



wwPDB EM Validation Summary Report ⓘ

Sep 10, 2026 – 10:09 pm BST

PDB ID : 8CMO / pdb_00008cmo
EMDB ID : EMD-16732
Title : Cryo-EM structure of the Photosystem I - LHCI supercomplex from Coelastrella sp.
Authors : Fadeeva, M.; Klaiman, D.; Nelson, N.; Khozin-Goldberg, I.; Zorin, B.
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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

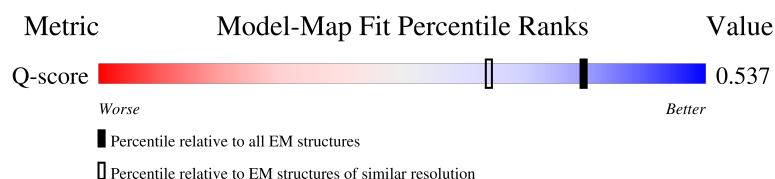
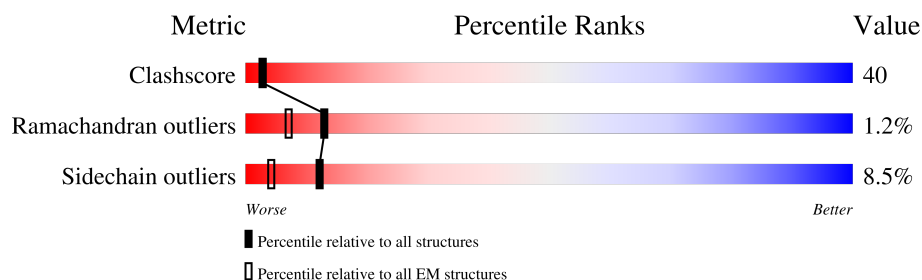
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11740 (2.31 - 3.31)

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	

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Mol	Chain	Length	Quality of chain
5	E	61	
6	F	165	
7	G	93	
8	I	41	
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
22	CLA	3	312	-	-	X	-
22	CLA	3	313	-	-	X	-
22	CLA	5	307	-	-	X	-
22	CLA	5	308	-	-	X	-
22	CLA	6	309	-	-	X	-
22	CLA	8	305	-	-	X	-
22	CLA	A	812	-	-	X	-
22	CLA	A	814	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	816	-	-	X	-
22	CLA	A	821	-	-	X	-
22	CLA	A	822	-	-	X	-
22	CLA	A	823	-	-	X	-
22	CLA	B	811	-	-	X	-
22	CLA	B	812	X	-	-	-
22	CLA	B	815	-	-	X	-
22	CLA	B	825	-	-	X	-
22	CLA	B	827	-	-	X	-
22	CLA	B	842	-	-	X	-
22	CLA	F	304	-	-	X	-
22	CLA	Z	303	-	-	X	-
22	CLA	Z	309	-	-	X	-
22	CLA	Z	313	-	-	X	-
24	BCR	3	304	-	X	-	-
24	BCR	3	307	-	X	-	-
24	BCR	4	804	-	-	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	848	-	X	-	-
24	BCR	B	853	-	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	4	816	-	-	X	-
39	CHL	6	315	-	-	X	-
39	CHL	8	315	-	-	X	-
39	CHL	9	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		

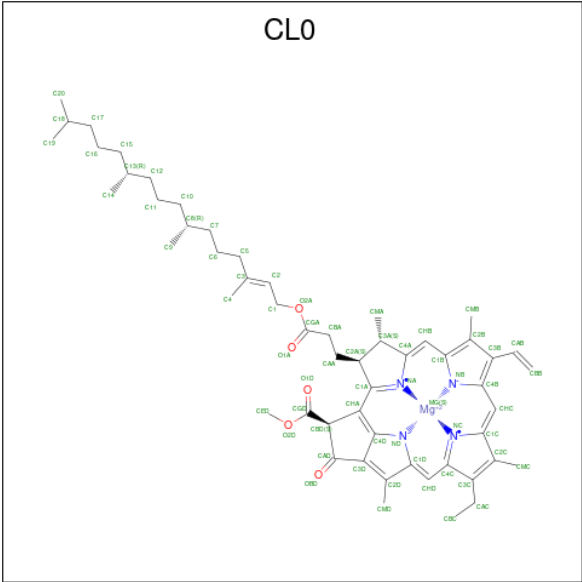
- Molecule 19 is a protein called Light-harvesting protein of photosystem I Lhca9.

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.

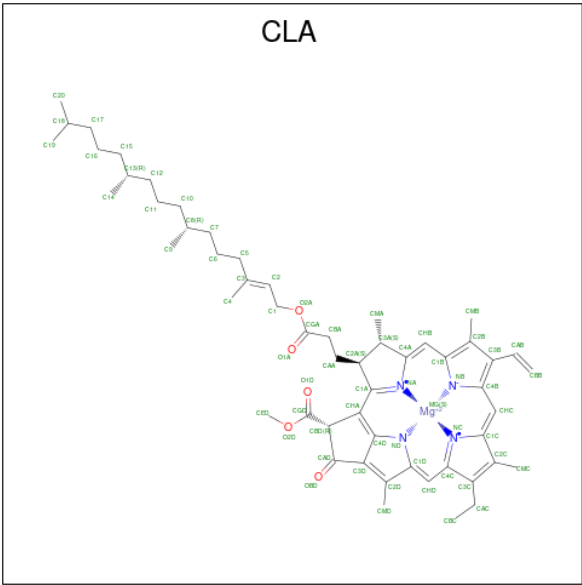
Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	70	Total	C	N	O	S	0	0
			525	336	90	94	5		

- Molecule 21 is CHLOROPHYLL A ISOMER (CCD ID: 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 (CCD ID: 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 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 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 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	A	1	Total 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 52	C 42	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 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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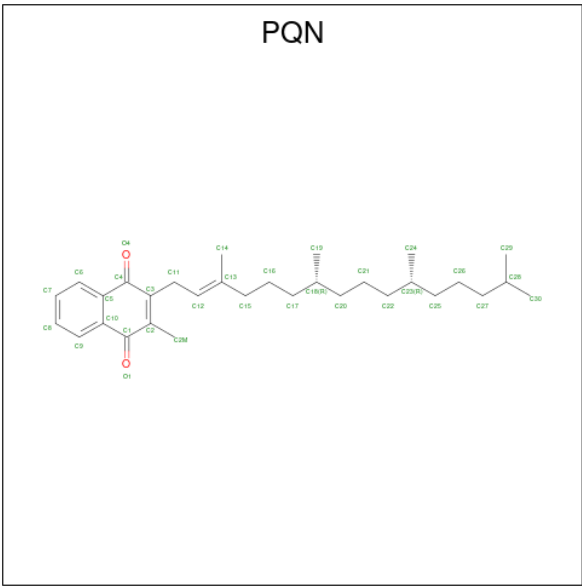
Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	5	1	Total 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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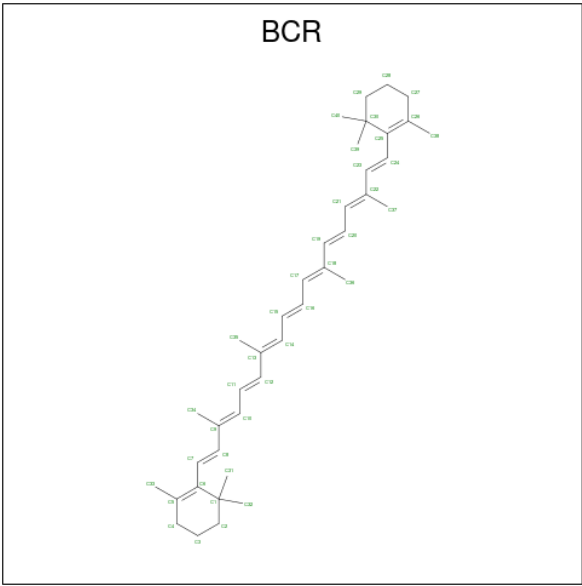
Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			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 (CCD ID: 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 (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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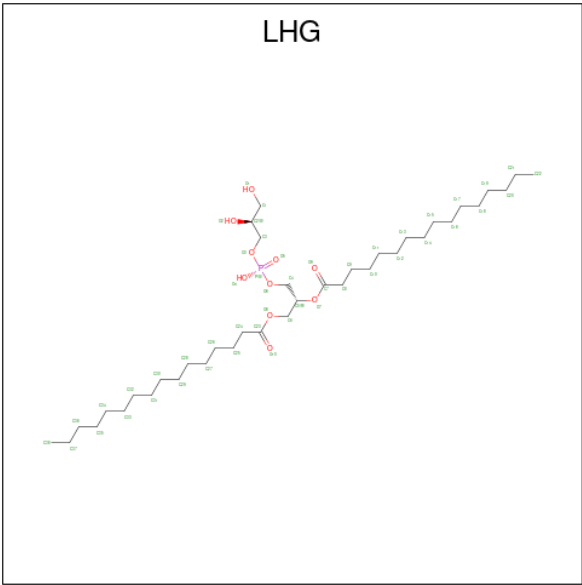
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 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 (CCD ID: 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

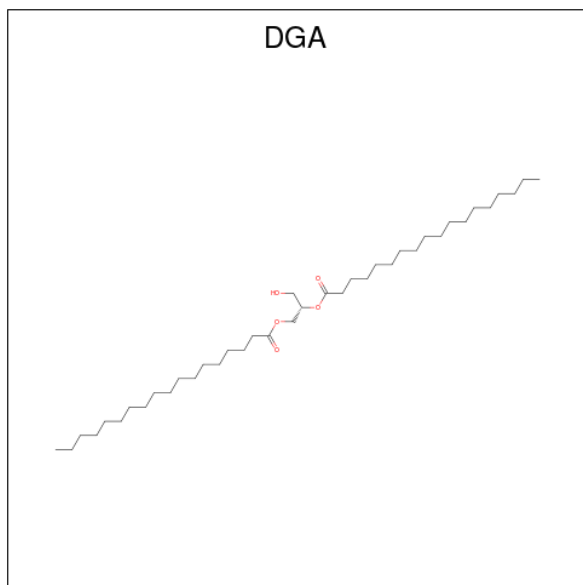
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Mol	Chain	Residues	Atoms				AltConf
25	B	1	Total 23	C 12	O 10	P 1	0
25	B	1	Total 20	C 9	O 10	P 1	0
25	1	1	Total 43	C 32	O 10	P 1	0
25	Z	1	Total 43	C 32	O 10	P 1	0
25	3	1	Total 20	C 9	O 10	P 1	0
25	7	1	Total 37	C 26	O 10	P 1	0
25	8	1	Total 38	C 27	O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

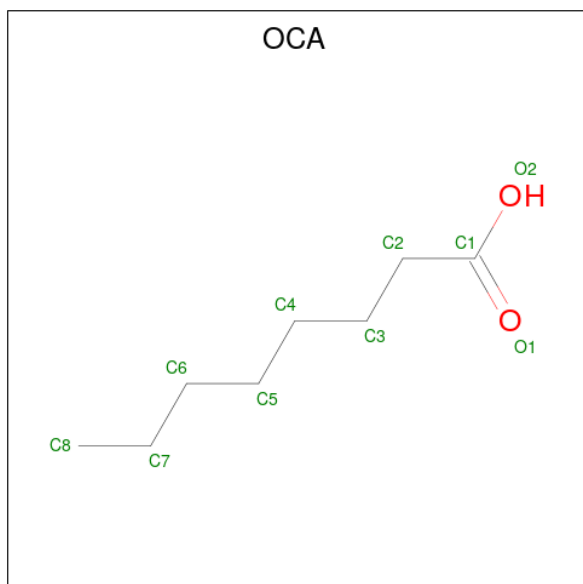
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			23	15	7	1	
26	8	1	Total	C	O	P	0
			29	21	7	1	

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



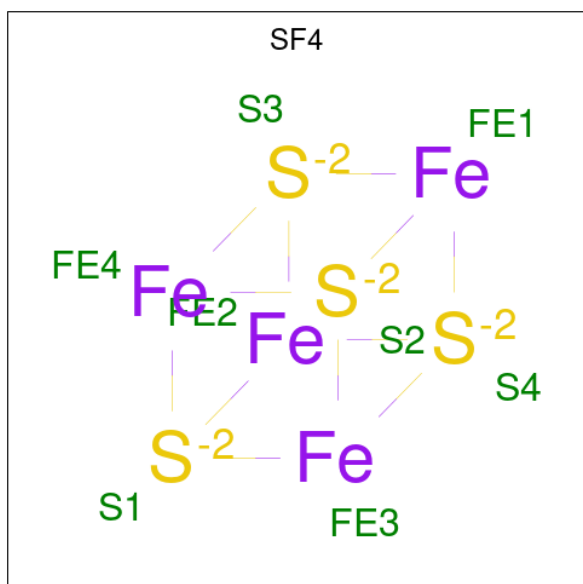
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O		0
			40	35	5		

- Molecule 28 is OCTANOIC ACID (CAPRYLIC ACID) (CCD ID: 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 (CCD ID: SF4) (formula: Fe_4S_4).

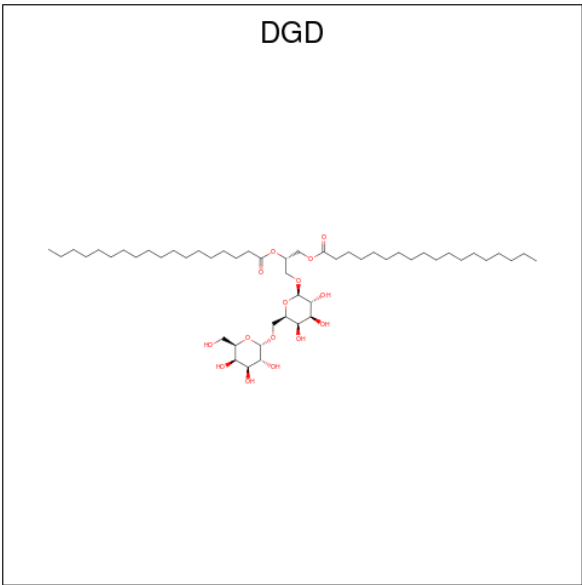


Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is CALCIUM ION (CCD ID: CA) (formula: Ca).

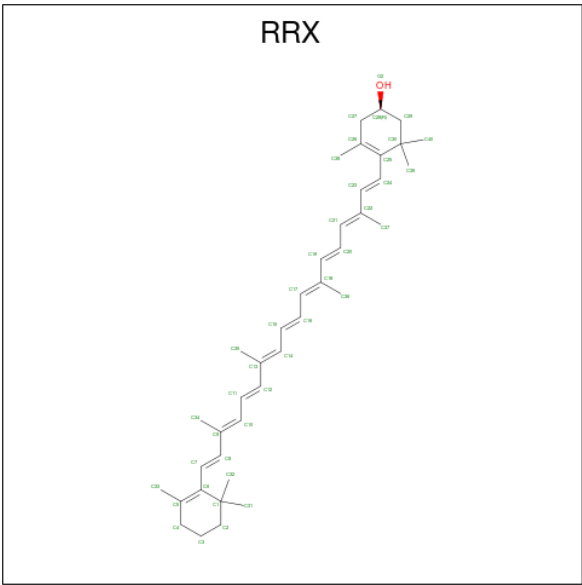
Mol	Chain	Residues	Atoms		AltConf
30	B	1	Total	Ca	0
			1	1	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$).



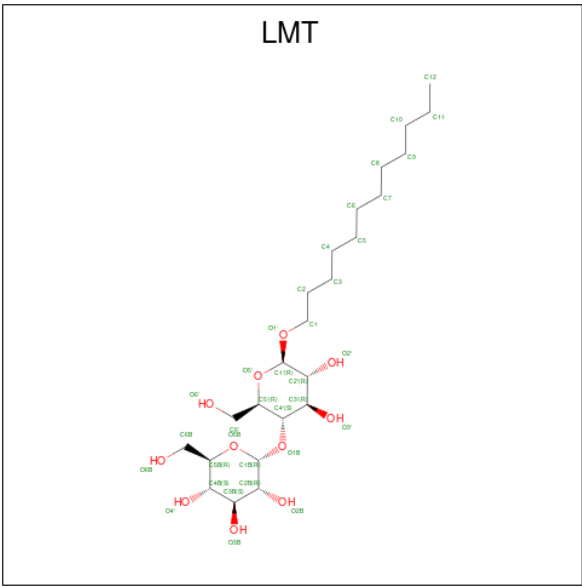
Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			61	46	15	
31	1	1	Total	C	O	0
			51	36	15	
31	3	1	Total	C	O	0
			51	36	15	

- Molecule 32 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



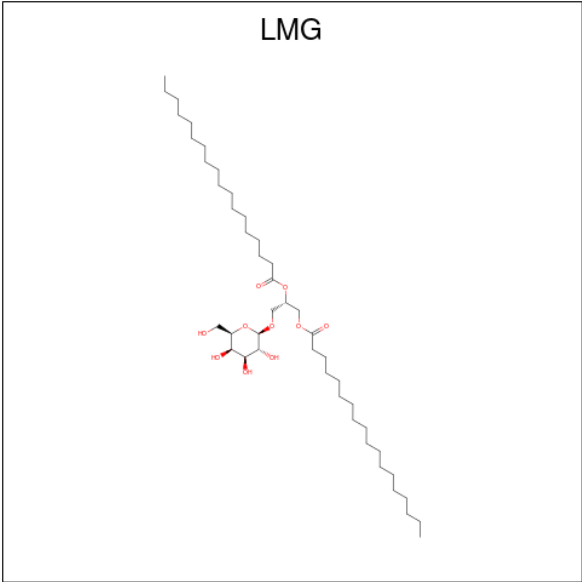
Mol	Chain	Residues	Atoms			AltConf
32	F	1	Total	C	O	0
			41	40	1	

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



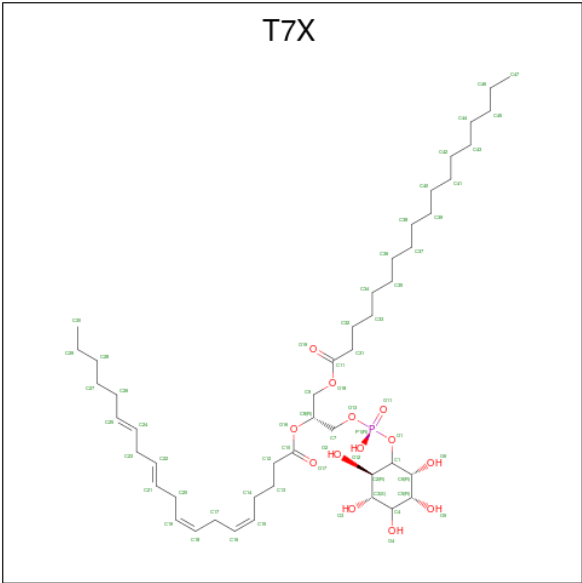
Mol	Chain	Residues	Atoms			AltConf
33	F	1	Total	C	O	0
			35	24	11	
33	G	1	Total	C	O	0
			35	24	11	
33	1	1	Total	C	O	0
			35	24	11	
33	4	1	Total	C	O	0
			35	24	11	
33	4	1	Total	C	O	0
			35	24	11	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



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	

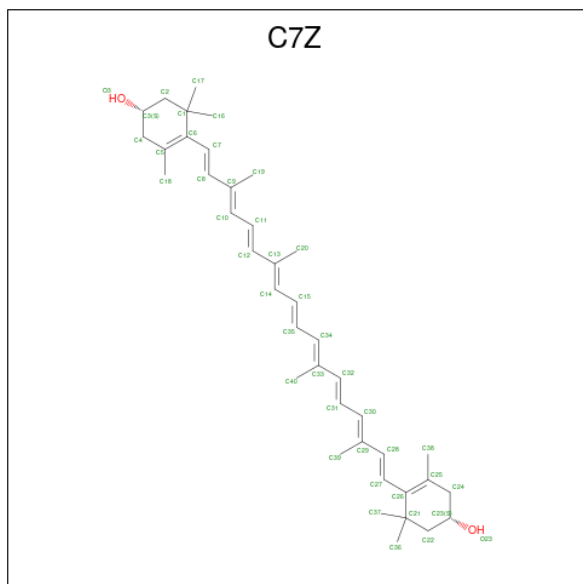
- Molecule 35 is Phosphatidylinositol (CCD ID: T7X) (formula: C₄₇H₈₃O₁₃P).



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

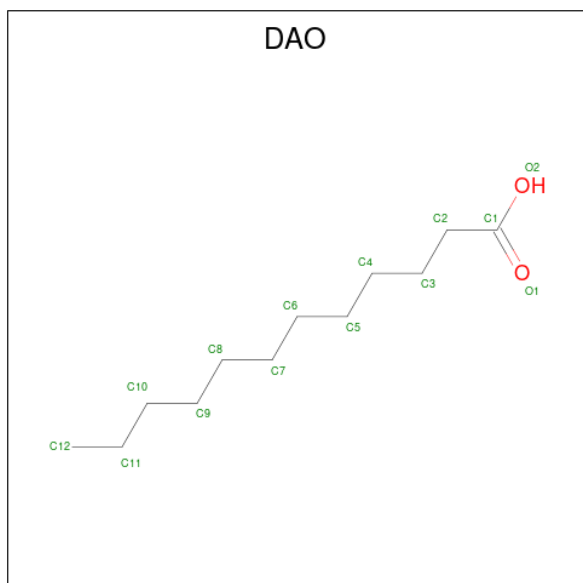
- Molecule 36 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},

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 (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



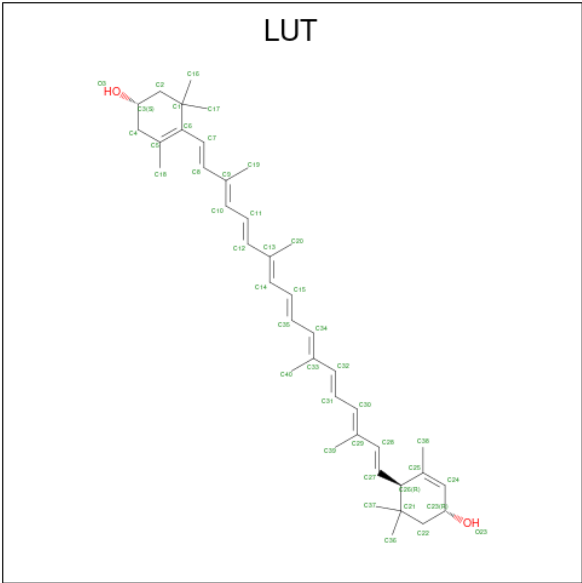
Mol	Chain	Residues	Atoms			AltConf
36	J	1	Total	C	O	0
			42	40	2	
36	5	1	Total	C	O	0
			42	40	2	

- Molecule 37 is LAURIC ACID (CCD ID: 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 (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



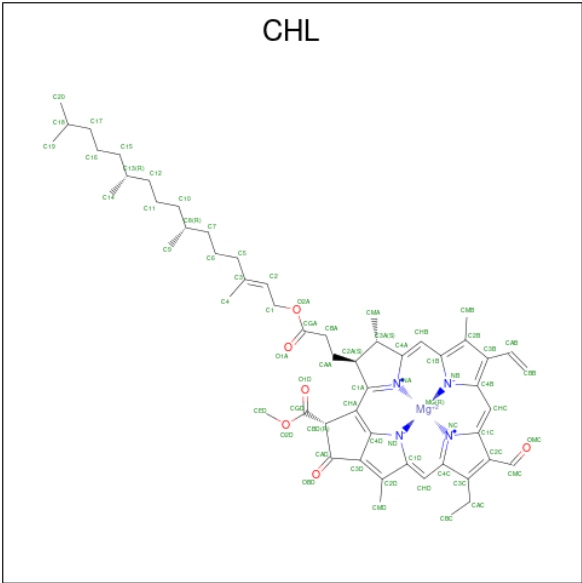
Mol	Chain	Residues	Atoms			AltConf
38	1	1	Total	C	O	0
			42	40	2	
38	1	1	Total	C	O	0
			42	40	2	
38	Z	1	Total	C	O	0
			42	40	2	
38	Z	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	3	1	Total	C	O	0
			42	40	2	
38	7	1	Total	C	O	0
			42	40	2	
38	7	1	Total	C	O	0
			42	40	2	
38	8	1	Total	C	O	0
			42	40	2	
38	8	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
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 (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



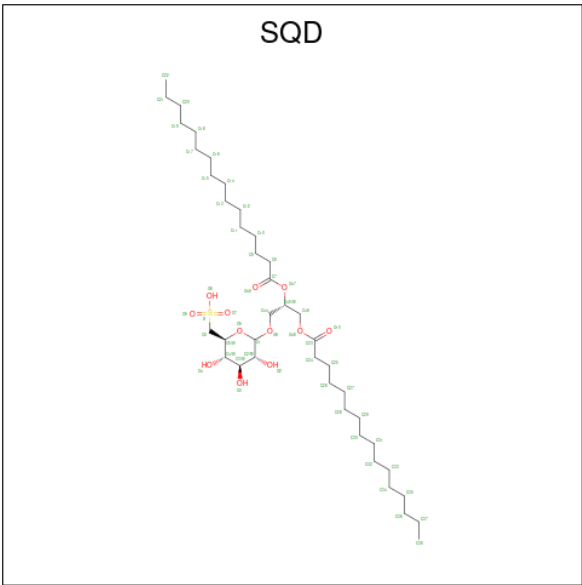
Mol	Chain	Residues	Atoms					AltConf
39	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
39	Z	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
39	Z	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

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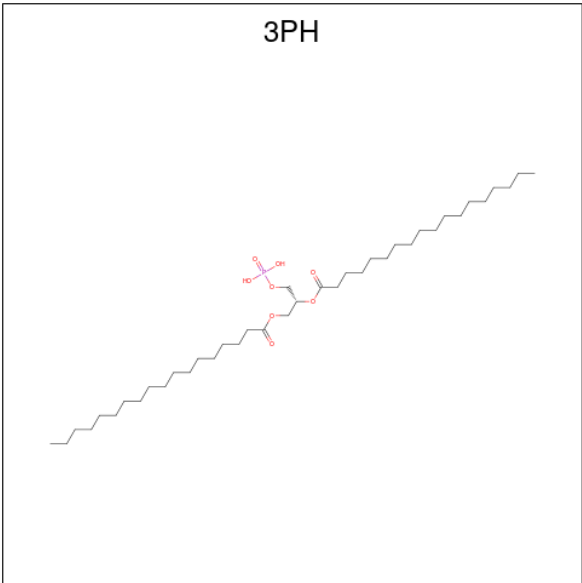
Mol	Chain	Residues	Atoms					AltConf
39	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	7	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
39	8	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
39	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
39	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
39	4	1	Total	C	Mg	N	O	0
			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	
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 (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



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 (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



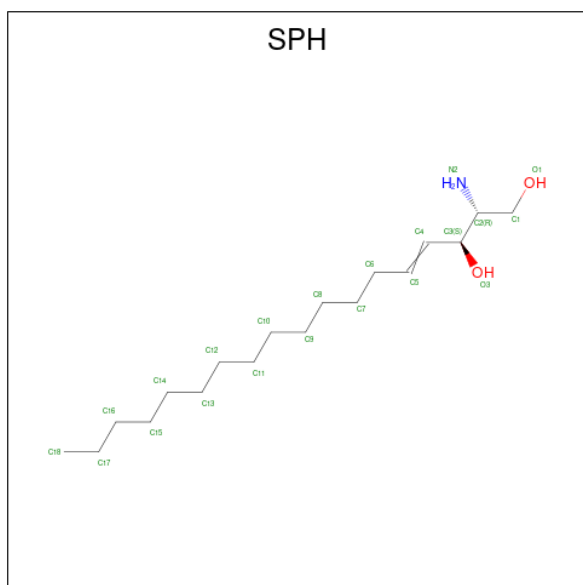
Mol	Chain	Residues	Atoms				AltConf
41	7	1	Total	C	O	P	0
			39	30	8	1	
41	8	1	Total	C	O	P	0
			30	21	8	1	

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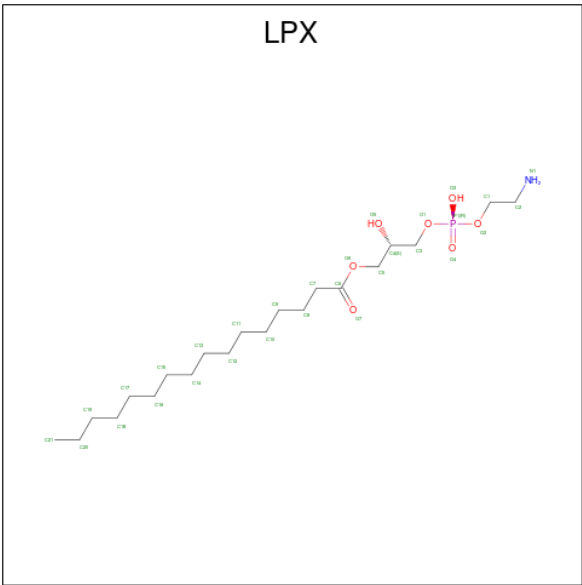
Mol	Chain	Residues	Atoms				AltConf
41	5	1	Total	C	O	P	0
			23	14	8	1	
41	6	1	Total	C	O	P	0
			29	20	8	1	

- Molecule 42 is SPHINGOSINE (CCD ID: 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 (CCD ID: LPX) (formula: $C_{21}H_{44}NO_7P$).



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	
44	1	1	Total	O	0
			1	1	
44	Z	1	Total	O	0
			1	1	
44	3	2	Total	O	0
			2	2	
44	7	4	Total	O	0
			4	4	
44	8	4	Total	O	0
			4	4	

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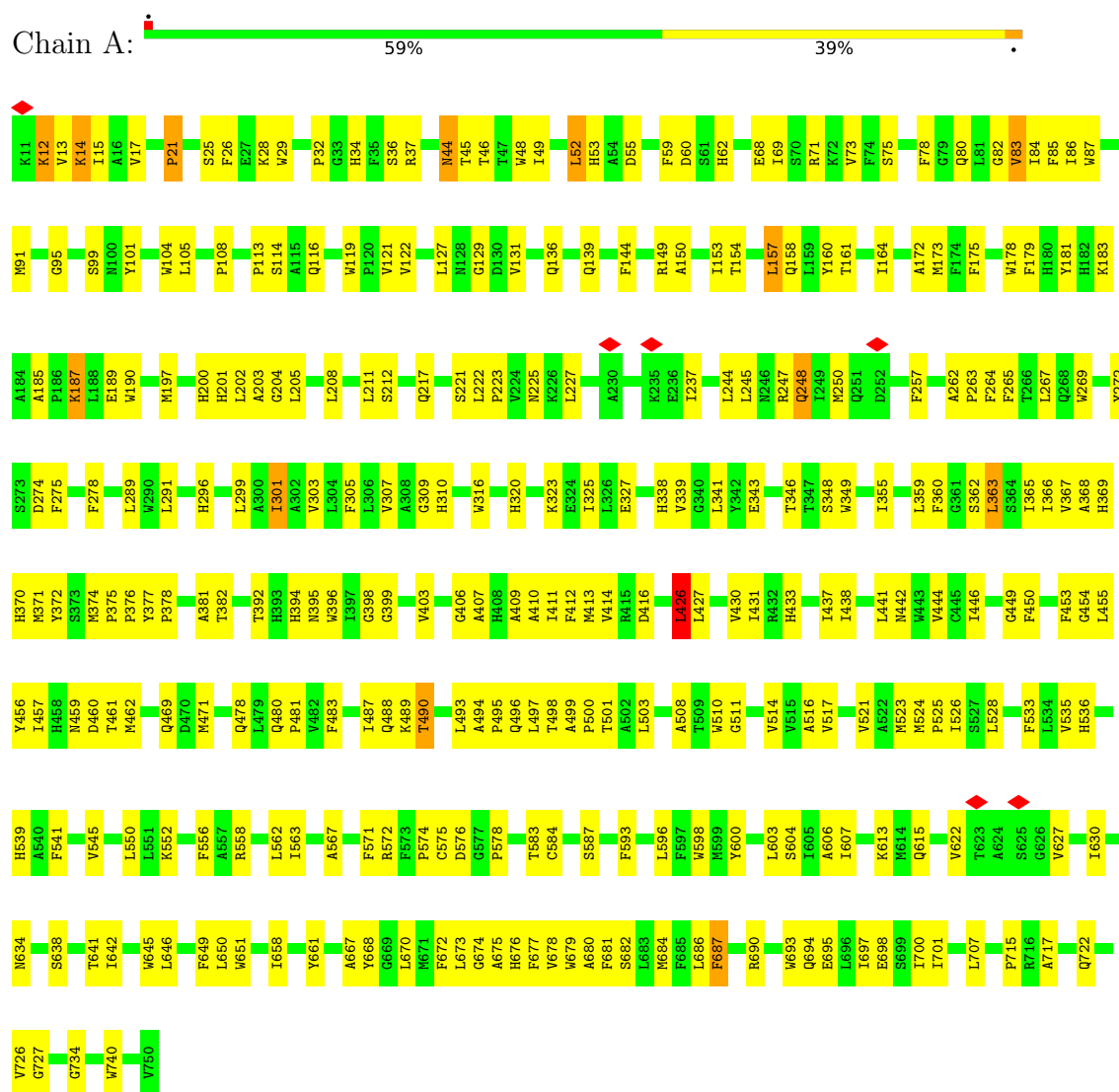
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Mol	Chain	Residues	Atoms		AltConf
44	4	5	Total 5	O 5	0
44	5	5	Total 5	O 5	0
44	6	3	Total 3	O 3	0
44	2	1	Total 1	O 1	0

3 Residue-property plots

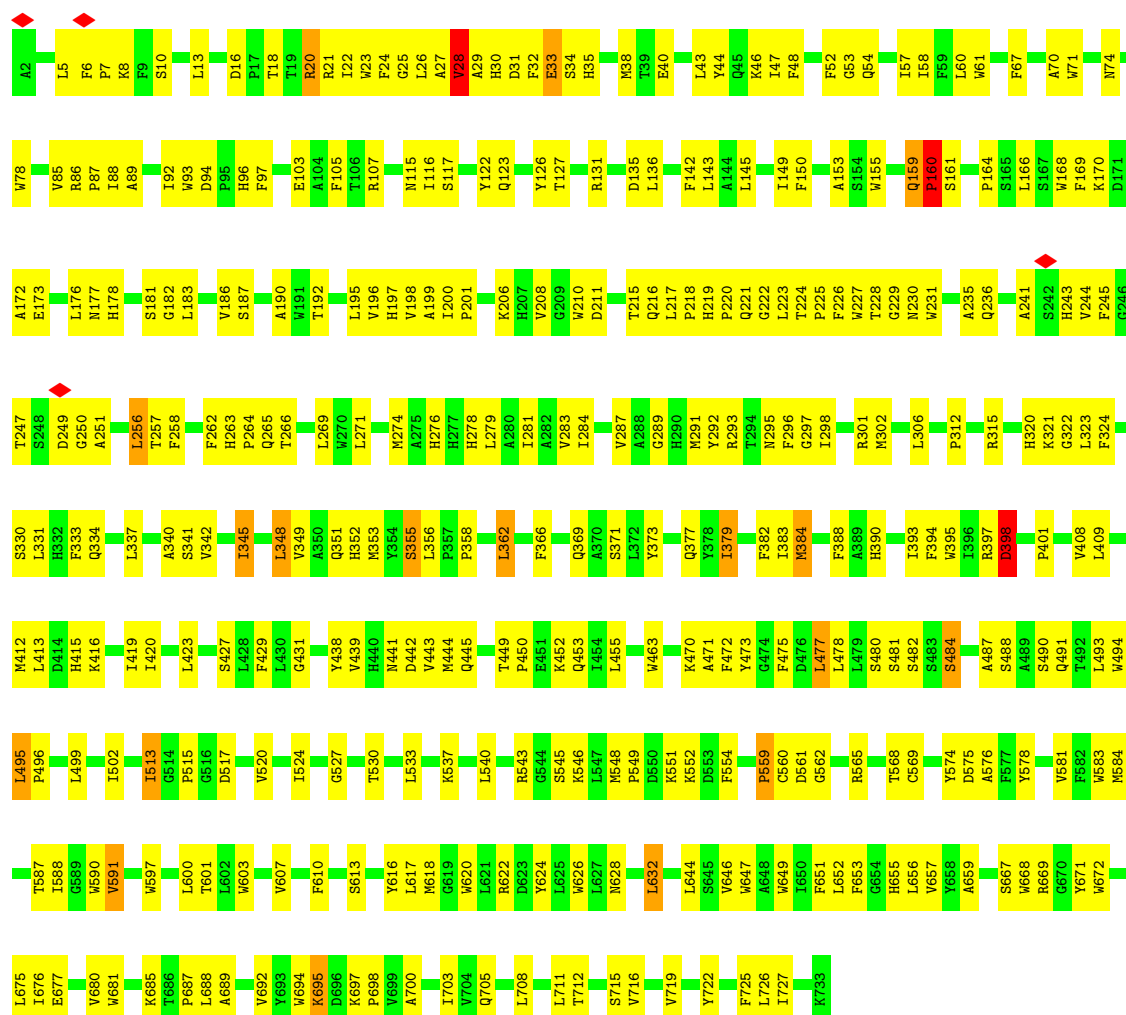
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



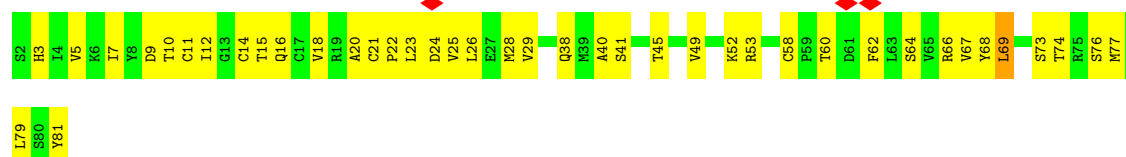
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 PsaB





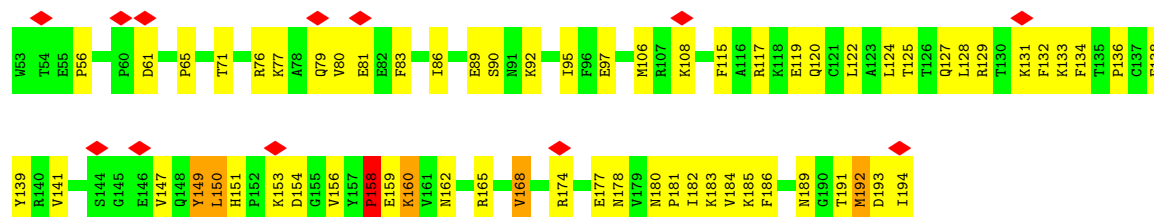
• Molecule 3: Photosystem I subunit VII Psac

Chain C: 49% 50%

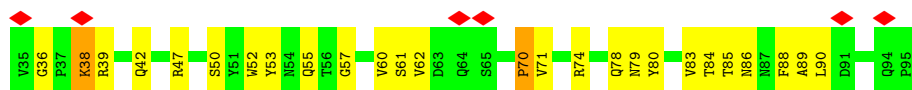


• Molecule 4: Photosystem I reaction center subunit II Psad

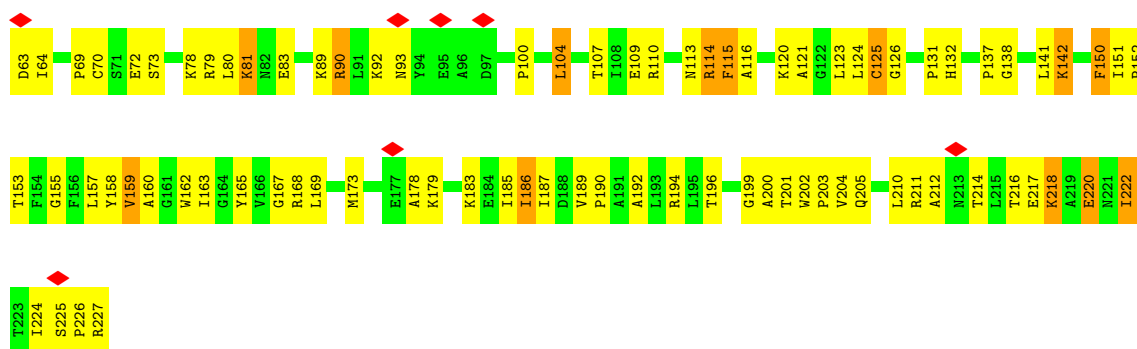
Chain D: 8% 55% 41%



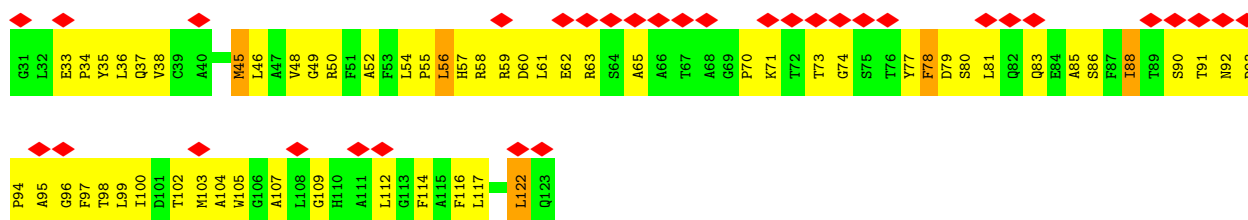
- Molecule 5: Photosystem I reaction center subunit IV PsaE



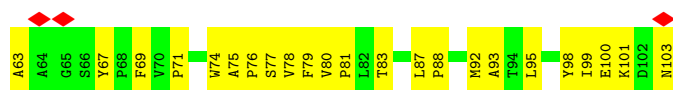
- Molecule 6: Photosystem I reaction center subunit III PsaF



- Molecule 7: Photosystem I reaction center subunit V PsaG



- Molecule 8: Photosystem I reaction center subunit VIII PsaI



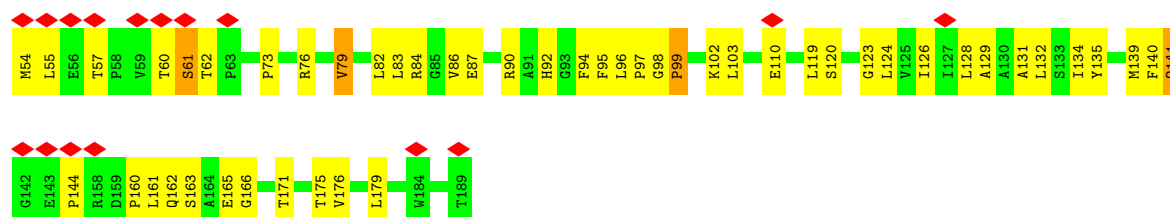
- Molecule 9: Photosystem I subunit IX PsaJ



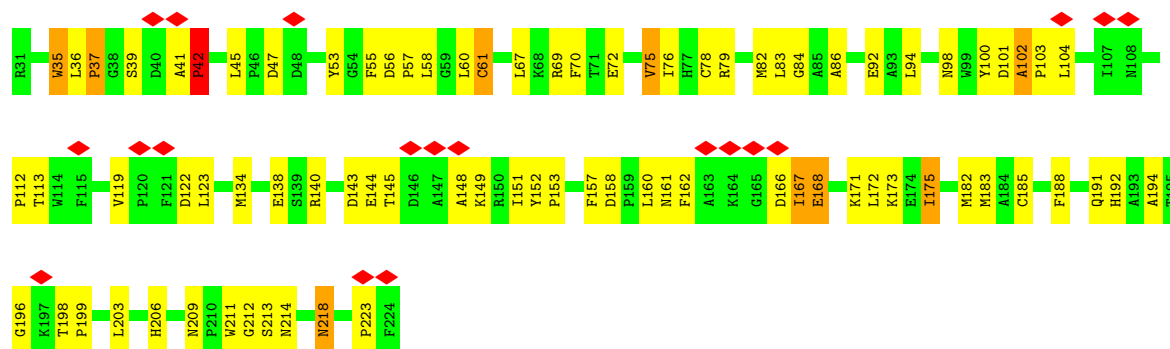
- Molecule 10: Photosystem I reaction center subunit X psaK



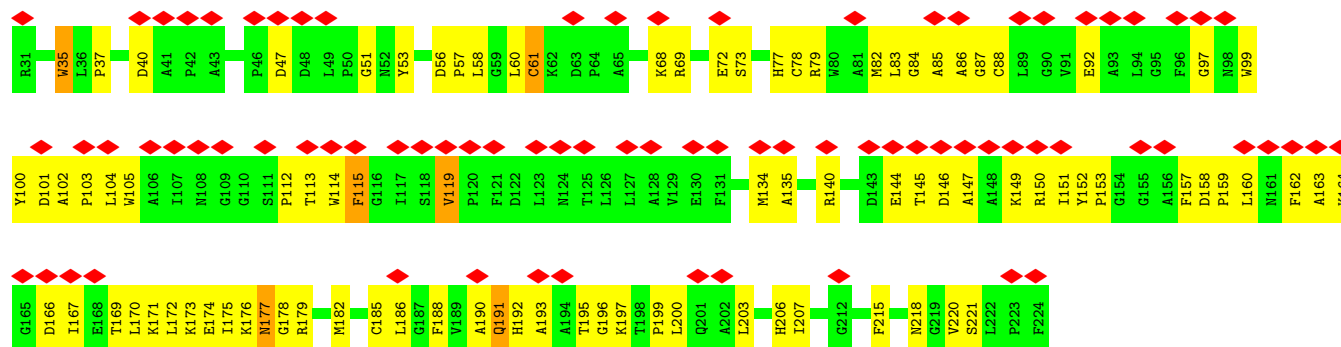
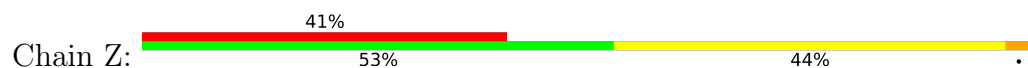
- Molecule 11: Photosystem I reaction centre subunit XI PsaL



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

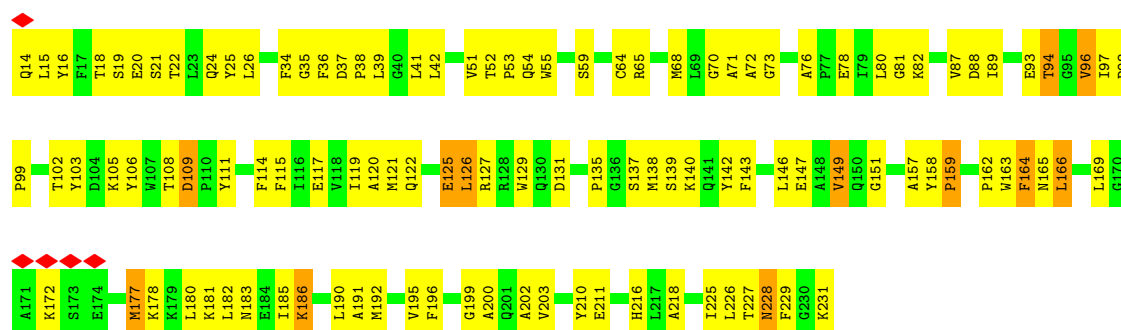


- Molecule 12: Light-harvesting protein of photosystem I Lhca1

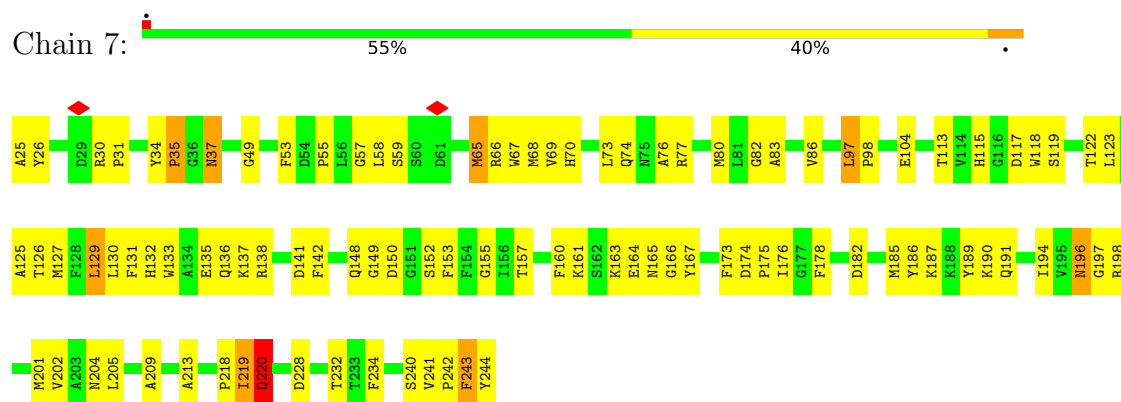


- Molecule 13: Light-harvesting protein of photosystem I Lhca3





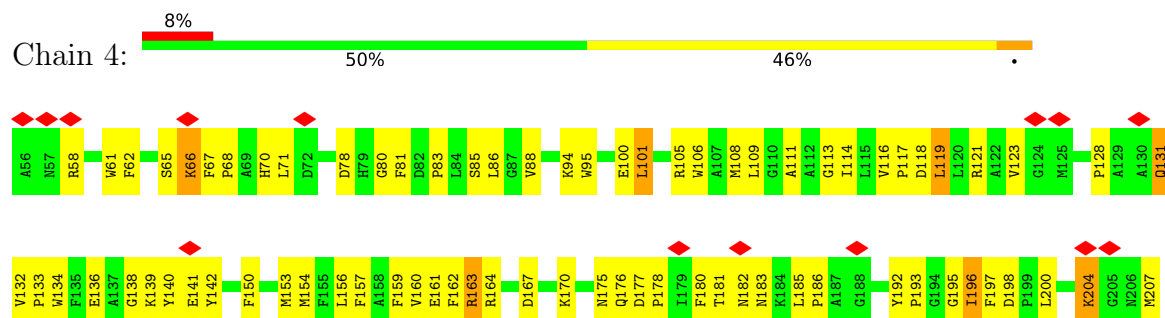
- Molecule 14: Light-harvesting protein of photosystem I Lhca7



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

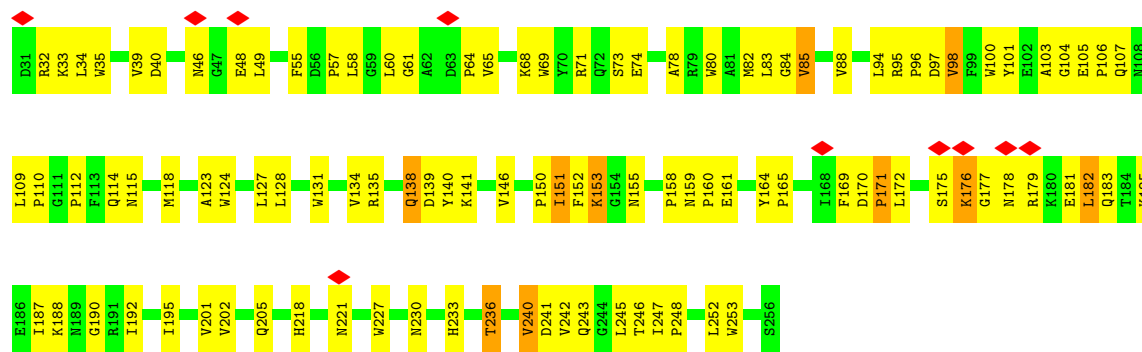


- Molecule 16: Light-harvesting protein of photosystem I Lhca4

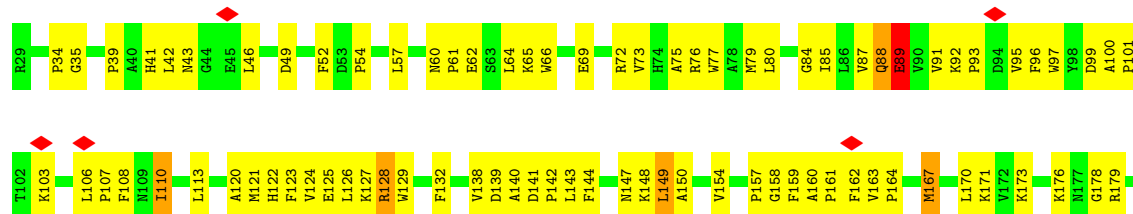




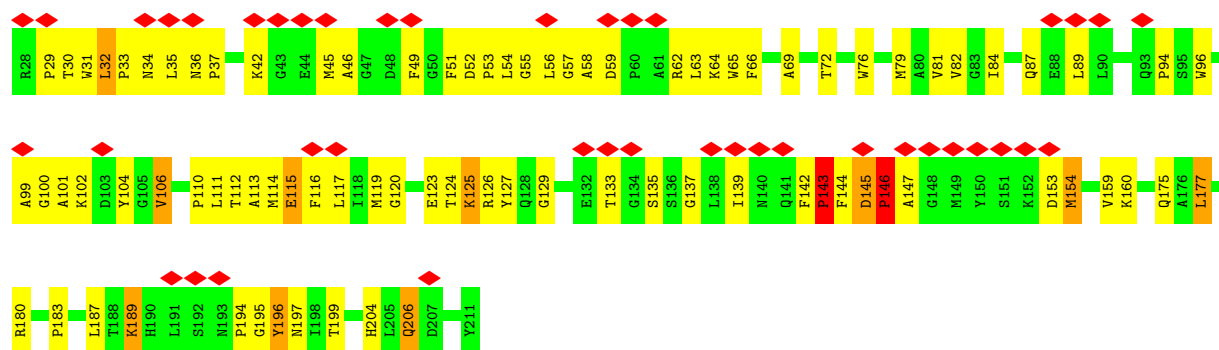
- Molecule 17: Light-harvesting protein of photosystem I Lhca5



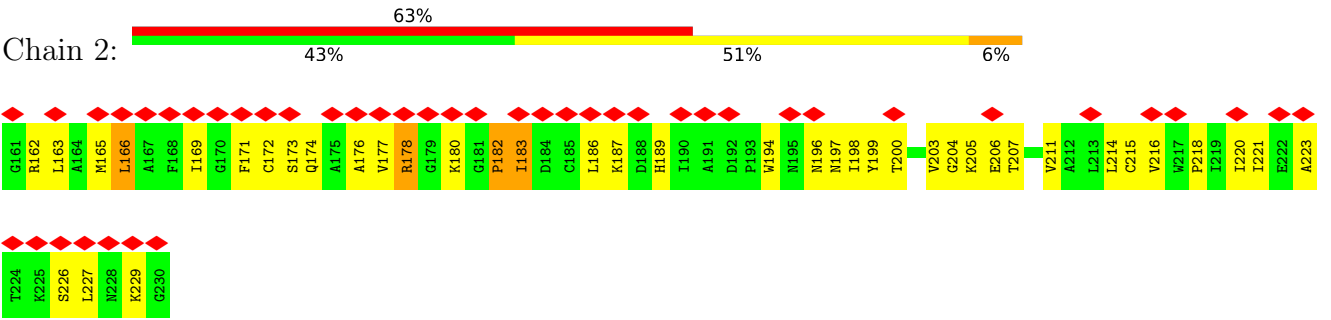
- Molecule 18: Light-harvesting protein of photosystem I Lhca6



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



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



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	TFS 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 ($\text{\AA}$)	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 ($\text{\AA}$)	0.651, 0.651, 0.651	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.91	0/6016	1.13	8/8200 (0.1%)
2	B	0.92	0/6010	1.13	3/8207 (0.0%)
3	C	0.98	0/613	1.15	0/830
4	D	0.89	0/1159	1.17	1/1569 (0.1%)
5	E	0.98	0/495	1.09	0/675
6	F	0.92	0/1292	1.25	3/1755 (0.2%)
7	G	0.95	0/706	1.20	1/960 (0.1%)
8	I	0.97	0/320	1.11	0/443
9	J	0.96	0/329	1.20	0/452
10	K	1.00	0/625	1.27	0/848
11	L	0.97	0/919	1.26	0/1253
12	1	0.91	0/1501	1.28	3/2045 (0.1%)
12	Z	0.78	0/1501	1.03	1/2045 (0.0%)
13	3	0.93	0/1747	1.21	2/2376 (0.1%)
14	7	0.93	0/1765	1.22	1/2407 (0.0%)
15	8	0.94	0/1643	1.24	2/2226 (0.1%)
16	4	0.92	0/1648	1.19	0/2240
17	5	0.92	0/1819	1.21	0/2480
18	6	0.92	0/1824	1.14	1/2488 (0.0%)
19	9	0.85	0/1456	1.30	5/1975 (0.3%)
20	2	0.96	0/535	1.24	0/726
All	All	0.92	0/33923	1.18	31/46200 (0.1%)

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	9	143	PRO	CA-N-CD	-11.78	95.51	112.00
12	1	42	PRO	CA-N-CD	-9.96	98.06	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	9	189	LYS	N-CA-C	-7.90	105.61	114.62
19	9	143	PRO	CB-CA-C	7.80	124.43	111.56
19	9	146	PRO	CA-N-CD	-7.61	101.35	112.00

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	295	0
2	B	5800	0	5556	371	0
3	C	603	0	587	41	0
4	D	1129	0	1127	46	0
5	E	484	0	477	25	0
6	F	1265	0	1292	75	0
7	G	690	0	671	69	0
8	I	308	0	310	31	0
9	J	319	0	327	23	0
10	K	617	0	635	54	0
11	L	897	0	891	48	0
12	1	1457	0	1406	79	0
12	Z	1457	0	1406	119	0
13	3	1695	0	1641	143	0
14	7	1705	0	1601	104	0
15	8	1602	0	1600	138	0
16	4	1598	0	1569	116	0
17	5	1764	0	1709	126	0
18	6	1762	0	1740	180	0
19	9	1416	0	1392	104	0
20	2	525	0	539	46	0
21	A	65	0	72	7	0
22	1	698	0	678	106	0
22	2	146	0	112	30	0
22	3	749	0	722	153	0
22	4	590	0	511	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	5	910	0	851	191	0
22	6	824	0	800	183	0
22	7	905	0	848	123	0
22	8	555	0	502	111	0
22	9	528	0	451	66	0
22	A	2640	0	2709	508	0
22	B	2340	0	2333	452	0
22	F	240	0	245	60	0
22	G	96	0	70	26	0
22	J	42	0	30	1	0
22	K	205	0	166	28	0
22	L	180	0	180	37	0
22	Z	679	0	631	147	0
23	A	33	0	46	10	0
23	B	33	0	46	5	0
24	3	160	0	224	59	0
24	4	40	0	56	26	0
24	5	80	0	112	30	0
24	6	80	0	112	35	0
24	7	40	0	56	14	0
24	8	40	0	56	14	0
24	A	240	0	336	98	0
24	B	280	0	392	103	0
24	F	40	0	56	14	0
24	G	40	0	56	12	0
24	I	40	0	56	12	0
24	J	40	0	56	18	0
24	K	40	0	55	12	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	19	0
25	5	37	0	44	7	0
25	6	49	0	74	11	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	13	0
25	B	76	0	64	15	0
25	Z	43	0	56	9	0
26	8	29	0	39	7	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	6	0
29	C	16	0	0	7	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	7	0
33	4	70	0	92	9	0
33	F	35	0	46	5	0
33	G	35	0	46	10	0
34	F	35	0	40	1	0
34	J	29	0	28	10	0
35	J	49	0	0	2	0
36	5	42	0	0	1	0
36	J	42	0	0	2	0
37	K	14	0	23	8	0
38	1	84	0	112	26	0
38	3	84	0	112	28	0
38	4	84	0	112	34	0
38	5	84	0	112	32	0
38	6	84	0	112	24	0
38	7	84	0	112	29	0
38	8	84	0	112	28	0
38	9	84	0	112	33	0
38	Z	84	0	112	36	0
39	1	48	0	32	8	0
39	2	51	0	36	8	0
39	3	66	0	69	14	0
39	4	192	0	130	42	0
39	5	160	0	134	31	0
39	6	206	0	156	51	0
39	7	54	0	42	9	0
39	8	180	0	165	44	0
39	9	108	0	95	35	0
39	Z	99	0	68	23	0
40	1	48	0	62	12	0
41	5	23	0	19	3	0
41	6	29	0	31	5	0
41	7	39	0	51	14	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	4003	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 40.

The worst 5 of 4003 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
24:3:306:BCR:H21C	22:3:318:CLA:H91	1.25	1.06
24:5:304:BCR:H19C	22:5:319:CLA:HBA2	1.40	1.04
19:9:53:PRO:HD2	38:9:302:LUT:H23	1.42	1.02
38:6:304:LUT:H28	22:6:310:CLA:H61	1.39	1.02

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%)	36	64
2	B	730/732 (100%)	683 (94%)	42 (6%)	5 (1%)	18	45
3	C	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
4	D	140/142 (99%)	124 (89%)	13 (9%)	3 (2%)	5	18
5	E	59/61 (97%)	50 (85%)	8 (14%)	1 (2%)	7	23
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	17
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%)	11	34
11	L	119/123 (97%)	106 (89%)	11 (9%)	2 (2%)	7	23
12	1	192/194 (99%)	165 (86%)	23 (12%)	4 (2%)	5	18
12	Z	192/194 (99%)	181 (94%)	10 (5%)	1 (0%)	24	53
13	3	216/218 (99%)	195 (90%)	18 (8%)	3 (1%)	9	27
14	7	218/220 (99%)	202 (93%)	12 (6%)	4 (2%)	6	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%)	6	22
18	6	224/226 (99%)	212 (95%)	11 (5%)	1 (0%)	30	58
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%)	13	31

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%)	574 (95%)	28 (5%)	23	55
2	B	596/596 (100%)	566 (95%)	30 (5%)	22	53
3	C	70/70 (100%)	69 (99%)	1 (1%)	59	84
4	D	122/122 (100%)	107 (88%)	15 (12%)	4	15
5	E	54/54 (100%)	52 (96%)	2 (4%)	30	63
6	F	128/128 (100%)	101 (79%)	27 (21%)	1	3
7	G	69/69 (100%)	63 (91%)	6 (9%)	9	29
8	I	33/33 (100%)	33 (100%)	0	100	100
9	J	35/35 (100%)	34 (97%)	1 (3%)	37	71
10	K	60/60 (100%)	54 (90%)	6 (10%)	7	23
11	L	90/90 (100%)	76 (84%)	14 (16%)	2	8
12	1	144/144 (100%)	125 (87%)	19 (13%)	4	13
12	Z	144/144 (100%)	134 (93%)	10 (7%)	14	39
13	3	173/173 (100%)	159 (92%)	14 (8%)	11	32
14	7	169/169 (100%)	156 (92%)	13 (8%)	12	34
15	8	162/162 (100%)	137 (85%)	25 (15%)	2	9
16	4	162/162 (100%)	141 (87%)	21 (13%)	4	13
17	5	185/185 (100%)	166 (90%)	19 (10%)	7	22
18	6	184/184 (100%)	172 (94%)	12 (6%)	15	42
19	9	143/143 (100%)	125 (87%)	18 (13%)	4	14
20	2	57/57 (100%)	50 (88%)	7 (12%)	4	15
All	All	3382/3382 (100%)	3094 (92%)	288 (8%)	12	30

5 of 288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	4	257	SER
20	2	205	LYS

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Mol	Chain	Res	Type
17	5	97	ASP
18	6	211	MET
6	F	211	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
13	3	141	GLN
16	4	98	GLN
13	3	222	ASN
14	7	191	GLN
16	4	242	ASN

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	B	812	2	63,67,73	1.41	6 (9%)	75,105,113	1.95	18 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	I	4001	-	41,41,41	4.78	27 (65%)	56,56,56	2.58	19 (33%)
22	CLA	A	855	44	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
22	CLA	7	322	15	59,63,73	1.46	6 (10%)	71,101,113	2.04	19 (26%)
25	LHG	B	850	22	22,22,48	0.56	0	25,28,54	1.26	2 (8%)
22	CLA	2	301	-	59,63,73	1.46	6 (10%)	71,101,113	2.09	17 (23%)
38	LUT	7	301	-	42,43,43	6.06	28 (66%)	51,60,60	1.95	13 (25%)
39	CHL	4	819	16	47,51,74	0.94	2 (4%)	52,86,114	1.50	11 (21%)
22	CLA	5	311	17	59,63,73	1.47	7 (11%)	71,101,113	2.05	19 (26%)
22	CLA	7	306	14	69,73,73	1.35	6 (8%)	83,113,113	2.00	19 (22%)
38	LUT	Z	302	-	42,43,43	6.09	27 (64%)	51,60,60	2.05	13 (25%)
22	CLA	A	837	1	55,59,73	1.52	6 (10%)	66,96,113	2.12	18 (27%)
22	CLA	B	817	2	61,65,73	1.44	6 (9%)	73,103,113	2.02	17 (23%)
22	CLA	B	824	2	63,67,73	1.42	6 (9%)	75,105,113	2.06	19 (25%)
22	CLA	9	311	19	50,54,73	1.58	6 (12%)	60,90,113	2.07	16 (26%)
22	CLA	1	307	12	64,68,73	1.41	7 (10%)	77,107,113	2.03	18 (23%)
22	CLA	9	304	-	49,53,73	1.61	6 (12%)	59,89,113	2.07	15 (25%)
22	CLA	A	809	1	59,63,73	1.46	6 (10%)	71,101,113	2.07	21 (29%)
22	CLA	A	811	1,22	69,73,73	1.35	7 (10%)	83,113,113	1.90	19 (22%)
38	LUT	6	304	-	42,43,43	6.08	28 (66%)	51,60,60	2.05	13 (25%)
22	CLA	7	314	44	54,58,73	1.52	5 (9%)	65,95,113	2.18	19 (29%)
23	PQN	A	843	-	34,34,34	0.37	0	42,45,45	1.20	6 (14%)
39	CHL	Z	311	12	55,59,74	0.89	1 (1%)	62,96,114	1.50	14 (22%)
22	CLA	A	828	-	69,73,73	1.35	6 (8%)	83,113,113	1.95	17 (20%)
22	CLA	8	309	15	69,73,73	1.36	7 (10%)	83,113,113	1.93	19 (22%)
22	CLA	3	318	13	64,68,73	1.40	6 (9%)	77,107,113	2.01	20 (25%)
22	CLA	4	812	16	59,63,73	1.46	6 (10%)	71,101,113	2.07	19 (26%)
38	LUT	1	303	-	42,43,43	6.07	28 (66%)	51,60,60	2.06	12 (23%)
22	CLA	3	310	13	69,73,73	1.36	7 (10%)	83,113,113	2.01	22 (26%)
22	CLA	3	309	13	50,54,73	1.59	7 (14%)	60,90,113	2.04	16 (26%)
22	CLA	1	305	12	49,53,73	1.60	7 (14%)	59,89,113	2.08	18 (30%)
22	CLA	3	320	13	50,54,73	1.61	6 (12%)	60,90,113	2.14	15 (25%)
31	DGD	1	319	-	52,52,67	0.89	2 (3%)	66,66,81	0.97	4 (6%)
41	3PH	6	324	-	28,28,47	1.09	4 (14%)	32,33,52	1.20	2 (6%)
37	DAO	K	201	-	13,13,13	0.59	0	13,13,13	0.56	0
24	BCR	6	305	-	41,41,41	4.79	26 (63%)	56,56,56	2.49	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	9	305	19	64,68,73	1.46	8 (12%)	77,107,113	2.36	24 (31%)
24	BCR	A	844	-	41,41,41	4.78	27 (65%)	56,56,56	3.12	23 (41%)
25	LHG	5	324	22	36,36,48	0.44	0	39,42,54	1.12	3 (7%)
22	CLA	B	828	2	69,73,73	1.36	6 (8%)	83,113,113	1.93	19 (22%)
33	LMT	4	801	-	36,36,36	0.36	0	47,47,47	0.72	1 (2%)
22	CLA	6	310	18	69,73,73	1.35	7 (10%)	83,113,113	1.92	20 (24%)
22	CLA	B	839	2	56,60,73	1.50	7 (12%)	67,97,113	2.14	20 (29%)
22	CLA	F	304	6	69,73,73	1.35	6 (8%)	83,113,113	1.97	19 (22%)
22	CLA	B	818	2	69,73,73	1.34	7 (10%)	83,113,113	1.93	19 (22%)
38	LUT	6	303	-	42,43,43	6.11	27 (64%)	51,60,60	1.92	16 (31%)
22	CLA	A	831	1	54,58,73	1.53	6 (11%)	65,95,113	2.15	19 (29%)
24	BCR	L	204	-	41,41,41	4.78	27 (65%)	56,56,56	2.34	18 (32%)
22	CLA	A	830	1	69,73,73	1.36	6 (8%)	83,113,113	1.93	18 (21%)
22	CLA	4	818	44	55,59,73	1.52	6 (10%)	66,96,113	2.20	21 (31%)
22	CLA	5	308	17	65,69,73	1.39	7 (10%)	78,108,113	1.99	20 (25%)
22	CLA	B	840	44	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
25	LHG	6	323	22	48,48,48	0.38	0	51,54,54	1.09	3 (5%)
33	LMT	F	307	-	36,36,36	0.38	0	47,47,47	0.64	0
39	CHL	5	317	44	55,59,74	0.86	2 (3%)	62,96,114	1.37	13 (20%)
26	NKP	A	851	-	22,22,28	0.37	0	24,26,32	0.39	0
22	CLA	B	820	2	64,68,73	1.41	6 (9%)	77,107,113	1.96	19 (24%)
22	CLA	A	816	44	60,64,73	1.45	7 (11%)	72,102,113	2.12	21 (29%)
22	CLA	5	323	44	50,54,73	1.57	6 (12%)	60,90,113	2.14	16 (26%)
22	CLA	A	822	1	59,63,73	1.47	7 (11%)	71,101,113	2.12	18 (25%)
22	CLA	A	825	44	69,73,73	1.36	6 (8%)	83,113,113	1.96	19 (22%)
21	CL0	A	801	-	69,73,73	2.36	22 (31%)	83,113,113	2.57	22 (26%)
22	CLA	1	316	12	69,73,73	1.41	7 (10%)	83,113,113	1.89	19 (22%)
22	CLA	3	311	13	64,68,73	1.41	6 (9%)	77,107,113	1.99	20 (25%)
34	LMG	F	308	-	35,35,55	0.46	0	43,43,63	1.38	5 (11%)
39	CHL	6	316	-	55,59,74	0.90	2 (3%)	62,96,114	1.46	13 (20%)
22	CLA	B	825	2	69,73,73	1.35	6 (8%)	83,113,113	1.92	19 (22%)
22	CLA	B	808	2	69,73,73	1.36	6 (8%)	83,113,113	1.92	19 (22%)
22	CLA	1	313	44	69,73,73	1.36	6 (8%)	83,113,113	1.99	20 (24%)
22	CLA	8	310	44	64,68,73	1.41	6 (9%)	77,107,113	2.03	19 (24%)
22	CLA	1	306	-	69,73,73	1.35	6 (8%)	83,113,113	1.97	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	2	304	44	50,54,73	1.58	6 (12%)	60,90,113	2.06	15 (25%)
38	LUT	5	303	-	42,43,43	6.11	28 (66%)	51,60,60	2.00	14 (27%)
22	CLA	9	313	19	54,58,73	1.53	6 (11%)	65,95,113	2.16	19 (29%)
22	CLA	Z	308	-	65,69,73	1.39	6 (9%)	78,108,113	1.99	19 (24%)
38	LUT	4	803	-	42,43,43	6.06	28 (66%)	51,60,60	2.15	13 (25%)
22	CLA	3	314	25	64,68,73	1.40	6 (9%)	77,107,113	1.99	18 (23%)
22	CLA	B	831	2	62,66,73	1.44	7 (11%)	74,104,113	2.05	18 (24%)
25	LHG	Z	317	22	42,42,48	0.41	0	45,48,54	1.08	3 (6%)
24	BCR	B	849	-	41,41,41	4.81	27 (65%)	56,56,56	2.35	21 (37%)
22	CLA	A	832	1	69,73,73	1.35	6 (8%)	83,113,113	1.90	20 (24%)
22	CLA	A	815	1	69,73,73	1.35	6 (8%)	83,113,113	1.95	18 (21%)
22	CLA	B	830	-	69,73,73	1.35	6 (8%)	83,113,113	1.91	18 (21%)
22	CLA	B	837	2	55,59,73	1.52	6 (10%)	66,96,113	2.16	19 (28%)
24	BCR	3	306	-	41,41,41	4.80	27 (65%)	56,56,56	2.28	17 (30%)
22	CLA	Z	315	-	50,54,73	1.58	6 (12%)	60,90,113	2.09	15 (25%)
22	CLA	5	318	17	69,73,73	1.34	6 (8%)	83,113,113	1.90	18 (21%)
22	CLA	6	317	18	54,58,73	1.53	6 (11%)	65,95,113	2.15	17 (26%)
22	CLA	1	304	-	69,73,73	1.36	6 (8%)	83,113,113	1.93	19 (22%)
22	CLA	8	314	15	50,54,73	1.58	6 (12%)	60,90,113	2.02	15 (25%)
22	CLA	B	838	2	69,73,73	1.34	6 (8%)	83,113,113	1.88	17 (20%)
24	BCR	A	846	-	41,41,41	4.80	27 (65%)	56,56,56	2.47	22 (39%)
22	CLA	F	305	-	49,53,73	1.60	7 (14%)	59,89,113	2.04	15 (25%)
39	CHL	8	312	-	60,64,74	0.86	2 (3%)	68,102,114	1.33	12 (17%)
43	LPX	8	319	-	29,29,29	0.29	0	31,33,33	0.35	0
41	3PH	5	325	-	22,22,47	1.22	4 (18%)	26,27,52	1.28	2 (7%)
22	CLA	6	319	44	65,69,73	1.39	6 (9%)	78,108,113	2.02	19 (24%)
22	CLA	A	827	1	69,73,73	1.36	6 (8%)	83,113,113	1.95	21 (25%)
25	LHG	A	850	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
22	CLA	L	203	-	54,58,73	1.54	6 (11%)	65,95,113	2.15	18 (27%)
24	BCR	B	847	-	41,41,41	4.78	27 (65%)	56,56,56	2.46	21 (37%)
22	CLA	A	833	1	69,73,73	1.35	6 (8%)	83,113,113	1.95	20 (24%)
22	CLA	1	310	25	64,68,73	1.40	7 (10%)	77,107,113	1.99	18 (23%)
25	LHG	1	317	22	42,42,48	0.45	0	45,48,54	1.18	3 (6%)
22	CLA	1	309	-	65,69,73	1.38	7 (10%)	78,108,113	2.02	18 (23%)
22	CLA	5	322	17	69,73,73	1.36	6 (8%)	83,113,113	1.92	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	6	322	18	69,73,73	1.36	6 (8%)	83,113,113	1.96	19 (22%)
22	CLA	A	803	1	69,73,73	1.35	6 (8%)	83,113,113	1.95	19 (22%)
22	CLA	4	806	16	56,60,73	1.51	7 (12%)	67,97,113	2.18	20 (29%)
38	LUT	4	802	-	42,43,43	6.08	28 (66%)	51,60,60	2.02	12 (23%)
22	CLA	B	819	2	63,67,73	1.41	6 (9%)	75,105,113	2.04	21 (28%)
24	BCR	A	856	-	41,41,41	4.77	27 (65%)	56,56,56	2.50	23 (41%)
39	CHL	8	315	44	70,74,74	0.78	2 (2%)	80,114,114	1.26	12 (15%)
22	CLA	7	317	-	62,66,73	1.42	6 (9%)	74,104,113	2.03	18 (24%)
22	CLA	1	314	12	69,73,73	1.34	6 (8%)	83,113,113	1.90	18 (21%)
22	CLA	5	310	17	69,73,73	1.35	6 (8%)	83,113,113	1.96	19 (22%)
22	CLA	A	839	1	55,59,73	1.52	7 (12%)	66,96,113	2.15	19 (28%)
22	CLA	8	311	25	54,58,73	1.53	6 (11%)	65,95,113	2.12	17 (26%)
22	CLA	B	821	44	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
22	CLA	7	312	14	64,68,73	1.40	6 (9%)	77,107,113	1.99	19 (24%)
22	CLA	3	313	44	69,73,73	1.34	6 (8%)	83,113,113	1.94	18 (21%)
33	LMT	G	204	-	36,36,36	0.39	0	47,47,47	0.74	2 (4%)
22	CLA	5	319	44	59,63,73	1.45	6 (10%)	71,101,113	2.09	19 (26%)
38	LUT	Z	301	-	42,43,43	6.07	27 (64%)	51,60,60	1.99	14 (27%)
22	CLA	A	829	-	69,73,73	1.36	6 (8%)	83,113,113	1.89	17 (20%)
22	CLA	L	202	11	69,73,73	1.35	6 (8%)	83,113,113	1.92	19 (22%)
26	NKP	8	318	-	28,28,28	0.33	0	31,32,32	0.34	0
31	DGD	3	301	-	52,52,67	0.89	2 (3%)	66,66,81	1.06	4 (6%)
22	CLA	7	304	14	64,68,73	1.40	6 (9%)	77,107,113	2.08	21 (27%)
22	CLA	A	813	1	69,73,73	1.36	5 (7%)	83,113,113	1.95	20 (24%)
22	CLA	6	314	18	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
24	BCR	3	304	-	41,41,41	4.82	27 (65%)	56,56,56	3.07	28 (50%)
22	CLA	F	301	44	69,73,73	1.35	6 (8%)	83,113,113	1.97	21 (25%)
22	CLA	A	834	1	69,73,73	1.36	6 (8%)	83,113,113	1.91	19 (22%)
41	3PH	8	320	-	29,29,47	1.06	4 (13%)	33,34,52	1.16	2 (6%)
22	CLA	B	809	2	69,73,73	1.36	7 (10%)	83,113,113	1.92	18 (21%)
22	CLA	B	811	2	69,73,73	1.35	6 (8%)	83,113,113	1.97	20 (24%)
22	CLA	F	302	2	69,73,73	1.34	7 (10%)	83,113,113	1.94	20 (24%)
22	CLA	Z	304	12	49,53,73	1.61	6 (12%)	59,89,113	2.02	14 (23%)
40	SQD	1	318	-	47,48,54	0.83	0	56,59,65	0.96	3 (5%)
24	BCR	6	306	-	41,41,41	4.77	27 (65%)	56,56,56	2.79	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SF4	C	102	3	0,12,12	-	-	-		
39	CHL	2	303	-	55,59,74	0.87	1 (1%)	62,96,114	1.45	14 (22%)
22	CLA	B	823	2	59,63,73	1.46	7 (11%)	71,101,113	2.05	20 (28%)
42	SPH	7	321	-	19,20,20	0.65	1 (5%)	18,21,21	1.15	0
22	CLA	3	315	13	49,53,73	1.68	6 (12%)	59,89,113	2.11	14 (23%)
22	CLA	A	836	-	59,63,73	1.46	7 (11%)	71,101,113	2.04	20 (28%)
22	CLA	A	824	1	69,73,73	1.35	6 (8%)	83,113,113	1.91	19 (22%)
22	CLA	A	842	25	56,60,73	1.50	7 (12%)	67,97,113	2.14	19 (28%)
39	CHL	9	312	-	70,74,74	0.78	2 (2%)	80,114,114	1.40	11 (13%)
22	CLA	6	307	18	64,68,73	1.41	7 (10%)	77,107,113	2.00	18 (23%)
39	CHL	5	321	17	47,51,74	0.95	2 (4%)	52,86,114	1.47	11 (21%)
27	DGA	A	852	-	39,39,43	1.14	3 (7%)	41,41,45	1.32	3 (7%)
39	CHL	6	315	44	60,64,74	0.83	2 (3%)	68,102,114	1.32	12 (17%)
22	CLA	7	315	14	54,58,73	1.53	7 (12%)	65,95,113	2.17	19 (29%)
24	BCR	3	305	-	41,41,41	4.78	27 (65%)	56,56,56	2.19	19 (33%)
22	CLA	5	326	18	59,63,73	1.45	6 (10%)	71,101,113	2.07	20 (28%)
24	BCR	A	848	-	41,41,41	4.78	27 (65%)	56,56,56	2.42	22 (39%)
22	CLA	4	815	16	54,58,73	1.53	6 (11%)	65,95,113	2.15	16 (24%)
22	CLA	6	313	25	59,63,73	1.47	6 (10%)	71,101,113	2.05	18 (25%)
25	LHG	A	849	22	34,34,48	0.44	0	37,40,54	1.14	3 (8%)
22	CLA	6	308	18	56,60,73	1.49	6 (10%)	67,97,113	2.18	21 (31%)
22	CLA	A	802	44	69,73,73	1.35	6 (8%)	83,113,113	1.98	19 (22%)
22	CLA	9	309	25	59,63,73	1.48	6 (10%)	71,101,113	2.11	15 (21%)
25	LHG	9	315	22	32,32,48	0.48	0	35,38,54	1.05	3 (8%)
39	CHL	6	320	18	47,51,74	0.94	2 (4%)	52,86,114	1.49	11 (21%)
22	CLA	7	309	-	60,64,73	1.45	6 (10%)	72,102,113	2.09	20 (27%)
22	CLA	B	827	44	69,73,73	1.35	6 (8%)	83,113,113	1.97	19 (22%)
22	CLA	3	322	14	69,73,73	1.35	7 (10%)	83,113,113	1.91	18 (21%)
22	CLA	A	808	1	69,73,73	1.34	6 (8%)	83,113,113	1.97	19 (22%)
22	CLA	4	810	44	54,58,73	1.53	6 (11%)	65,95,113	2.16	20 (30%)
22	CLA	6	301	44	64,68,73	1.41	7 (10%)	77,107,113	2.03	20 (25%)
39	CHL	9	314	-	46,50,74	1.05	3 (6%)	51,85,114	1.50	12 (23%)
22	CLA	8	307	15	69,73,73	1.35	7 (10%)	83,113,113	2.00	18 (21%)
22	CLA	4	805	16	64,68,73	1.45	8 (12%)	77,107,113	1.89	18 (23%)
22	CLA	A	835	1	69,73,73	1.35	6 (8%)	83,113,113	1.90	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	815	2	69,73,73	1.36	5 (7%)	83,113,113	1.99	20 (24%)
22	CLA	2	302	20	49,53,73	1.60	6 (12%)	59,89,113	2.12	17 (28%)
38	LUT	5	302	-	42,43,43	6.07	28 (66%)	51,60,60	1.96	14 (27%)
29	SF4	C	101	3	0,12,12	-	-	-		
22	CLA	6	321	-	50,54,73	1.58	6 (12%)	60,90,113	2.07	15 (25%)
22	CLA	7	305	-	54,58,73	1.53	6 (11%)	65,95,113	2.18	19 (29%)
22	CLA	A	814	1	64,68,73	1.40	6 (9%)	77,107,113	2.03	20 (25%)
22	CLA	5	307	17	64,68,73	1.40	7 (10%)	77,107,113	2.00	18 (23%)
22	CLA	B	835	2	54,58,73	1.53	7 (12%)	65,95,113	2.22	19 (29%)
22	CLA	A	804	22	49,53,73	1.60	6 (12%)	59,89,113	2.07	16 (27%)
22	CLA	B	805	-	69,73,73	1.35	6 (8%)	83,113,113	1.94	20 (24%)
22	CLA	A	810	1	69,73,73	1.35	7 (10%)	83,113,113	1.93	18 (21%)
22	CLA	5	313	25	65,69,73	1.40	7 (10%)	78,108,113	2.02	19 (24%)
24	BCR	A	847	-	41,41,41	4.80	27 (65%)	56,56,56	2.38	20 (35%)
39	CHL	4	814	44	55,59,74	0.86	2 (3%)	62,96,114	1.42	14 (22%)
24	BCR	3	307	-	41,41,41	4.78	27 (65%)	56,56,56	3.25	27 (48%)
22	CLA	A	805	1	69,73,73	1.35	7 (10%)	83,113,113	1.94	19 (22%)
22	CLA	9	310	19	49,53,73	1.60	7 (14%)	59,89,113	2.16	16 (27%)
25	LHG	B	851	-	19,19,48	0.87	1 (5%)	20,24,54	1.36	1 (5%)
38	LUT	8	302	-	42,43,43	6.02	28 (66%)	51,60,60	1.96	13 (25%)
22	CLA	A	826	44	54,58,73	1.53	6 (11%)	65,95,113	2.16	18 (27%)
22	CLA	A	819	1	69,73,73	1.35	6 (8%)	83,113,113	1.90	18 (21%)
22	CLA	A	806	1	69,73,73	1.36	6 (8%)	83,113,113	1.92	18 (21%)
22	CLA	B	822	2	60,64,73	1.46	6 (10%)	72,102,113	2.01	18 (25%)
22	CLA	B	829	2	61,65,73	1.44	6 (9%)	73,103,113	2.06	20 (27%)
22	CLA	5	301	44	60,64,73	1.45	6 (10%)	72,102,113	2.06	19 (26%)
28	OCA	A	853	-	9,9,9	0.70	0	9,9,9	0.70	0
25	LHG	4	820	22	48,48,48	0.42	0	51,54,54	1.04	4 (7%)
34	LMG	J	101	-	29,29,55	0.53	0	37,37,63	1.12	3 (8%)
25	LHG	8	317	22	37,37,48	0.43	0	40,43,54	1.03	2 (5%)
22	CLA	Z	313	44	69,73,73	1.37	6 (8%)	83,113,113	1.95	20 (24%)
22	CLA	G	201	7	54,58,73	1.54	5 (9%)	65,95,113	2.18	20 (30%)
22	CLA	6	311	18	59,63,73	1.47	6 (10%)	71,101,113	2.01	18 (25%)
22	CLA	4	808	16	64,68,73	1.40	7 (10%)	77,107,113	1.99	19 (24%)
22	CLA	8	306	15	55,59,73	1.52	6 (10%)	66,96,113	2.08	19 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	5	316	44	70,74,74	0.78	1 (1%)	80,114,114	1.23	13 (16%)
22	CLA	9	303	19	64,68,73	1.45	6 (9%)	77,107,113	2.09	22 (28%)
23	PQN	B	843	-	34,34,34	0.37	0	42,45,45	1.13	3 (7%)
22	CLA	Z	307	12	59,63,73	1.48	6 (10%)	71,101,113	2.12	19 (26%)
33	LMT	4	822	-	36,36,36	0.45	0	47,47,47	1.17	3 (6%)
22	CLA	6	312	18	69,73,73	1.36	7 (10%)	83,113,113	1.95	20 (24%)
22	CLA	8	305	15	64,68,73	1.41	5 (7%)	77,107,113	2.01	18 (23%)
22	CLA	Z	310	12	54,58,73	1.52	6 (11%)	65,95,113	2.11	19 (29%)
22	CLA	B	813	-	60,64,73	1.45	6 (10%)	72,102,113	2.11	19 (26%)
22	CLA	1	308	12	59,63,73	1.47	7 (11%)	71,101,113	2.15	18 (25%)
22	CLA	K	203	44	59,63,73	1.47	6 (10%)	71,101,113	2.08	19 (26%)
22	CLA	1	311	12	50,54,73	1.58	7 (14%)	60,90,113	2.16	14 (23%)
22	CLA	1	315	-	50,54,73	1.59	6 (12%)	60,90,113	2.07	15 (25%)
22	CLA	A	812	1	69,73,73	1.35	7 (10%)	83,113,113	1.94	19 (22%)
22	CLA	A	821	44	69,73,73	1.35	6 (8%)	83,113,113	1.90	18 (21%)
22	CLA	7	324	14	64,68,73	1.41	6 (9%)	77,107,113	2.02	20 (25%)
22	CLA	8	313	44	54,58,73	1.53	6 (11%)	65,95,113	2.14	18 (27%)
32	RRX	F	306	-	42,42,42	5.06	25 (59%)	57,58,58	2.59	23 (40%)
22	CLA	J	103	9	46,50,73	1.66	6 (13%)	55,85,113	2.13	17 (30%)
22	CLA	3	308	13	69,73,73	1.36	7 (10%)	83,113,113	1.97	19 (22%)
38	LUT	3	302	-	42,43,43	6.05	28 (66%)	51,60,60	2.02	13 (25%)
39	CHL	3	317	-	70,74,74	0.77	1 (1%)	80,114,114	1.29	10 (12%)
22	CLA	9	308	19	54,58,73	1.53	6 (11%)	65,95,113	2.13	20 (30%)
24	BCR	B	845	-	41,41,41	4.78	27 (65%)	56,56,56	2.39	20 (35%)
38	LUT	1	302	-	42,43,43	6.10	28 (66%)	51,60,60	2.08	12 (23%)
22	CLA	5	312	44	54,58,73	1.53	6 (11%)	65,95,113	2.11	18 (27%)
36	C7Z	5	306	-	43,43,43	5.32	27 (62%)	58,60,60	2.37	22 (37%)
22	CLA	B	833	2	69,73,73	1.35	6 (8%)	83,113,113	1.92	19 (22%)
22	CLA	7	311	14	47,51,73	1.62	6 (12%)	56,86,113	2.13	16 (28%)
22	CLA	B	816	-	64,68,73	1.40	6 (9%)	77,107,113	1.98	18 (23%)
22	CLA	A	818	1	64,68,73	1.40	7 (10%)	77,107,113	2.06	19 (24%)
33	LMT	1	301	-	36,36,36	0.37	0	47,47,47	0.84	0
38	LUT	9	302	-	42,43,43	6.07	28 (66%)	51,60,60	1.87	12 (23%)
38	LUT	8	303	-	42,43,43	6.07	28 (66%)	51,60,60	1.97	14 (27%)
24	BCR	5	304	-	41,41,41	4.78	25 (60%)	56,56,56	2.54	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SF4	B	802	2,1	0,12,12	-	-	-		
22	CLA	9	307	19	59,63,73	1.47	7 (11%)	71,101,113	2.01	18 (25%)
24	BCR	J	104	-	41,41,41	4.76	27 (65%)	56,56,56	2.38	20 (35%)
22	CLA	Z	306	12	64,68,73	1.41	7 (10%)	77,107,113	1.99	19 (24%)
39	CHL	Z	312	-	52,56,74	0.91	2 (3%)	58,92,114	1.37	11 (18%)
24	BCR	G	203	-	41,41,41	4.79	27 (65%)	56,56,56	2.41	22 (39%)
22	CLA	A	807	1	64,68,73	1.40	6 (9%)	77,107,113	2.00	17 (22%)
24	BCR	A	845	-	41,41,41	4.77	27 (65%)	56,56,56	2.50	24 (42%)
22	CLA	Z	316	12	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
22	CLA	G	202	7	50,54,73	1.58	6 (12%)	60,90,113	2.07	16 (26%)
39	CHL	1	312	-	52,56,74	0.91	1 (1%)	58,92,114	1.39	10 (17%)
22	CLA	Z	303	12	69,73,73	1.35	6 (8%)	83,113,113	1.97	20 (24%)
38	LUT	3	303	-	42,43,43	6.06	28 (66%)	51,60,60	2.00	13 (25%)
35	T7X	J	102	-	49,49,61	0.91	4 (8%)	59,61,73	0.94	3 (5%)
25	LHG	B	803	-	32,32,48	0.46	0	35,38,54	1.18	3 (8%)
24	BCR	5	305	-	41,41,41	4.80	27 (65%)	56,56,56	2.67	22 (39%)
39	CHL	6	318	-	60,64,74	0.86	2 (3%)	68,102,114	1.36	12 (17%)
22	CLA	B	832	2	54,58,73	1.53	6 (11%)	65,95,113	2.14	19 (29%)
25	LHG	4	821	-	31,31,48	0.48	0	34,37,54	1.19	3 (8%)
22	CLA	B	841	2	69,73,73	1.35	6 (8%)	83,113,113	1.99	19 (22%)
24	BCR	B	848	-	41,41,41	4.79	27 (65%)	56,56,56	6.79	24 (42%)
22	CLA	5	315	17	69,73,73	1.36	6 (8%)	83,113,113	1.94	19 (22%)
22	CLA	L	201	2	69,73,73	1.34	6 (8%)	83,113,113	1.97	19 (22%)
38	LUT	9	301	-	42,43,43	6.08	28 (66%)	51,60,60	1.96	12 (23%)
42	SPH	7	320	-	19,20,20	0.63	0	18,21,21	1.10	0
22	CLA	K	202	10	50,54,73	1.60	6 (12%)	60,90,113	2.10	17 (28%)
22	CLA	9	306	19	66,70,73	1.39	6 (9%)	79,109,113	2.04	20 (25%)
22	CLA	5	314	17	49,53,73	1.59	6 (12%)	59,89,113	2.07	15 (25%)
41	3PH	7	319	-	38,38,47	0.94	4 (10%)	42,43,52	1.13	2 (4%)
39	CHL	7	313	44	58,62,74	0.85	2 (3%)	65,99,114	1.34	13 (20%)
39	CHL	4	813	44	55,59,74	0.90	2 (3%)	62,96,114	1.39	12 (19%)
22	CLA	4	807	16	69,73,73	1.36	7 (10%)	83,113,113	1.98	18 (21%)
22	CLA	8	316	15	50,54,73	1.58	7 (14%)	60,90,113	2.05	15 (25%)
38	LUT	7	302	-	42,43,43	6.08	28 (66%)	51,60,60	2.06	15 (29%)
22	CLA	3	312	13	69,73,73	1.36	7 (10%)	83,113,113	1.93	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	Z	309	25	64,68,73	1.40	6 (9%)	77,107,113	1.99	18 (23%)
24	BCR	8	304	-	41,41,41	4.80	27 (65%)	56,56,56	2.43	21 (37%)
22	CLA	5	309	-	60,64,73	1.45	7 (11%)	72,102,113	2.17	20 (27%)
22	CLA	7	308	14	65,69,73	1.41	7 (10%)	78,108,113	1.98	19 (24%)
22	CLA	4	817	16	45,49,73	1.66	6 (13%)	54,84,113	2.17	17 (31%)
22	CLA	7	310	25	69,73,73	1.35	6 (8%)	83,113,113	1.93	17 (20%)
22	CLA	A	838	1	69,73,73	1.35	6 (8%)	83,113,113	1.97	19 (22%)
22	CLA	A	840	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	18 (21%)
22	CLA	Z	305	-	60,64,73	1.45	6 (10%)	72,102,113	2.04	17 (23%)
31	DGD	B	852	-	62,62,67	1.12	6 (9%)	76,76,81	0.96	3 (3%)
22	CLA	B	807	2	49,53,73	1.60	6 (12%)	59,89,113	2.06	16 (27%)
22	CLA	4	809	16	55,59,73	1.53	7 (12%)	66,96,113	2.09	19 (28%)
24	BCR	7	303	-	41,41,41	4.78	27 (65%)	56,56,56	2.39	21 (37%)
22	CLA	4	811	25	59,63,73	1.46	6 (10%)	71,101,113	2.10	19 (26%)
22	CLA	3	319	-	59,63,73	1.46	6 (10%)	71,101,113	2.06	18 (25%)
22	CLA	3	316	13	56,60,73	1.50	6 (10%)	67,97,113	2.11	19 (28%)
22	CLA	A	823	1	69,73,73	1.34	7 (10%)	83,113,113	1.96	19 (22%)
39	CHL	4	816	44	51,55,74	0.94	2 (3%)	57,91,114	1.41	8 (14%)
24	BCR	4	804	-	41,41,41	4.82	26 (63%)	56,56,56	2.25	20 (35%)
22	CLA	Z	314	12	55,59,73	1.50	6 (10%)	66,96,113	2.11	18 (27%)
22	CLA	K	204	10	53,57,73	1.54	6 (11%)	62,93,113	2.19	19 (30%)
24	BCR	B	853	-	41,41,41	4.83	27 (65%)	56,56,56	2.40	22 (39%)
22	CLA	7	307	14	69,73,73	1.36	7 (10%)	83,113,113	1.97	17 (20%)
22	CLA	B	814	2	64,68,73	1.39	6 (9%)	77,107,113	2.00	17 (22%)
22	CLA	6	309	44	69,73,73	1.36	7 (10%)	83,113,113	2.01	20 (24%)
25	LHG	3	321	22	19,19,48	1.07	1 (5%)	20,24,54	1.53	1 (5%)
25	LHG	7	318	22	36,36,48	0.43	0	39,42,54	1.14	3 (7%)
24	BCR	B	846	-	41,41,41	4.79	27 (65%)	56,56,56	2.40	22 (39%)
22	CLA	A	854	-	69,73,73	1.35	6 (8%)	83,113,113	1.90	18 (21%)
22	CLA	B	810	2	60,64,73	1.44	5 (8%)	72,102,113	2.12	22 (30%)
22	CLA	K	205	10	59,63,73	1.57	8 (13%)	71,101,113	2.16	17 (23%)
22	CLA	A	820	1	64,68,73	1.41	6 (9%)	77,107,113	1.96	19 (24%)
24	BCR	F	303	-	41,41,41	4.81	27 (65%)	56,56,56	2.21	18 (32%)
22	CLA	5	320	-	54,58,73	1.60	7 (12%)	65,95,113	2.13	17 (26%)
24	BCR	K	206	-	41,41,41	4.79	27 (65%)	56,56,56	2.50	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	6	302	16	64,68,73	1.40	6 (9%)	77,107,113	1.96	18 (23%)
39	CHL	8	301	12	62,66,74	0.85	2 (3%)	70,104,114	1.40	13 (18%)
22	CLA	A	841	1	69,73,73	1.35	6 (8%)	83,113,113	1.96	19 (22%)
22	CLA	B	834	2	62,66,73	1.43	6 (9%)	74,104,113	2.04	19 (25%)
22	CLA	A	817	-	64,68,73	1.41	7 (10%)	77,107,113	2.03	18 (23%)
22	CLA	B	806	44	69,73,73	1.36	6 (8%)	83,113,113	1.95	18 (21%)
22	CLA	B	842	25	69,73,73	1.35	6 (8%)	83,113,113	1.94	18 (21%)
22	CLA	7	323	15	69,73,73	1.35	6 (8%)	83,113,113	1.96	20 (24%)
22	CLA	B	801	2	69,73,73	1.35	6 (8%)	83,113,113	1.86	18 (21%)
22	CLA	B	836	-	49,53,73	1.59	6 (12%)	59,89,113	2.06	17 (28%)
22	CLA	8	308	15	66,70,73	1.38	6 (9%)	79,109,113	1.98	19 (24%)
22	CLA	B	826	44	69,73,73	1.36	6 (8%)	83,113,113	1.95	20 (24%)
36	C7Z	J	105	-	43,43,43	5.34	27 (62%)	58,60,60	2.21	21 (36%)
24	BCR	B	844	-	41,41,41	4.79	26 (63%)	56,56,56	2.77	24 (42%)
22	CLA	7	316	44	46,50,73	1.65	6 (13%)	55,85,113	2.14	17 (30%)

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	B	812	2	1/1/14/20	15/29/105/115	-
24	BCR	I	4001	-	-	14/29/63/63	0/2/2/2
22	CLA	A	855	44	-	18/39/115/115	-
22	CLA	7	322	15	-	9/27/103/115	-
25	LHG	B	850	22	-	16/26/26/53	-
22	CLA	2	301	-	-	11/27/103/115	-
38	LUT	7	301	-	-	9/29/67/67	0/2/2/2
39	CHL	4	819	16	-	0/14/90/117	-
22	CLA	5	311	17	-	11/27/103/115	-
22	CLA	7	306	14	-	16/39/115/115	-
38	LUT	Z	302	-	-	7/29/67/67	0/2/2/2
22	CLA	A	837	1	-	10/23/99/115	-
22	CLA	B	817	2	-	18/30/106/115	-
22	CLA	B	824	2	-	19/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	9	311	19	-	5/17/93/115	-
22	CLA	1	307	12	-	18/33/109/115	-
22	CLA	9	304	-	-	5/15/91/115	-
22	CLA	A	809	1	-	7/27/103/115	-
22	CLA	A	811	1,22	-	20/39/115/115	-
38	LUT	6	304	-	-	6/29/67/67	0/2/2/2
22	CLA	7	314	44	-	7/21/97/115	-
23	PQN	A	843	-	-	8/23/43/43	0/2/2/2
39	CHL	Z	311	12	-	10/23/99/117	-
22	CLA	A	828	-	-	21/39/115/115	-
22	CLA	8	309	15	-	17/39/115/115	-
22	CLA	3	318	13	-	11/33/109/115	-
22	CLA	4	812	16	-	10/27/103/115	-
38	LUT	1	303	-	-	8/29/67/67	0/2/2/2
22	CLA	3	310	13	-	14/39/115/115	-
22	CLA	3	309	13	-	6/17/93/115	-
22	CLA	1	305	12	-	6/15/91/115	-
22	CLA	3	320	13	-	7/17/93/115	-
31	DGD	1	319	-	-	14/40/80/95	0/2/2/2
41	3PH	6	324	-	-	11/30/30/49	-
37	DAO	K	201	-	-	1/11/11/11	-
24	BCR	6	305	-	-	13/29/63/63	0/2/2/2
22	CLA	9	305	19	-	20/33/109/115	-
24	BCR	A	844	-	-	13/29/63/63	0/2/2/2
25	LHG	5	324	22	-	24/41/41/53	-
22	CLA	B	828	2	-	18/39/115/115	-
33	LMT	4	801	-	-	1/21/61/61	0/2/2/2
22	CLA	6	310	18	-	18/39/115/115	-
22	CLA	B	839	2	-	11/24/100/115	-
22	CLA	F	304	6	-	24/39/115/115	-
22	CLA	B	818	2	-	15/39/115/115	-
38	LUT	6	303	-	-	9/29/67/67	0/2/2/2
22	CLA	A	831	1	-	10/21/97/115	-
24	BCR	L	204	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	830	1	-	14/39/115/115	-
22	CLA	4	818	44	-	12/23/99/115	-
22	CLA	5	308	17	-	17/35/111/115	-
22	CLA	B	840	44	-	9/39/115/115	-
25	LHG	6	323	22	-	38/53/53/53	-
33	LMT	F	307	-	-	8/21/61/61	0/2/2/2
39	CHL	5	317	44	-	7/23/99/117	-
26	NKP	A	851	-	-	9/22/22/28	-
22	CLA	B	820	2	-	18/33/109/115	-
22	CLA	A	816	44	-	14/29/105/115	-
22	CLA	5	323	44	-	9/17/93/115	-
22	CLA	A	822	1	-	12/27/103/115	-
22	CLA	A	825	44	-	16/39/115/115	-
21	CL0	A	801	-	-	13/39/115/115	-
22	CLA	1	316	12	-	22/39/115/115	-
22	CLA	3	311	13	-	13/33/109/115	-
34	LMG	F	308	-	-	16/30/50/70	0/1/1/1
39	CHL	6	316	-	-	10/23/99/117	-
22	CLA	B	825	2	-	19/39/115/115	-
22	CLA	B	808	2	-	15/39/115/115	-
22	CLA	1	313	44	-	12/39/115/115	-
22	CLA	8	310	44	-	15/33/109/115	-
22	CLA	1	306	-	-	18/39/115/115	-
22	CLA	2	304	44	-	9/17/93/115	-
38	LUT	5	303	-	-	6/29/67/67	0/2/2/2
22	CLA	9	313	19	-	6/21/97/115	-
22	CLA	Z	308	-	-	14/35/111/115	-
38	LUT	4	803	-	-	8/29/67/67	0/2/2/2
22	CLA	3	314	25	-	19/33/109/115	-
22	CLA	B	831	2	-	17/31/107/115	-
25	LHG	Z	317	22	-	27/47/47/53	-
24	BCR	B	849	-	-	13/29/63/63	0/2/2/2
22	CLA	A	832	1	-	17/39/115/115	-
22	CLA	A	815	1	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	830	-	-	13/39/115/115	-
22	CLA	B	837	2	-	9/23/99/115	-
24	BCR	3	306	-	-	13/29/63/63	0/2/2/2
22	CLA	Z	315	-	-	10/17/93/115	-
22	CLA	5	318	17	-	14/39/115/115	-
22	CLA	6	317	18	-	10/21/97/115	-
22	CLA	1	304	-	-	13/39/115/115	-
22	CLA	8	314	15	-	10/17/93/115	-
22	CLA	B	838	2	-	15/39/115/115	-
24	BCR	A	846	-	-	13/29/63/63	0/2/2/2
22	CLA	F	305	-	-	6/15/91/115	-
39	CHL	8	312	-	-	10/29/105/117	-
43	LPX	8	319	-	-	6/31/31/31	-
41	3PH	5	325	-	-	5/24/24/49	-
22	CLA	6	319	44	-	17/35/111/115	-
22	CLA	A	827	1	-	17/39/115/115	-
25	LHG	A	850	-	-	29/53/53/53	-
22	CLA	L	203	-	-	7/21/97/115	-
24	BCR	B	847	-	-	11/29/63/63	0/2/2/2
22	CLA	A	833	1	-	14/39/115/115	-
22	CLA	1	310	25	-	17/33/109/115	-
25	LHG	1	317	22	-	22/47/47/53	-
22	CLA	1	309	-	-	13/35/111/115	-
22	CLA	5	322	17	-	11/39/115/115	-
22	CLA	6	322	18	-	15/39/115/115	-
22	CLA	A	803	1	-	12/39/115/115	-
22	CLA	4	806	16	-	12/24/100/115	-
38	LUT	4	802	-	-	10/29/67/67	0/2/2/2
22	CLA	B	819	2	-	15/32/108/115	-
24	BCR	A	856	-	-	16/29/63/63	0/2/2/2
39	CHL	8	315	44	-	13/41/117/117	-
22	CLA	7	317	-	-	15/31/107/115	-
22	CLA	1	314	12	-	13/39/115/115	-
22	CLA	5	310	17	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	839	1	-	10/23/99/115	-
22	CLA	8	311	25	-	10/21/97/115	-
22	CLA	B	821	44	-	18/39/115/115	-
22	CLA	7	312	14	-	18/33/109/115	-
22	CLA	3	313	44	-	17/39/115/115	-
33	LMT	G	204	-	-	6/21/61/61	0/2/2/2
22	CLA	5	319	44	-	13/27/103/115	-
38	LUT	Z	301	-	-	7/29/67/67	0/2/2/2
22	CLA	A	829	-	-	11/39/115/115	-
22	CLA	L	202	11	-	21/39/115/115	-
26	NKP	8	318	-	-	7/28/28/28	-
31	DGD	3	301	-	-	12/40/80/95	0/2/2/2
22	CLA	7	304	14	-	13/33/109/115	-
22	CLA	A	813	1	-	14/39/115/115	-
22	CLA	6	314	18	-	15/39/115/115	-
24	BCR	3	304	-	-	10/29/63/63	0/2/2/2
22	CLA	F	301	44	-	13/39/115/115	-
22	CLA	A	834	1	-	15/39/115/115	-
41	3PH	8	320	-	-	13/31/31/49	-
22	CLA	B	809	2	-	19/39/115/115	-
22	CLA	B	811	2	-	15/39/115/115	-
22	CLA	F	302	2	-	17/39/115/115	-
22	CLA	Z	304	12	-	6/15/91/115	-
40	SQD	1	318	-	-	12/43/63/69	0/1/1/1
24	BCR	6	306	-	-	16/29/63/63	0/2/2/2
39	CHL	2	303	-	-	8/23/99/117	-
29	SF4	C	102	3	-	-	0/6/5/5
22	CLA	B	823	2	-	13/27/103/115	-
42	SPH	7	321	-	-	11/21/21/21	-
22	CLA	3	315	13	-	8/15/91/115	-
22	CLA	A	836	-	-	12/27/103/115	-
22	CLA	A	824	1	-	17/39/115/115	-
22	CLA	A	842	25	-	12/24/100/115	-
39	CHL	9	312	-	-	16/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	307	18	-	12/33/109/115	-
39	CHL	5	321	17	-	4/14/90/117	-
27	DGA	A	852	-	-	23/41/41/45	-
39	CHL	6	315	44	-	12/29/105/117	-
22	CLA	7	315	14	-	8/21/97/115	-
24	BCR	3	305	-	-	14/29/63/63	0/2/2/2
22	CLA	5	326	18	-	8/27/103/115	-
24	BCR	A	848	-	-	15/29/63/63	0/2/2/2
22	CLA	4	815	16	-	8/21/97/115	-
22	CLA	6	313	25	-	9/27/103/115	-
25	LHG	A	849	22	-	27/39/39/53	-
22	CLA	6	308	18	-	8/24/100/115	-
22	CLA	A	802	44	-	17/39/115/115	-
22	CLA	9	309	25	-	9/27/103/115	-
25	LHG	9	315	22	-	20/37/37/53	-
39	CHL	6	320	18	-	1/14/90/117	-
22	CLA	7	309	-	-	14/29/105/115	-
22	CLA	B	827	44	-	14/39/115/115	-
22	CLA	3	322	14	-	14/39/115/115	-
22	CLA	A	808	1	-	19/39/115/115	-
22	CLA	4	810	44	-	8/21/97/115	-
22	CLA	6	301	44	-	18/33/109/115	-
39	CHL	9	314	-	-	0/12/88/117	-
22	CLA	8	307	15	-	12/39/115/115	-
22	CLA	4	805	16	-	15/33/109/115	-
22	CLA	A	835	1	-	13/39/115/115	-
22	CLA	B	815	2	-	13/39/115/115	-
22	CLA	2	302	20	-	8/15/91/115	-
38	LUT	5	302	-	-	9/29/67/67	0/2/2/2
29	SF4	C	101	3	-	-	0/6/5/5
22	CLA	6	321	-	-	6/17/93/115	-
22	CLA	7	305	-	-	6/21/97/115	-
22	CLA	A	814	1	-	19/33/109/115	-
22	CLA	5	307	17	-	14/33/109/115	-
22	CLA	B	835	2	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	804	22	-	6/15/91/115	-
22	CLA	B	805	-	-	16/39/115/115	-
22	CLA	A	810	1	-	17/39/115/115	-
22	CLA	5	313	25	-	12/35/111/115	-
24	BCR	A	847	-	-	16/29/63/63	0/2/2/2
39	CHL	4	814	44	-	11/23/99/117	-
24	BCR	3	307	-	-	13/29/63/63	0/2/2/2
22	CLA	A	805	1	-	19/39/115/115	-
22	CLA	9	310	19	-	6/15/91/115	-
25	LHG	B	851	-	-	15/22/22/53	-
38	LUT	8	302	-	-	8/29/67/67	0/2/2/2
22	CLA	A	826	44	-	6/21/97/115	-
22	CLA	A	819	1	-	12/39/115/115	-
22	CLA	A	806	1	-	16/39/115/115	-
22	CLA	B	822	2	-	17/29/105/115	-
22	CLA	B	829	2	-	15/30/106/115	-
22	CLA	5	301	44	-	13/29/105/115	-
28	OCA	A	853	-	-	3/7/7/7	-
25	LHG	4	820	22	-	30/53/53/53	-
34	LMG	J	101	-	-	7/24/44/70	0/1/1/1
25	LHG	8	317	22	-	27/42/42/53	-
22	CLA	Z	313	44	-	13/39/115/115	-
22	CLA	G	201	7	-	10/21/97/115	-
22	CLA	6	311	18	-	12/27/103/115	-
22	CLA	4	808	16	-	16/33/109/115	-
22	CLA	8	306	15	-	9/23/99/115	-
39	CHL	5	316	44	-	12/41/117/117	-
22	CLA	9	303	19	-	13/33/109/115	-
23	PQN	B	843	-	-	9/23/43/43	0/2/2/2
22	CLA	Z	307	12	-	10/27/103/115	-
33	LMT	4	822	-	-	6/21/61/61	0/2/2/2
22	CLA	6	312	18	-	15/39/115/115	-
22	CLA	8	305	15	-	14/33/109/115	-
22	CLA	Z	310	12	-	10/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	813	-	-	14/29/105/115	-
22	CLA	1	308	12	-	13/27/103/115	-
22	CLA	K	203	44	-	9/27/103/115	-
22	CLA	1	311	12	-	8/17/93/115	-
22	CLA	1	315	-	-	7/17/93/115	-
22	CLA	A	812	1	-	16/39/115/115	-
22	CLA	A	821	44	-	12/39/115/115	-
22	CLA	7	324	14	-	23/33/109/115	-
22	CLA	8	313	44	-	7/21/97/115	-
32	RRX	F	306	-	-	15/29/65/65	0/2/2/2
22	CLA	J	103	9	-	5/12/88/115	-
22	CLA	3	308	13	-	18/39/115/115	-
38	LUT	3	302	-	-	4/29/67/67	0/2/2/2
39	CHL	3	317	-	-	13/41/117/117	-
22	CLA	9	308	19	-	8/21/97/115	-
24	BCR	B	845	-	-	16/29/63/63	0/2/2/2
38	LUT	1	302	-	-	9/29/67/67	0/2/2/2
22	CLA	5	312	44	-	6/21/97/115	-
36	C7Z	5	306	-	-	13/29/67/67	0/2/2/2
22	CLA	B	833	2	-	19/39/115/115	-
22	CLA	7	311	14	-	6/13/89/115	-
22	CLA	B	816	-	-	13/33/109/115	-
22	CLA	A	818	1	-	15/33/109/115	-
33	LMT	1	301	-	-	4/21/61/61	0/2/2/2
38	LUT	9	302	-	-	4/29/67/67	0/2/2/2
38	LUT	8	303	-	-	3/29/67/67	0/2/2/2
24	BCR	5	304	-	-	14/29/63/63	0/2/2/2
29	SF4	B	802	2,1	-	-	0/6/5/5
22	CLA	9	307	19	-	10/27/103/115	-
24	BCR	J	104	-	-	14/29/63/63	0/2/2/2
22	CLA	Z	306	12	-	20/33/109/115	-
39	CHL	Z	312	-	-	10/20/96/117	-
24	BCR	G	203	-	-	15/29/63/63	0/2/2/2
22	CLA	A	807	1	-	17/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	A	845	-	-	14/29/63/63	0/2/2/2
22	CLA	Z	316	12	-	21/39/115/115	-
22	CLA	G	202	7	-	8/17/93/115	-
39	CHL	1	312	-	-	4/20/96/117	-
22	CLA	Z	303	12	-	16/39/115/115	-
38	LUT	3	303	-	-	7/29/67/67	0/2/2/2
35	T7X	J	102	-	-	17/44/68/80	0/1/1/1
25	LHG	B	803	-	-	22/37/37/53	-
24	BCR	5	305	-	-	13/29/63/63	0/2/2/2
39	CHL	6	318	-	-	9/29/105/117	-
22	CLA	B	832	2	-	6/21/97/115	-
25	LHG	4	821	-	-	16/36/36/53	-
22	CLA	B	841	2	-	13/39/115/115	-
24	BCR	B	848	-	-	16/29/63/63	0/2/2/2
22	CLA	5	315	17	-	14/39/115/115	-
22	CLA	L	201	2	-	17/39/115/115	-
38	LUT	9	301	-	-	5/29/67/67	0/2/2/2
42	SPH	7	320	-	-	11/21/21/21	-
22	CLA	K	202	10	-	10/17/93/115	-
22	CLA	9	306	19	-	14/36/112/115	-
22	CLA	5	314	17	-	6/15/91/115	-
41	3PH	7	319	-	-	17/40/40/49	-
39	CHL	7	313	44	-	7/27/103/117	-
39	CHL	4	813	44	-	7/23/99/117	-
22	CLA	4	807	16	-	12/39/115/115	-
22	CLA	8	316	15	-	11/17/93/115	-
38	LUT	7	302	-	-	5/29/67/67	0/2/2/2
22	CLA	3	312	13	-	12/39/115/115	-
22	CLA	Z	309	25	-	16/33/109/115	-
24	BCR	8	304	-	-	12/29/63/63	0/2/2/2
22	CLA	5	309	-	-	17/29/105/115	-
22	CLA	7	308	14	-	16/35/111/115	-
22	CLA	4	817	16	-	2/10/86/115	-
22	CLA	7	310	25	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	838	1	-	15/39/115/115	-
22	CLA	A	840	-	-	18/39/115/115	-
22	CLA	Z	305	-	-	12/29/105/115	-
31	DGD	B	852	-	-	11/50/90/95	0/2/2/2
22	CLA	B	807	2	-	8/15/91/115	-
22	CLA	4	809	16	-	5/23/99/115	-
24	BCR	7	303	-	-	16/29/63/63	0/2/2/2
22	CLA	4	811	25	-	9/27/103/115	-
22	CLA	3	319	-	-	9/27/103/115	-
22	CLA	3	316	13	-	8/24/100/115	-
22	CLA	A	823	1	-	15/39/115/115	-
39	CHL	4	816	44	-	7/19/95/117	-
24	BCR	4	804	-	-	14/29/63/63	0/2/2/2
22	CLA	Z	314	12	-	9/23/99/115	-
22	CLA	K	204	10	-	12/20/96/115	-
24	BCR	B	853	-	-	17/29/63/63	0/2/2/2
22	CLA	7	307	14	-	14/39/115/115	-
22	CLA	B	814	2	-	19/33/109/115	-
22	CLA	6	309	44	-	17/39/115/115	-
25	LHG	3	321	22	-	11/22/22/53	-
25	LHG	7	318	22	-	25/41/41/53	-
24	BCR	B	846	-	-	17/29/63/63	0/2/2/2
22	CLA	A	854	-	-	13/39/115/115	-
22	CLA	B	810	2	-	11/29/105/115	-
22	CLA	K	205	10	-	17/27/103/115	-
22	CLA	A	820	1	-	21/33/109/115	-
24	BCR	F	303	-	-	15/29/63/63	0/2/2/2
22	CLA	5	320	-	-	11/21/97/115	-
24	BCR	K	206	-	-	13/29/63/63	0/2/2/2
22	CLA	6	302	16	-	17/33/109/115	-
39	CHL	8	301	12	-	5/32/108/117	-
22	CLA	A	841	1	-	10/39/115/115	-
22	CLA	B	834	2	-	15/31/107/115	-
22	CLA	A	817	-	-	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	806	44	-	12/39/115/115	-
22	CLA	B	842	25	-	17/39/115/115	-
22	CLA	7	323	15	-	19/39/115/115	-
22	CLA	B	801	2	-	15/39/115/115	-
22	CLA	B	836	-	-	6/15/91/115	-
22	CLA	8	308	15	-	15/36/112/115	-
22	CLA	B	826	44	-	17/39/115/115	-
36	C7Z	J	105	-	-	13/29/67/67	0/2/2/2
24	BCR	B	844	-	-	12/29/63/63	0/2/2/2
22	CLA	7	316	44	-	6/12/88/115	-

The worst 5 of 2818 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 5260 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

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	B	812	CLA	C13

5 of 4136 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

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Mol	Chain	Res	Type	Atoms
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 2926 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	812	CLA	14	0
24	I	4001	BCR	12	0
22	A	855	CLA	14	0
22	7	322	CLA	15	0
25	B	850	LHG	4	0
22	2	301	CLA	17	0
38	7	301	LUT	14	0
39	4	819	CHL	9	0
22	5	311	CLA	13	0
22	7	306	CLA	11	0
38	Z	302	LUT	13	0
22	A	837	CLA	9	0
22	B	817	CLA	17	0
22	B	824	CLA	18	0
22	9	311	CLA	5	0
22	1	307	CLA	17	0
22	9	304	CLA	2	0
22	A	809	CLA	15	0
22	A	811	CLA	15	0
38	6	304	LUT	13	0
22	7	314	CLA	3	0
23	A	843	PQN	10	0
39	Z	311	CHL	11	0
22	A	828	CLA	14	0
22	8	309	CLA	14	0
22	3	318	CLA	18	0
22	4	812	CLA	4	0
38	1	303	LUT	18	0
22	3	310	CLA	7	0
22	3	309	CLA	7	0
22	1	305	CLA	10	0
22	3	320	CLA	10	0
31	1	319	DGD	10	0
41	6	324	3PH	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	K	201	DAO	8	0
24	6	305	BCR	19	0
22	9	305	CLA	6	0
24	A	844	BCR	30	0
25	5	324	LHG	7	0
22	B	828	CLA	20	0
33	4	801	LMT	7	0
22	6	310	CLA	15	0
22	B	839	CLA	16	0
22	F	304	CLA	27	0
22	B	818	CLA	13	0
38	6	303	LUT	11	0
22	A	831	CLA	5	0
24	L	204	BCR	17	0
22	A	830	CLA	9	0
22	4	818	CLA	9	0
22	5	308	CLA	23	0
22	B	840	CLA	16	0
25	6	323	LHG	11	0
33	F	307	LMT	5	0
39	5	317	CHL	8	0
26	A	851	NKP	3	0
22	B	820	CLA	11	0
22	A	816	CLA	23	0
22	5	323	CLA	9	0
22	A	822	CLA	26	0
22	A	825	CLA	18	0
21	A	801	CL0	7	0
22	1	316	CLA	5	0
22	3	311	CLA	14	0
34	F	308	LMG	1	0
39	6	316	CHL	11	0
22	B	825	CLA	21	0
22	B	808	CLA	13	0
22	1	313	CLA	12	0
22	8	310	CLA	12	0
22	1	306	CLA	8	0
22	2	304	CLA	9	0
38	5	303	LUT	16	0
22	9	313	CLA	17	0
22	Z	308	CLA	12	0
38	4	803	LUT	19	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	314	CLA	12	0
22	B	831	CLA	10	0
25	Z	317	LHG	9	0
24	B	849	BCR	9	0
22	A	832	CLA	13	0
22	A	815	CLA	18	0
22	B	830	CLA	15	0
22	B	837	CLA	1	0
24	3	306	BCR	14	0
22	Z	315	CLA	10	0
22	5	318	CLA	18	0
22	6	317	CLA	11	0
22	1	304	CLA	14	0
22	8	314	CLA	6	0
22	B	838	CLA	14	0
24	A	846	BCR	11	0
22	F	305	CLA	9	0
39	8	312	CHL	14	0
43	8	319	LPX	7	0
41	5	325	3PH	3	0
22	6	319	CLA	11	0
22	A	827	CLA	17	0
25	A	850	LHG	8	0
22	L	203	CLA	6	0
24	B	847	BCR	20	0
22	A	833	CLA	18	0
22	1	310	CLA	10	0
25	1	317	LHG	8	0
22	1	309	CLA	4	0
22	5	322	CLA	10	0
22	6	322	CLA	17	0
22	A	803	CLA	7	0
22	4	806	CLA	8	0
38	4	802	LUT	15	0
22	B	819	CLA	15	0
24	A	856	BCR	24	0
39	8	315	CHL	21	0
22	7	317	CLA	4	0
22	1	314	CLA	19	0
22	5	310	CLA	13	0
22	A	839	CLA	8	0
22	8	311	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	821	CLA	13	0
22	7	312	CLA	4	0
22	3	313	CLA	22	0
33	G	204	LMT	10	0
22	5	319	CLA	13	0
38	Z	301	LUT	23	0
22	A	829	CLA	16	0
22	L	202	CLA	16	0
26	8	318	NKP	7	0
31	3	301	DGD	21	0
22	7	304	CLA	10	0
22	A	813	CLA	18	0
22	6	314	CLA	17	0
24	3	304	BCR	13	0
22	F	301	CLA	8	0
22	A	834	CLA	10	0
41	8	320	3PH	4	0
22	B	809	CLA	13	0
22	B	811	CLA	21	0
22	F	302	CLA	16	0
22	Z	304	CLA	19	0
40	1	318	SQD	12	0
24	6	306	BCR	16	0
29	C	102	SF4	5	0
39	2	303	CHL	8	0
22	B	823	CLA	14	0
42	7	321	SPH	8	0
22	3	315	CLA	8	0
22	A	836	CLA	13	0
22	A	824	CLA	16	0
22	A	842	CLA	6	0
39	9	312	CHL	24	0
22	6	307	CLA	20	0
39	5	321	CHL	6	0
27	A	852	DGA	20	0
39	6	315	CHL	21	0
22	7	315	CLA	10	0
24	3	305	BCR	15	0
22	5	326	CLA	17	0
24	A	848	BCR	7	0
22	4	815	CLA	12	0
22	6	313	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	849	LHG	5	0
22	6	308	CLA	15	0
22	A	802	CLA	12	0
25	9	315	LHG	2	0
39	6	320	CHL	13	0
22	7	309	CLA	9	0
22	B	827	CLA	23	0
22	3	322	CLA	15	0
22	A	808	CLA	14	0
22	4	810	CLA	17	0
22	6	301	CLA	20	0
39	9	314	CHL	13	0
22	8	307	CLA	15	0
22	4	805	CLA	17	0
22	A	835	CLA	15	0
22	B	815	CLA	23	0
22	2	302	CLA	5	0
38	5	302	LUT	16	0
29	C	101	SF4	2	0
22	6	321	CLA	6	0
22	7	305	CLA	6	0
22	A	814	CLA	23	0
22	5	307	CLA	24	0
22	B	835	CLA	10	0
22	A	804	CLA	14	0
22	B	805	CLA	11	0
22	A	810	CLA	20	0
22	5	313	CLA	12	0
24	A	847	BCR	14	0
39	4	814	CHL	5	0
24	3	307	BCR	19	0
22	A	805	CLA	15	0
22	9	310	CLA	1	0
25	B	851	LHG	3	0
38	8	302	LUT	16	0
22	A	826	CLA	7	0
22	A	819	CLA	8	0
22	A	806	CLA	10	0
22	B	822	CLA	11	0
22	B	829	CLA	12	0
22	5	301	CLA	12	0
25	4	820	LHG	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	J	101	LMG	10	0
25	8	317	LHG	7	0
22	Z	313	CLA	23	0
22	G	201	CLA	12	0
22	6	311	CLA	10	0
22	4	808	CLA	15	0
22	8	306	CLA	14	0
39	5	316	CHL	17	0
22	9	303	CLA	6	0
23	B	843	PQN	5	0
22	Z	307	CLA	10	0
33	4	822	LMT	2	0
22	6	312	CLA	13	0
22	8	305	CLA	24	0
22	Z	310	CLA	2	0
22	B	813	CLA	7	0
22	1	308	CLA	19	0
22	K	203	CLA	9	0
22	1	315	CLA	4	0
22	A	812	CLA	24	0
22	A	821	CLA	24	0
22	7	324	CLA	4	0
22	8	313	CLA	9	0
32	F	306	RRX	19	0
22	J	103	CLA	1	0
22	3	308	CLA	18	0
38	3	302	LUT	10	0
39	3	317	CHL	14	0
22	9	308	CLA	9	0
24	B	845	BCR	9	0
38	1	302	LUT	8	0
22	5	312	CLA	8	0
36	5	306	C7Z	1	0
22	B	833	CLA	12	0
22	7	311	CLA	1	0
22	B	816	CLA	12	0
22	A	818	CLA	11	0
33	1	301	LMT	7	0
38	9	302	LUT	17	0
38	8	303	LUT	12	0
24	5	304	BCR	20	0
29	B	802	SF4	6	0

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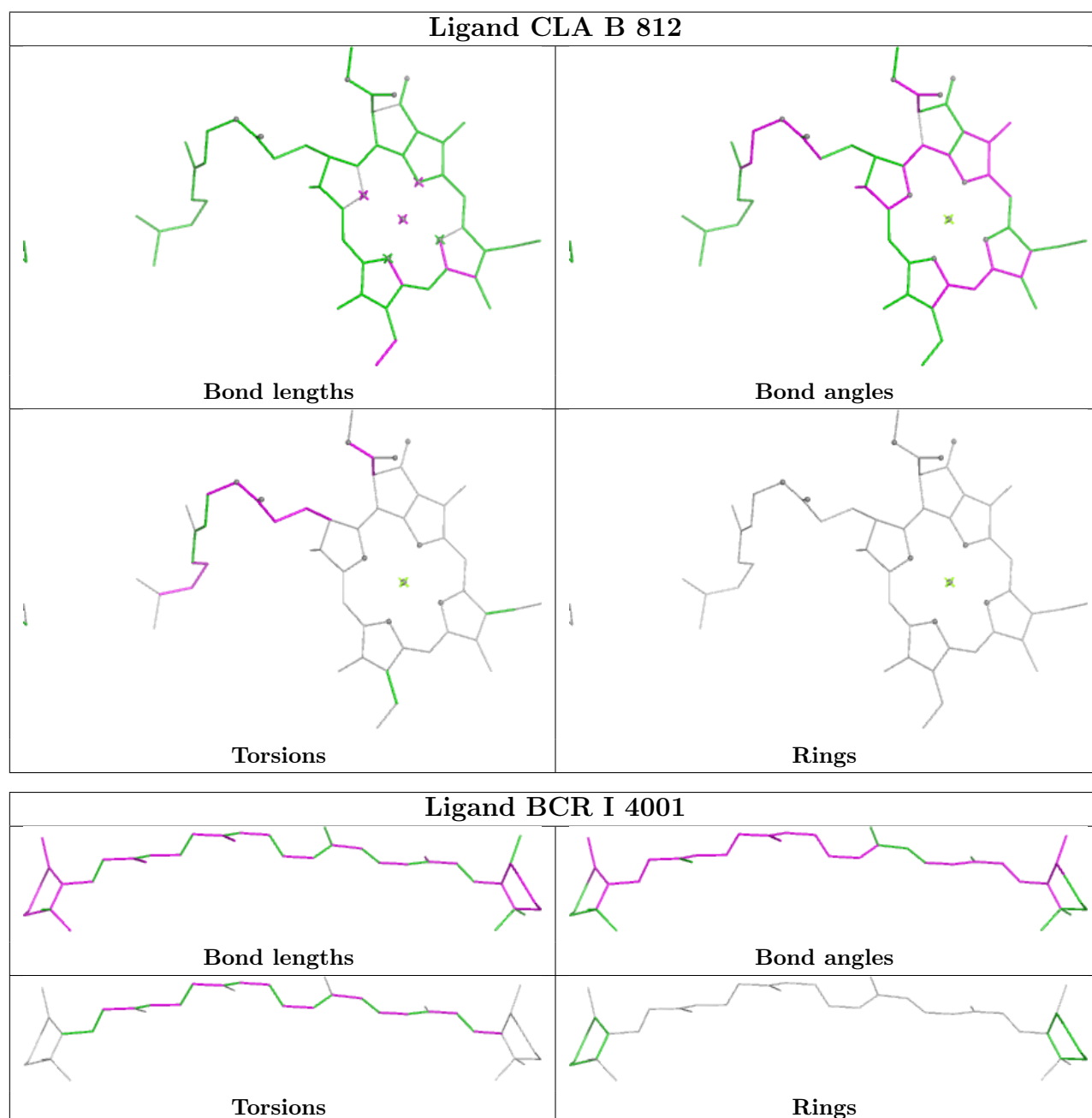
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24	J	104	BCR	18	0
22	Z	306	CLA	16	0
39	Z	312	CHL	12	0
24	G	203	BCR	12	0
22	A	807	CLA	15	0
24	A	845	BCR	20	0
22	Z	316	CLA	15	0
22	G	202	CLA	14	0
39	1	312	CHL	8	0
22	Z	303	CLA	29	0
38	3	303	LUT	18	0
35	J	102	T7X	2	0
25	B	803	LHG	8	0
24	5	305	BCR	10	0
39	6	318	CHL	12	0
22	B	832	CLA	9	0
25	4	821	LHG	4	0
22	B	841	CLA	15	0
24	B	848	BCR	15	0
22	5	315	CLA	19	0
22	L	201	CLA	15	0
38	9	301	LUT	16	0
42	7	320	SPH	4	0
22	K	202	CLA	9	0
22	9	306	CLA	15	0
22	5	314	CLA	7	0
41	7	319	3PH	14	0
39	7	313	CHL	9	0
39	4	813	CHL	12	0
22	4	807	CLA	12	0
22	8	316	CLA	3	0
38	7	302	LUT	15	0
22	3	312	CLA	24	0
22	Z	309	CLA	21	0
24	8	304	BCR	14	0
22	5	309	CLA	13	0
22	7	308	CLA	12	0
22	4	817	CLA	4	0
22	7	310	CLA	13	0
22	A	838	CLA	7	0
22	A	840	CLA	13	0

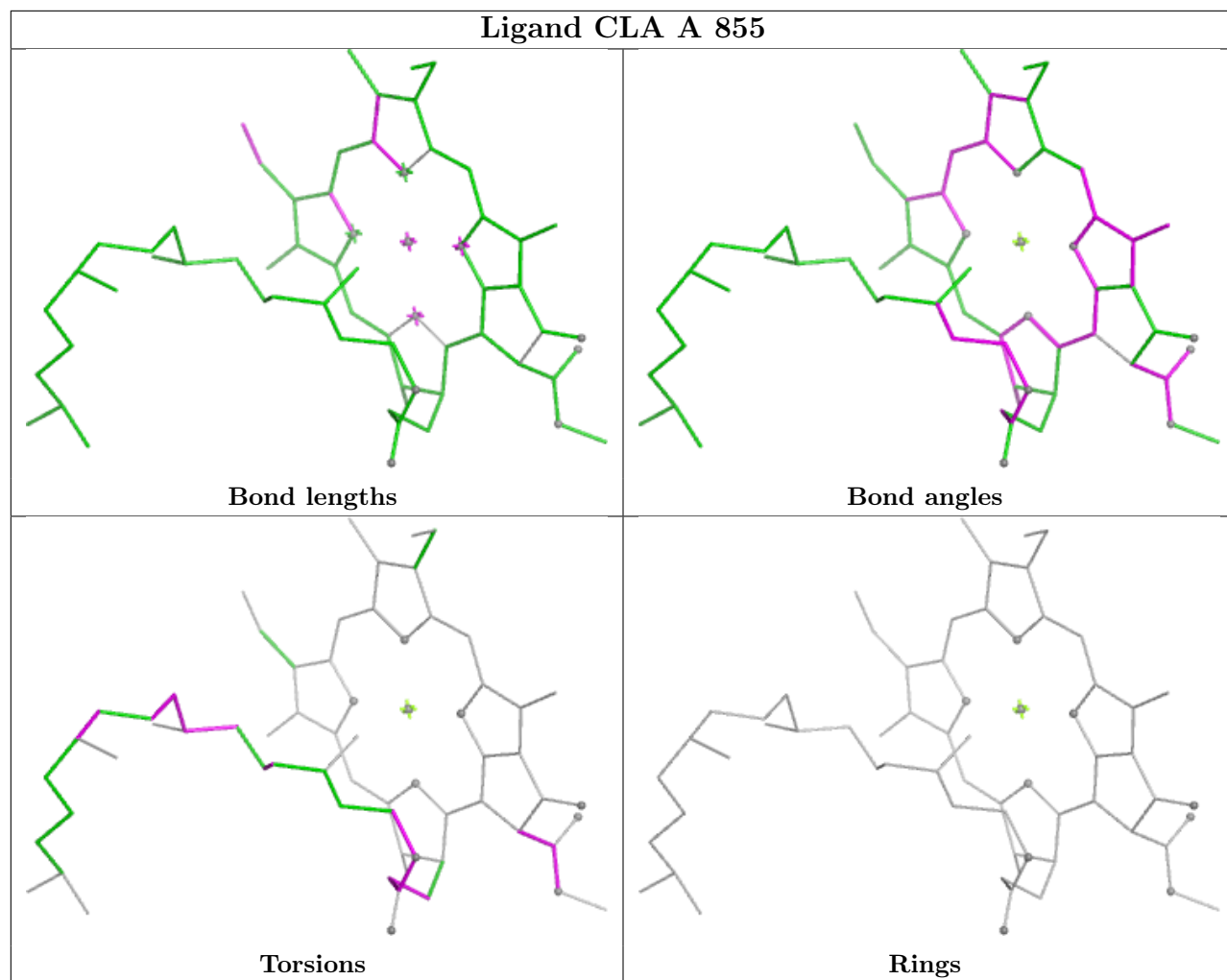
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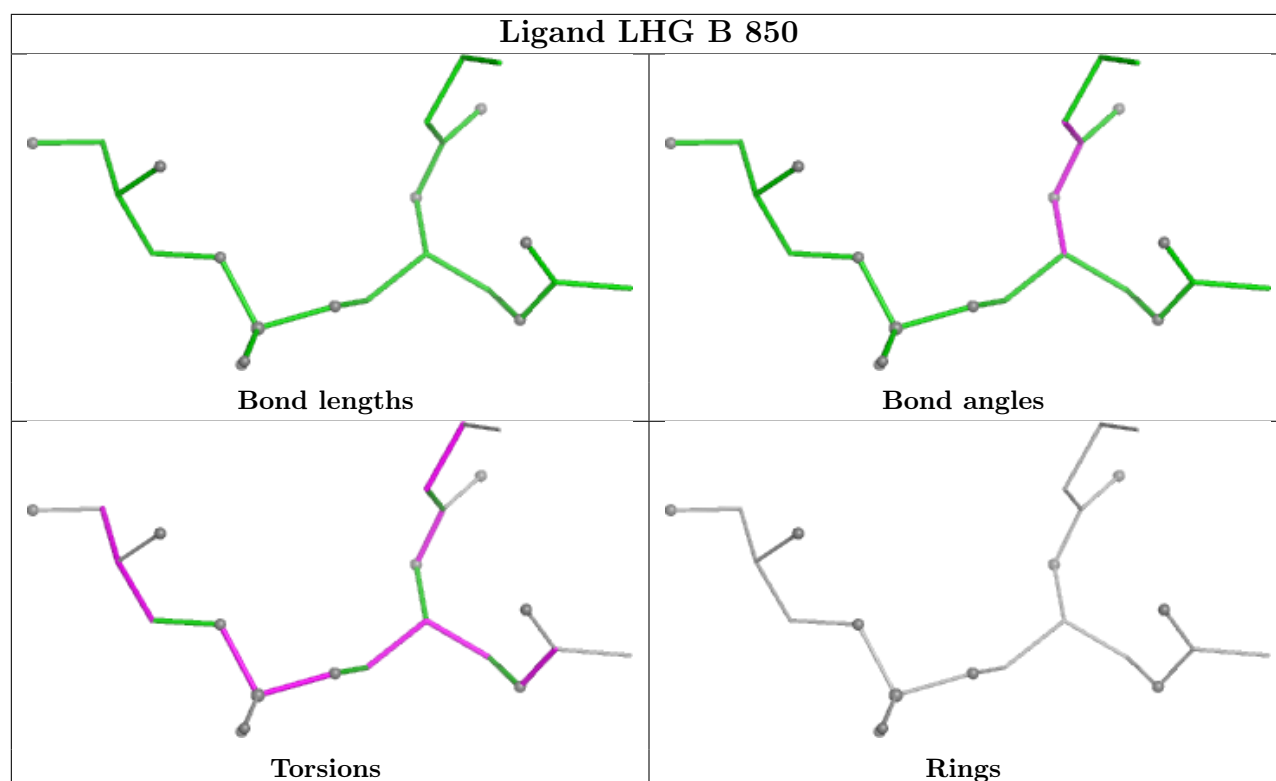
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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31	B	852	DGD	17	0
22	B	807	CLA	8	0
22	4	809	CLA	5	0
24	7	303	BCR	14	0
22	4	811	CLA	6	0
22	3	319	CLA	5	0
22	3	316	CLA	12	0
22	A	823	CLA	28	0
39	4	816	CHL	21	0
24	4	804	BCR	26	0
22	Z	314	CLA	6	0
22	K	204	CLA	6	0
24	B	853	BCR	20	0
22	7	307	CLA	18	0
22	B	814	CLA	16	0
22	6	309	CLA	21	0
25	3	321	LHG	1	0
25	7	318	LHG	10	0
24	B	846	BCR	12	0
22	A	854	CLA	10	0
22	B	810	CLA	13	0
22	K	205	CLA	4	0
22	A	820	CLA	8	0
24	F	303	BCR	14	0
22	5	320	CLA	11	0
24	K	206	BCR	12	0
22	6	302	CLA	16	0
39	8	301	CHL	11	0
22	A	841	CLA	16	0
22	B	834	CLA	11	0
22	A	817	CLA	14	0
22	B	806	CLA	19	0
22	B	842	CLA	24	0
22	7	323	CLA	16	0
22	B	801	CLA	13	0
22	B	836	CLA	7	0
22	8	308	CLA	11	0
22	B	826	CLA	12	0
36	J	105	C7Z	2	0
24	B	844	BCR	20	0
22	7	316	CLA	8	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.

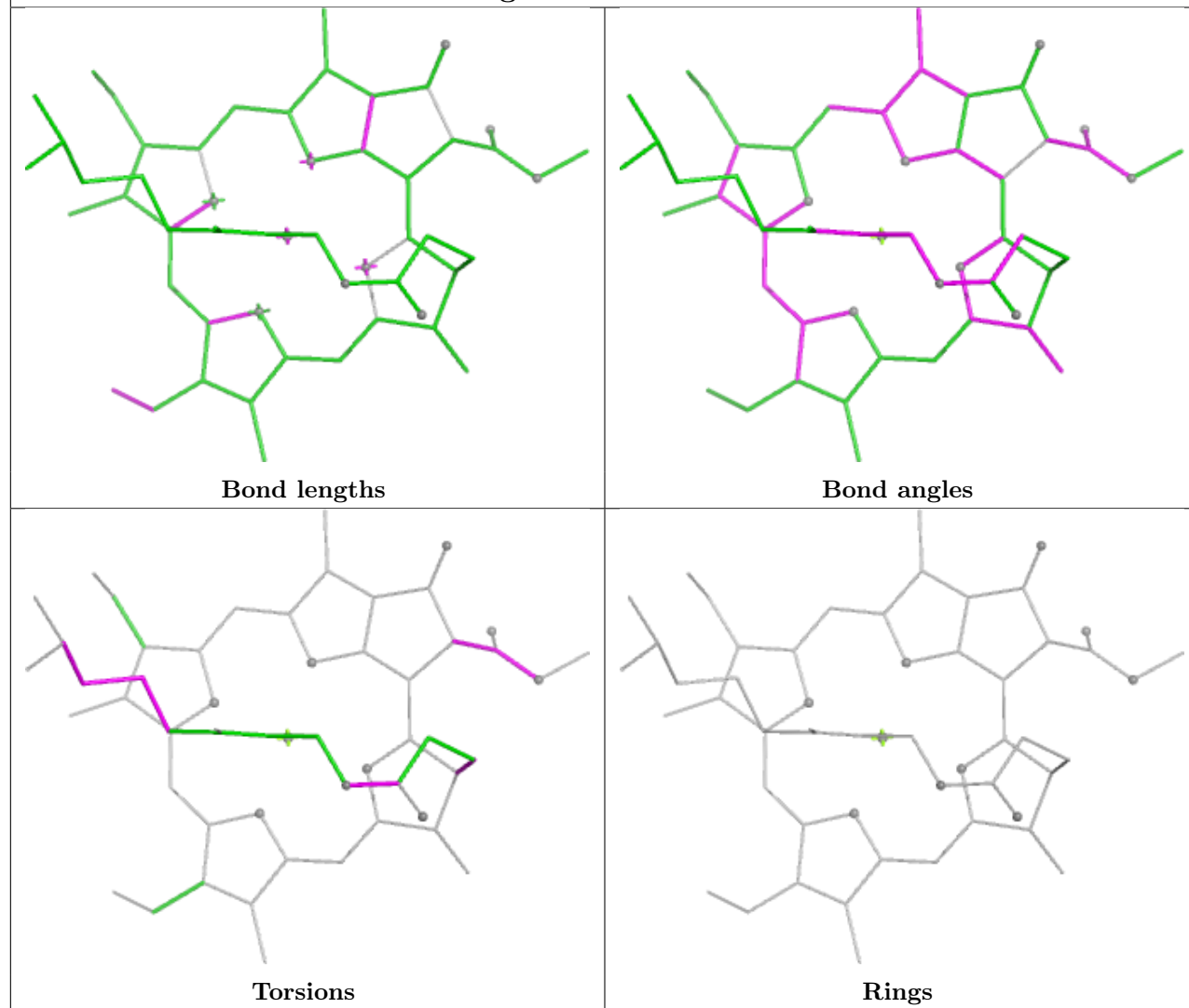




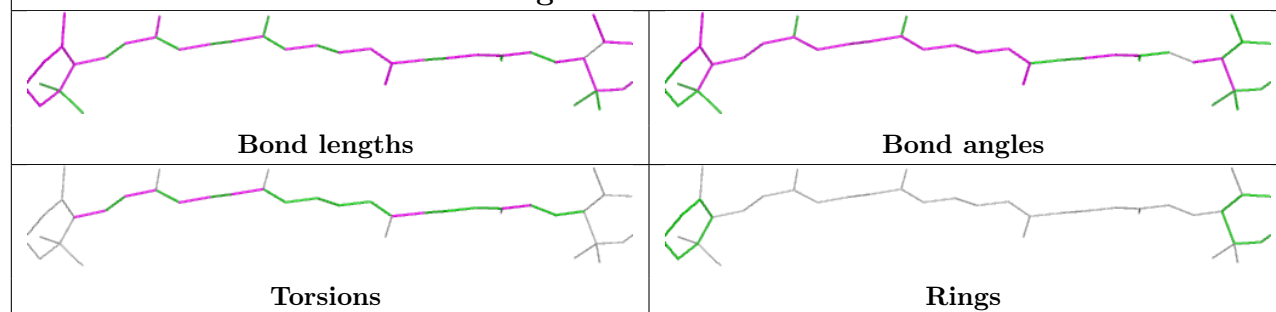




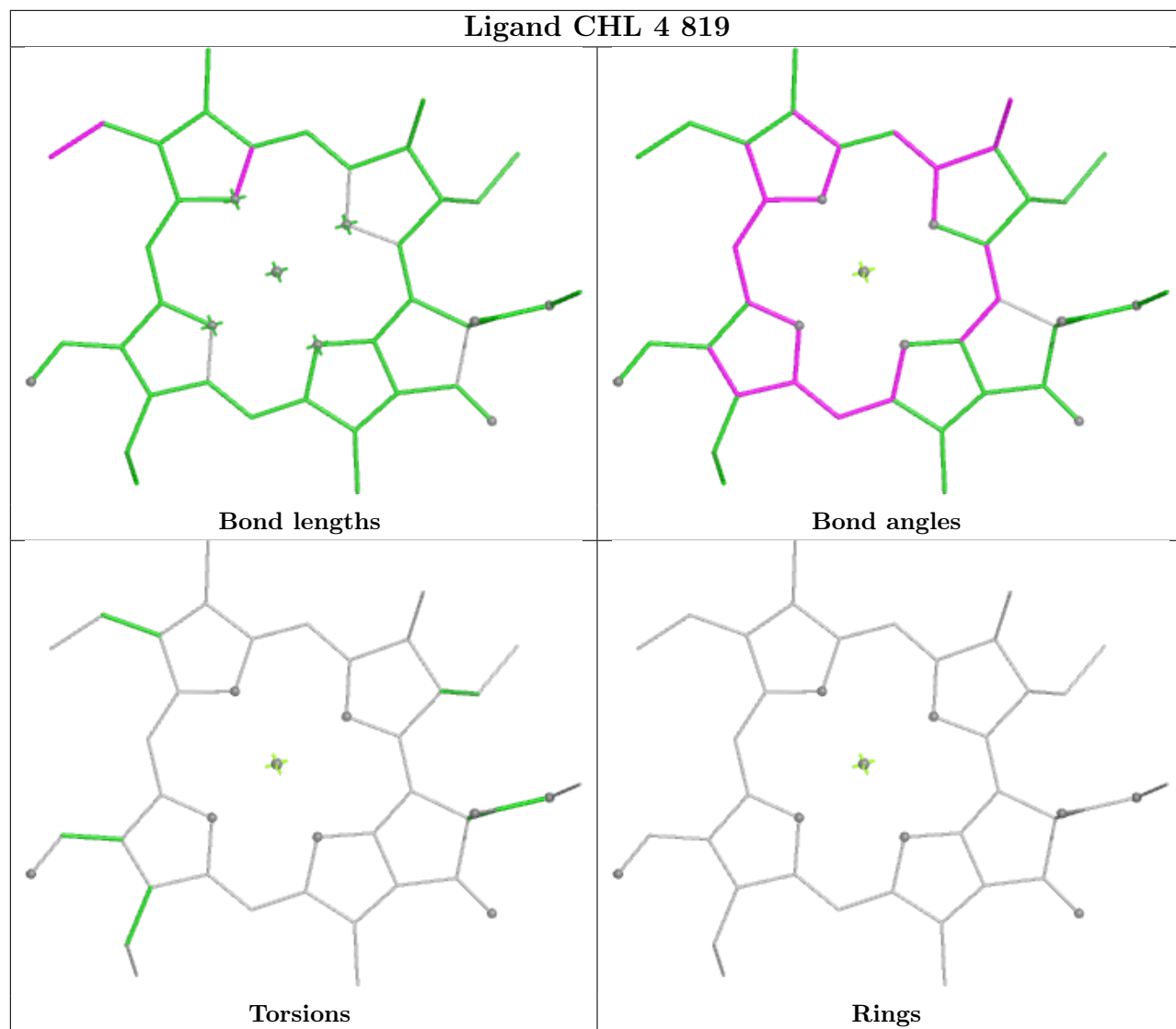
Ligand CLA 2 301



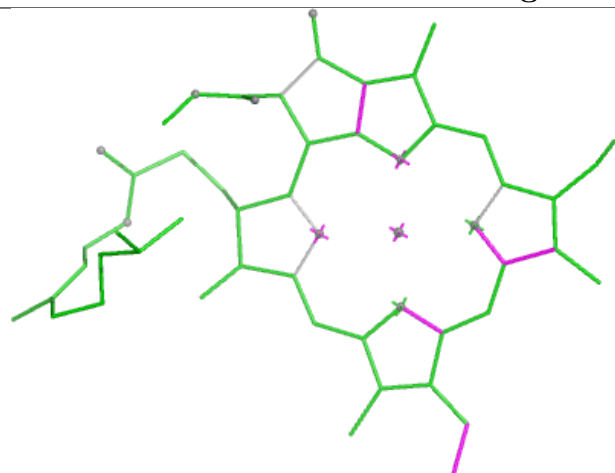
Ligand LUT 7 301



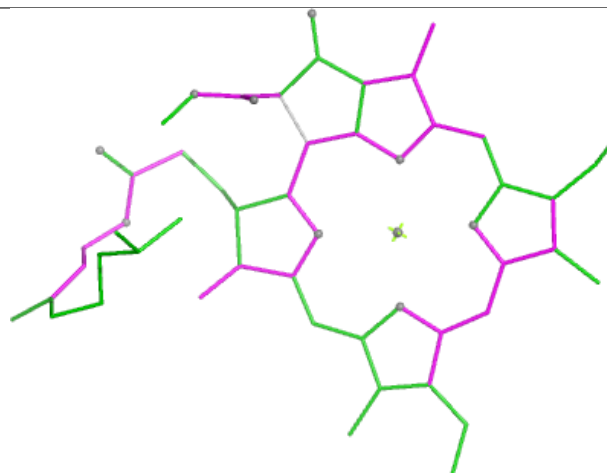
Ligand CHL 4 819



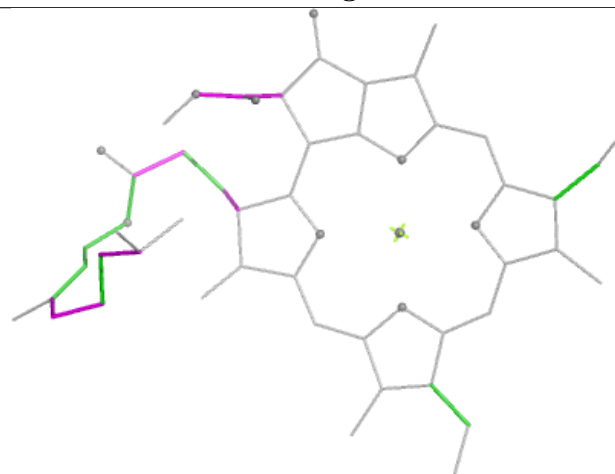
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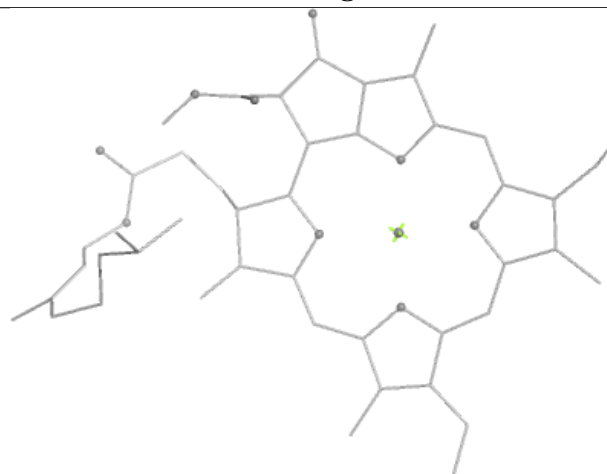
Bond lengths



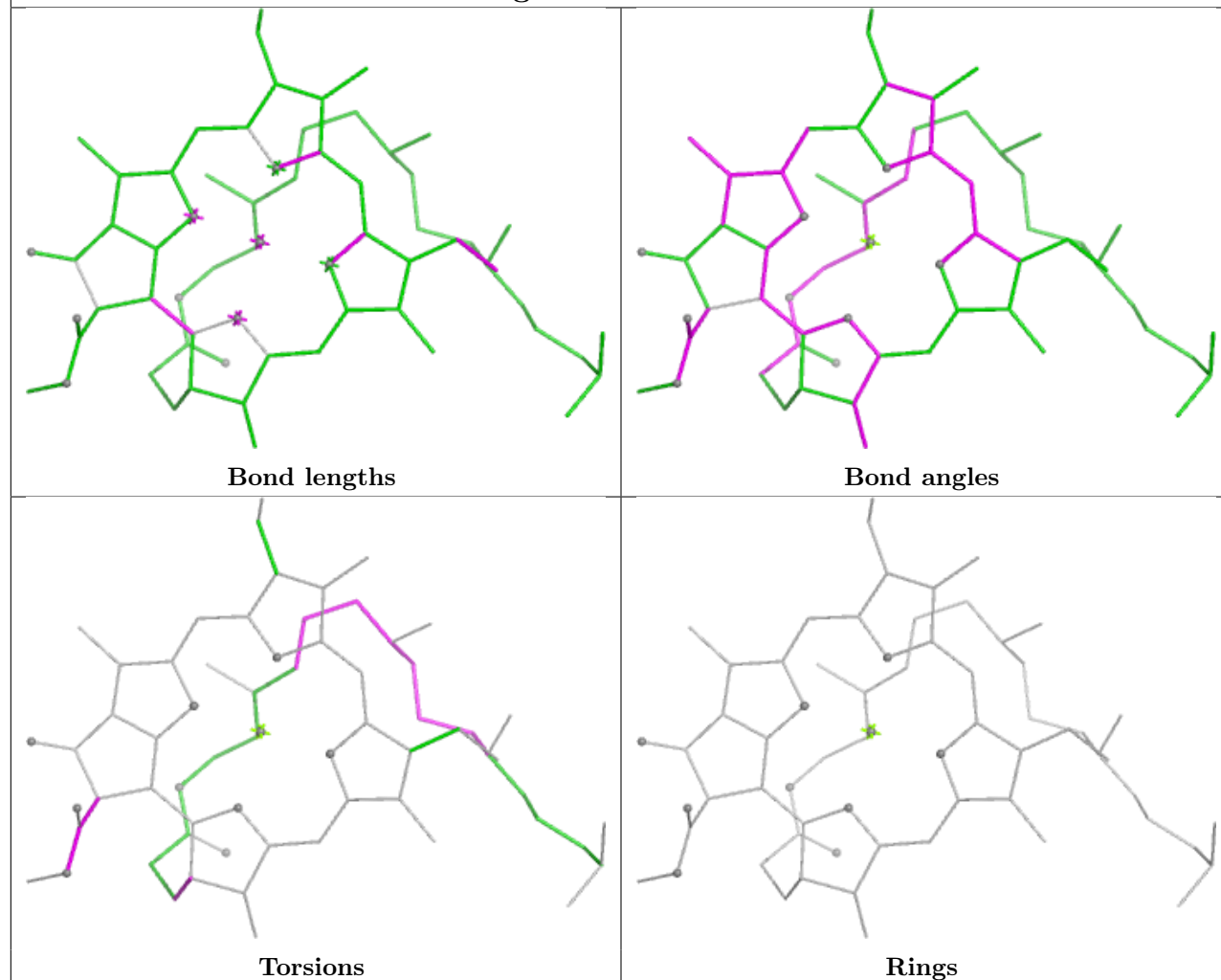
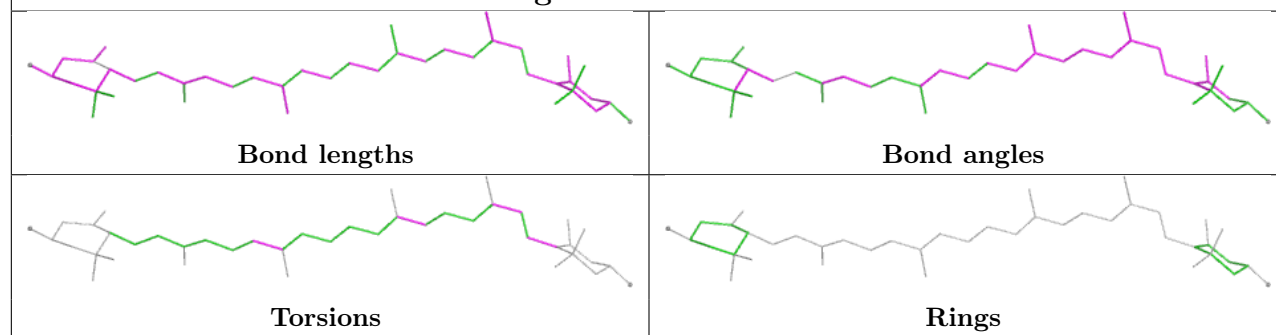
Bond angles

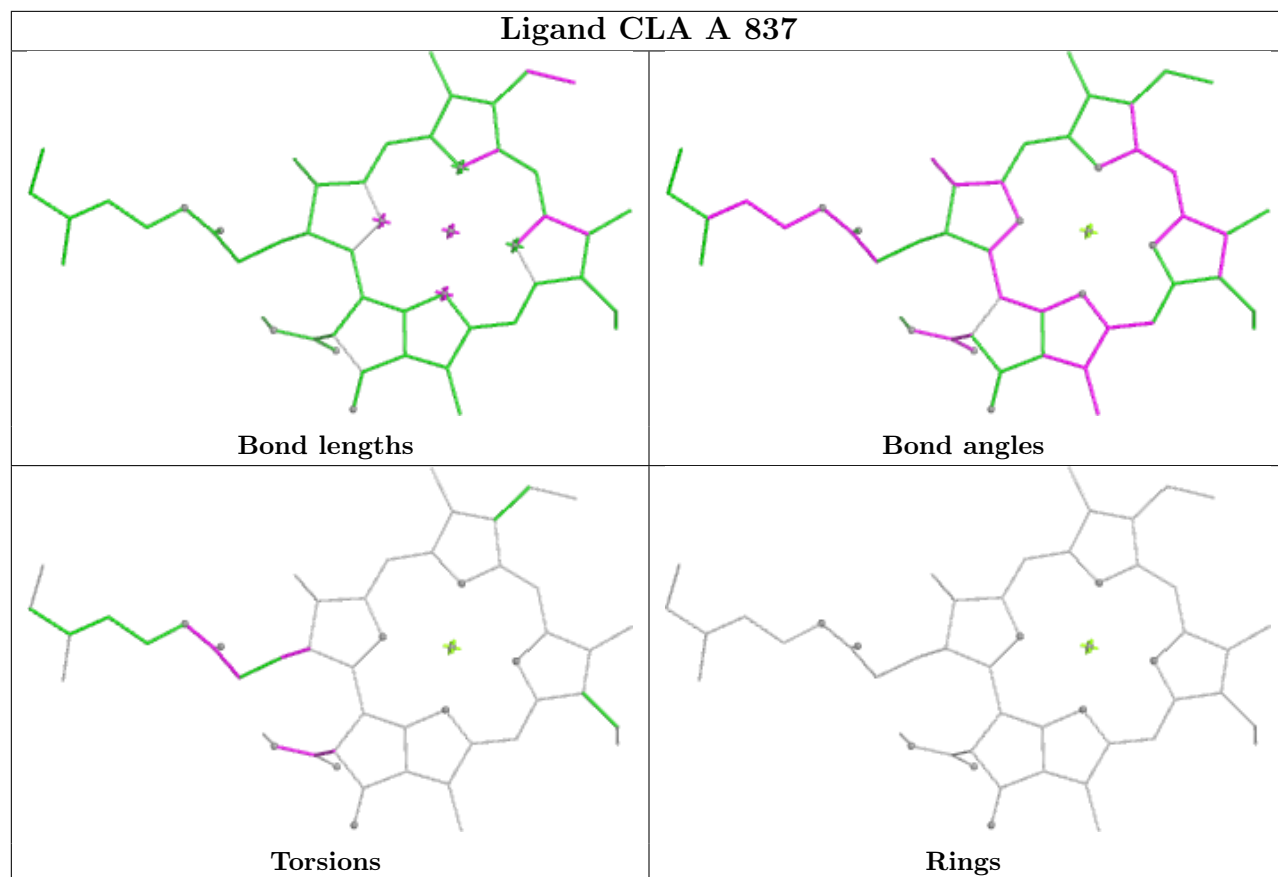


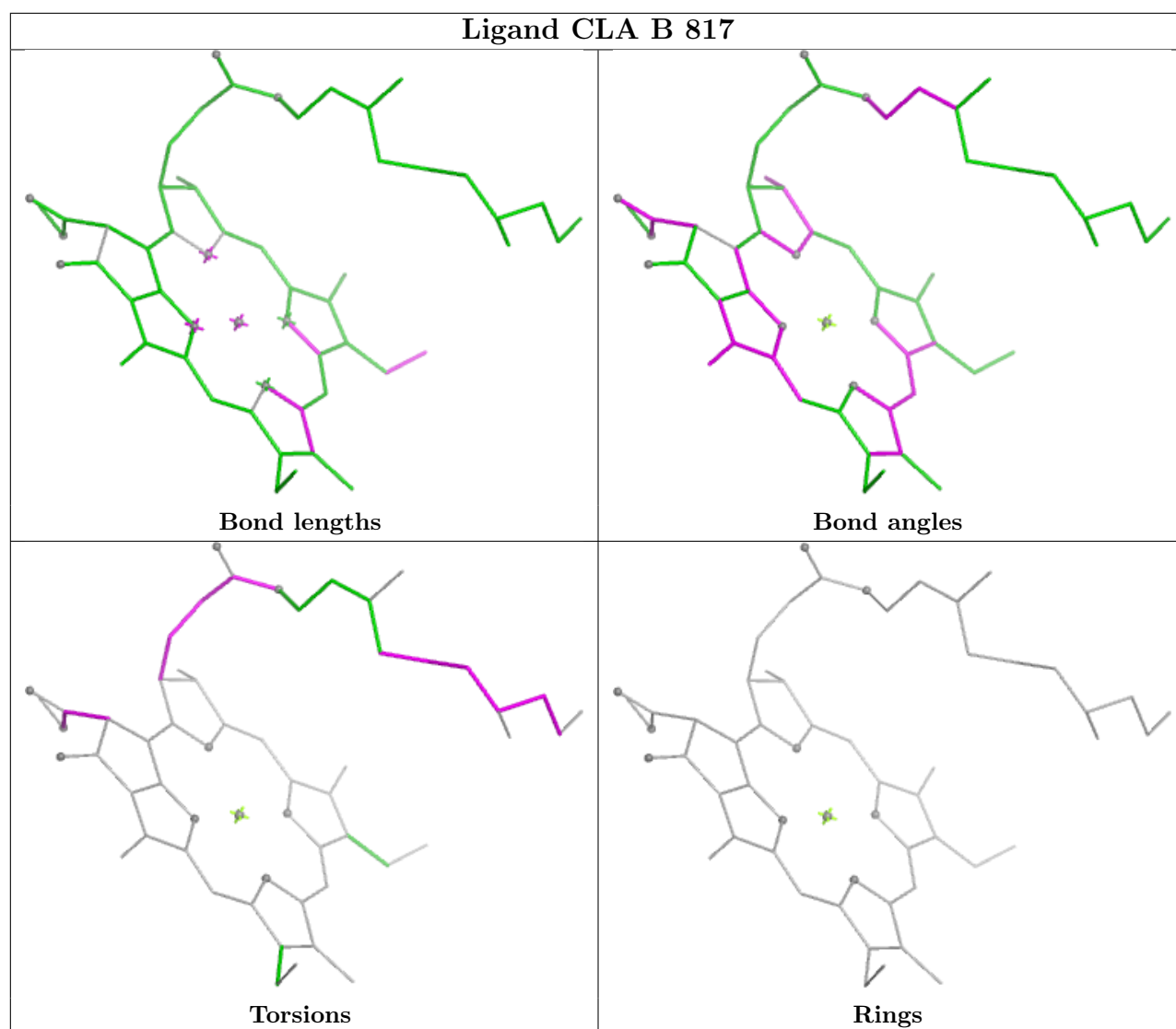
Torsions

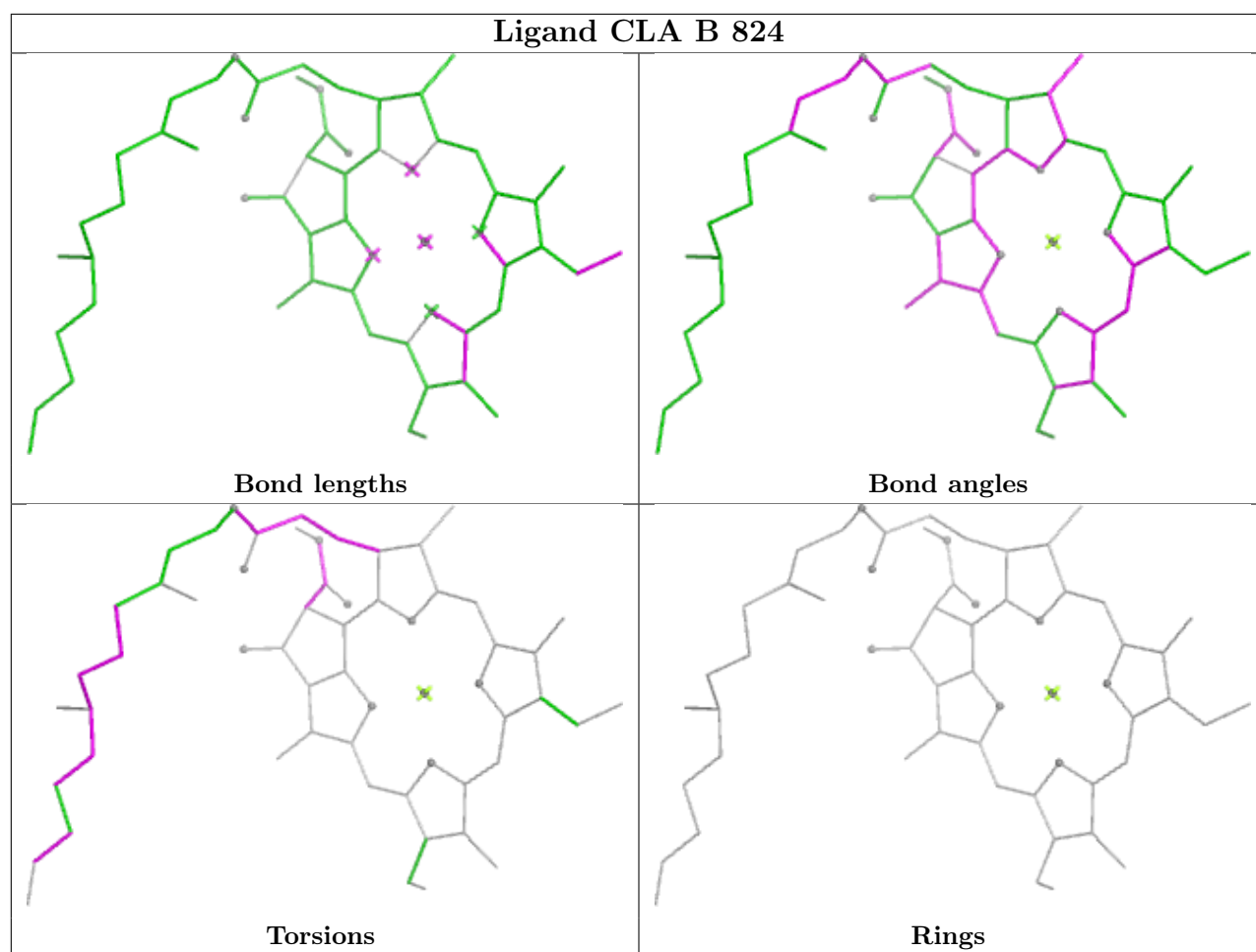


Rings

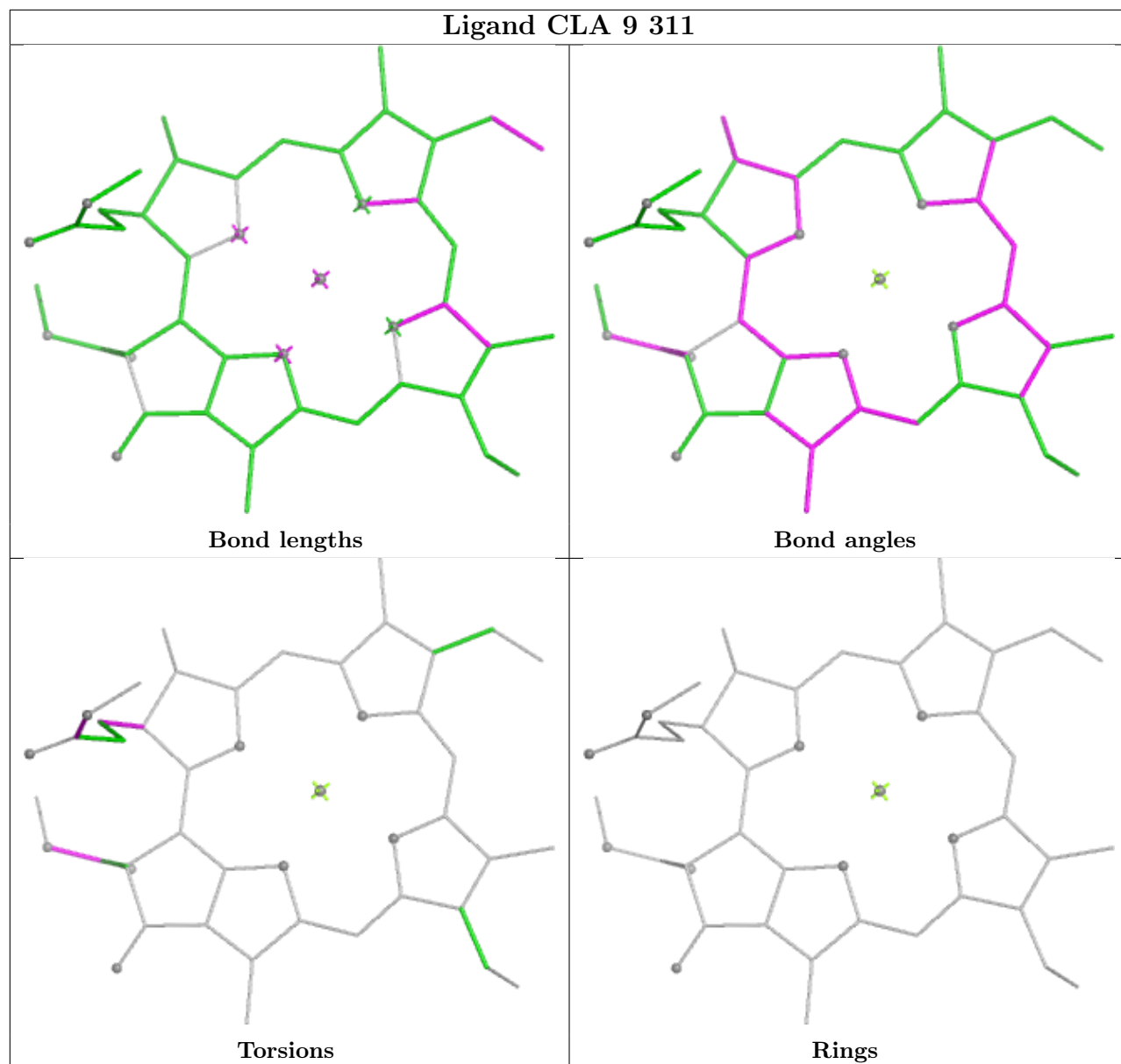
Ligand CLA 7 306**Ligand LUT Z 302**



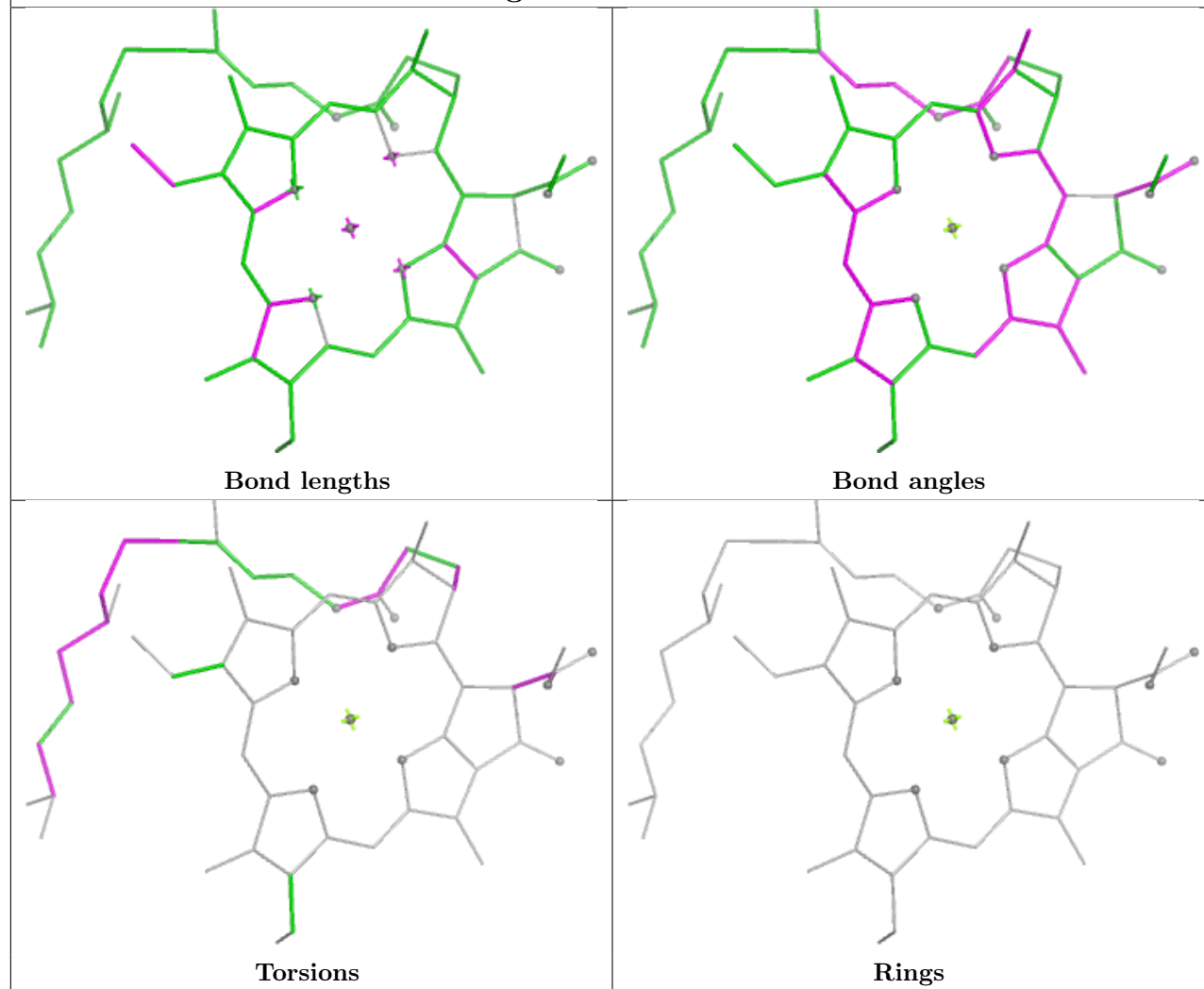




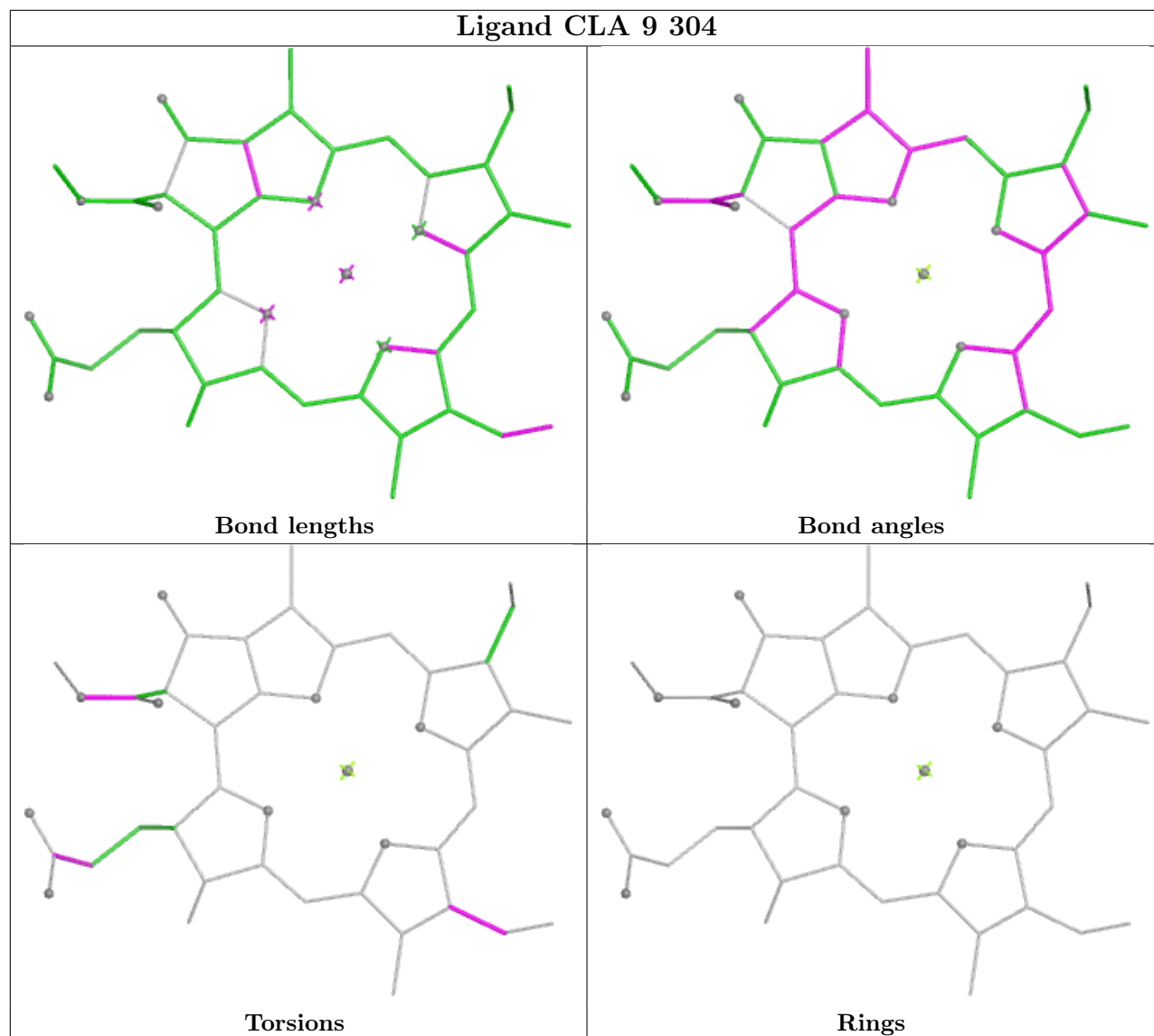
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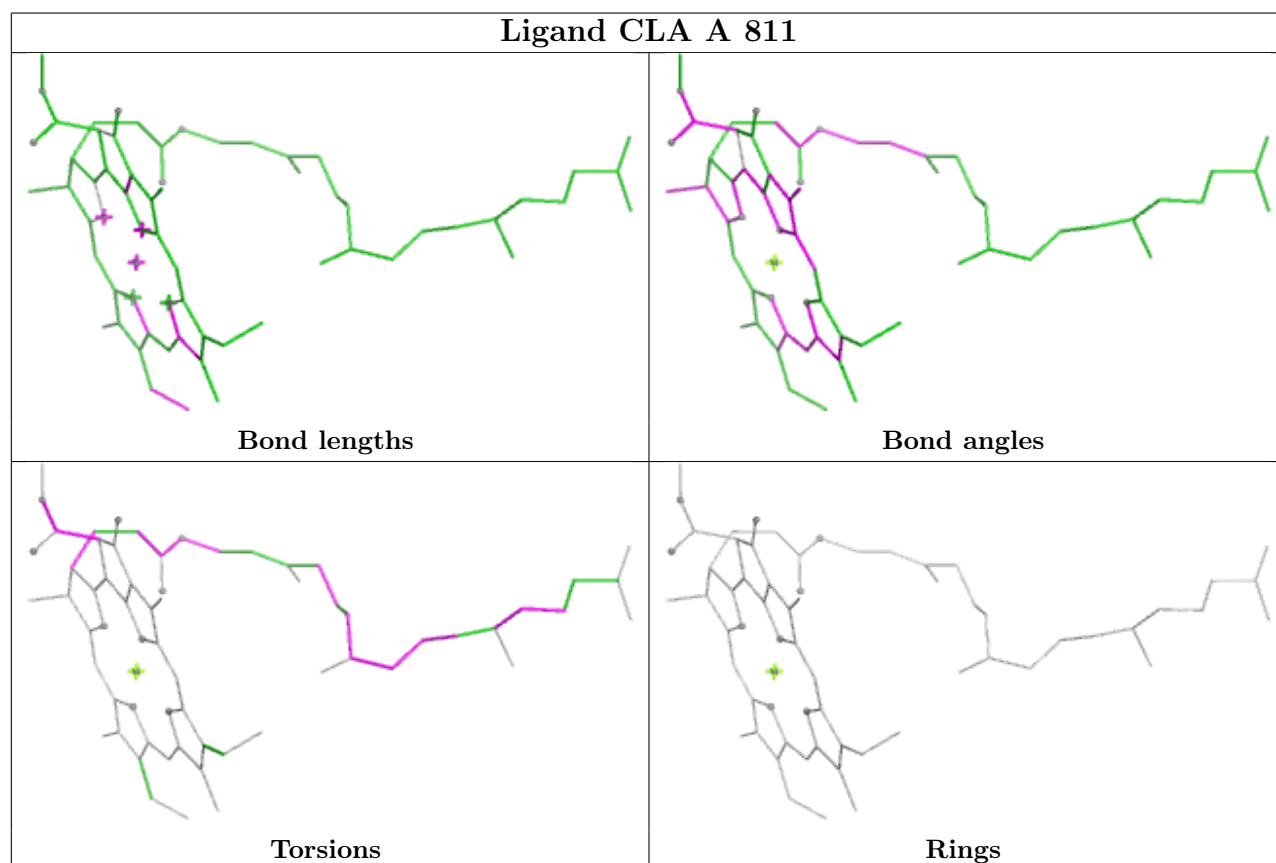
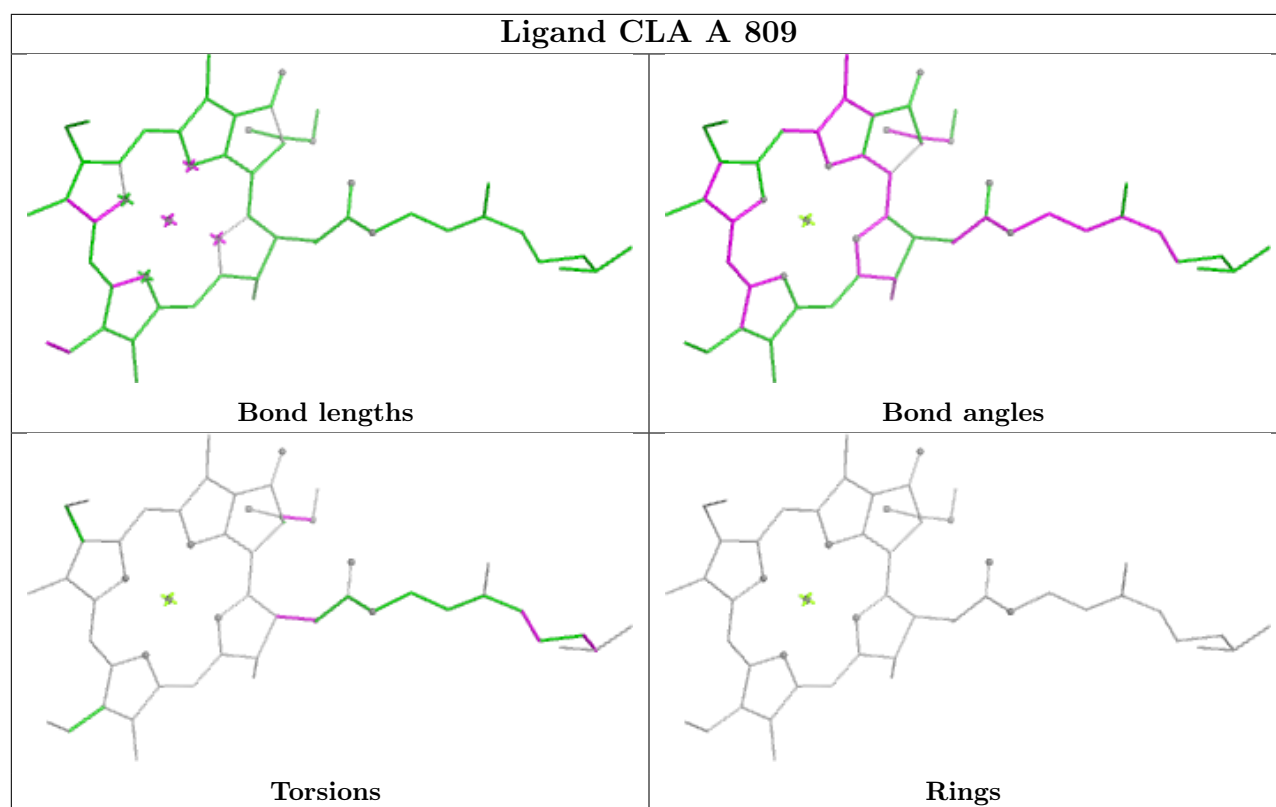


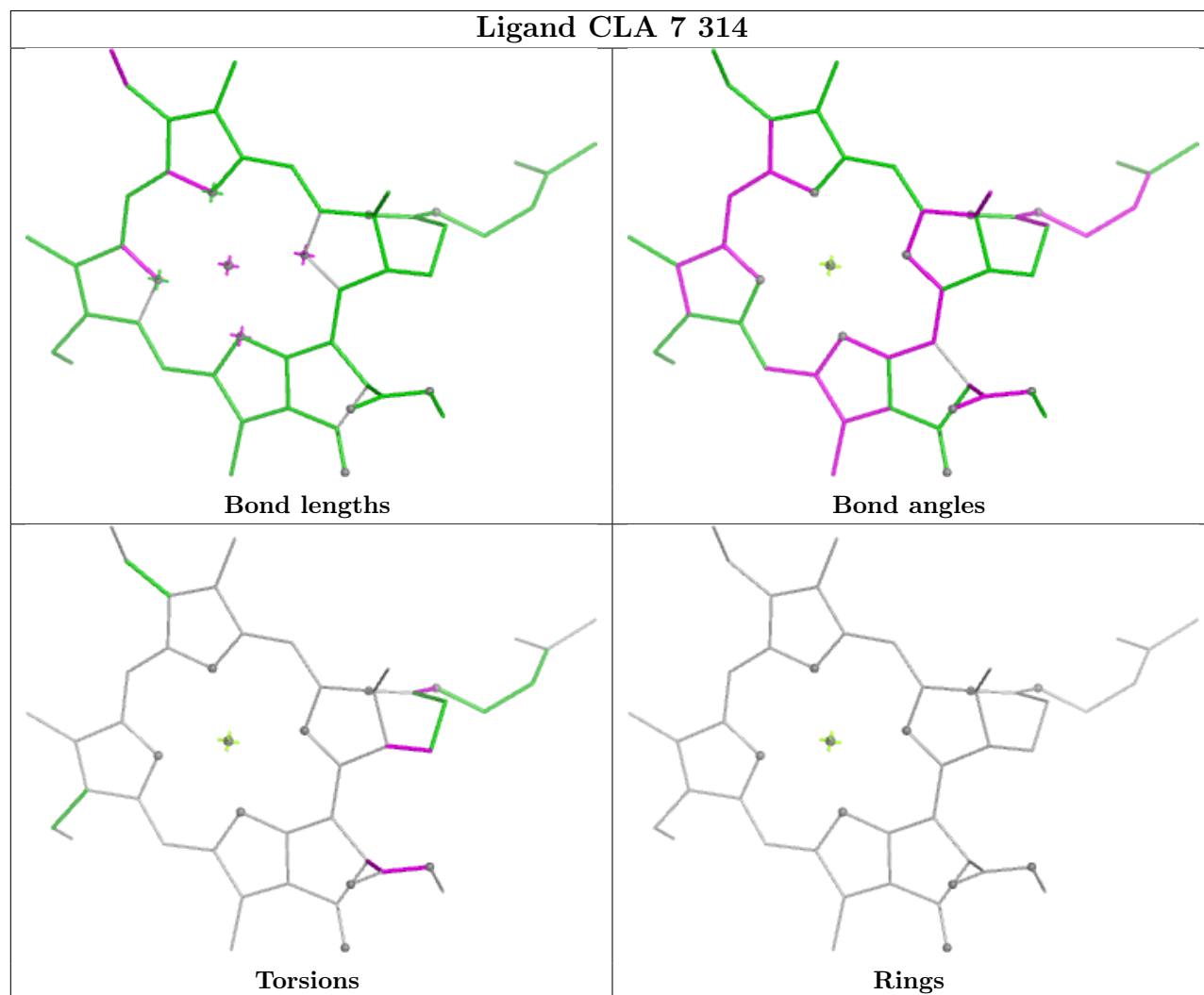
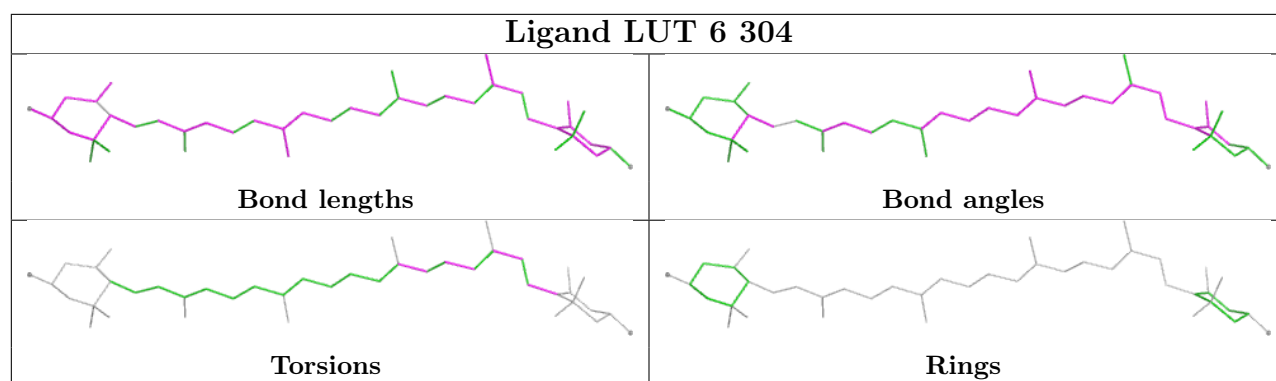
Ligand CLA 1 307

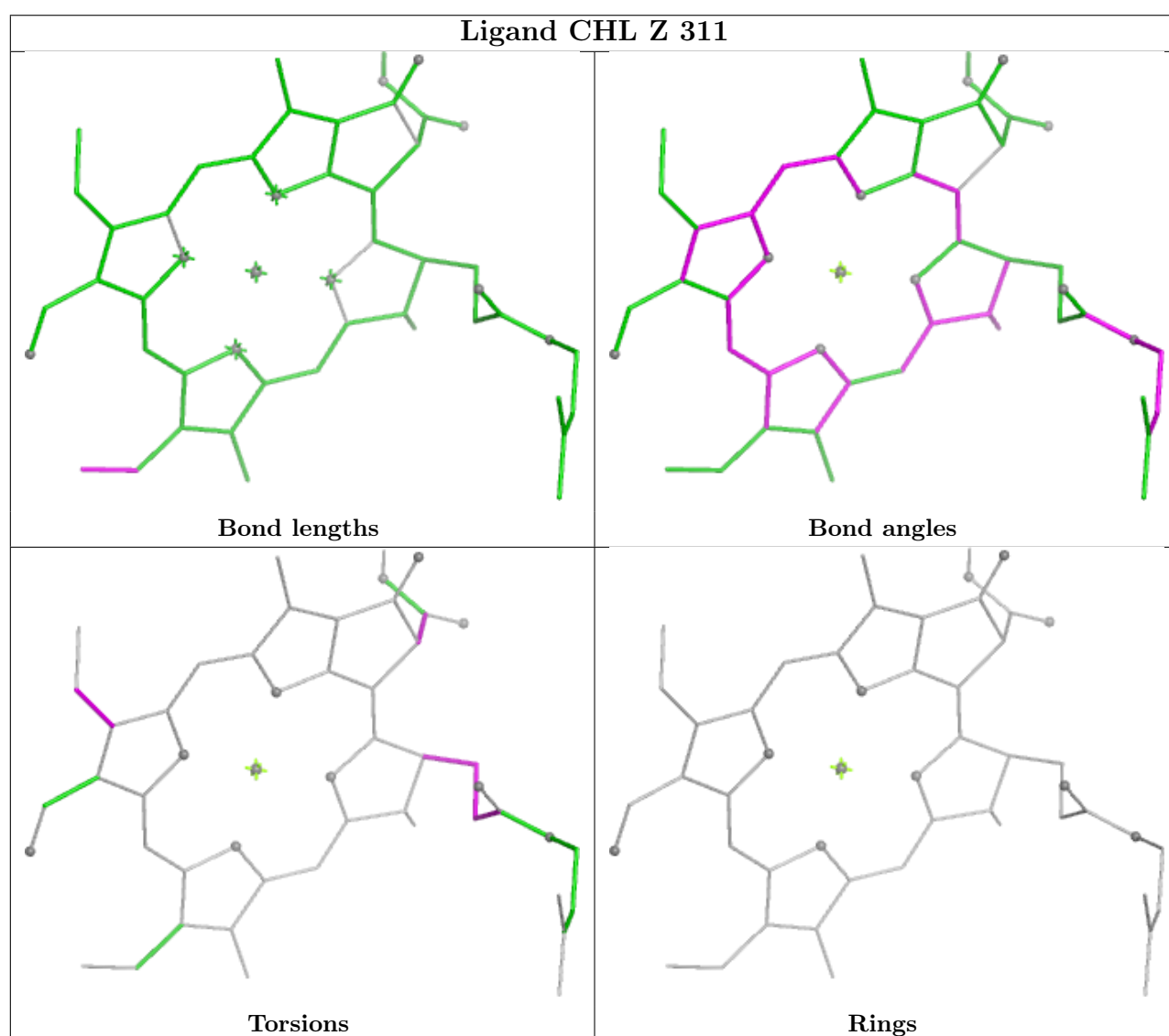
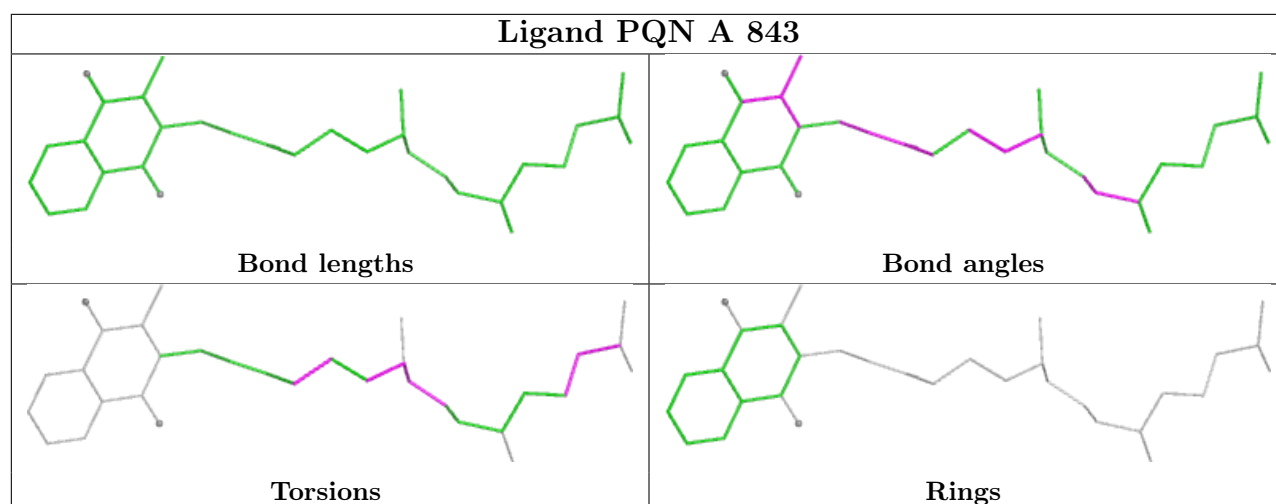


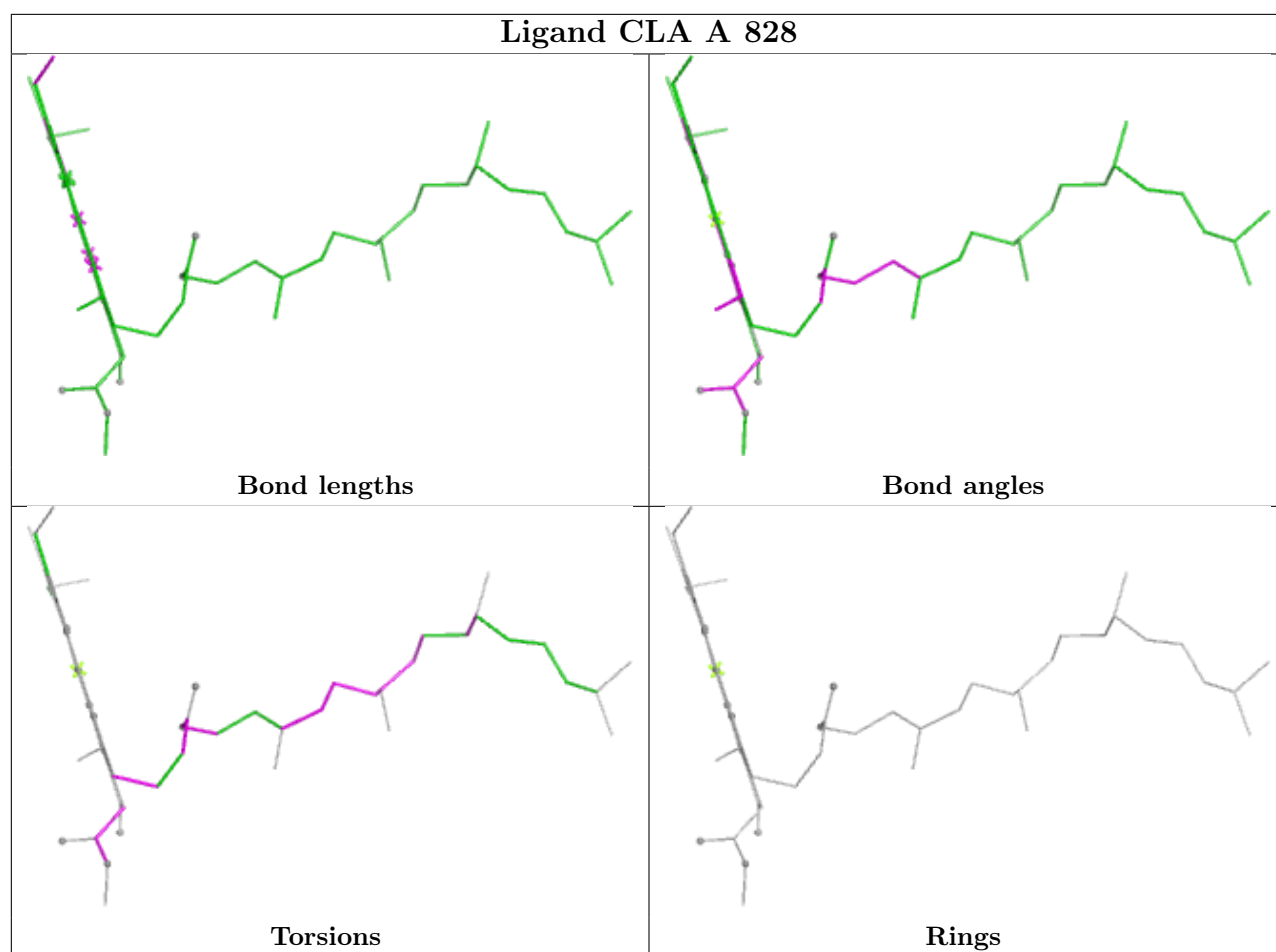
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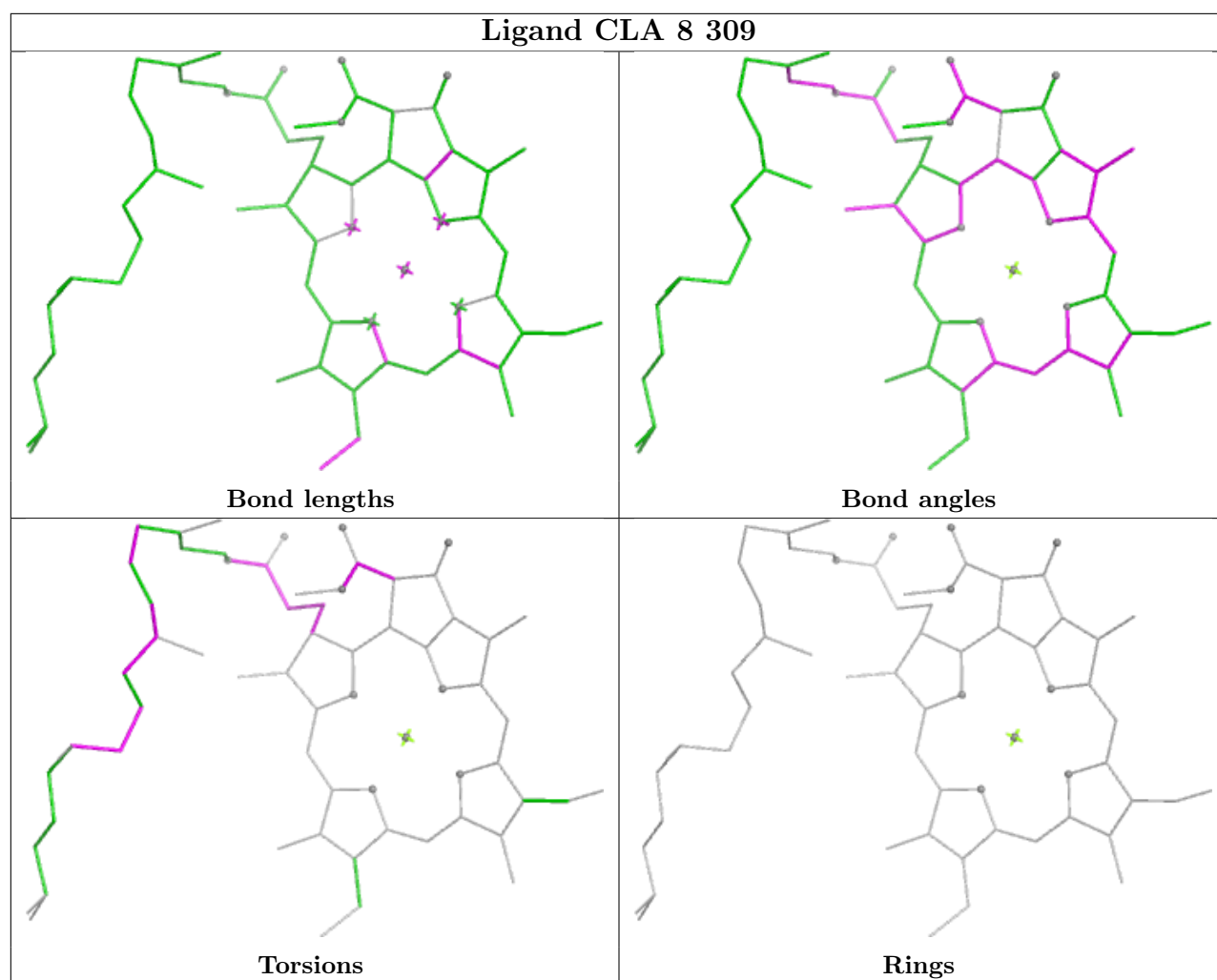


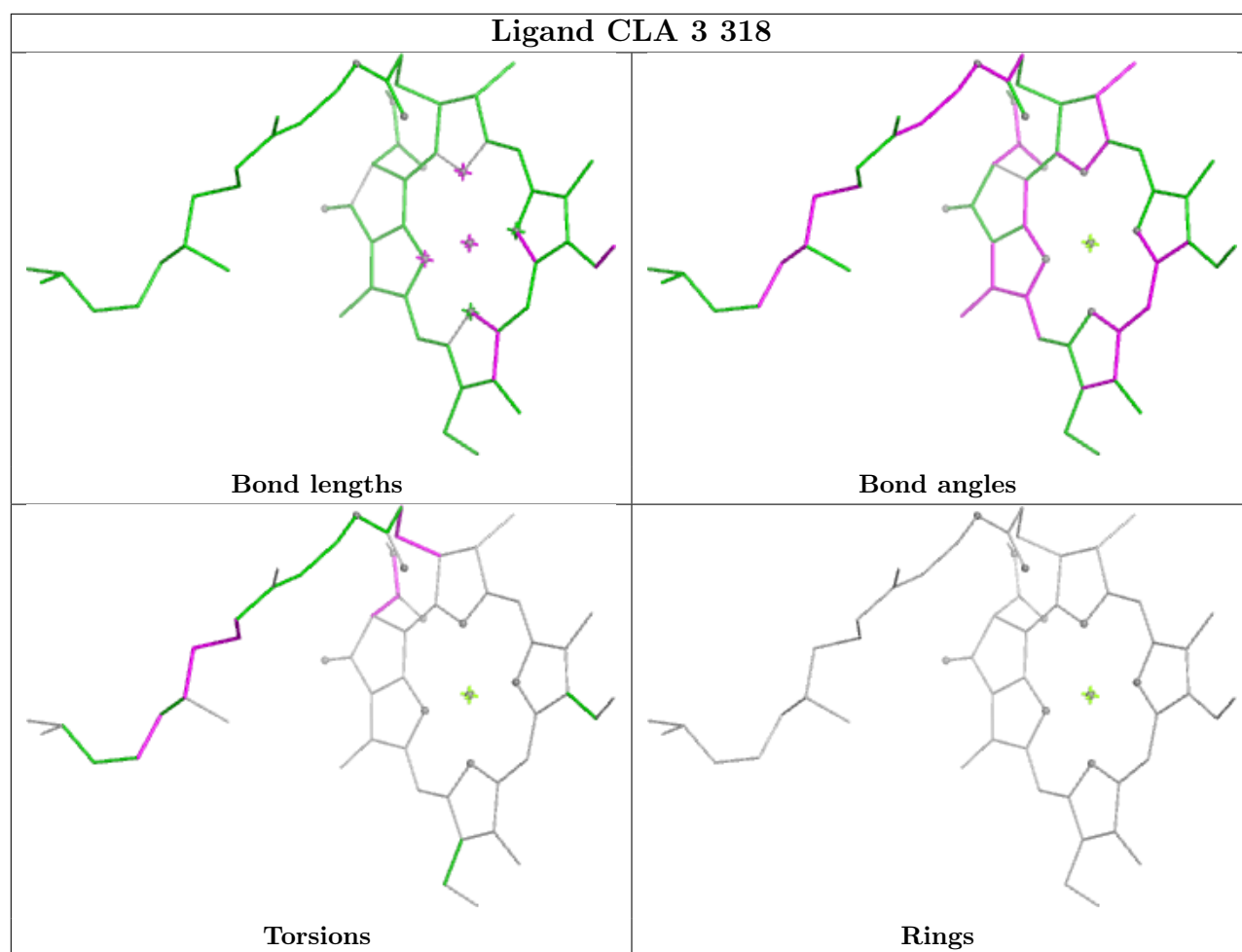




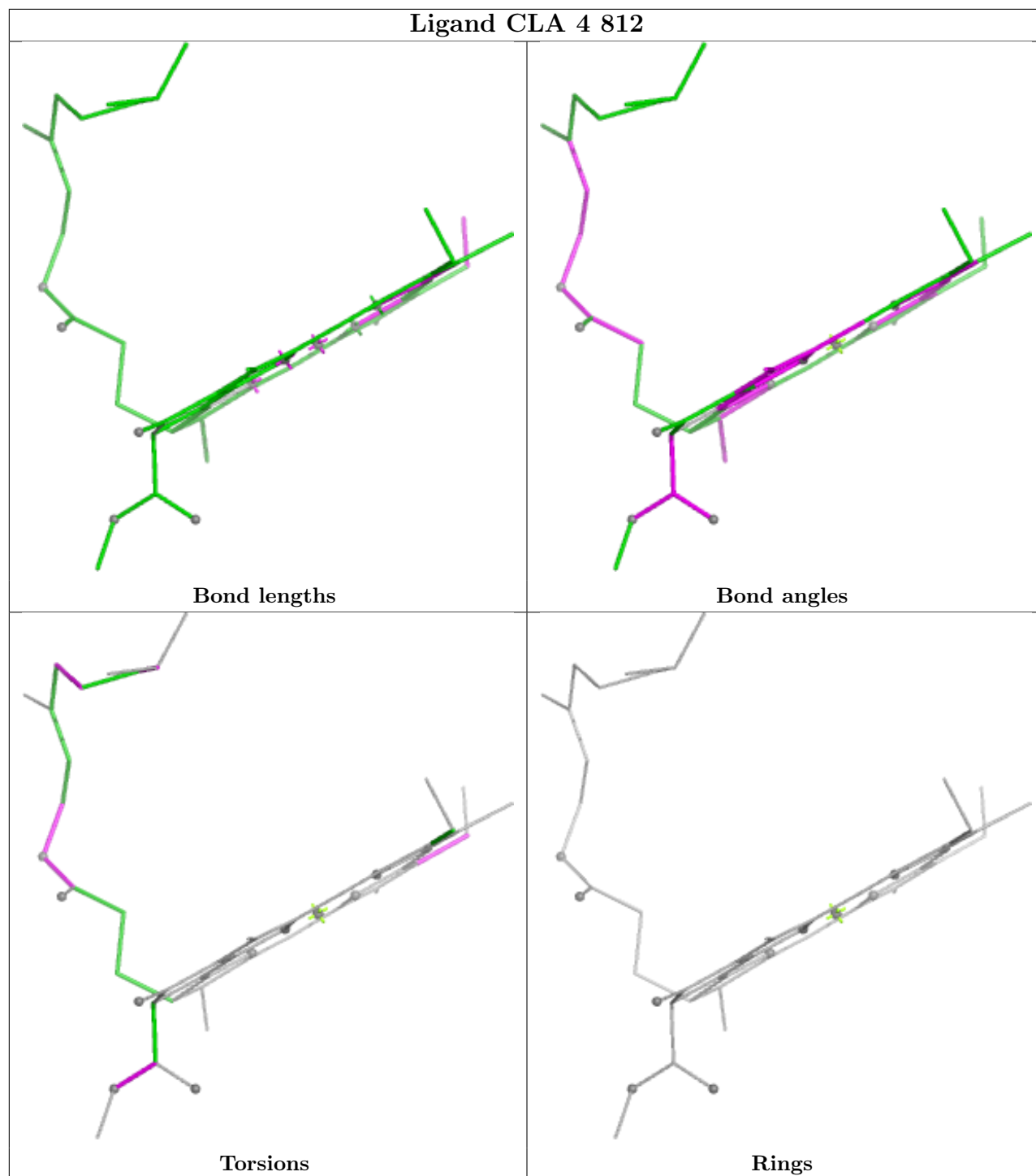


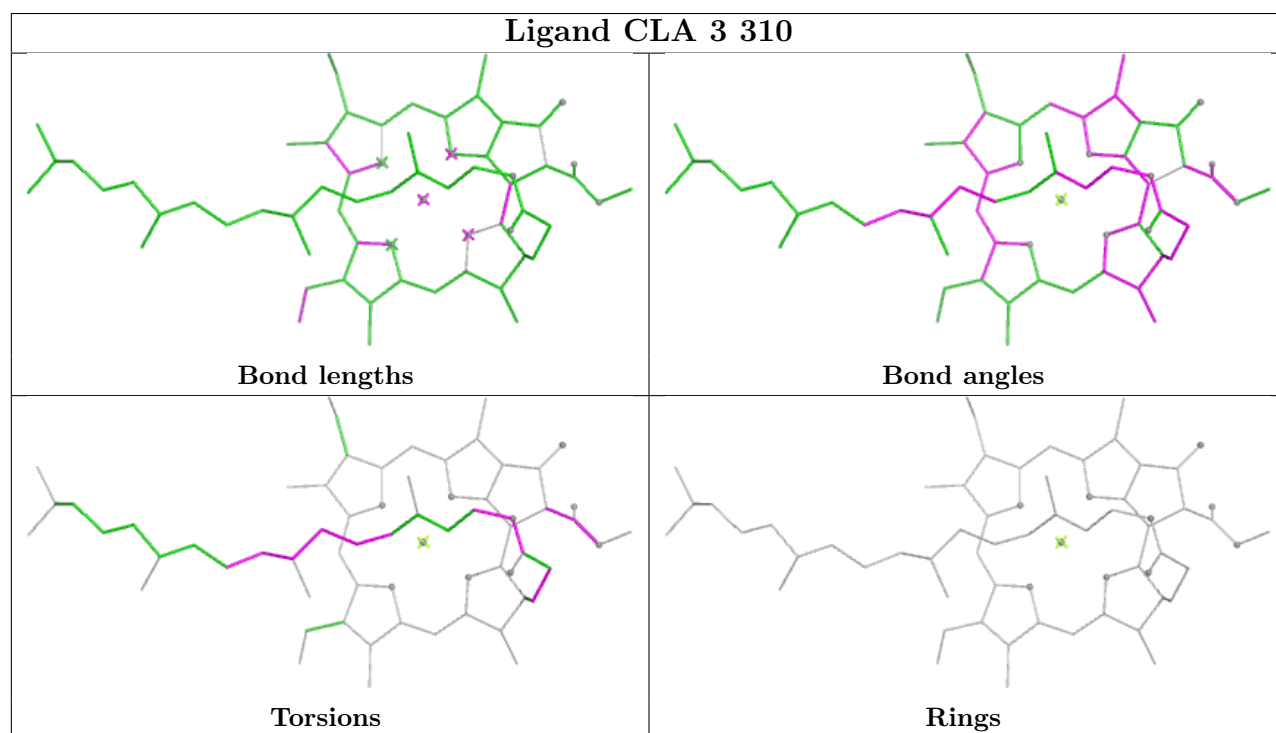
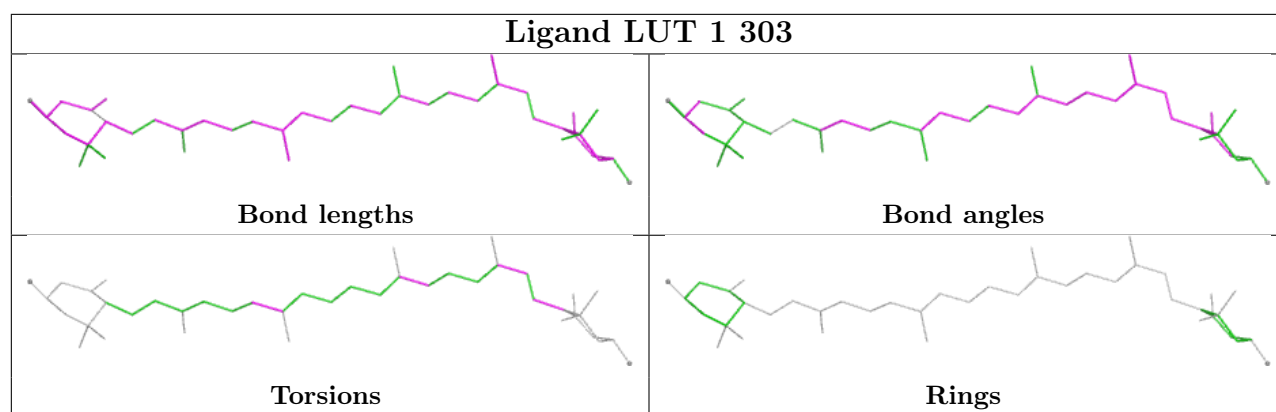


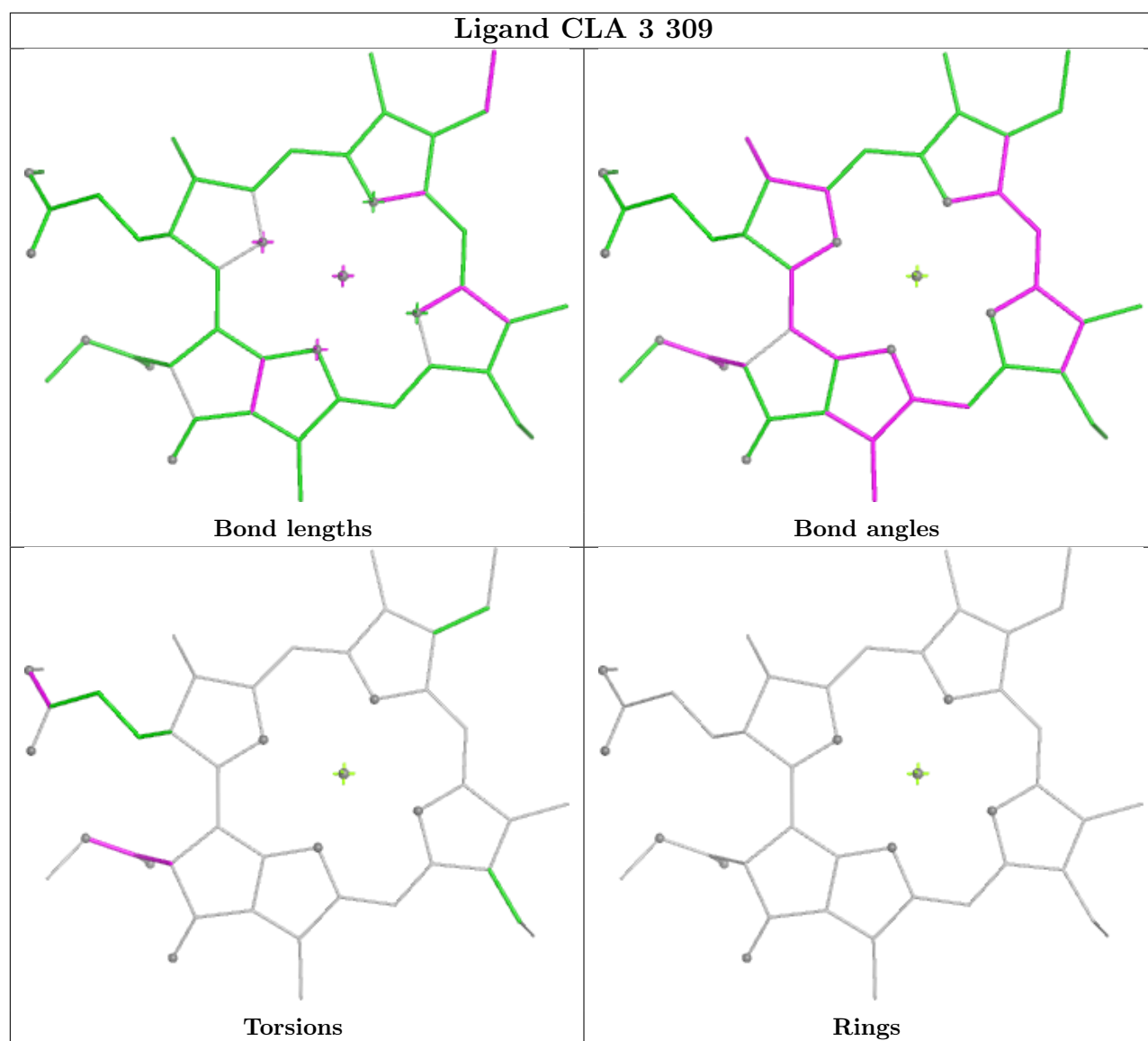




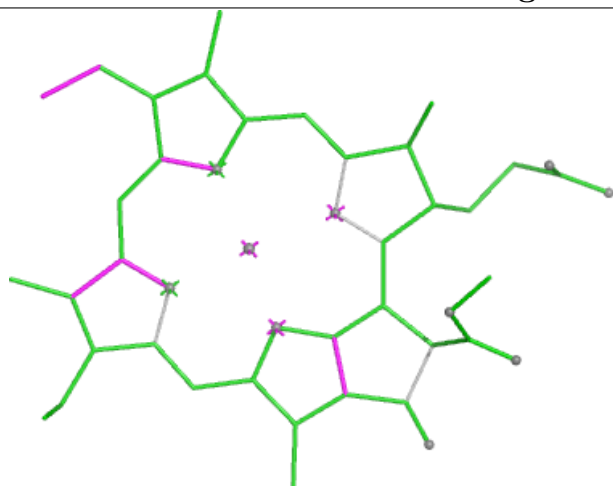
Ligand CLA 4 812



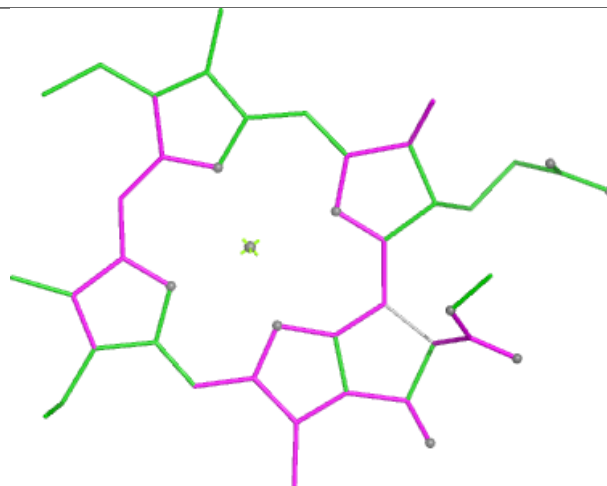




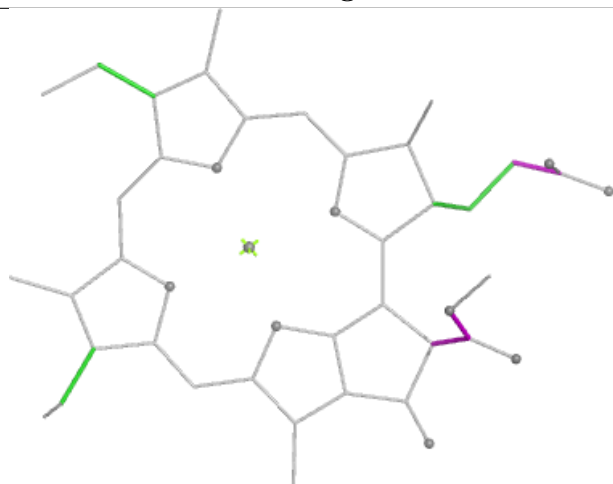
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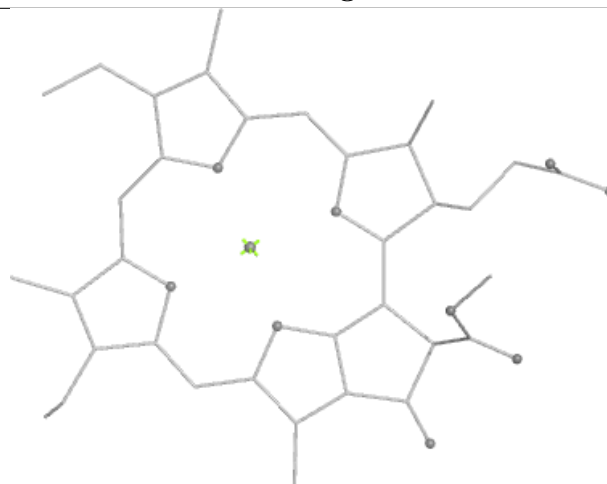
Bond lengths



Bond angles

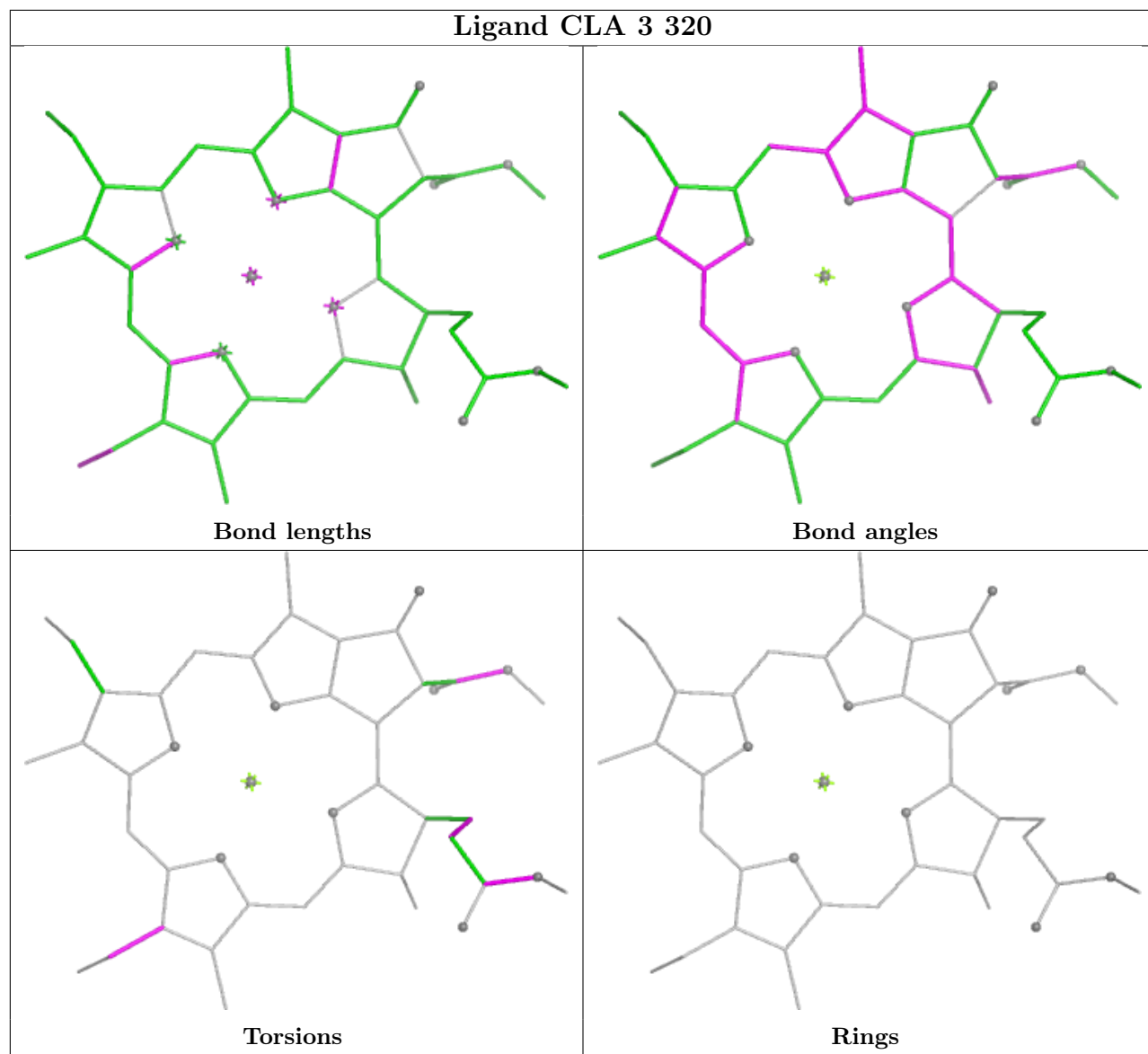


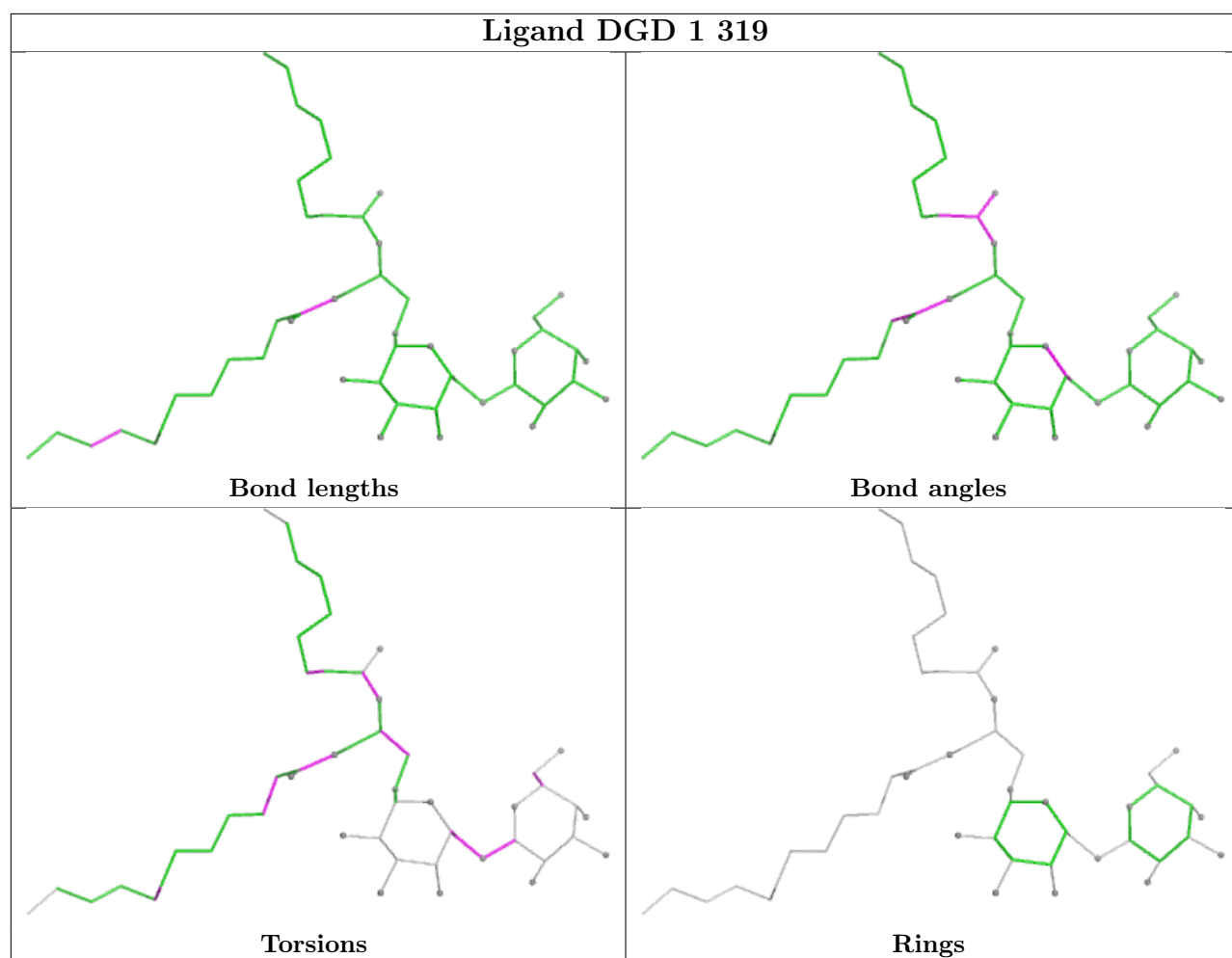
Torsions

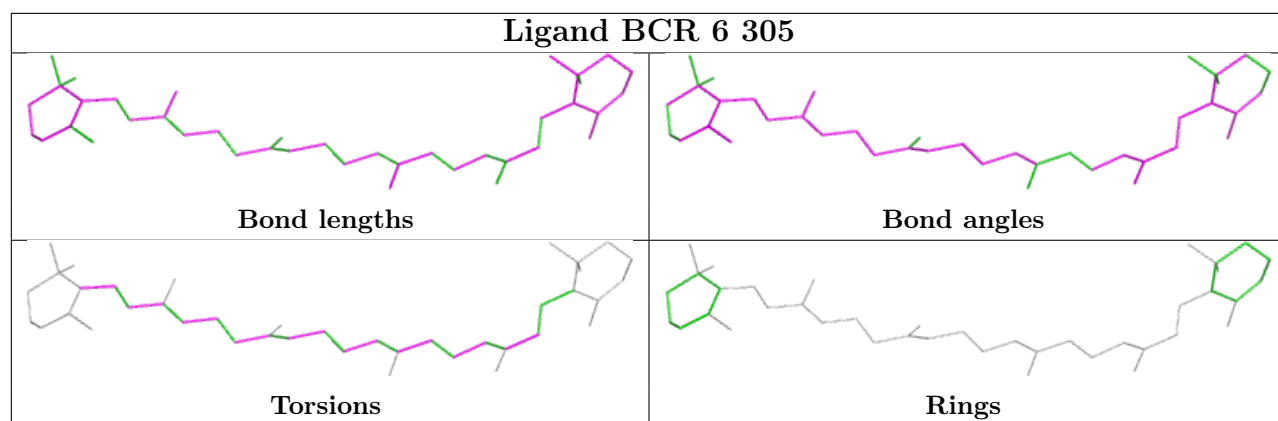
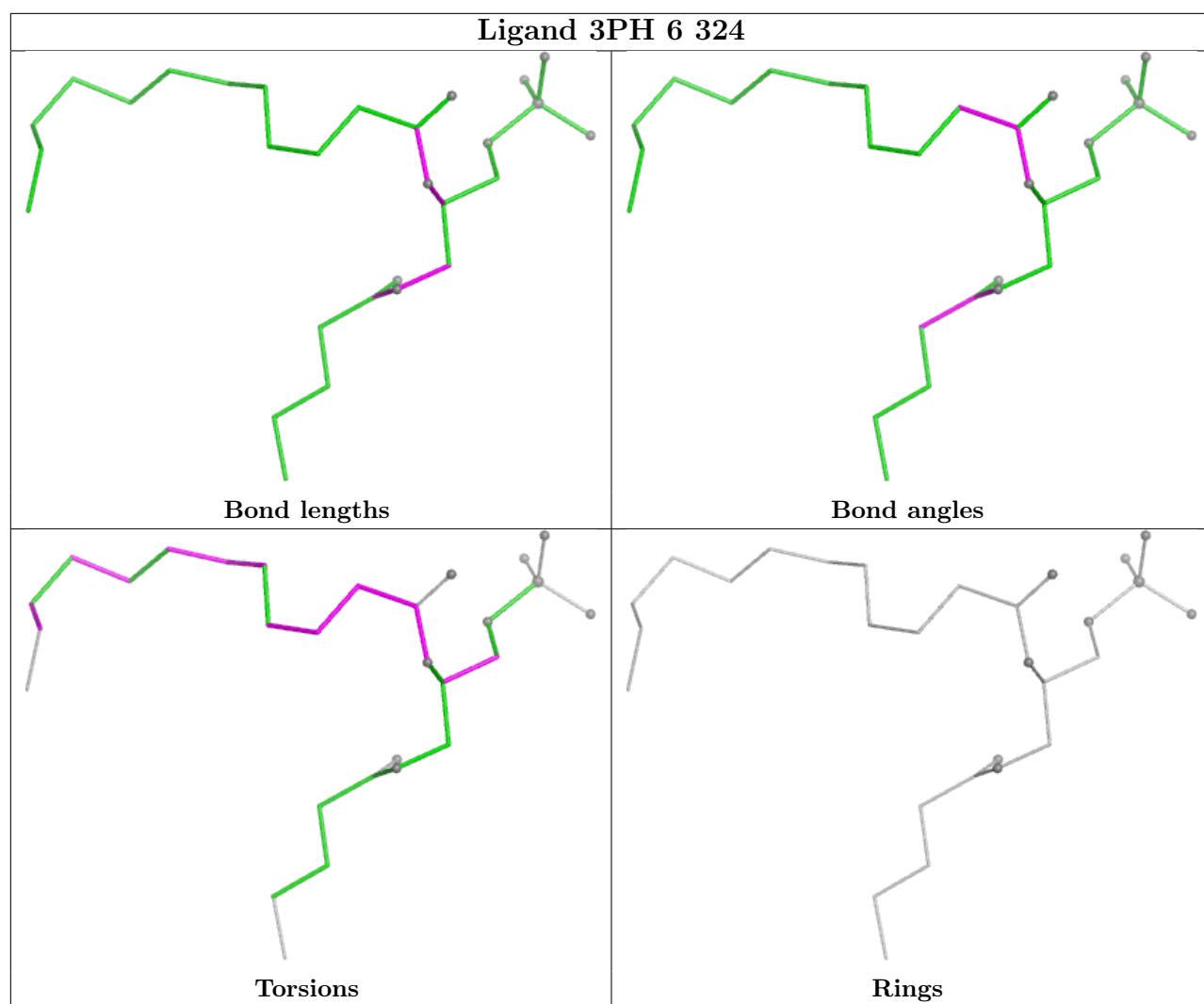


Rings

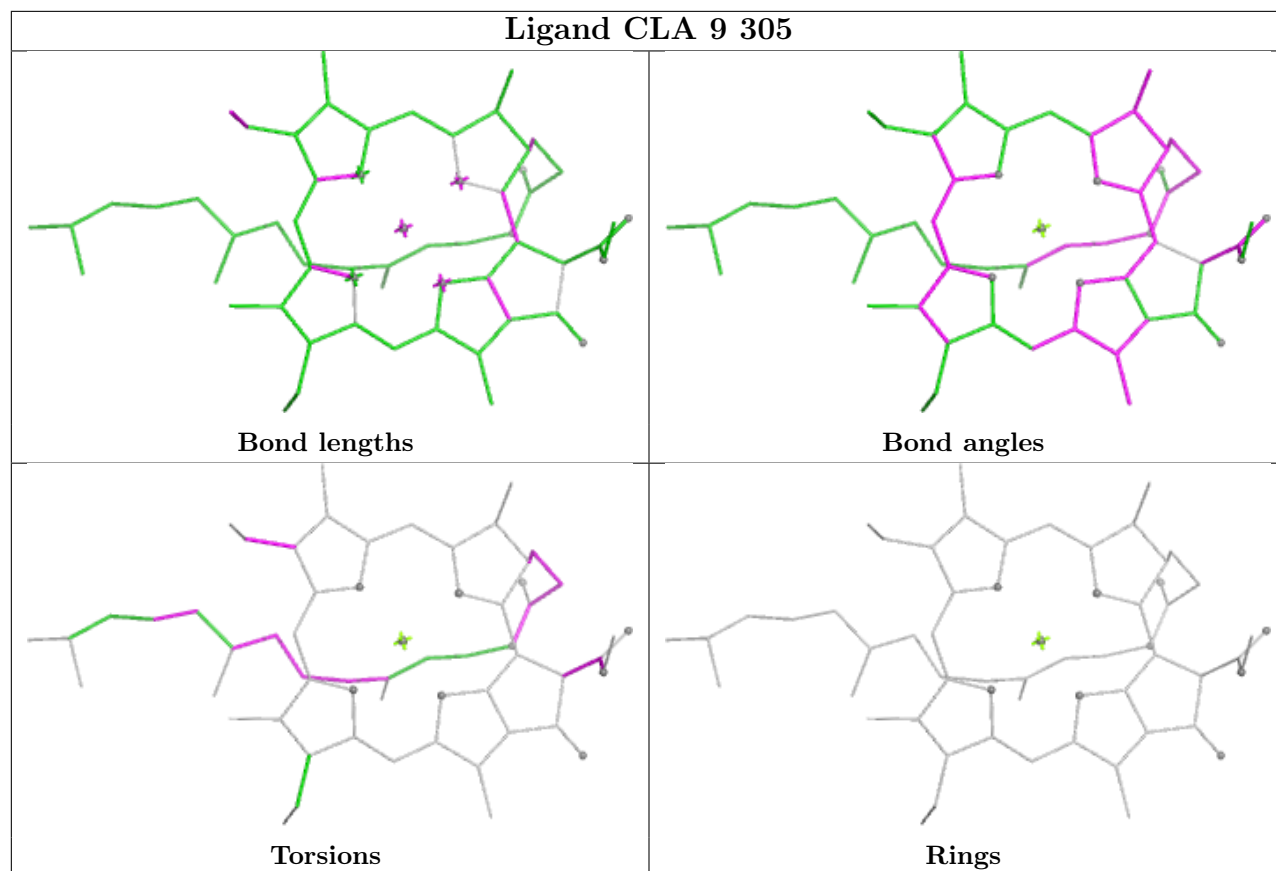
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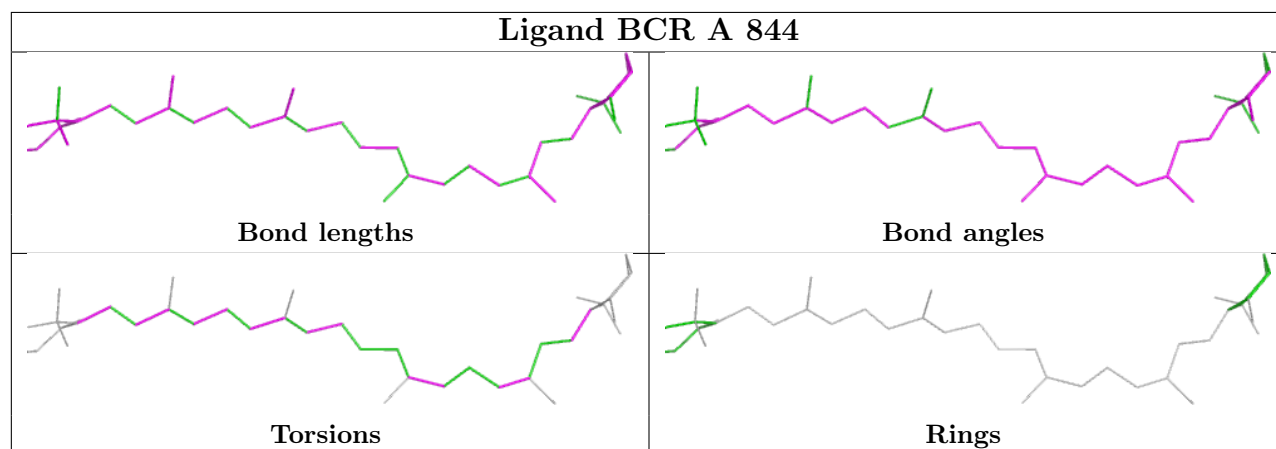


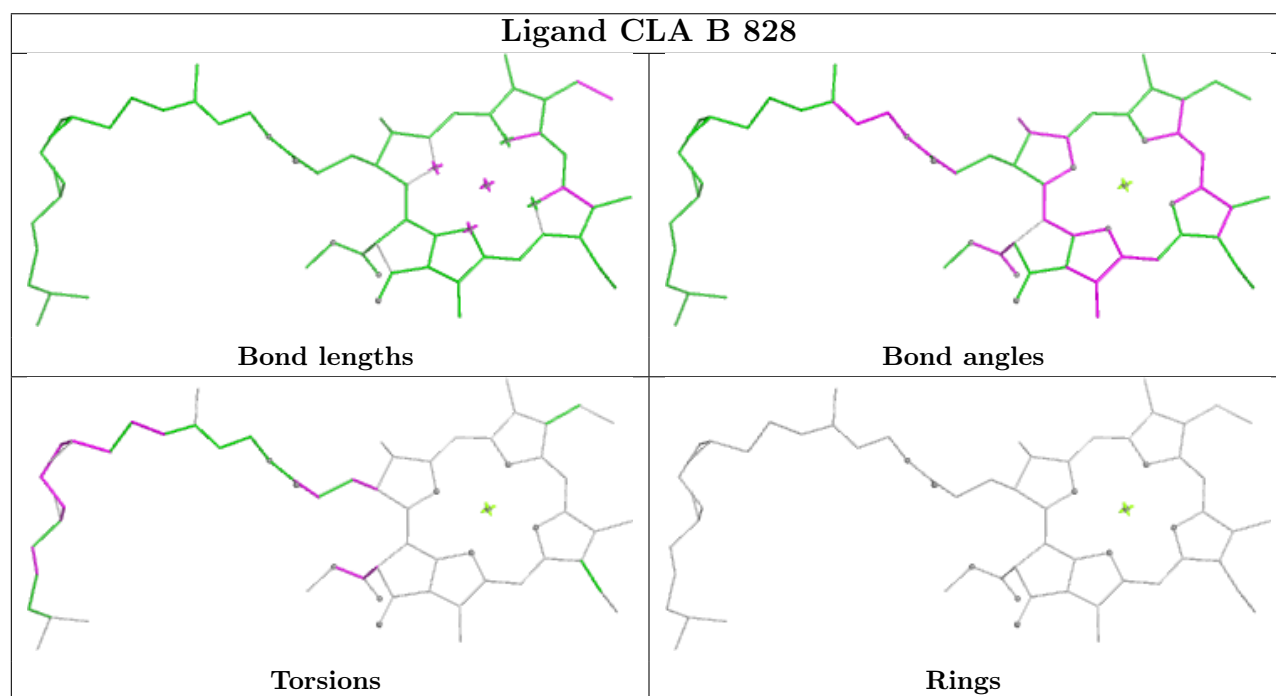
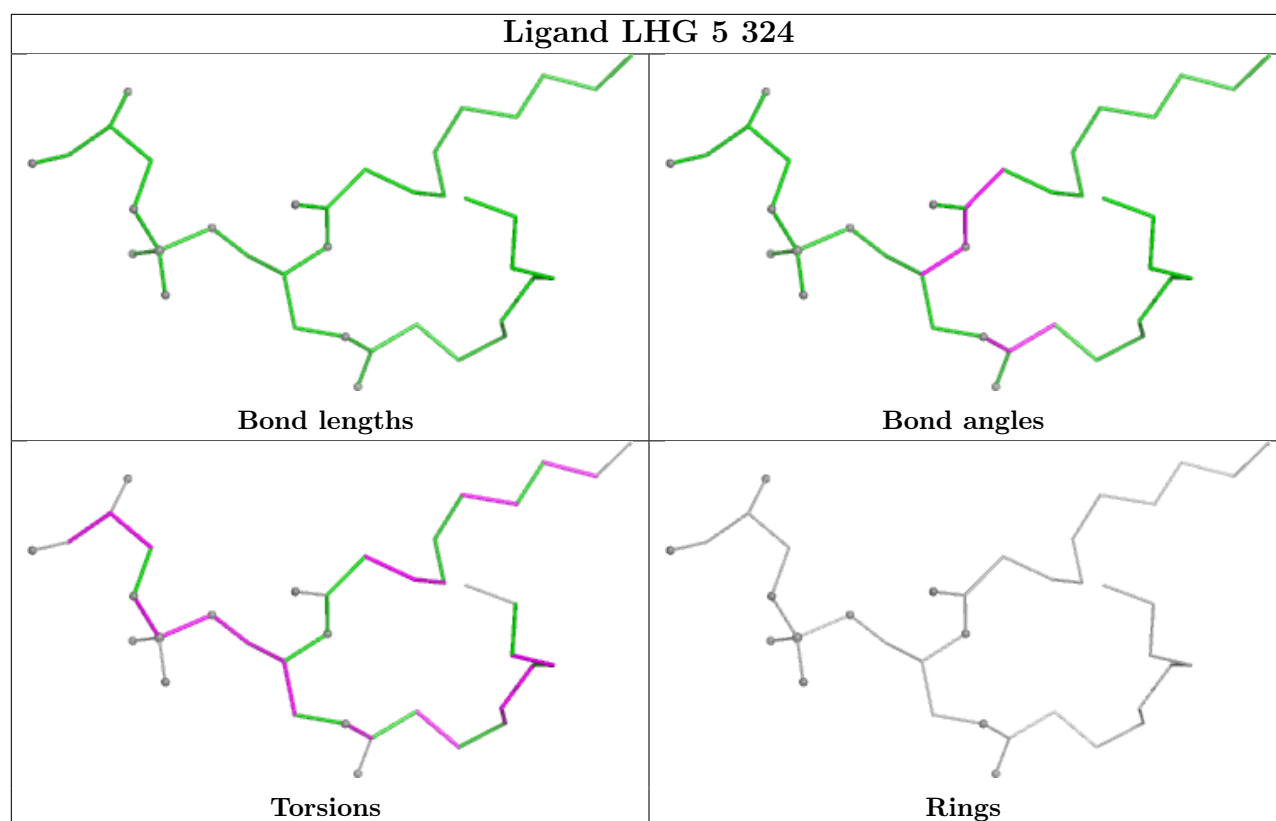


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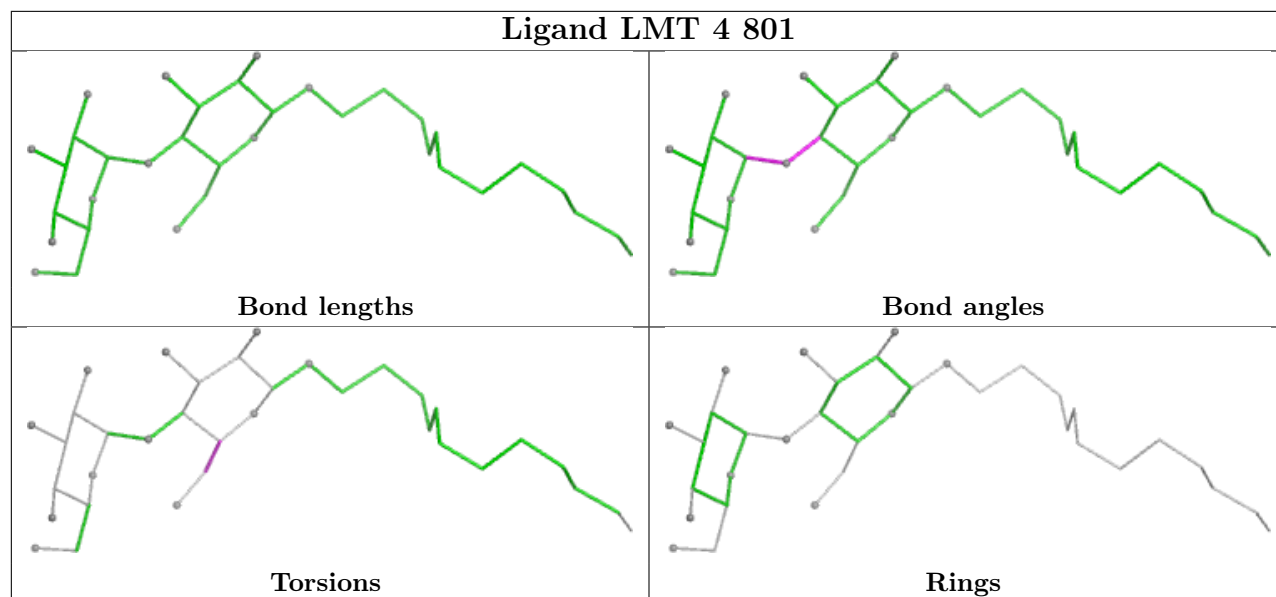


Ligand BCR A 844

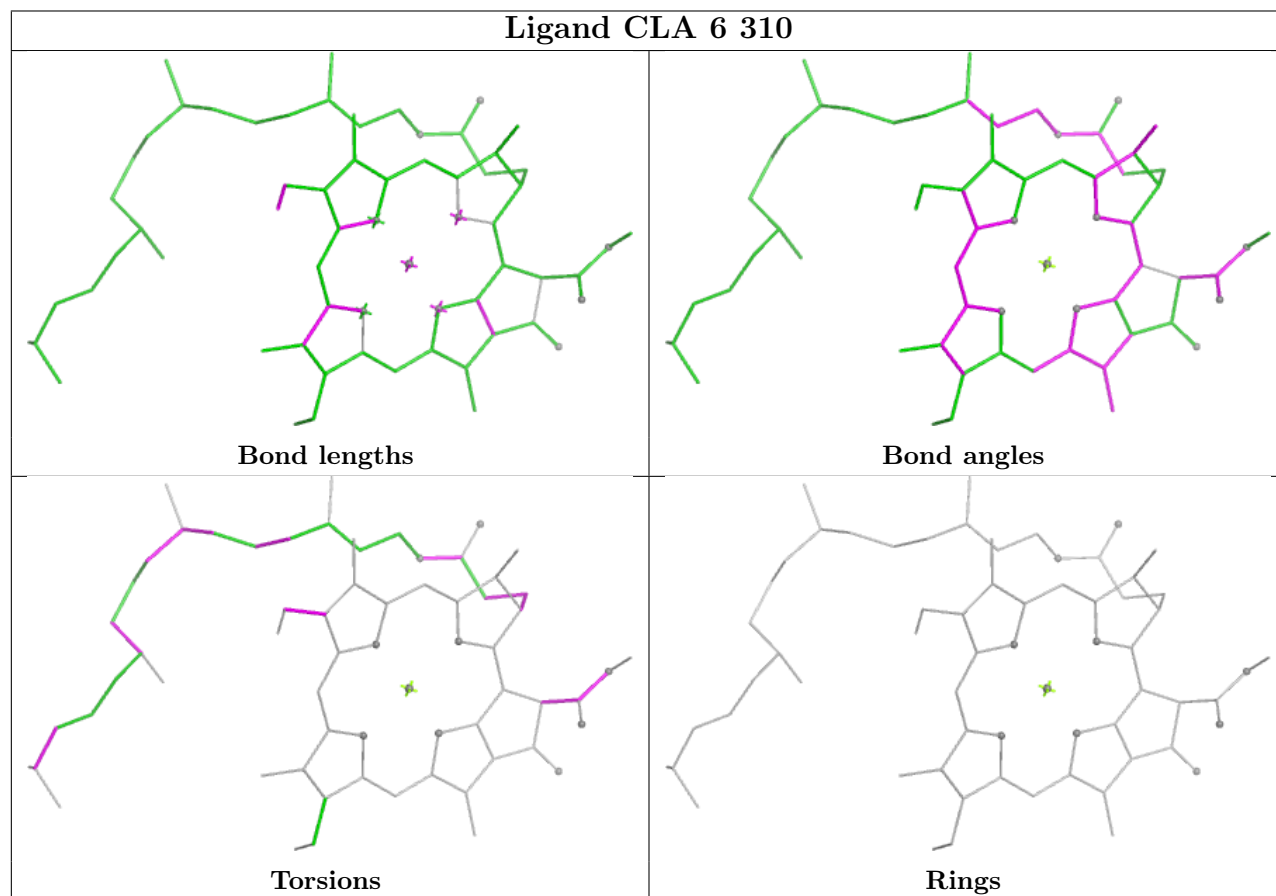


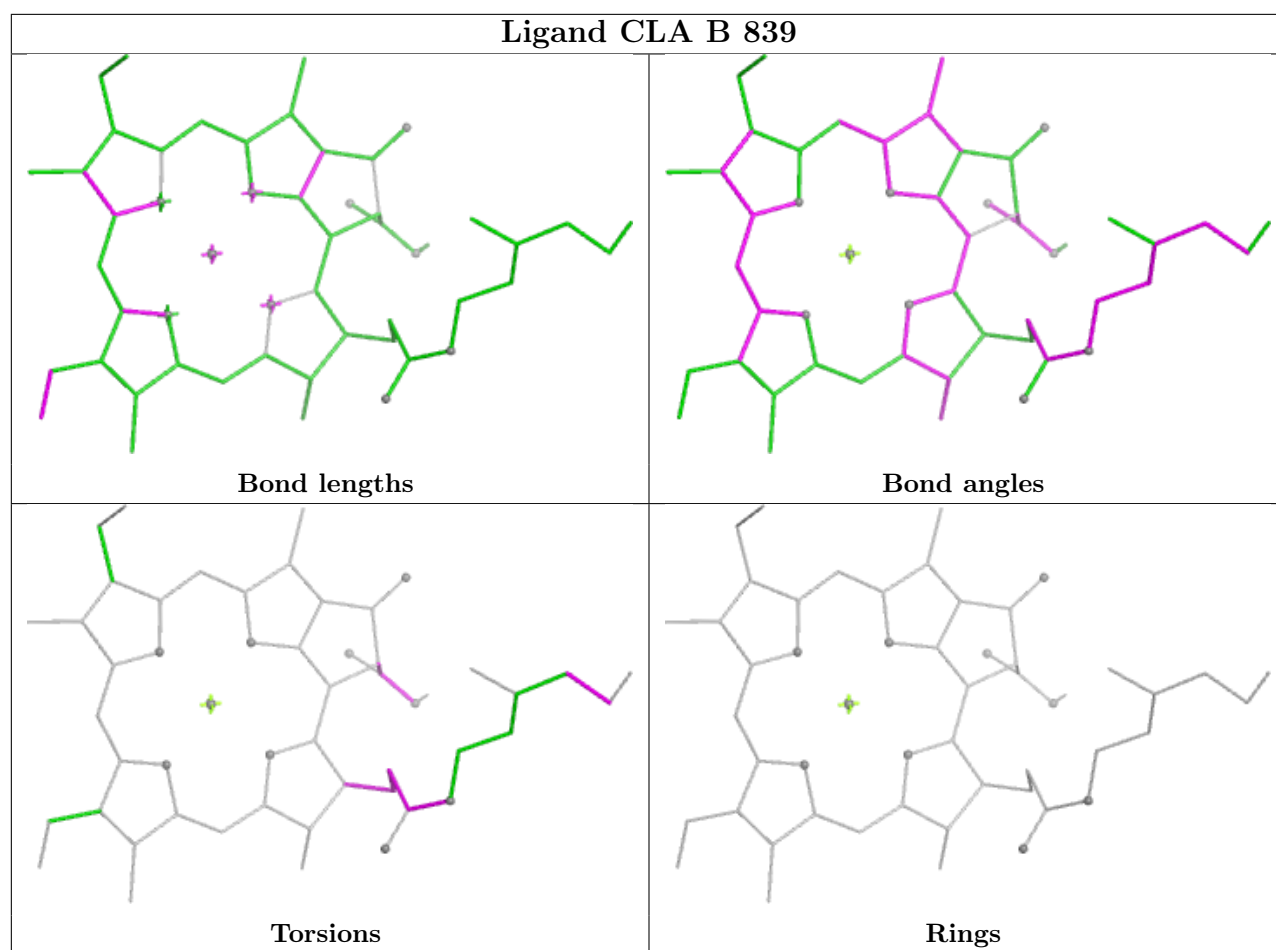


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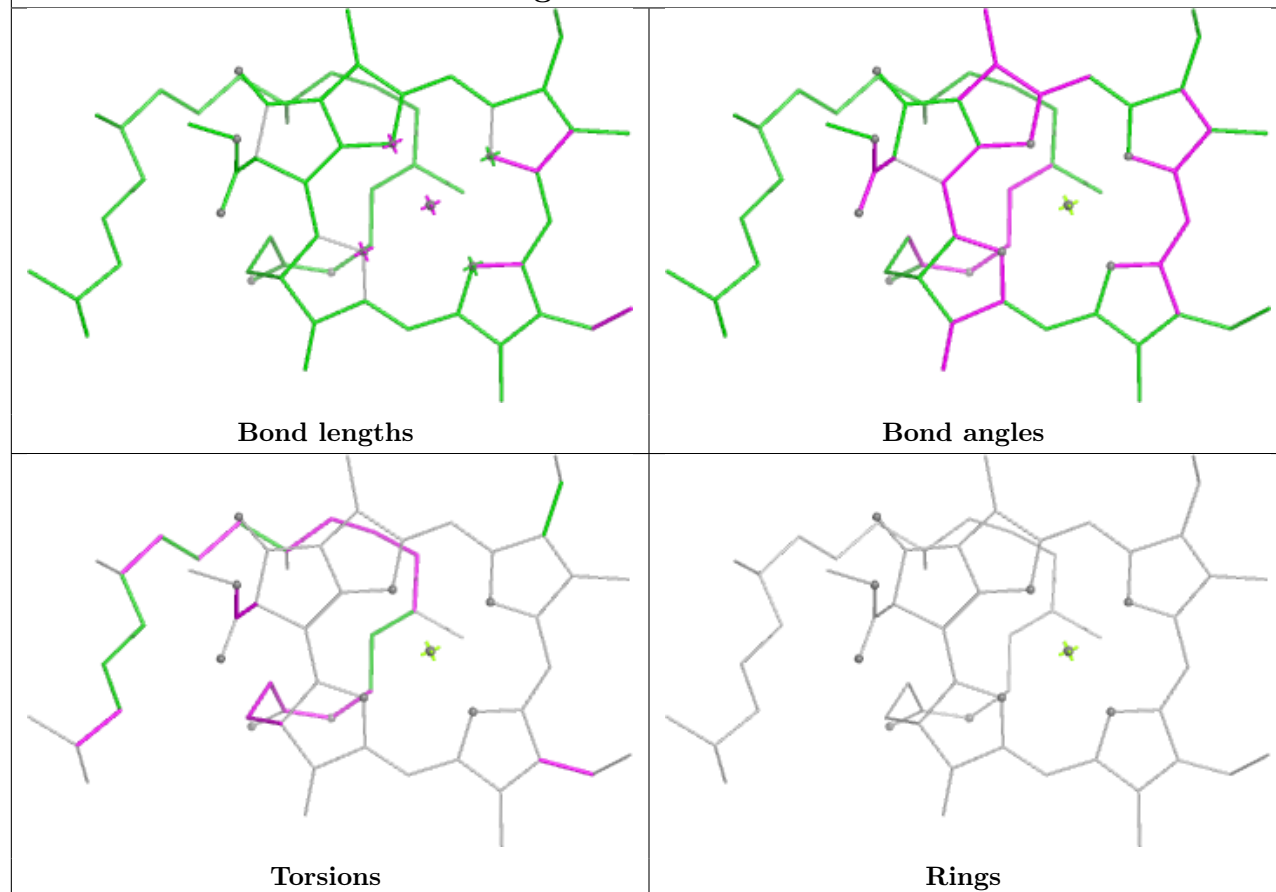


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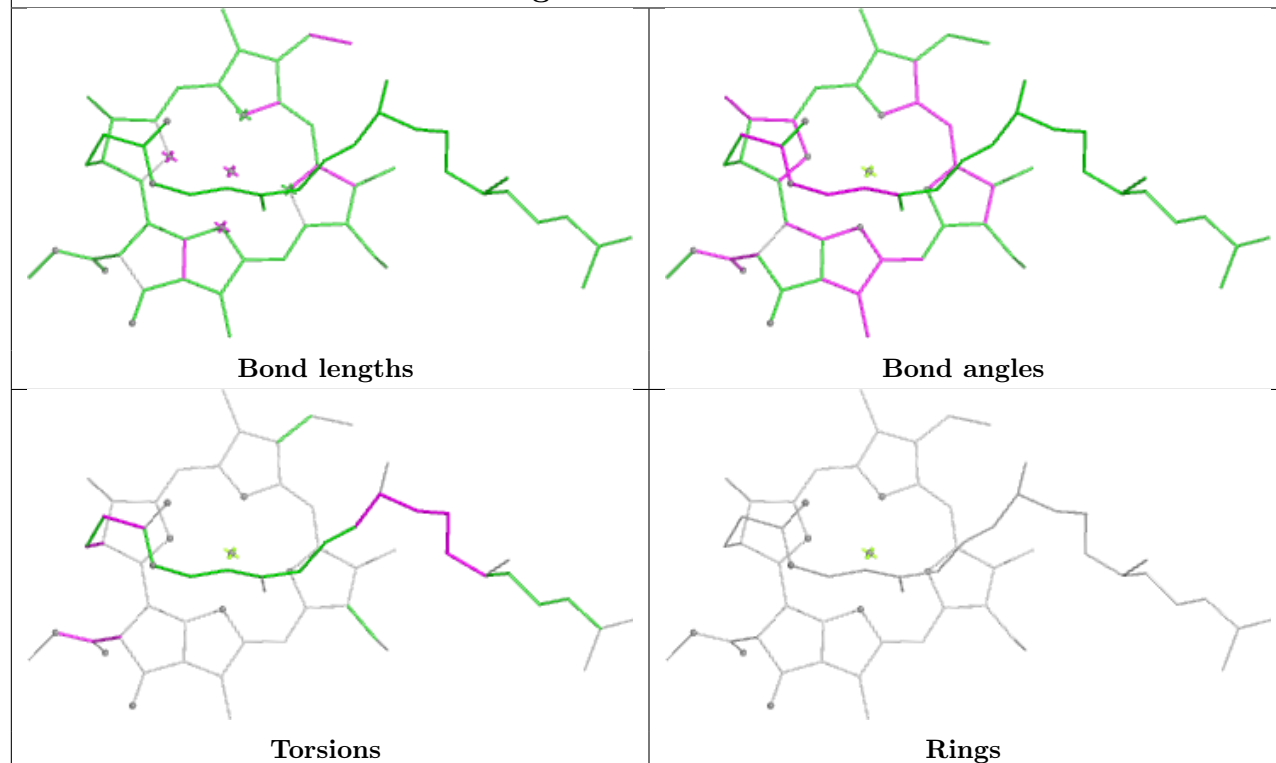


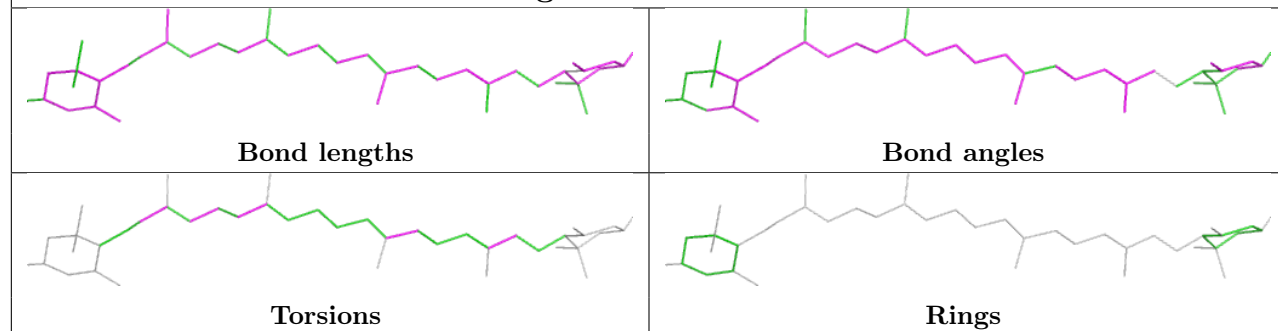
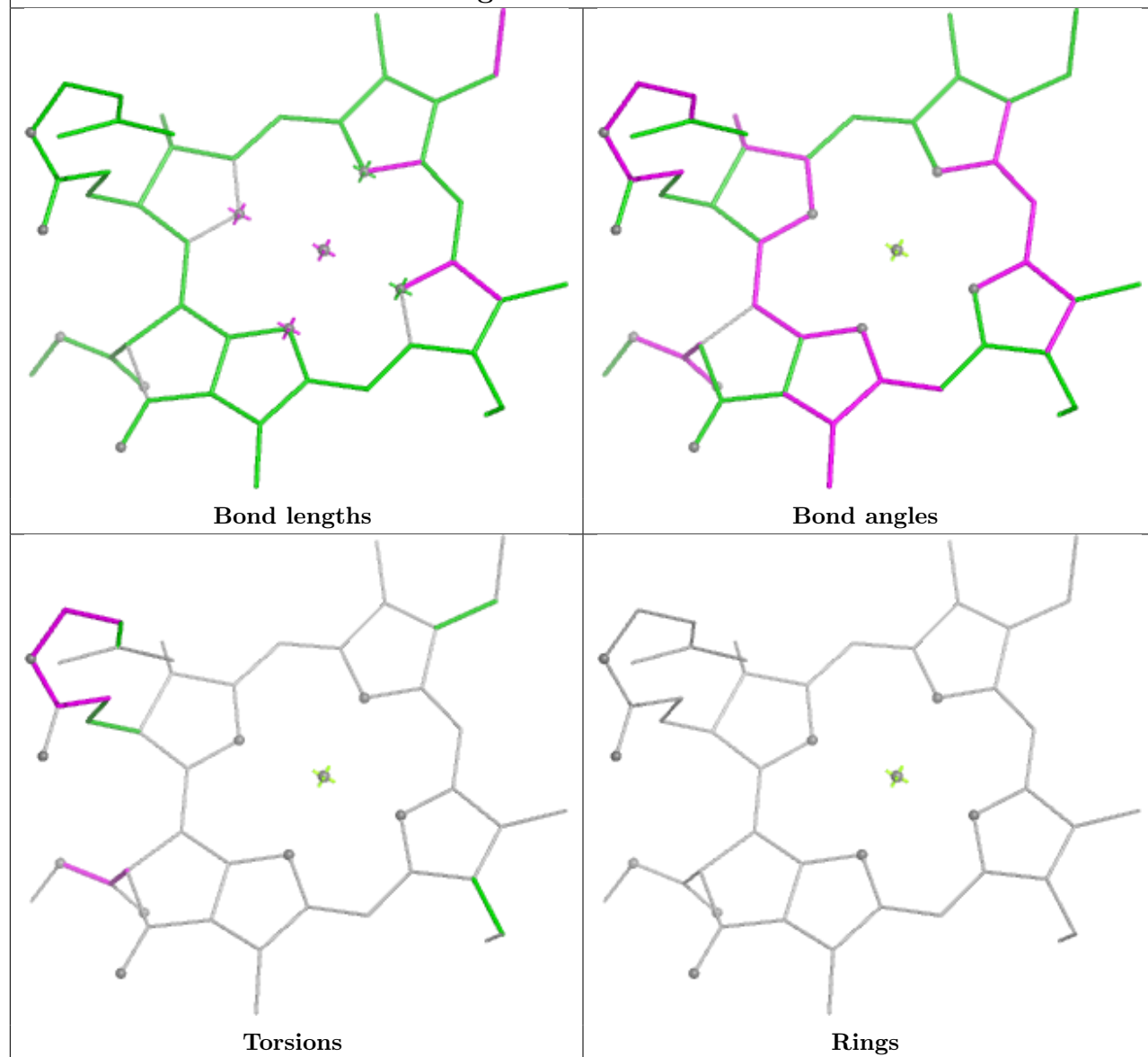


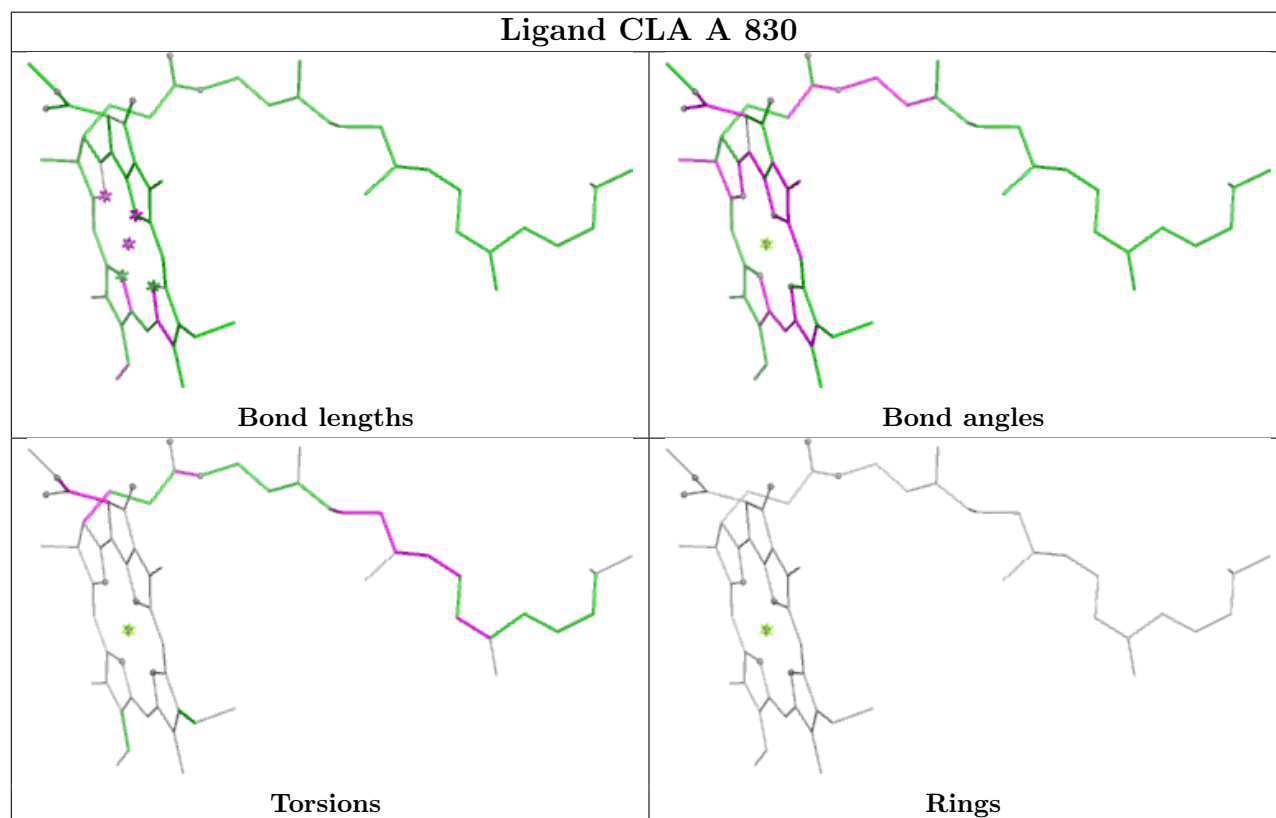
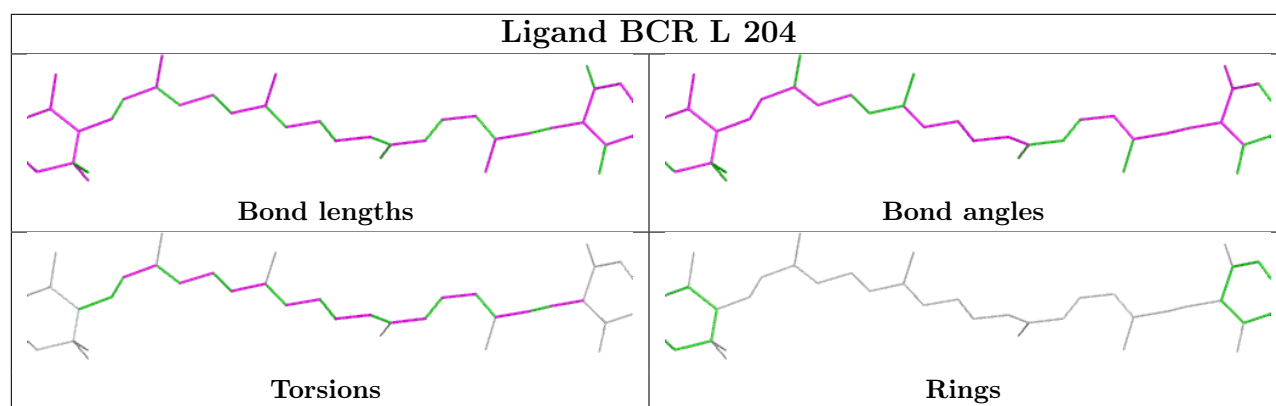
Ligand CLA F 304



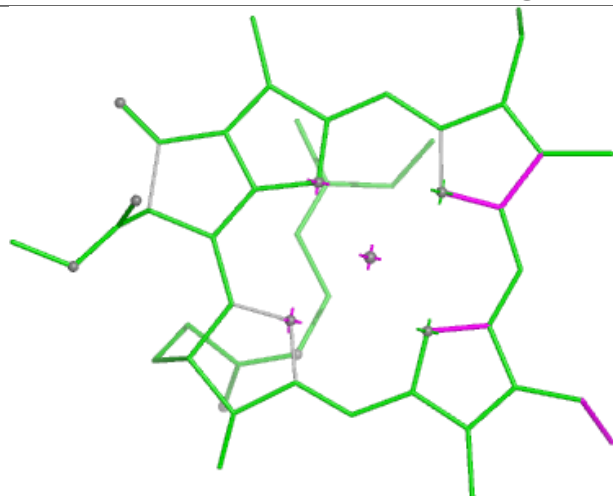
Ligand CLA B 818



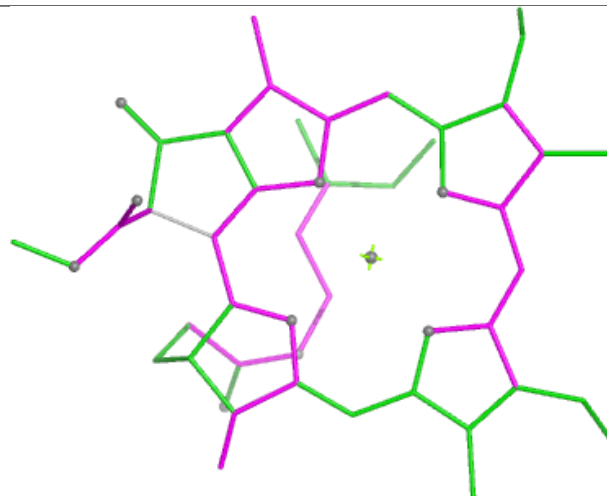
Ligand LUT 6 303**Ligand CLA A 831**



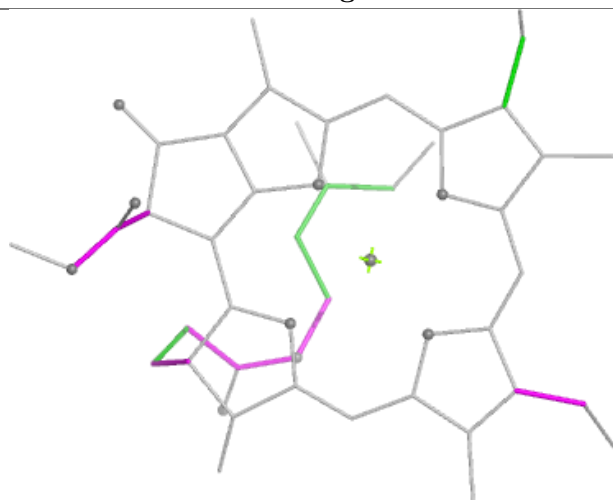
Ligand CLA 4 818



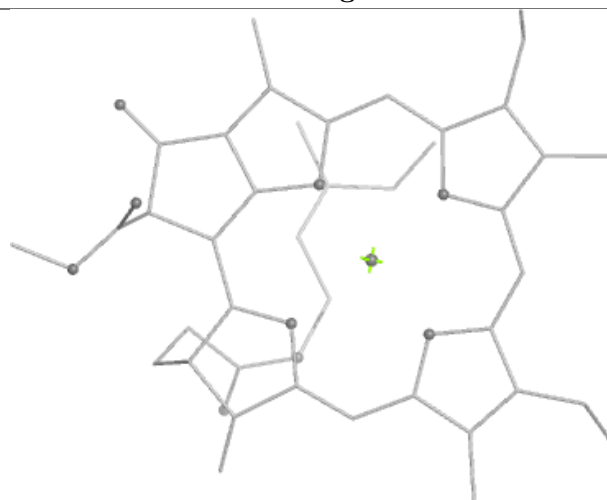
Bond lengths



Bond angles

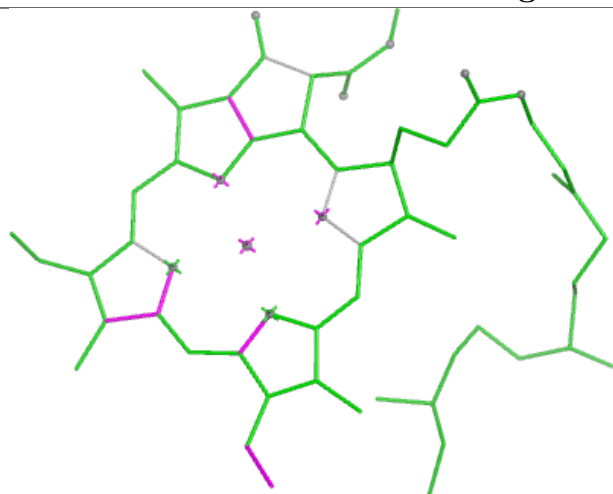


Torsions

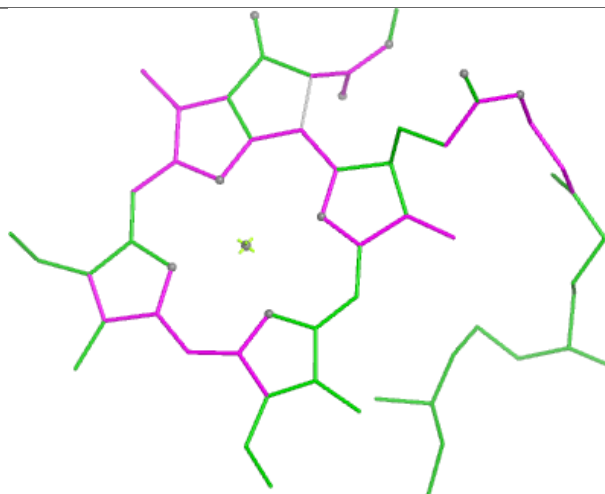


Rings

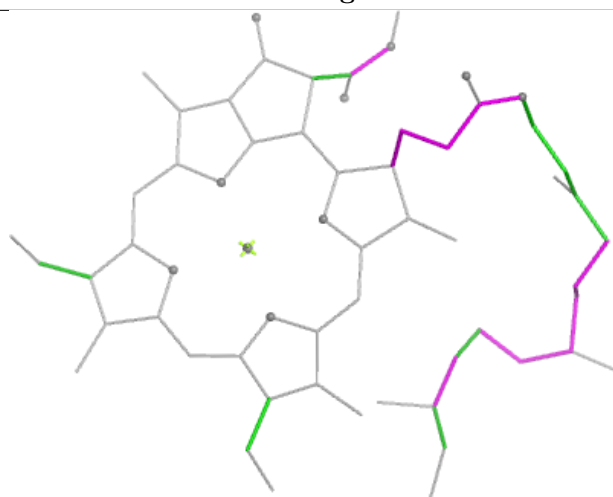
Ligand CLA 5 308



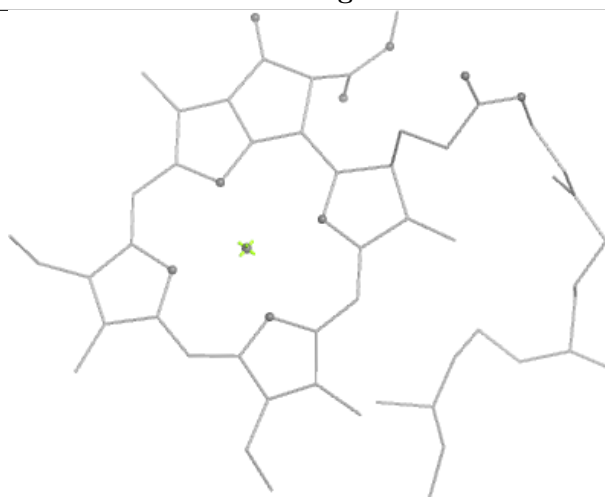
Bond lengths



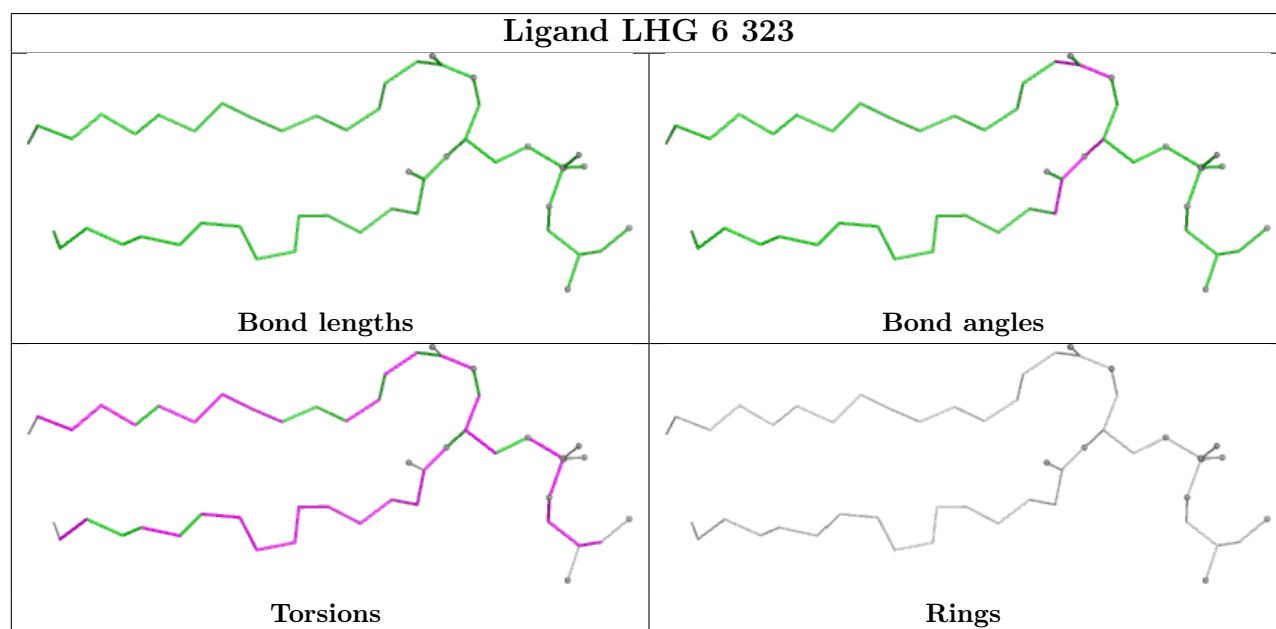
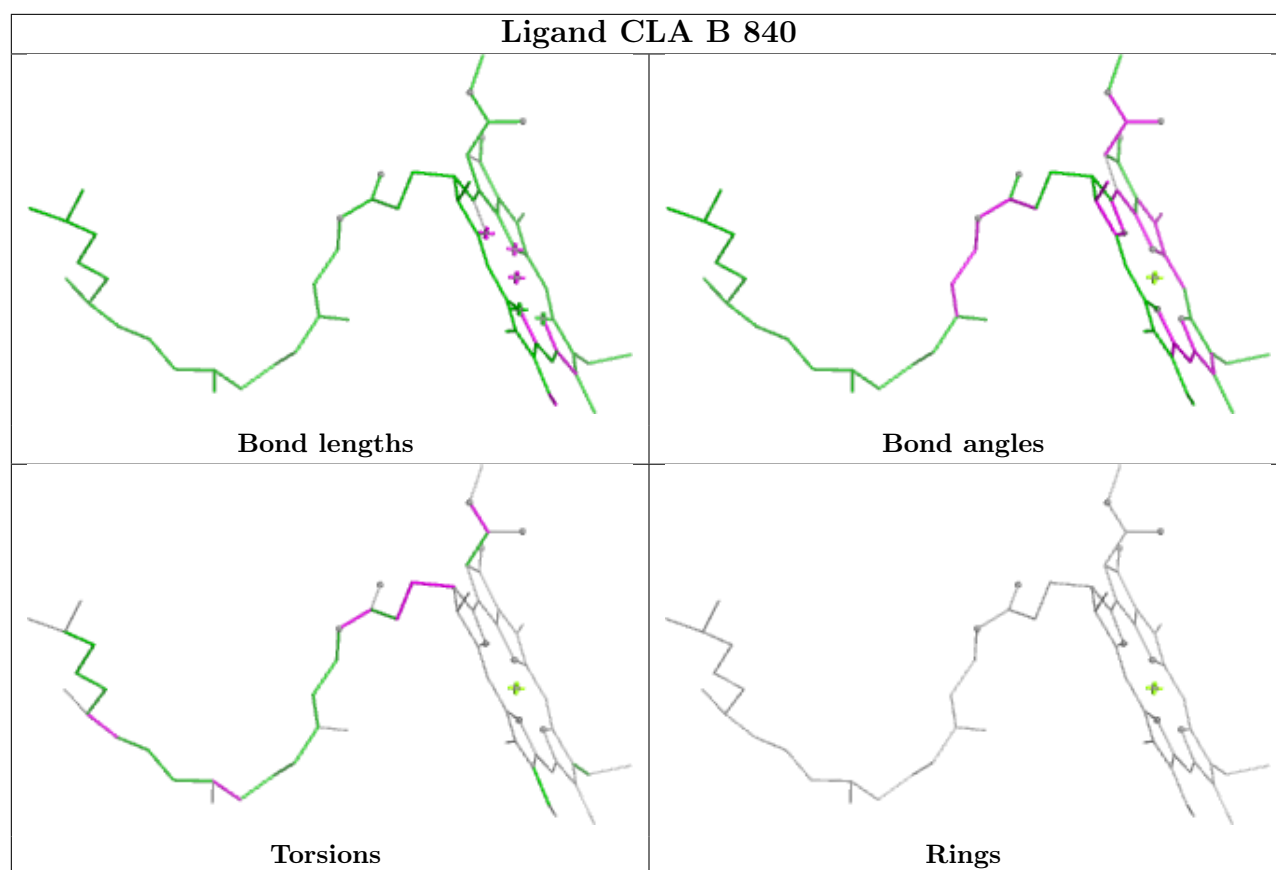
Bond angles

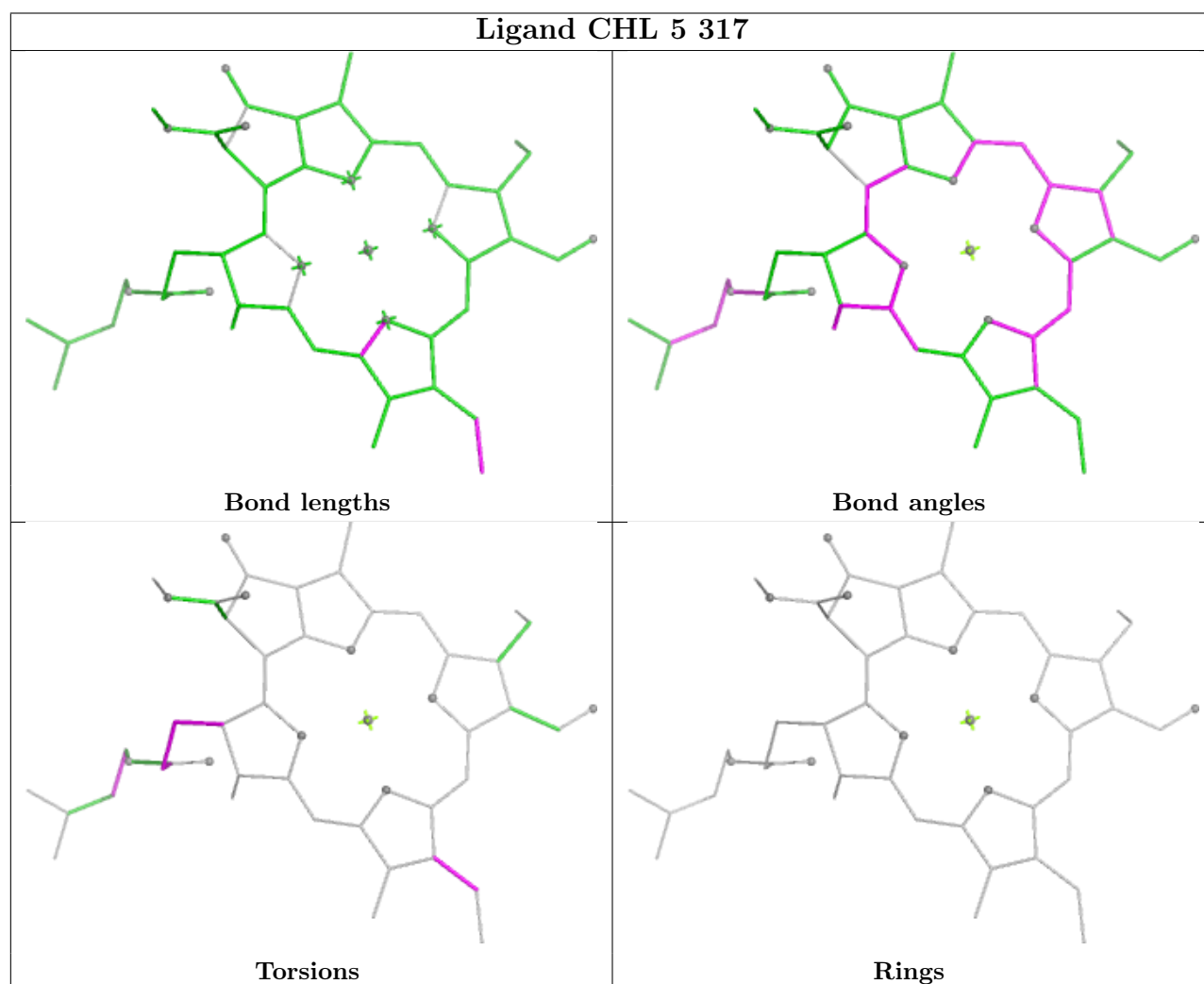
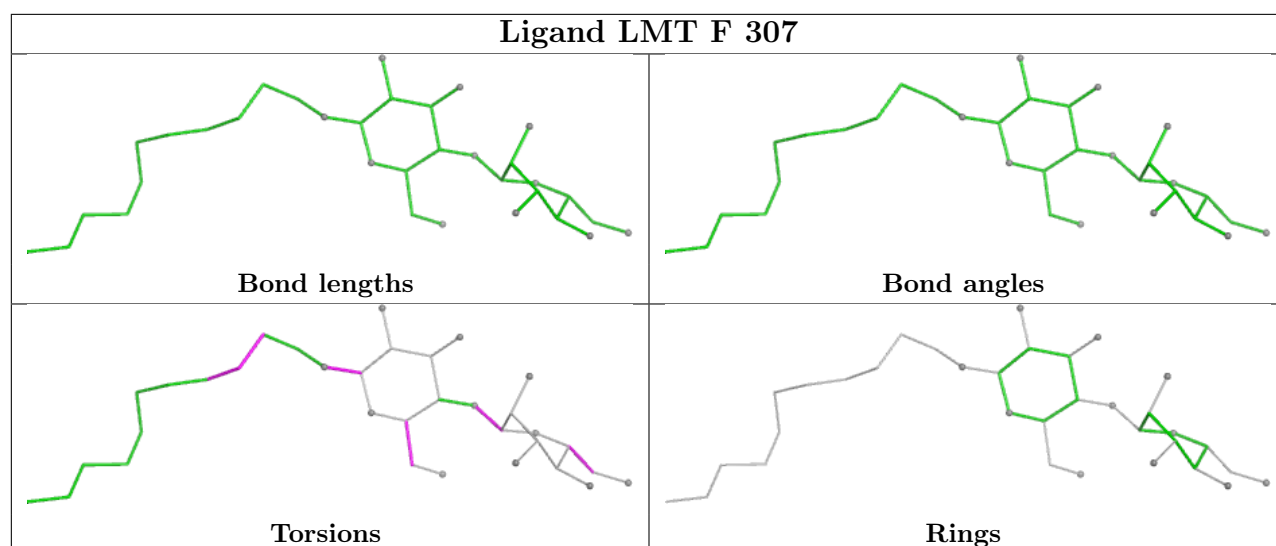


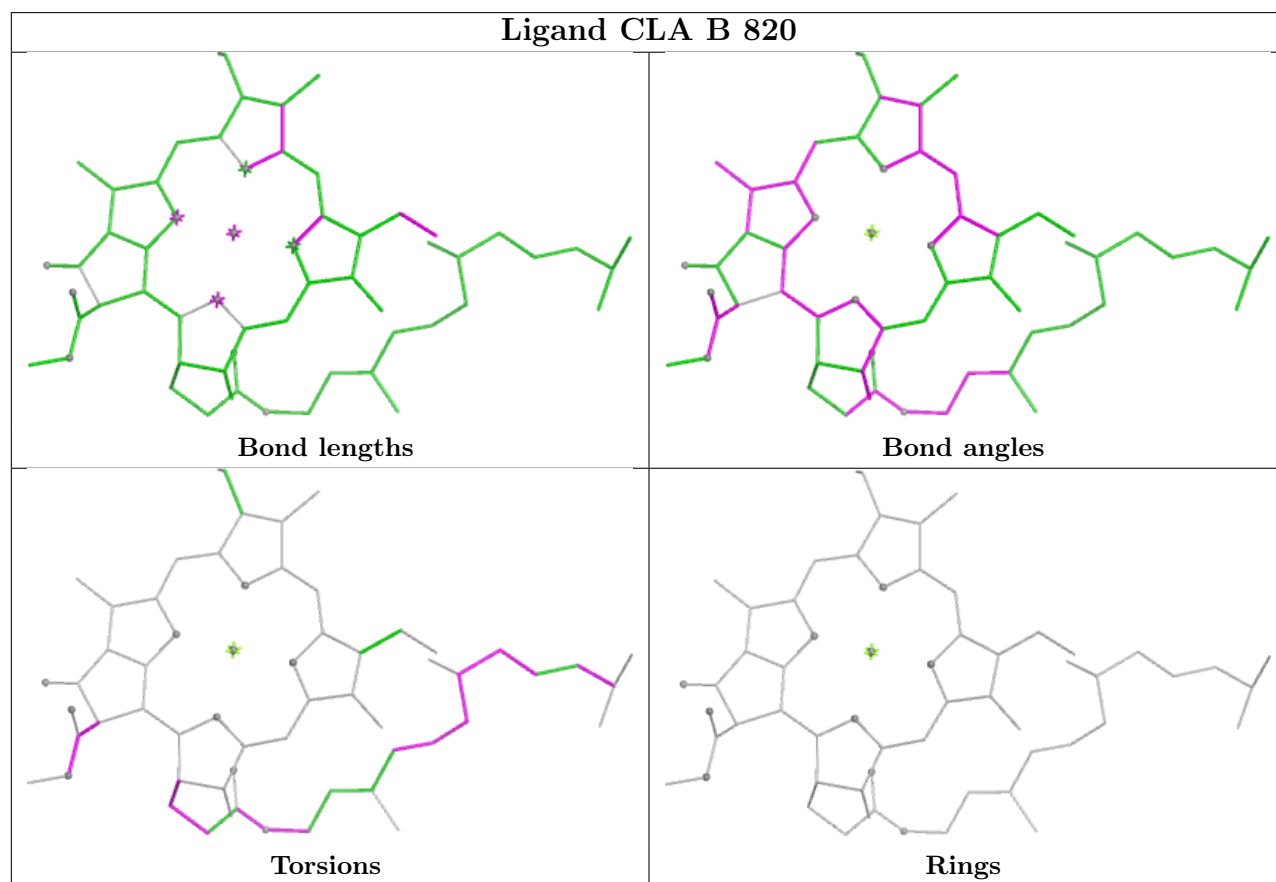
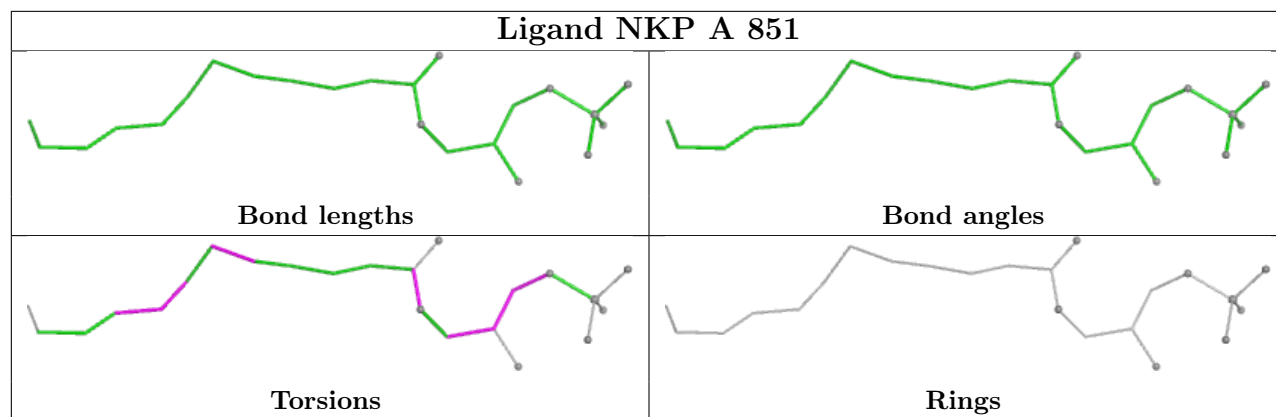
Torsions

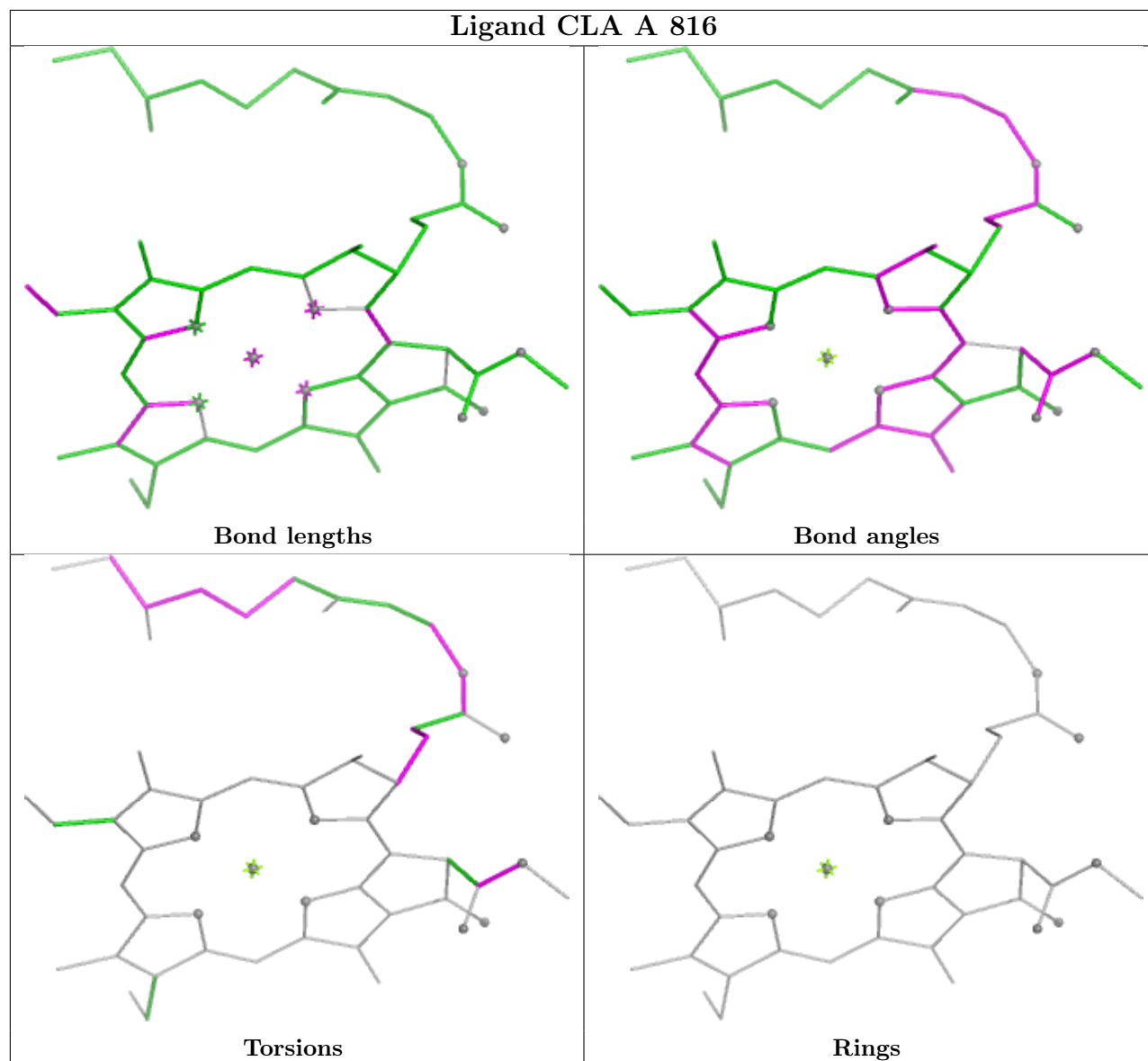


Rings

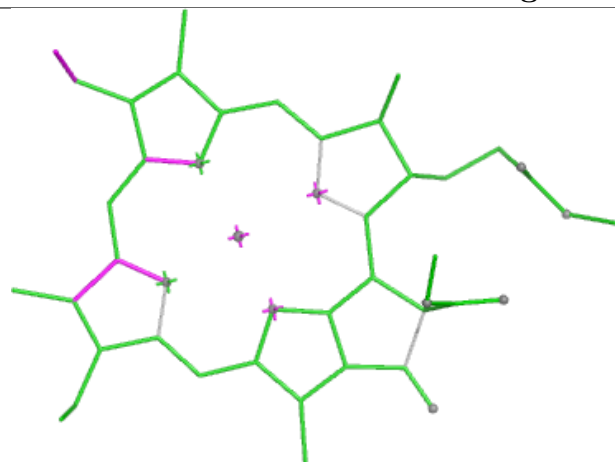




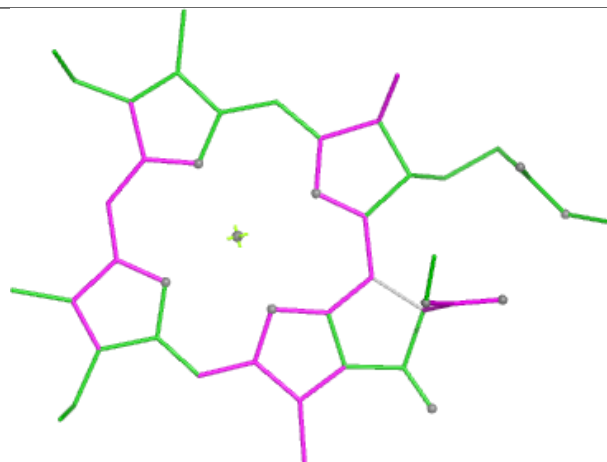




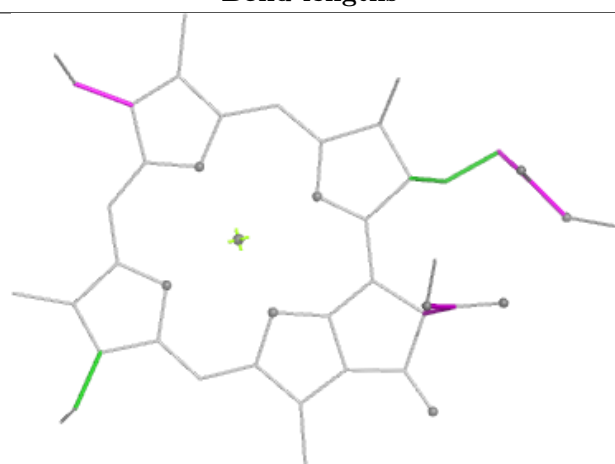
Ligand CLA 5 323



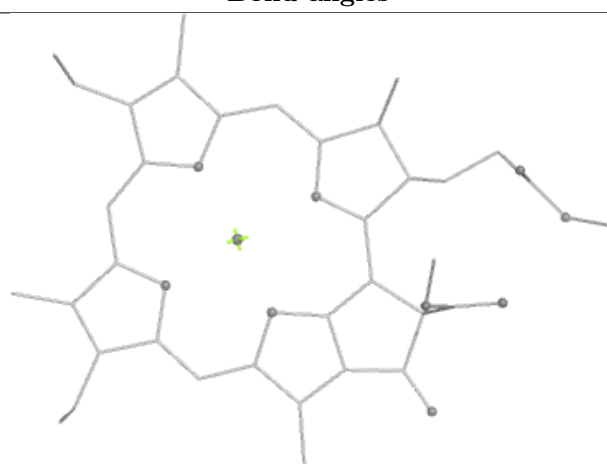
Bond lengths



Bond angles

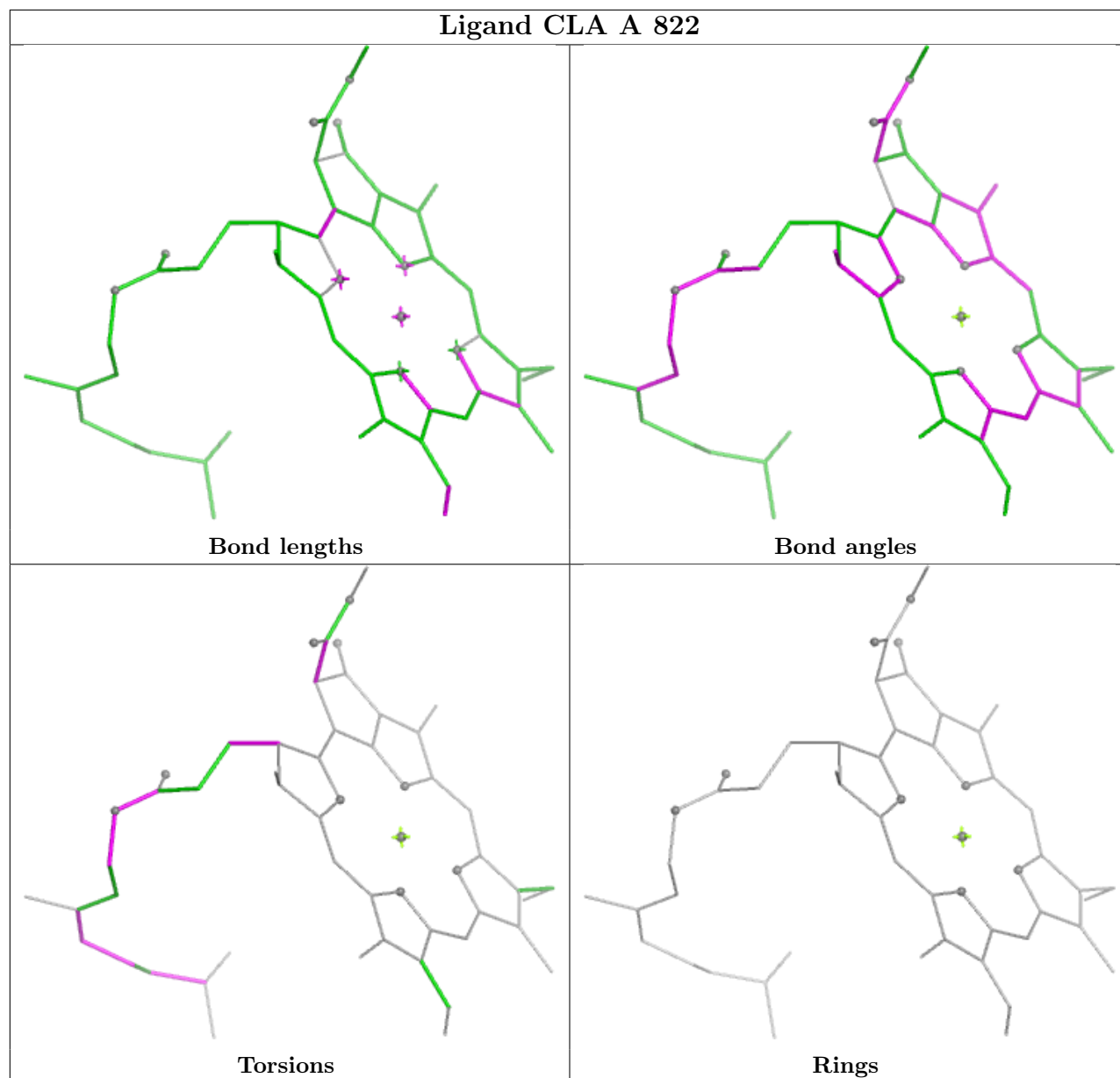


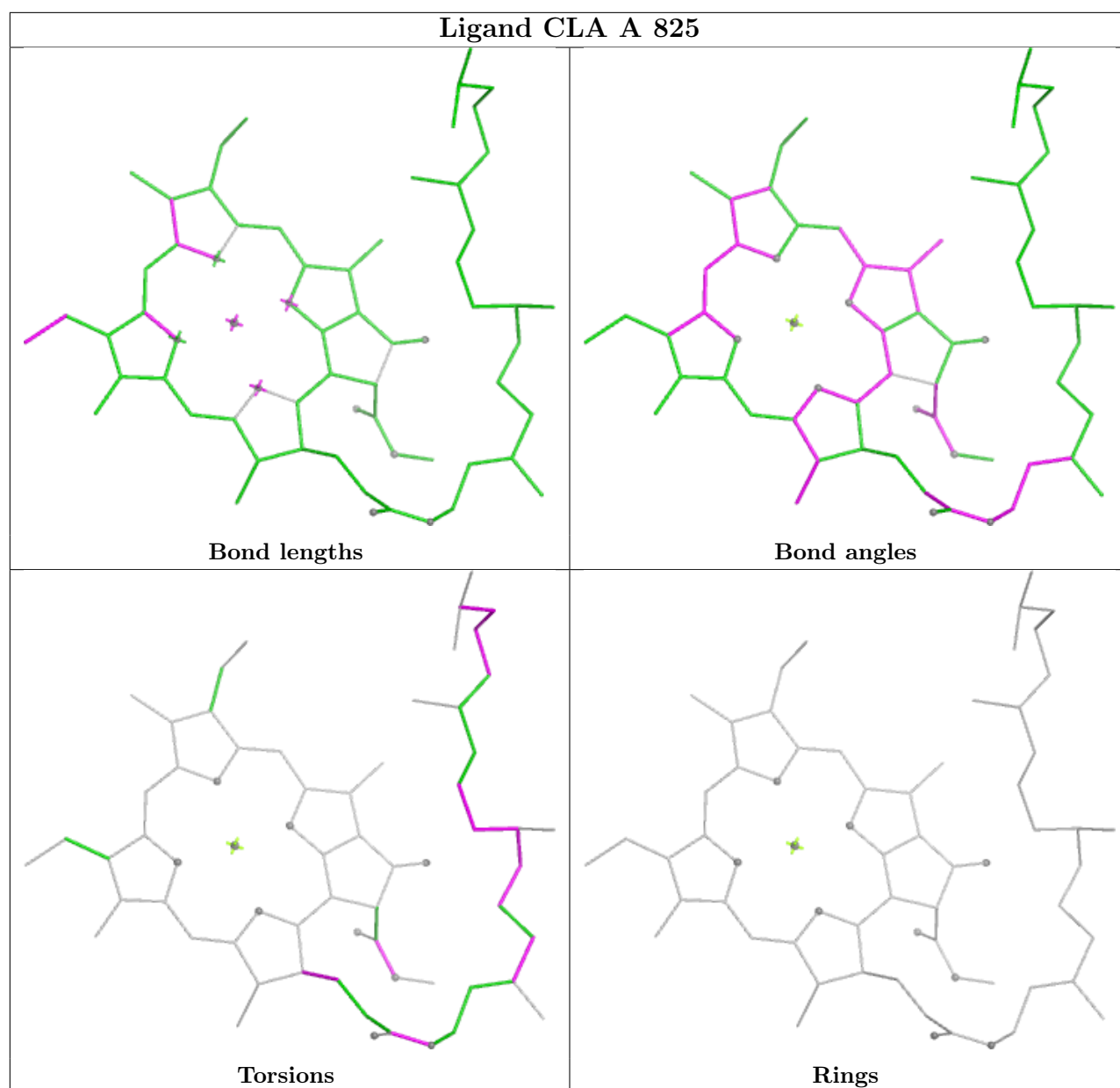
Torsions

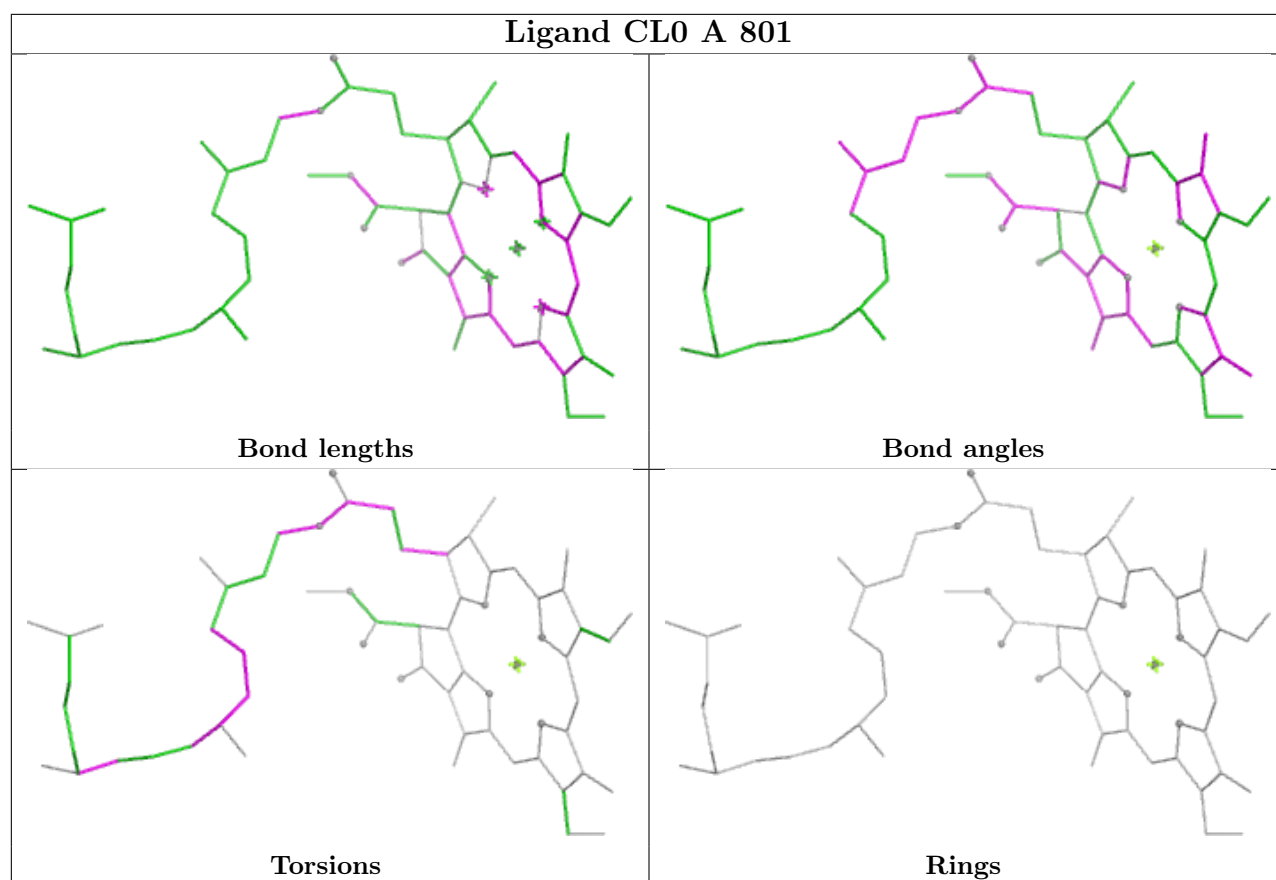


Rings

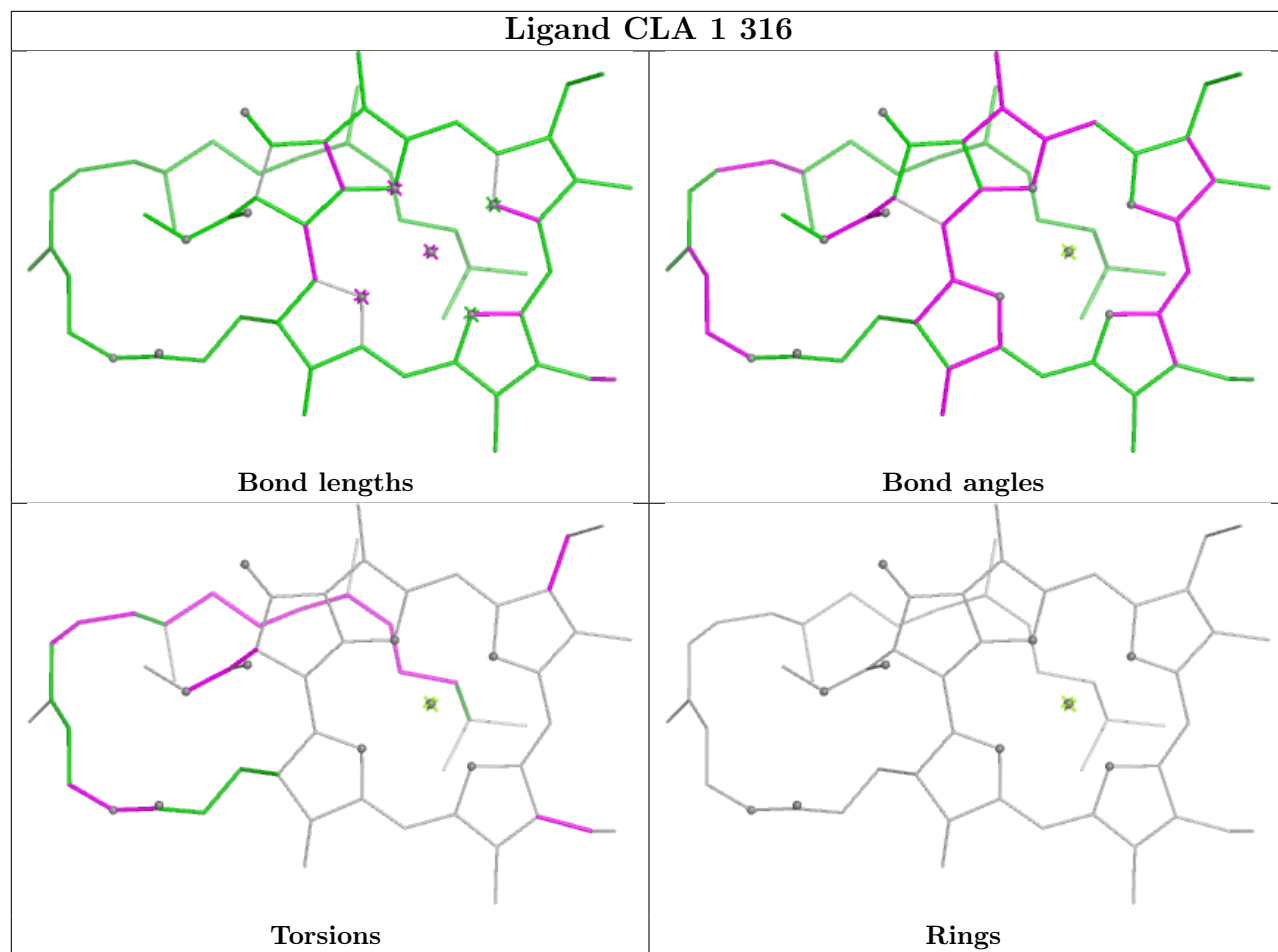
Ligand CLA A 822

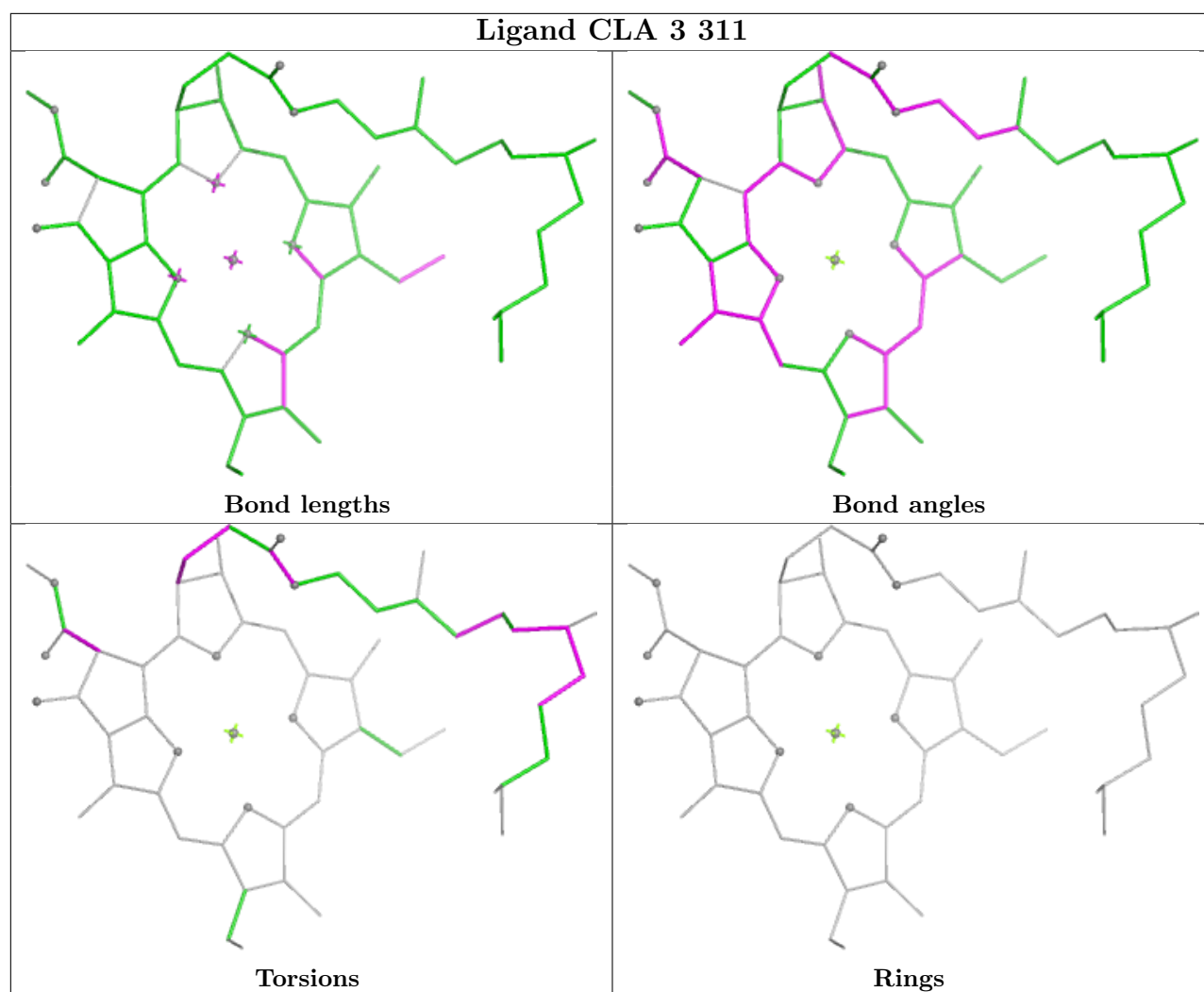


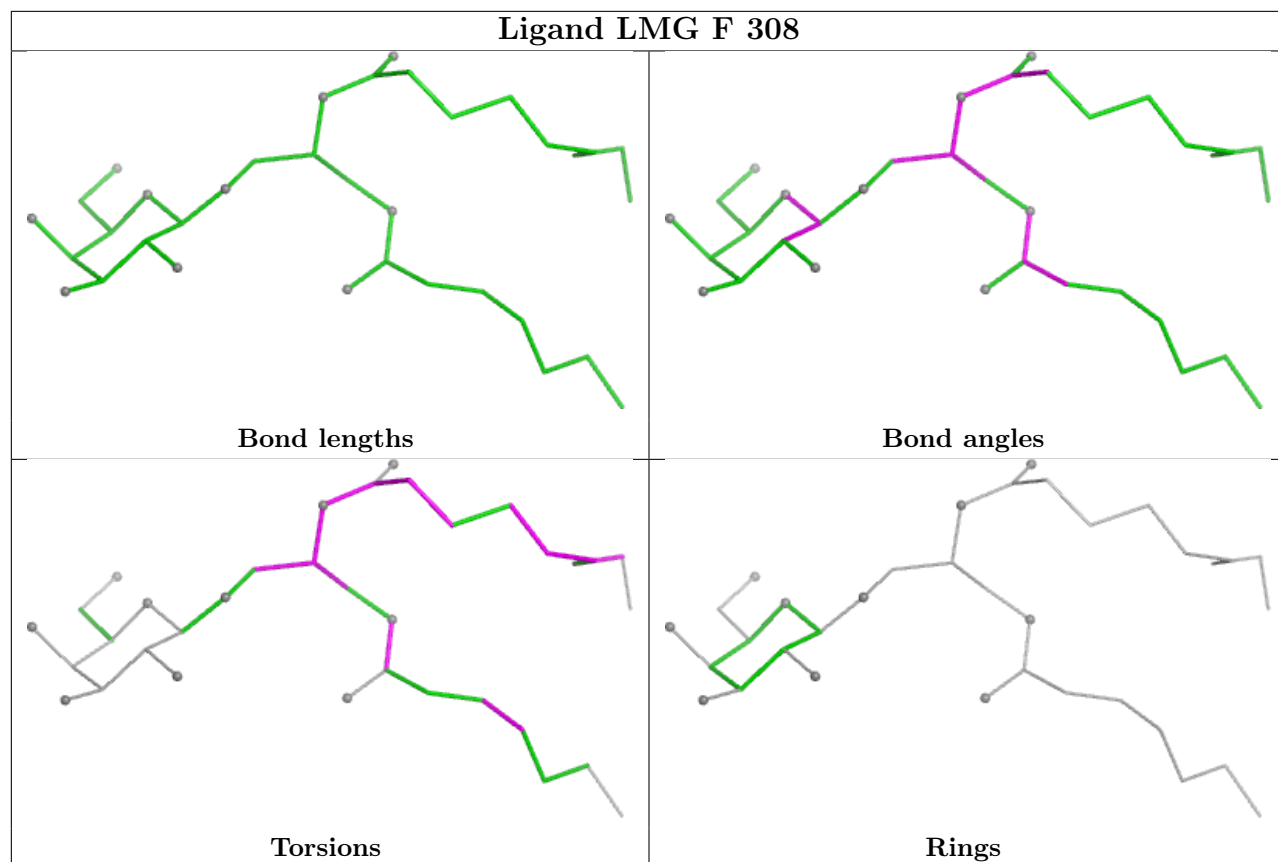




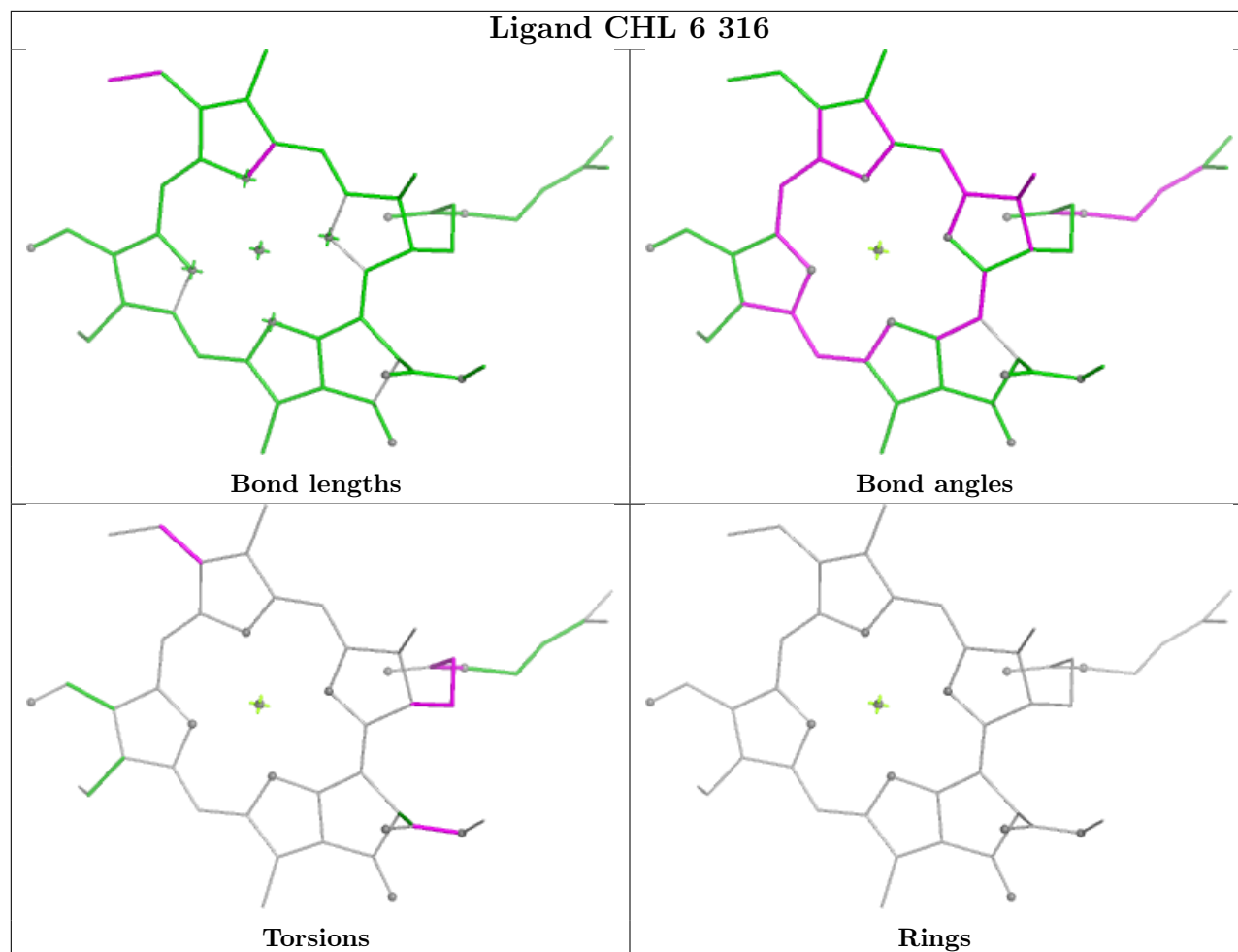
Ligand CLA 1 316

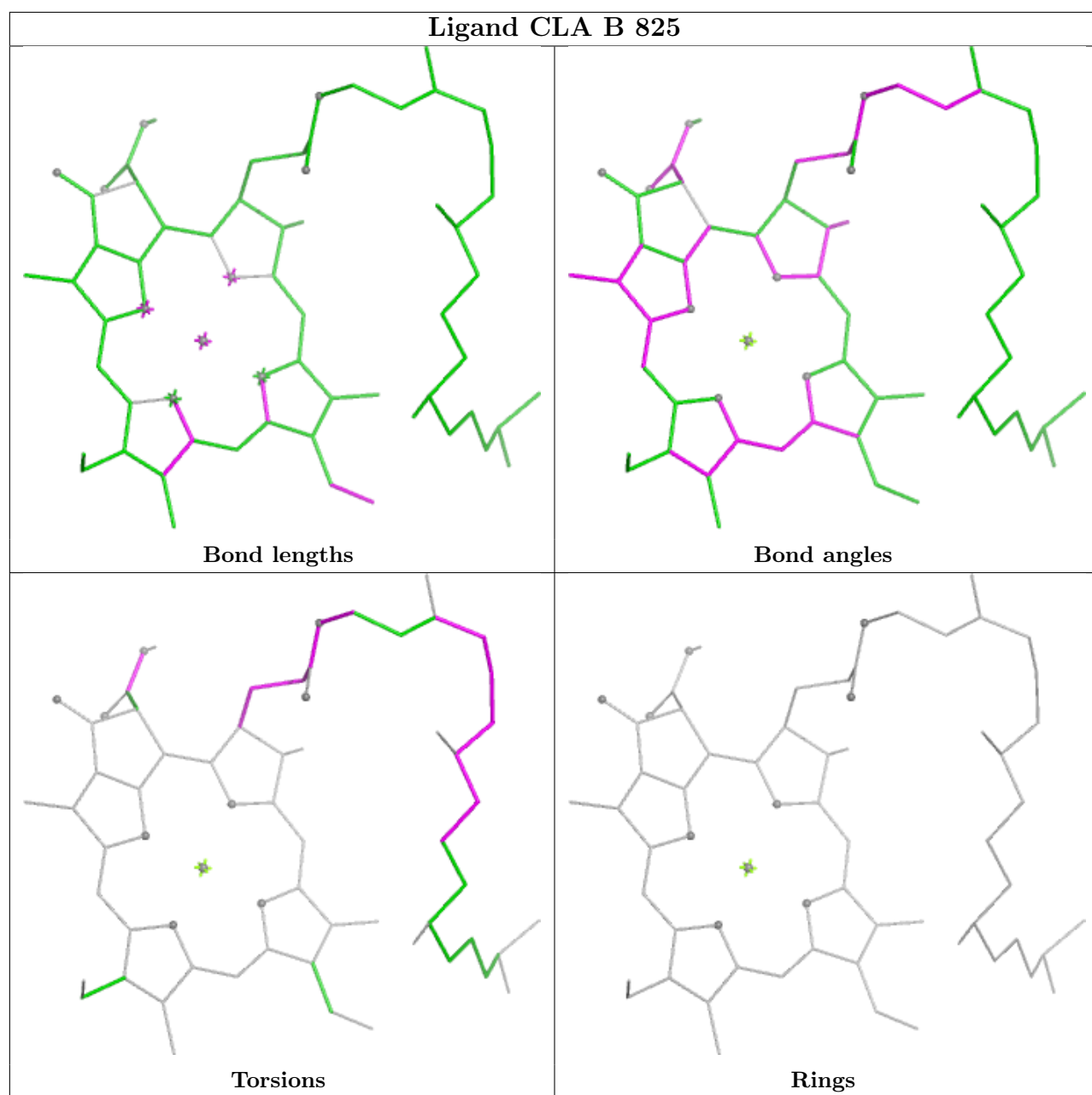




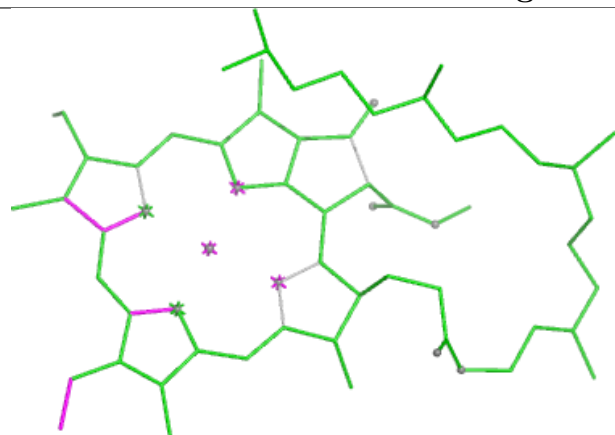


Ligand CHL 6 316

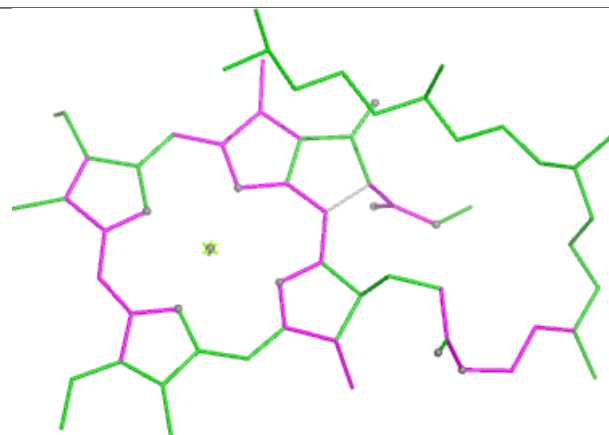




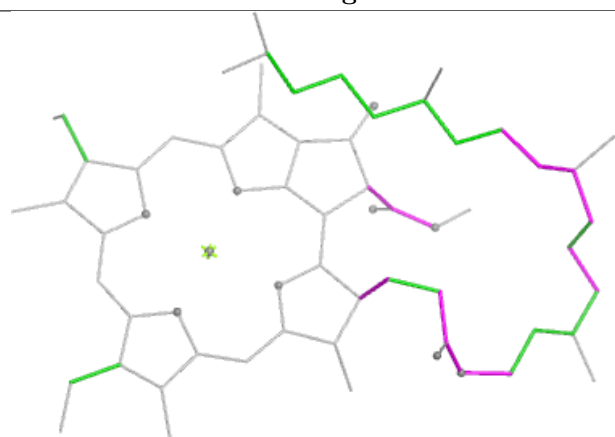
Ligand CLA B 808



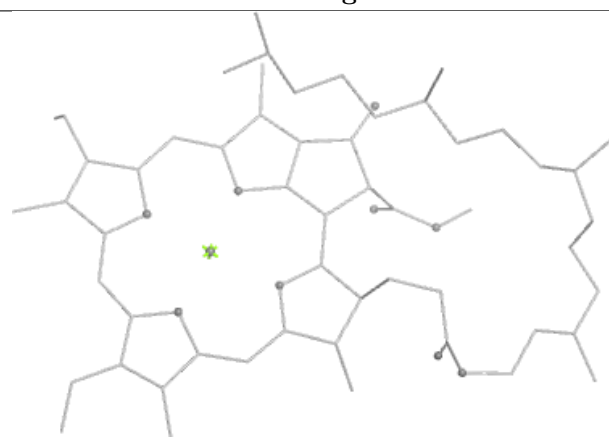
Bond lengths



Bond angles

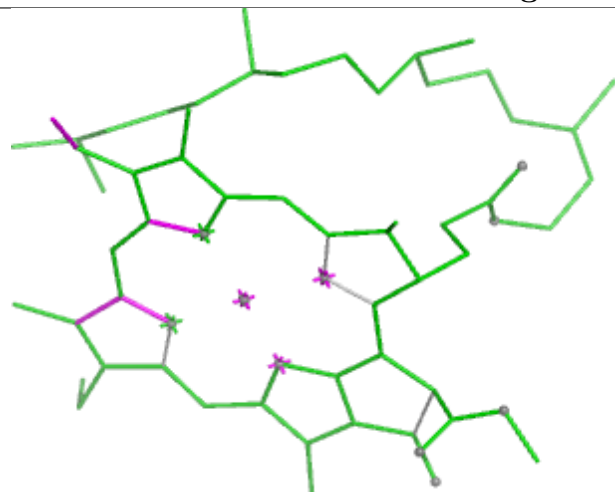


Torsions

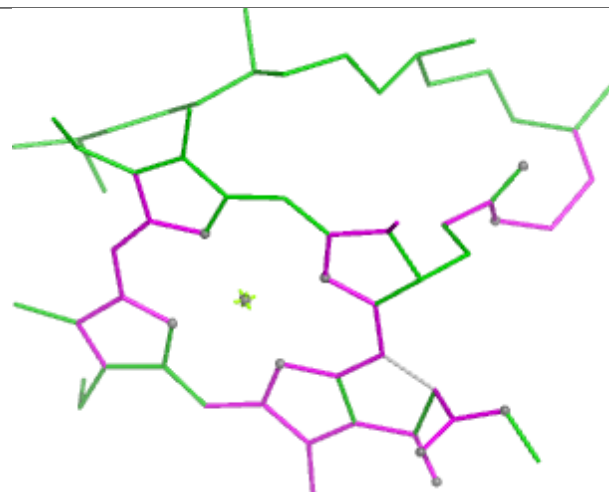


Rings

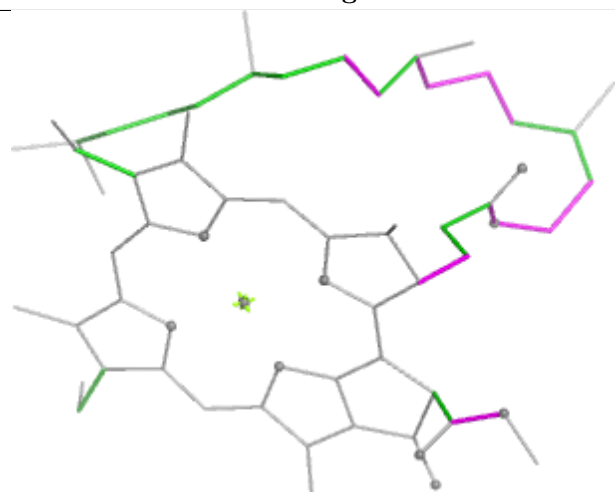
Ligand CLA 1 313



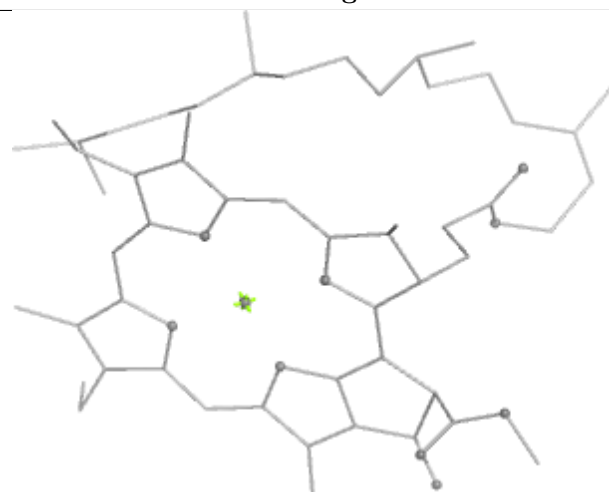
Bond lengths



Bond angles

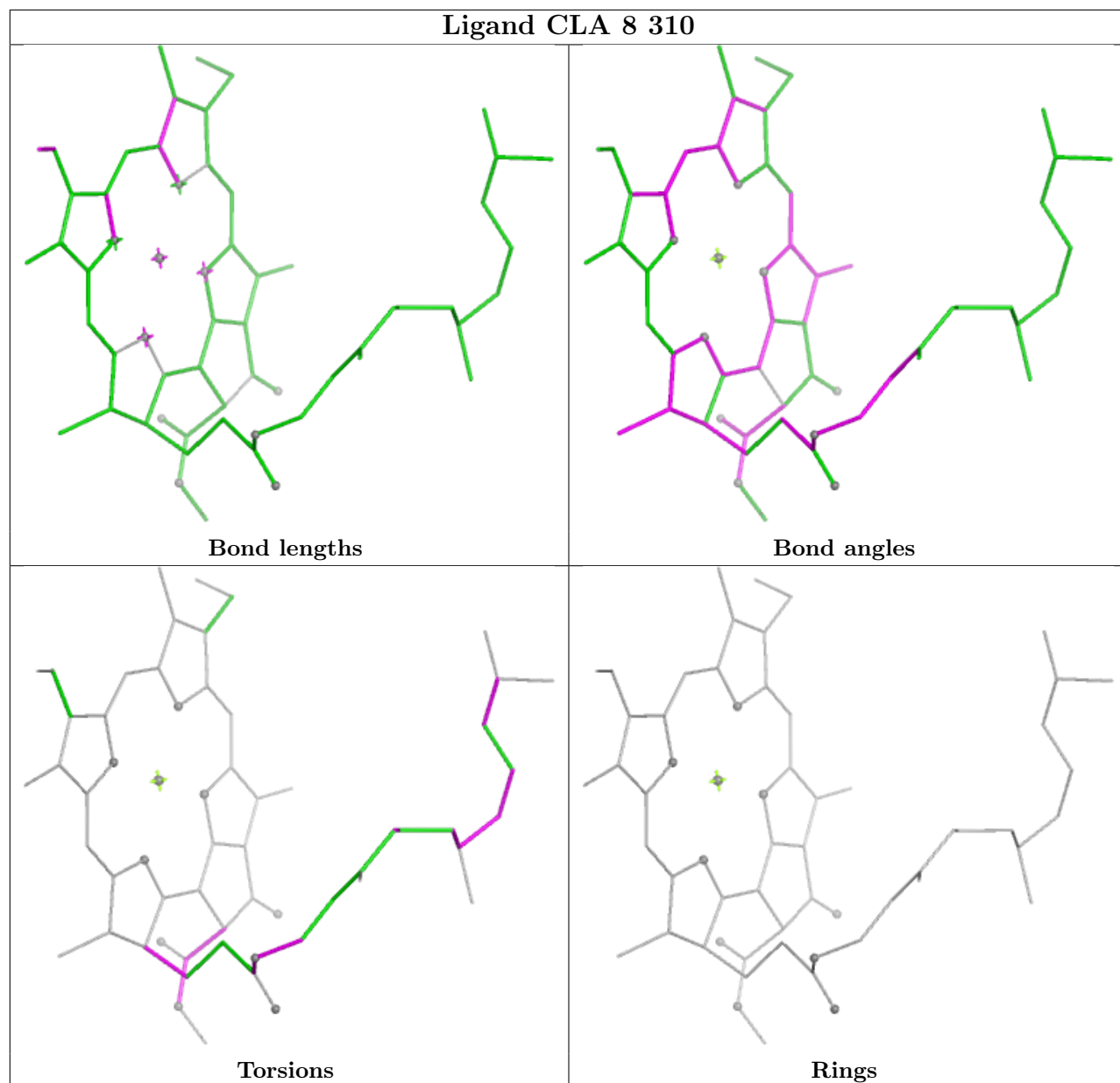


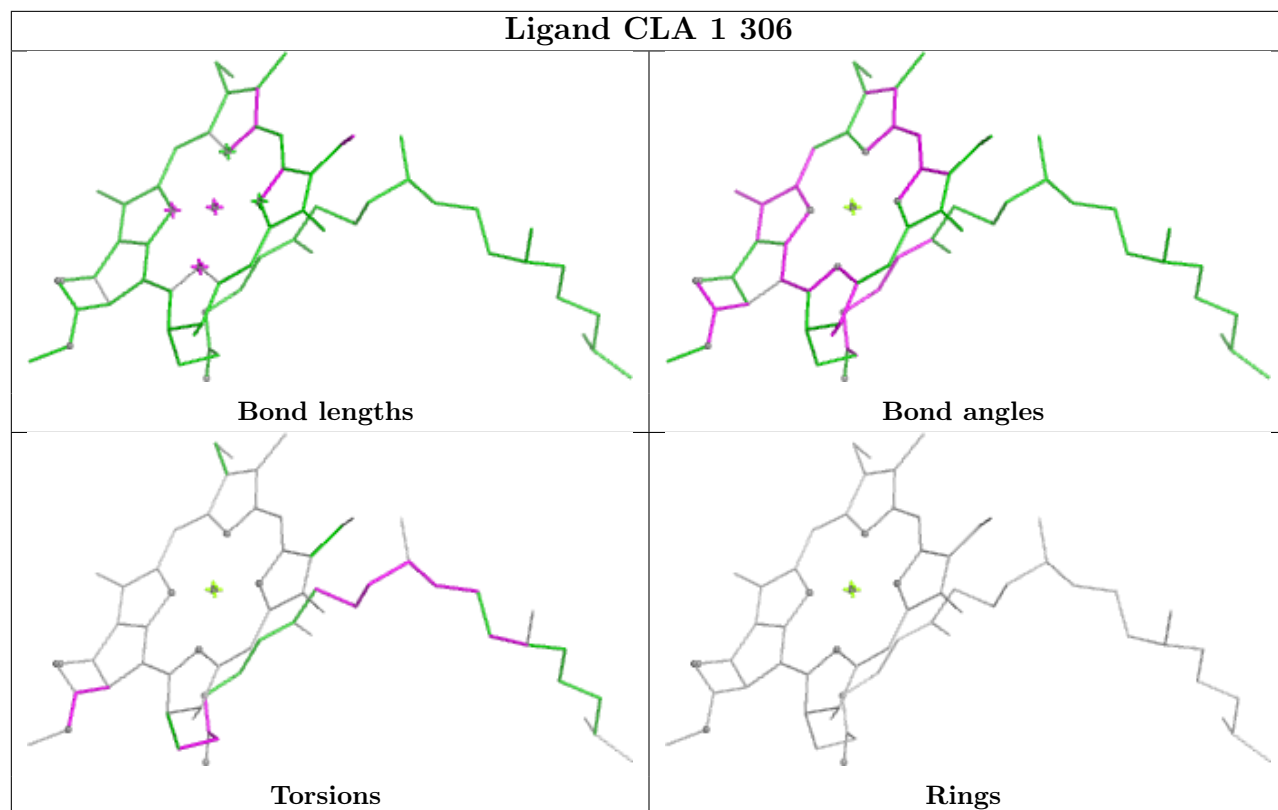
Torsions



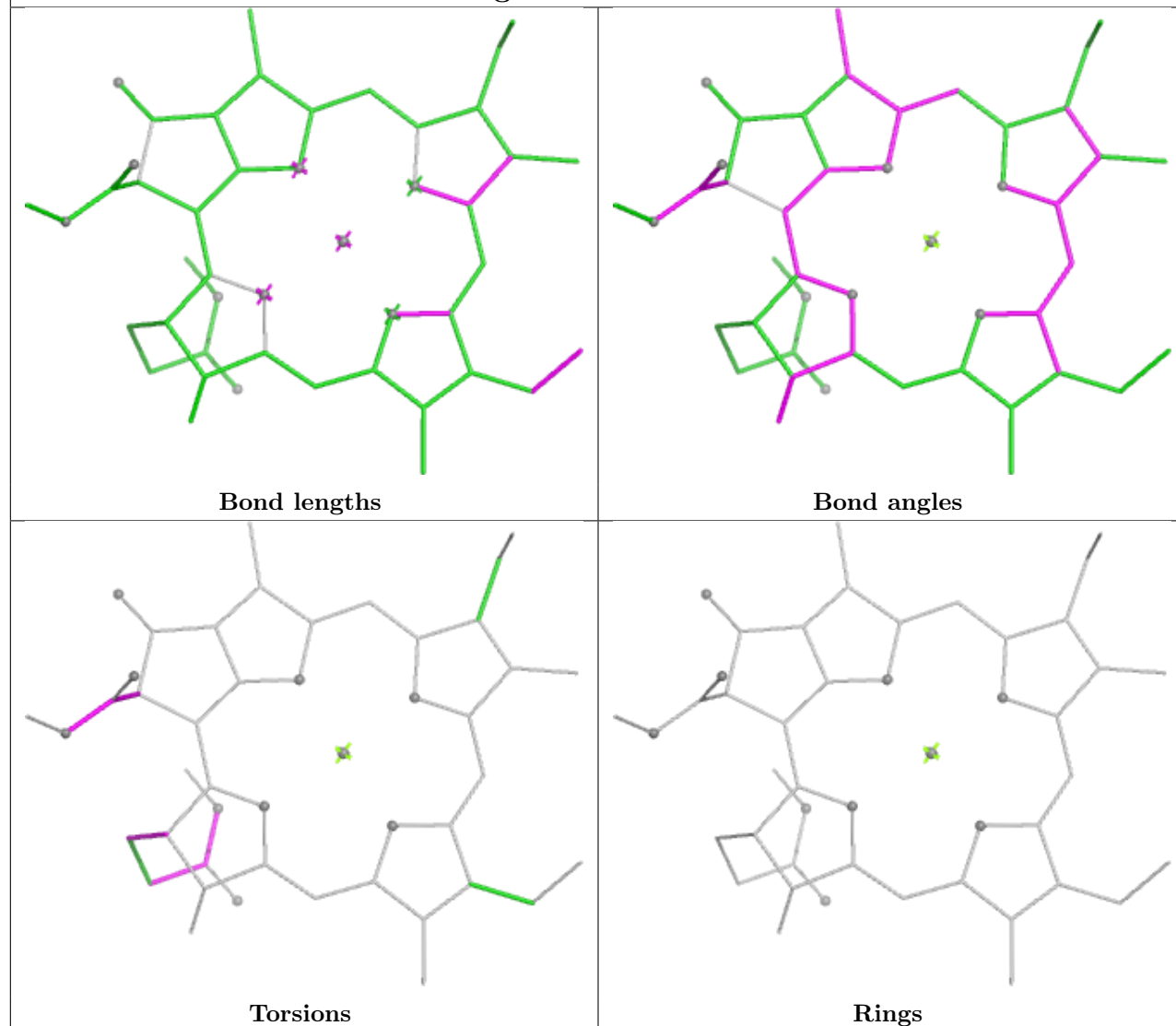
Rings

Ligand CLA 8 310

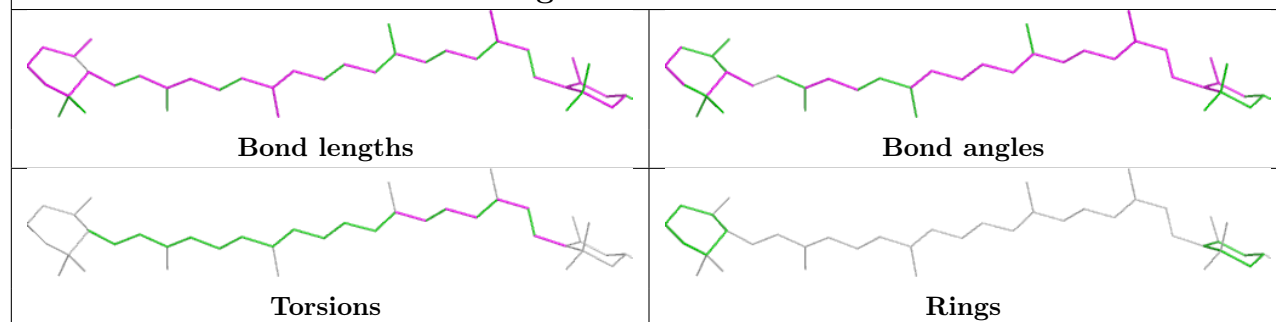




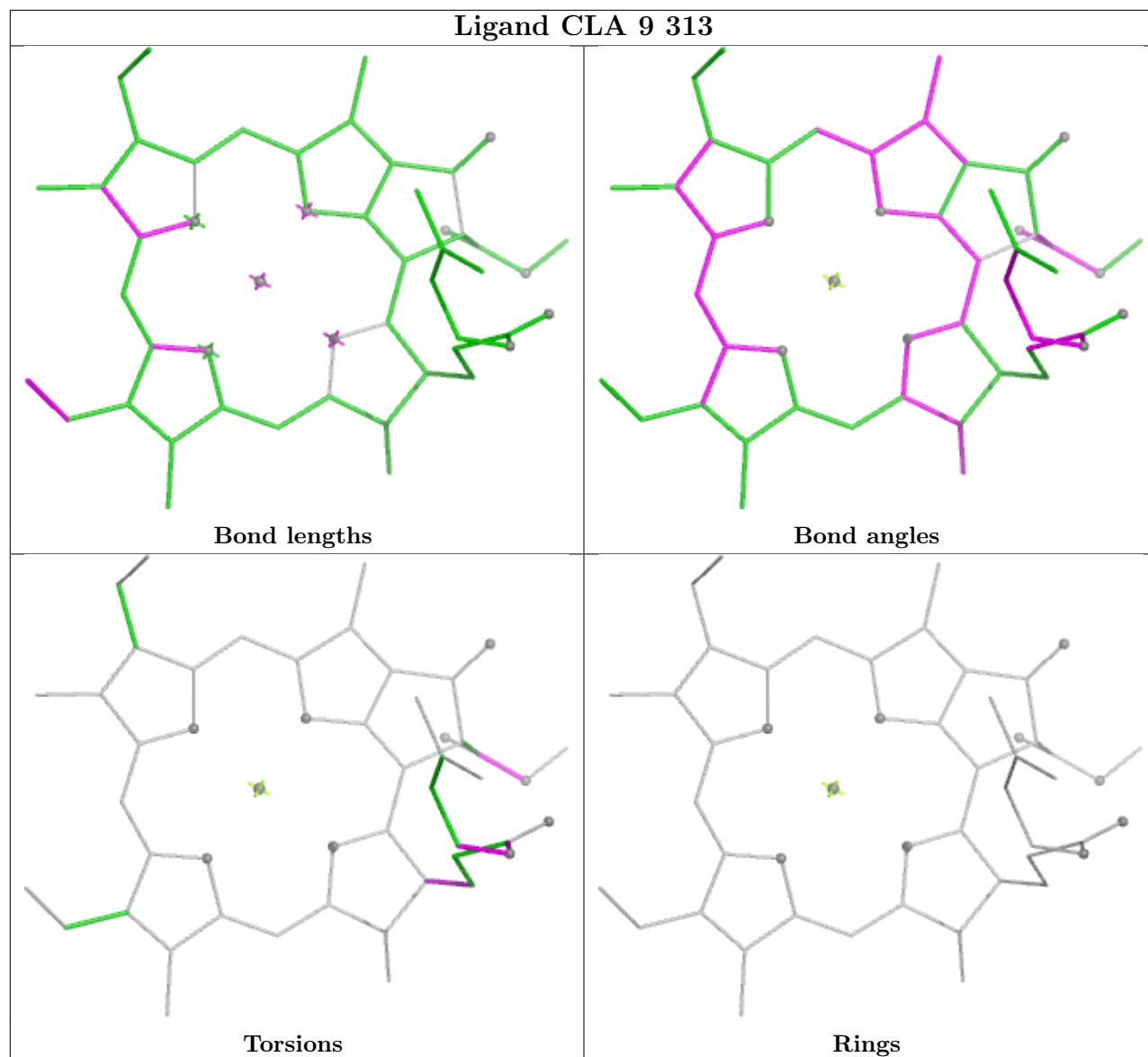
Ligand CLA 2 304

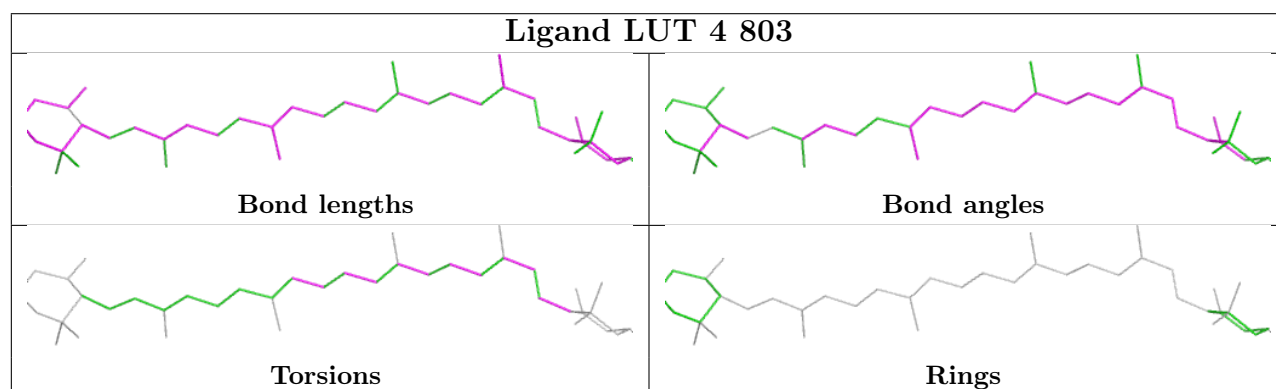
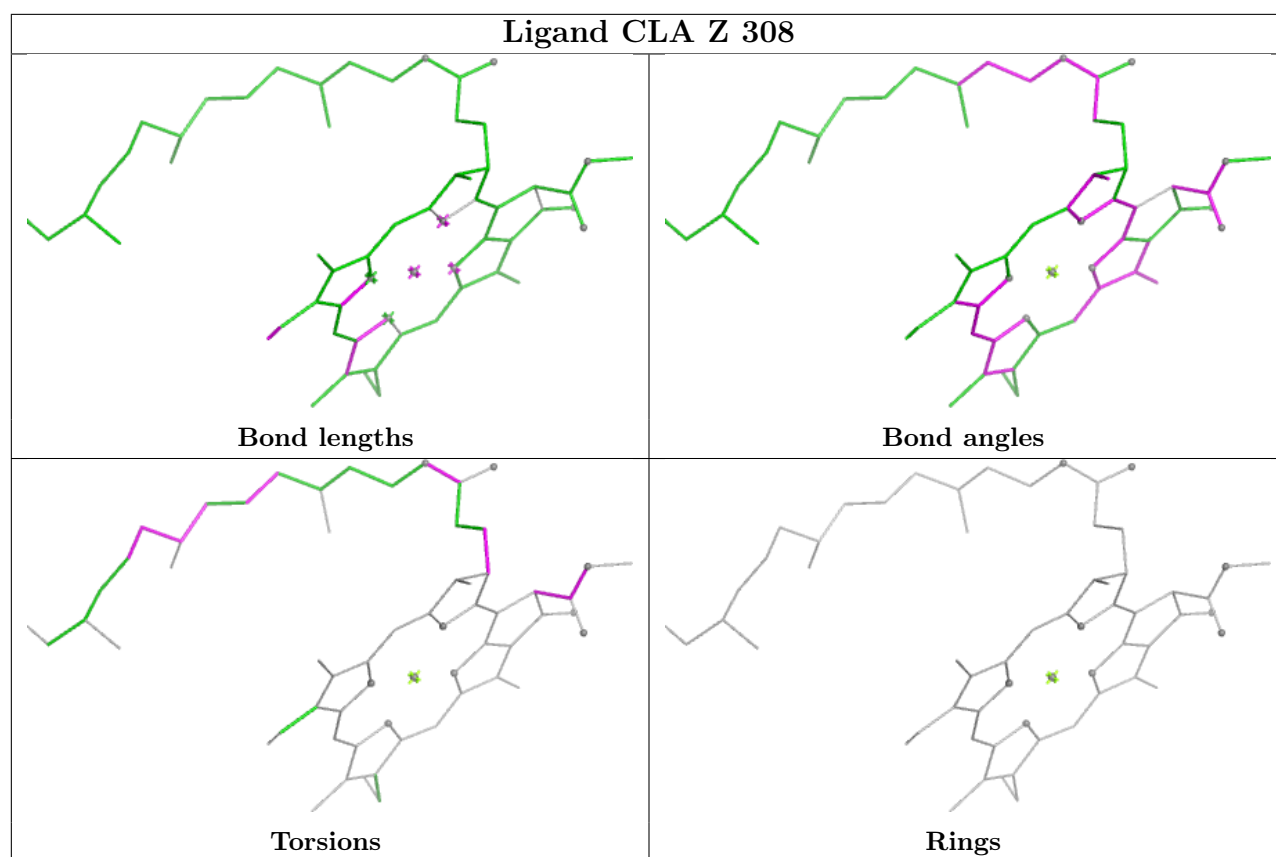


Ligand LUT 5 303

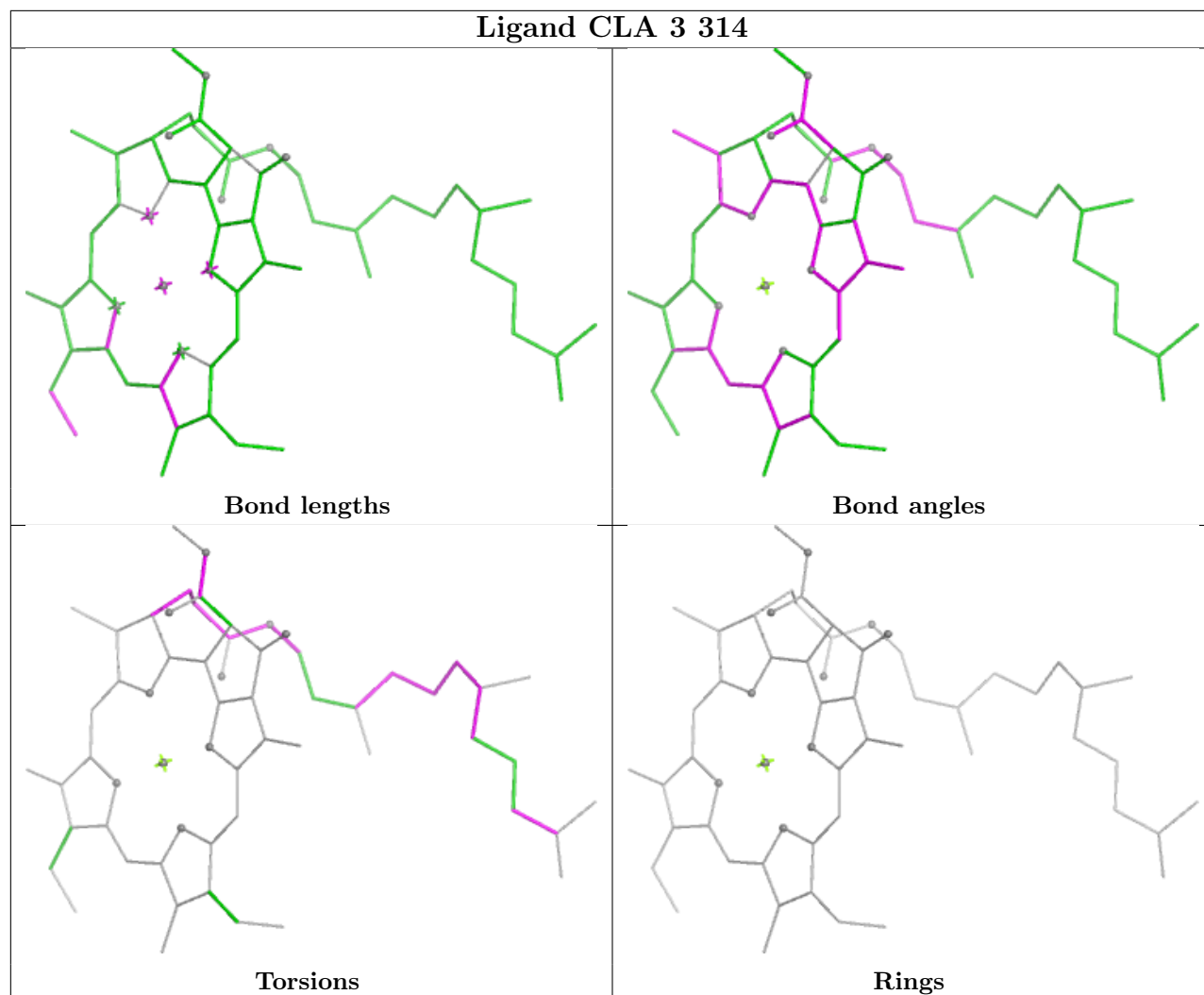


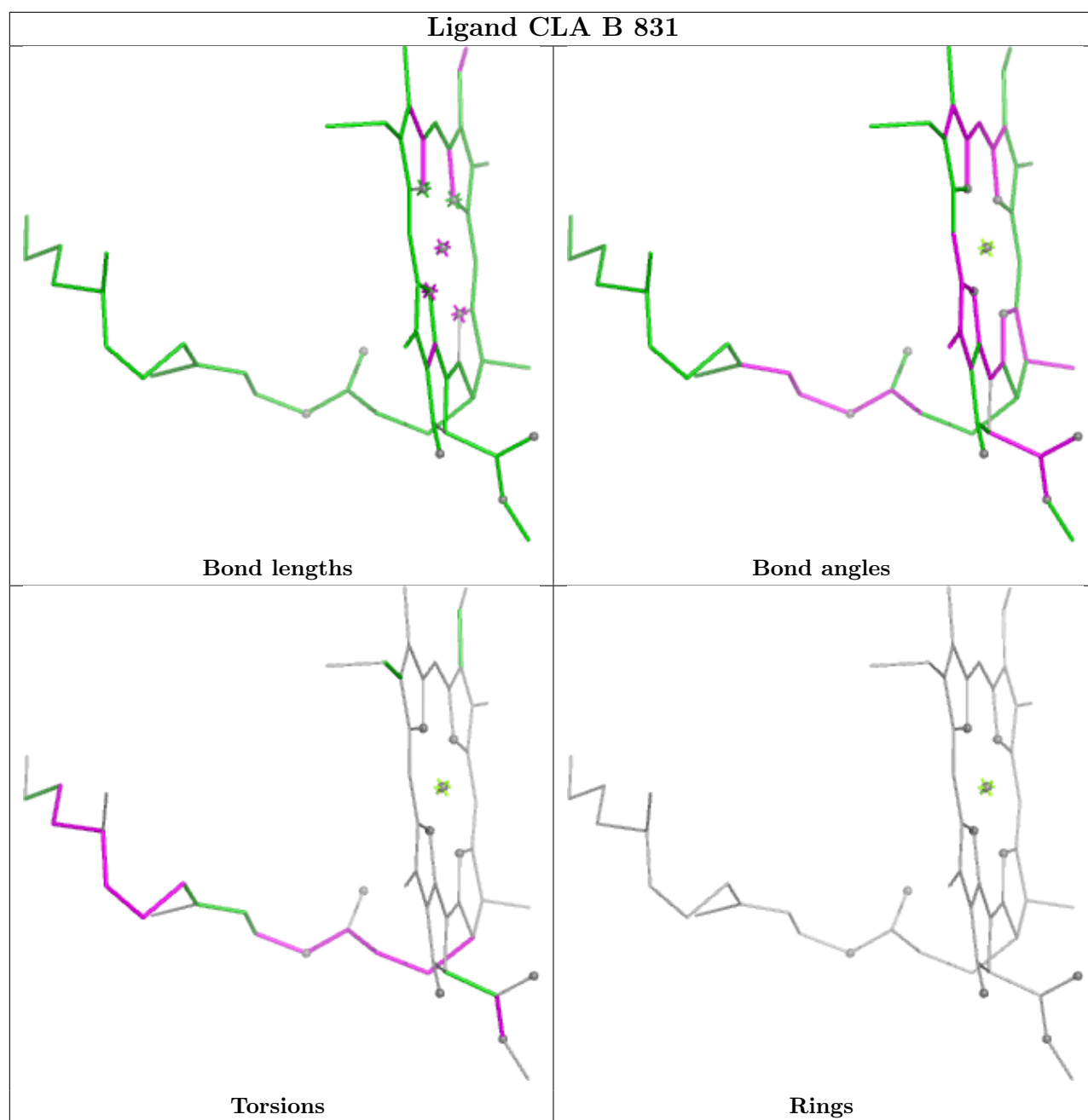
Ligand CLA 9 313

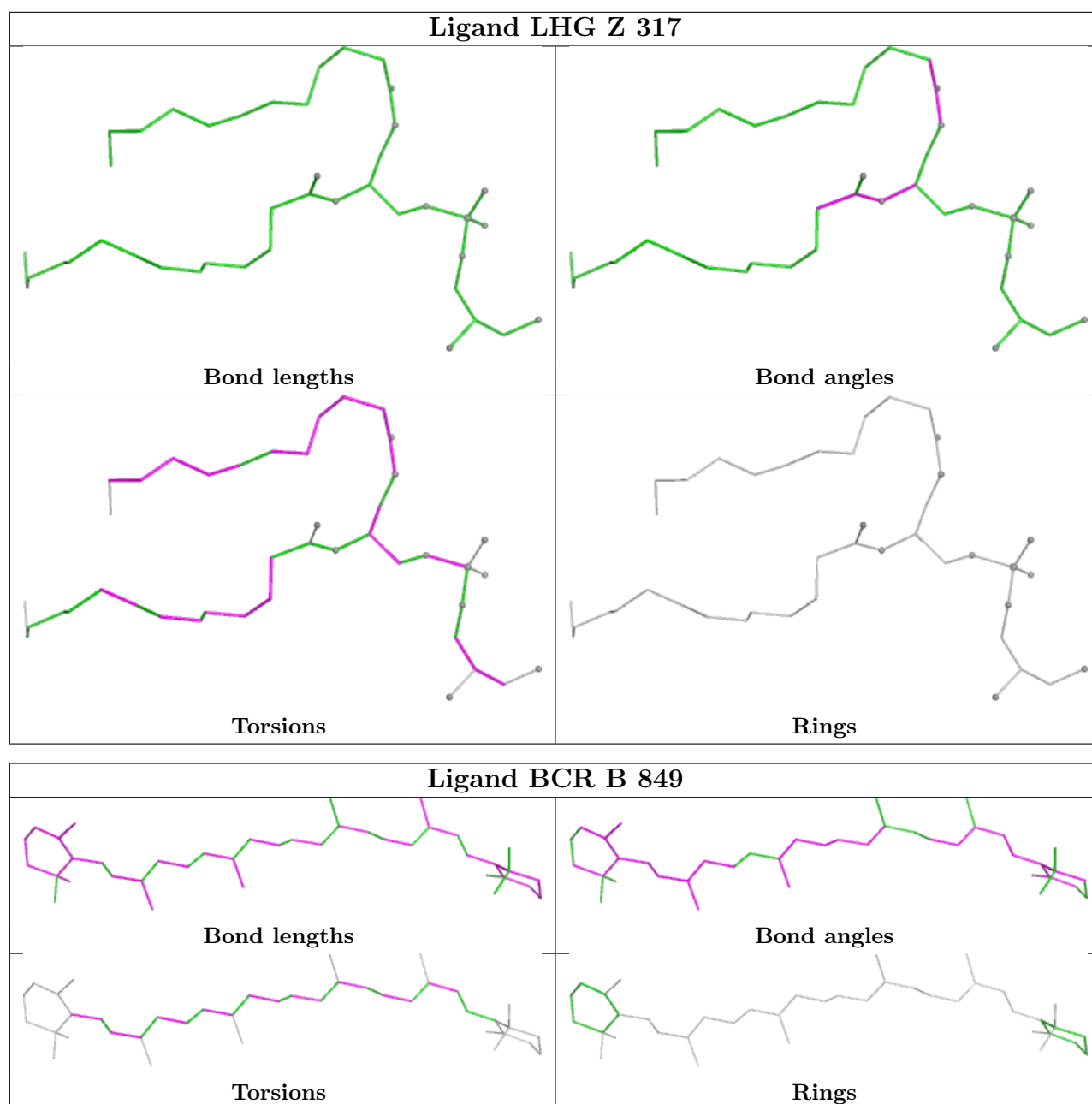


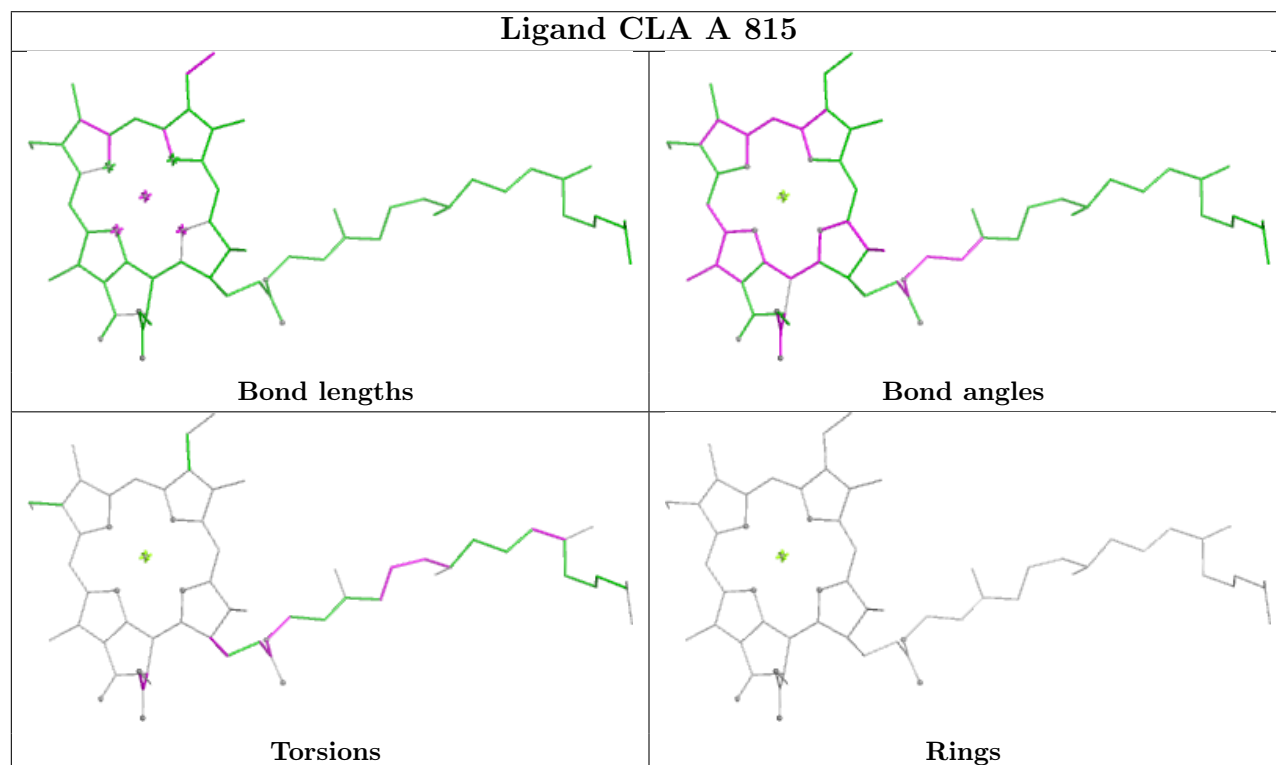
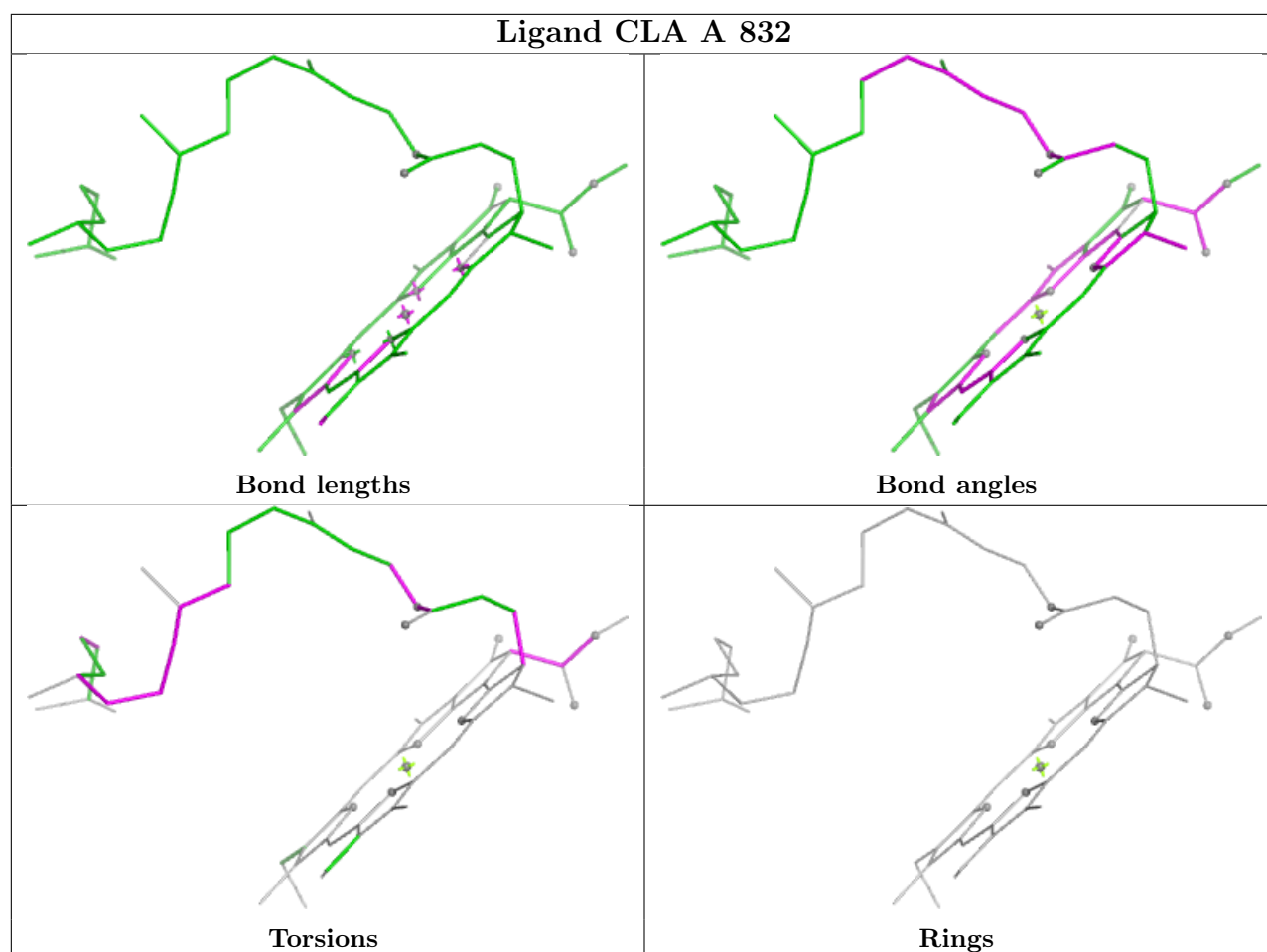


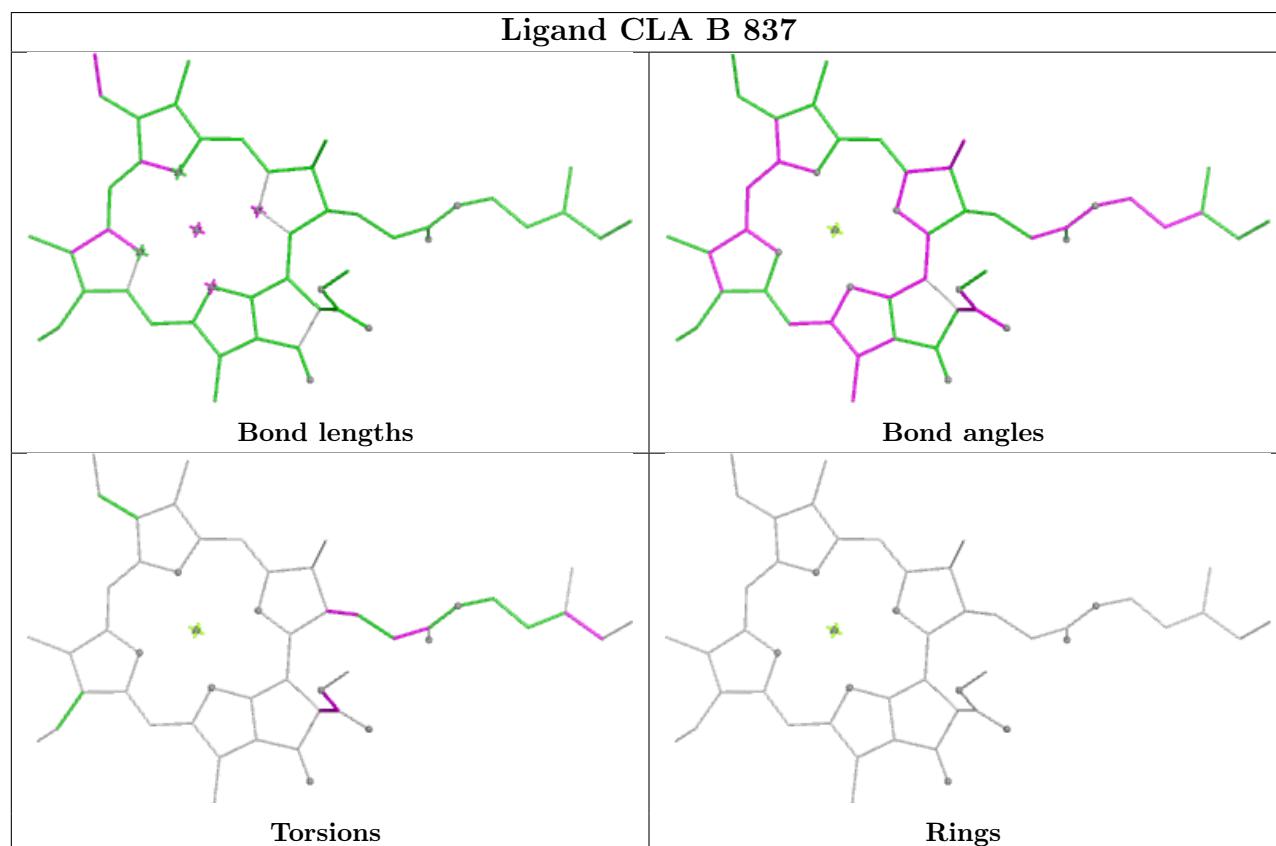
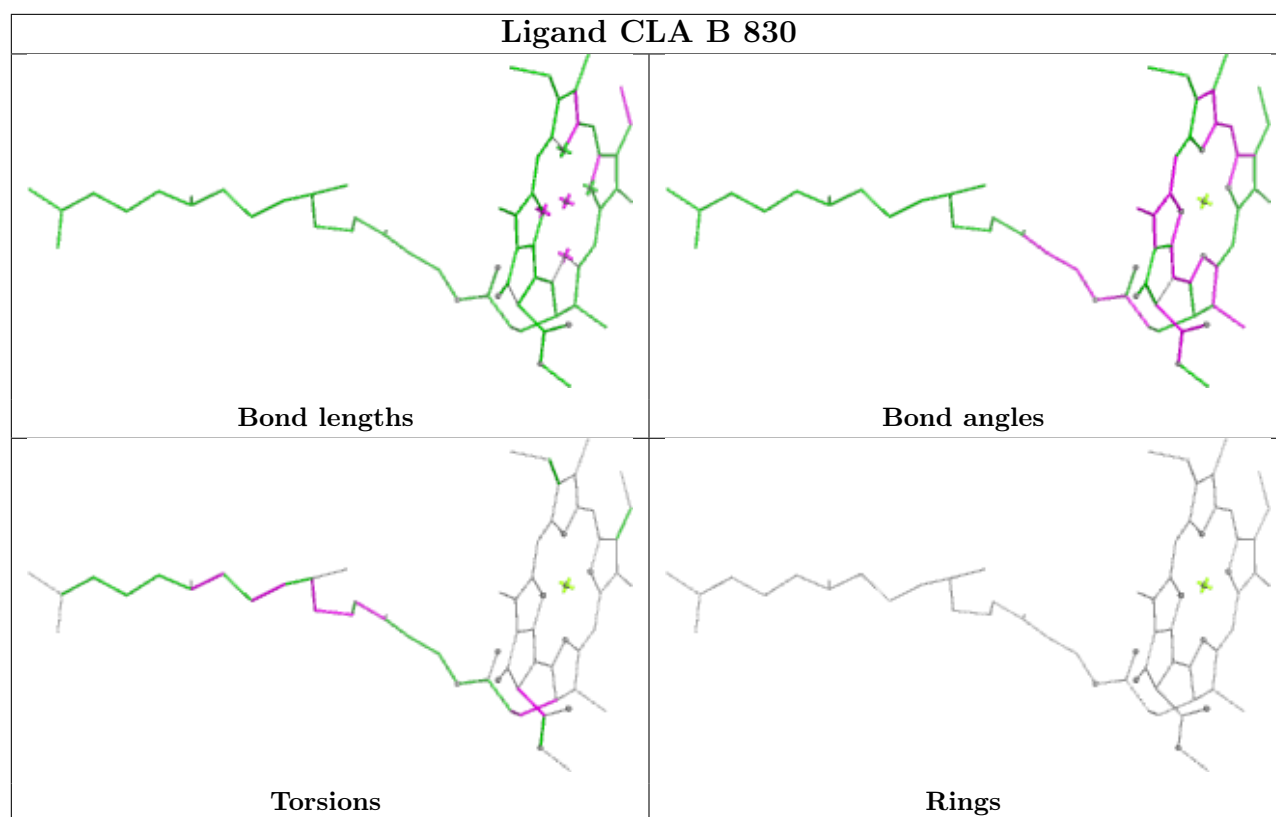
Ligand CLA 3 314

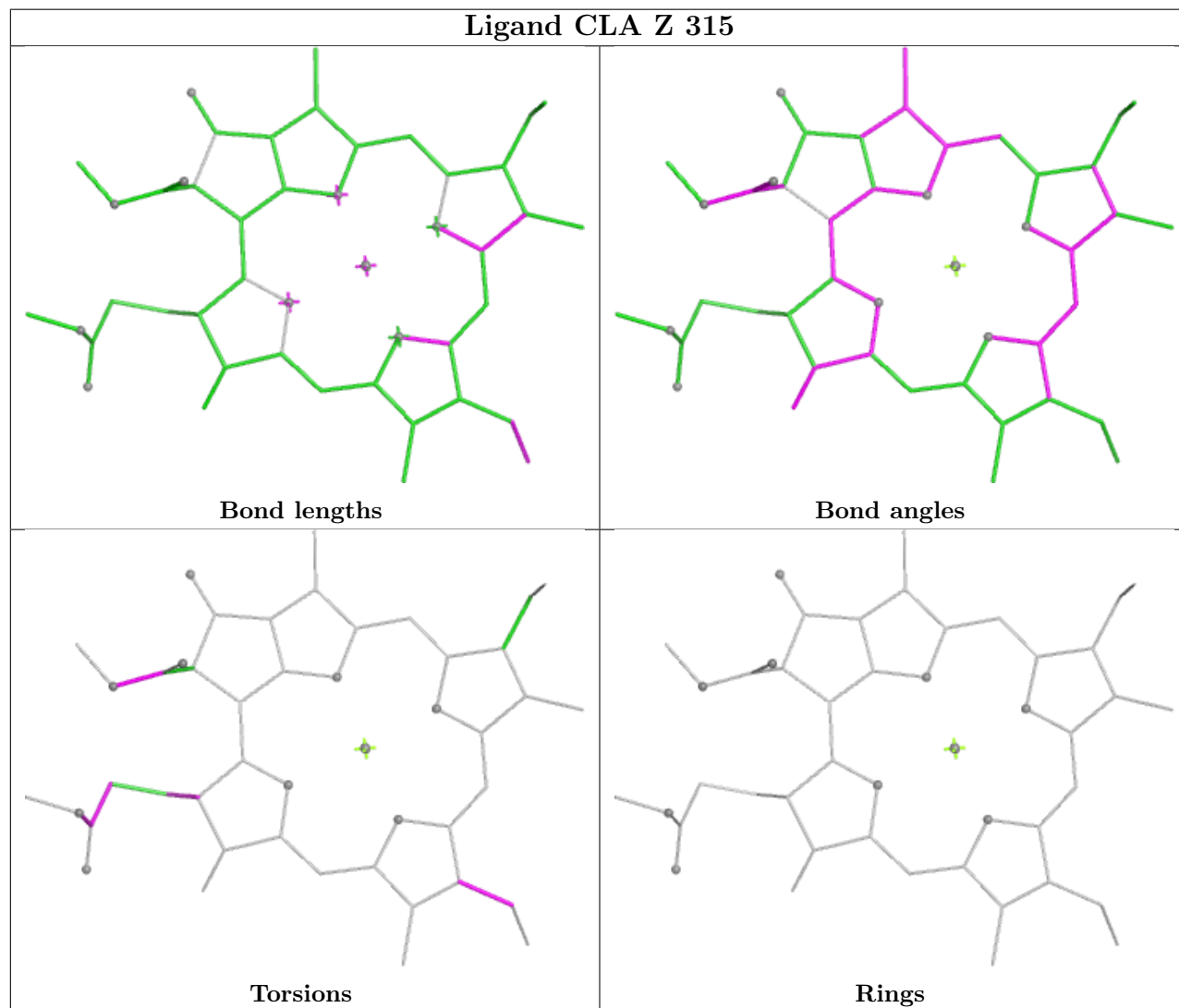
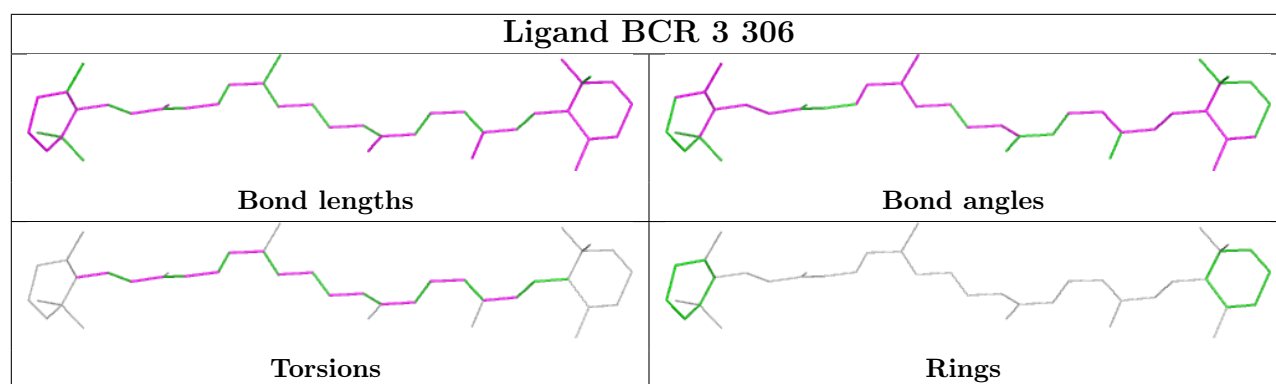




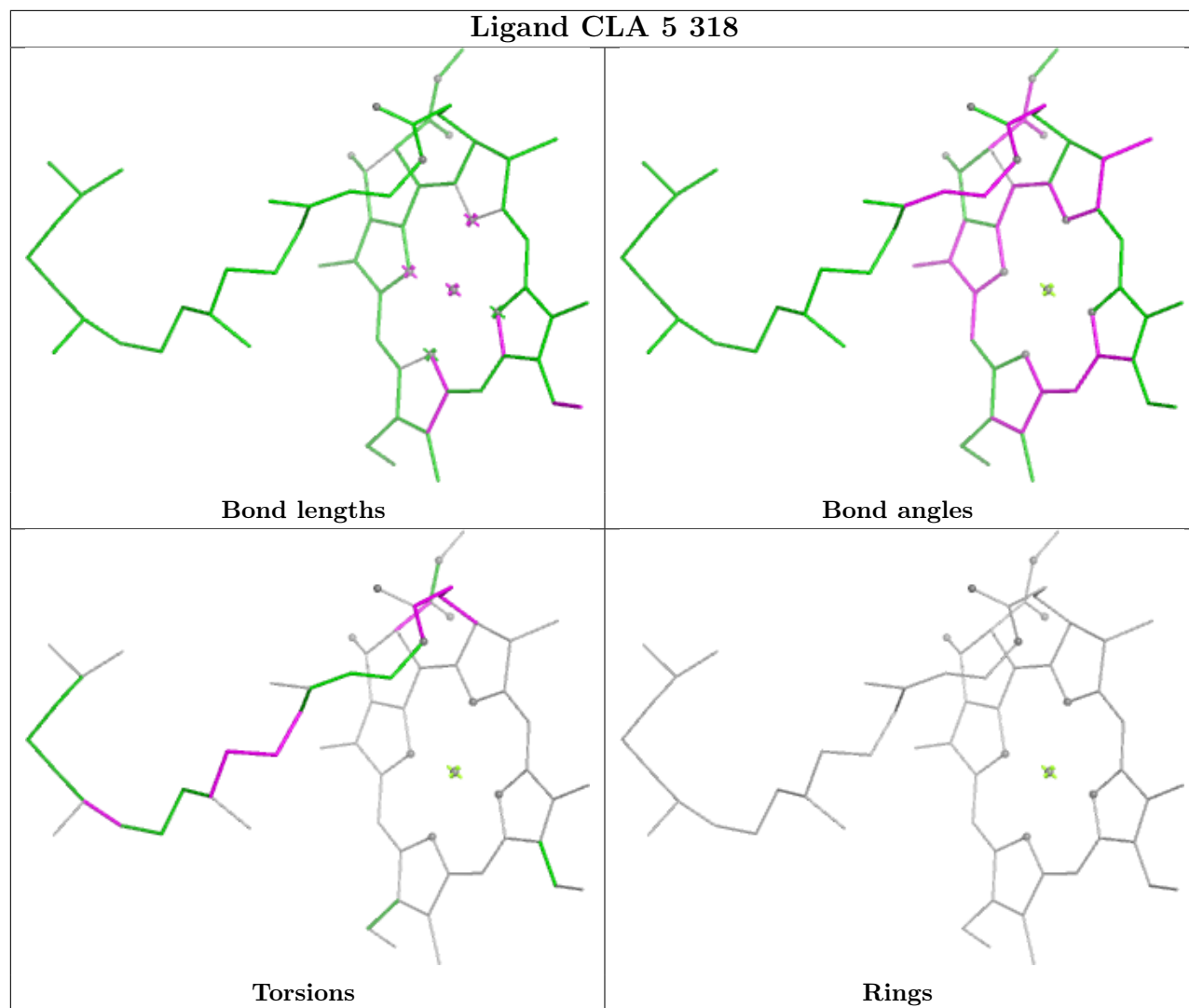




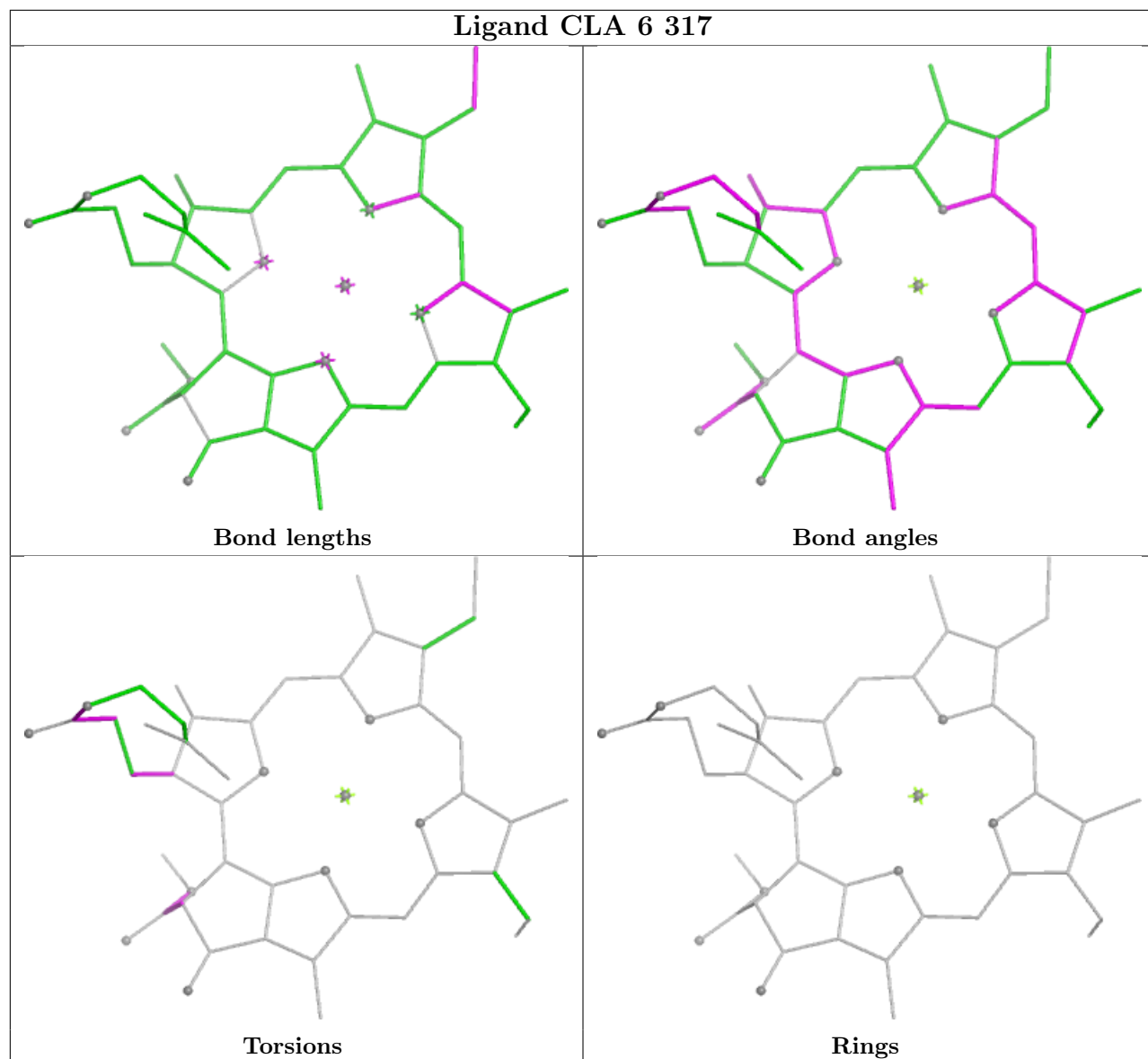


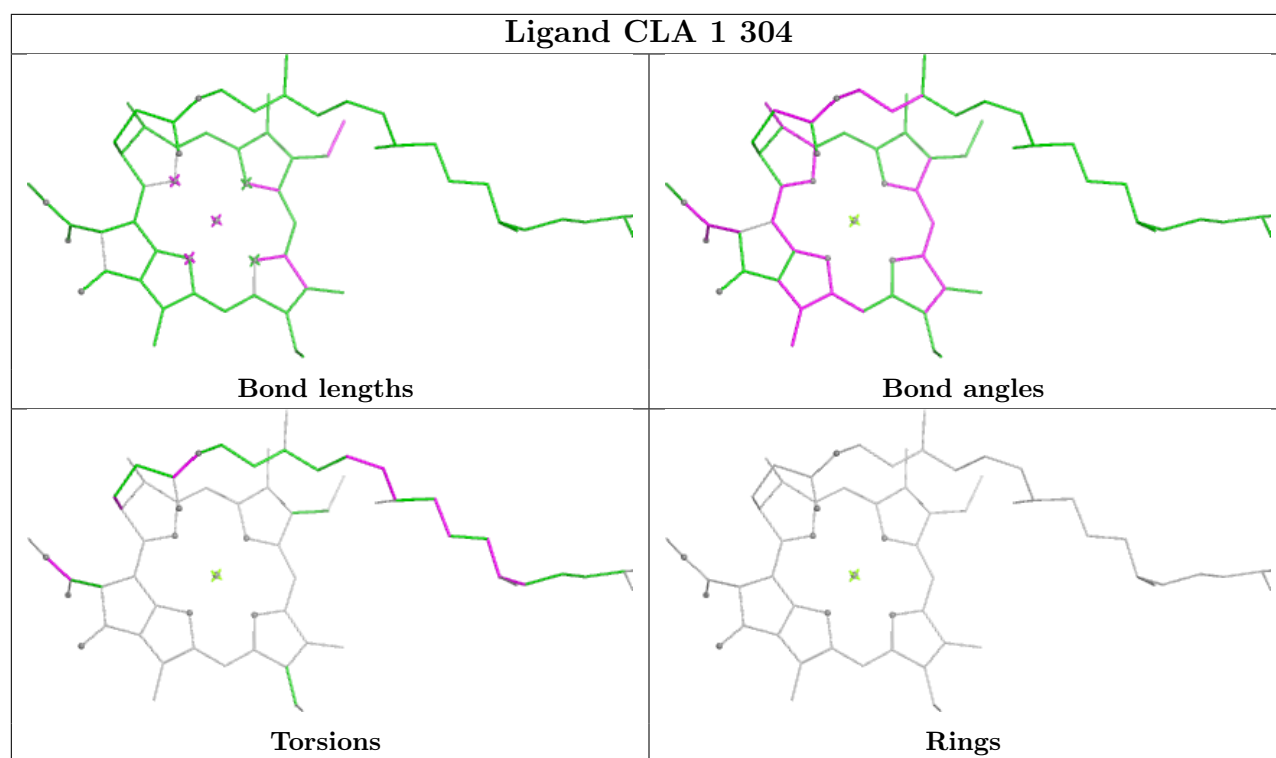


Ligand CLA 5 318

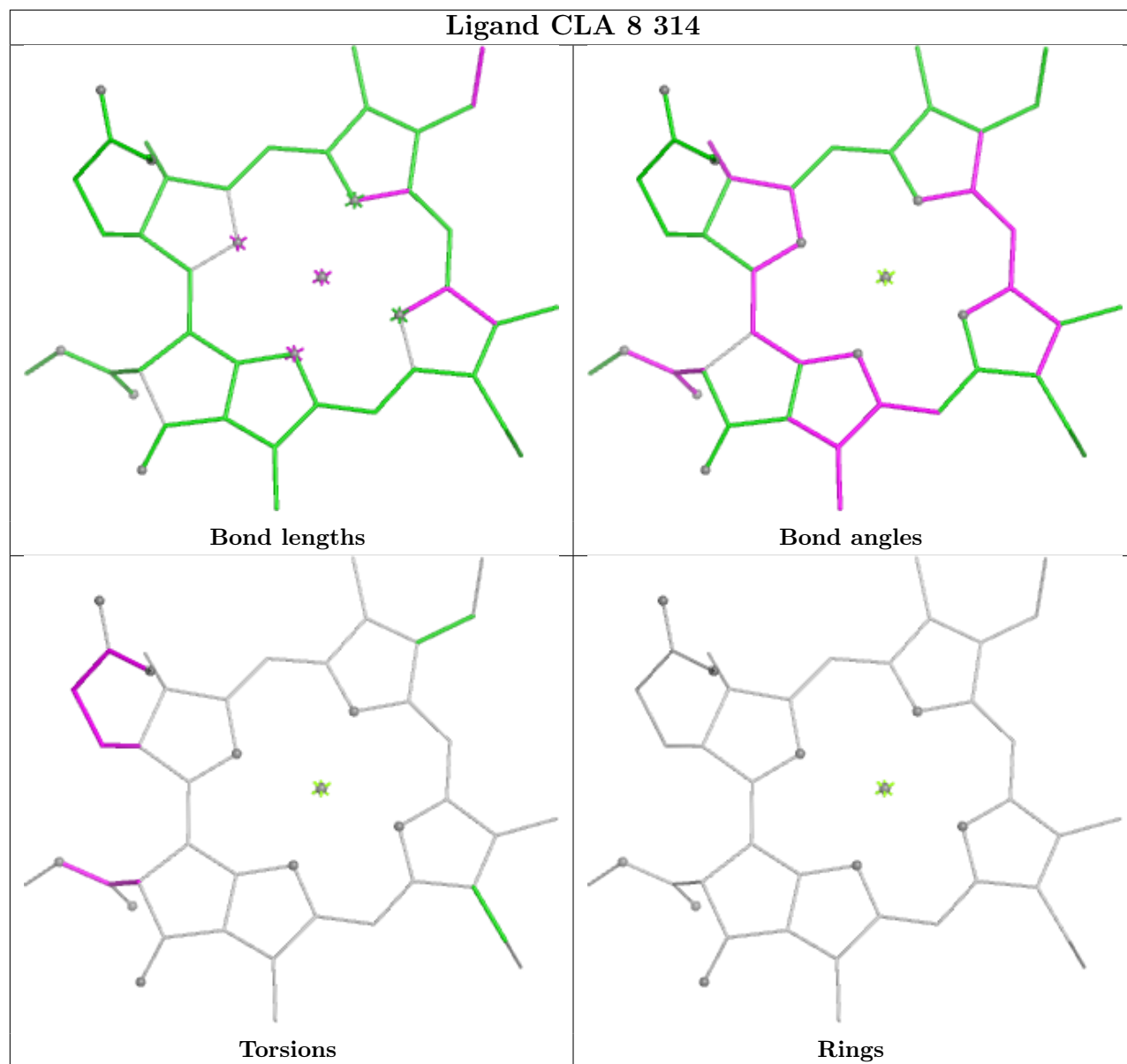


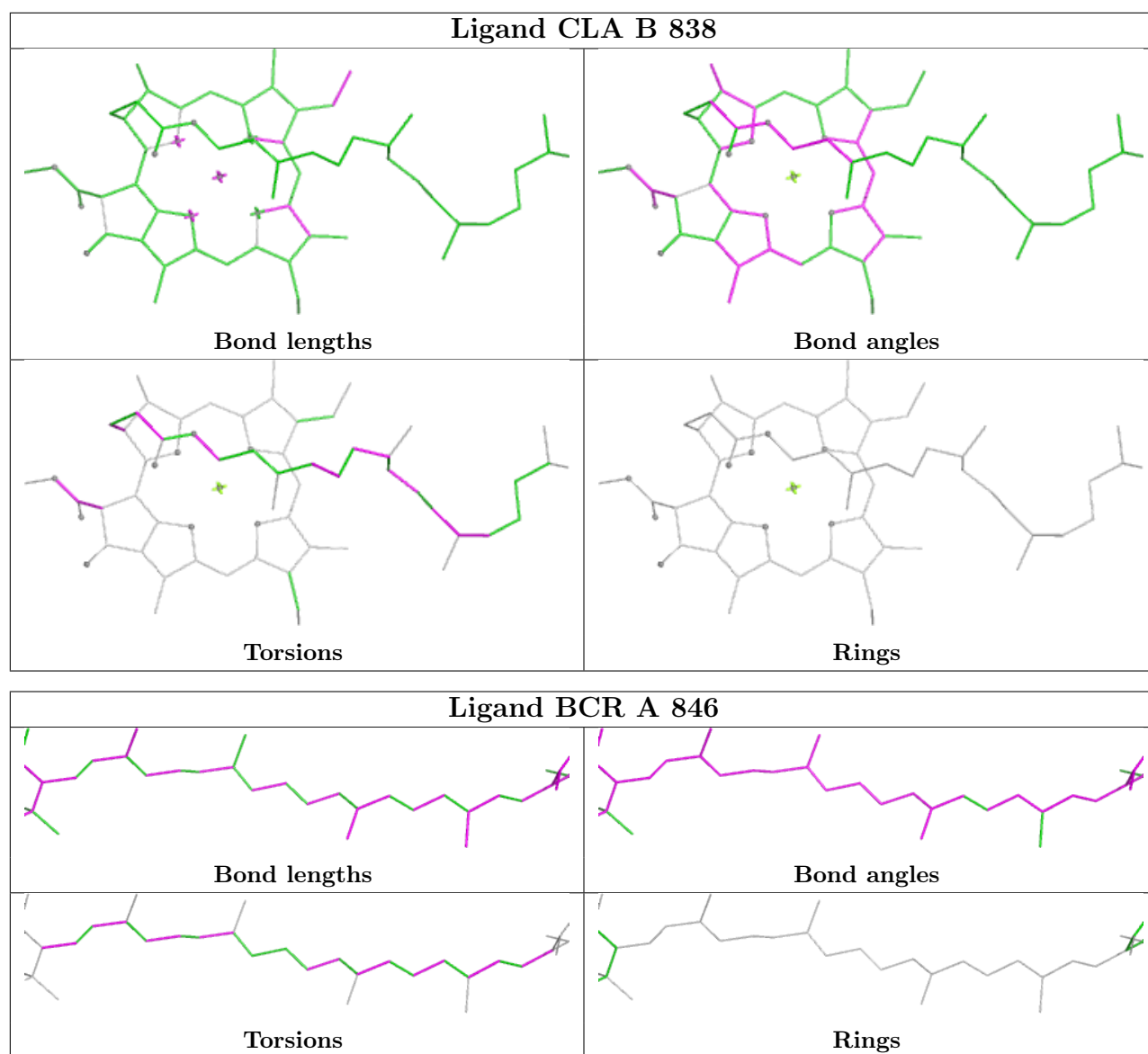
Ligand CLA 6 317



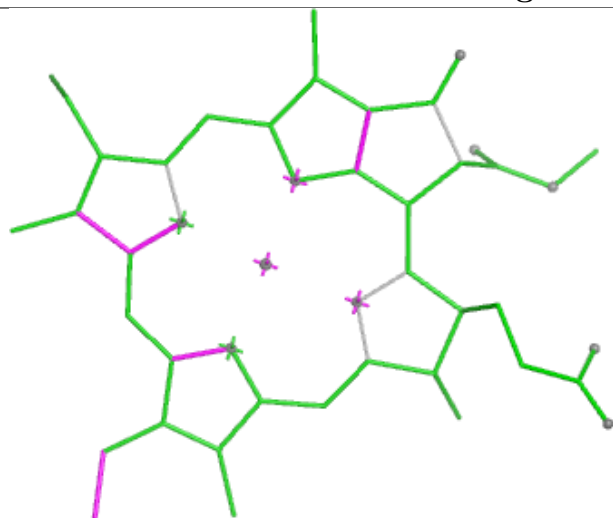


Ligand CLA 8 314

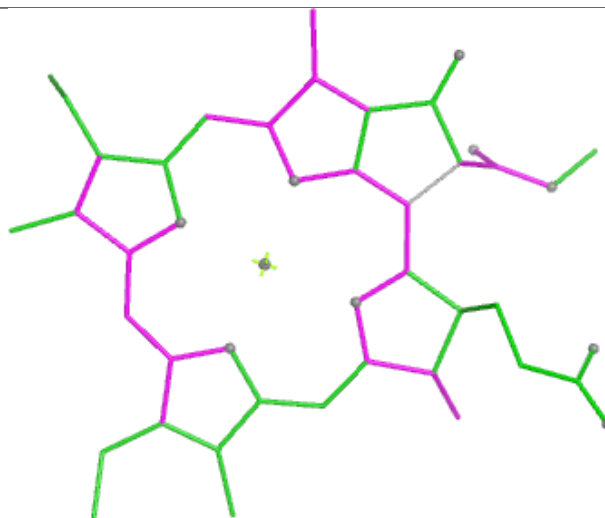




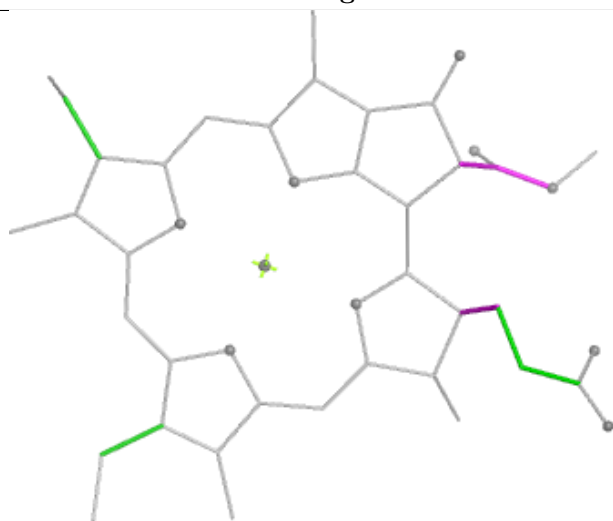
Ligand CLA F 305



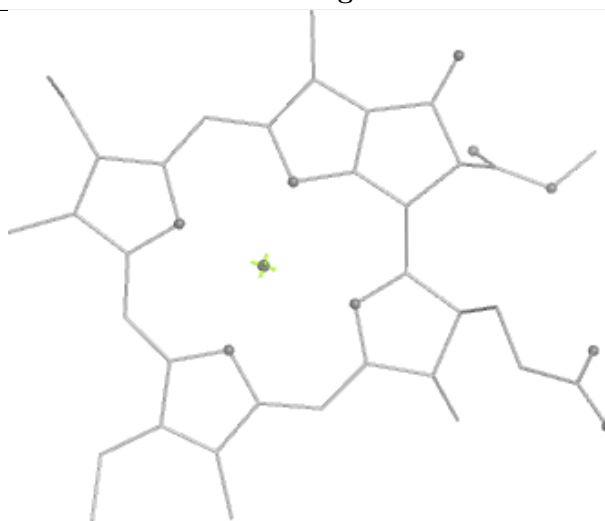
Bond lengths



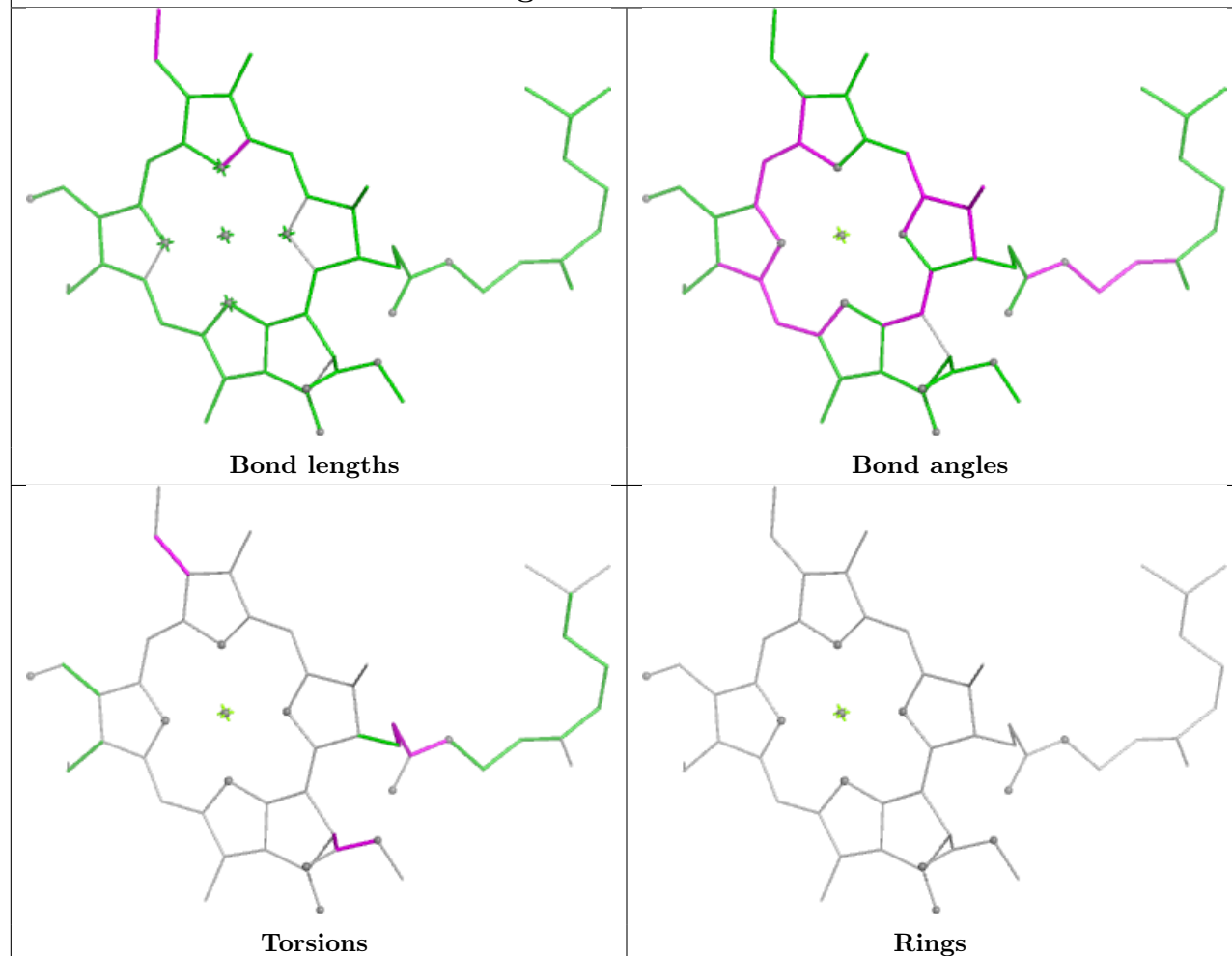
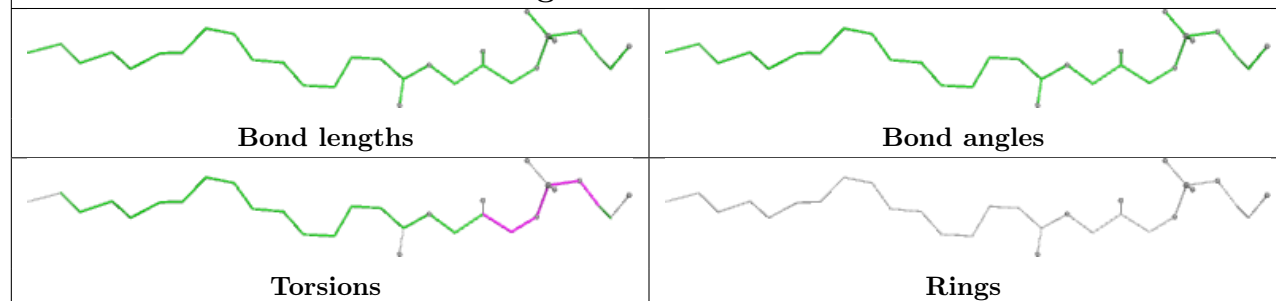
Bond angles



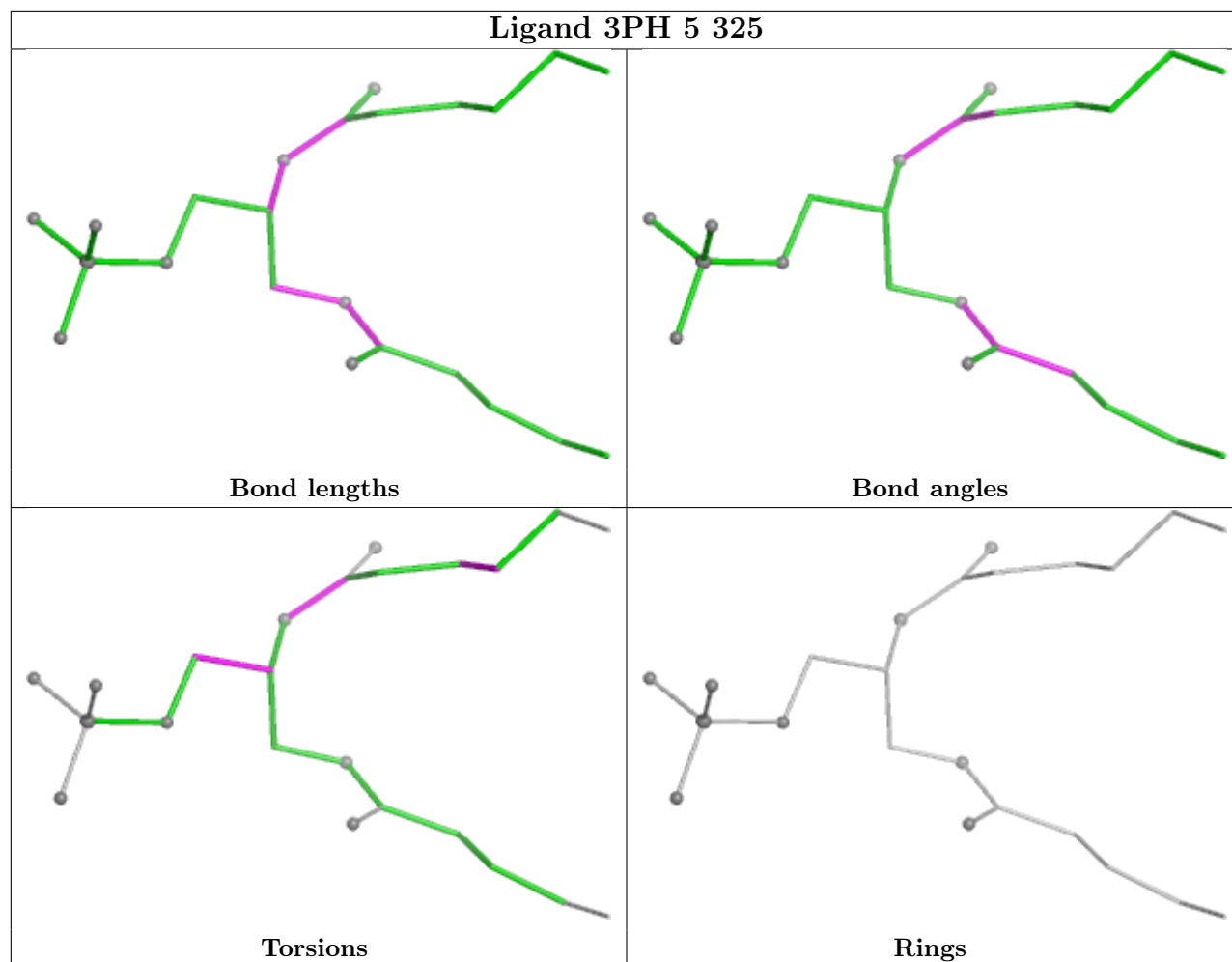
Torsions



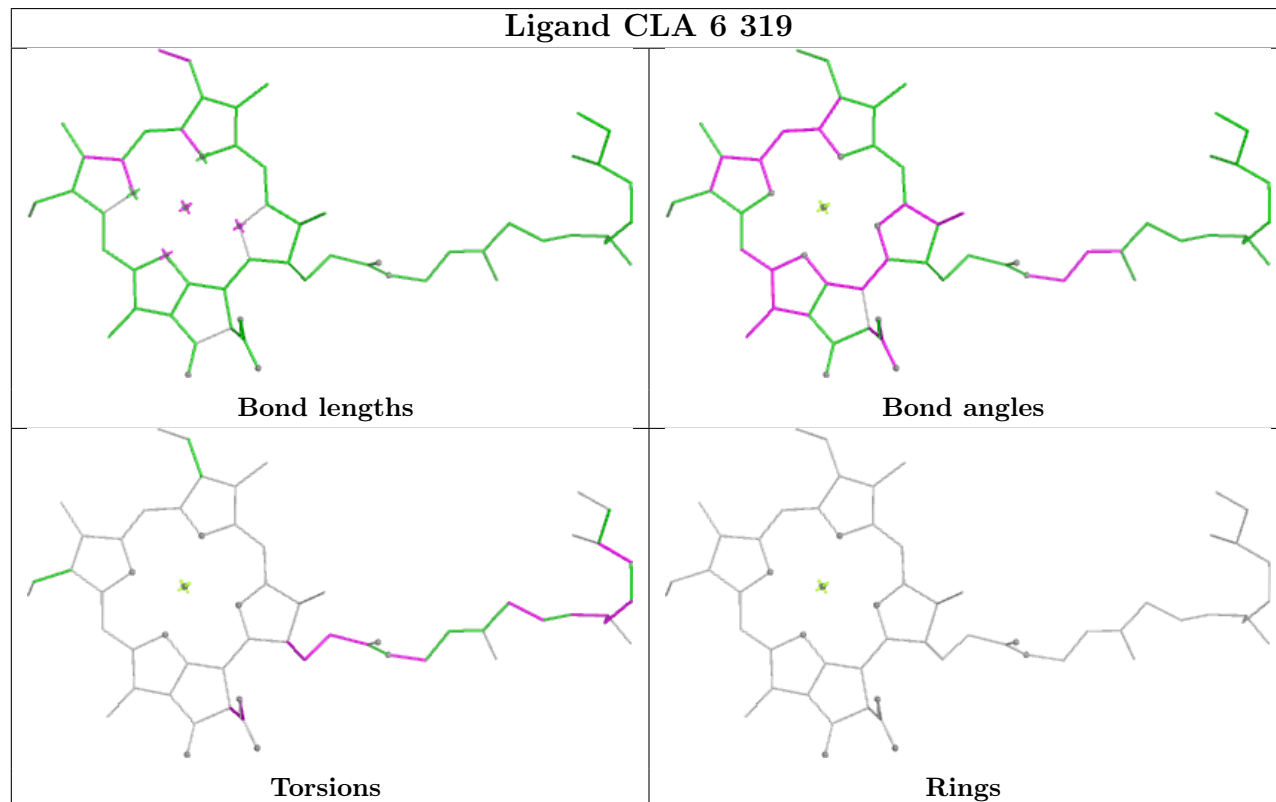
Rings

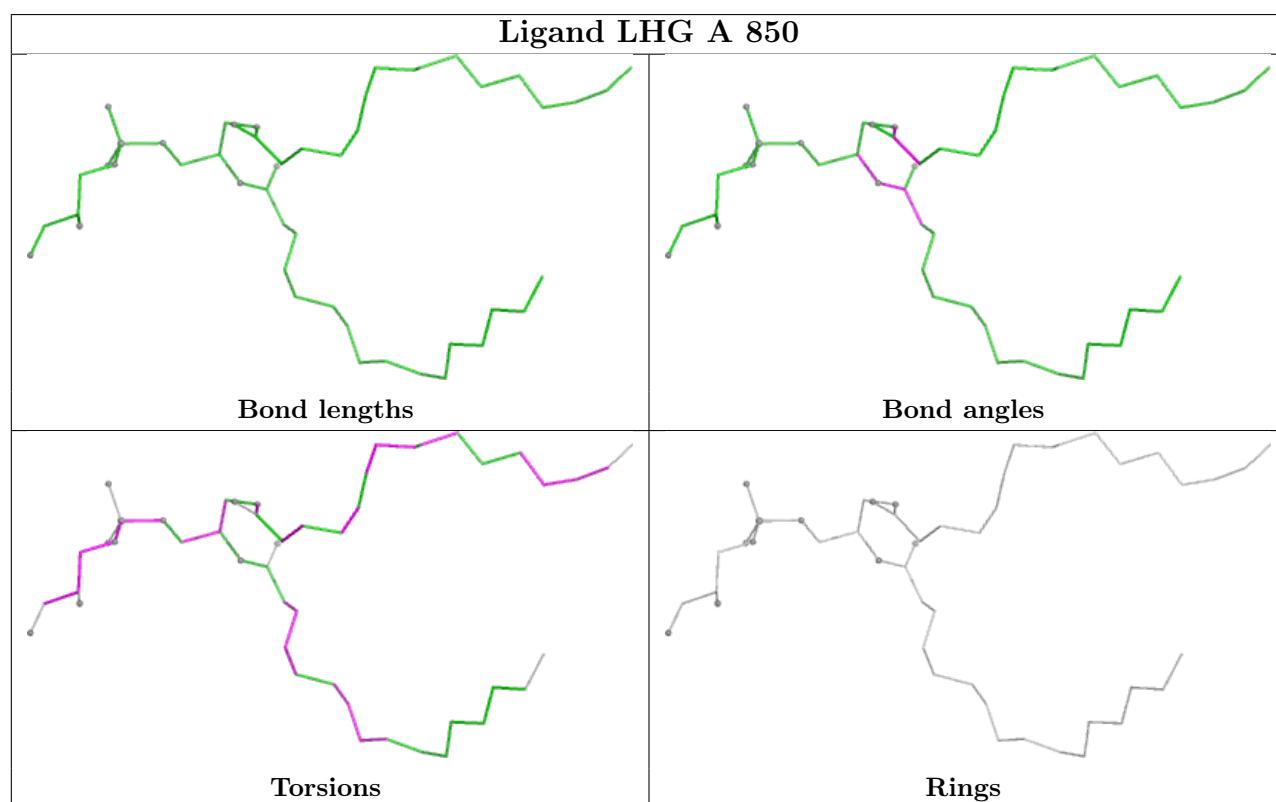
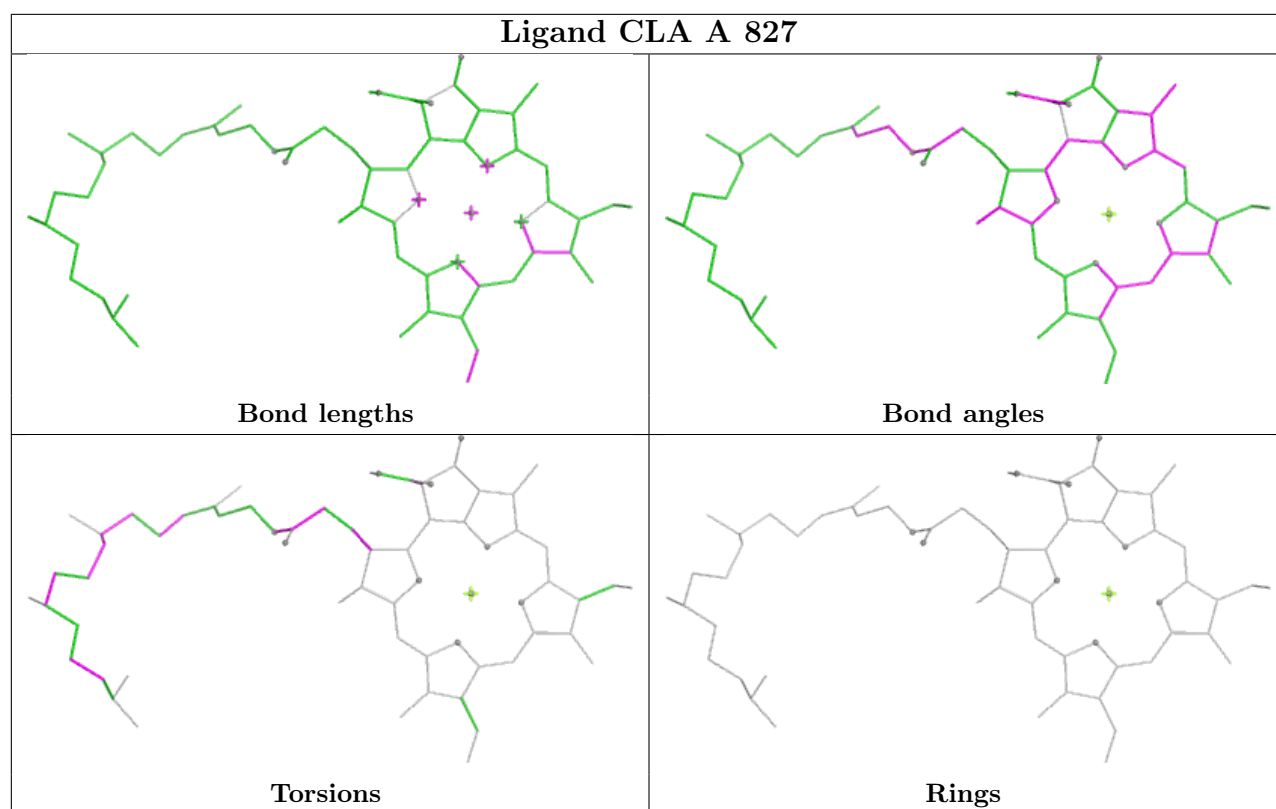
Ligand CHL 8 312**Ligand LPX 8 319**

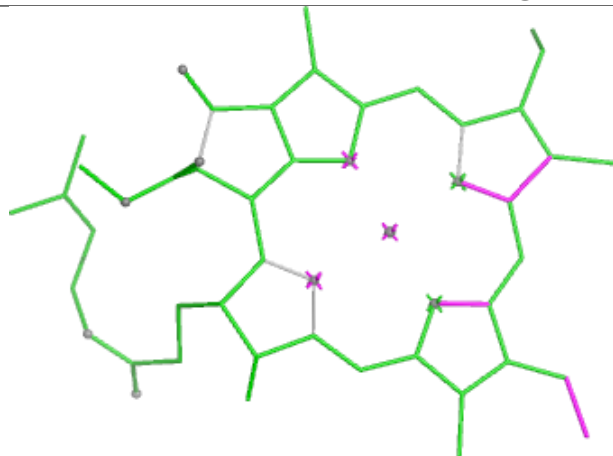
Ligand 3PH 5 325



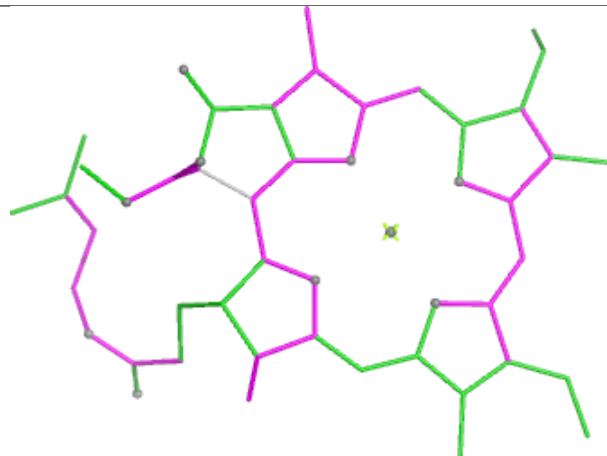
Ligand CLA 6 319



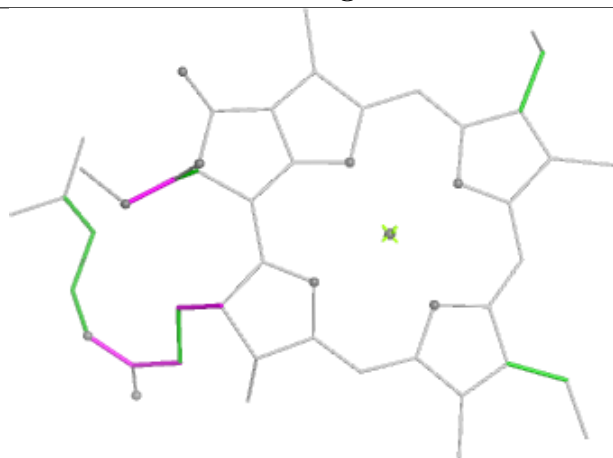


Ligand CLA L 203

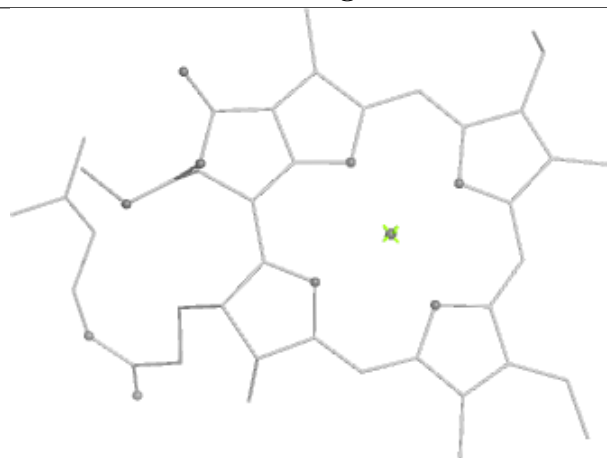
Bond lengths



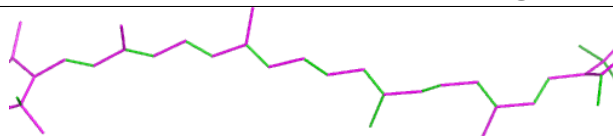
Bond angles



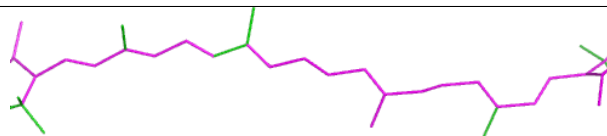
Torsions



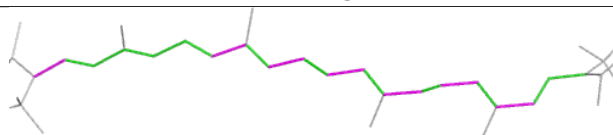
Rings

Ligand BCR B 847

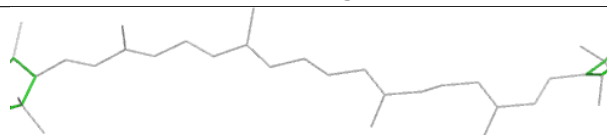
Bond lengths



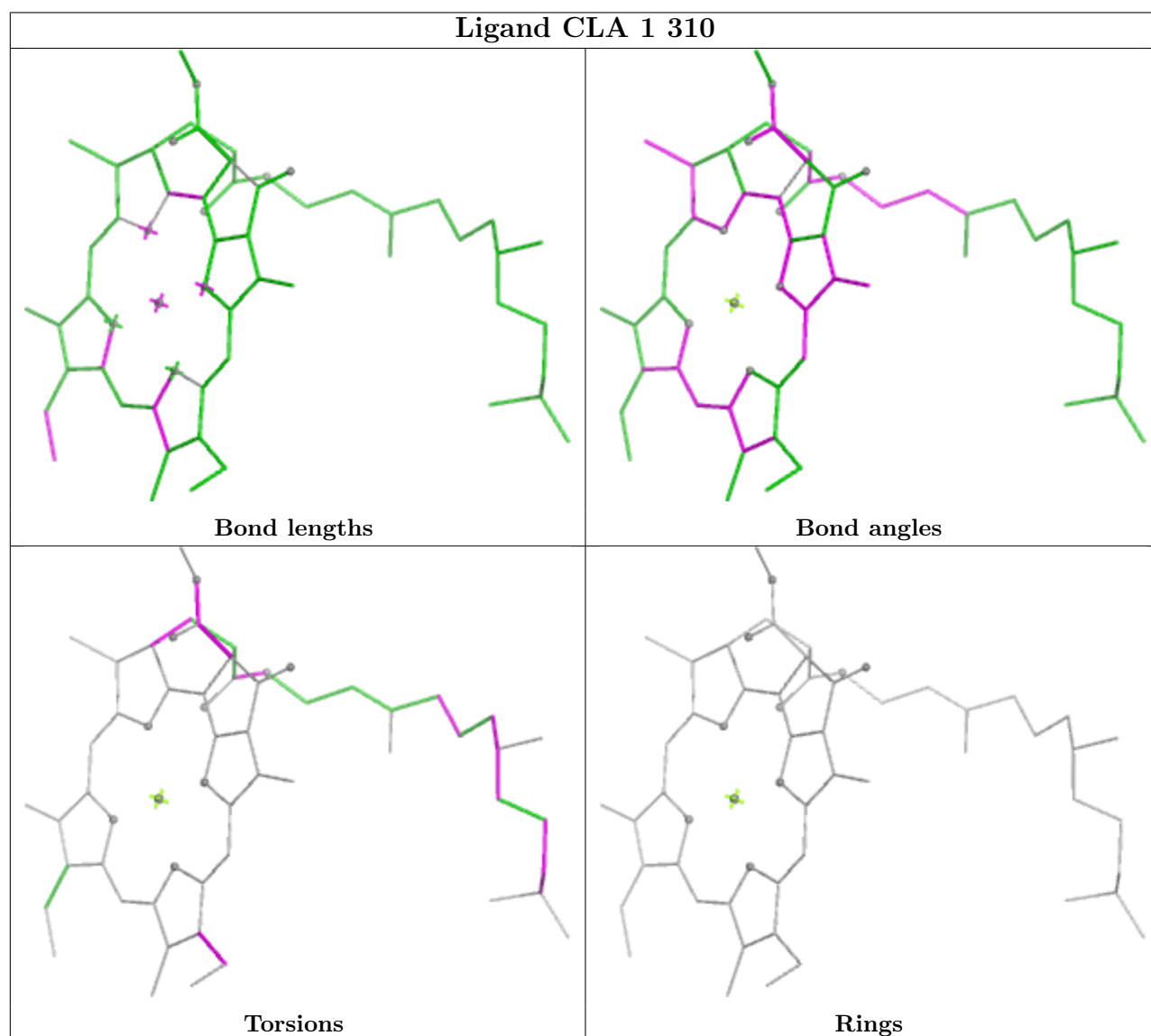
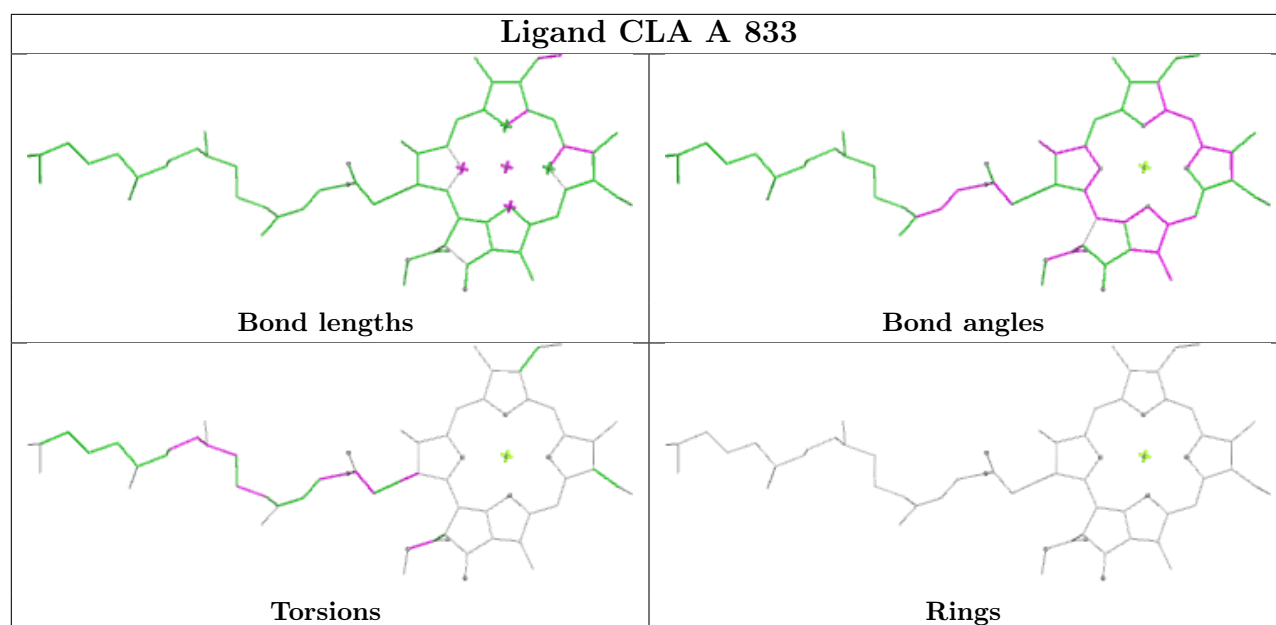
Bond angles

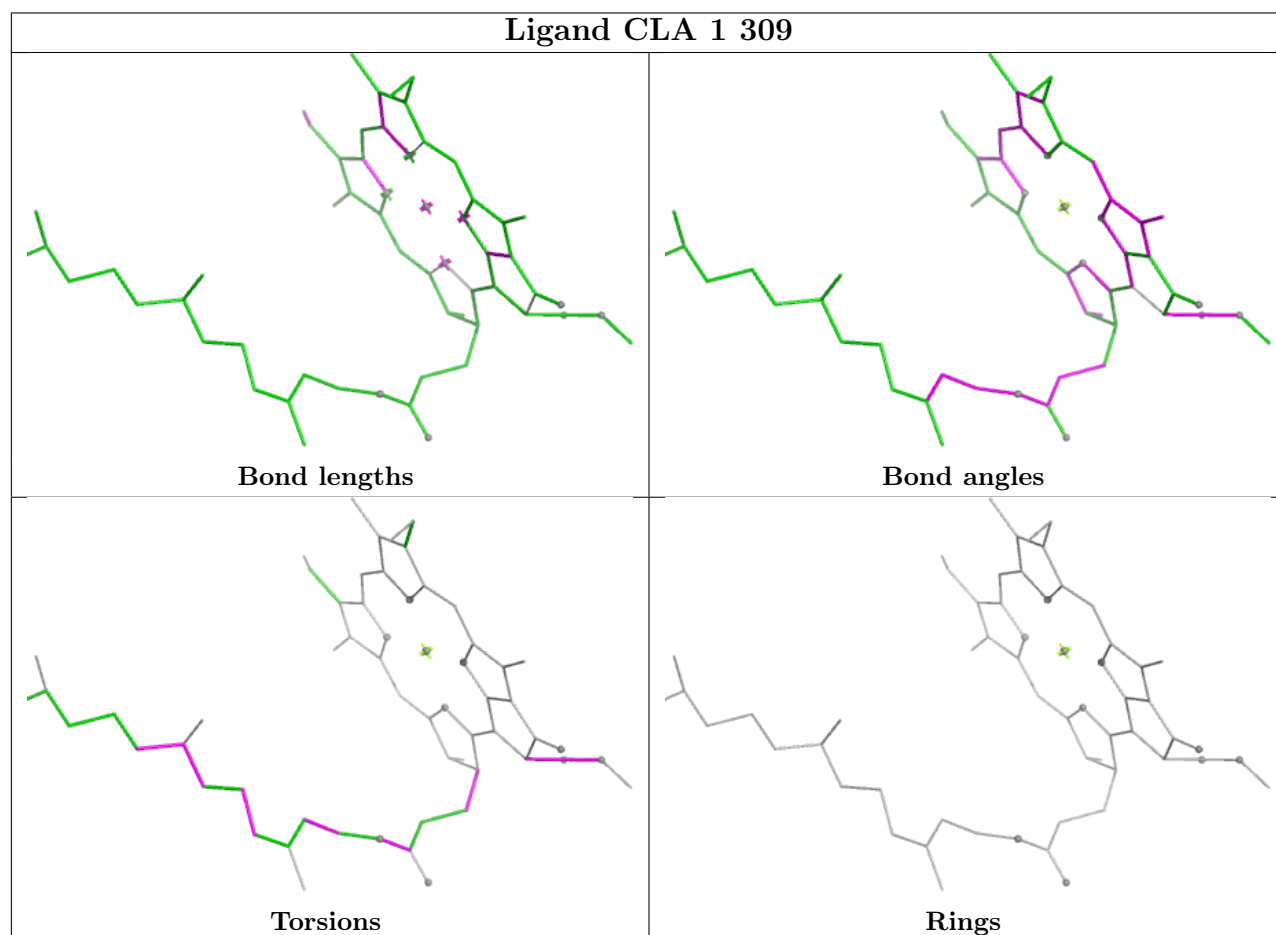
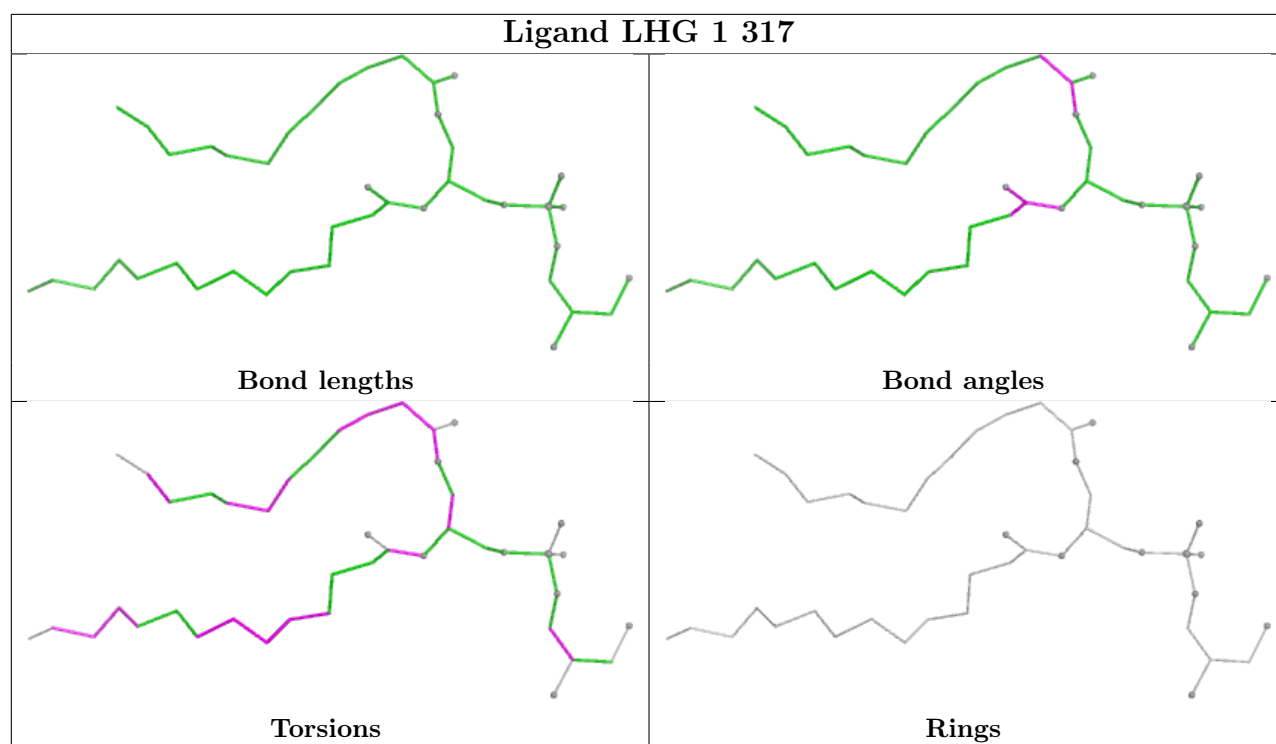


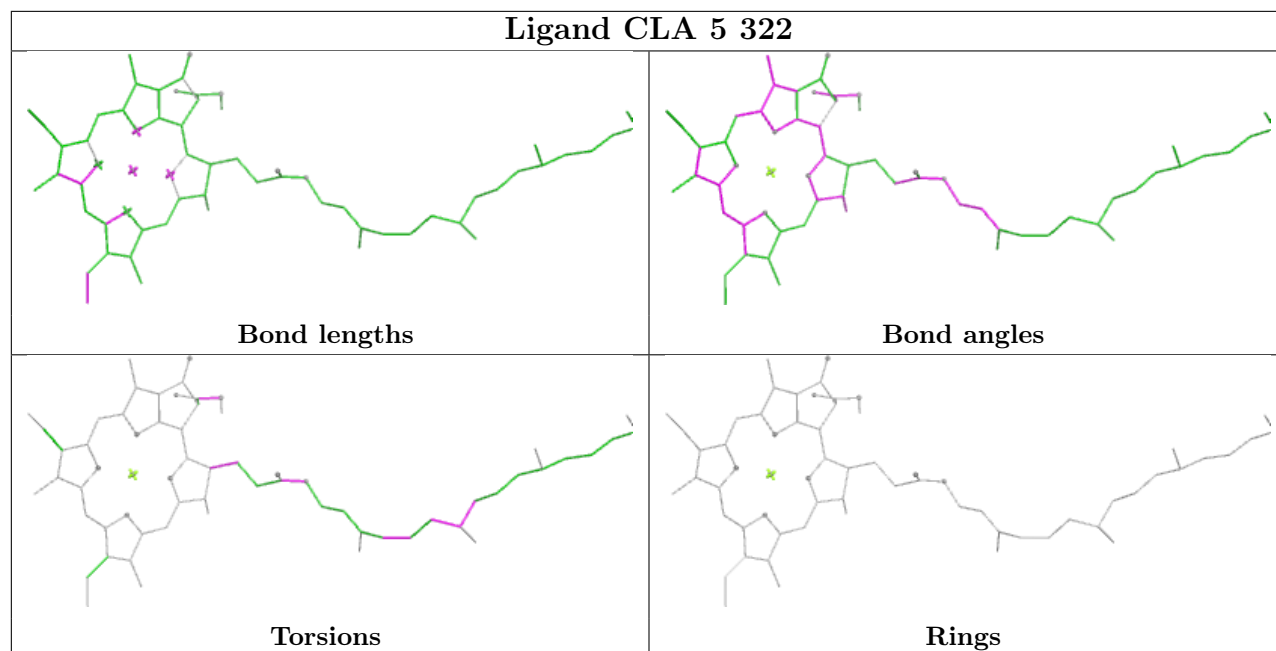
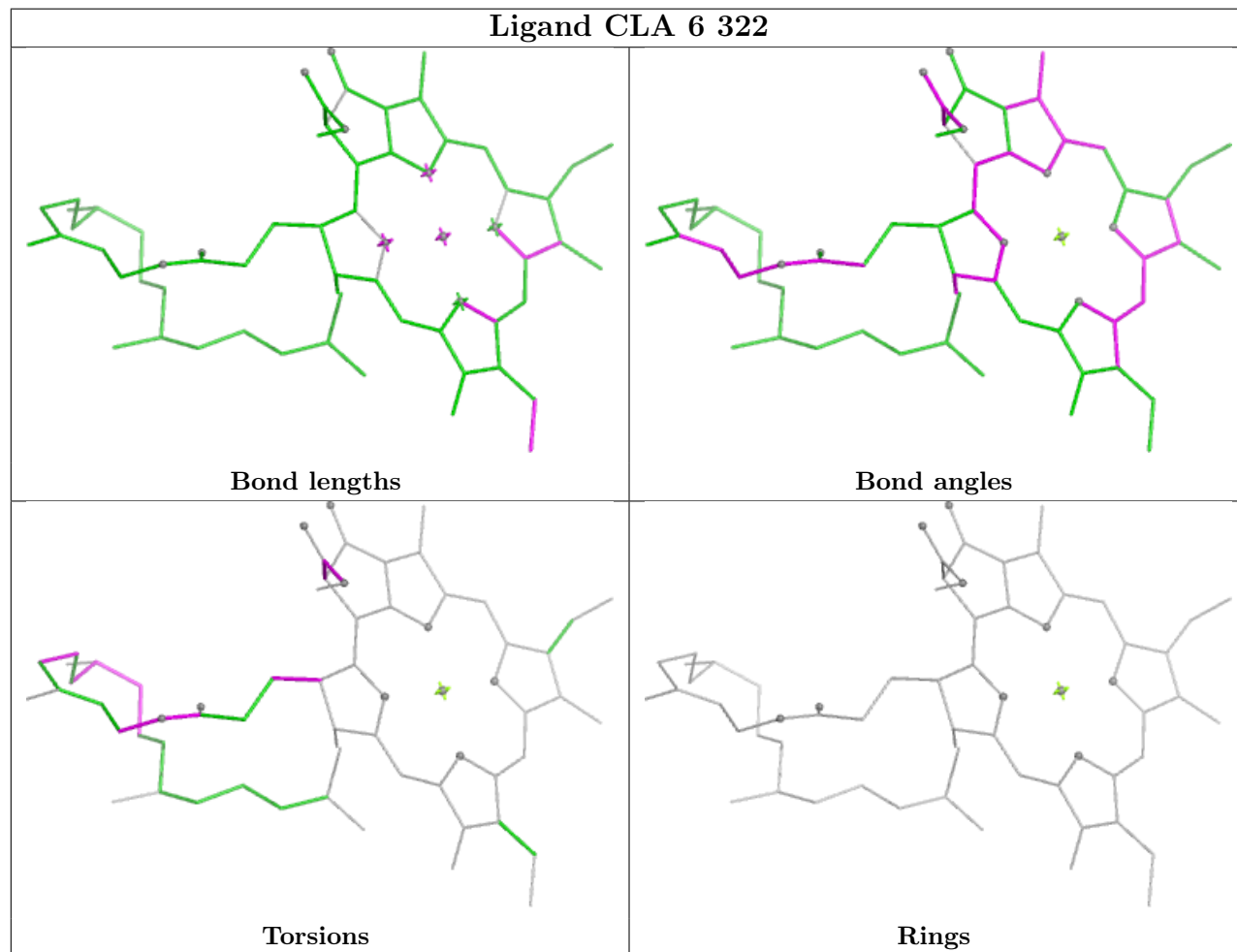
Torsions

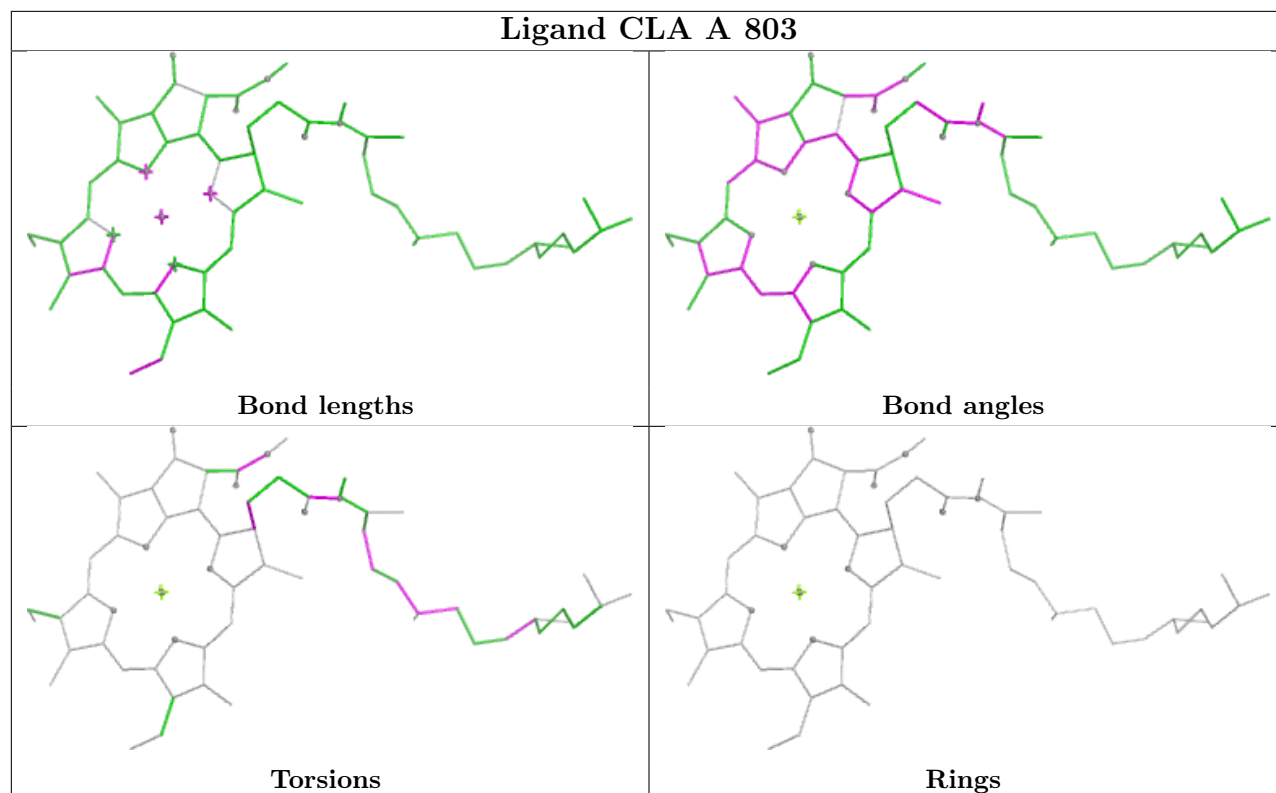
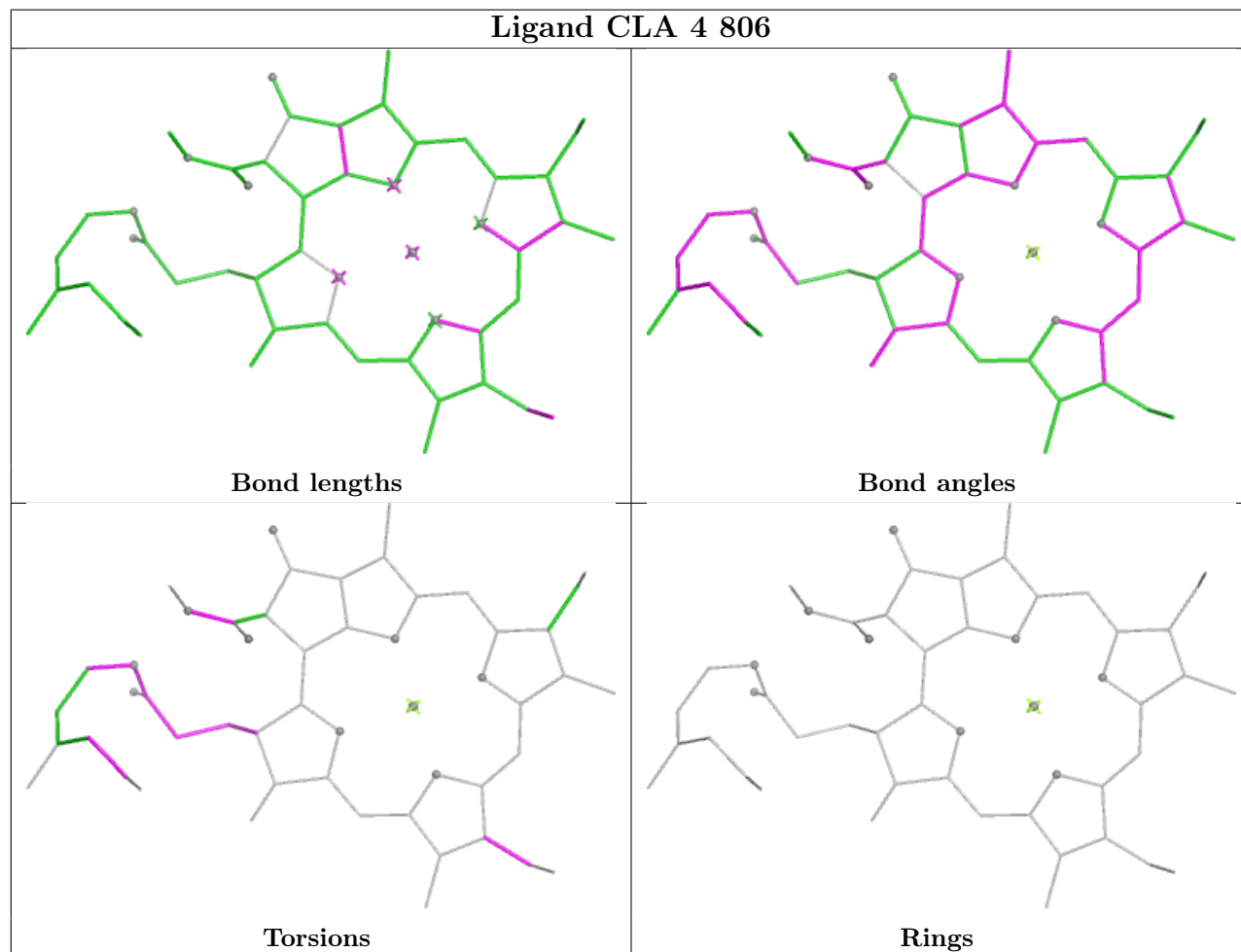


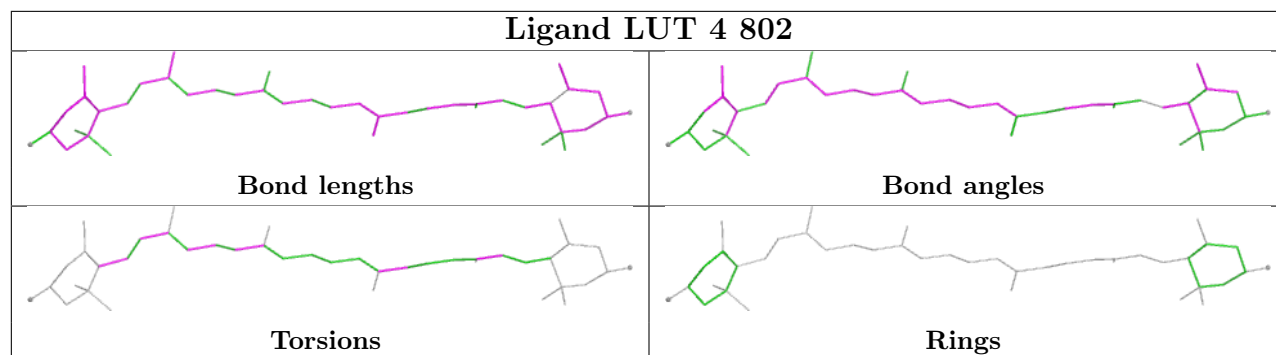
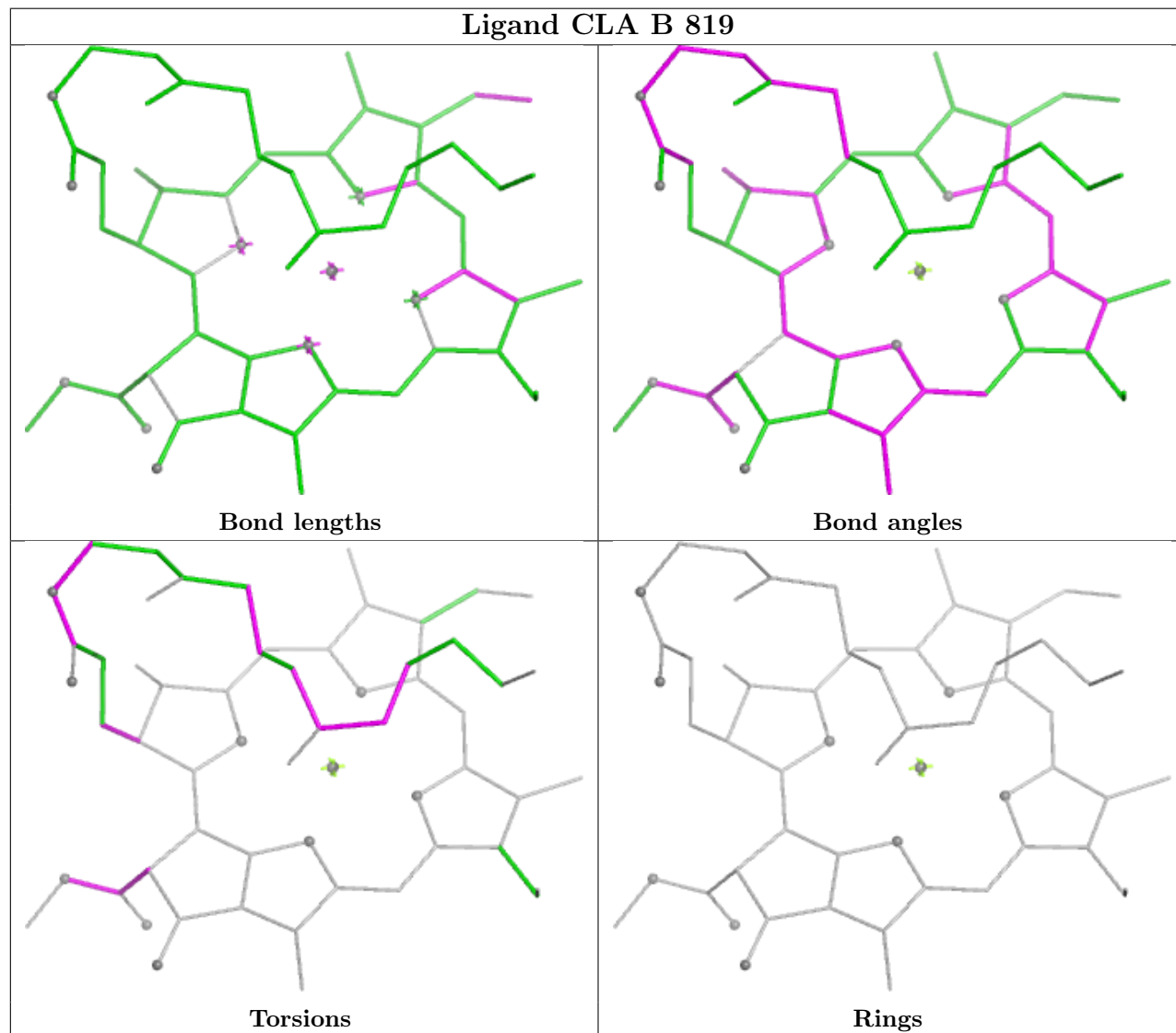
Rings

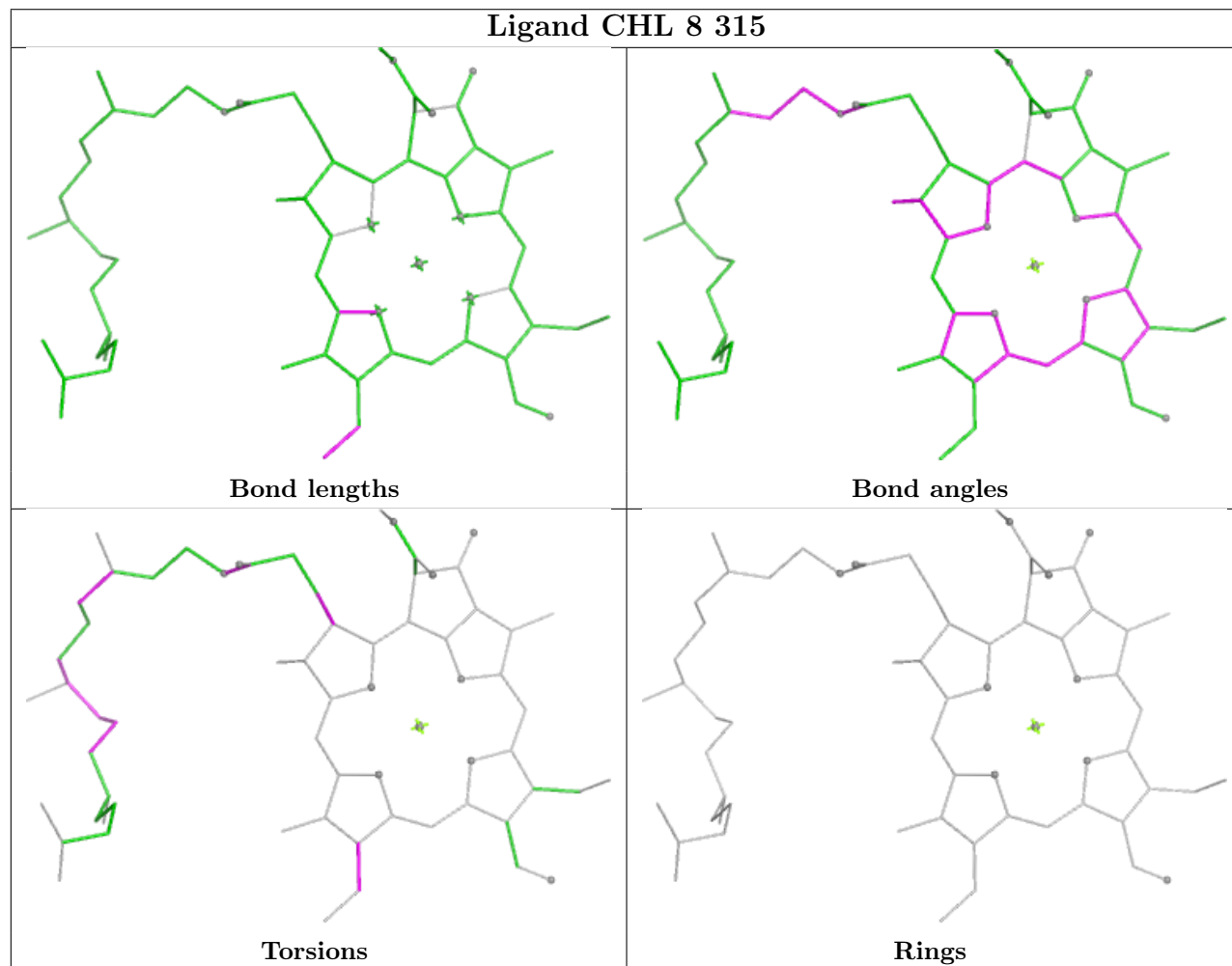
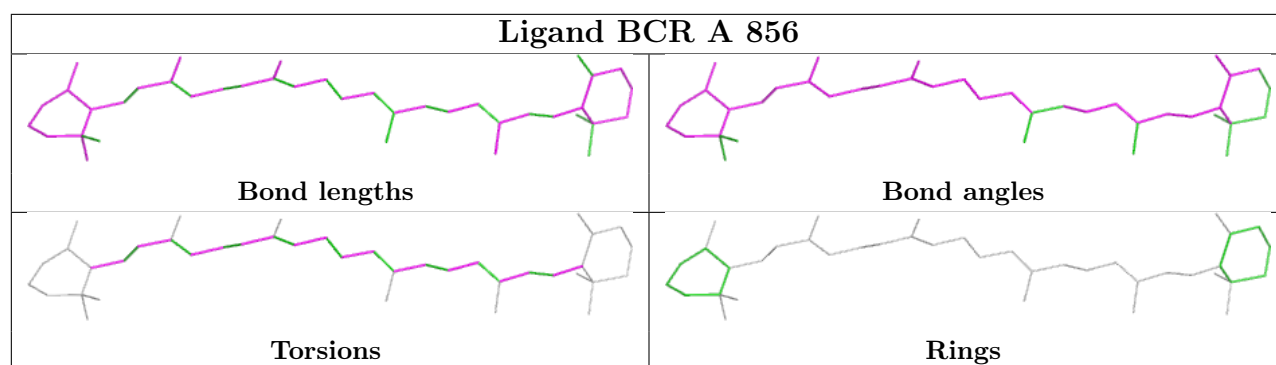




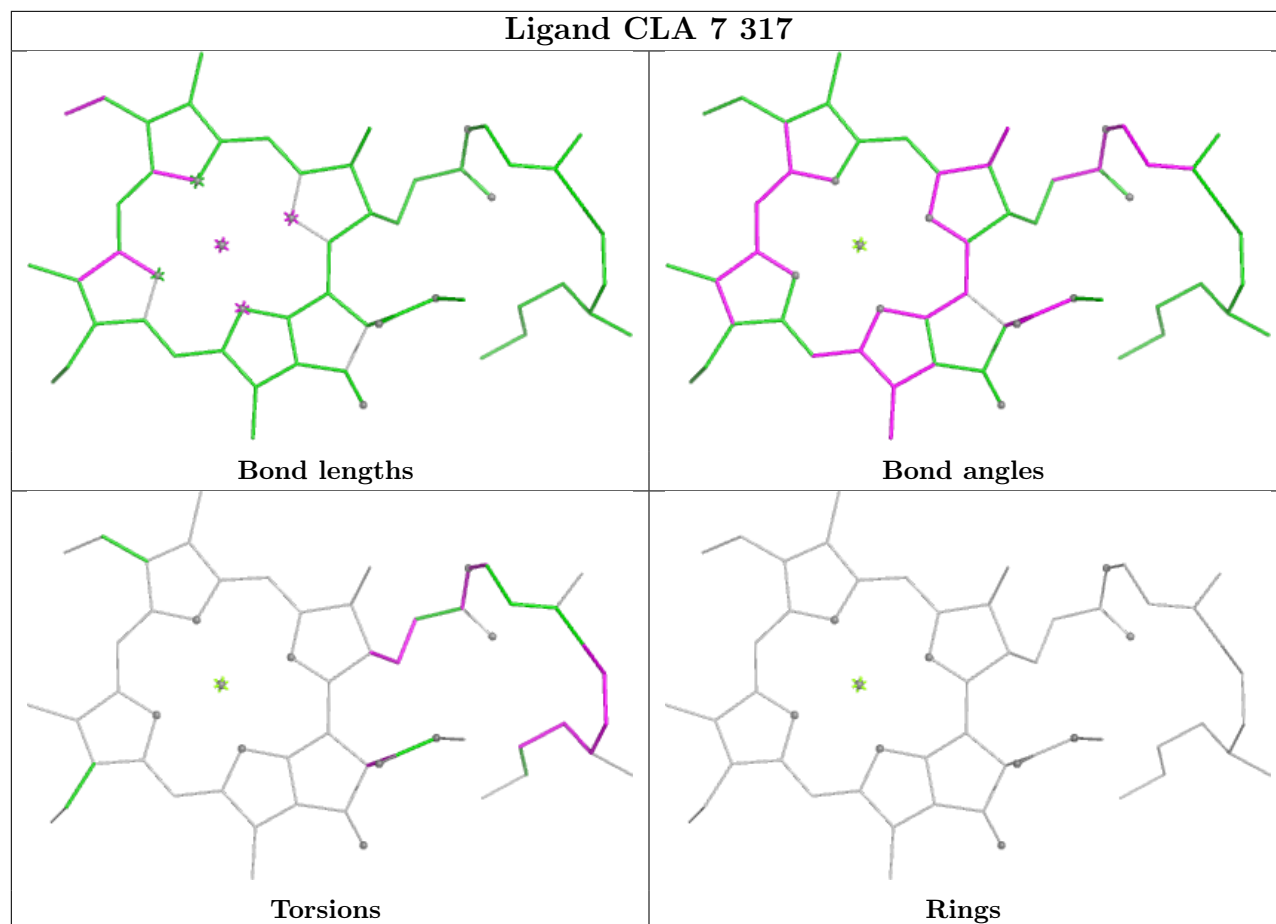
Ligand CLA 5 322**Ligand CLA 6 322**

Ligand CLA A 803**Ligand CLA 4 806**

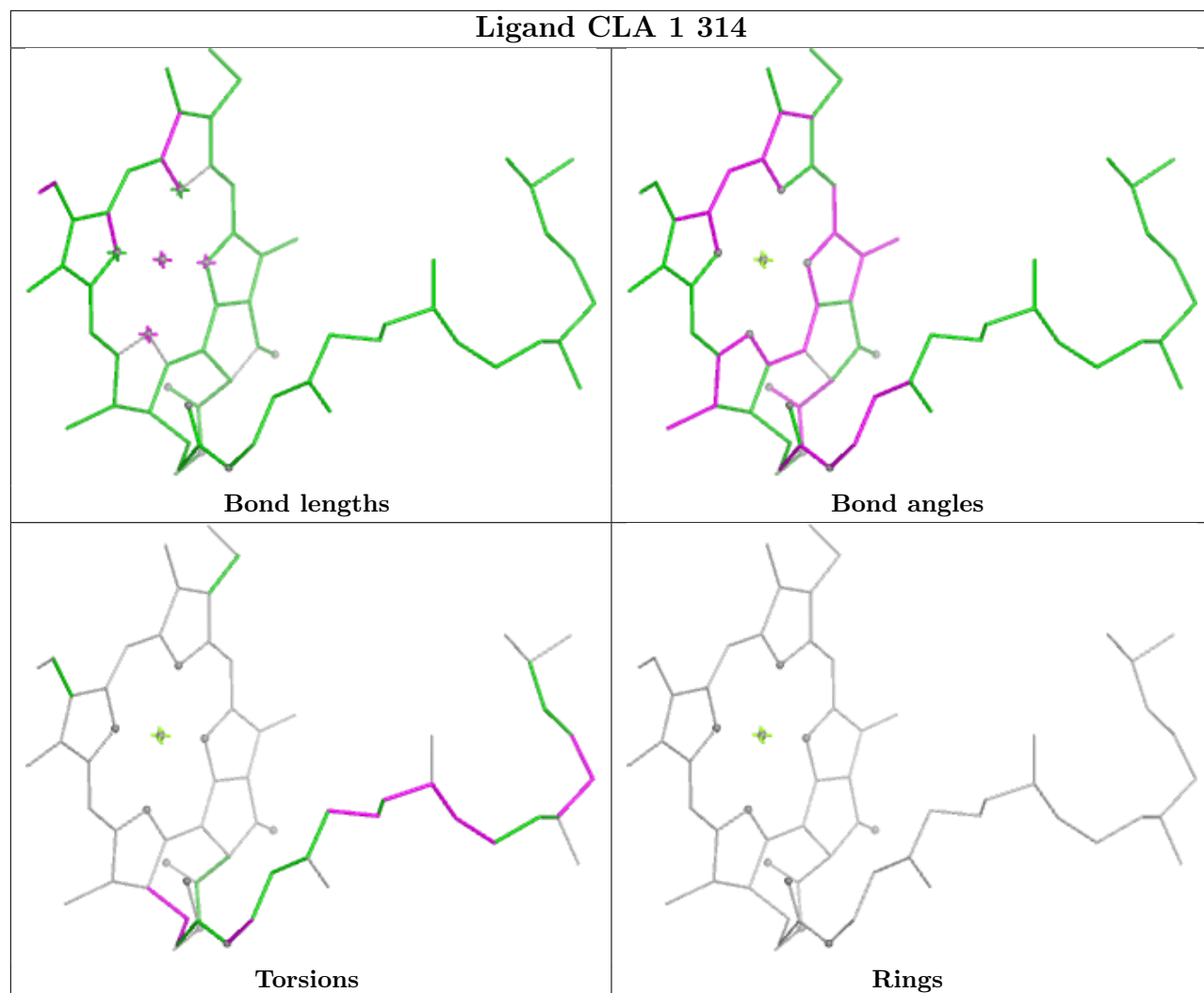
Ligand LUT 4 802**Ligand CLA B 819**

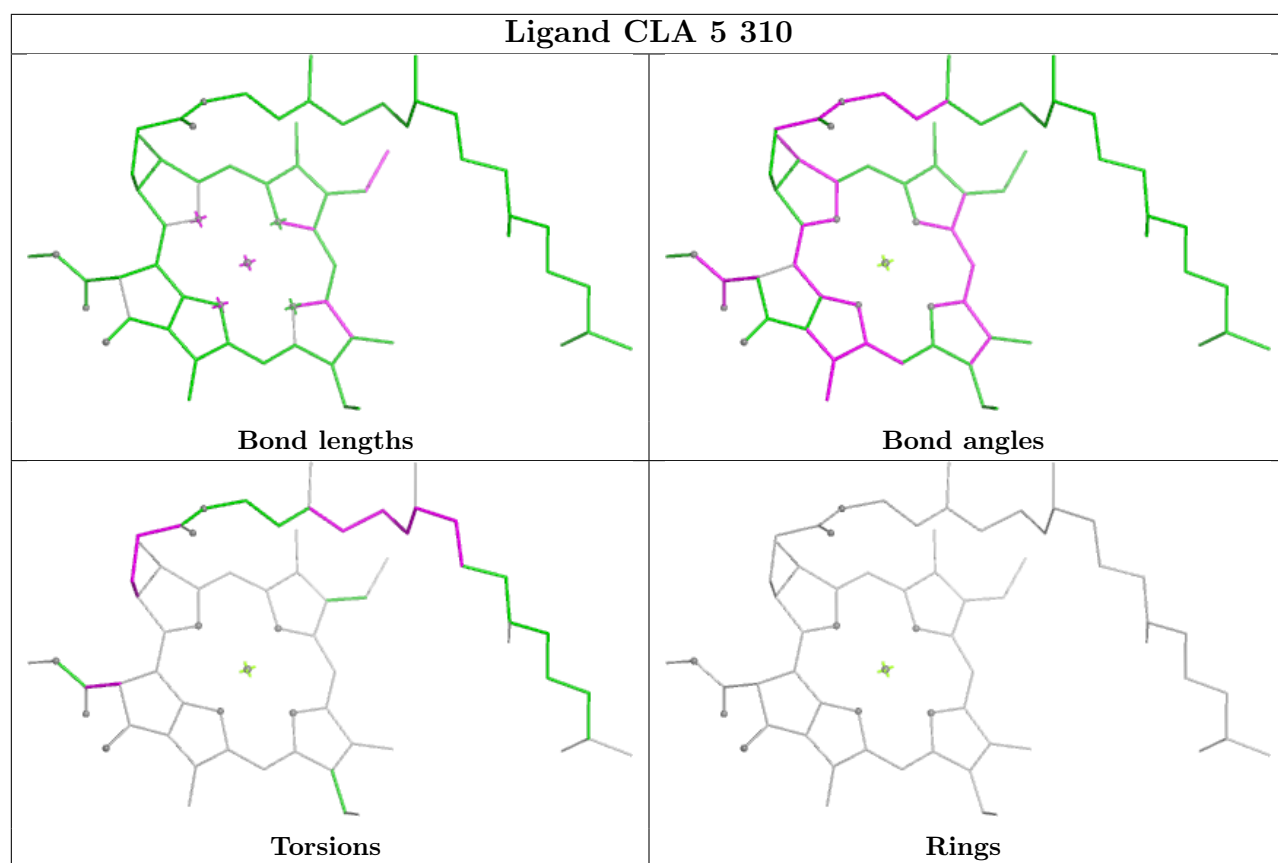


Ligand CLA 7 317

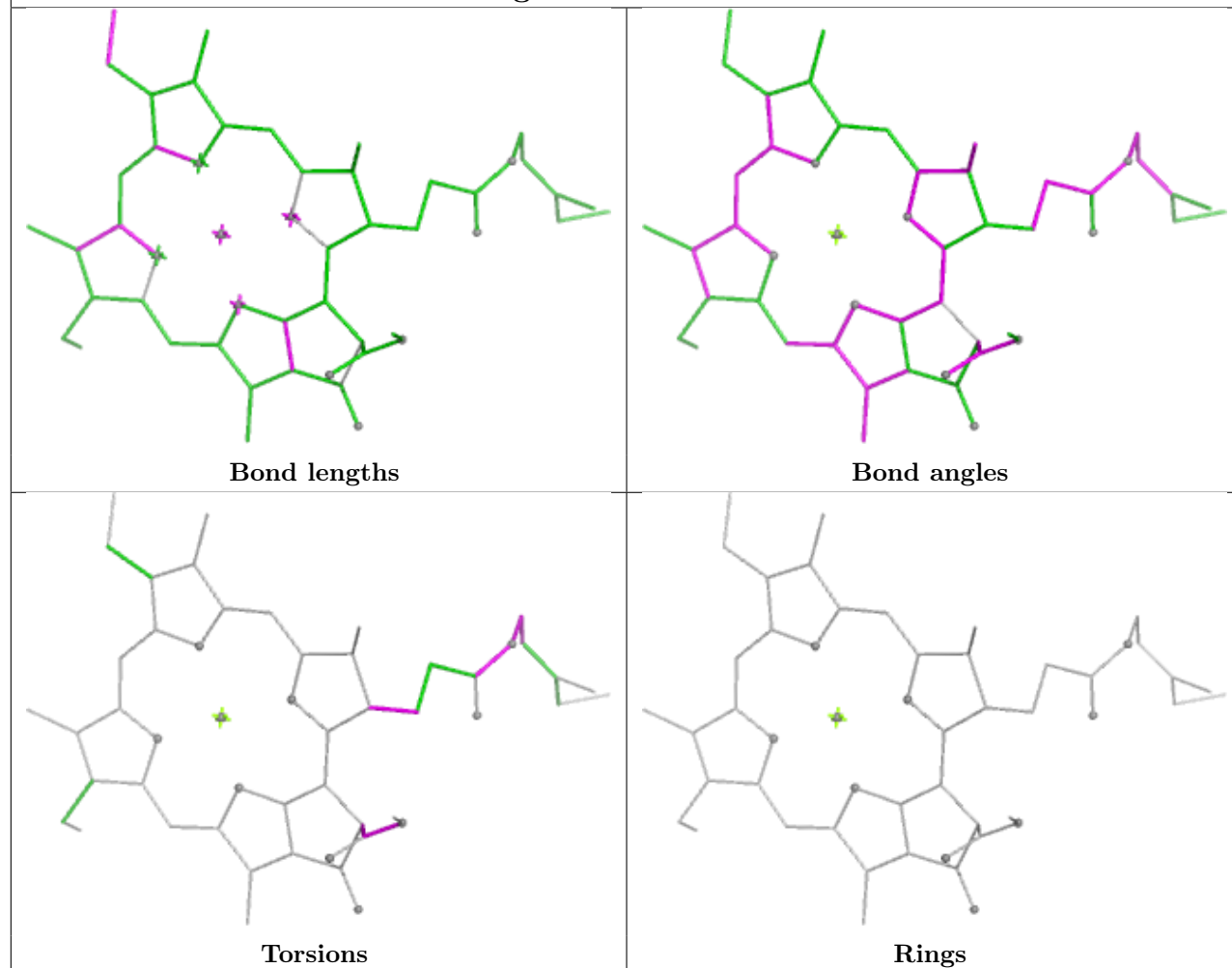


Ligand CLA 1 314

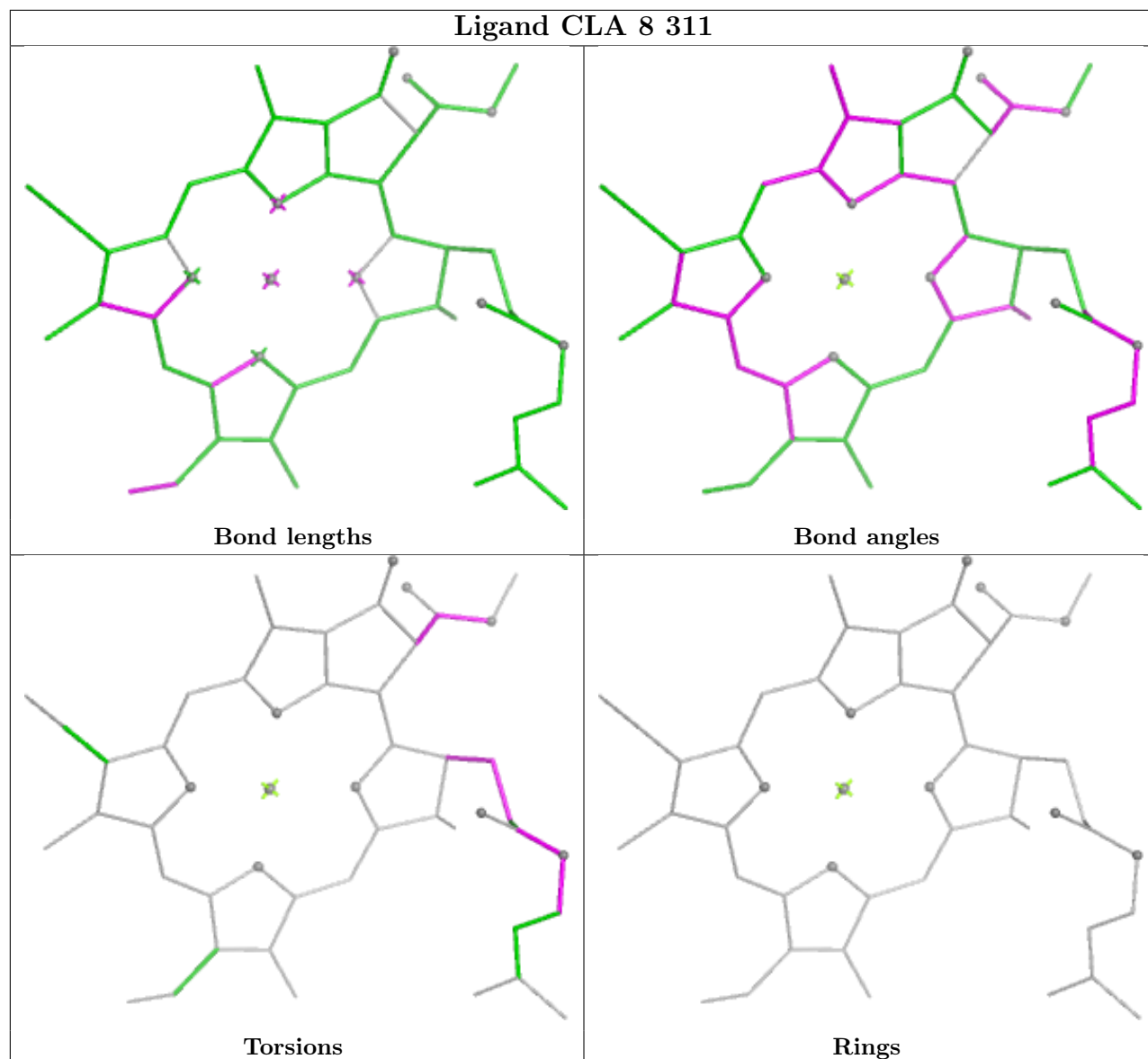




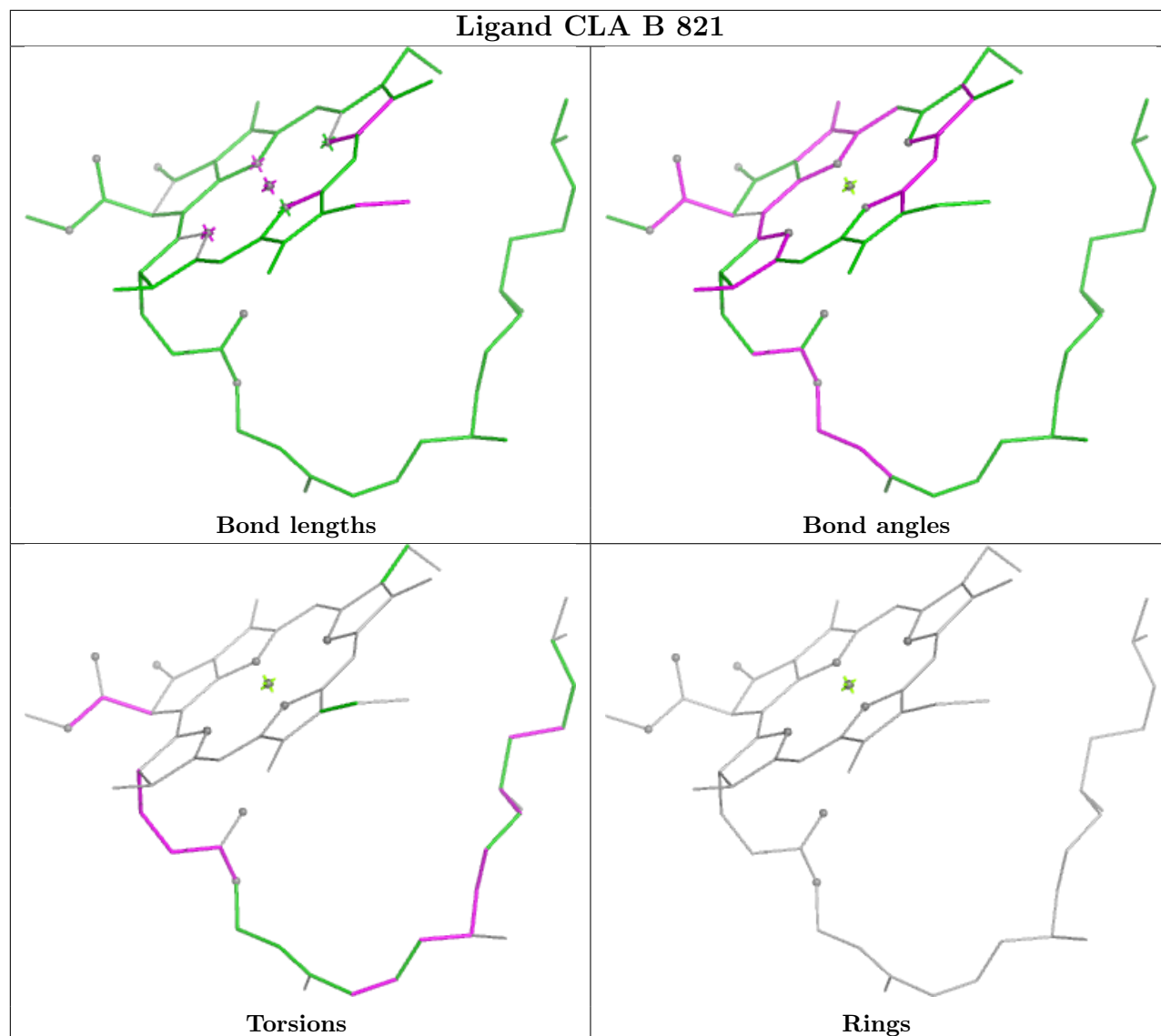
Ligand CLA A 839



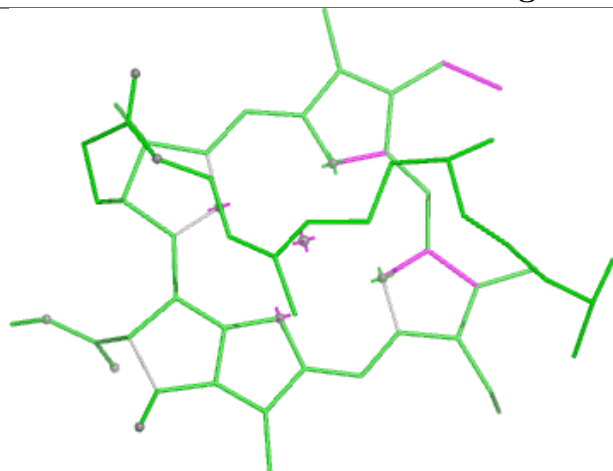
Ligand CLA 8 311



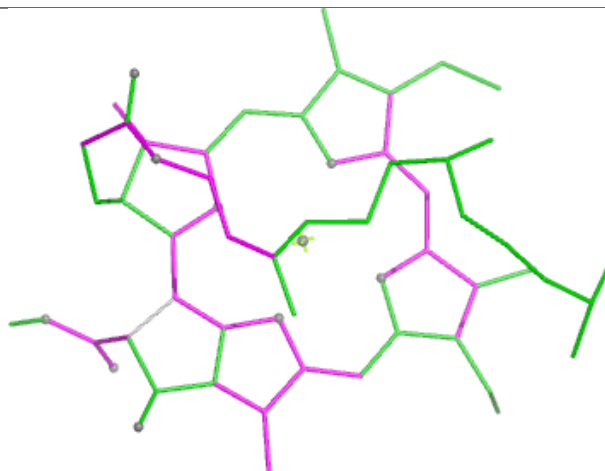
Ligand CLA B 821



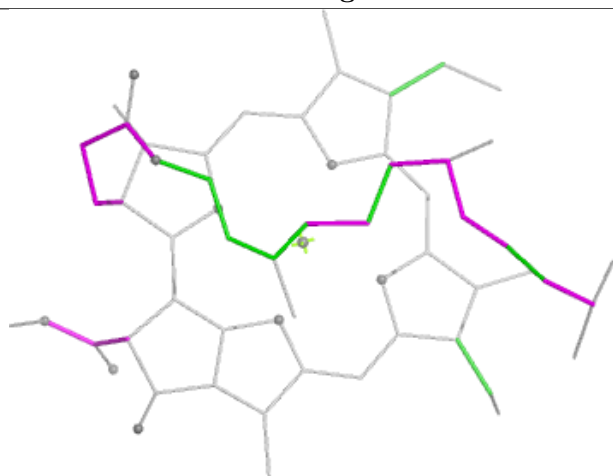
Ligand CLA 7 312



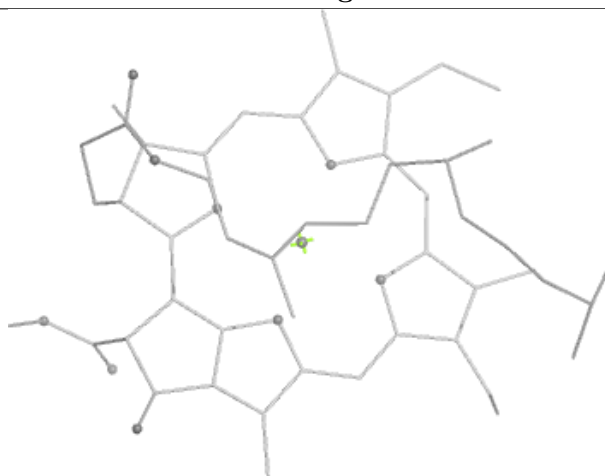
Bond lengths



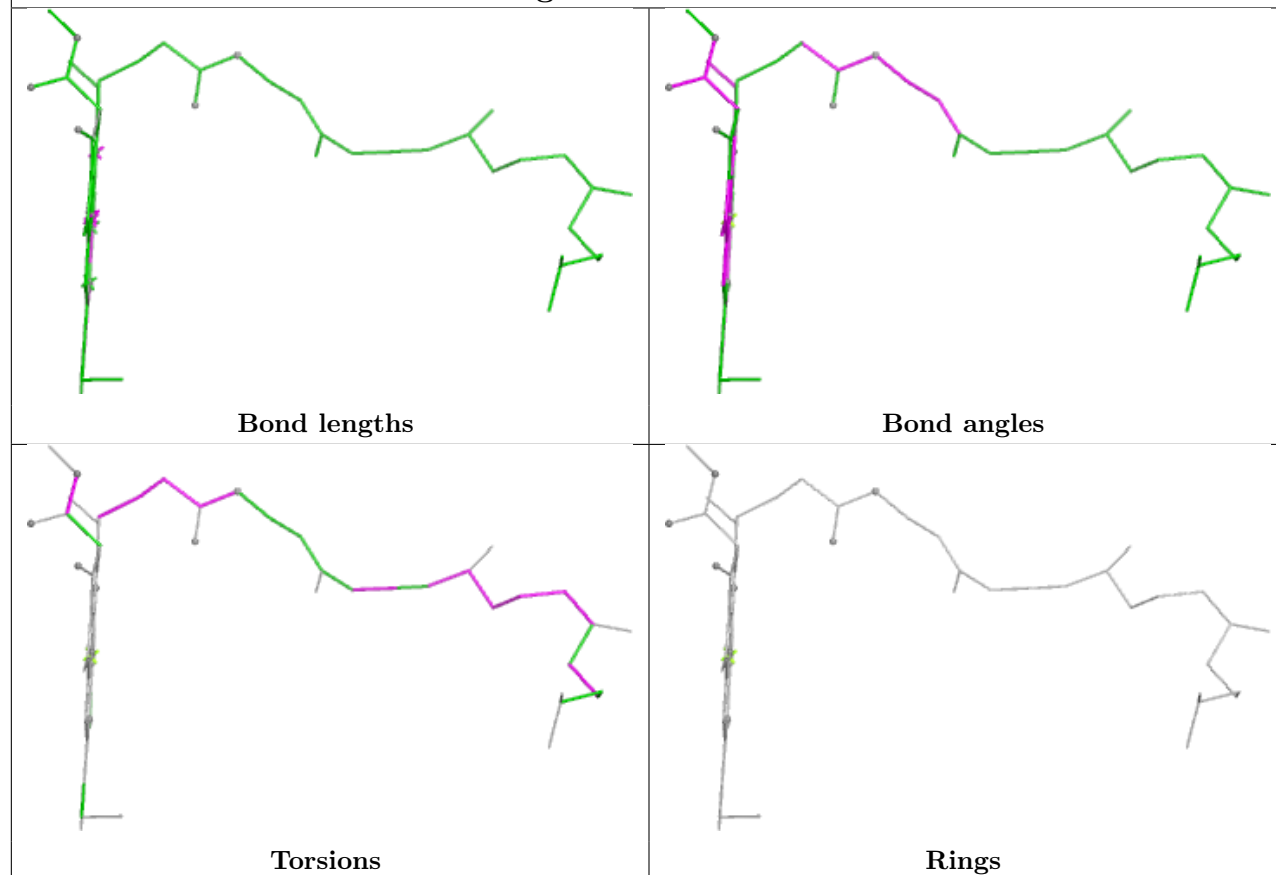
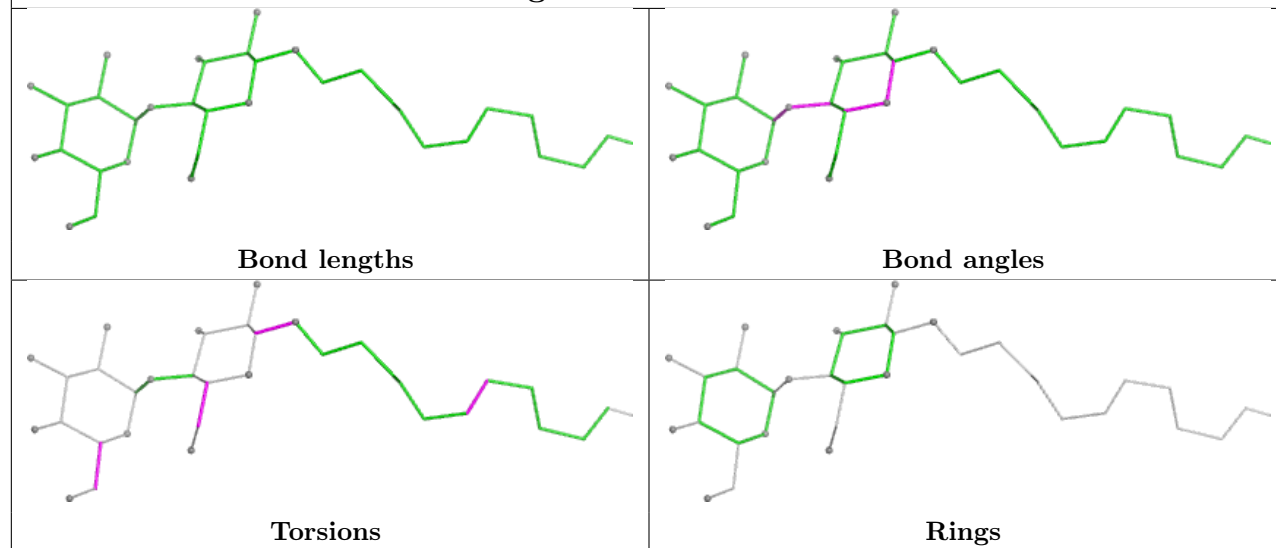
Bond angles

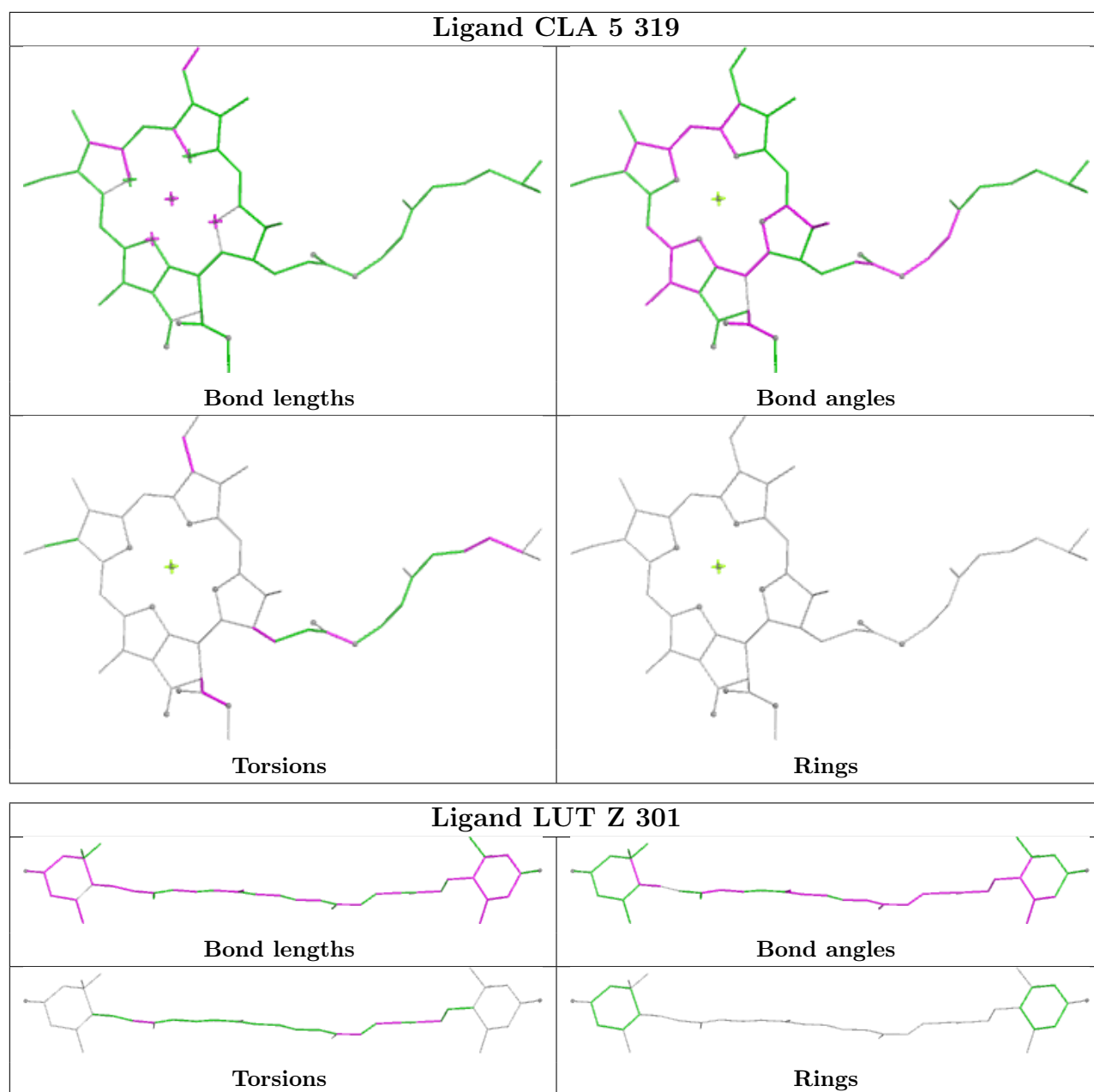


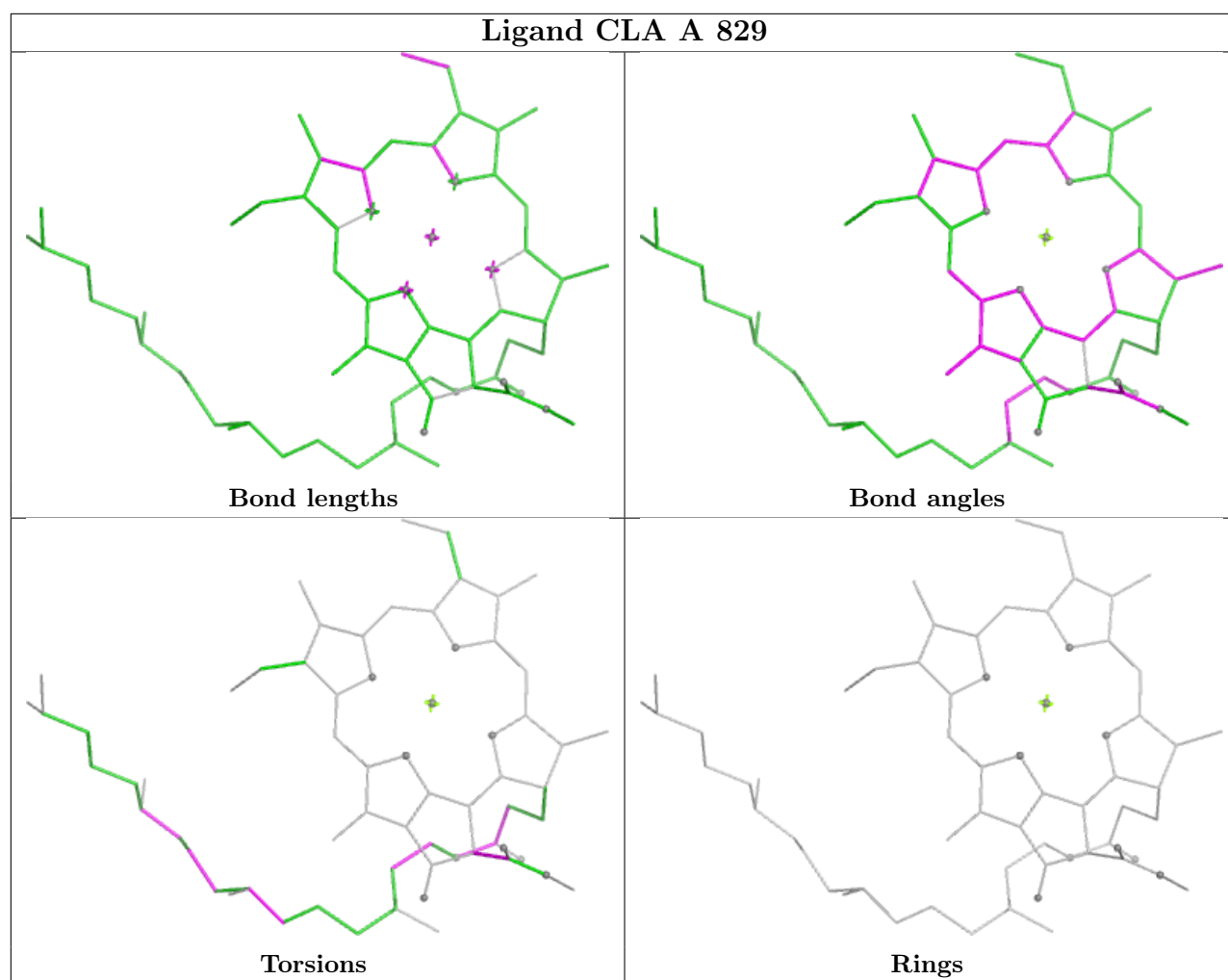
Torsions



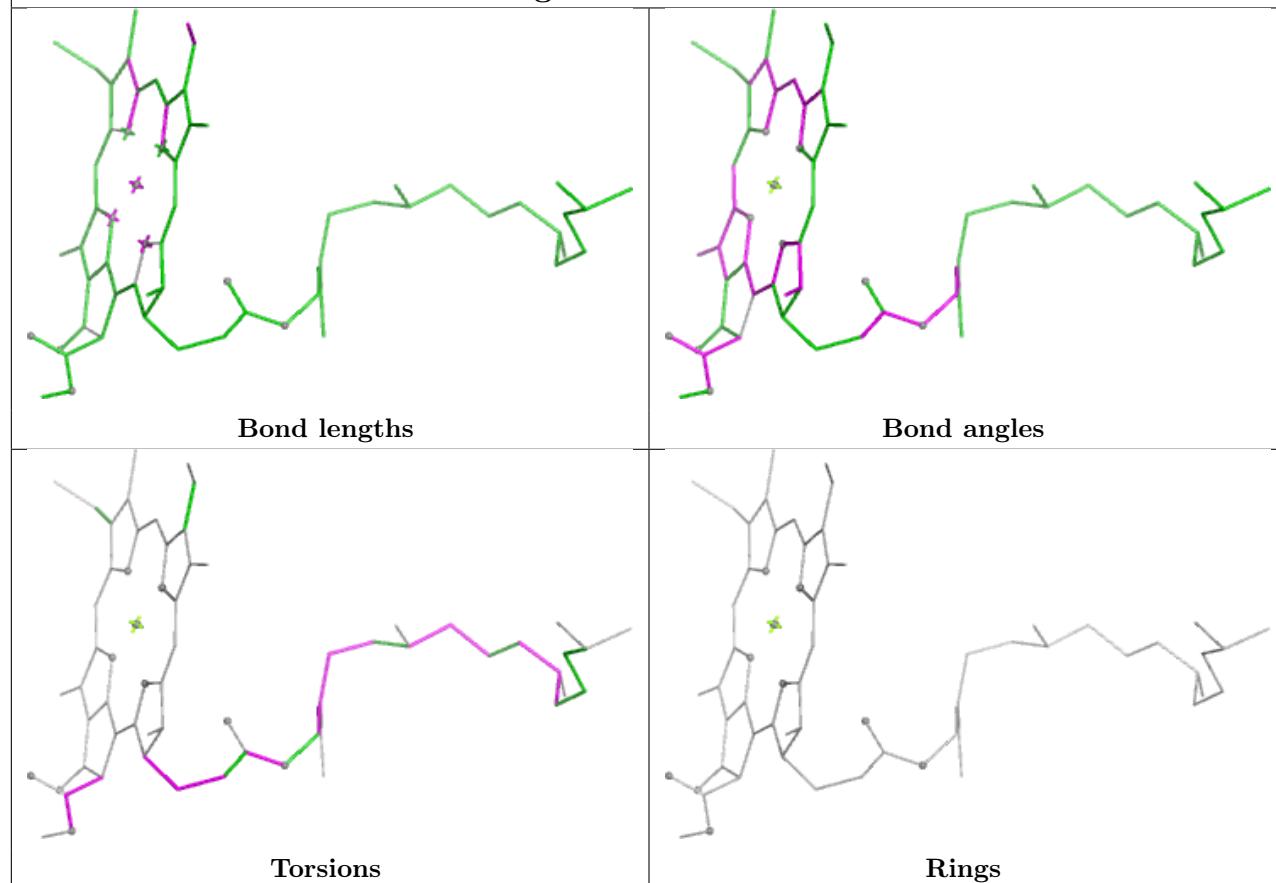
Rings

Ligand CLA 3 313**Ligand LMT G 204**

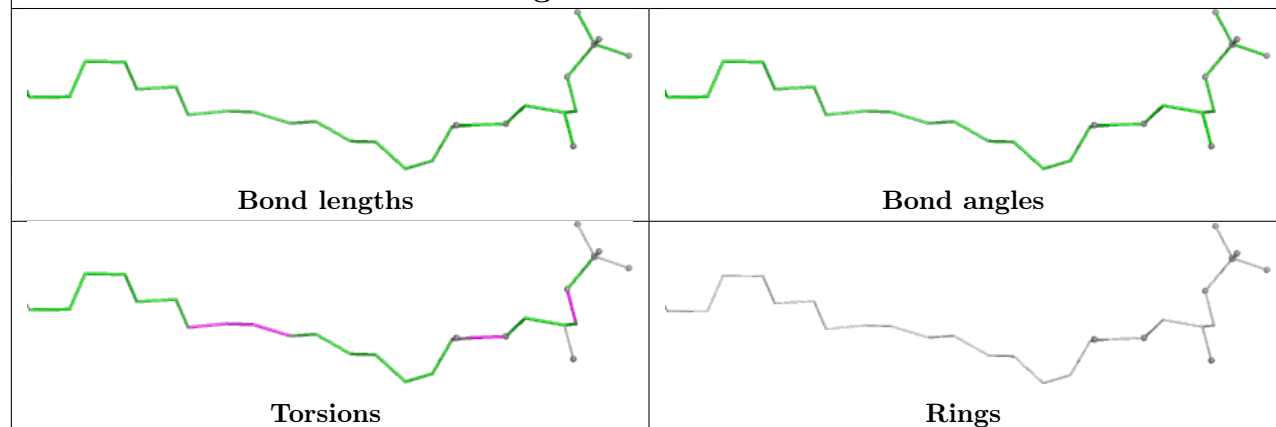


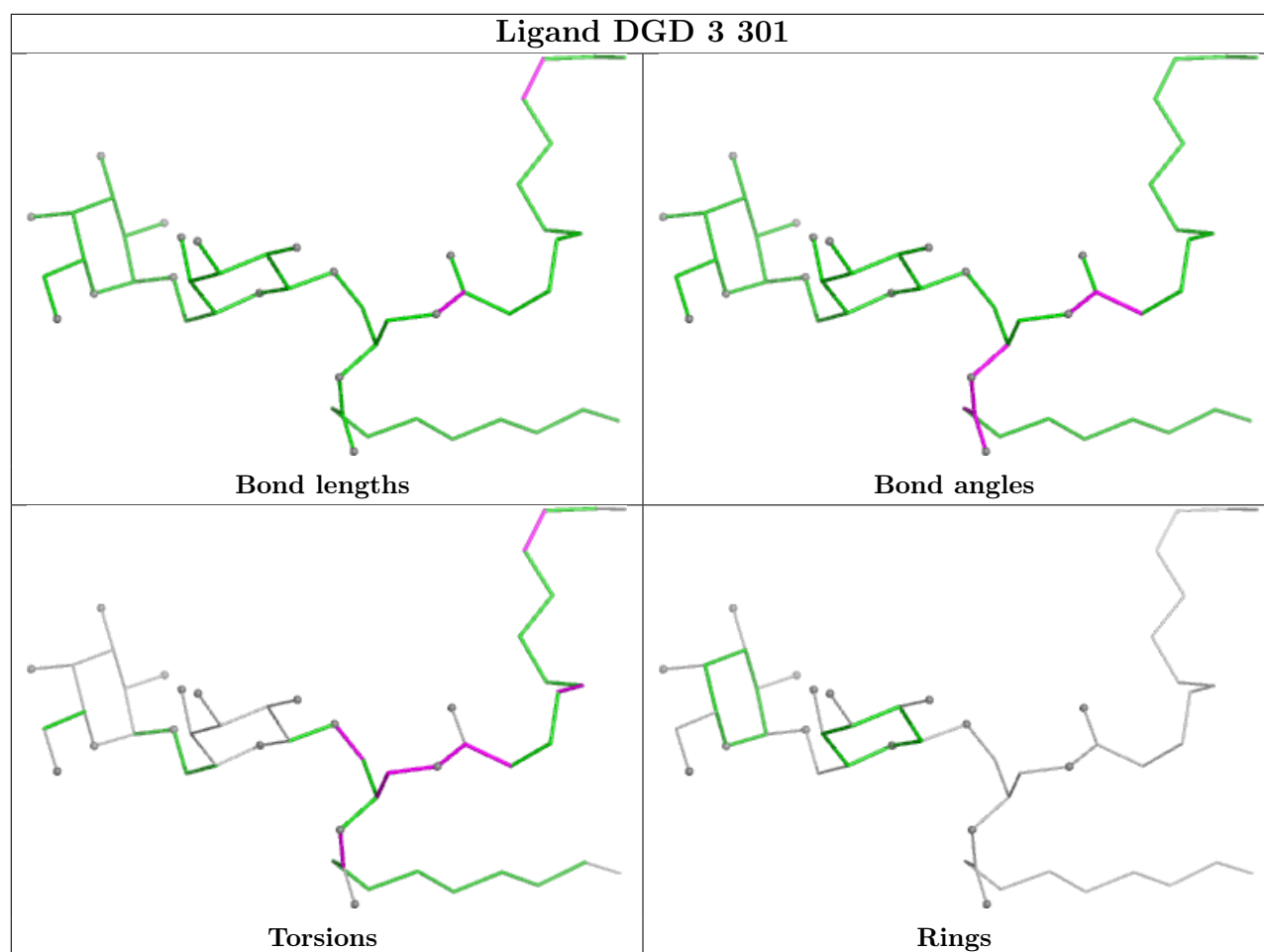


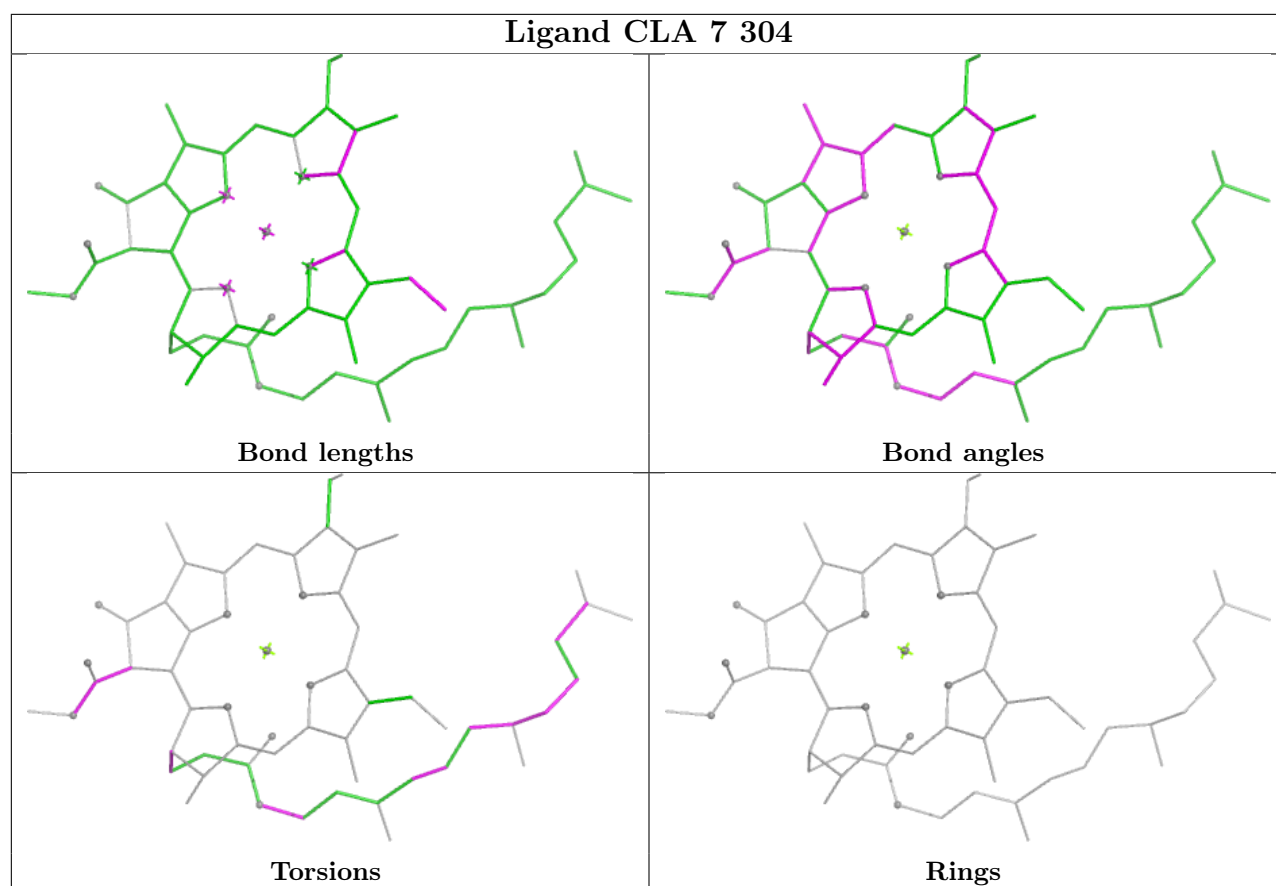
Ligand CLA L 202

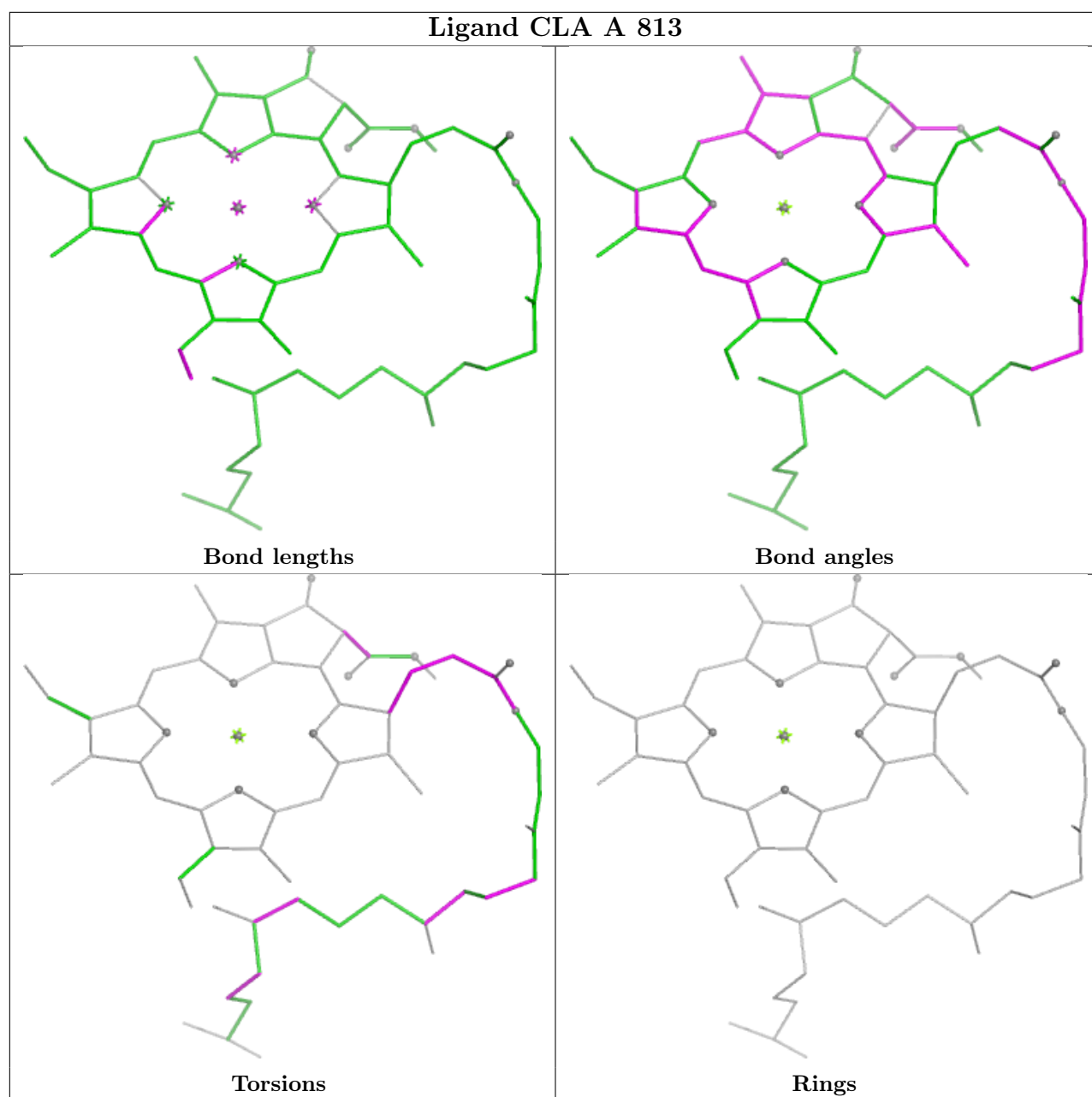


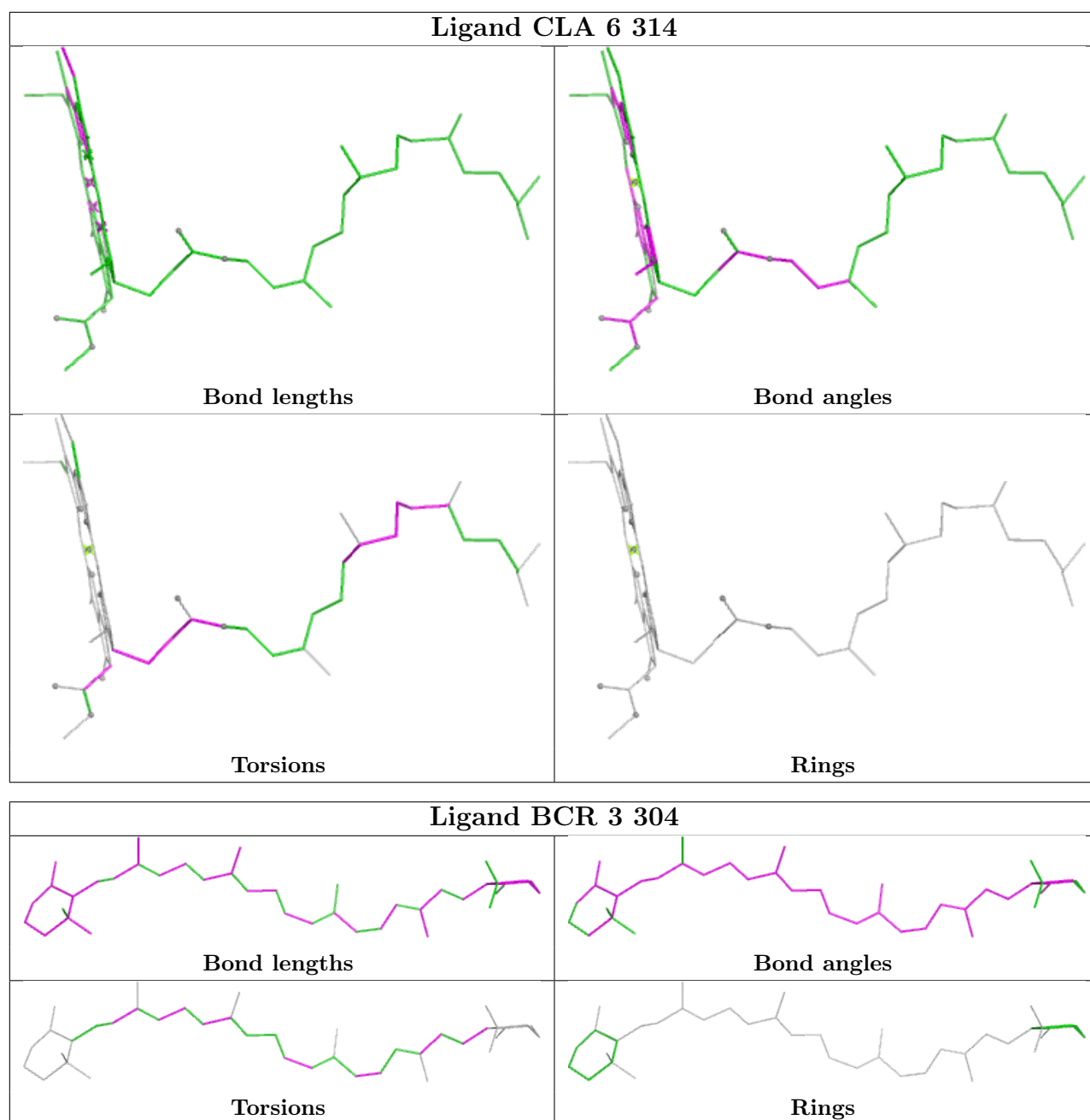
Ligand NKP 8 318

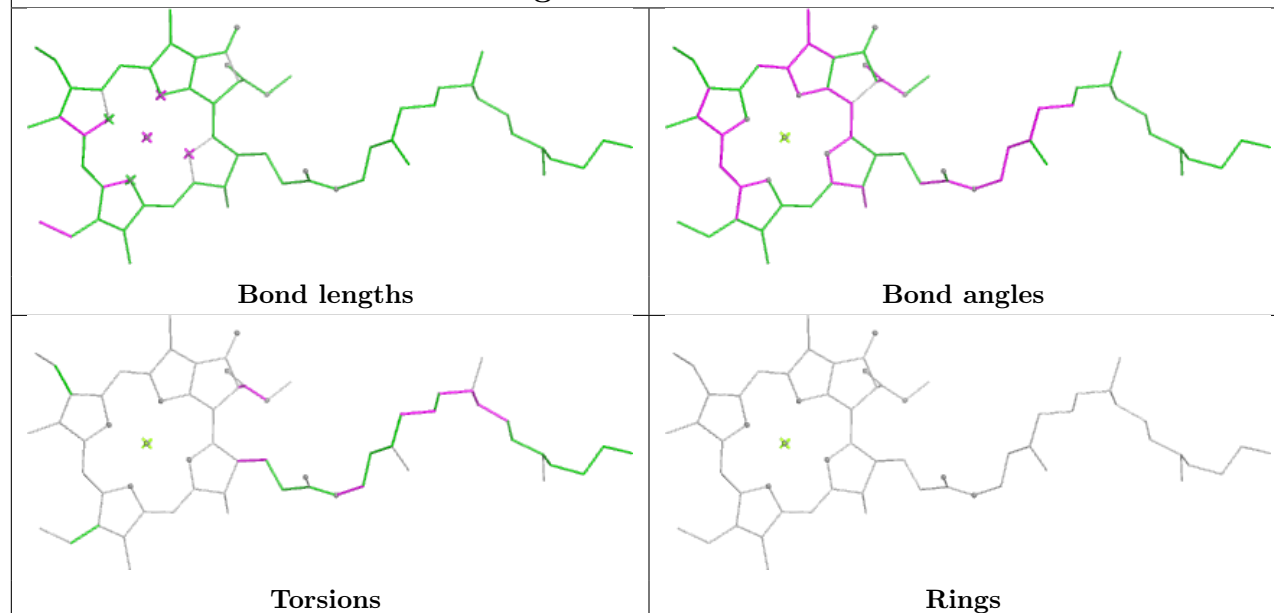
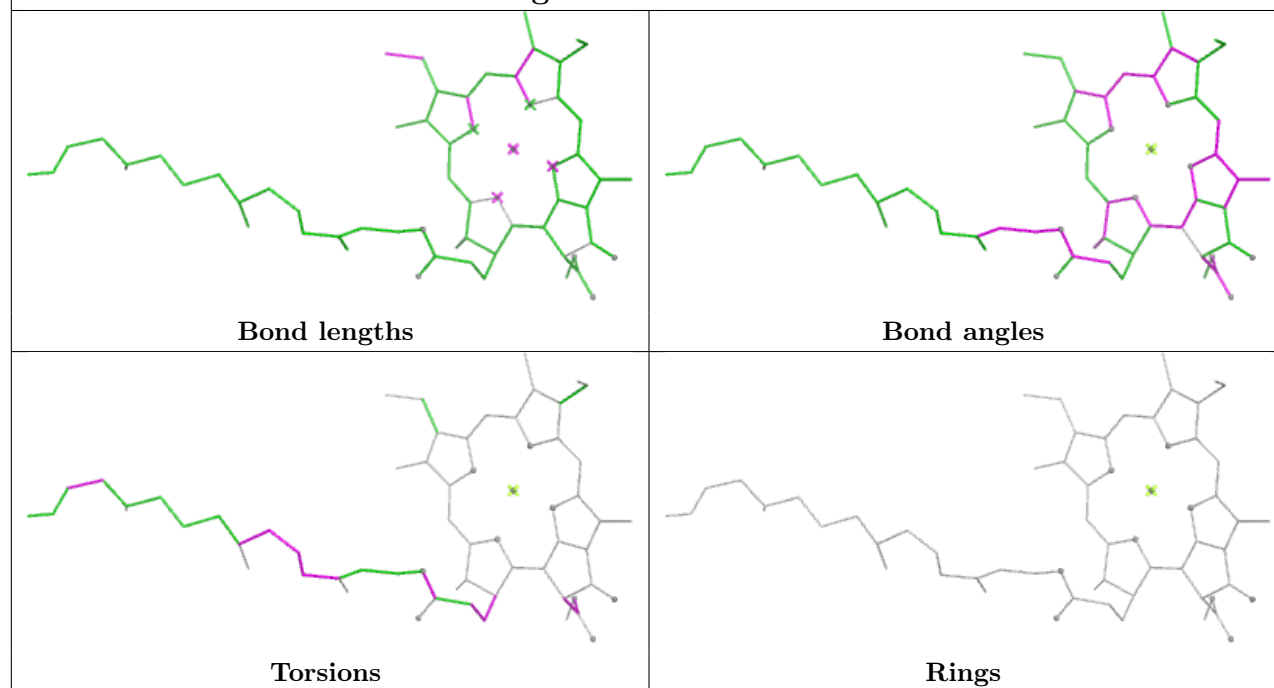


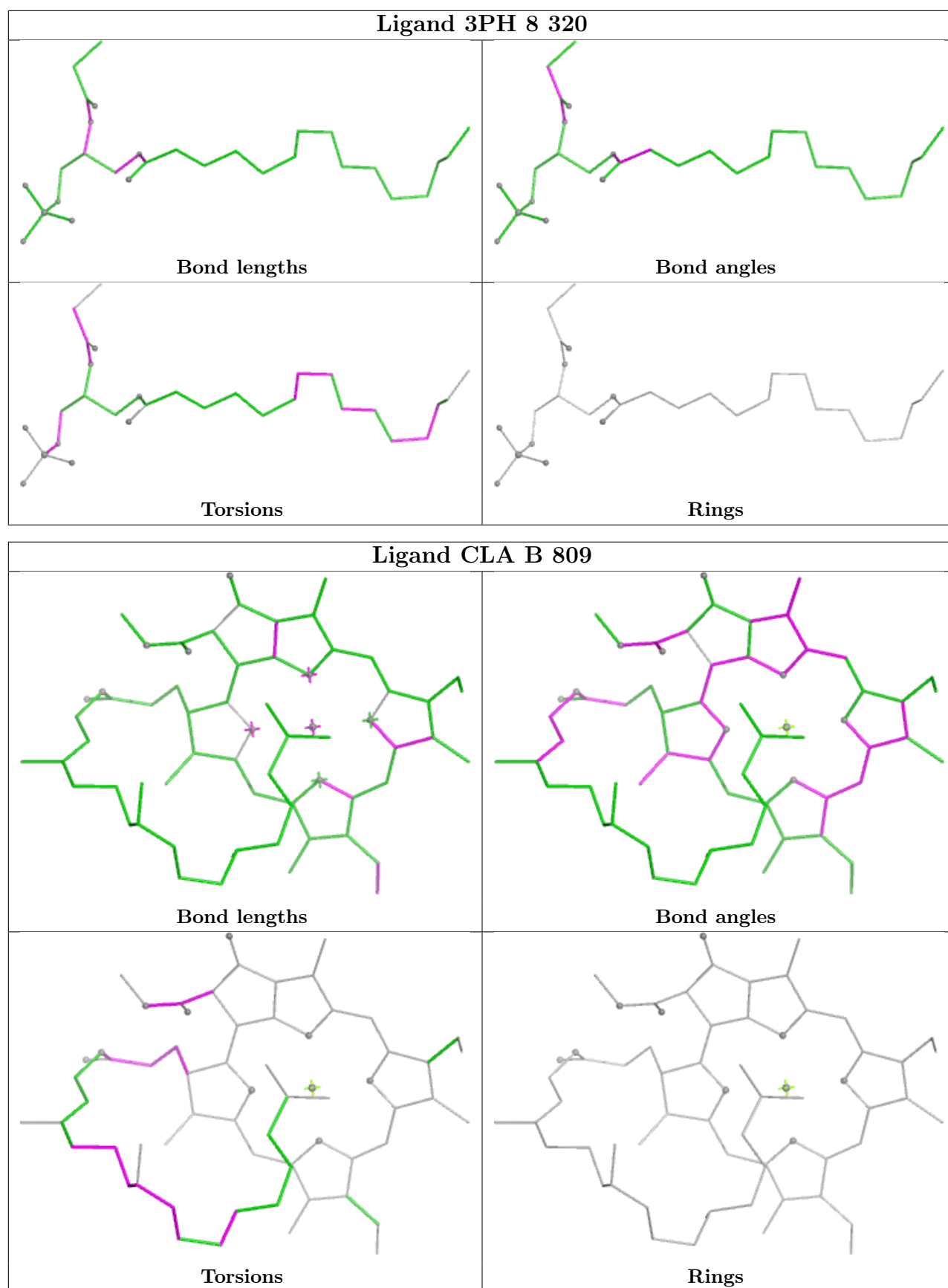




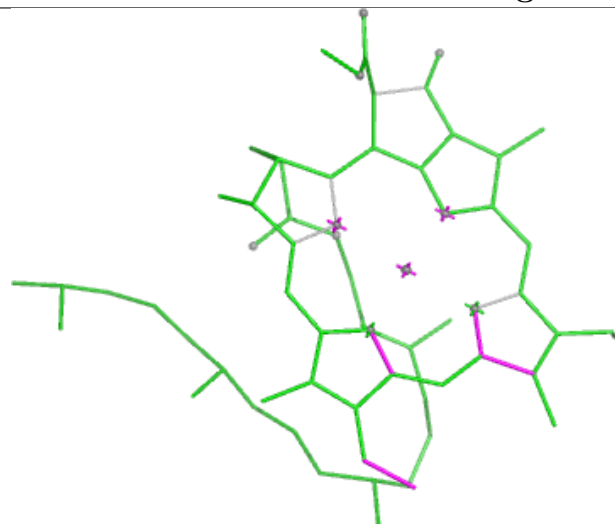




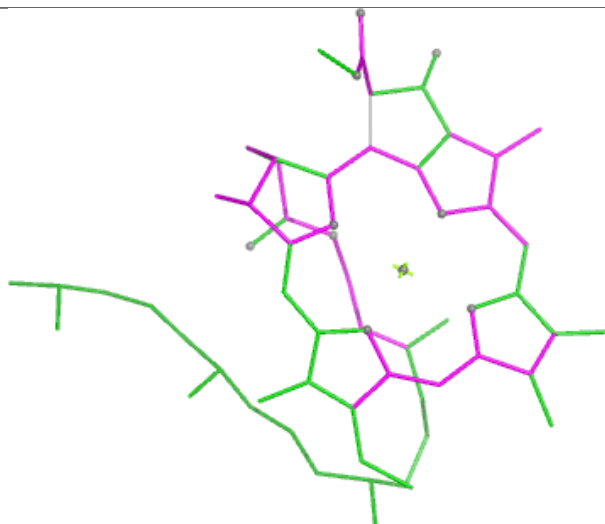
Ligand CLA F 301**Ligand CLA A 834**



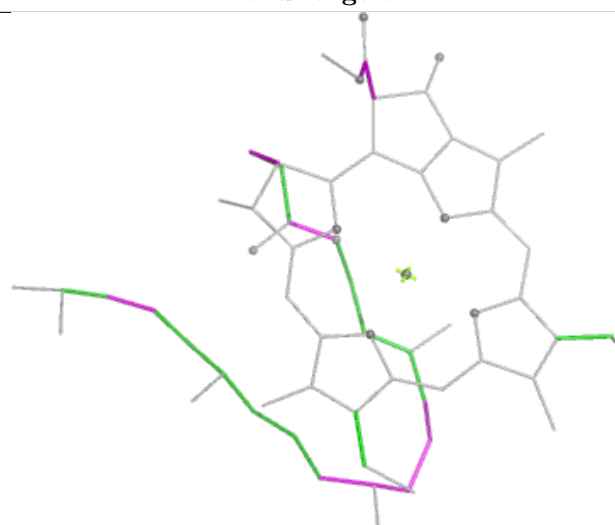
Ligand CLA B 811



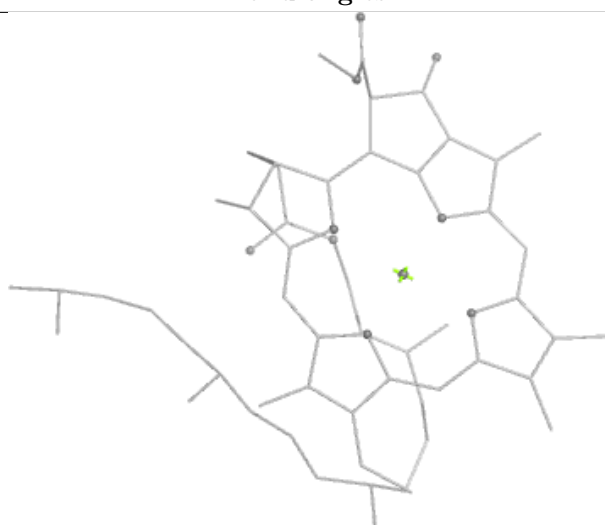
Bond lengths



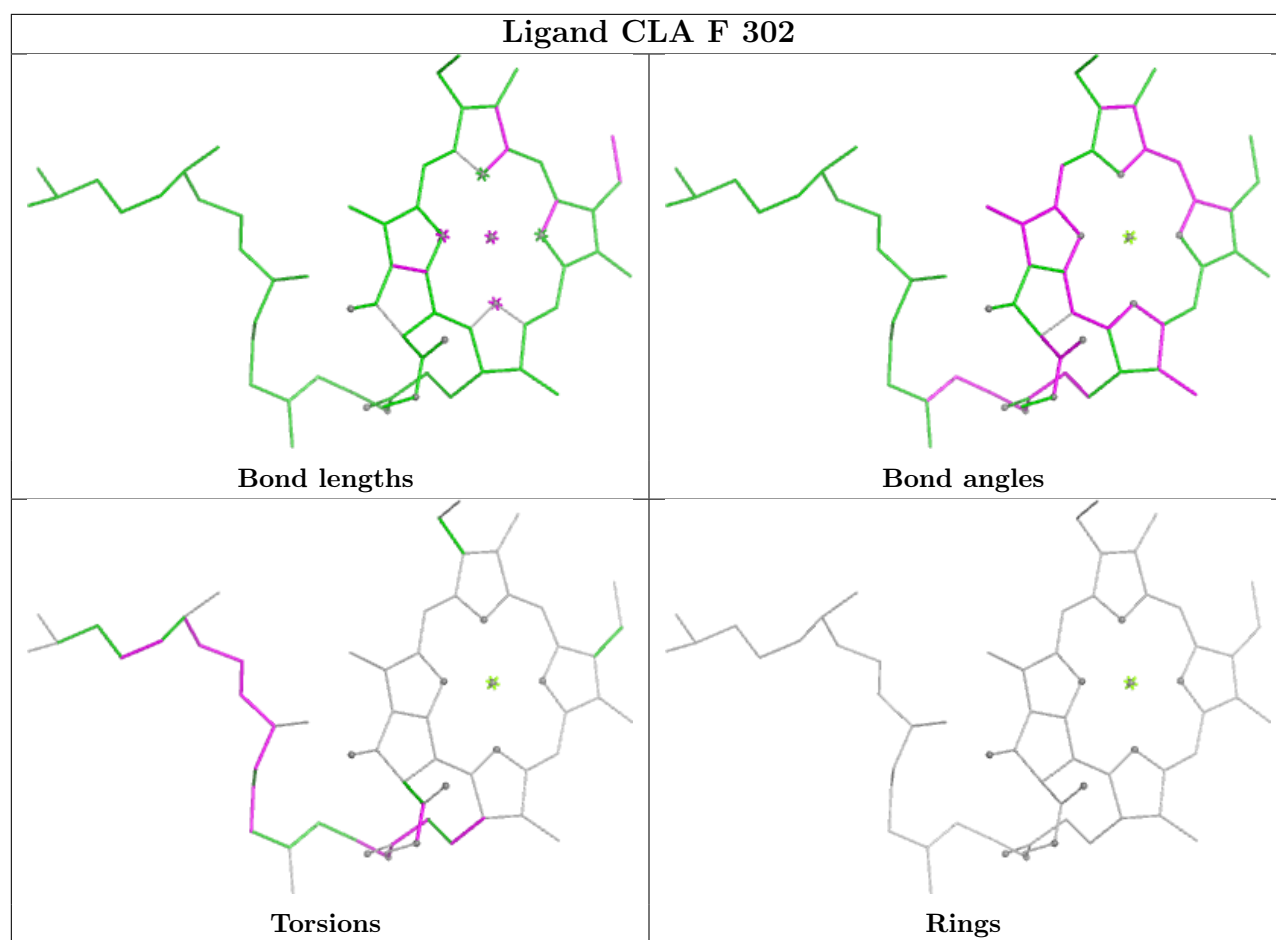
Bond angles



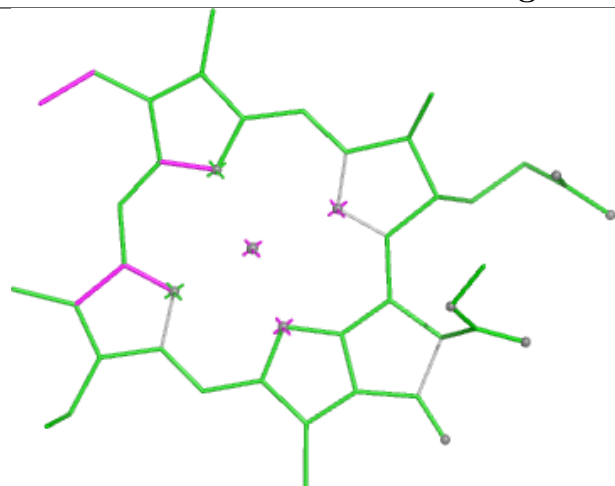
Torsions



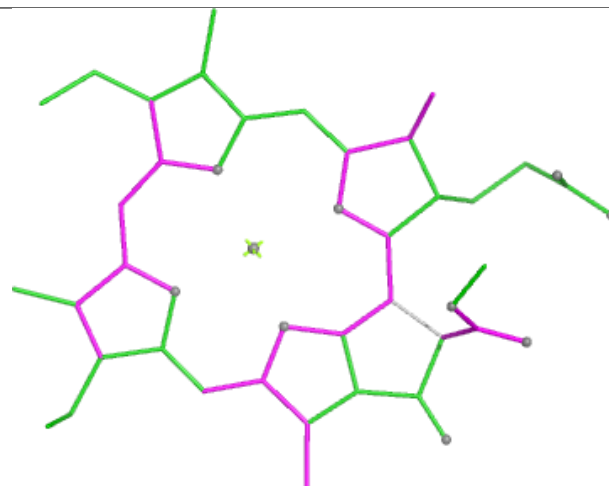
Rings



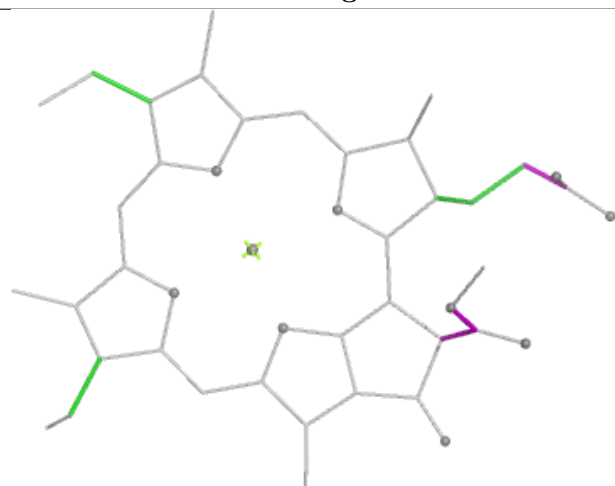
Ligand CLA Z 304



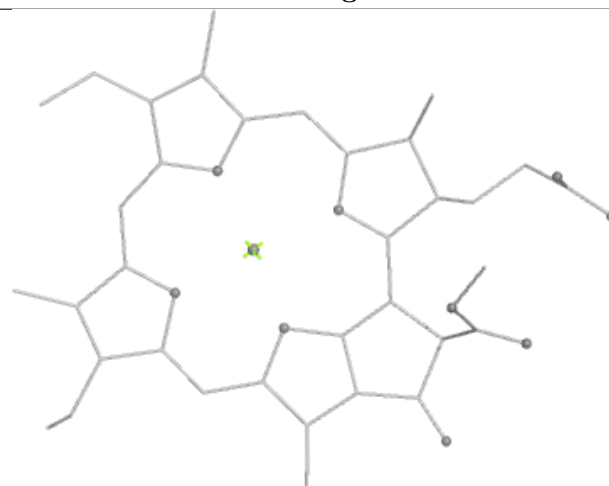
Bond lengths



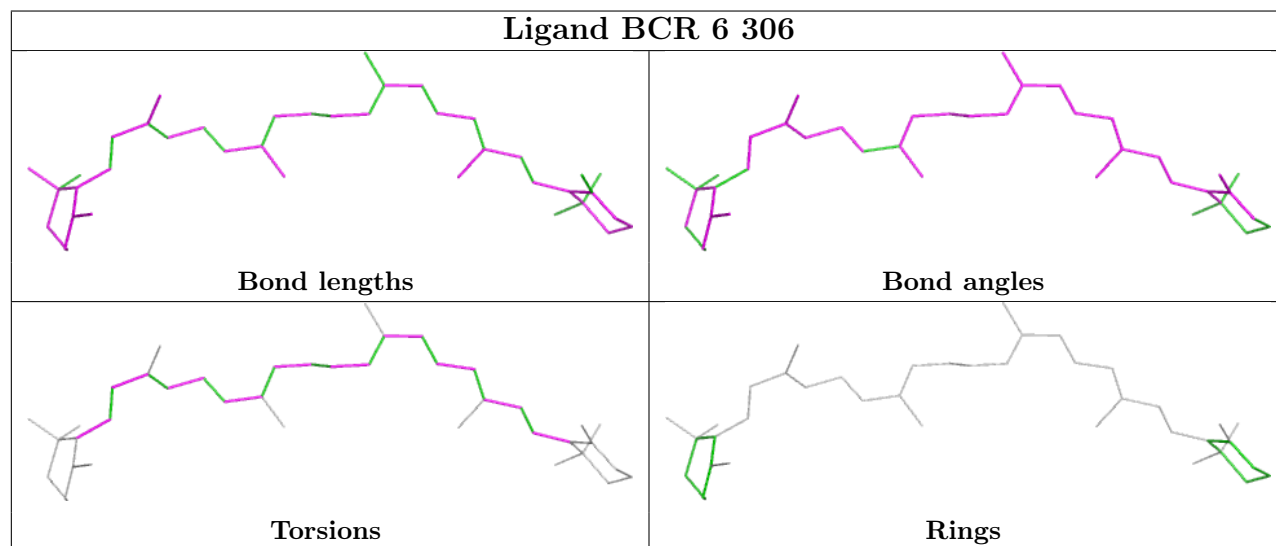
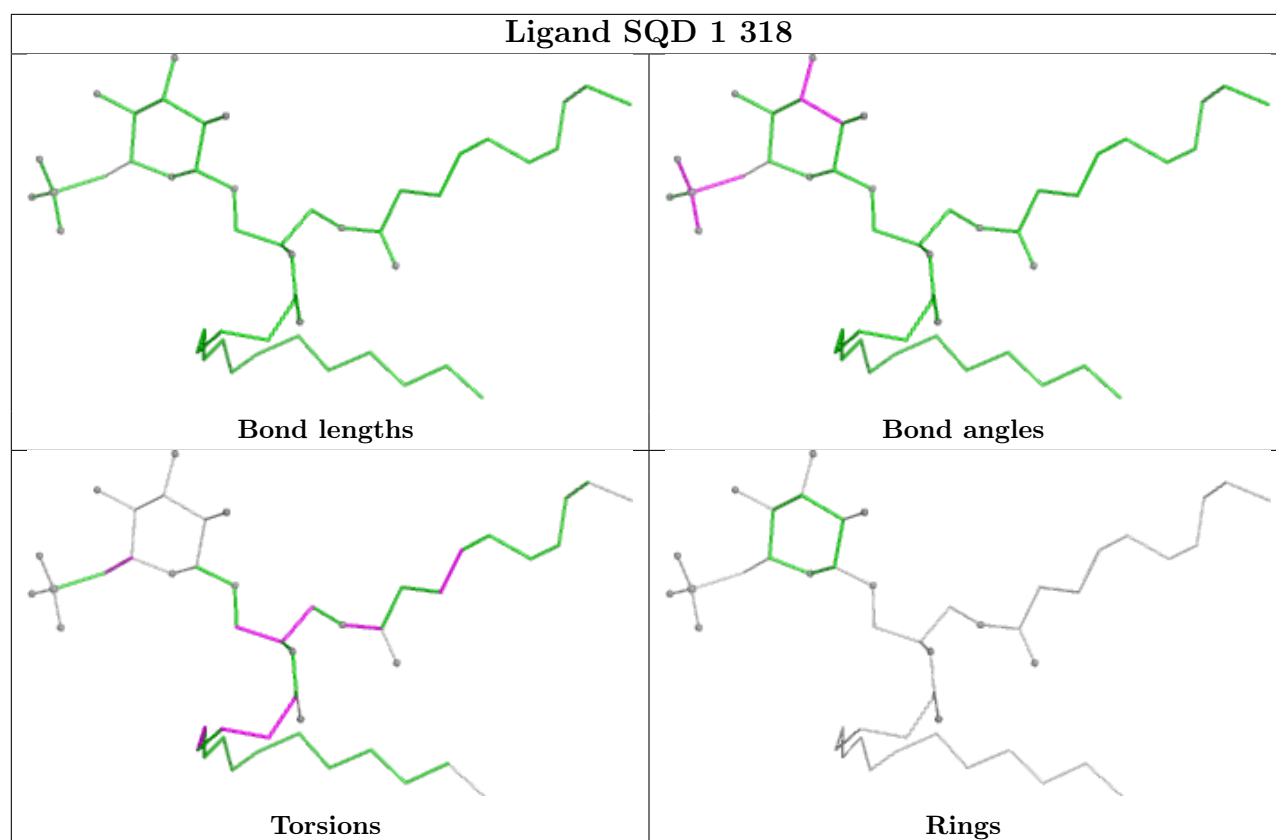
Bond angles



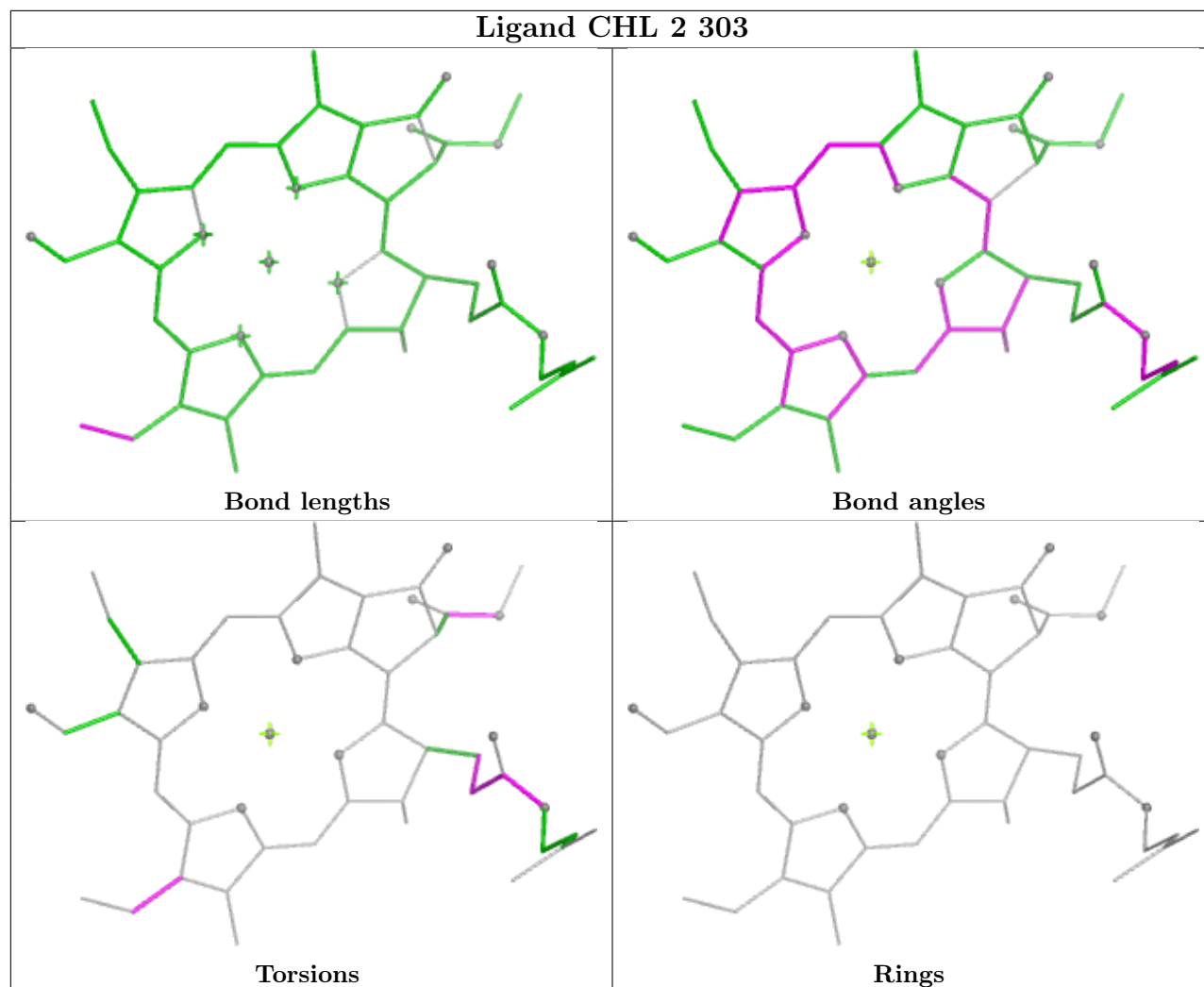
Torsions

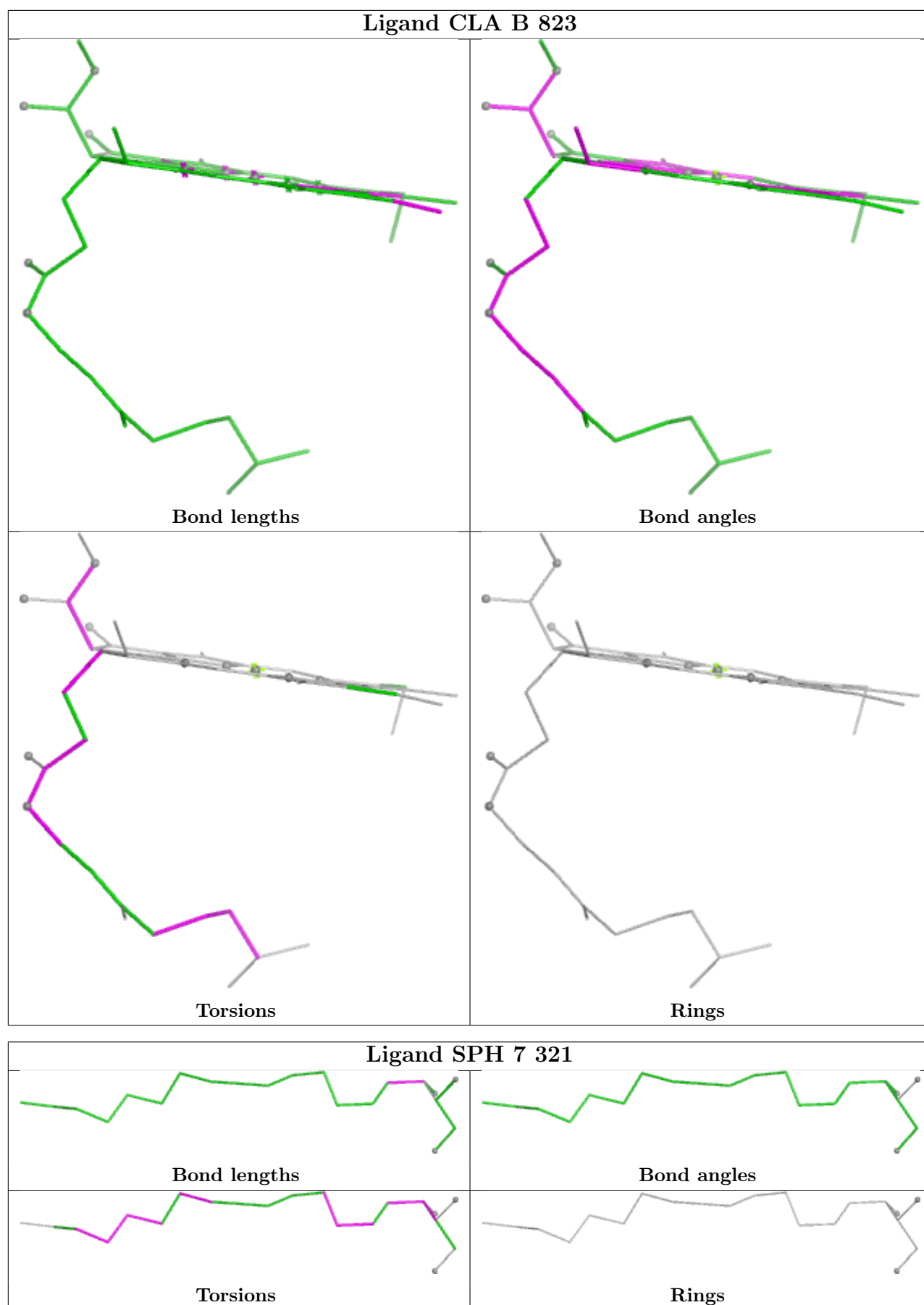


Rings

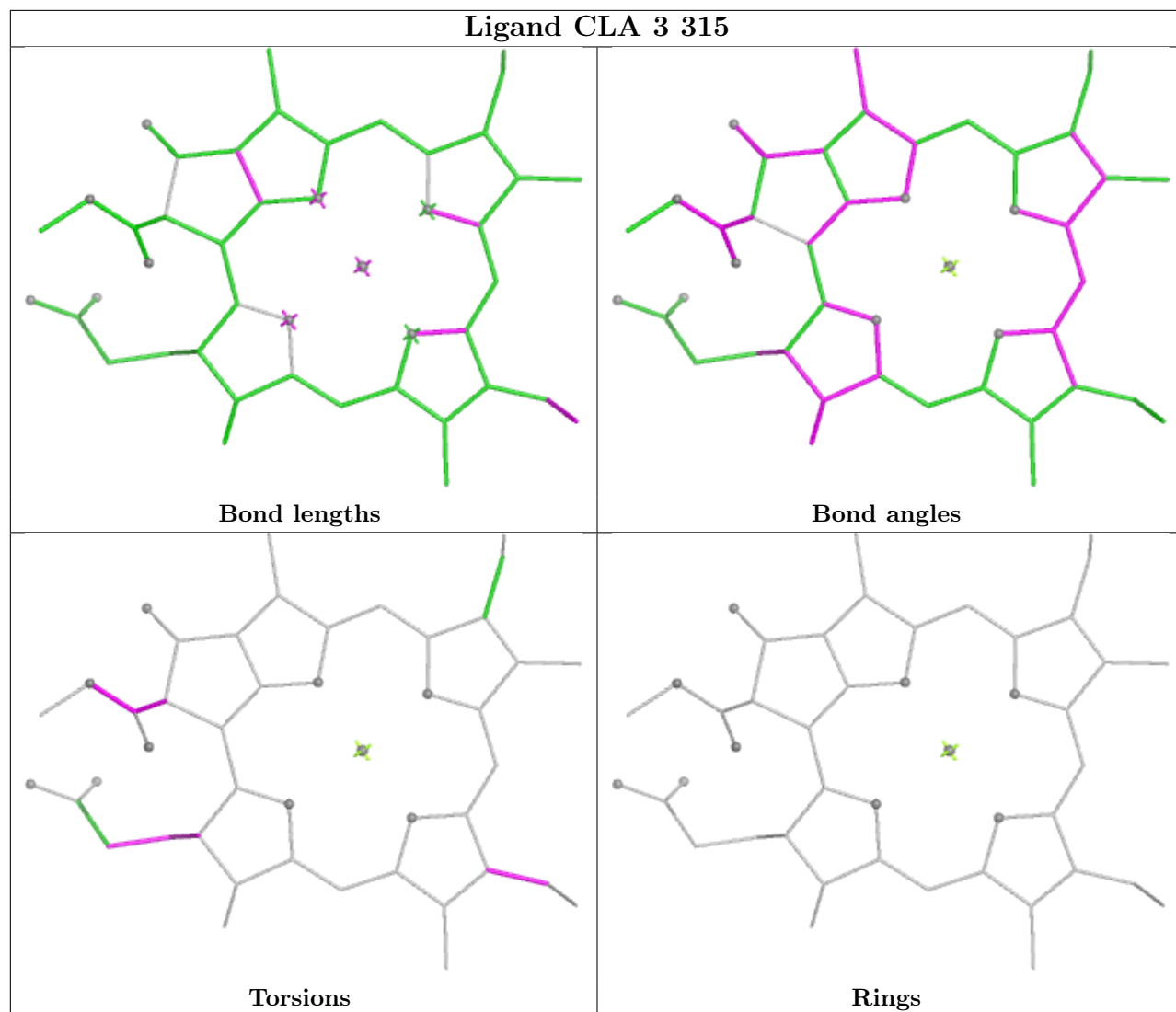


Ligand CHL 2 303

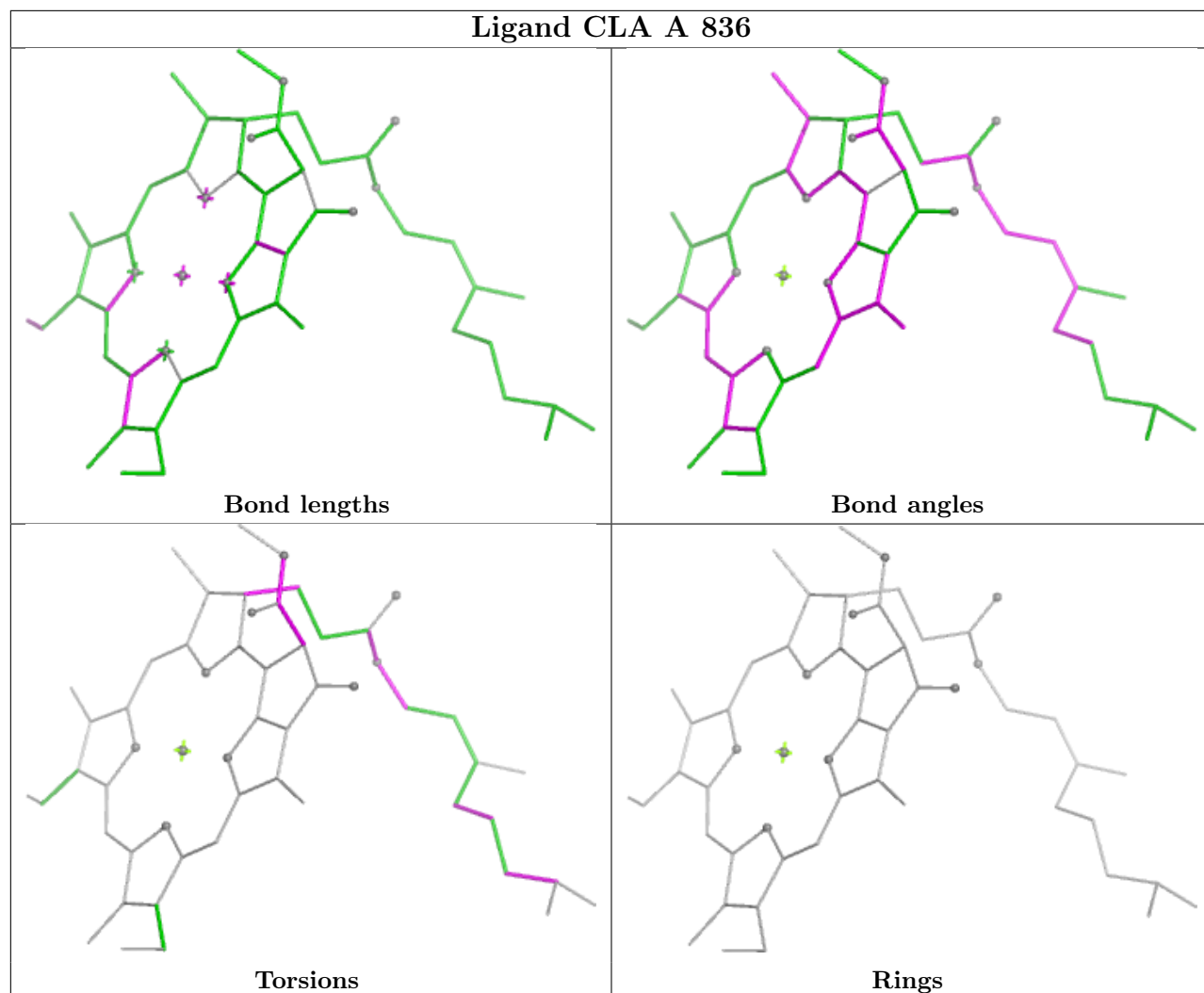


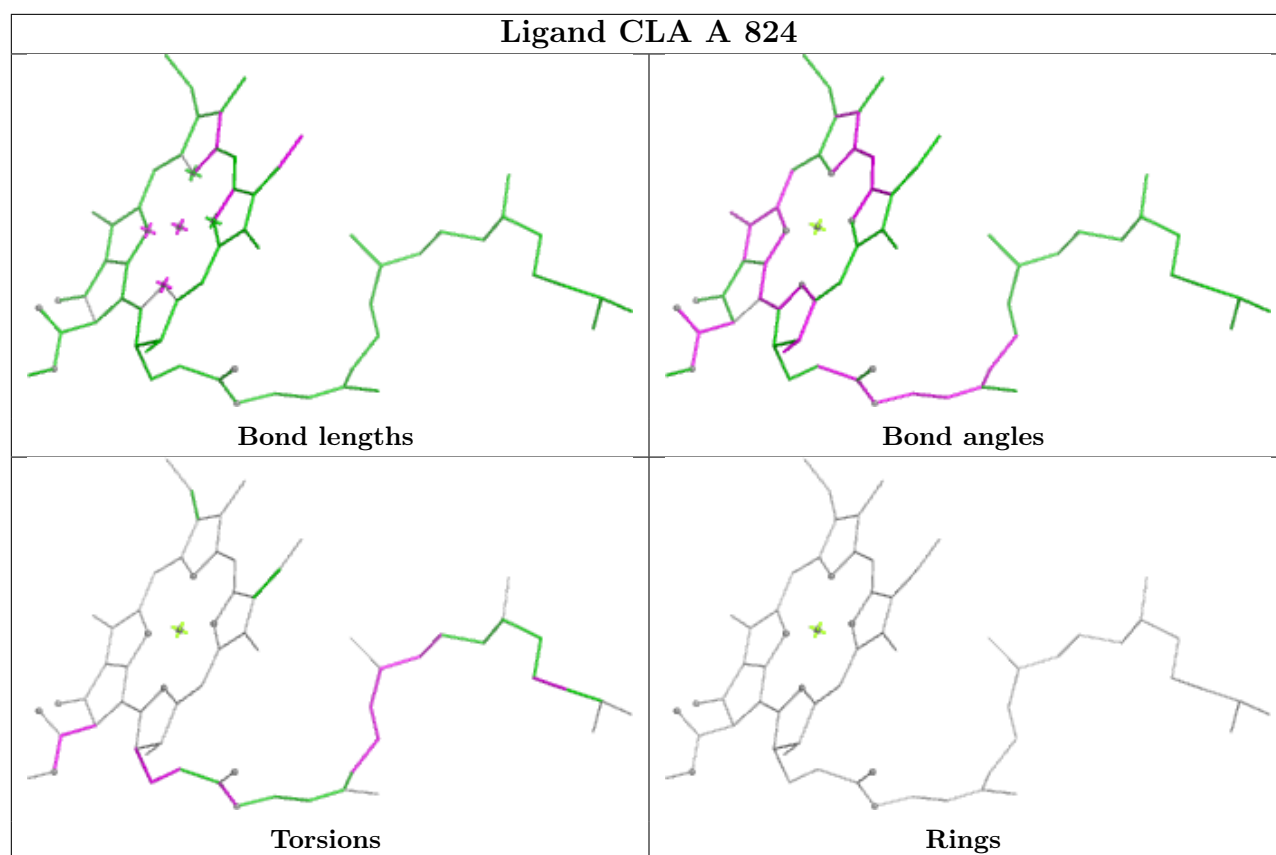


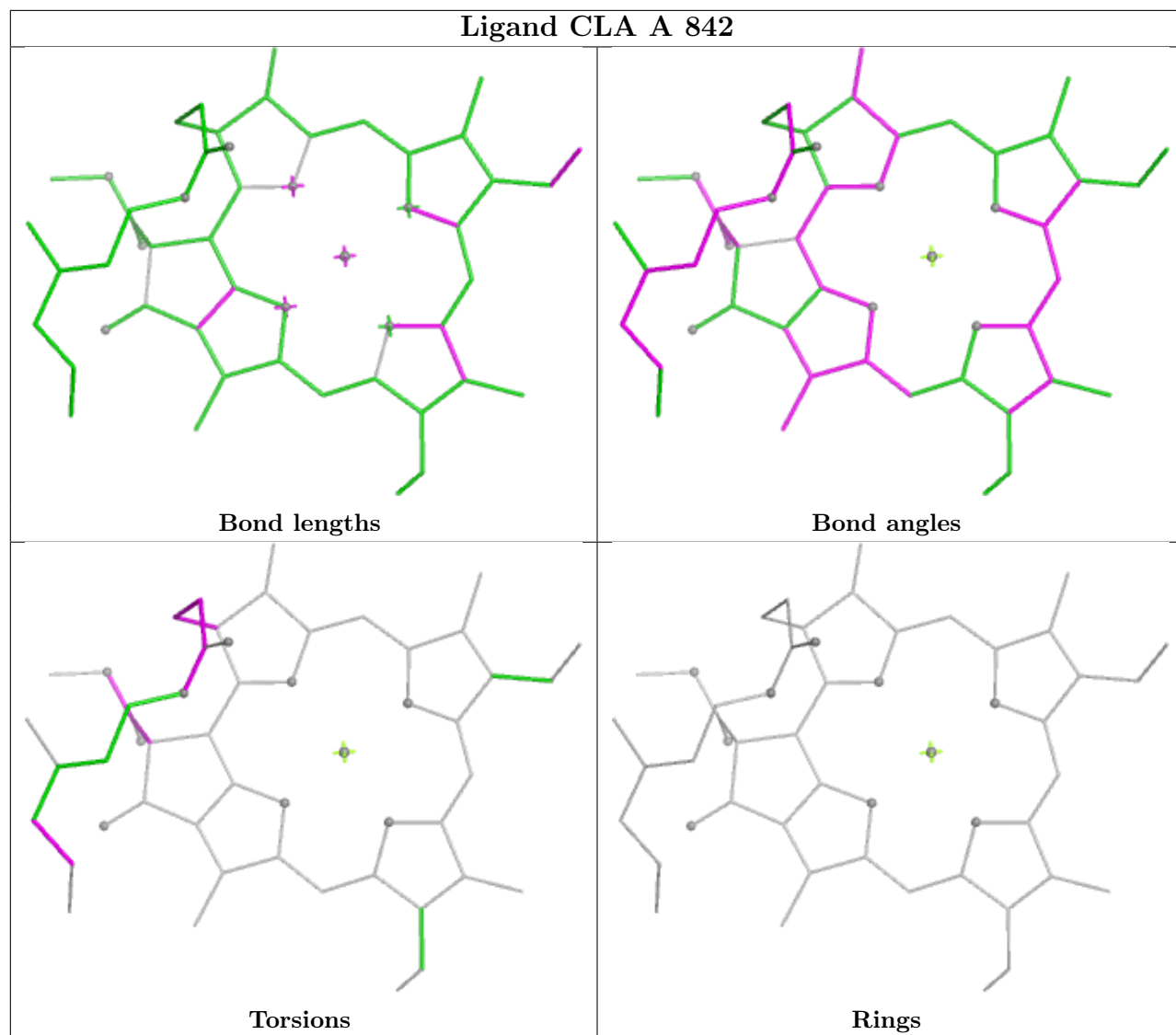
Ligand CLA 3 315



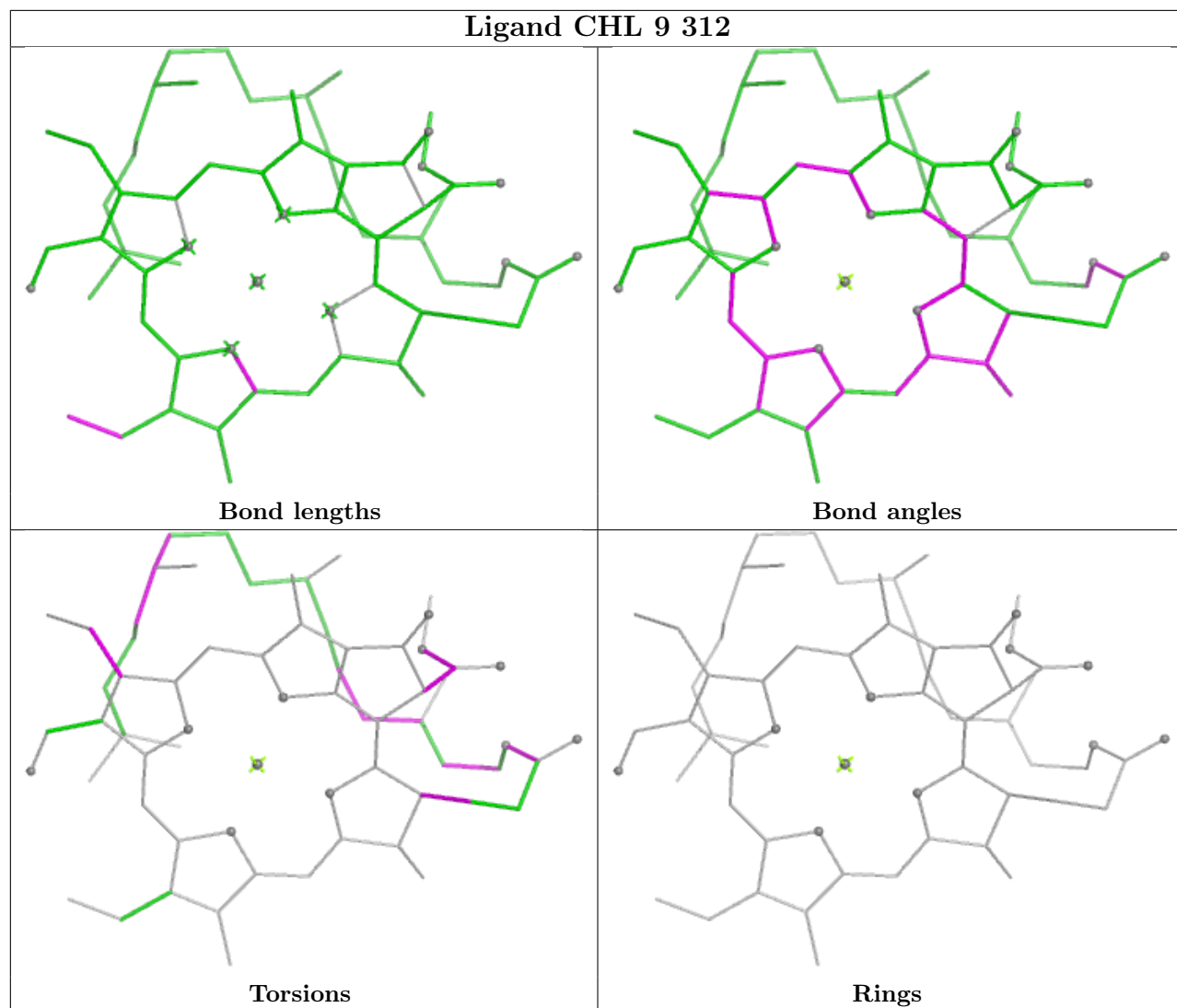
Ligand CLA A 836

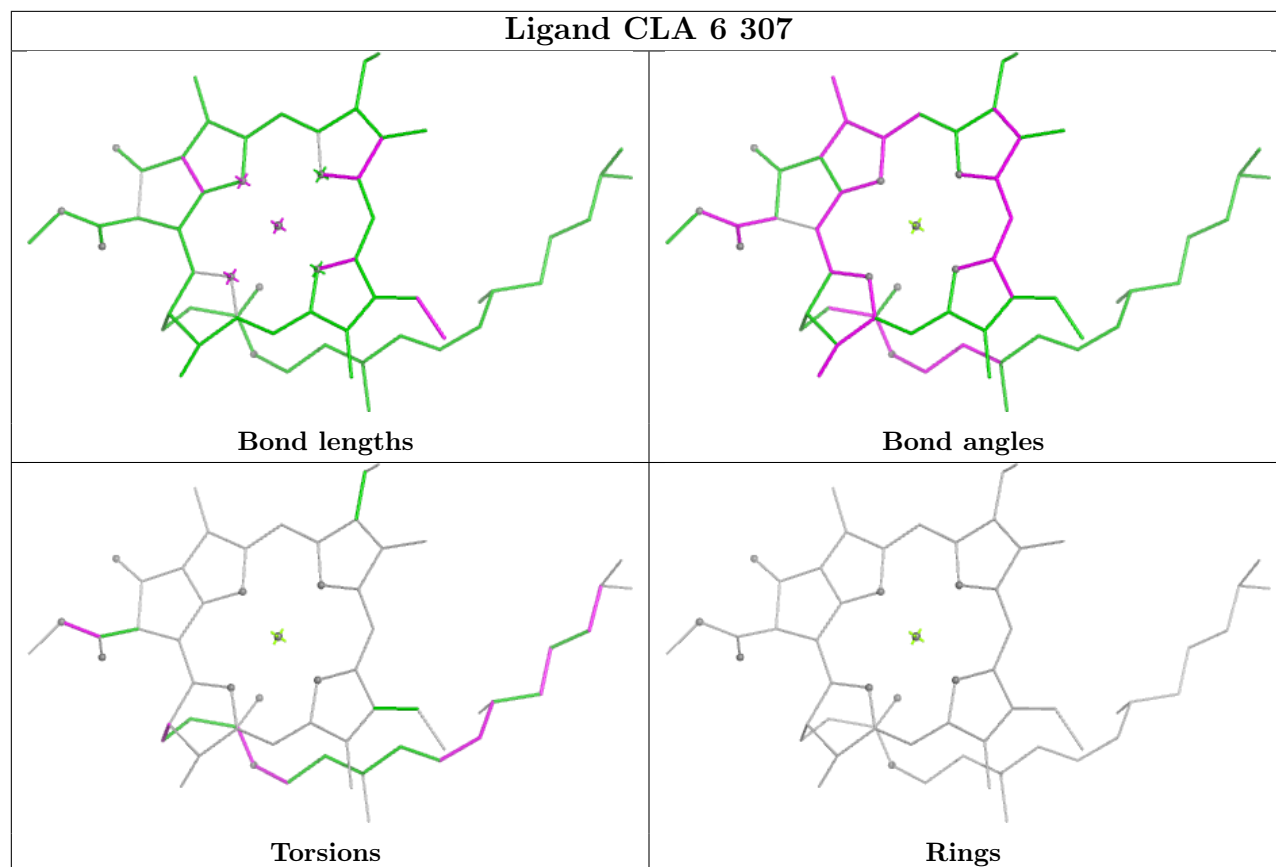




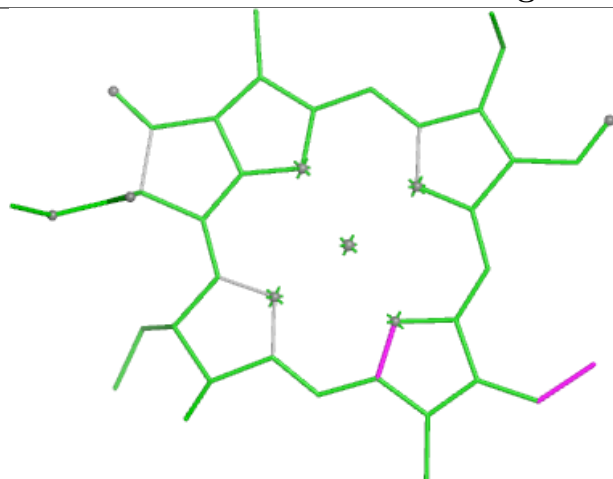


Ligand CHL 9 312

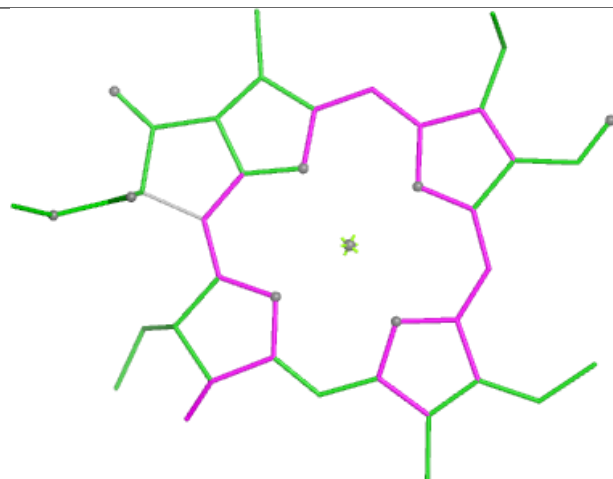




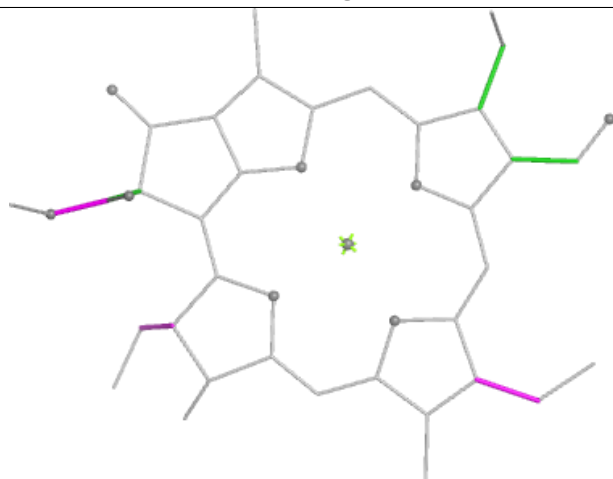
Ligand CHL 5 321



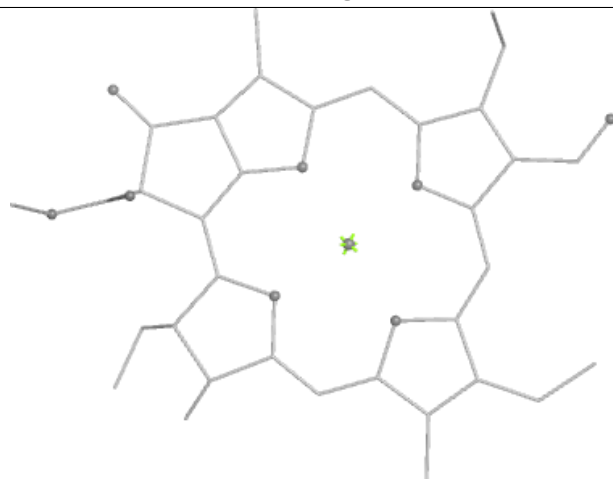
Bond lengths



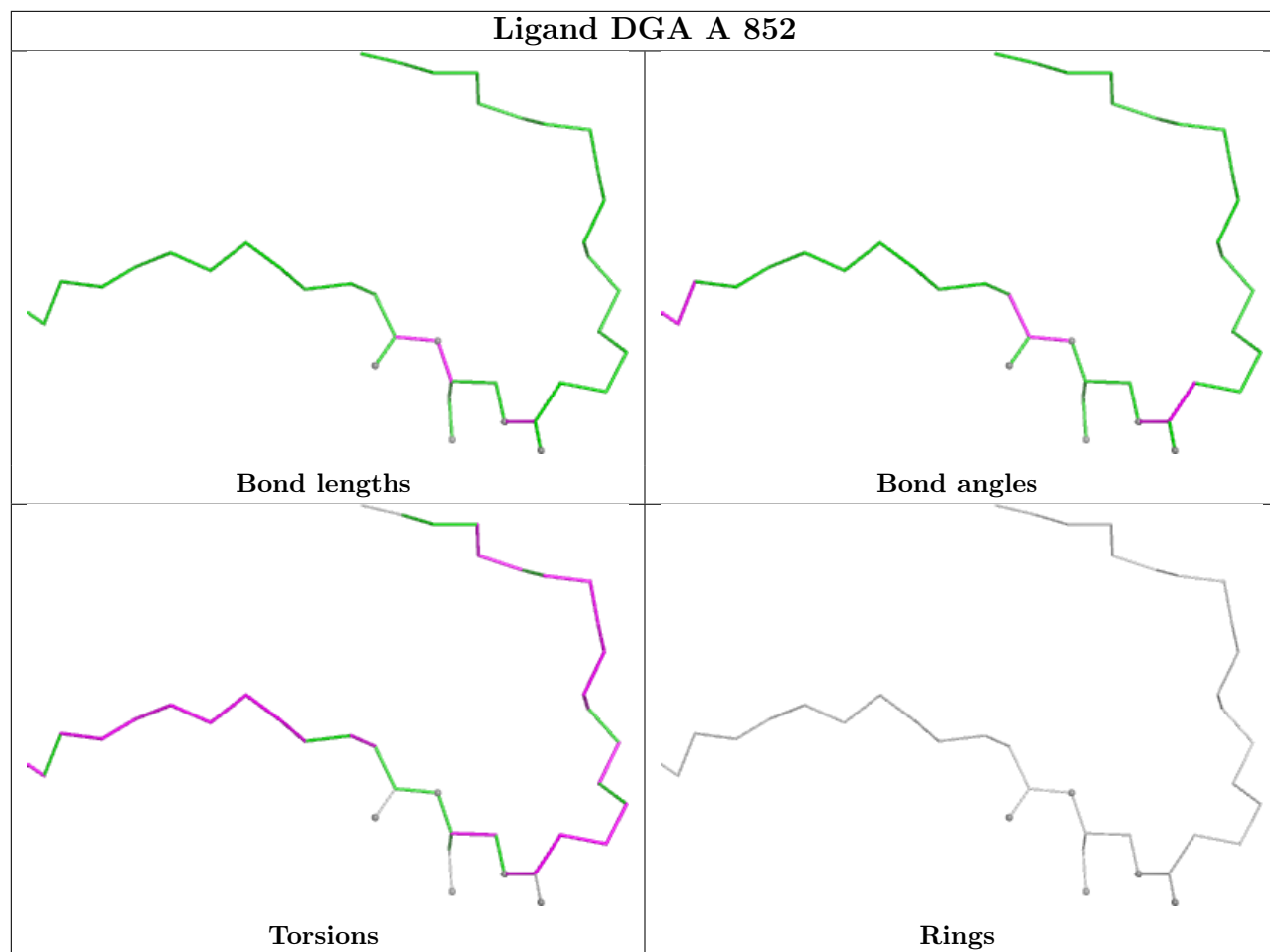
Bond angles



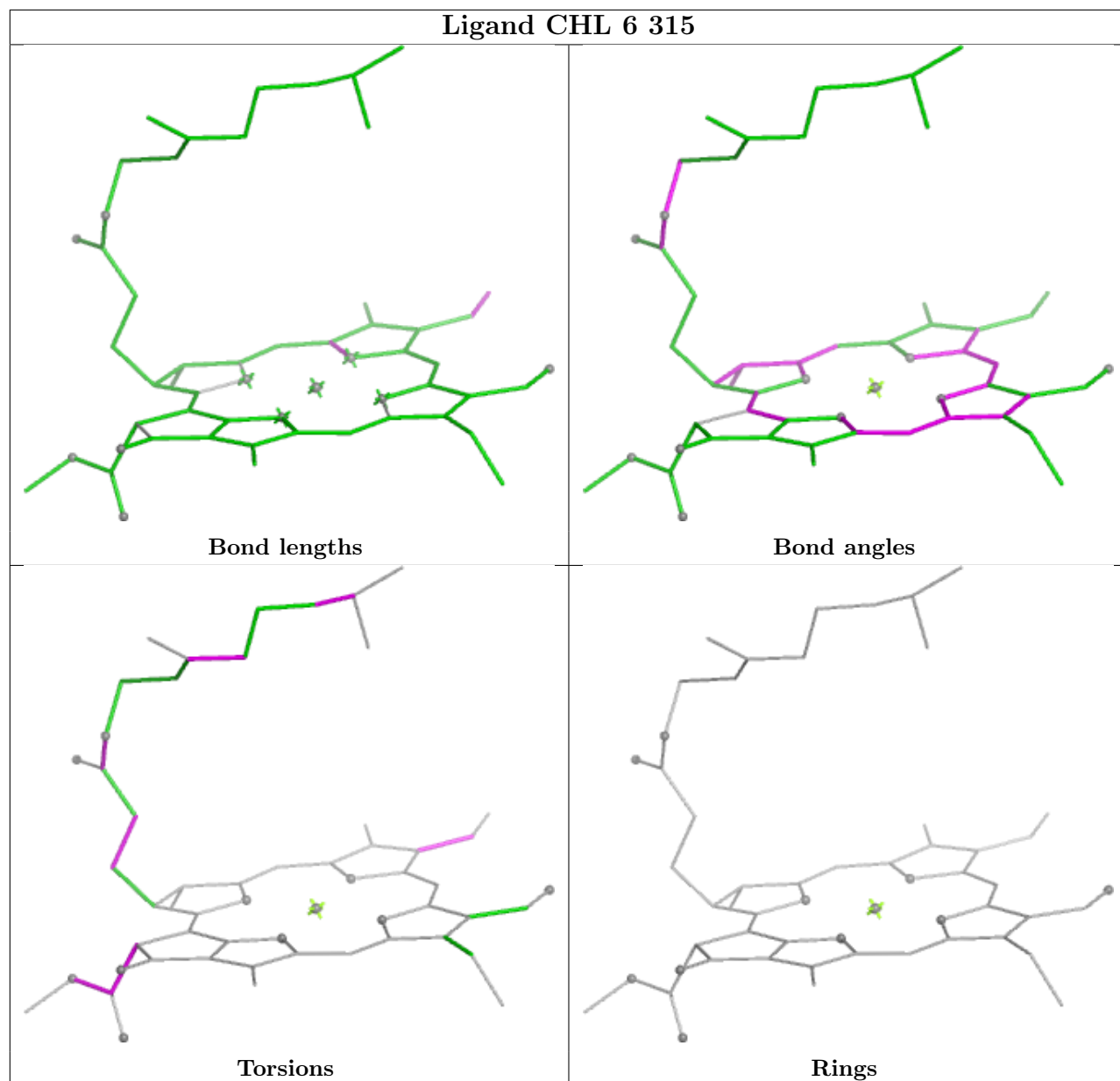
Torsions

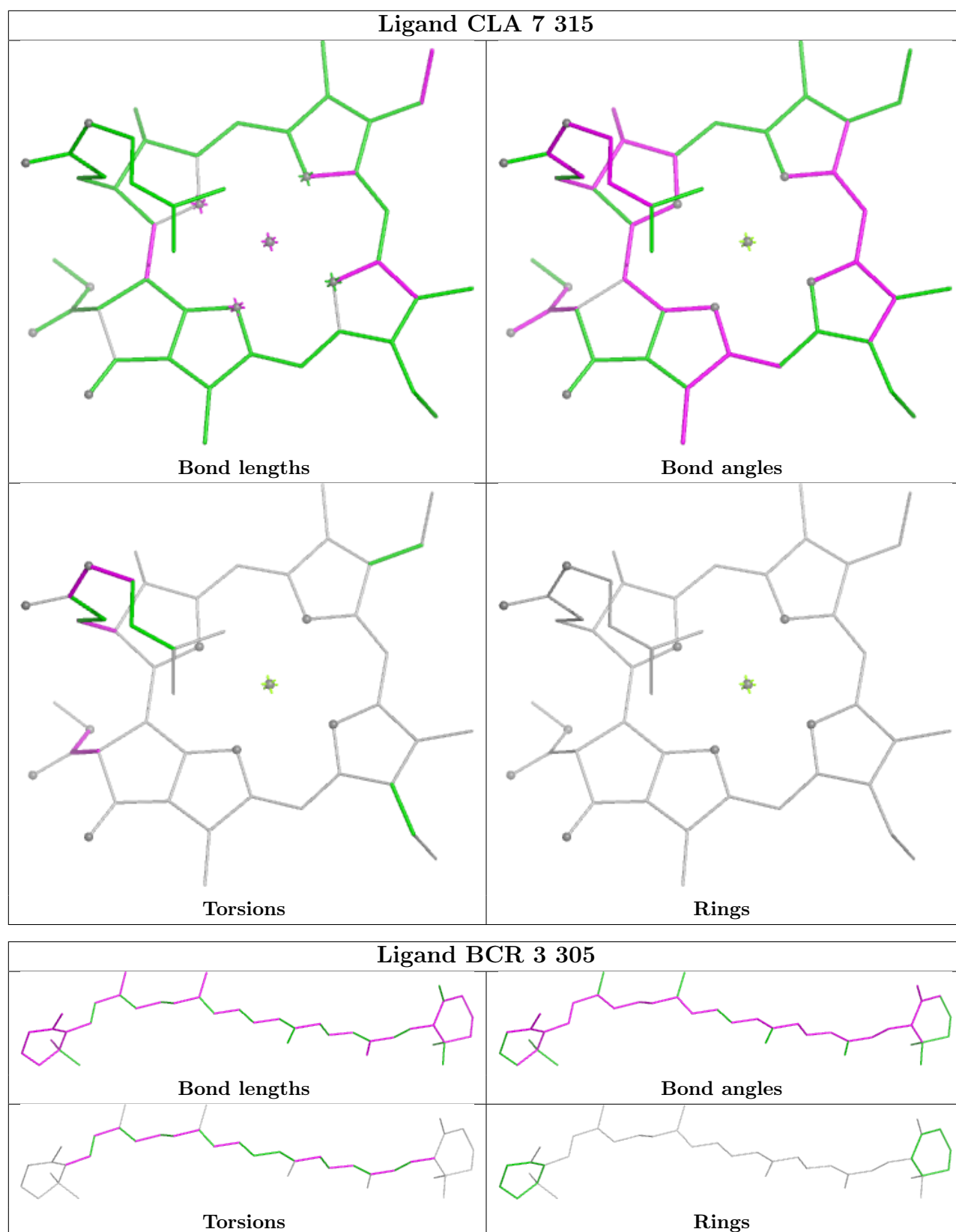


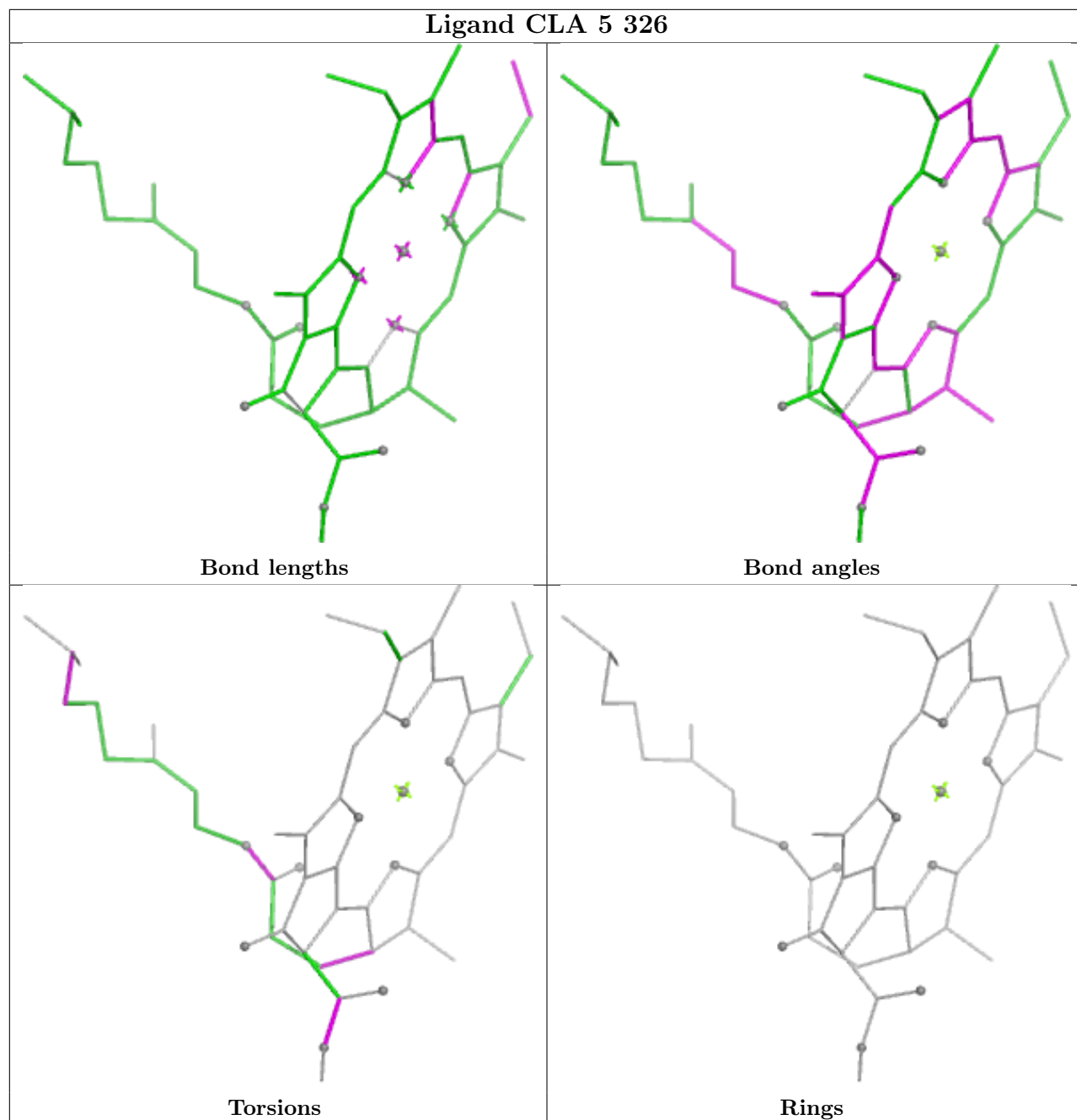
Rings

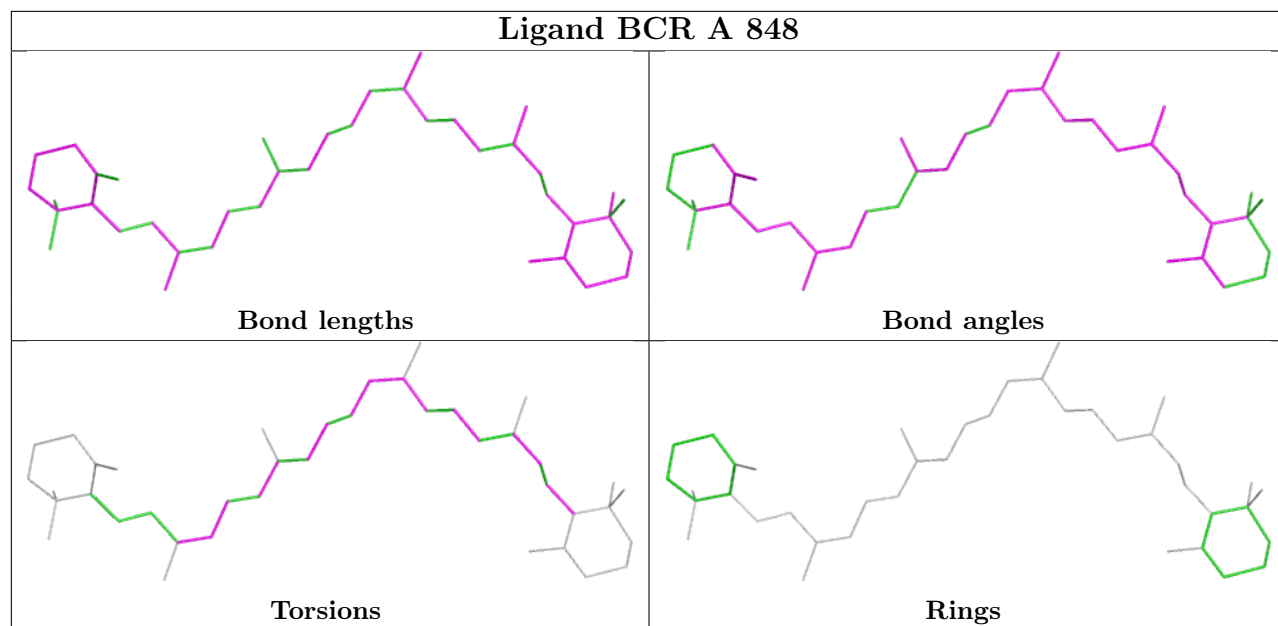


Ligand CHL 6 315

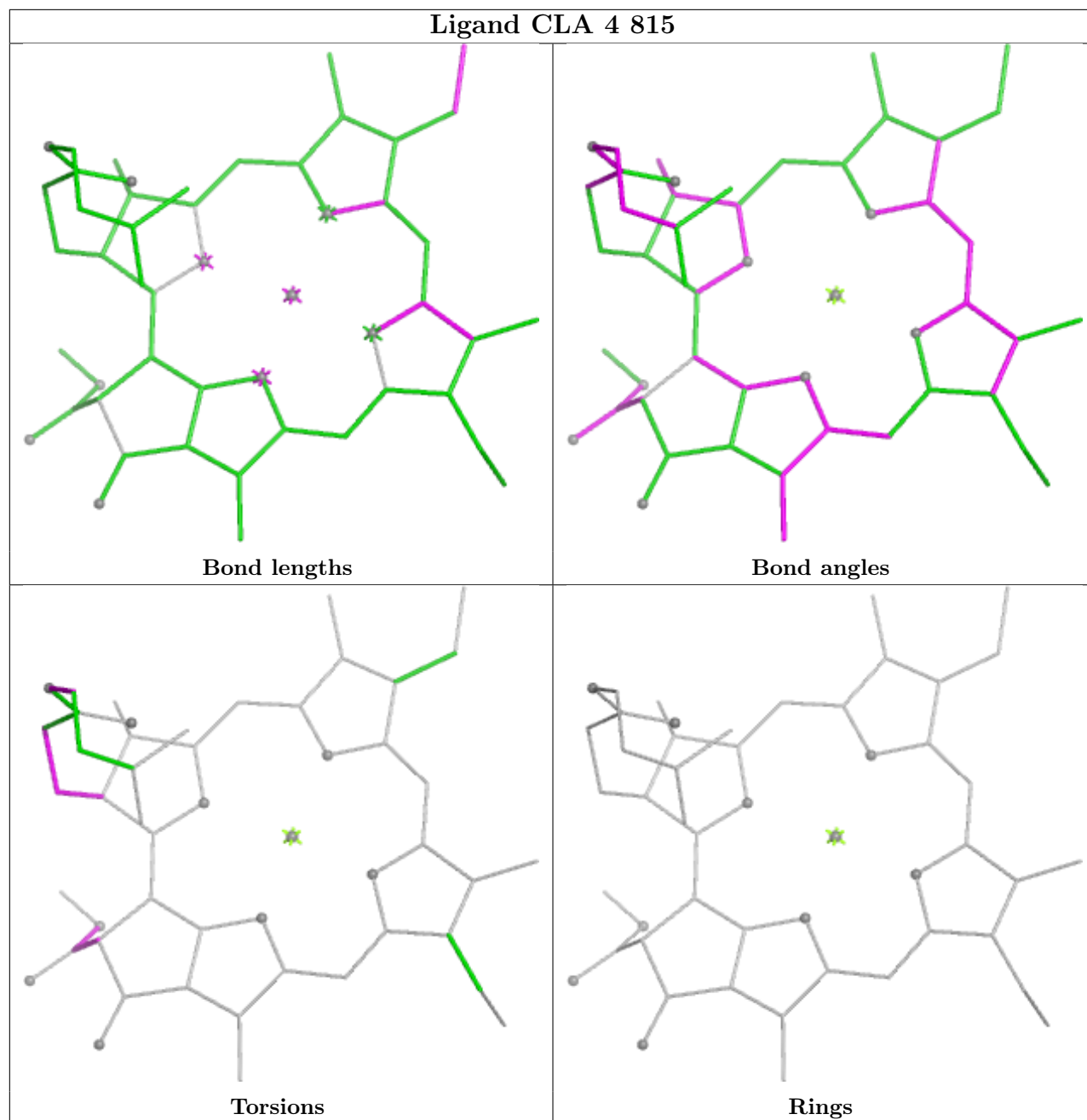




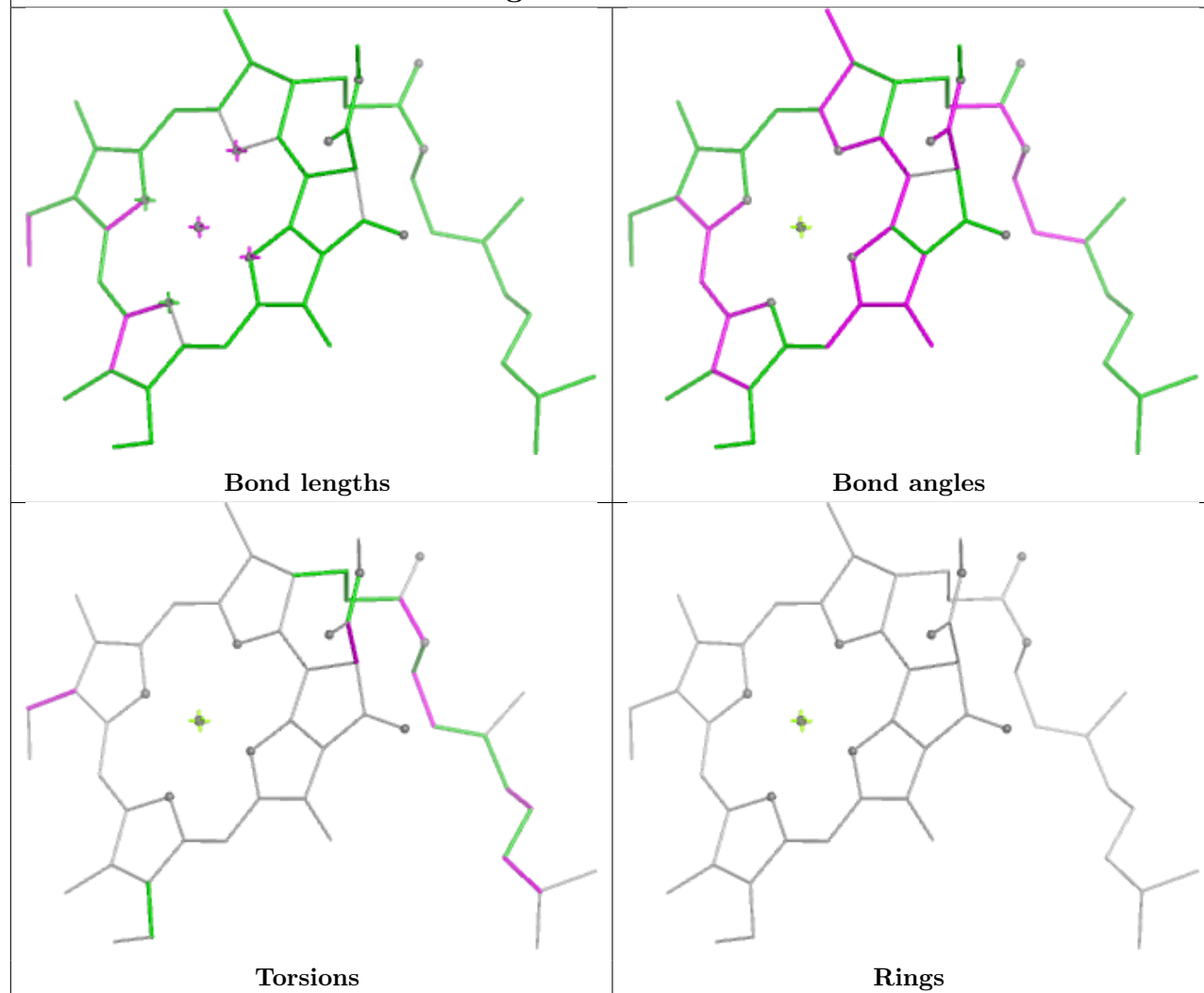




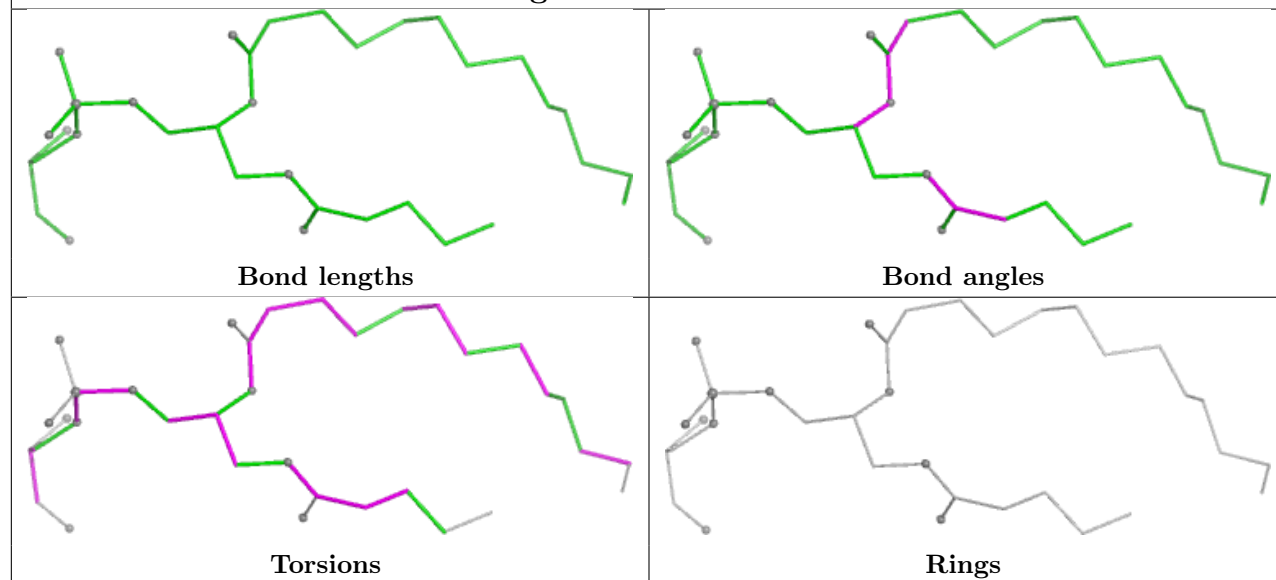
Ligand CLA 4 815



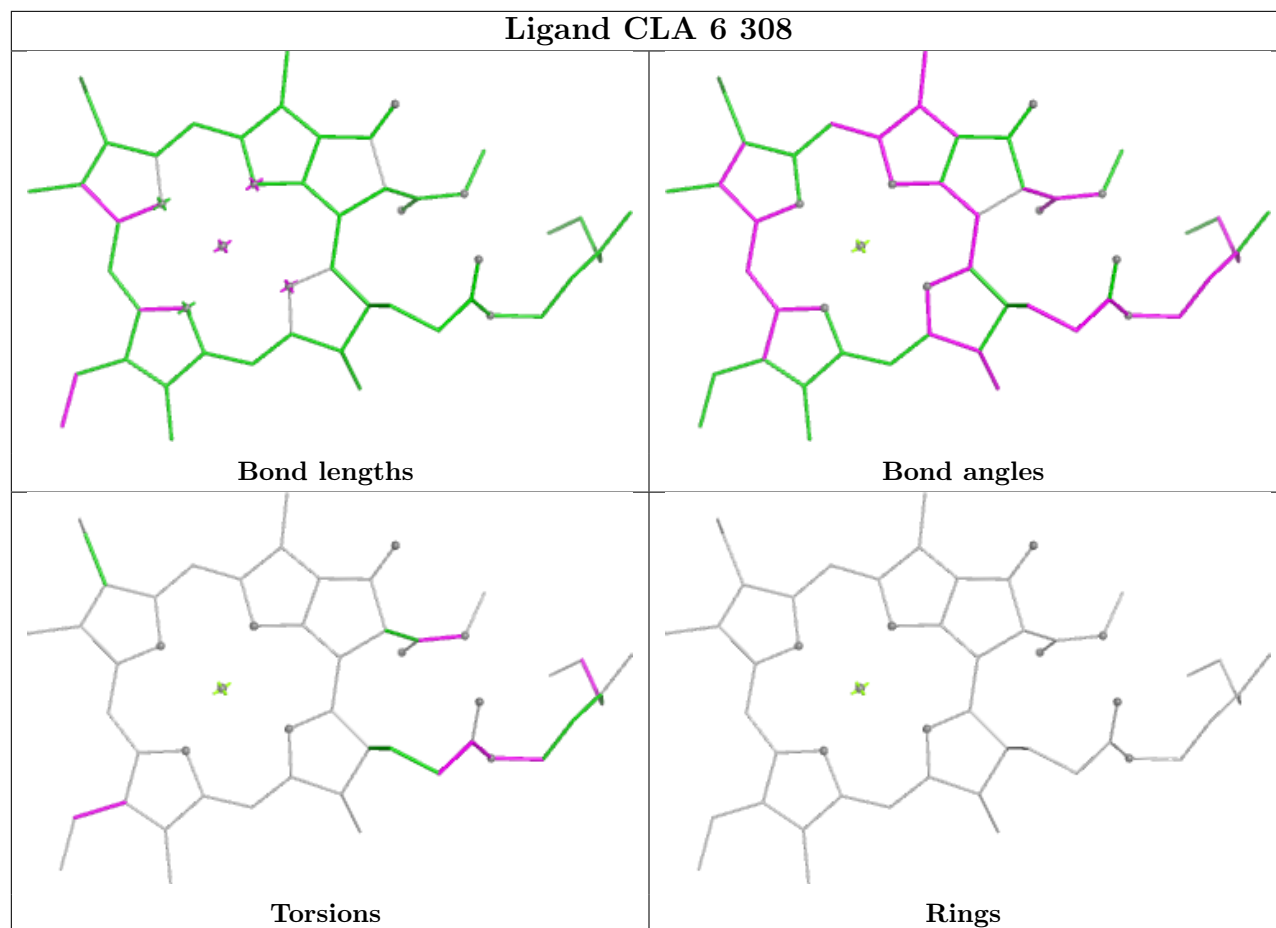
Ligand CLA 6 313



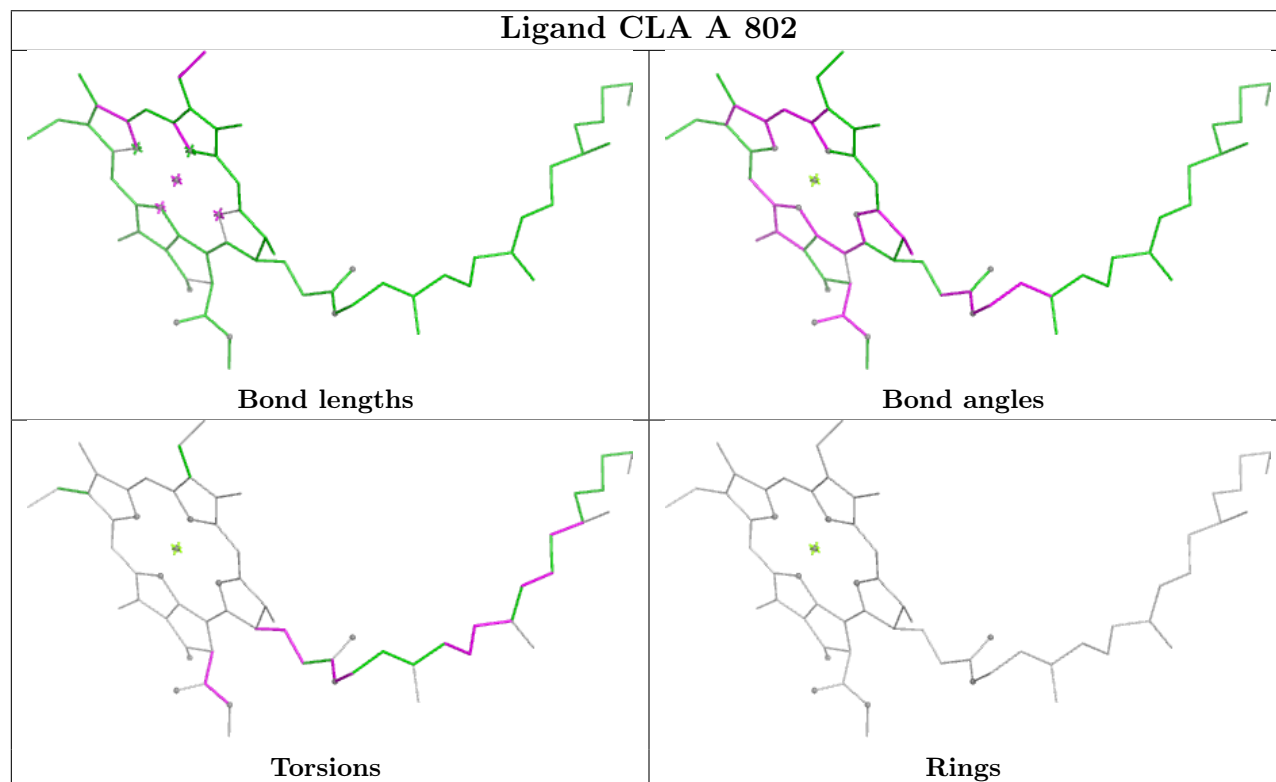
Ligand LHG A 849



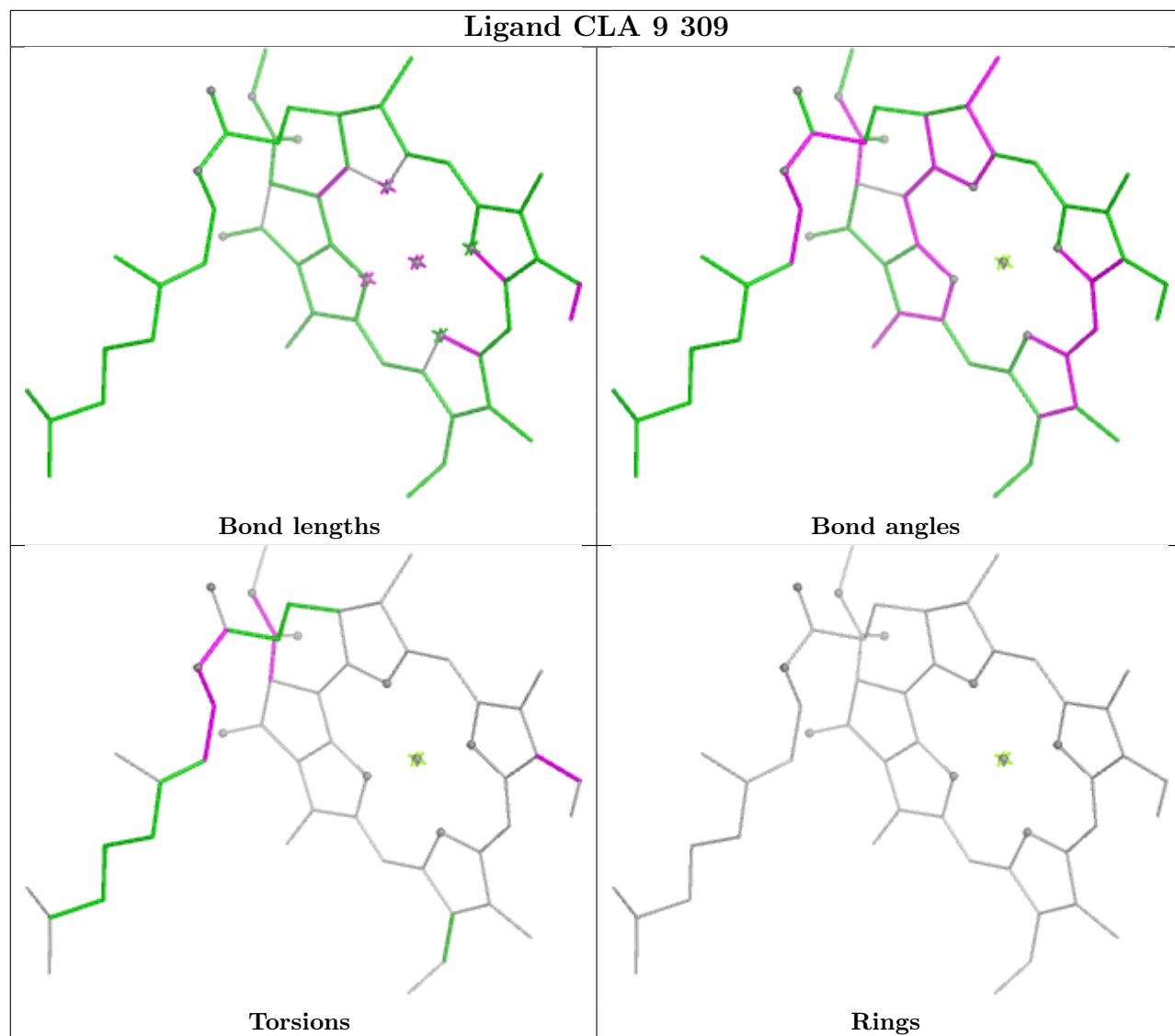
Ligand CLA 6 308

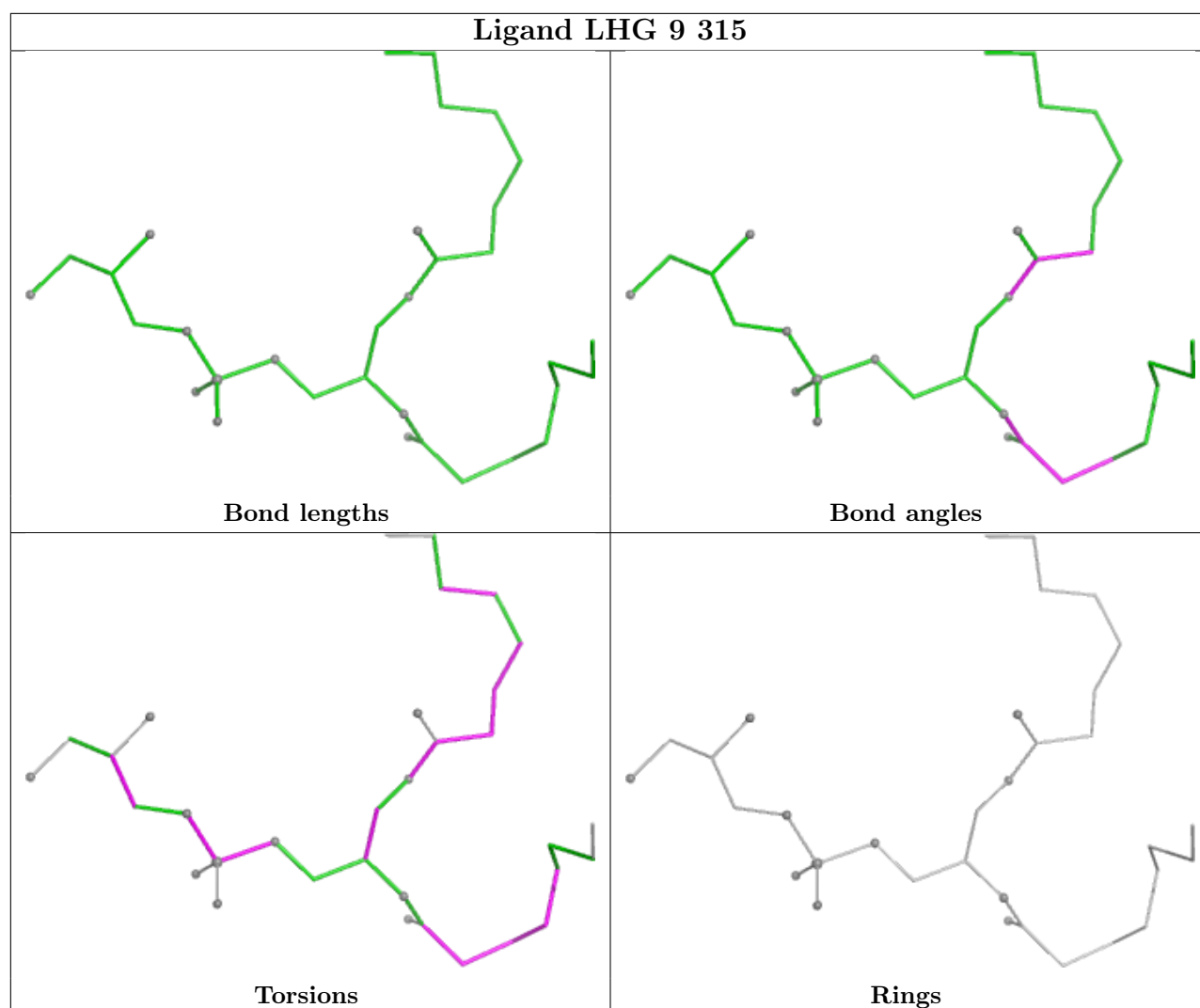


Ligand CLA A 802

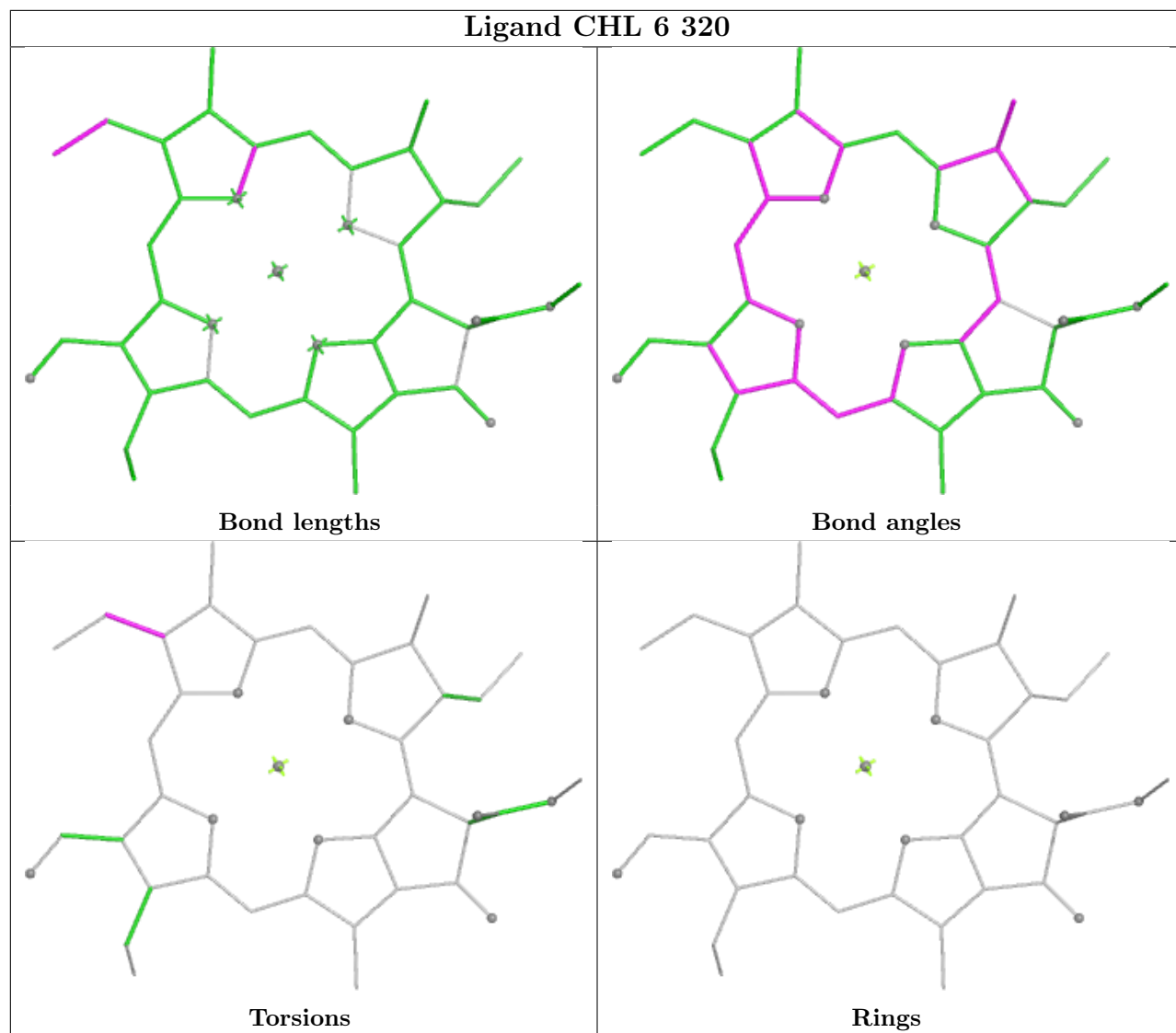


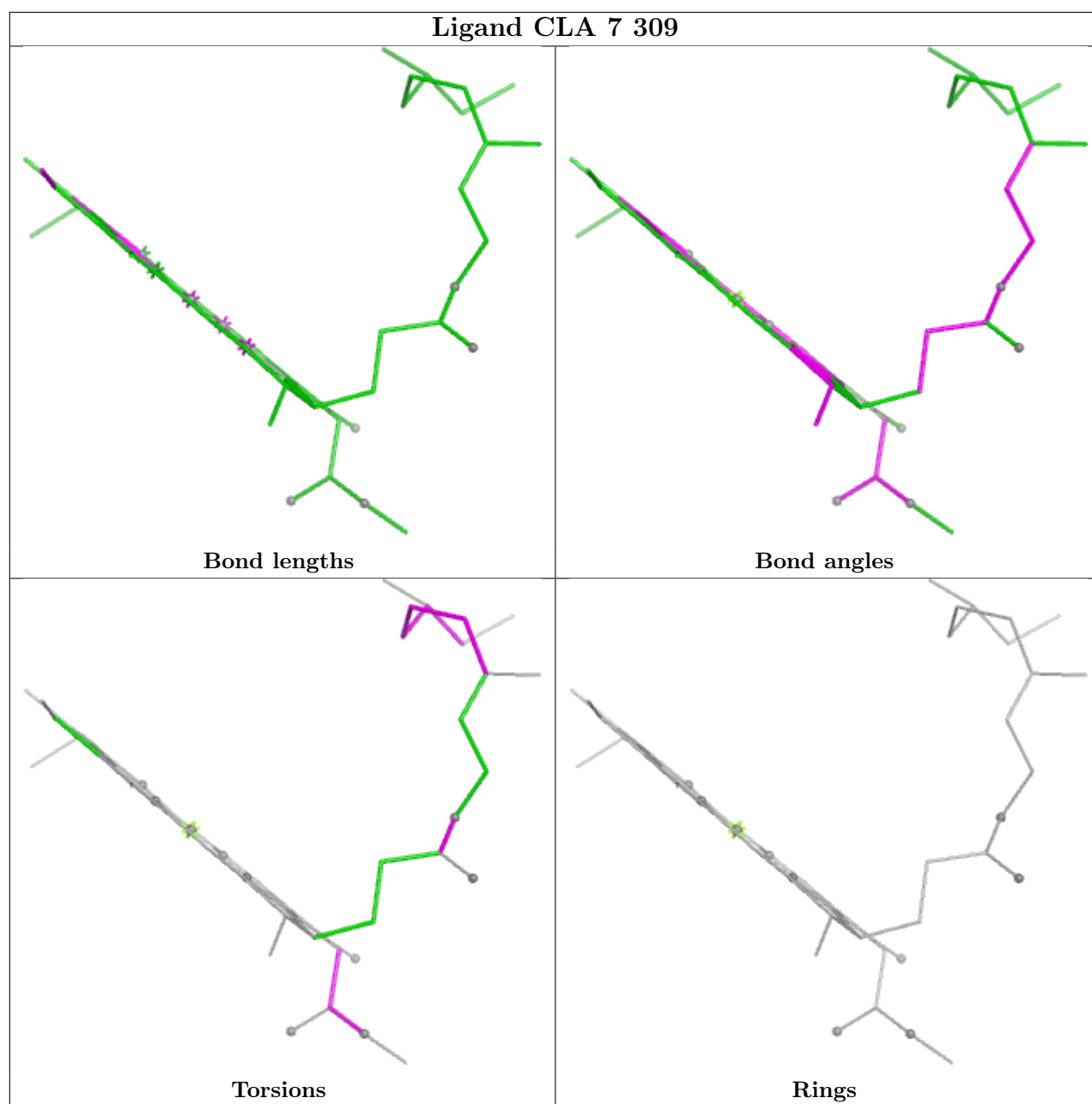
Ligand CLA 9 309

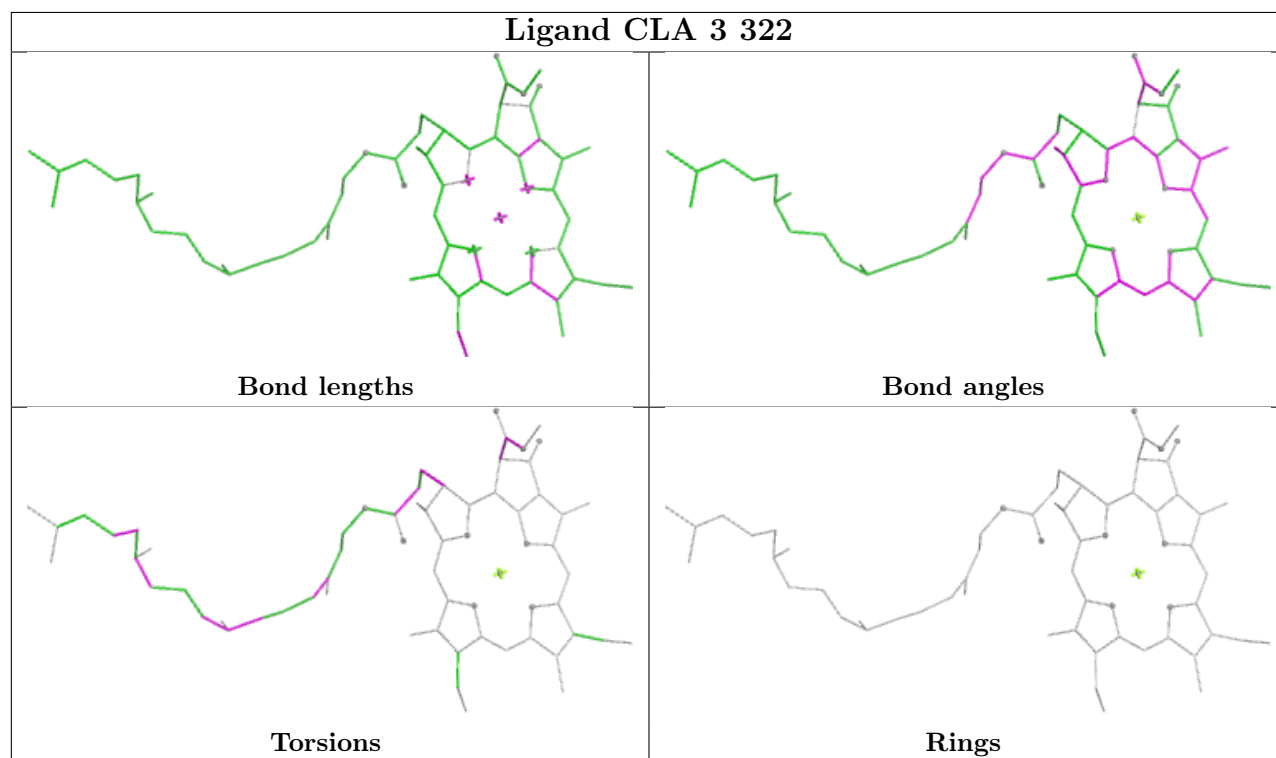
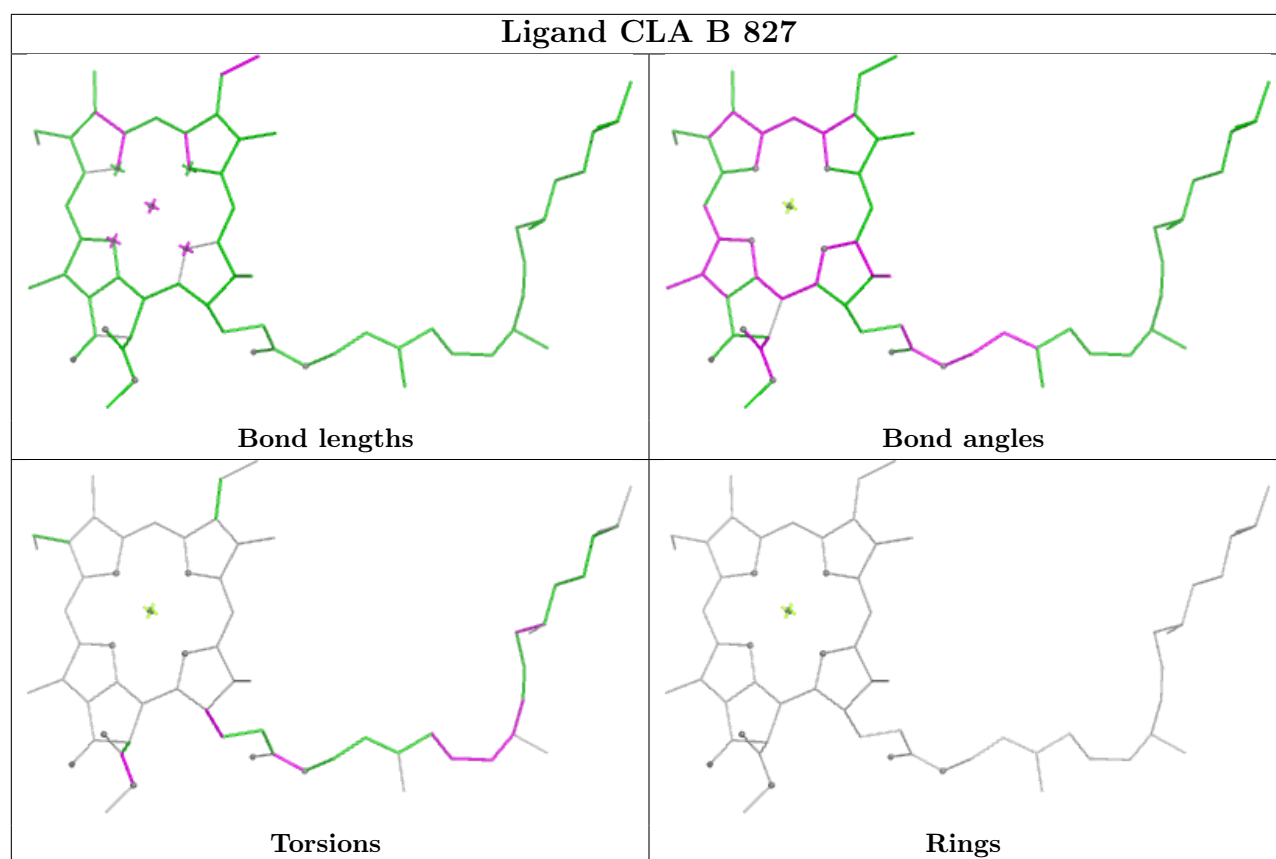


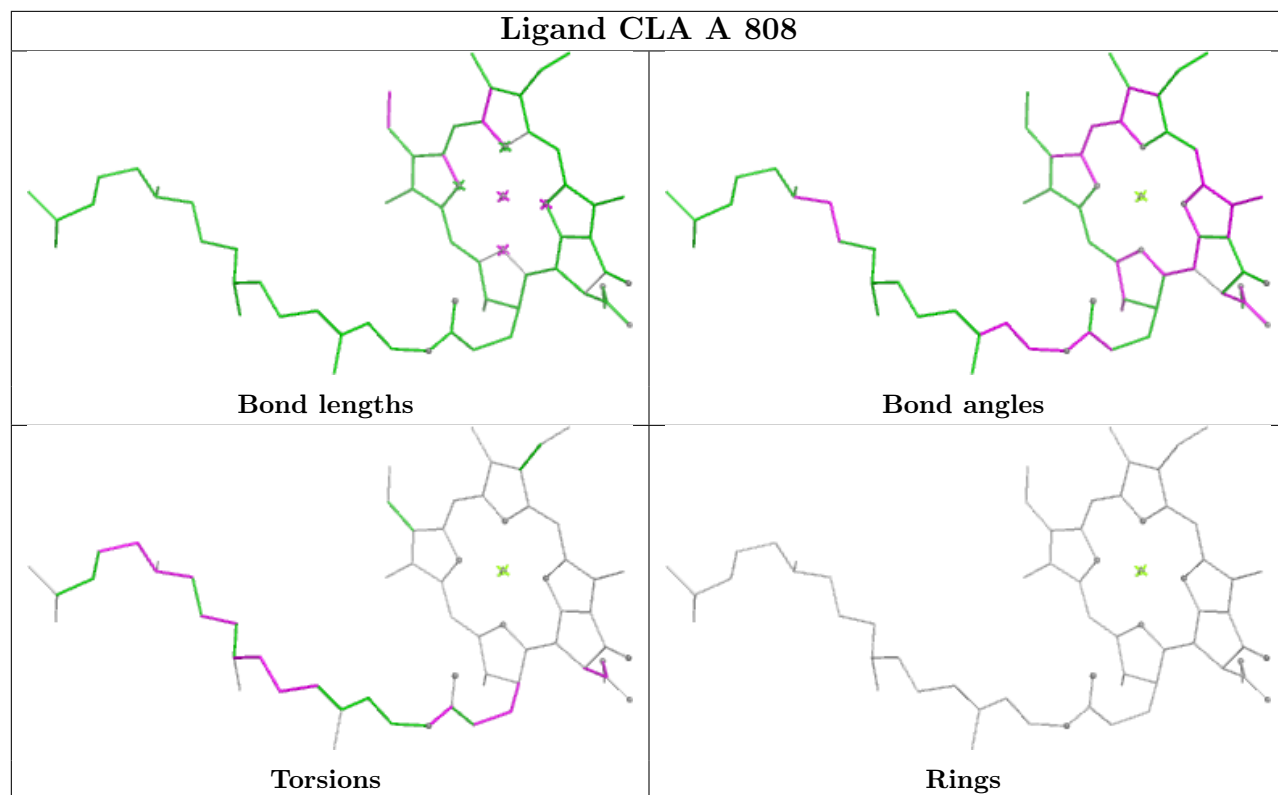


Ligand CHL 6 320

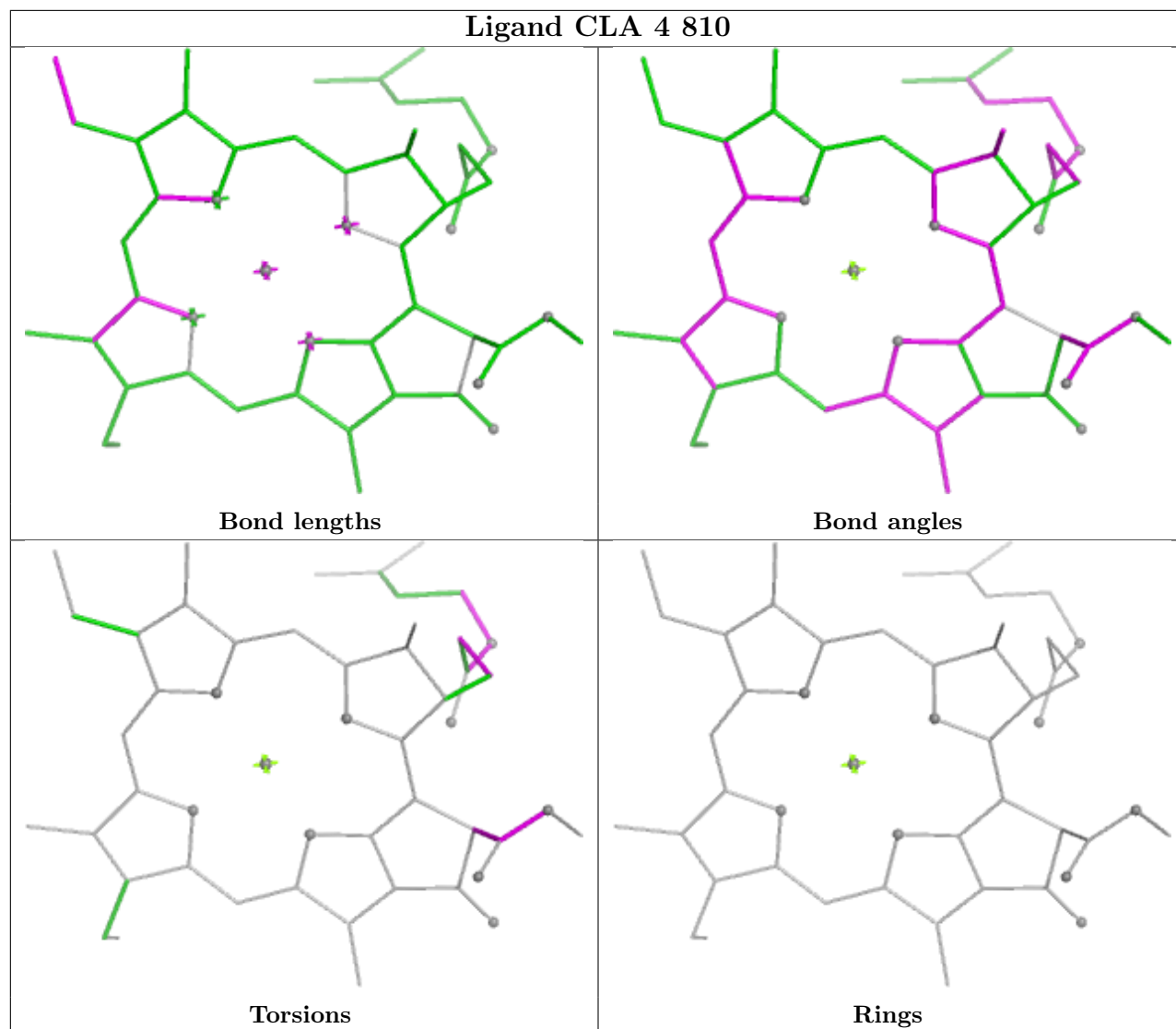




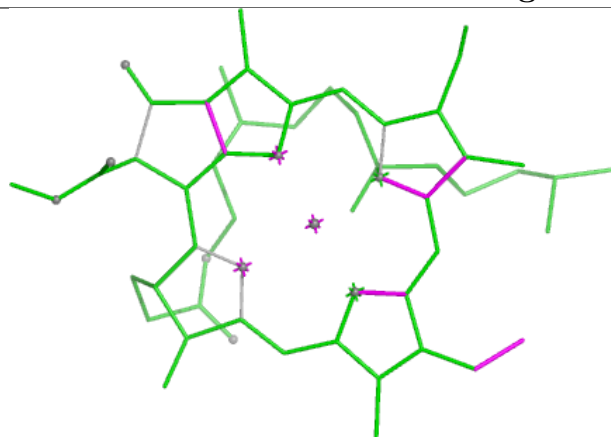




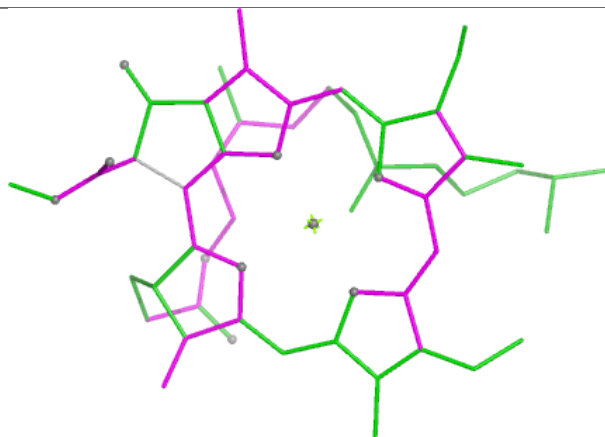
Ligand CLA 4 810



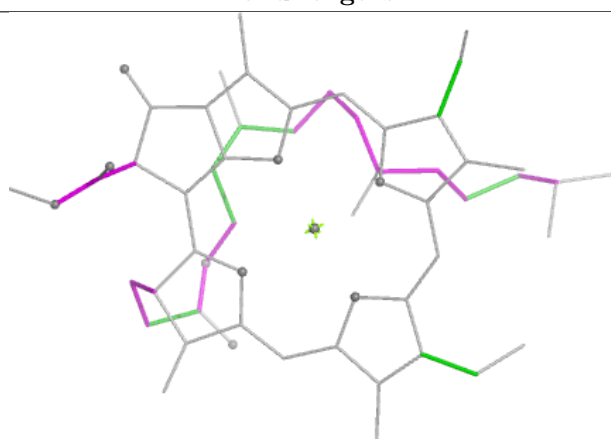
Ligand CLA 6 301



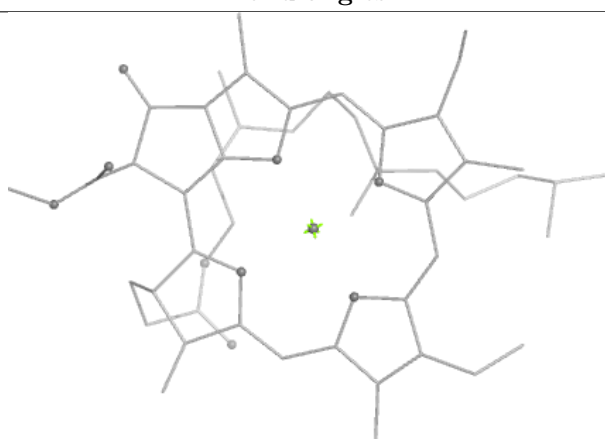
Bond lengths



Bond angles

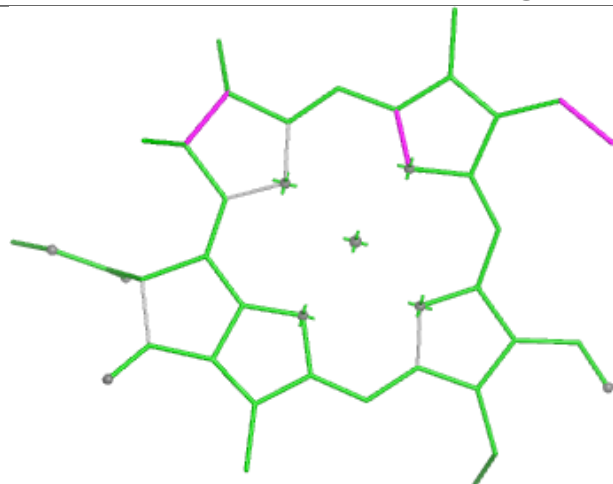


Torsions

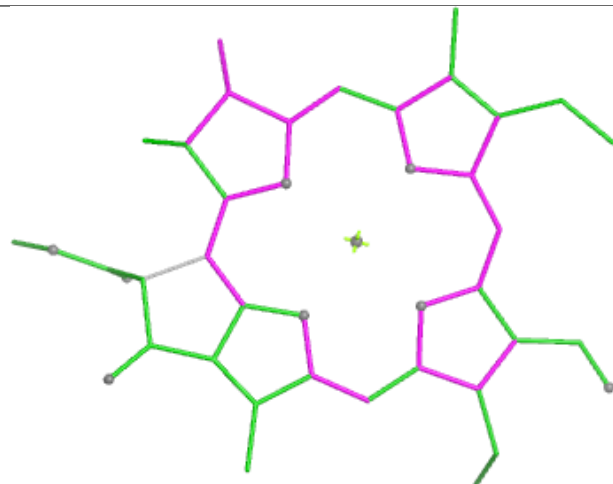


Rings

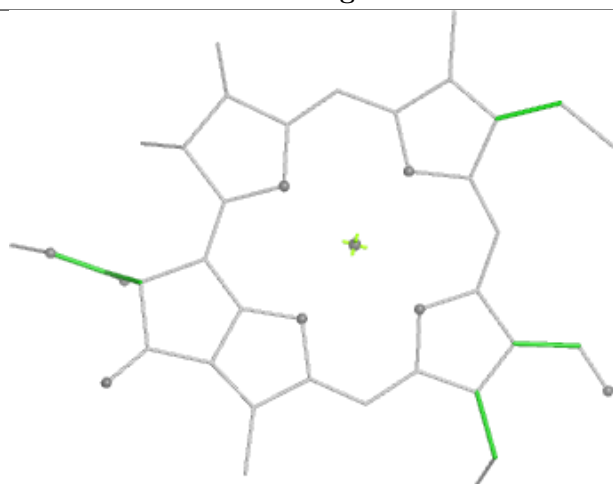
Ligand CHL 9 314



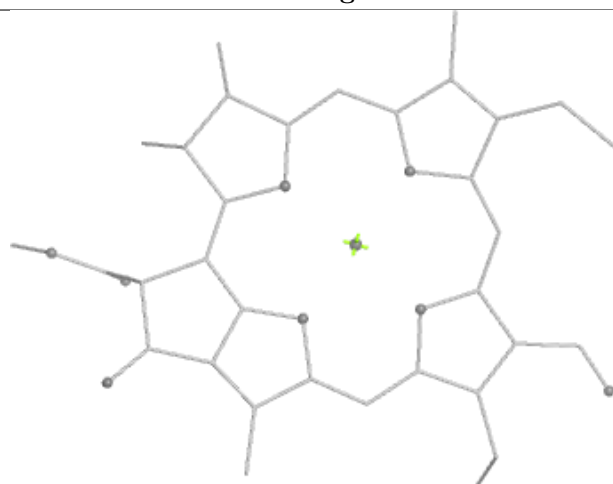
Bond lengths



Bond angles

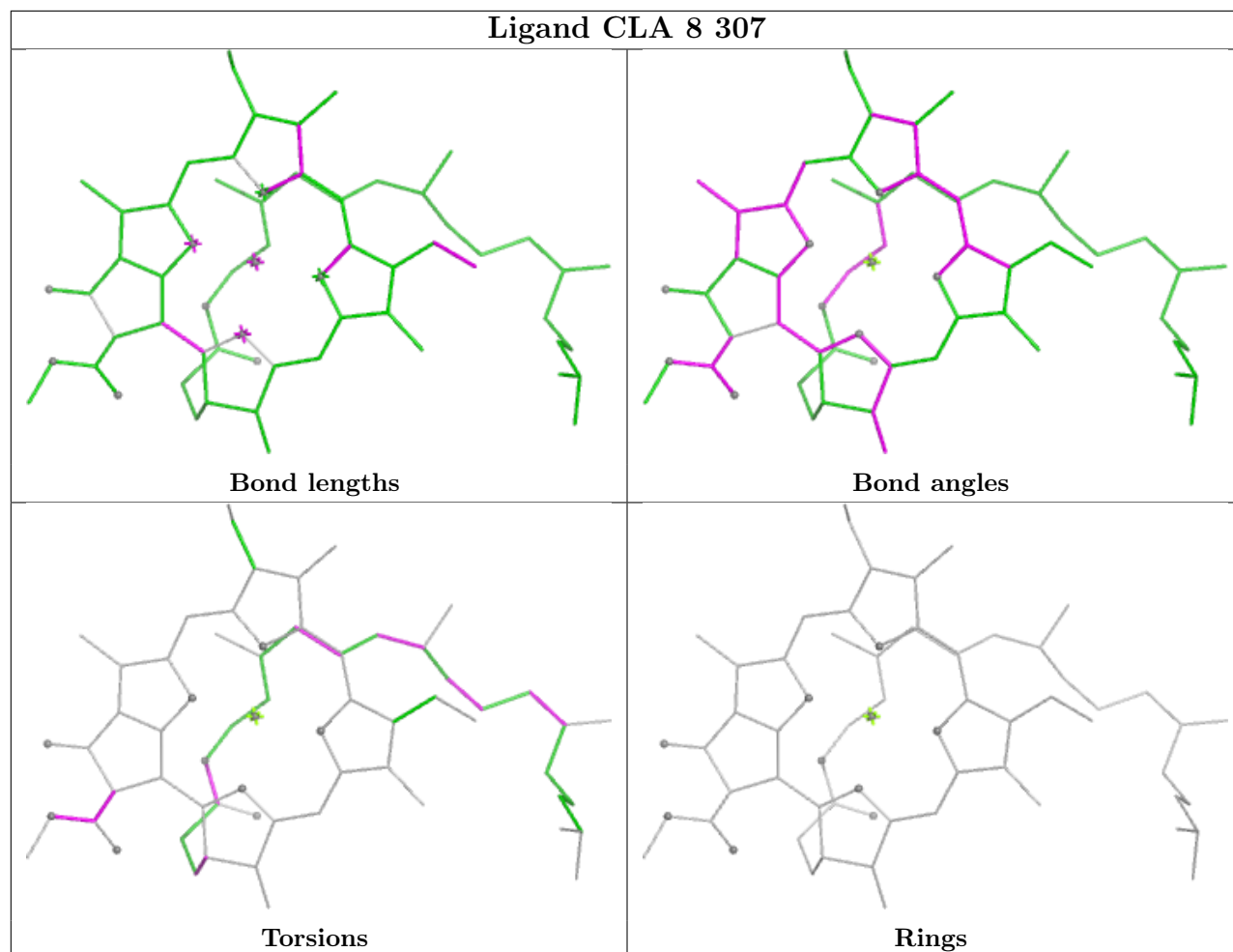


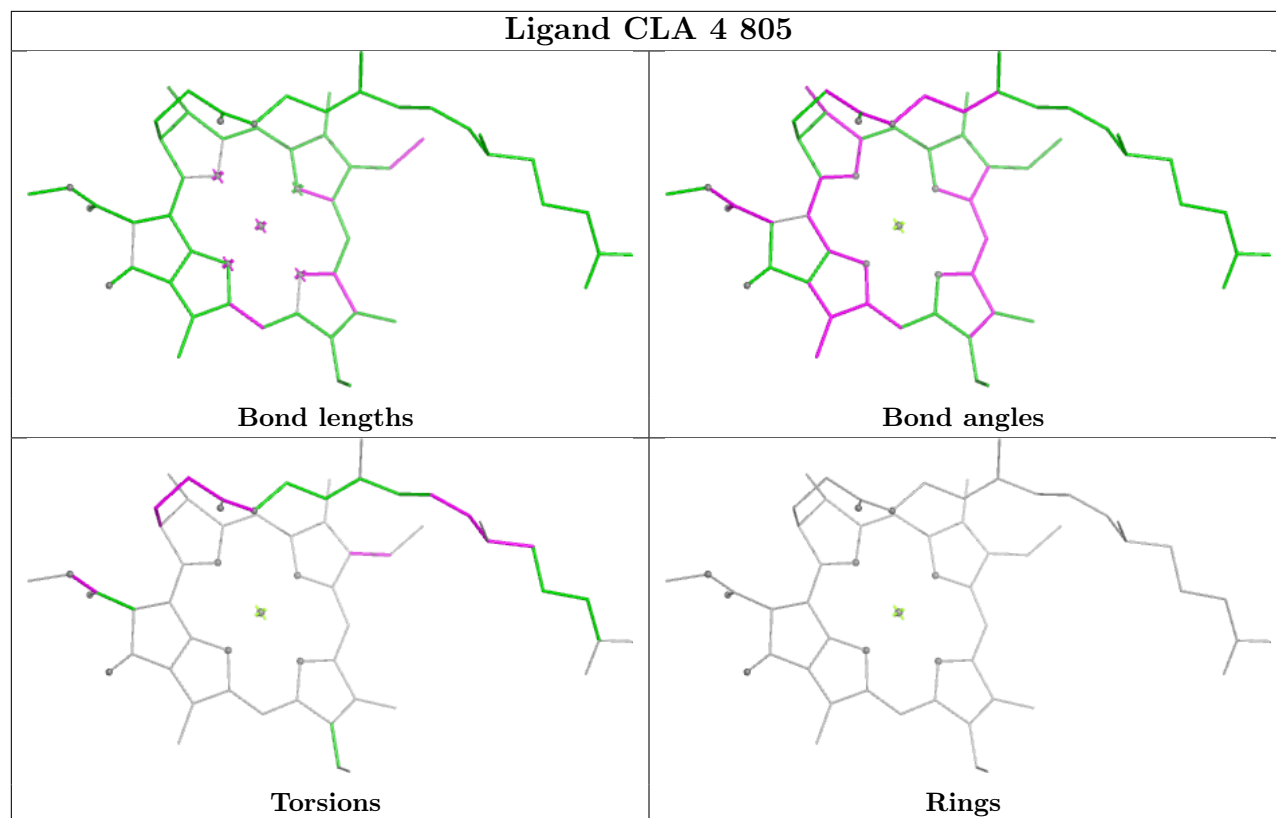
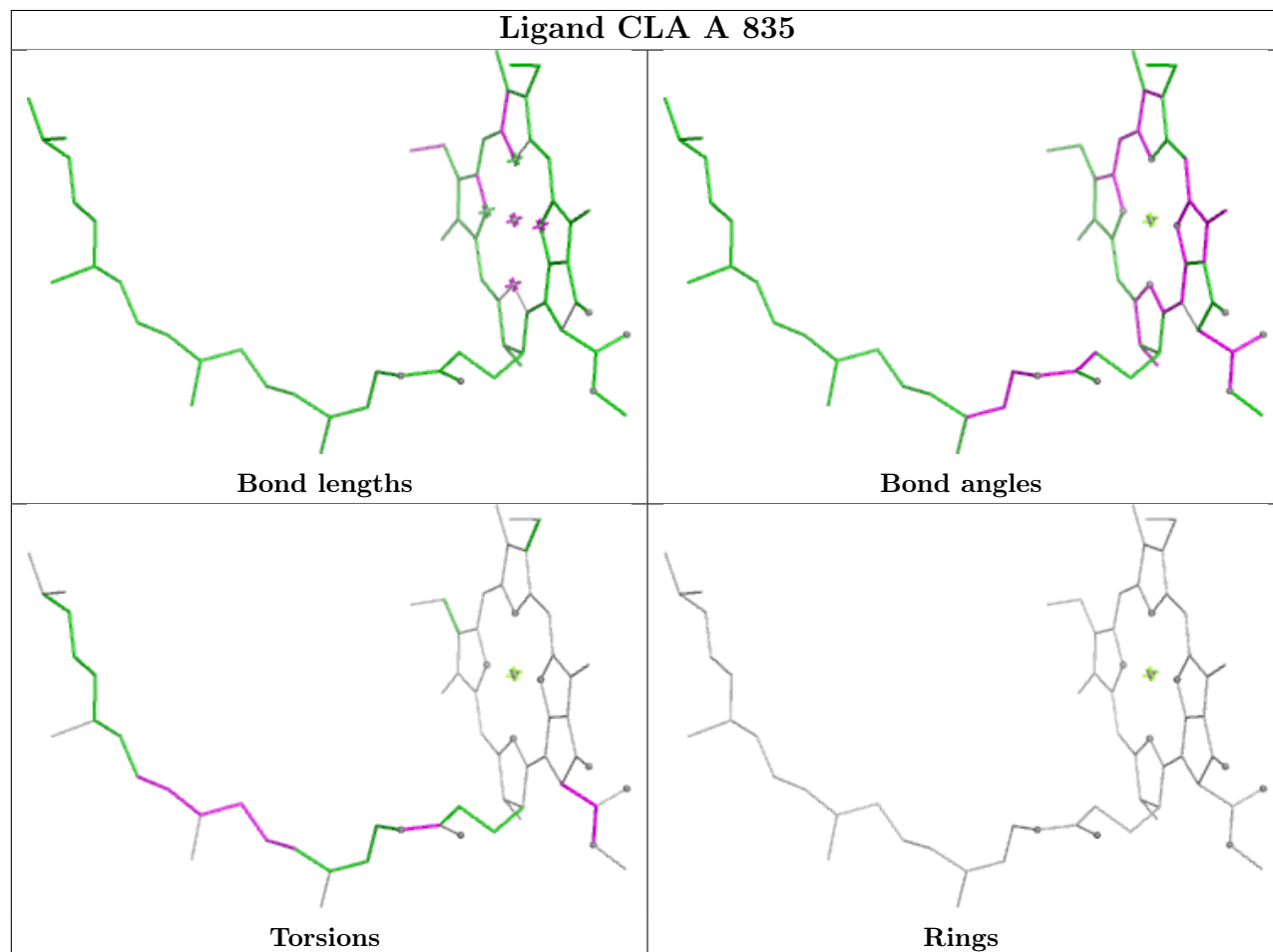
Torsions

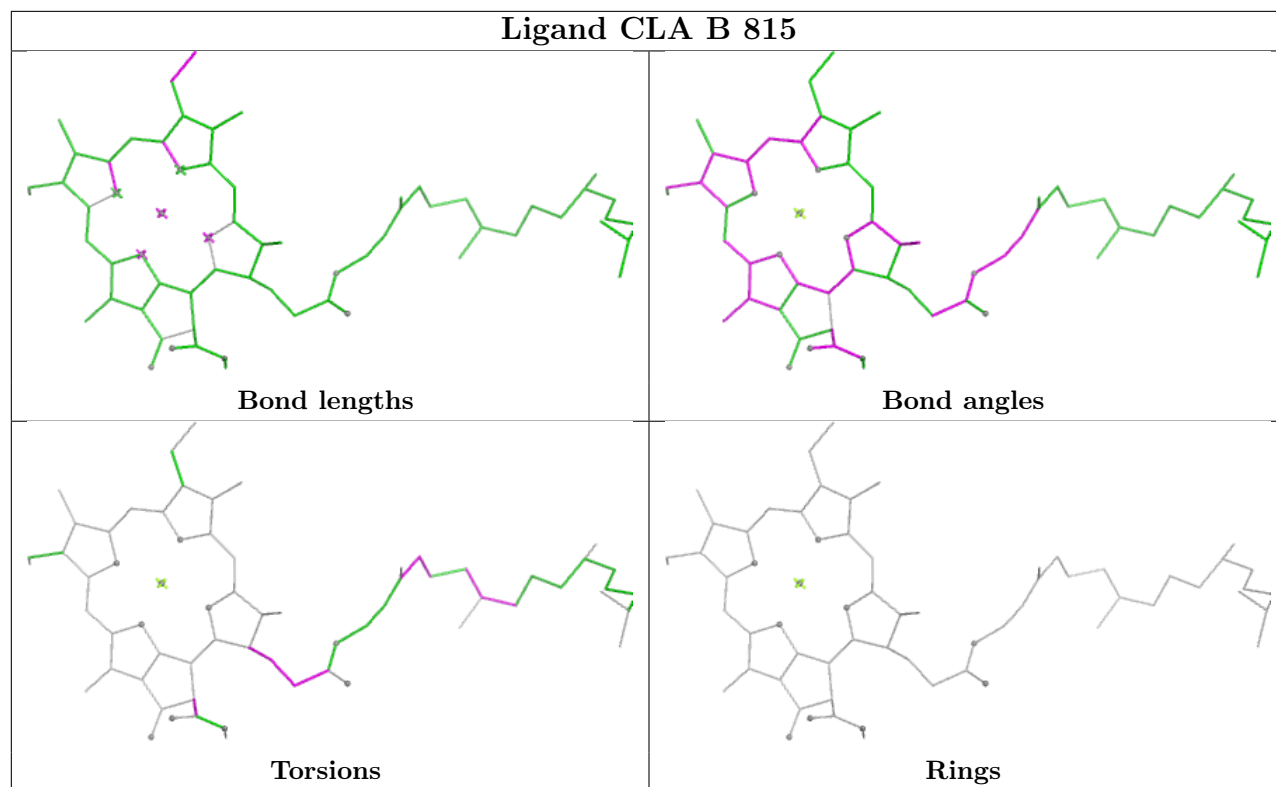


Rings

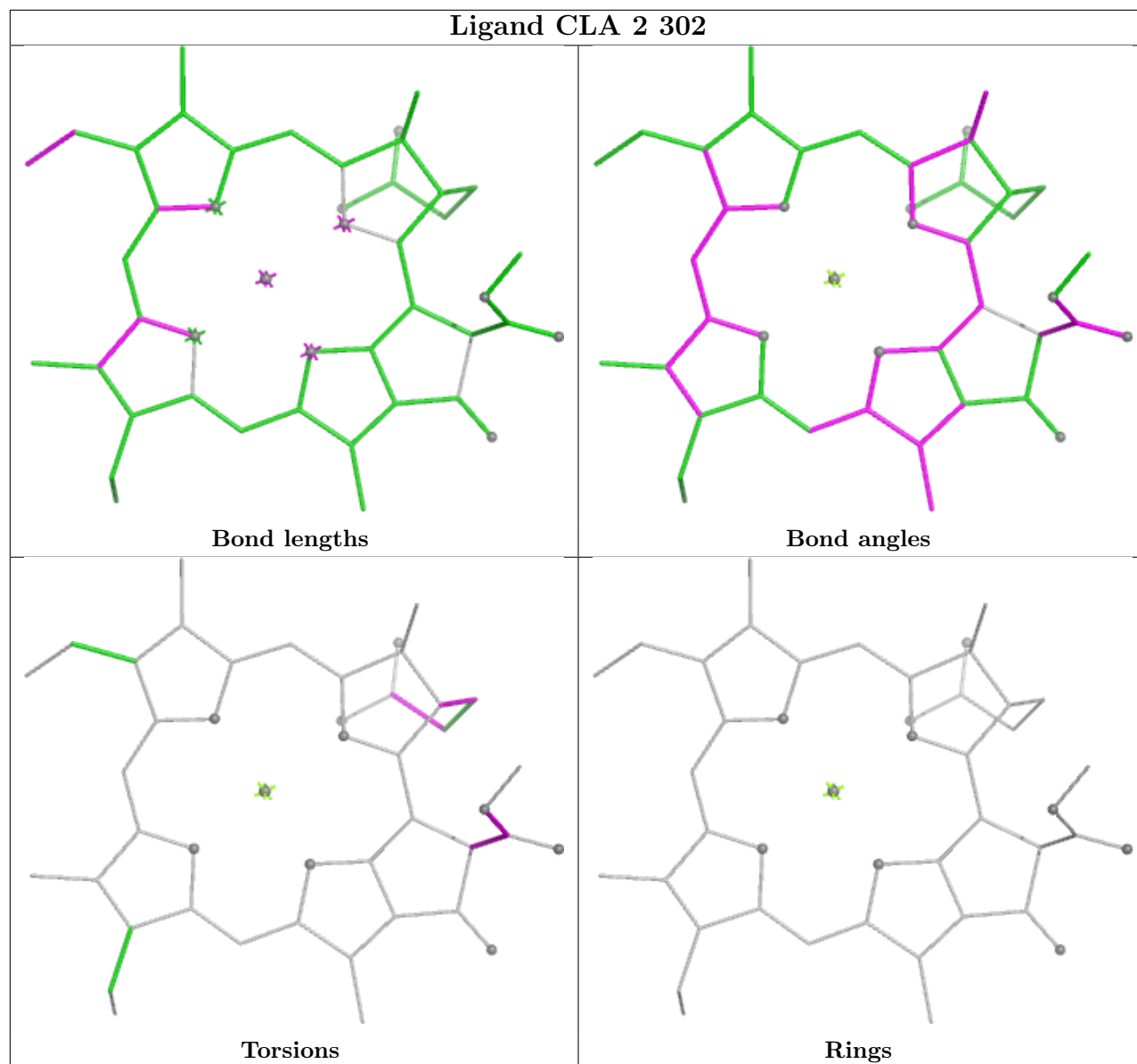
Ligand CLA 8 307



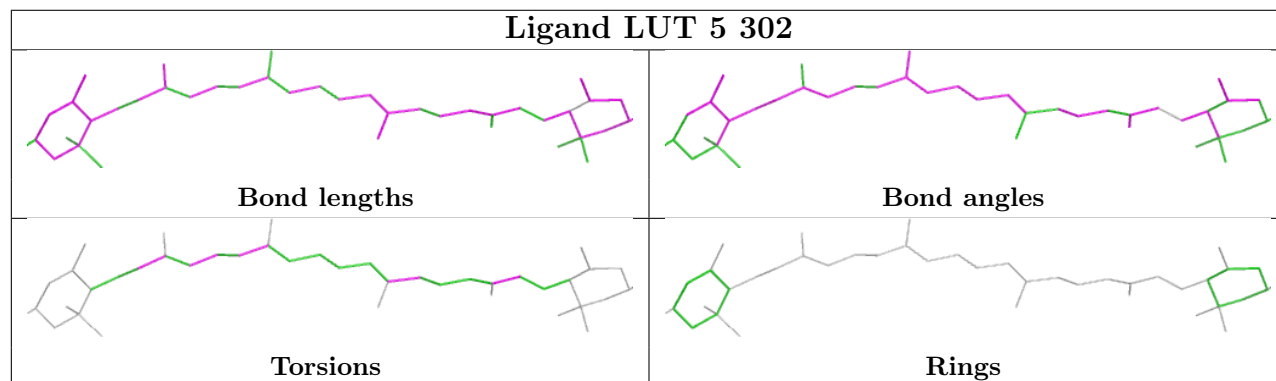
Ligand CLA 4 805**Ligand CLA A 835**



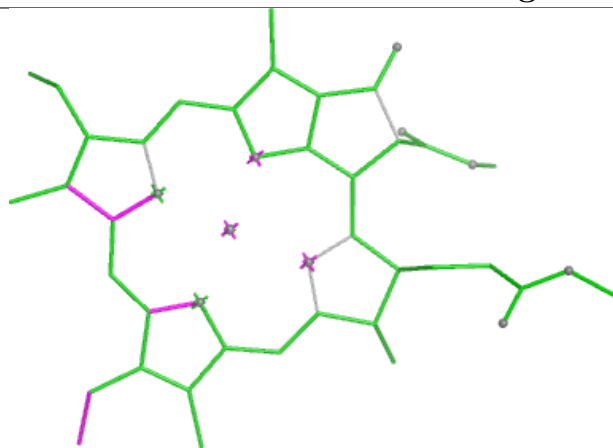
Ligand CLA 2 302



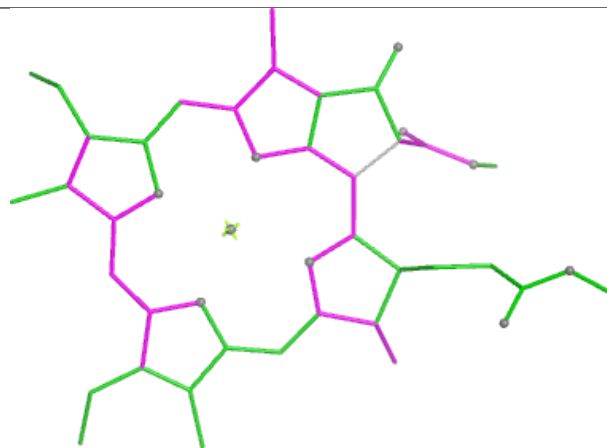
Ligand LUT 5 302



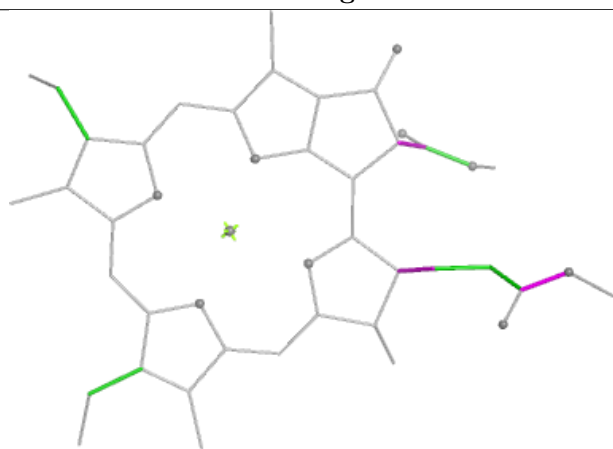
Ligand CLA 6 321



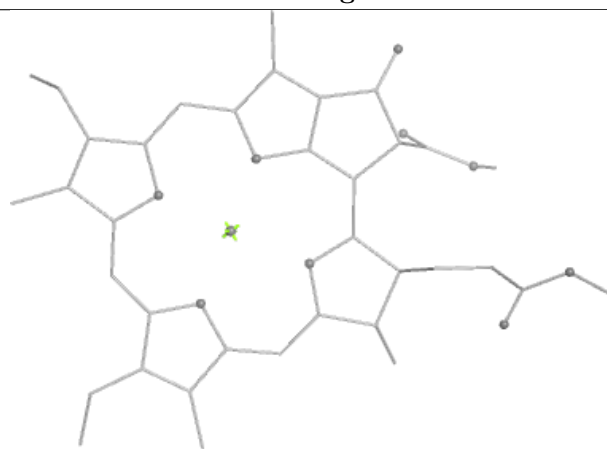
Bond lengths



Bond angles

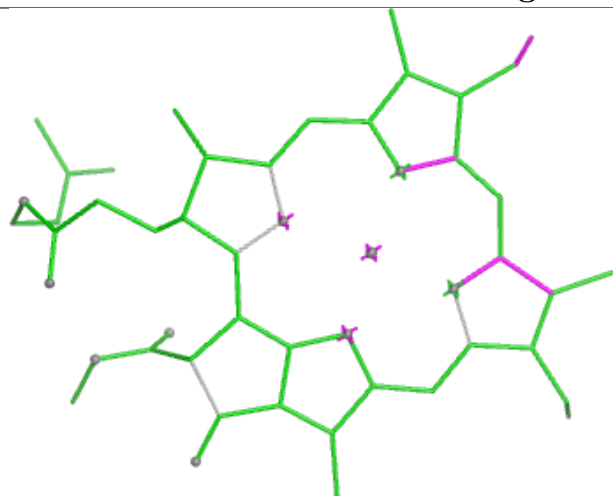


Torsions

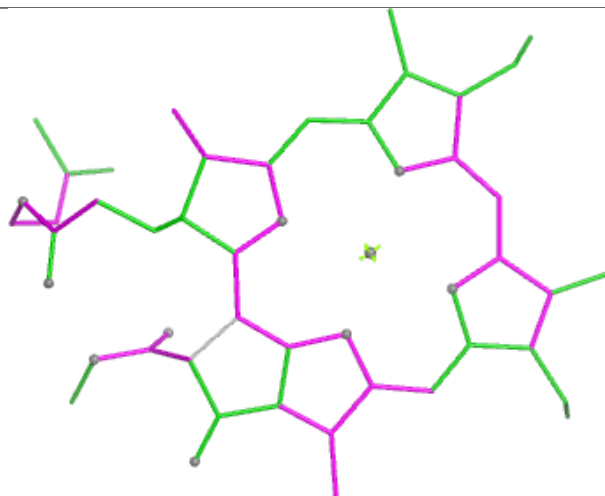


Rings

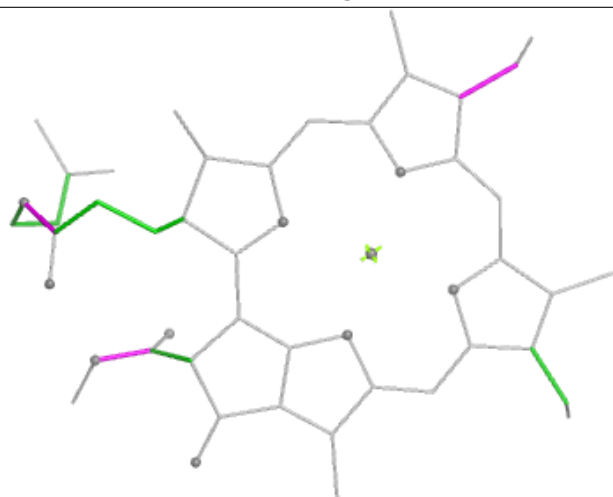
Ligand CLA 7 305



Bond lengths



Bond angles

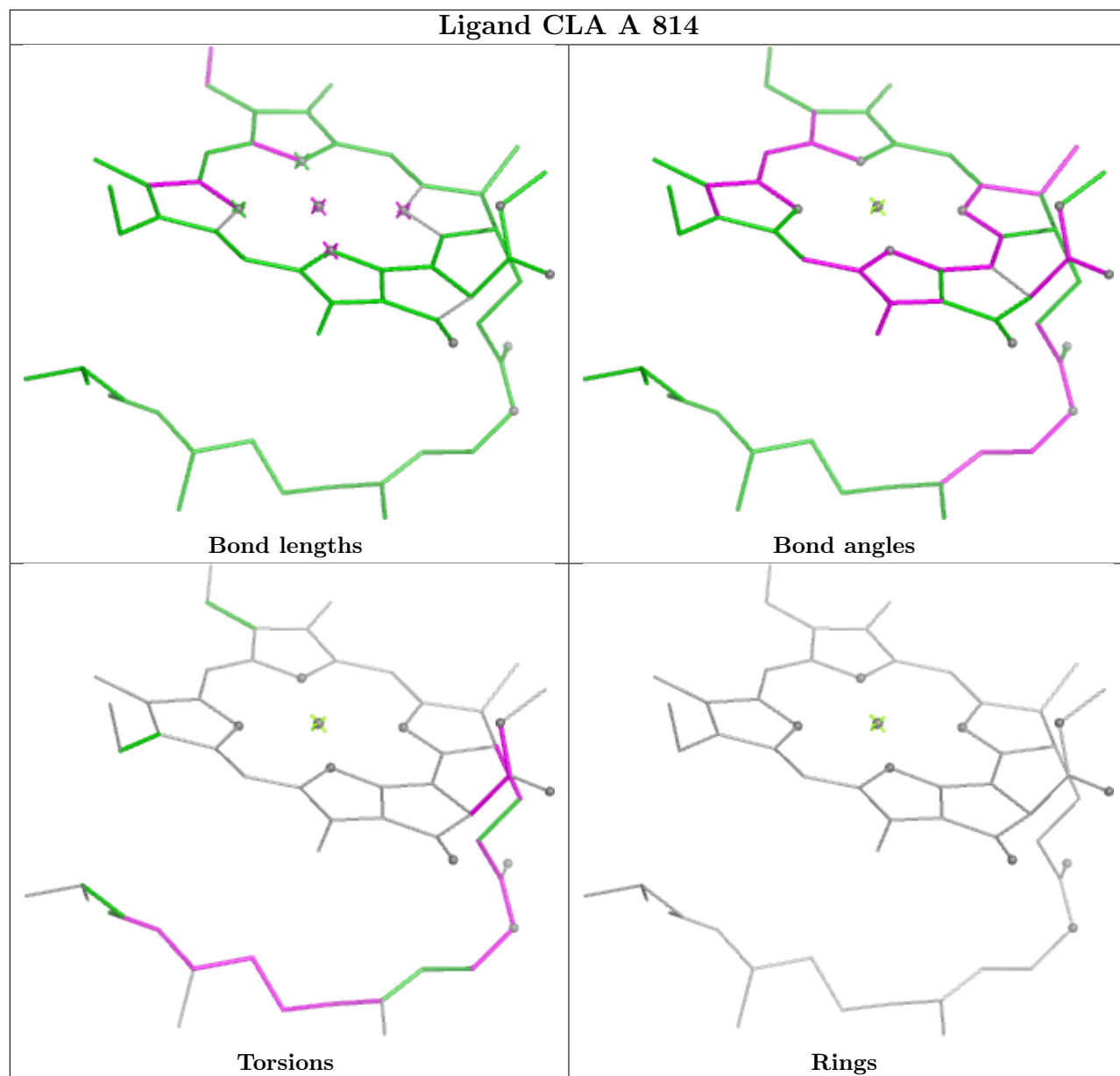


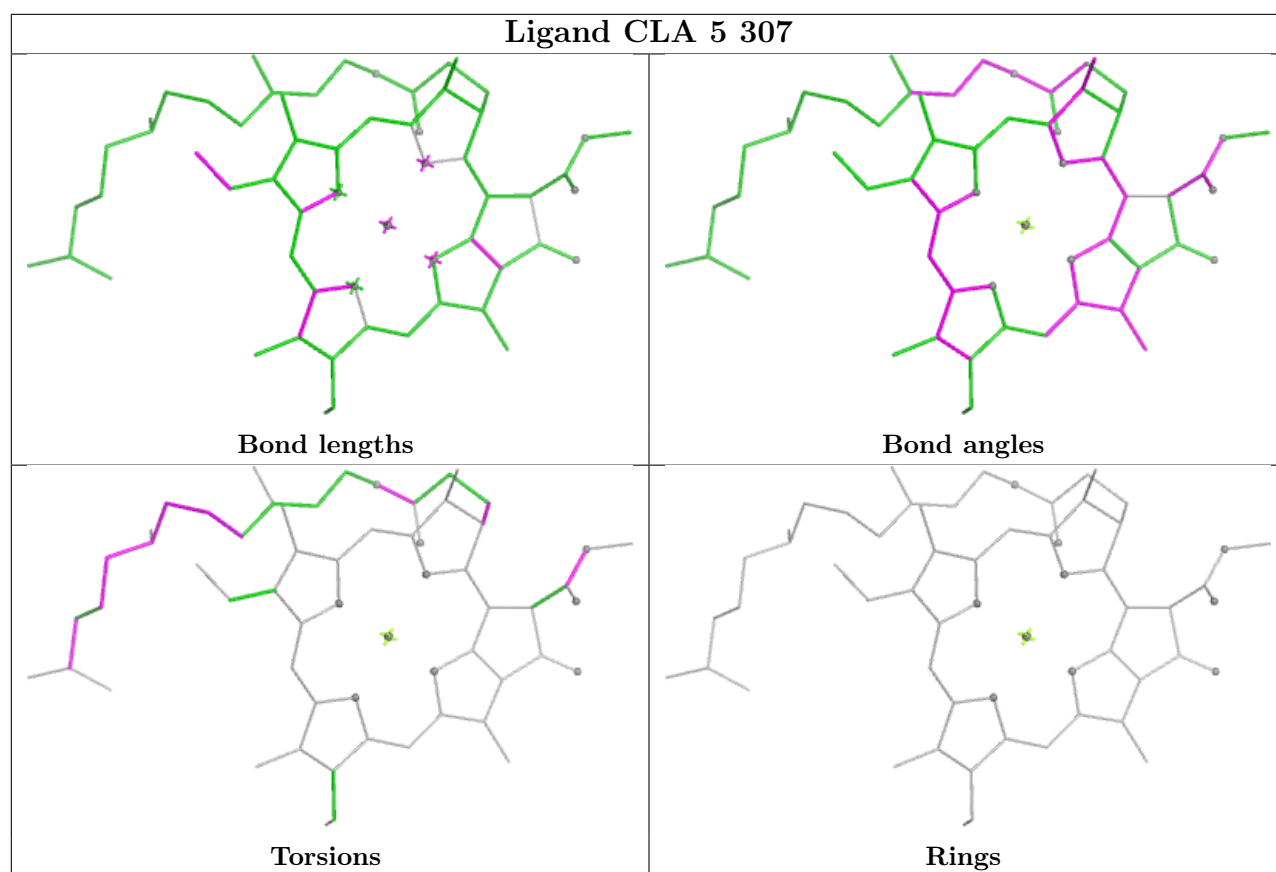
Torsions



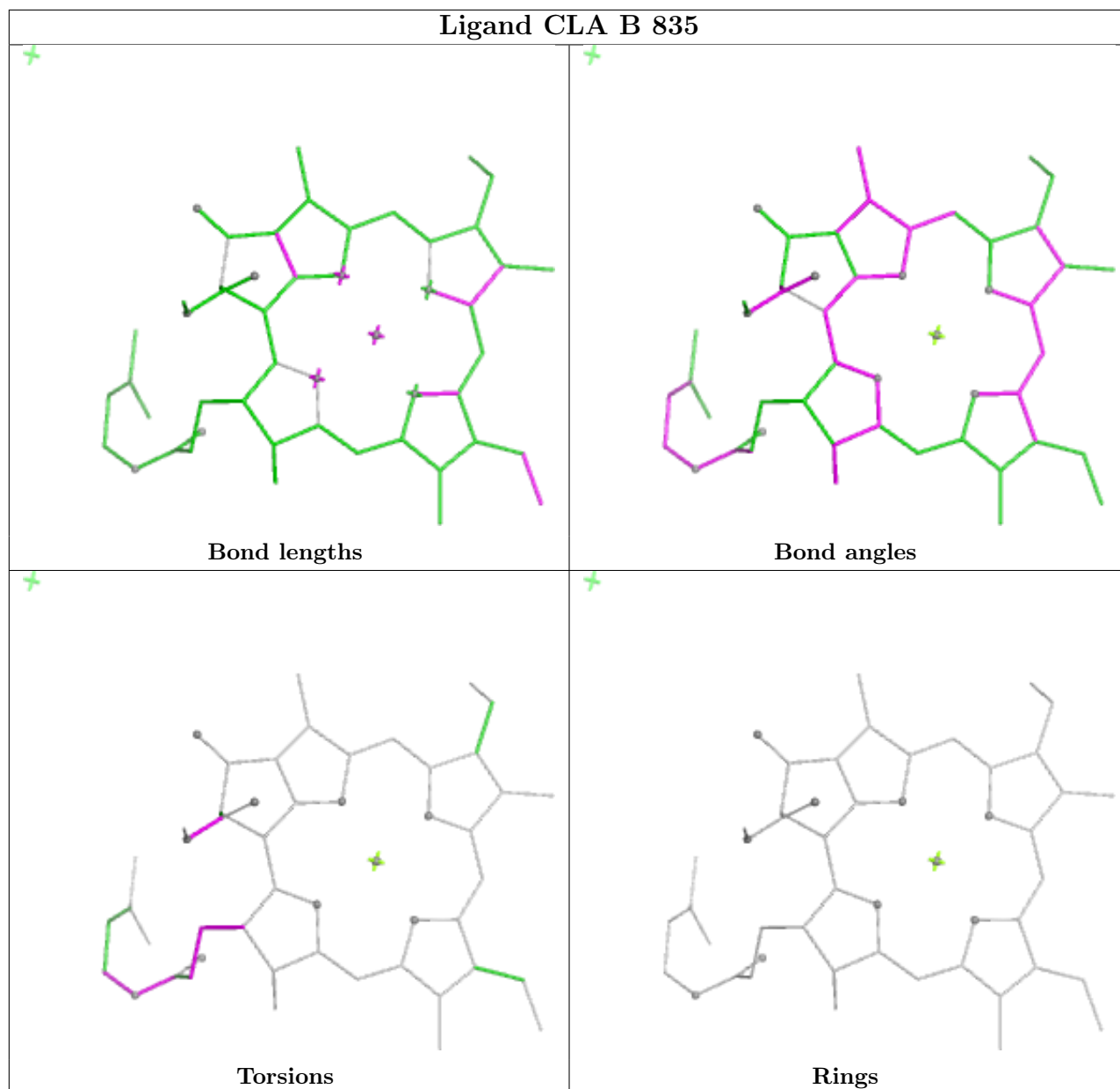
Rings

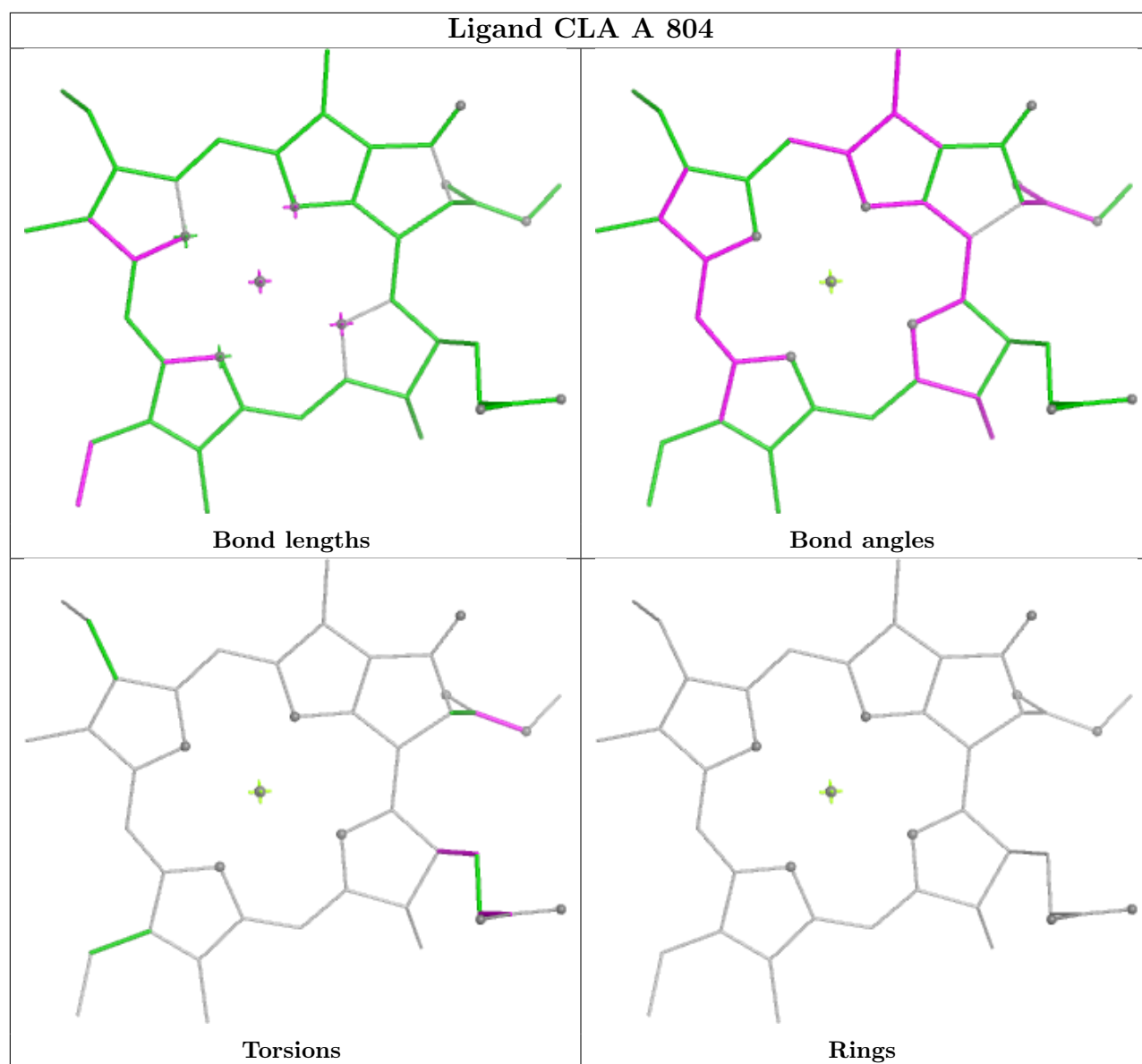
Ligand CLA A 814

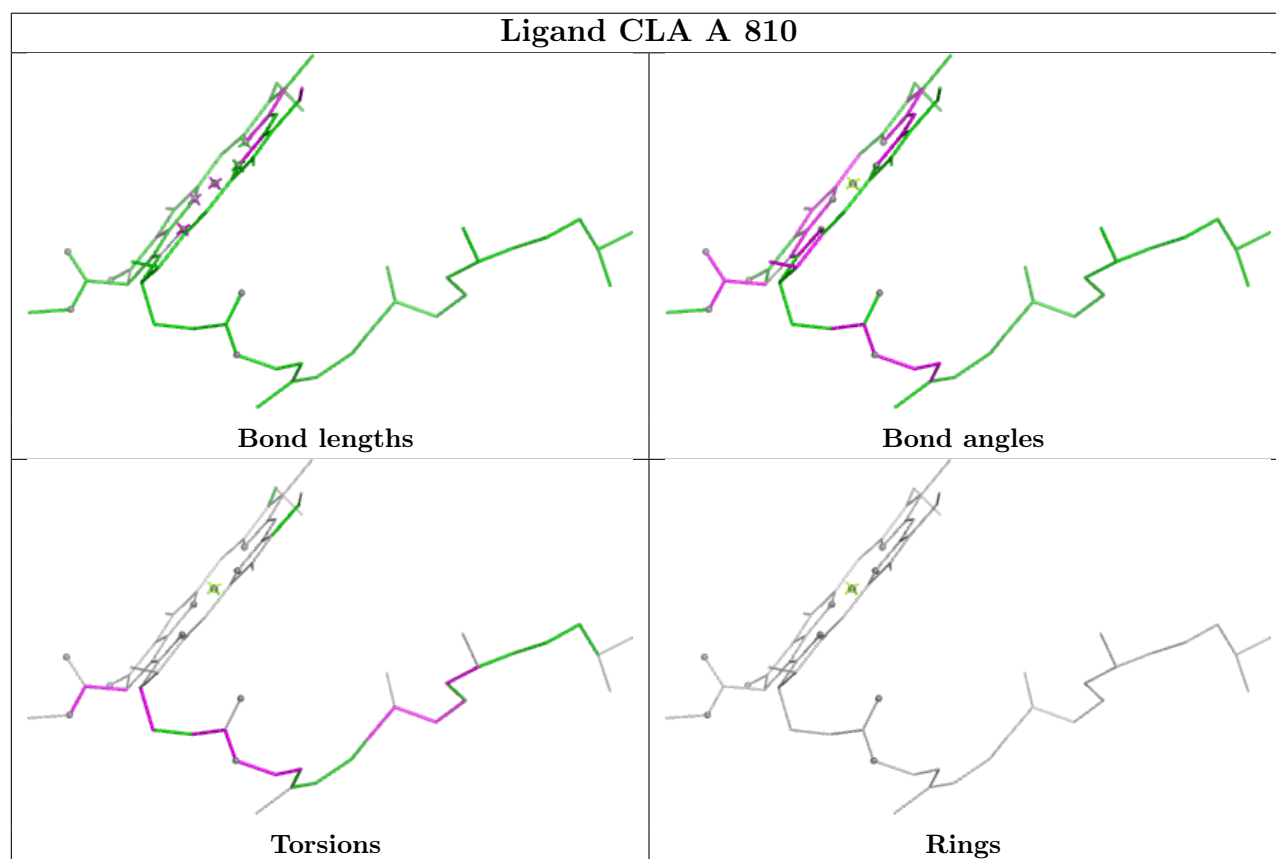
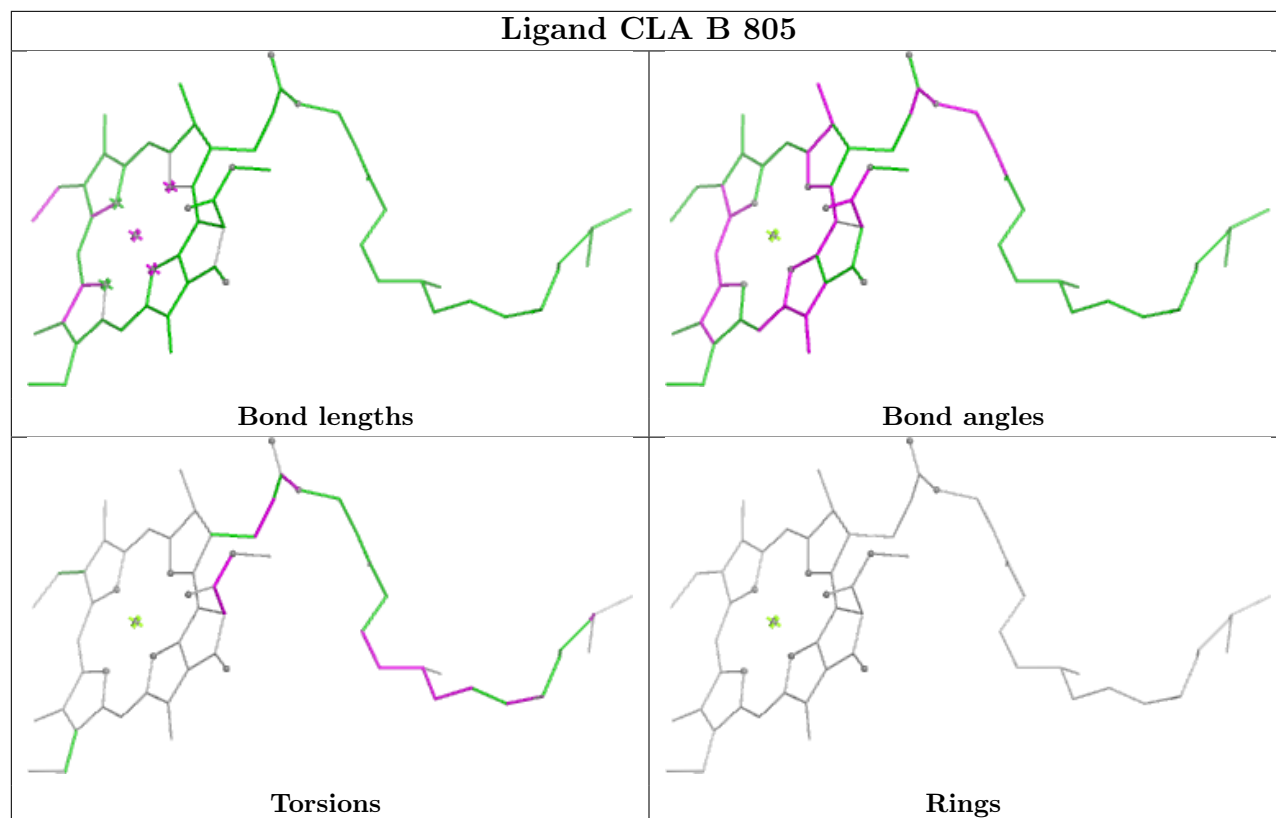


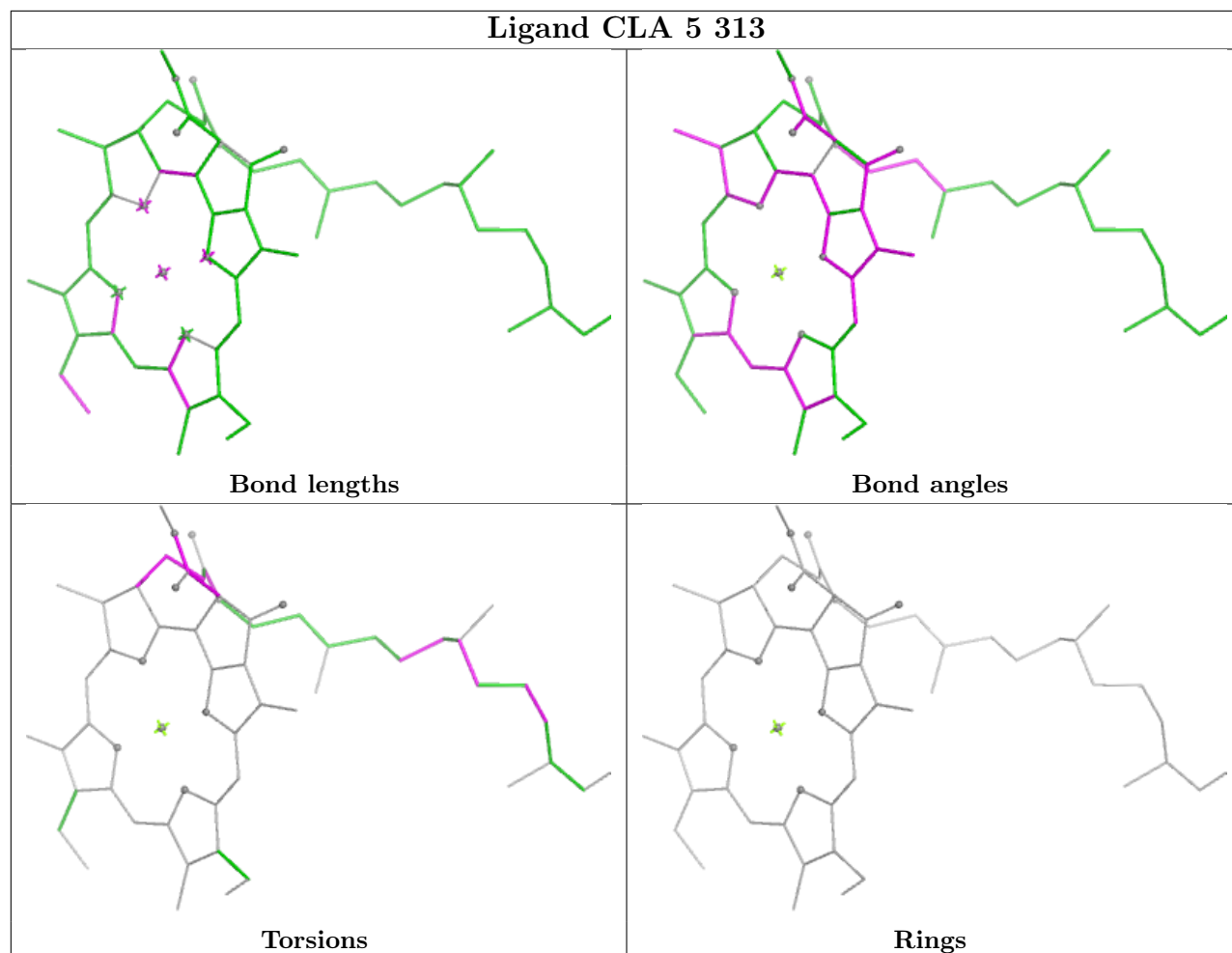
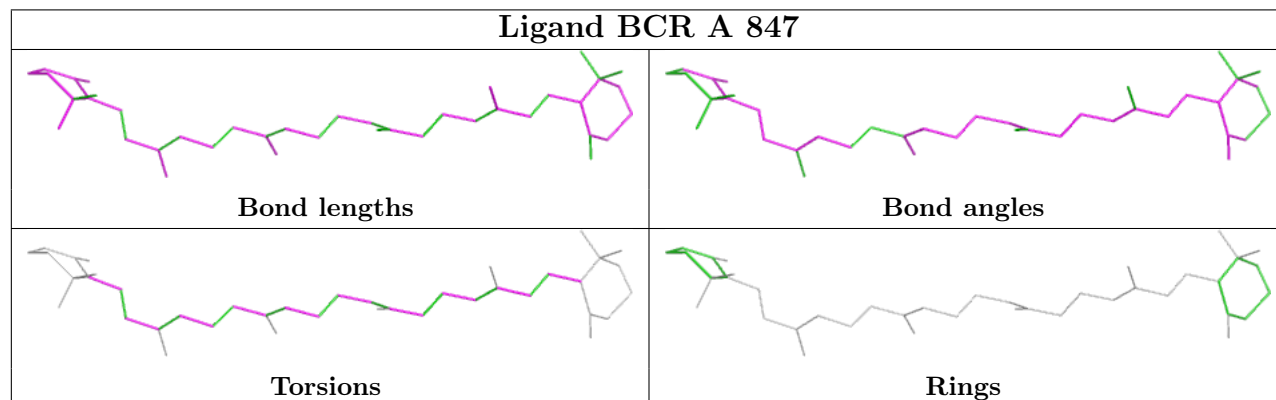


Ligand CLA B 835

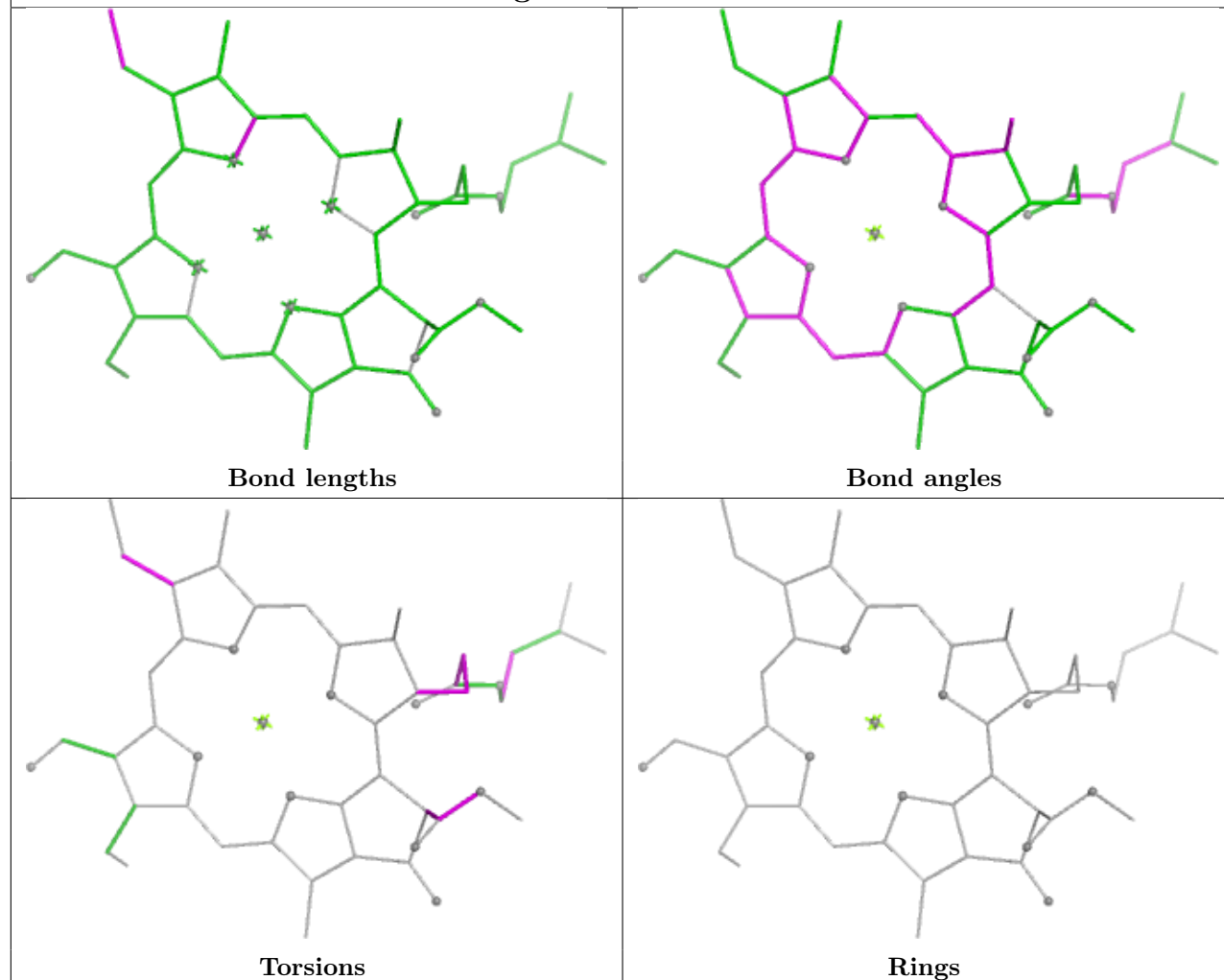




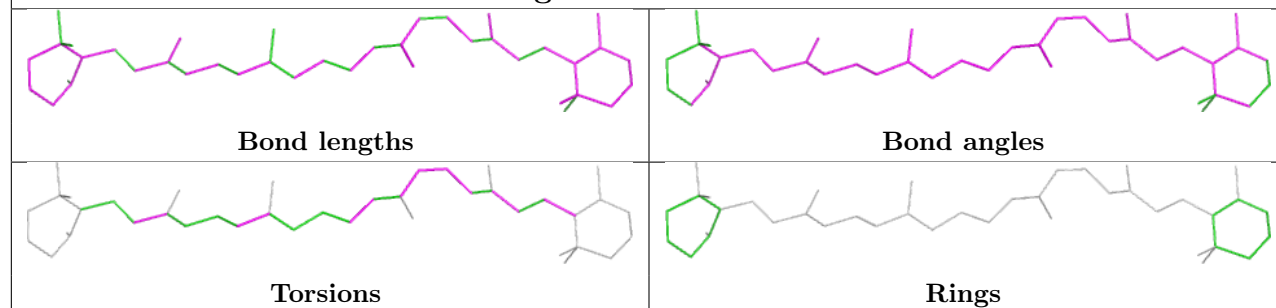


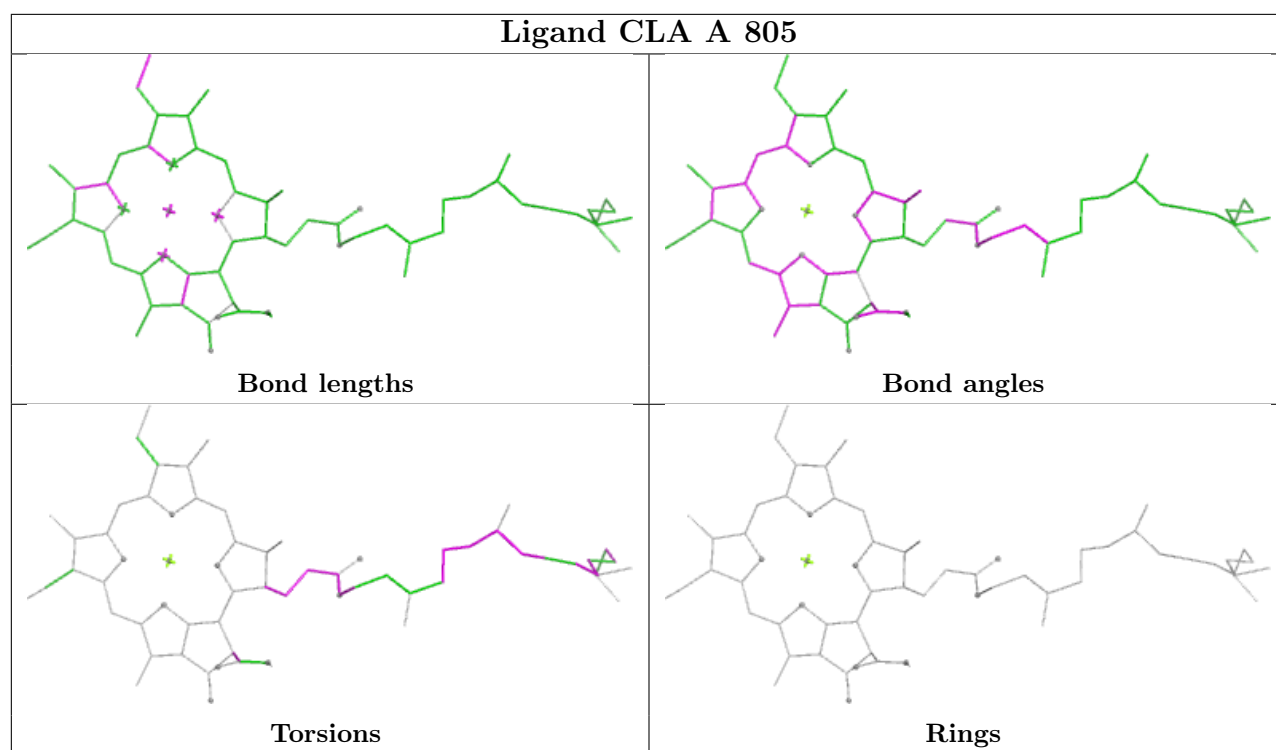
Ligand CLA 5 313**Ligand BCR A 847**

Ligand CHL 4 814

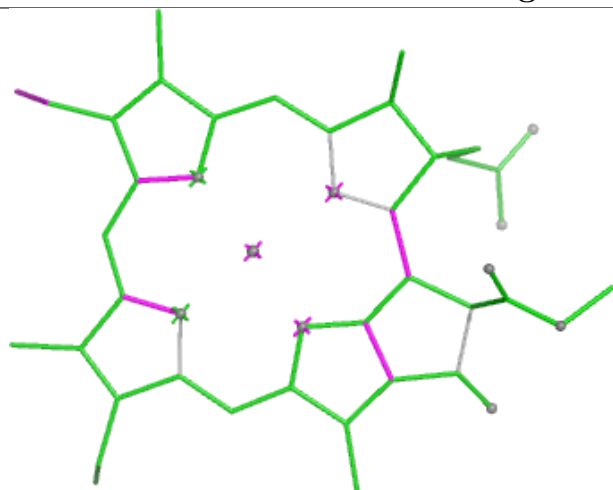


Ligand BCR 3 307

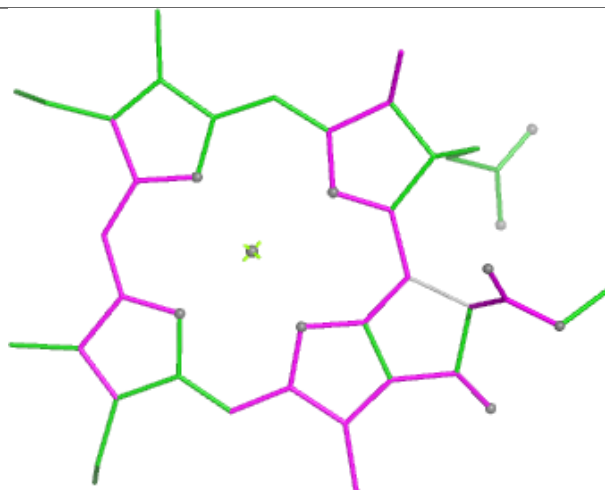




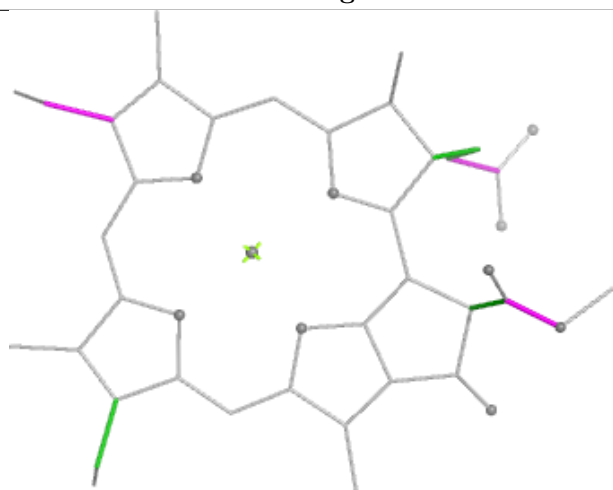
Ligand CLA 9 310



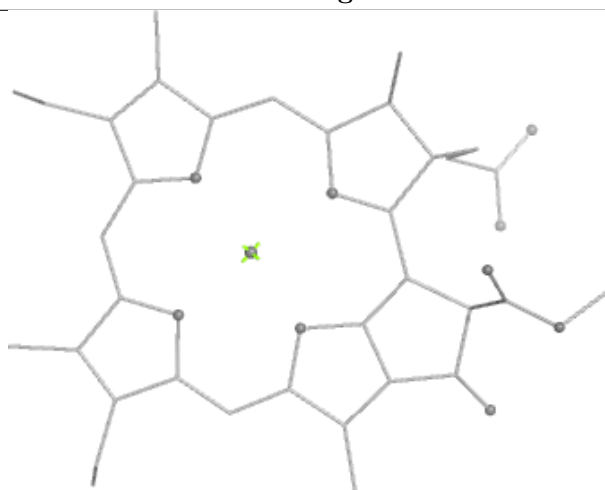
Bond lengths



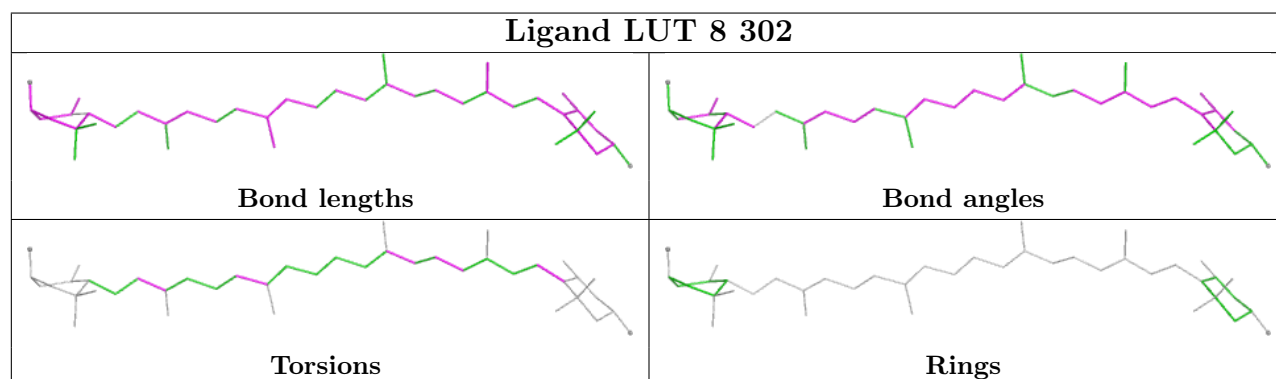
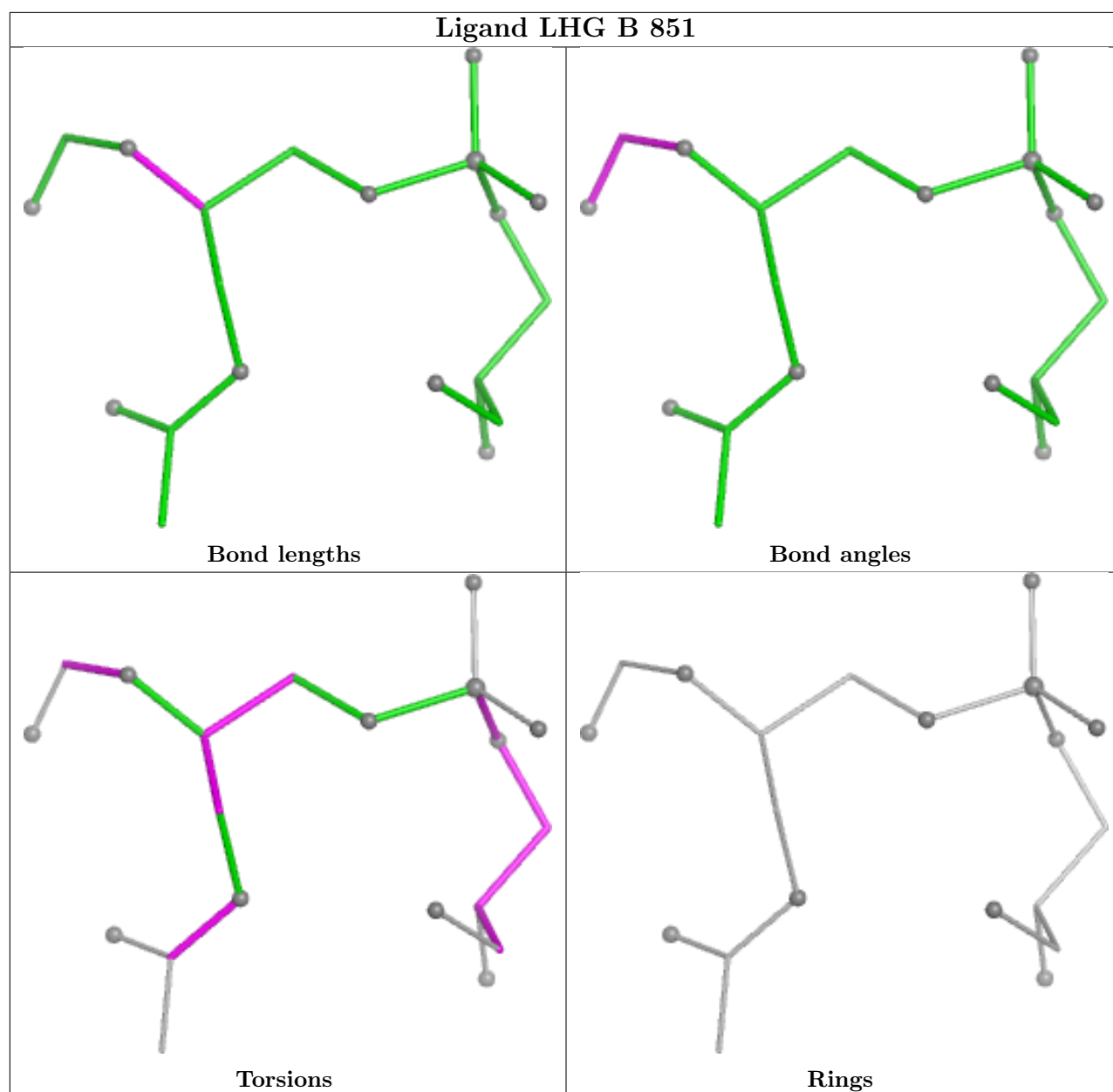
Bond angles



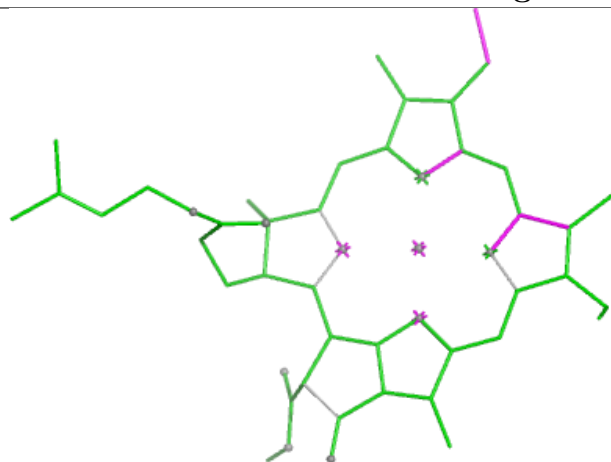
Torsions



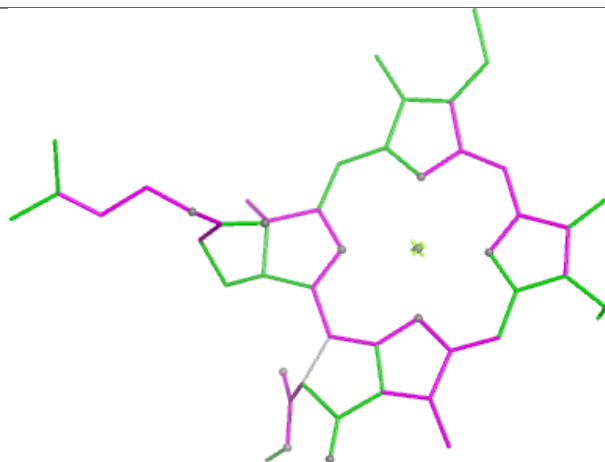
Rings



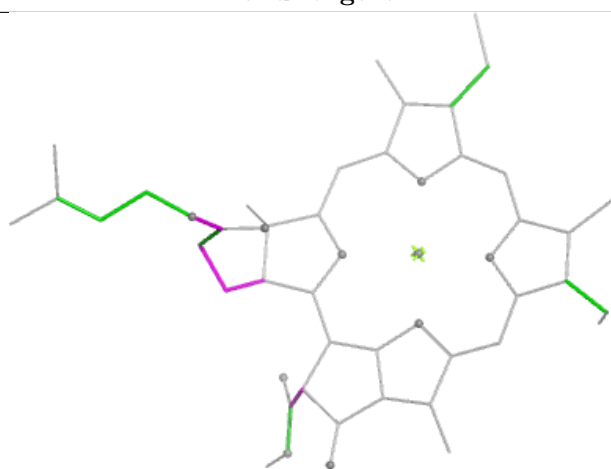
Ligand CLA A 826



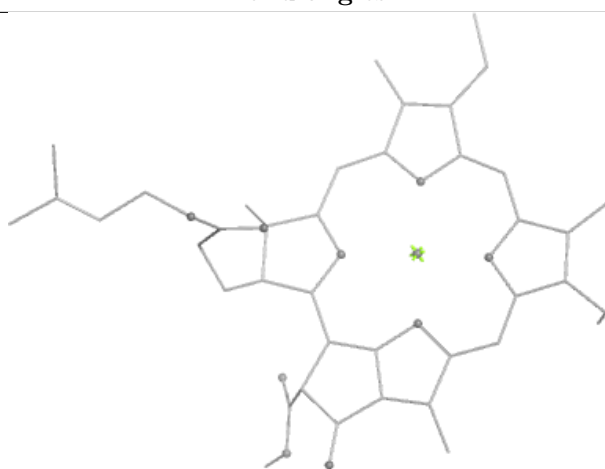
Bond lengths



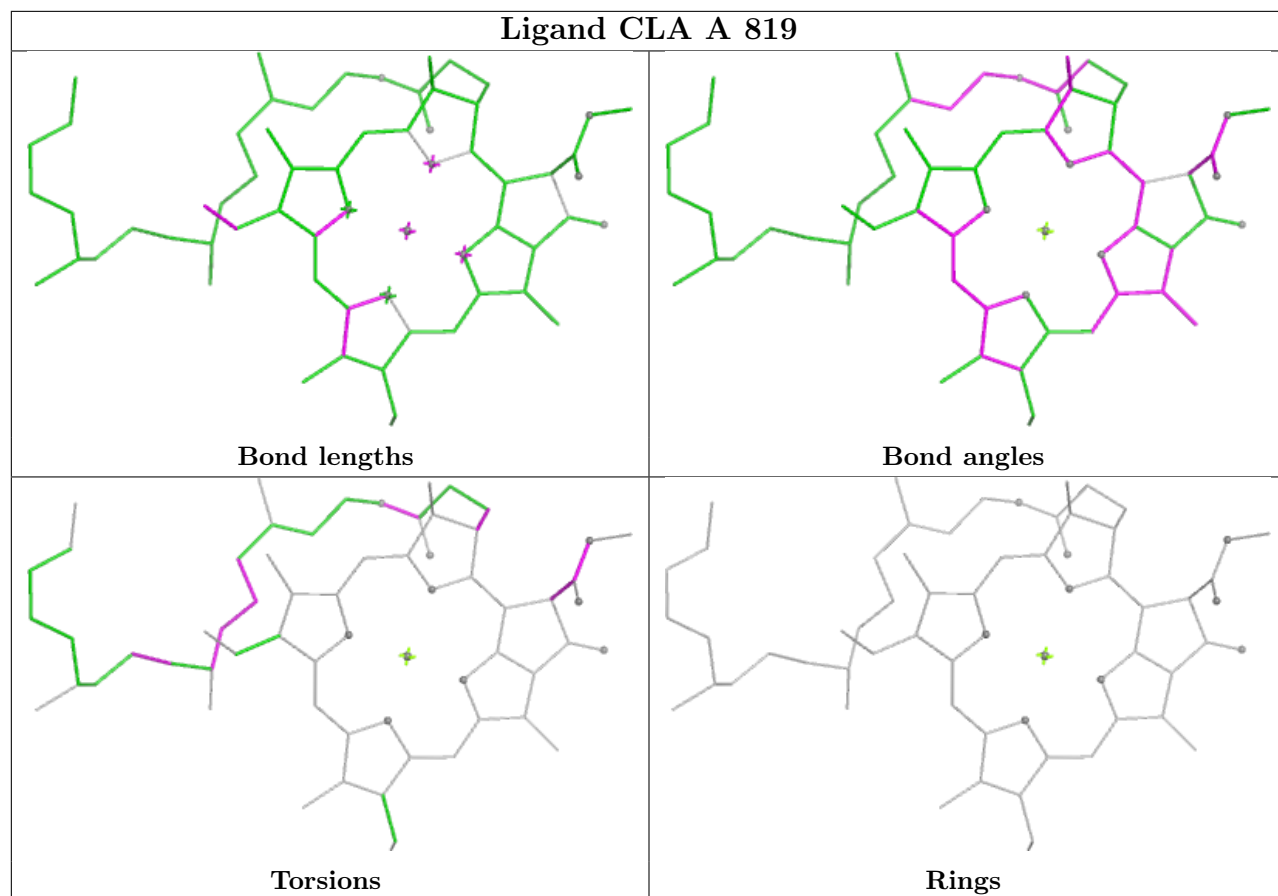
Bond angles



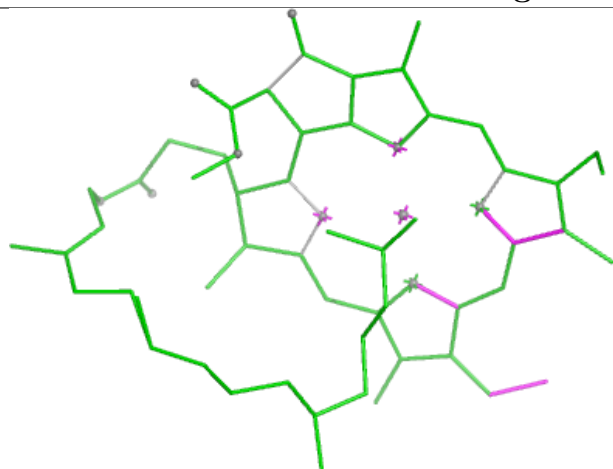
Torsions



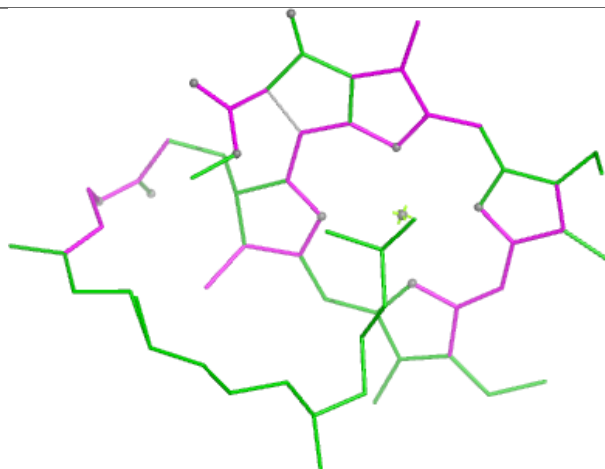
Rings



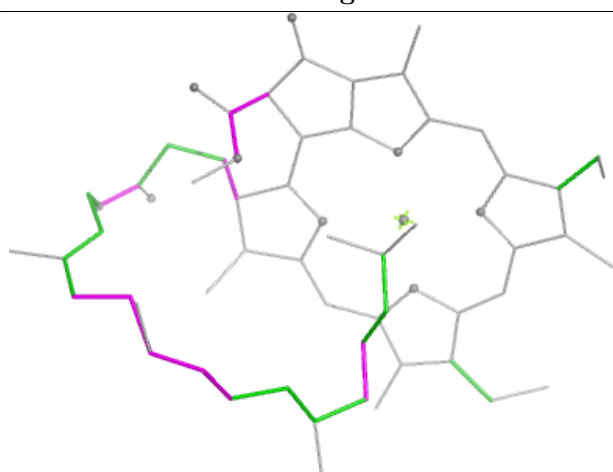
Ligand CLA A 806



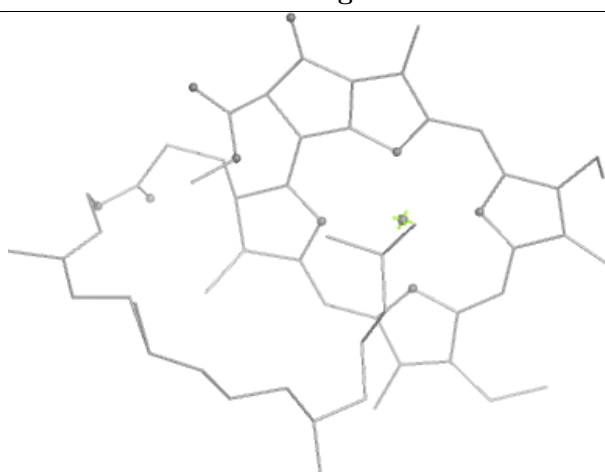
Bond lengths



Bond angles

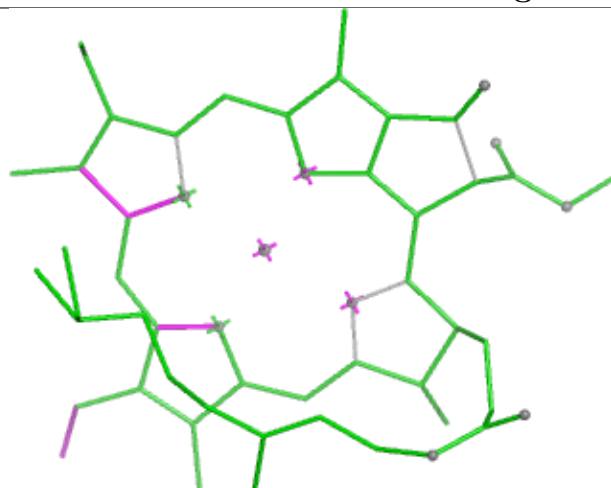


Torsions

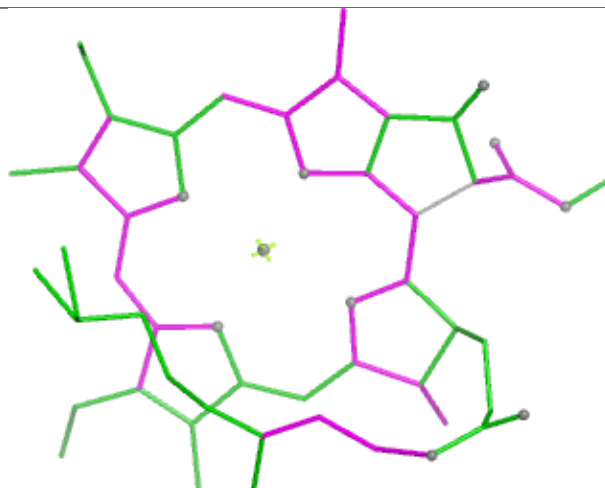


Rings

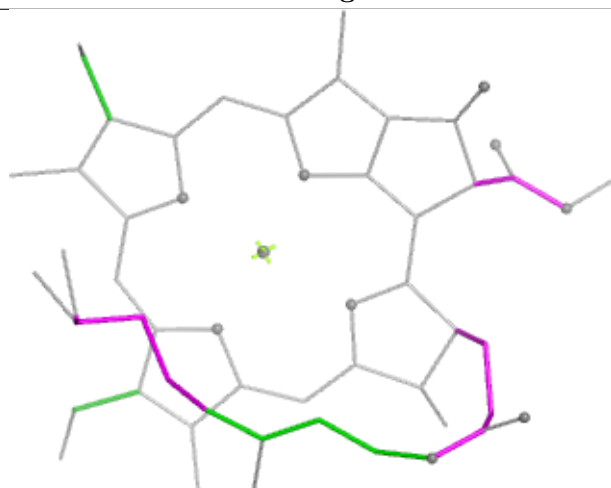
Ligand CLA B 822



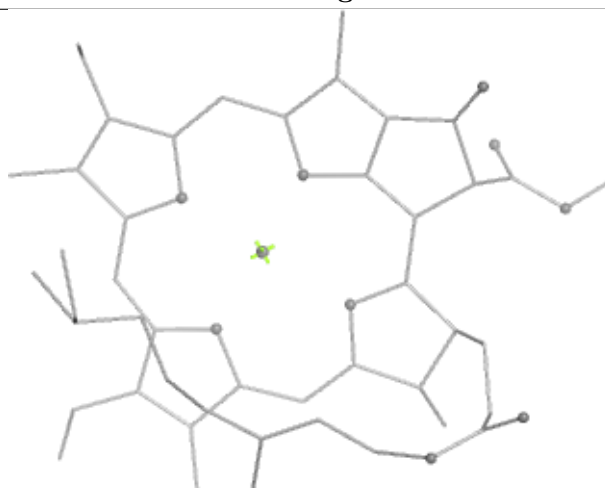
Bond lengths



Bond angles

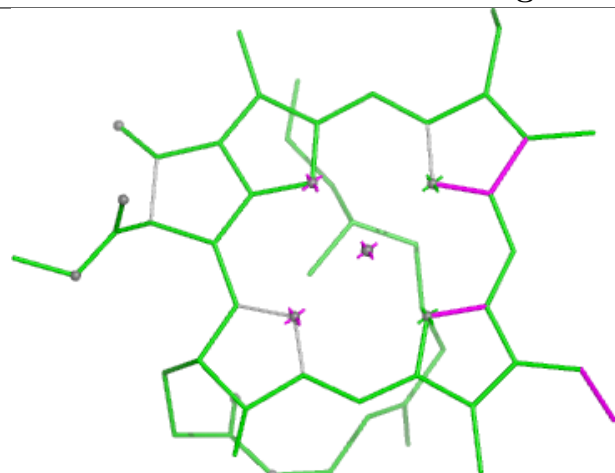


Torsions

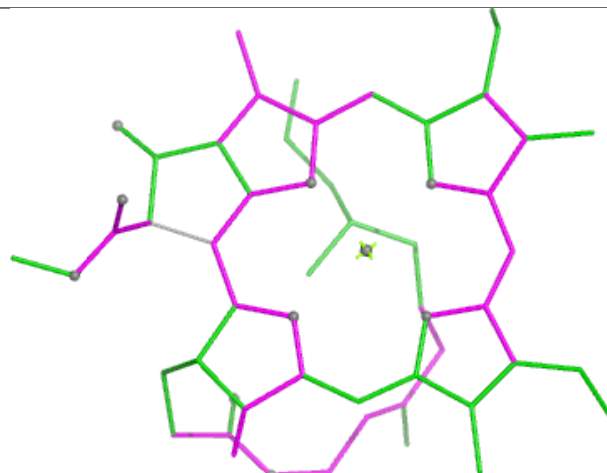


Rings

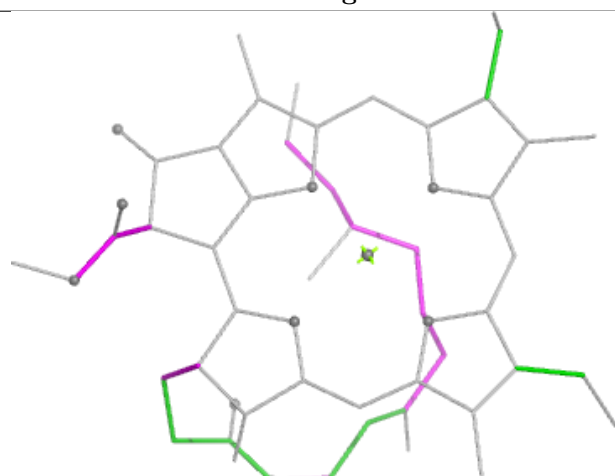
Ligand CLA B 829



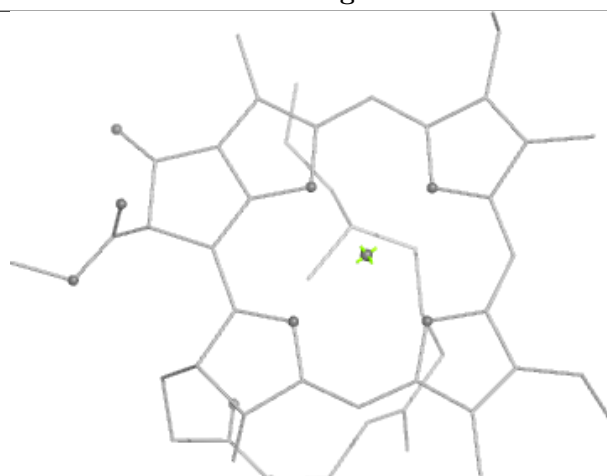
Bond lengths



Bond angles

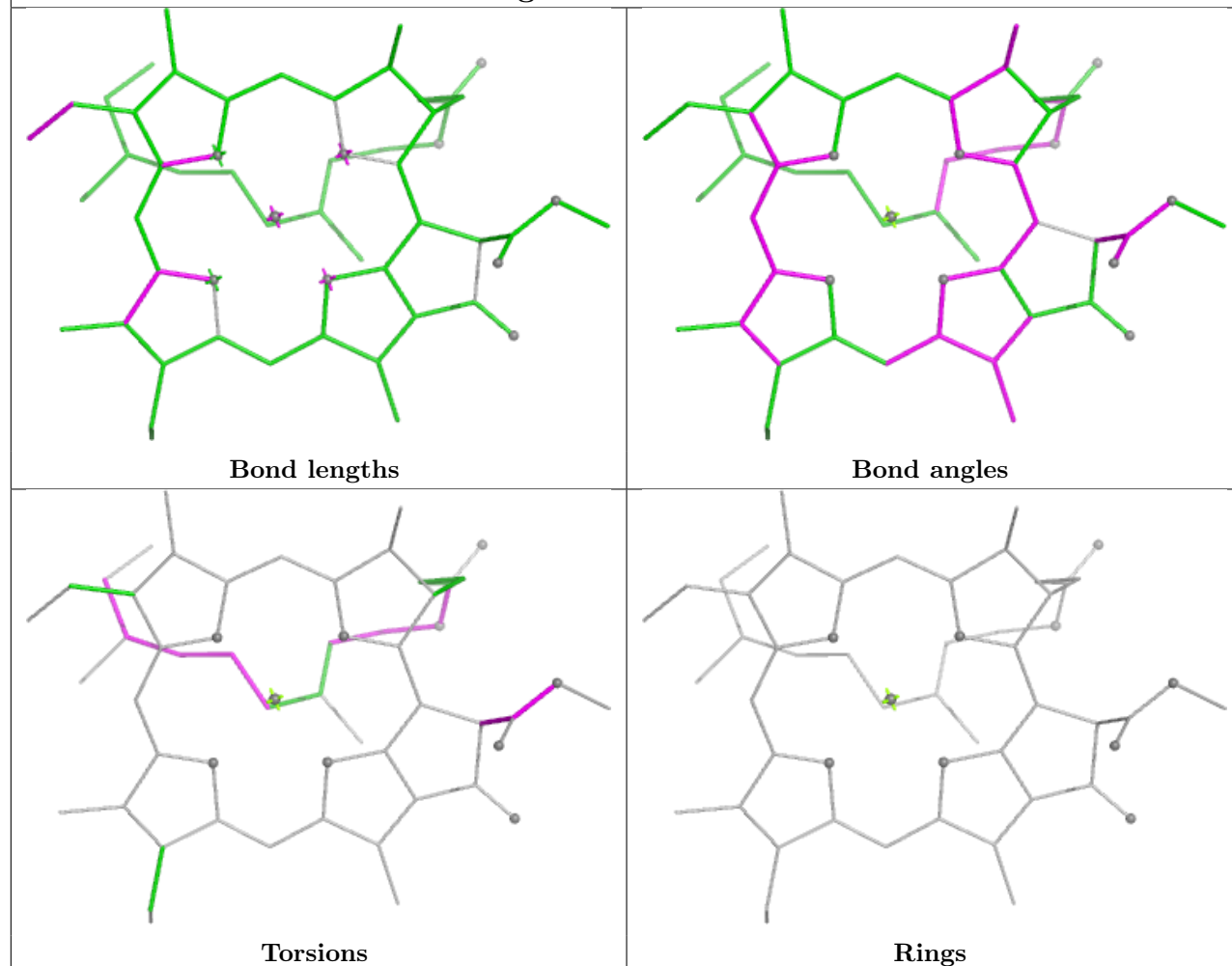


Torsions

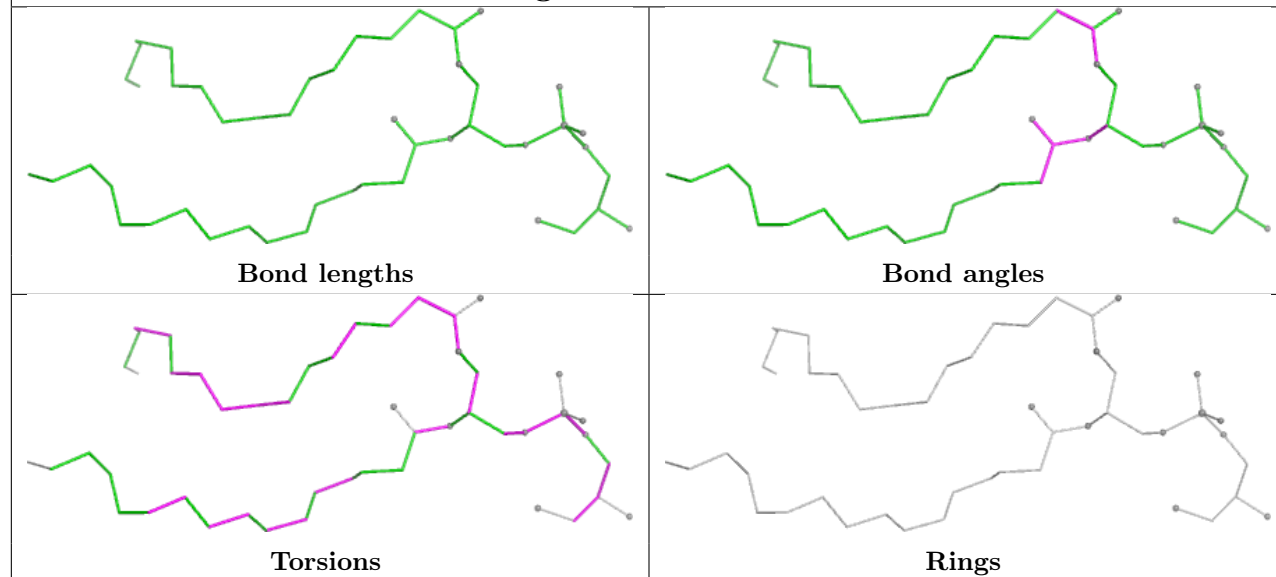


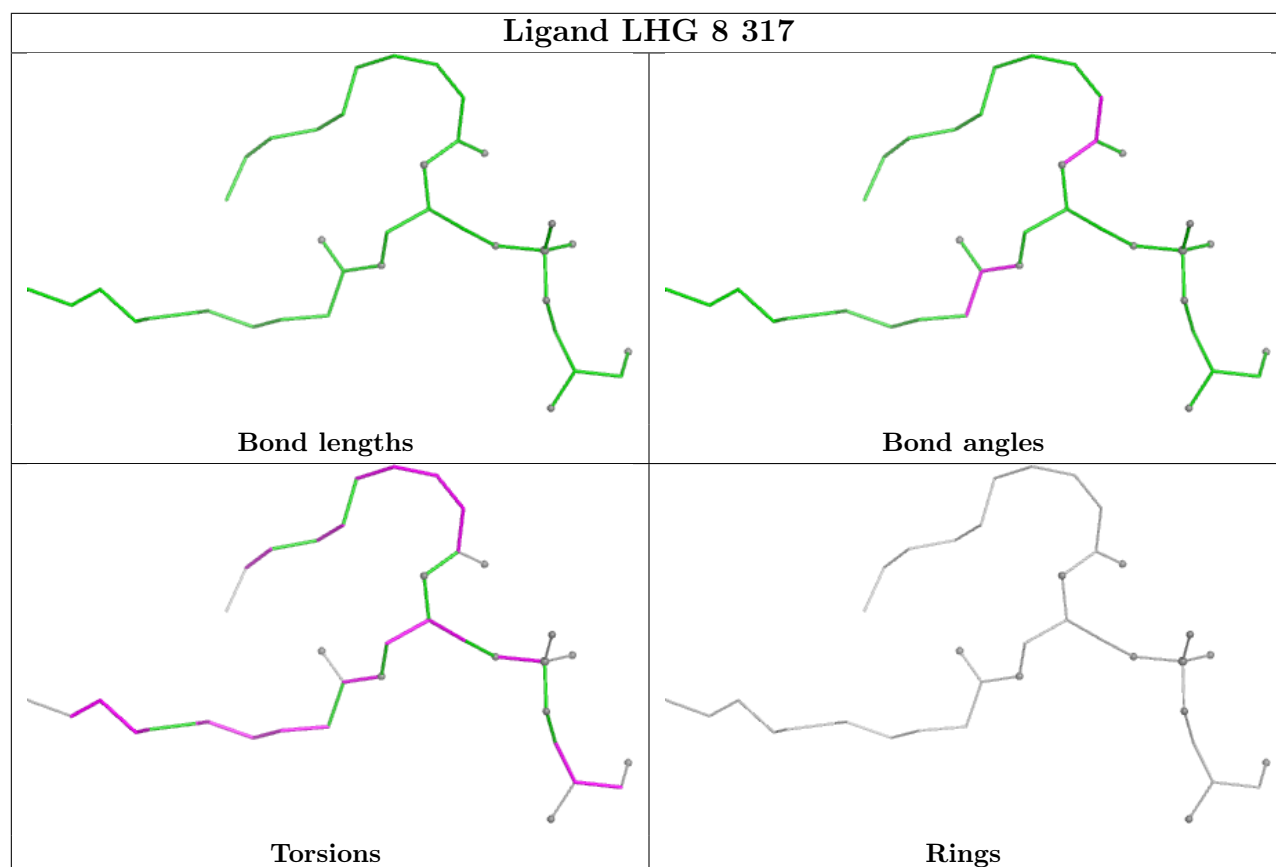
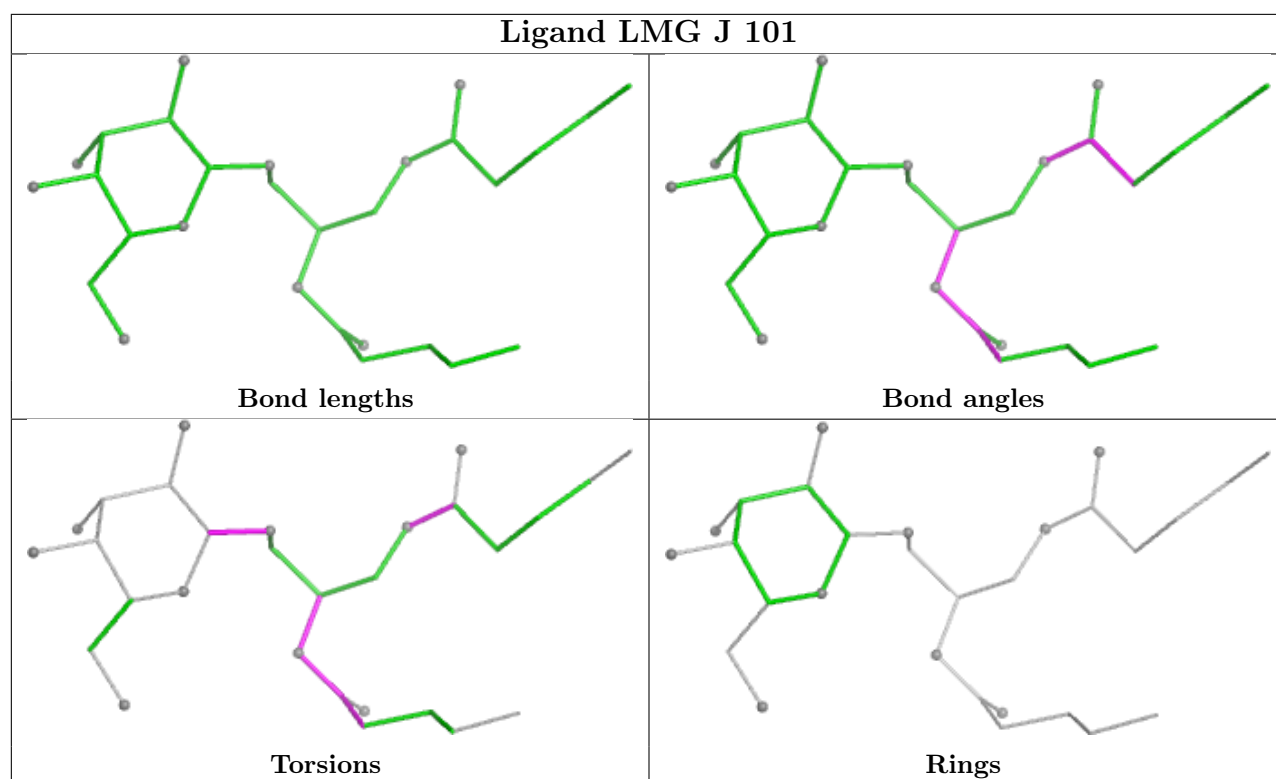
Rings

Ligand CLA 5 301

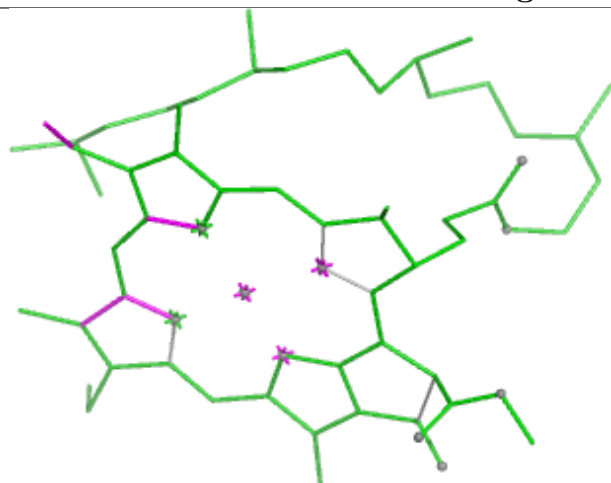


Ligand LHG 4 820

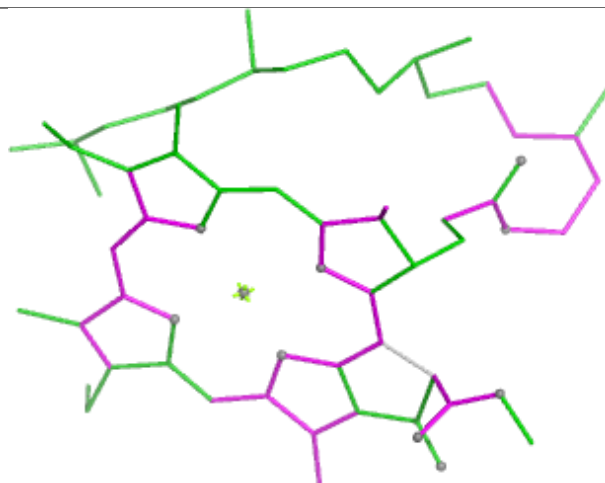




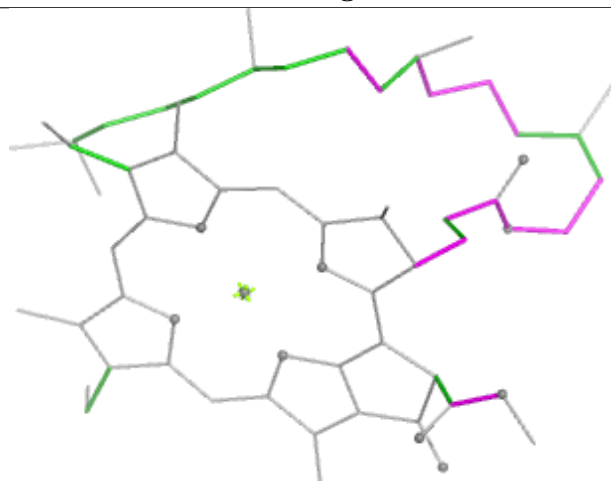
Ligand CLA Z 313



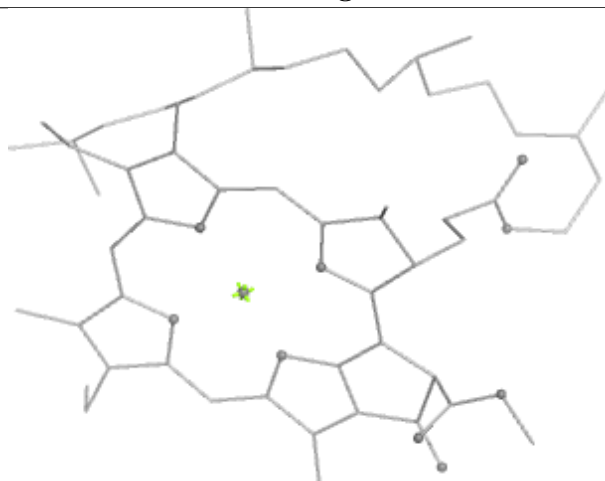
Bond lengths



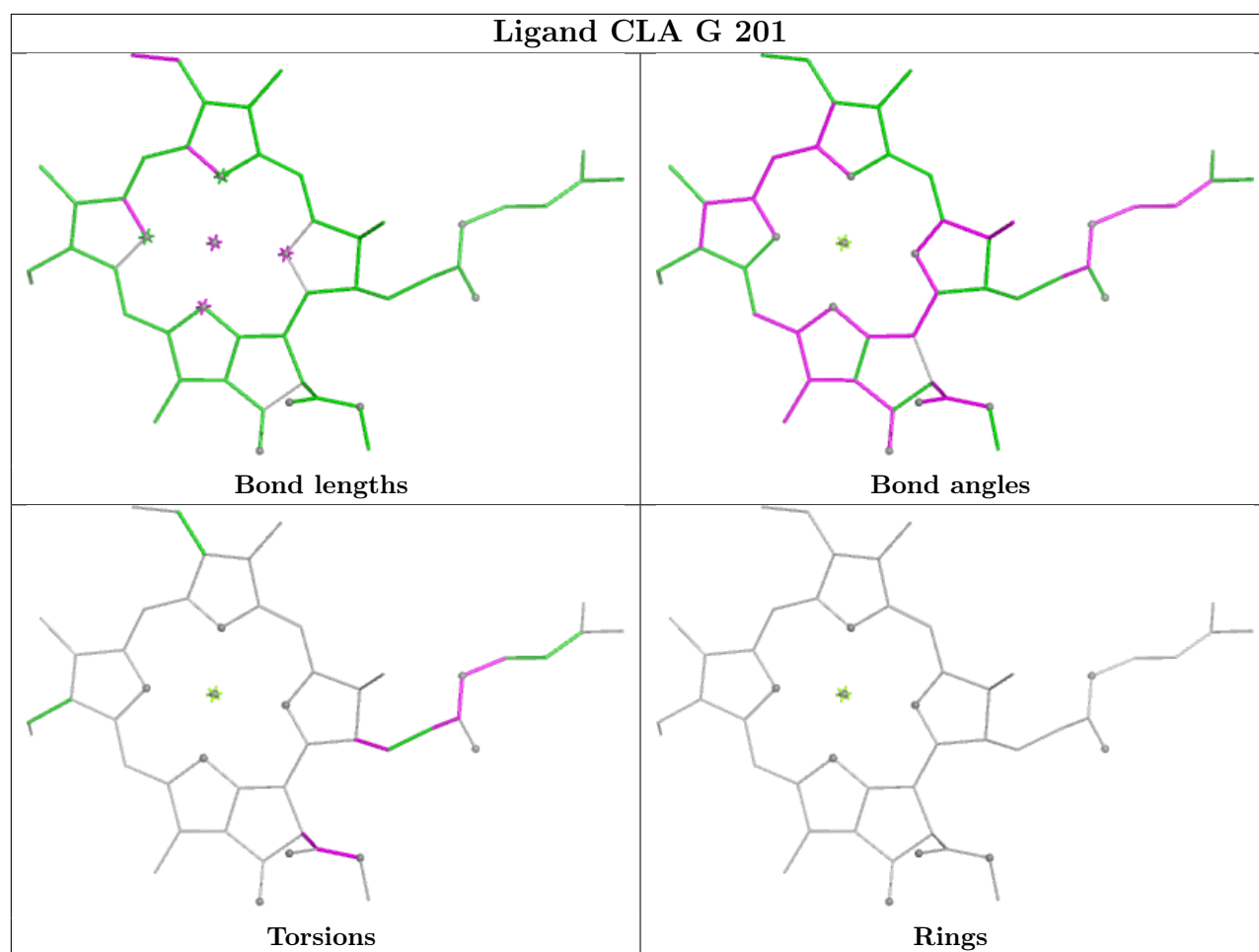
Bond angles



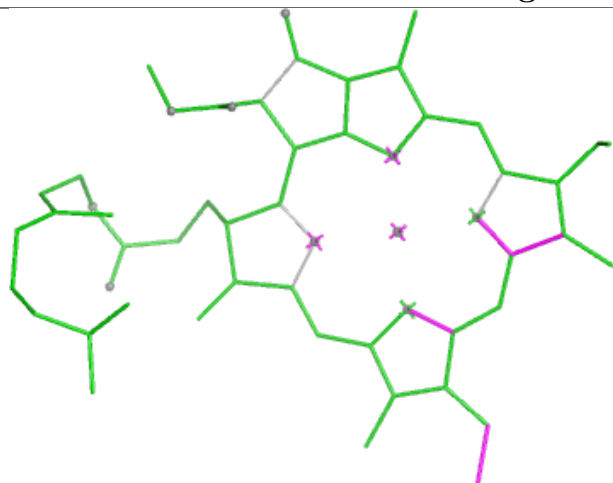
Torsions



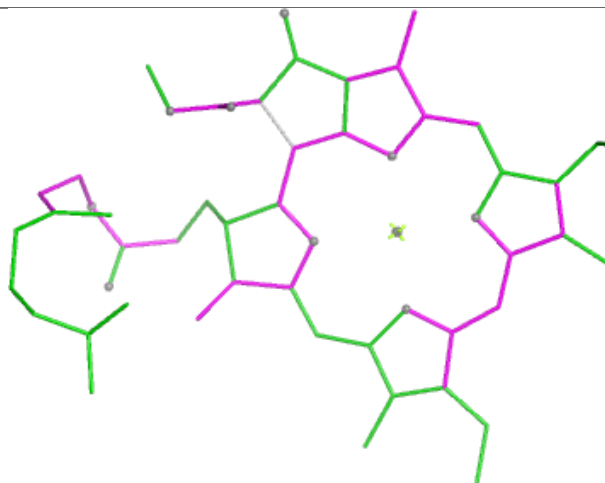
Rings



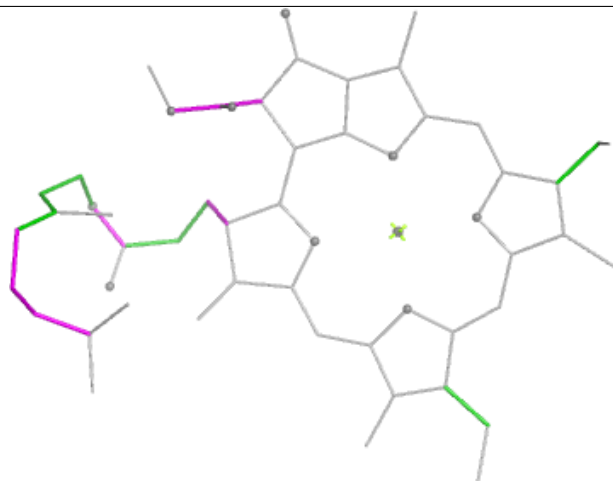
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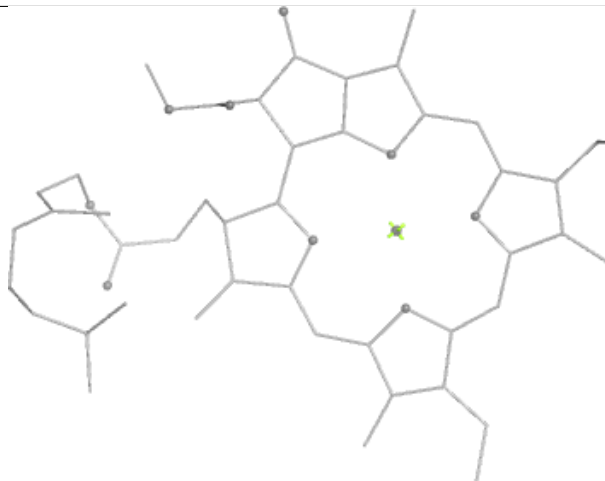
Bond lengths



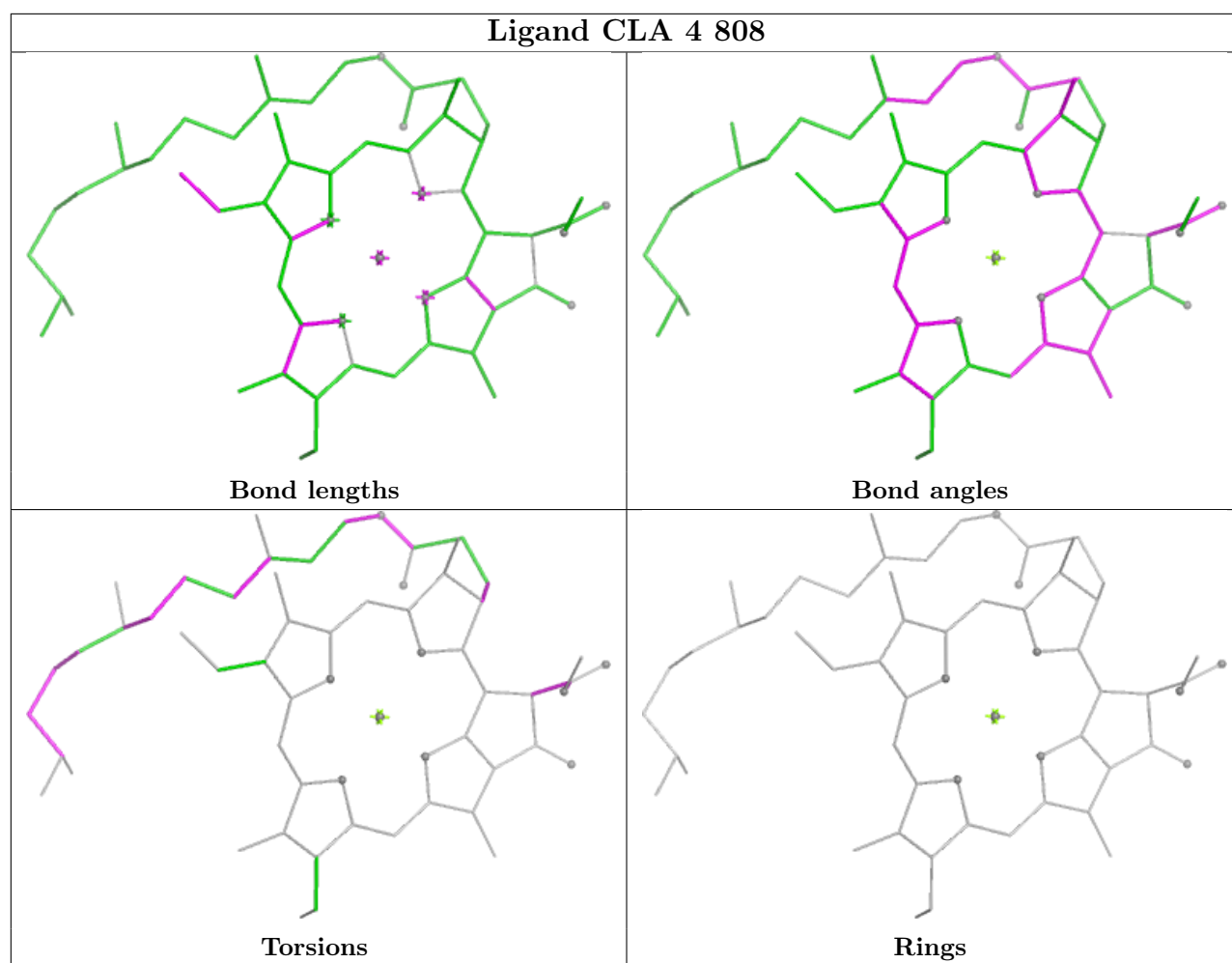
Bond angles



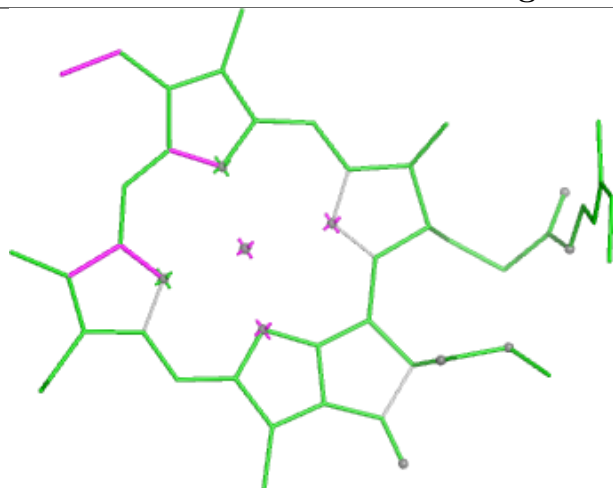
Torsions



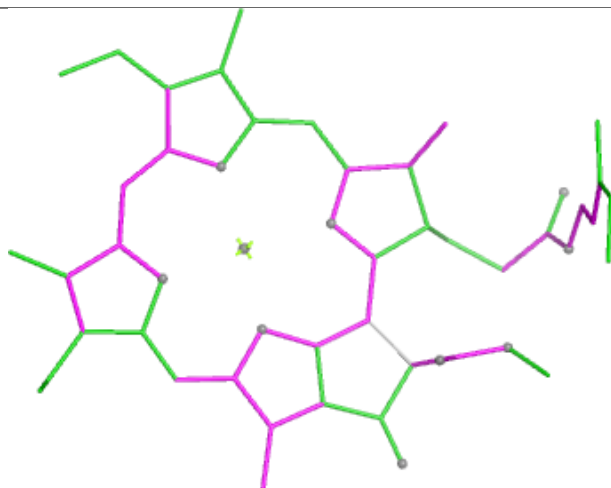
Rings



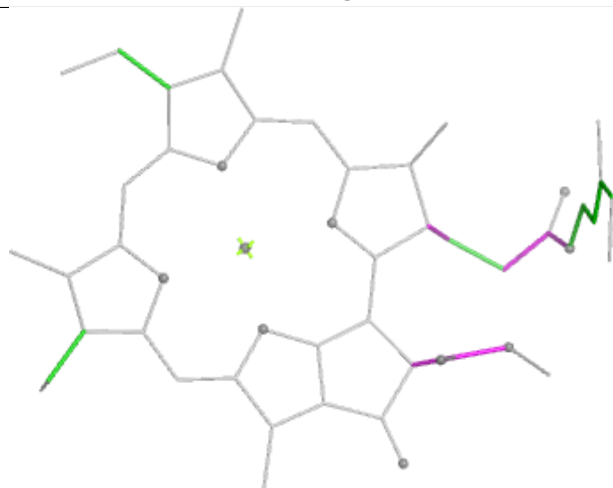
Ligand CLA 8 306



Bond lengths



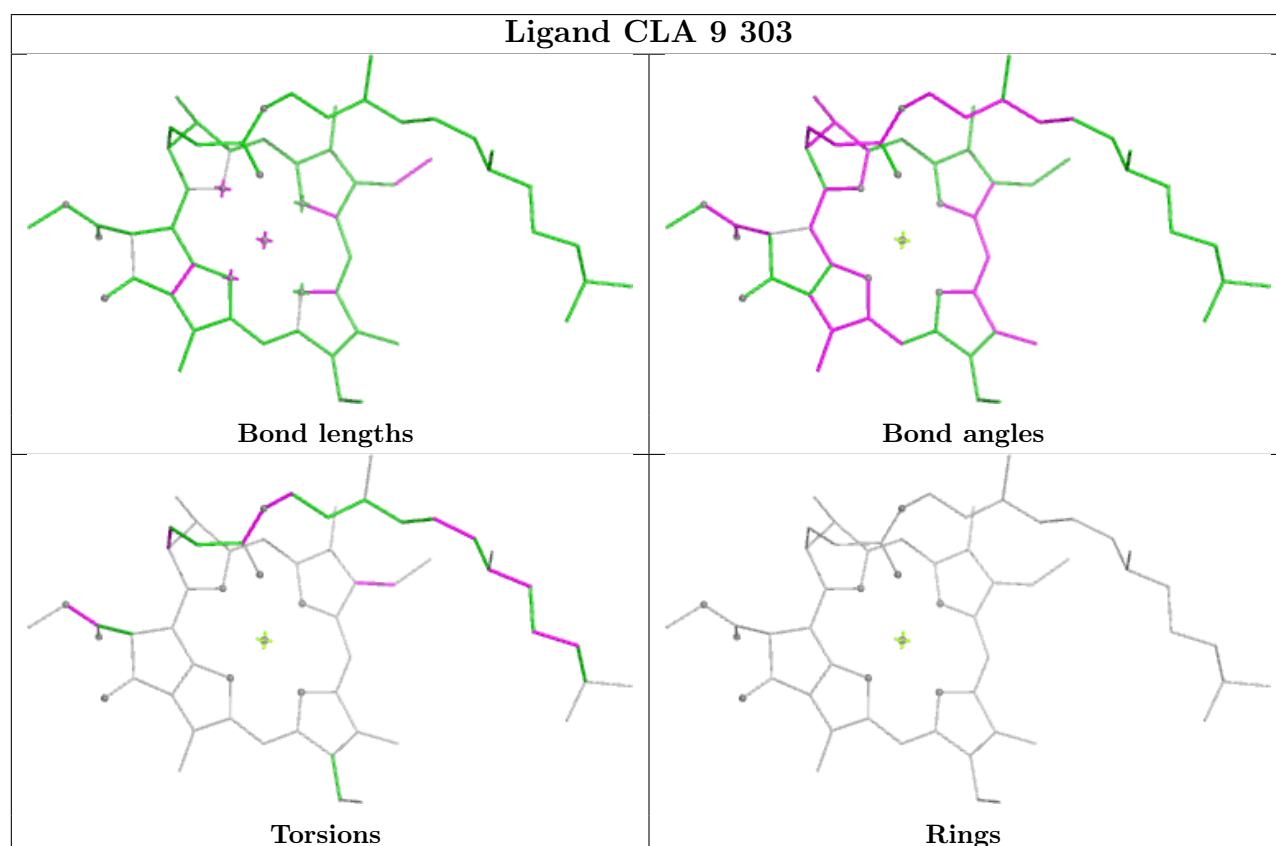
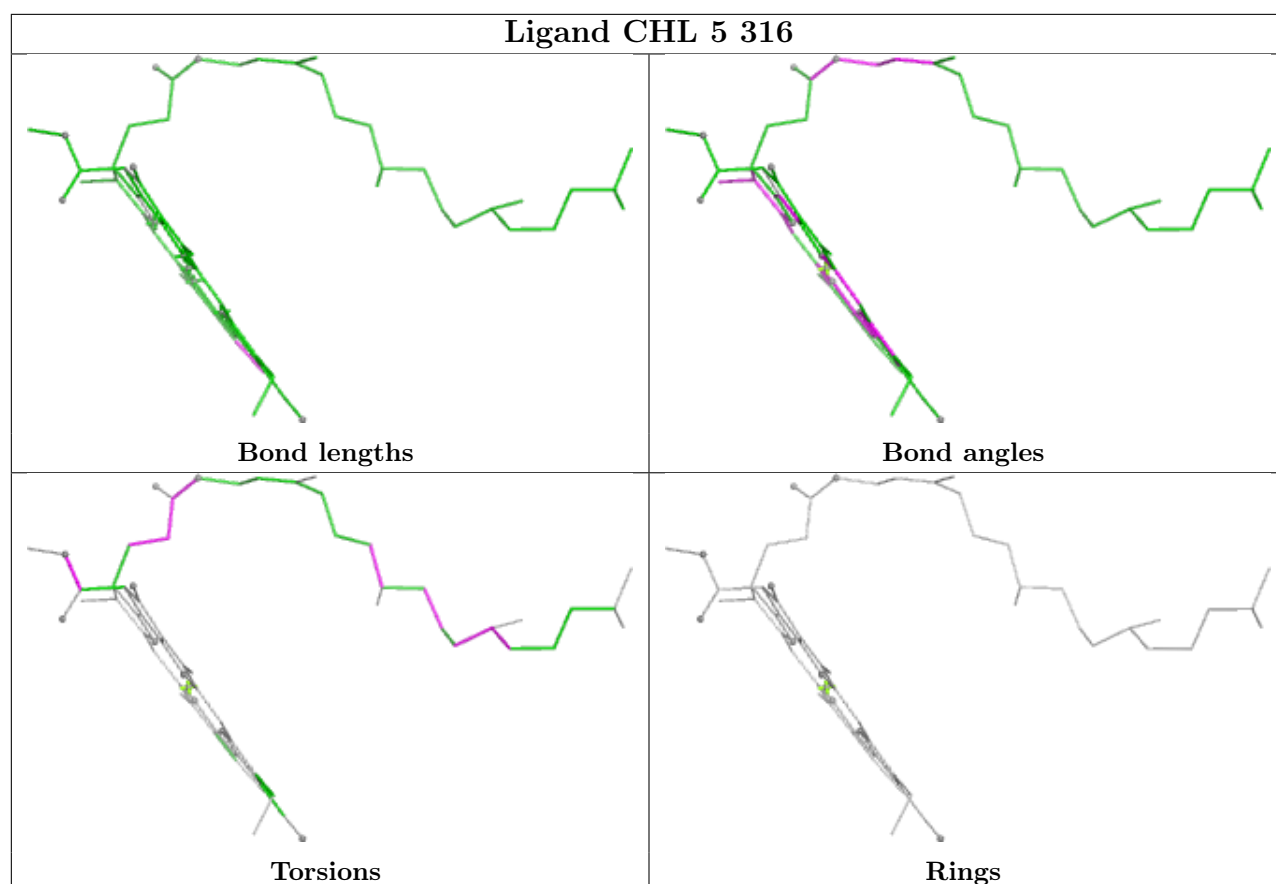
Bond angles

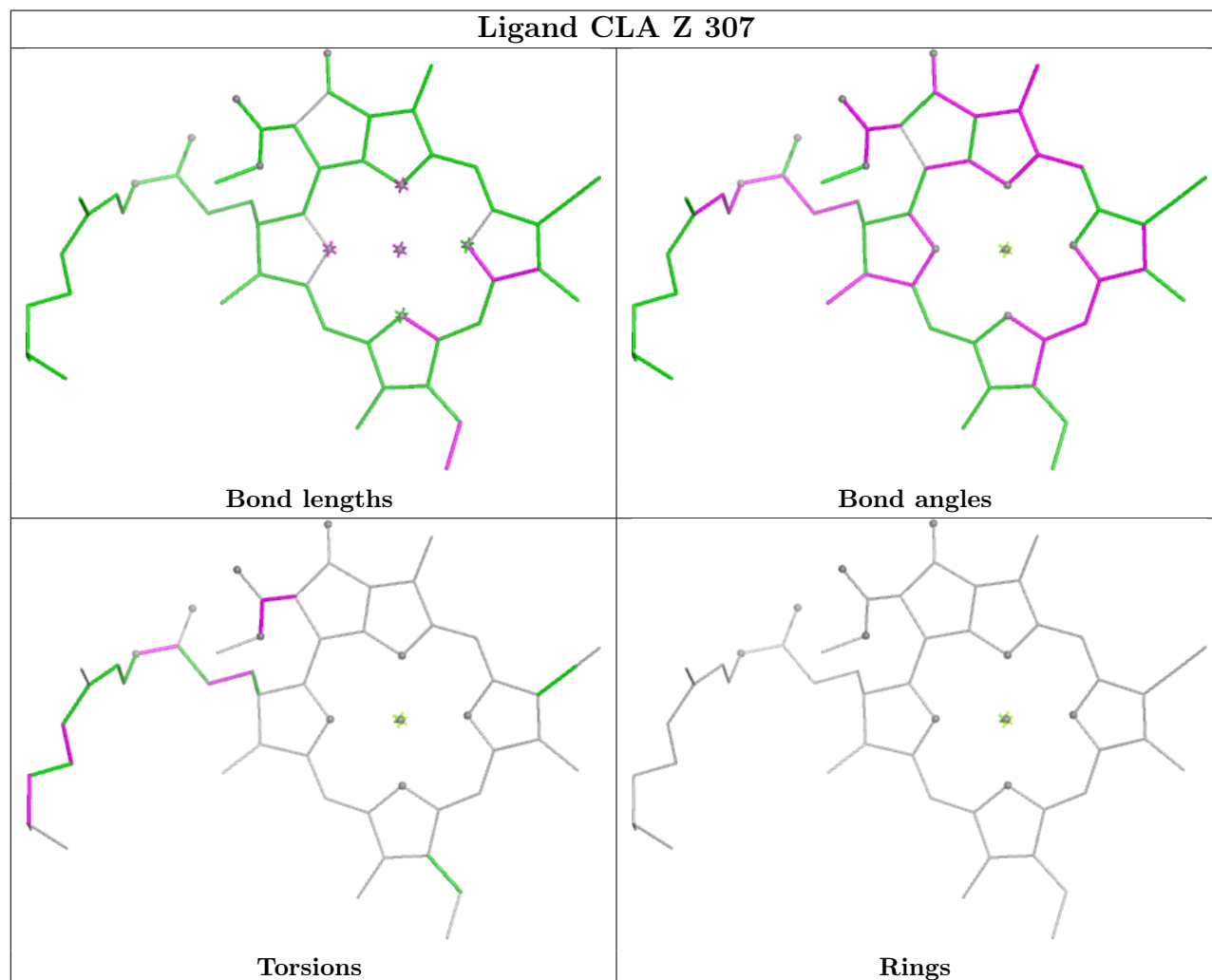
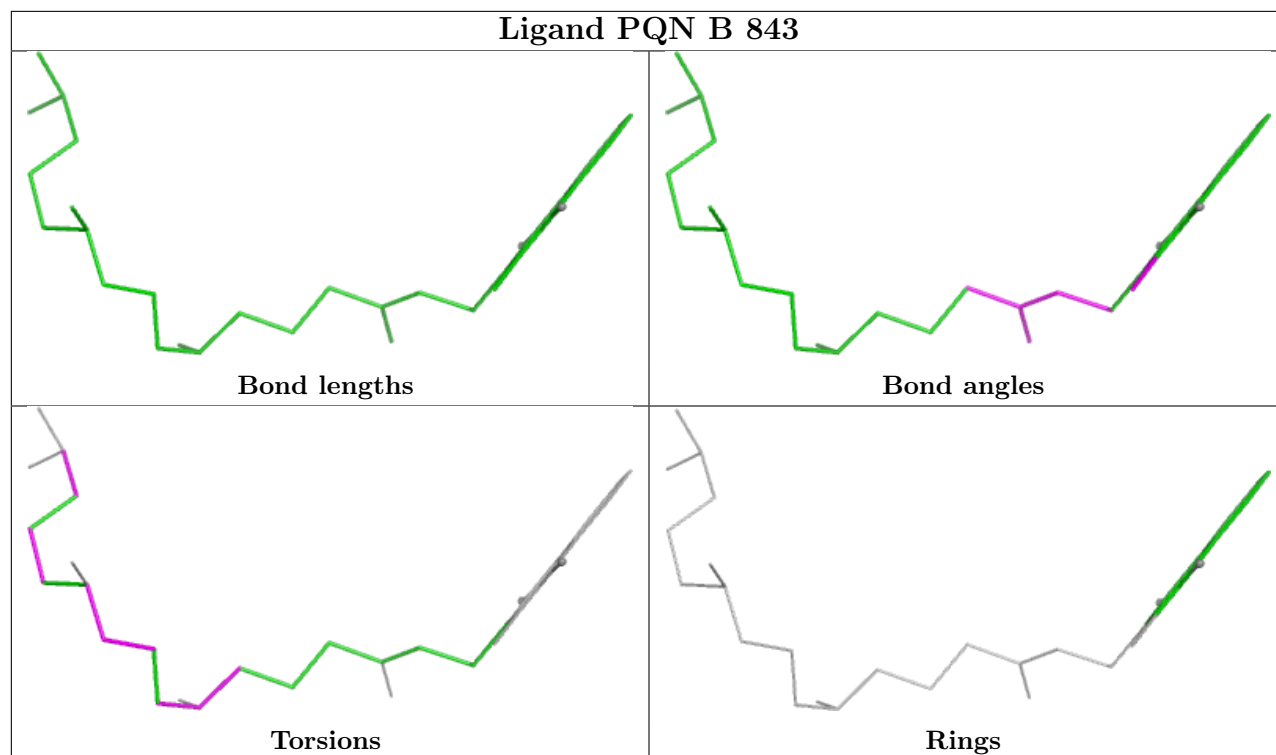


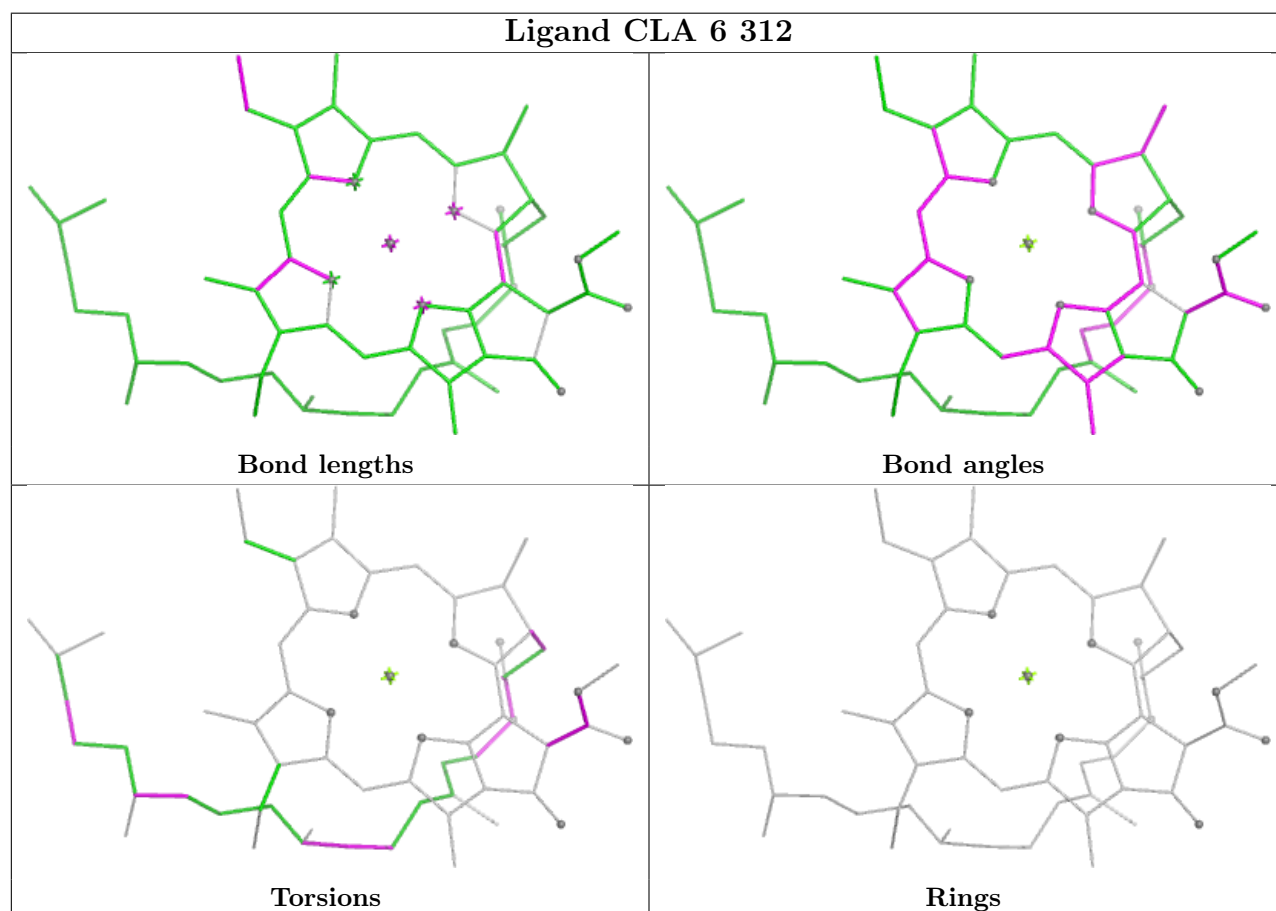
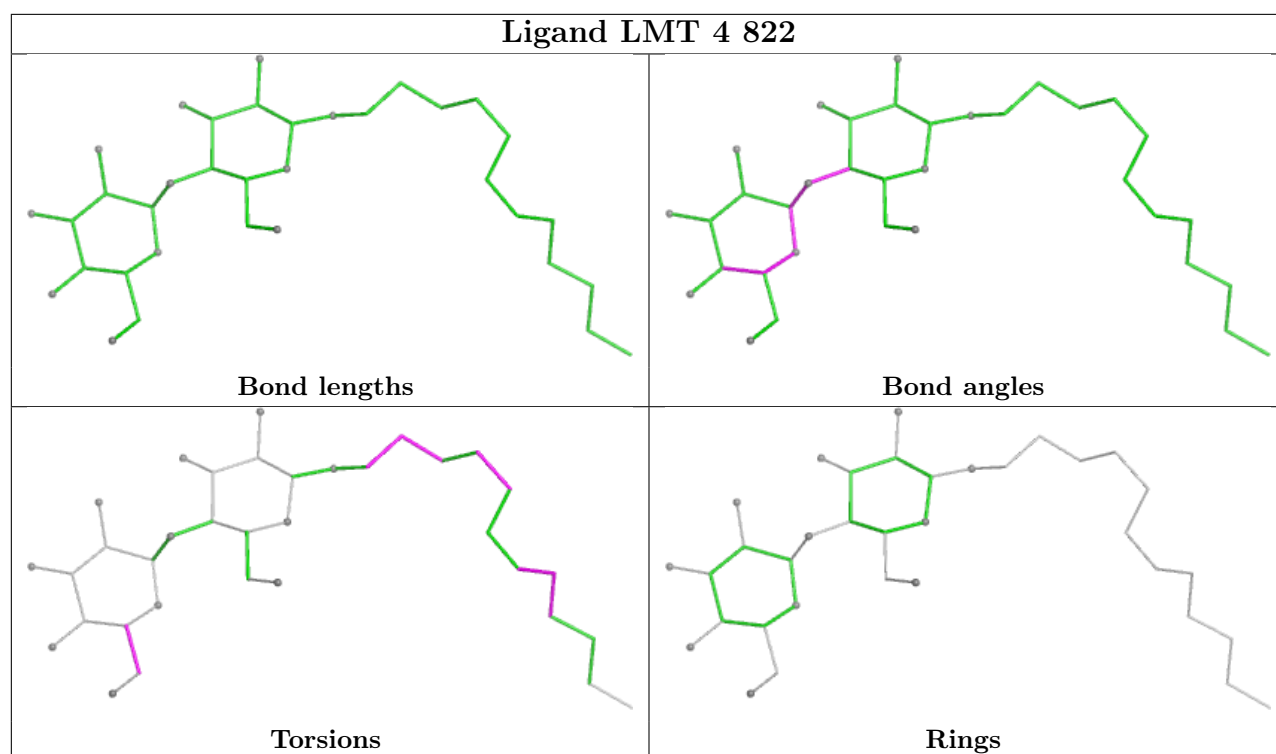
Torsions



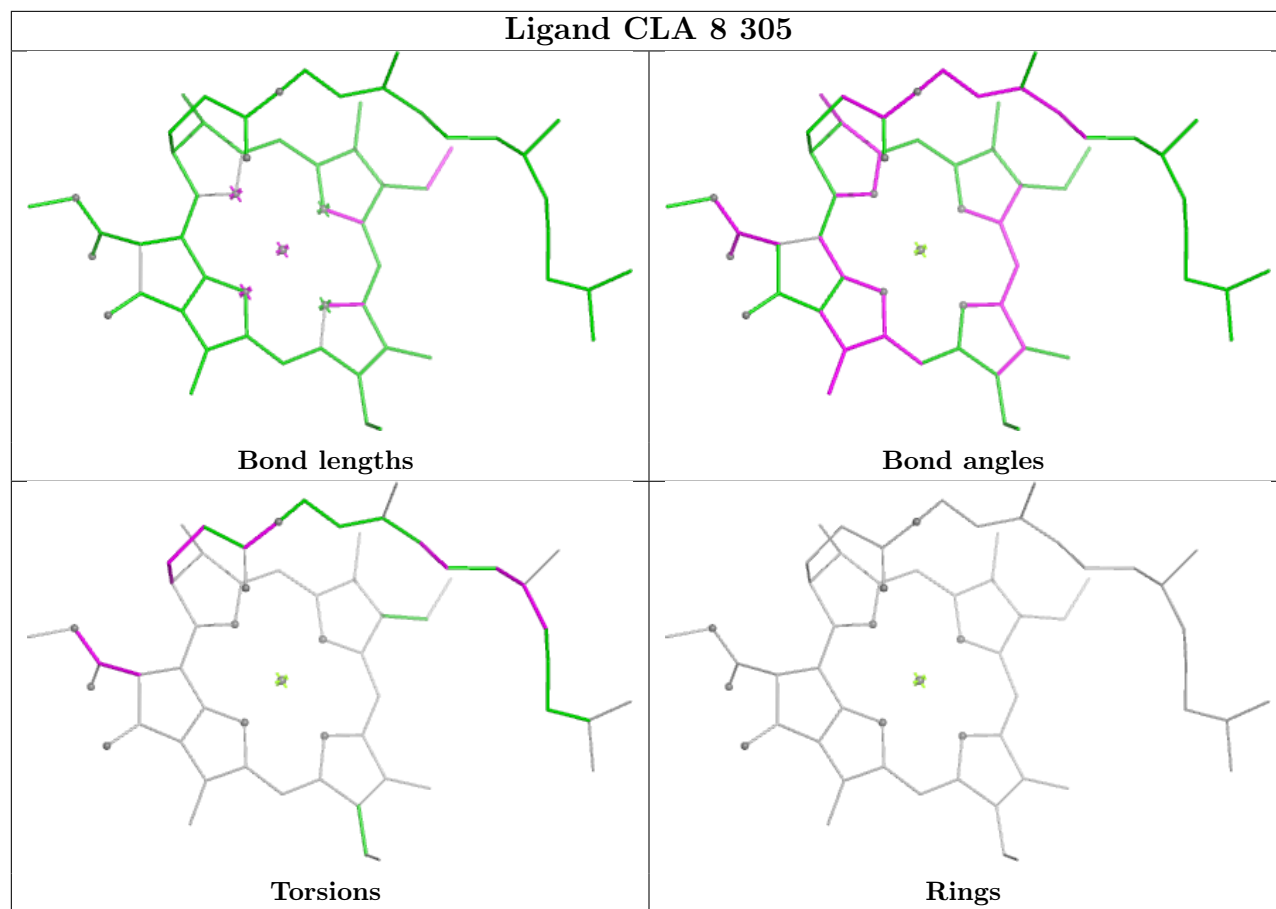
Rings



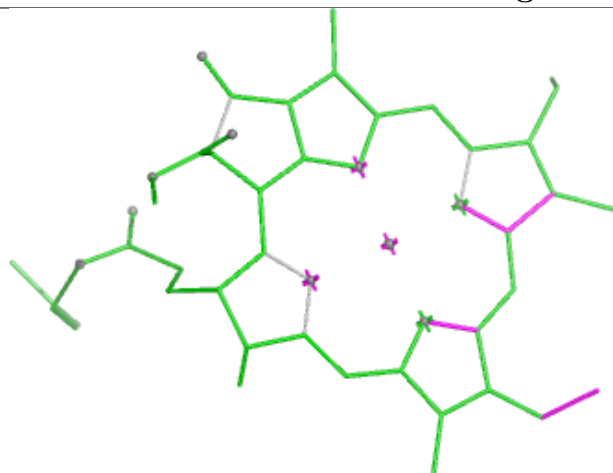




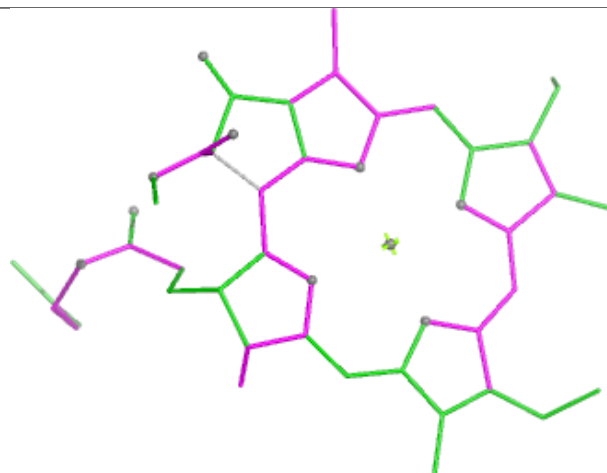
Ligand CLA 8 305



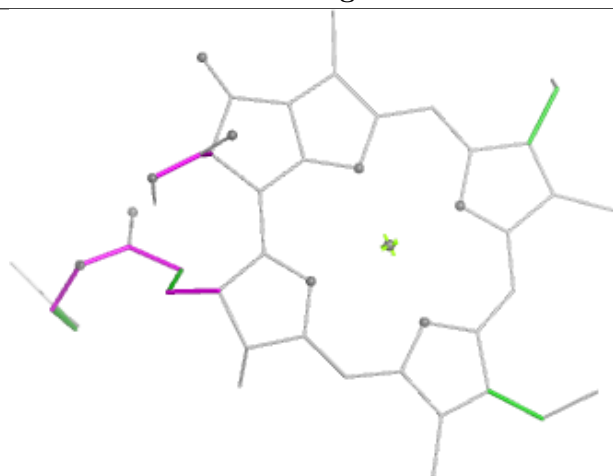
Ligand CLA Z 310



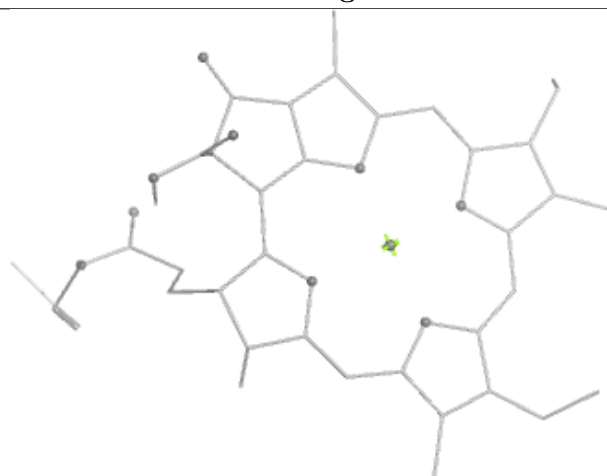
Bond lengths



Bond angles

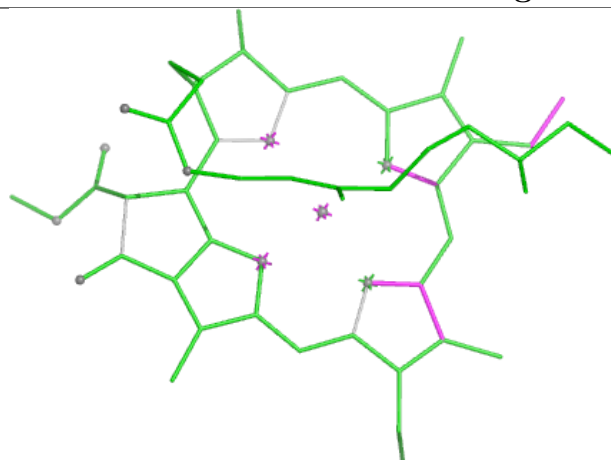


Torsions

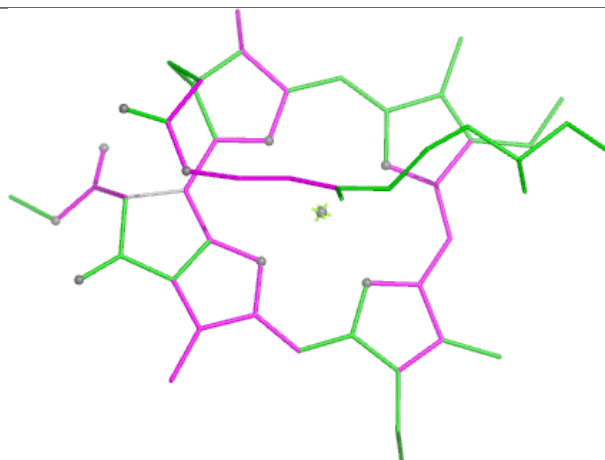


Rings

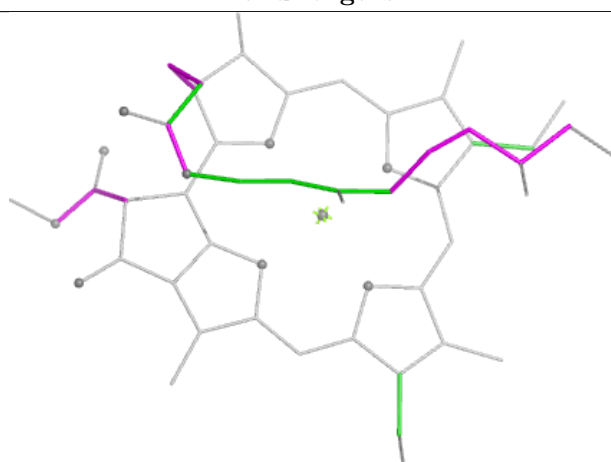
Ligand CLA B 813



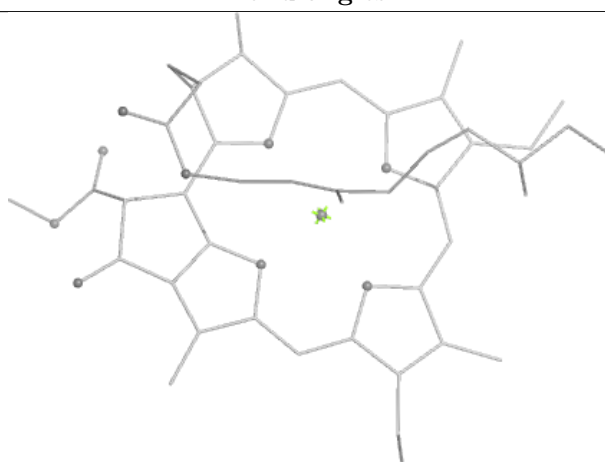
Bond lengths



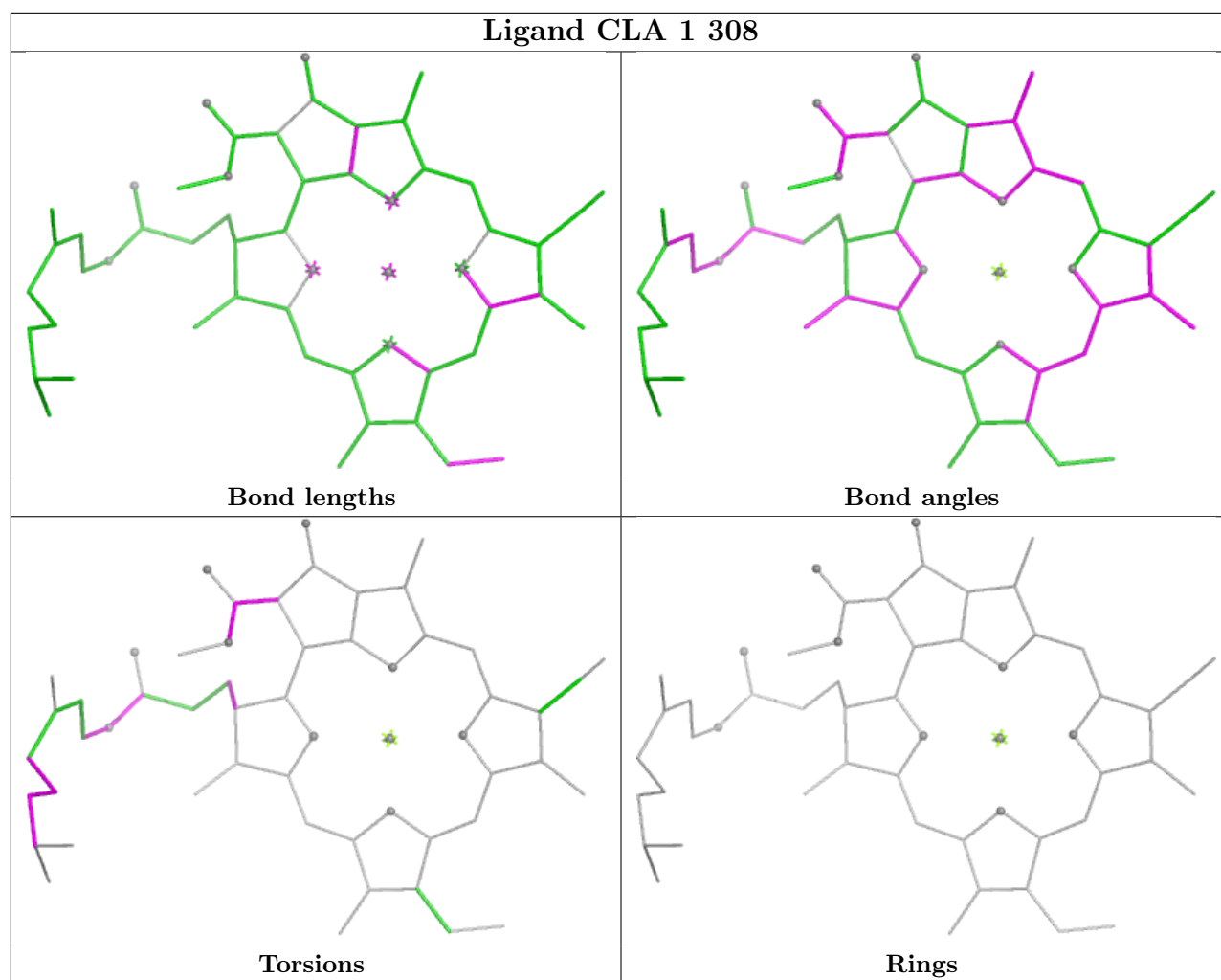
Bond angles

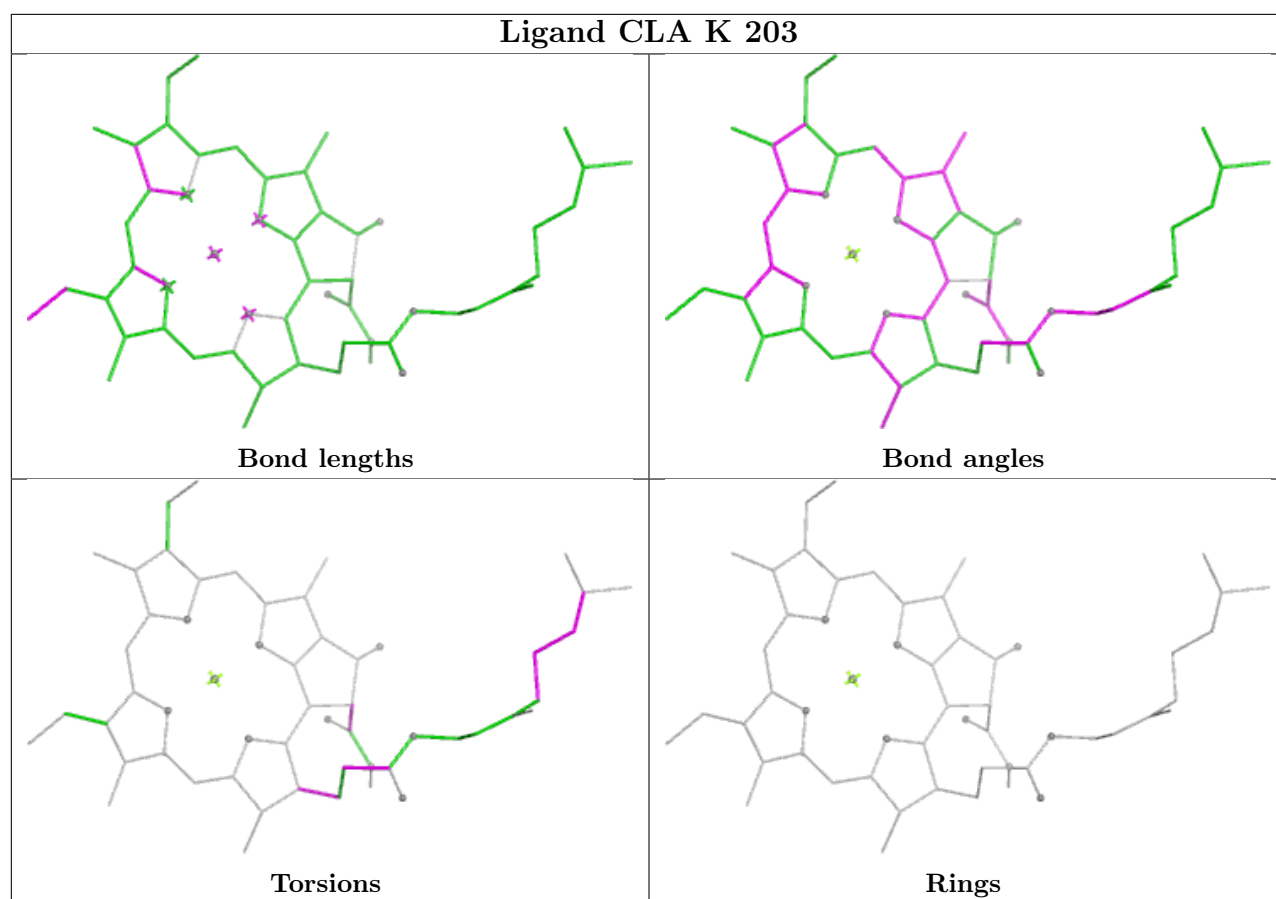


Torsions

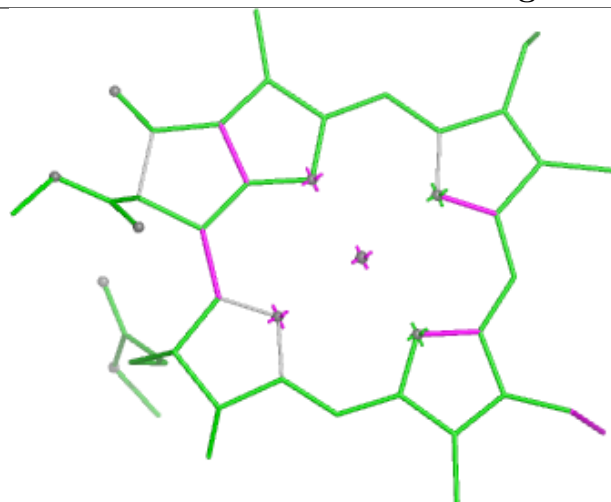


Rings

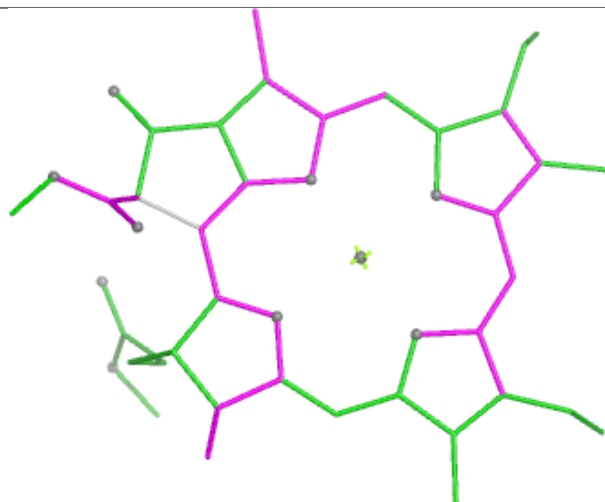




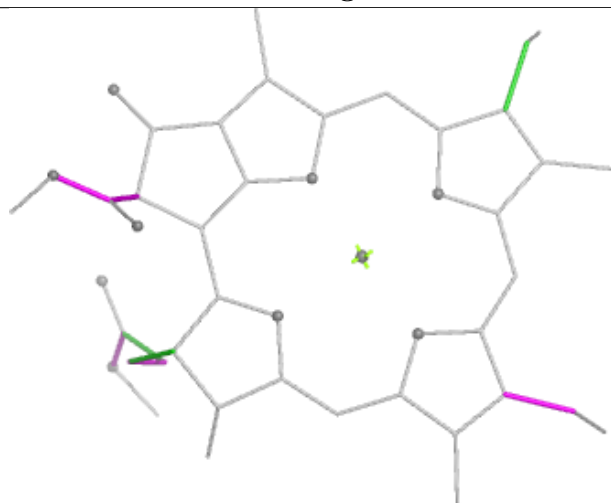
Ligand CLA 1 311



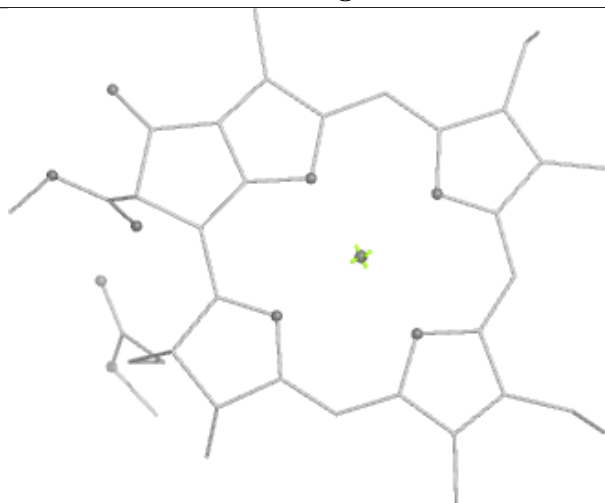
Bond lengths



Bond angles

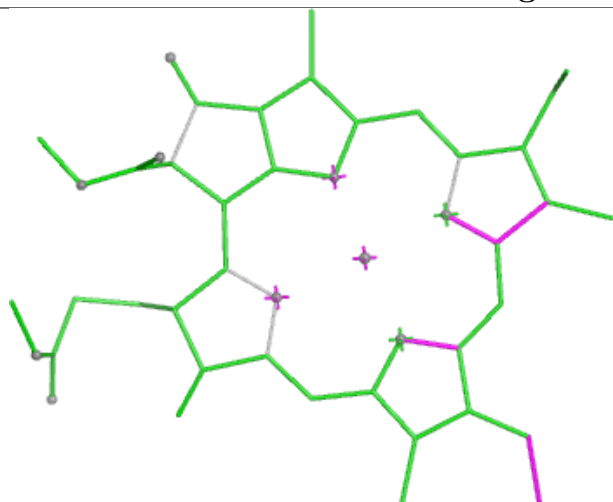


Torsions

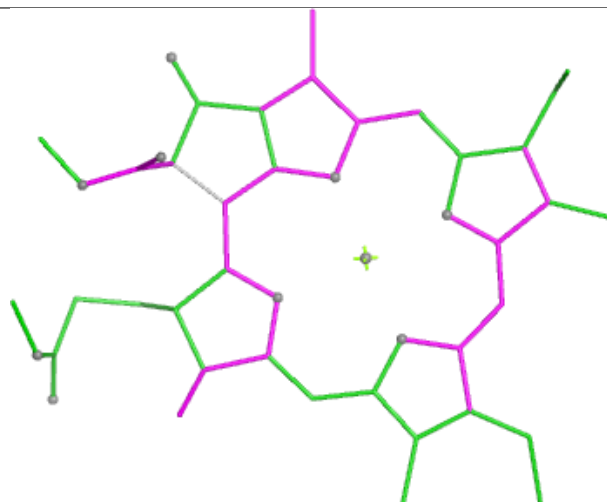


Rings

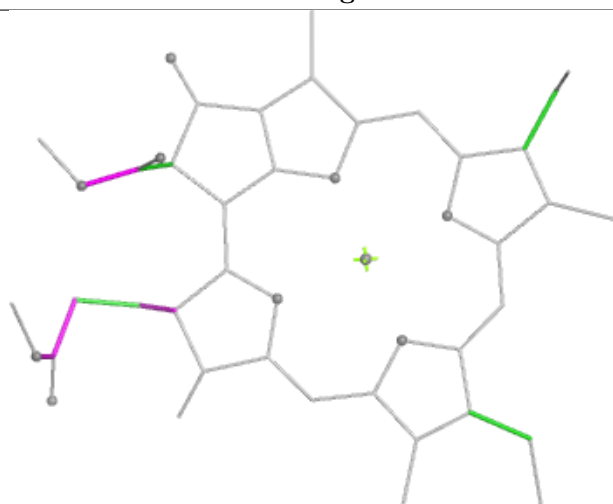
Ligand CLA 1 315



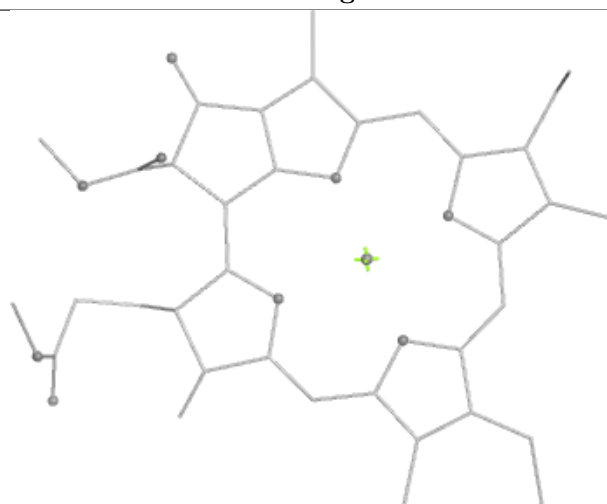
Bond lengths



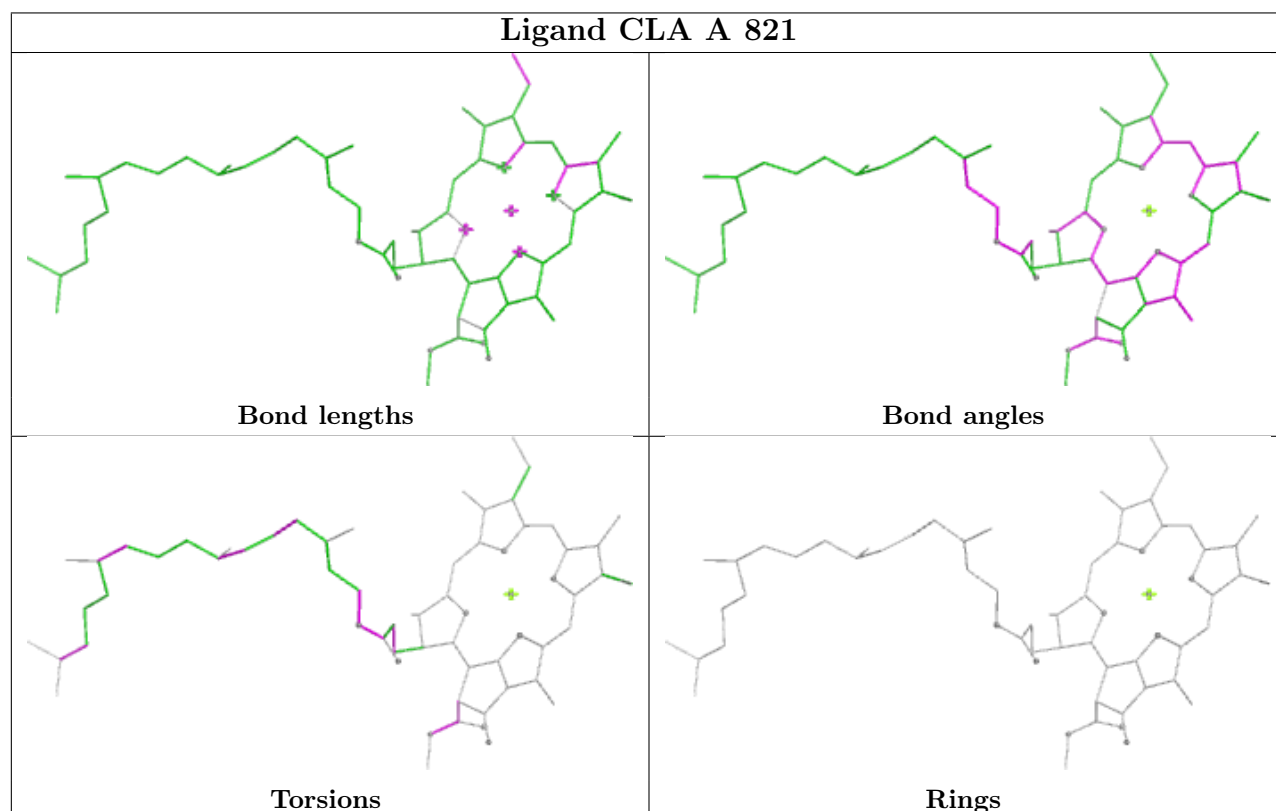
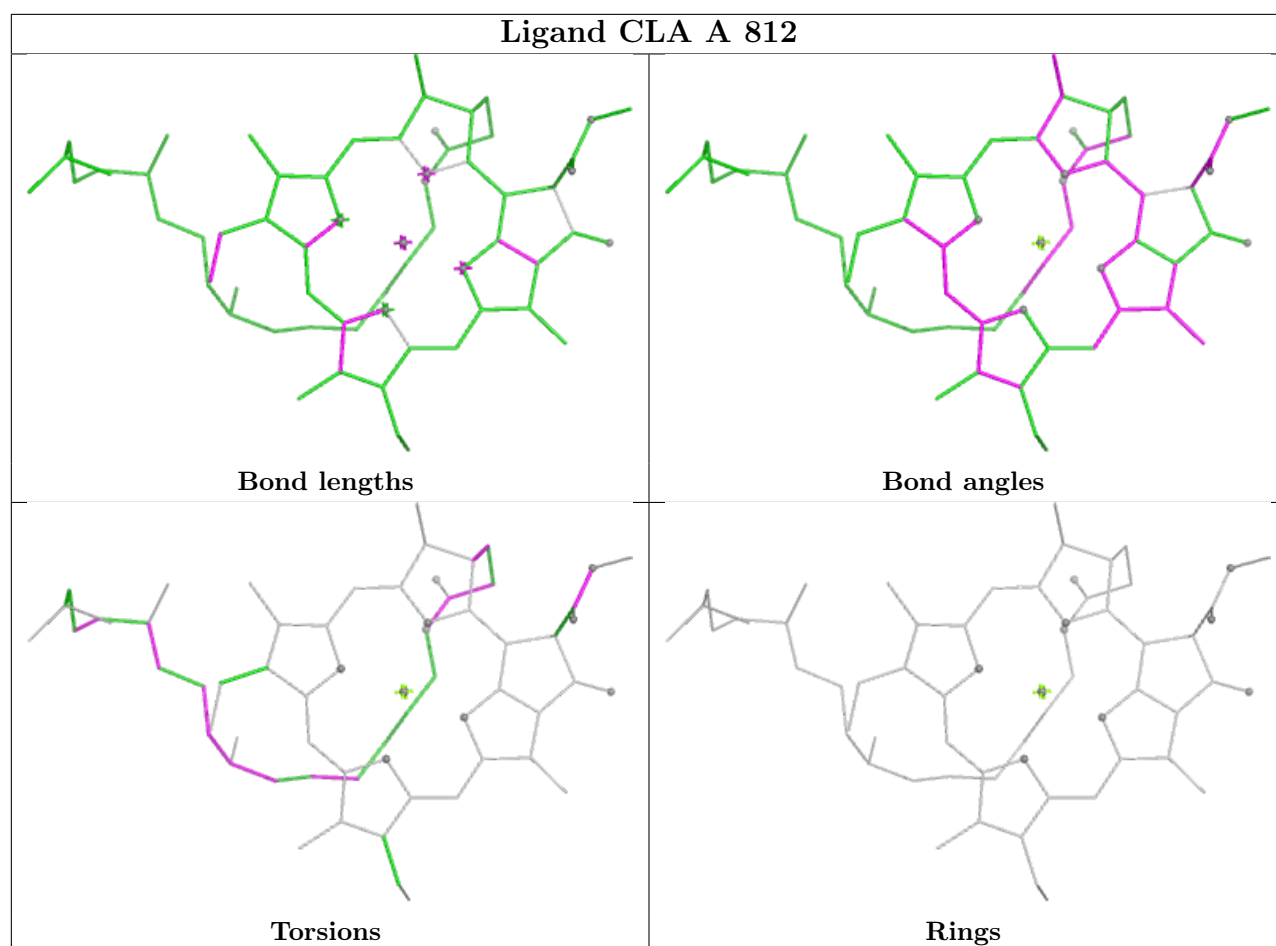
Bond angles



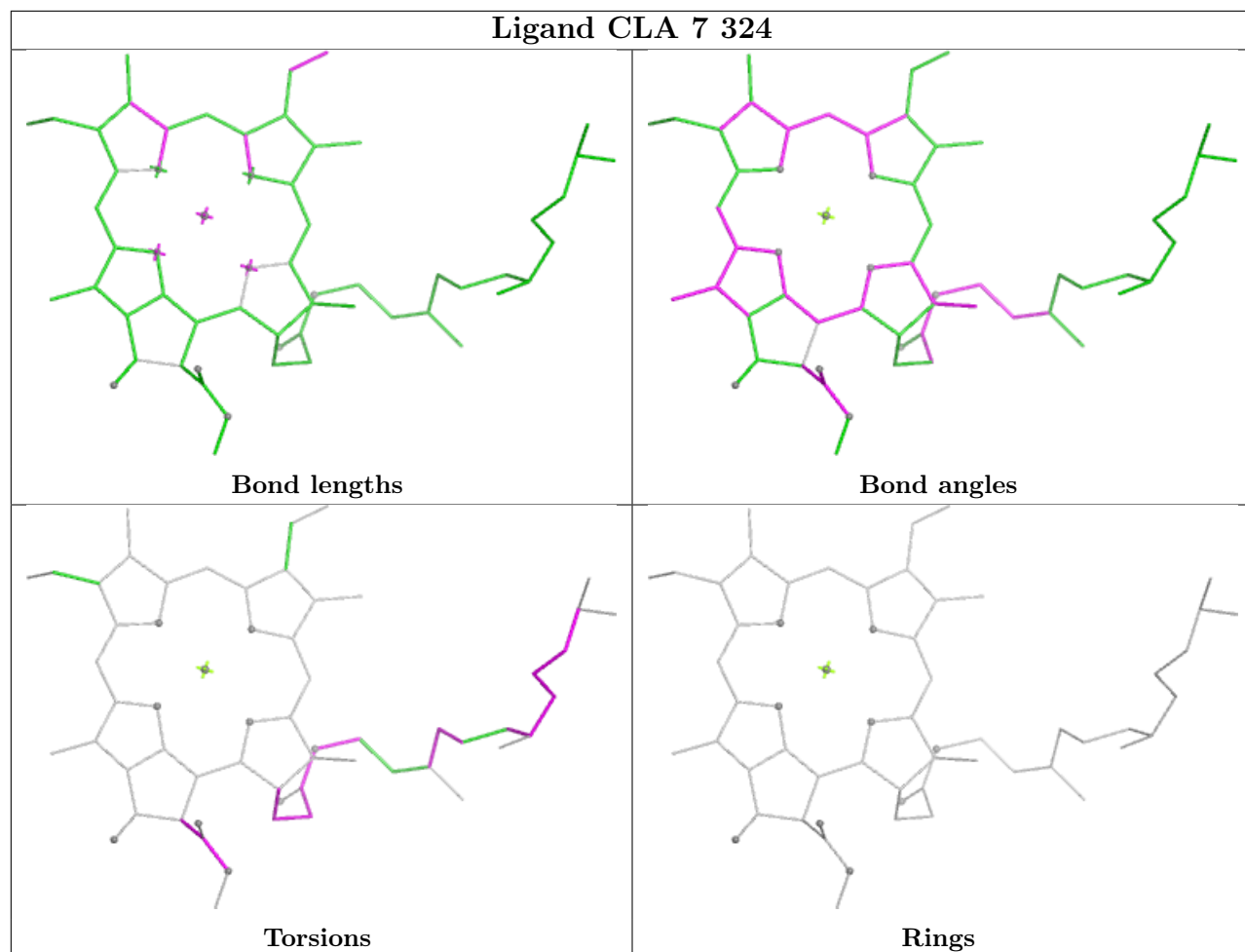
Torsions



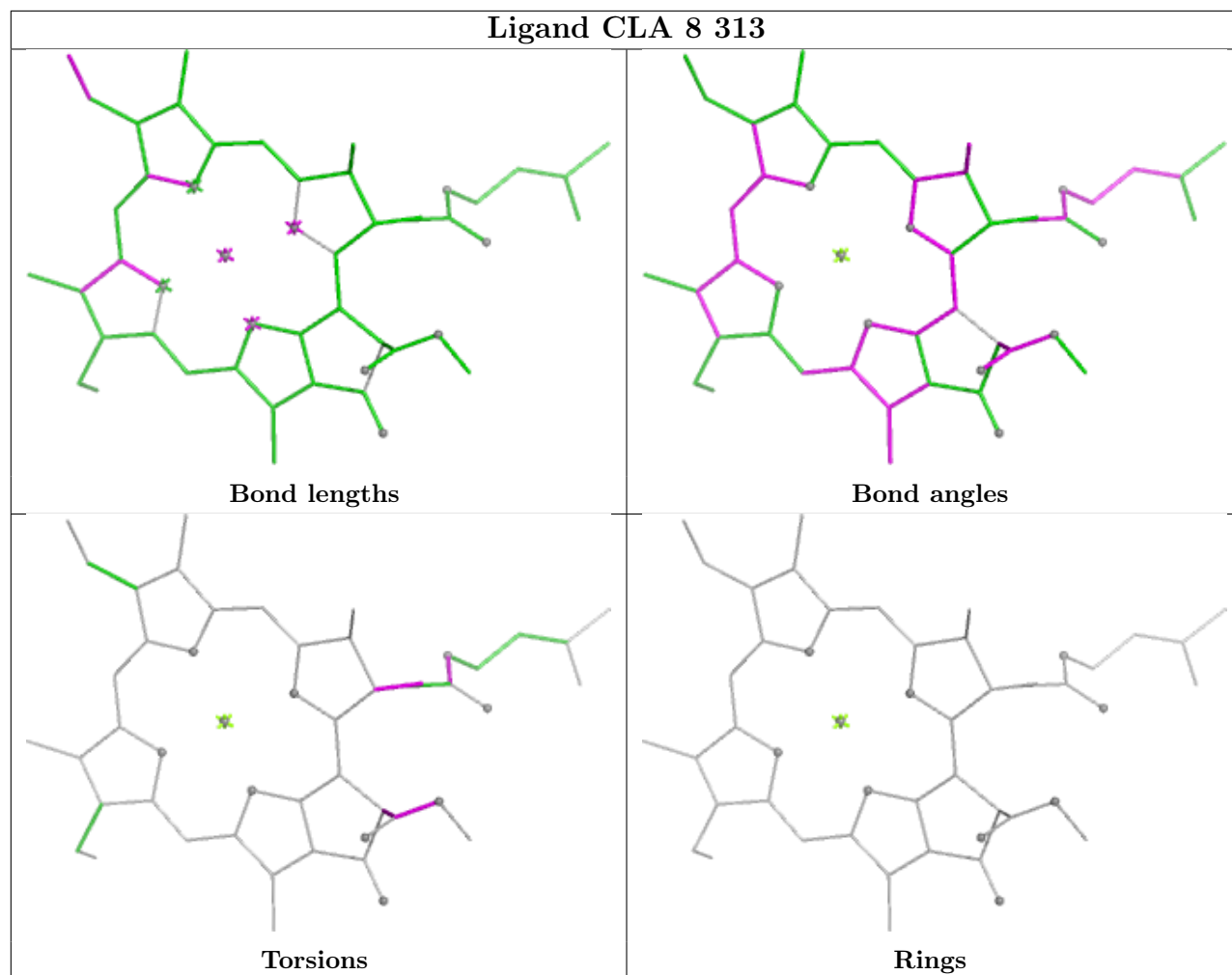
Rings

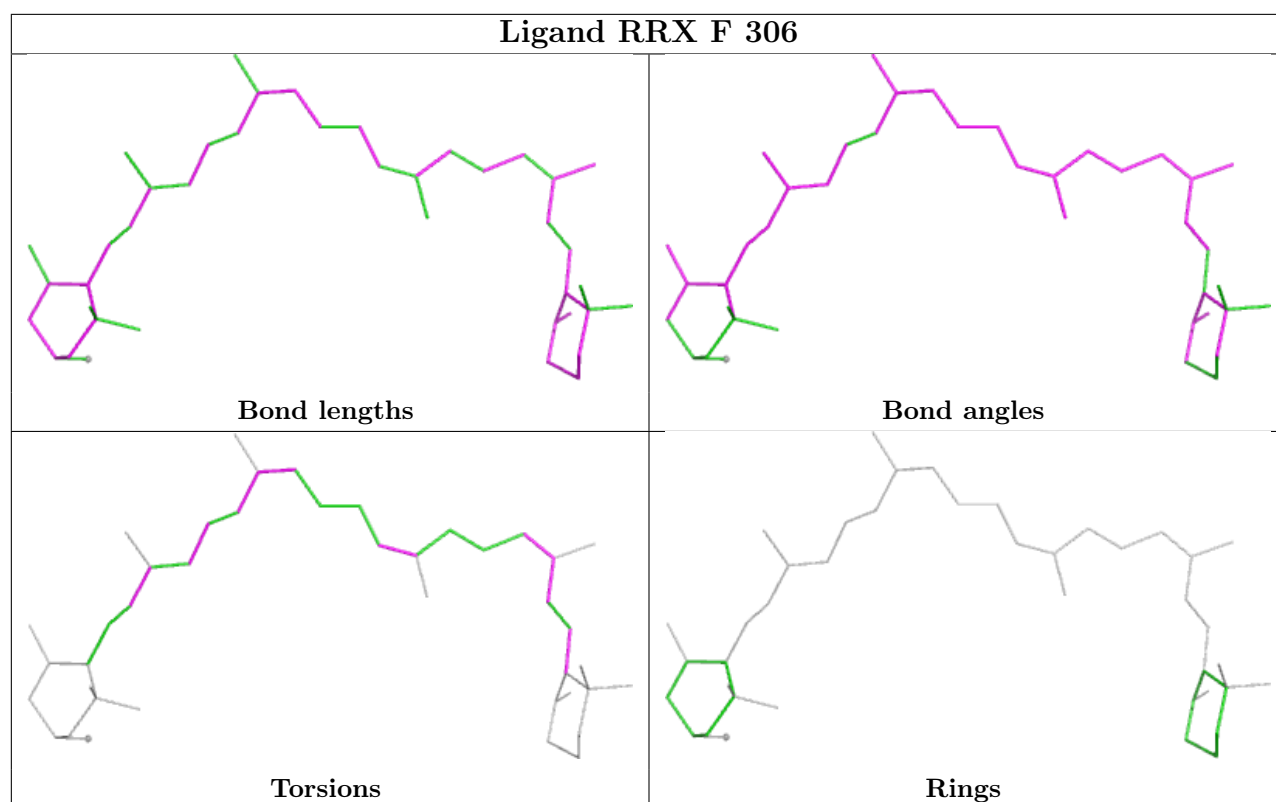


Ligand CLA 7 324

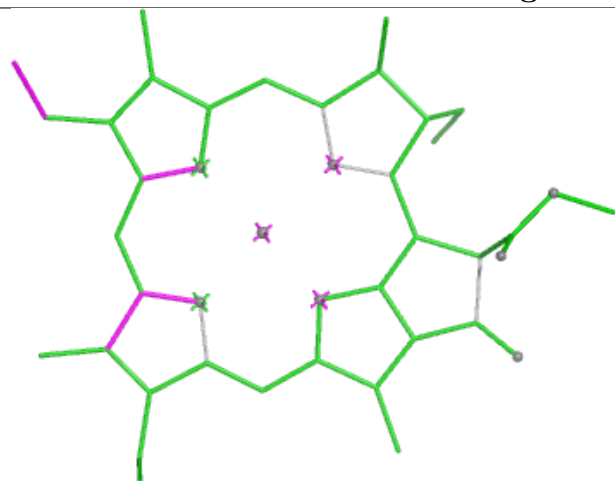


Ligand CLA 8 313

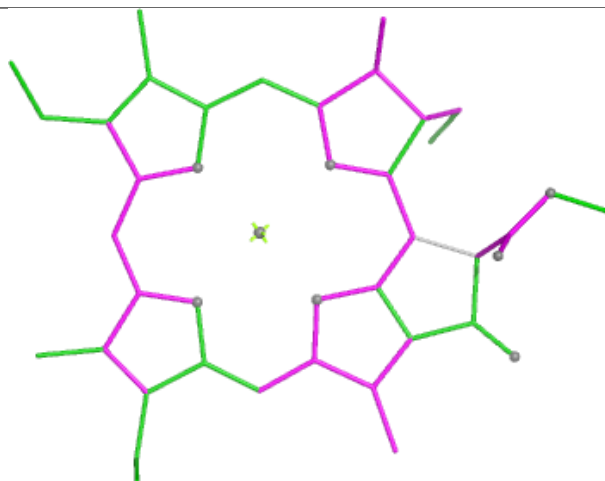




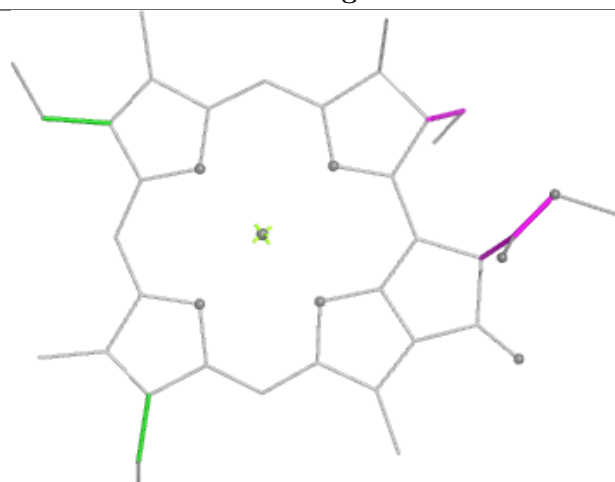
Ligand CLA J 103



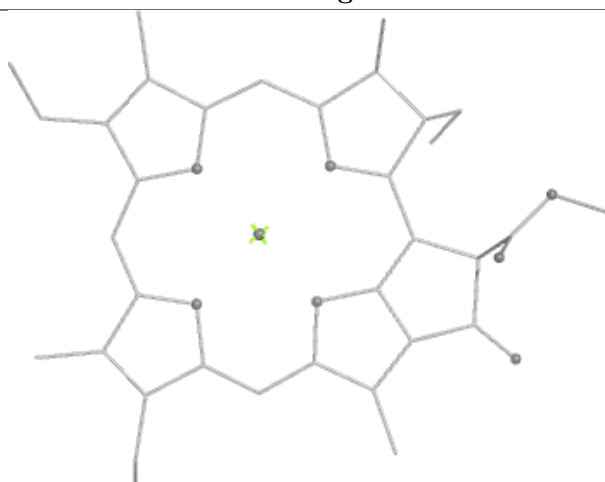
Bond lengths



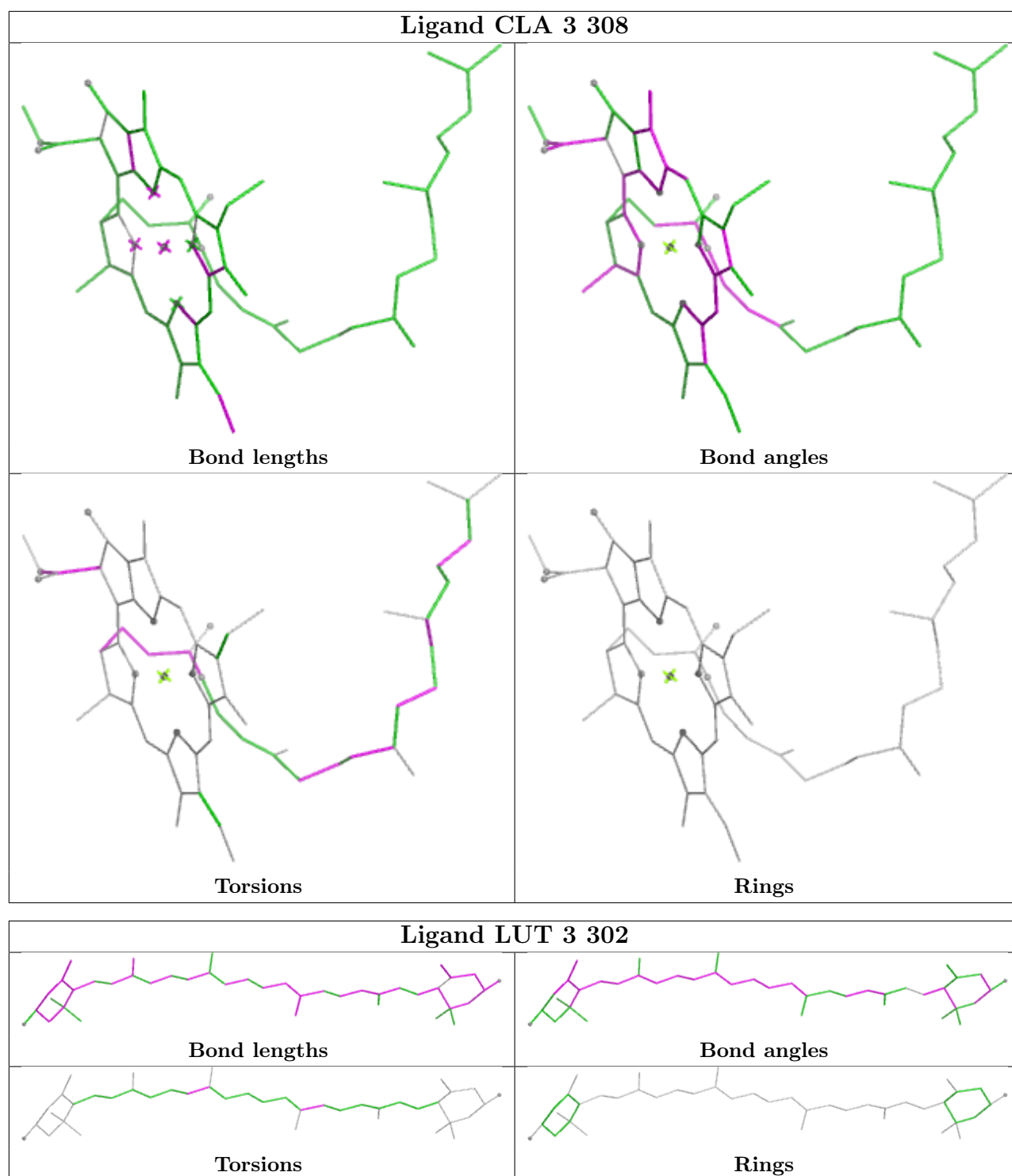
Bond angles

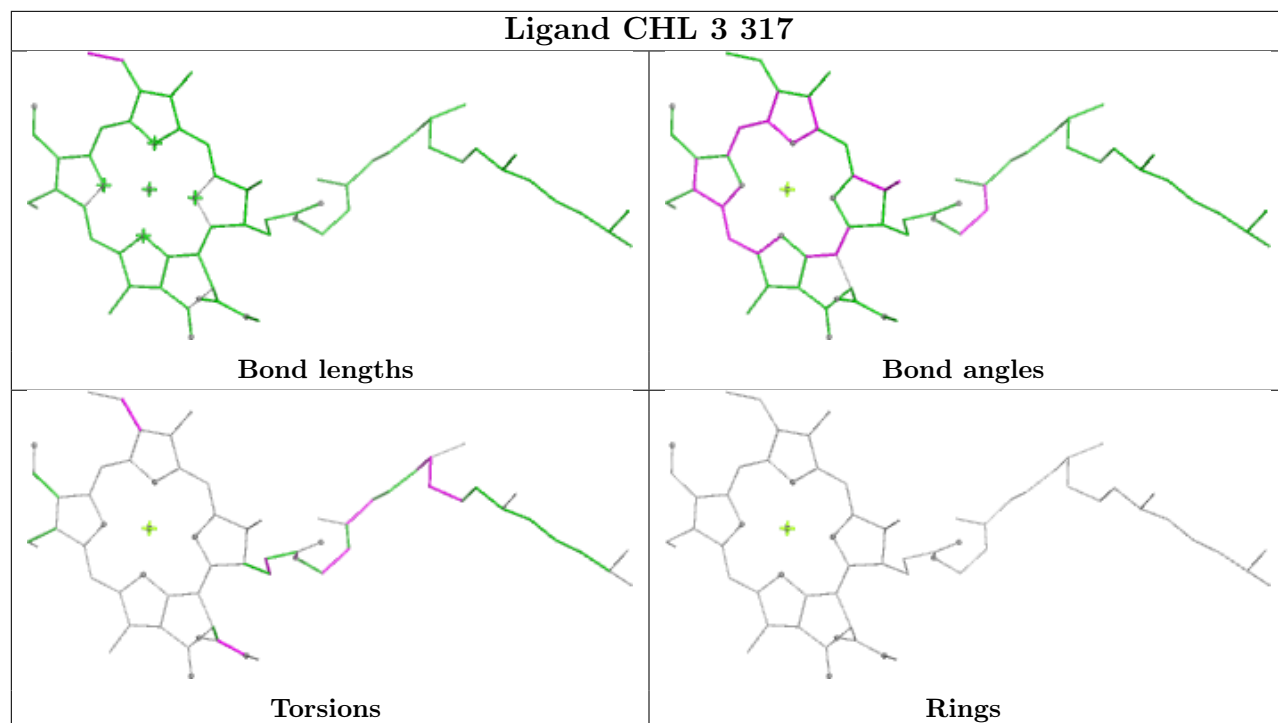


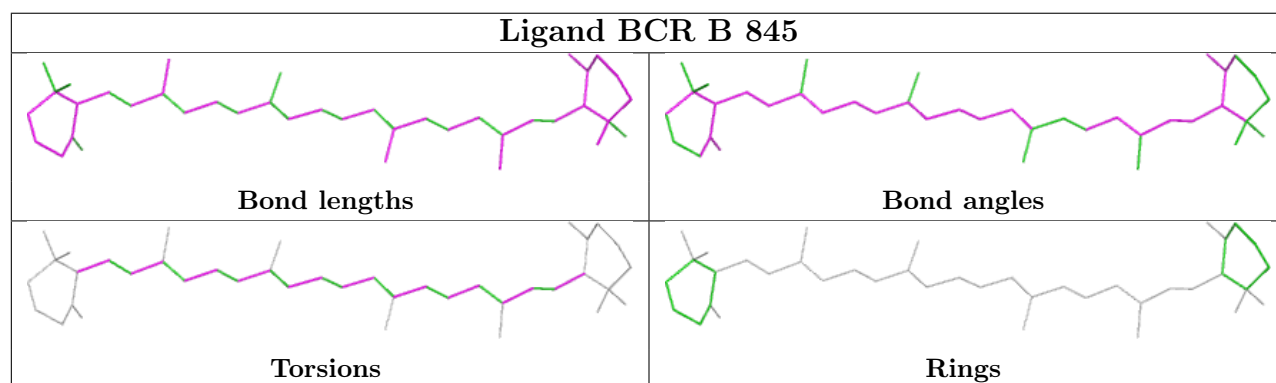
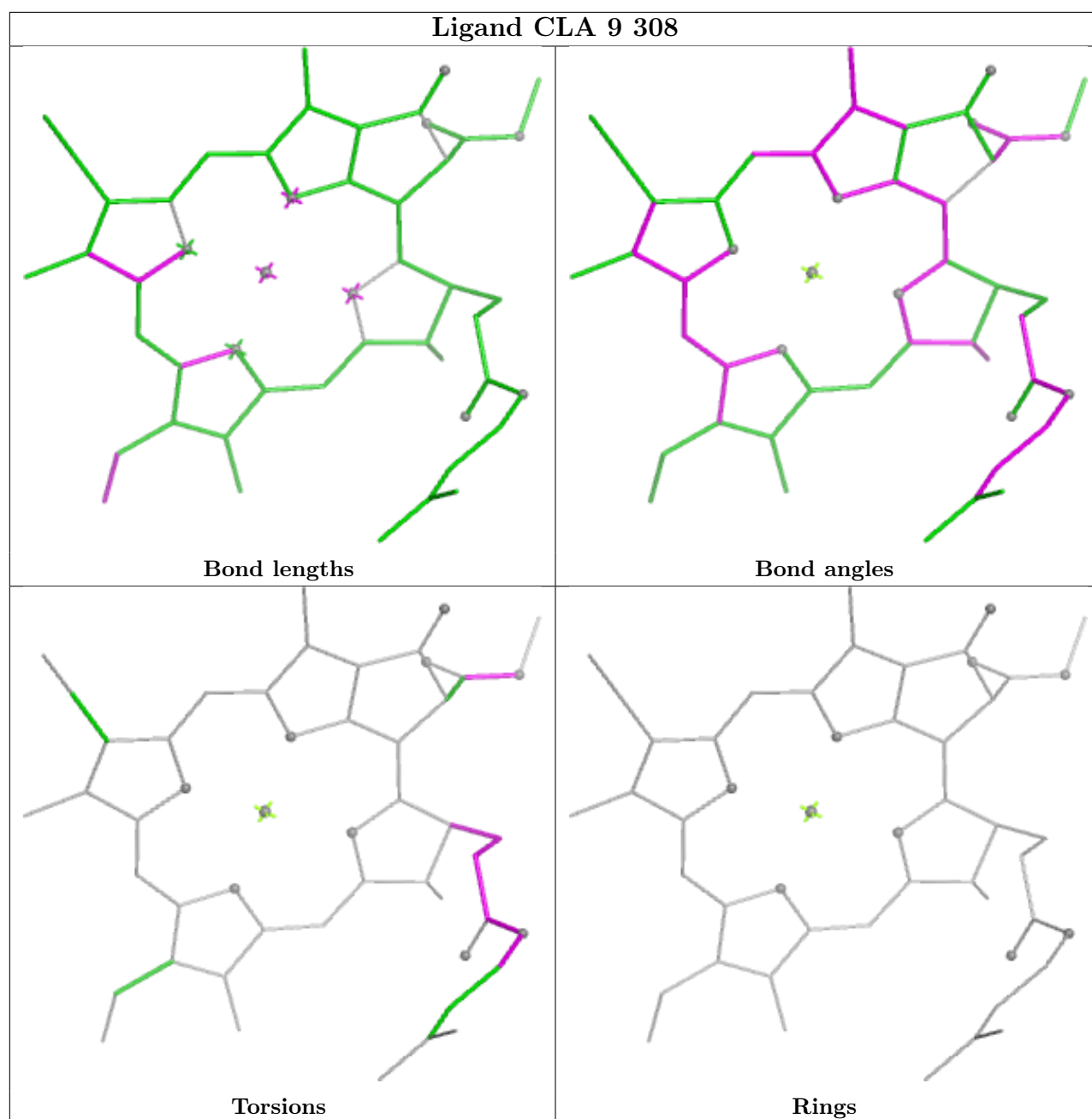
Torsions

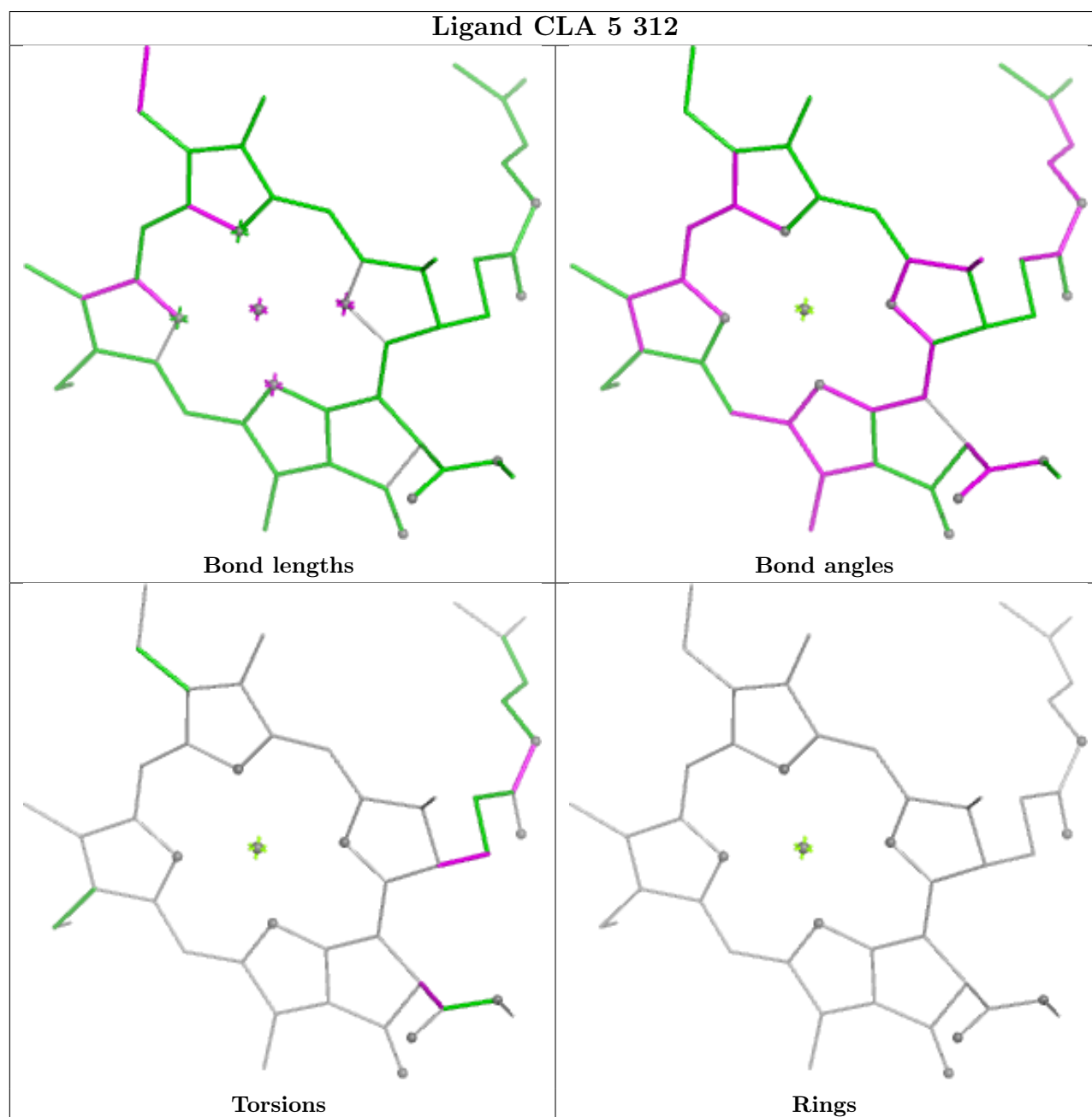
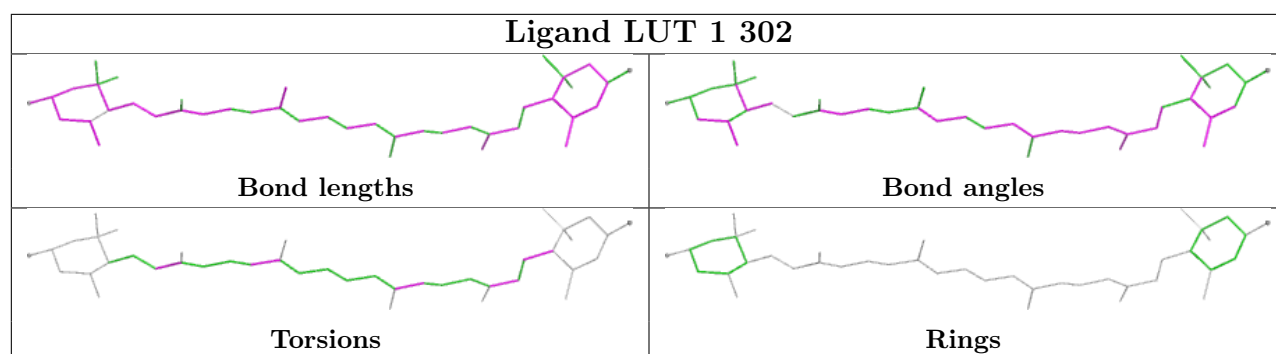


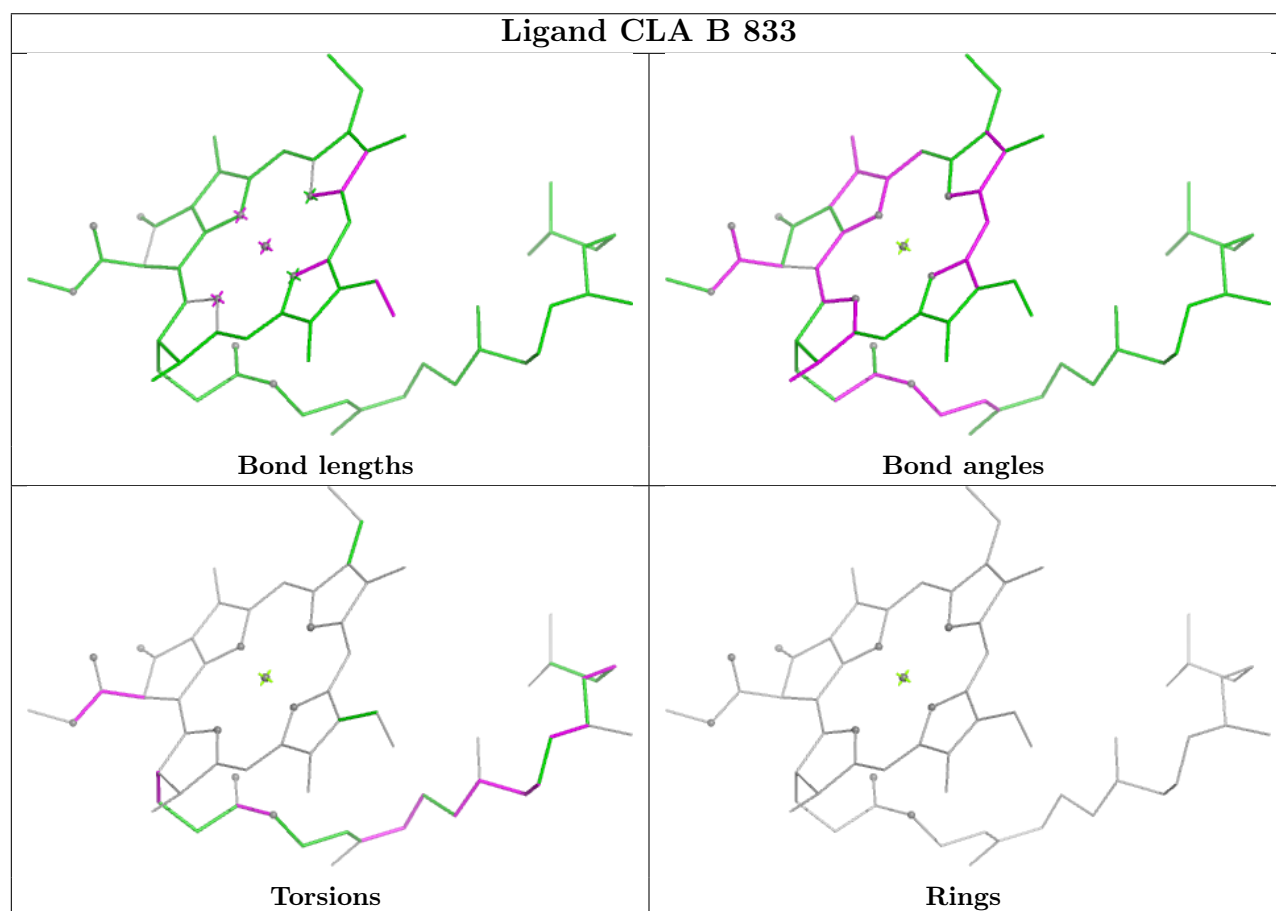
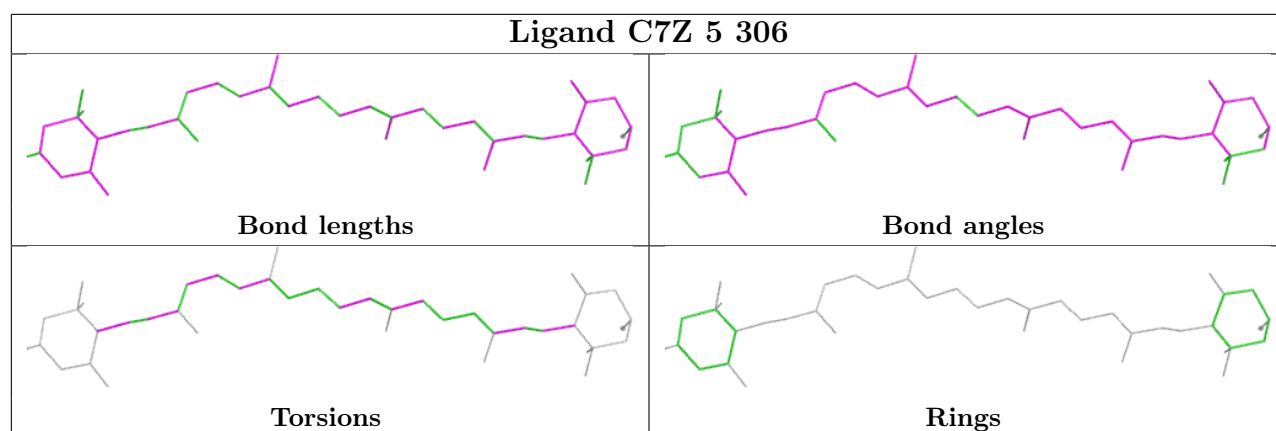
Rings



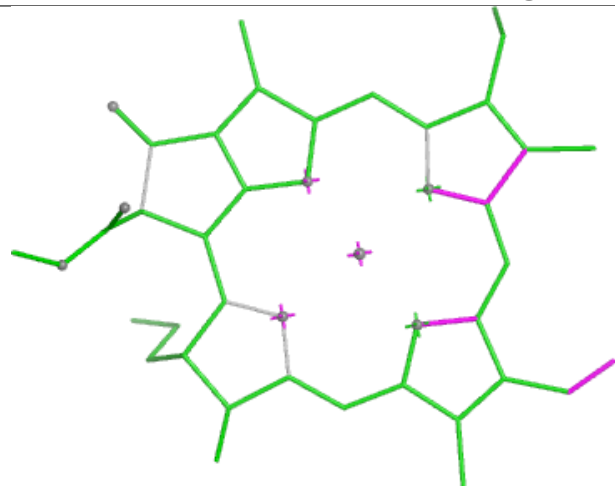




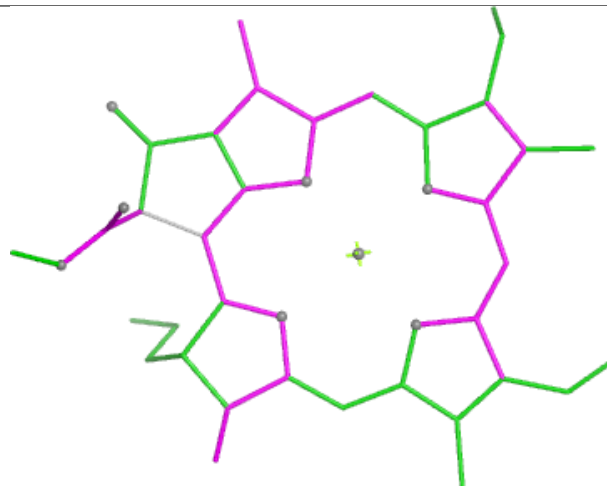




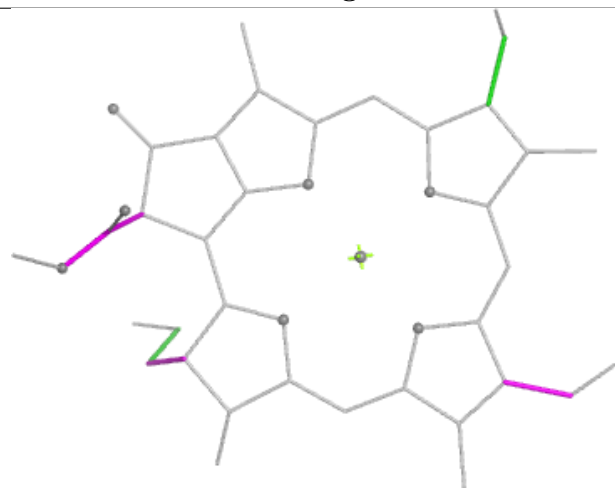
Ligand CLA 7 311



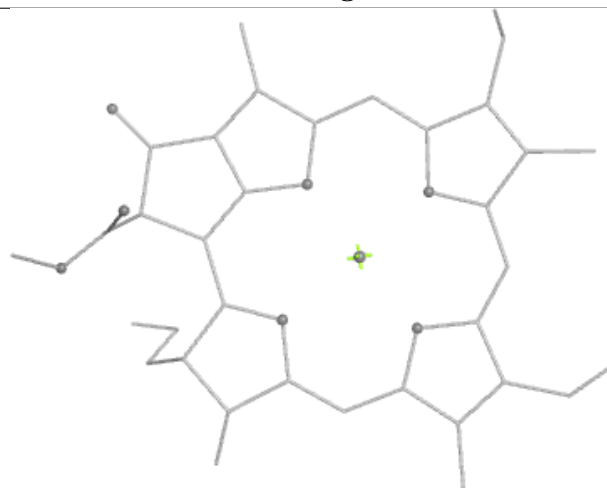
Bond lengths



Bond angles

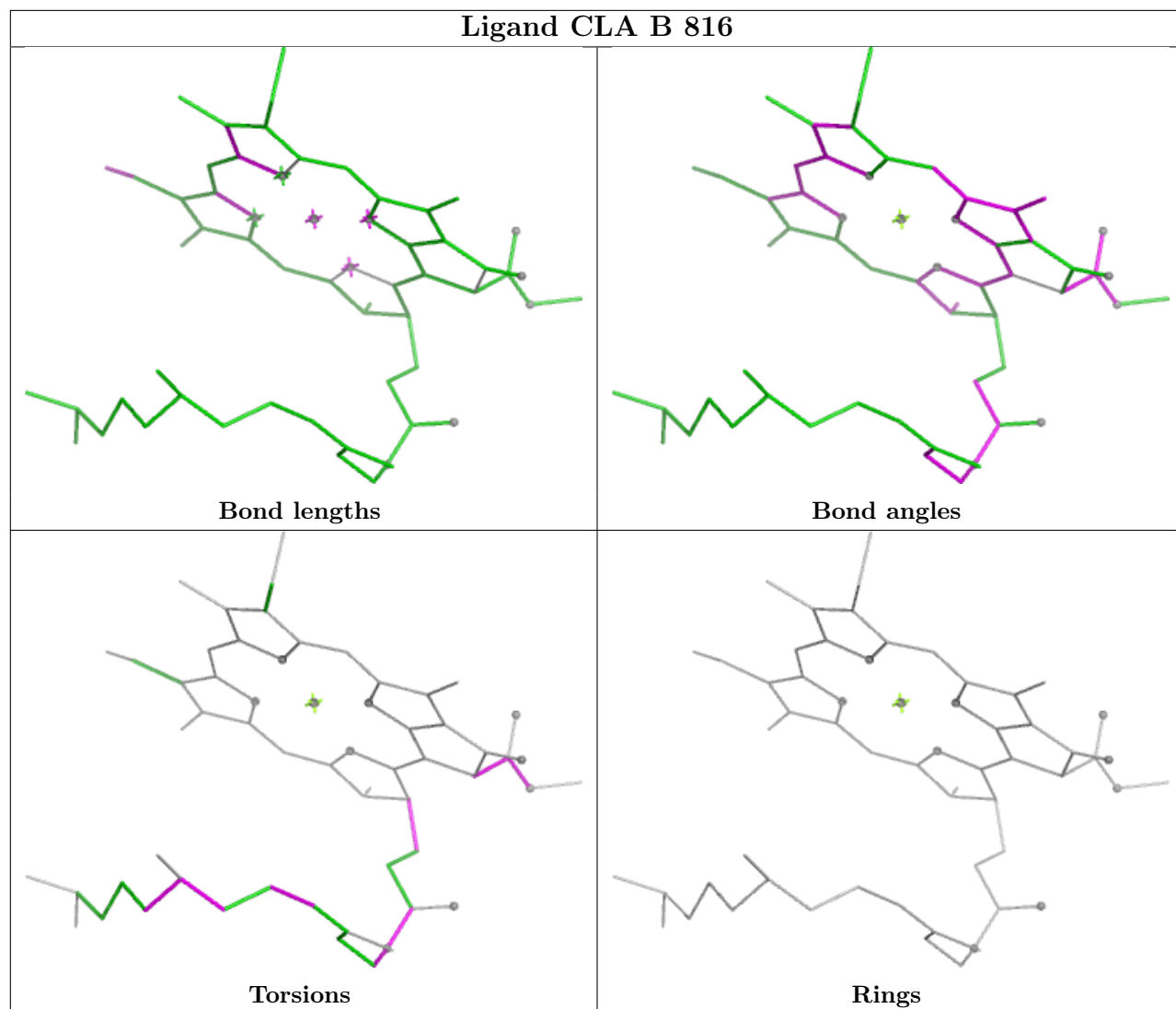


Torsions

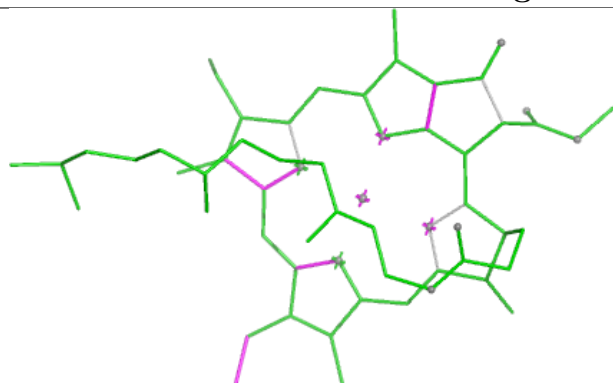


Rings

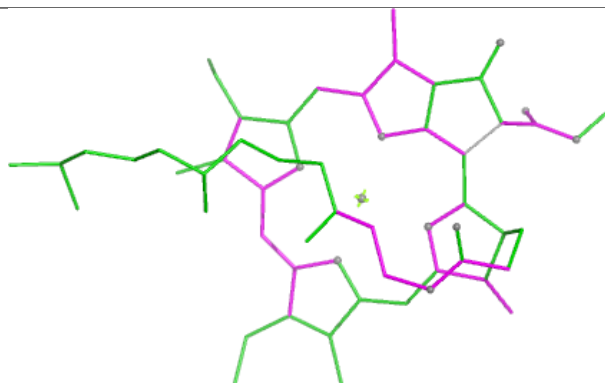
Ligand CLA B 816



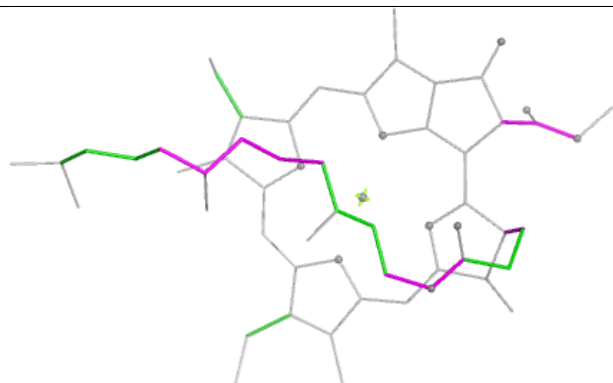
Ligand CLA A 818



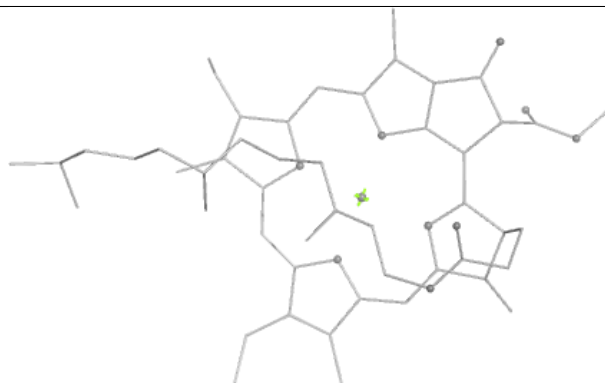
Bond lengths



Bond angles

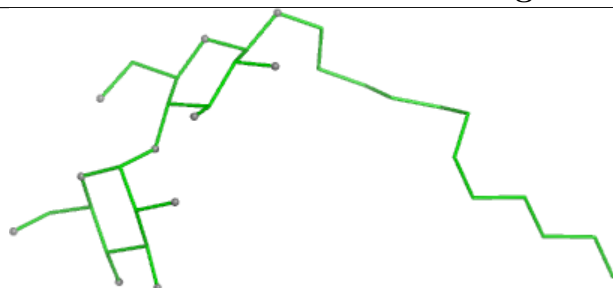


Torsions



Rings

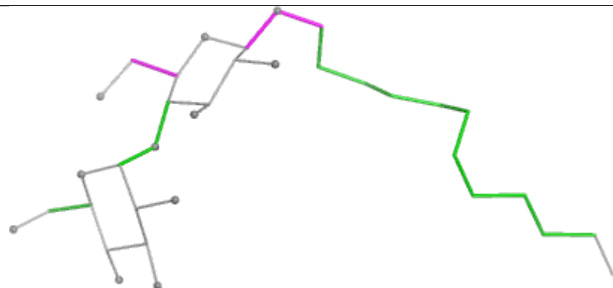
Ligand LMT 1 301



Bond lengths



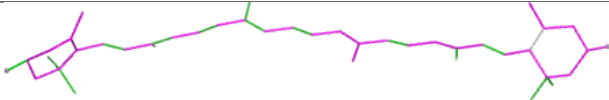
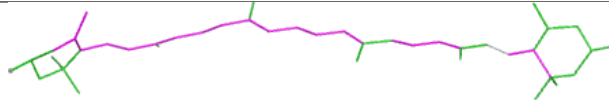
Bond angles

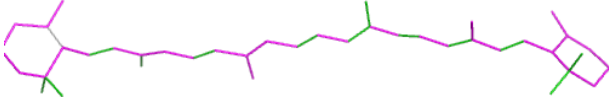
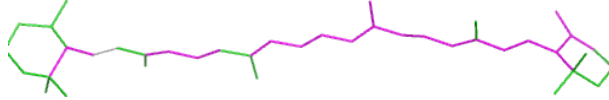


Torsions



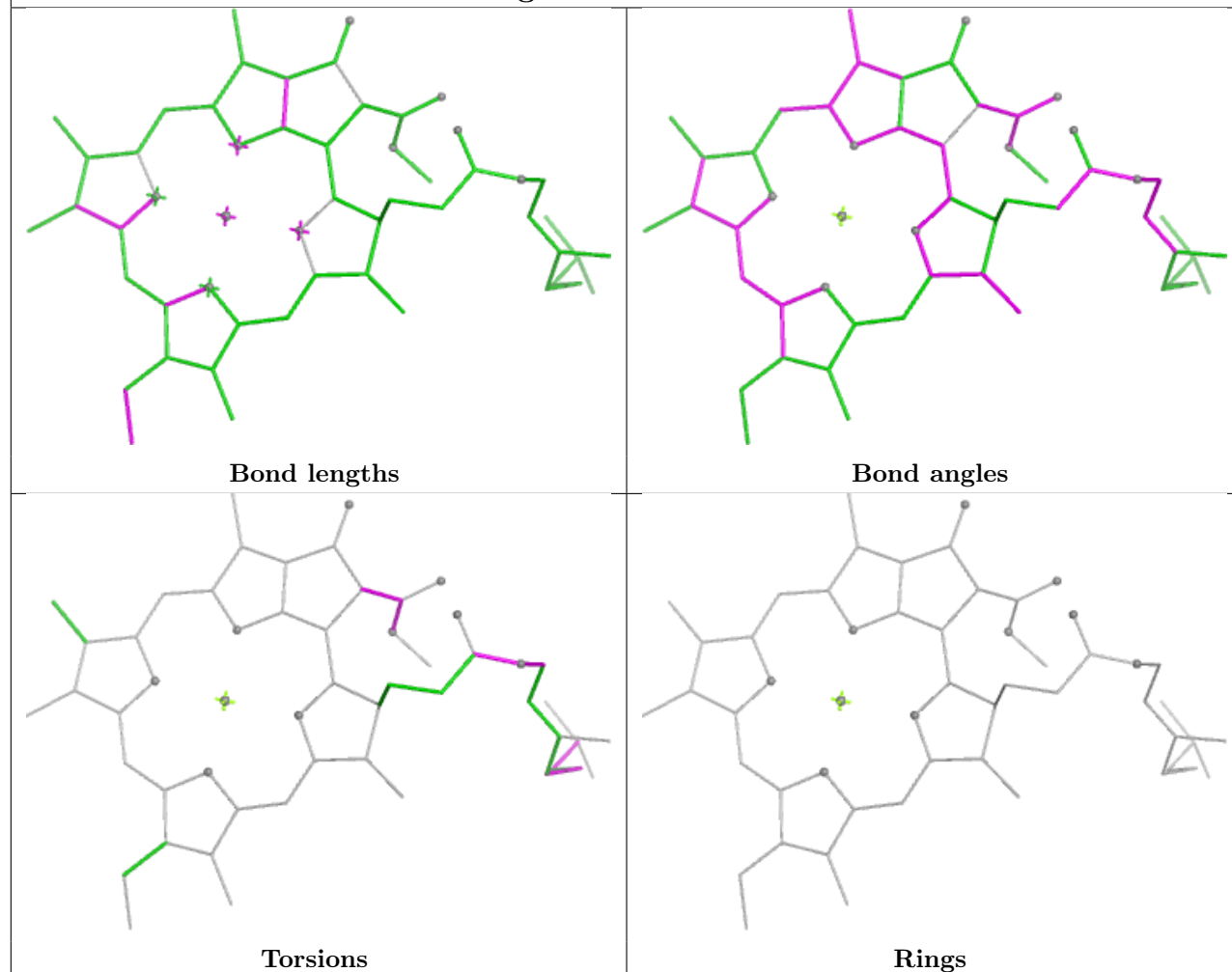
Rings

Ligand LUT 9 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

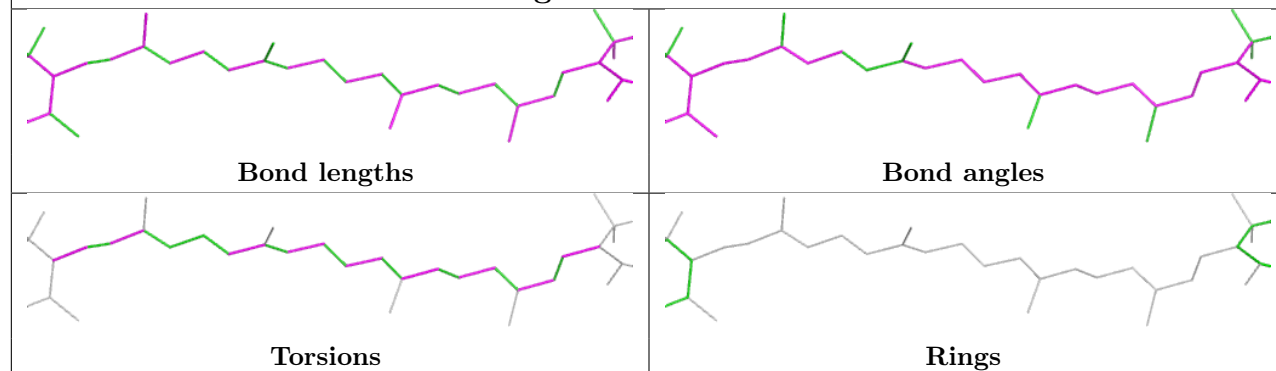
Ligand LUT 8 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 5 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

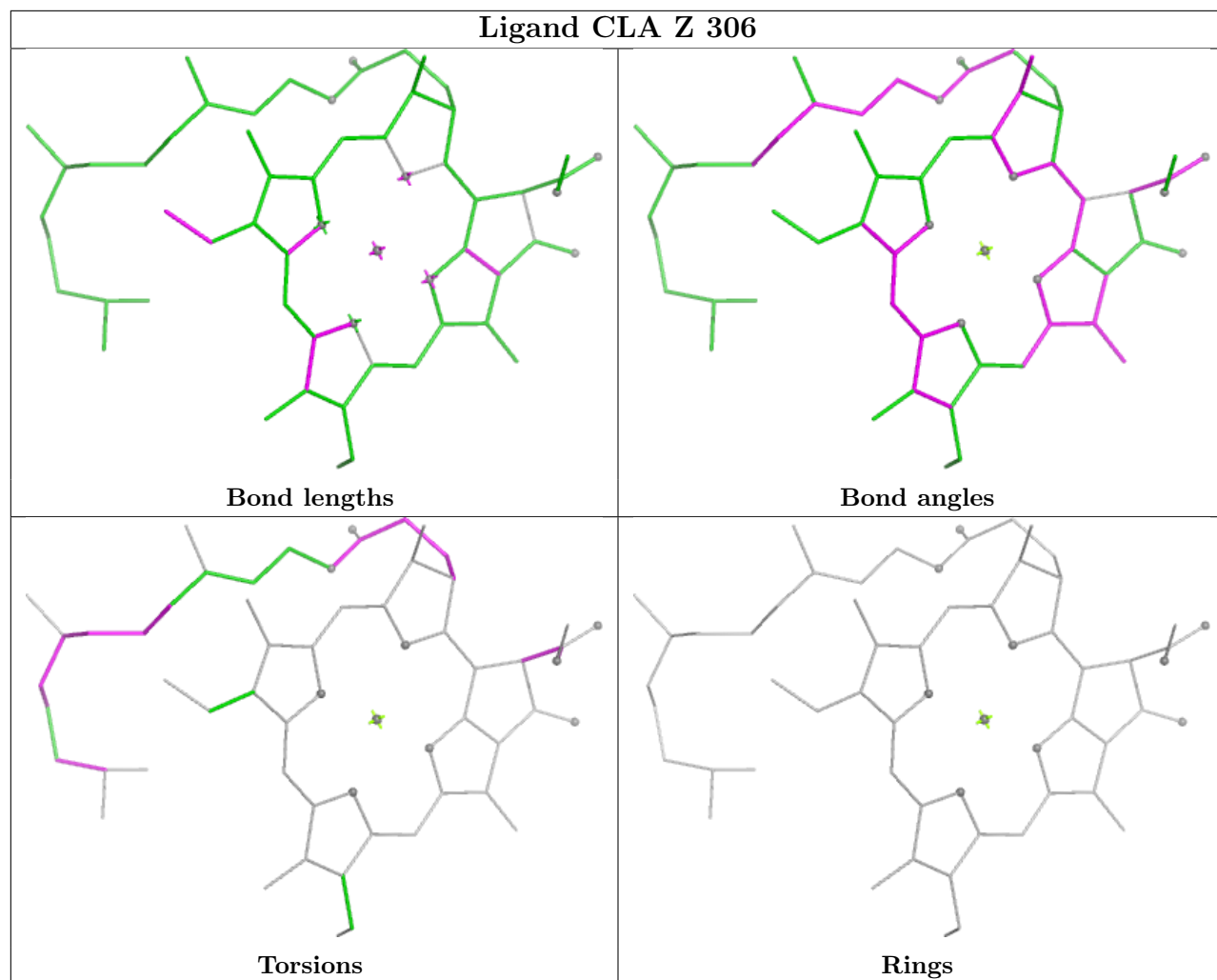
Ligand CLA 9 307



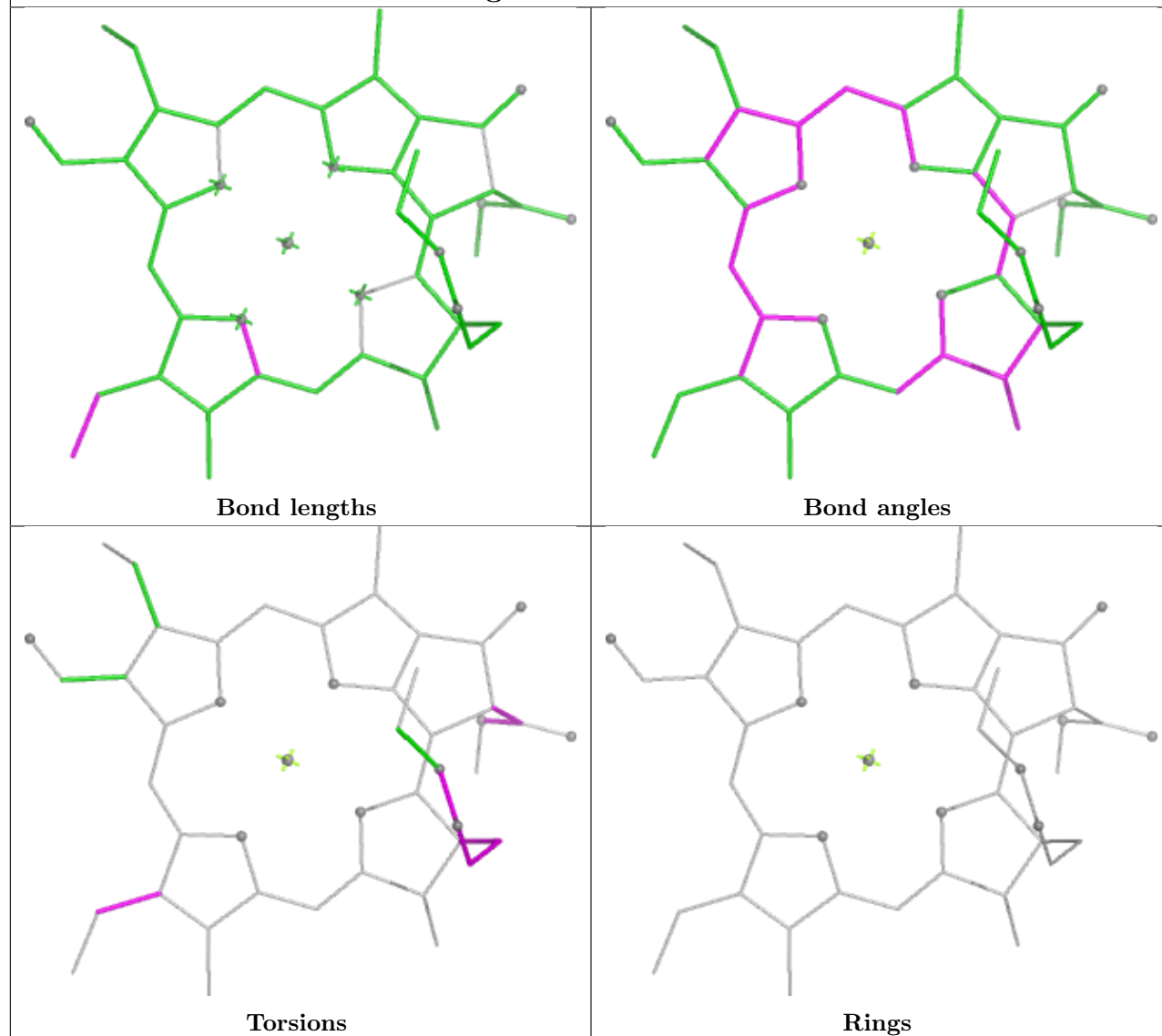
Ligand BCR J 104



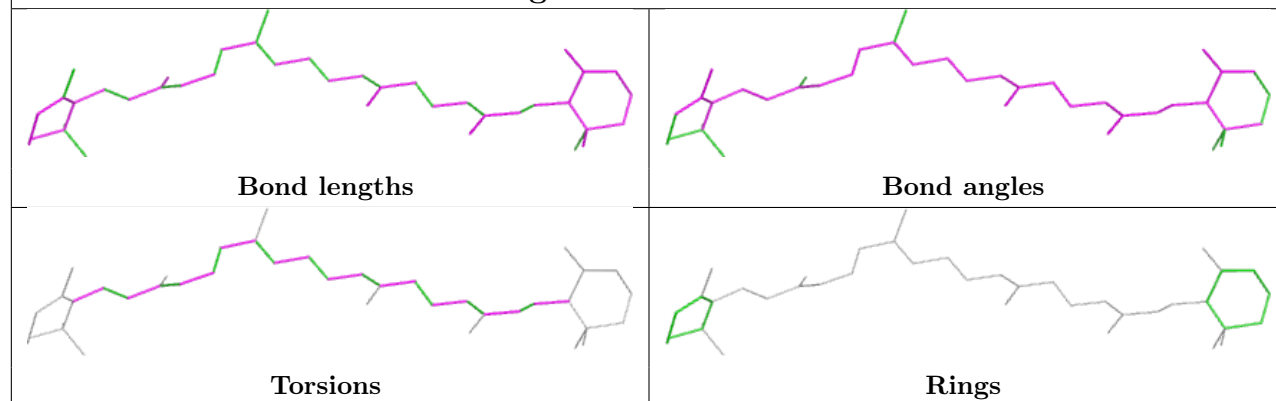
Ligand CLA Z 306

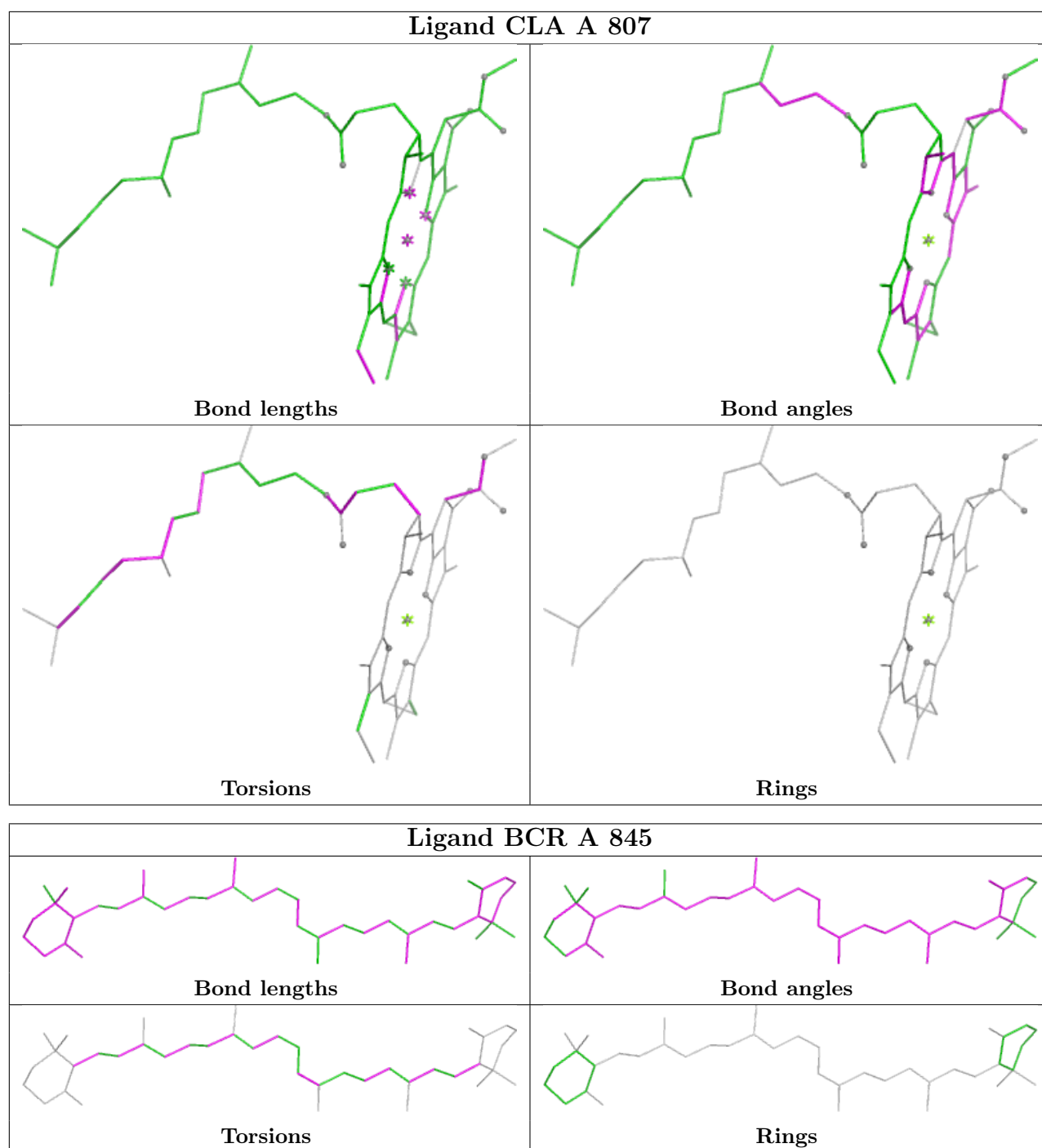


Ligand CHL Z 312

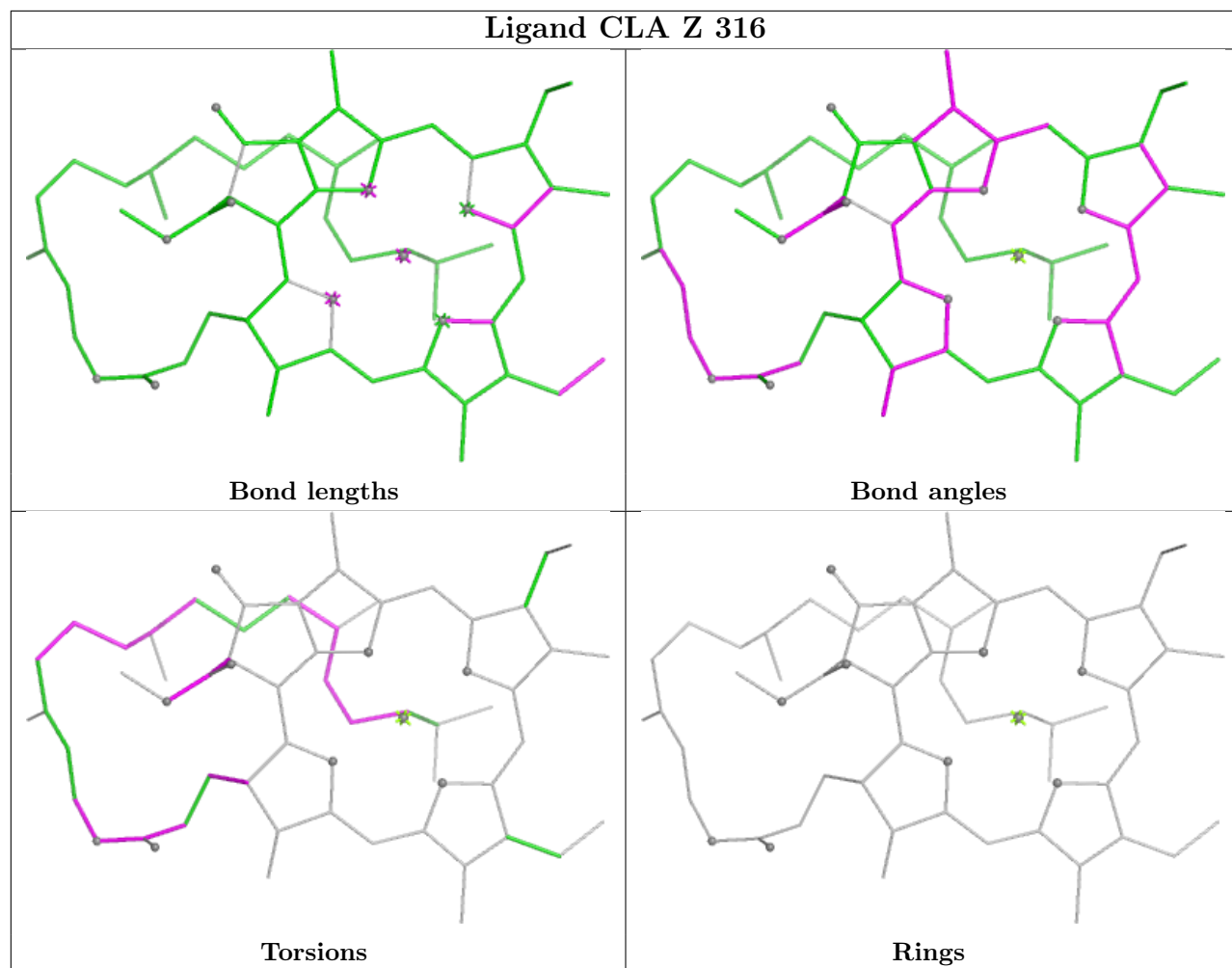


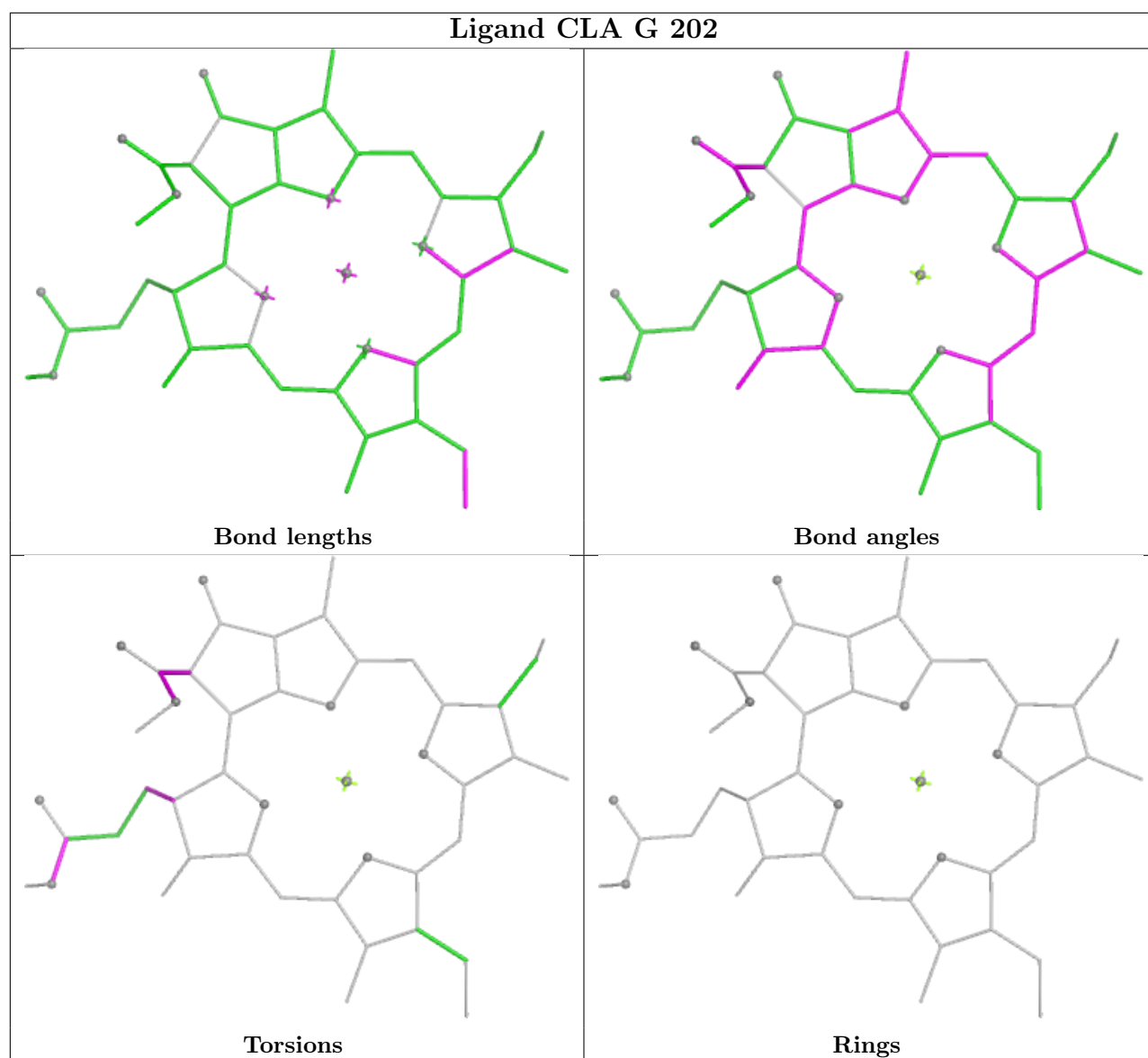
Ligand BCR G 203



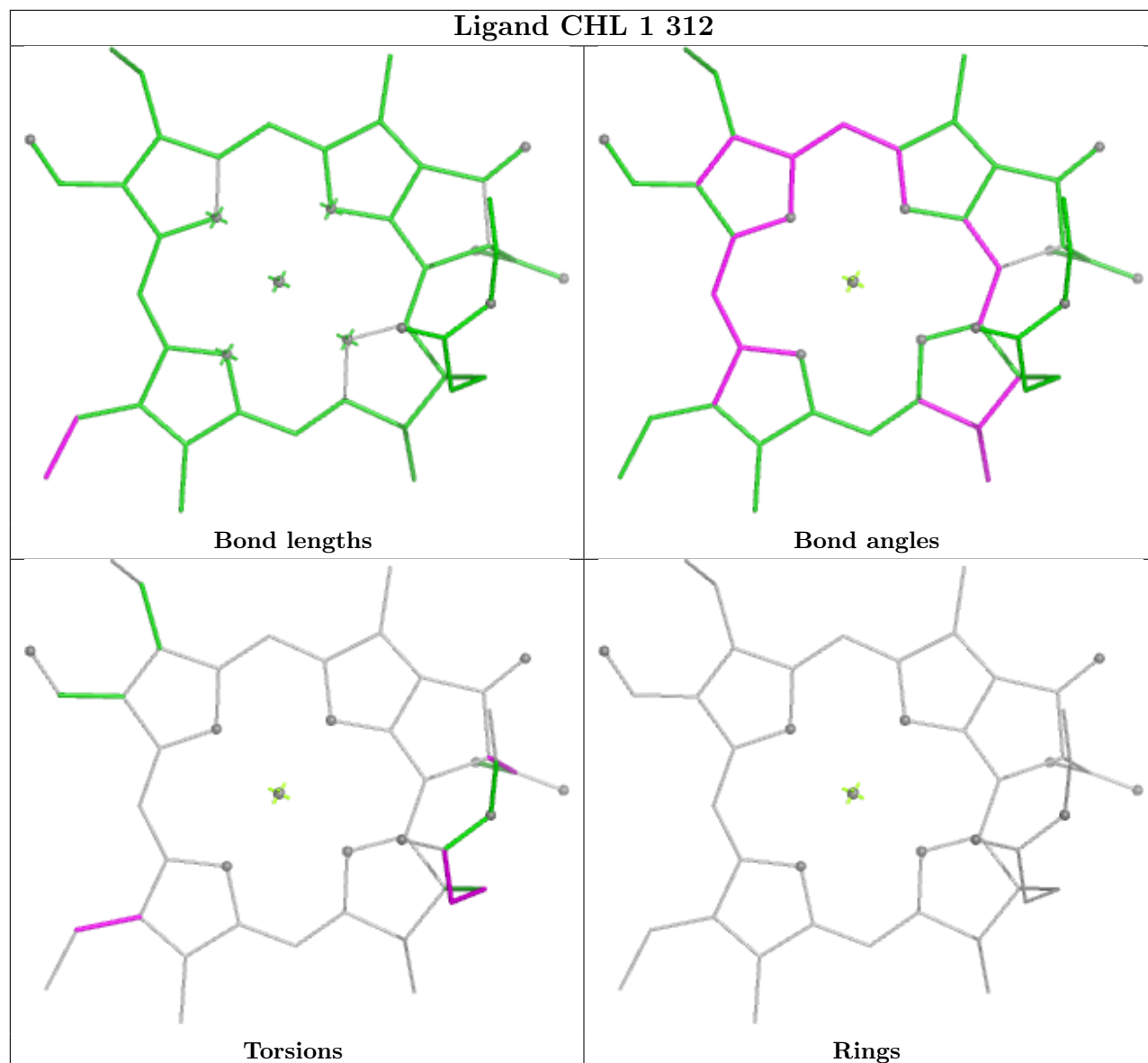


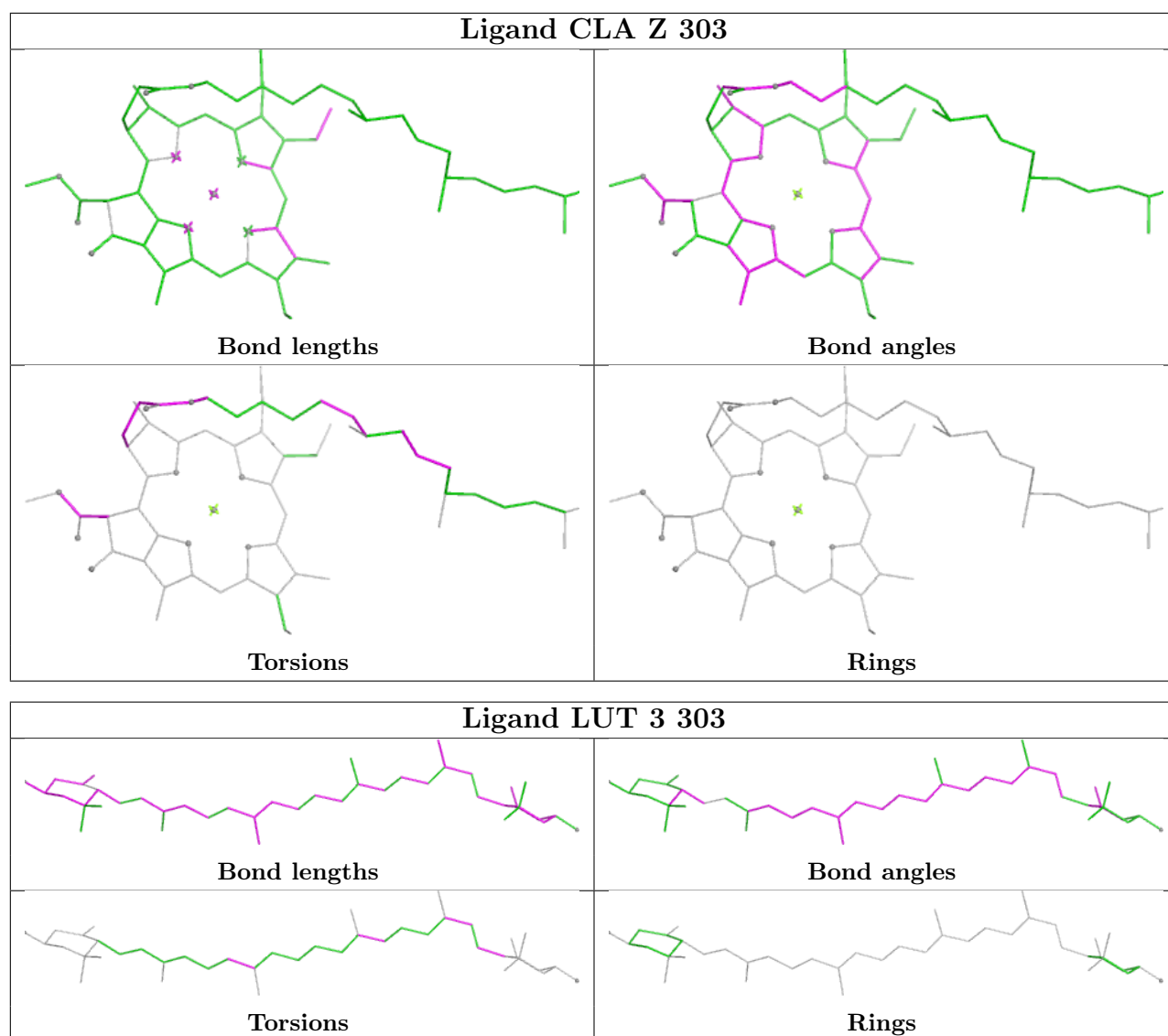
Ligand CLA Z 316

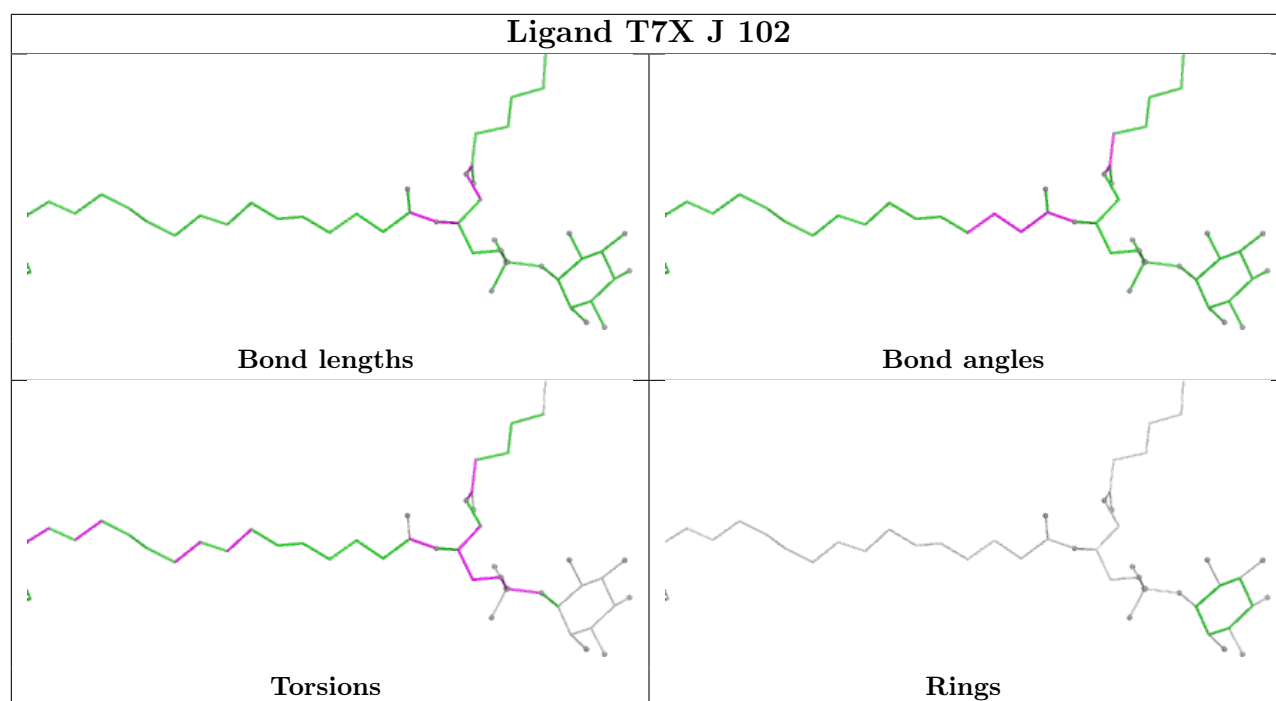


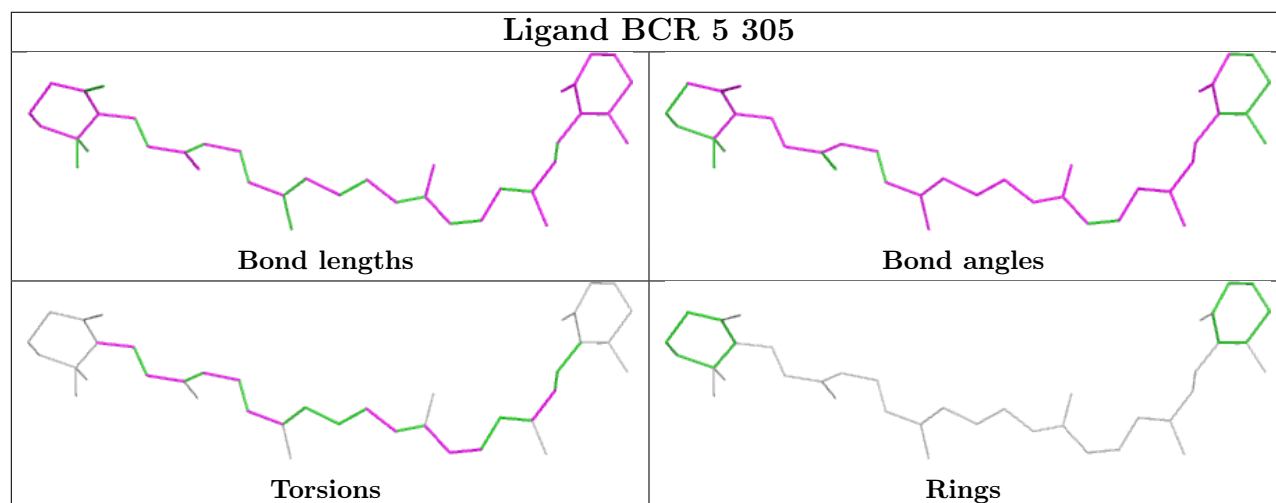
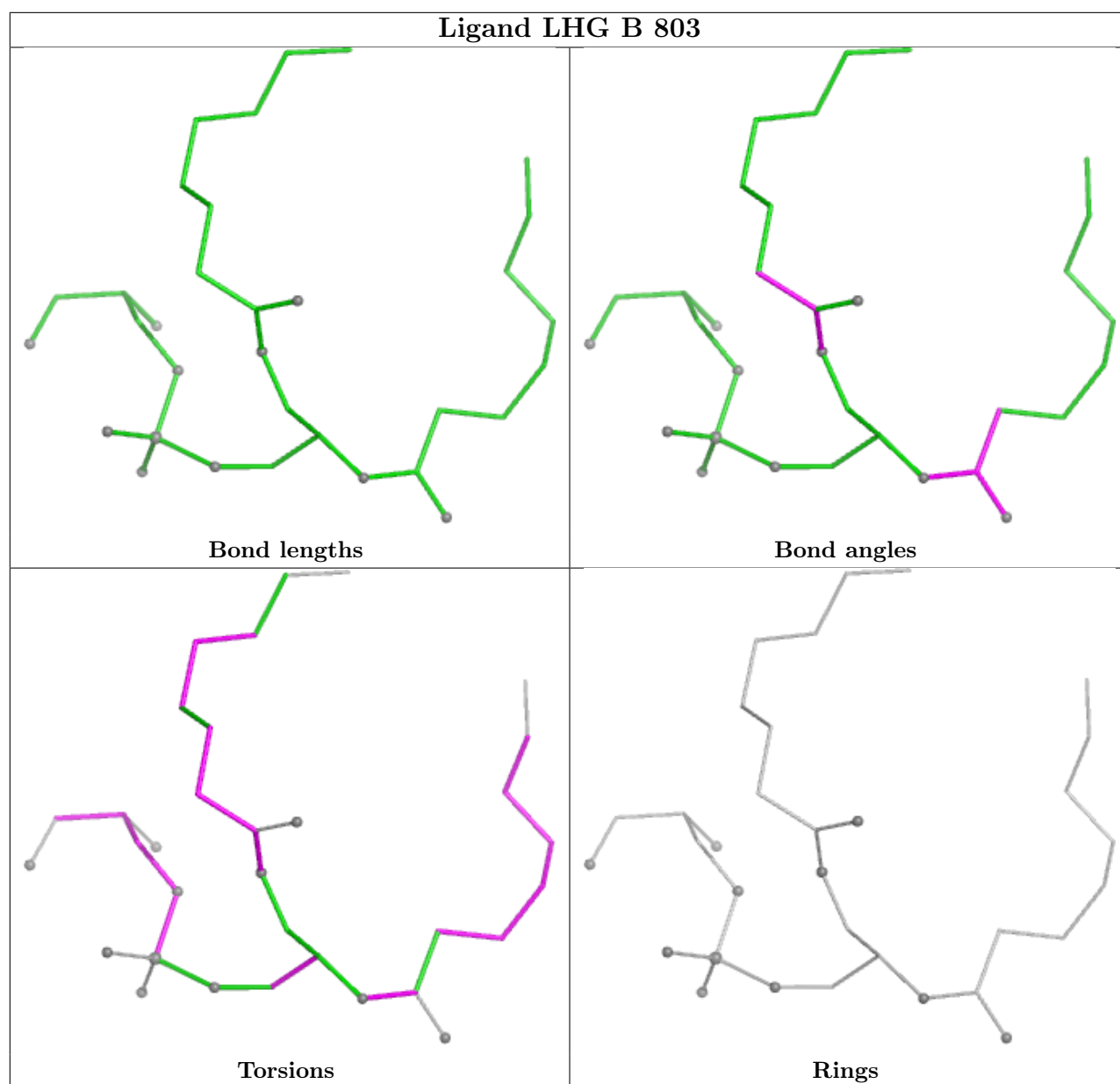


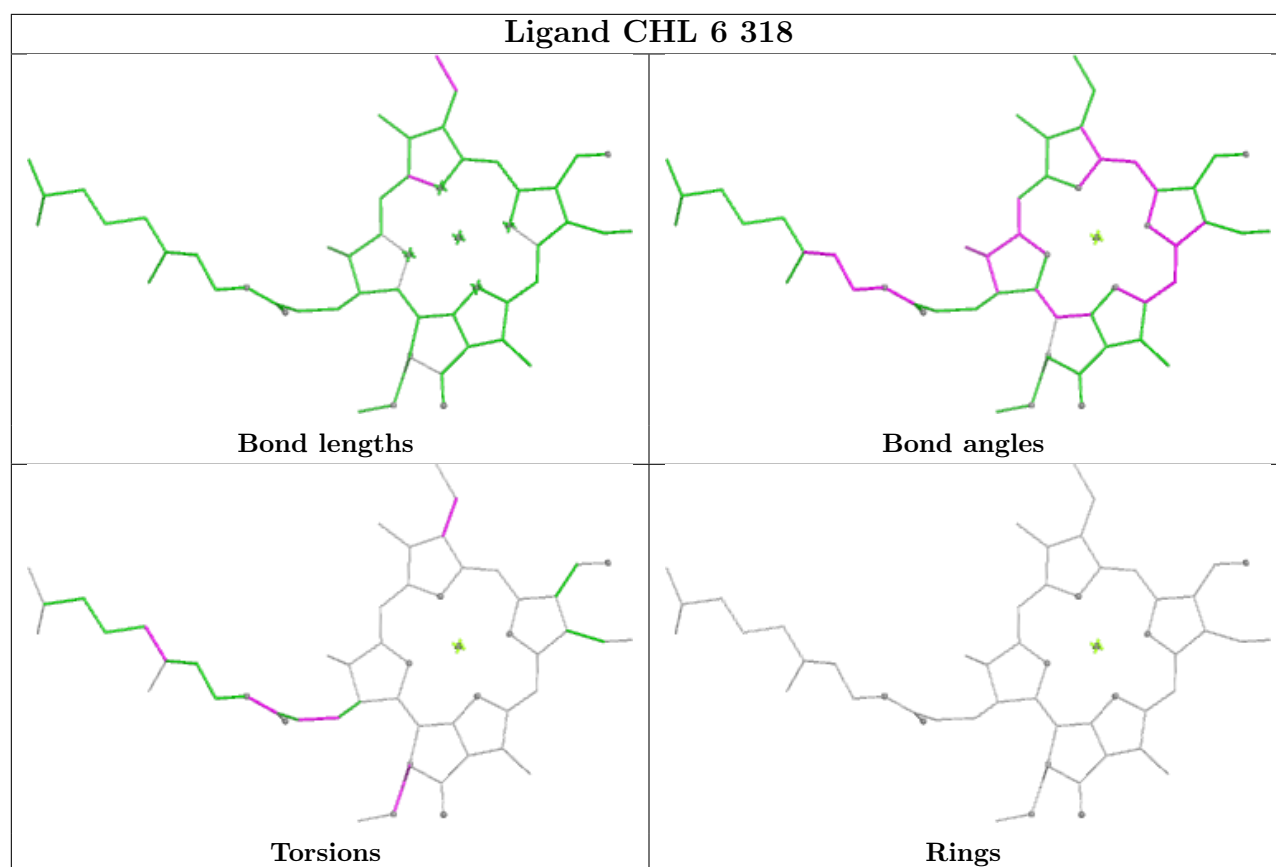
Ligand CHL 1 312



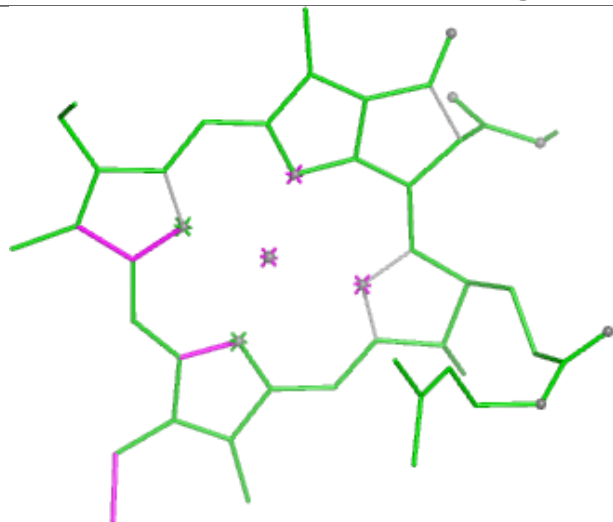




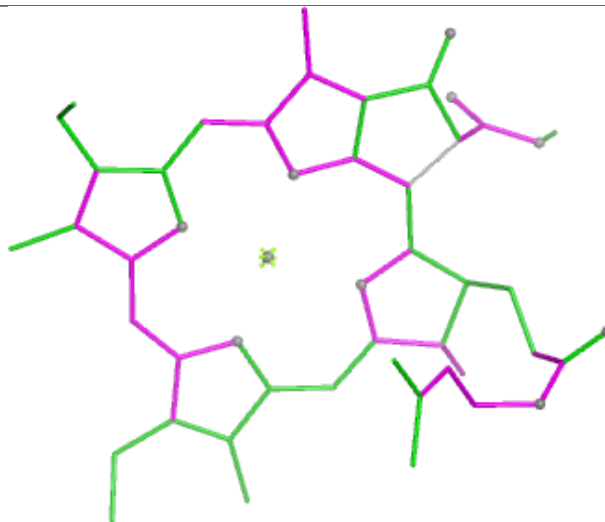




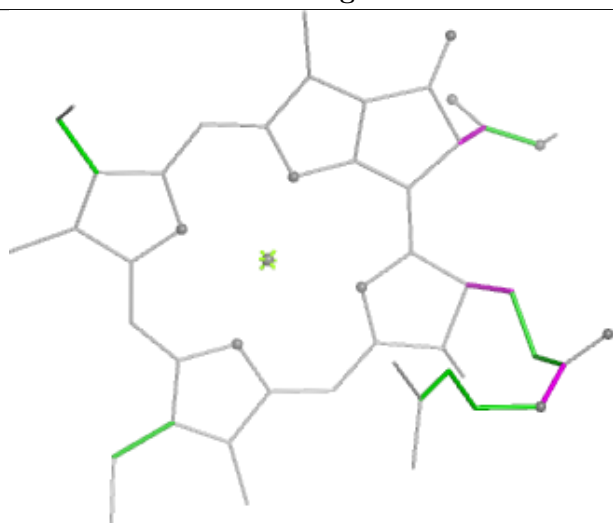
Ligand CLA B 832



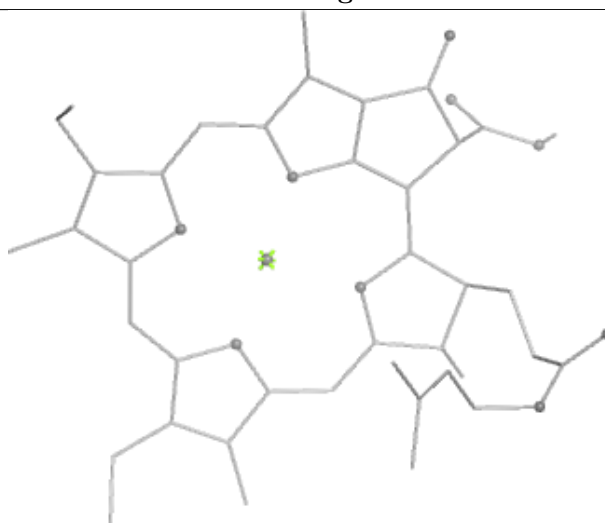
Bond lengths



Bond angles

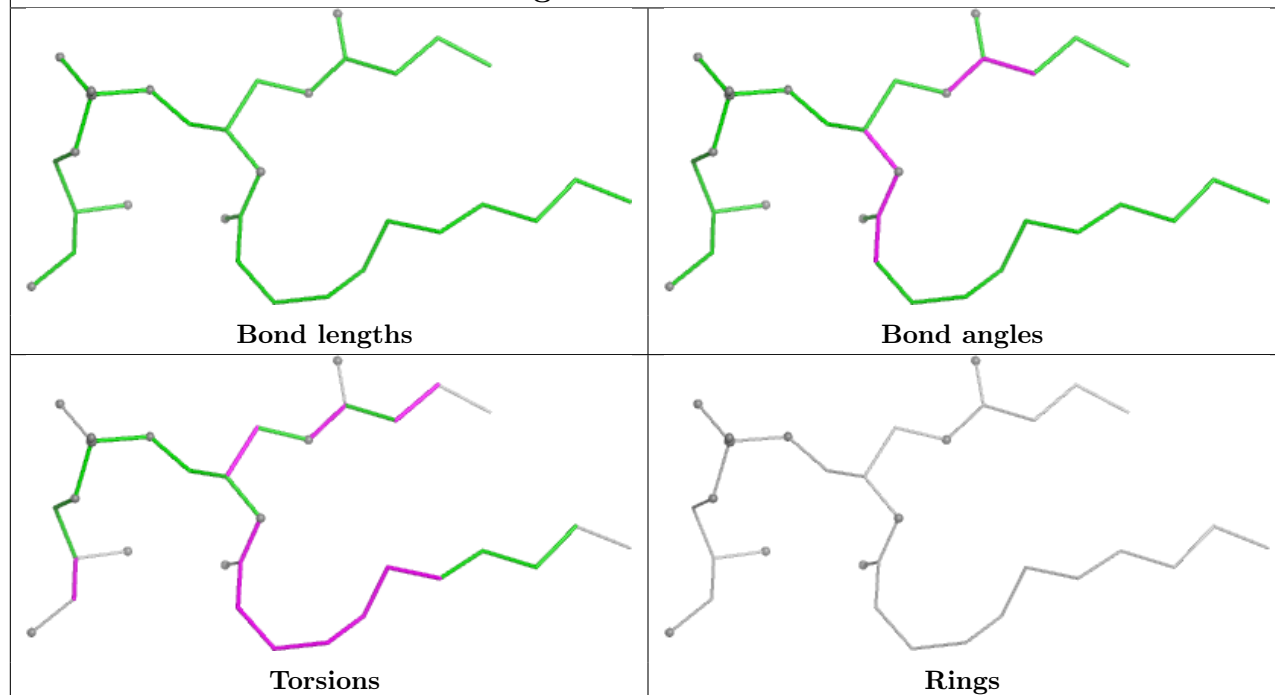


Torsions

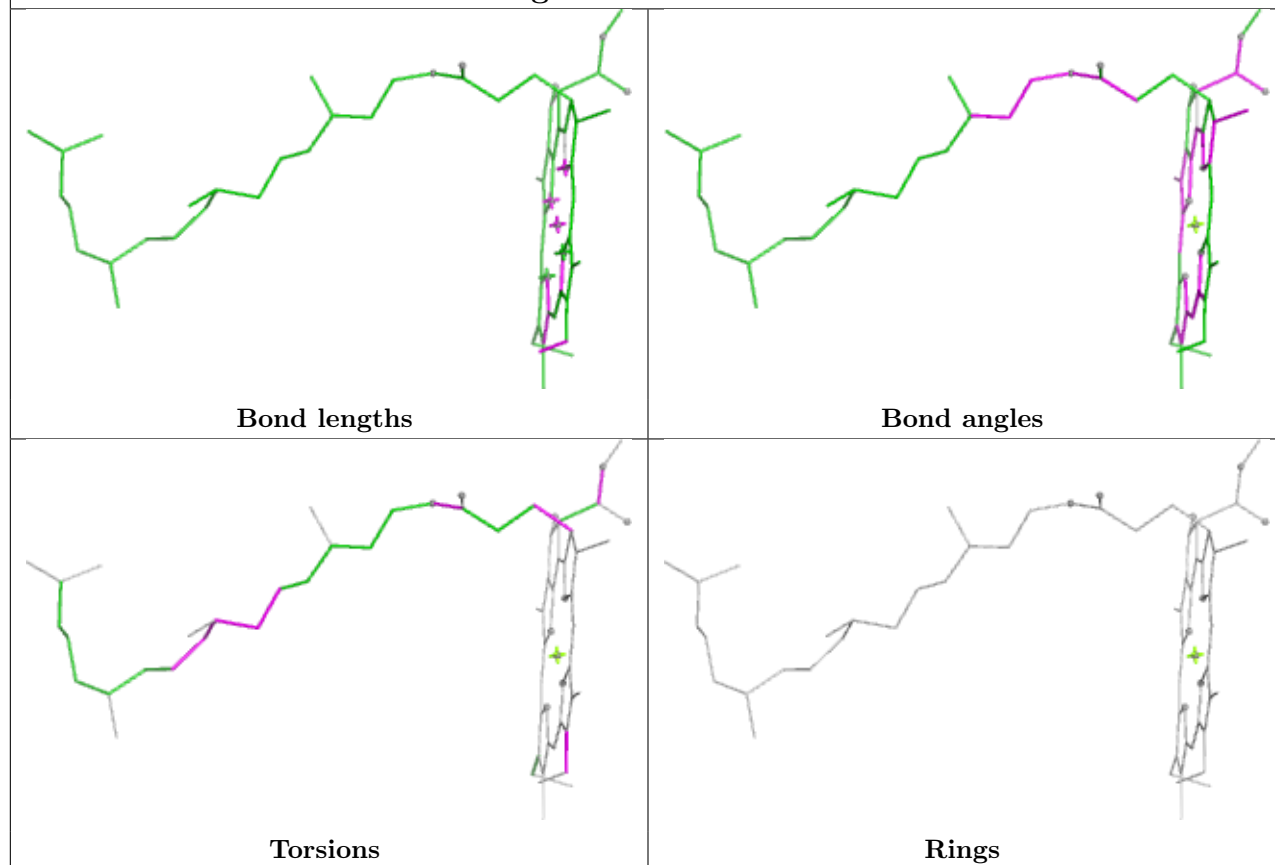


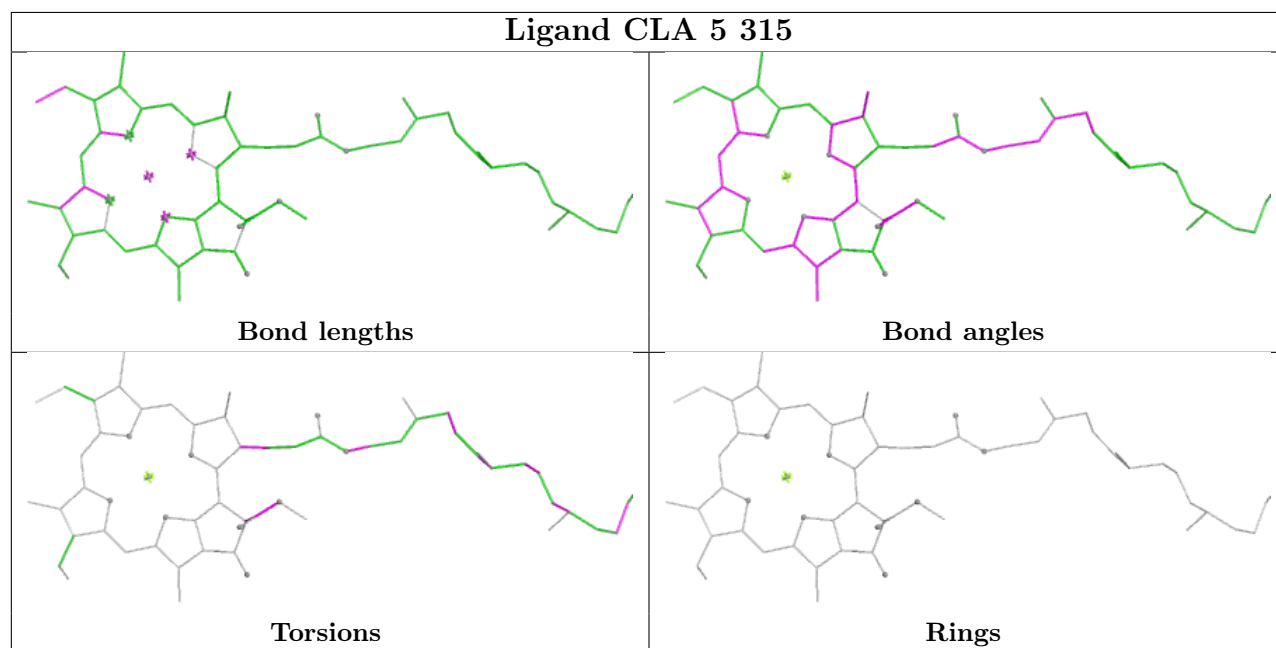
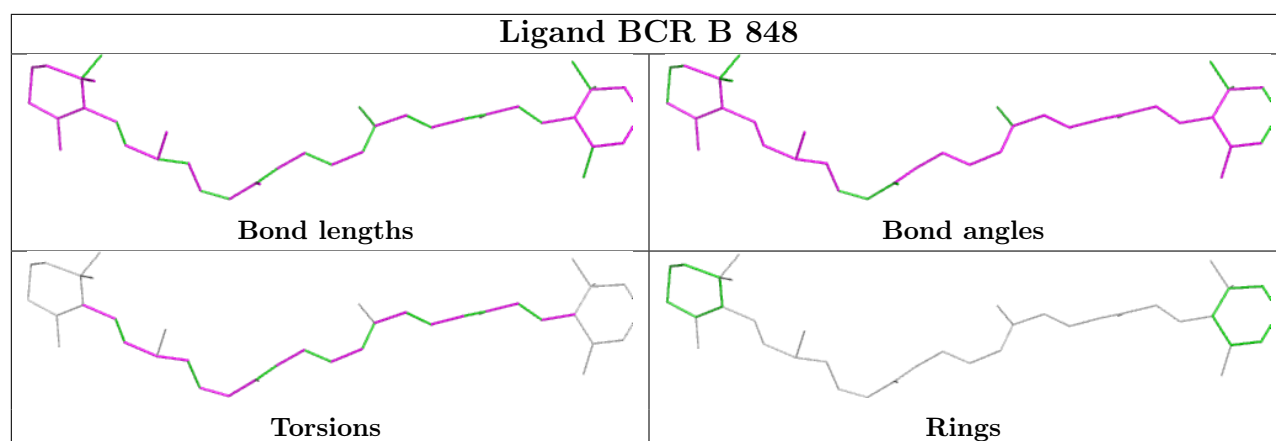
Rings

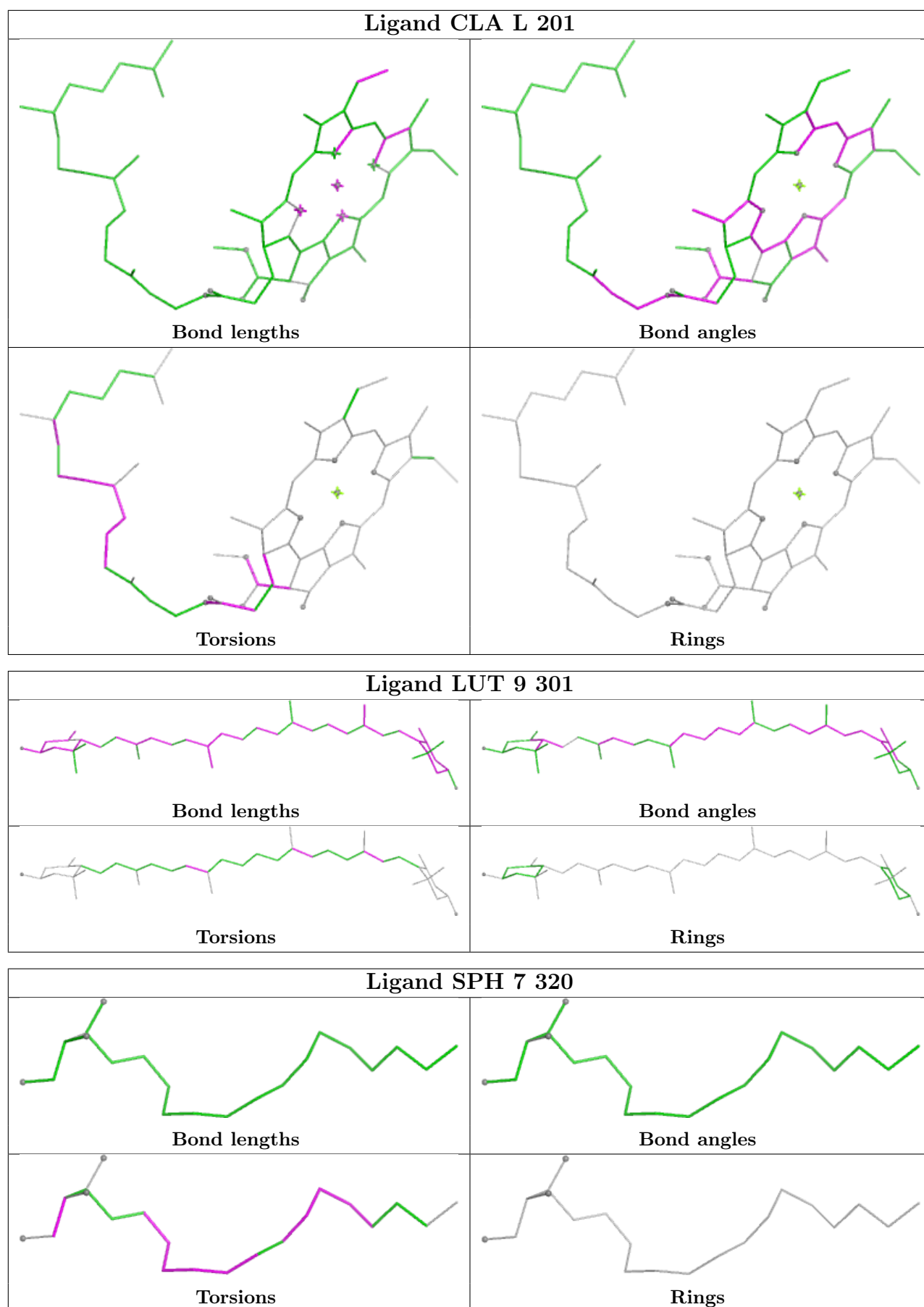
Ligand LHG 4 821

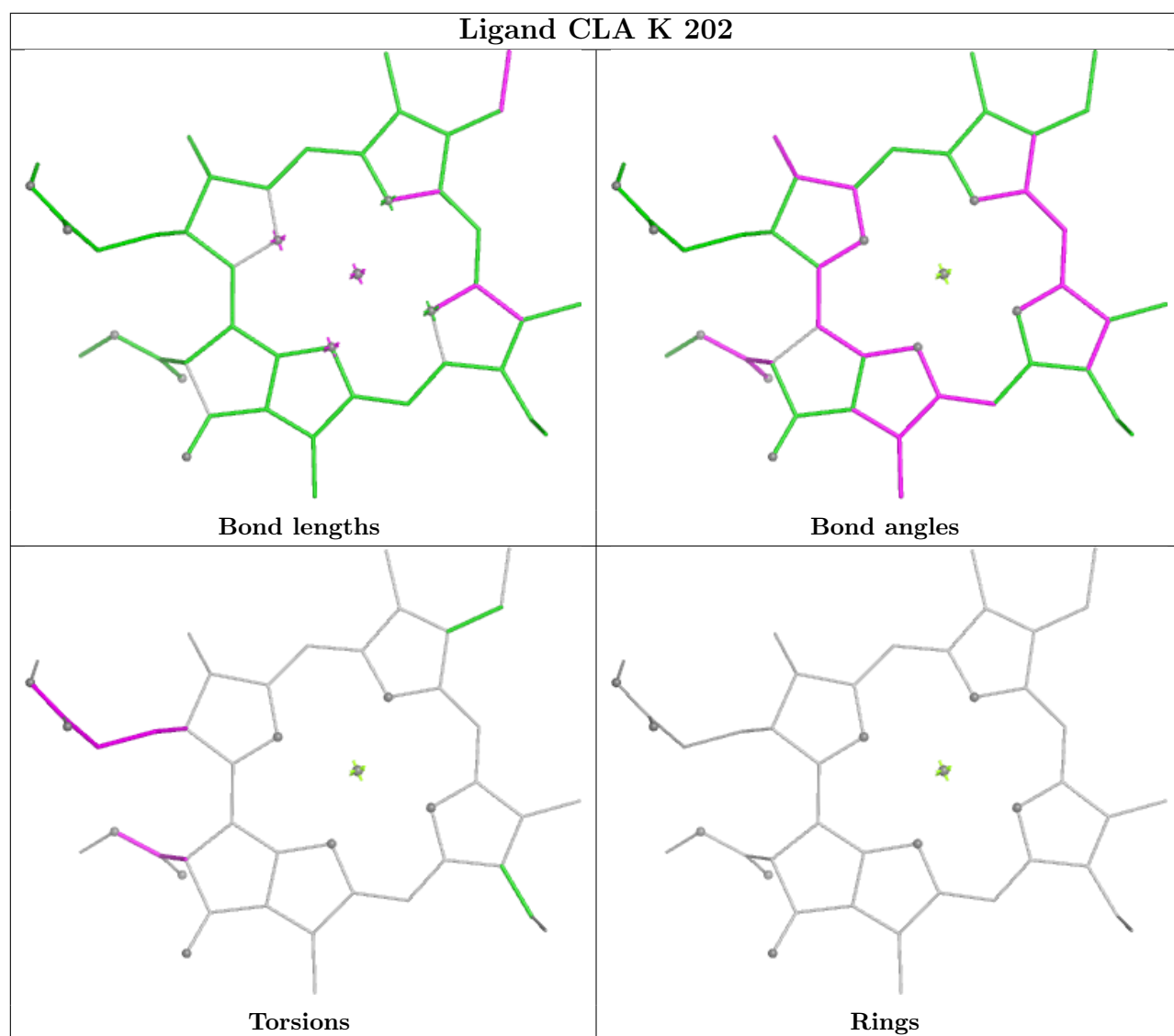


Ligand CLA B 841

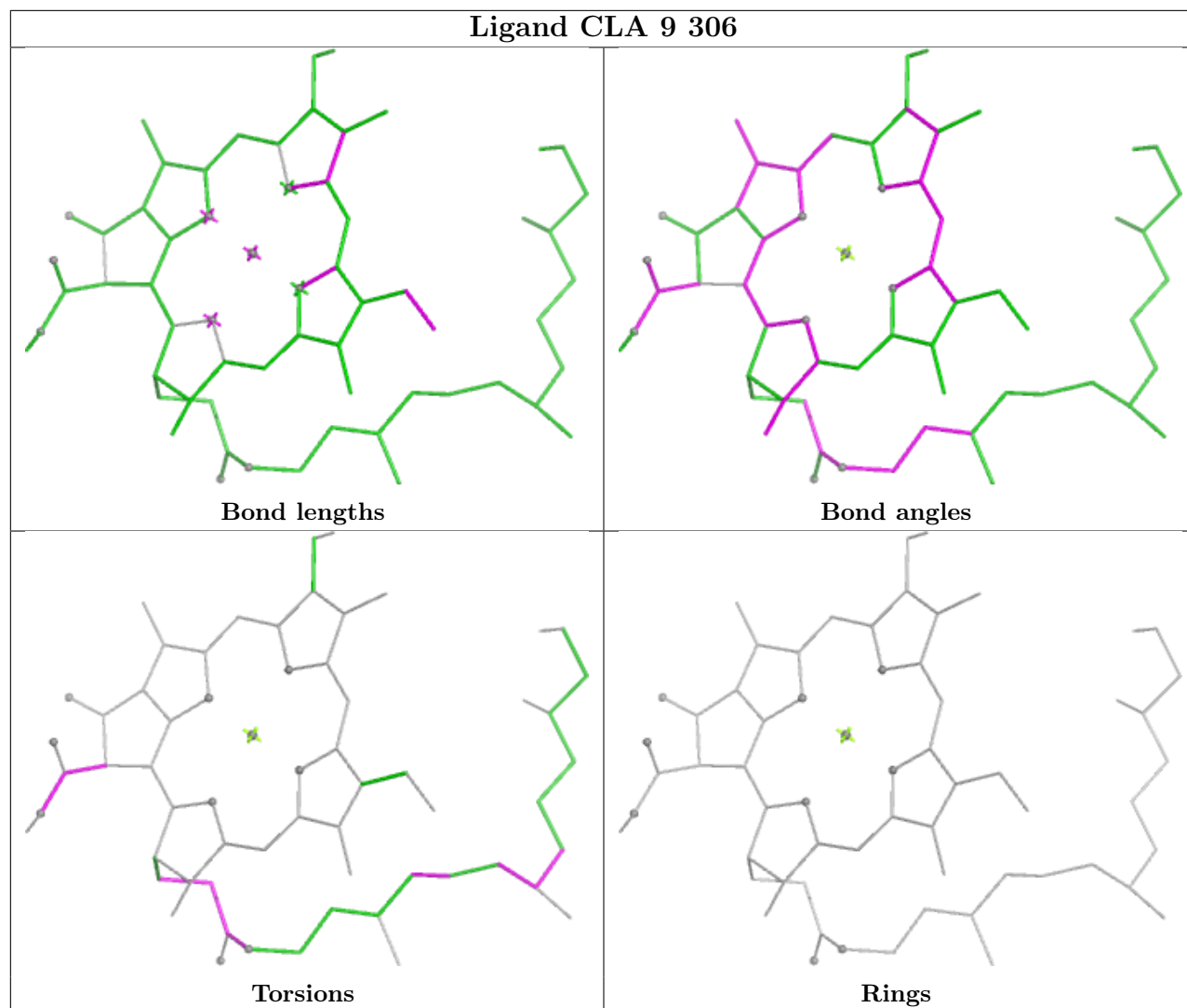




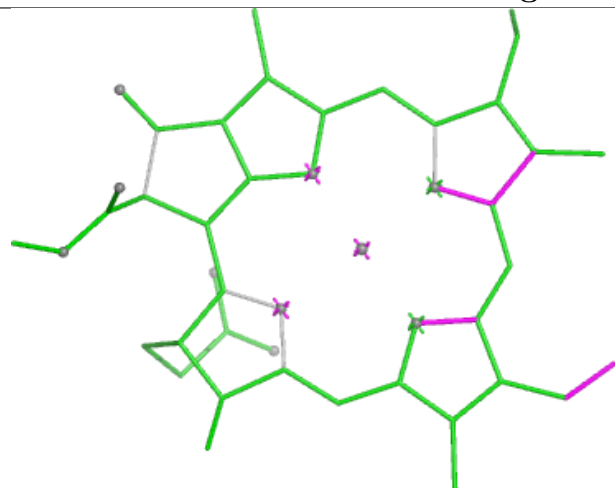




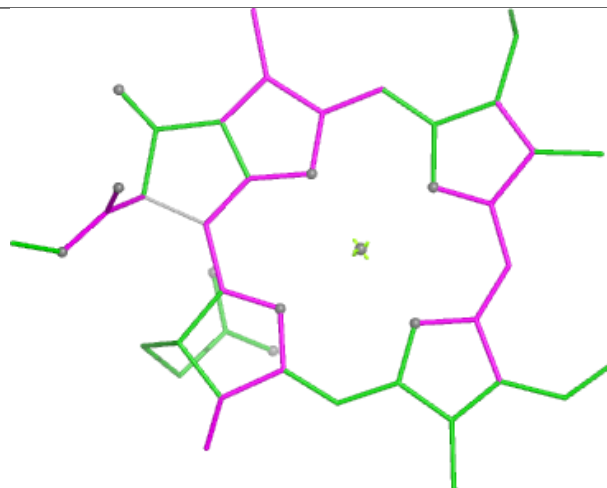
Ligand CLA 9 306



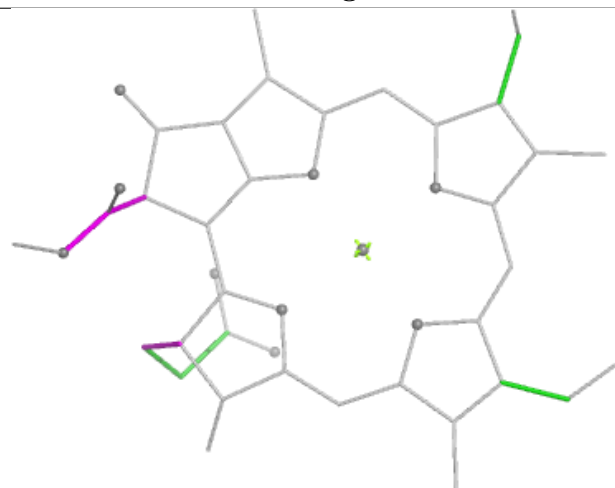
Ligand CLA 5 314



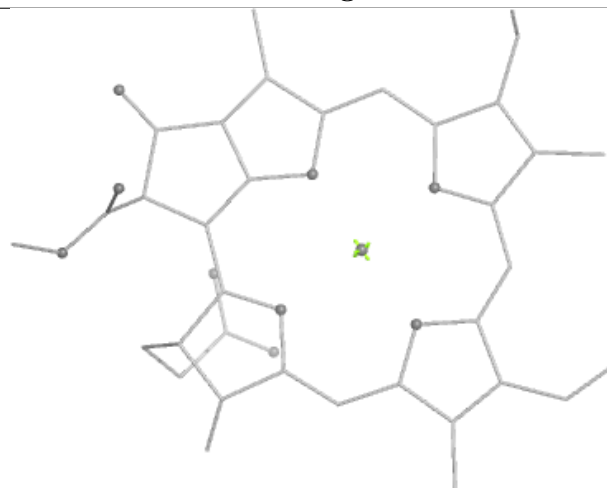
Bond lengths



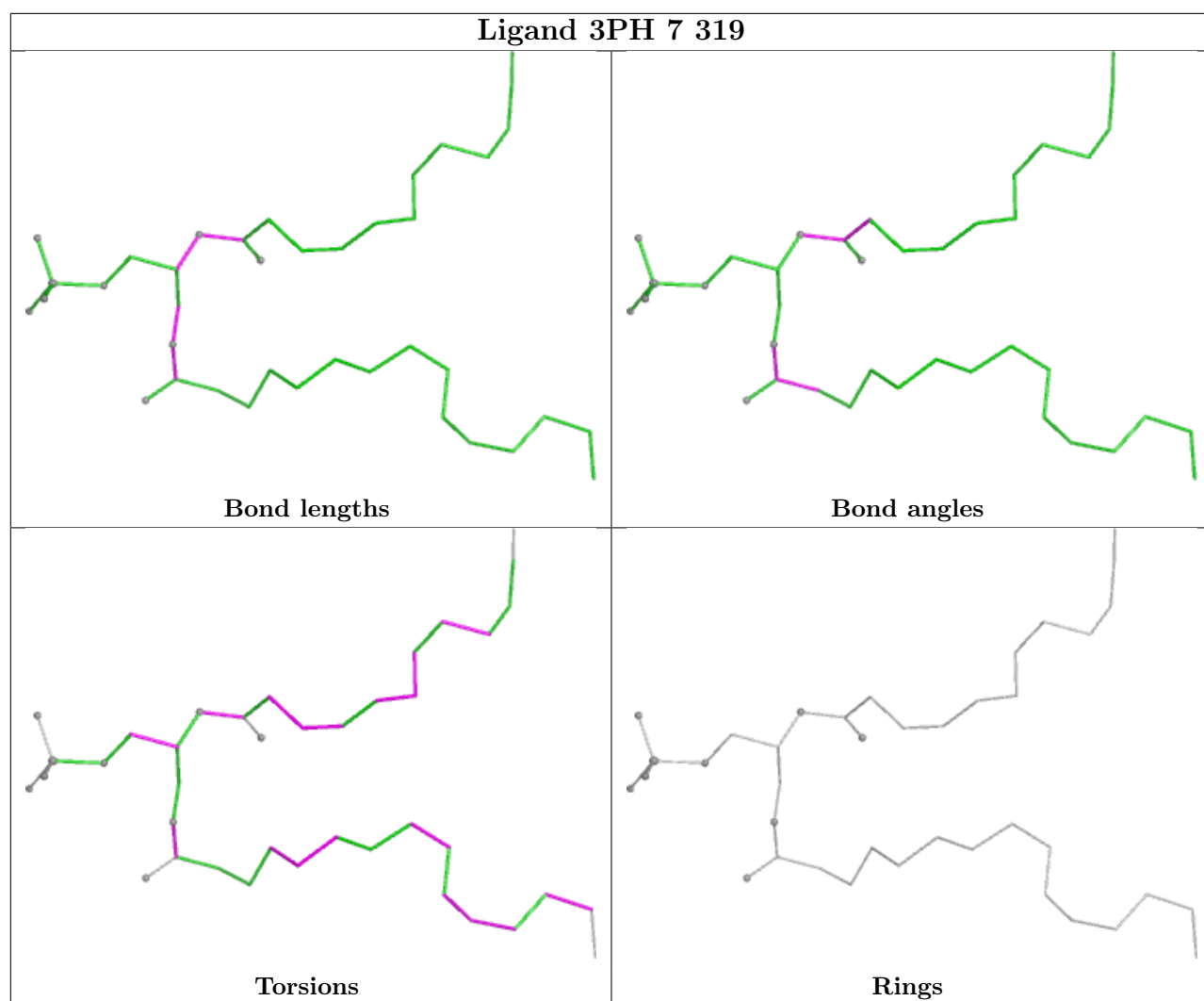
Bond angles



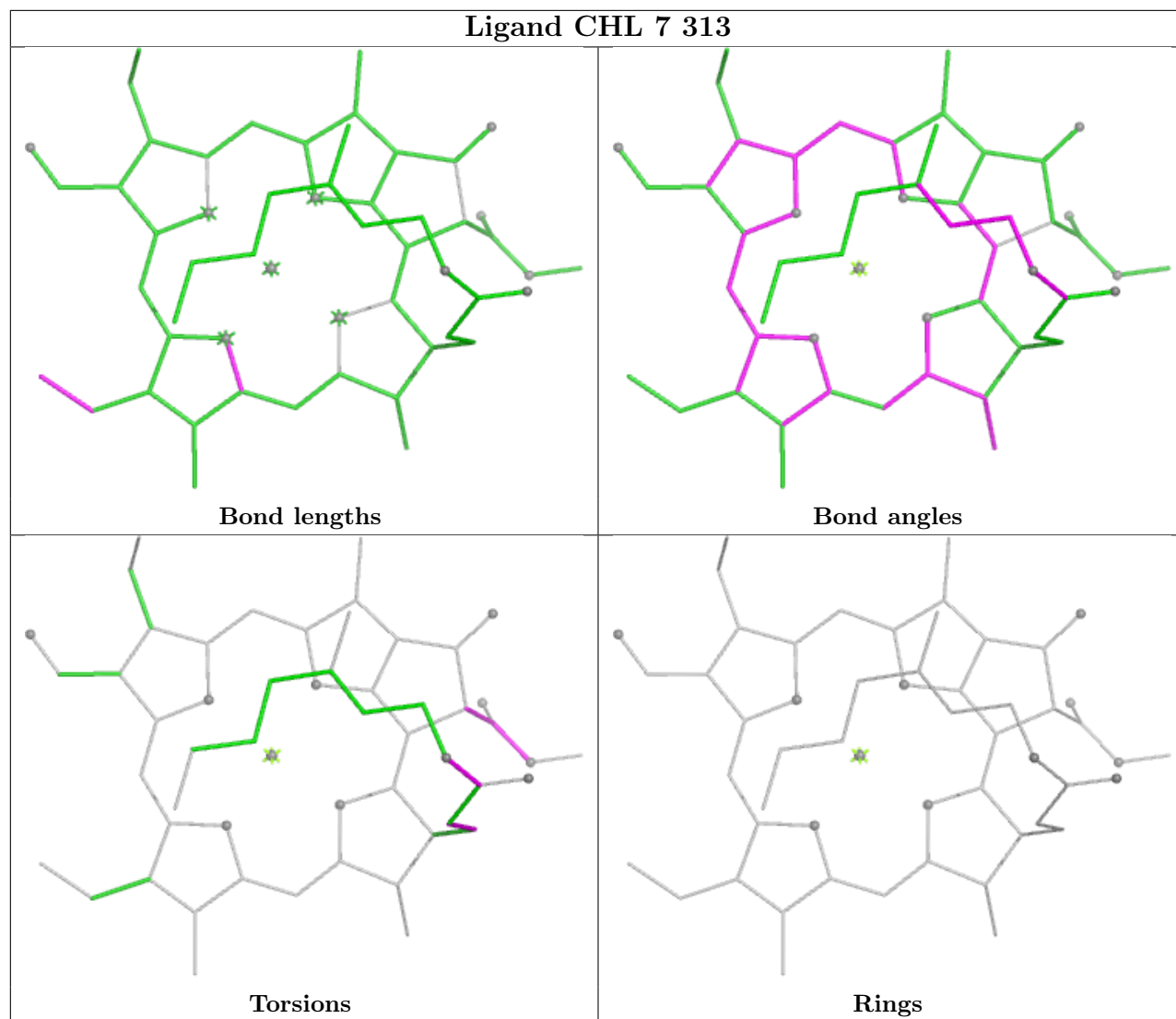
Torsions



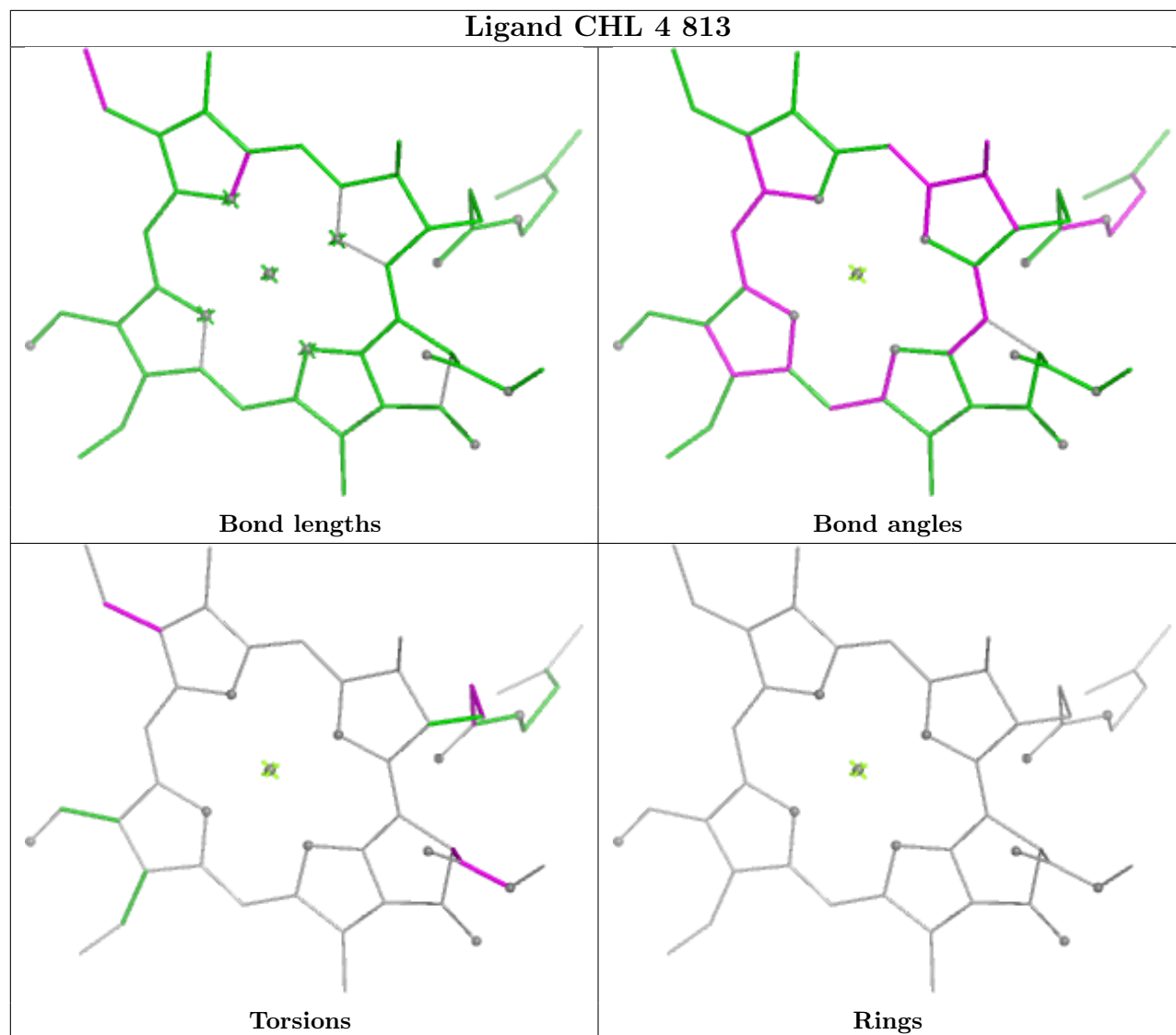
Rings



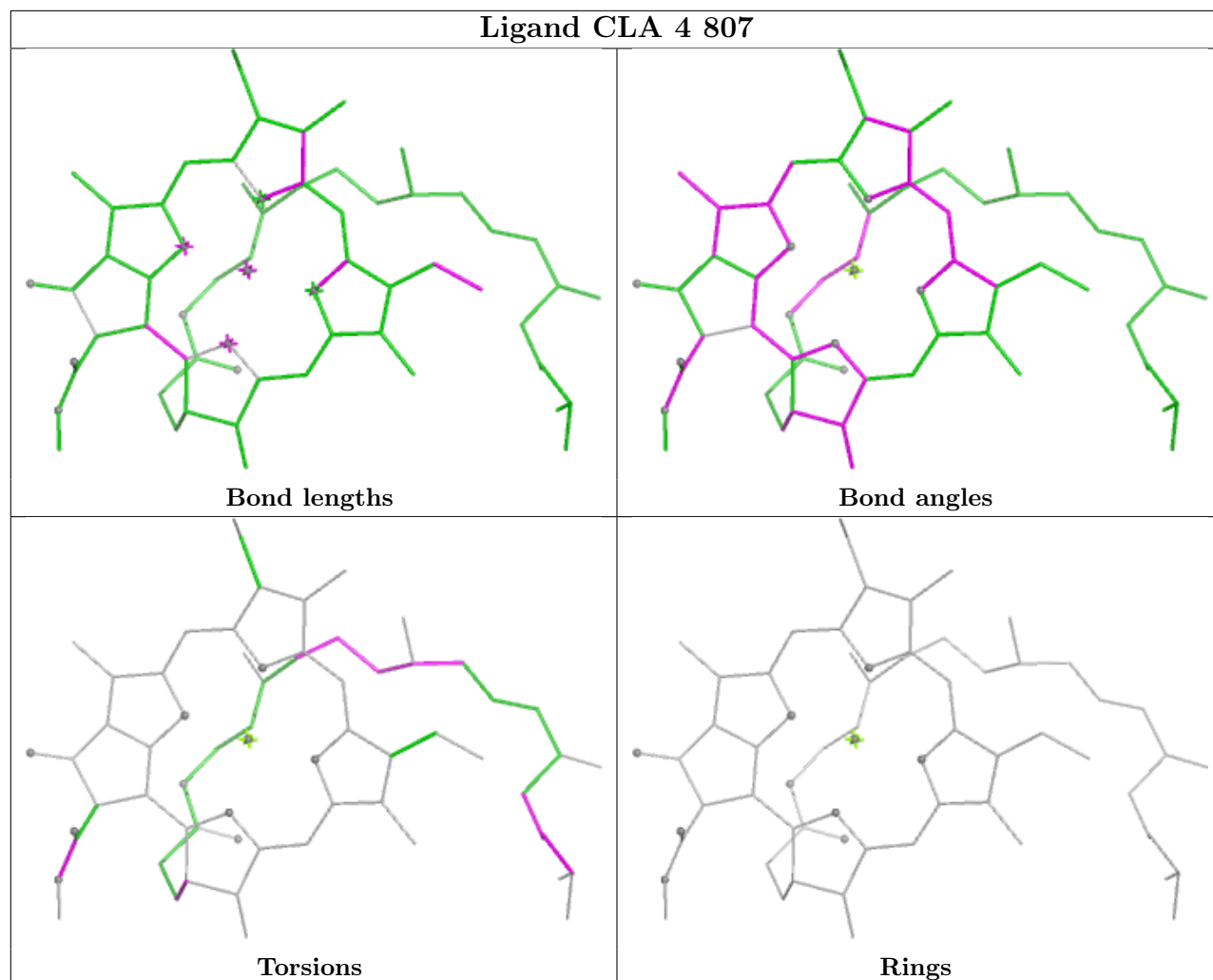
Ligand CHL 7 313



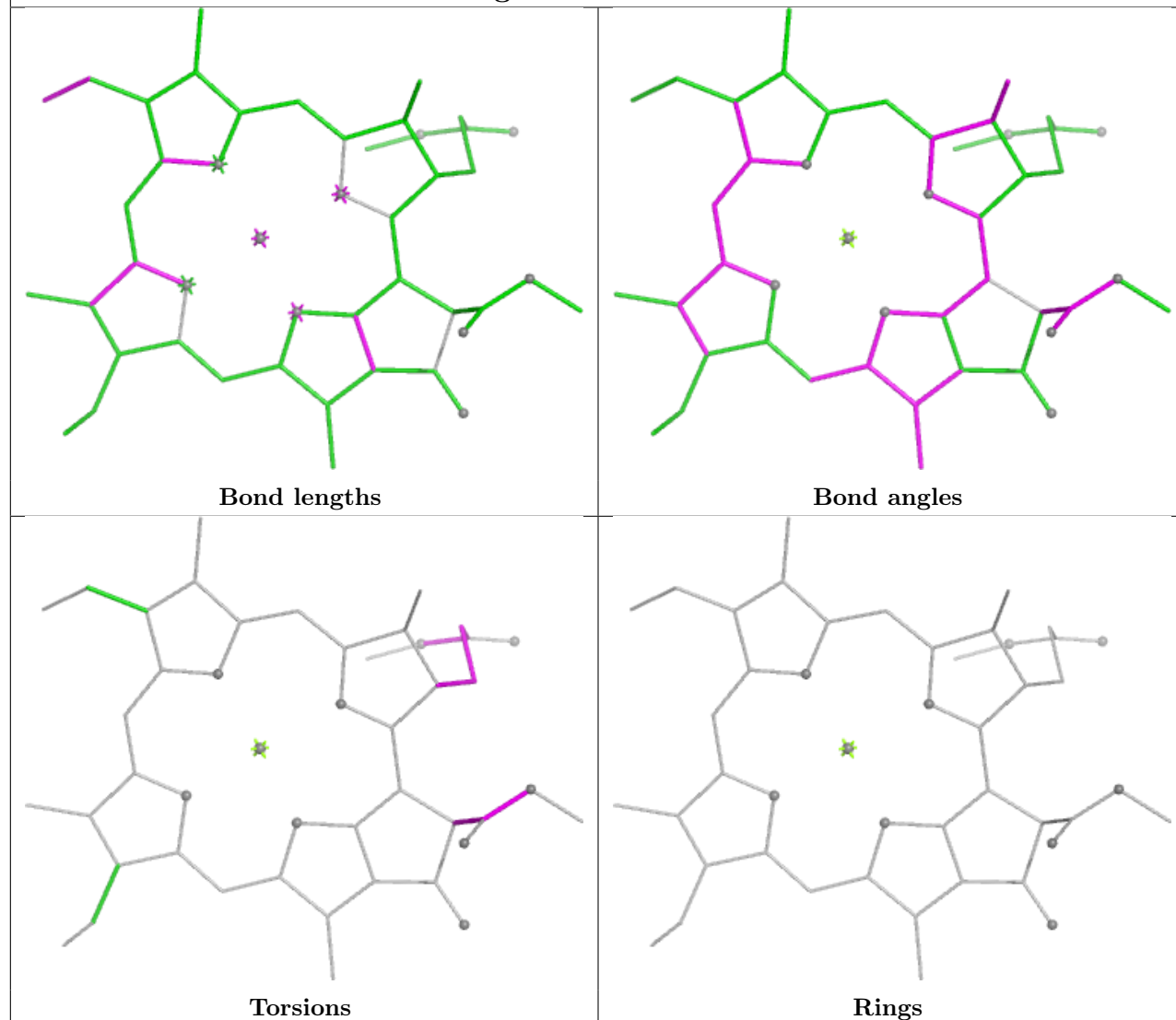
Ligand CHL 4 813



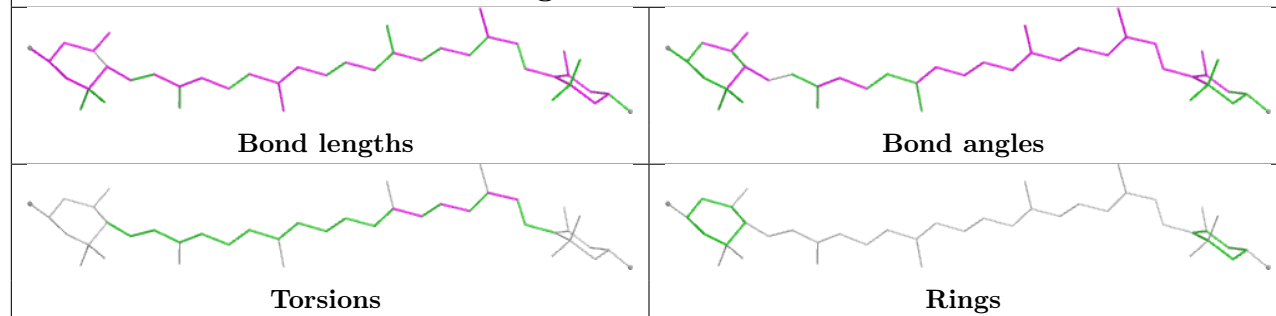
Ligand CLA 4 807

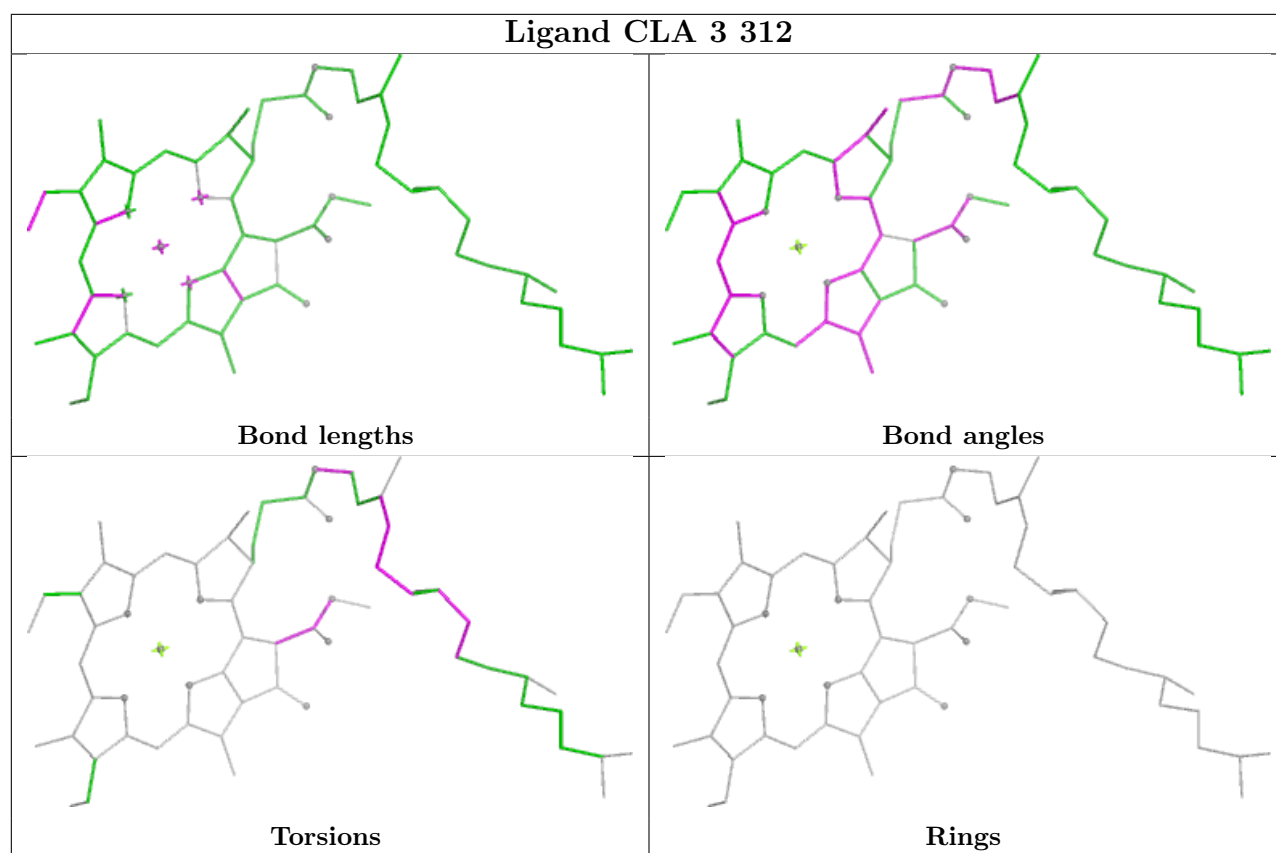


Ligand CLA 8 316

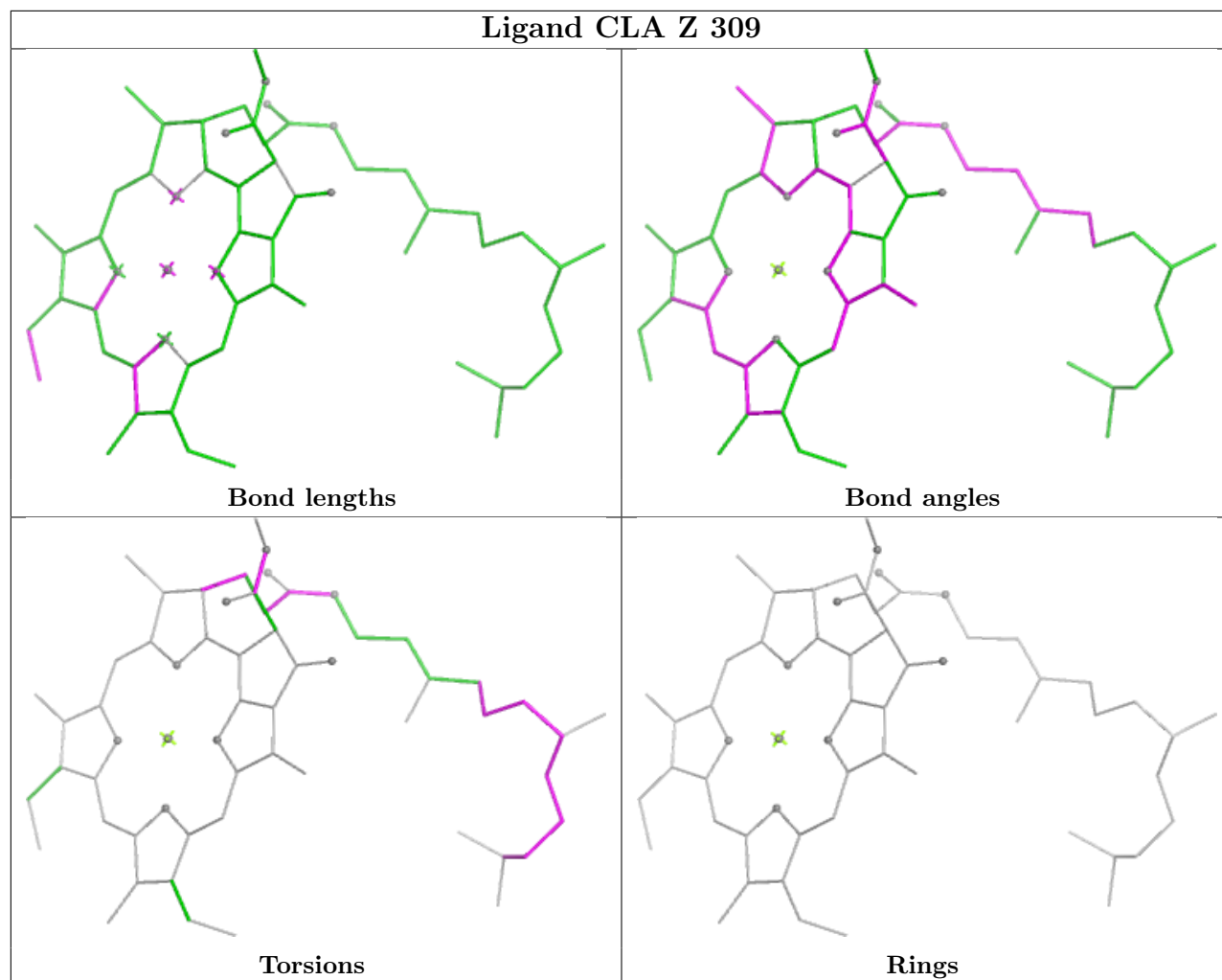


Ligand LUT 7 302

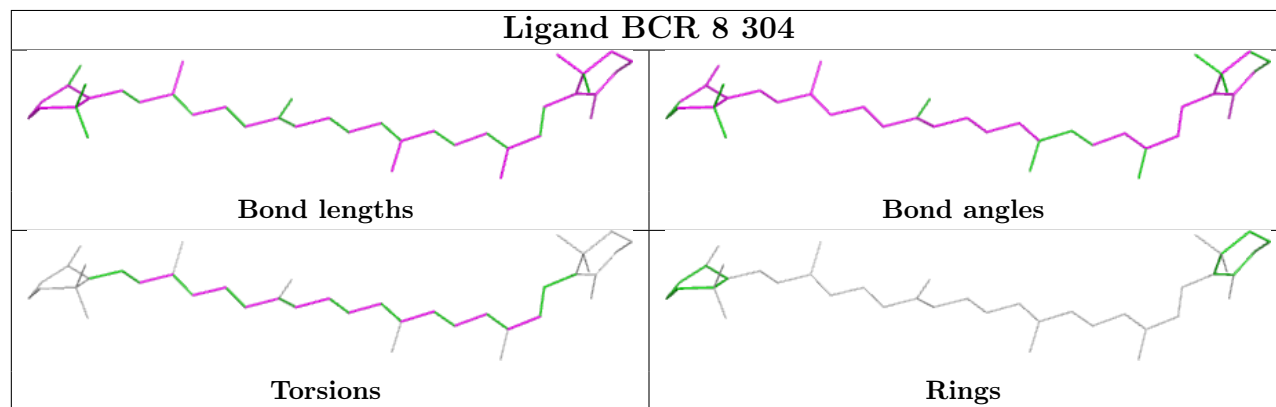


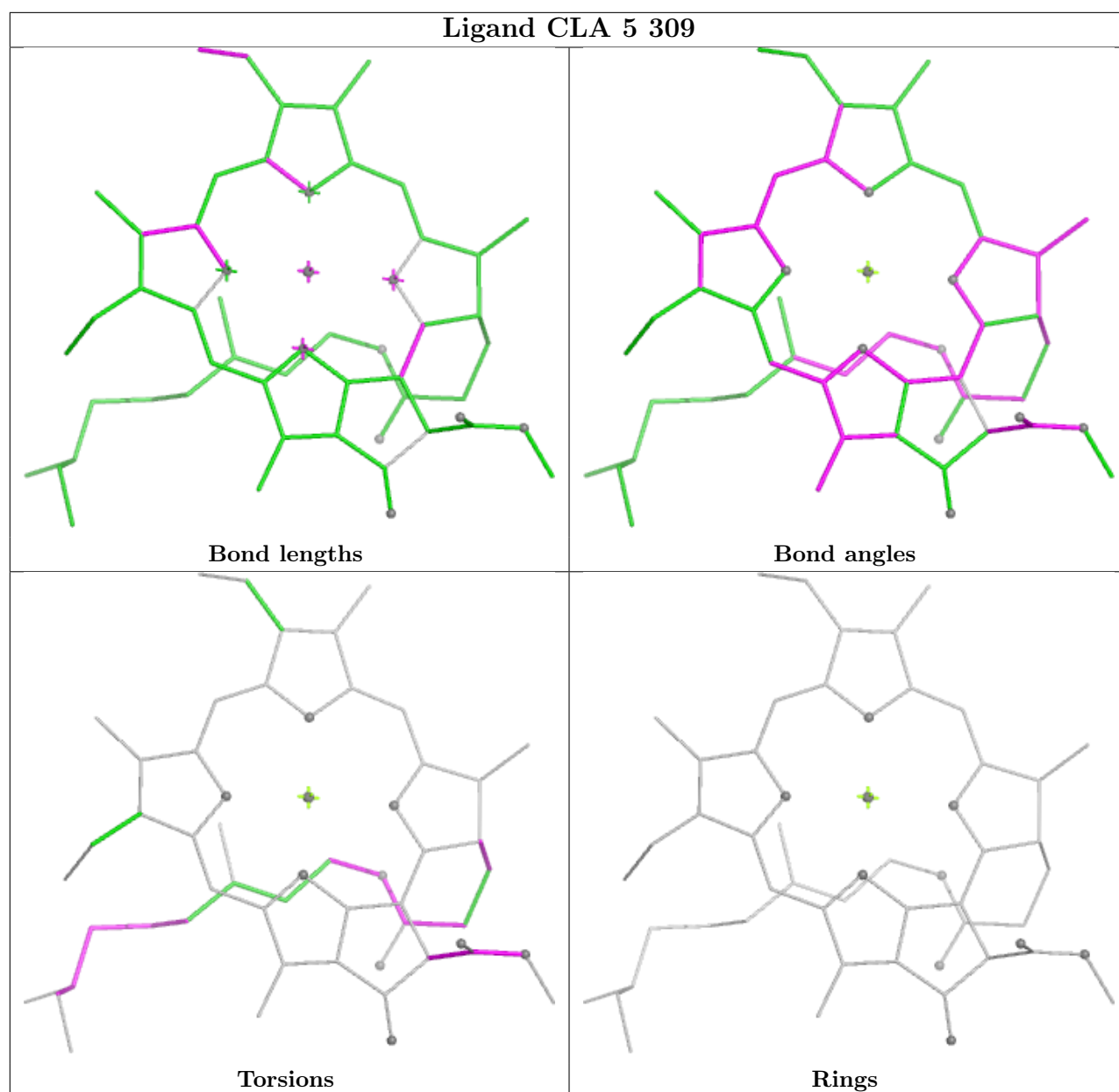


Ligand CLA Z 309

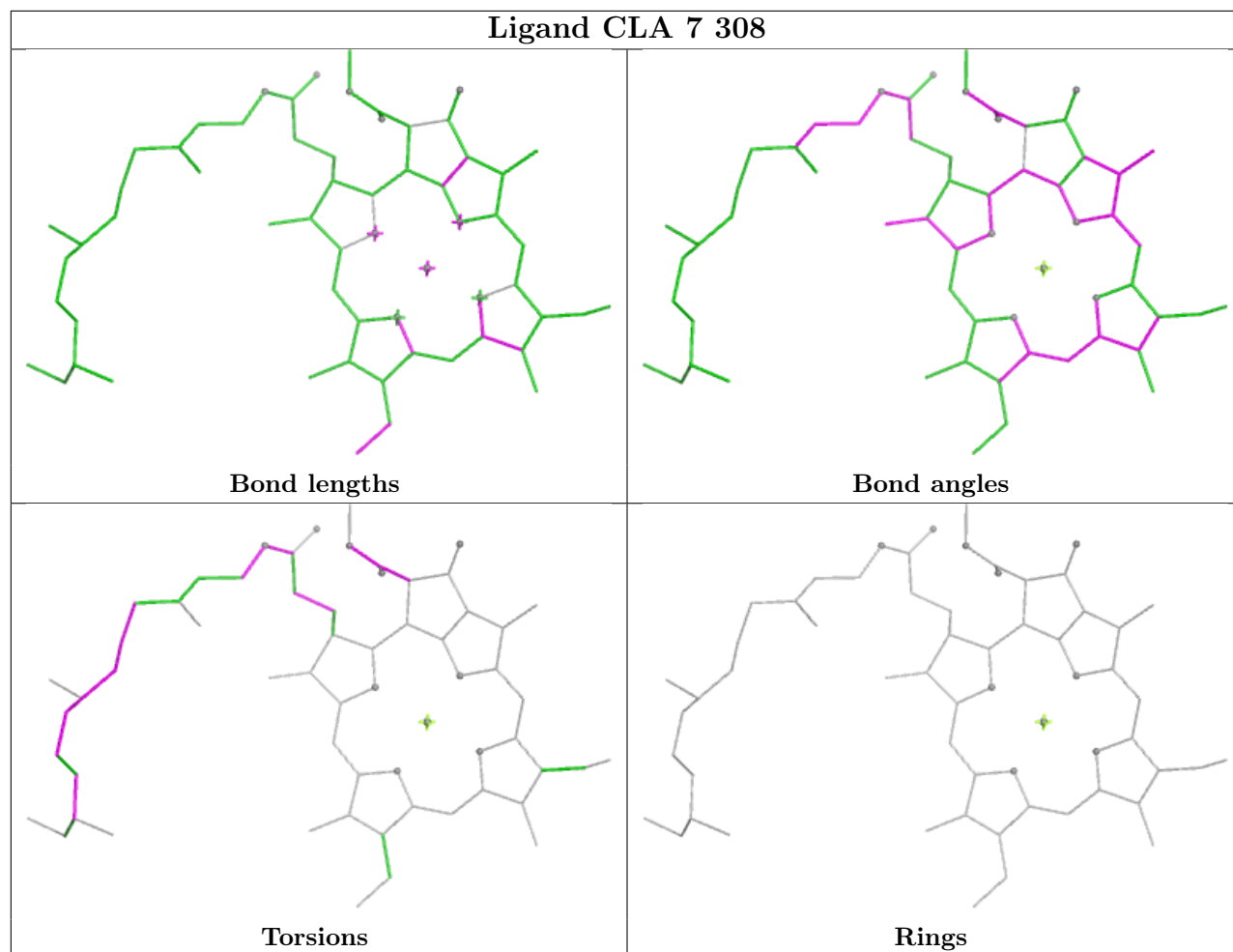


Ligand BCR 8 304

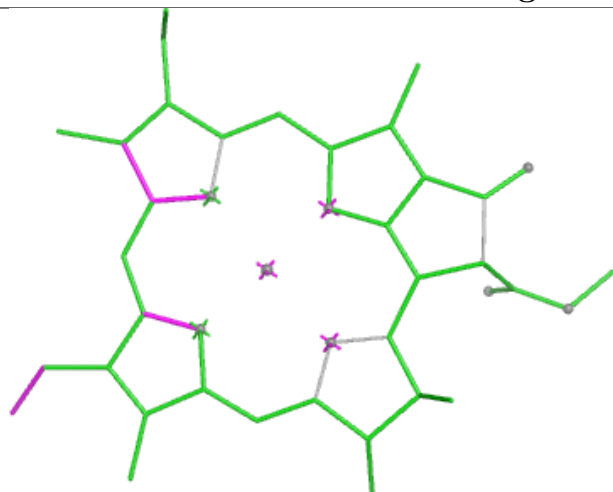




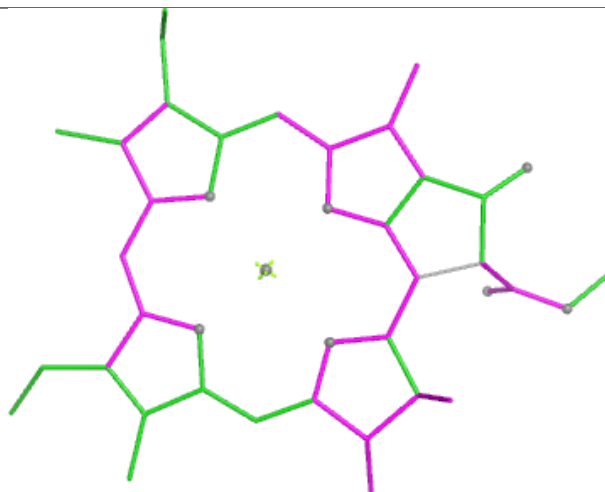
Ligand CLA 7 308



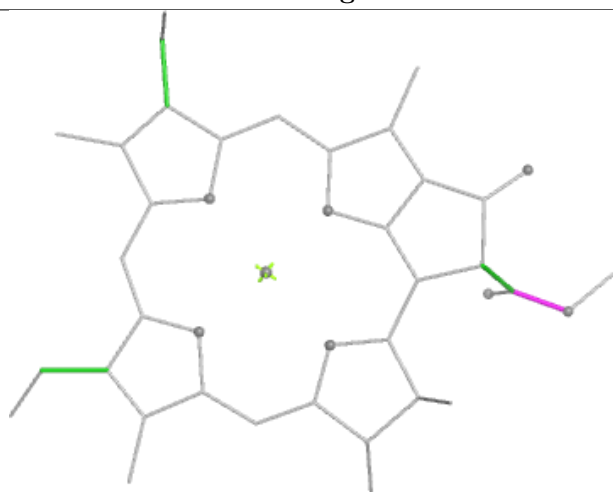
Ligand CLA 4 817



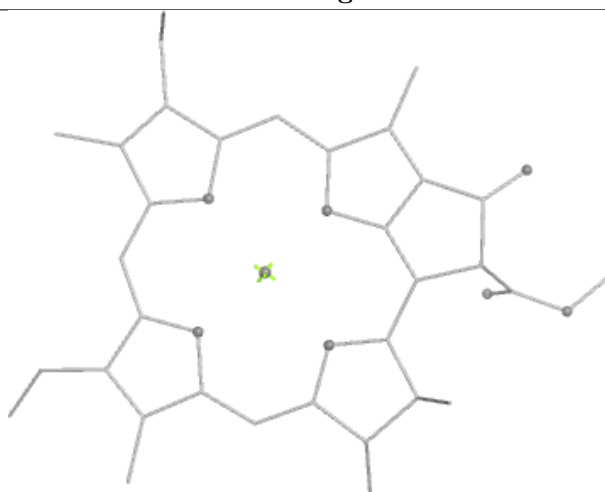
Bond lengths



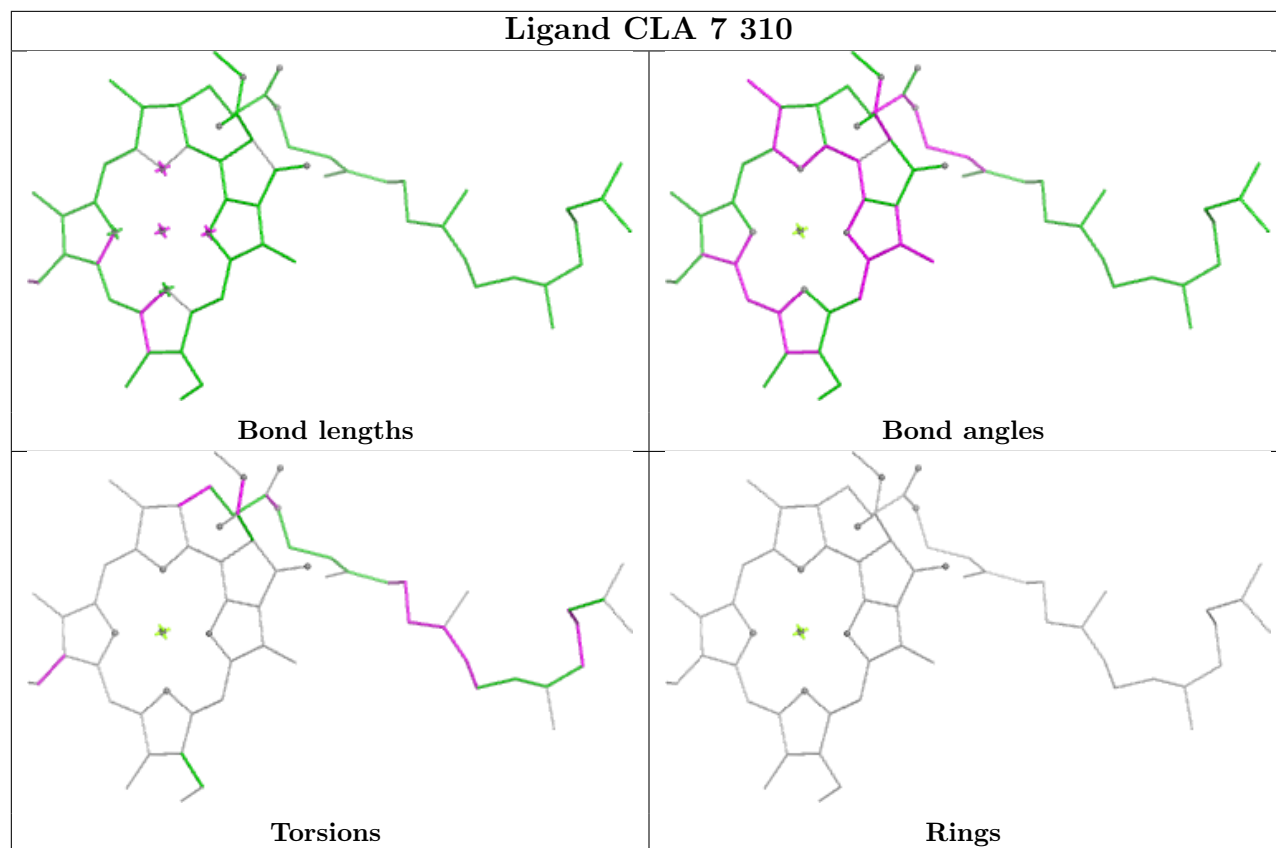
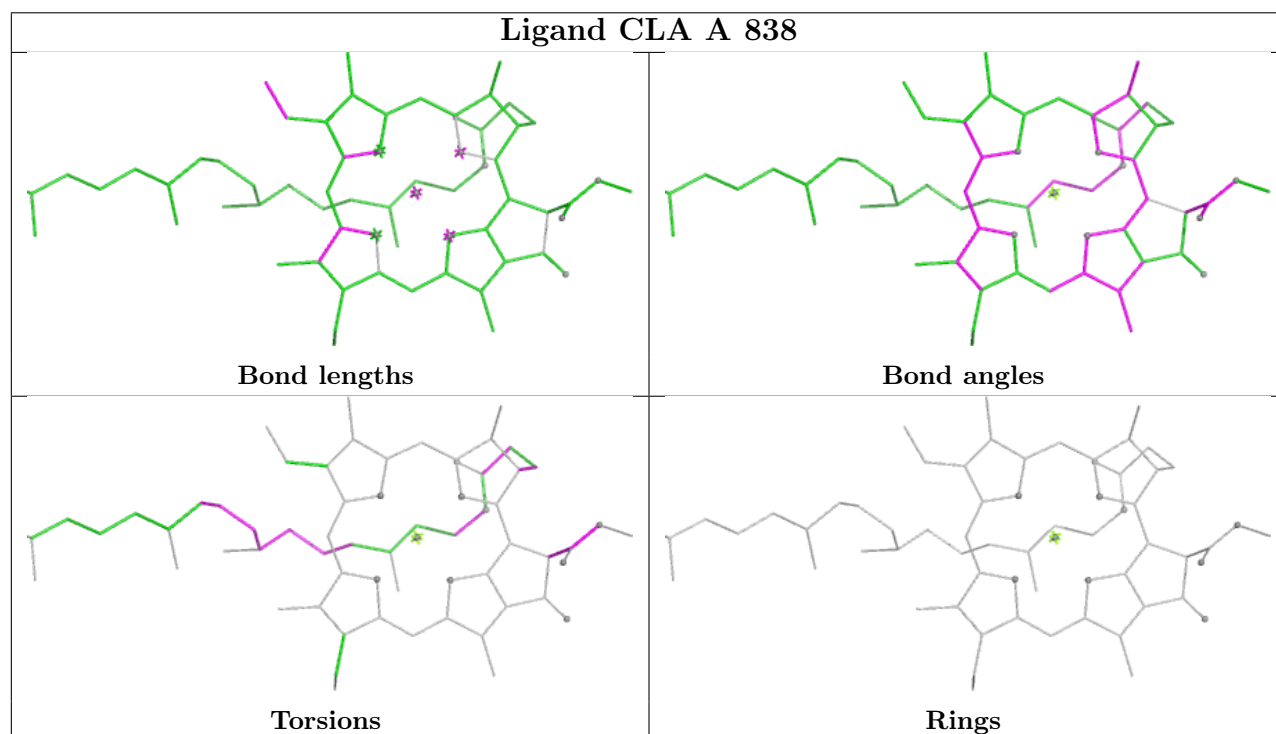
Bond angles



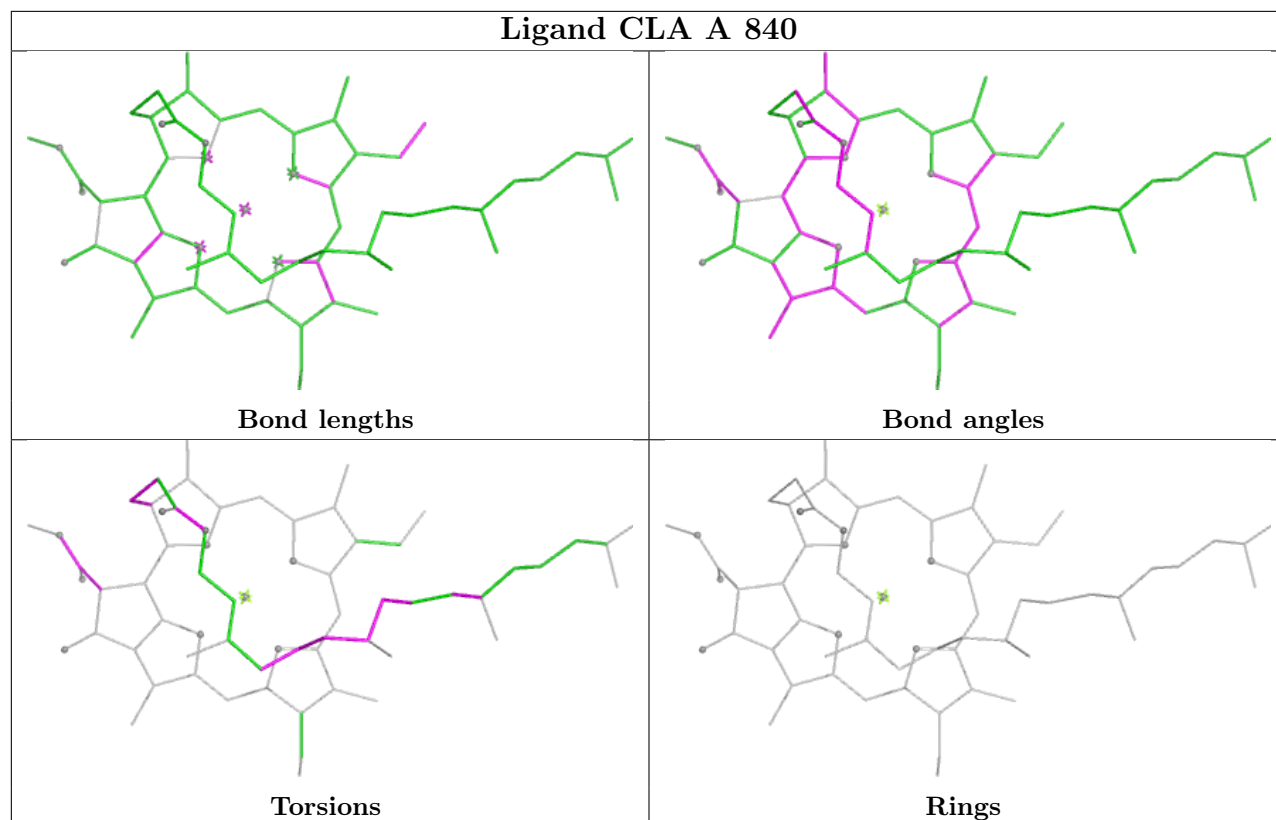
Torsions



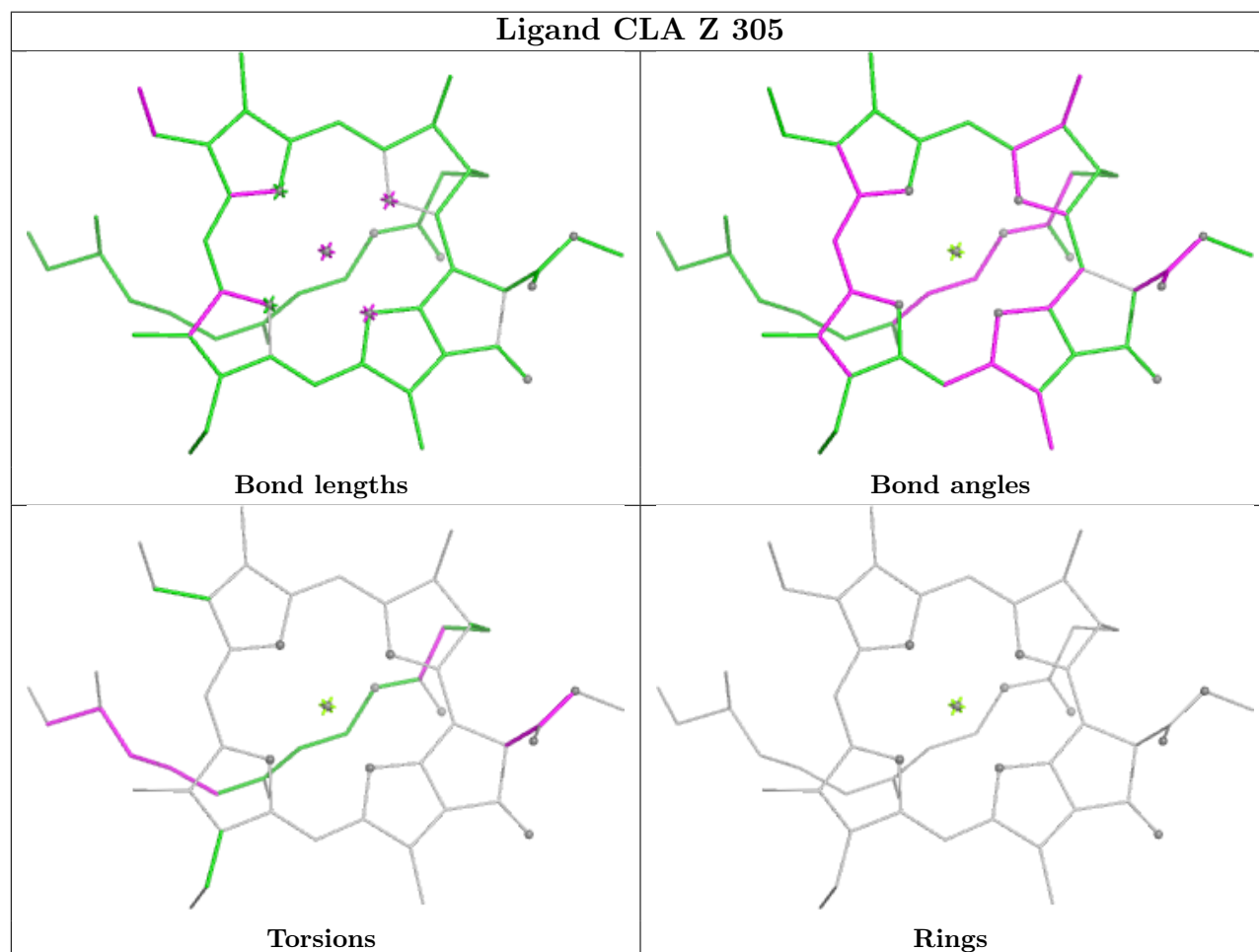
Rings

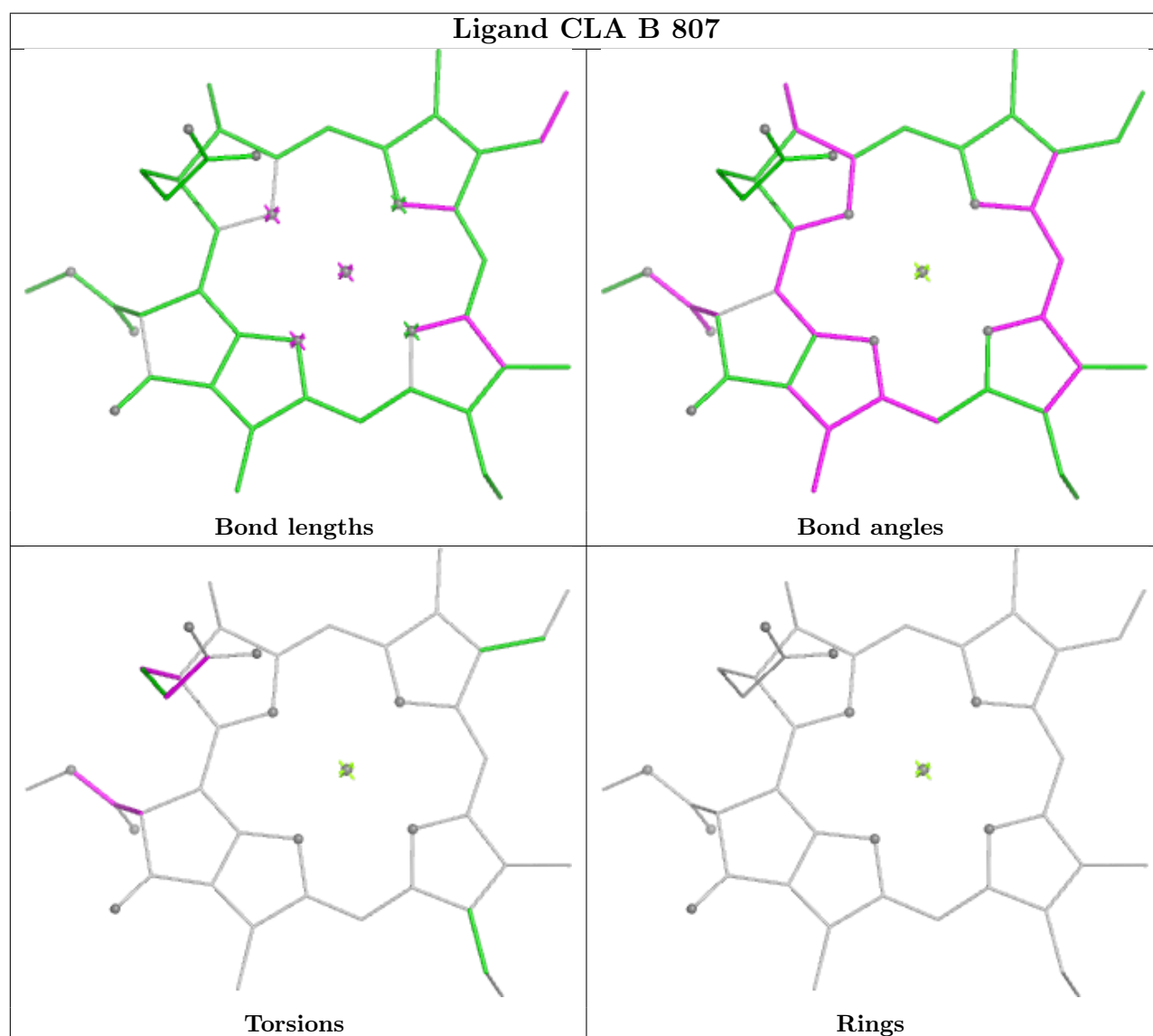
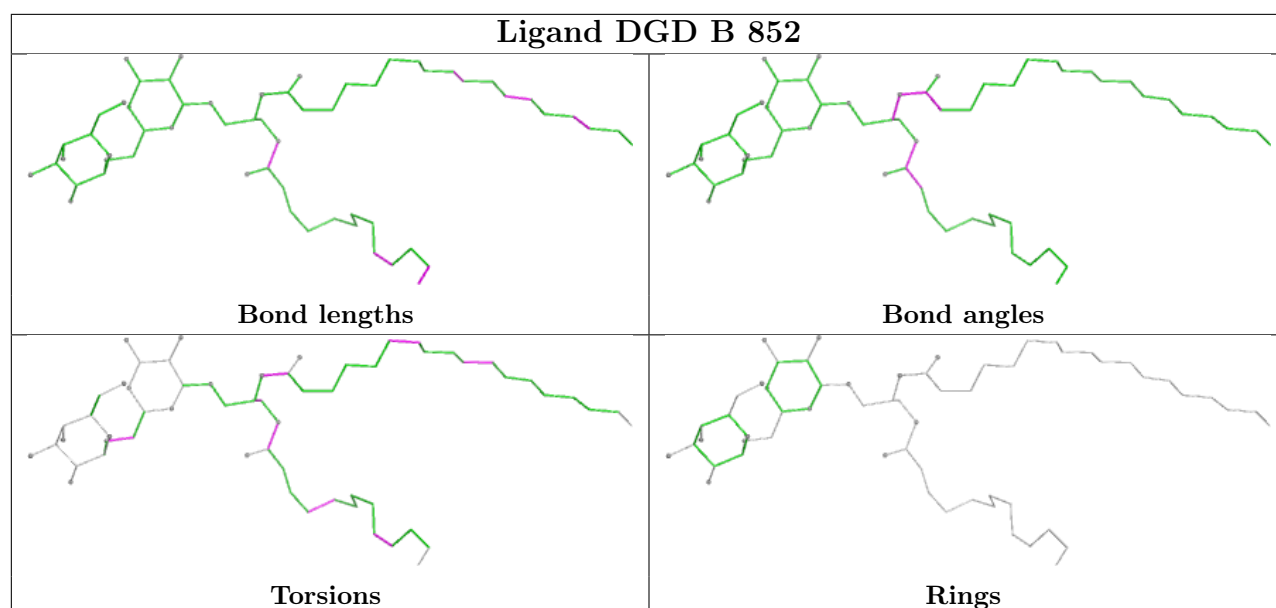
Ligand CLA 7 310**Ligand CLA A 838**

Ligand CLA A 840

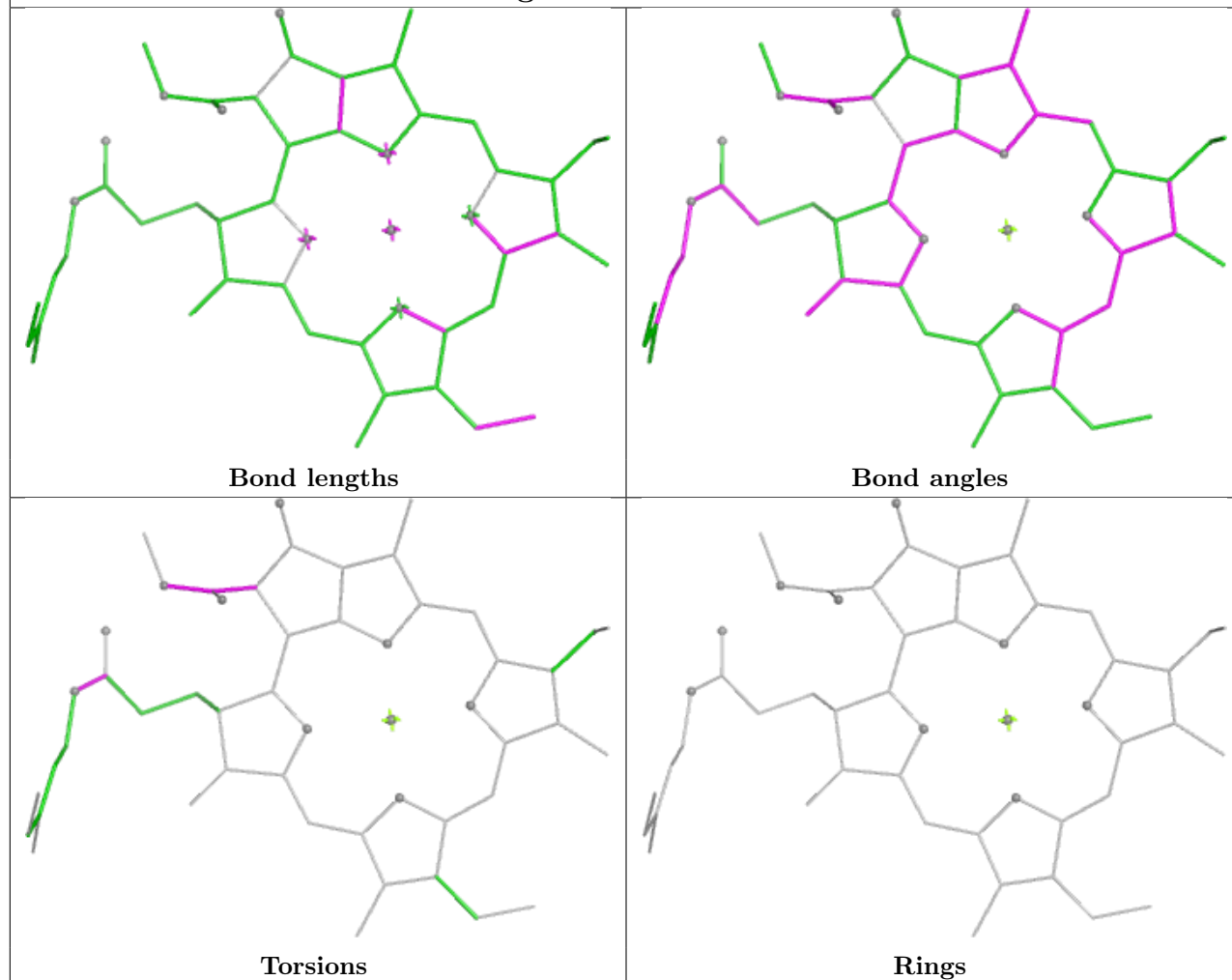


Ligand CLA Z 305

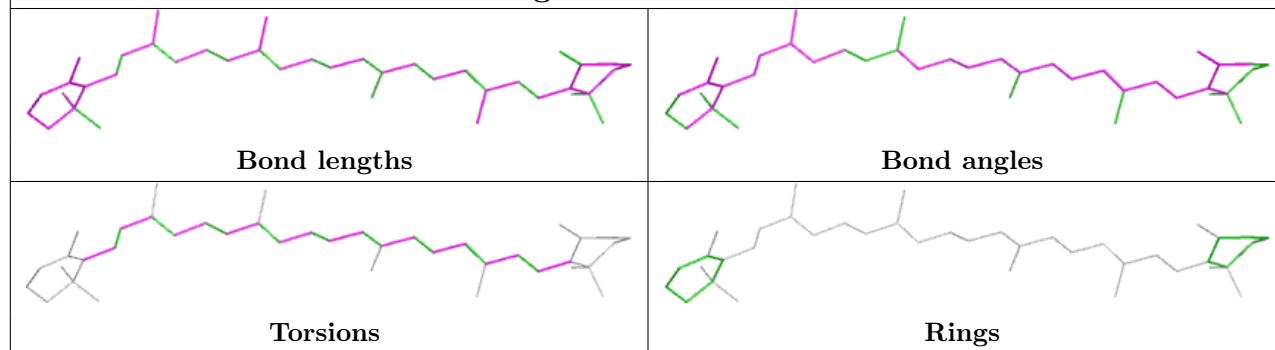




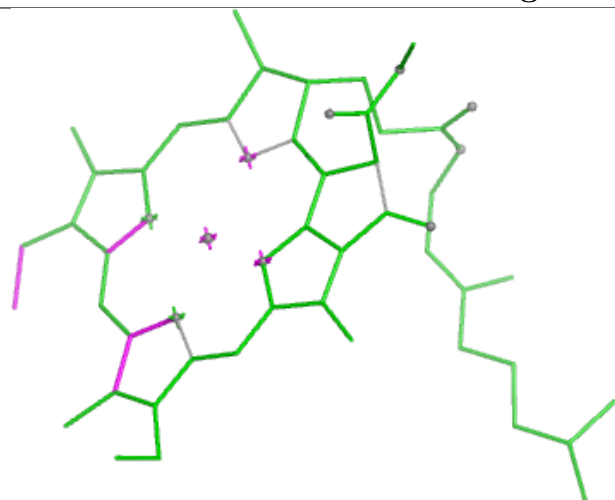
Ligand CLA 4 809



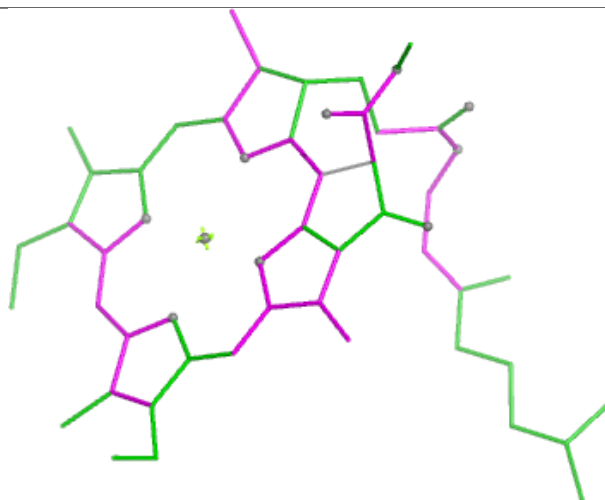
Ligand BCR 7 303



Ligand CLA 4 811



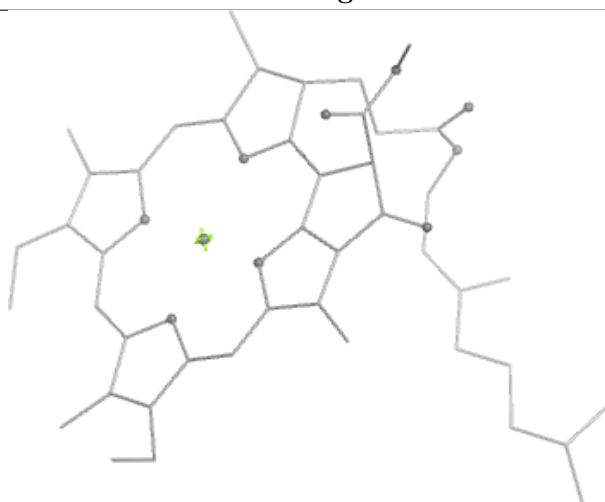
Bond lengths



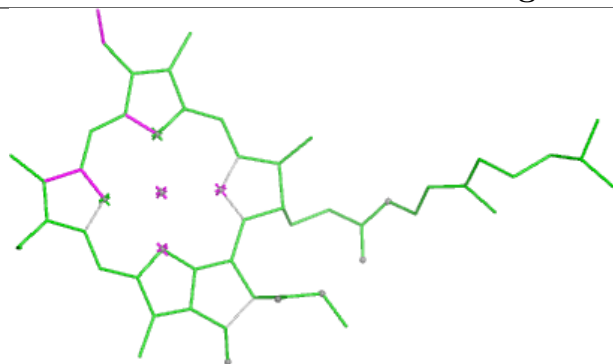
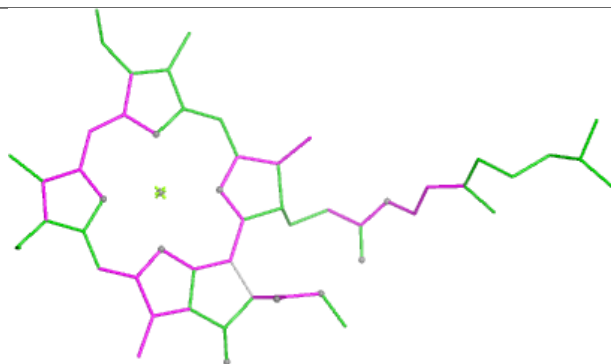
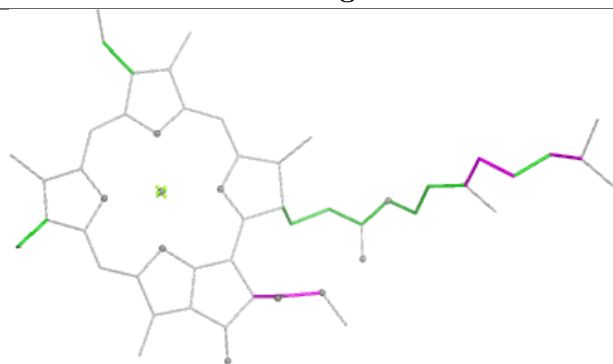
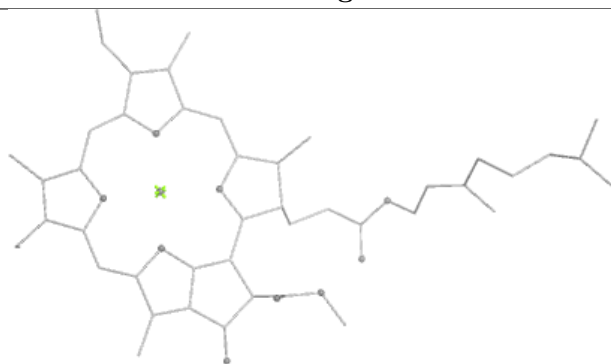
Bond angles



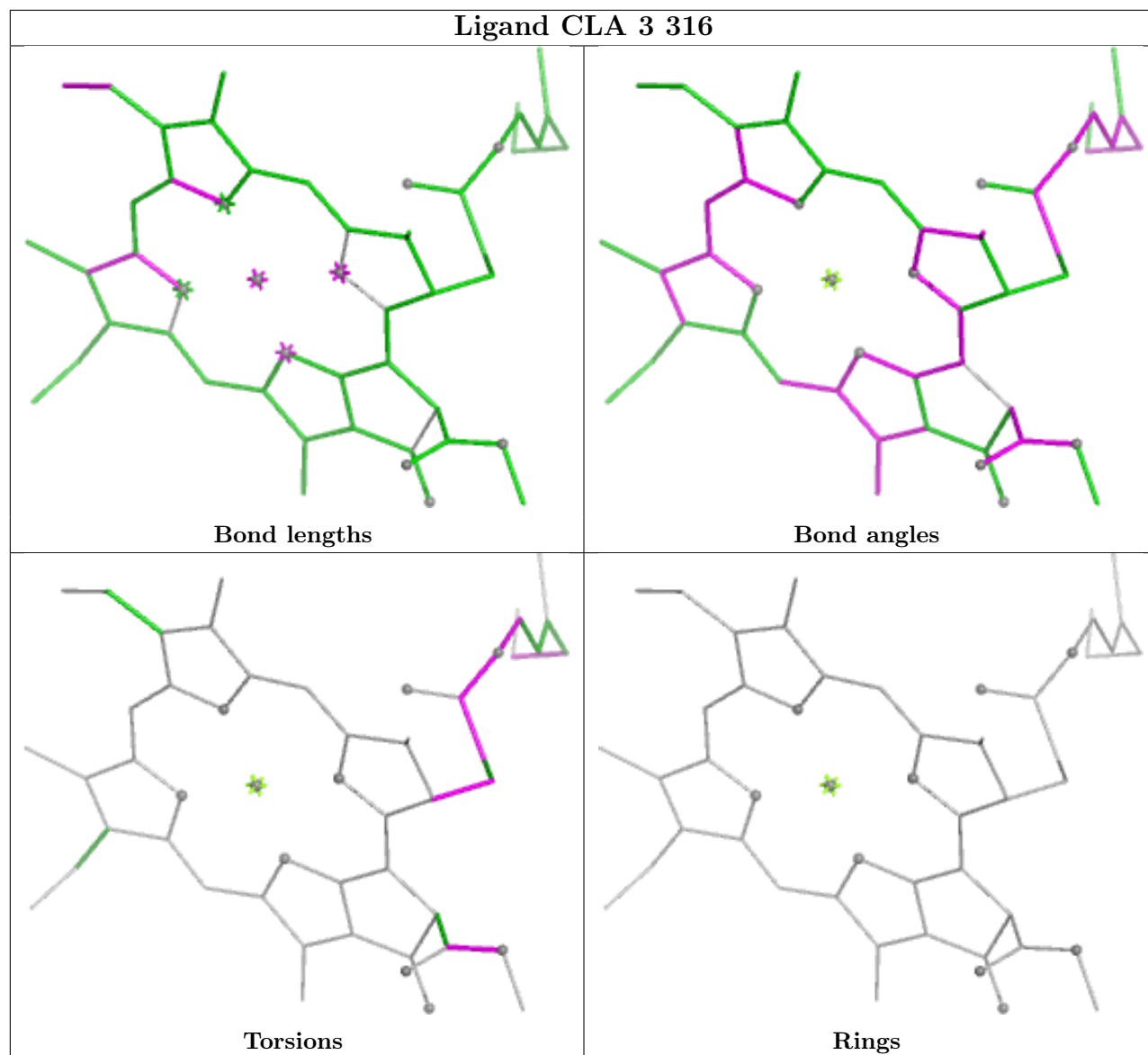
Torsions

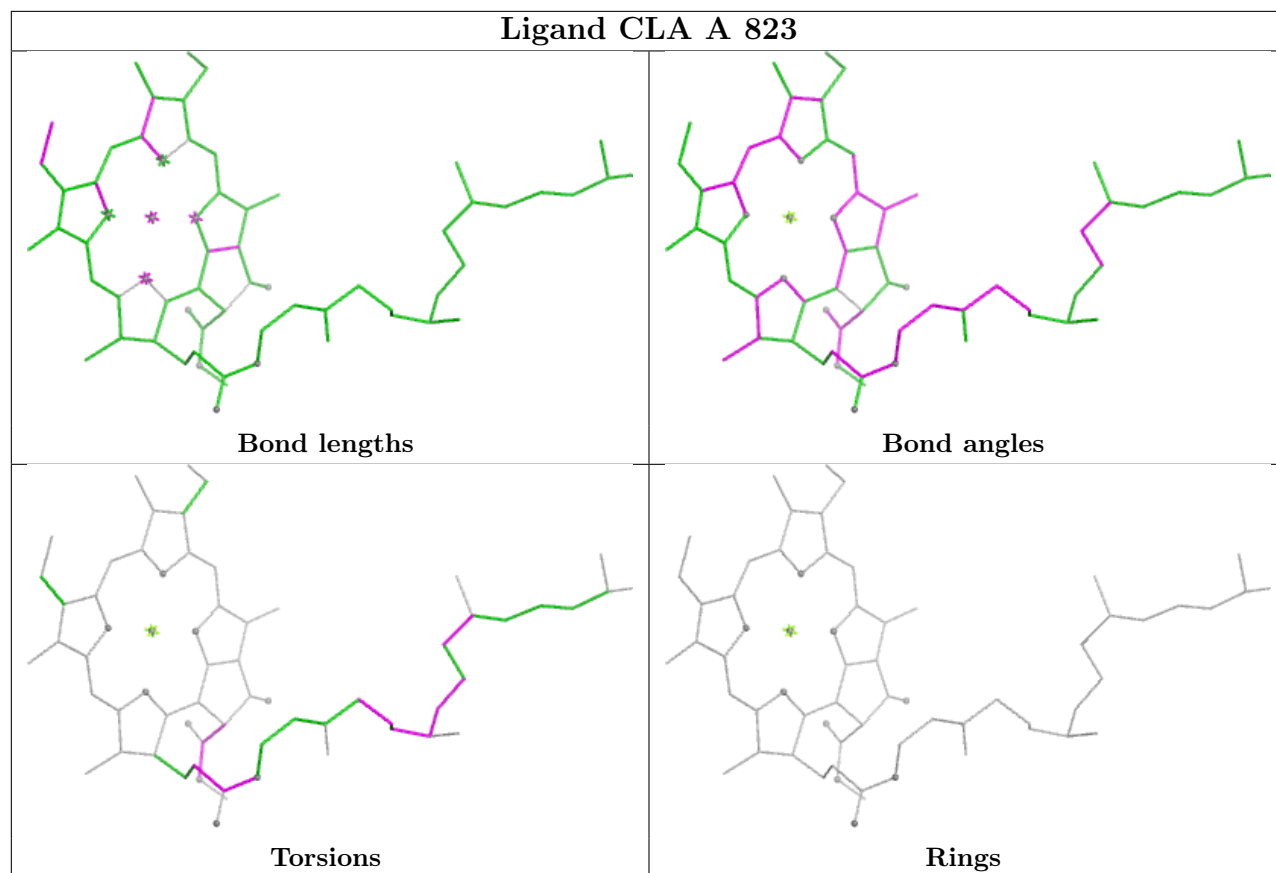


Rings

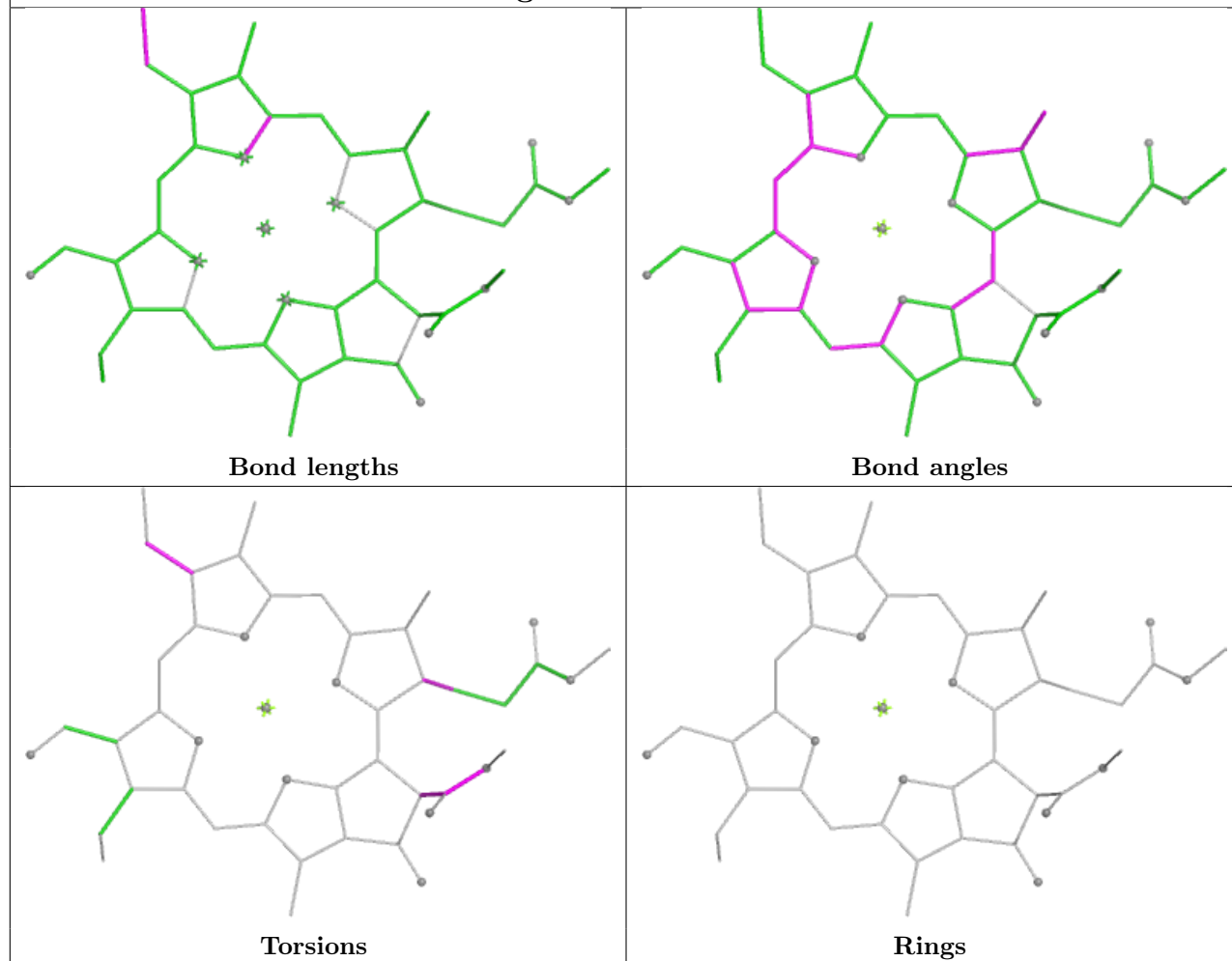
Ligand CLA 3 319**Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA 3 316

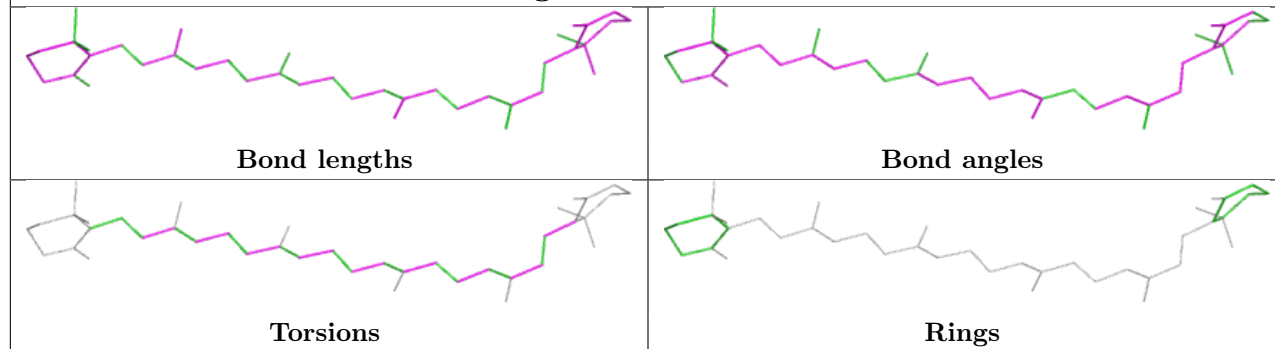




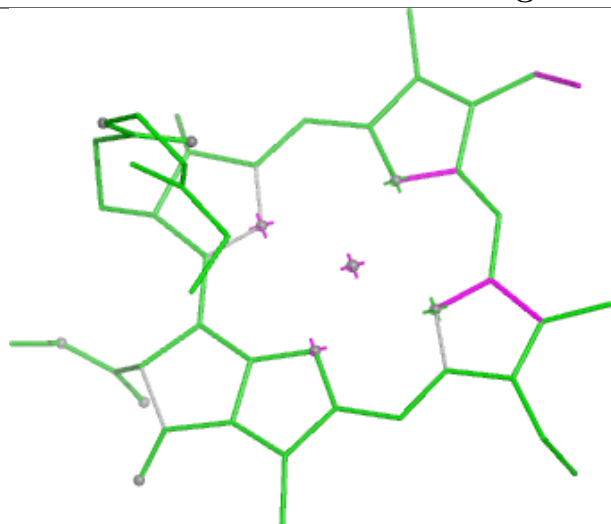
Ligand CHL 4 816



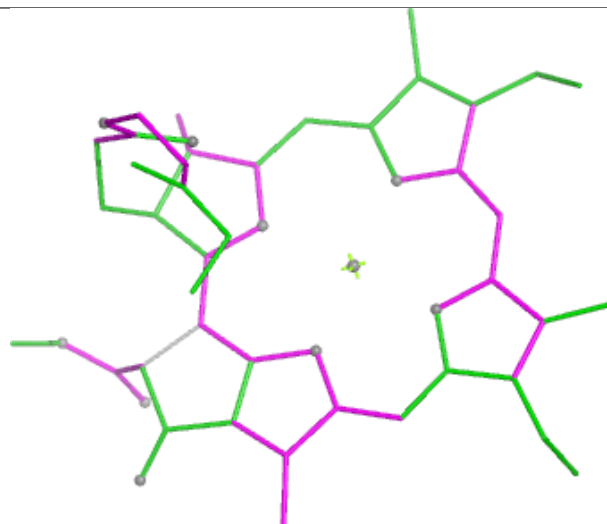
Ligand BCR 4 804



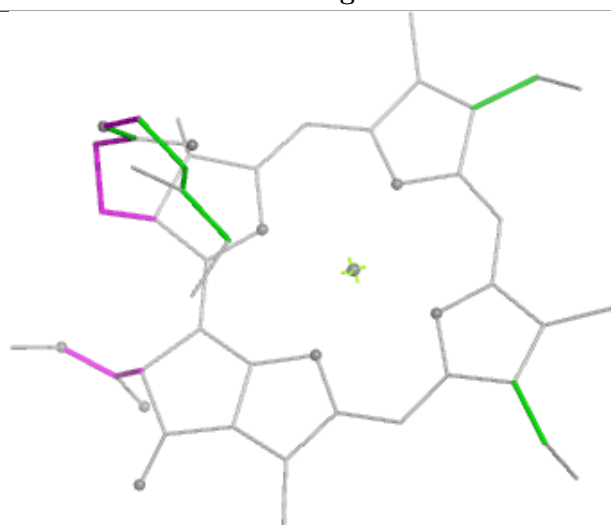
Ligand CLA Z 314



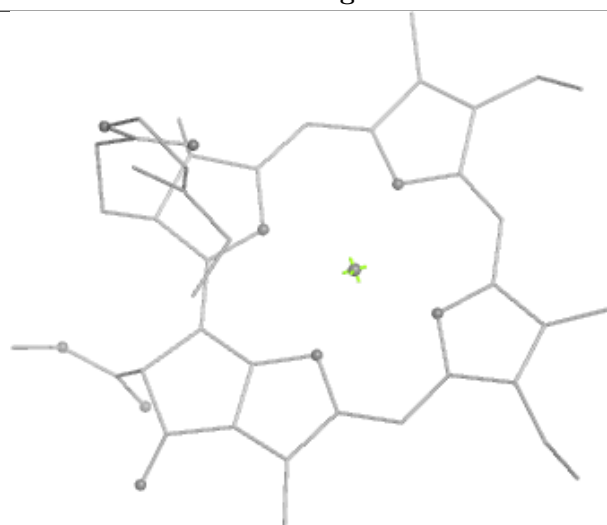
Bond lengths



Bond angles

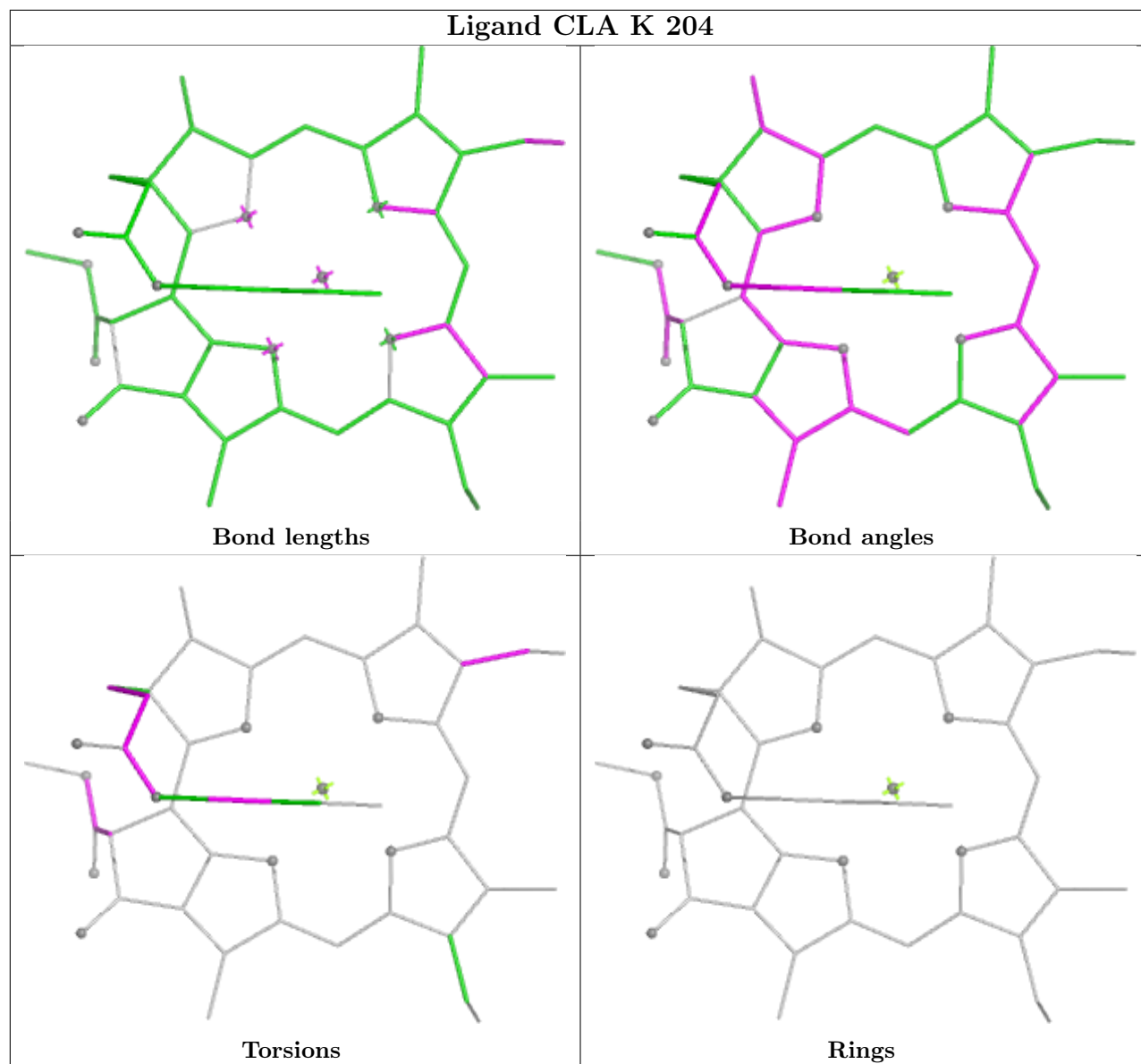


Torsions

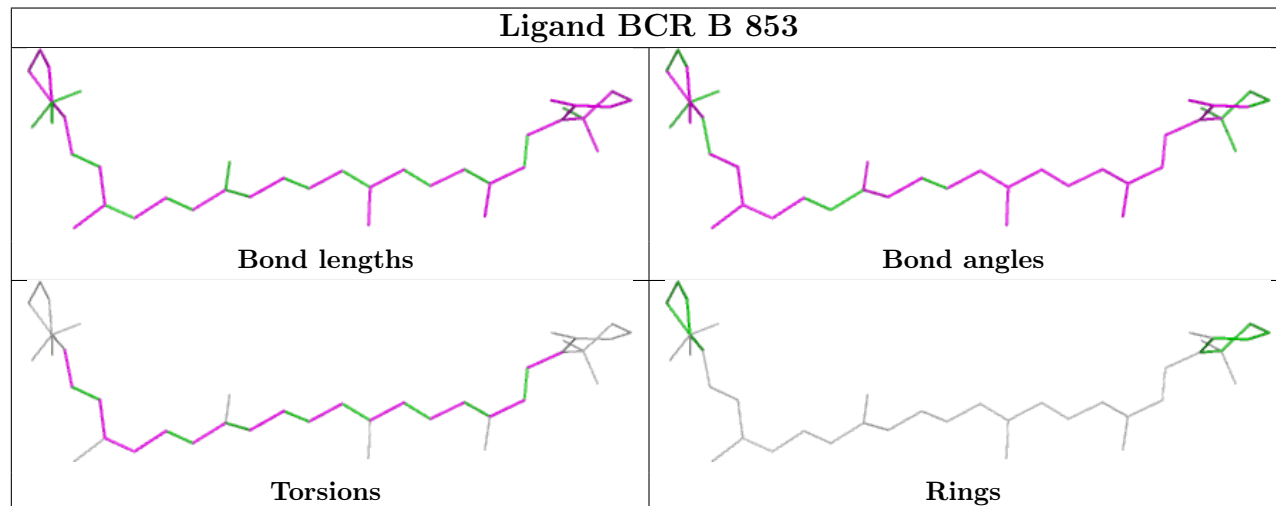


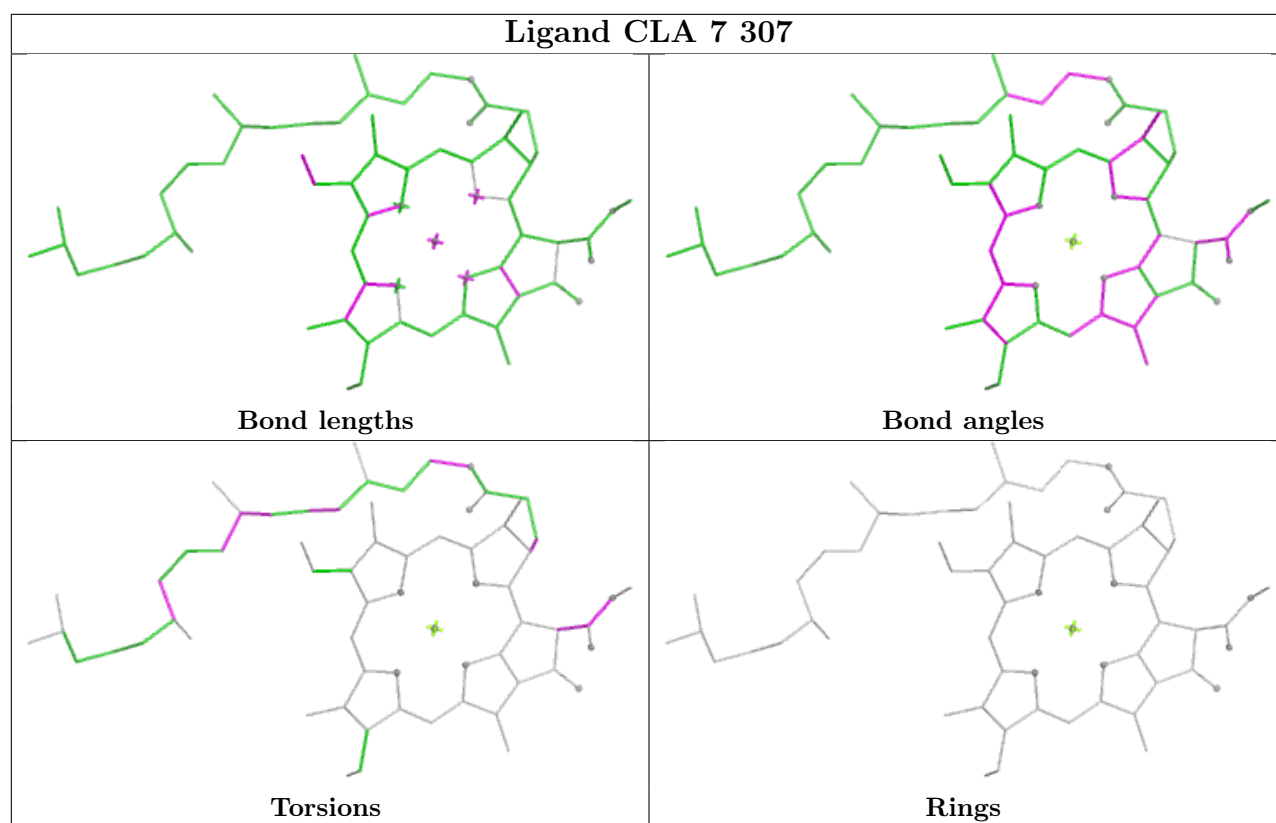
Rings

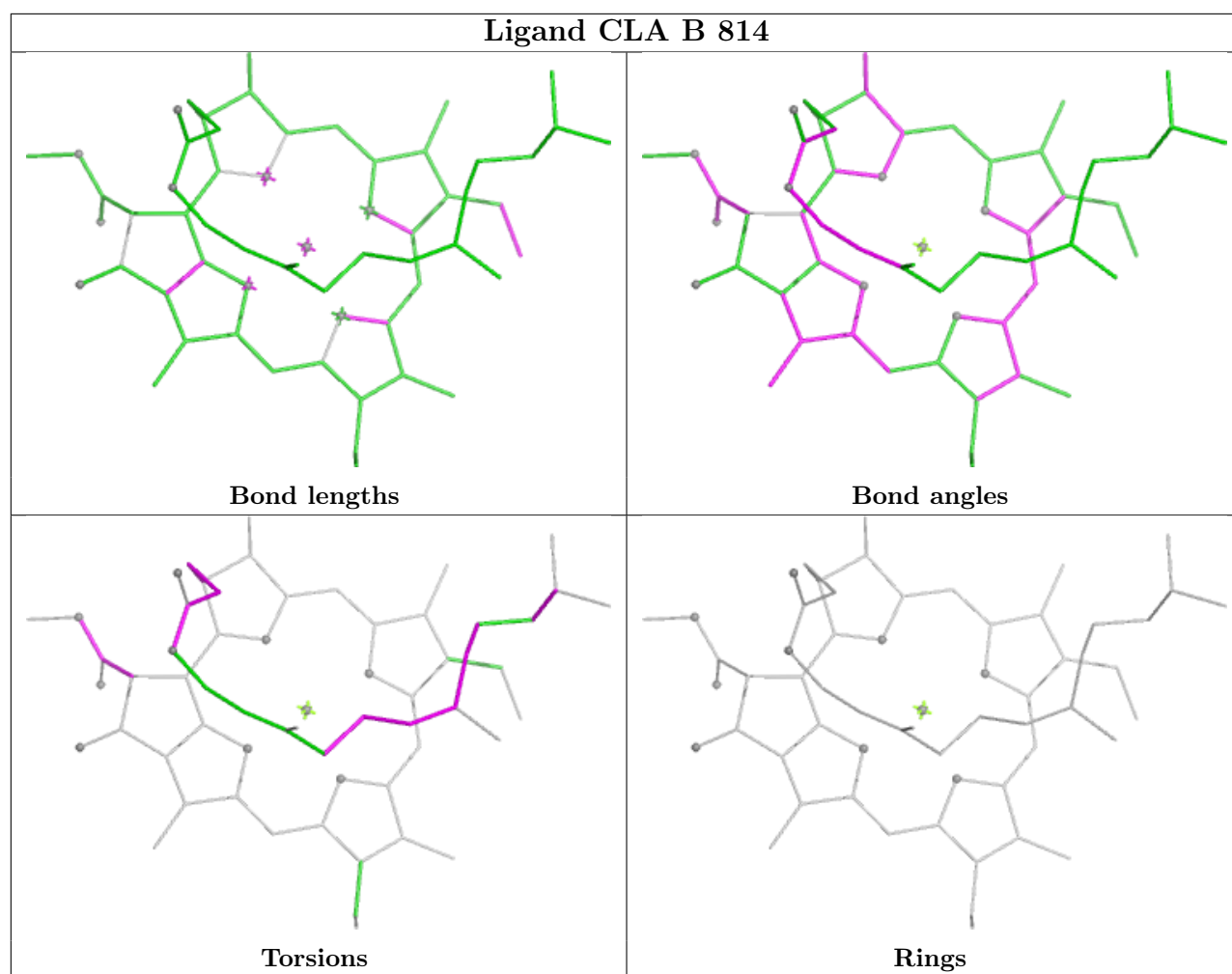
Ligand CLA K 204



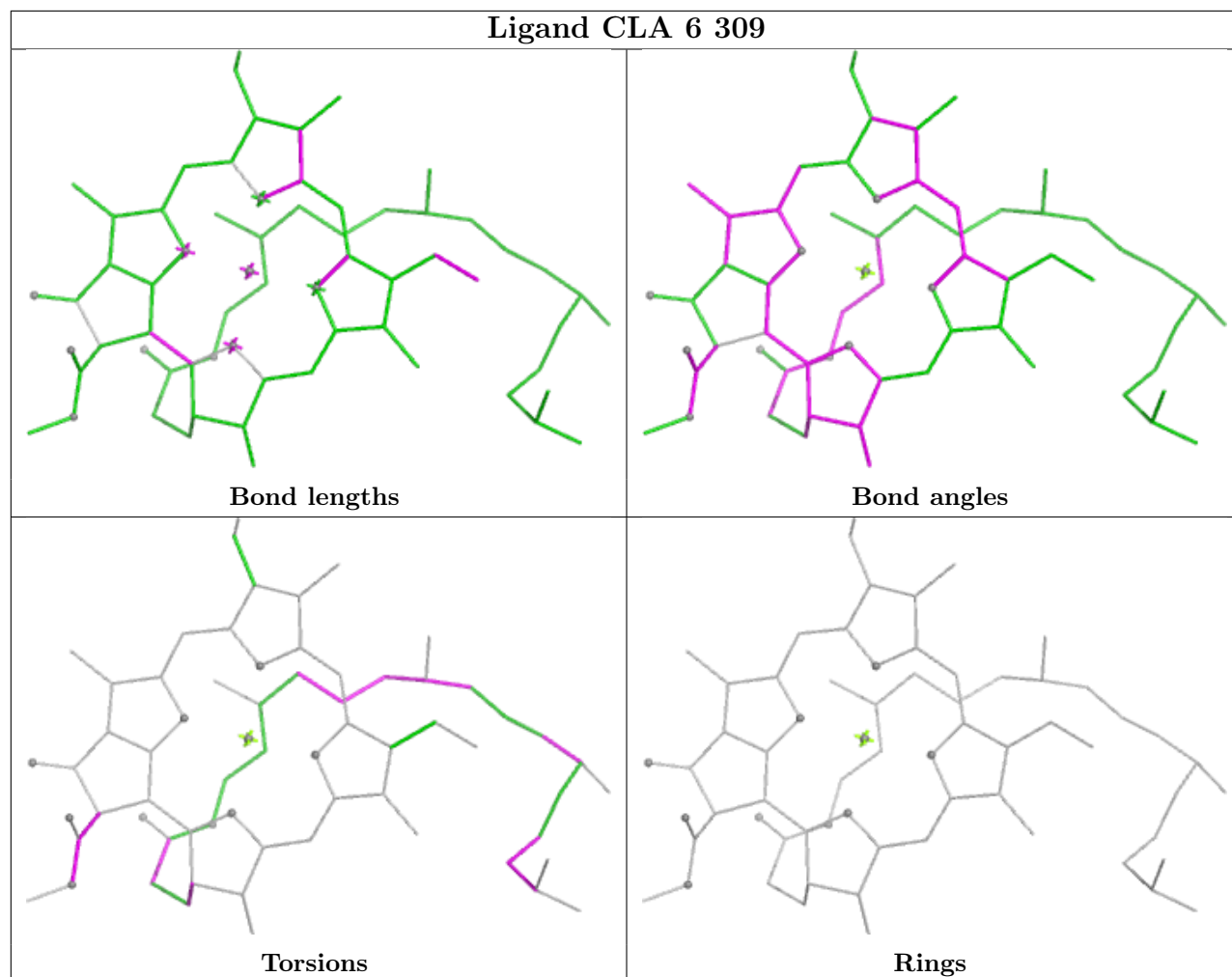
Ligand BCR B 853



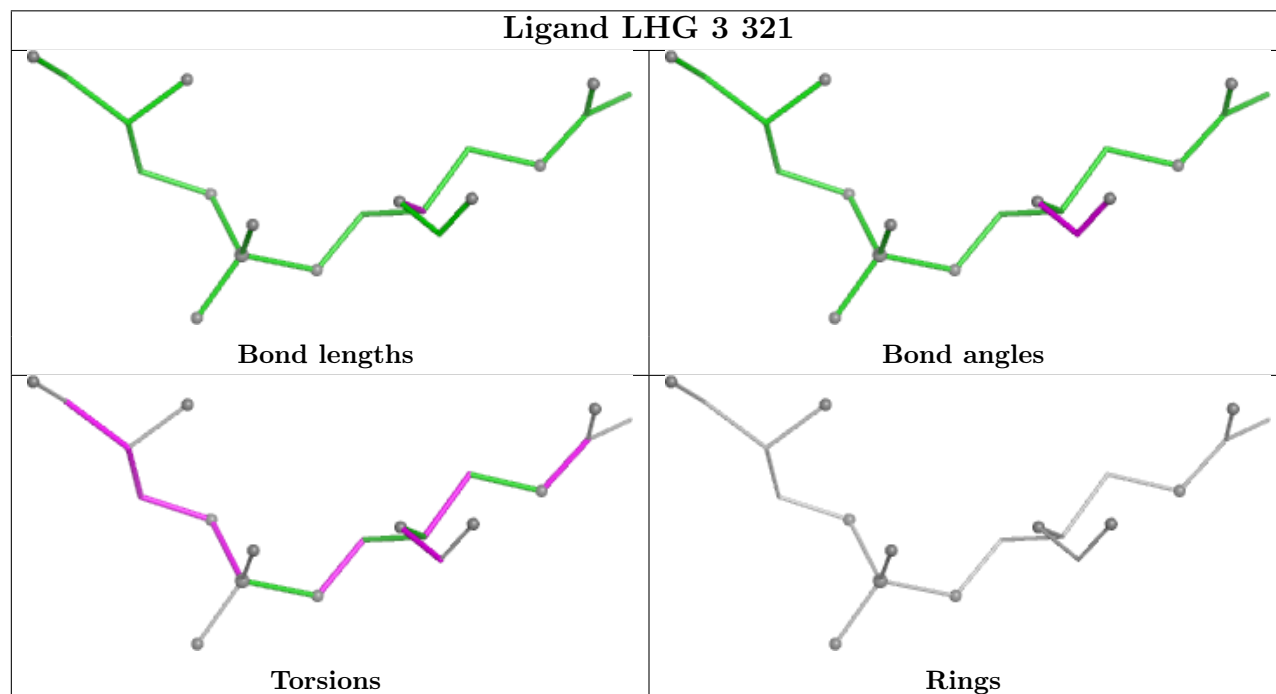


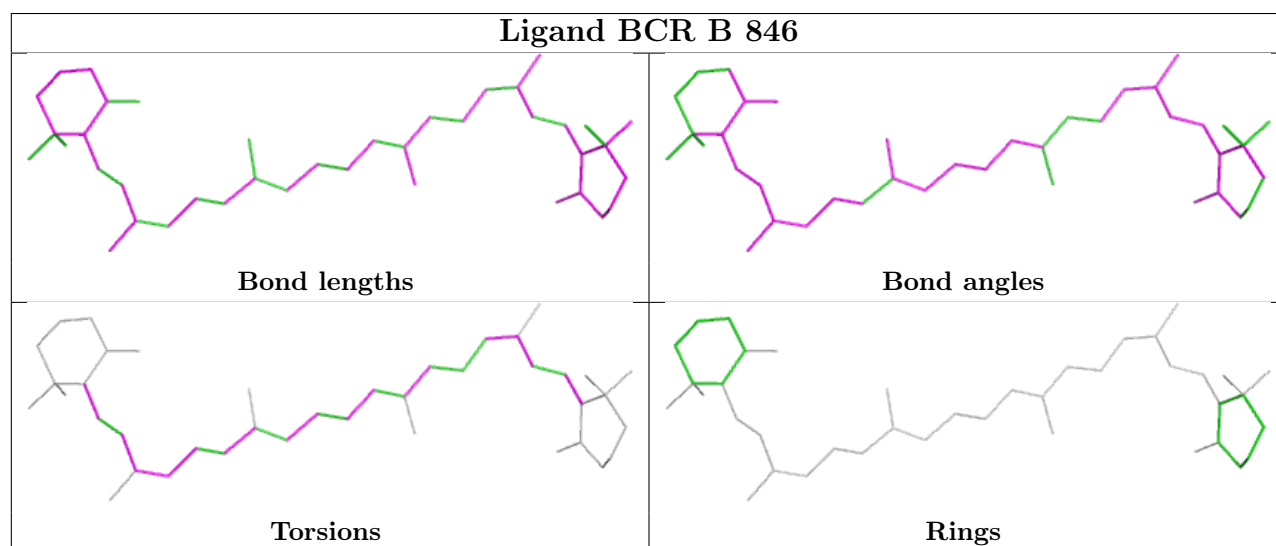
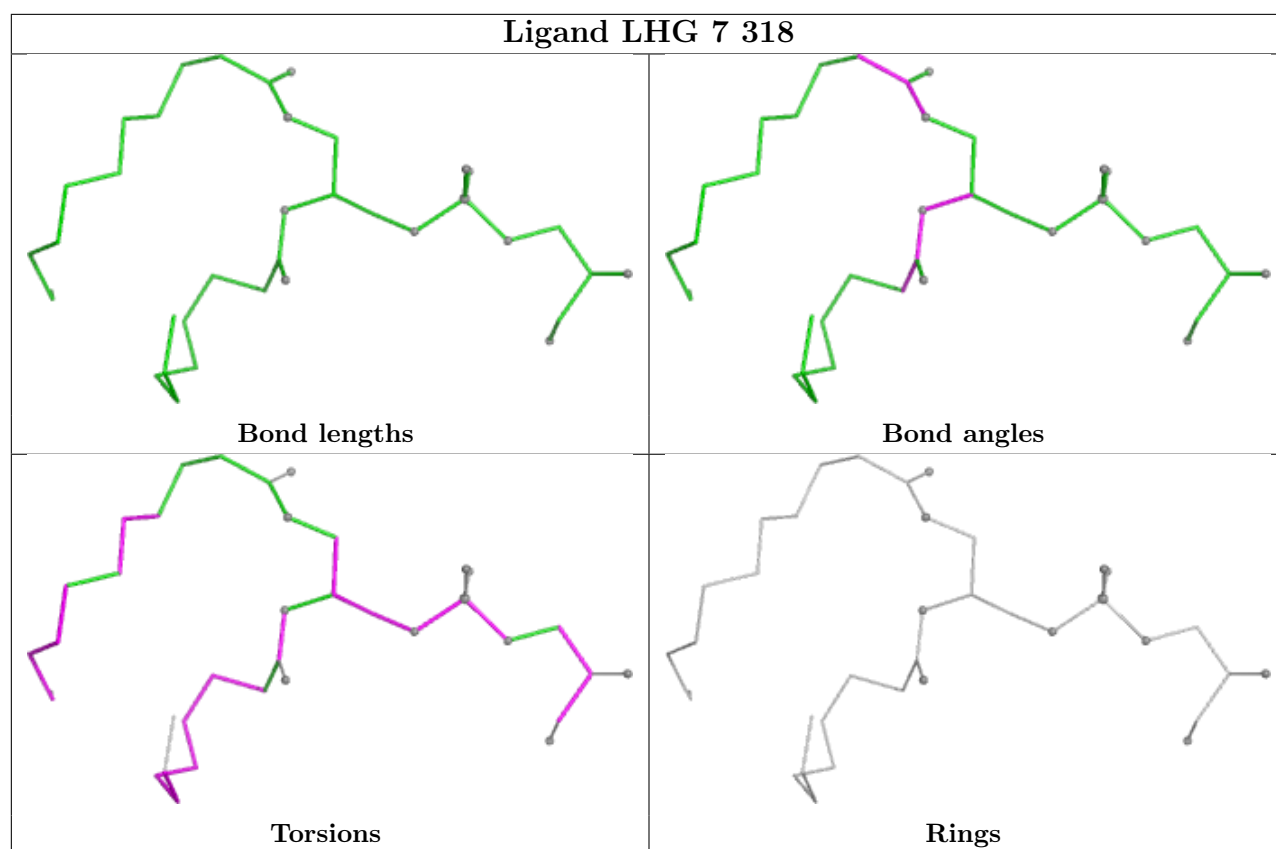


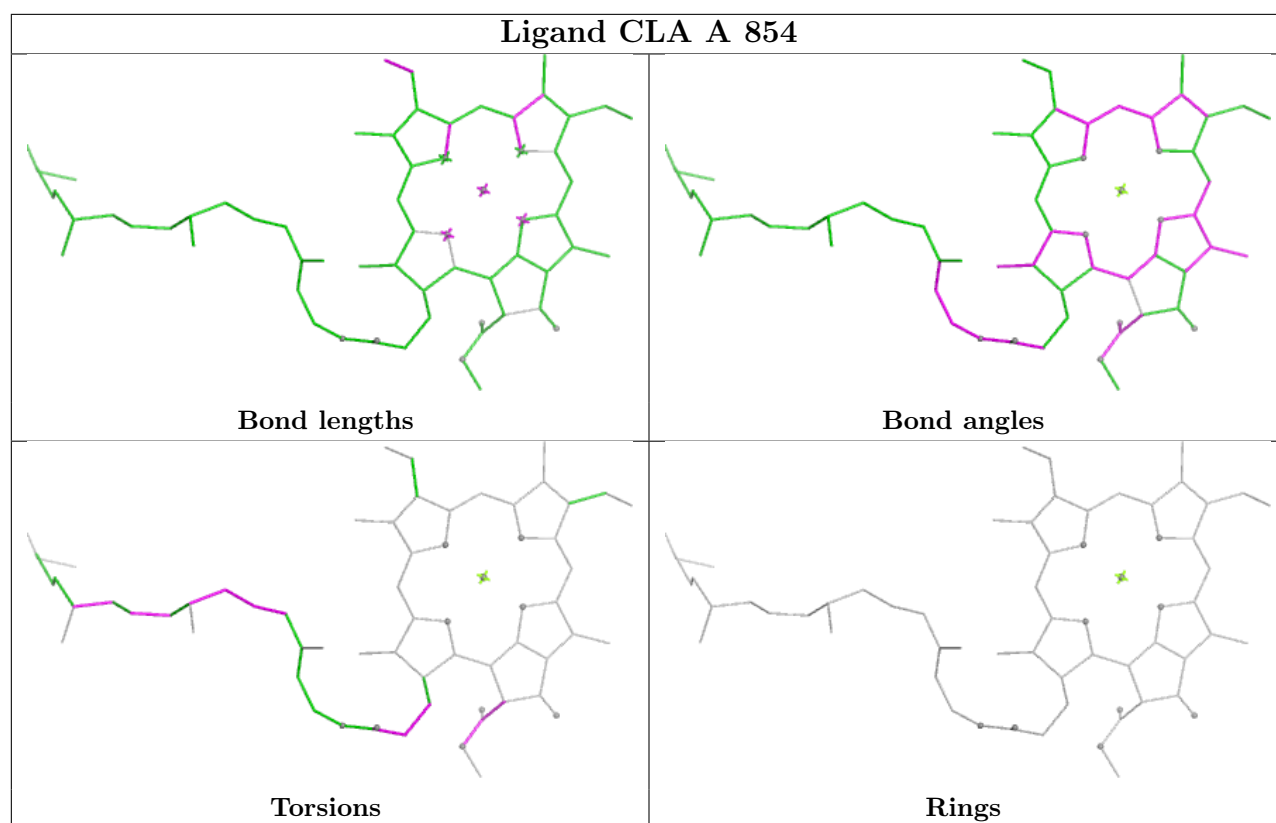
Ligand CLA 6 309



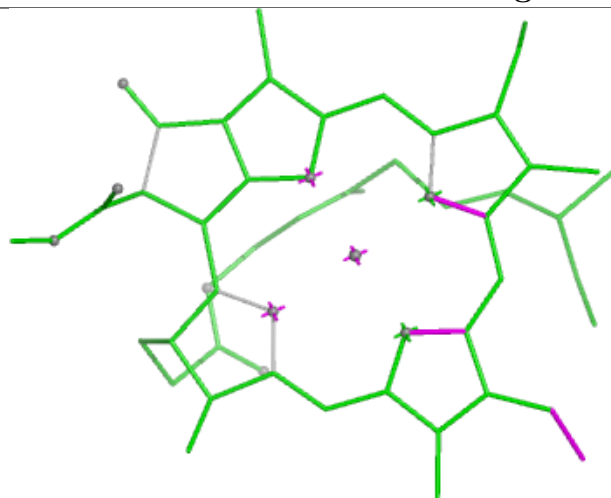
Ligand LHG 3 321



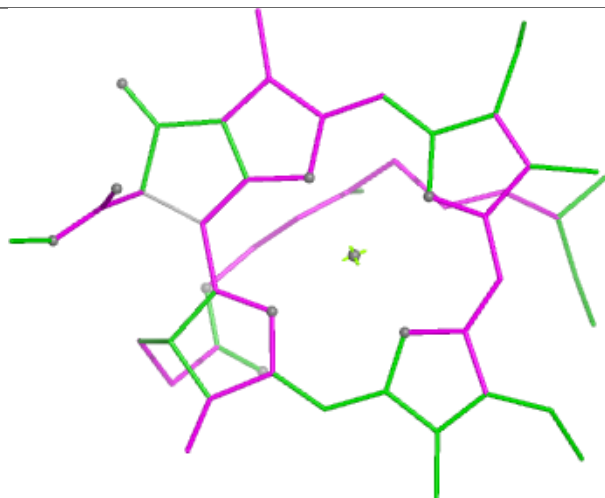




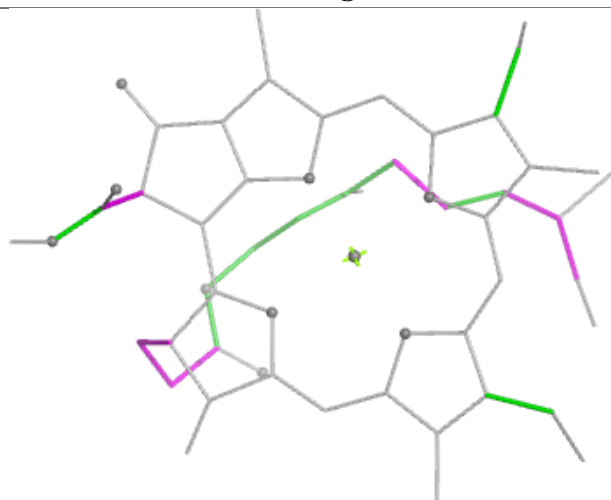
Ligand CLA B 810



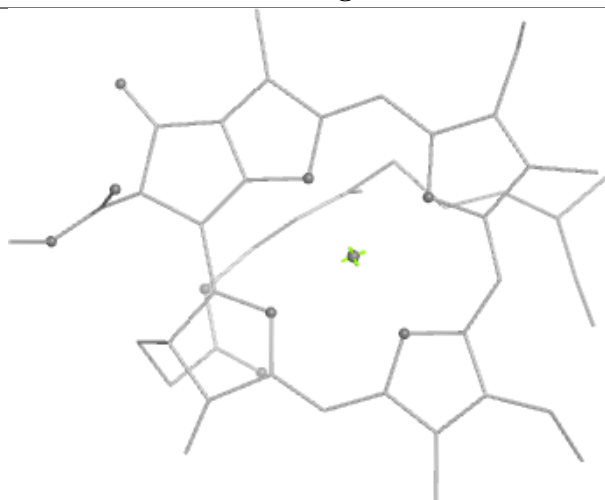
Bond lengths



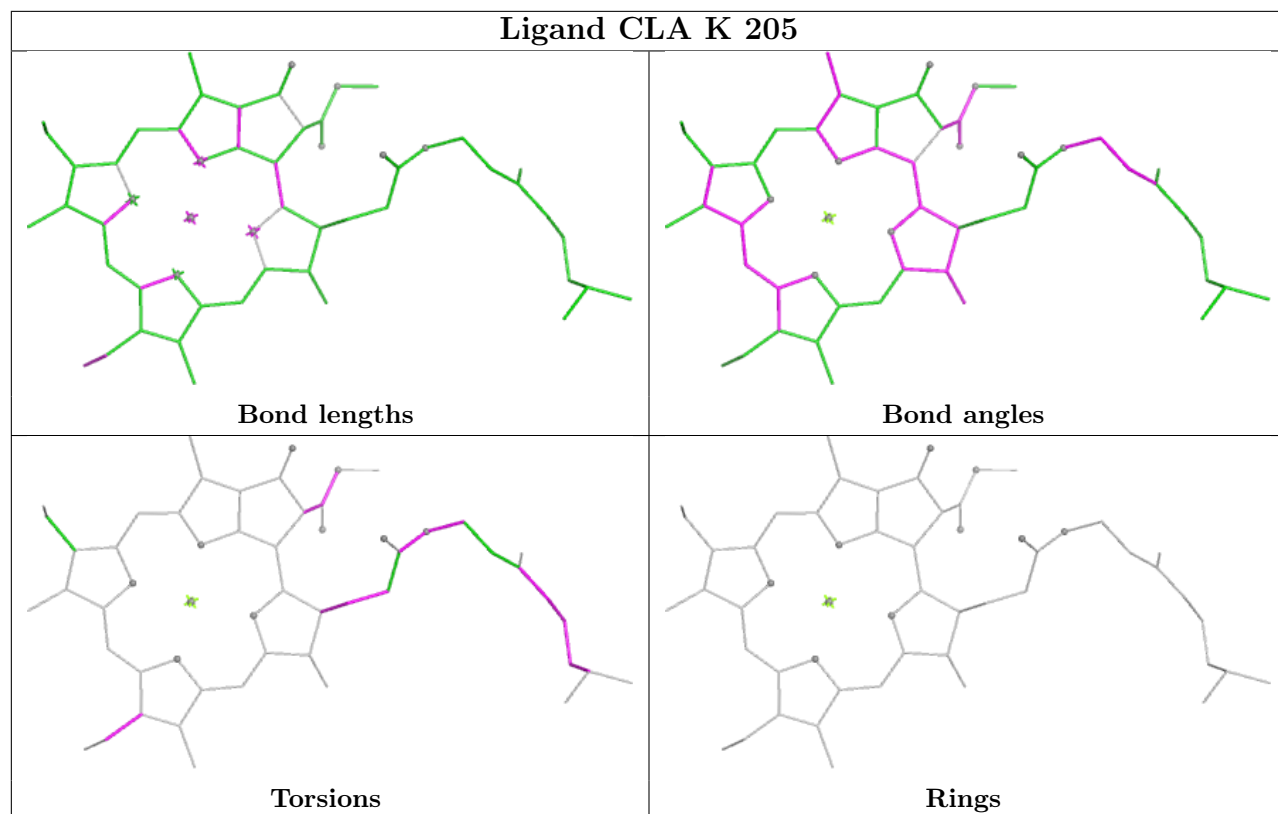
Bond angles



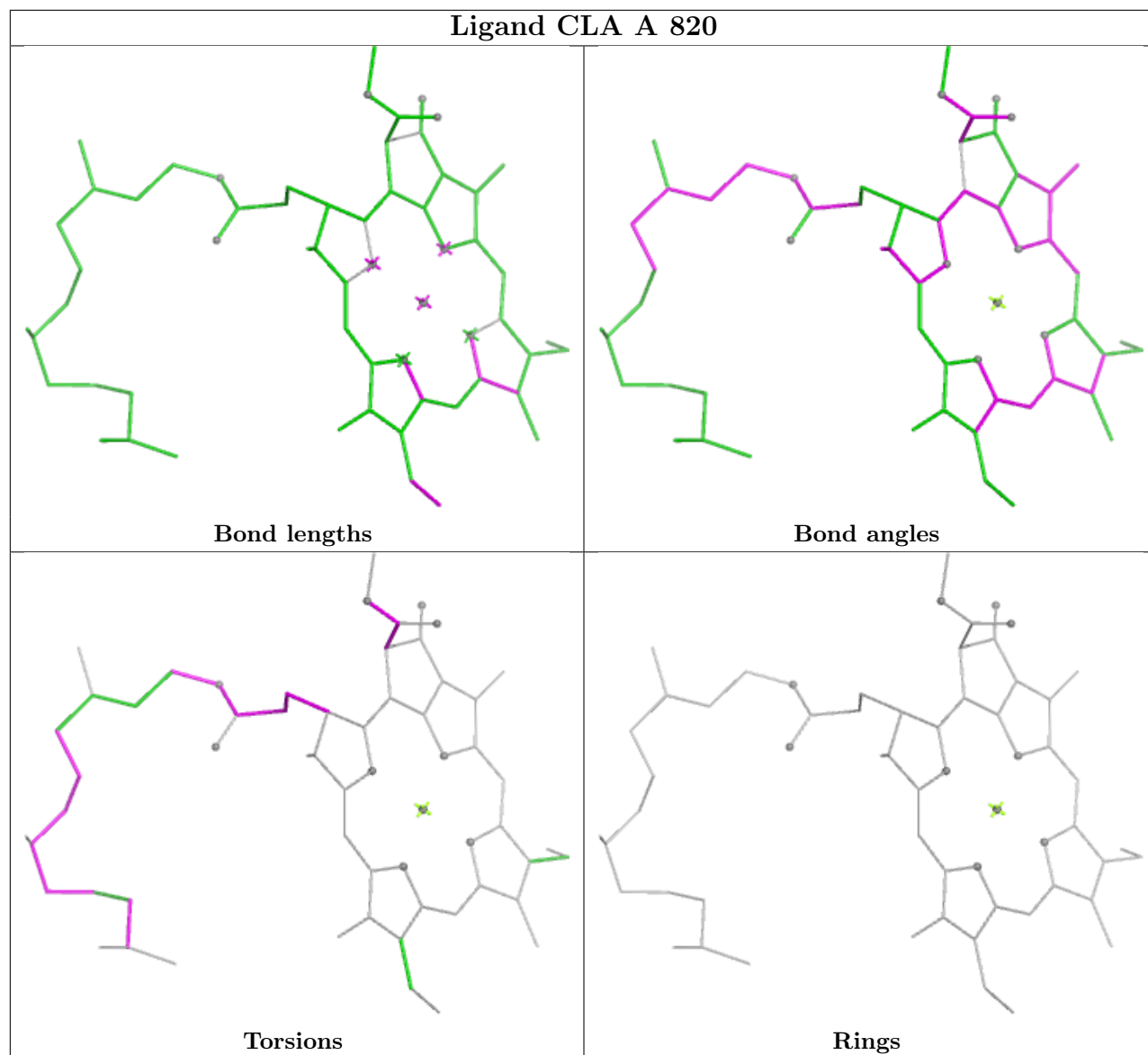
Torsions



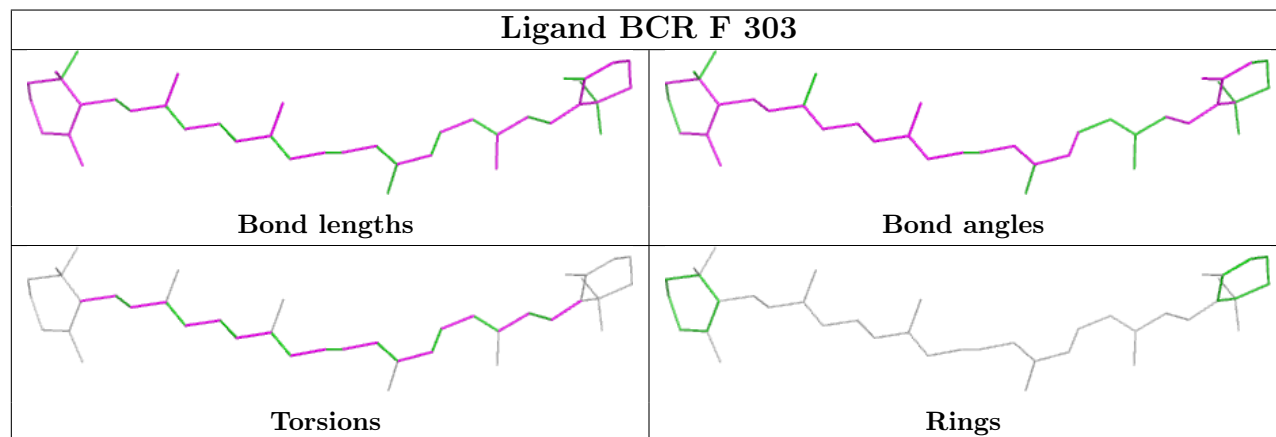
Rings



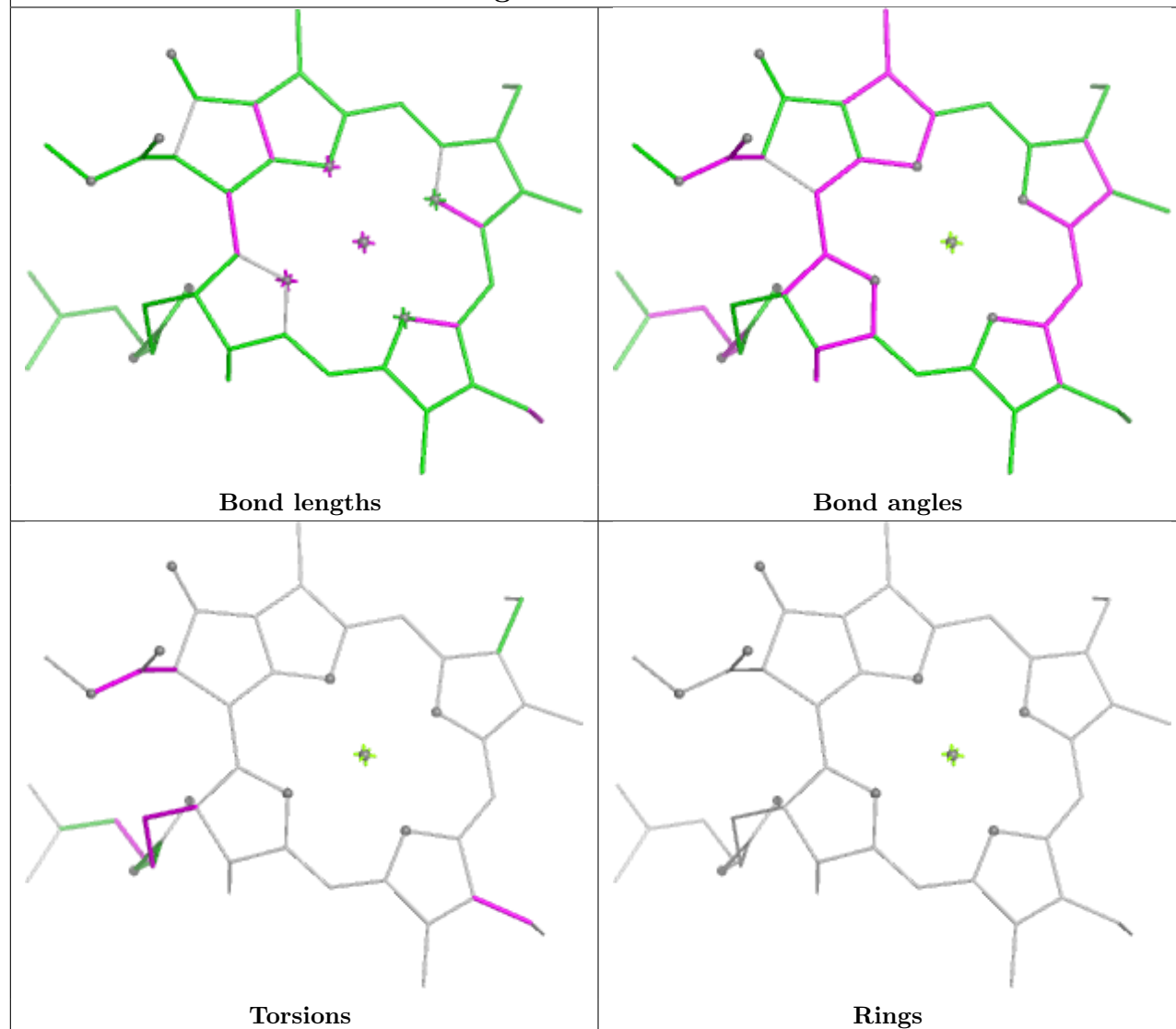
Ligand CLA A 820



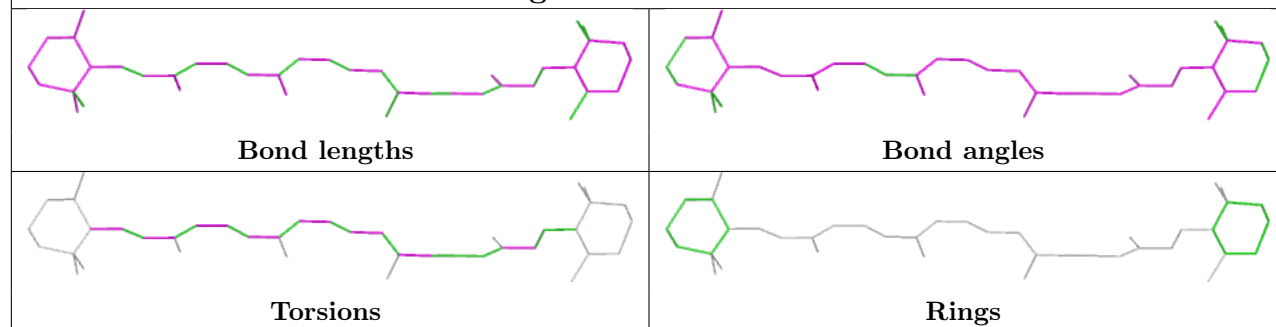
Ligand BCR F 303

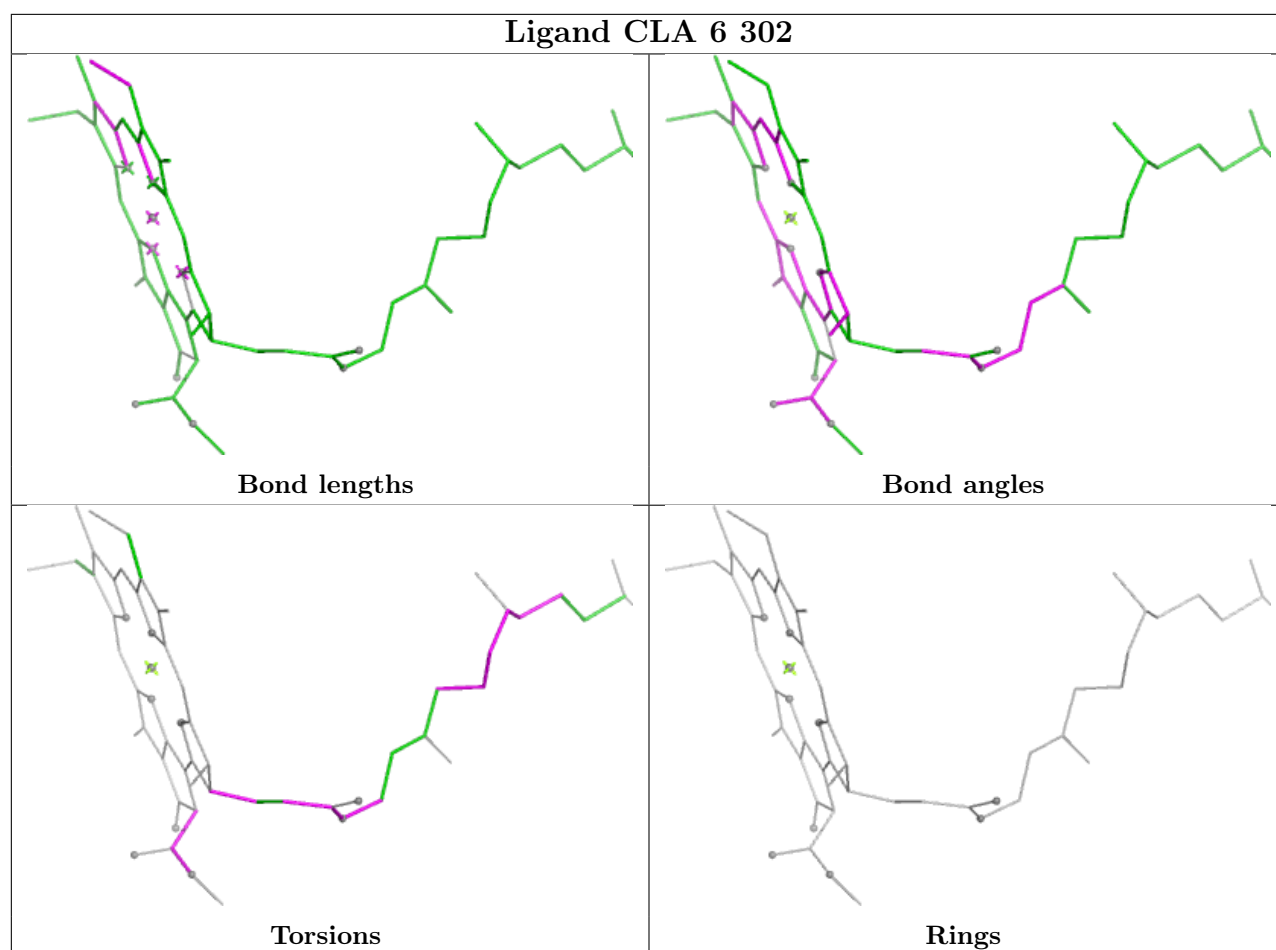


Ligand CLA 5 320

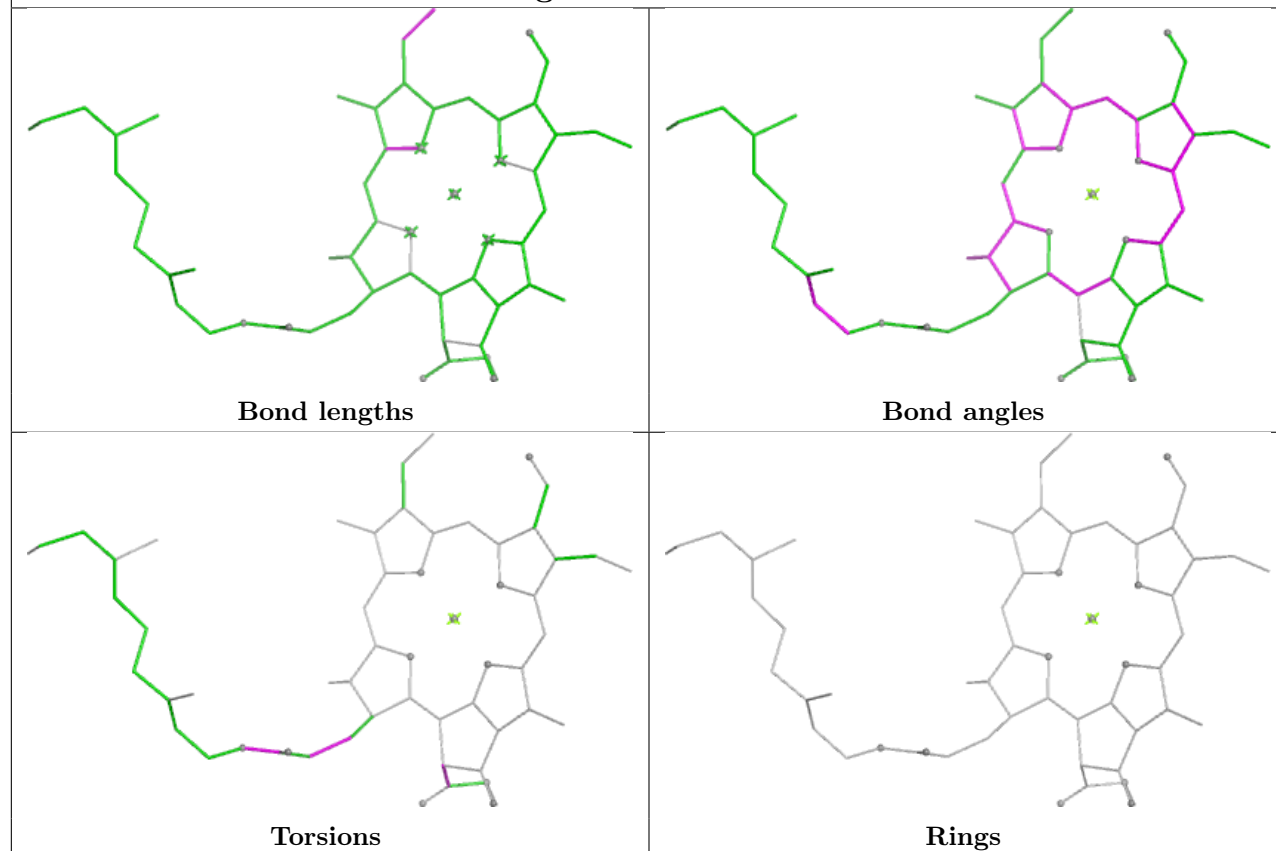


Ligand BCR K 206

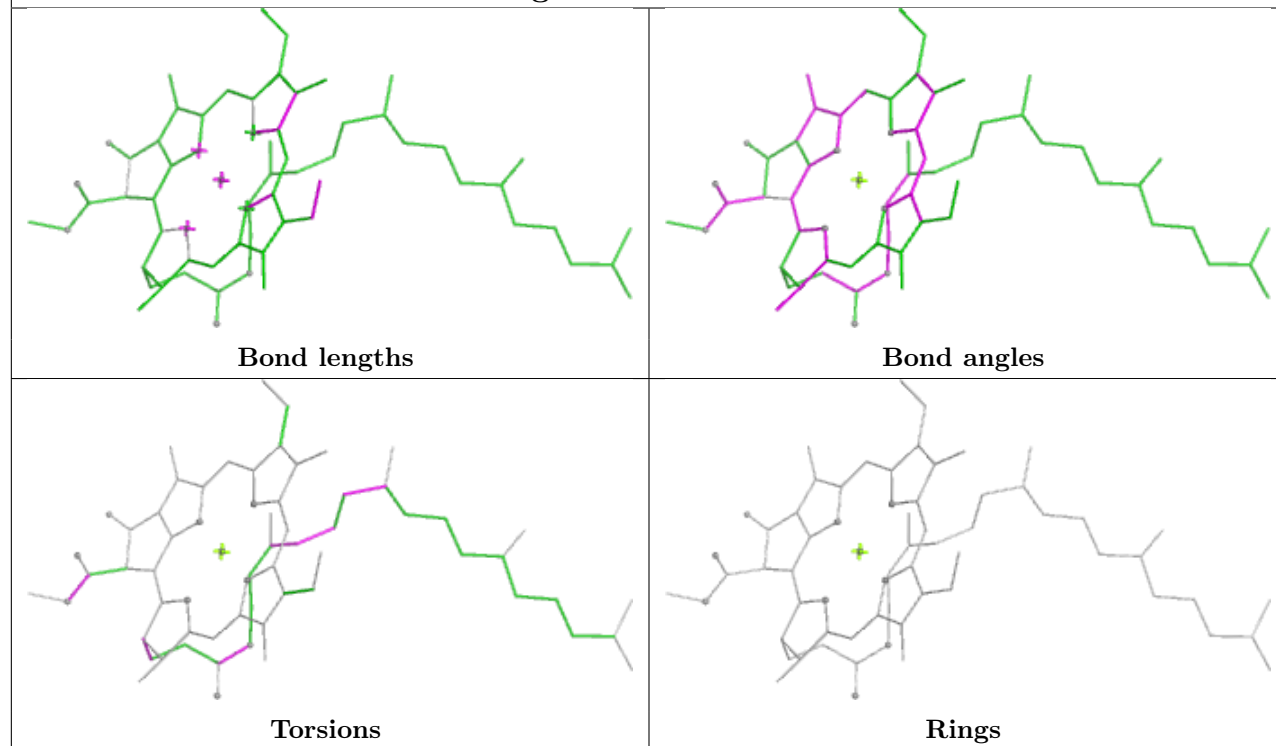


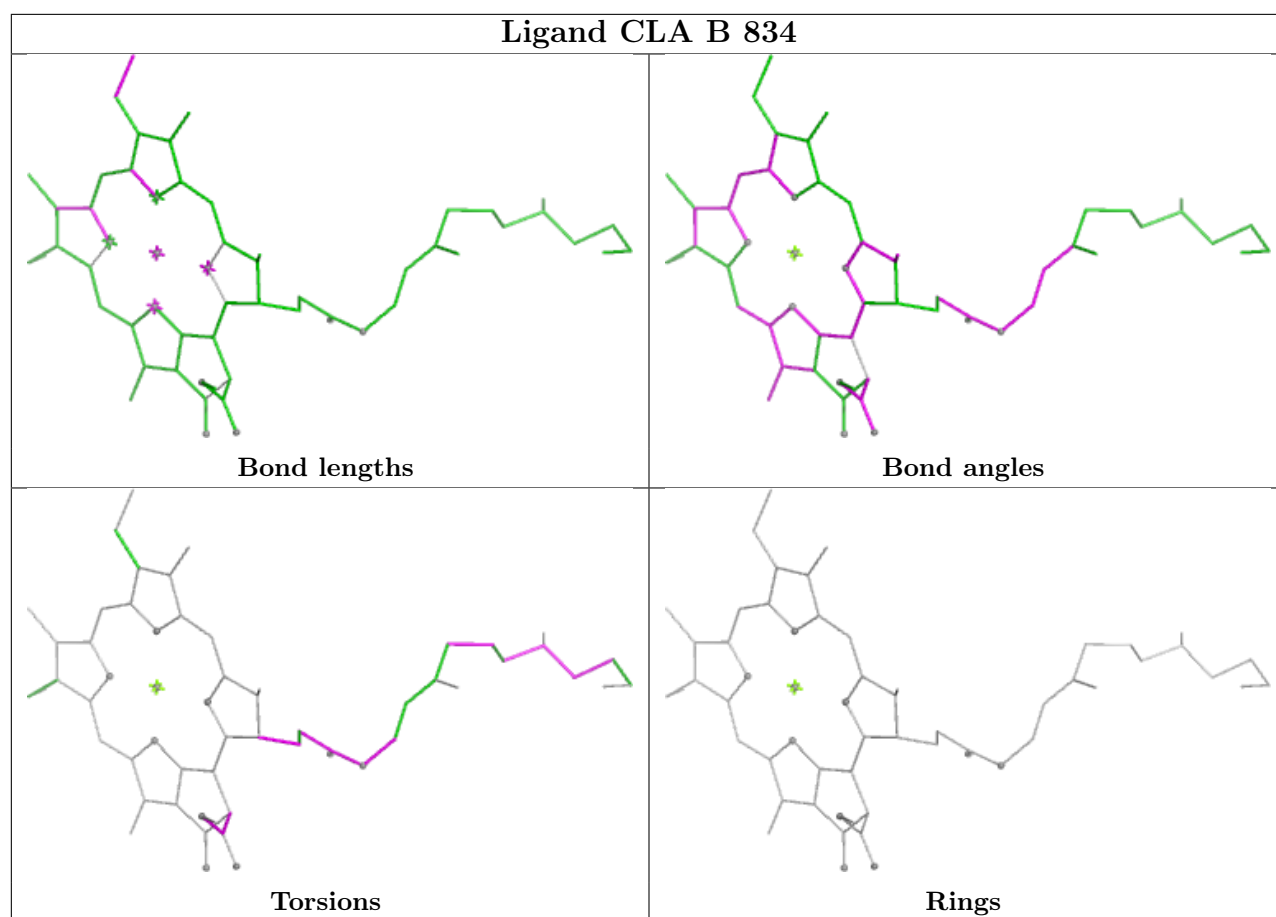


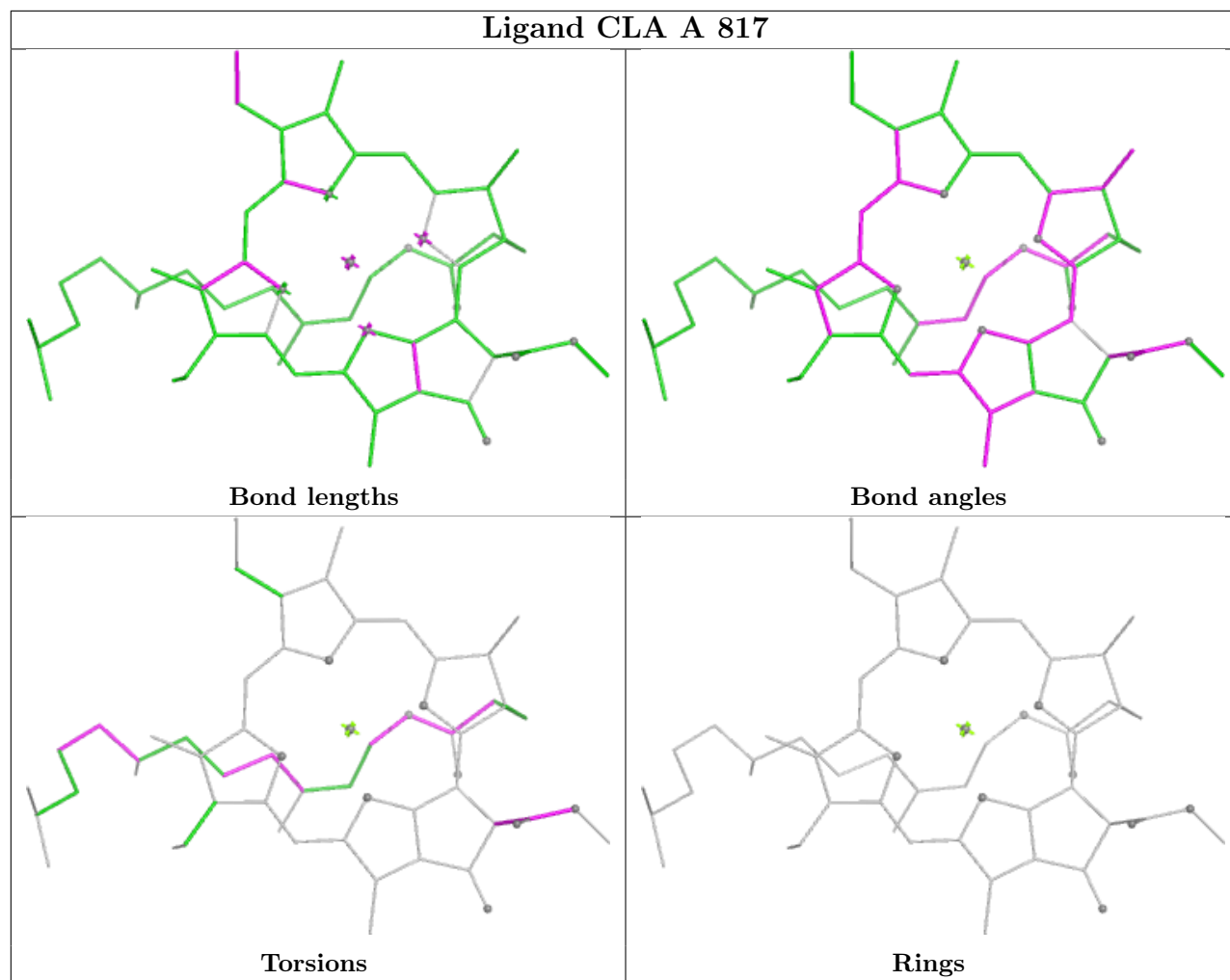
Ligand CHL 8 301

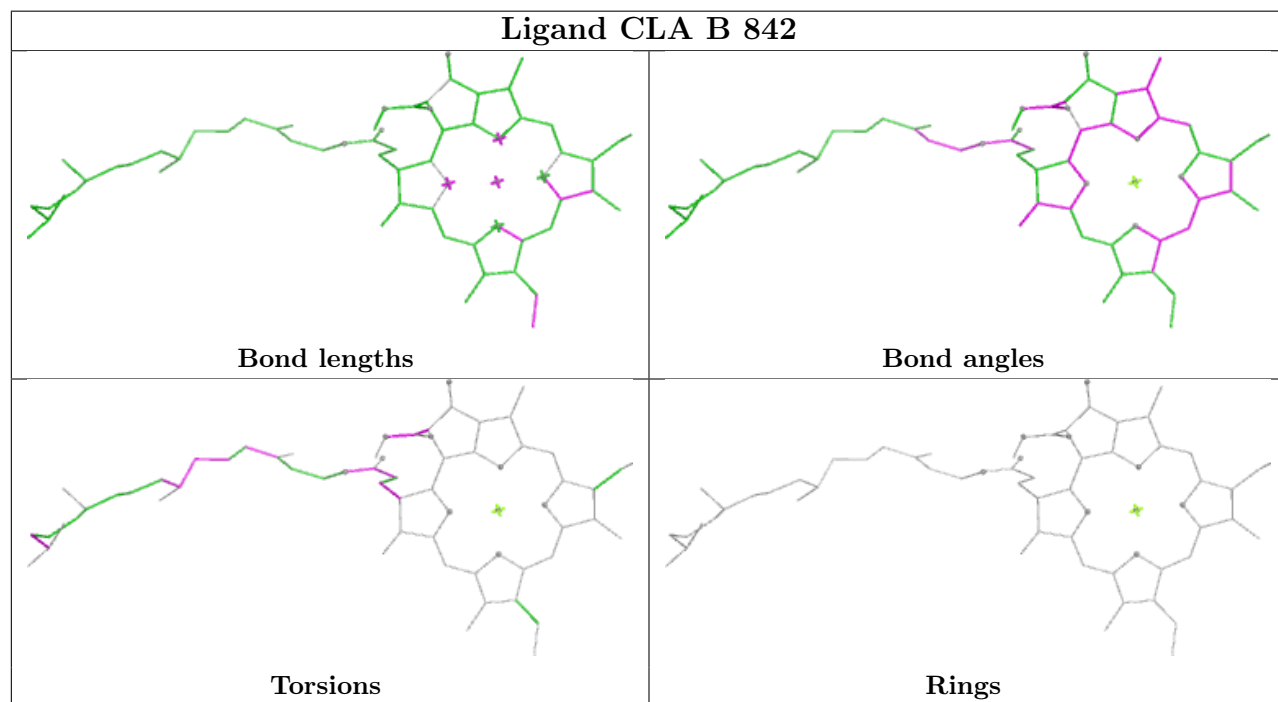
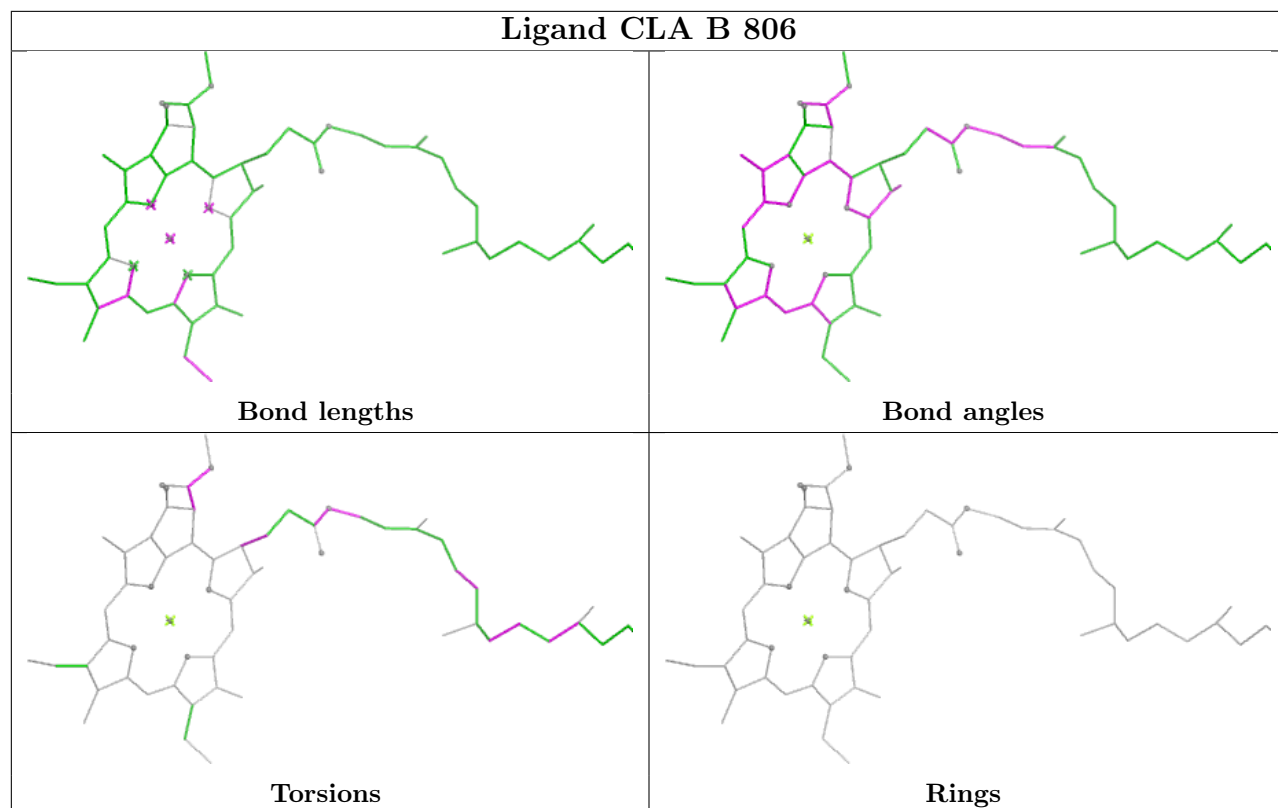


Ligand CLA A 841

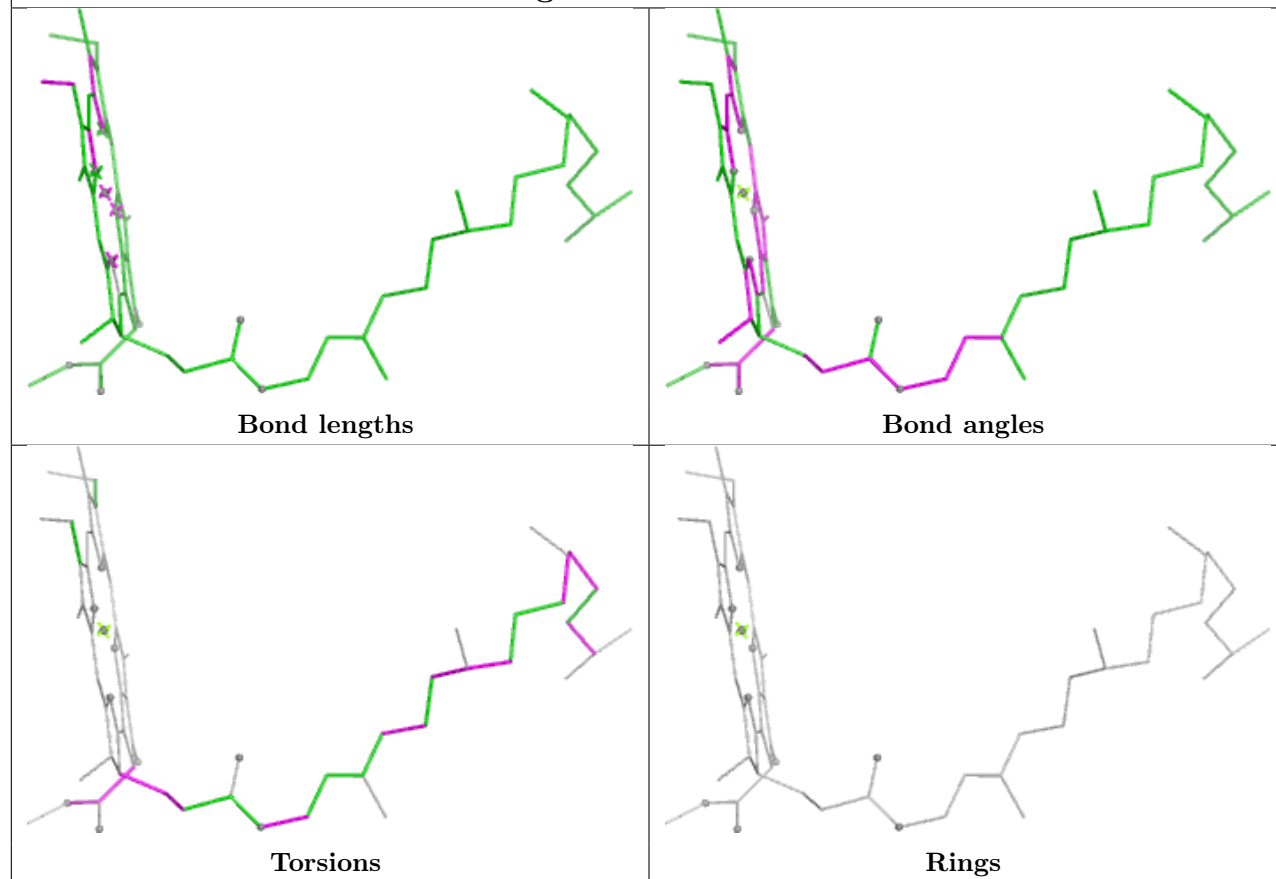




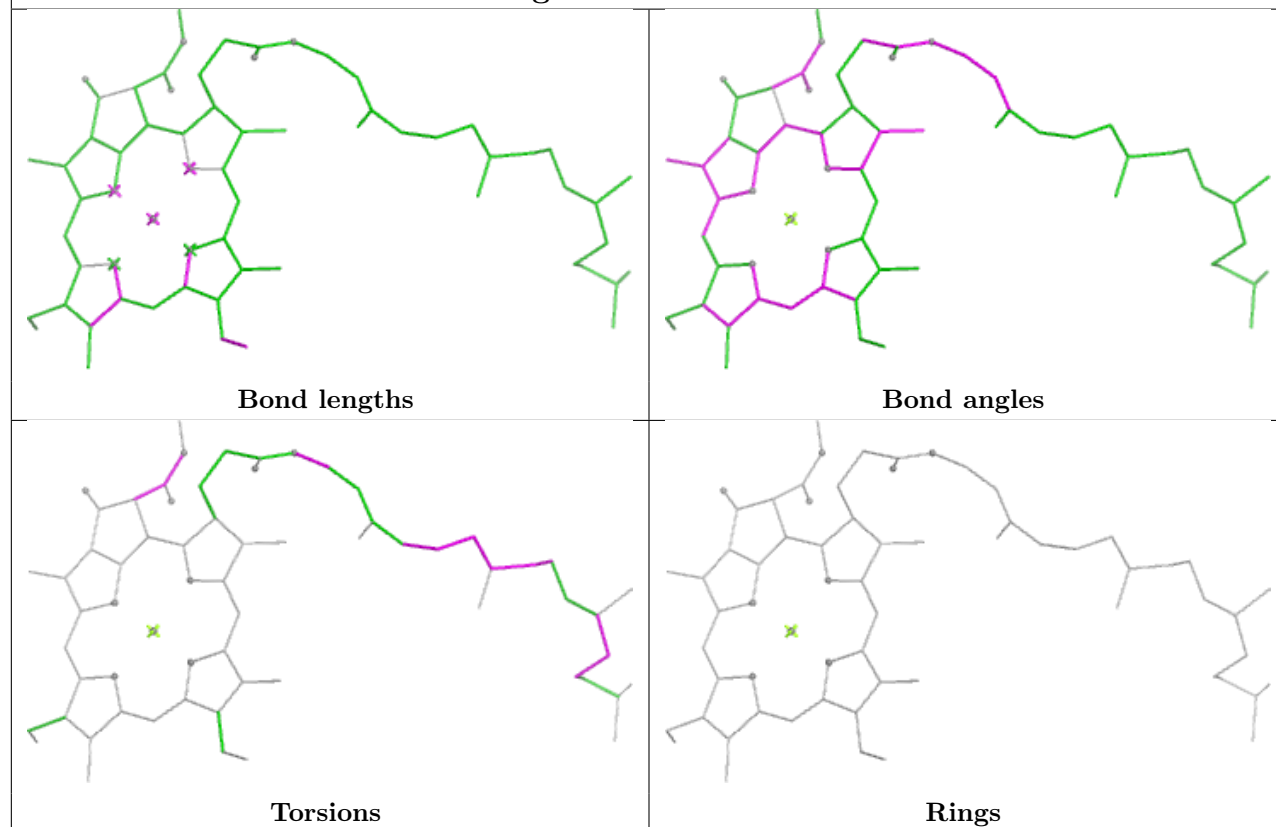




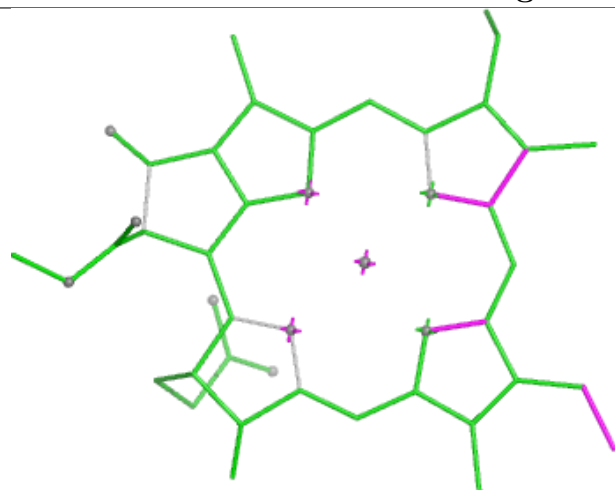
Ligand CLA 7 323



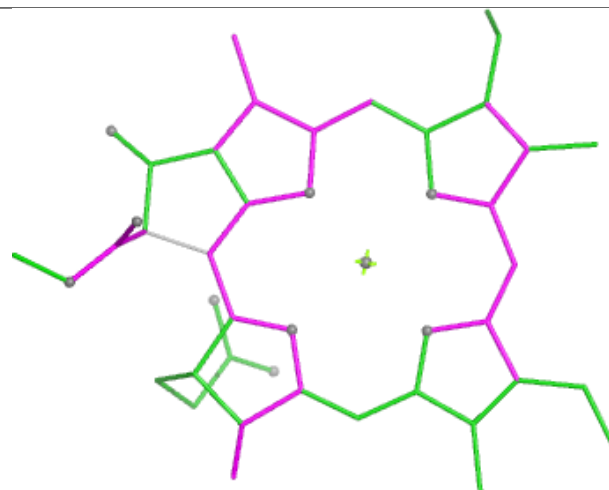
Ligand CLA B 801



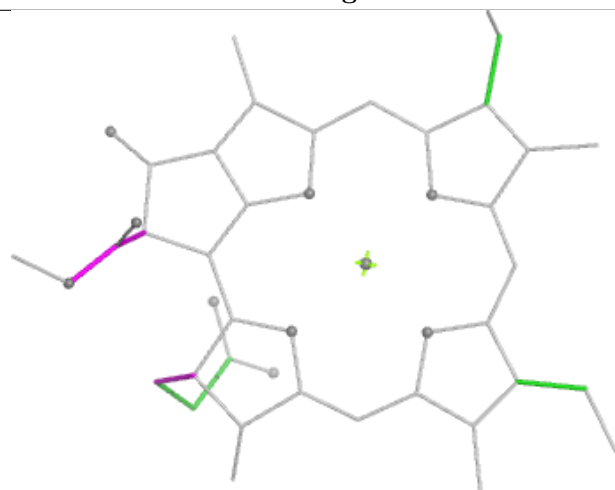
Ligand CLA B 836



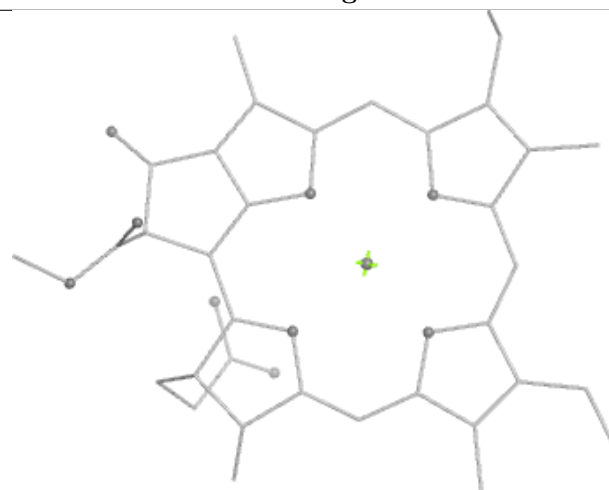
Bond lengths



Bond angles

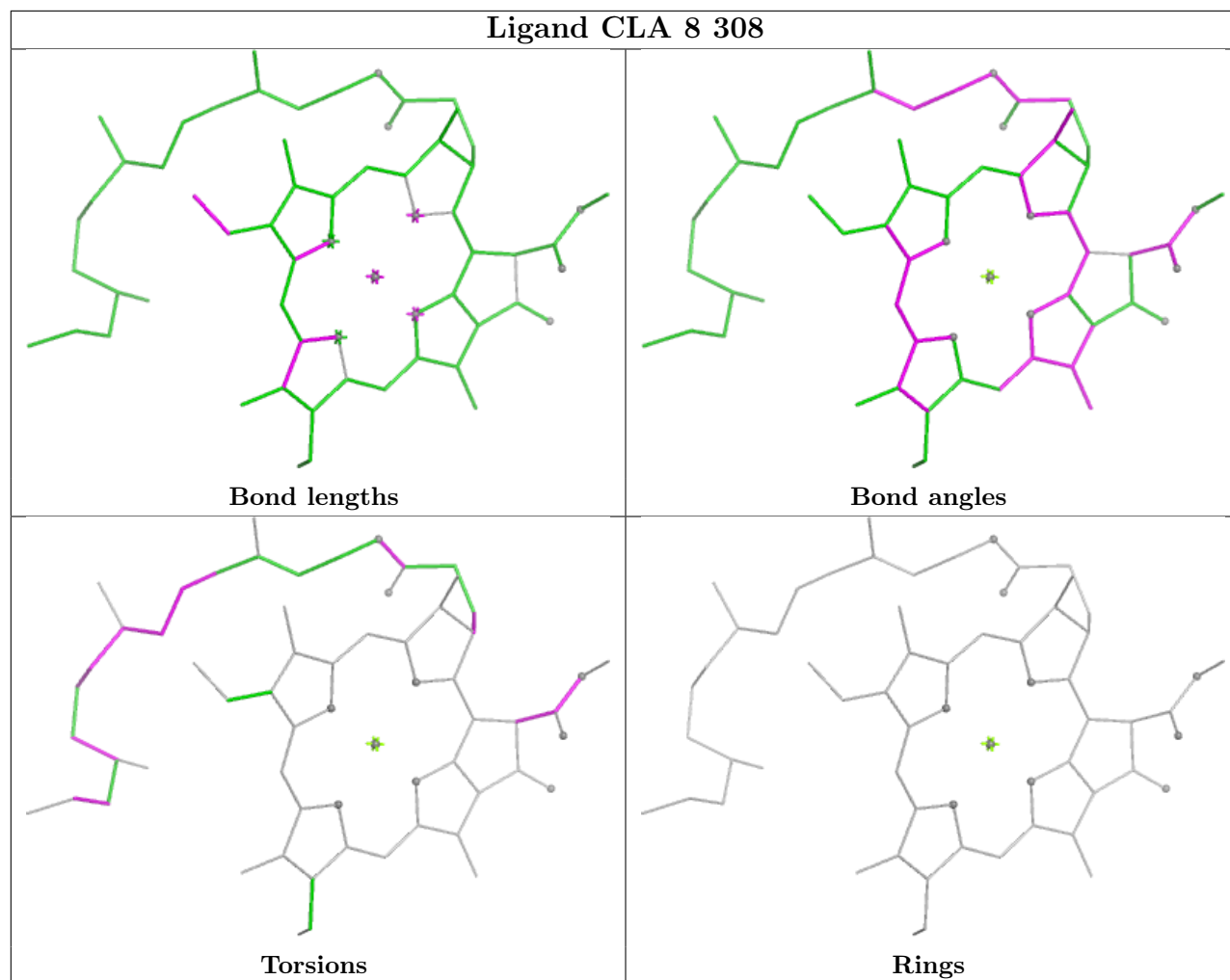


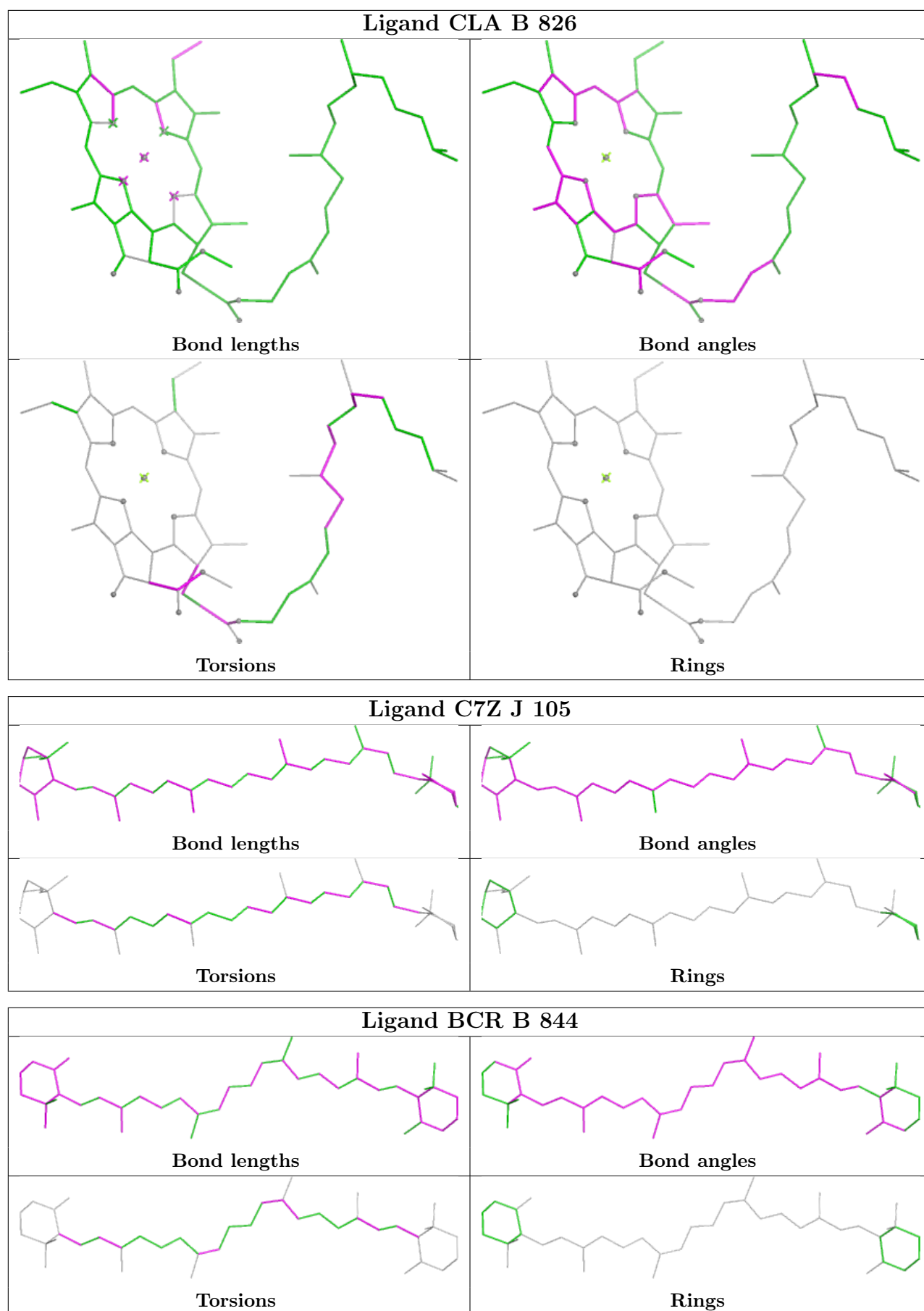
Torsions

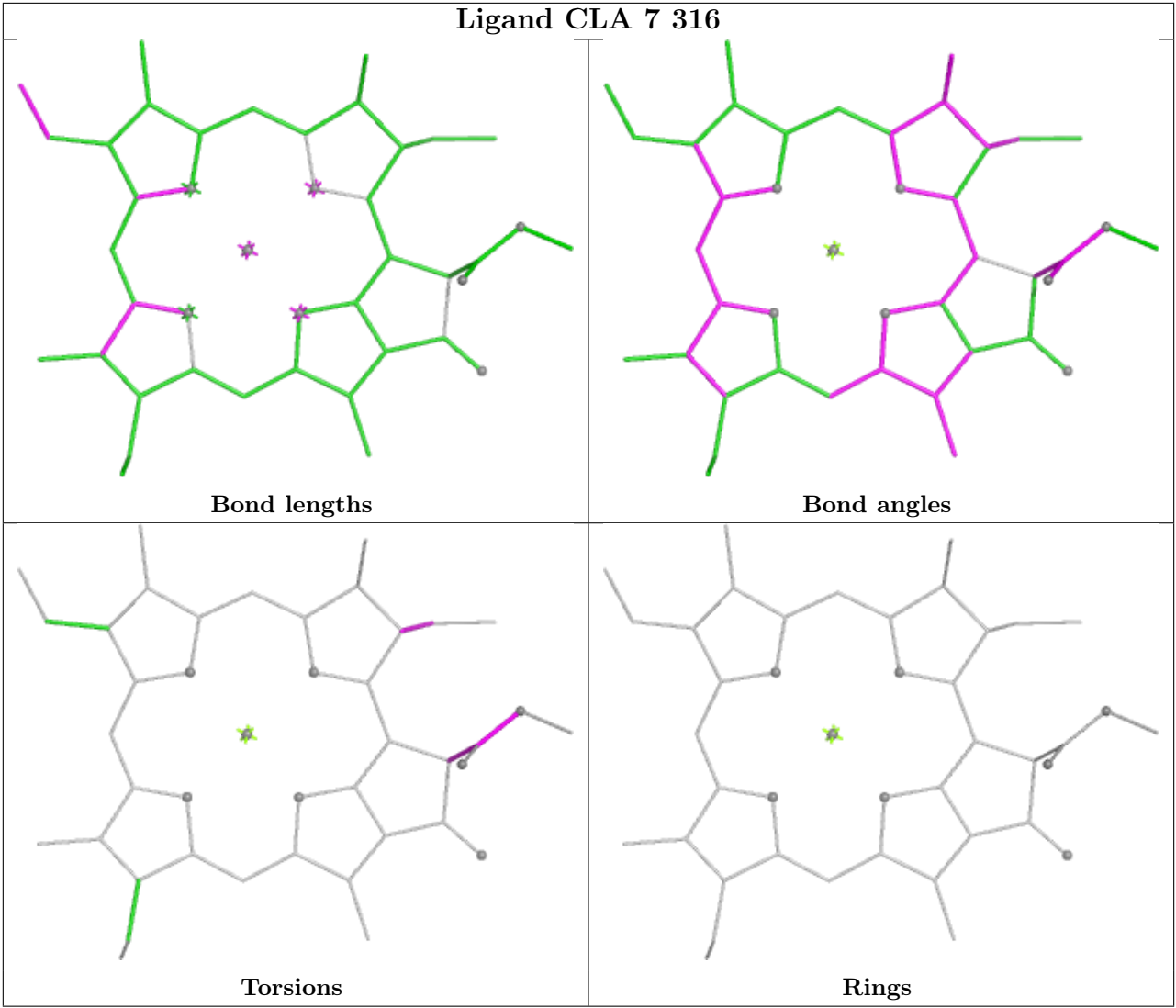


Rings

Ligand CLA 8 308







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

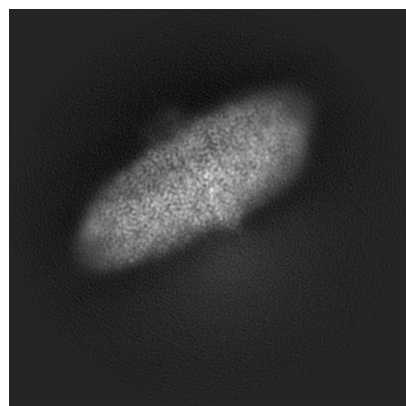
6 Map visualisation [i](#)

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.

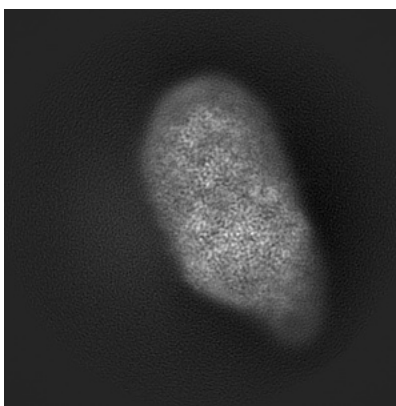
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

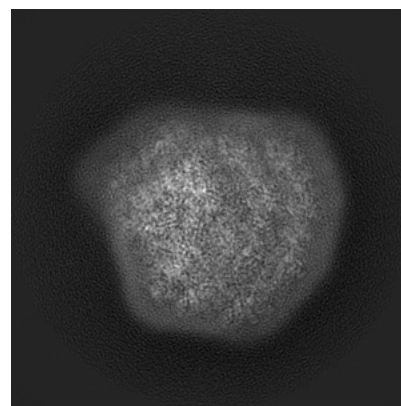
6.1.1 Primary map



X

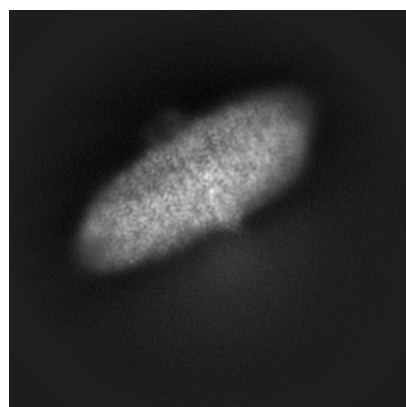


Y

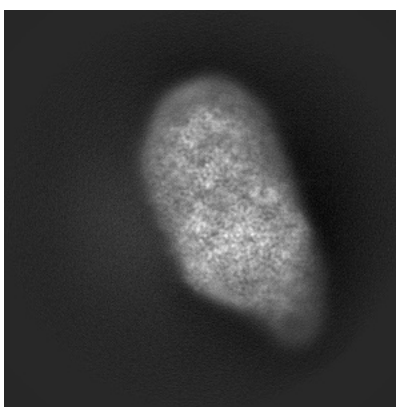


Z

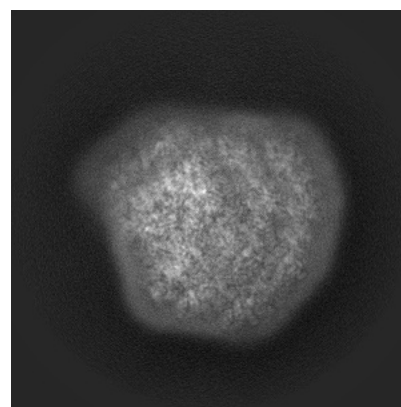
6.1.2 Raw map



X



Y

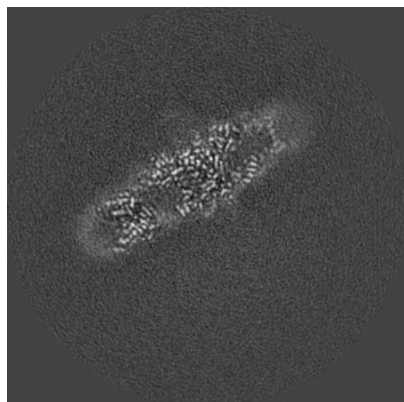


Z

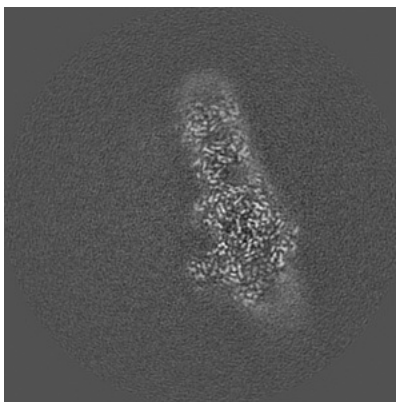
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

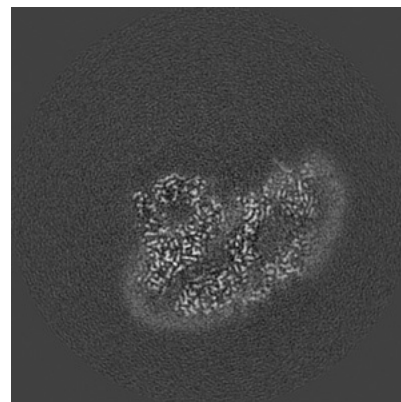
6.2.1 Primary map



X Index: 250

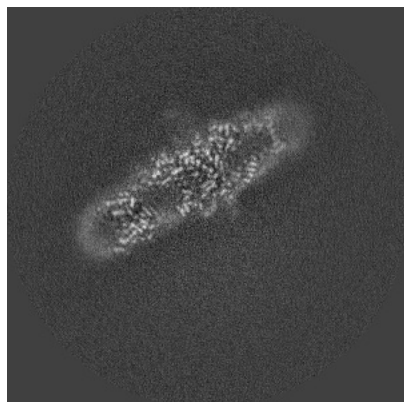


Y Index: 250

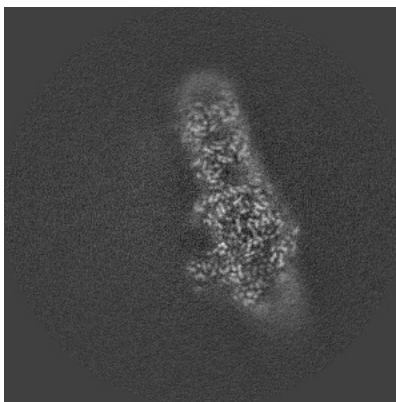


Z Index: 250

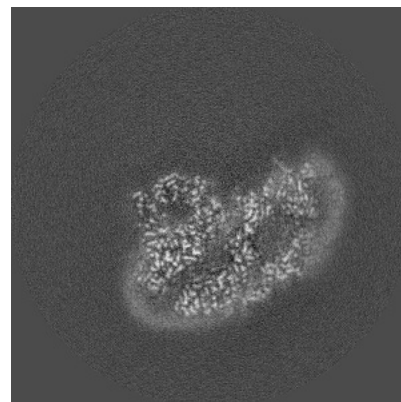
6.2.2 Raw map



X Index: 250



Y Index: 250

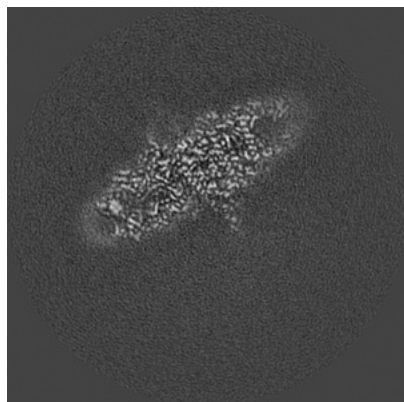


Z Index: 250

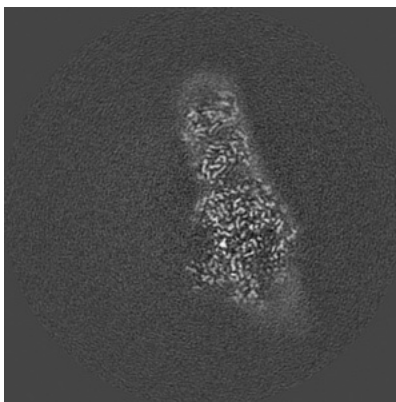
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

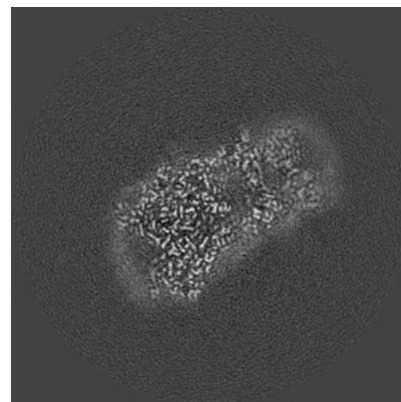
6.3.1 Primary map



X Index: 218

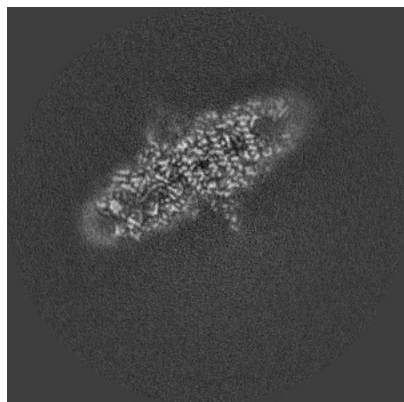


Y Index: 252

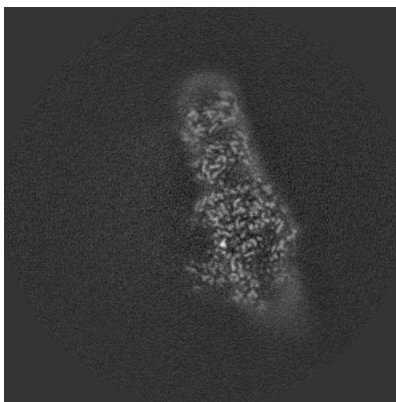


Z Index: 289

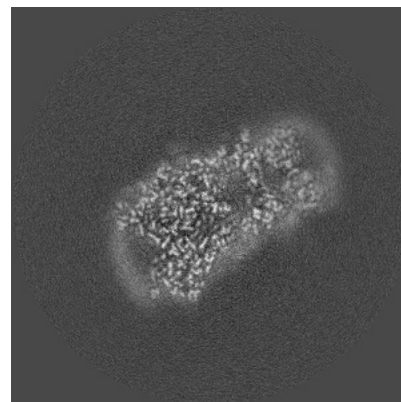
6.3.2 Raw map



X Index: 218



Y Index: 252

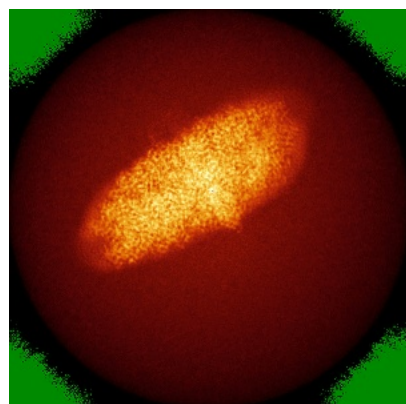


Z Index: 289

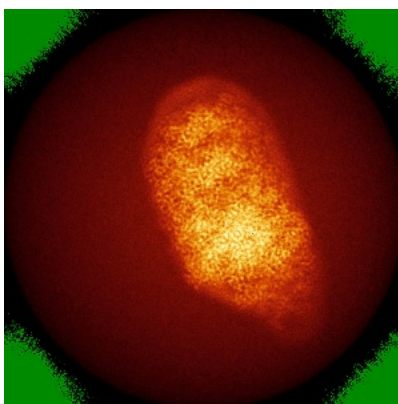
The images above show the largest variance slices of the map in three orthogonal directions.

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

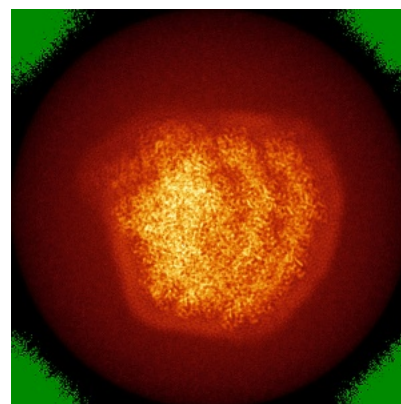
6.4.1 Primary map



X

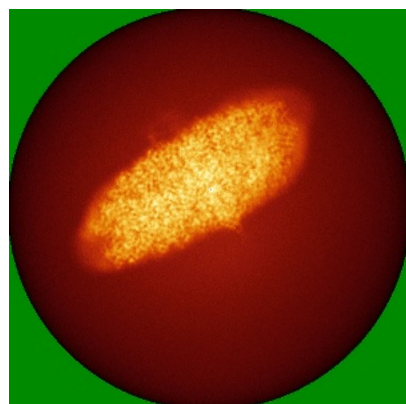


Y

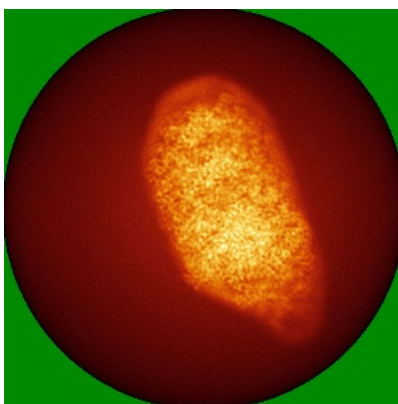


Z

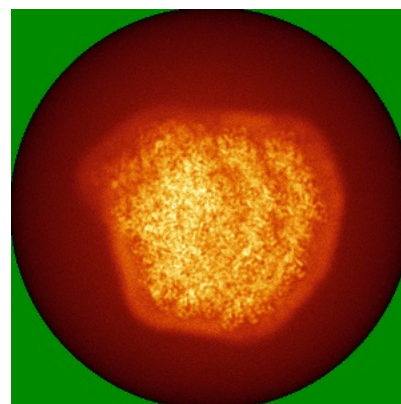
6.4.2 Raw map



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.

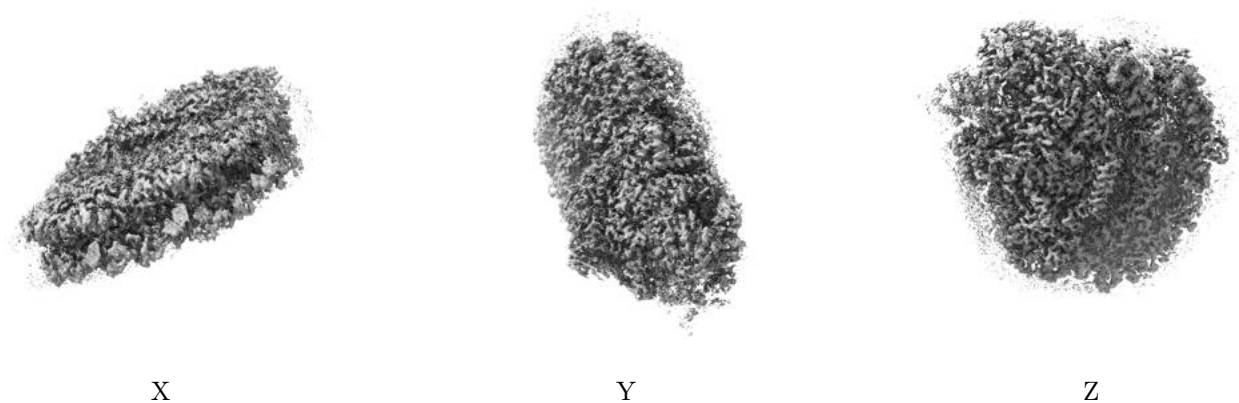
6.5 Orthogonal surface views [i](#)

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.

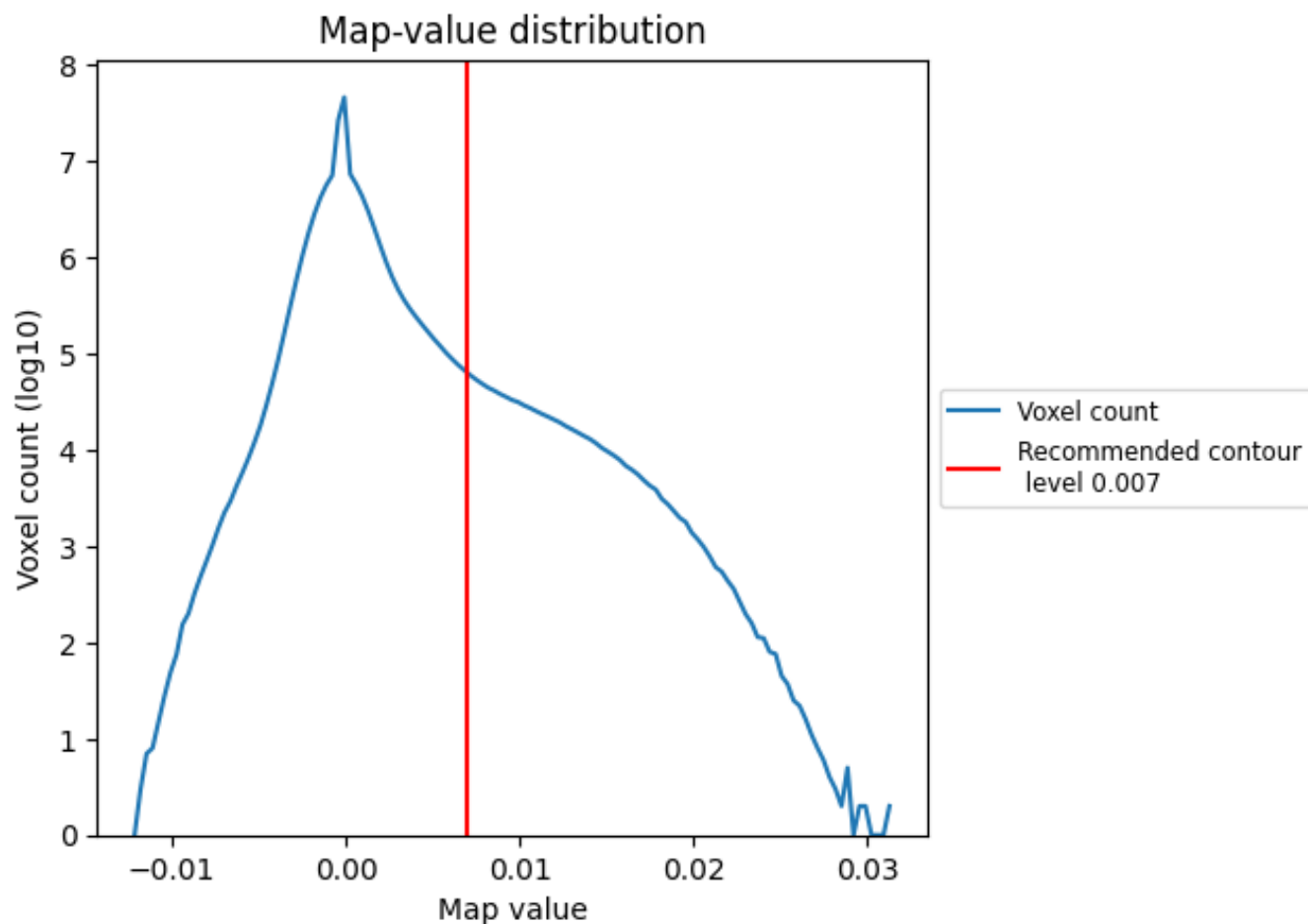
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

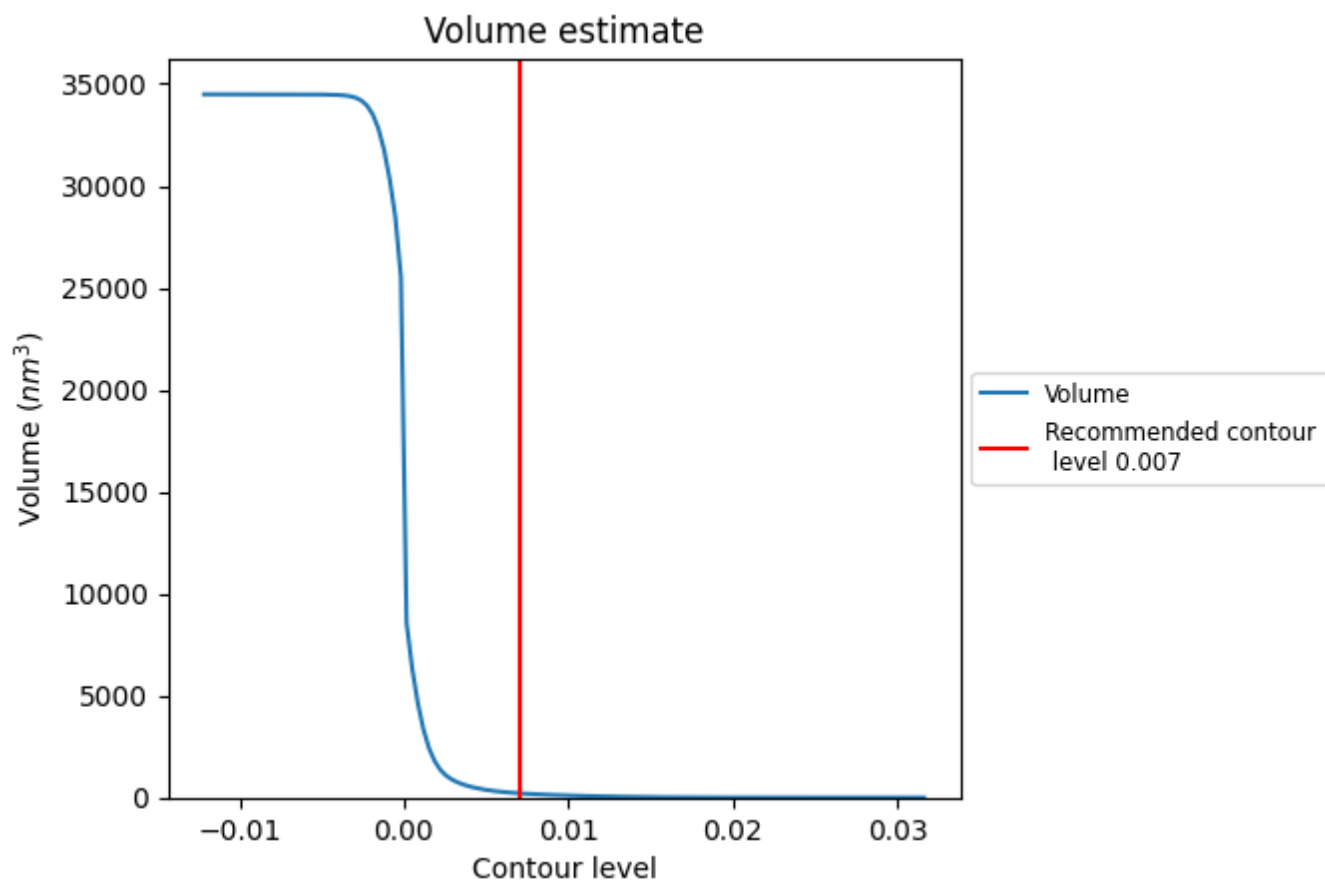
This section contains the results of statistical analysis of the map.

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.

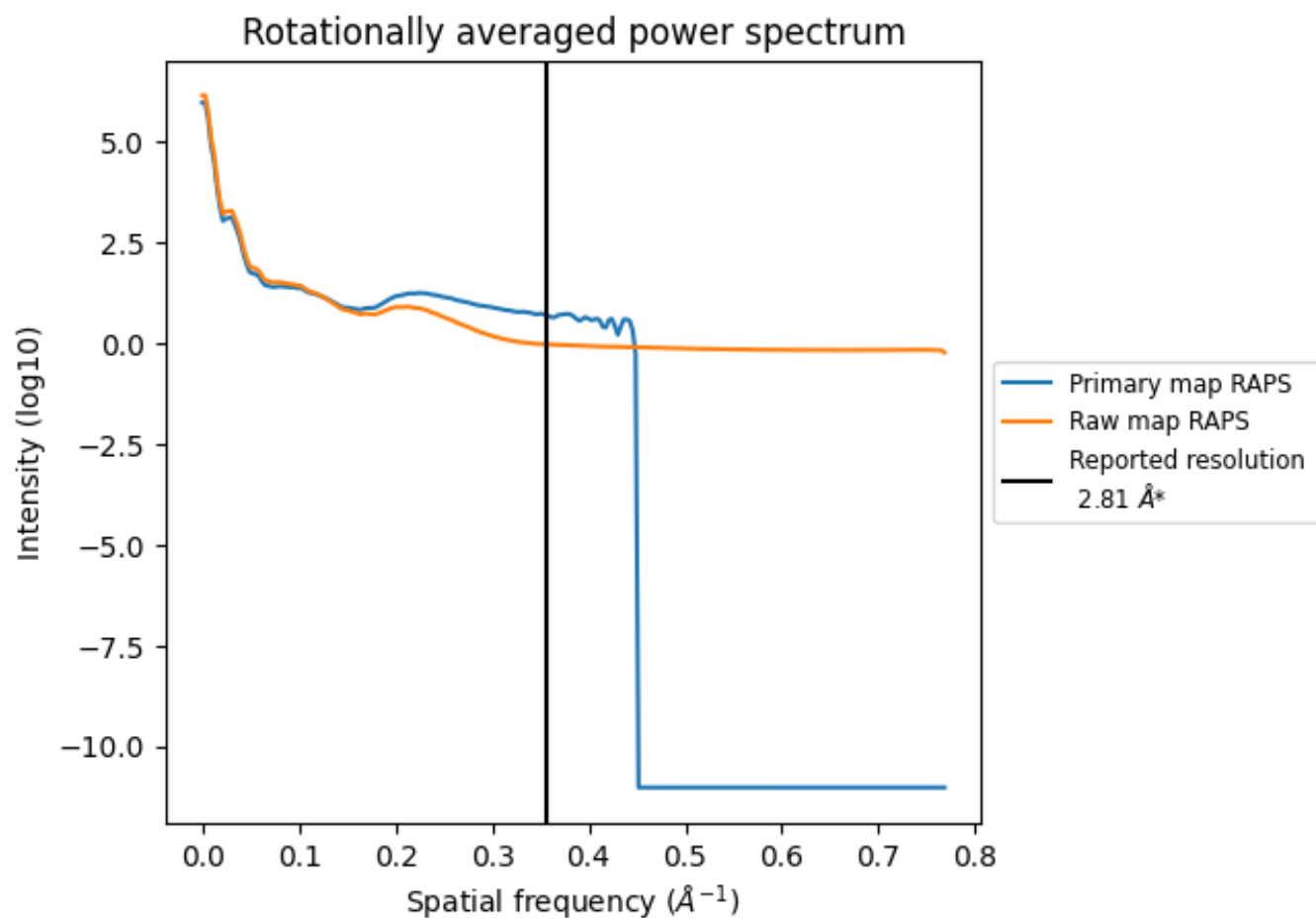
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm^3 ; 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 ⓘ

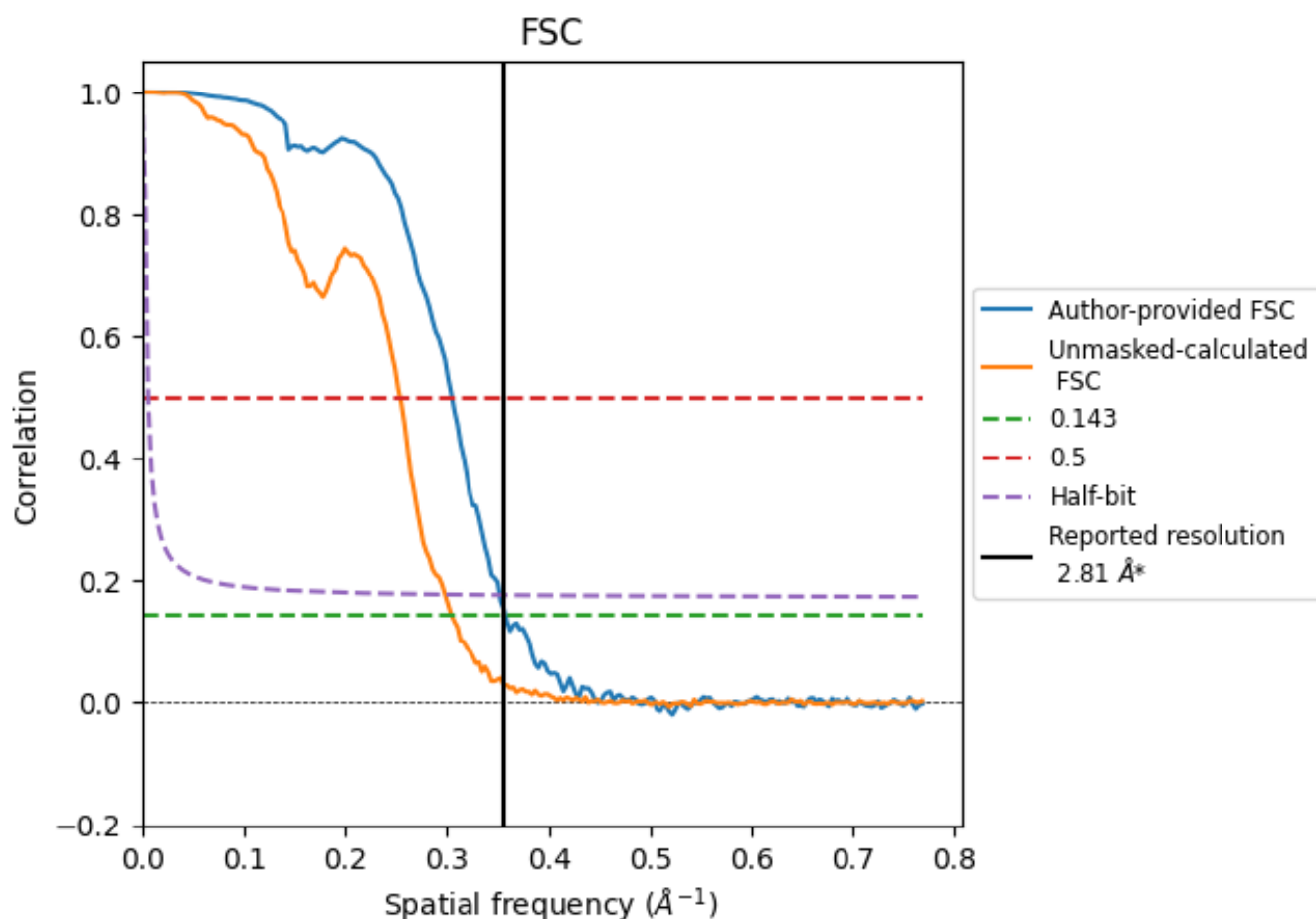


*Reported resolution corresponds to spatial frequency of 0.356 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

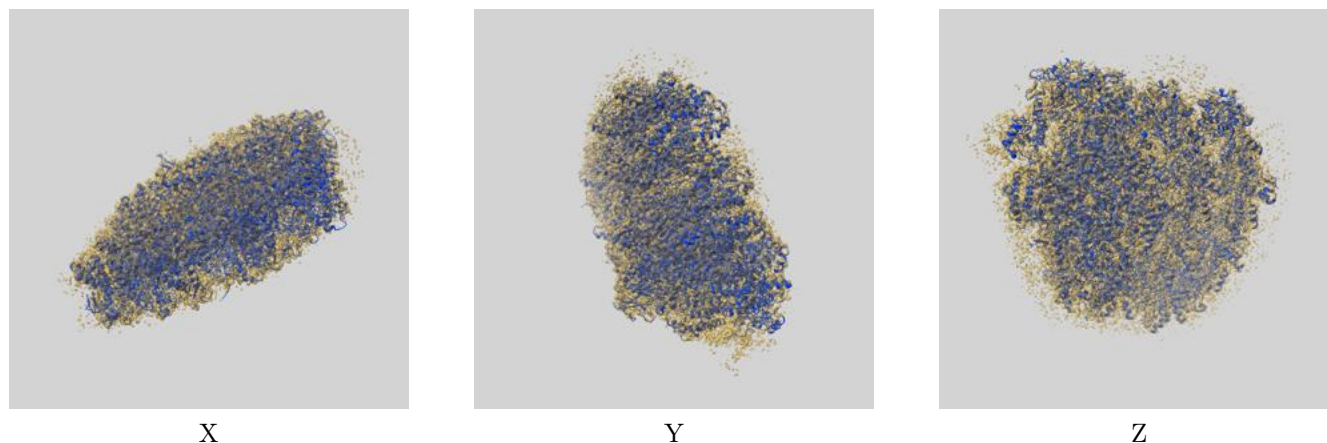
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.79	3.28	2.84
Unmasked-calculated*	3.28	3.94	3.36

*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](#)

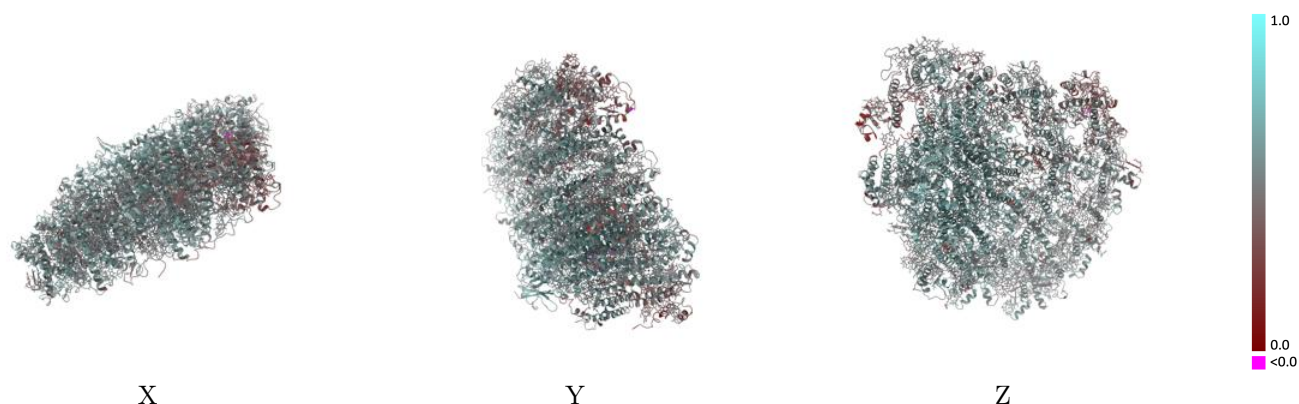
This section contains information regarding the fit between EMDB map EMD-16732 and PDB model 8CMO. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



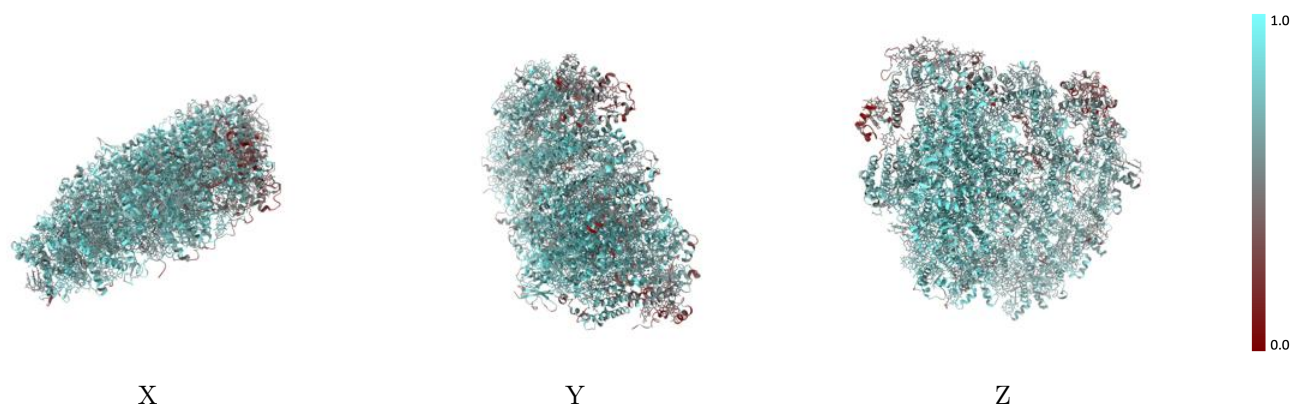
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



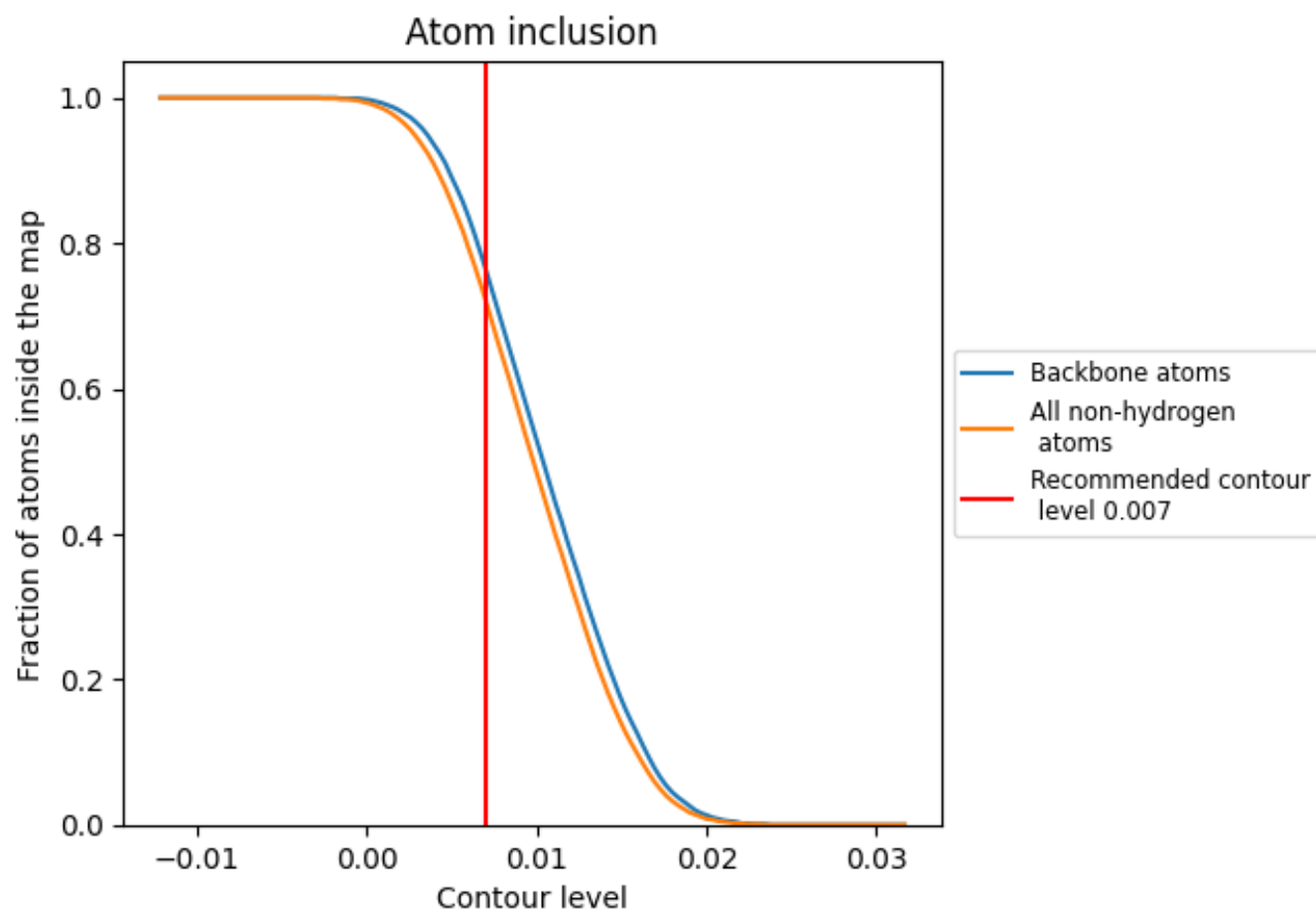
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.7200	0.5370
1	0.6350	0.4980
2	0.3310	0.3380
3	0.7710	0.5610
4	0.6470	0.5050
5	0.6780	0.5150
6	0.6810	0.5140
7	0.7840	0.5510
8	0.7410	0.5310
9	0.5380	0.4770
A	0.8270	0.5920
B	0.8210	0.5830
C	0.7720	0.6020
D	0.6520	0.5660
E	0.6830	0.5660
F	0.6980	0.5310
G	0.4660	0.4150
I	0.6720	0.5270
J	0.7000	0.5310
K	0.7110	0.5230
L	0.6550	0.5030
Z	0.4730	0.4100

