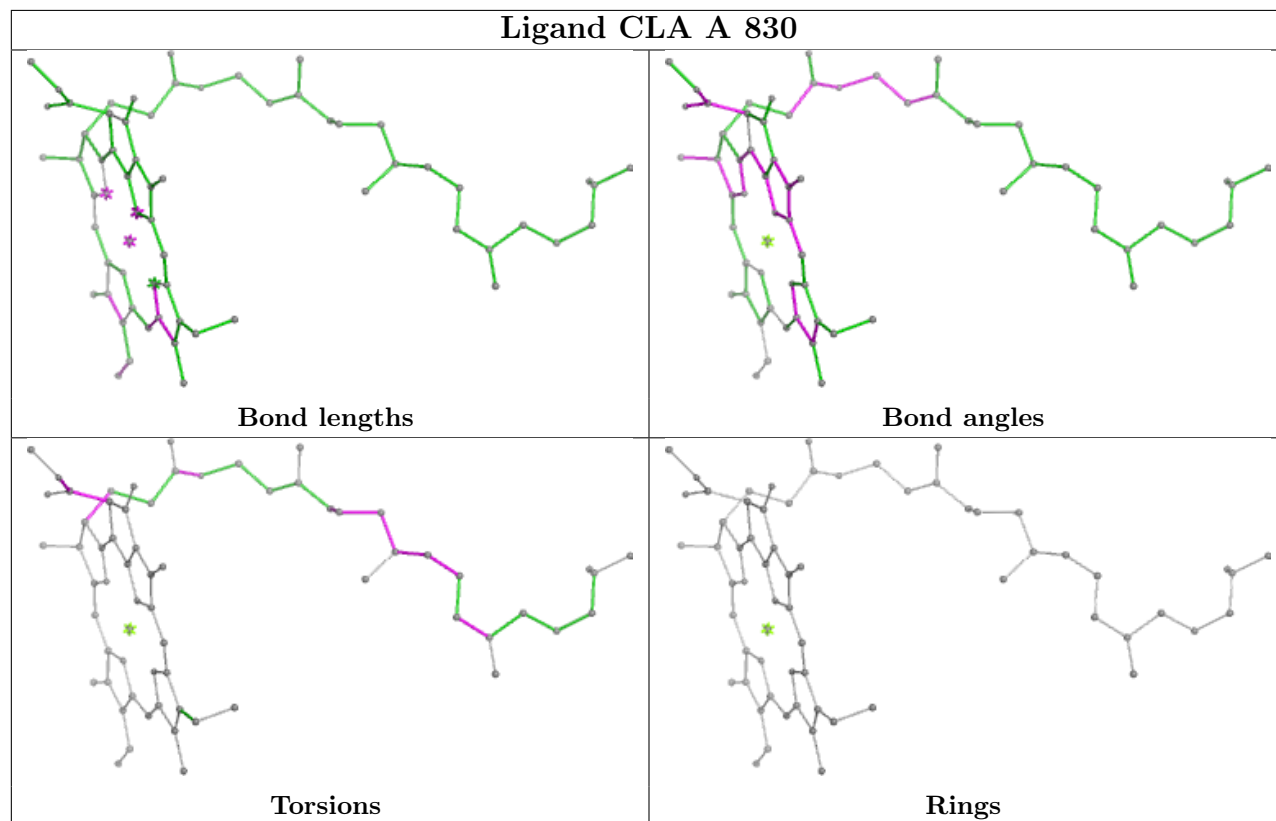


Ligand CLA 2 301

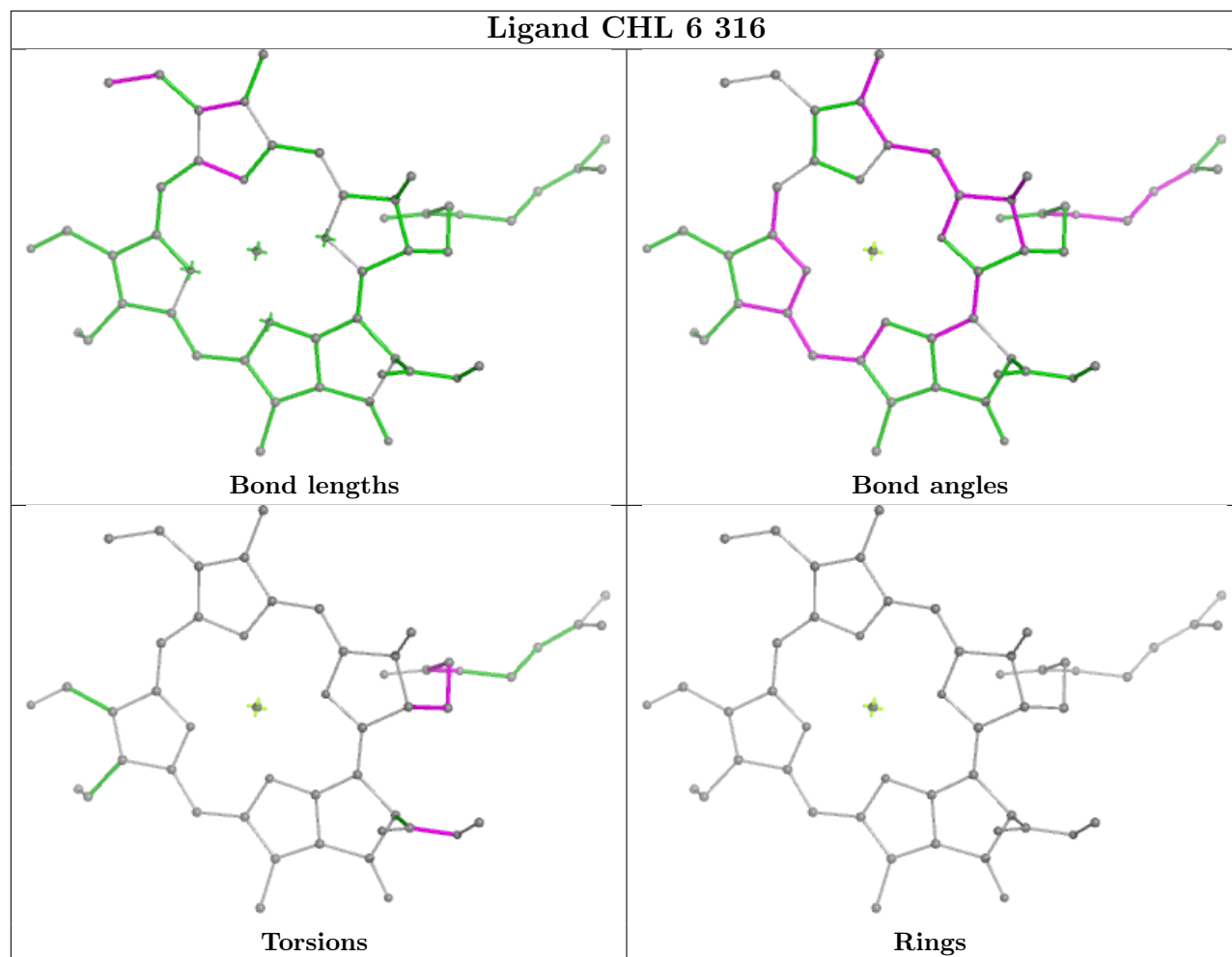


Ligand LUT 1 303

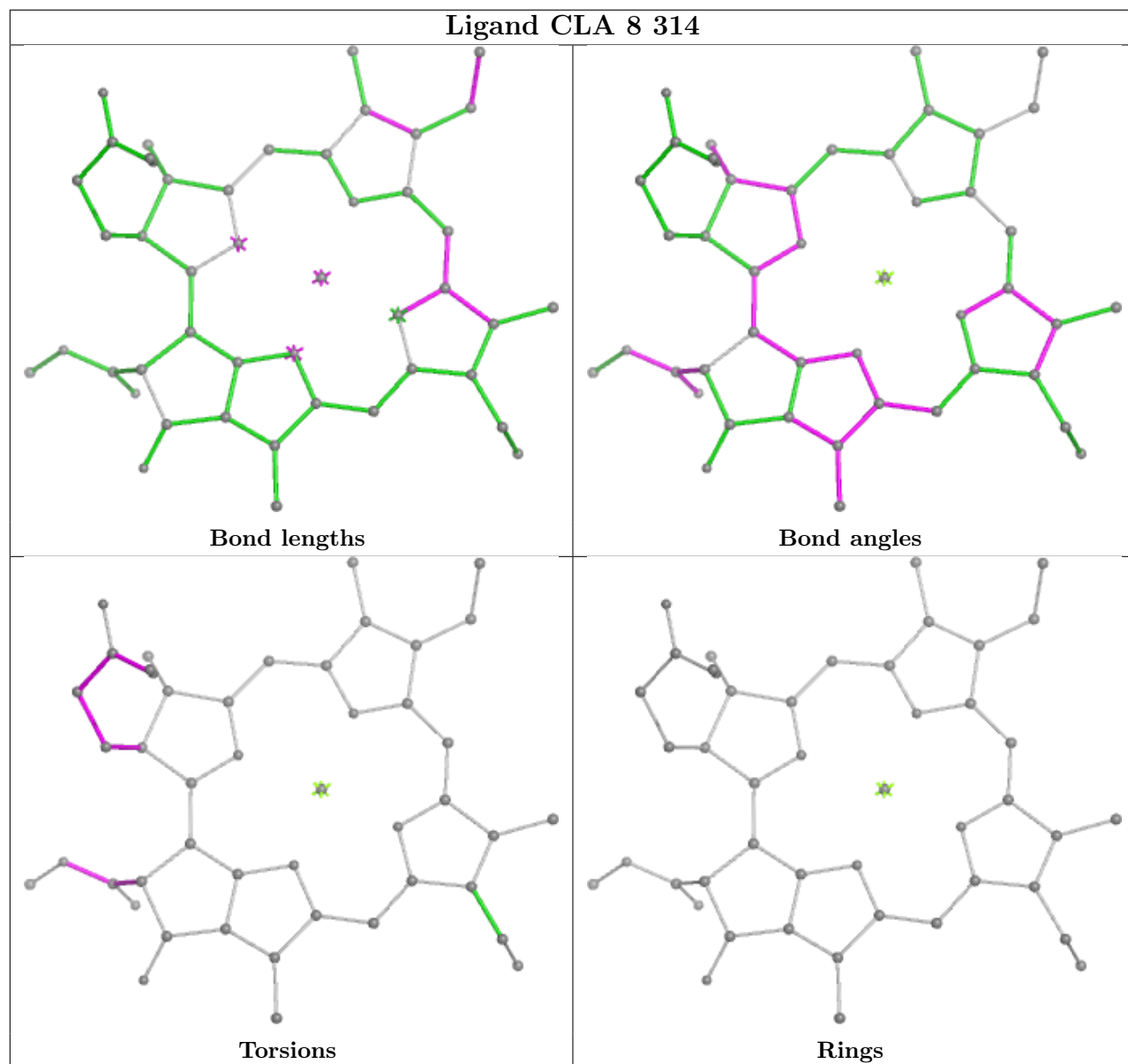


Ligand CLA 5 322**Ligand CLA A 830**

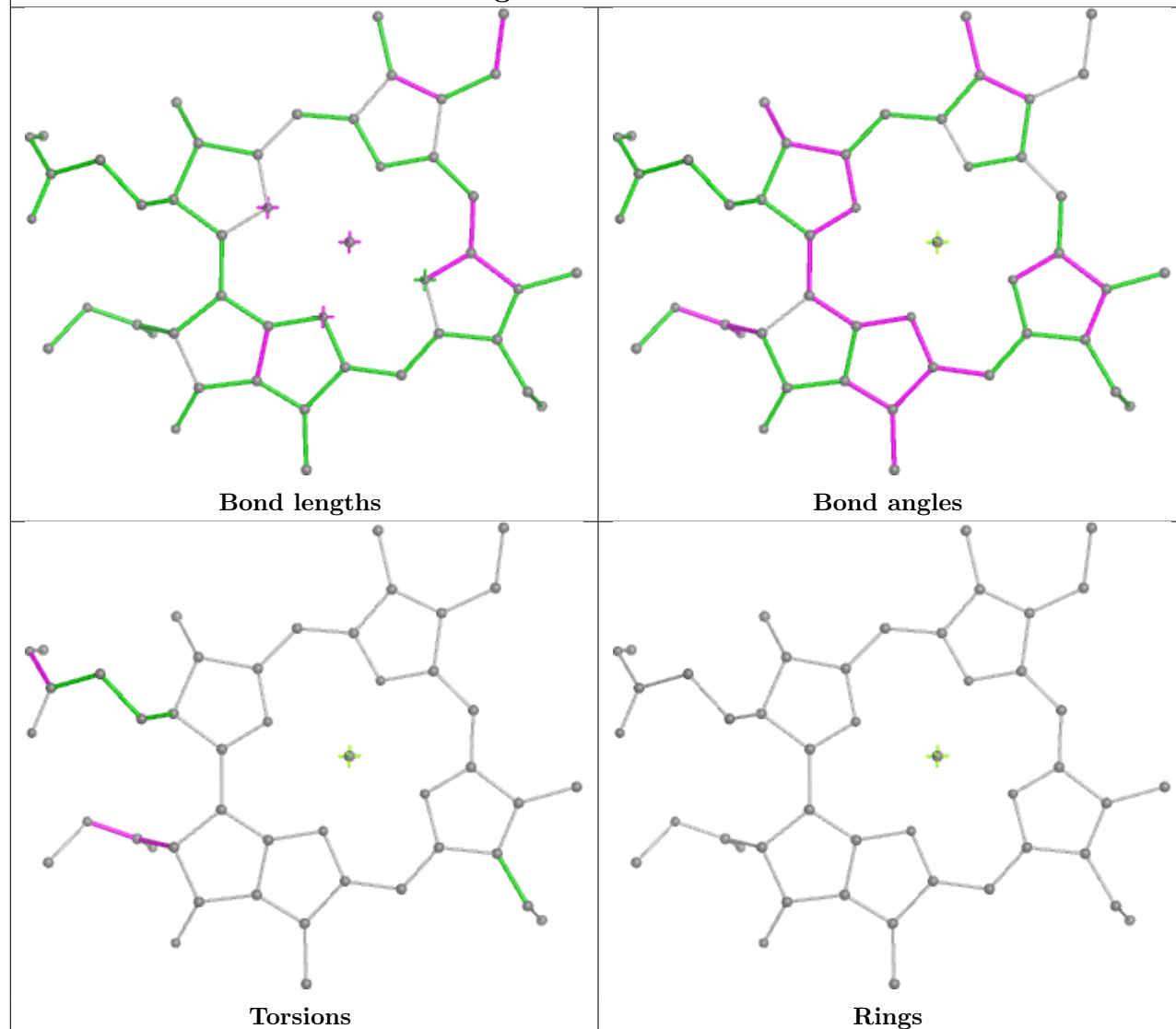
Ligand CHL 6 316



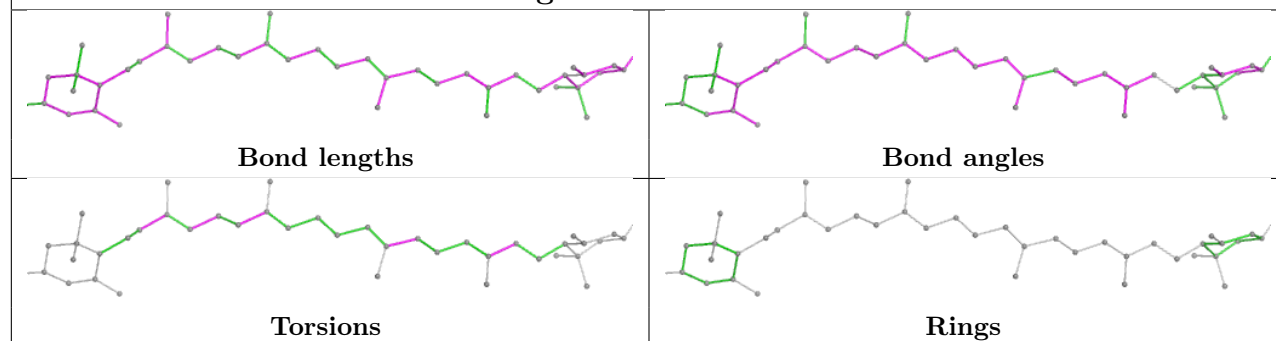
Ligand CLA 8 314



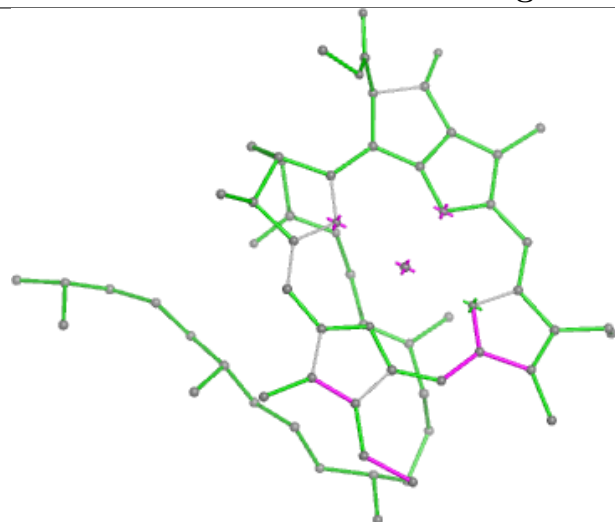
Ligand CLA 3 309



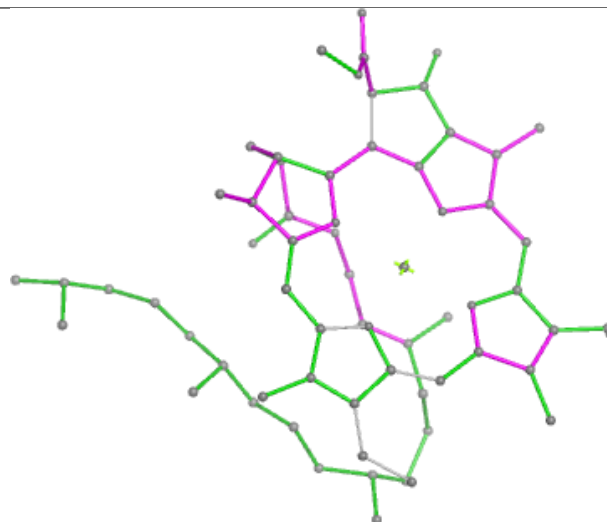
Ligand LUT 6 303



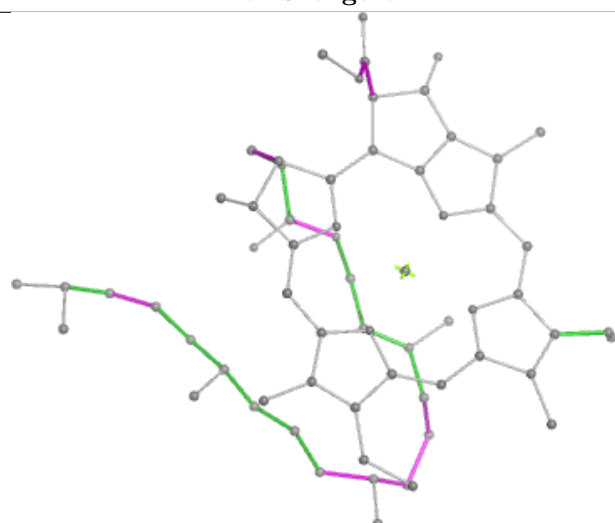
Ligand CLA B 811



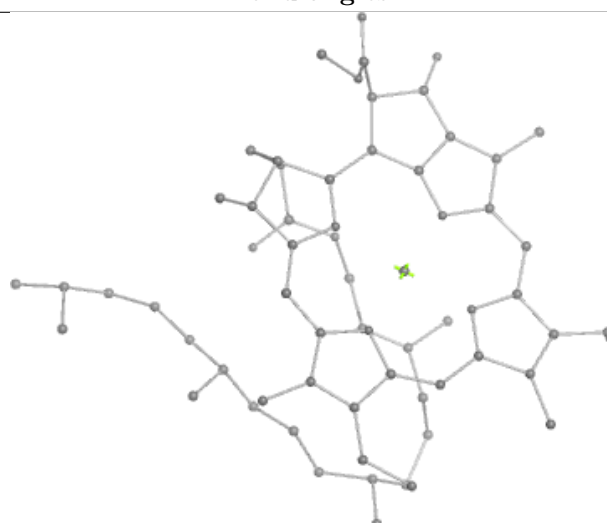
Bond lengths



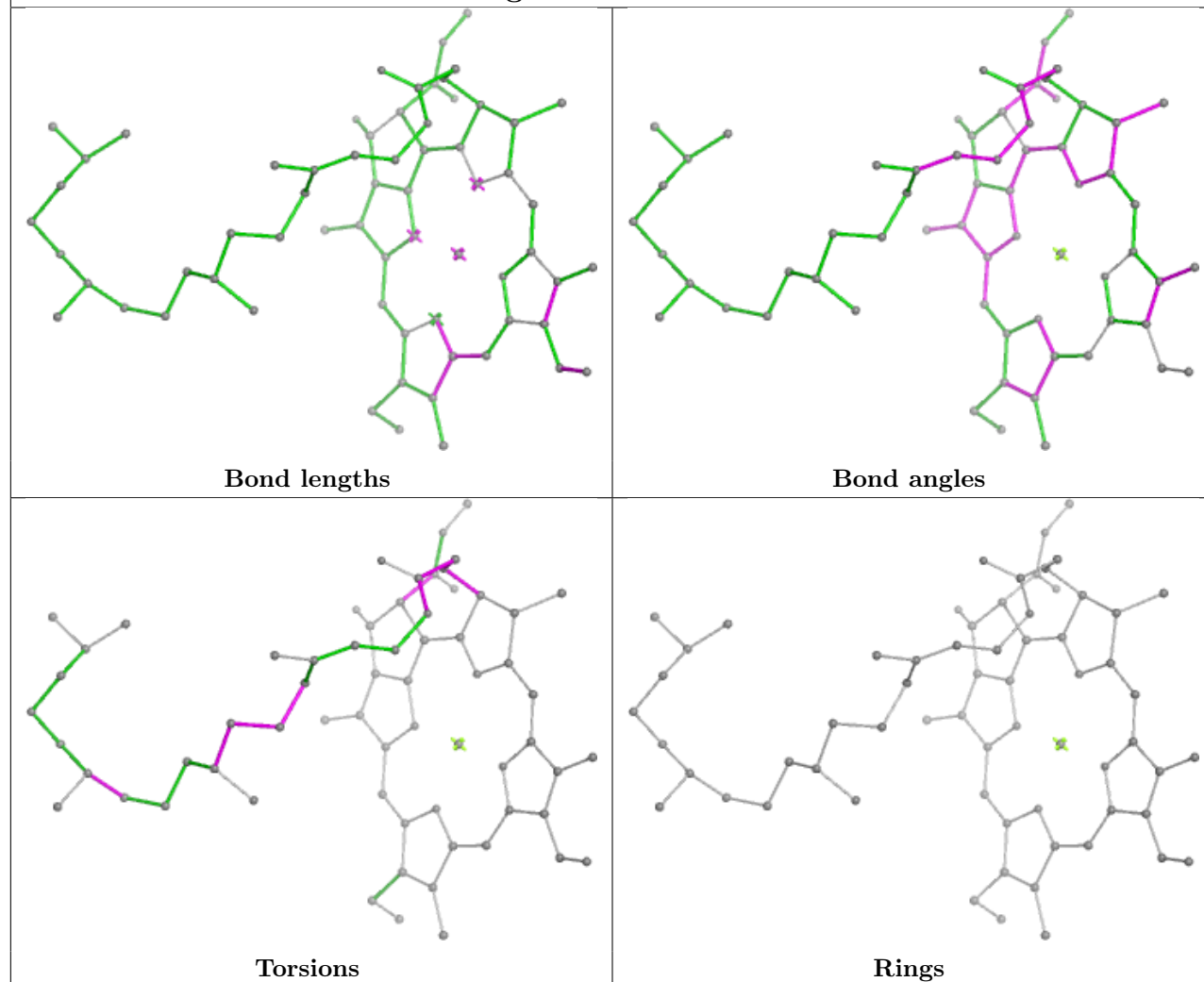
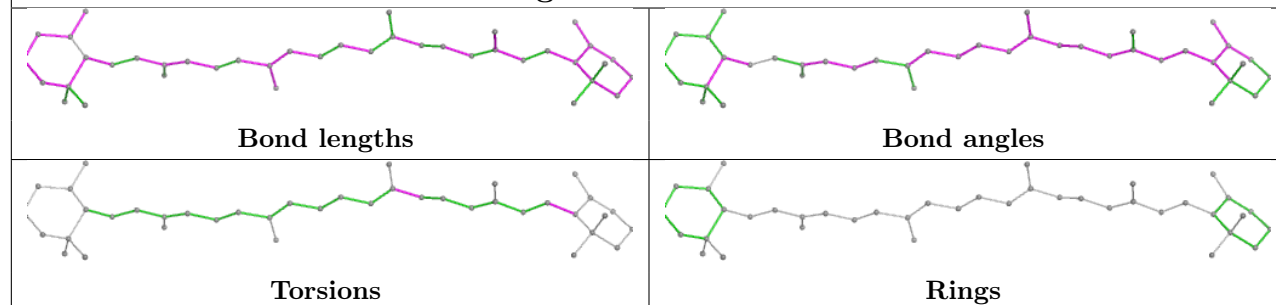
Bond angles



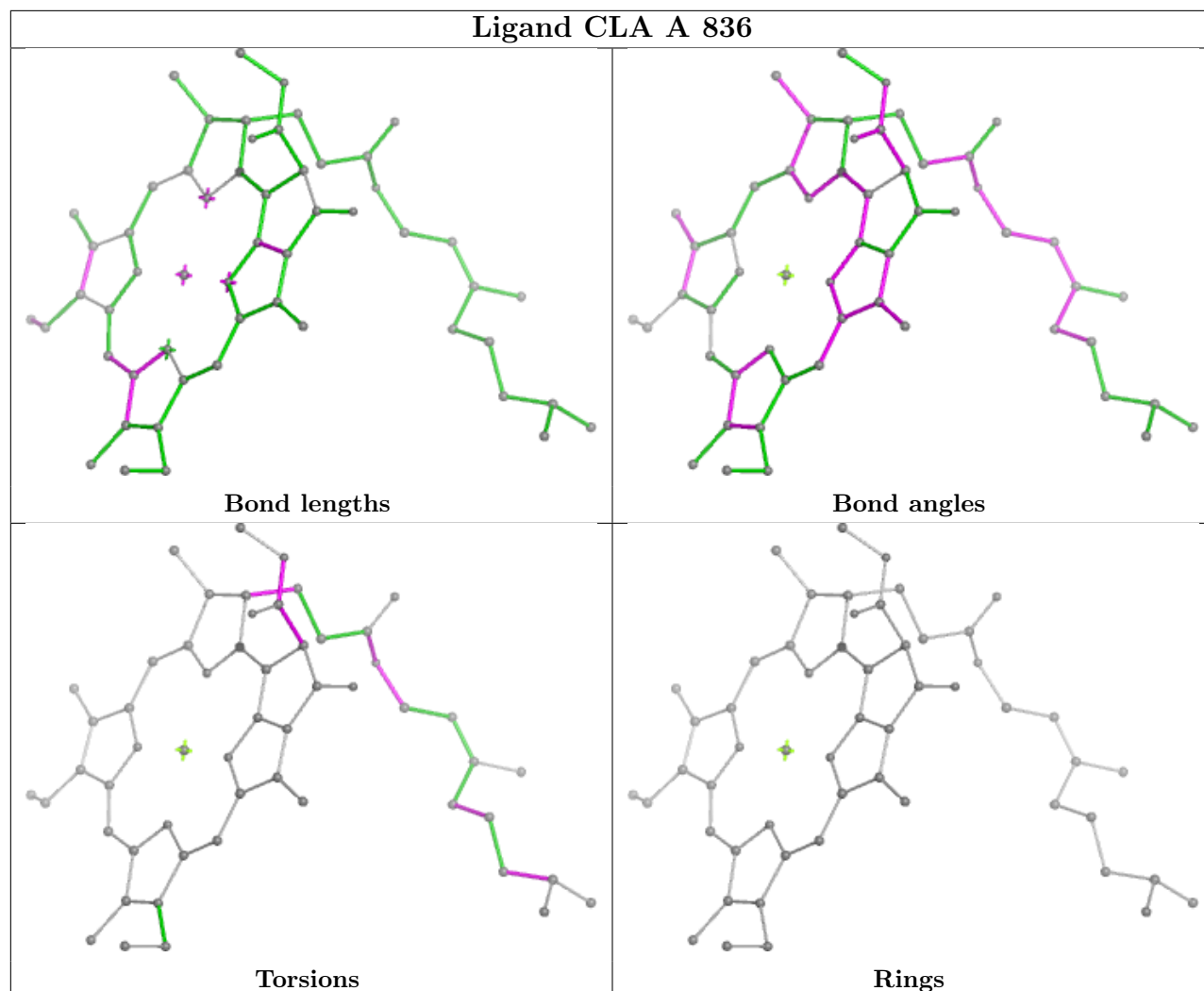
Torsions



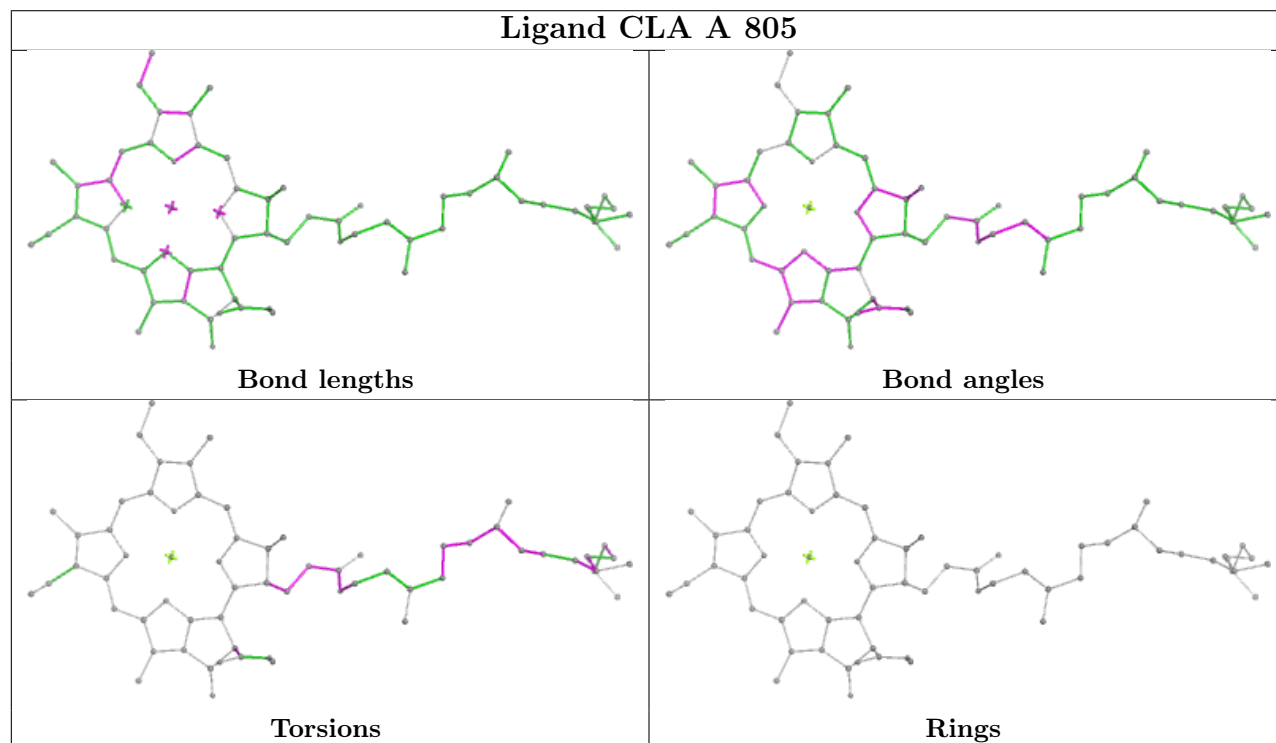
Rings

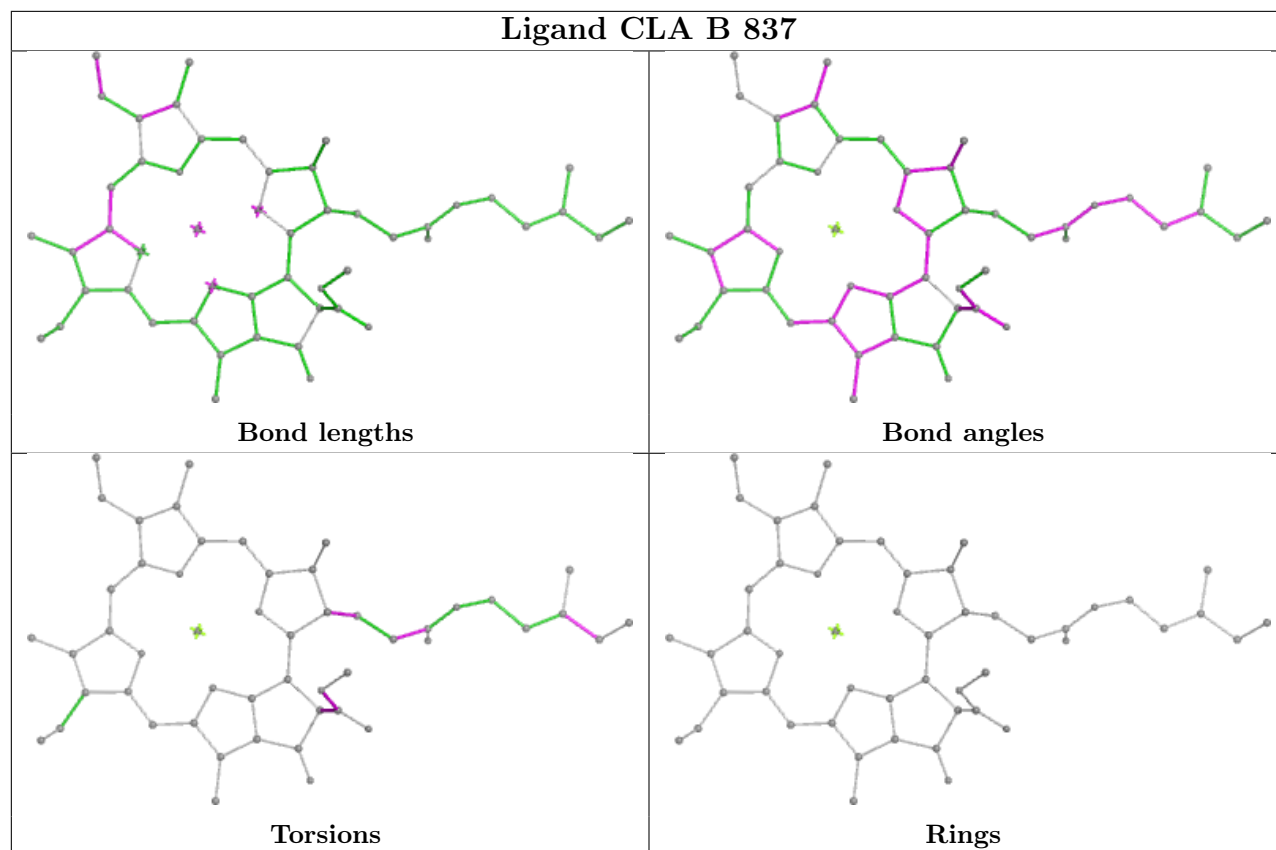
Ligand CLA 5 318**Ligand LUT 8 303**

Ligand CLA A 836

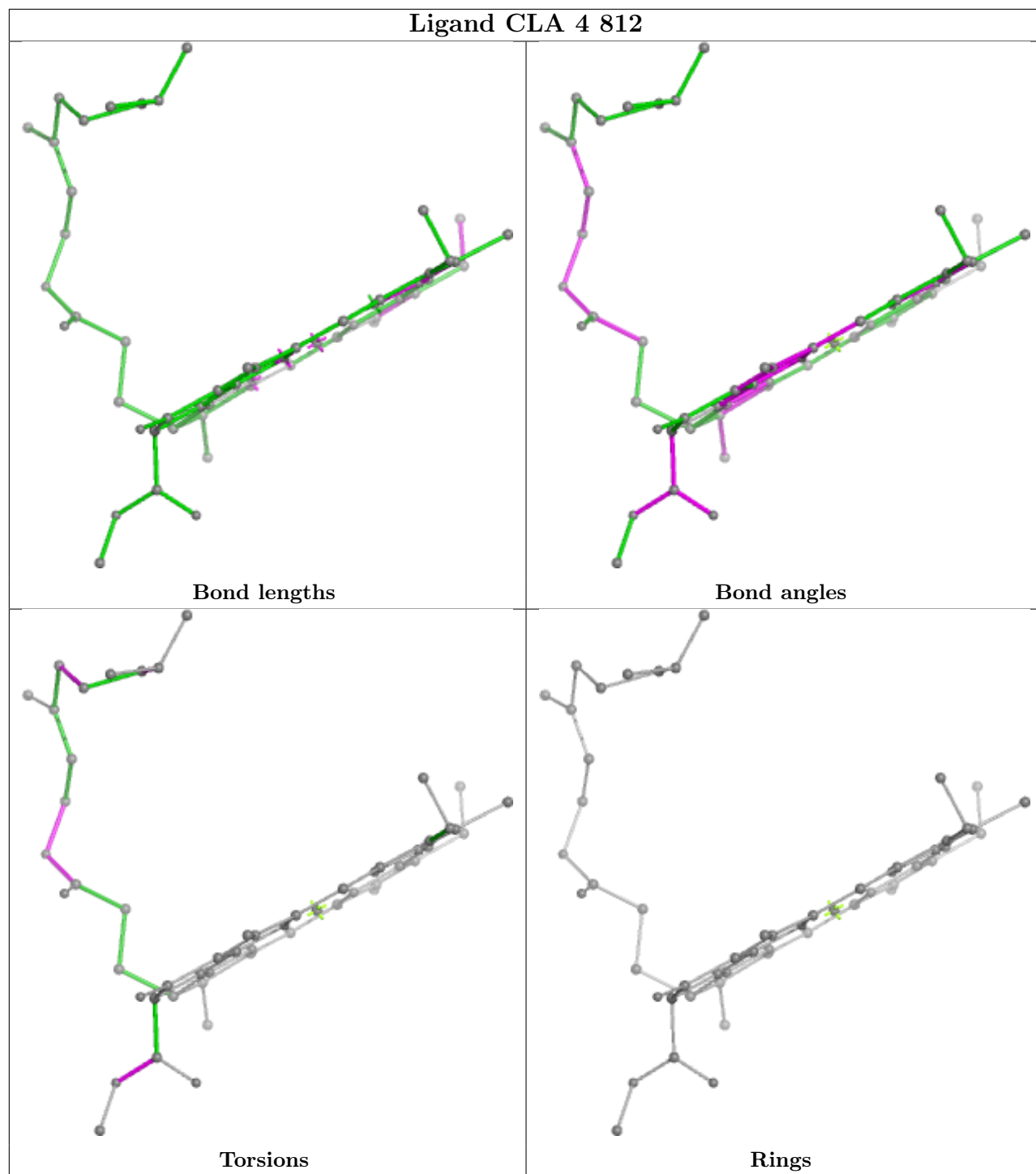


Ligand CLA A 805

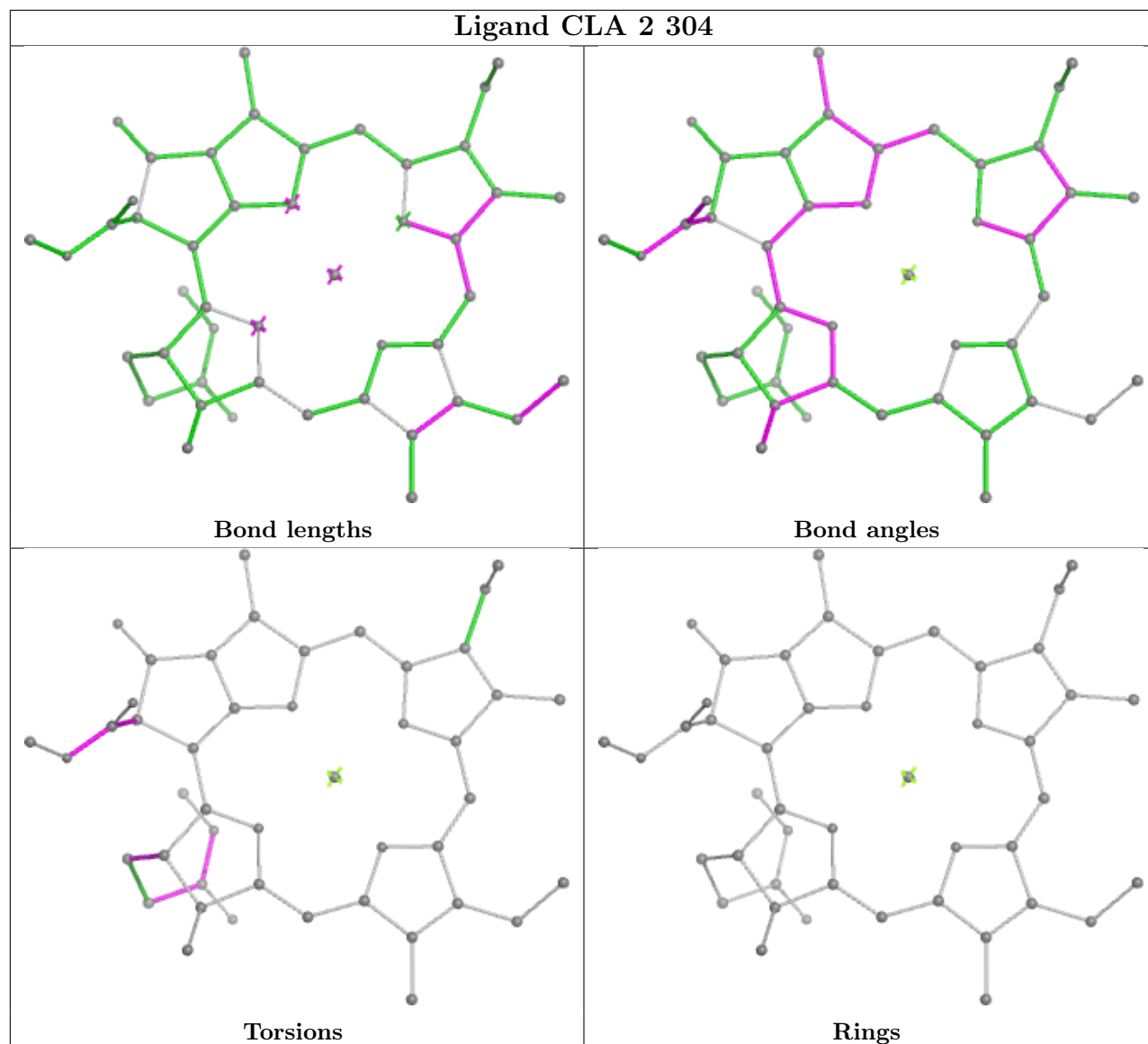




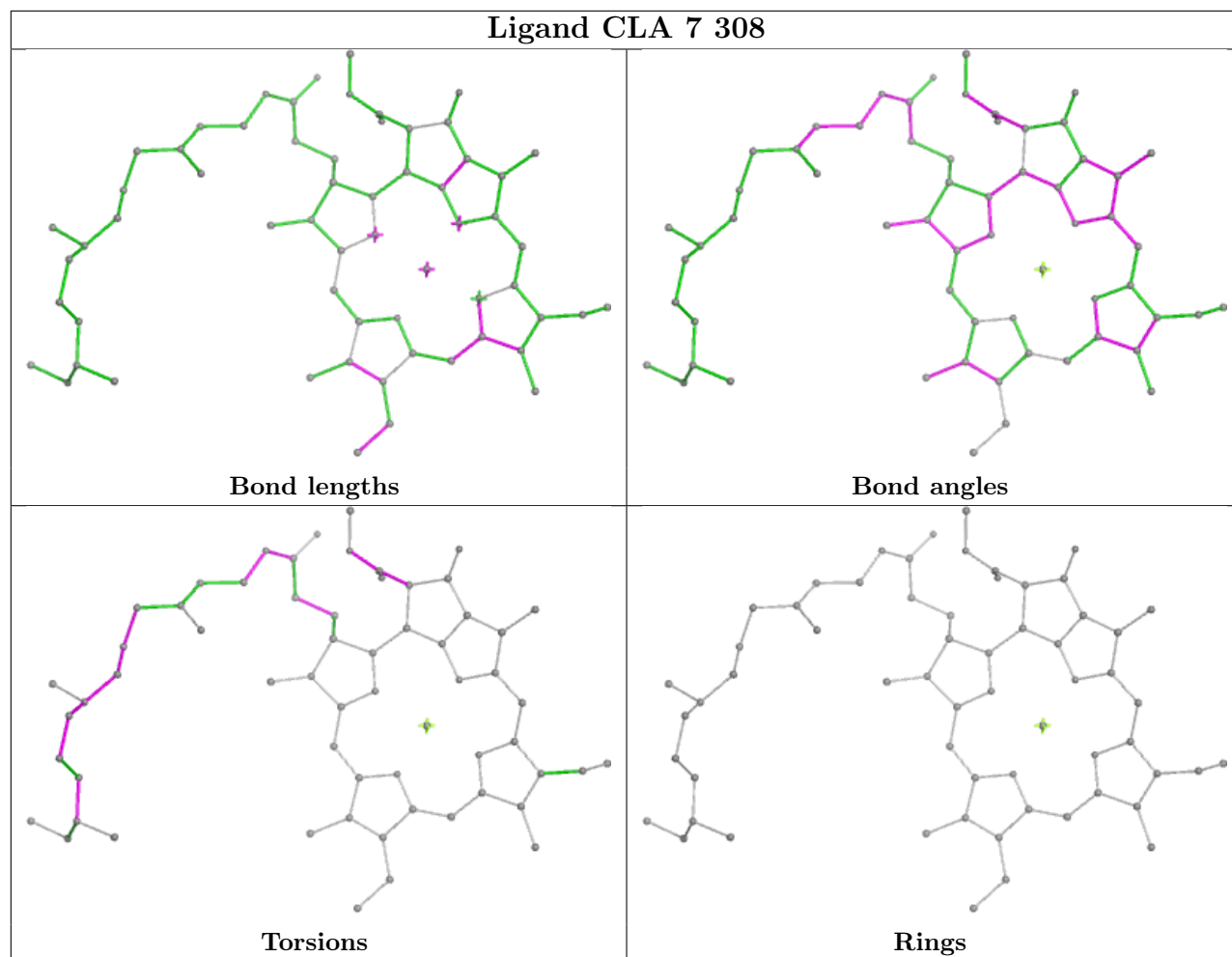
Ligand CLA 4 812



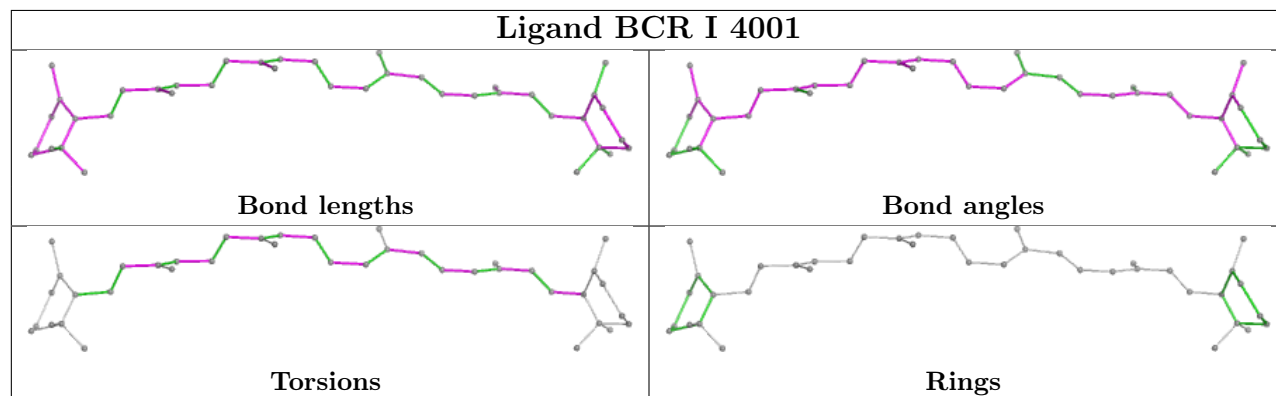
Ligand CLA 2 304

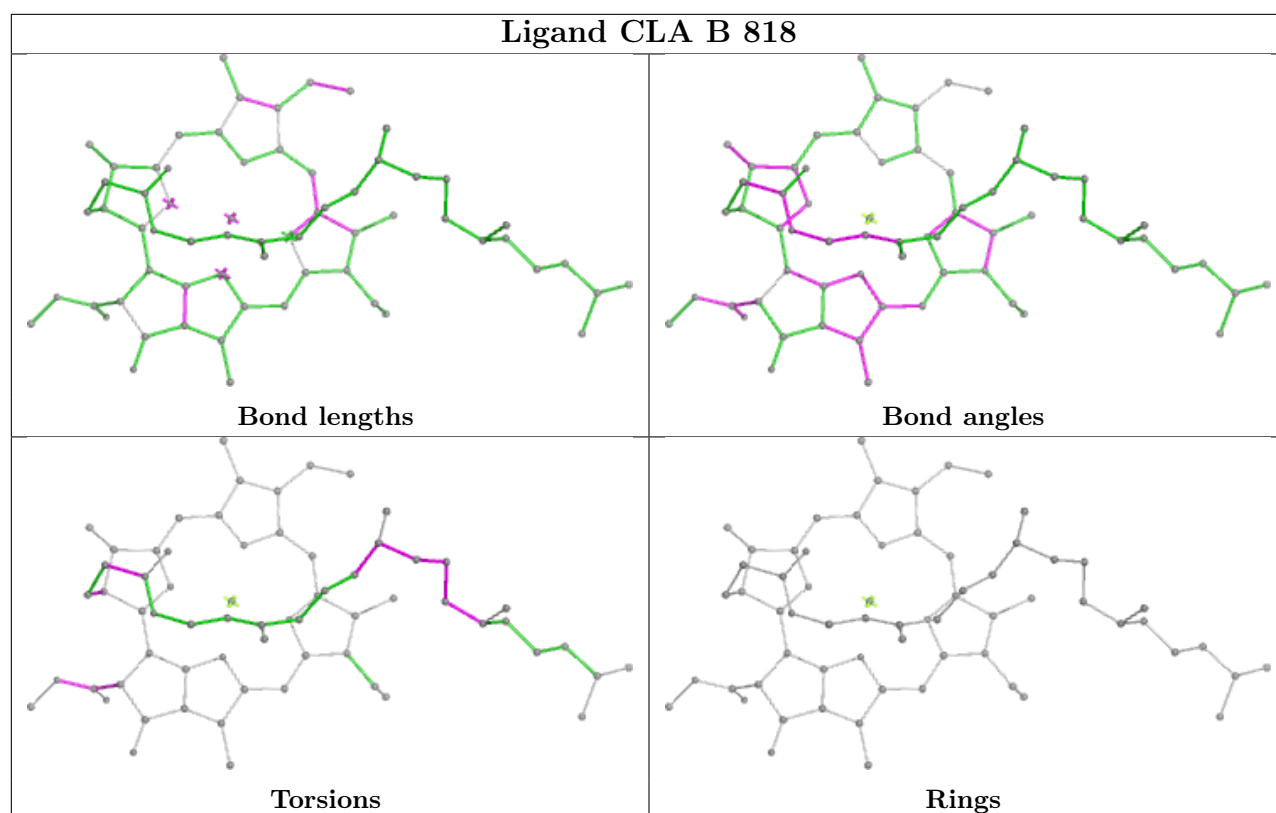


Ligand CLA 7 308

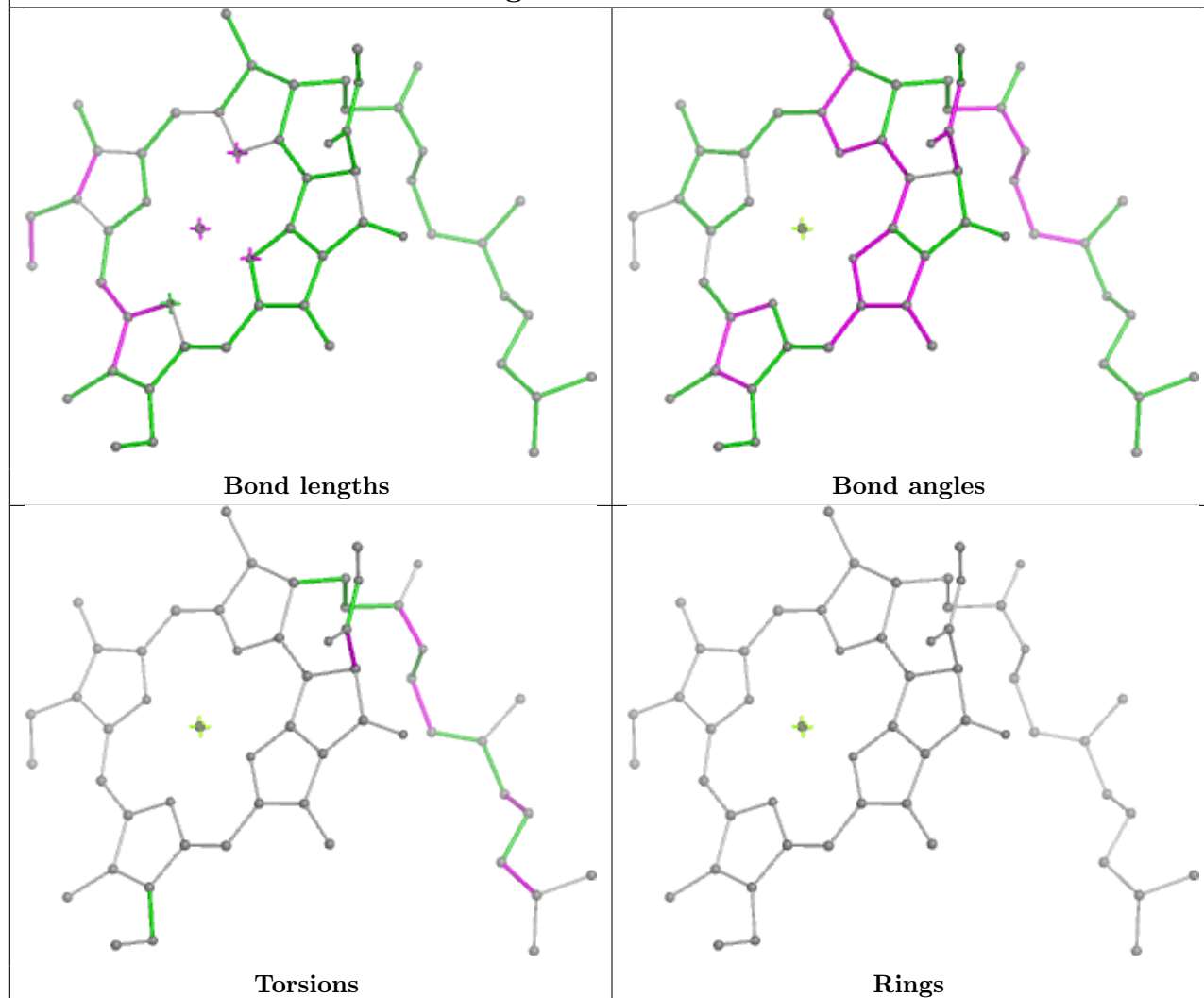


Ligand BCR I 4001

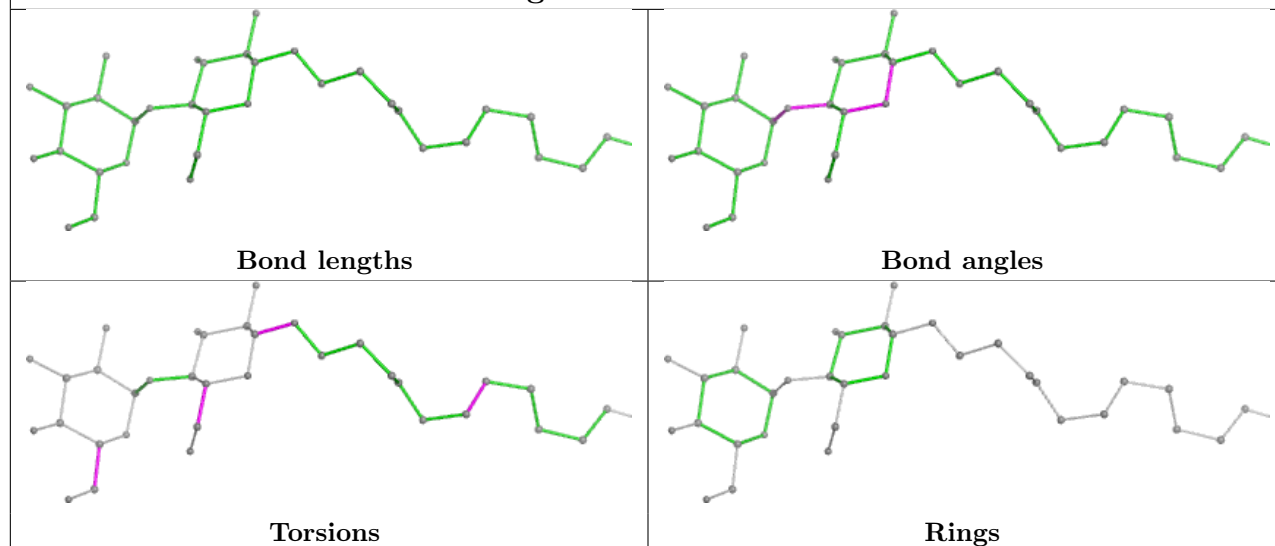


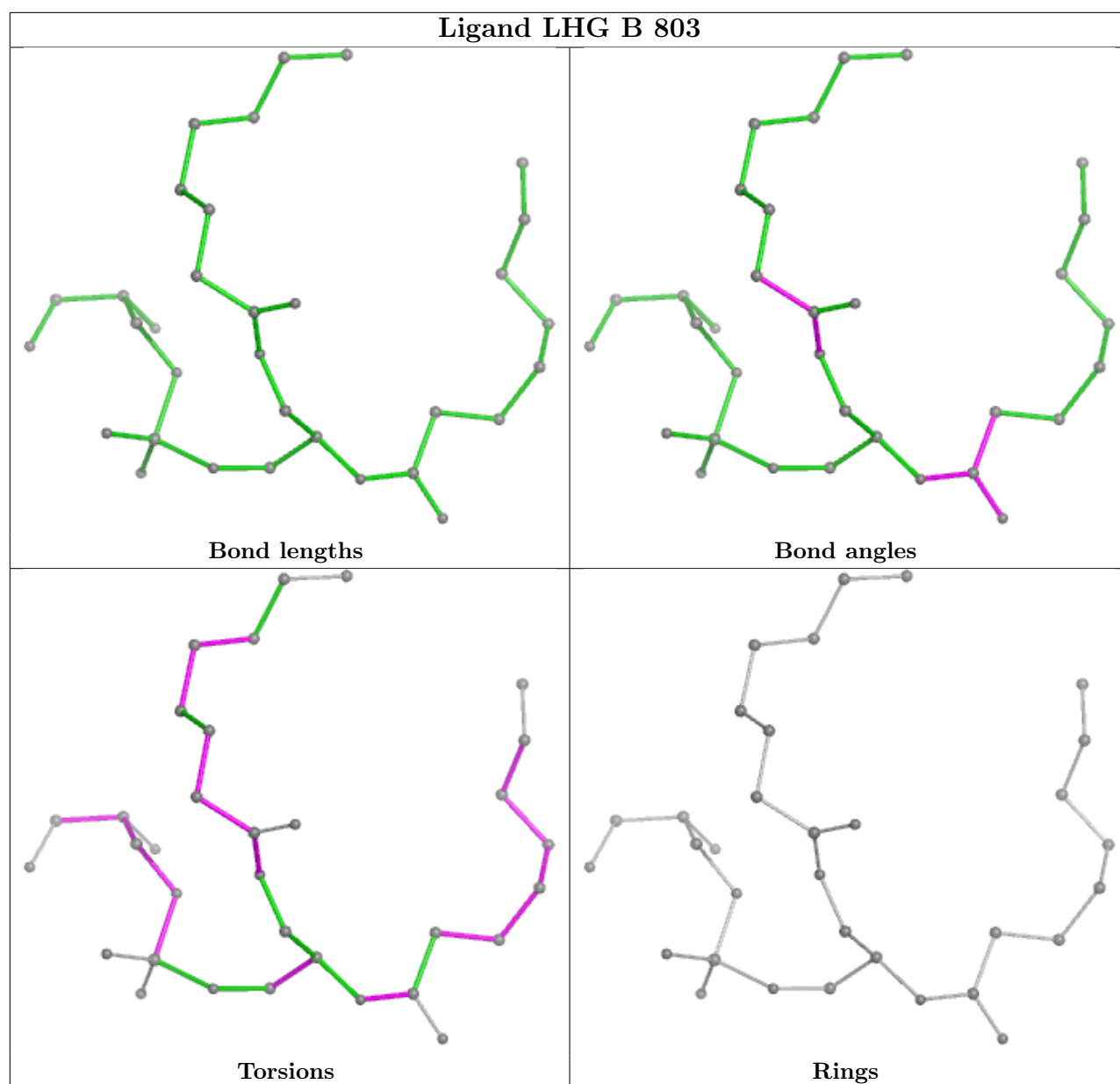


Ligand CLA 6 313

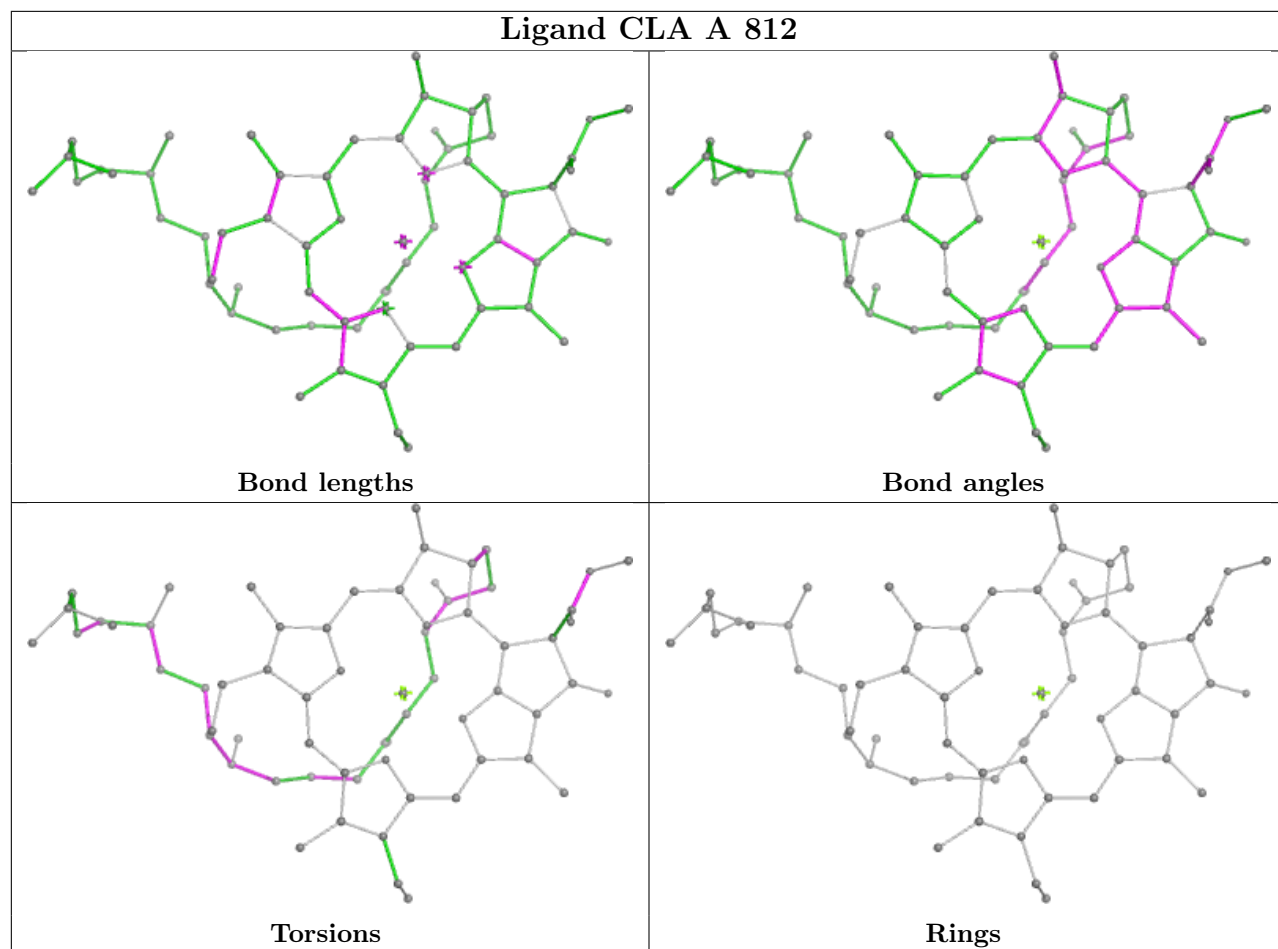


Ligand LMT G 204

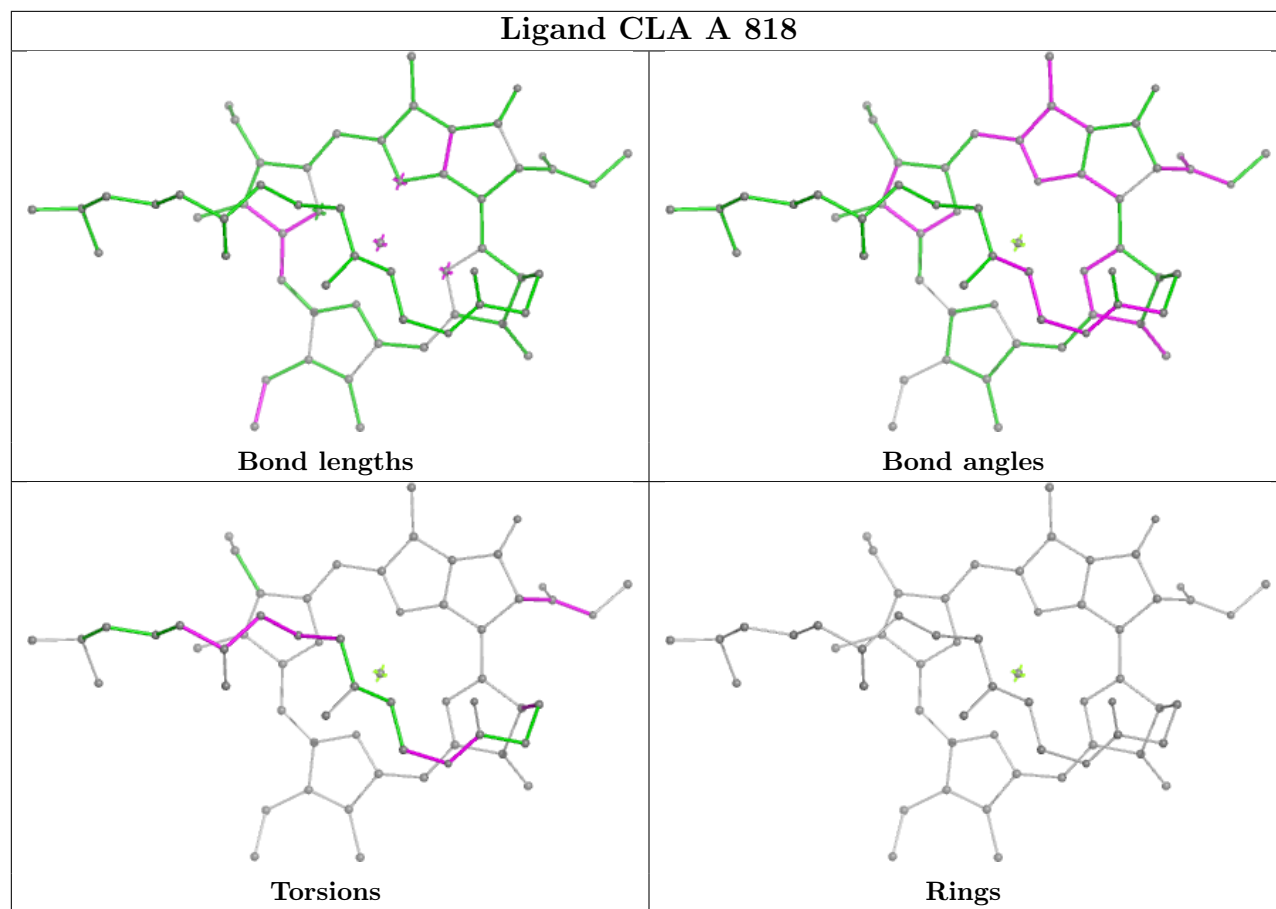




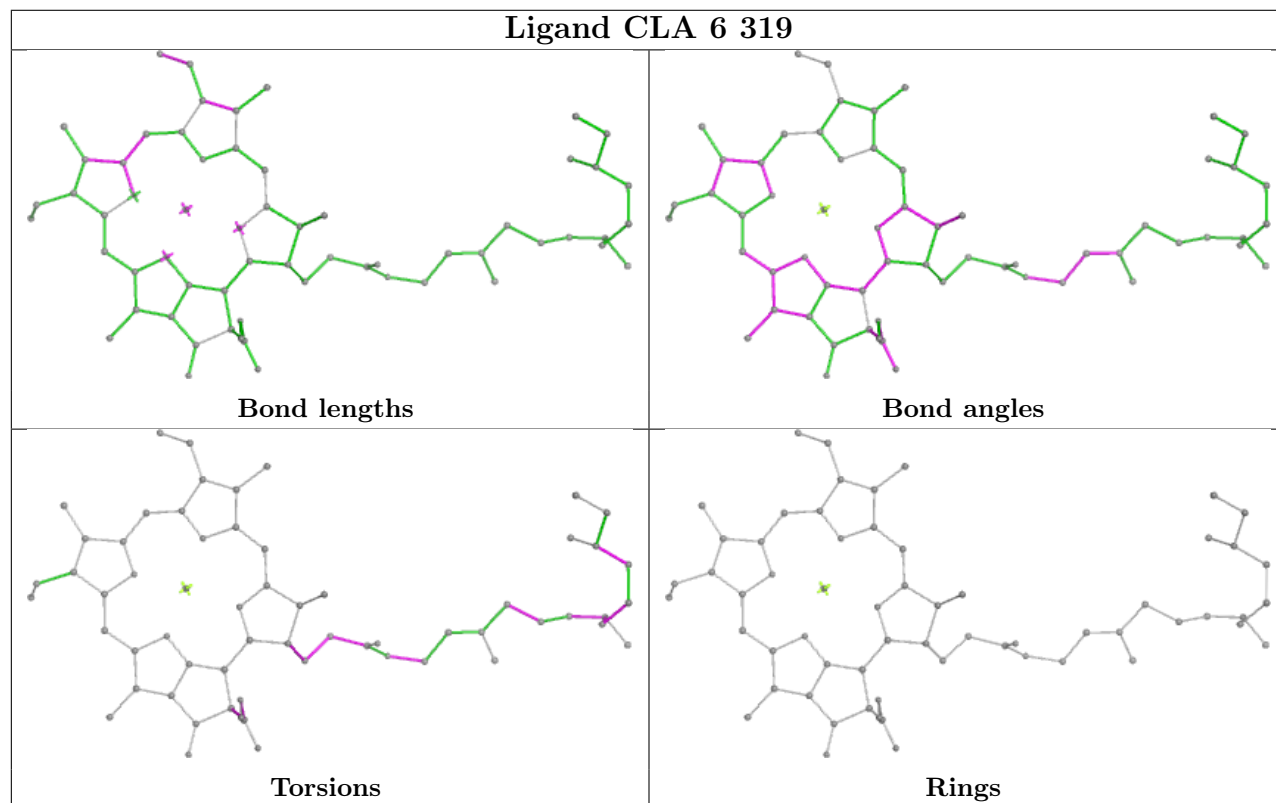
Ligand CLA A 812

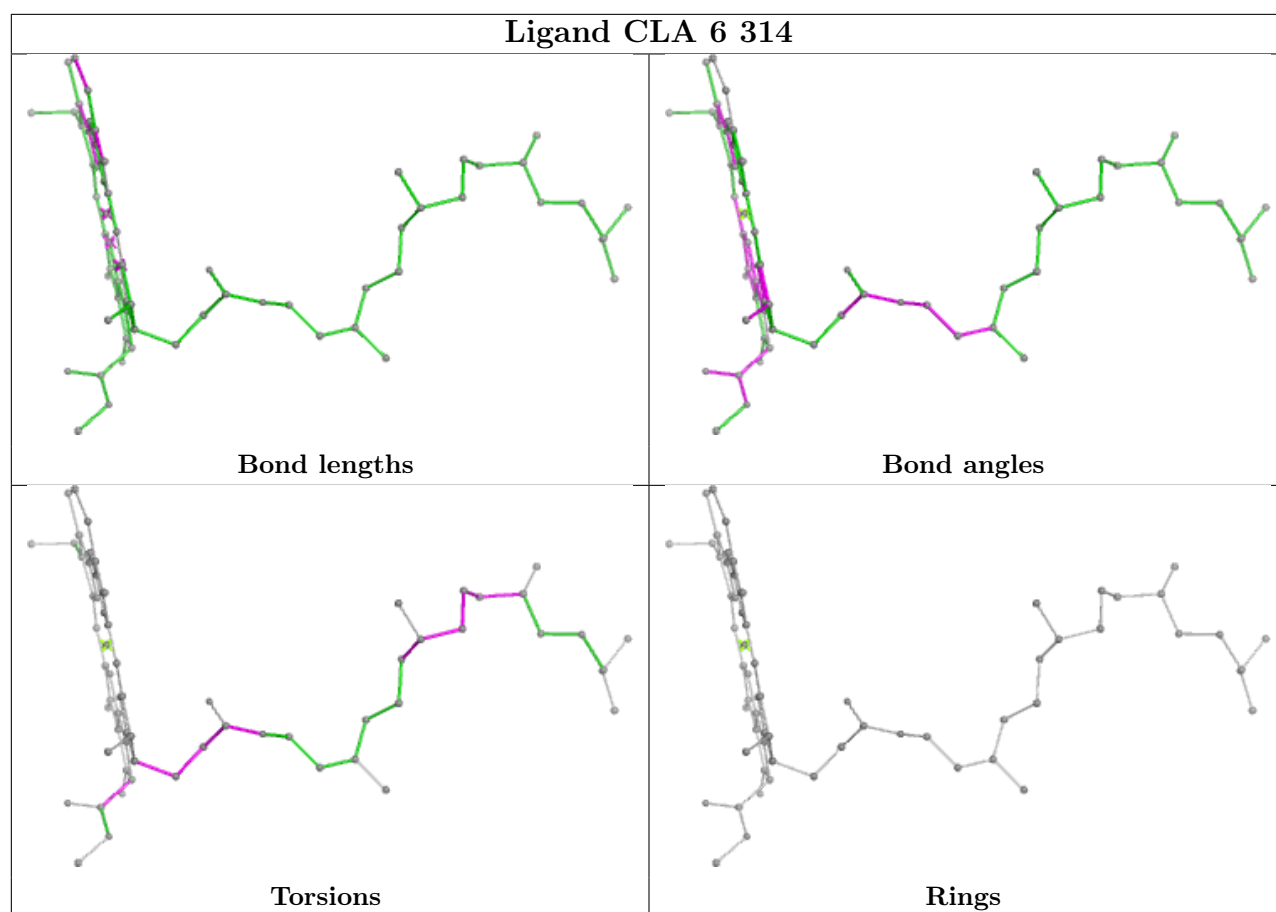


Ligand CLA A 818

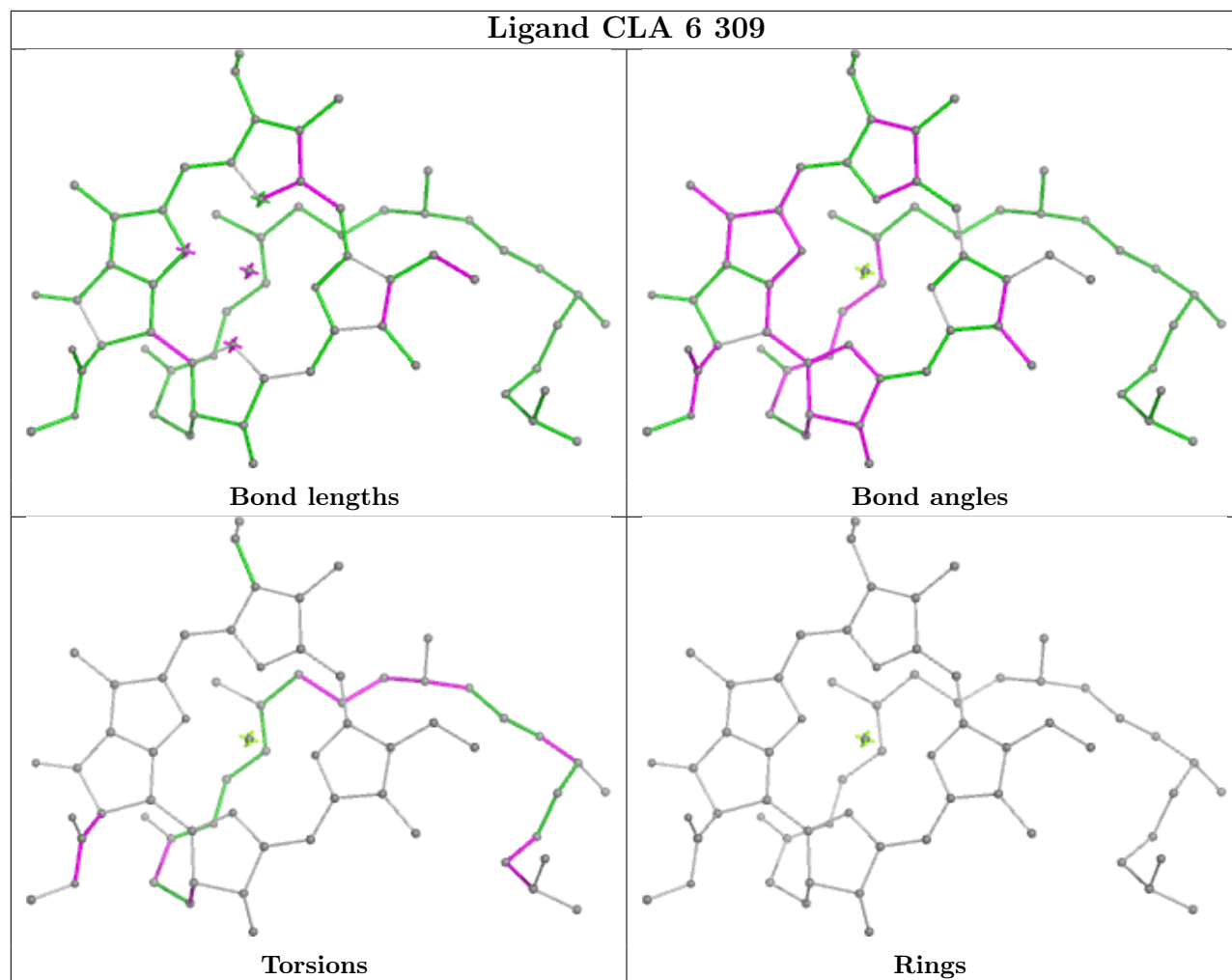


Ligand CLA 6 319

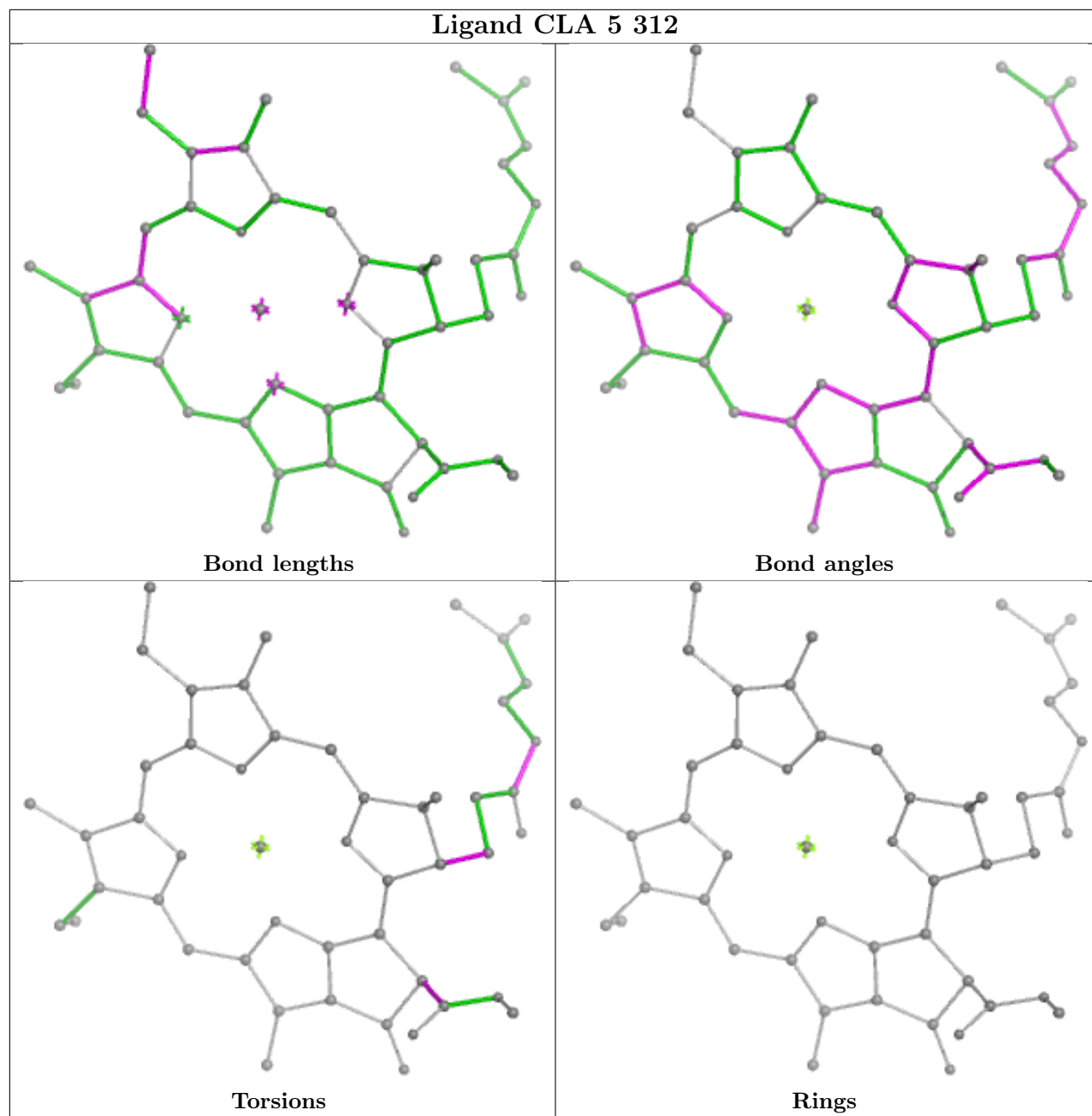


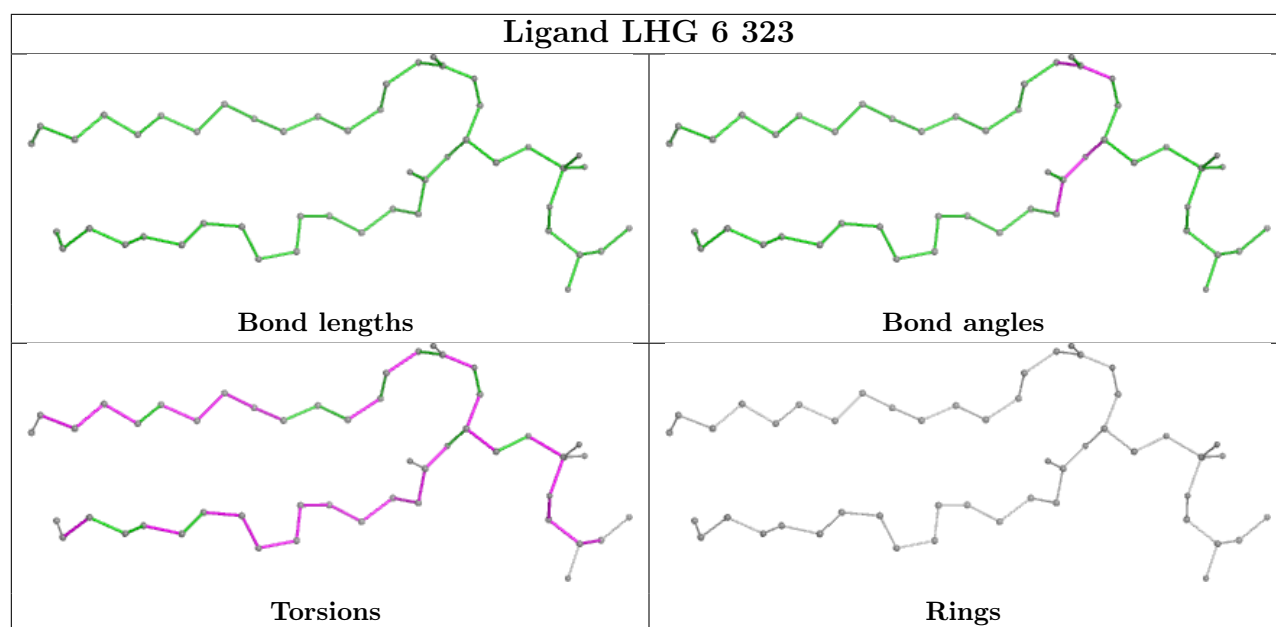


Ligand CLA 6 309

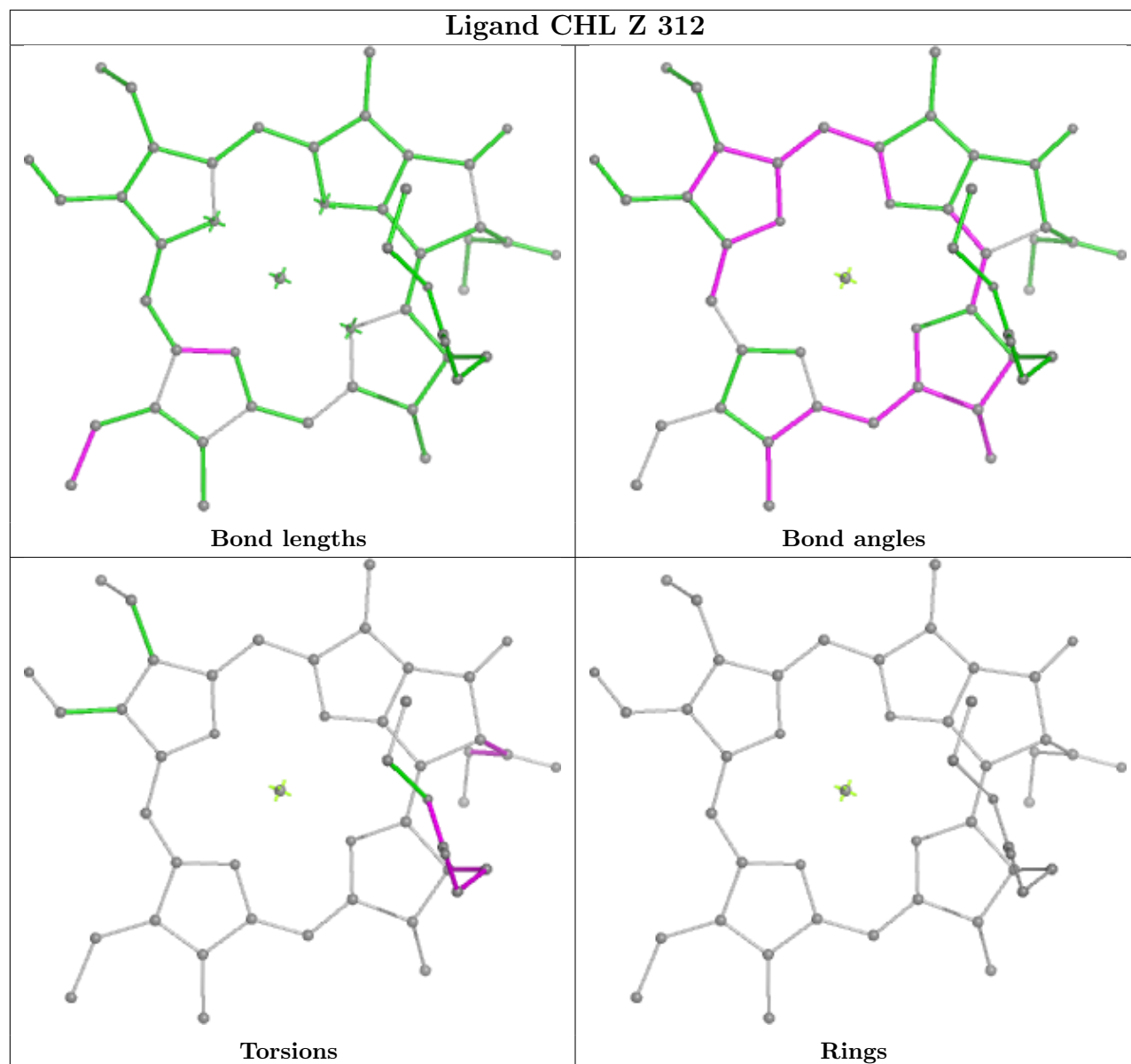


Ligand CLA 5 312

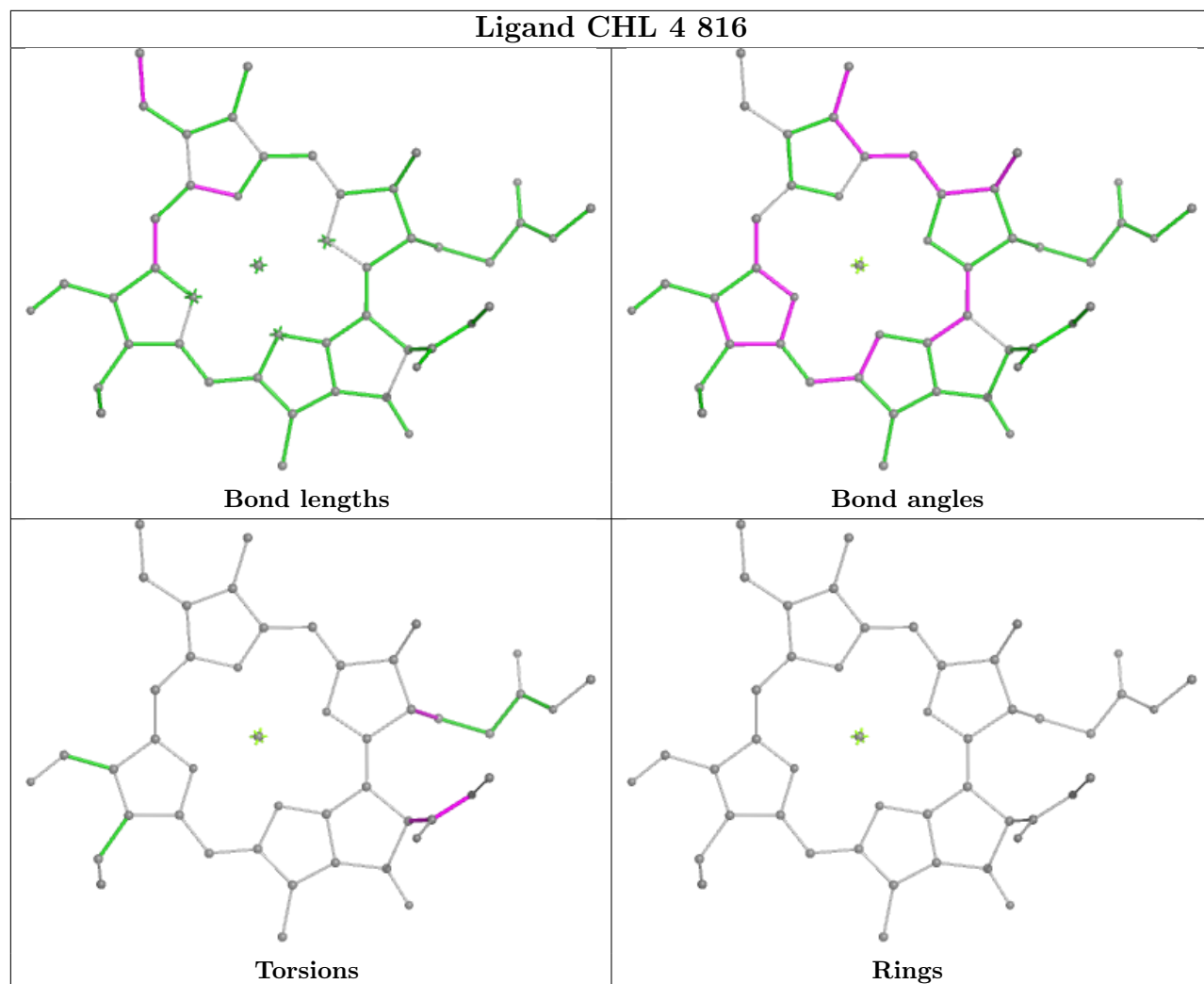


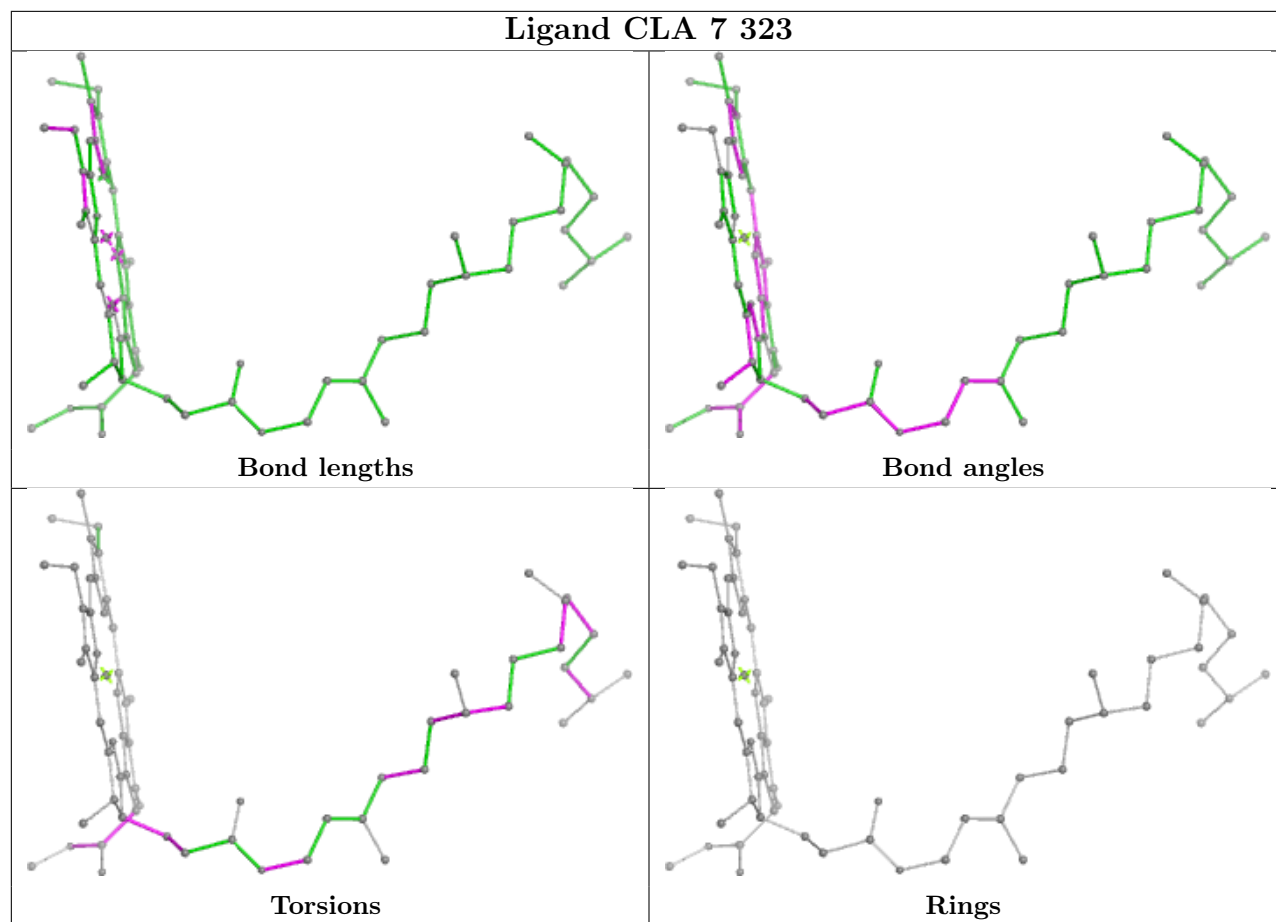


Ligand CHL Z 312

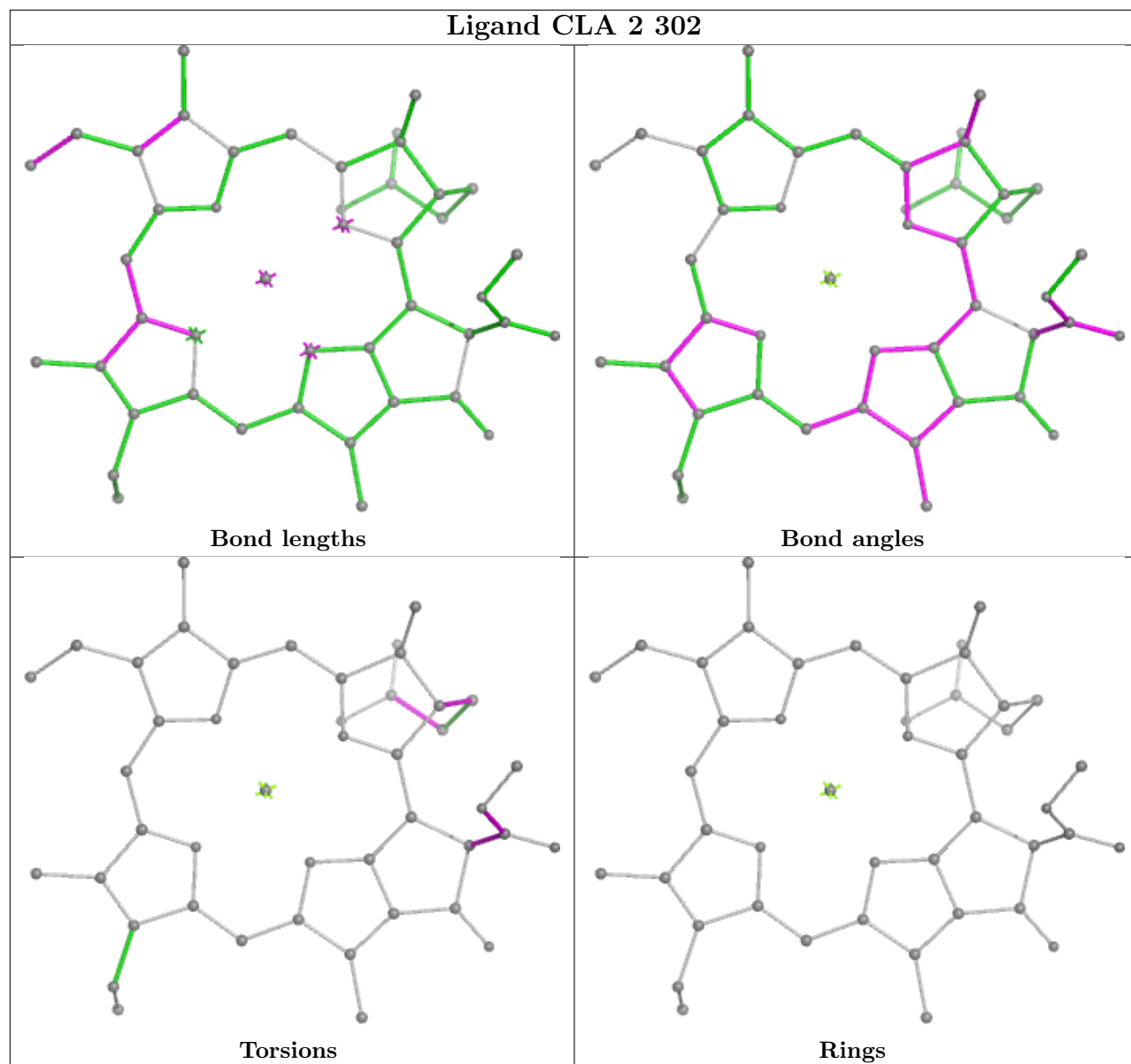


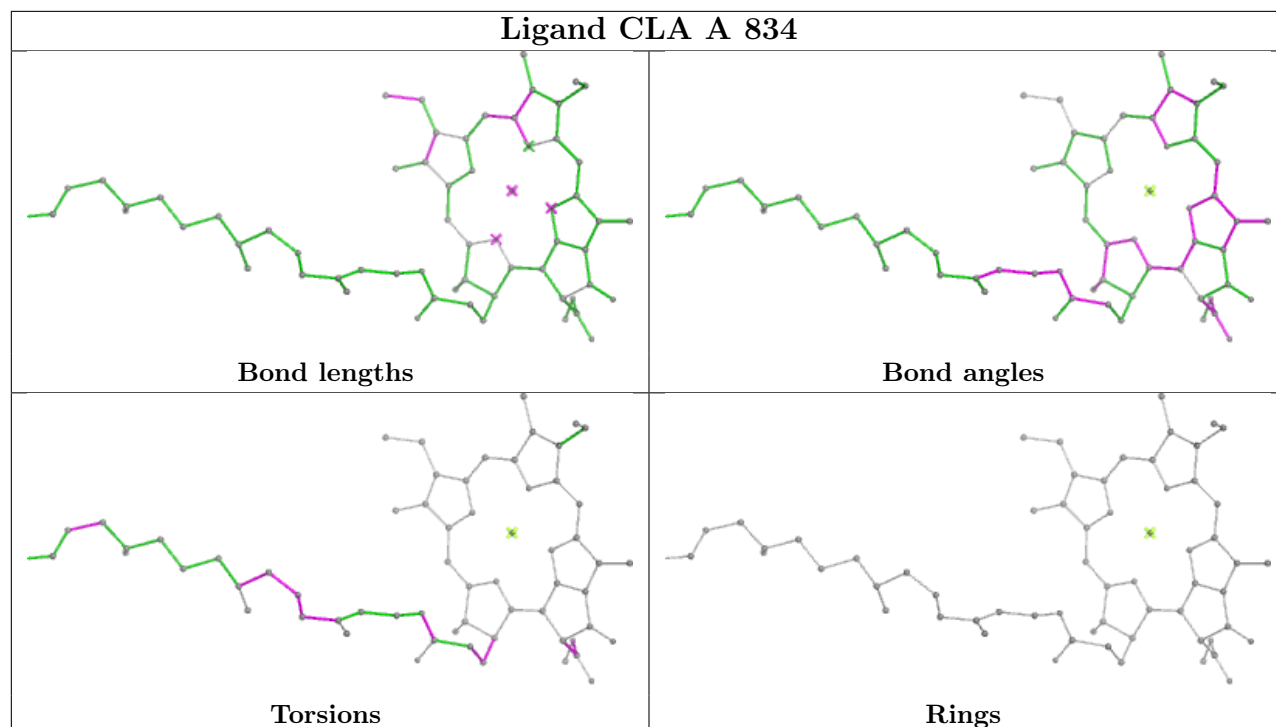
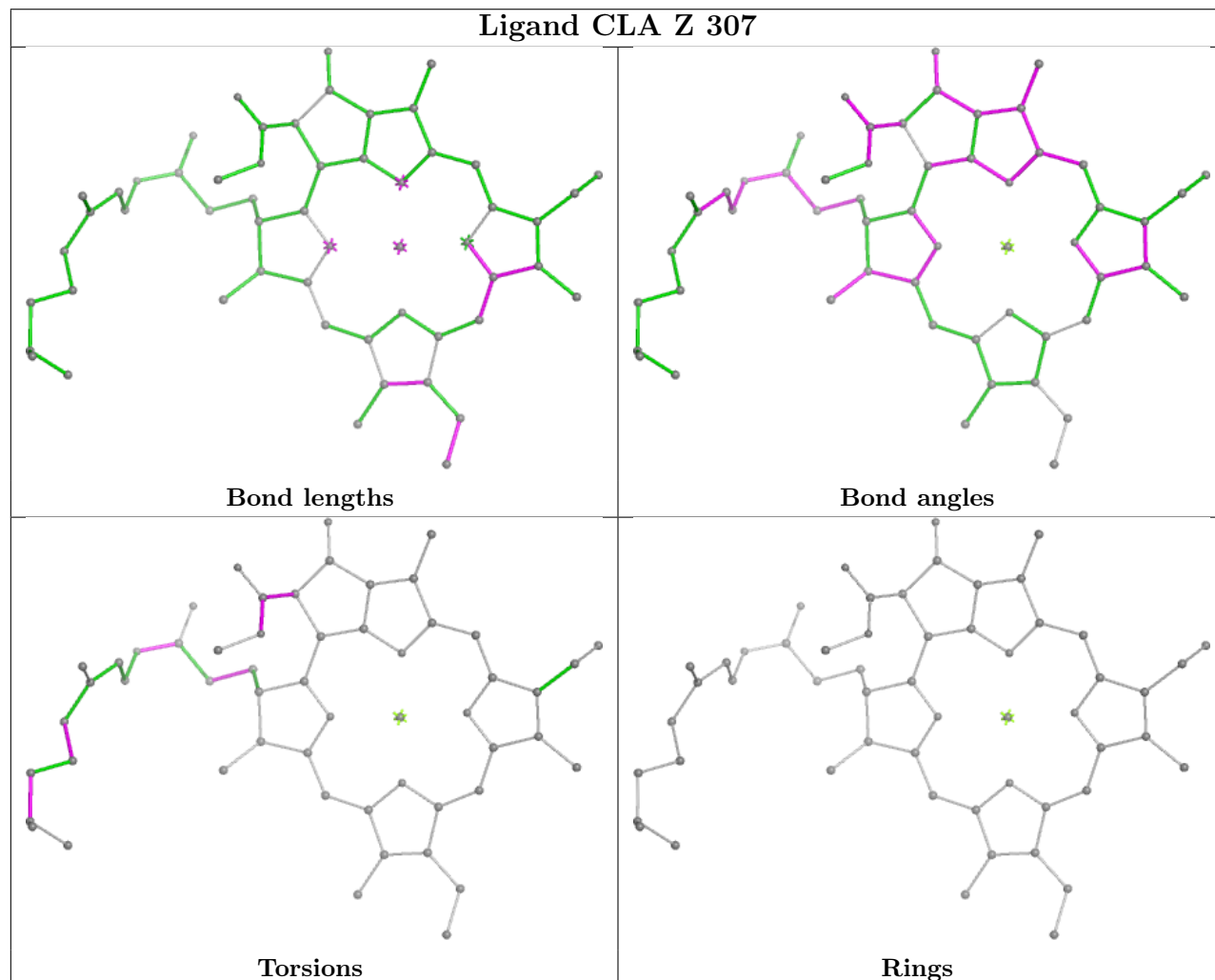
Ligand CHL 4 816

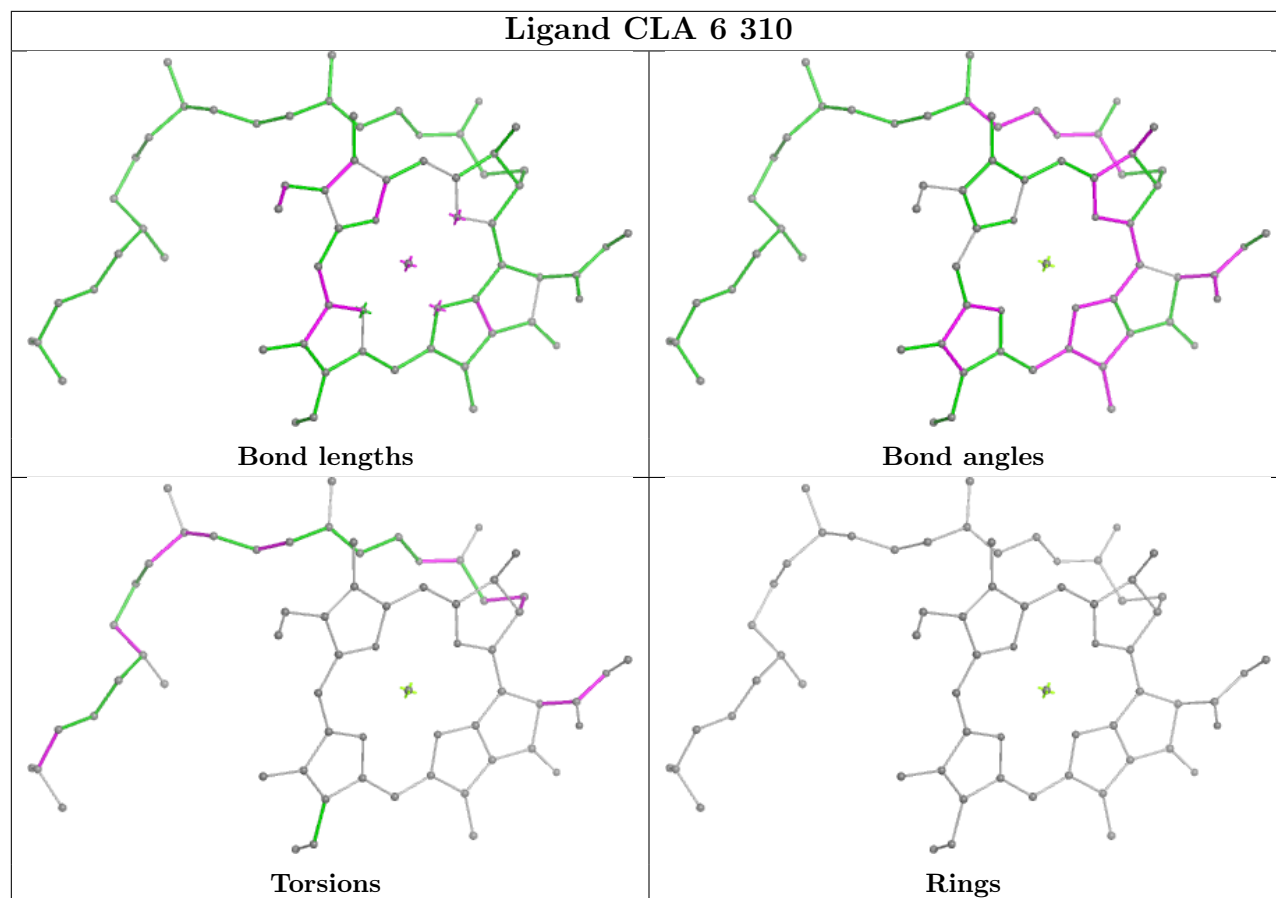




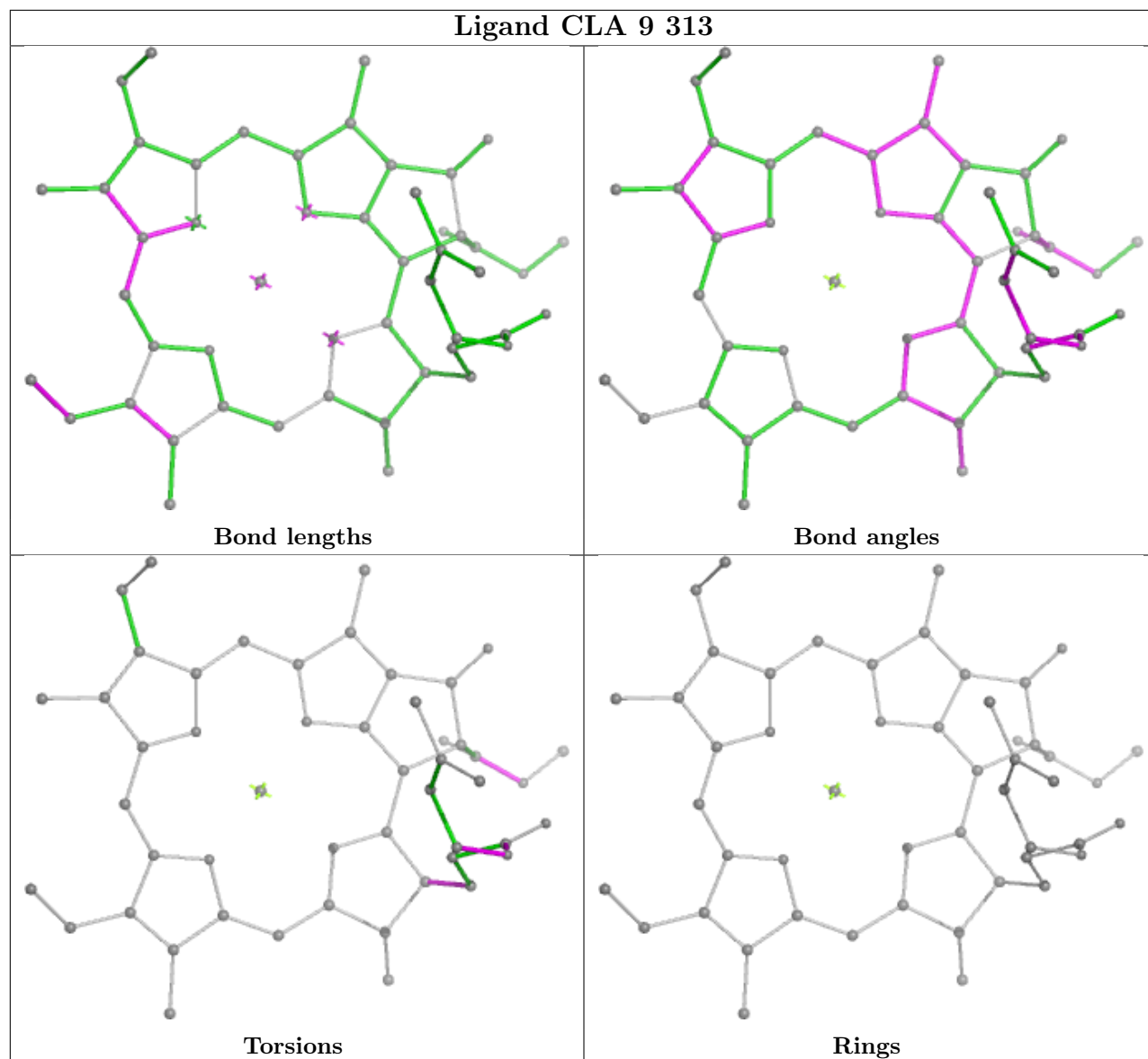
Ligand CLA 2 302



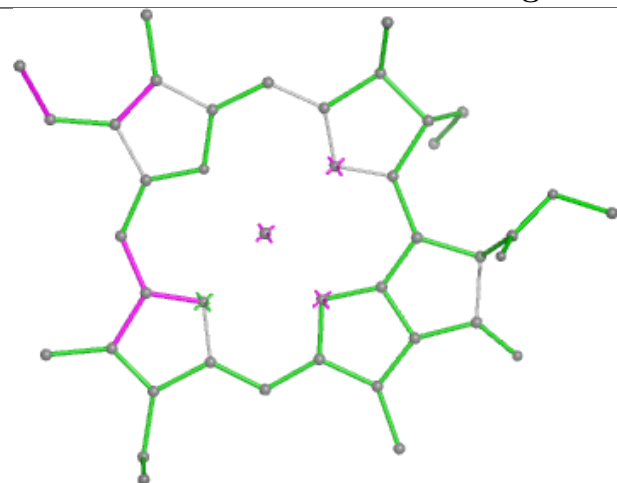
Ligand CLA A 834**Ligand CLA Z 307**

Ligand CLA 6 310

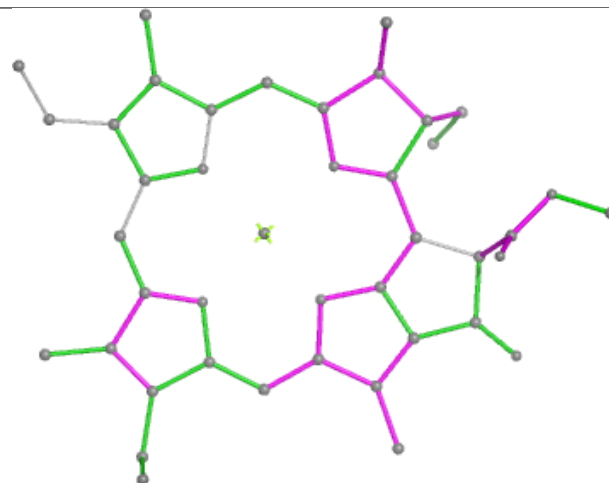
Ligand CLA 9 313



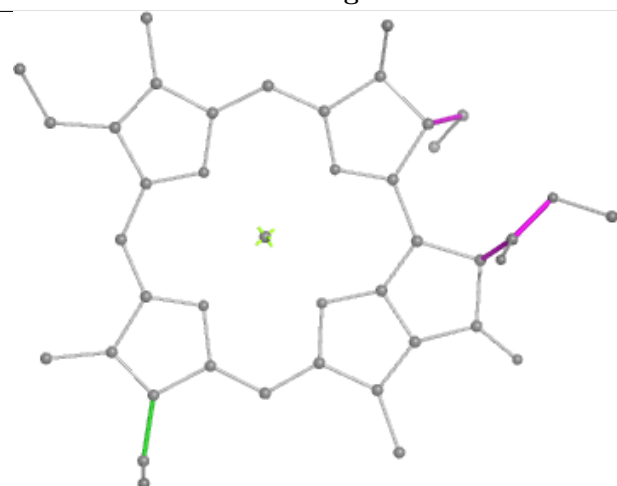
Ligand CLA J 103



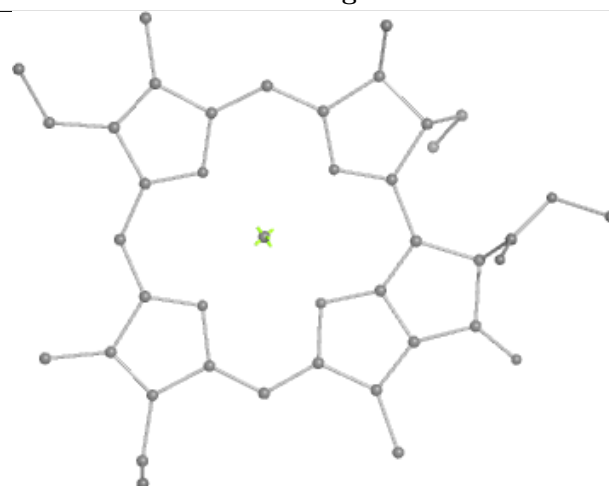
Bond lengths



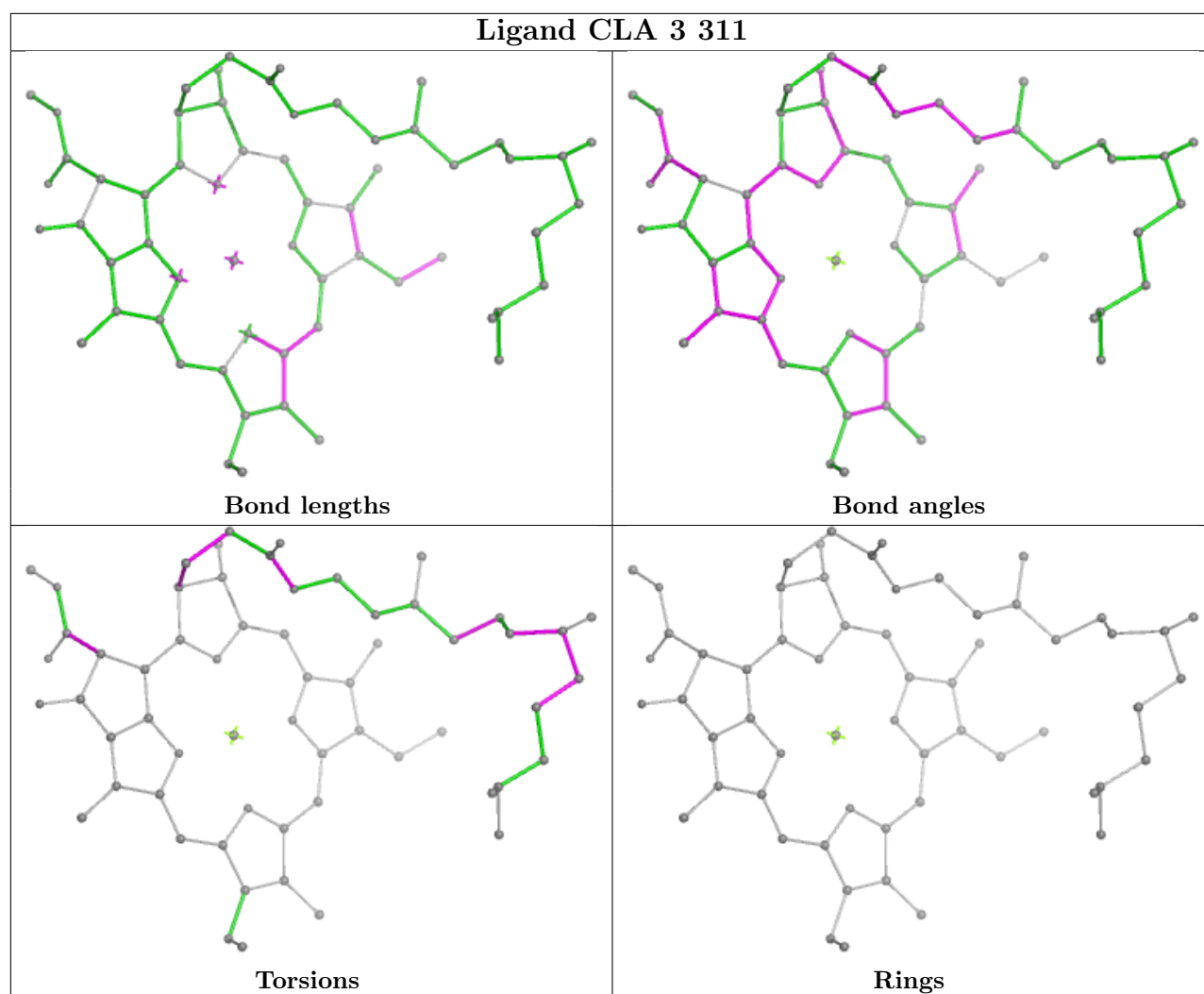
Bond angles

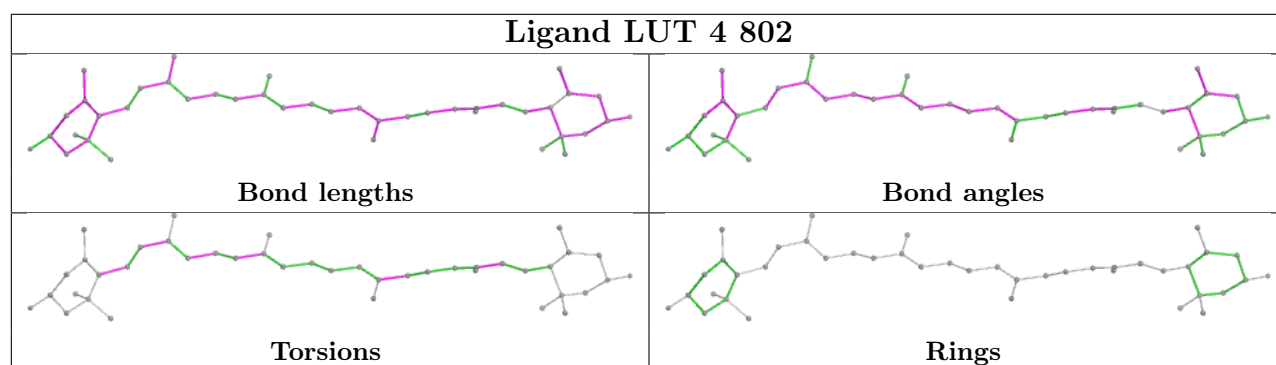
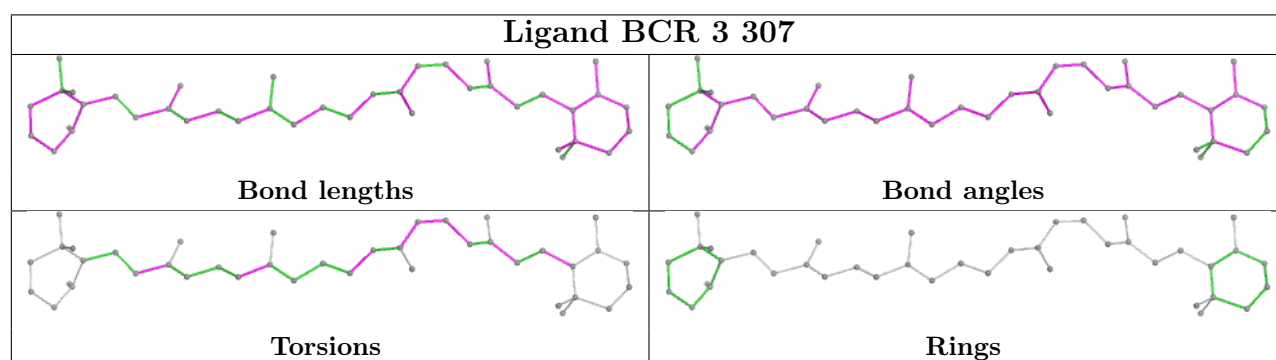
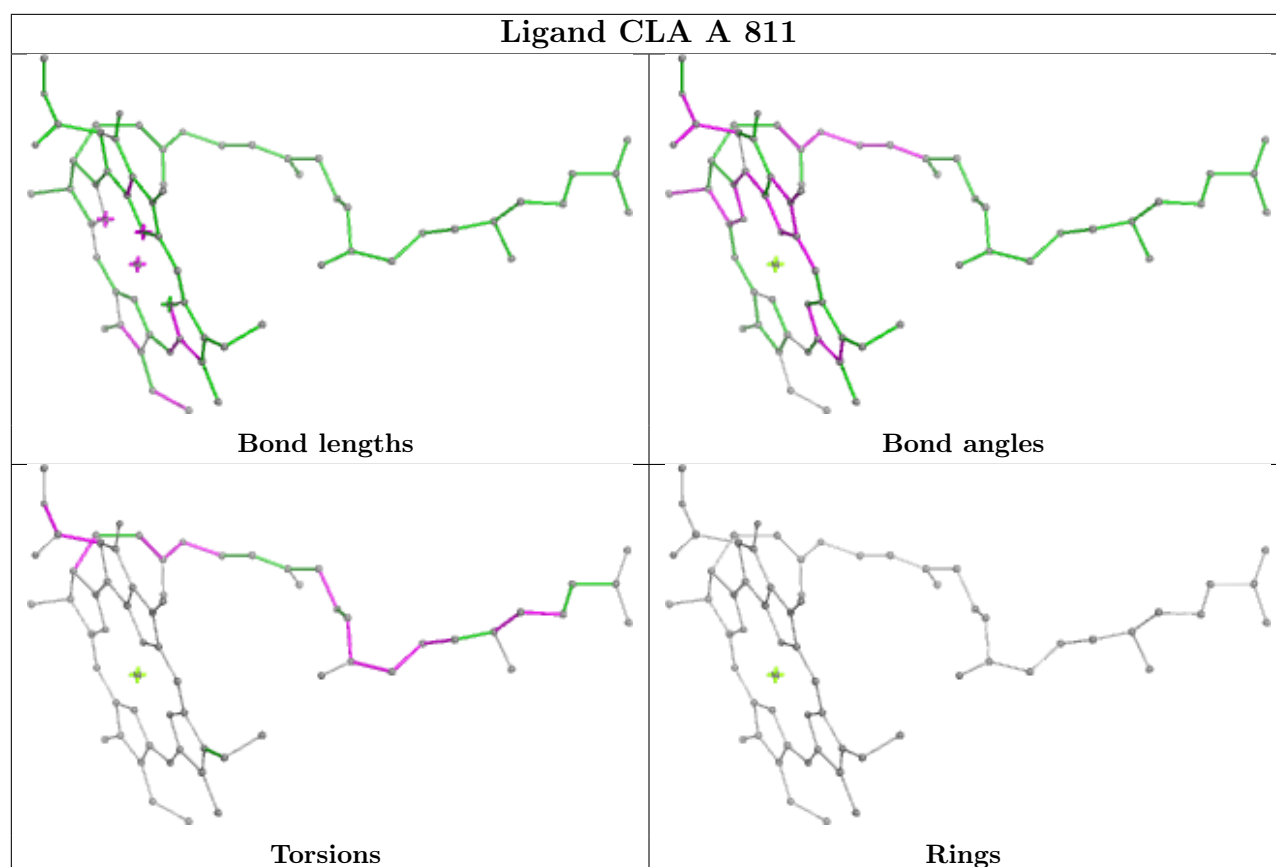


Torsions

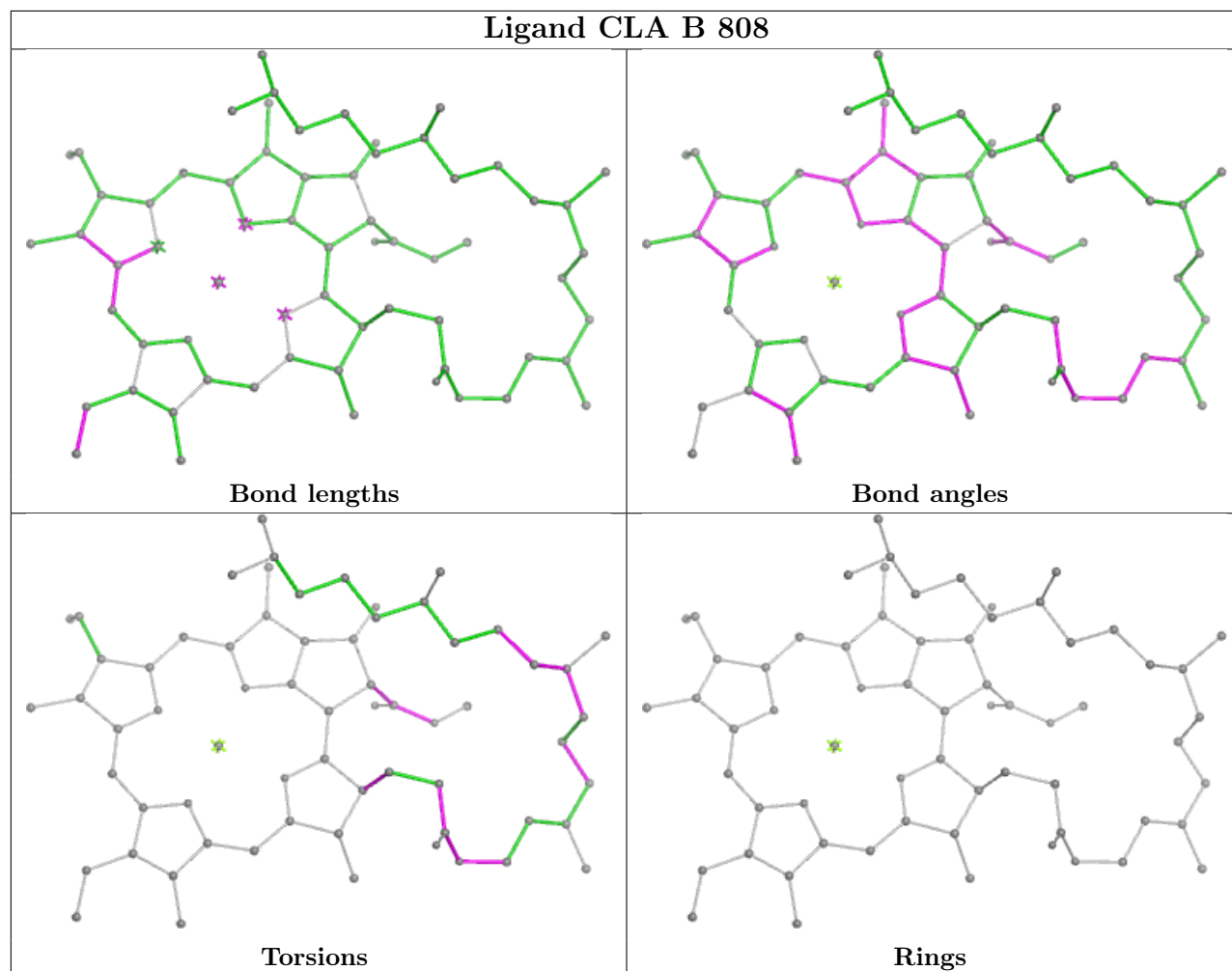


Rings

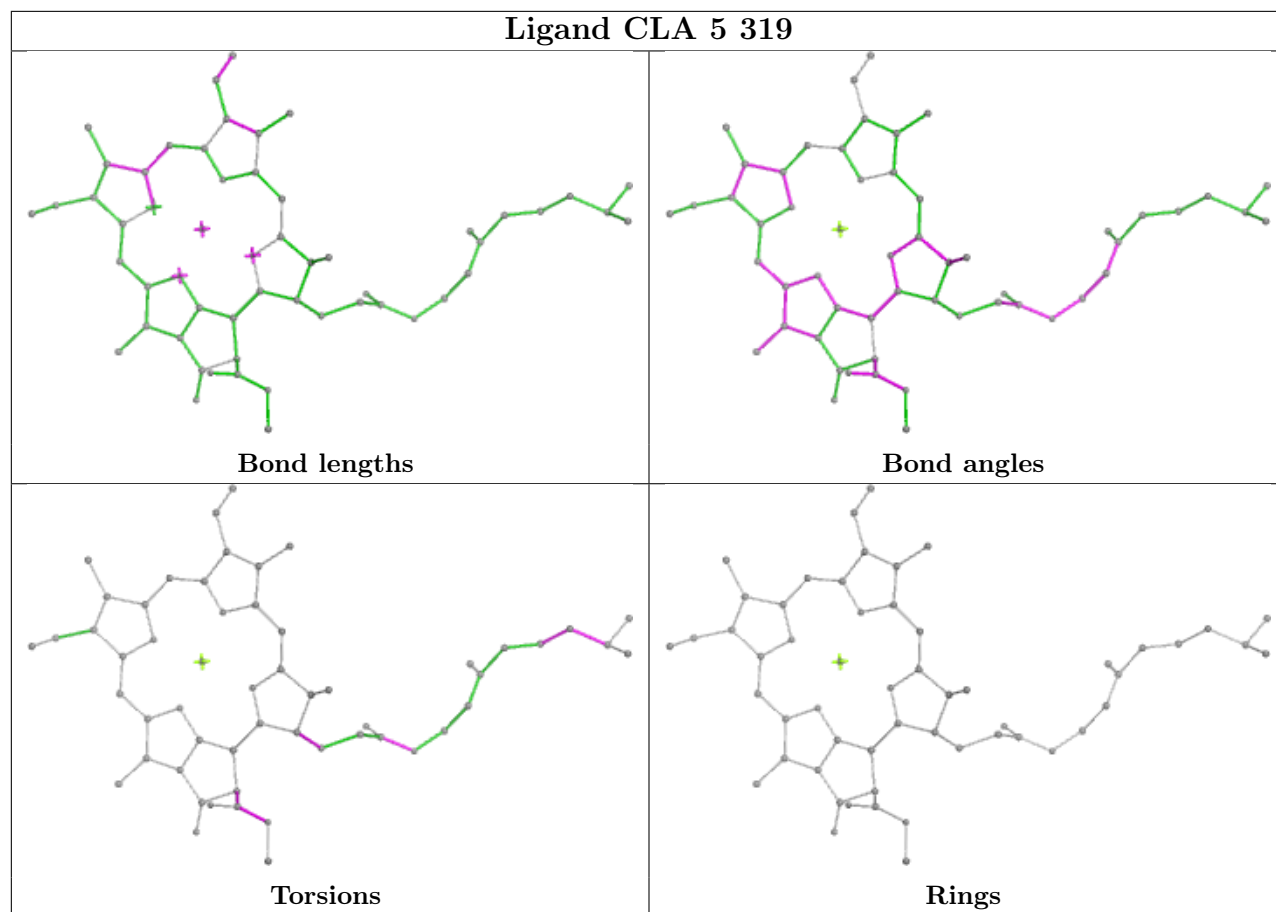




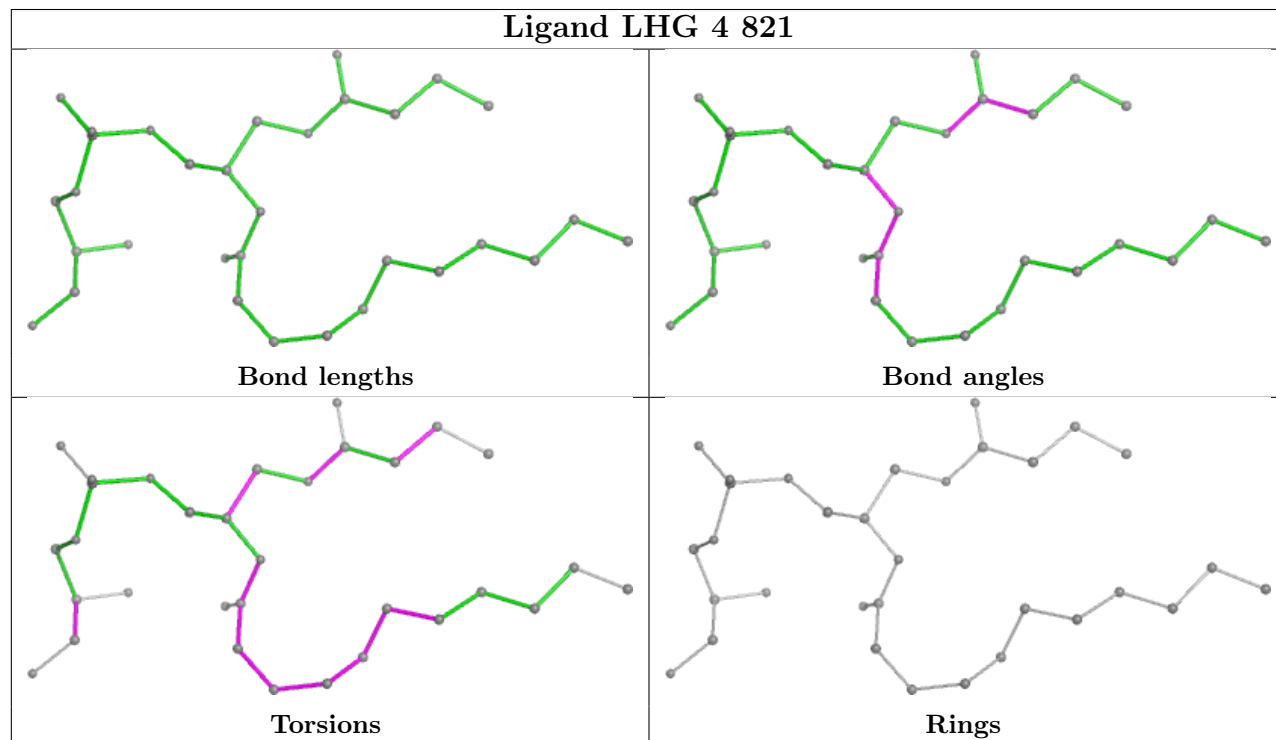
Ligand CLA B 808



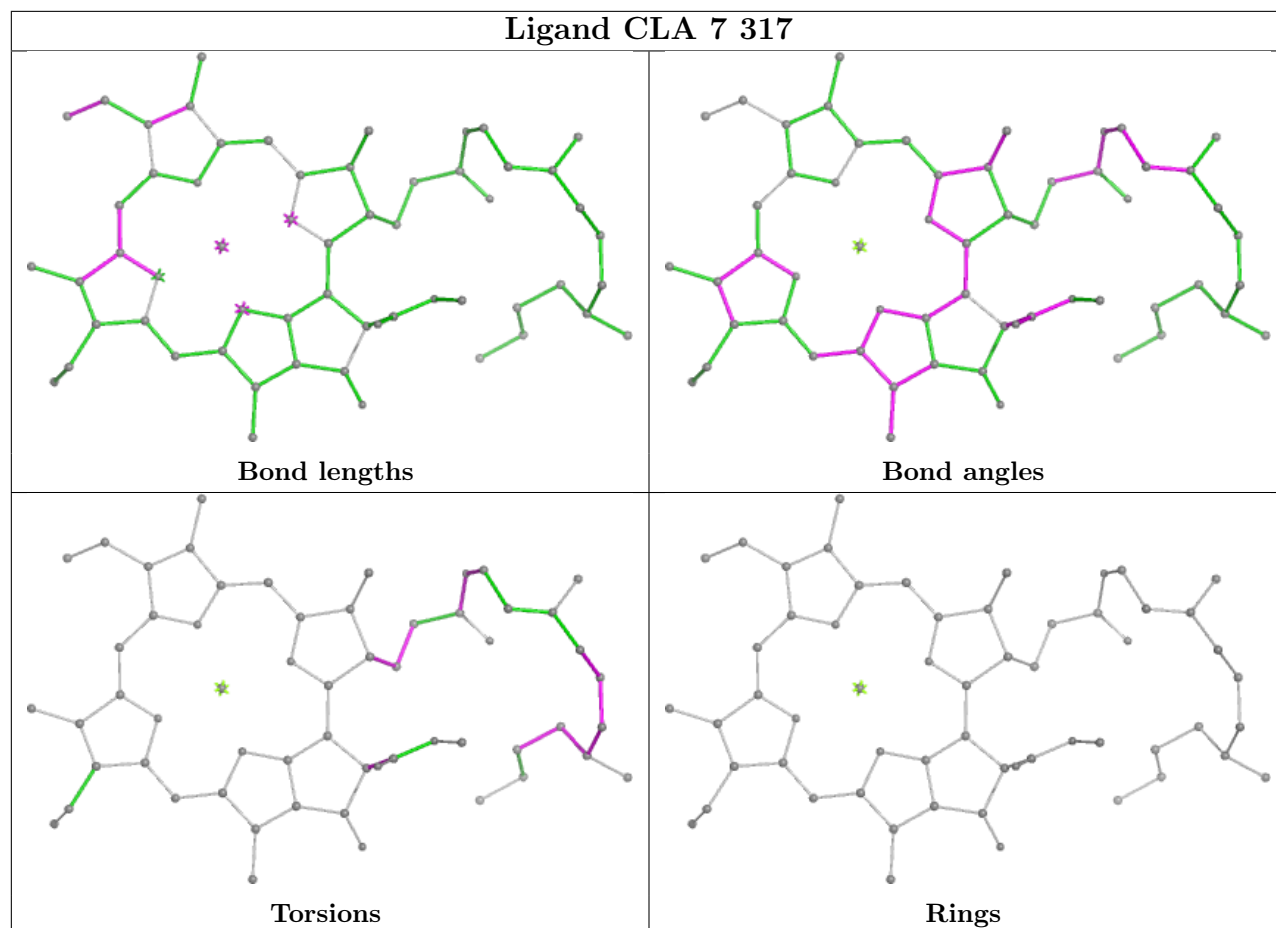
Ligand CLA 5 319



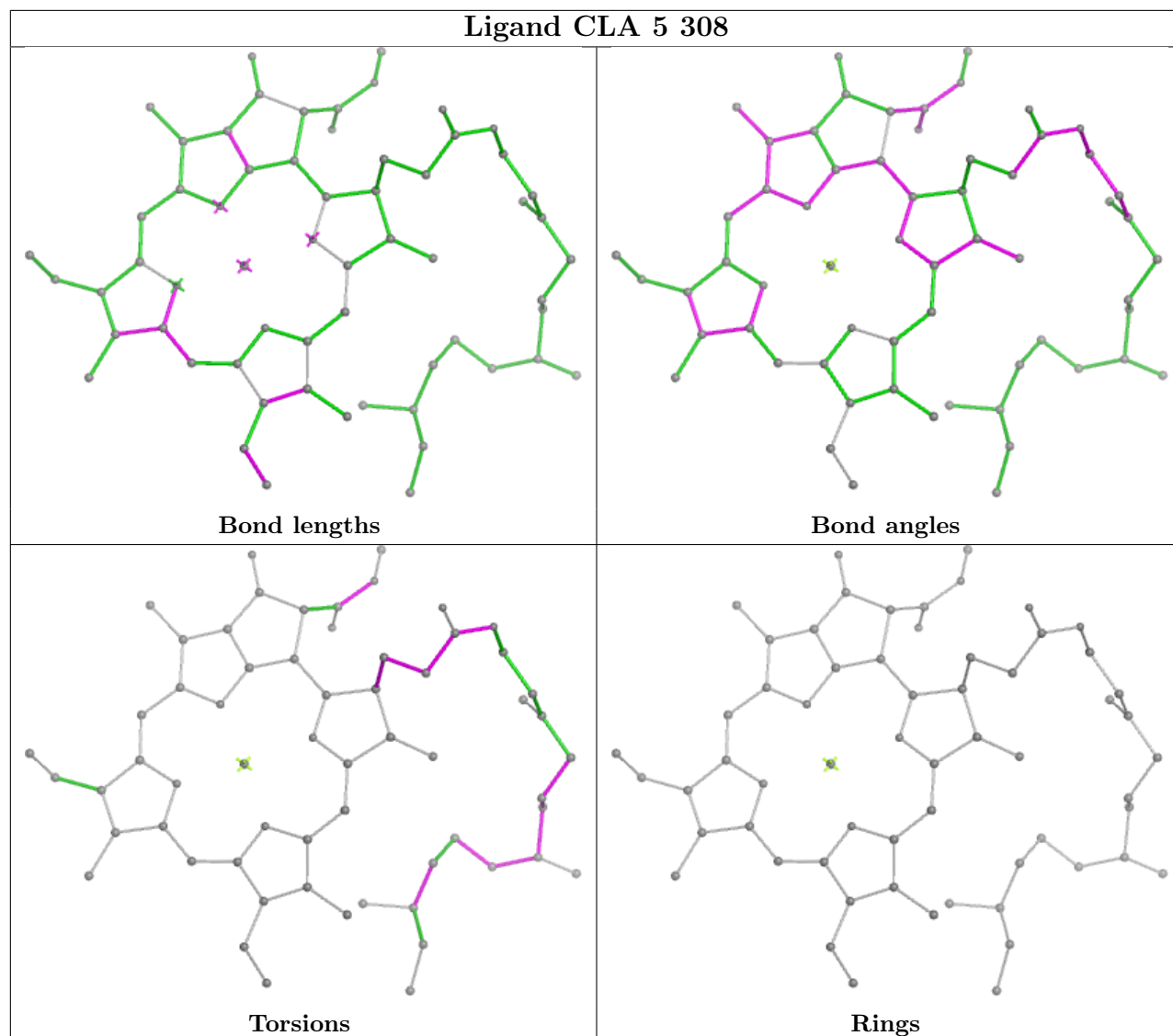
Ligand LHG 4 821



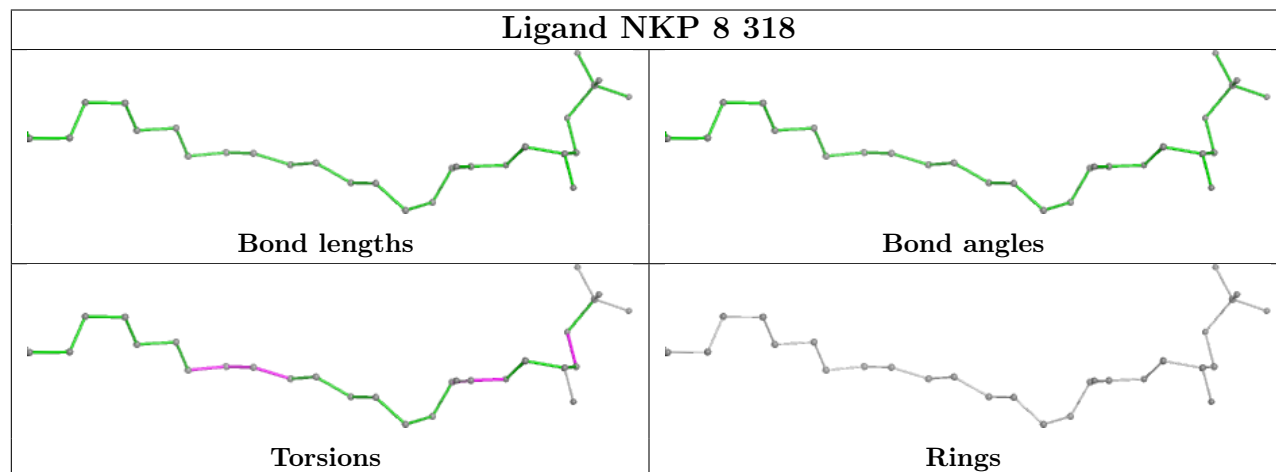
Ligand CLA 7 317



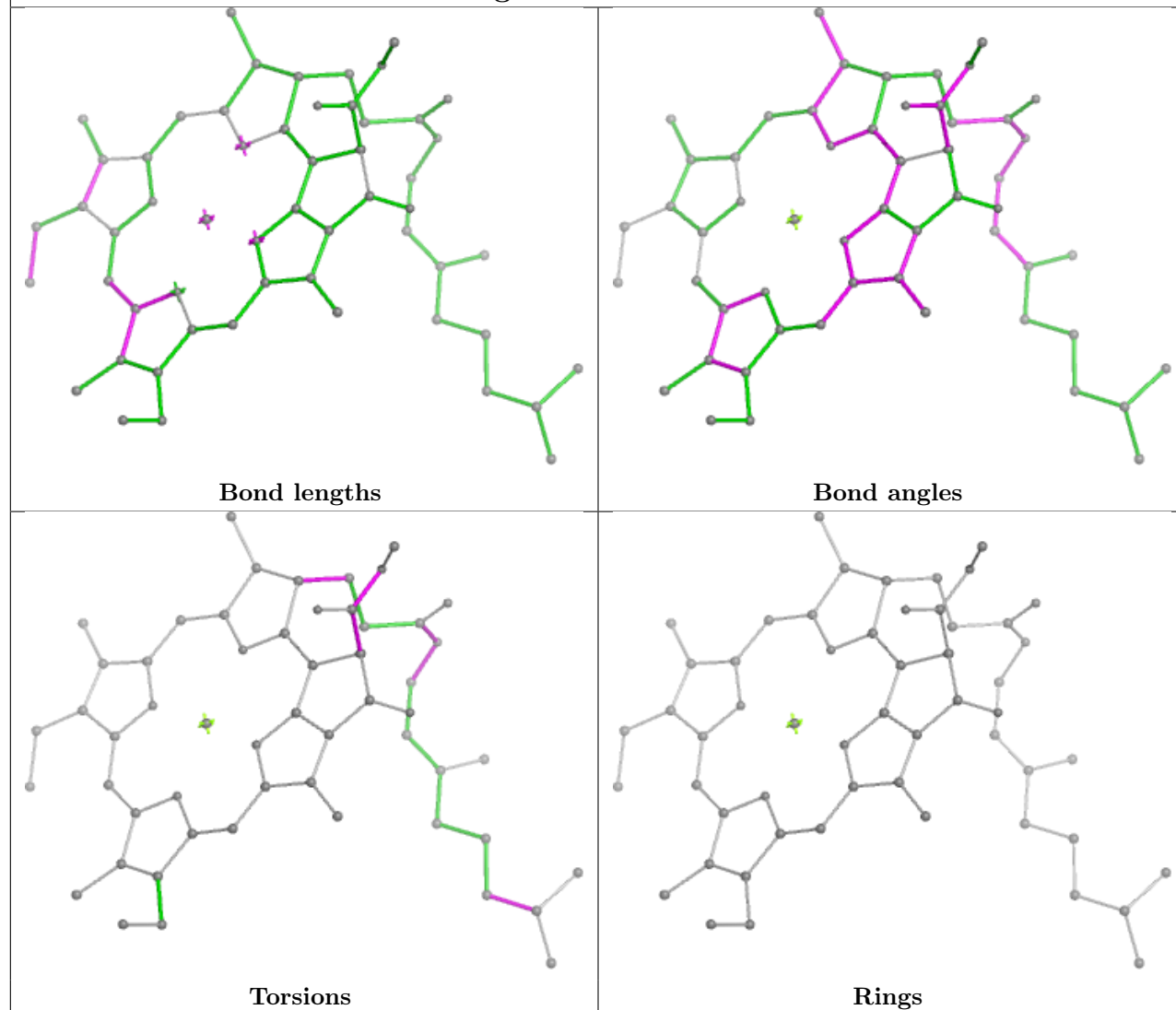
Ligand CLA 5 308



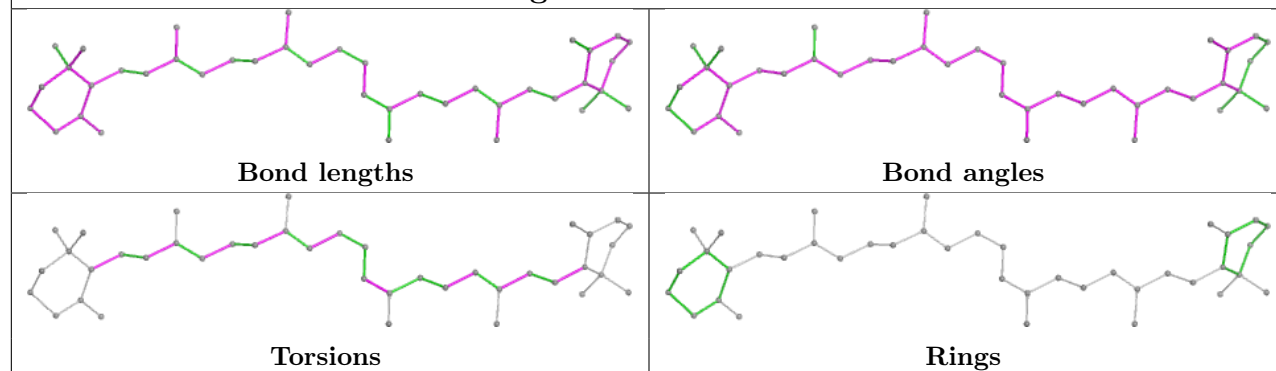
Ligand NKP 8 318

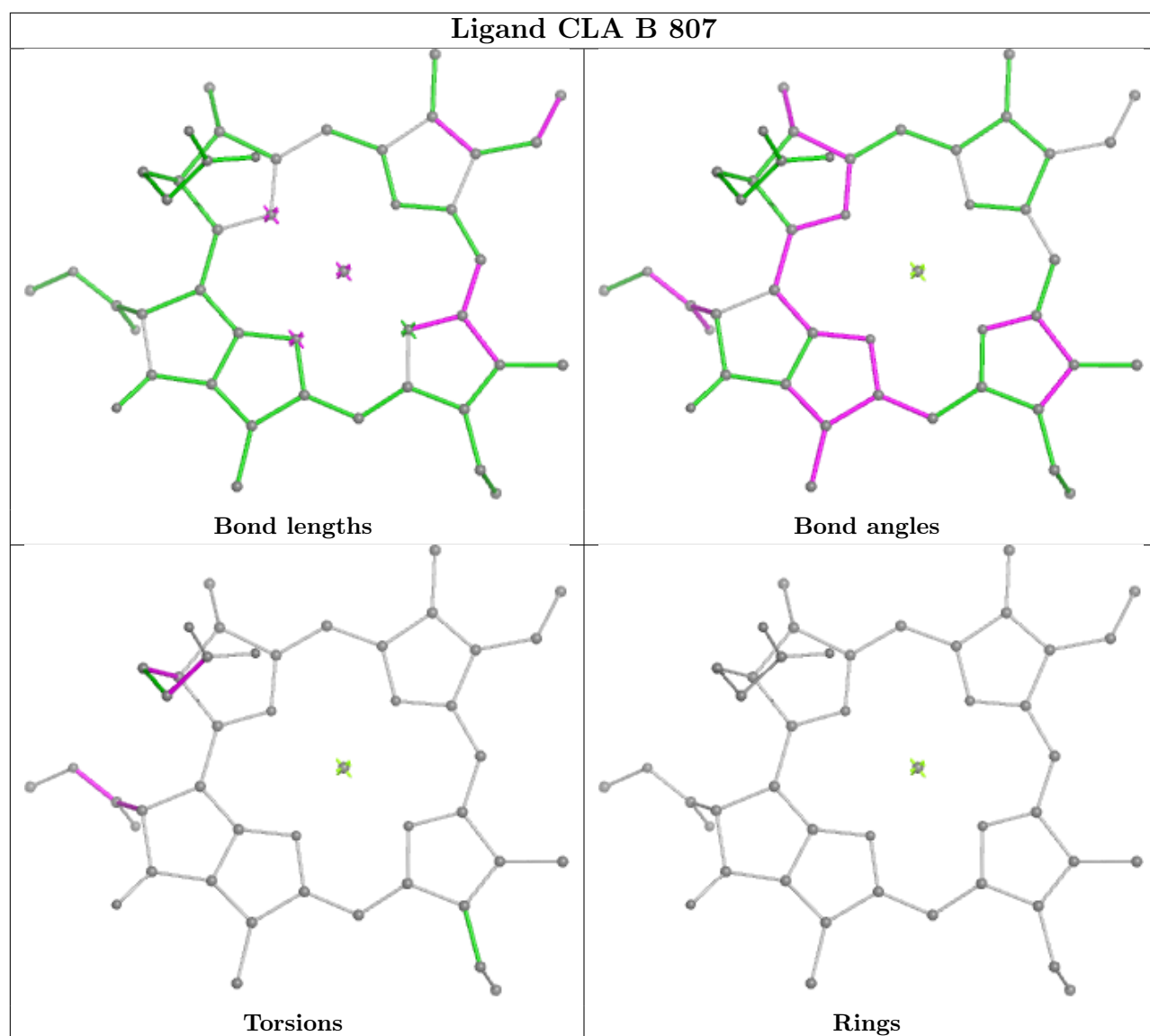


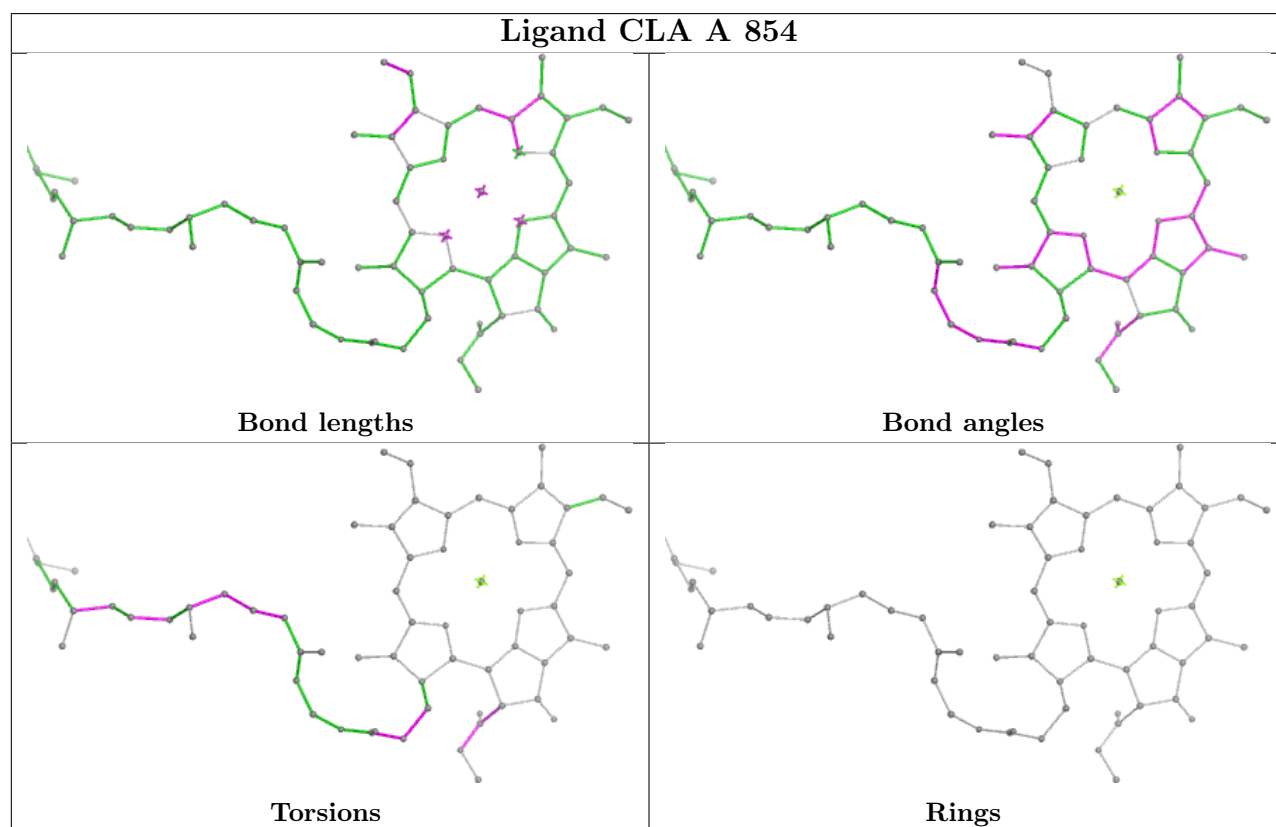
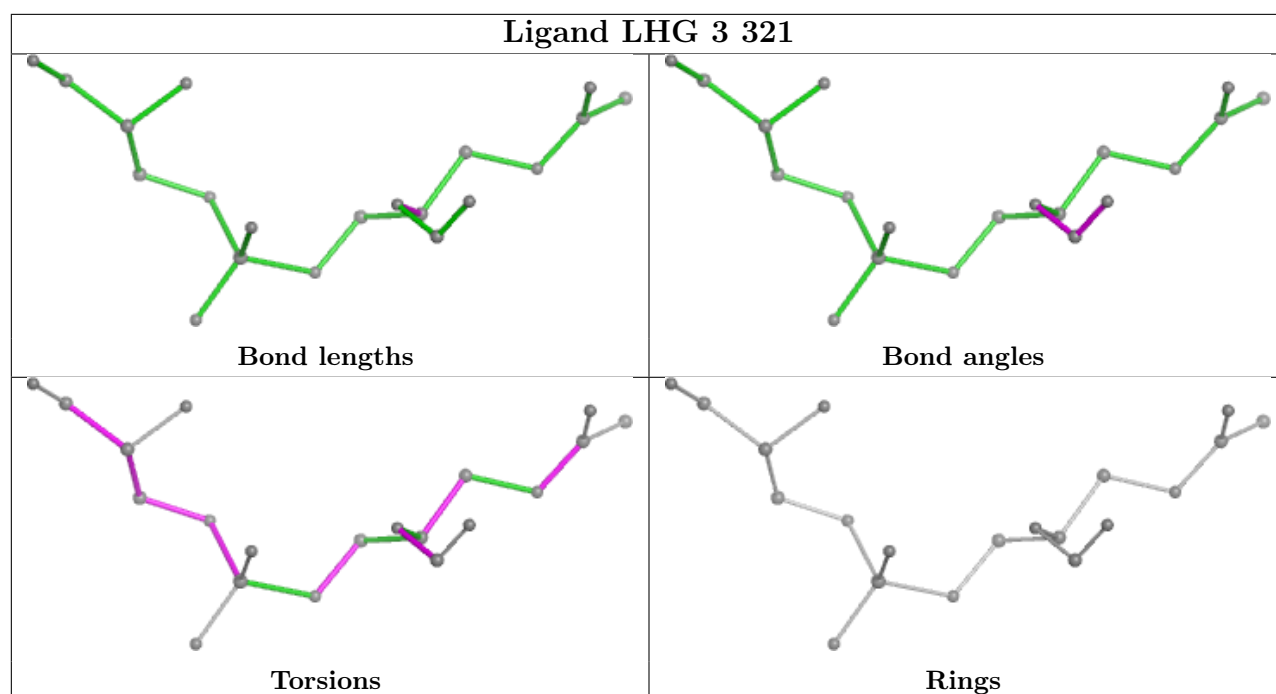
Ligand CLA 4 811

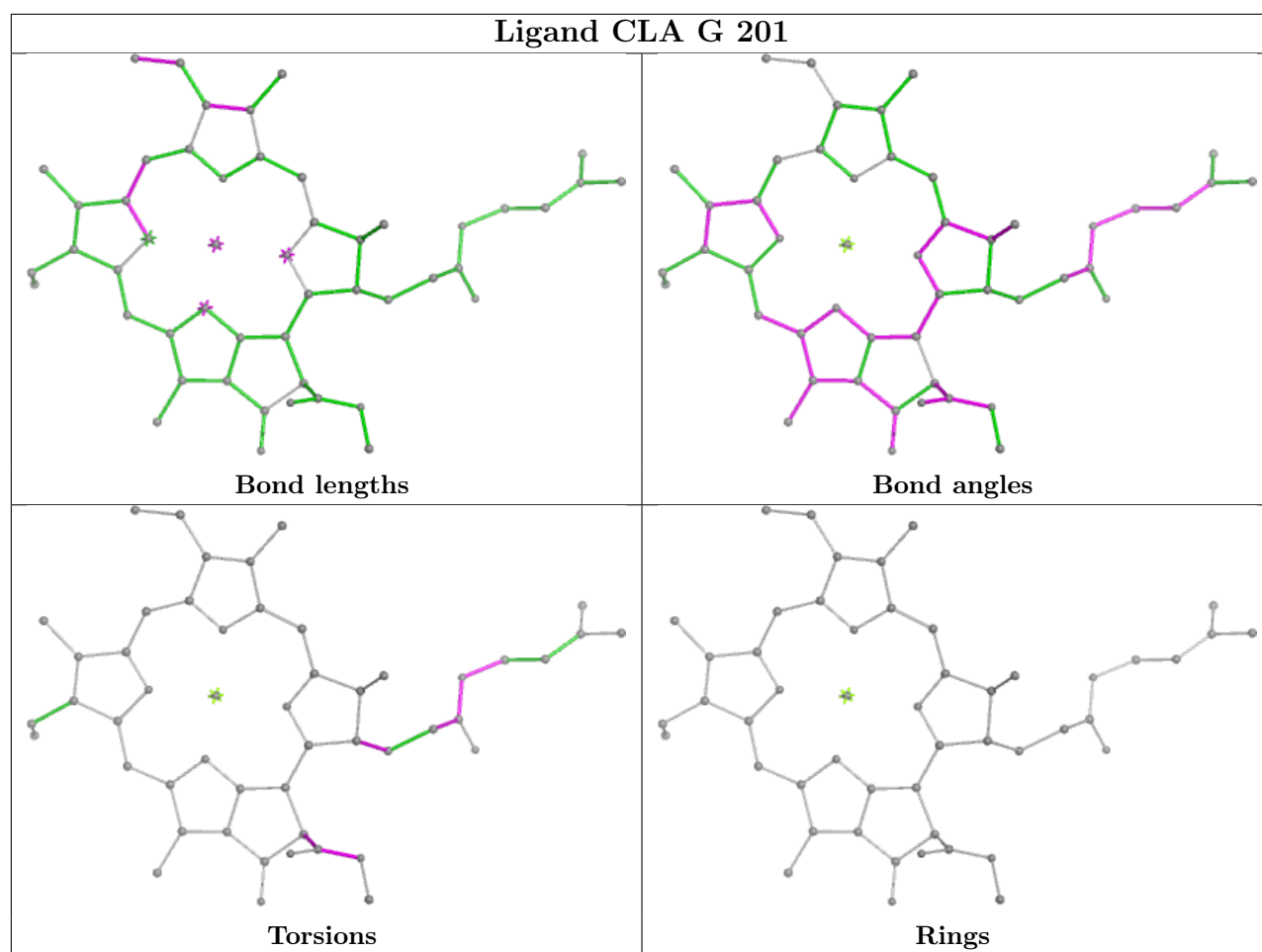


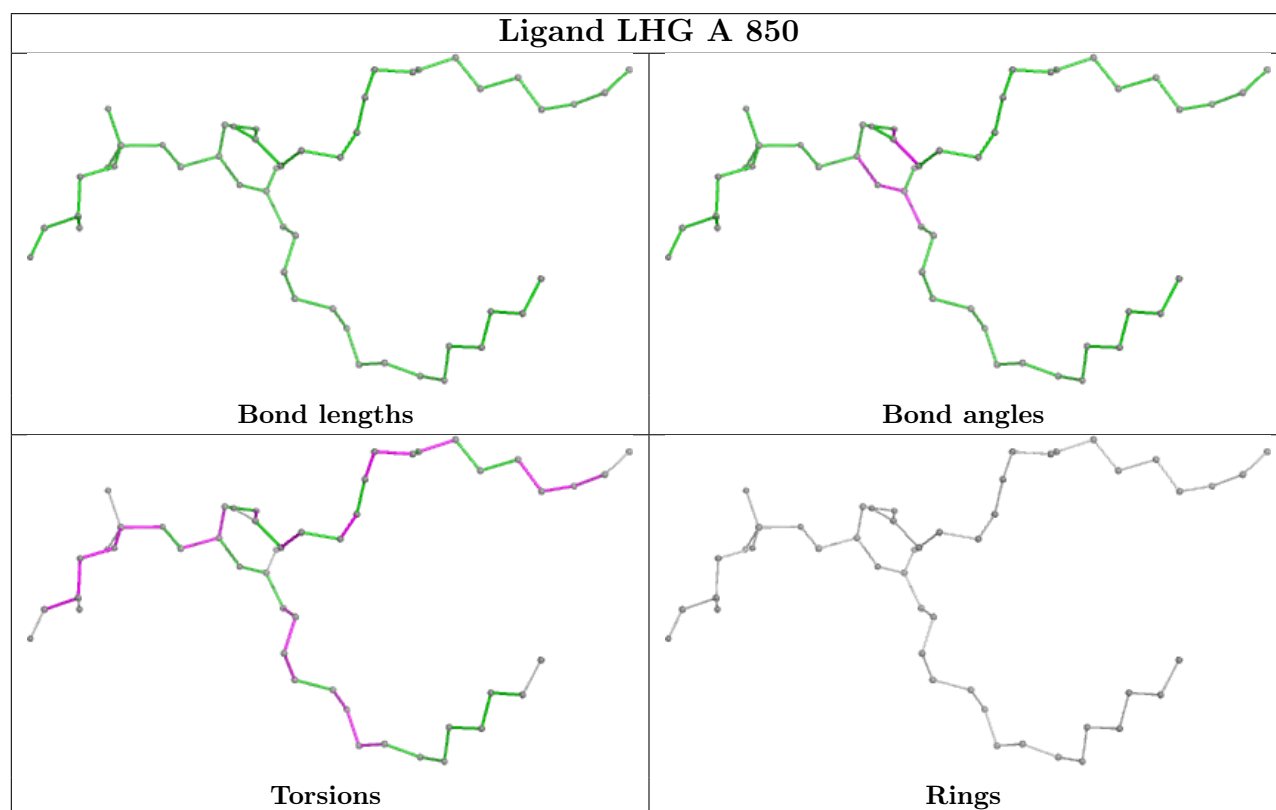
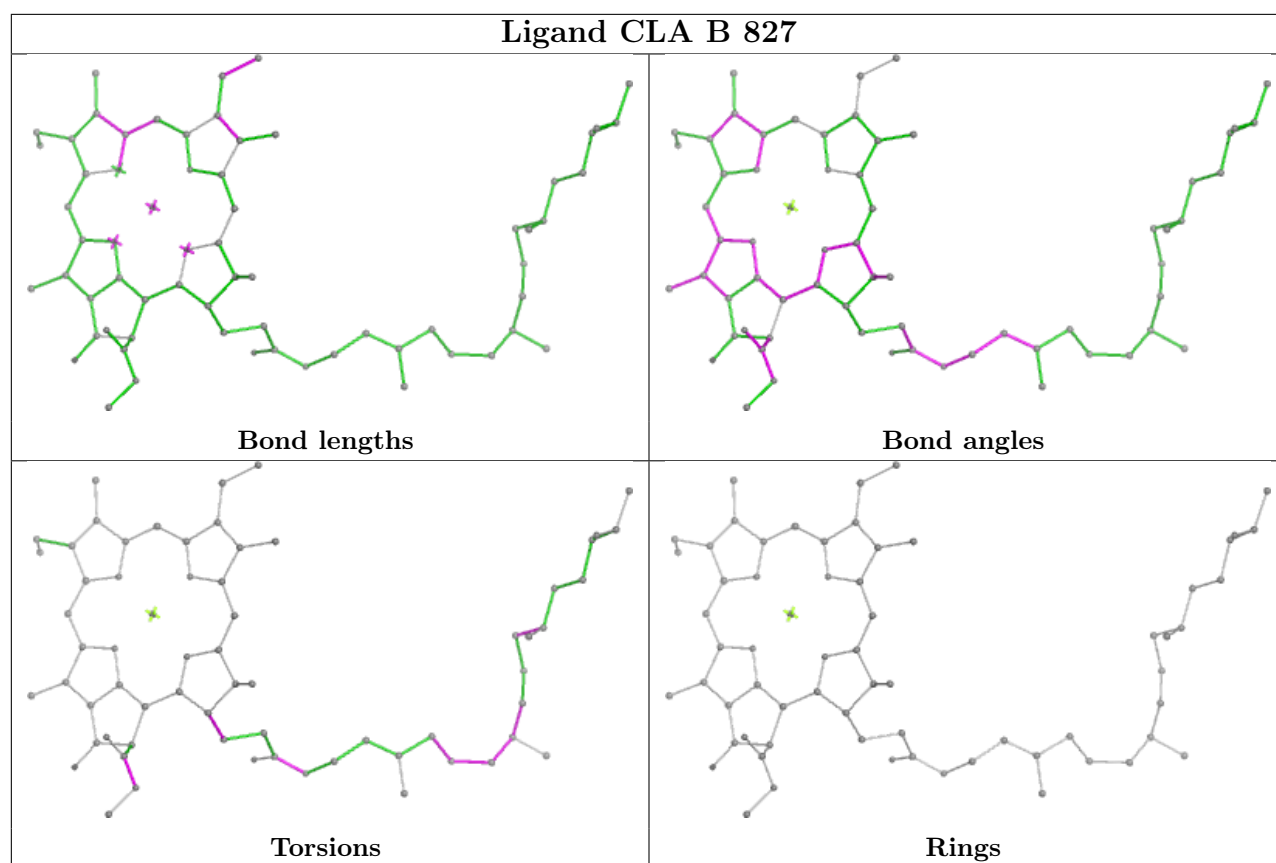
Ligand BCR A 845

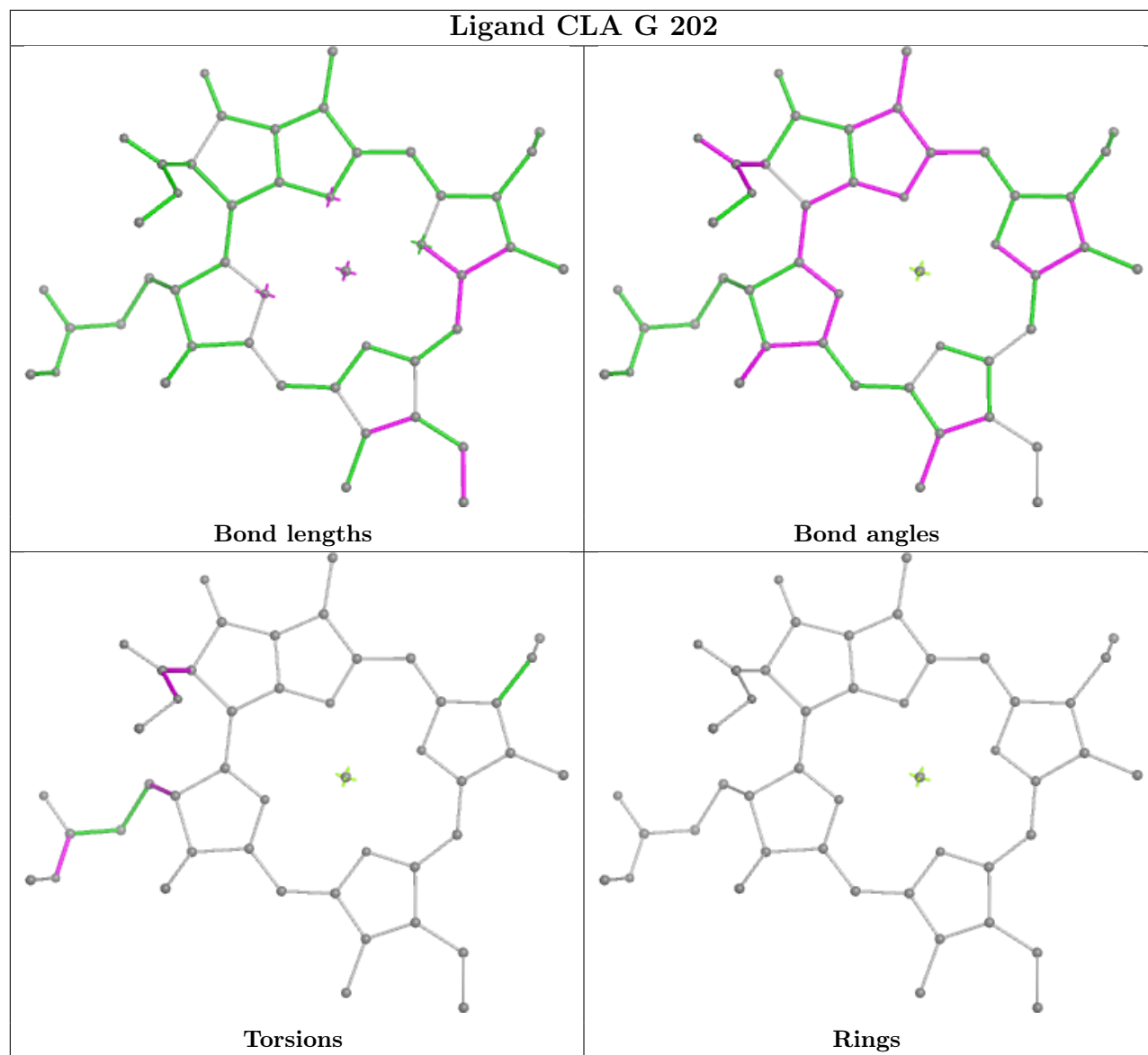




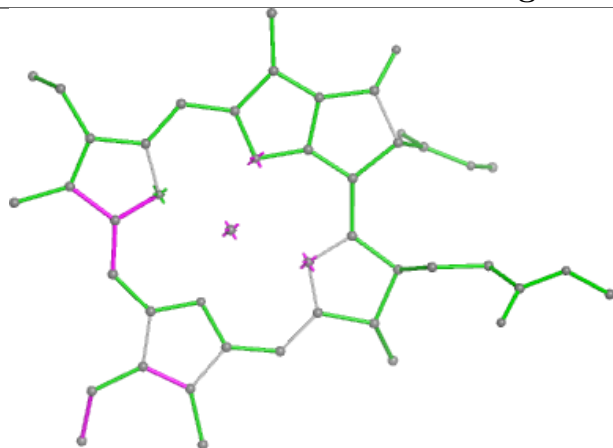




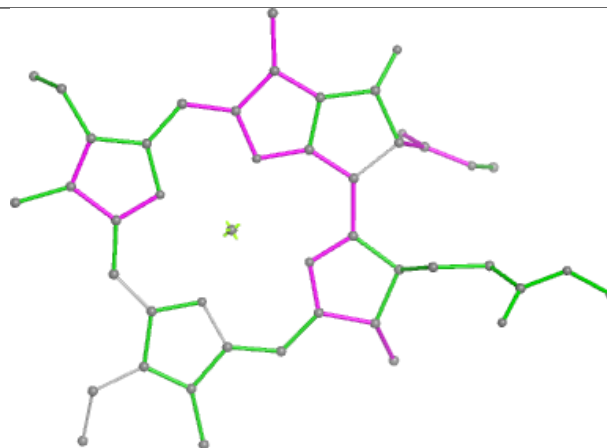




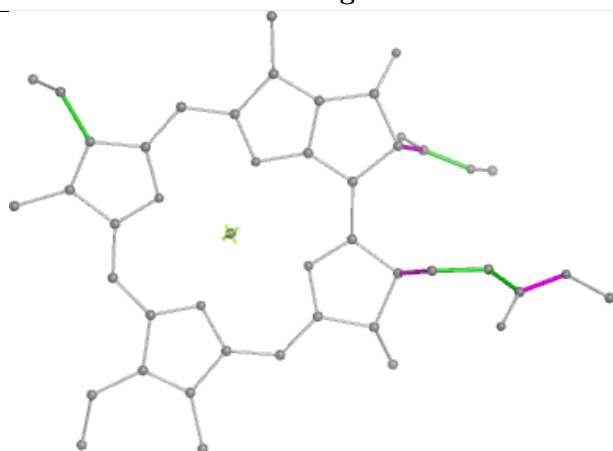
Ligand CLA 6 321



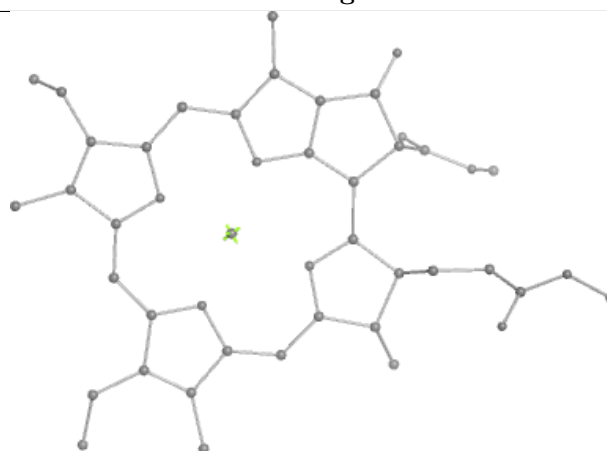
Bond lengths



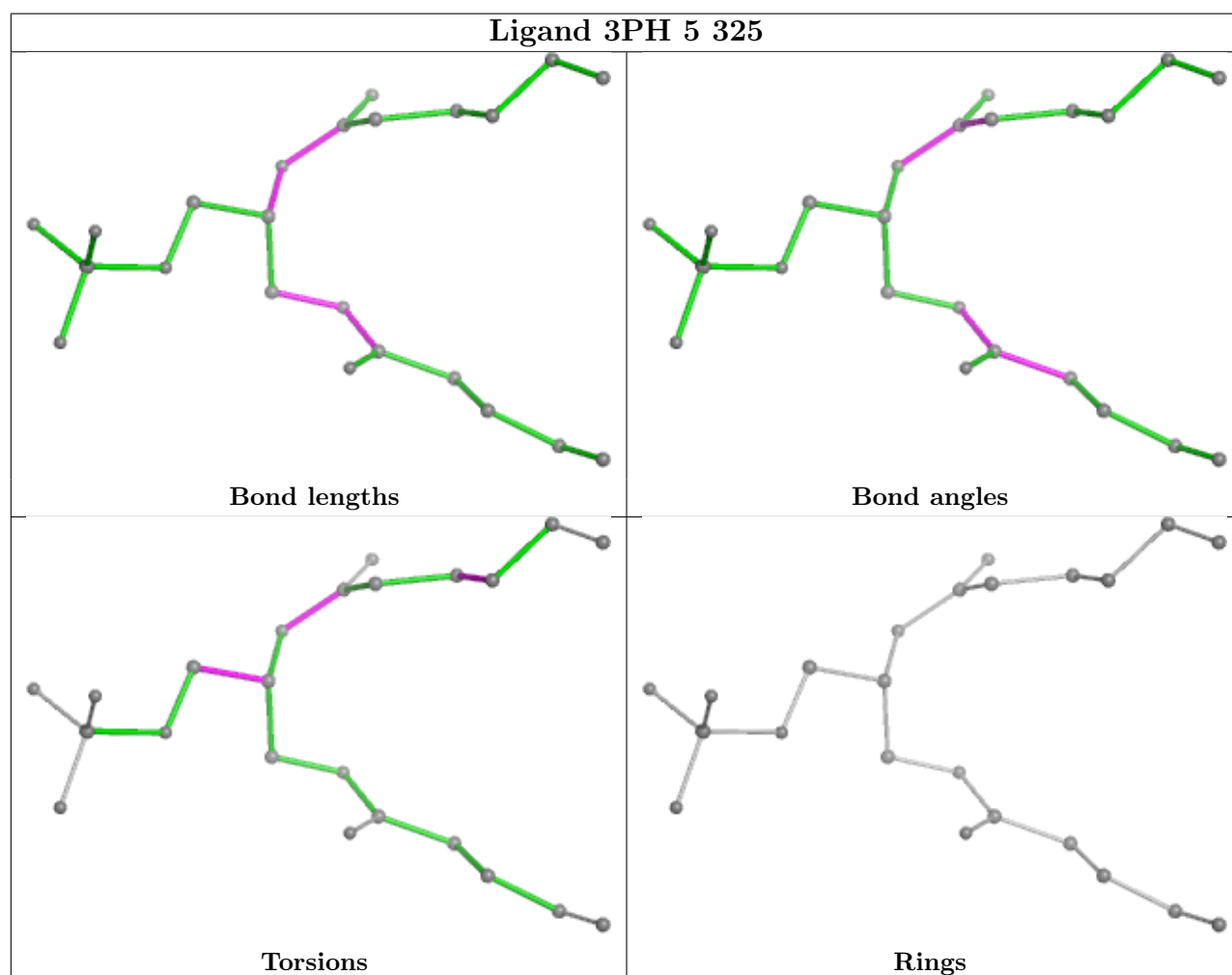
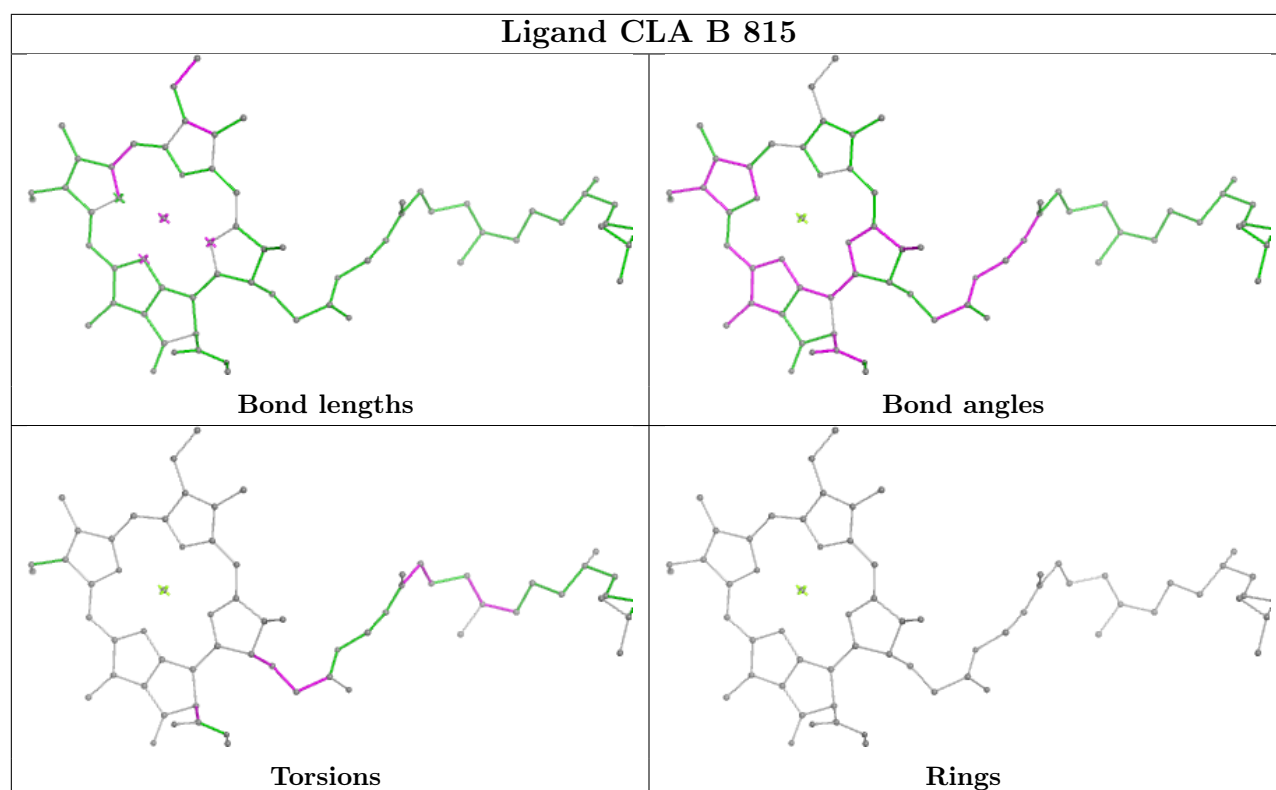
Bond angles

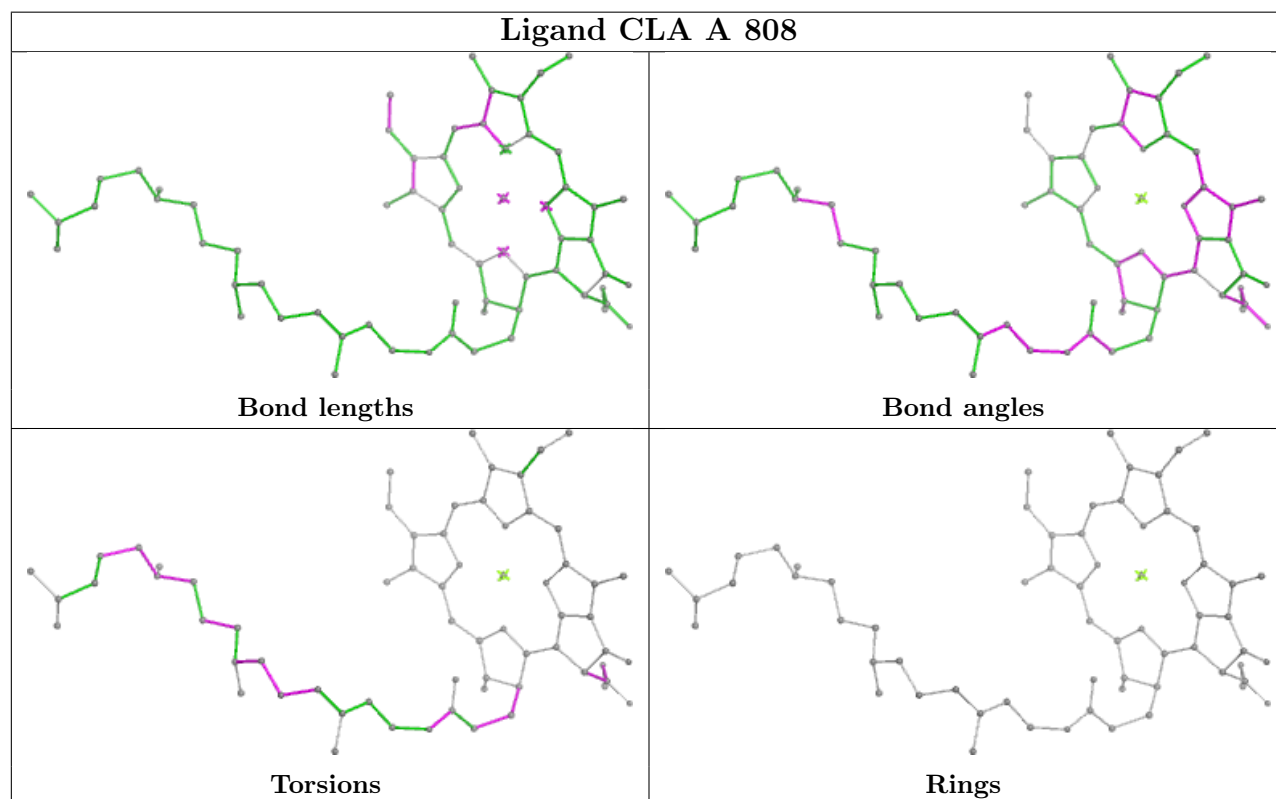
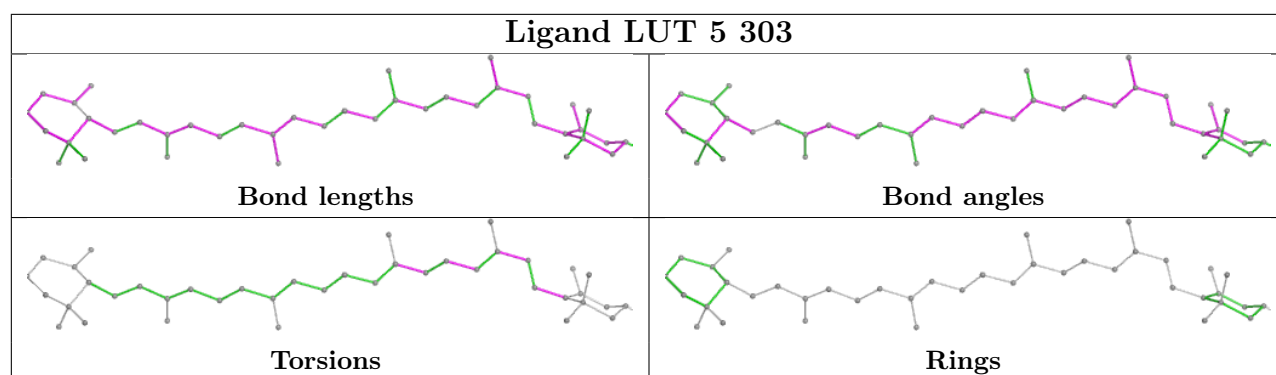


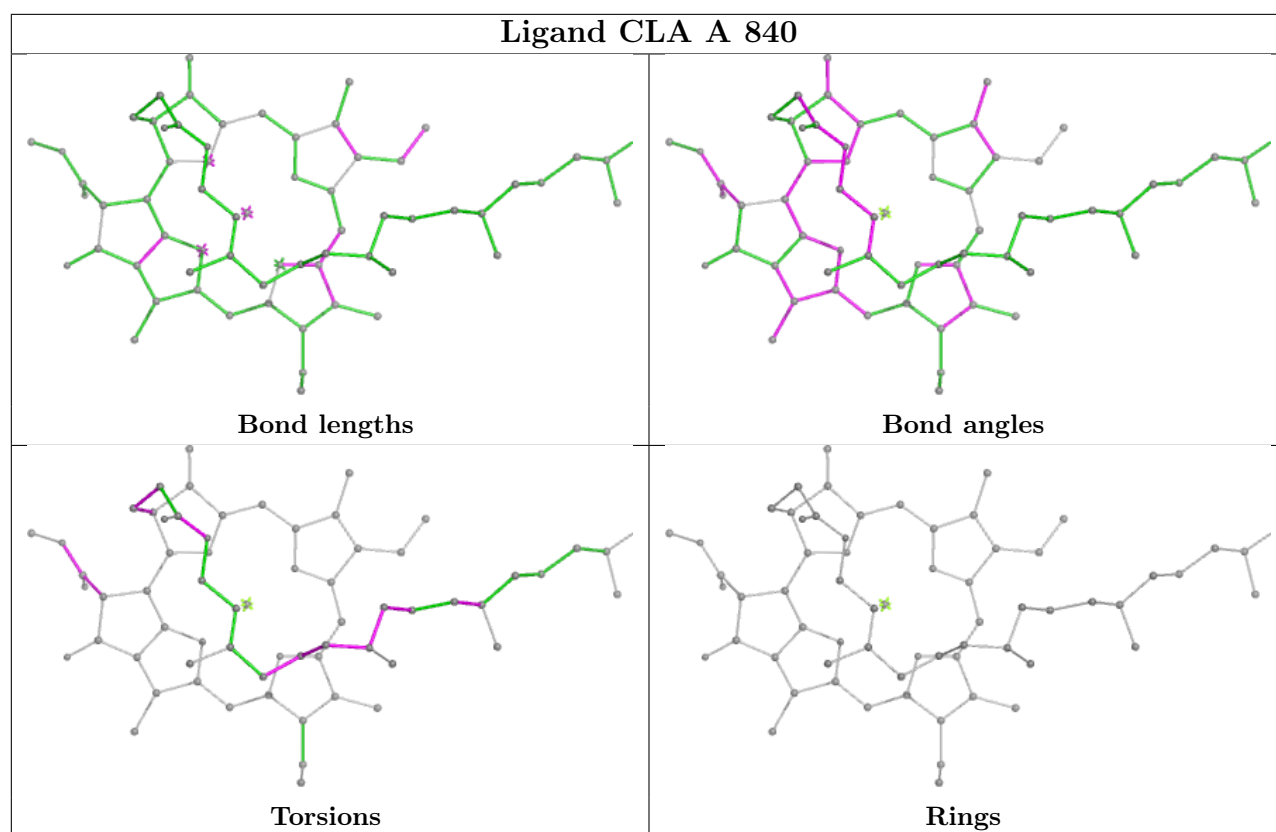
Torsions



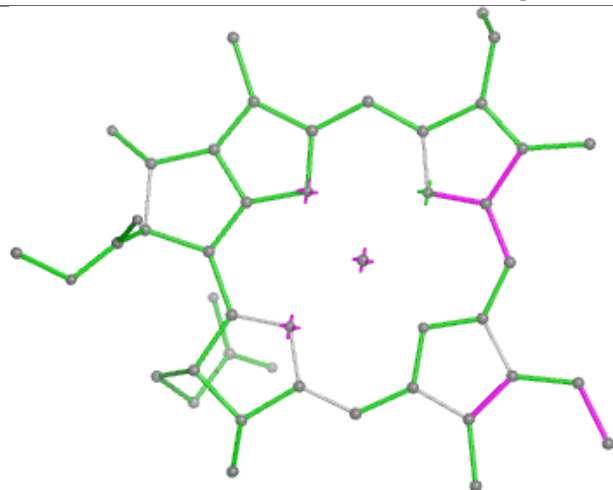
Rings



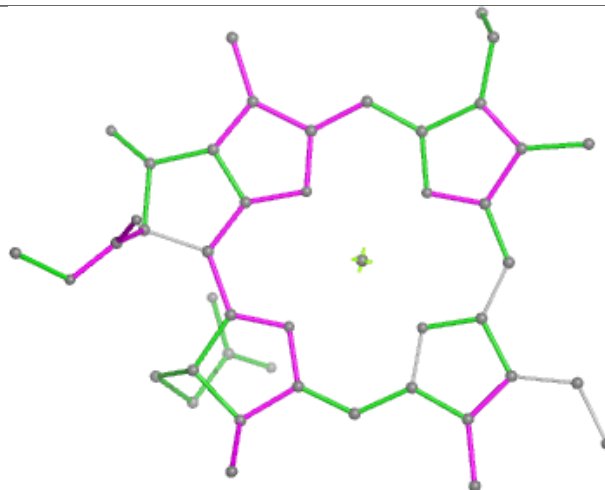




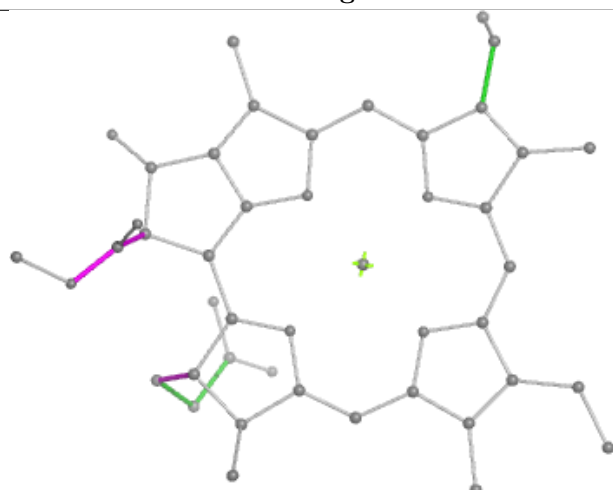
Ligand CLA B 836



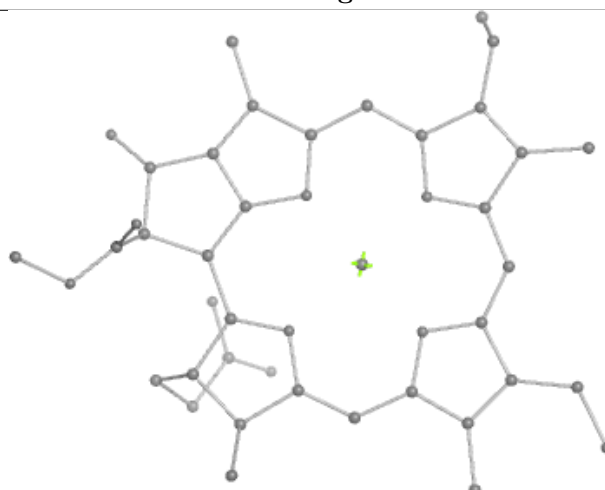
Bond lengths



Bond angles

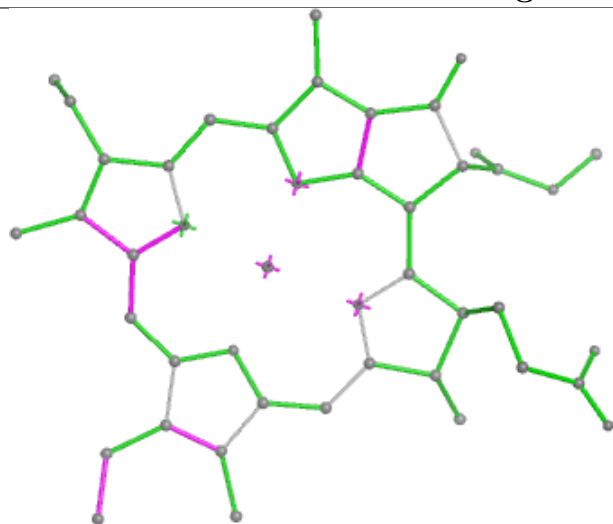


Torsions

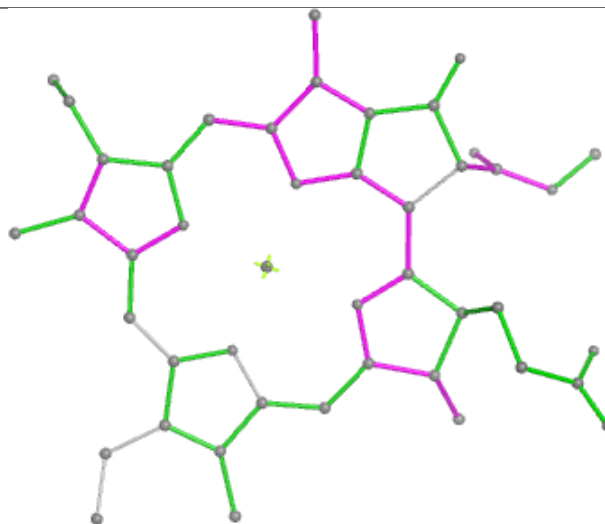


Rings

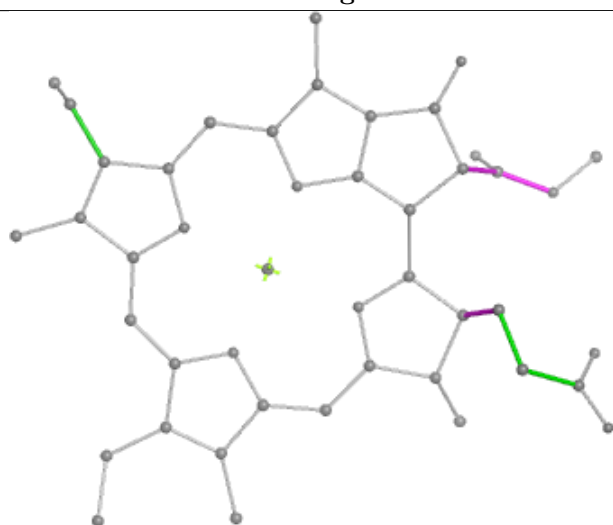
Ligand CLA F 305



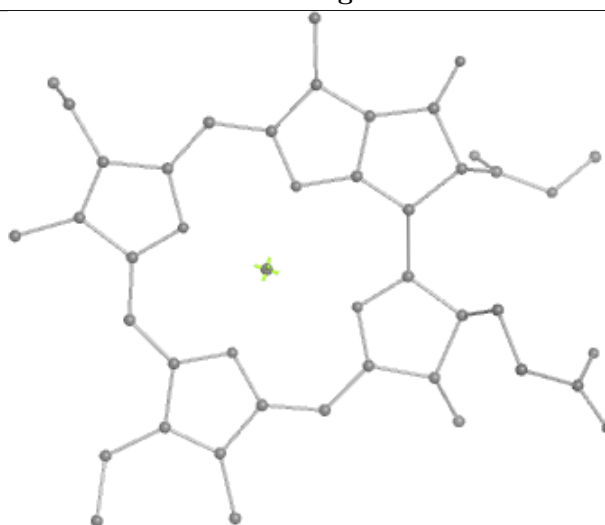
Bond lengths



Bond angles

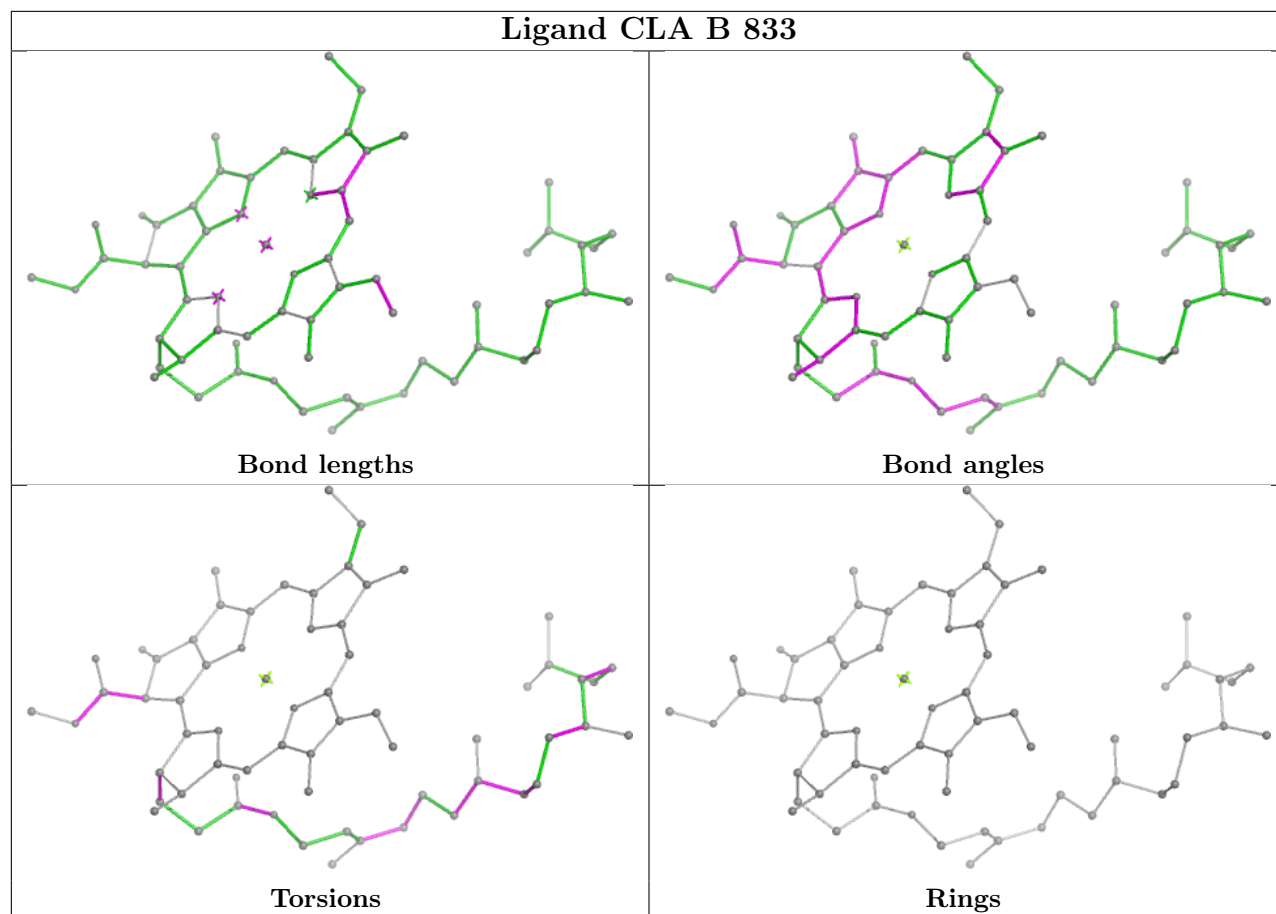


Torsions

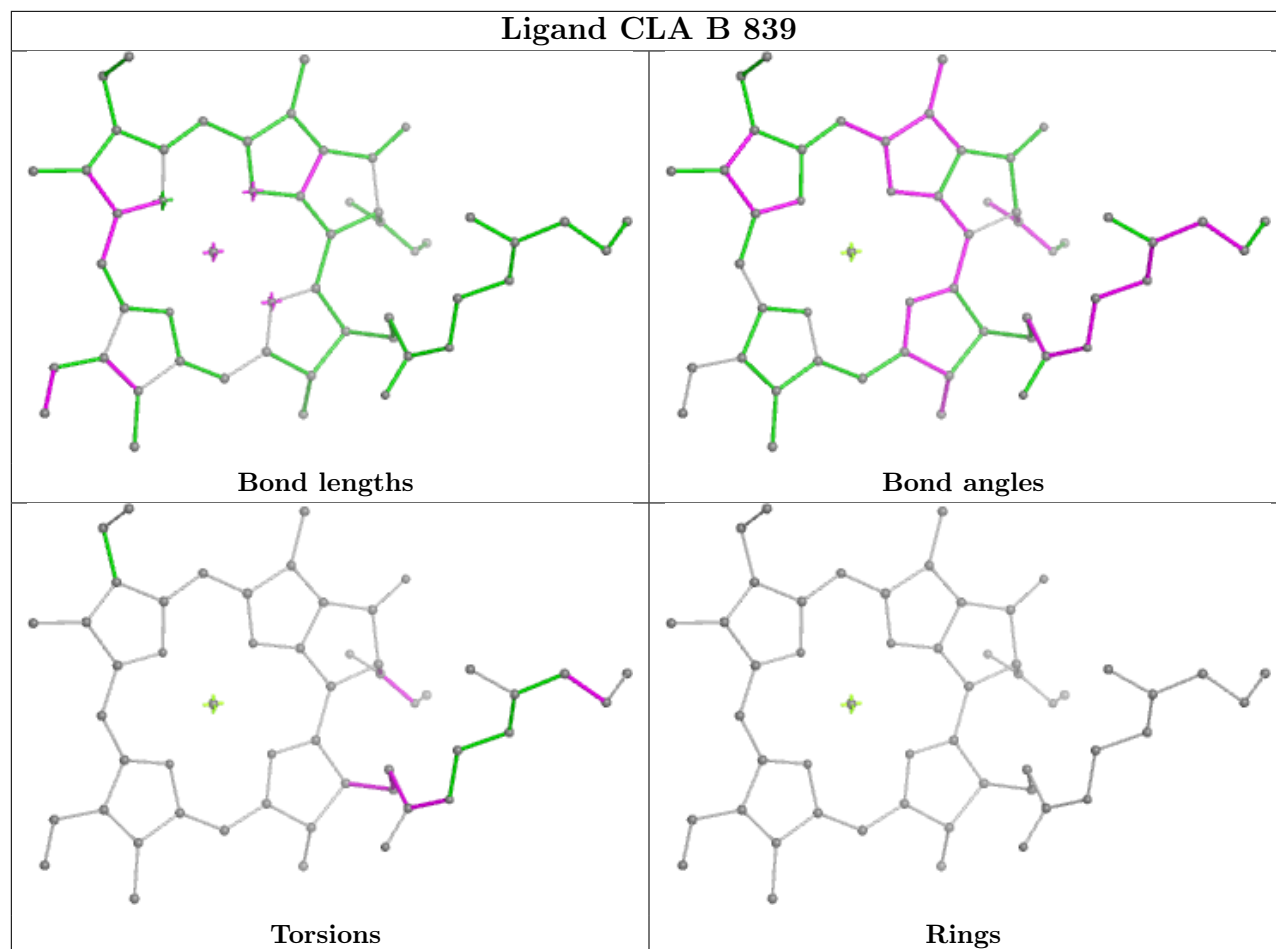


Rings

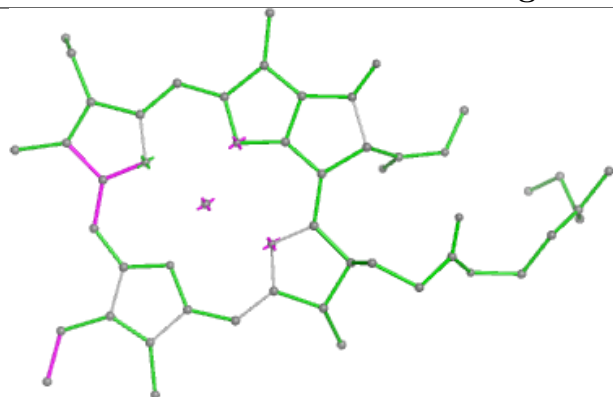
Ligand CLA B 833



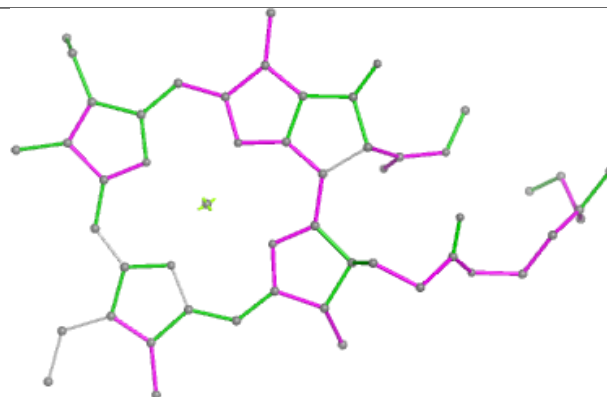
Ligand CLA B 839



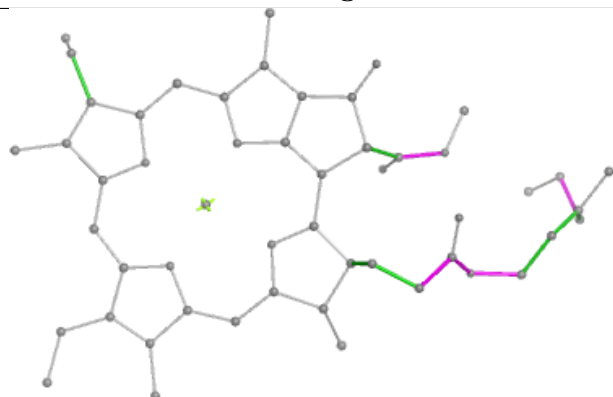
Ligand CLA 6 308



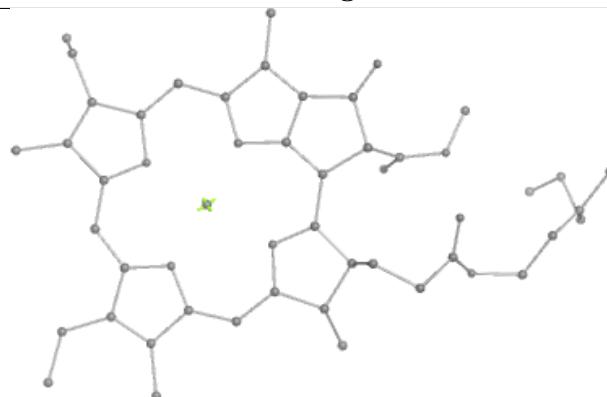
Bond lengths



Bond angles

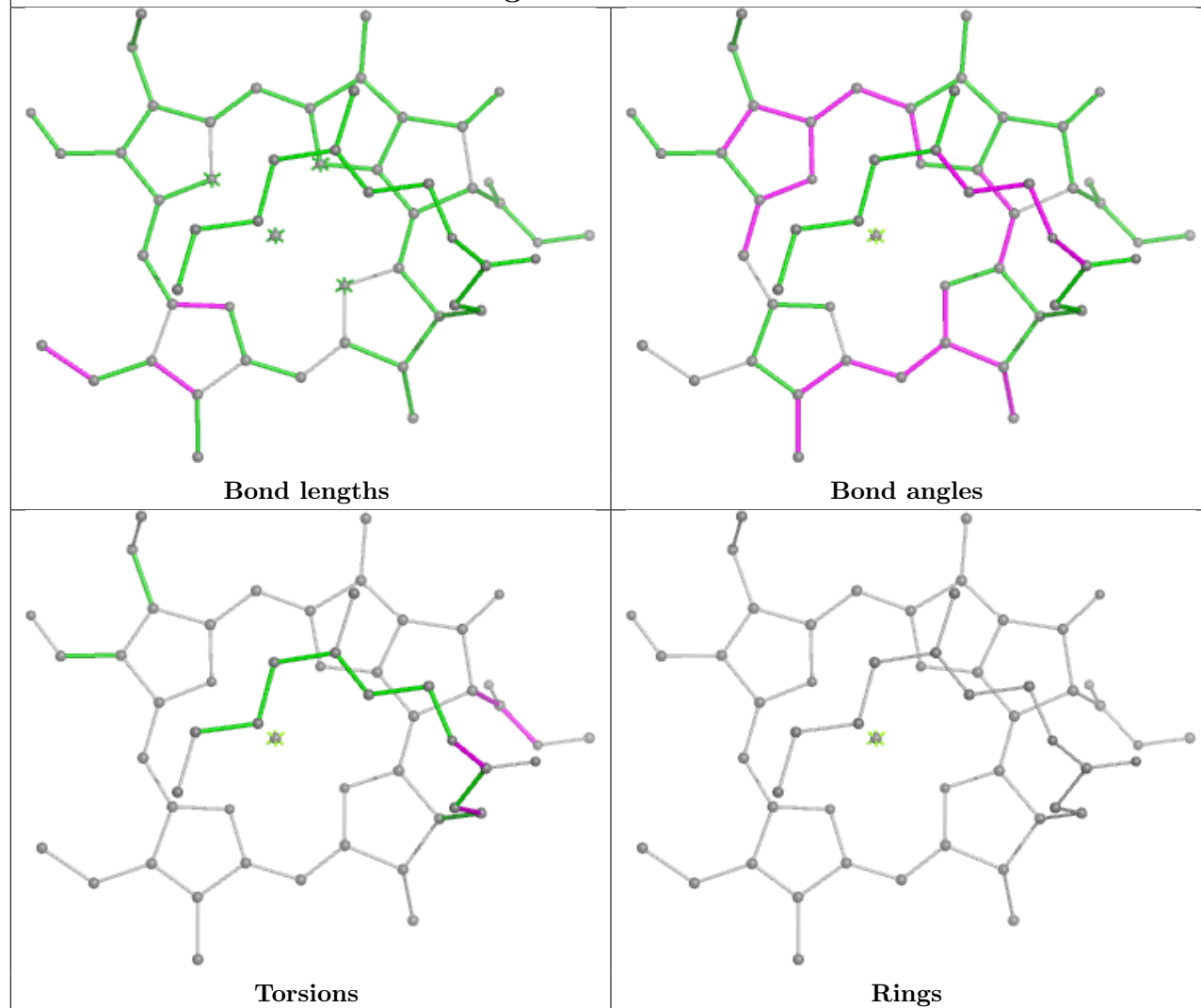


Torsions

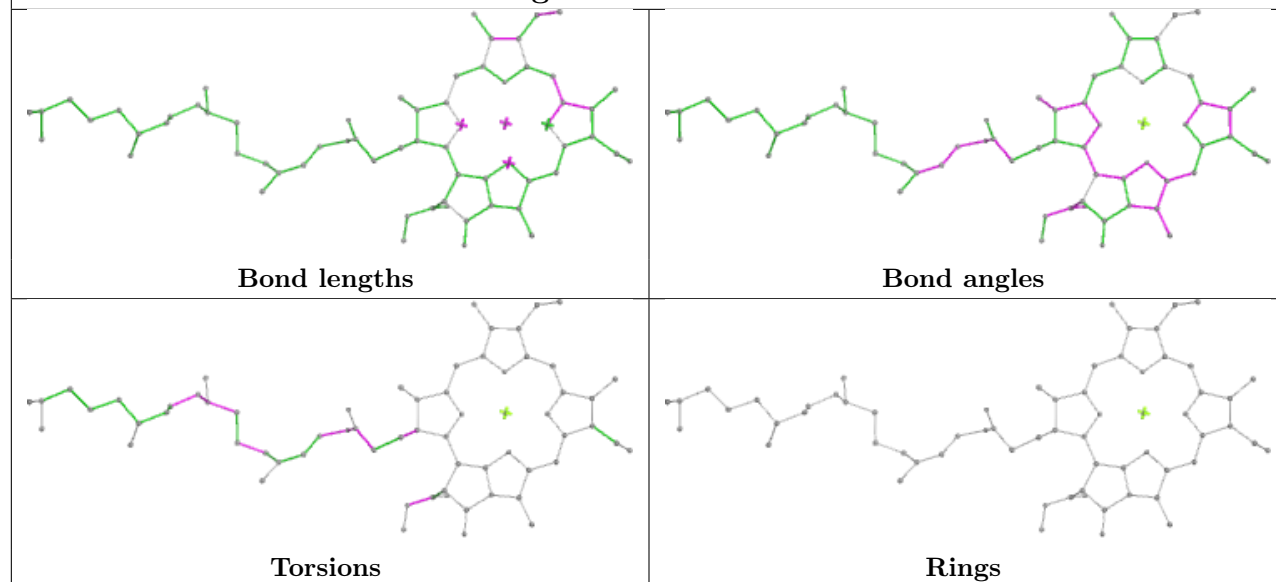


Rings

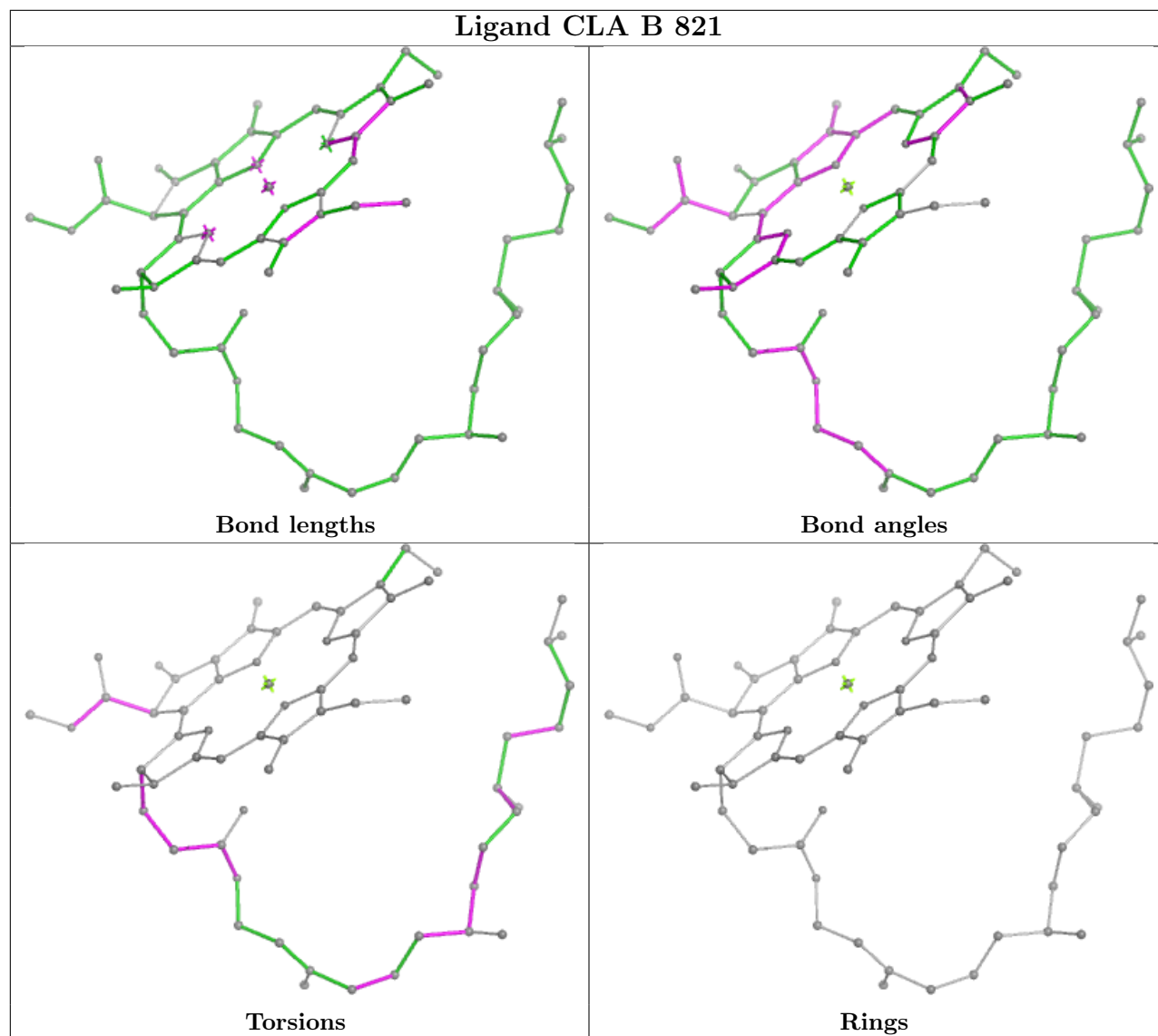
Ligand CHL 7 313



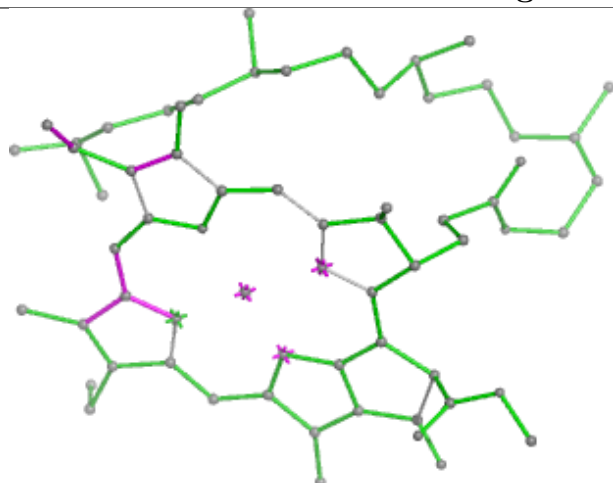
Ligand CLA A 833



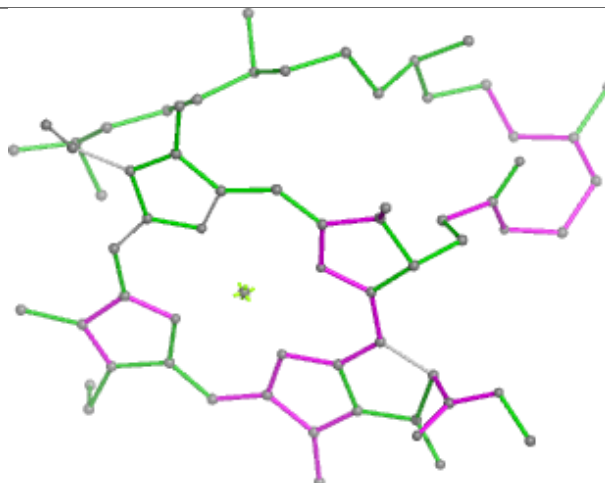
Ligand CLA B 821



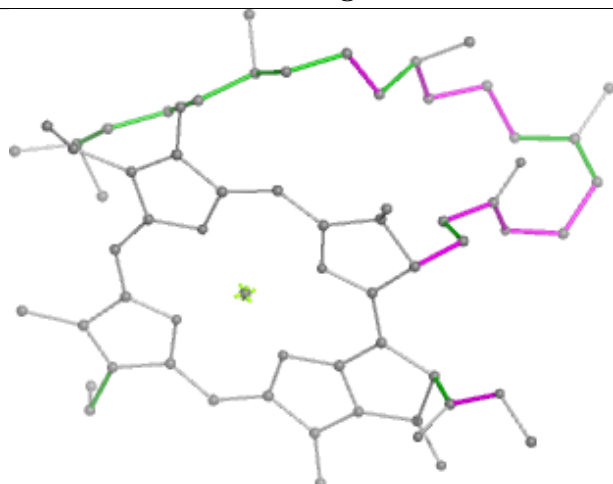
Ligand CLA Z 313



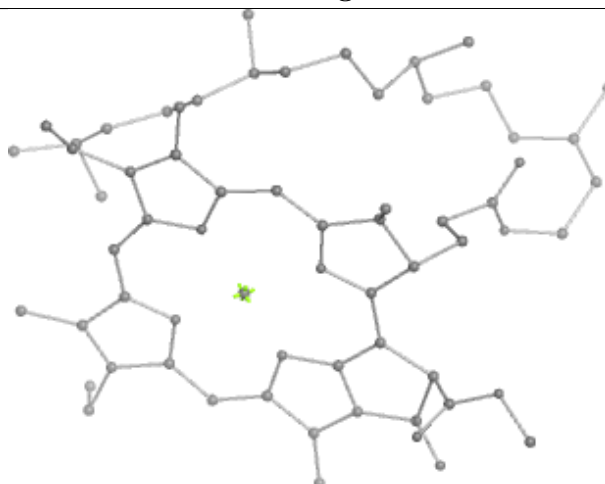
Bond lengths



Bond angles

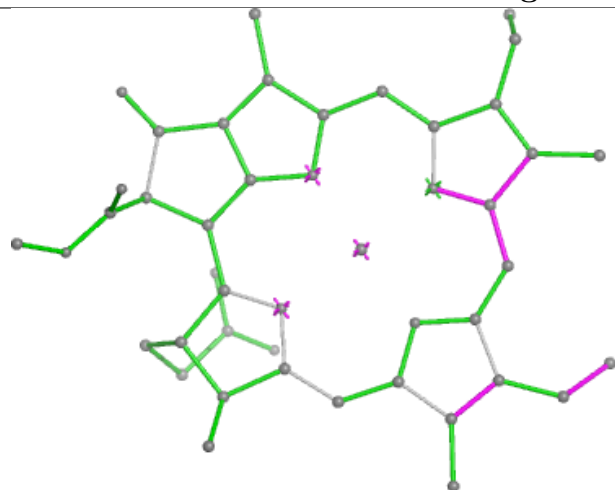


Torsions

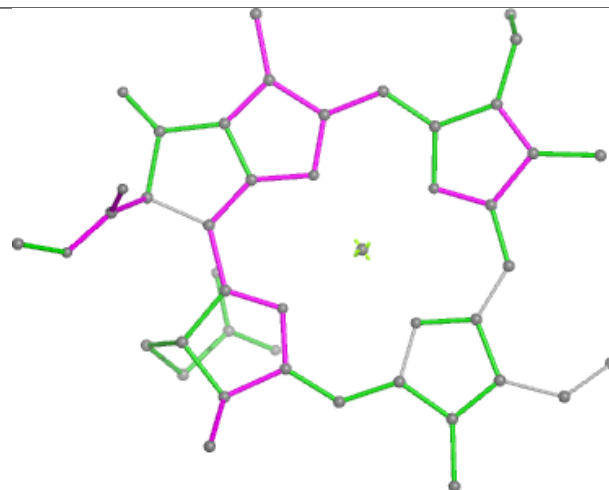


Rings

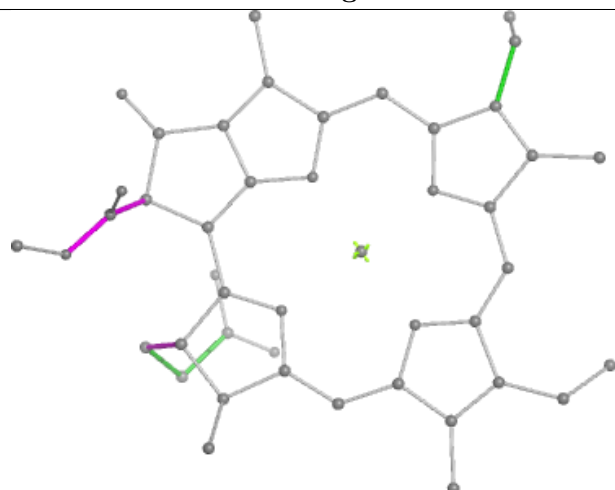
Ligand CLA 5 314



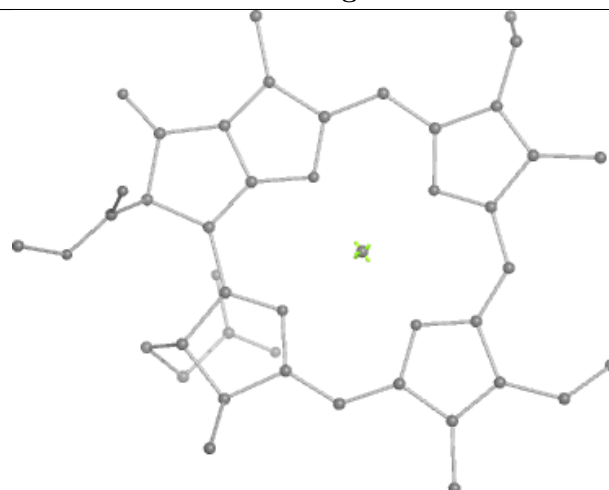
Bond lengths



Bond angles

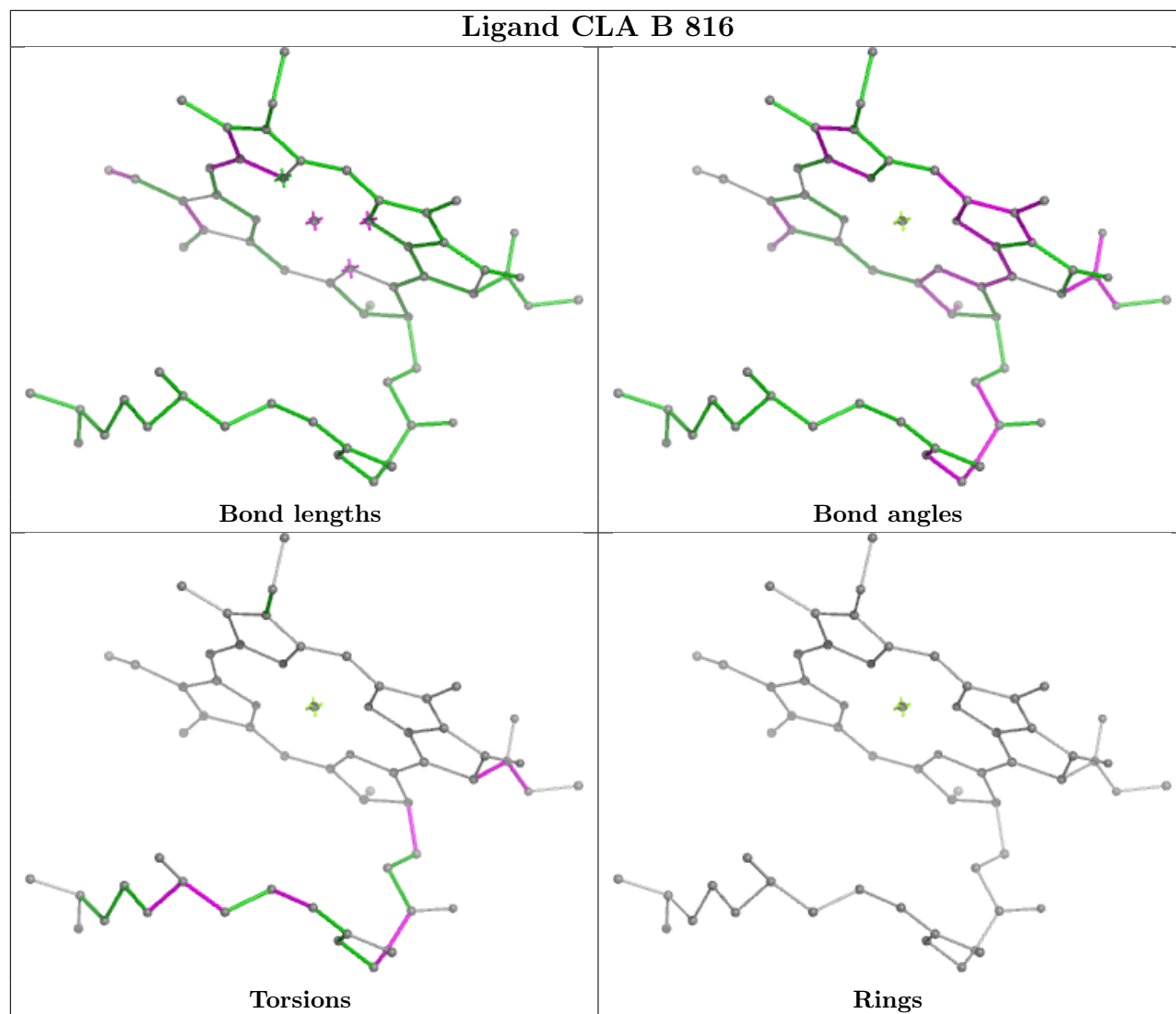


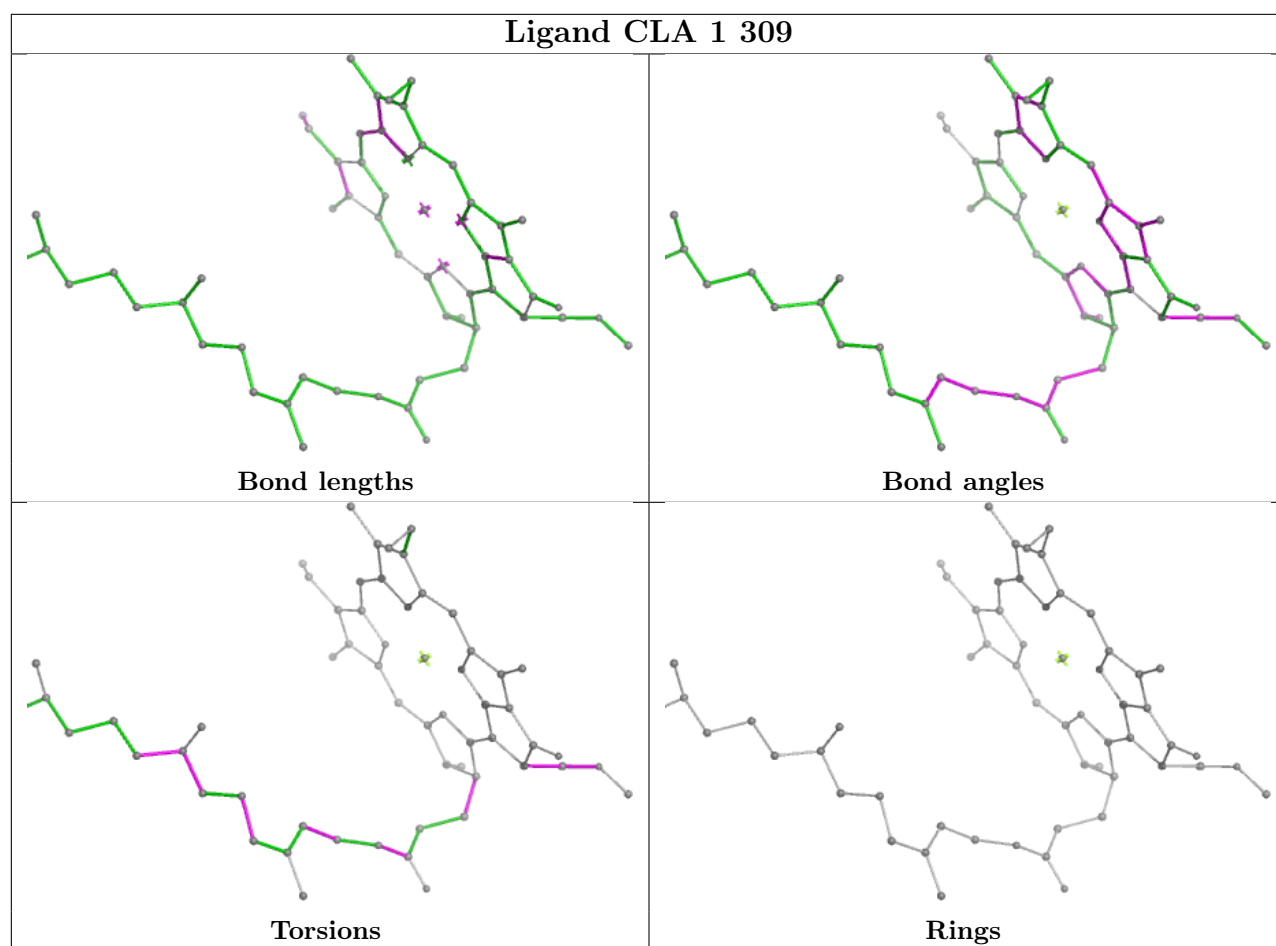
Torsions



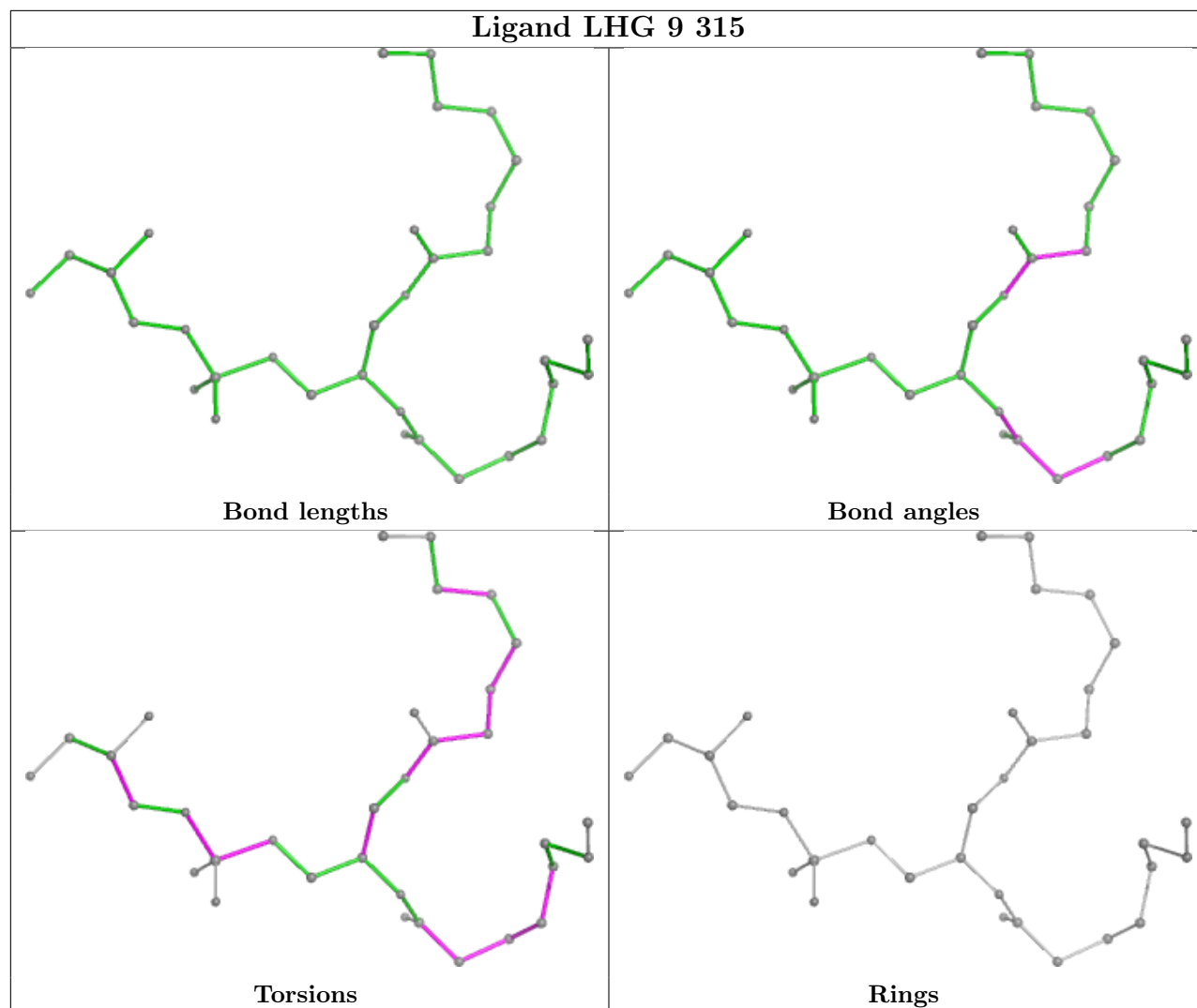
Rings

Ligand CLA B 816

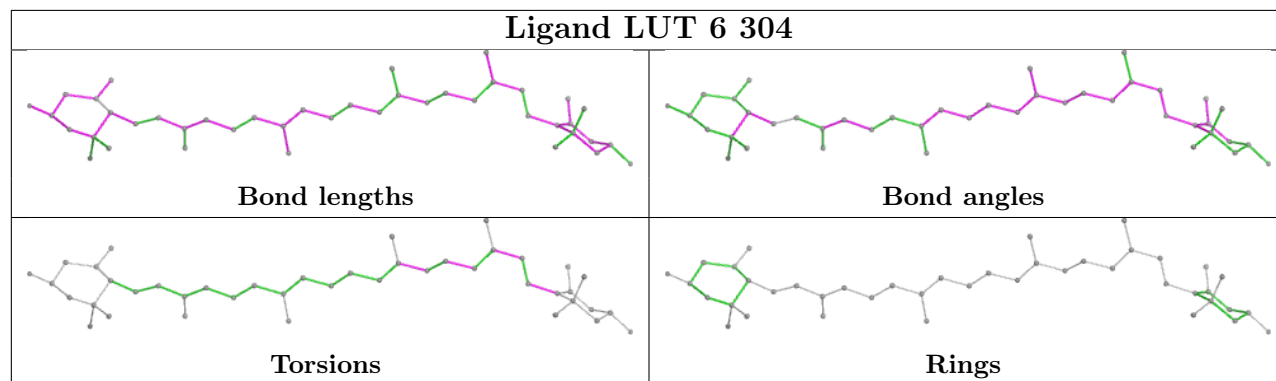


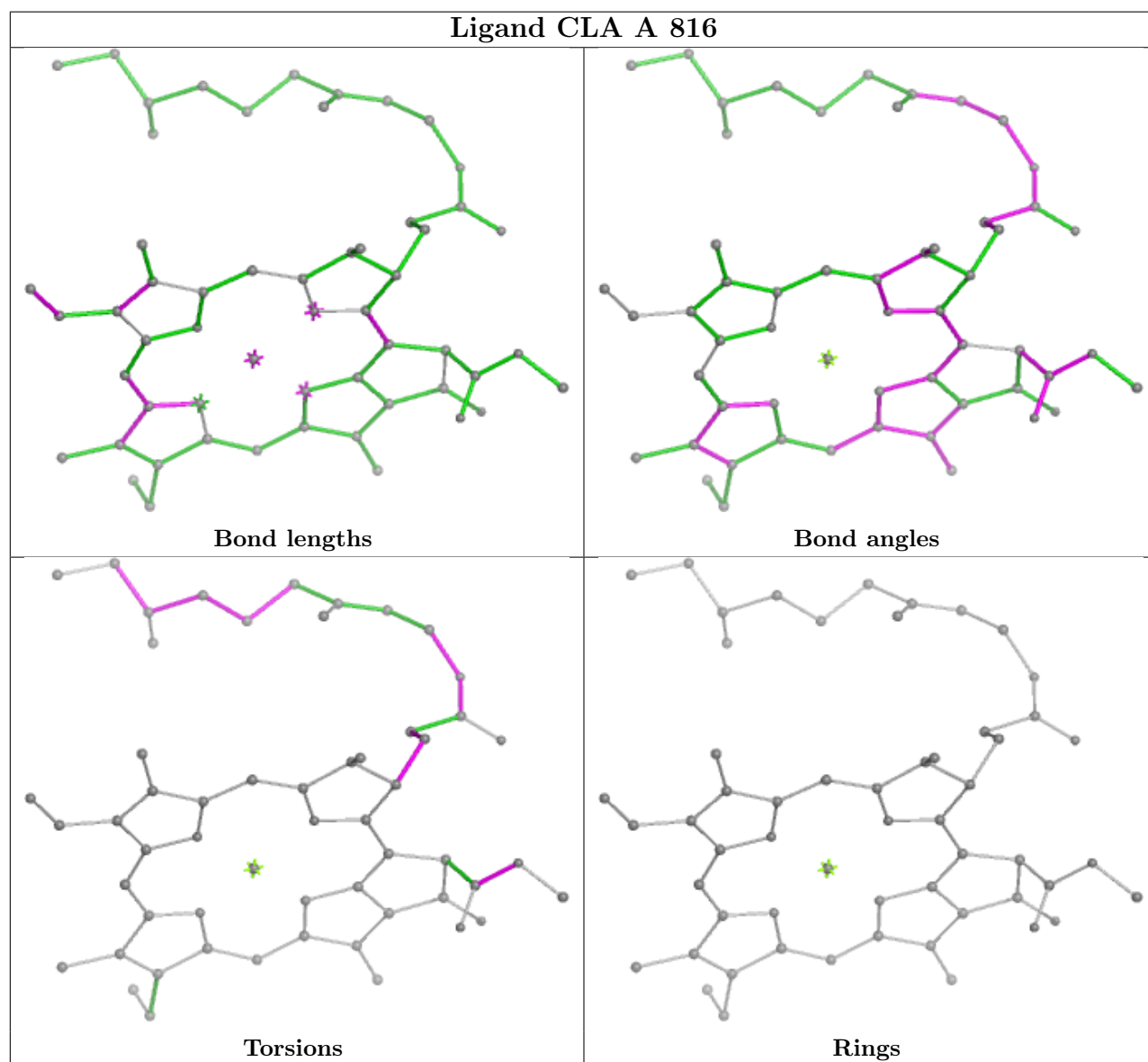
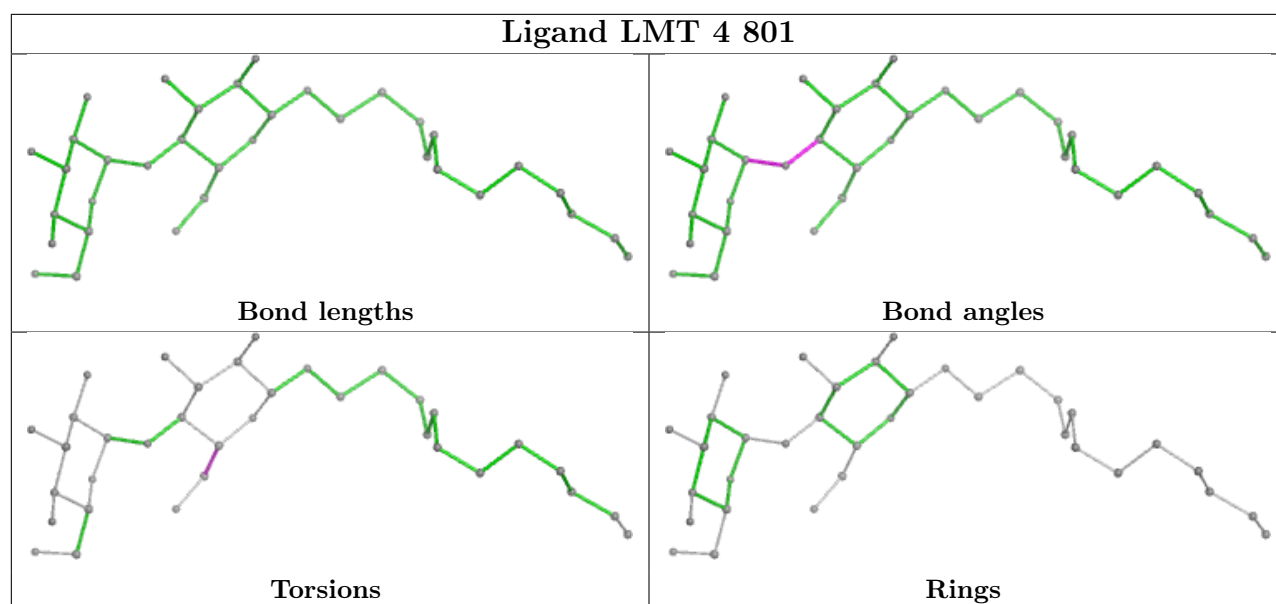


Ligand LHG 9 315

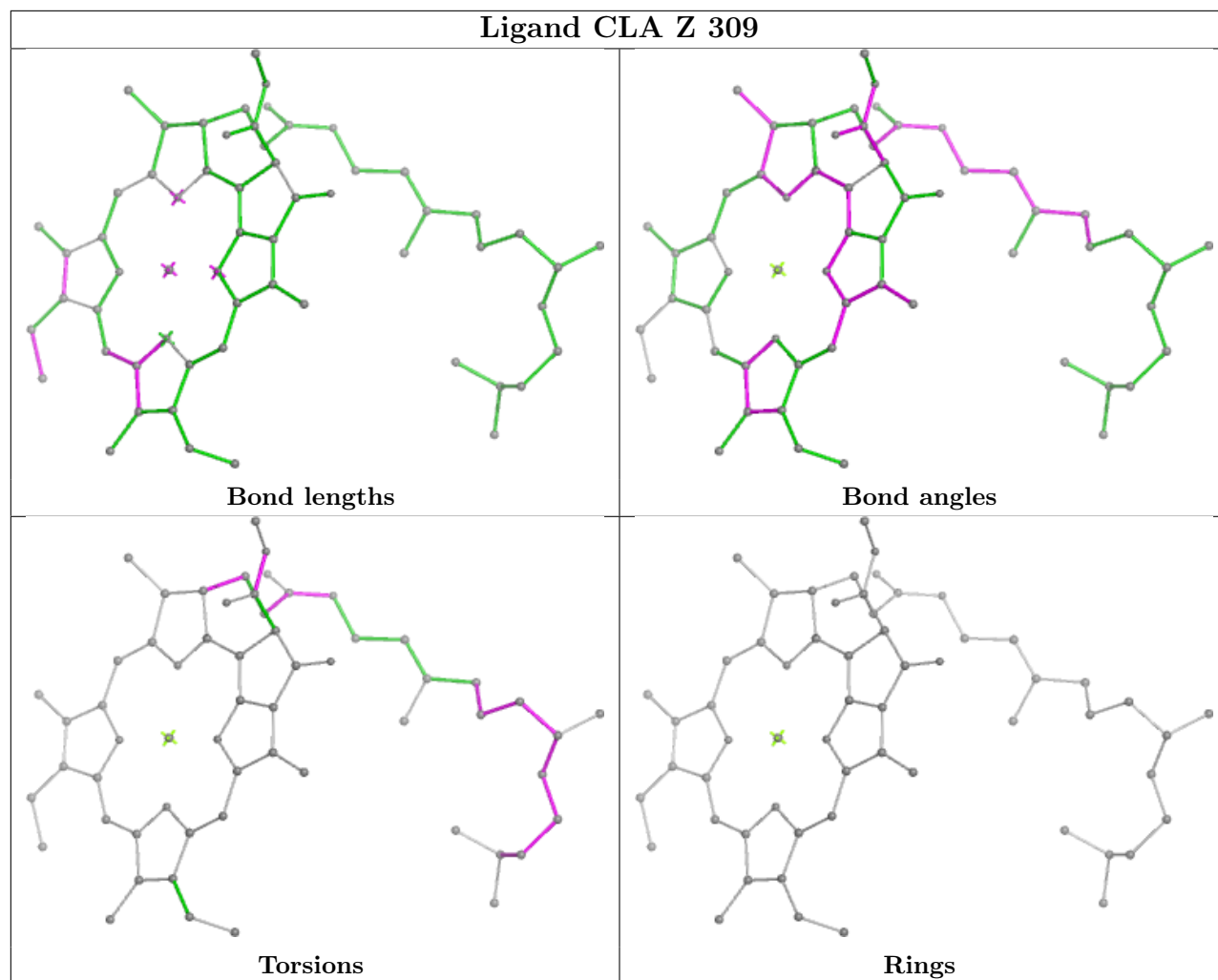


Ligand LUT 6 304

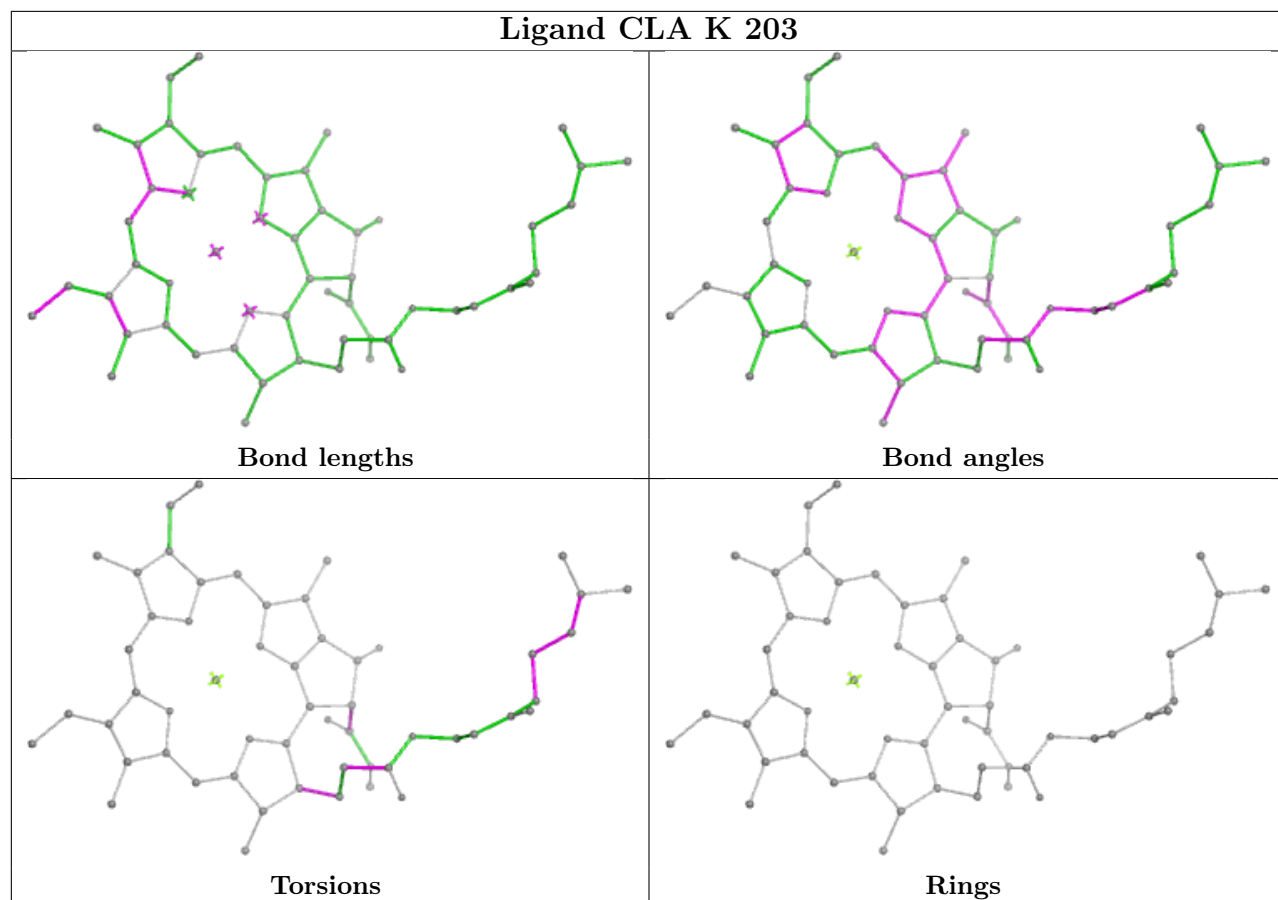




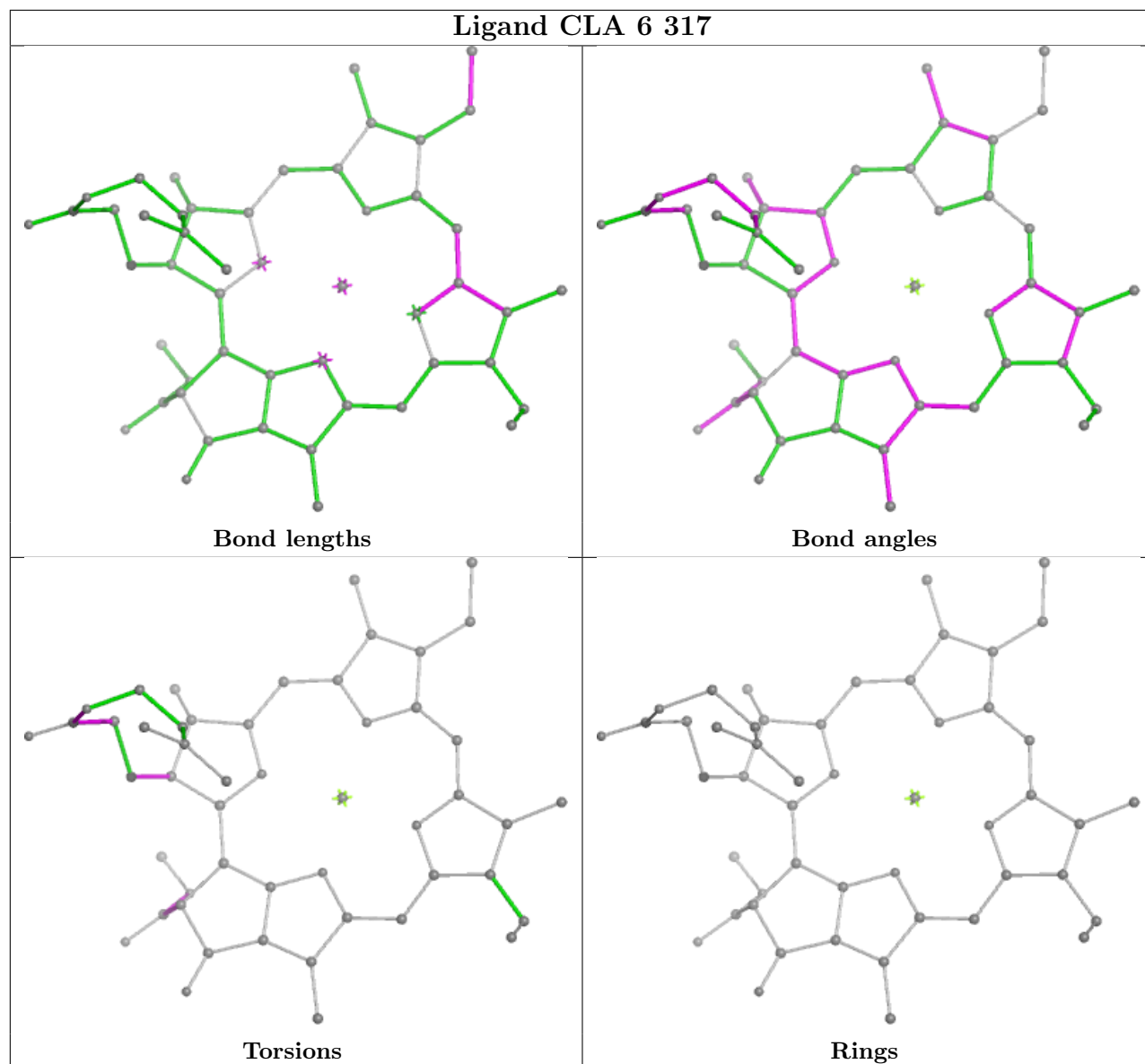
Ligand CLA Z 309

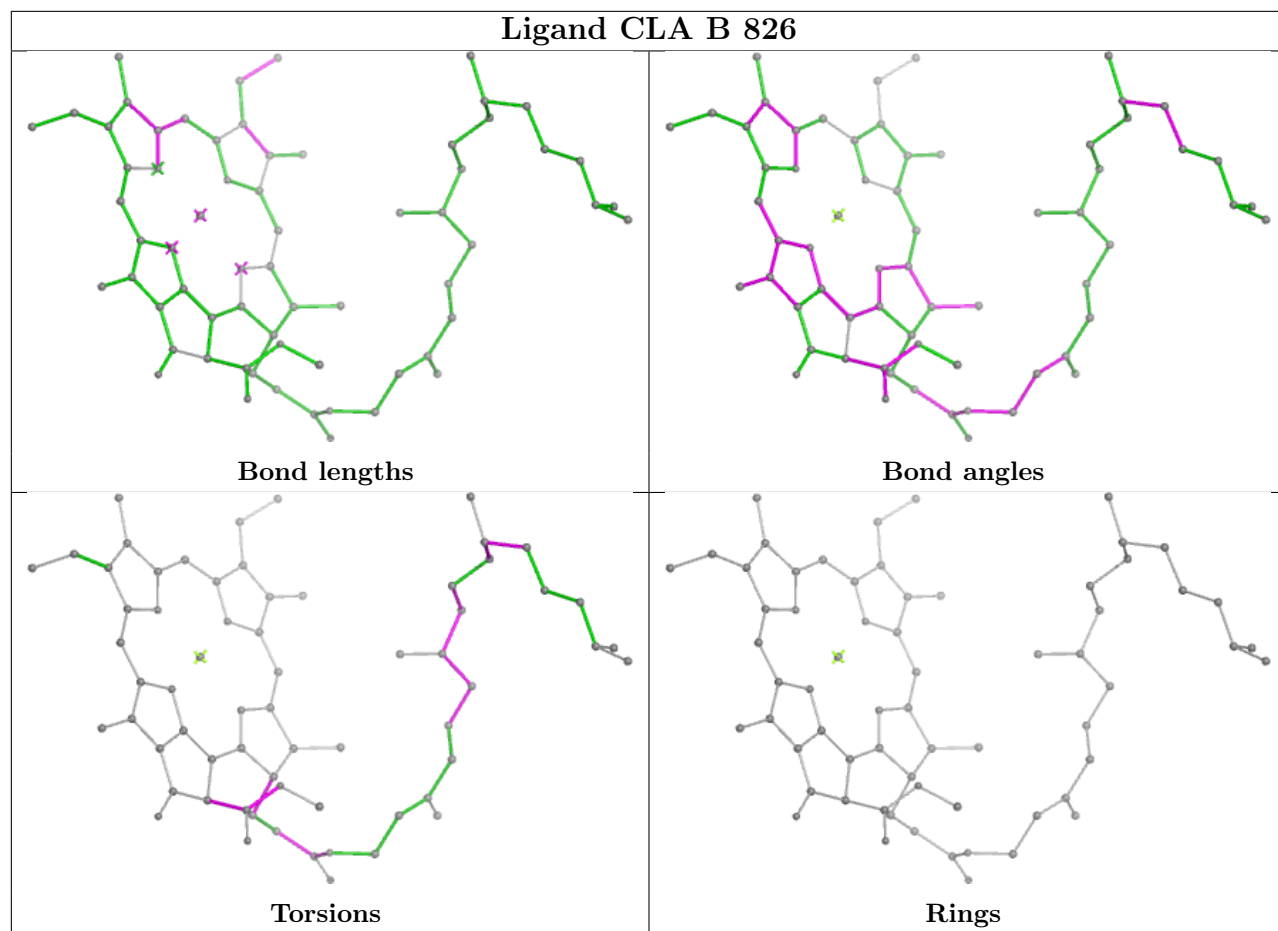


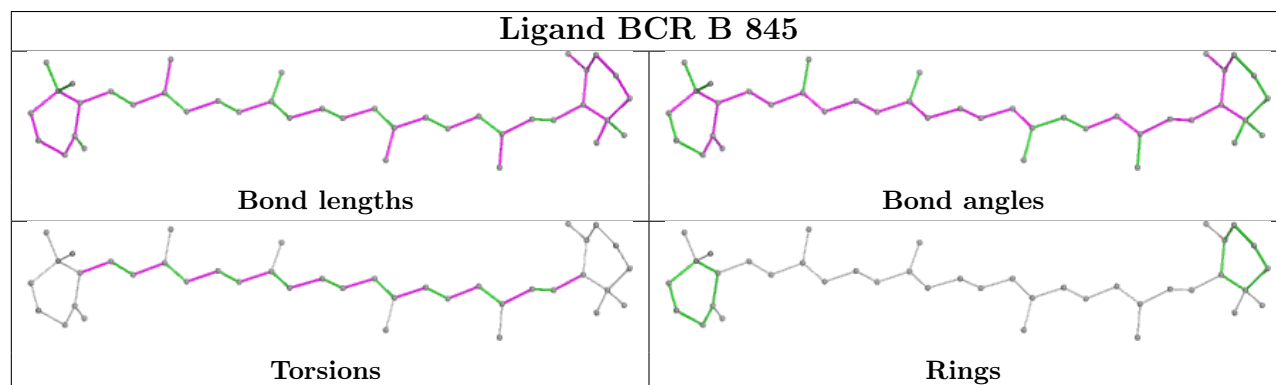
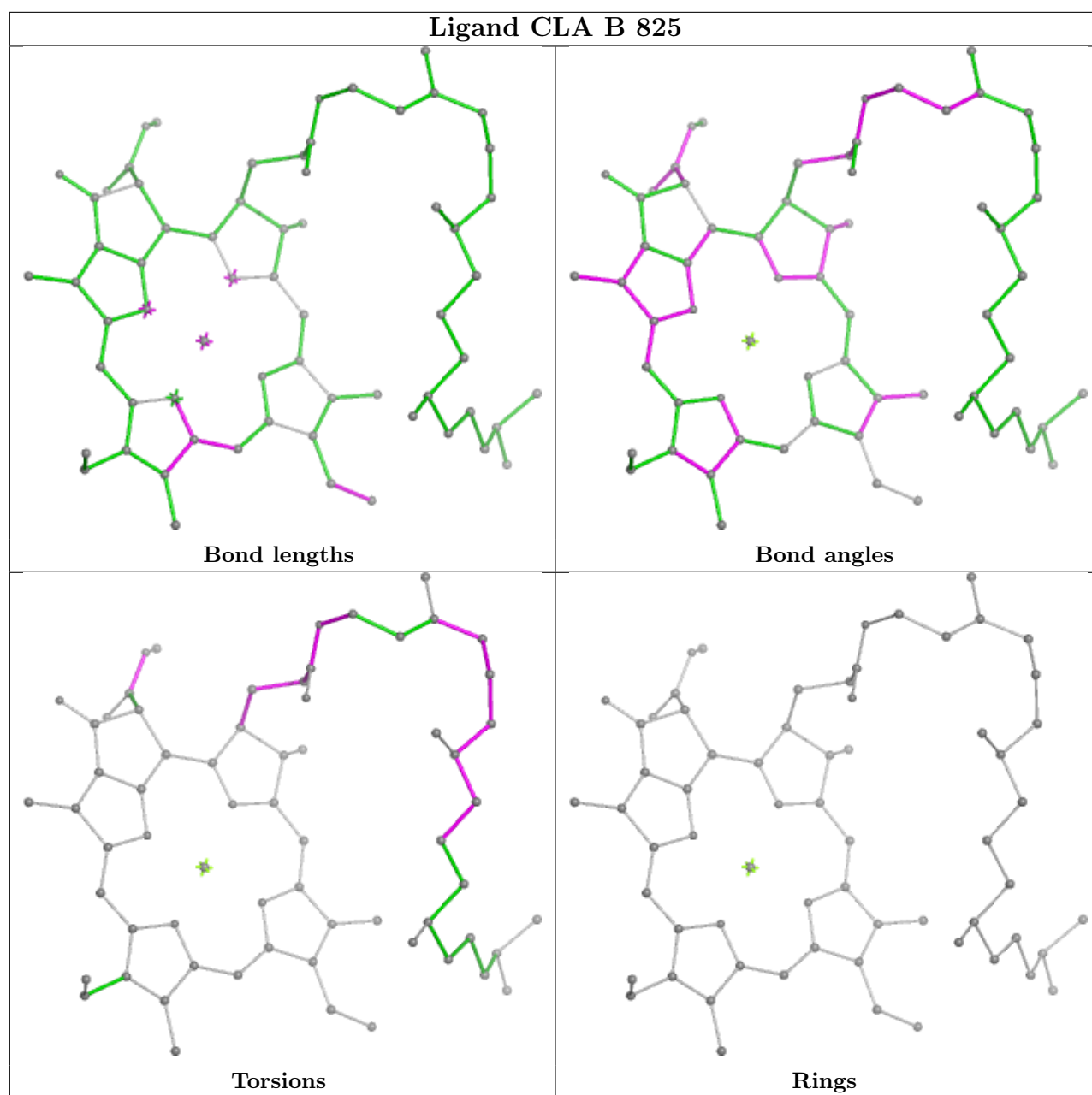
Ligand CLA K 203



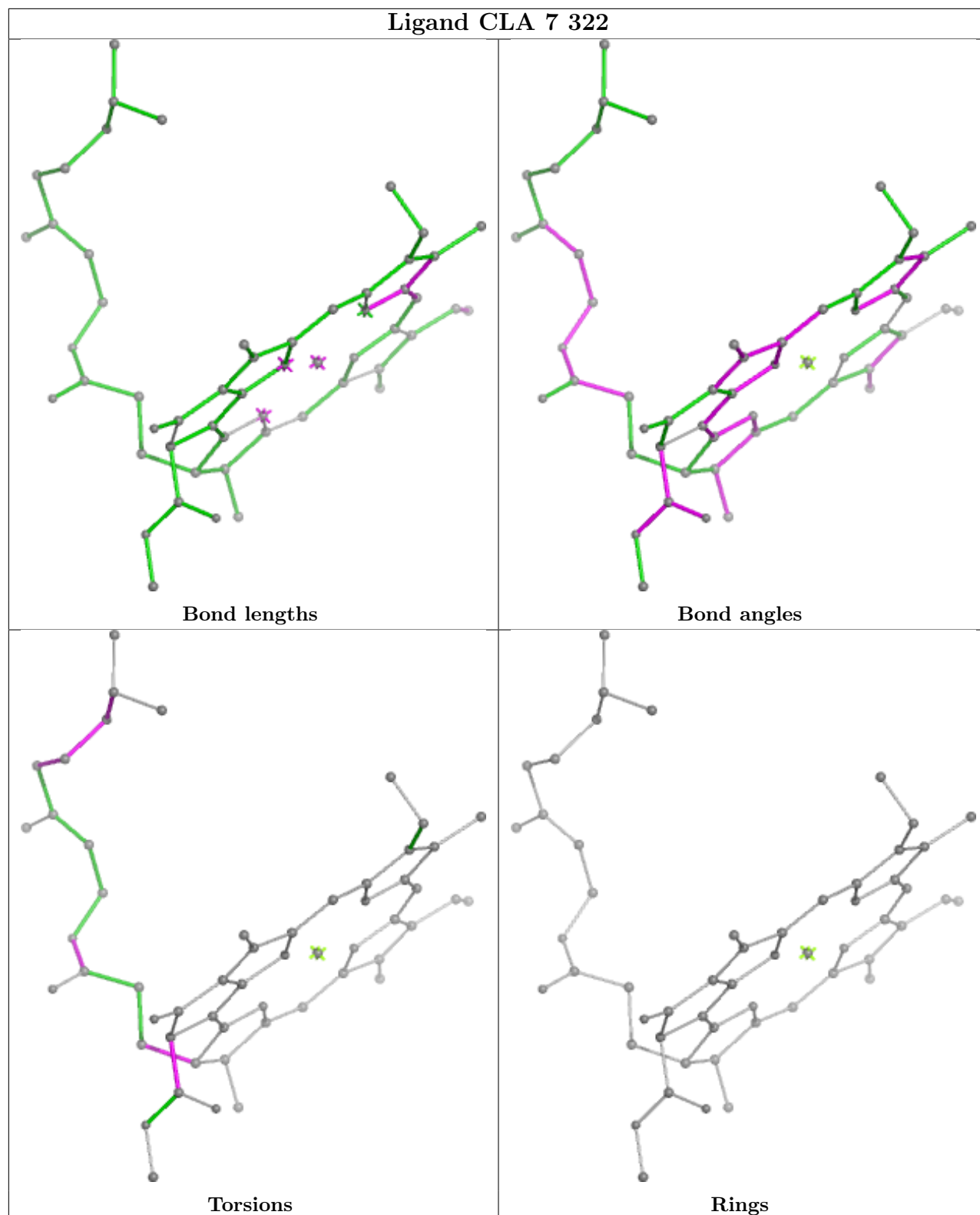
Ligand CLA 6 317

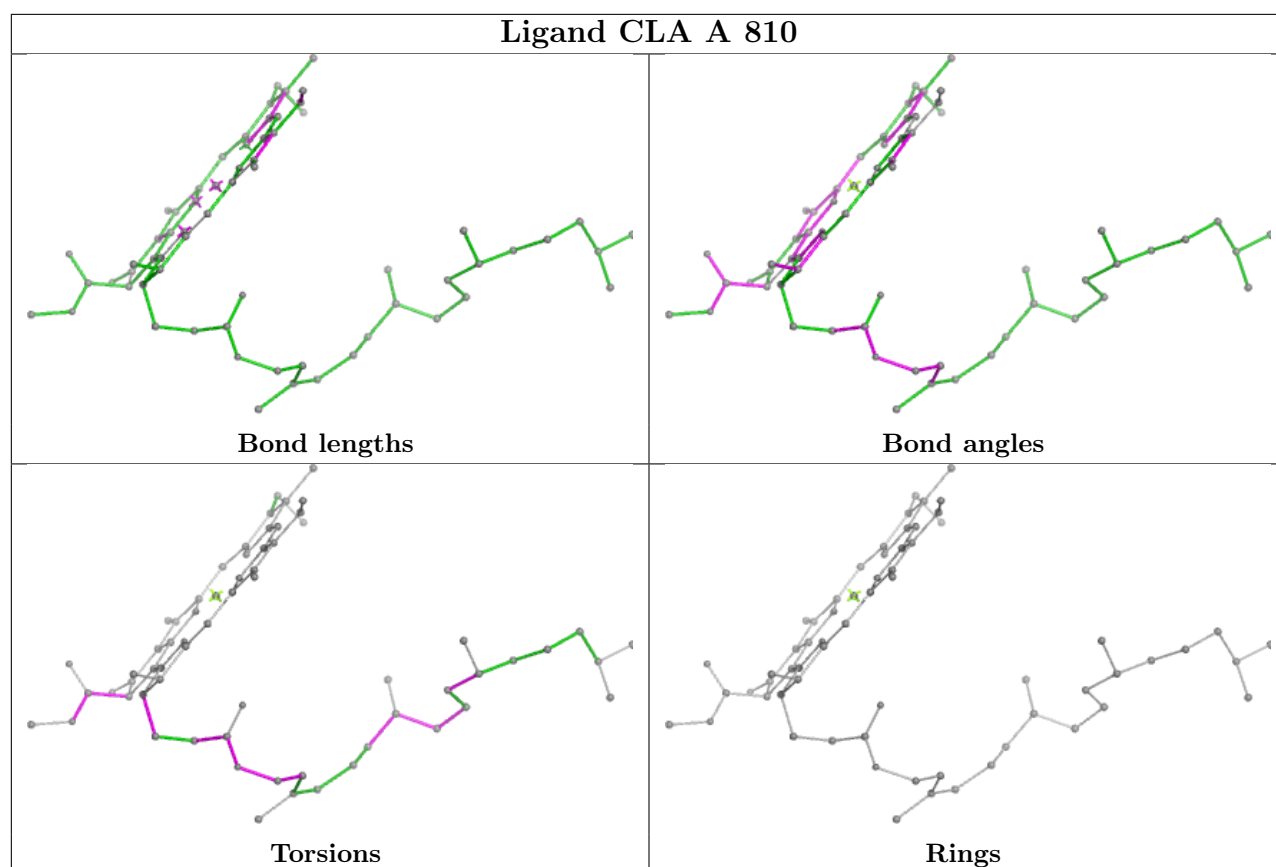




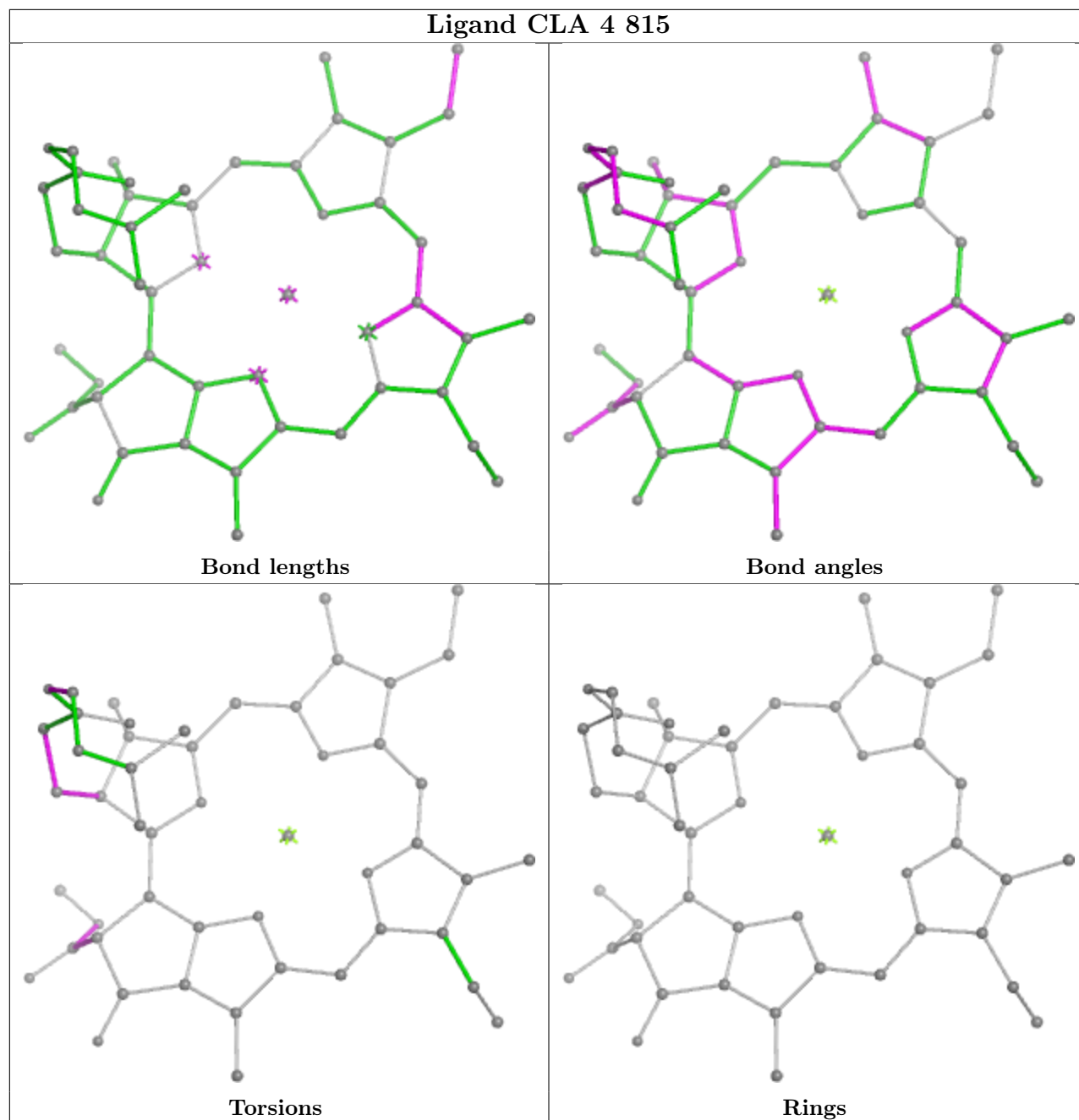


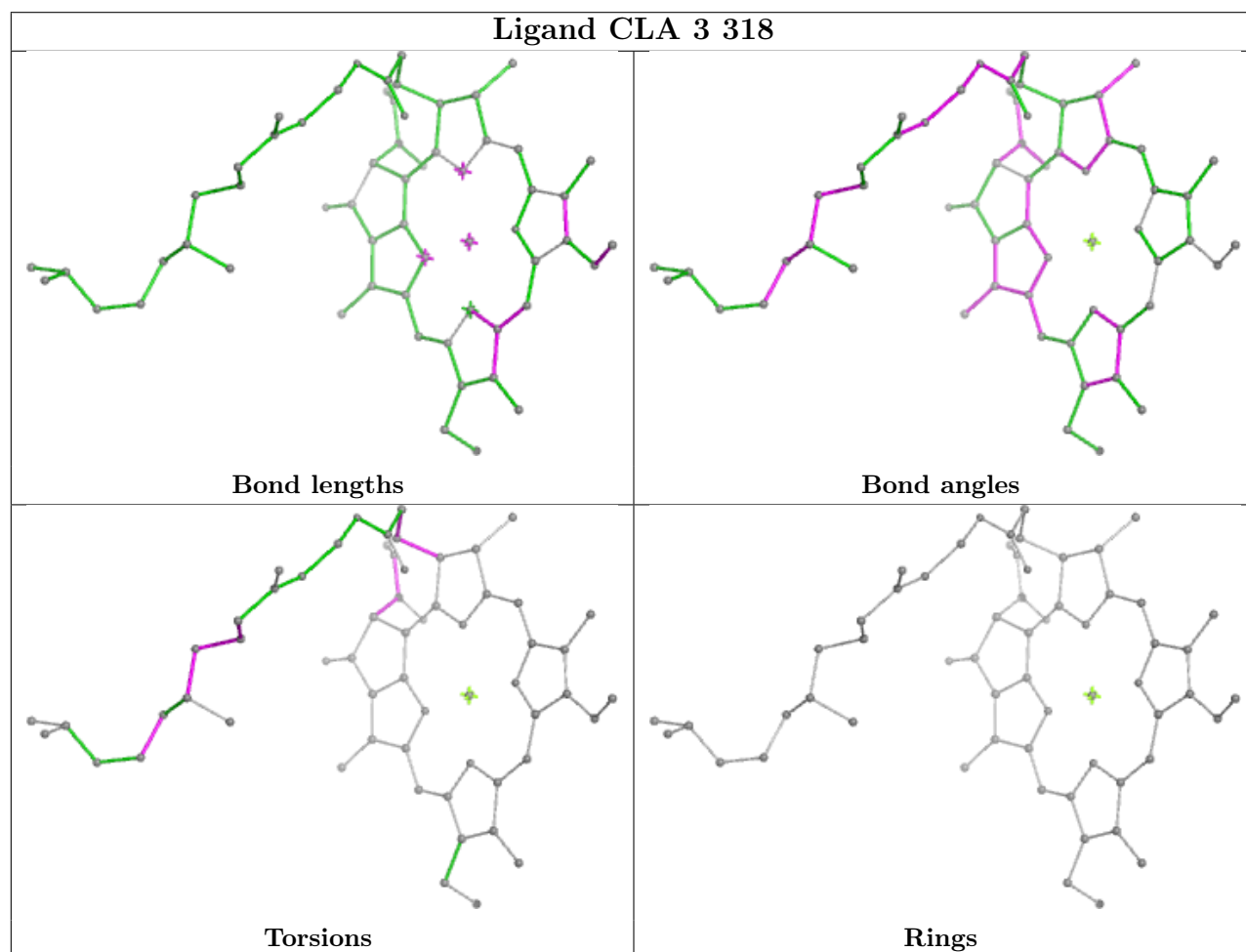
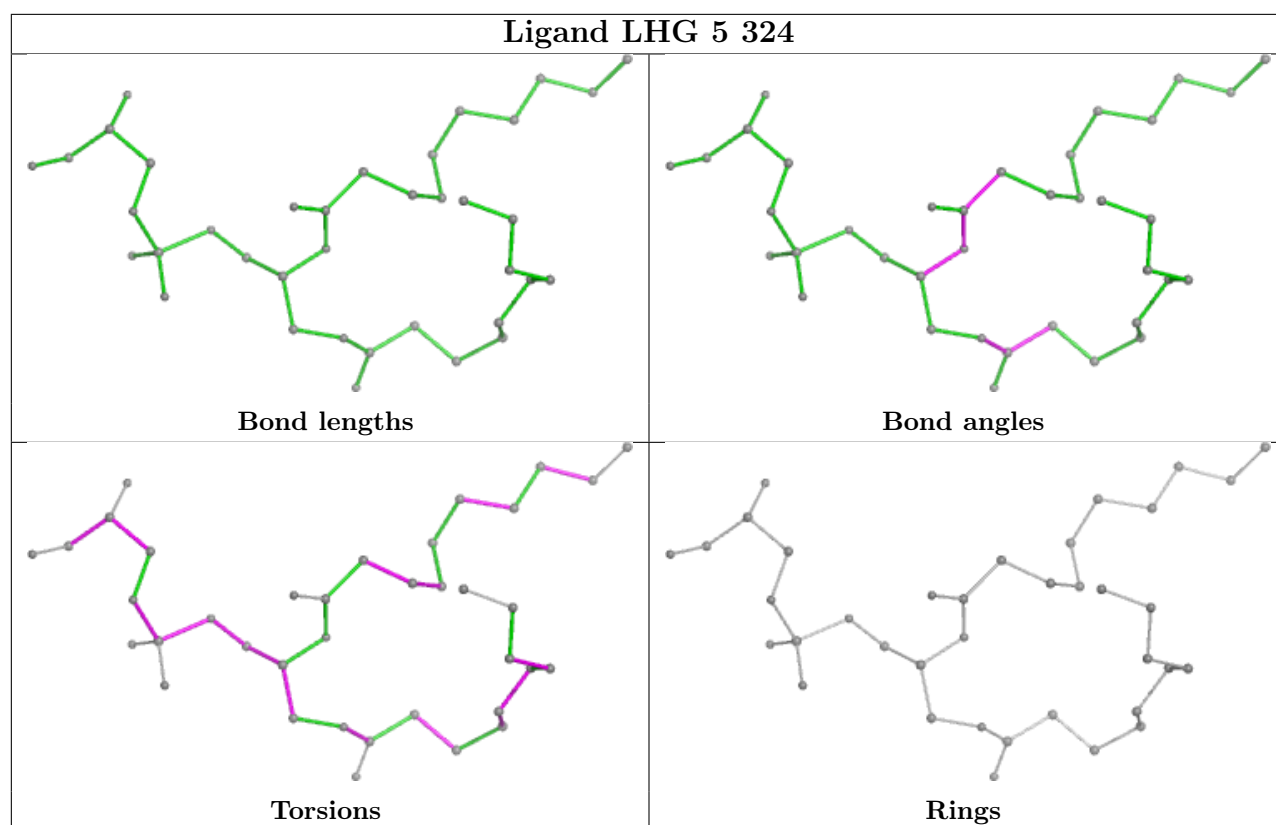
Ligand CLA 7 322

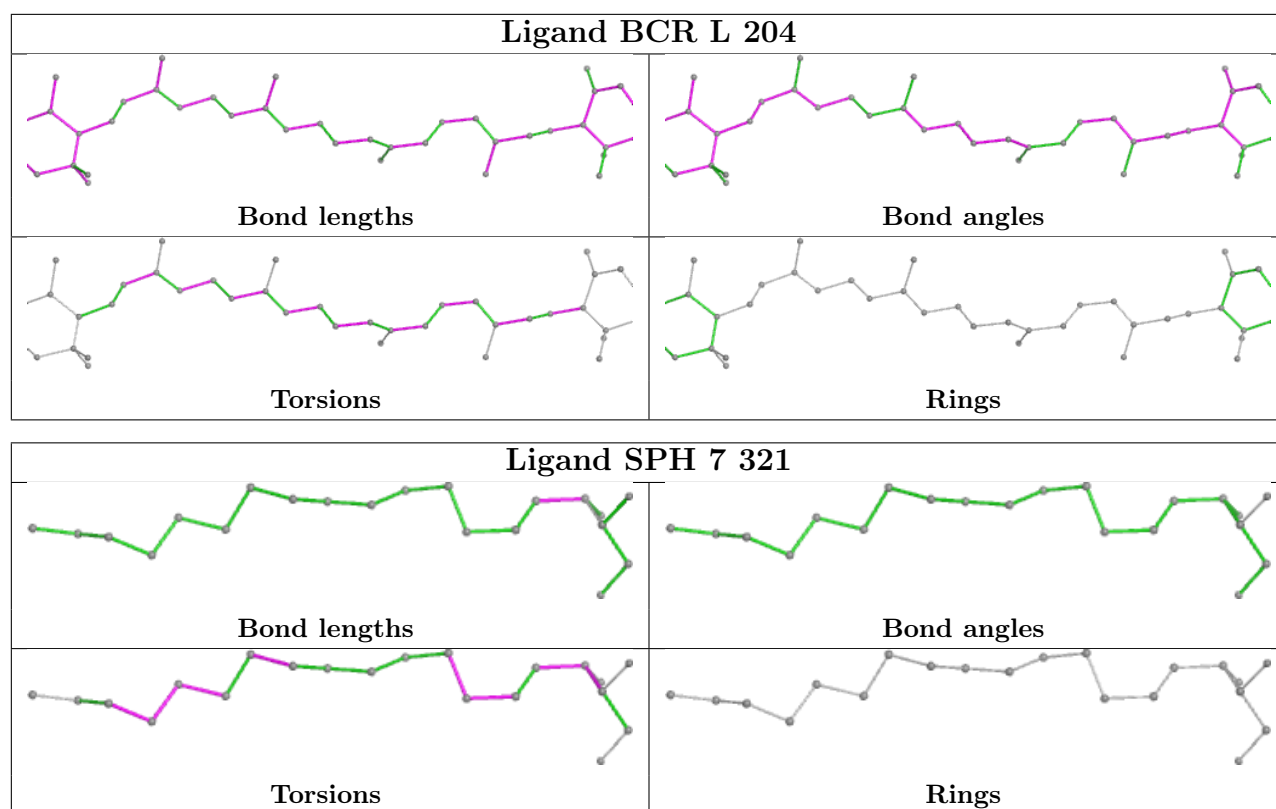




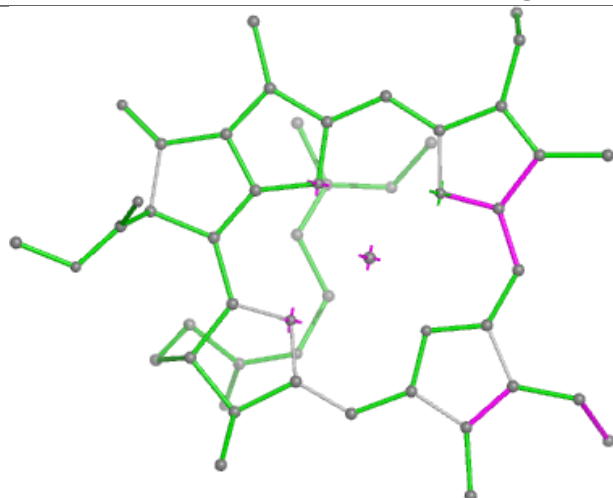
Ligand CLA 4 815



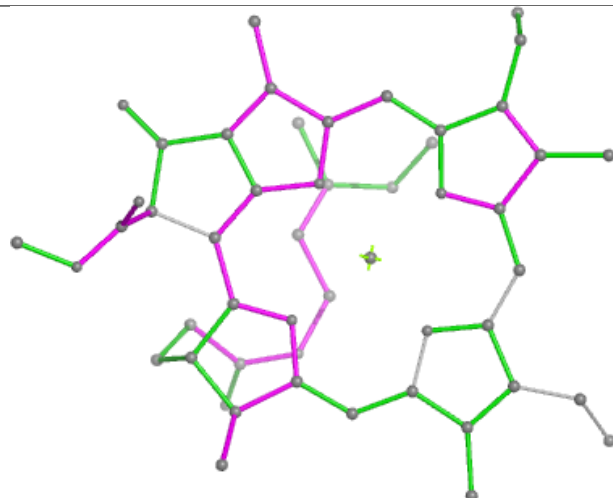




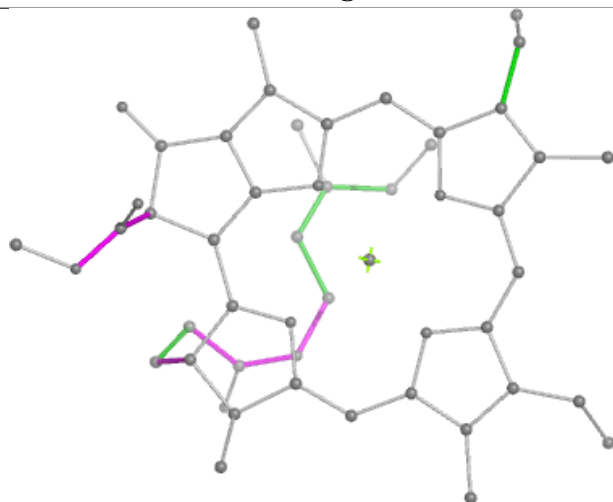
Ligand CLA 4 818



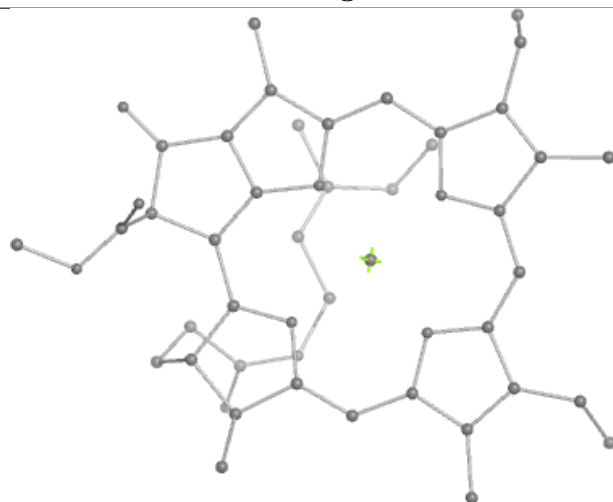
Bond lengths



Bond angles

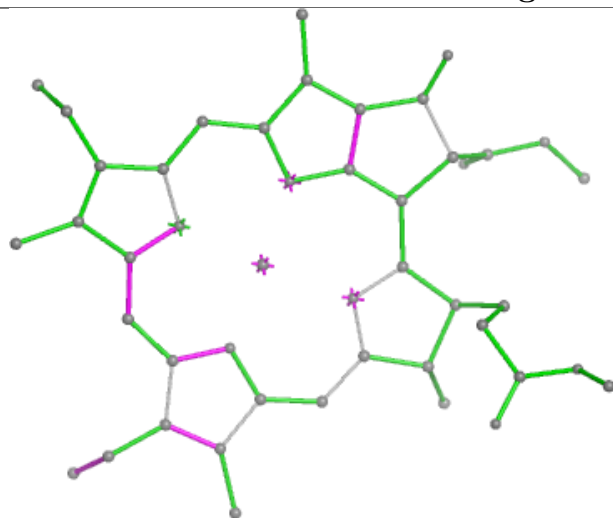


Torsions

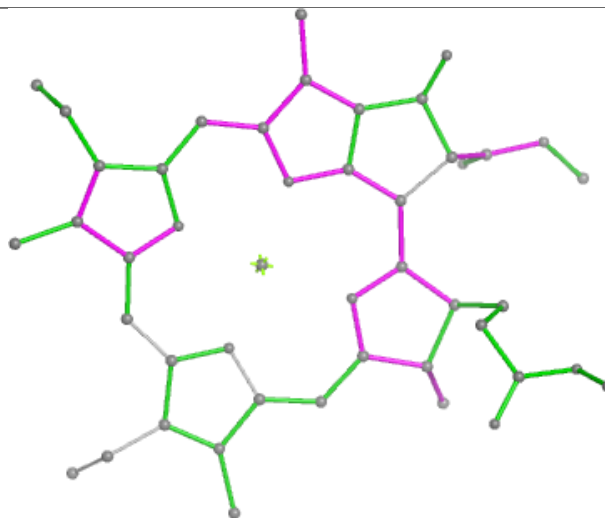


Rings

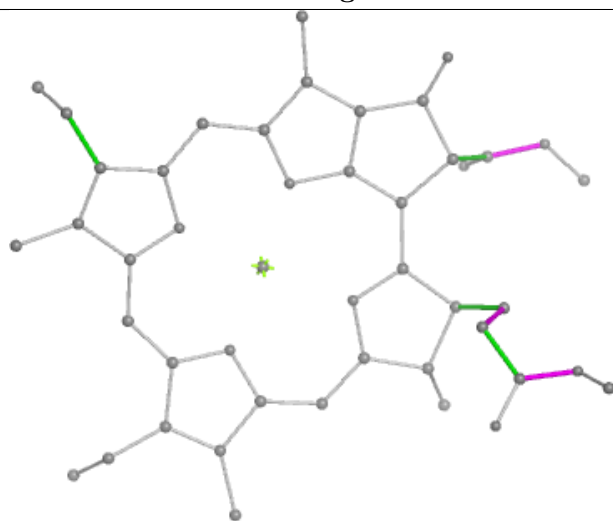
Ligand CLA 3 320



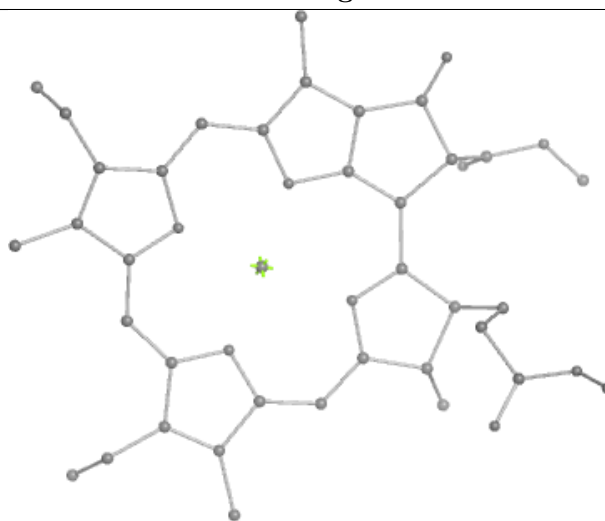
Bond lengths



Bond angles

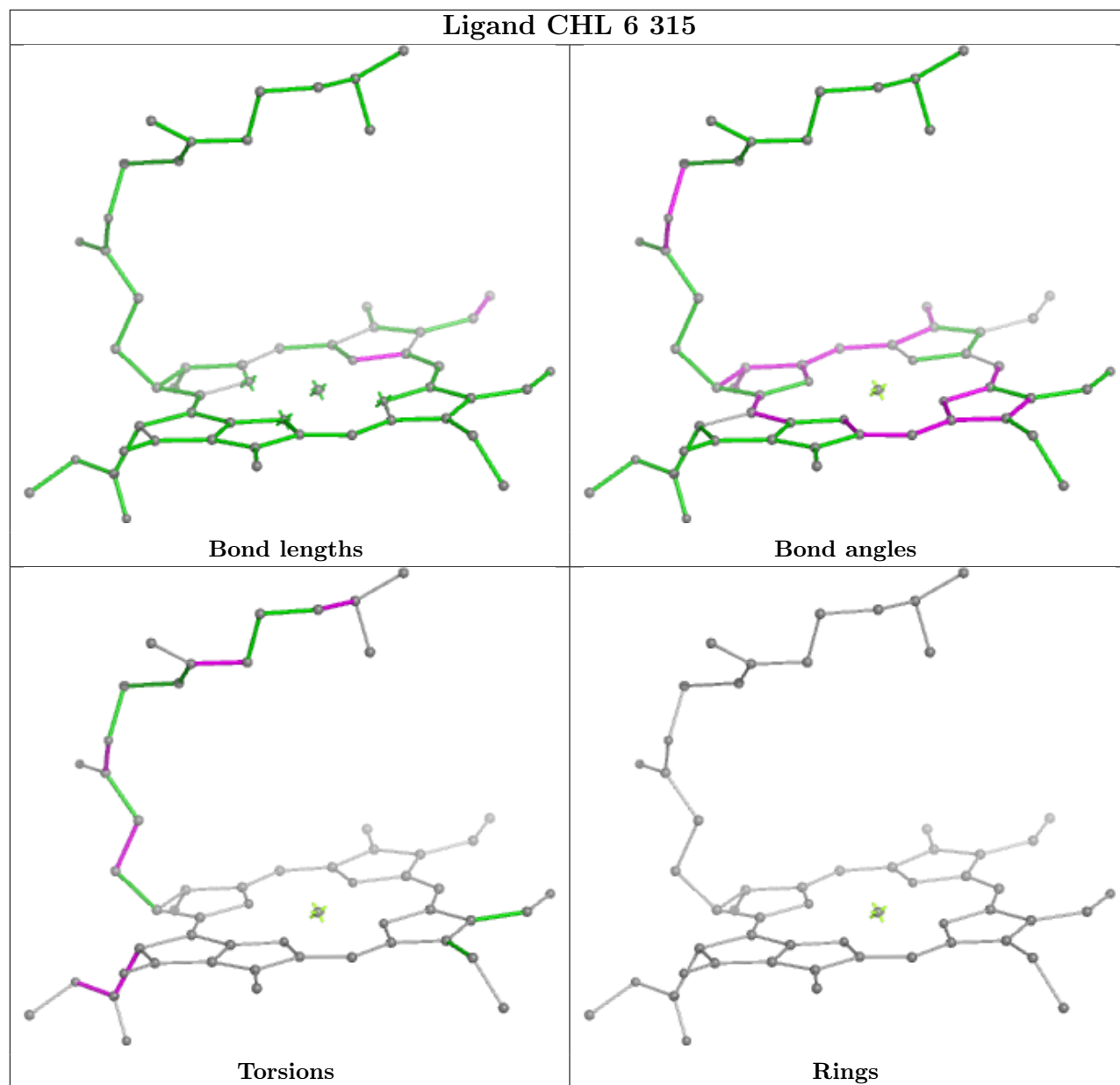


Torsions

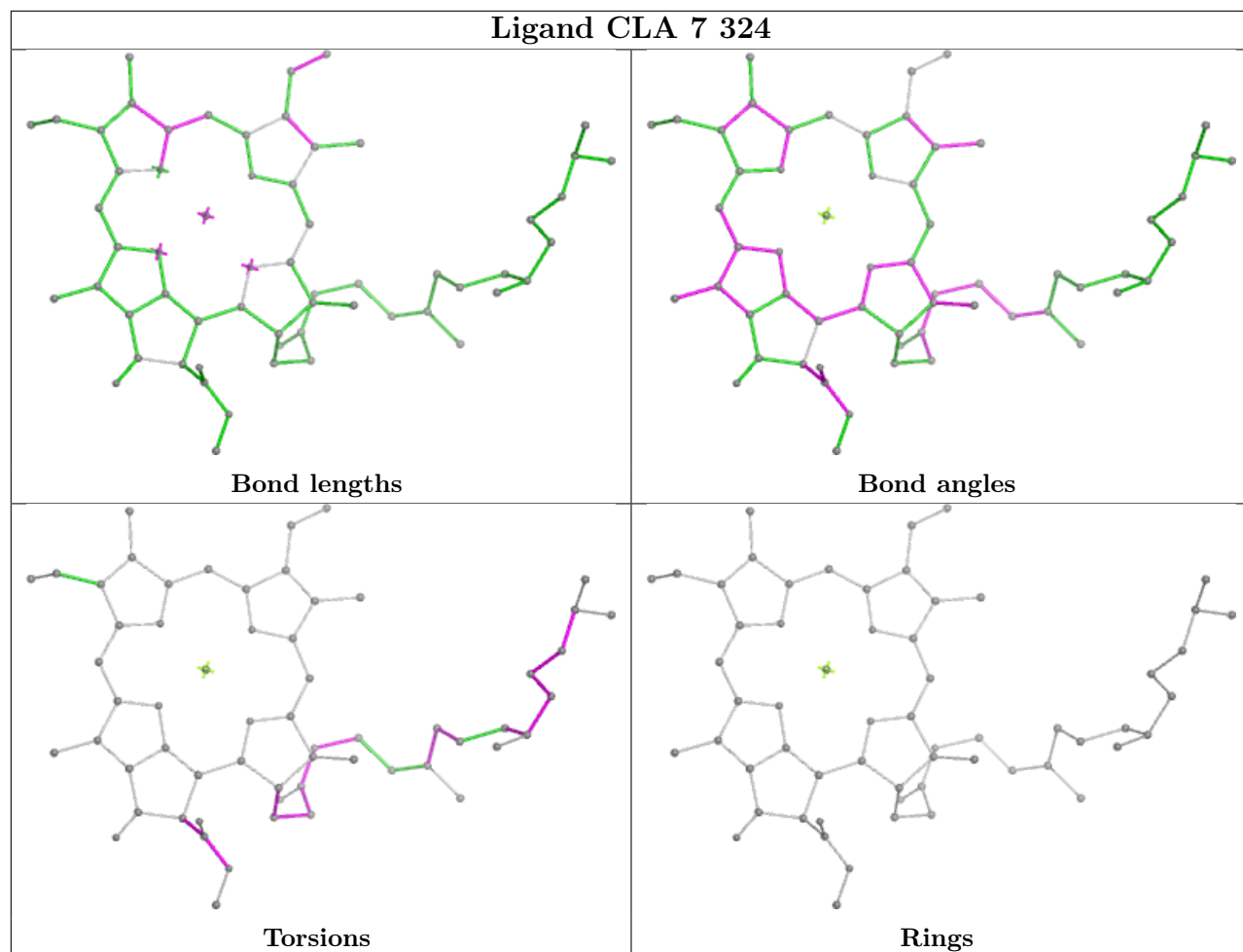


Rings

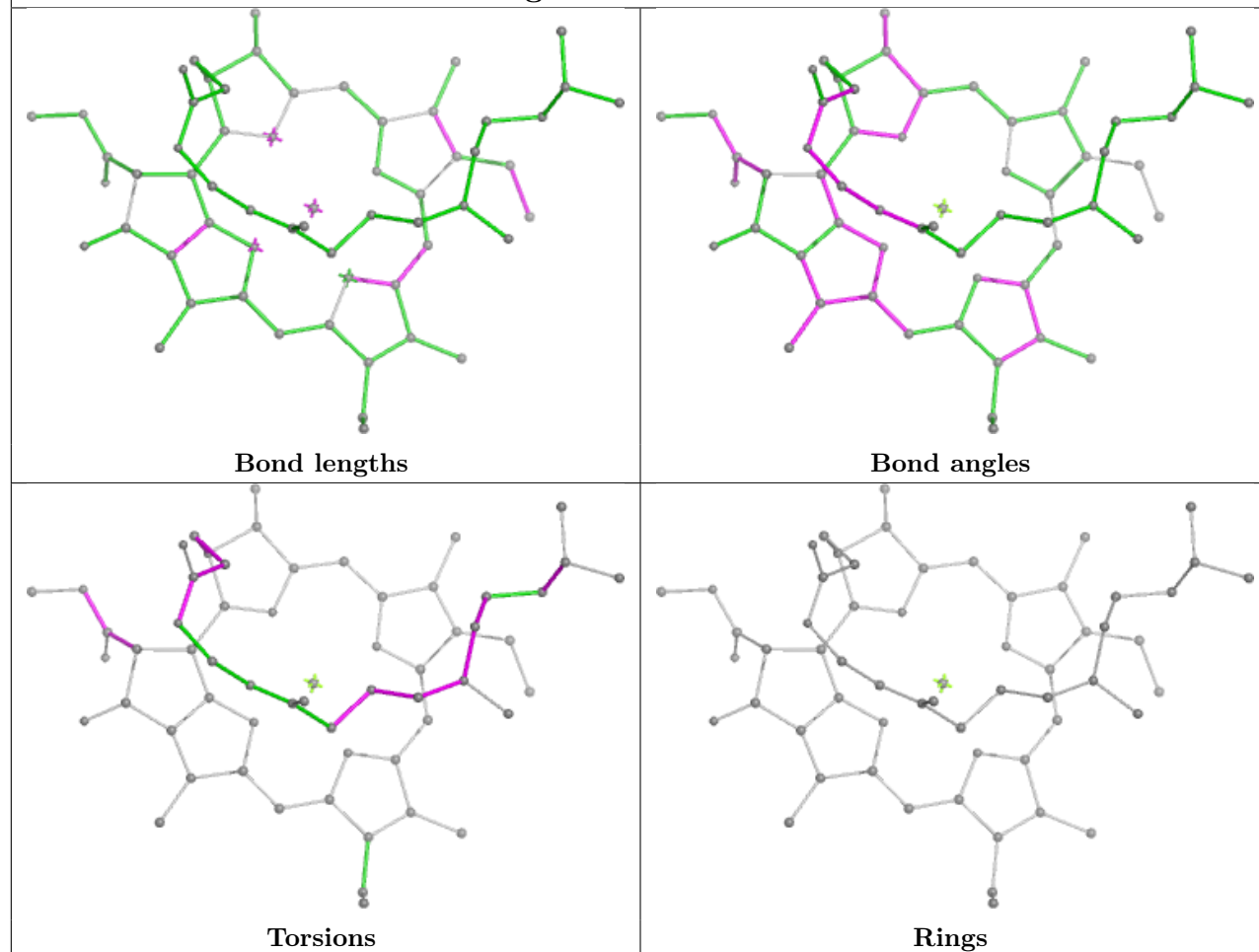
Ligand CHL 6 315



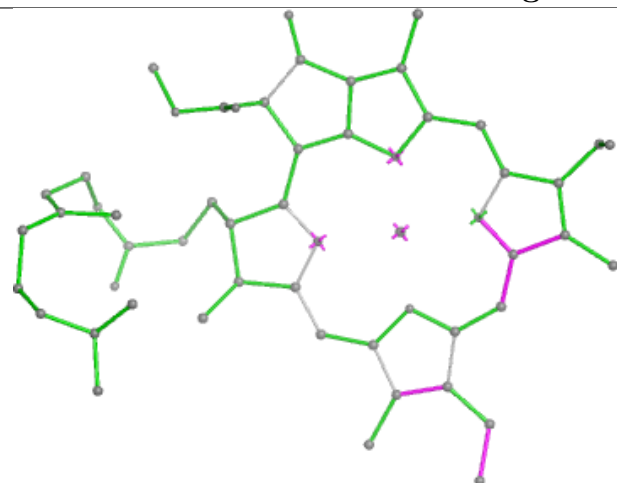
Ligand CLA 7 324



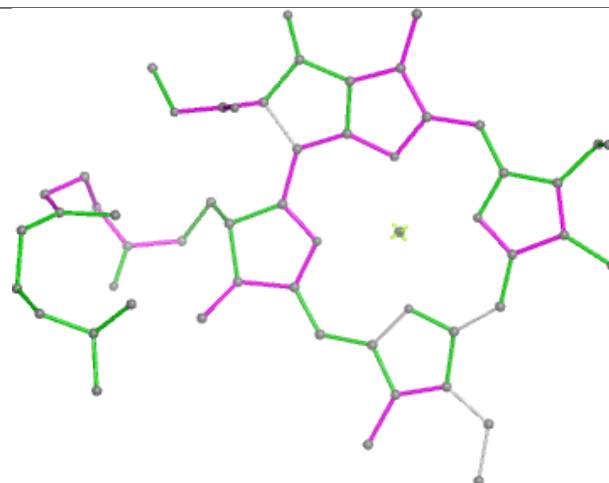
Ligand CLA B 814



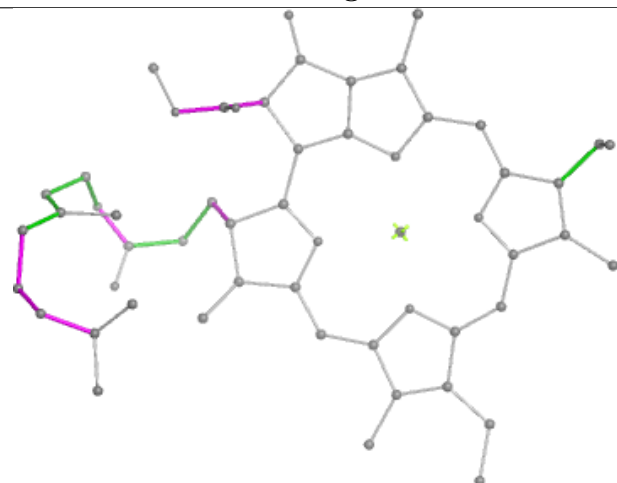
Ligand CLA 6 311



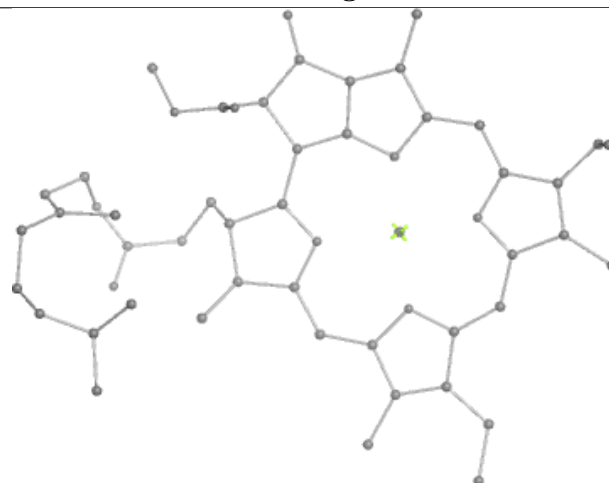
Bond lengths



Bond angles

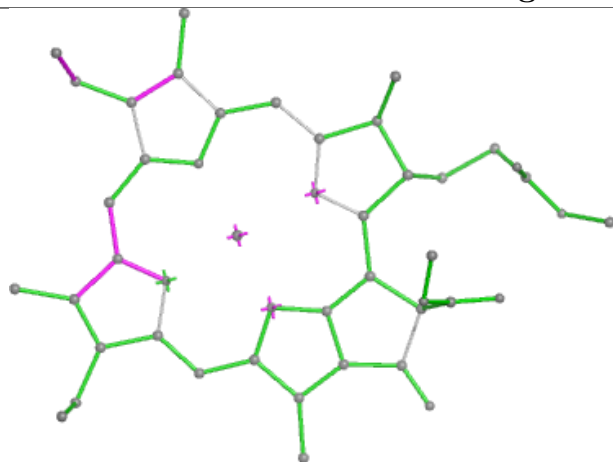


Torsions

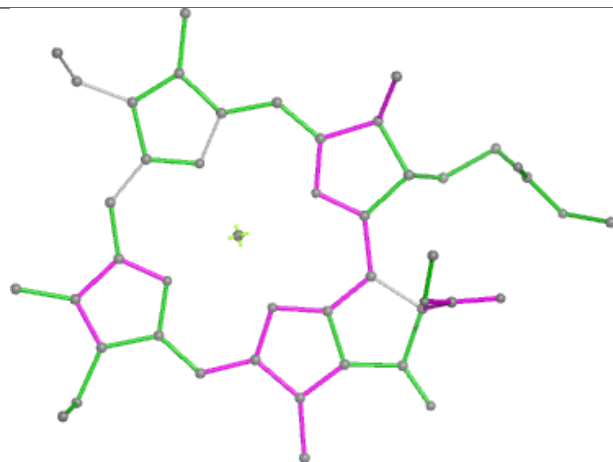


Rings

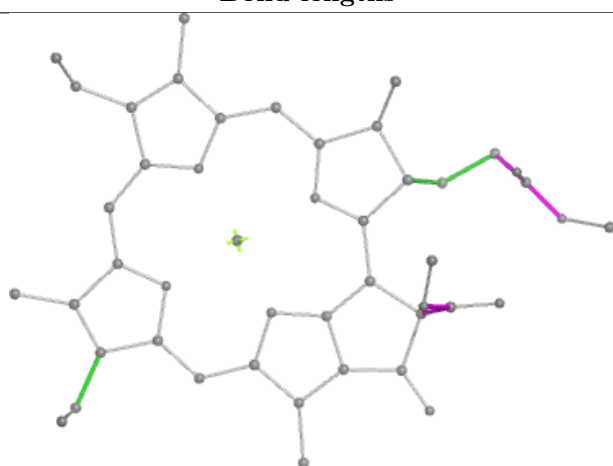
Ligand CLA 5 323



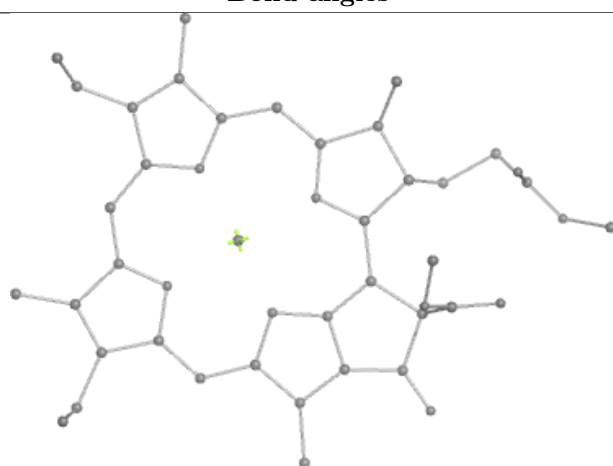
Bond lengths



Bond angles

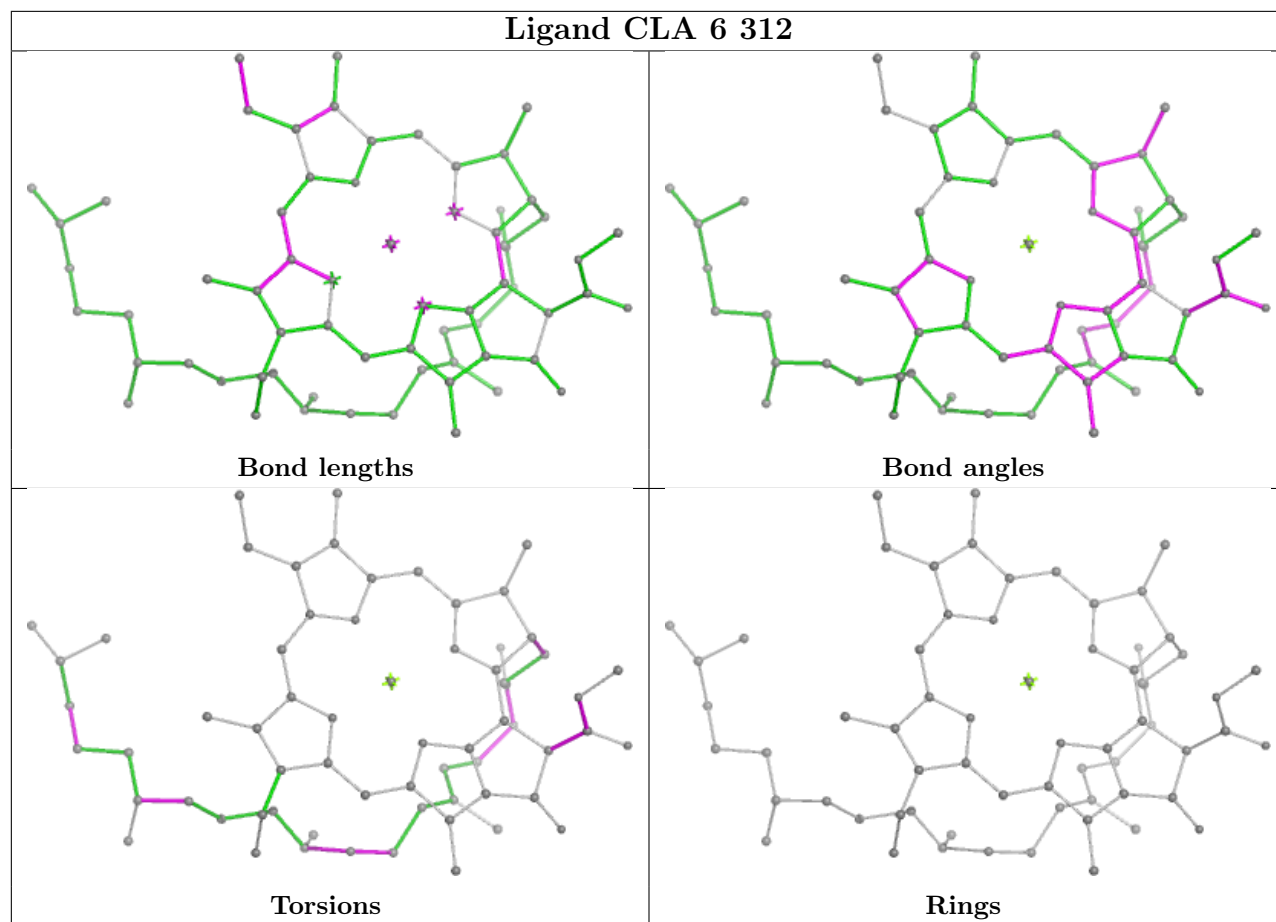


Torsions

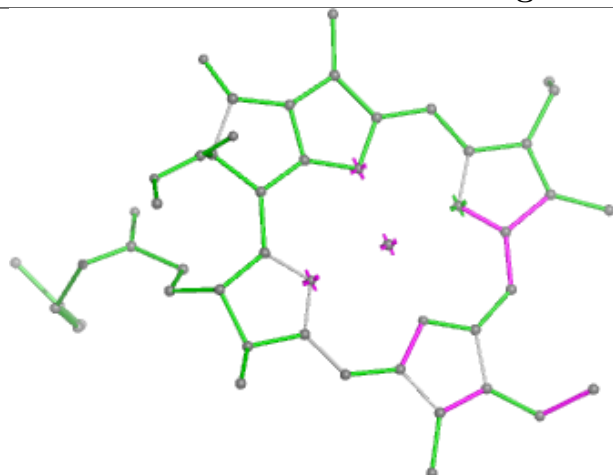


Rings

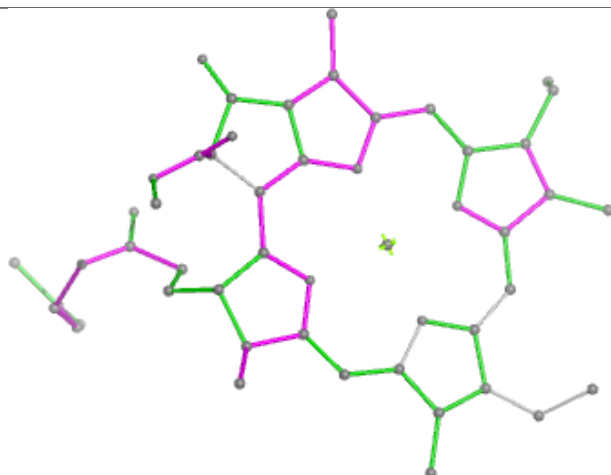
Ligand CLA 6 312



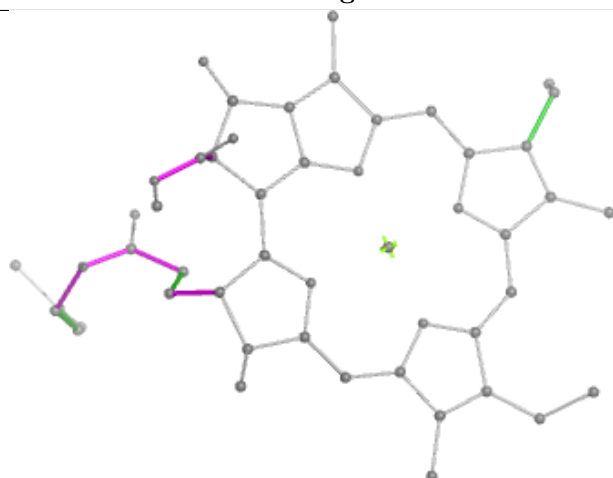
Ligand CLA Z 310



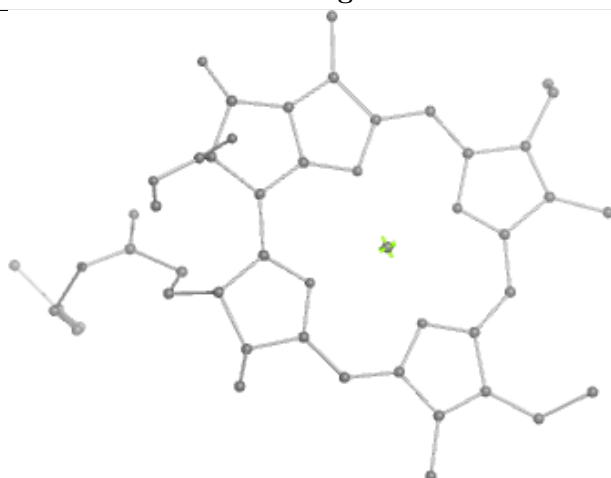
Bond lengths



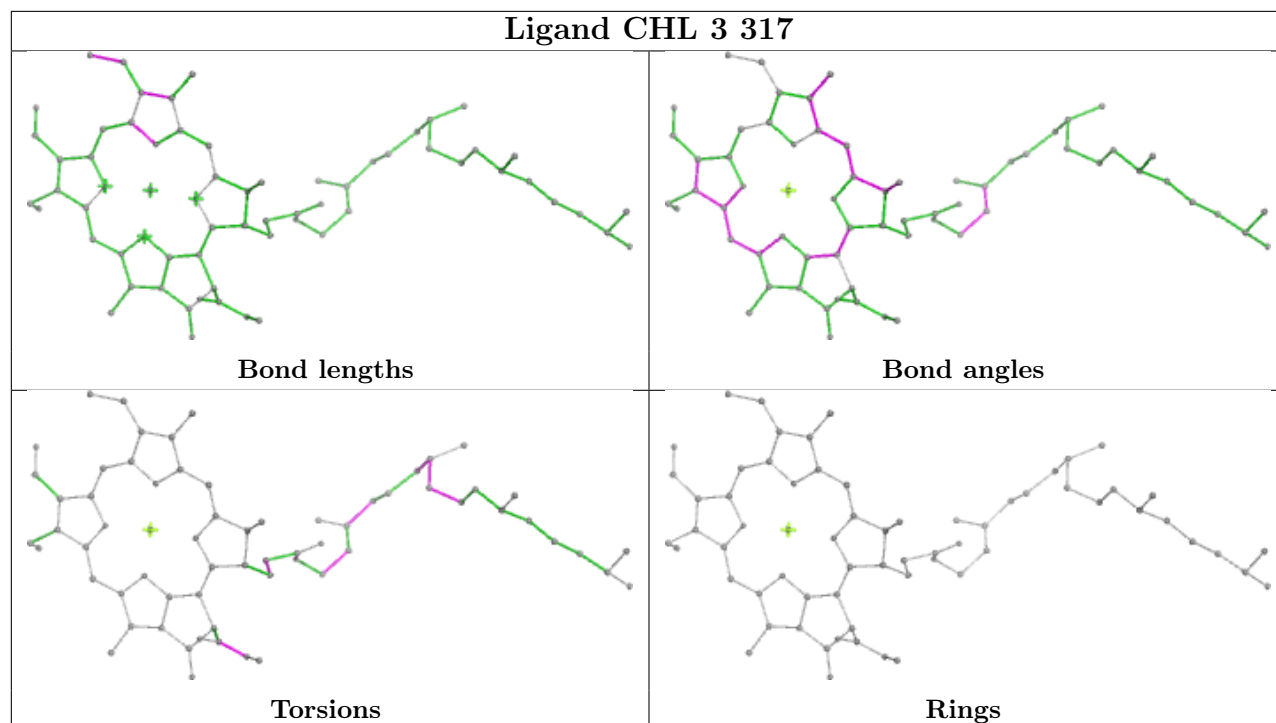
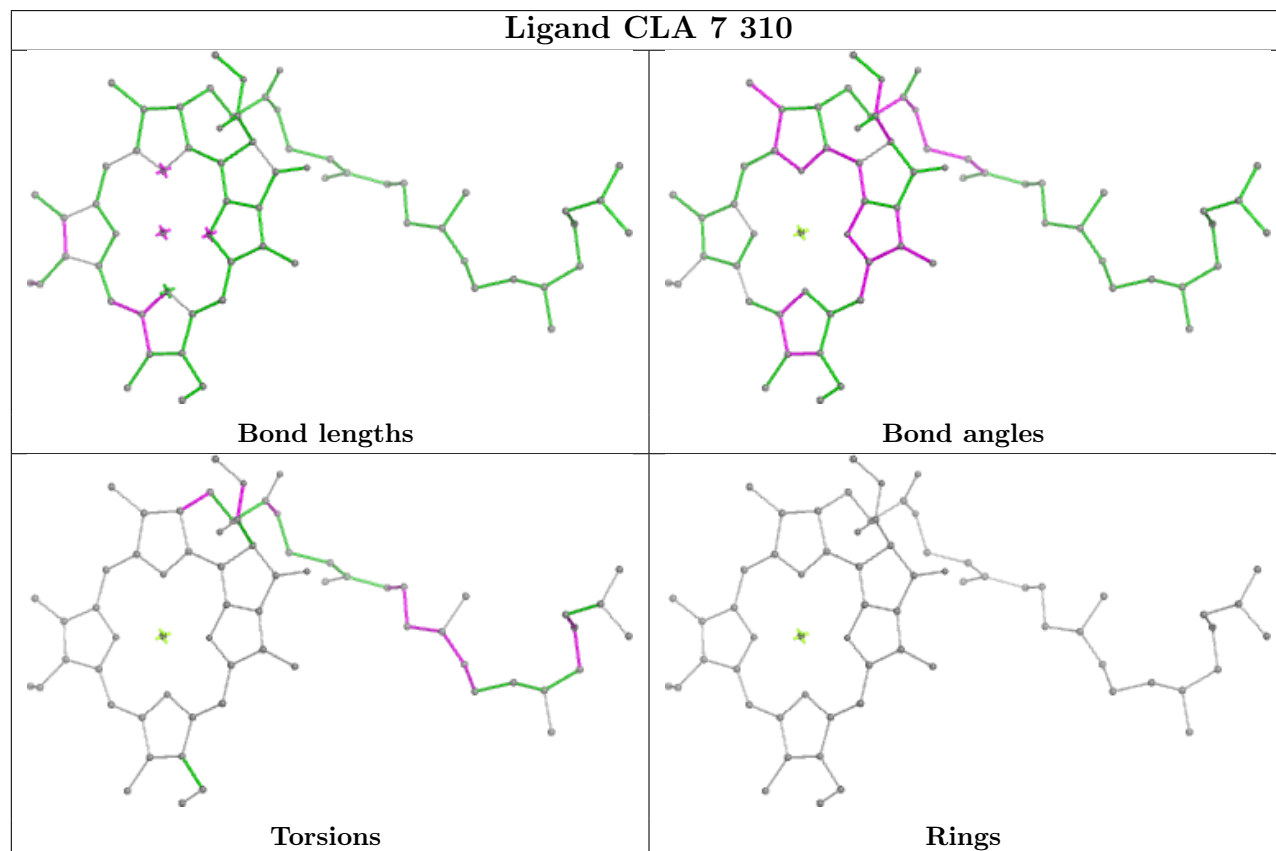
Bond angles

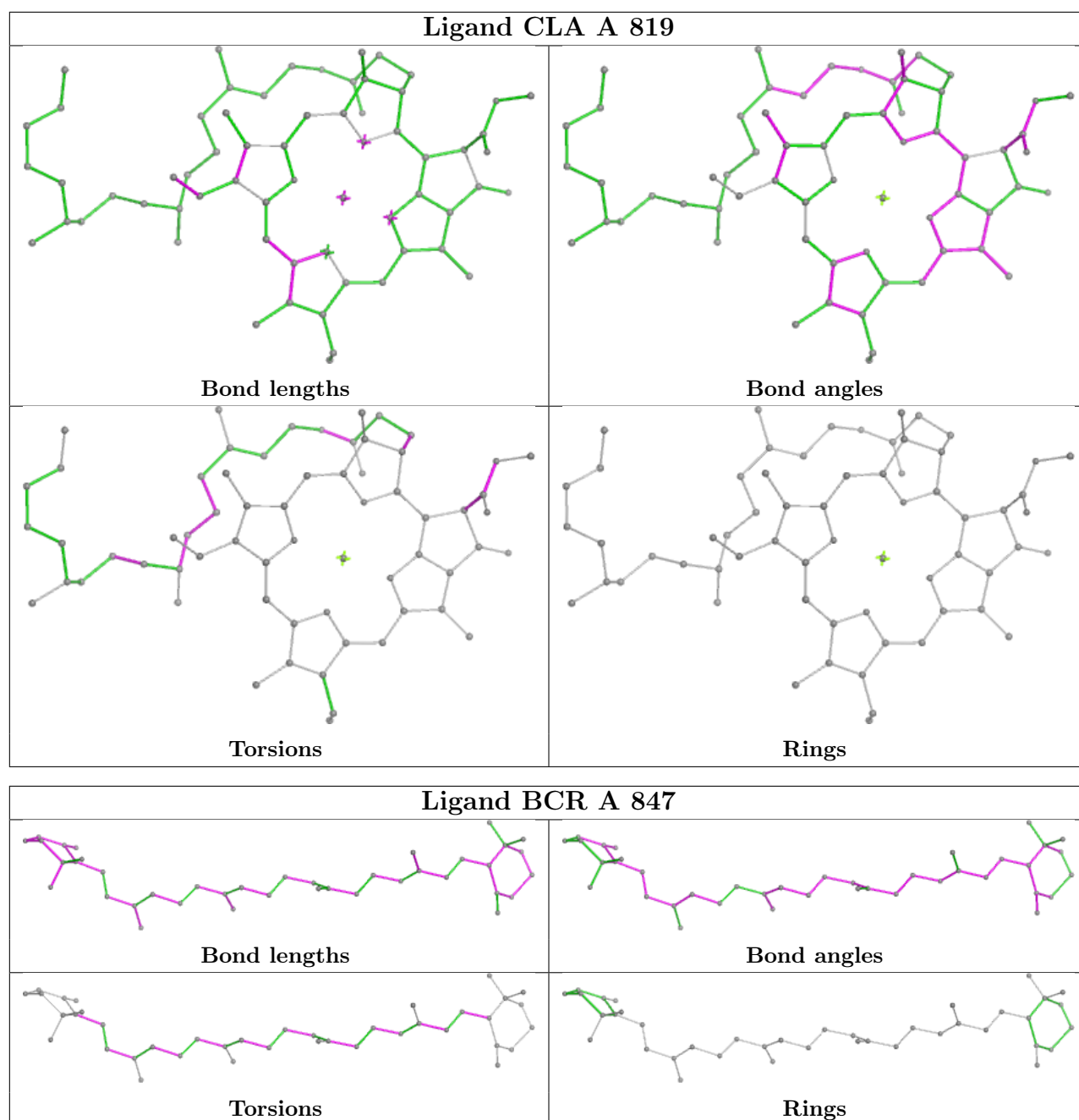


Torsions

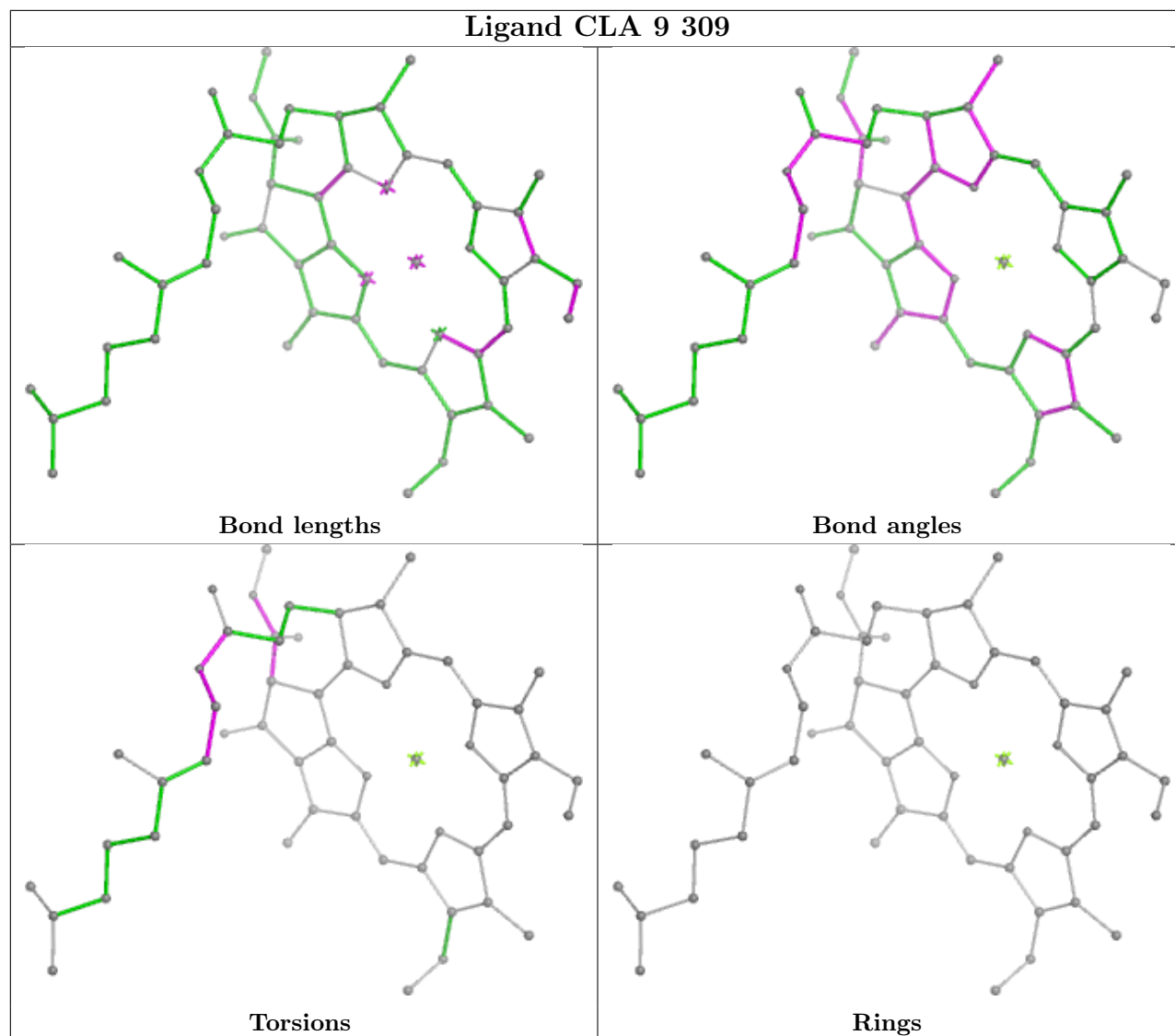


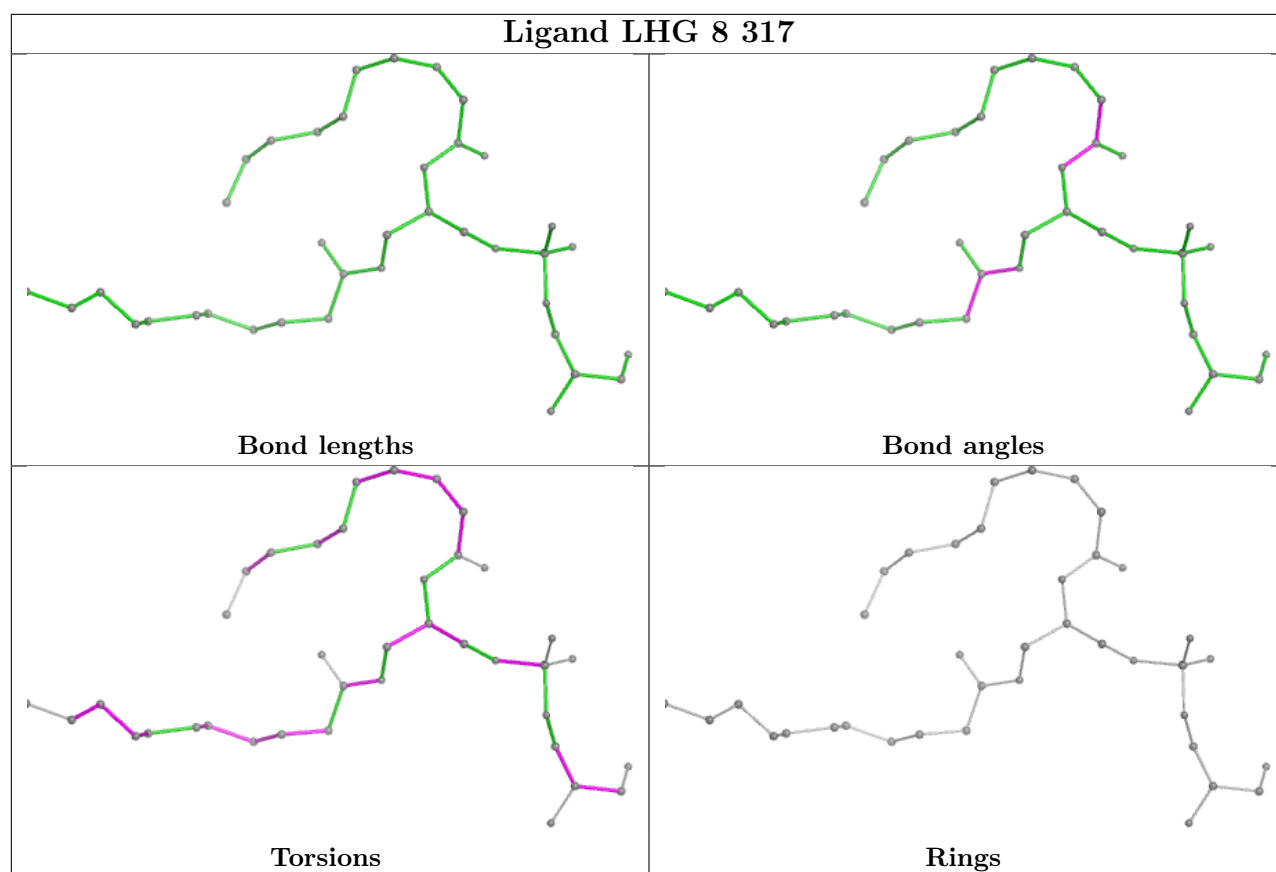
Rings

Ligand CHL 3 317**Ligand CLA 7 310**

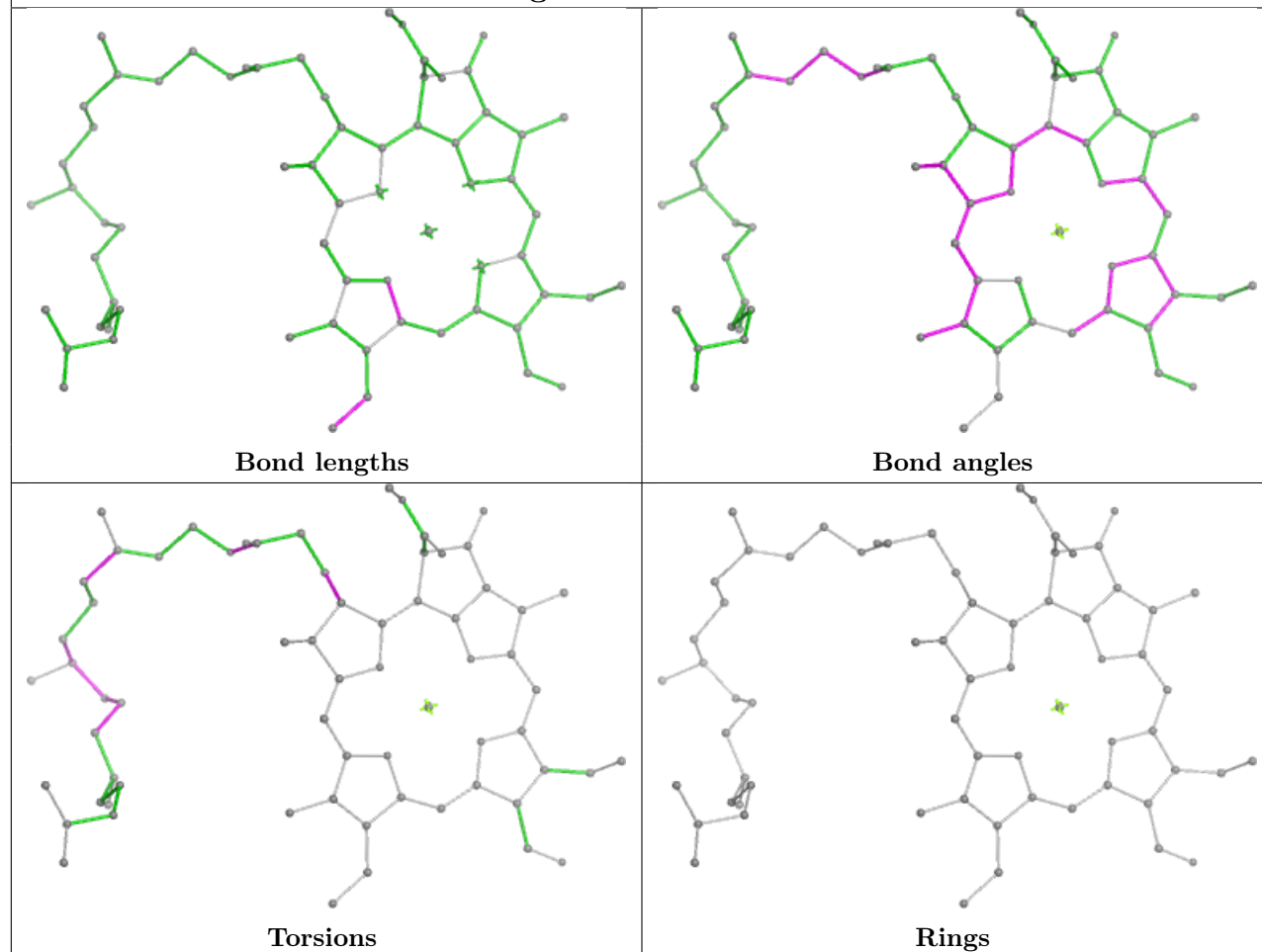


Ligand CLA 9 309

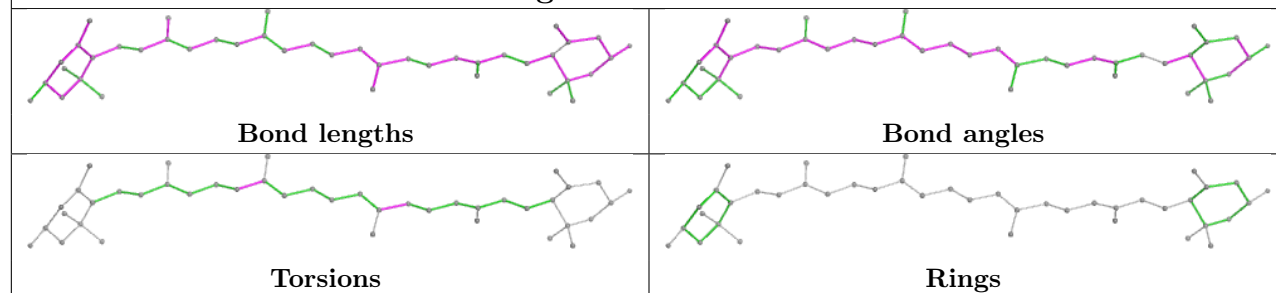




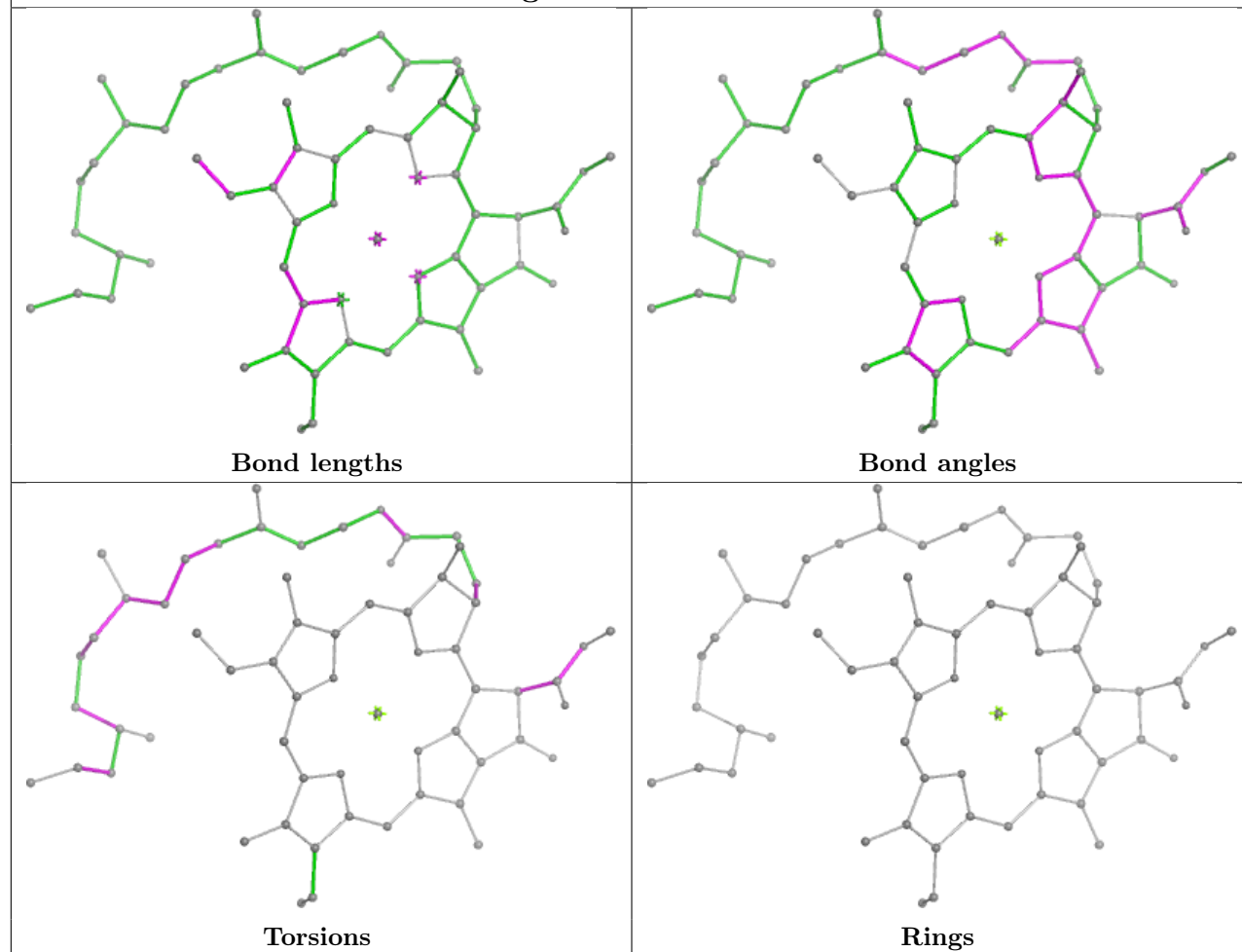
Ligand CHL 8 315



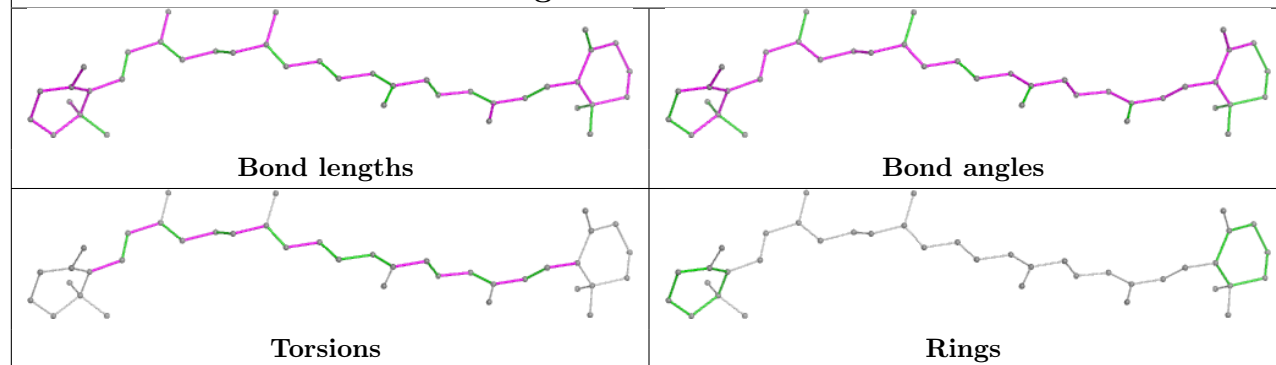
Ligand LUT 3 302



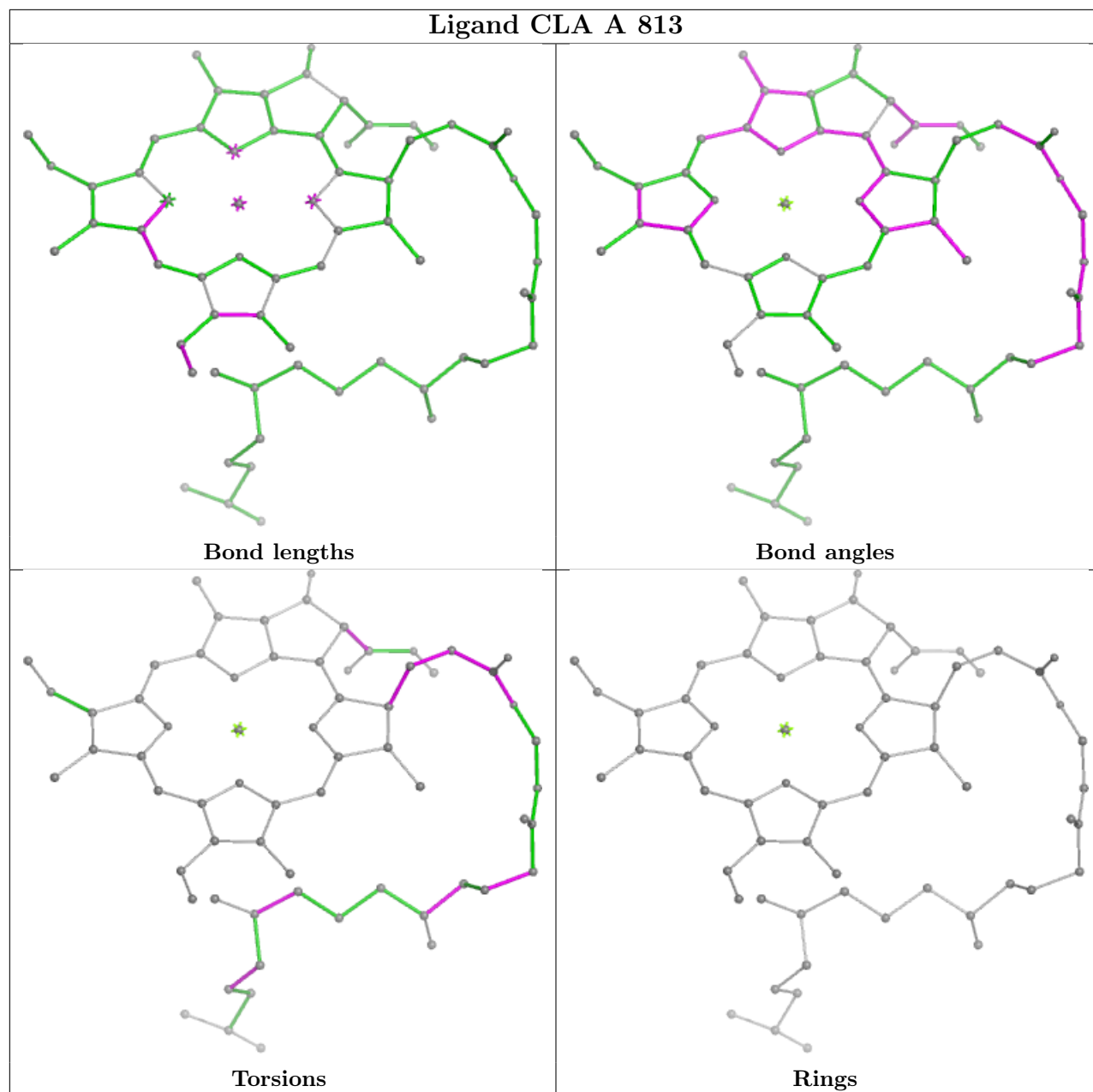
Ligand CLA 8 308

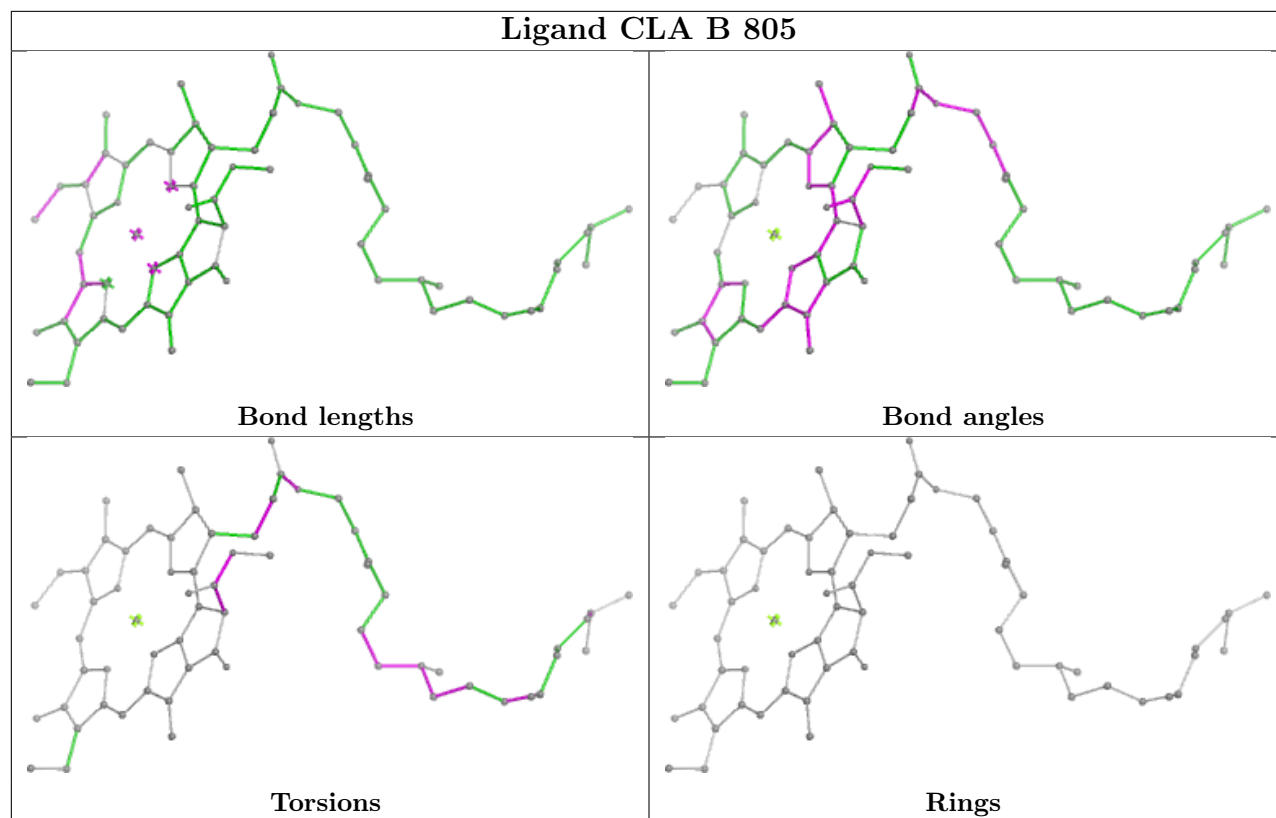


Ligand BCR 3 305

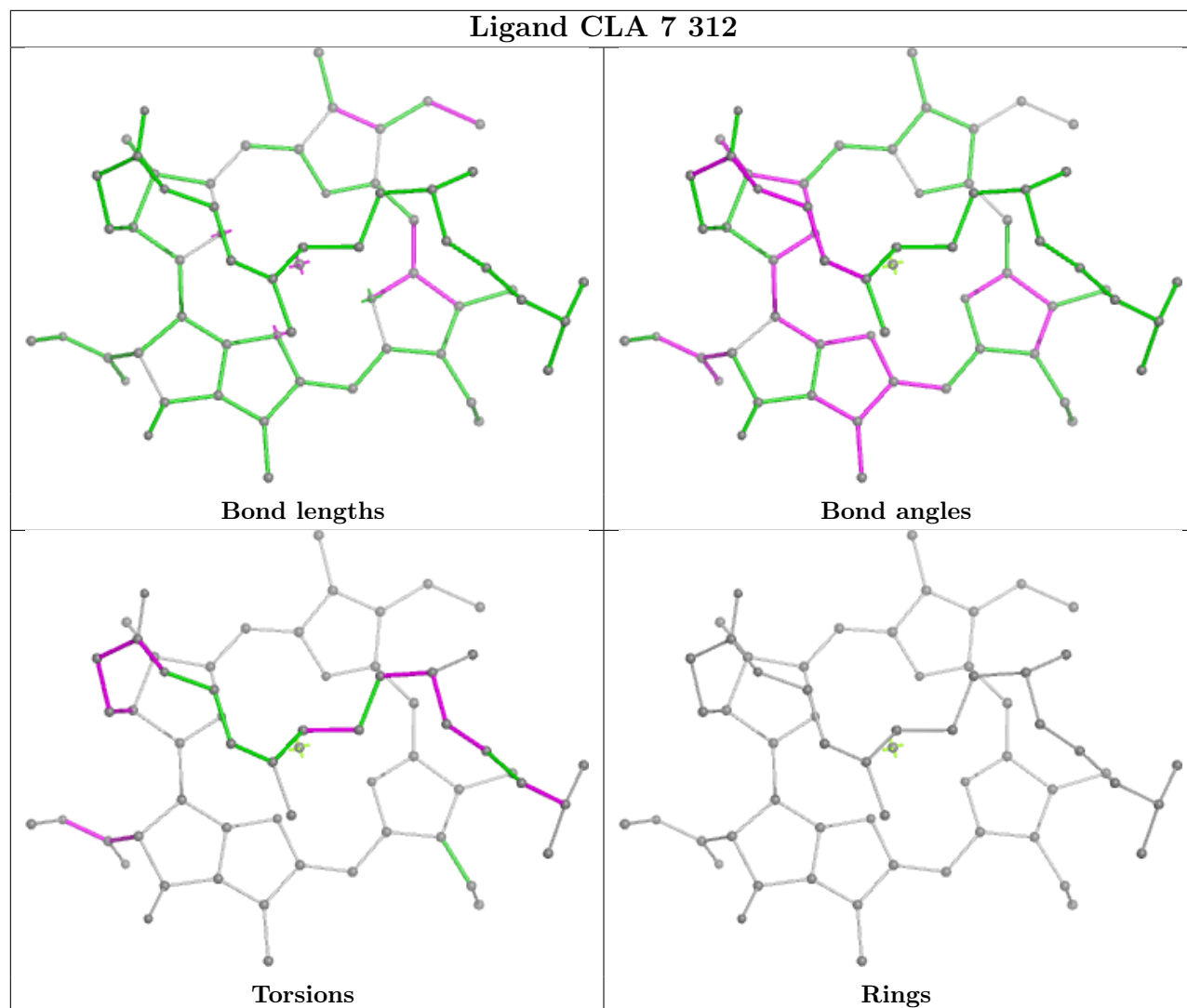


Ligand CLA A 813

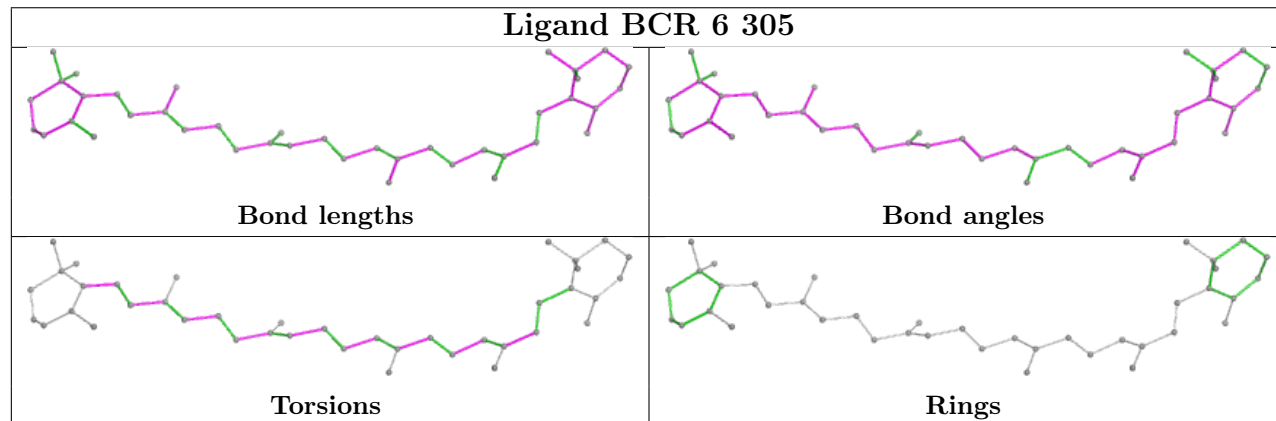


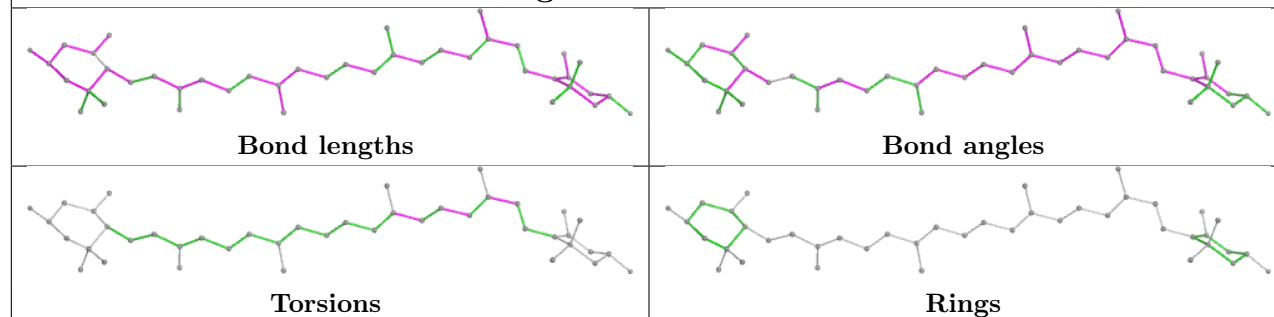
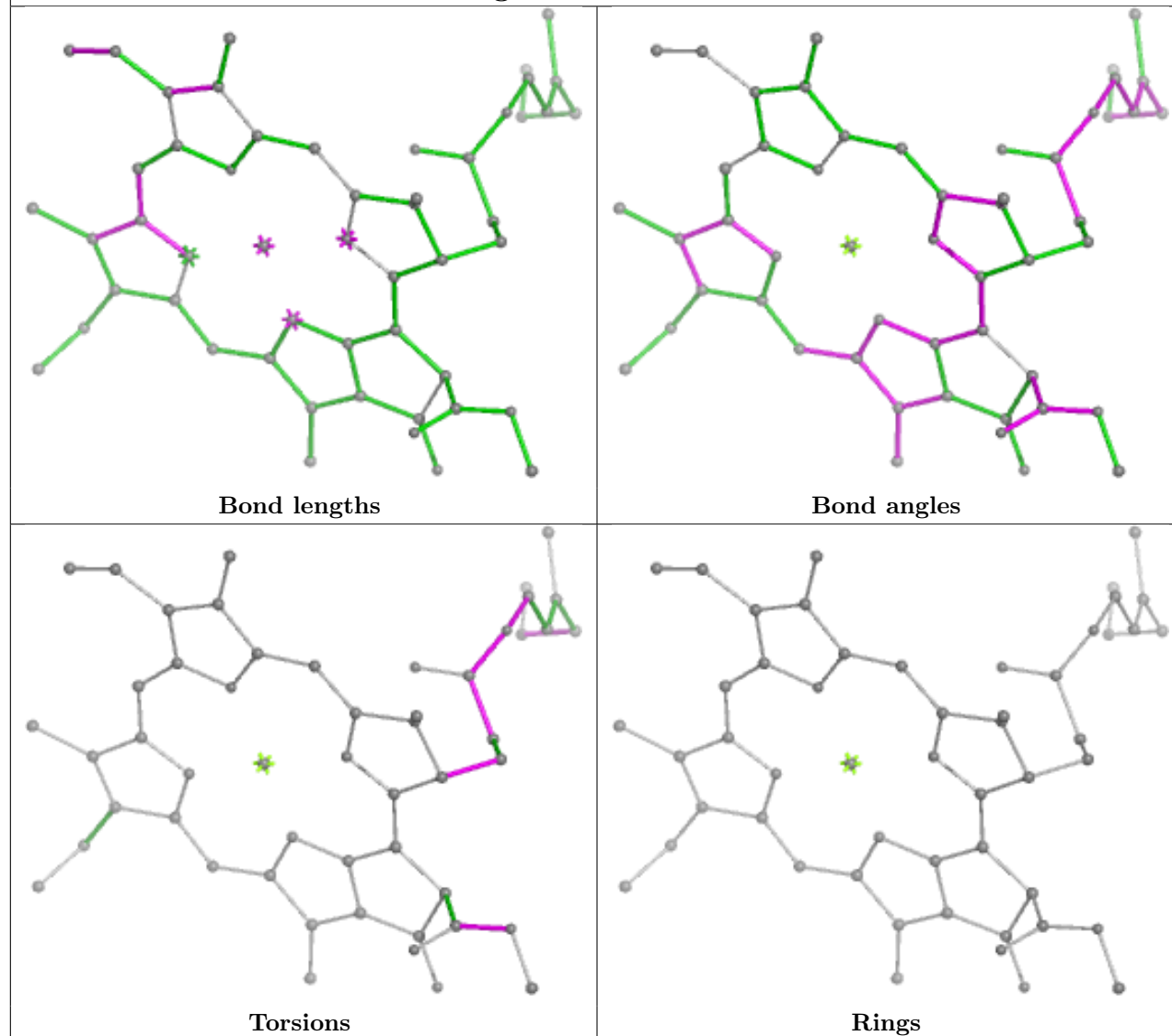


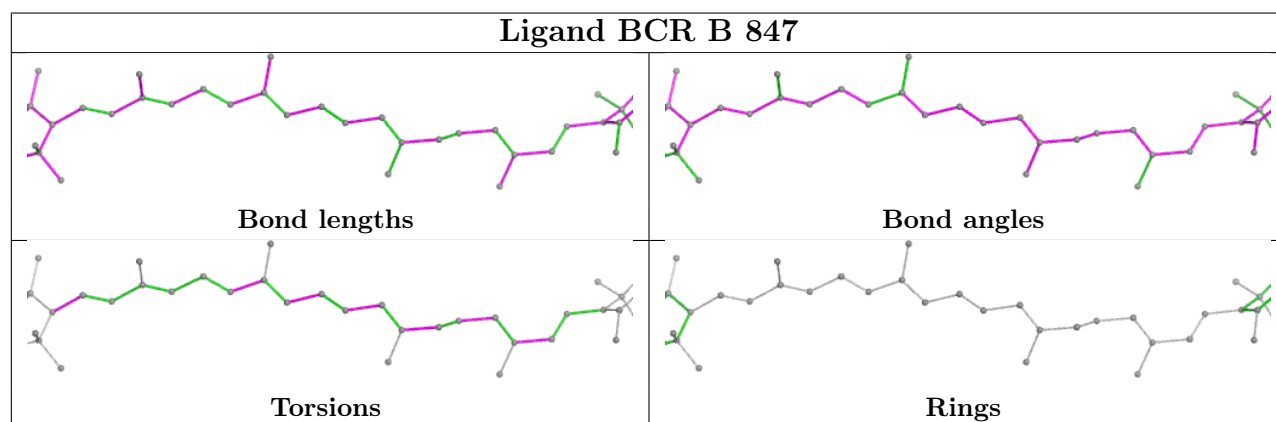
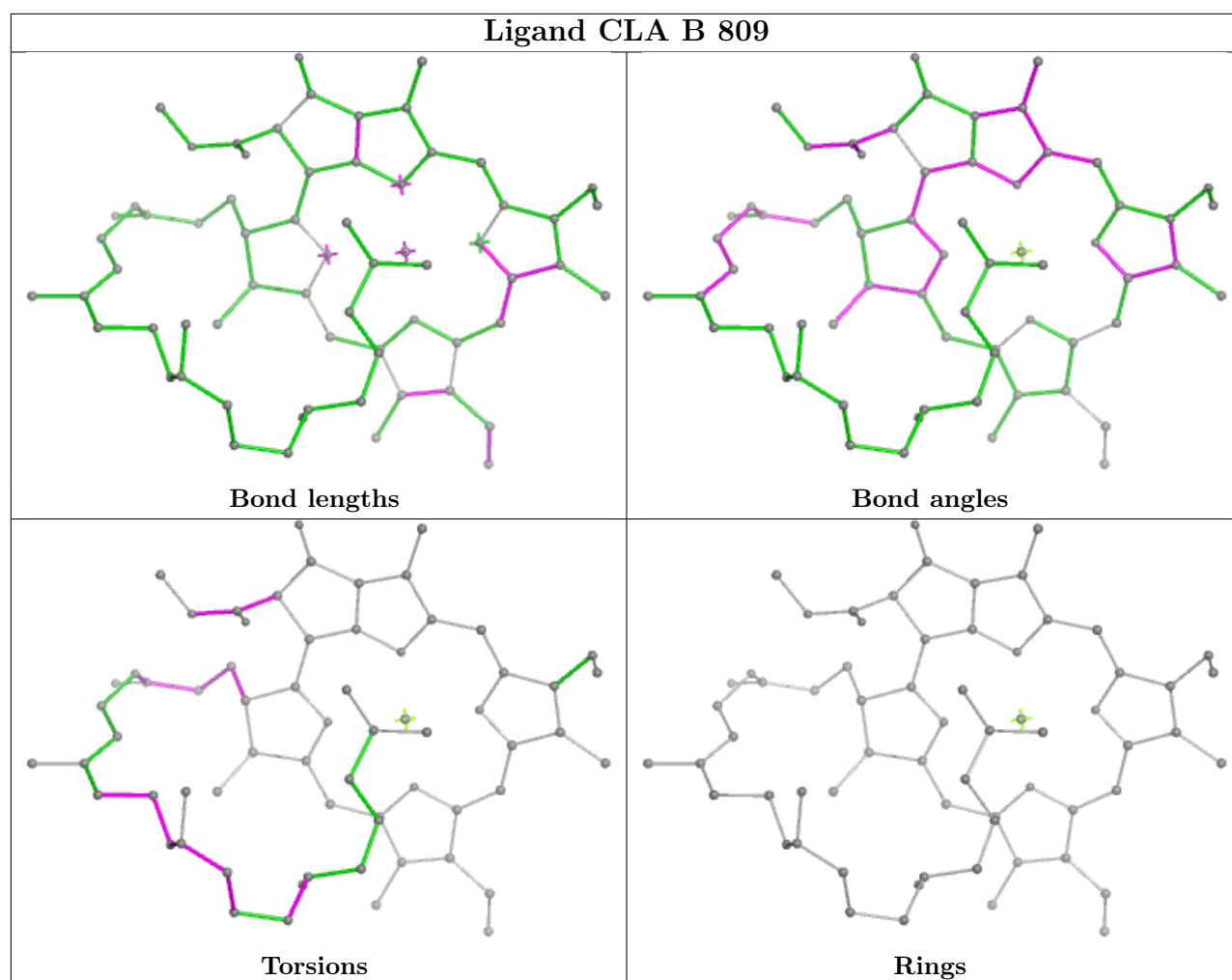
Ligand CLA 7 312

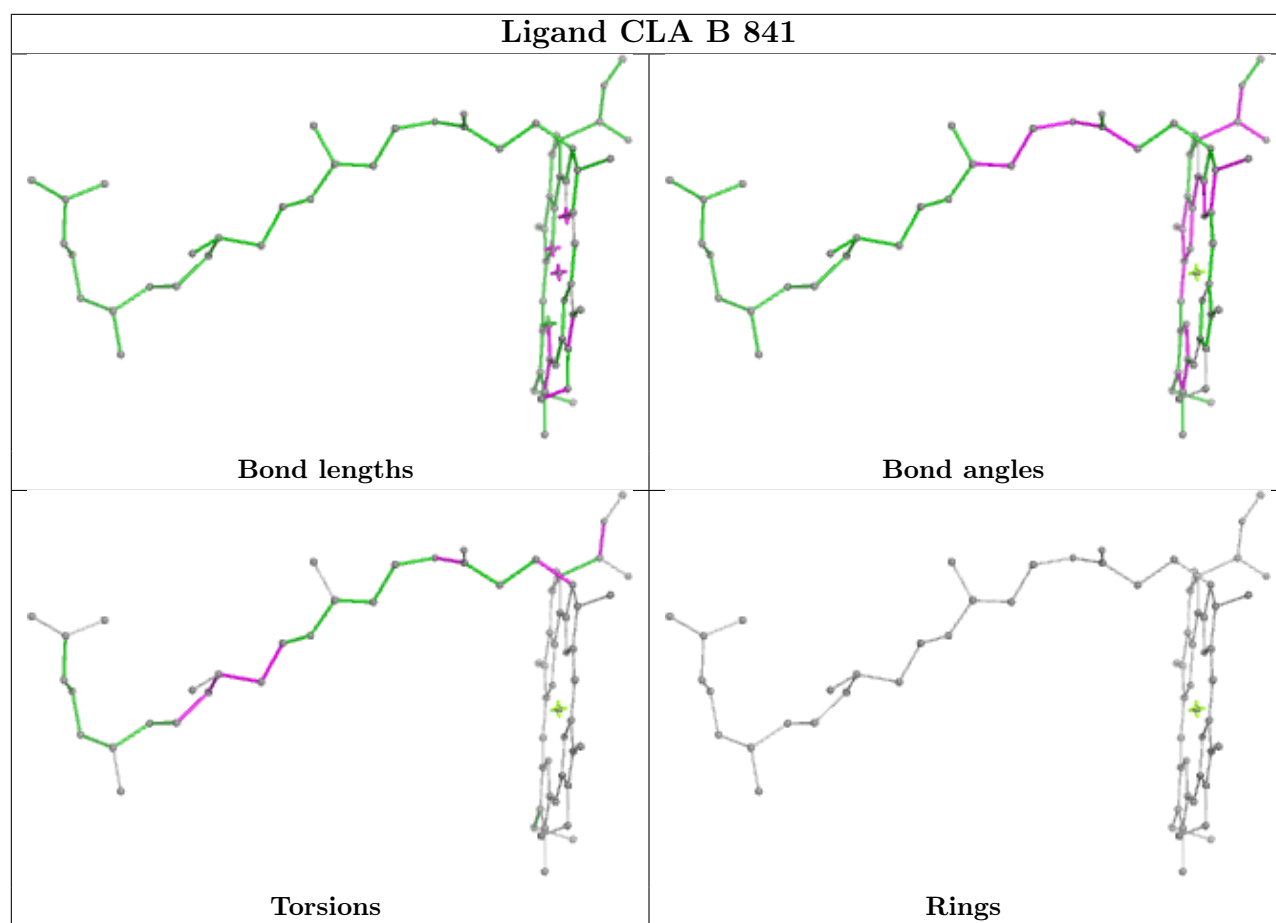


Ligand BCR 6 305

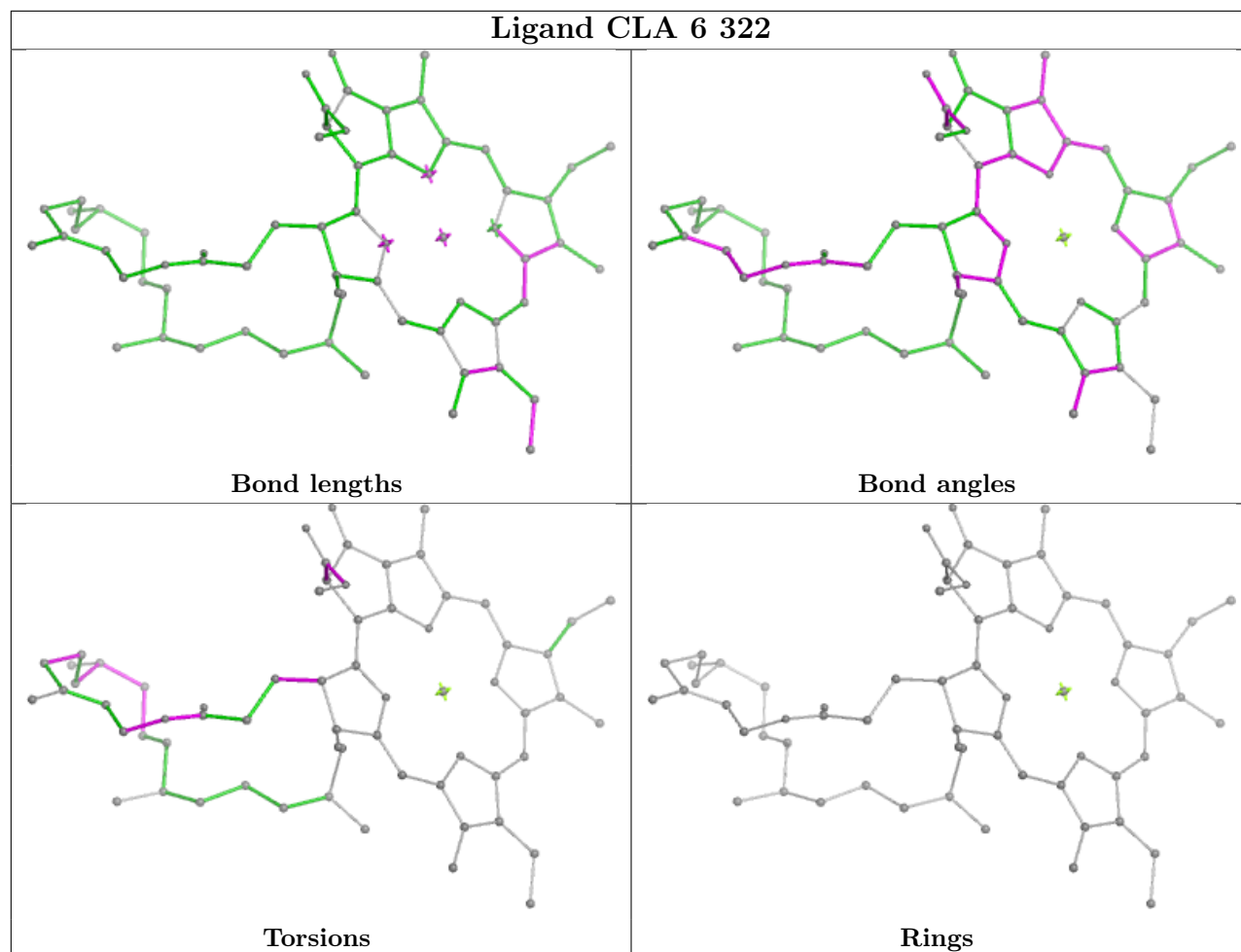


Ligand LUT 7 302**Ligand CLA 3 316**

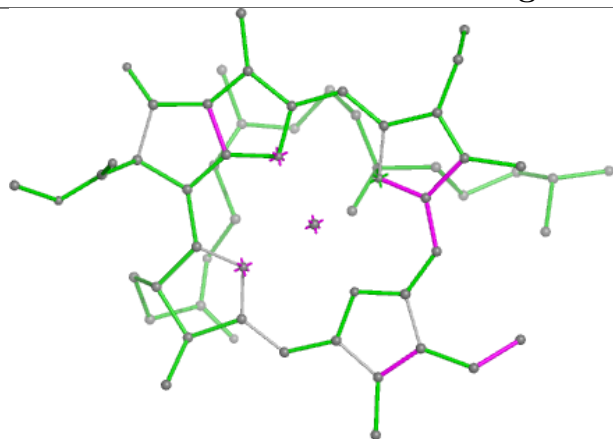




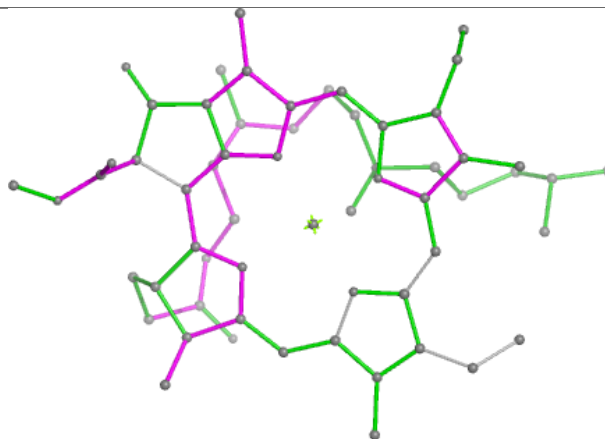
Ligand CLA 6 322



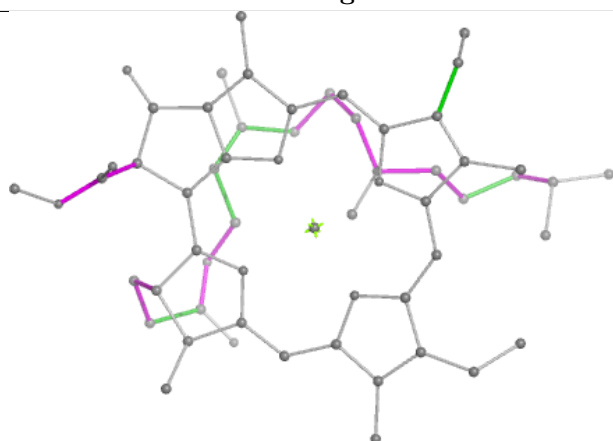
Ligand CLA 6 301



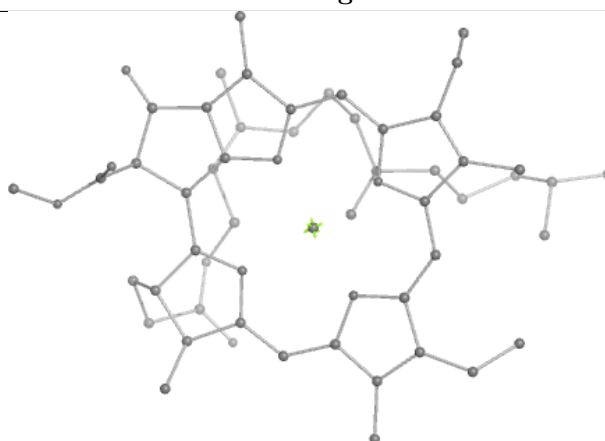
Bond lengths



Bond angles

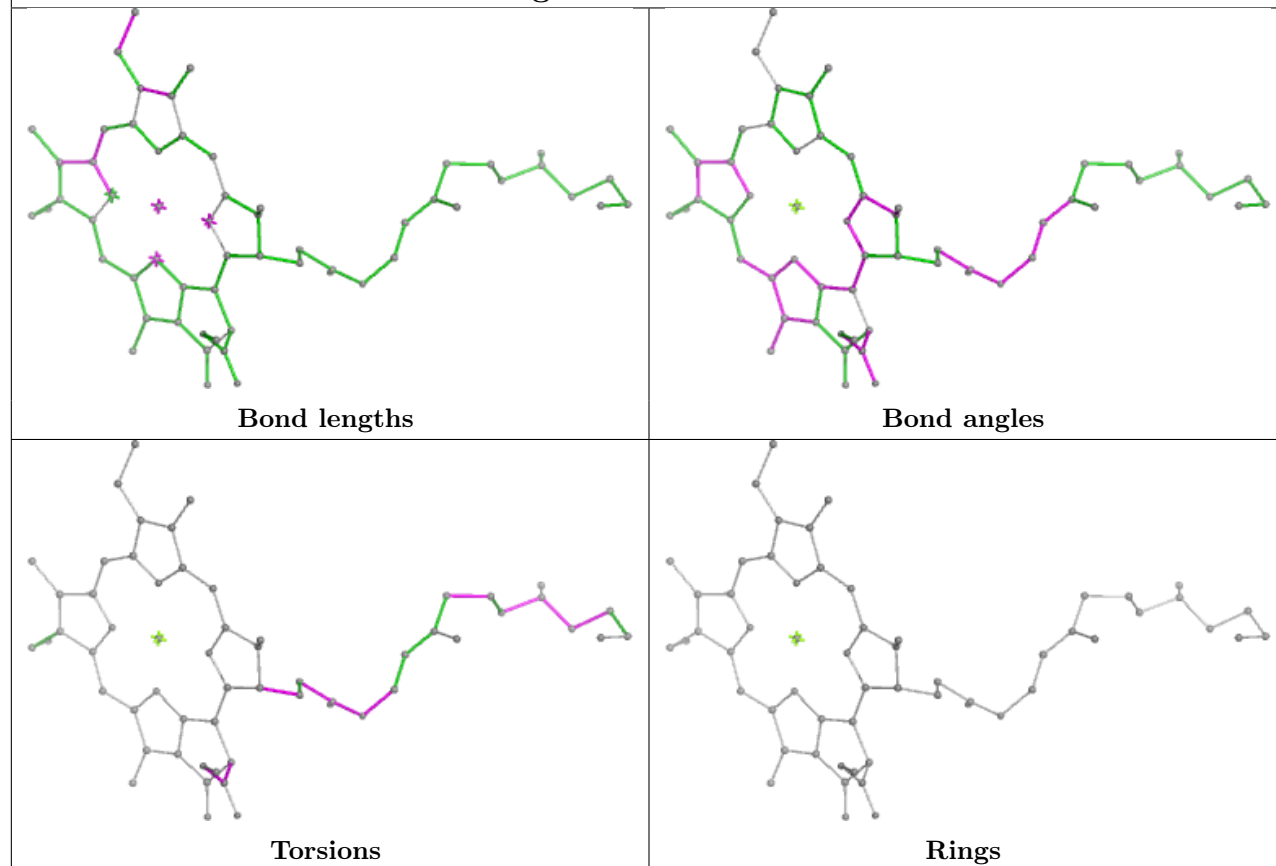


Torsions

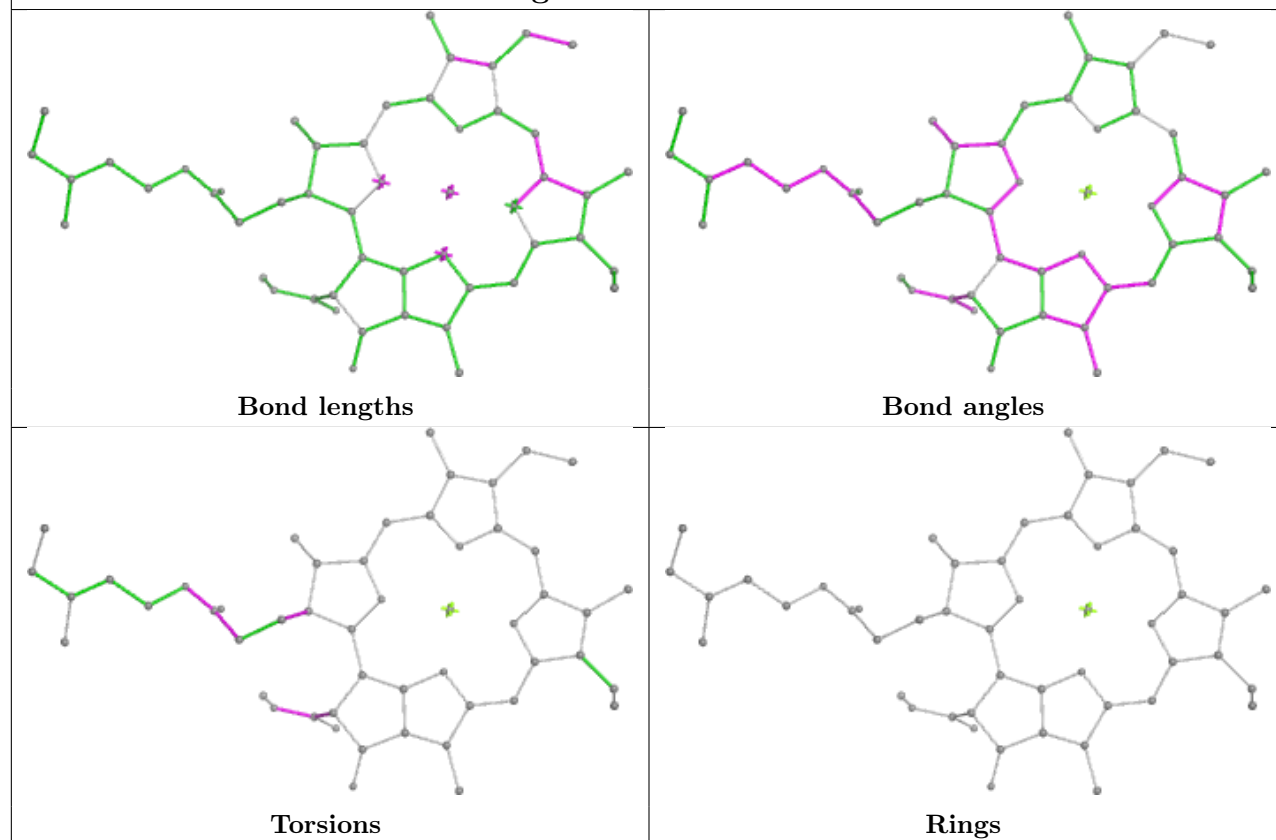


Rings

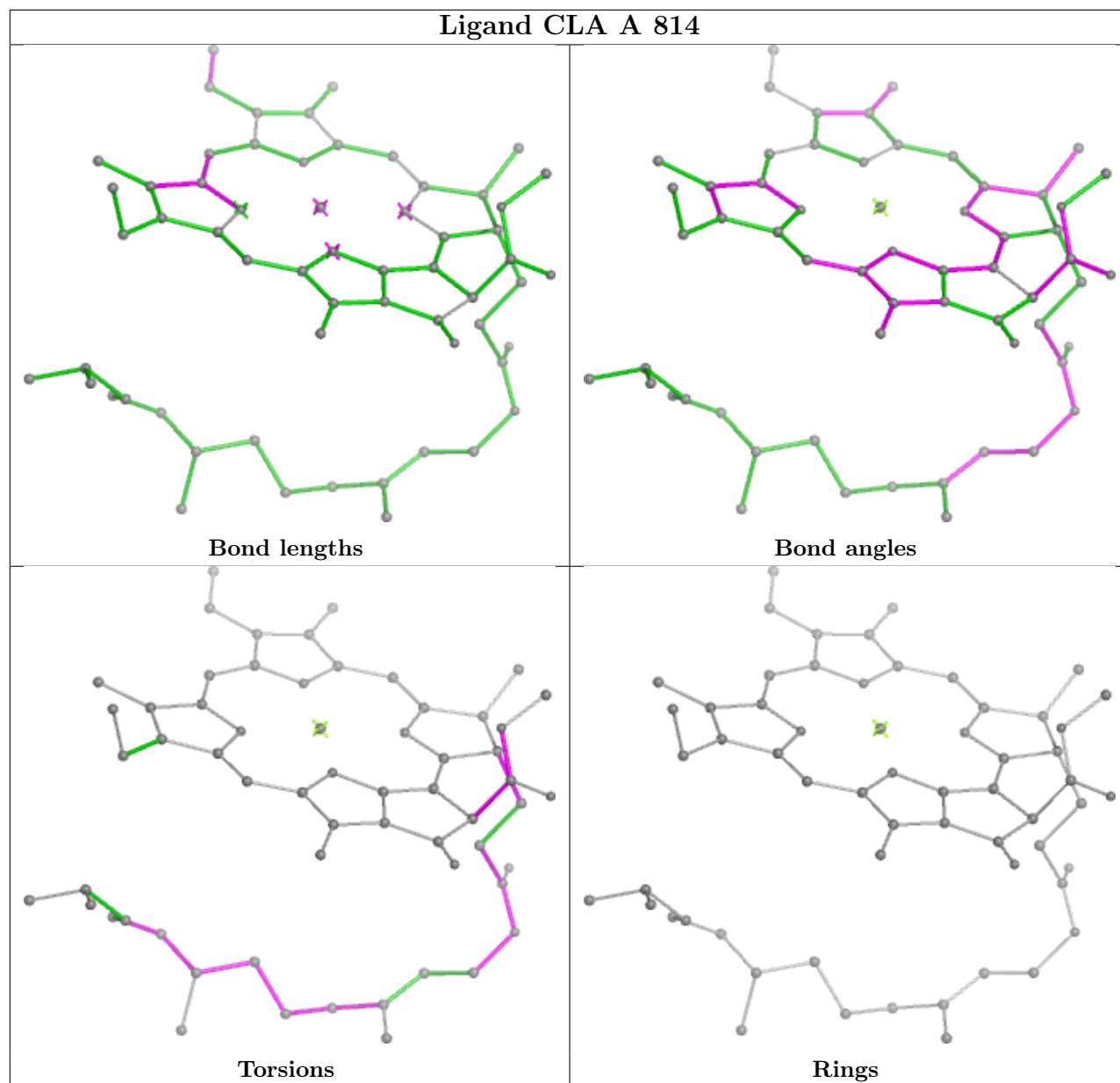
Ligand CLA B 834



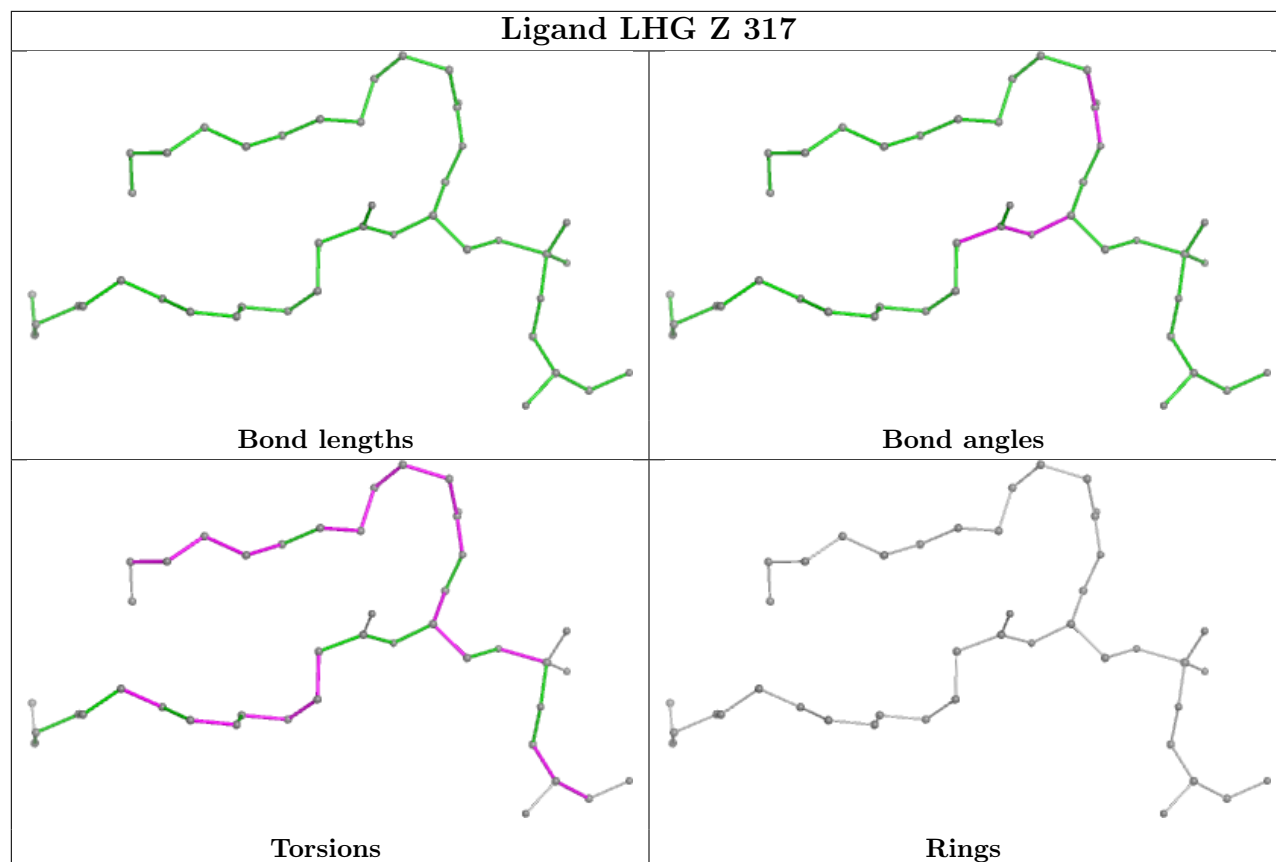
Ligand CLA A 837



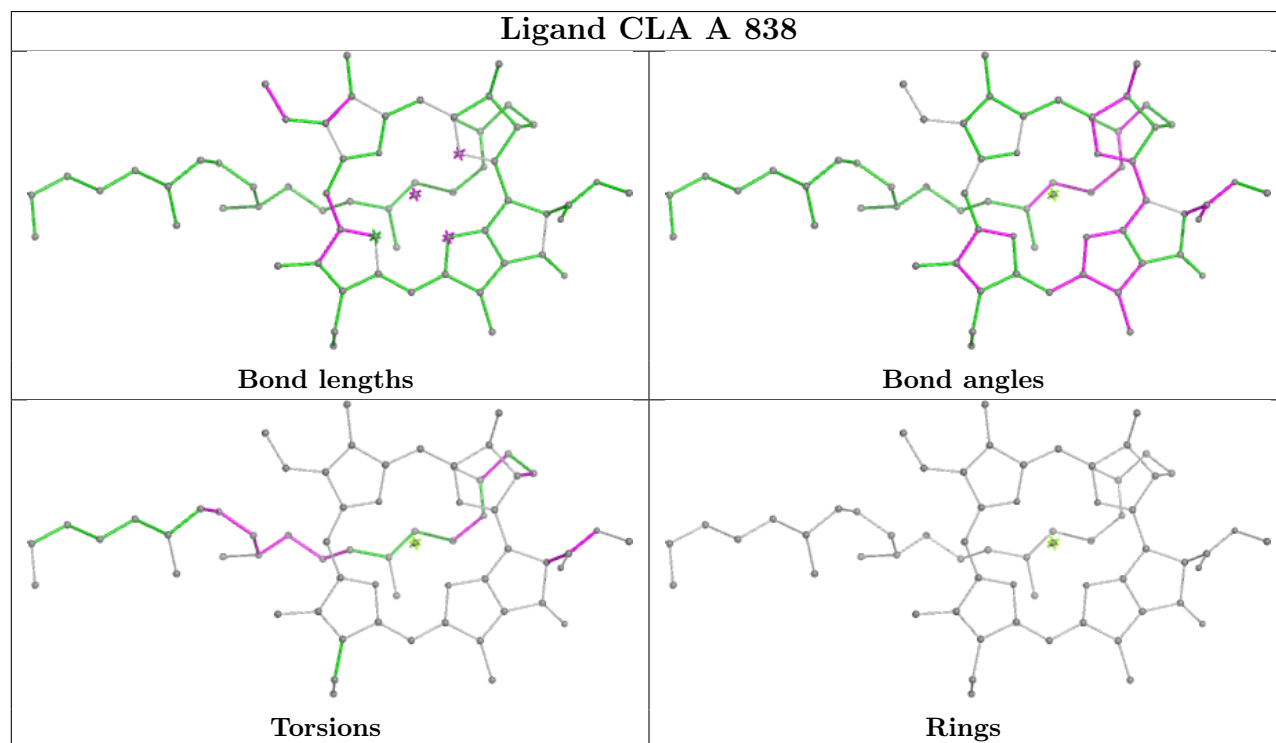
Ligand CLA A 814



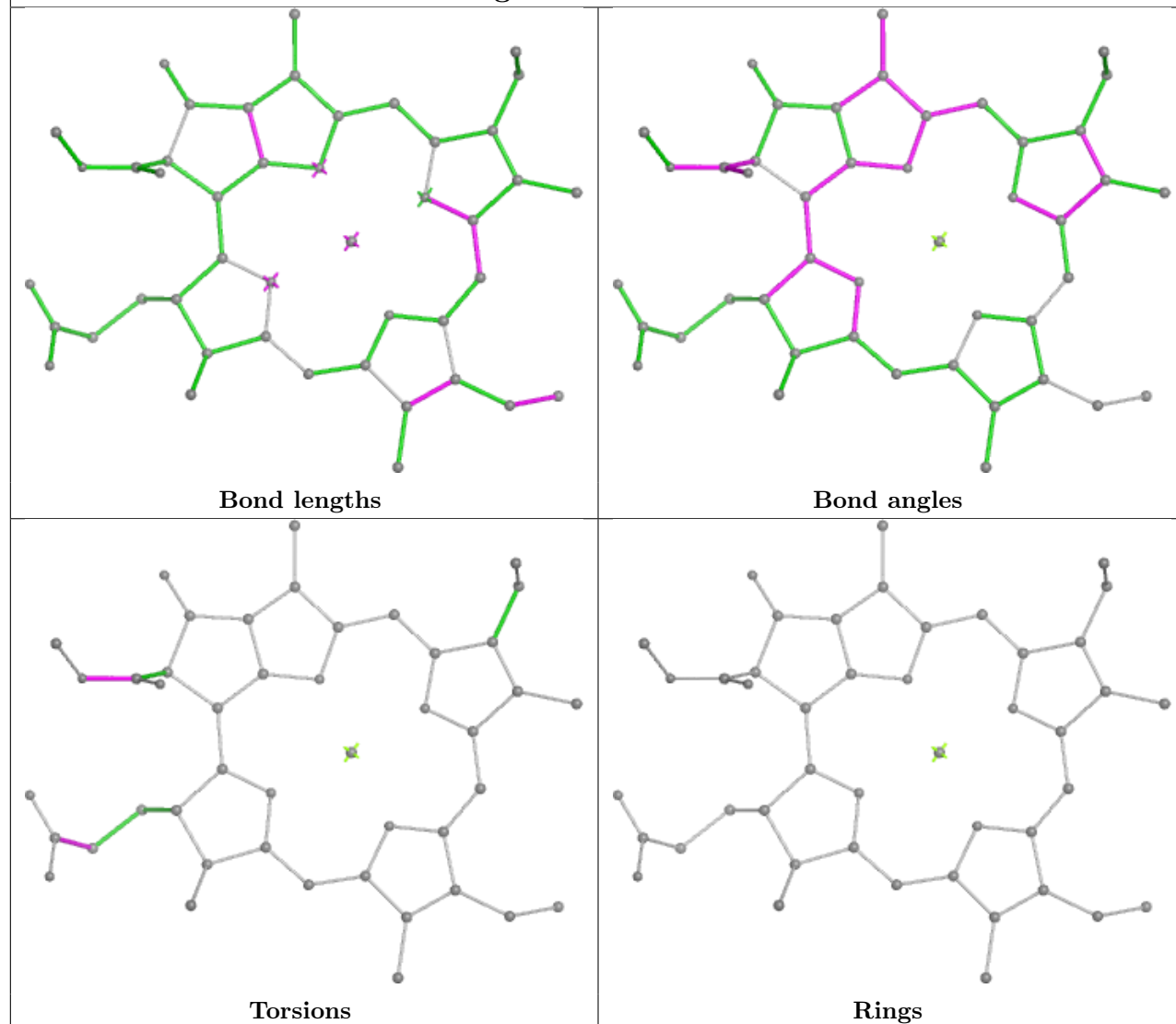
Ligand LHG Z 317



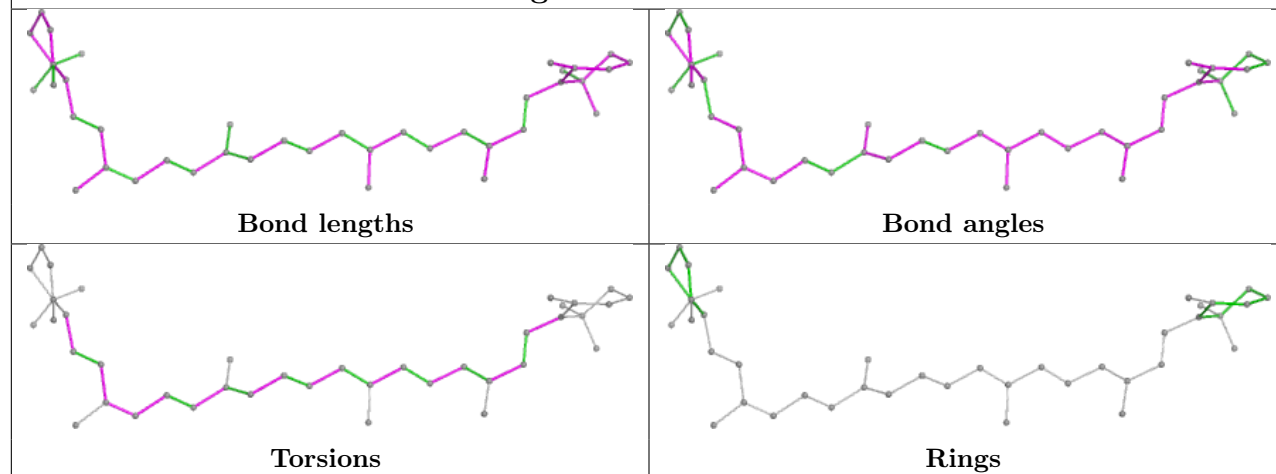
Ligand CLA A 838

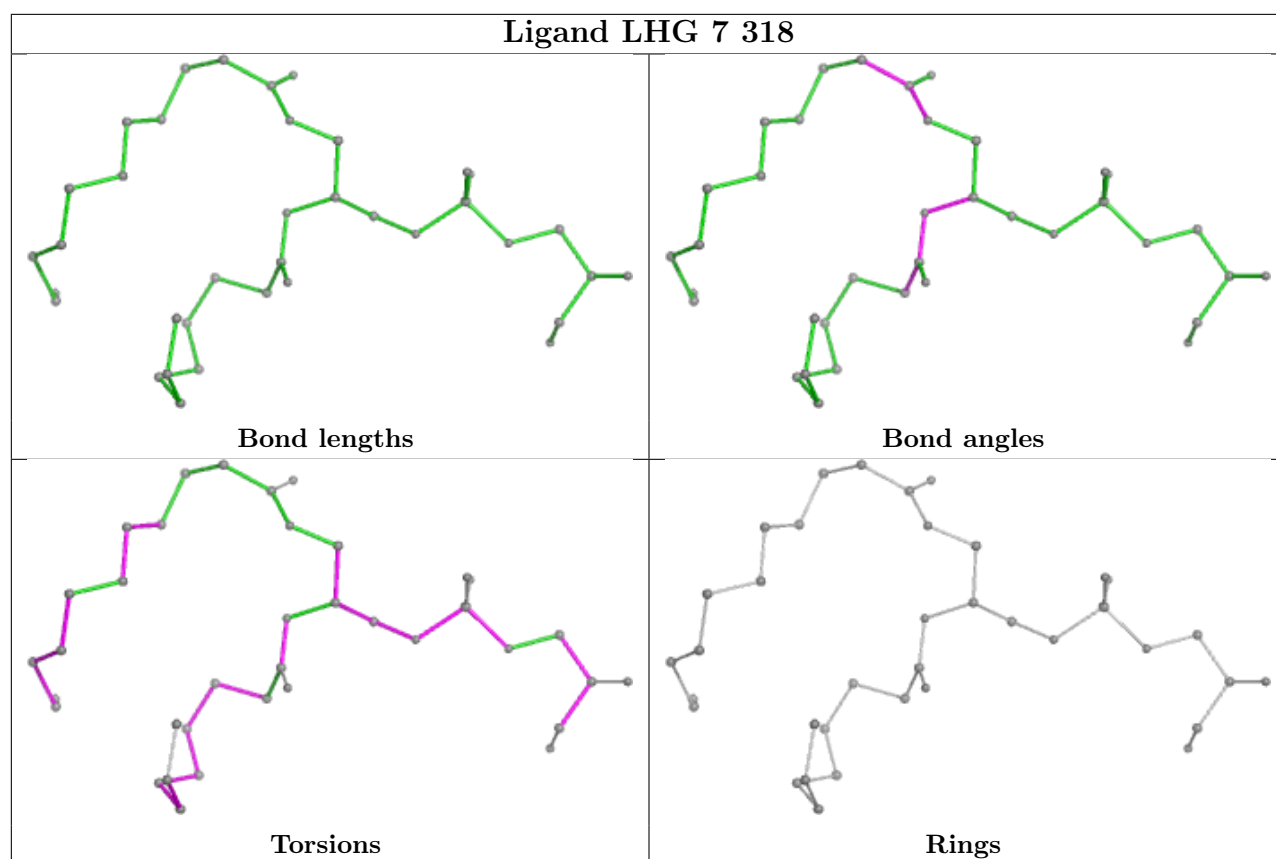


Ligand CLA 9 304

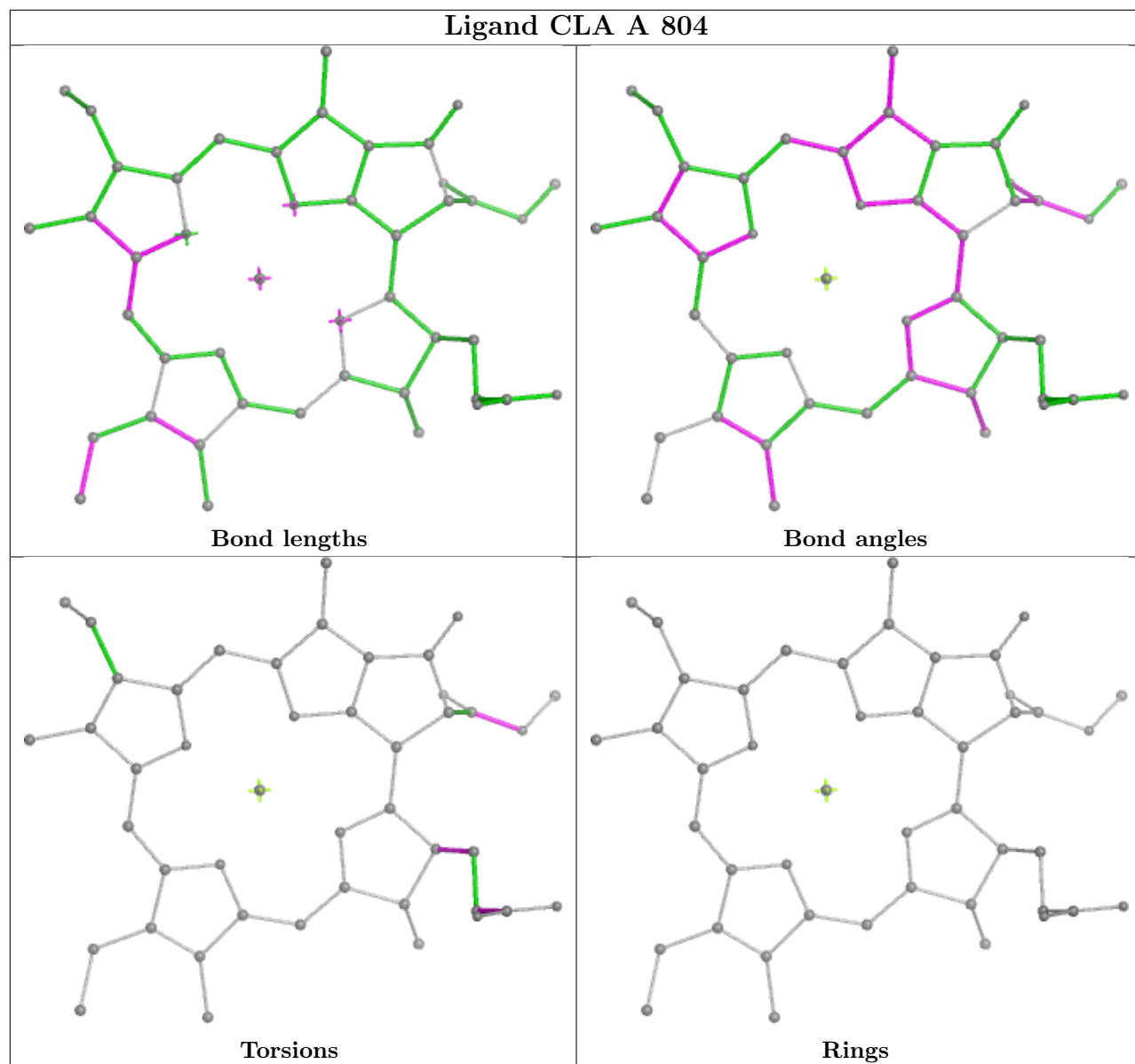


Ligand BCR B 853

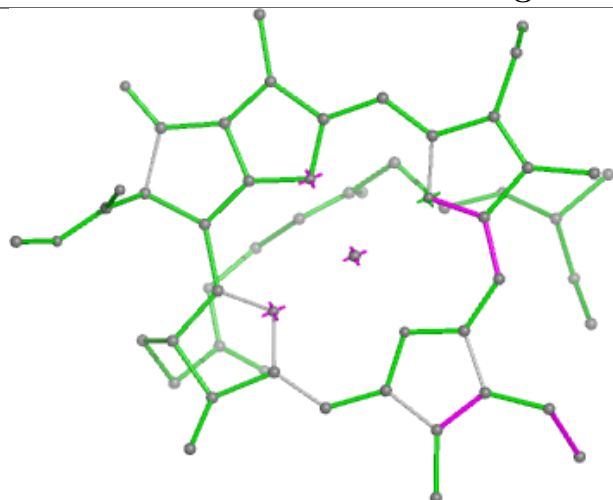




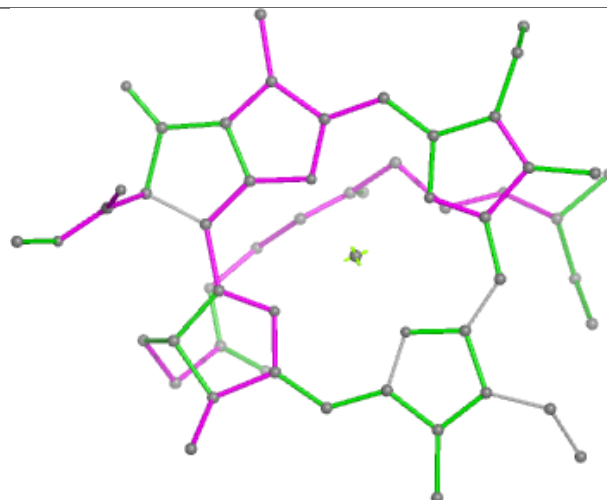
Ligand CLA A 804



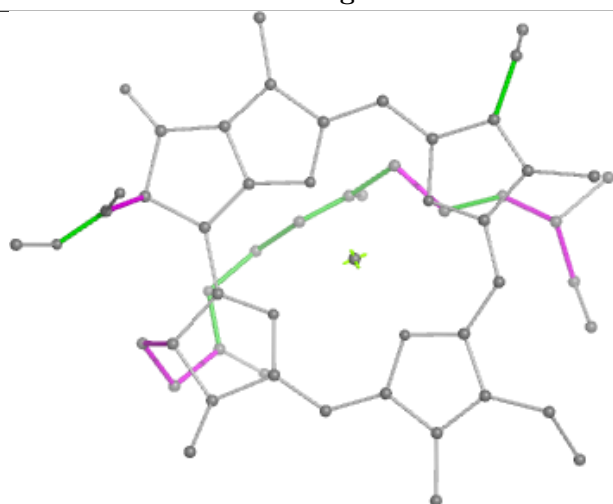
Ligand CLA B 810



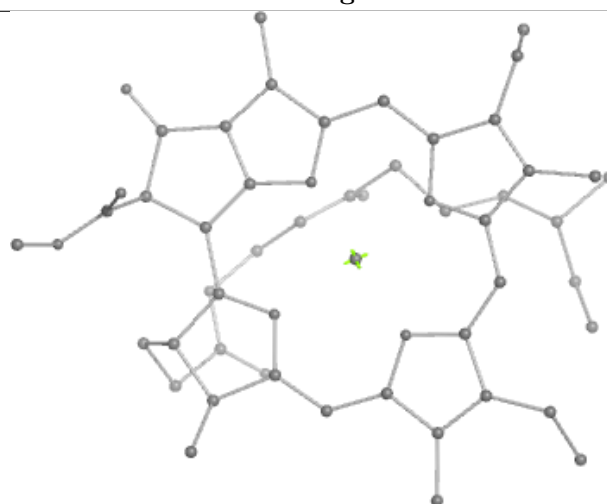
Bond lengths



Bond angles

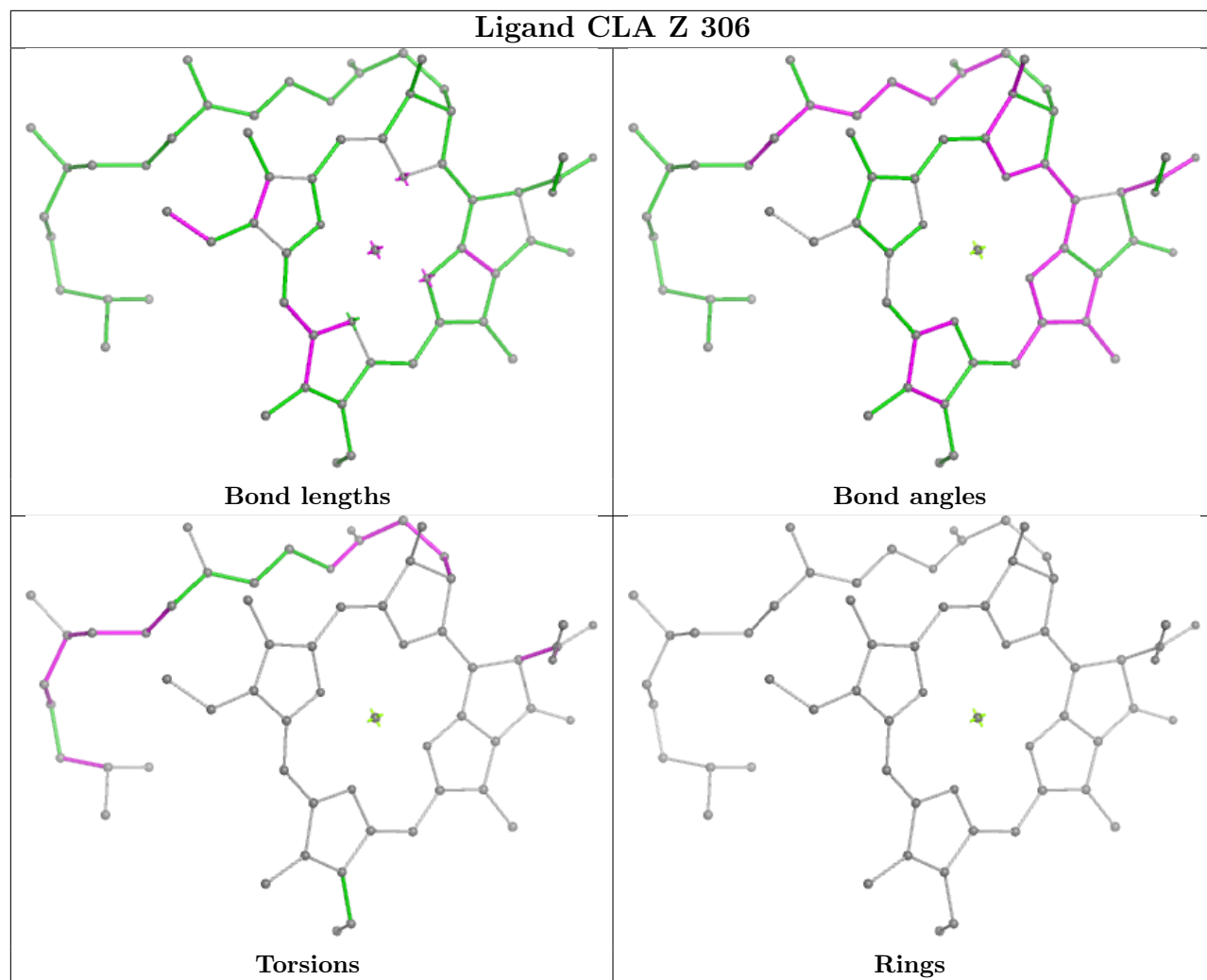


Torsions

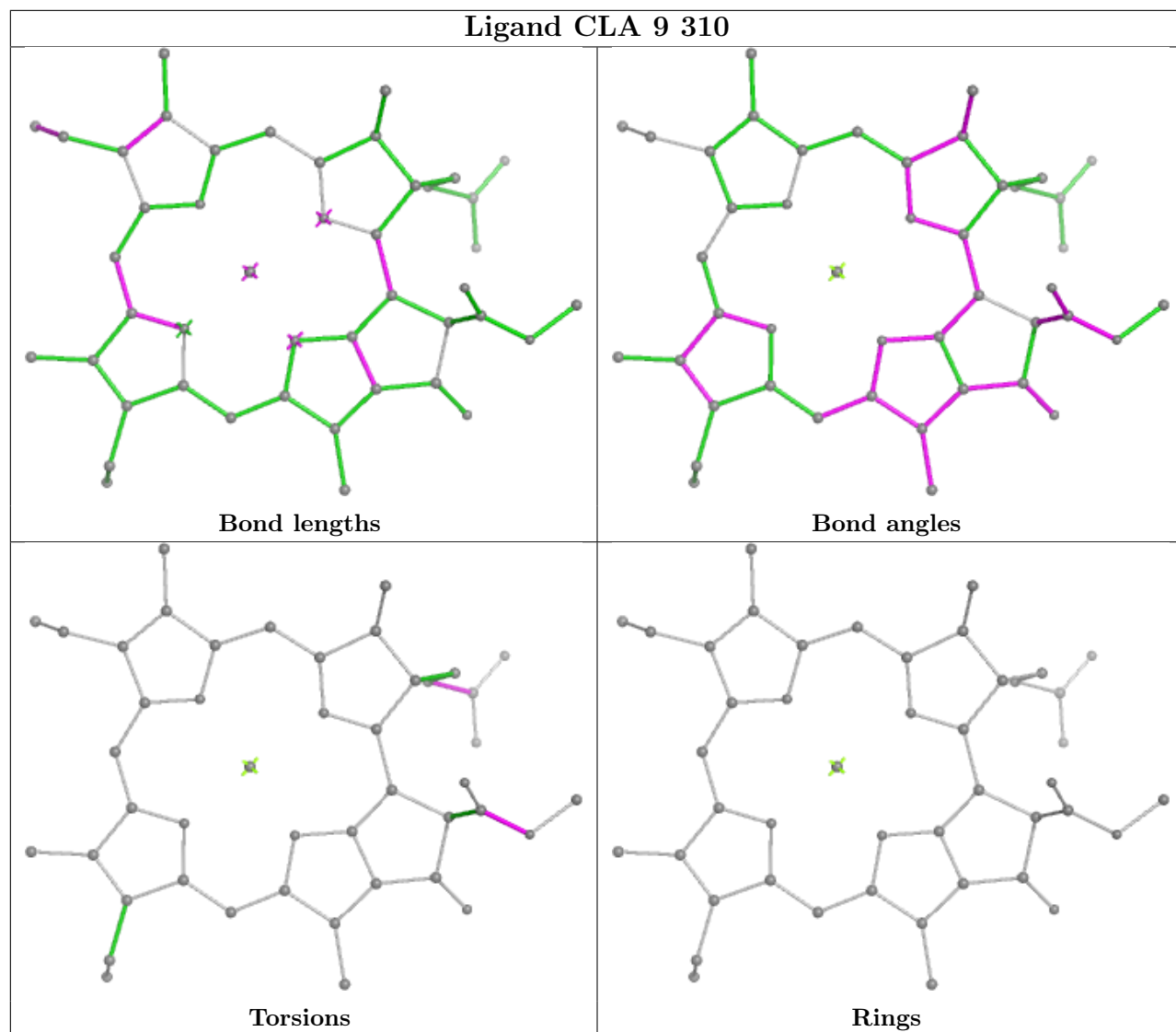


Rings

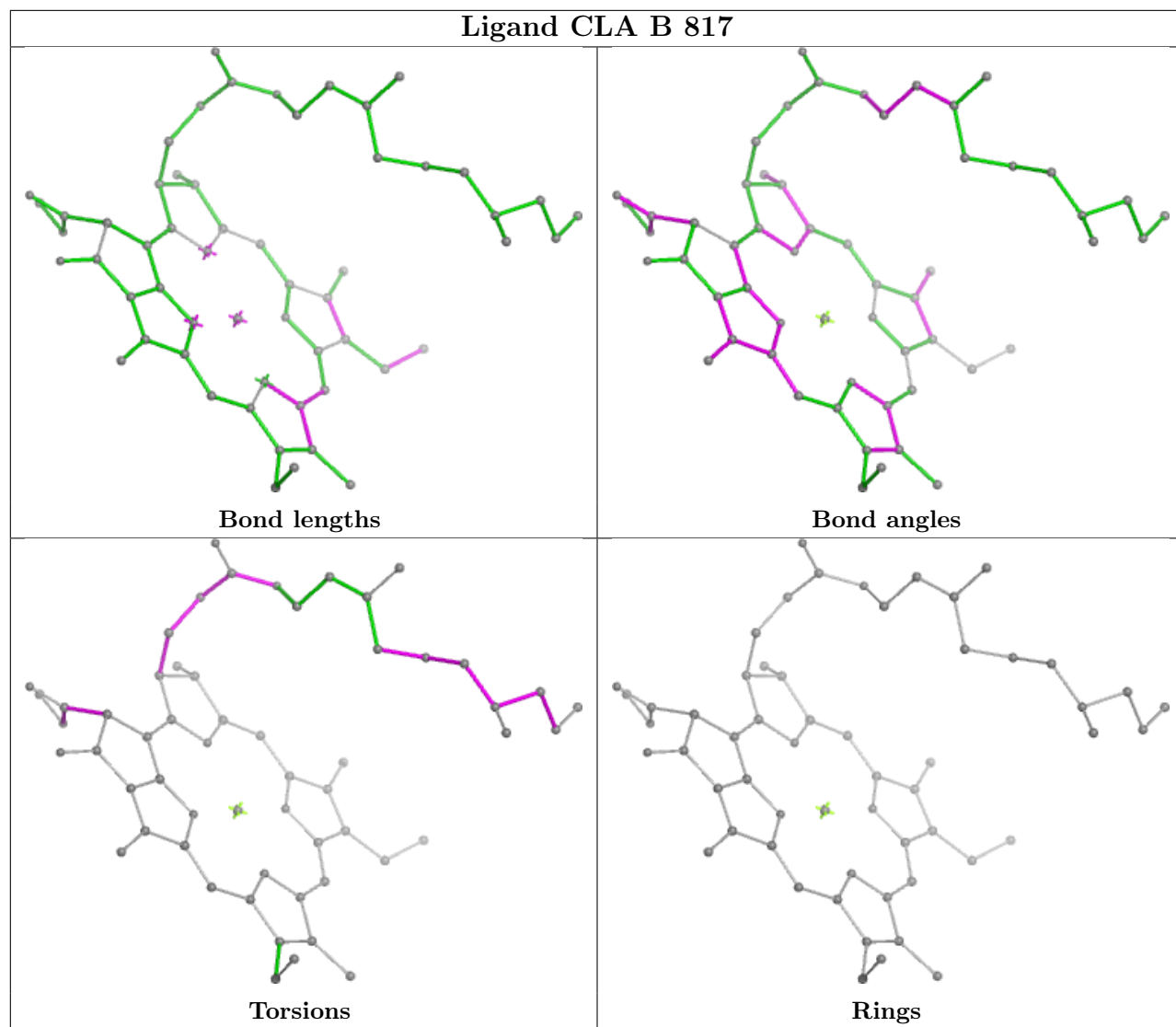
Ligand CLA Z 306

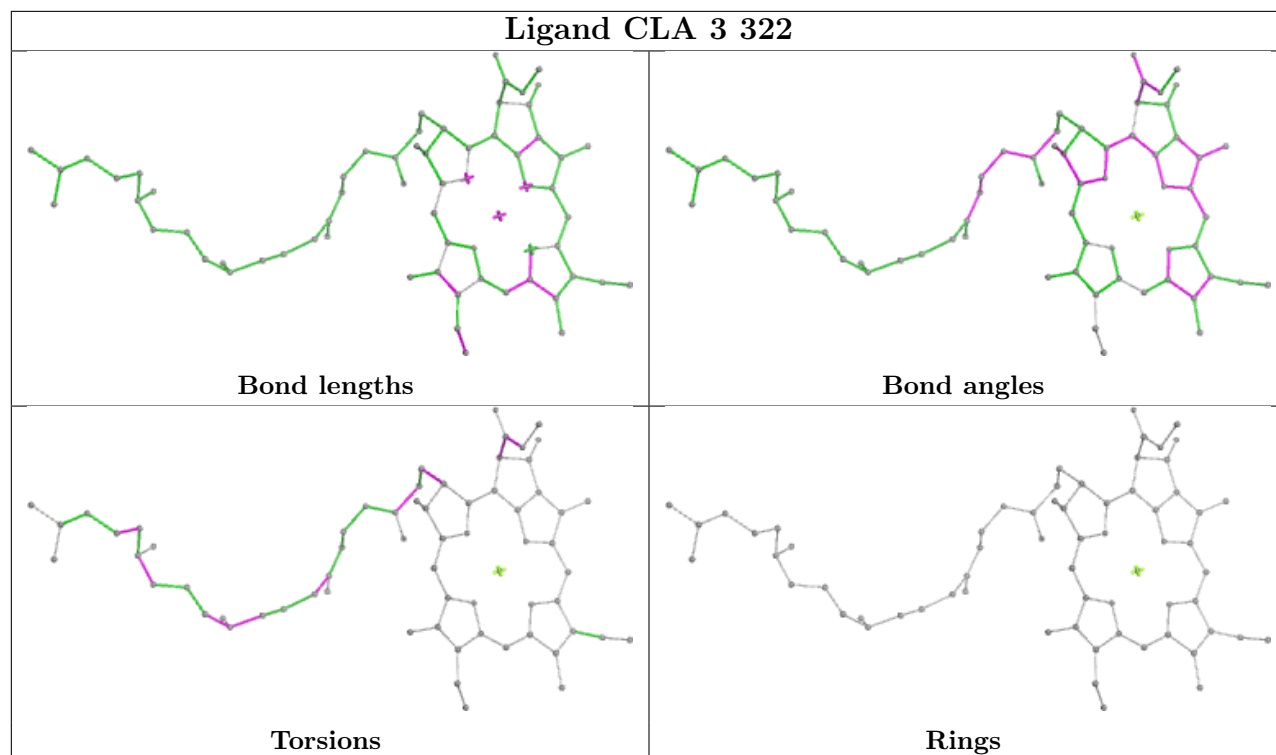
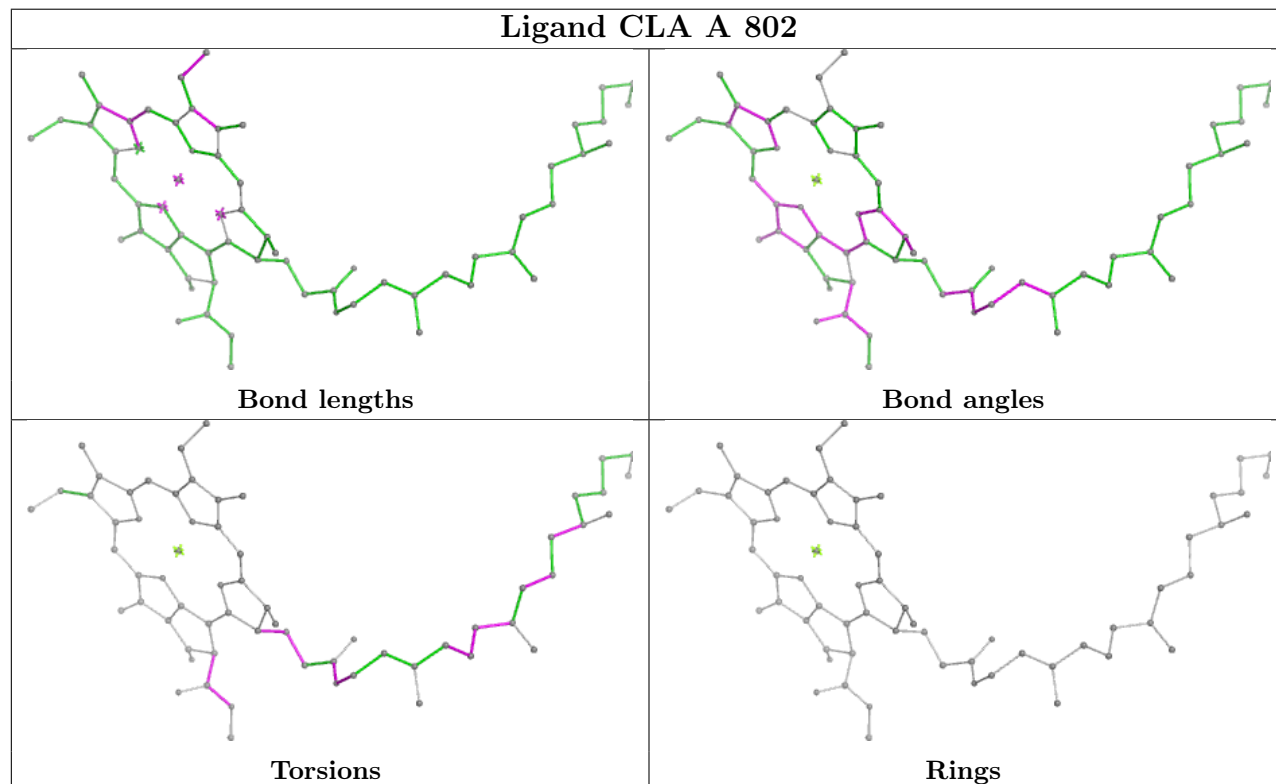


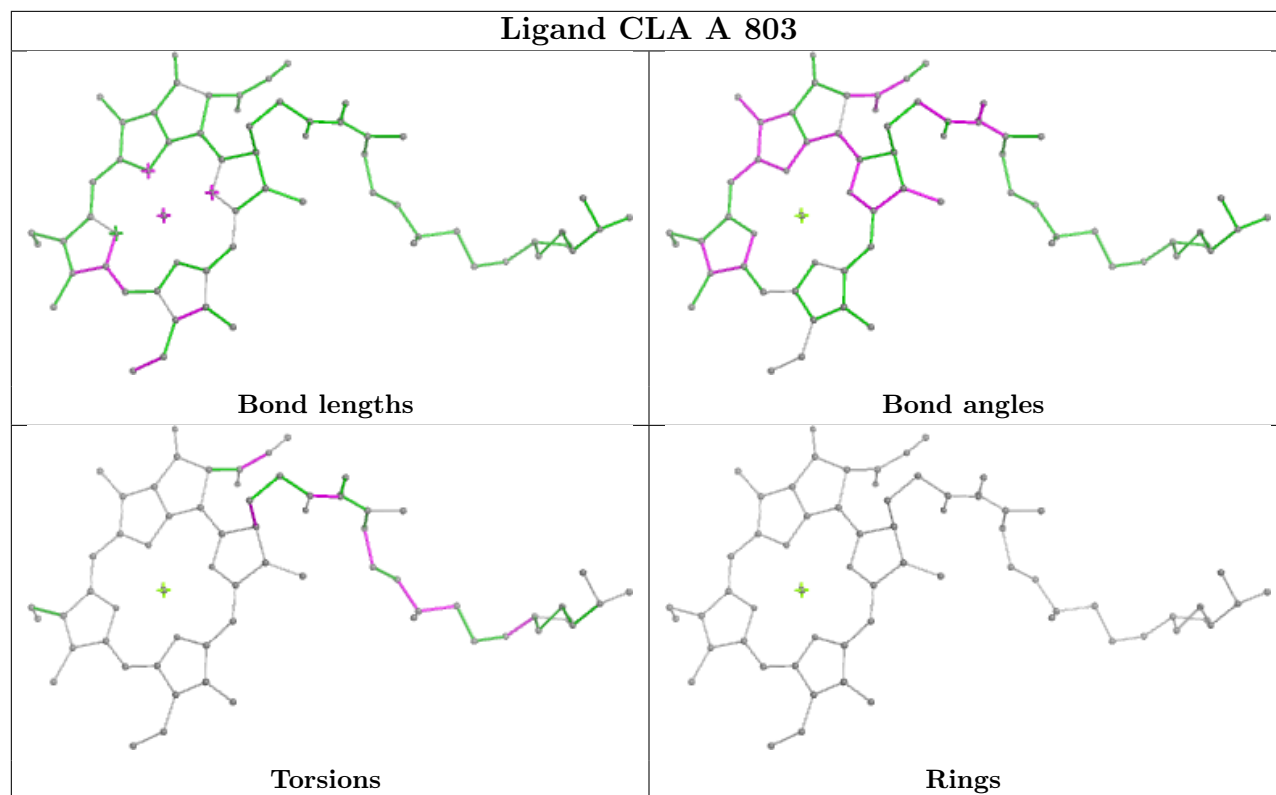
Ligand CLA 9 310



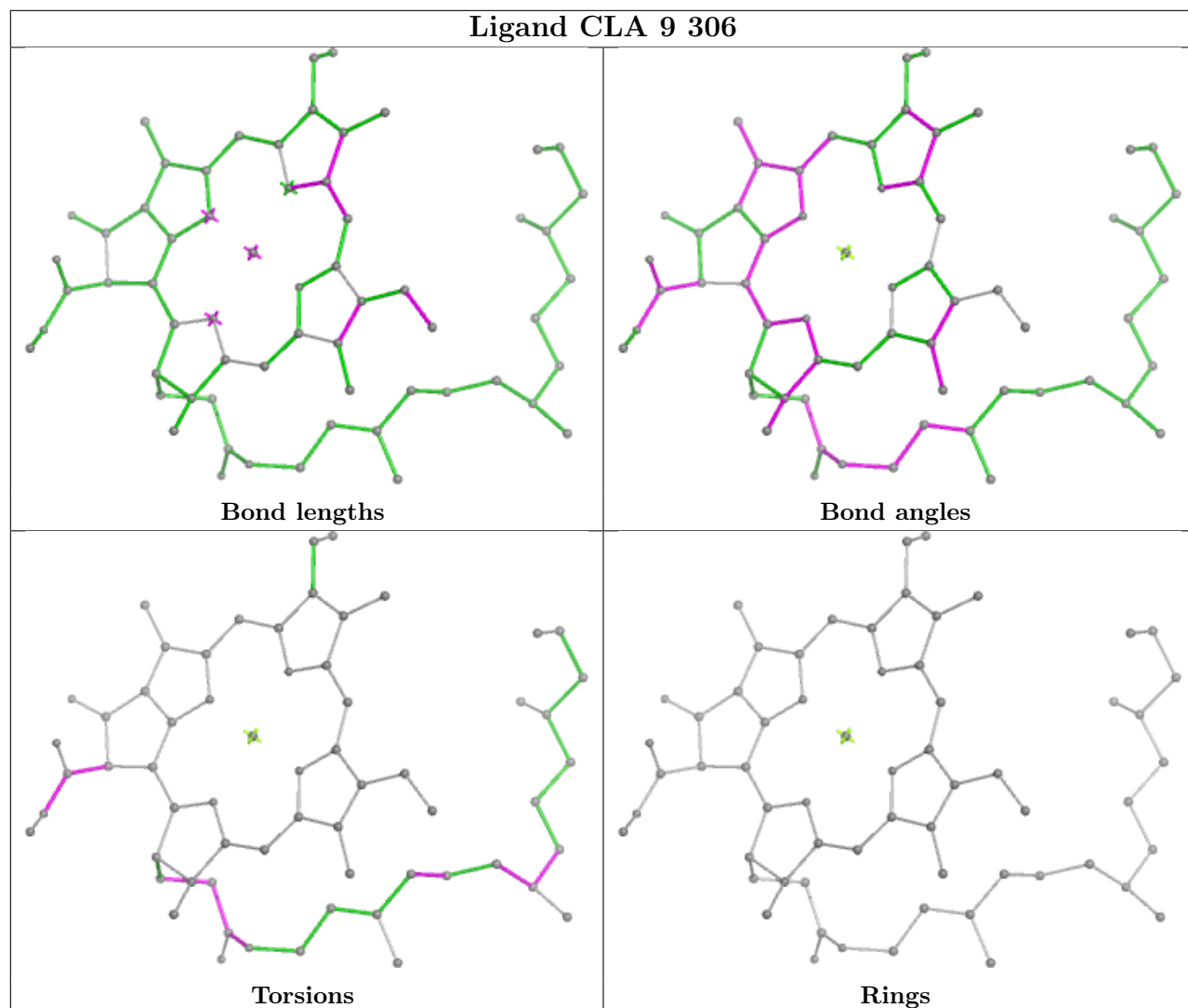
Ligand CLA B 817



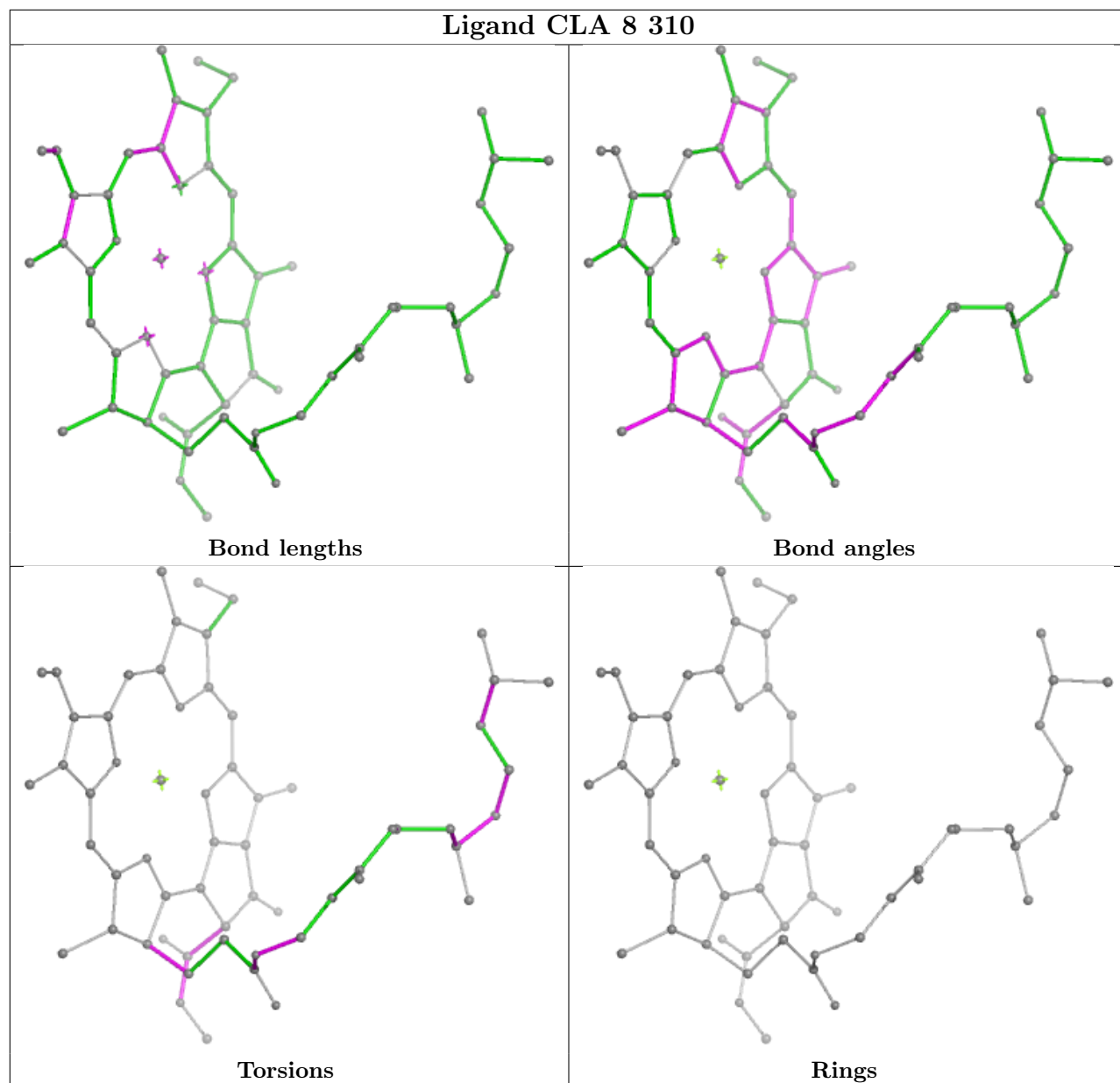
Ligand CLA 3 322**Ligand CLA A 802**

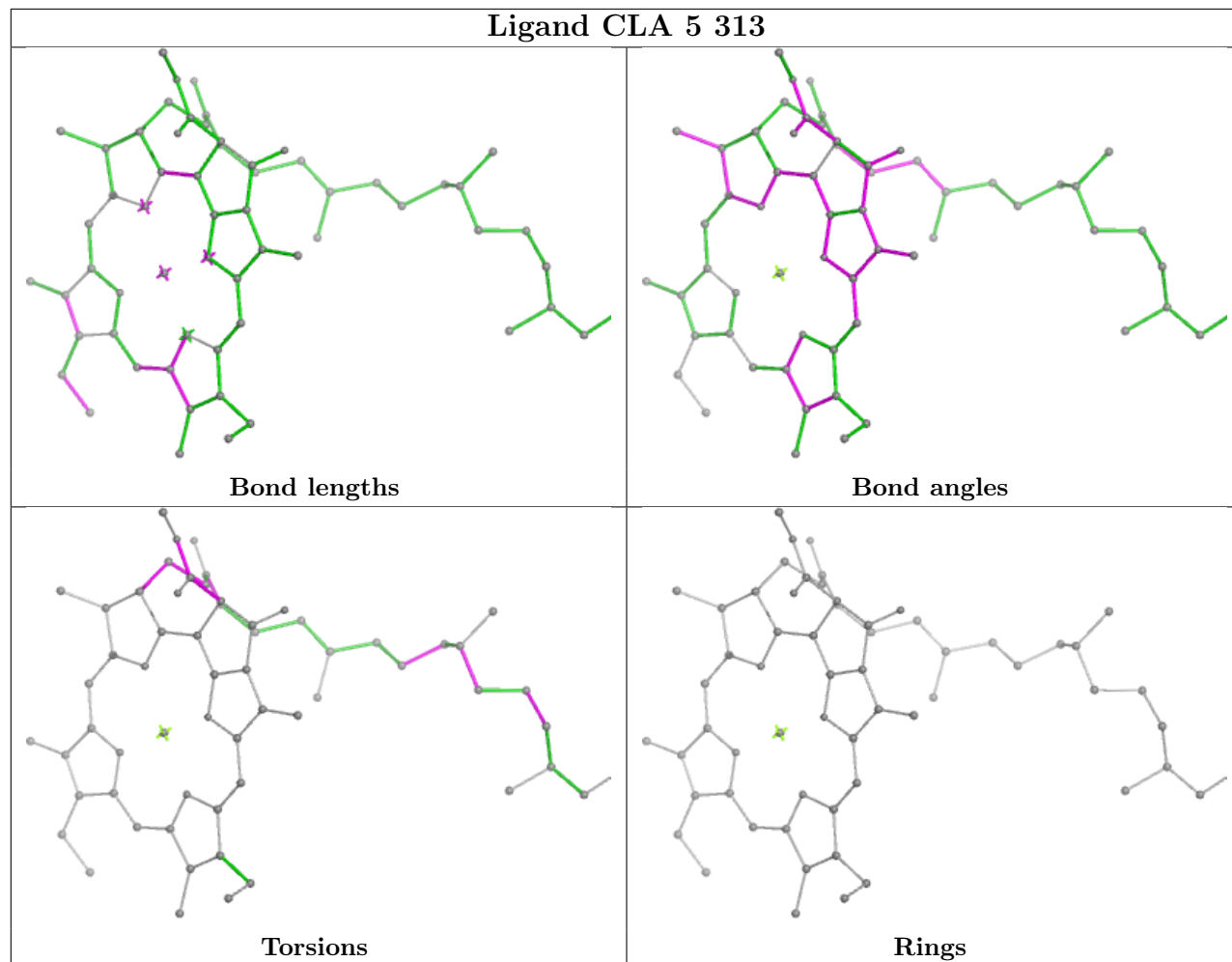
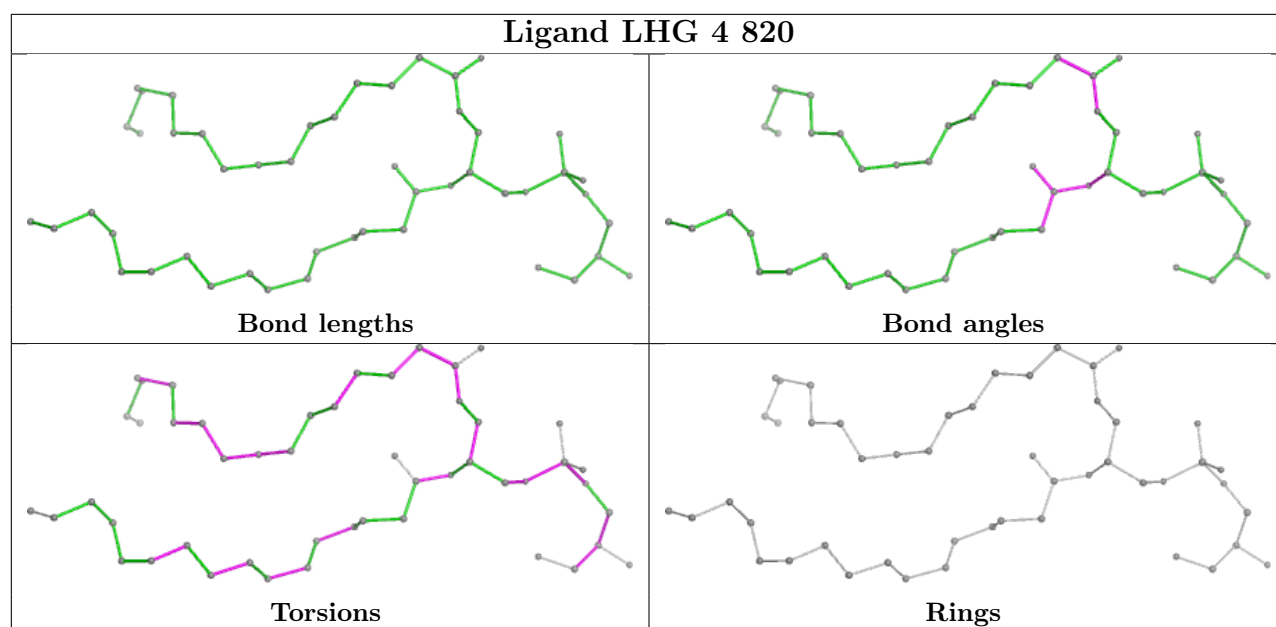


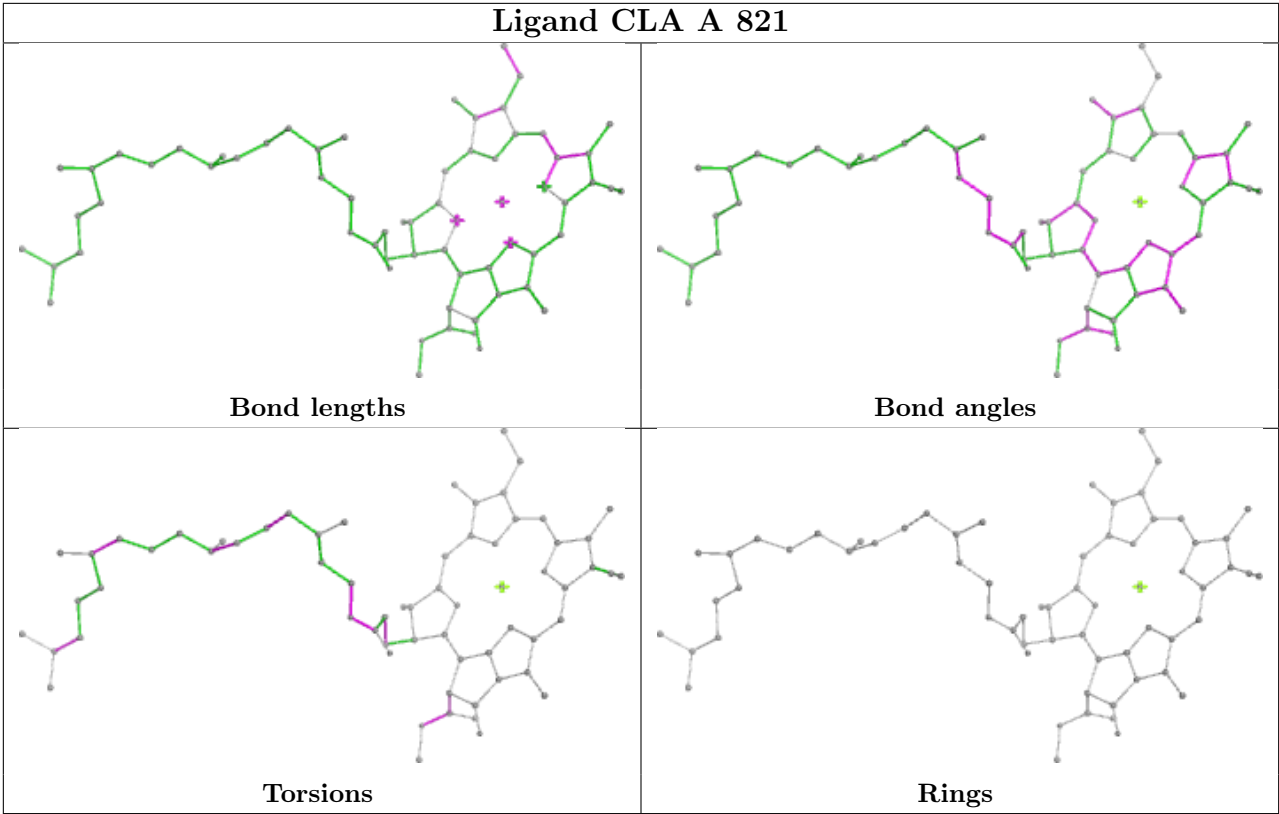
Ligand CLA 9 306



Ligand CLA 8 310







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	144:PRO	C	158:ARG	N	6.44

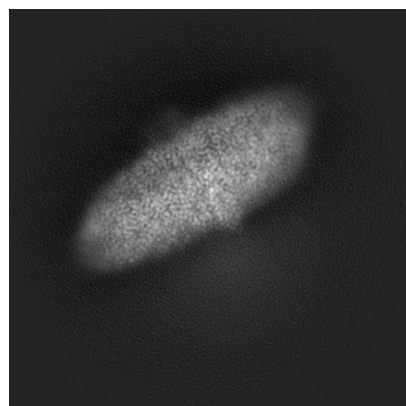
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16732. These allow visual inspection of the internal detail of the map and identification of artifacts.

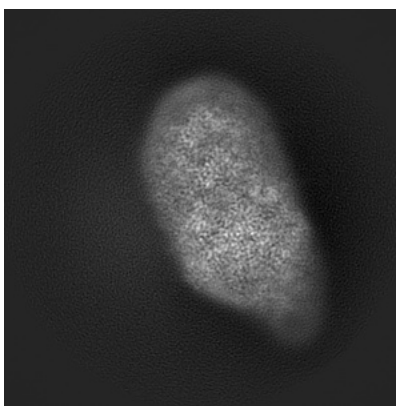
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

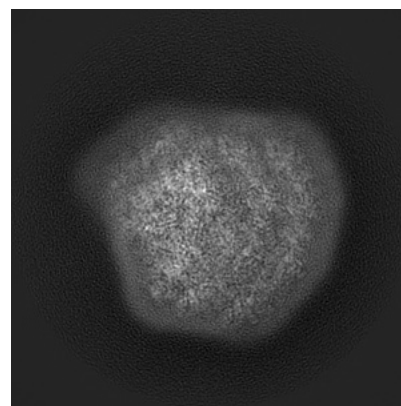
6.1.1 Primary map



X

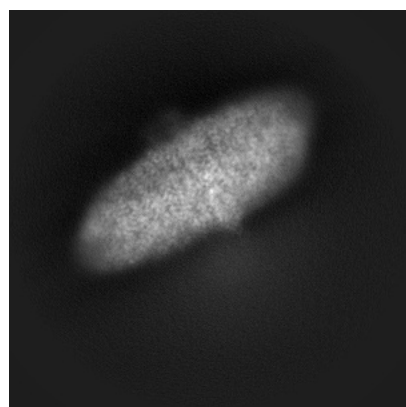


Y

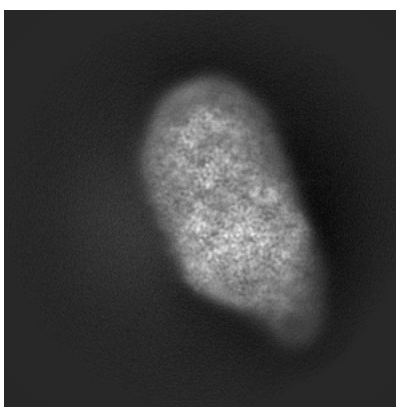


Z

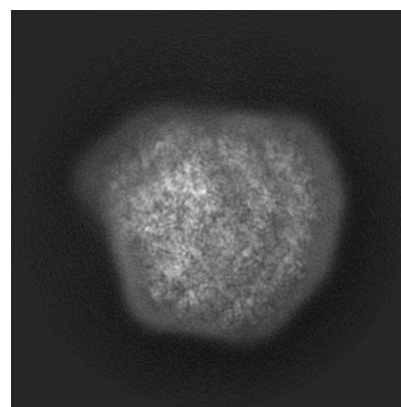
6.1.2 Raw map



X



Y

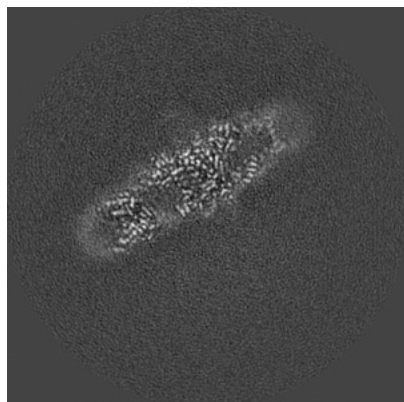


Z

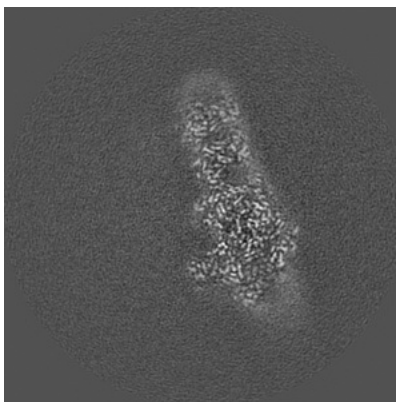
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

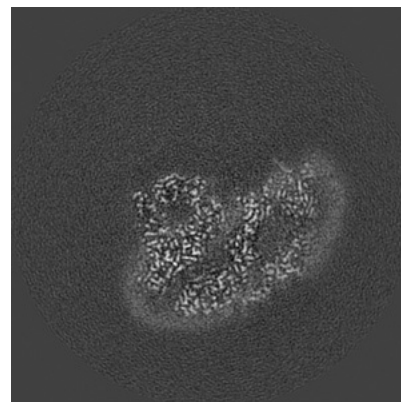
6.2.1 Primary map



X Index: 250

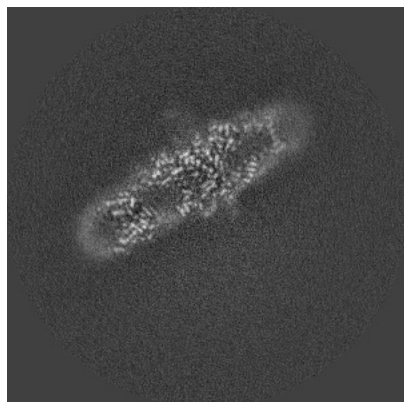


Y Index: 250

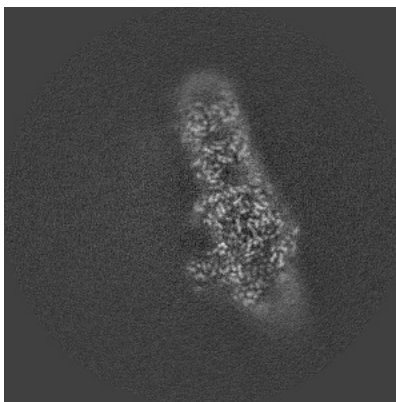


Z Index: 250

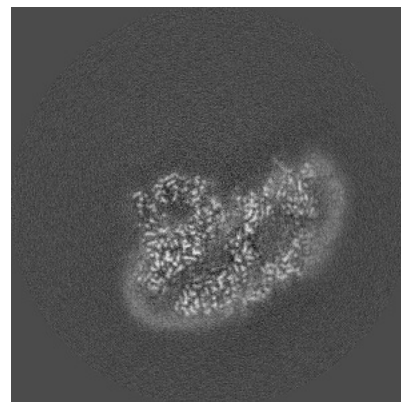
6.2.2 Raw map



X Index: 250



Y Index: 250

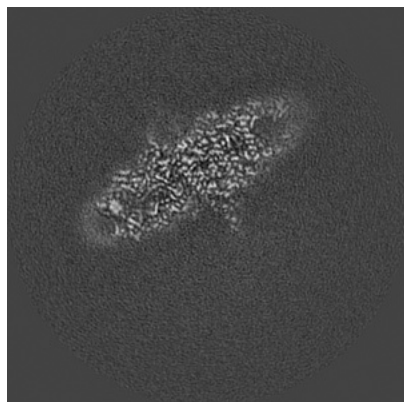


Z Index: 250

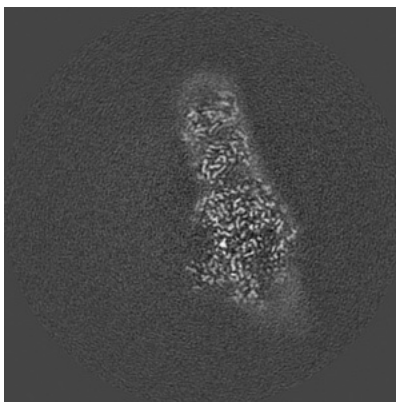
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

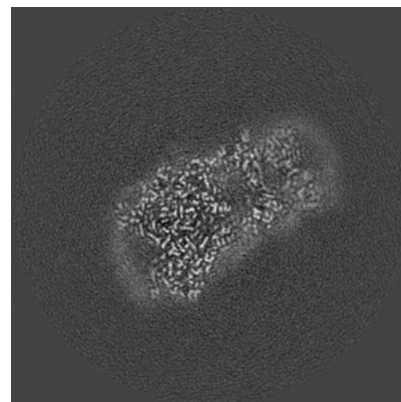
6.3.1 Primary map



X Index: 218

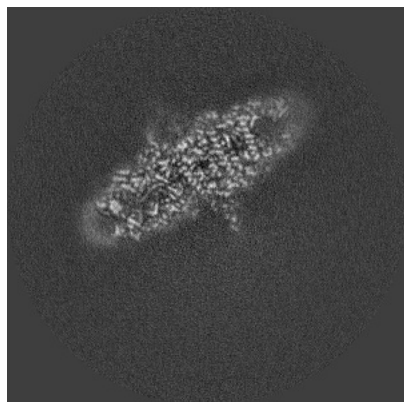


Y Index: 252

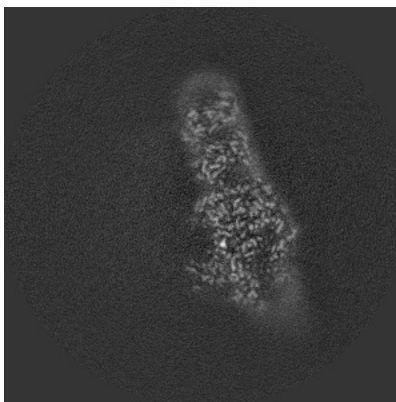


Z Index: 289

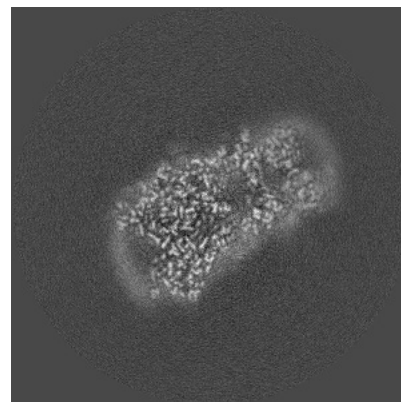
6.3.2 Raw map



X Index: 218



Y Index: 252

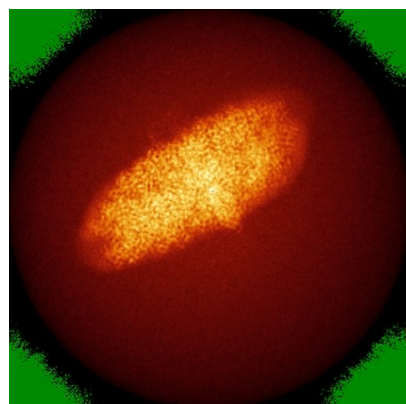


Z Index: 289

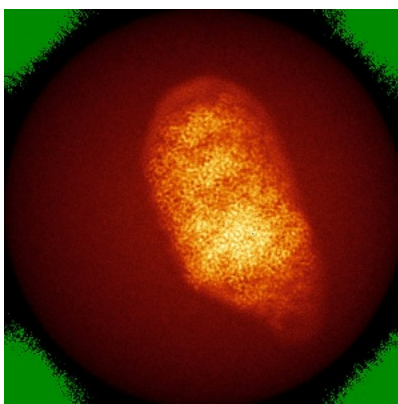
The images above show the largest variance slices of the map in three orthogonal directions.

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

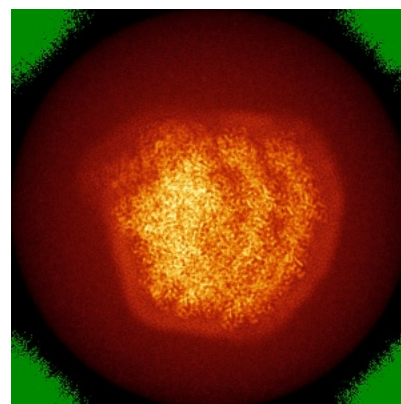
6.4.1 Primary map



X

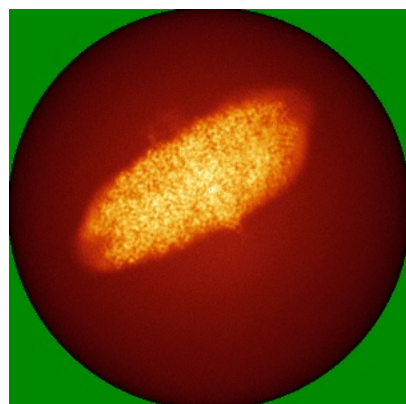


Y

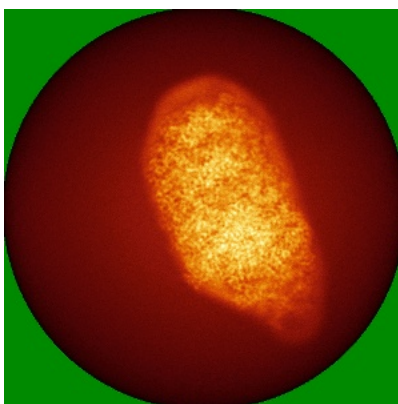


Z

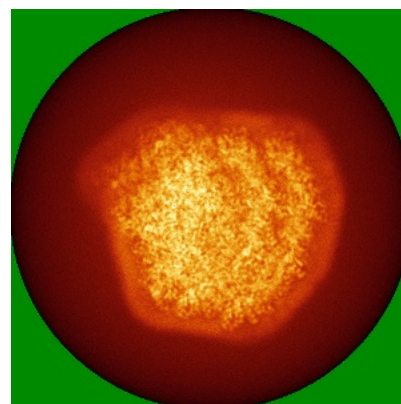
6.4.2 Raw map



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.

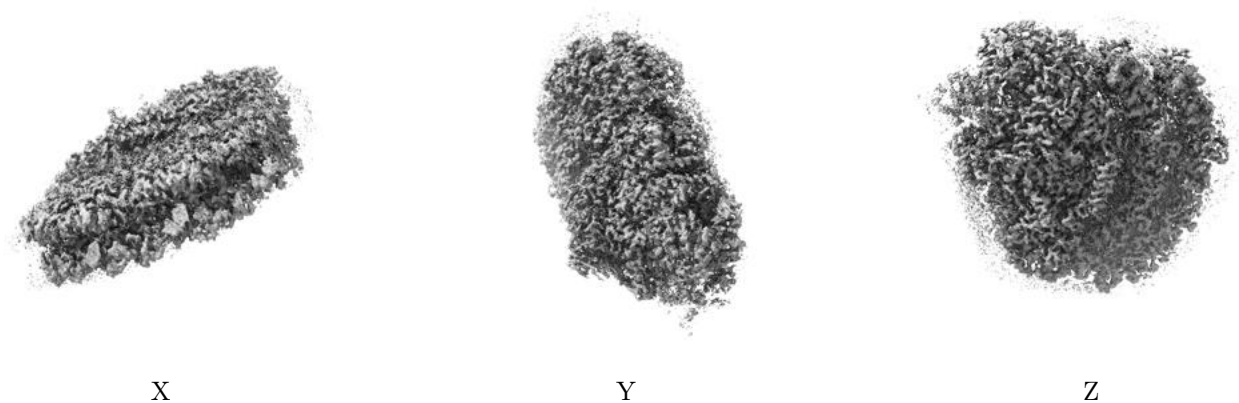
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. 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.

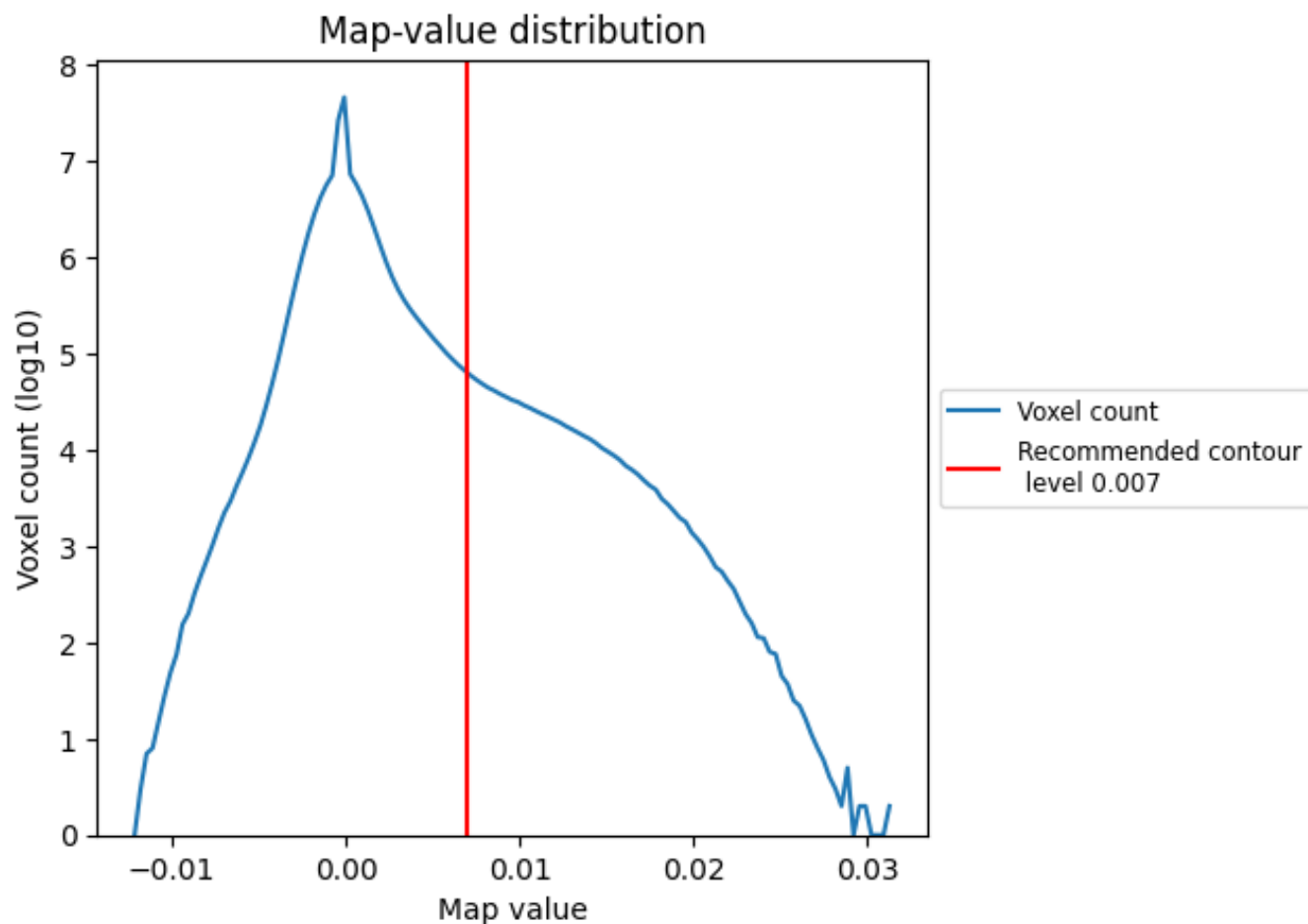
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

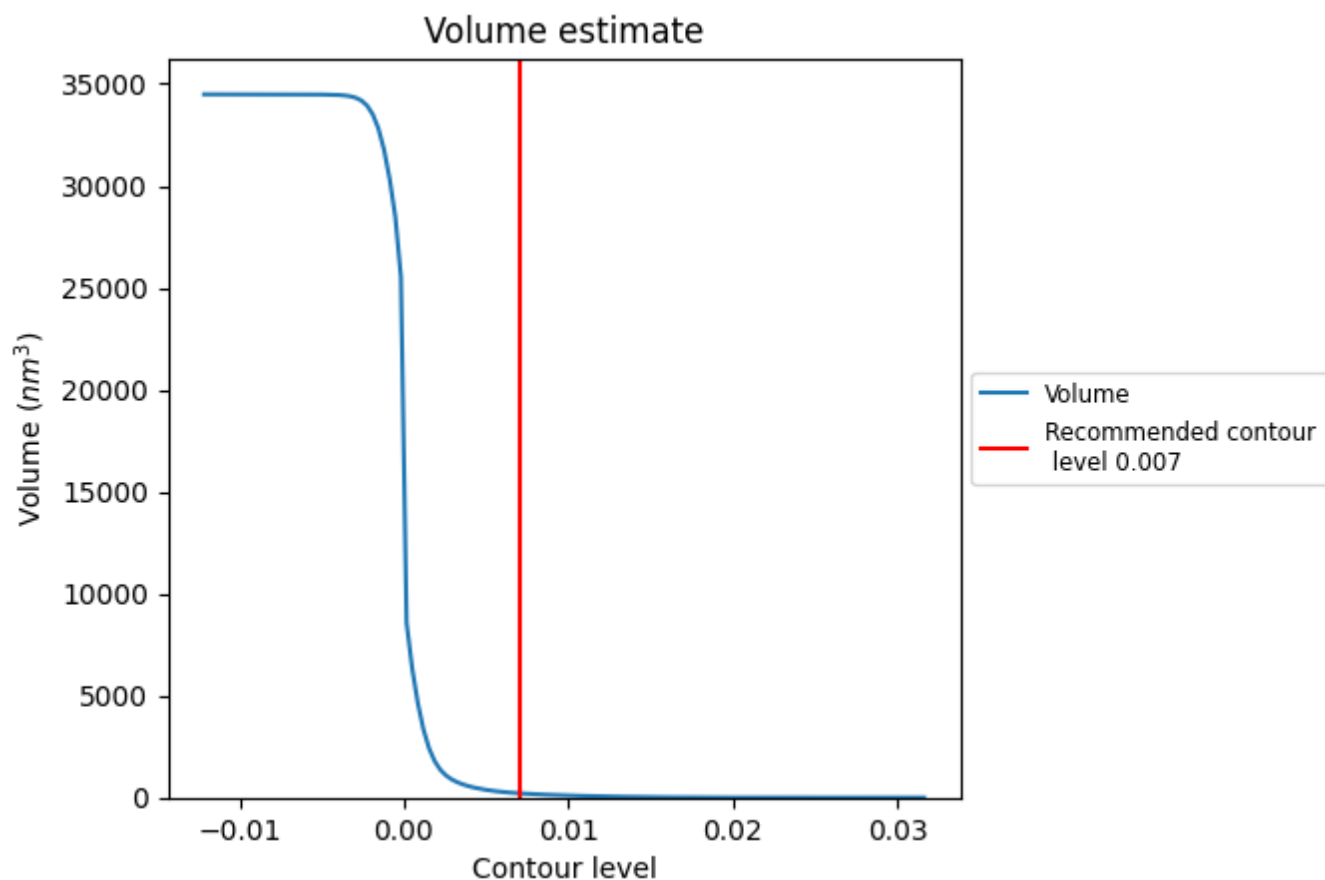
This section contains the results of statistical analysis of the map.

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.

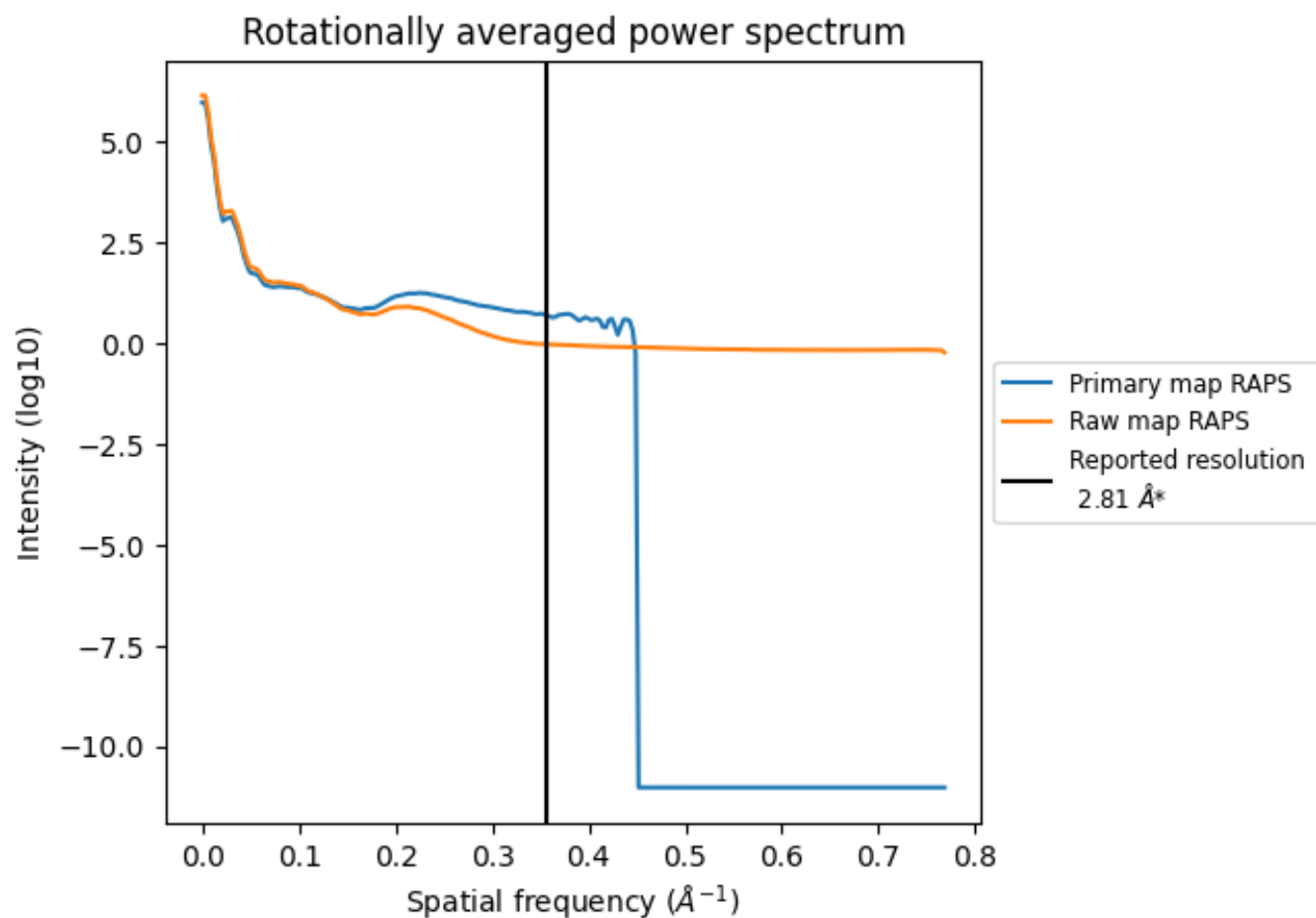
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm³; this corresponds to an approximate mass of 190 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 ⓘ

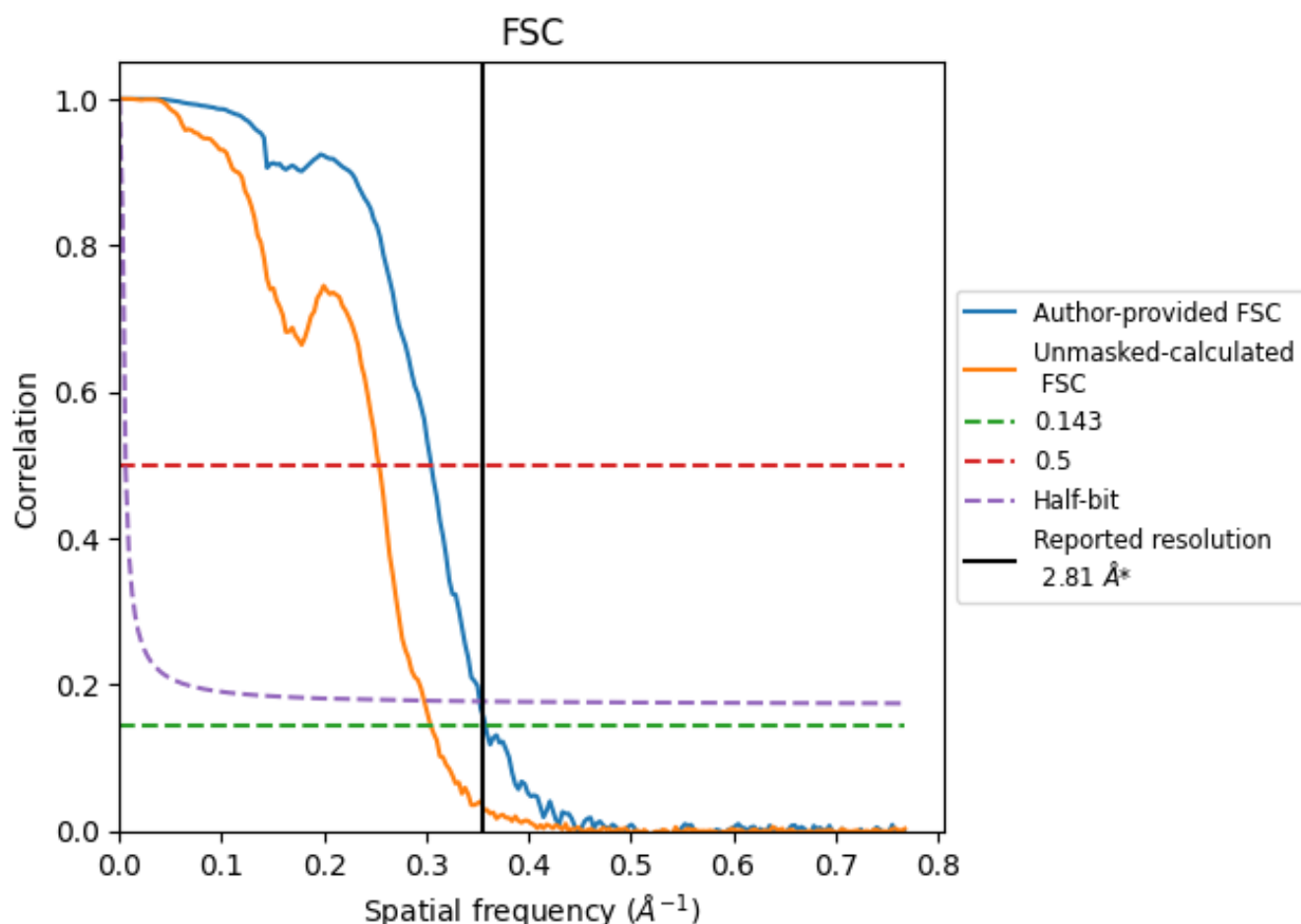


*Reported resolution corresponds to spatial frequency of 0.356 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.356 \AA^{-1}

8.2 Resolution estimates [i](#)

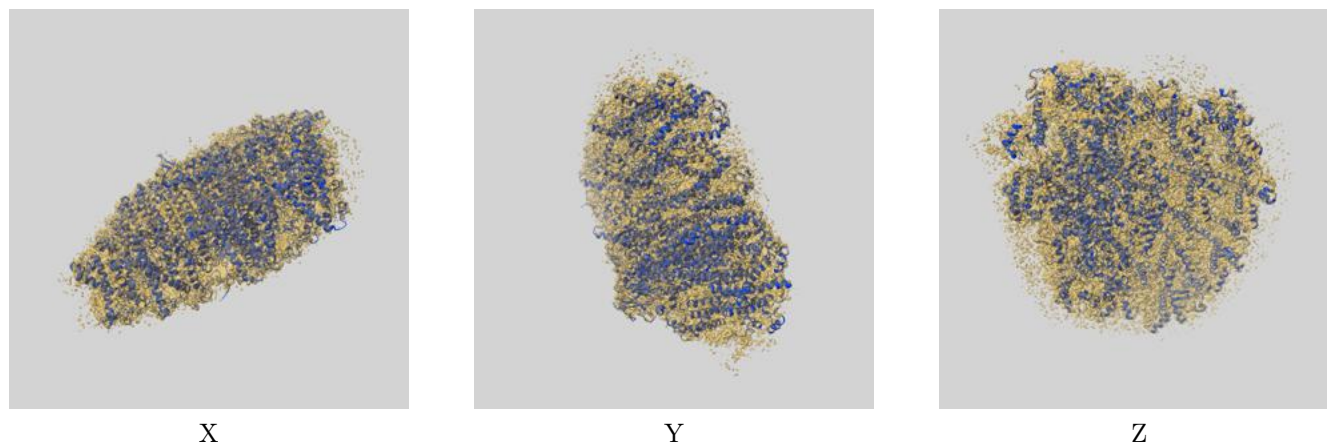
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.79	3.28	2.84
Unmasked-calculated*	3.28	3.94	3.36

*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 3.28 differs from the reported value 2.81 by more than 10 %

9 Map-model fit [i](#)

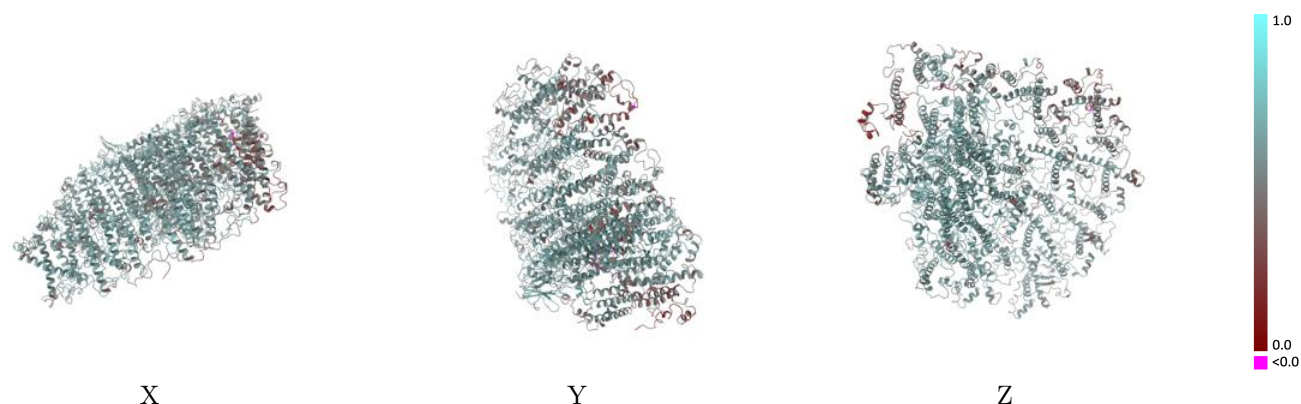
This section contains information regarding the fit between EMDB map EMD-16732 and PDB model 8CMO. Per-residue inclusion information can be found in section [3](#) on page [41](#).

9.1 Map-model overlay [i](#)



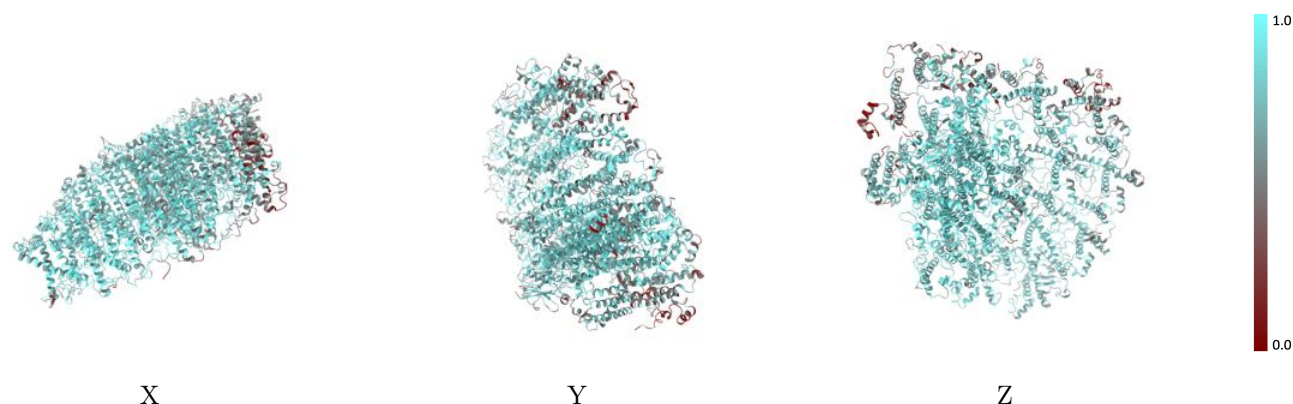
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



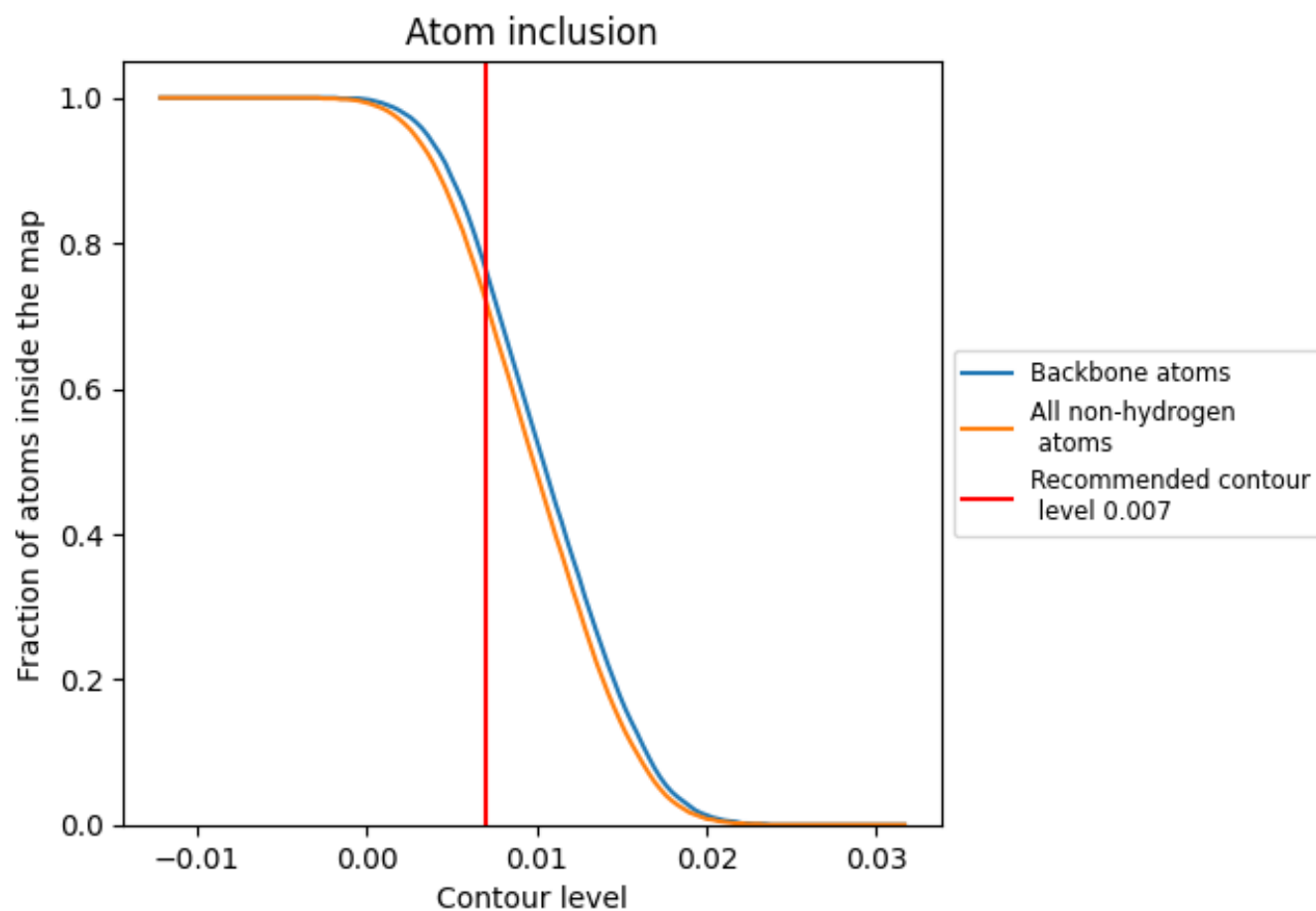
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7200	<div></div> 0.5370
1	<div></div> 0.6350	<div></div> 0.4980
2	<div></div> 0.3310	<div></div> 0.3380
3	<div></div> 0.7710	<div></div> 0.5610
4	<div></div> 0.6470	<div></div> 0.5050
5	<div></div> 0.6780	<div></div> 0.5150
6	<div></div> 0.6810	<div></div> 0.5140
7	<div></div> 0.7840	<div></div> 0.5510
8	<div></div> 0.7410	<div></div> 0.5310
9	<div></div> 0.5380	<div></div> 0.4770
A	<div></div> 0.8270	<div></div> 0.5920
B	<div></div> 0.8210	<div></div> 0.5830
C	<div></div> 0.7720	<div></div> 0.6020
D	<div></div> 0.6520	<div></div> 0.5660
E	<div></div> 0.6830	<div></div> 0.5660
F	<div></div> 0.6980	<div></div> 0.5310
G	<div></div> 0.4660	<div></div> 0.4150
I	<div></div> 0.6720	<div></div> 0.5270
J	<div></div> 0.7000	<div></div> 0.5310
K	<div></div> 0.7110	<div></div> 0.5230
L	<div></div> 0.6550	<div></div> 0.5030
Z	<div></div> 0.4730	<div></div> 0.4100

