



Full wwPDB EM Validation Report ⓘ

Sep 10, 2026 – 10:14 am BST

PDB ID : 8BCV / pdb_00008bcv
EMDB ID : EMD-15969
Title : Photosystem I assembly intermediate of Avena sativa
Authors : Naschberger, A.; Amunts, A.; Nelson, N.
Deposited on : 2022-10-17
Resolution : 2.20 Å(reported)

This is a Full wwPDB EM Validation 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:

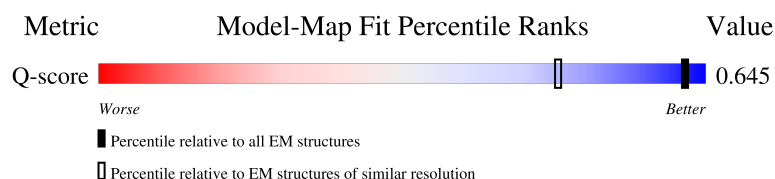
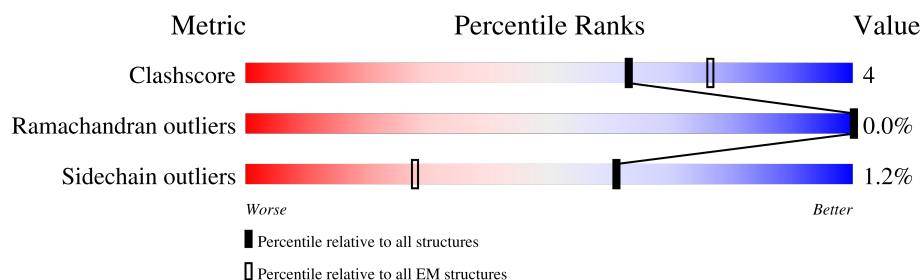
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.20 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	3184 (1.71 - 2.70)

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	750	
2	B	734	
3	C	81	
4	D	206	

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Mol	Chain	Length	Quality of chain
5	E	143	
6	H	94	
7	I	36	
8	L	213	
9	F	178	
10	G	144	
11	J	52	
12	K	130	
13	1	242	
14	2	207	
15	3	269	
16	4	256	

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 37485 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5840	3826	992	1003	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5864	3848	996	1007	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			605	372	104	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1124	722	196	203	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	67	Total	C	N	O	0	0
			533	340	94	99		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	94	Total	C	N	O	0	0
			715	469	114	132		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	33	Total	C	N	O	S	0	0
			258	178	38	41	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	159	Total	C	N	O	S	0	0
			1192	788	189	214	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	158	Total	C	N	O	S	0	0
			1238	804	210	221	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	94	Total	C	N	O	S	0	0
			721	467	121	133			

- Molecule 11 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	43	Total	C	N	O	S	0	0
			342	232	52	57	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit X.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	88	Total	C	N	O	S	0	0
			628	397	107	121	3		

- Molecule 13 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	196	Total	C	N	O	S	0	0
			1519	990	254	271	4		

- Molecule 14 is a protein called Chlorophyll a-b binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	207	Total	C	N	O	S	0	0
			1609	1050	263	292	4		

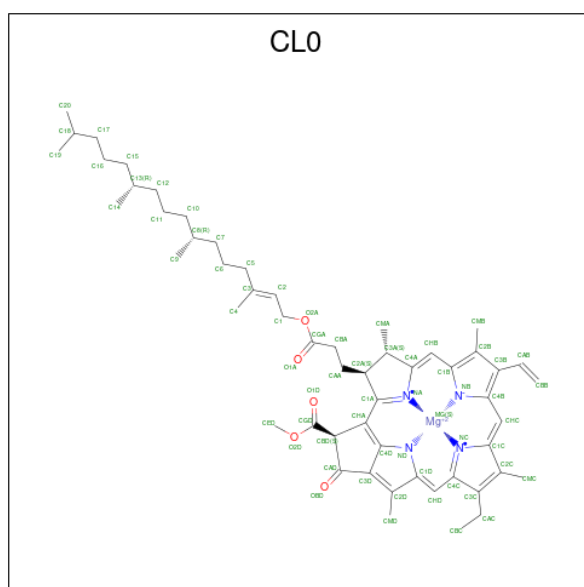
- Molecule 15 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	222	Total	C	N	O	S	0	0
			1725	1130	278	309	8		

- Molecule 16 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	199	Total	C	N	O	S	0	0
			1555	1012	257	282	4		

- Molecule 17 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	F	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	G	1	Total 57	C 47	Mg 1	N 4	O 5	0
18	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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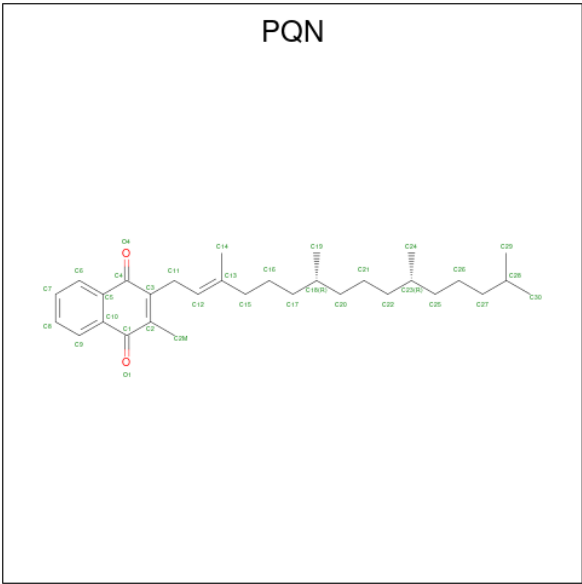
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18	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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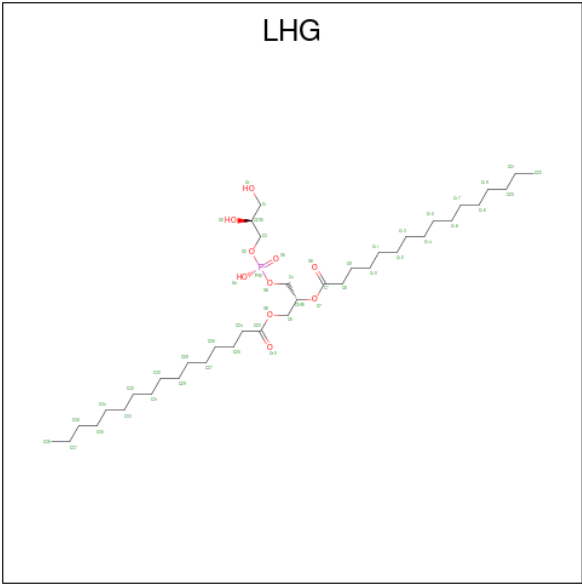
Mol	Chain	Residues	Atoms					AltConf
18	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Lig- and of Interest" by depositor).



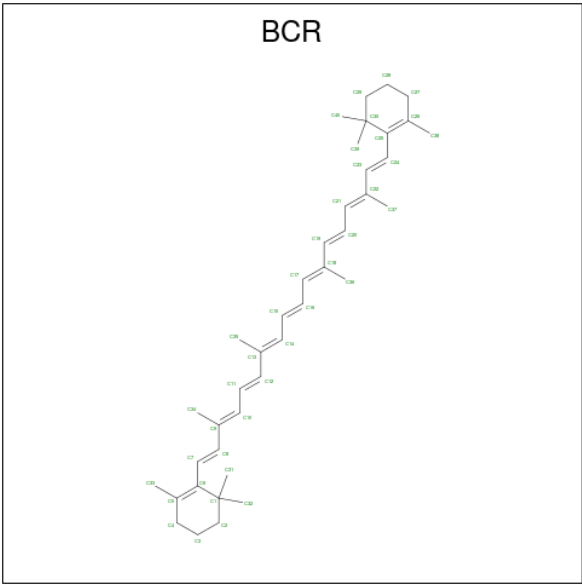
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			33	31	2	
19	B	1	Total	C	O	0
			33	31	2	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	A	1	Total	C	O	P	0
			31	20	10	1	
20	B	1	Total	C	O	P	0
			39	28	10	1	
20	B	1	Total	C	O	P	0
			49	38	10	1	
20	1	1	Total	C	O	P	0
			49	38	10	1	
20	2	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



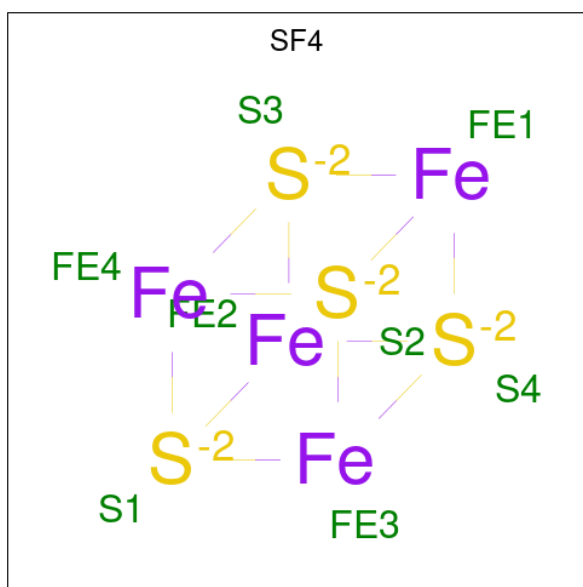
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	

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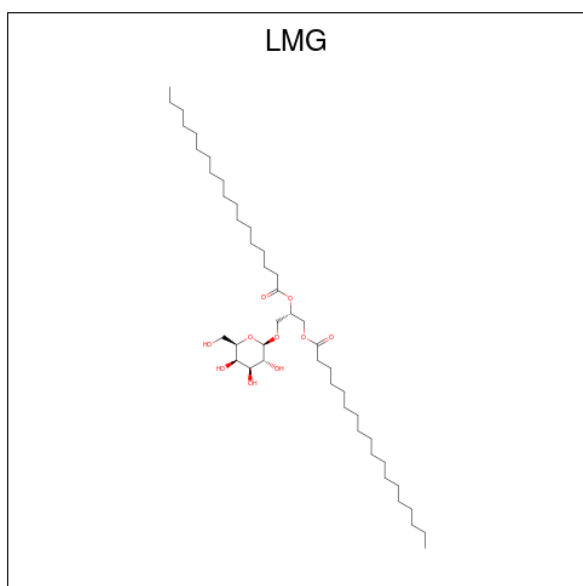
Mol	Chain	Residues	Atoms	AltConf
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	I	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	4	1	Total C 40 40	0

- Molecule 22 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



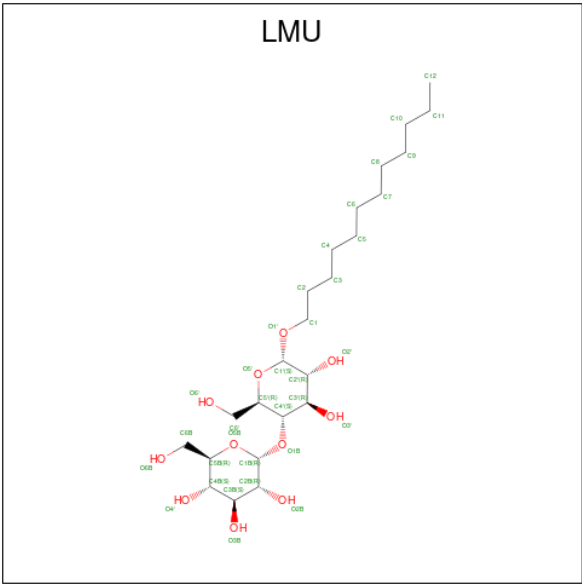
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			43	33	10	
23	F	1	Total	C	O	0
			30	20	10	
23	4	1	Total	C	O	0
			46	36	10	
23	4	1	Total	C	O	0
			45	35	10	

- Molecule 24 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



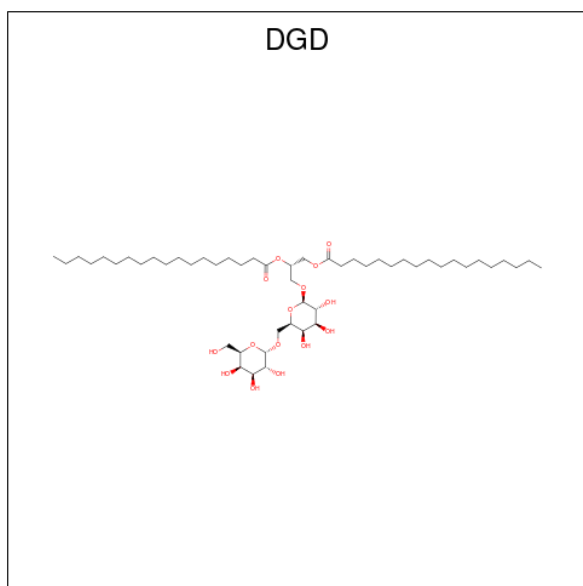
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			24	18	6	
24	A	1	Total	C	O	0
			35	24	11	
24	B	1	Total	C	O	0
			24	18	6	
24	H	1	Total	C	O	0
			24	18	6	
24	L	1	Total	C	O	0
			20	14	6	
24	F	1	Total	C	O	0
			35	24	11	
24	F	1	Total	C	O	0
			35	24	11	

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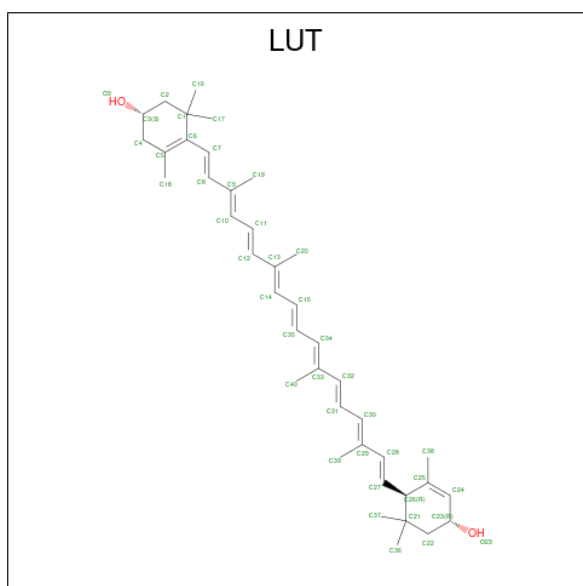
Mol	Chain	Residues	Atoms			AltConf
24	F	1	Total	C	O	0
			35	24	11	
24	F	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			35	24	11	
24	1	1	Total	C	O	0
			35	24	11	
24	1	1	Total	C	O	0
			35	24	11	
24	1	1	Total	C	O	0
			24	18	6	
24	2	1	Total	C	O	0
			35	24	11	
24	4	1	Total	C	O	0
			23	17	6	
24	4	1	Total	C	O	0
			35	24	11	
24	4	1	Total	C	O	0
			24	18	6	

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



Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			61	46	15	
25	J	1	Total	C	O	0
			58	43	15	
25	4	1	Total	C	O	0
			49	34	15	

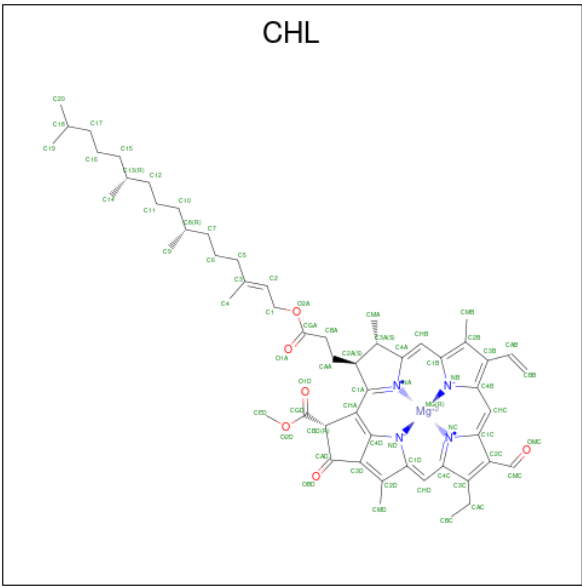
- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	J	1	Total	C	O	0
			42	40	2	
26	1	1	Total	C	O	0
			42	40	2	
26	1	1	Total	C	O	0
			42	40	2	
26	2	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	4	1	Total	C	O	0
			42	40	2	

- Molecule 27 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as

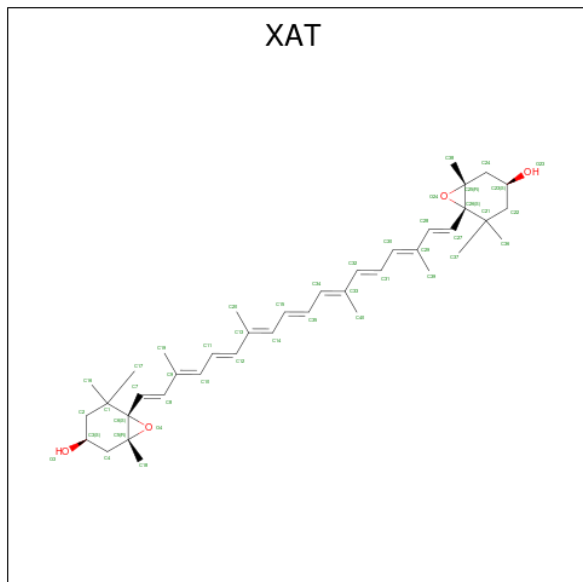
"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
27	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
27	2	1	Total 51	C 40	Mg 1	N 4	O 6	0
27	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
27	2	1	Total 51	C 40	Mg 1	N 4	O 6	0
27	2	1	Total 47	C 36	Mg 1	N 4	O 6	0
27	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
27	3	1	Total 51	C 40	Mg 1	N 4	O 6	0
27	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
27	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
27	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
27	4	1	Total 46	C 35	Mg 1	N 4	O 6	0

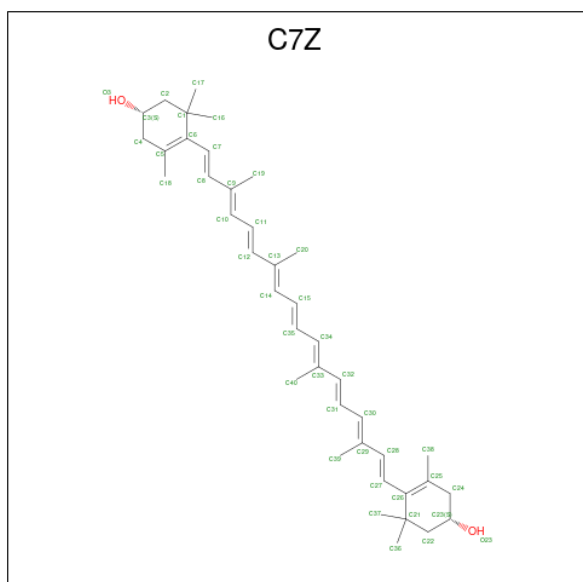
- Molecule 28 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA

,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



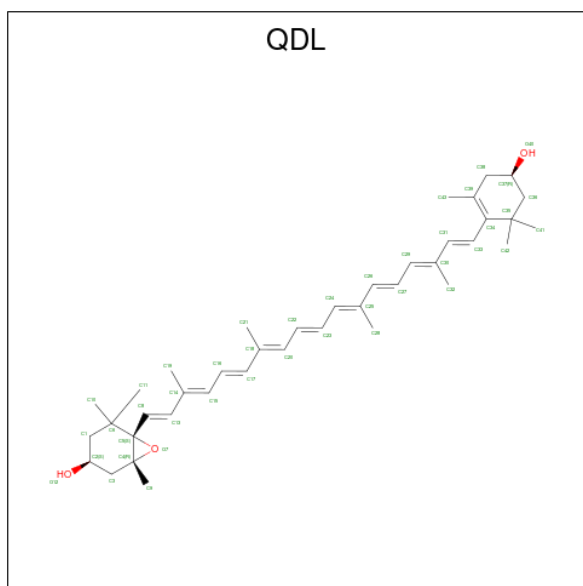
Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			44	40	4	
28	2	1	Total	C	O	0
			44	40	4	

- Molecule 29 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: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			42	40	2	

- Molecule 30 is Anthraxanthin (CCD ID: QDL) (formula: $C_{40}H_{56}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	4	1	Total	C	O	0
			43	40	3	

- Molecule 31 is water.

Mol	Chain	Residues	Atoms		AltConf
31	A	199	Total	O	0
			199	199	
31	B	267	Total	O	0
			267	267	
31	C	75	Total	O	0
			75	75	
31	D	58	Total	O	0
			58	58	
31	E	22	Total	O	0
			22	22	
31	H	7	Total	O	0
			7	7	
31	I	5	Total	O	0
			5	5	

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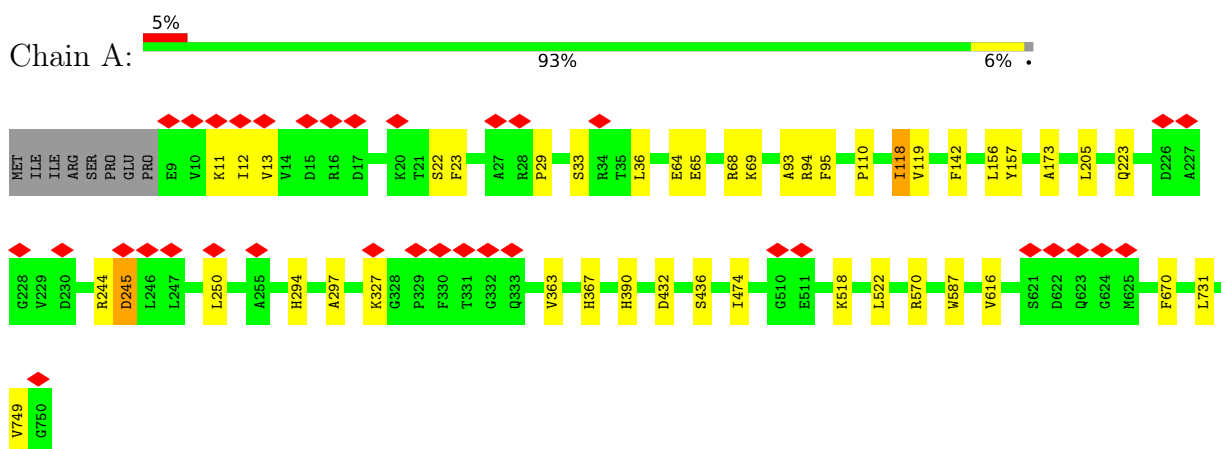
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Mol	Chain	Residues	Atoms		AltConf
31	L	12	Total 12	O 12	0
31	F	32	Total 32	O 32	0
31	G	2	Total 2	O 2	0
31	J	8	Total 8	O 8	0
31	K	2	Total 2	O 2	0
31	1	4	Total 4	O 4	0
31	2	4	Total 4	O 4	0
31	3	2	Total 2	O 2	0
31	4	4	Total 4	O 4	0

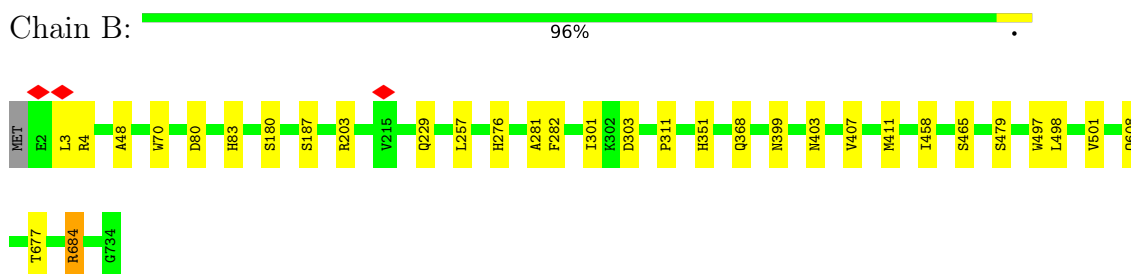
3 Residue-property plots [i](#)

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

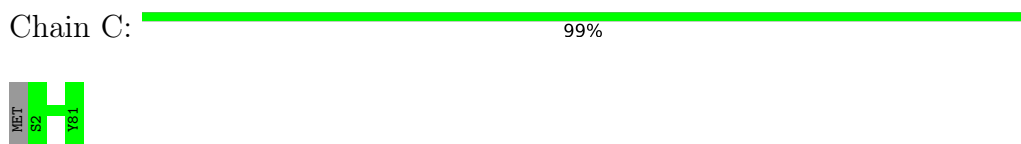
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

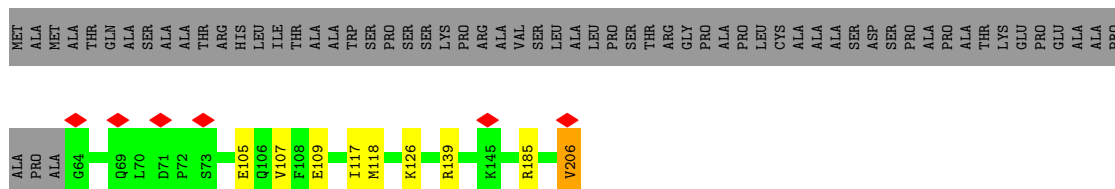


- Molecule 3: Photosystem I iron-sulfur center

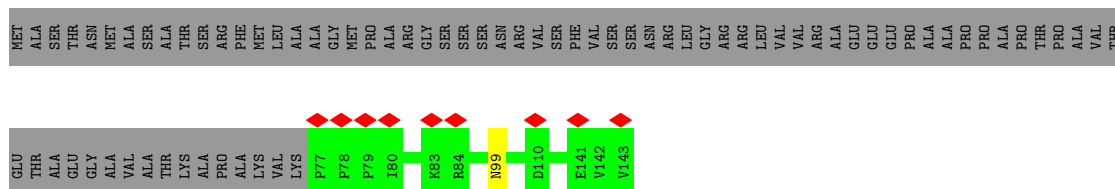


- Molecule 4: Photosystem I reaction center subunit II





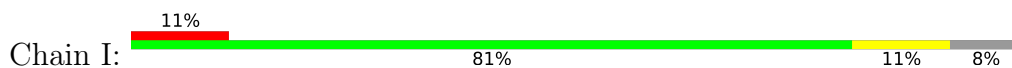
• Molecule 5: Photosystem I reaction center subunit IV



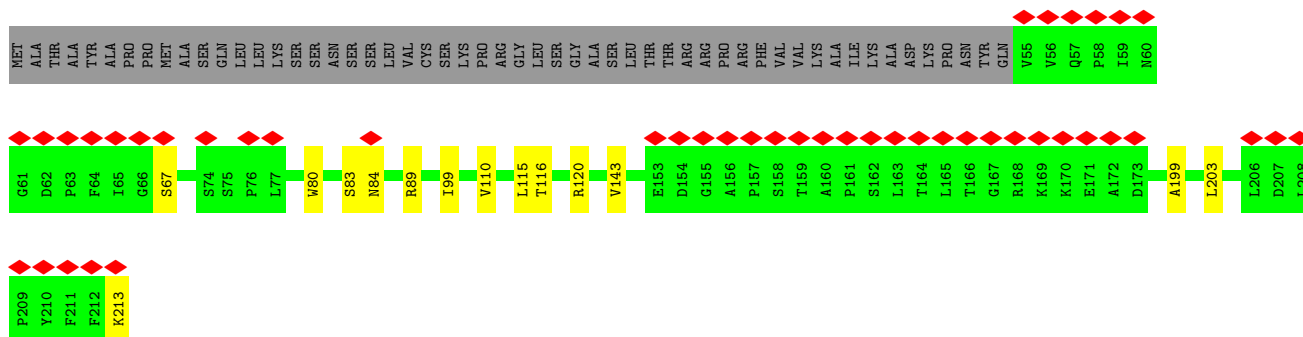
• Molecule 6: Photosystem I reaction center subunit VI



• Molecule 7: Photosystem I reaction center subunit VIII

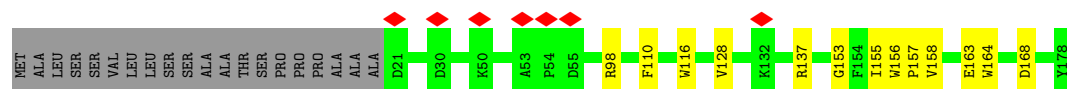


• Molecule 8: Photosystem I reaction center subunit XI



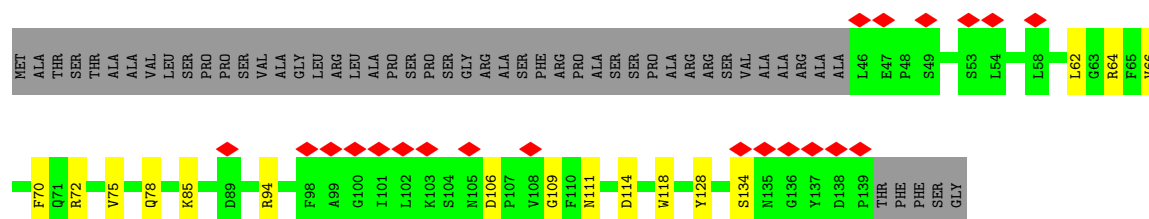
• Molecule 9: Photosystem I reaction center subunit III

Chain F: 



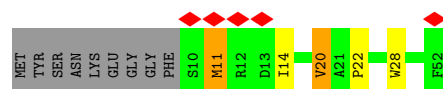
• Molecule 10: Photosystem I reaction center subunit V

Chain G: 

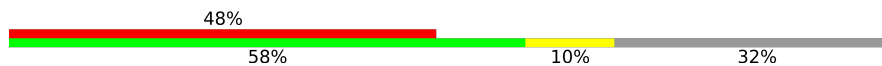


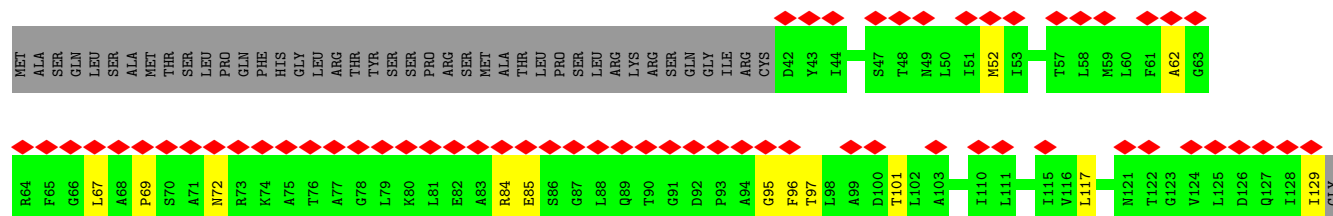
• Molecule 11: Photosystem I reaction center subunit IX

Chain J: 



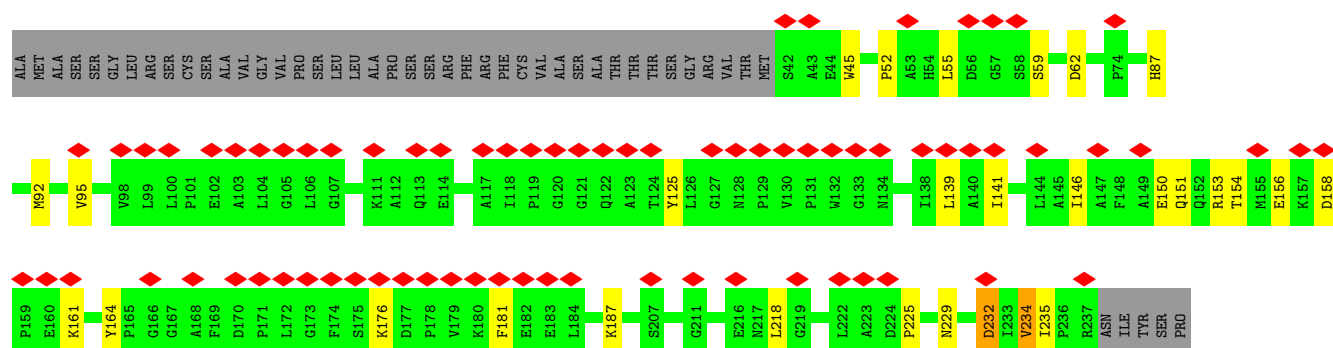
• Molecule 12: Photosystem I reaction center subunit X

Chain K: 

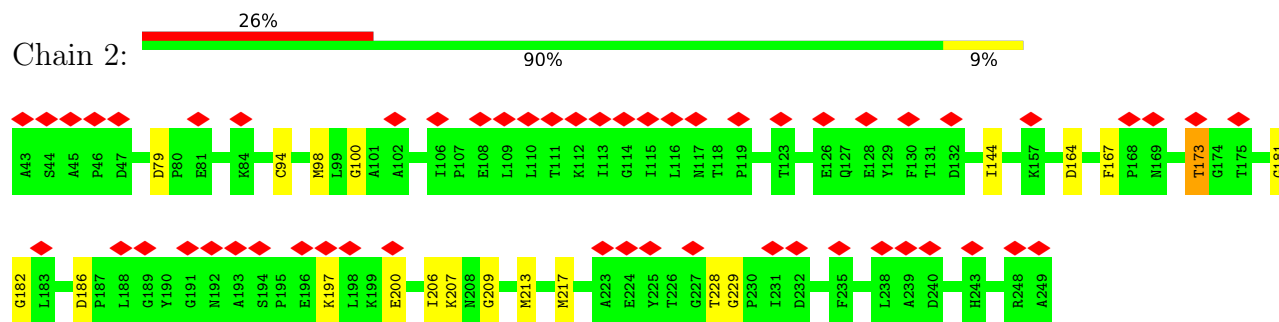


• Molecule 13: Chlorophyll a-b binding protein 1, chloroplastic

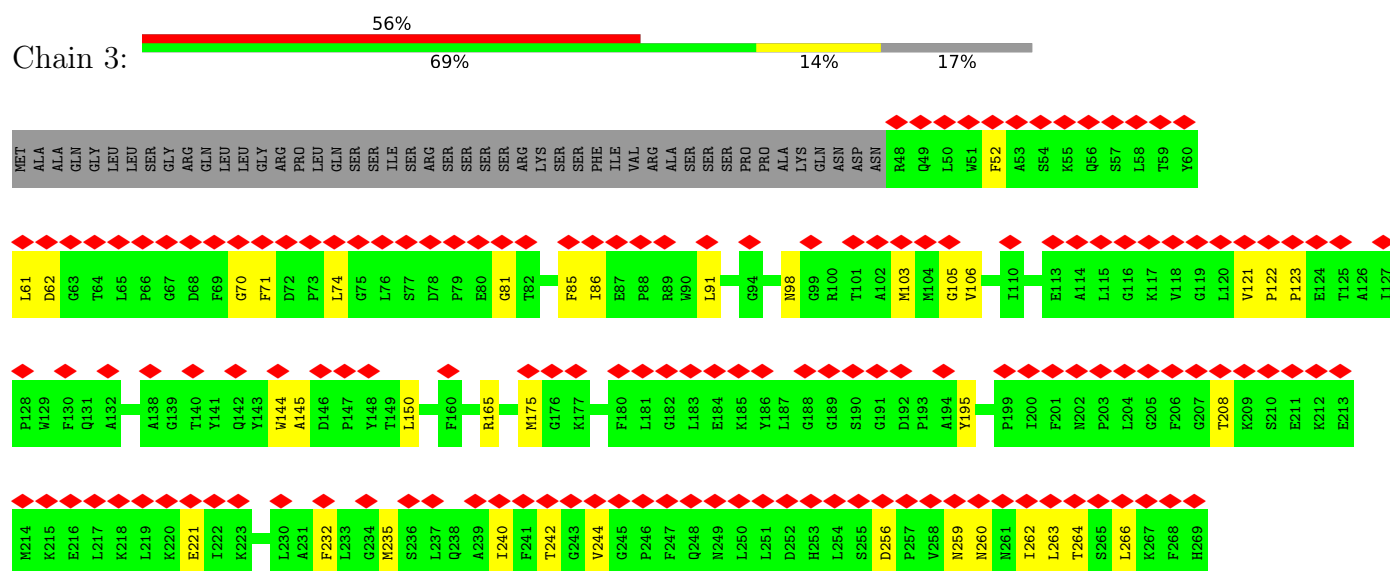
Chain 1: 



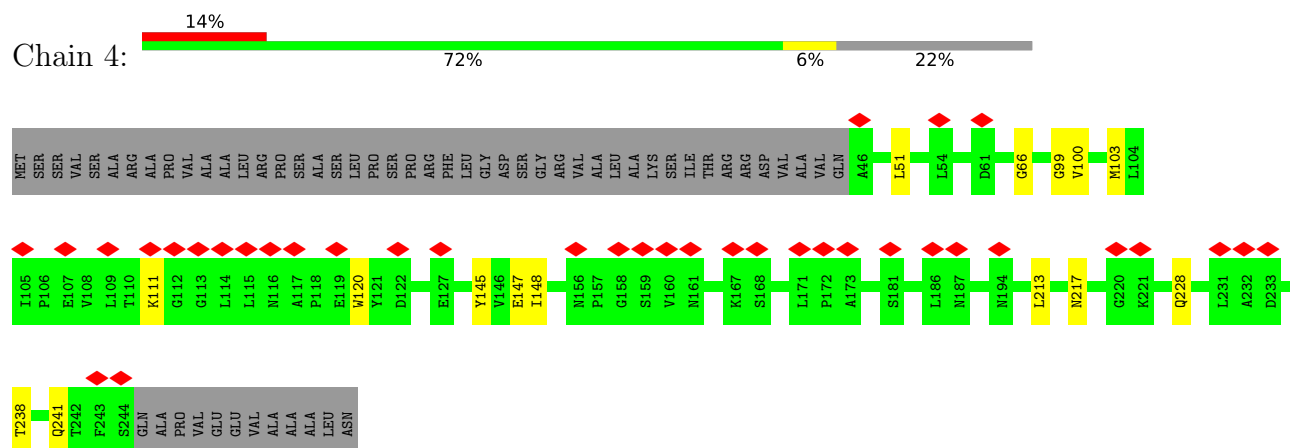
- Molecule 14: Chlorophyll a-b binding protein 2, chloroplastic



- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic



- Molecule 16: Chlorophyll a-b binding protein 4, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96997	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.346	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.434	Depositor
Minimum map value	-0.157	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	425.0, 425.0, 425.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.85, 0.85, 0.85	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, C7Z, QDL, LUT, BCR, CHL, CLA, LMU, CL0, DGD, LHG, SF4, LMG, PQN

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	0.20	0/6038	0.36	0/8237
2	B	0.20	0/6075	0.36	0/8297
3	C	0.16	0/616	0.41	0/834
4	D	0.14	0/1153	0.35	0/1557
5	E	0.11	0/546	0.29	0/743
6	H	0.12	0/737	0.31	0/1002
7	I	0.14	0/264	0.33	0/359
8	L	0.13	0/1227	0.32	0/1678
9	F	0.16	0/1269	0.30	0/1716
10	G	0.12	0/738	0.31	0/1004
11	J	0.14	0/352	0.35	0/479
12	K	0.10	0/633	0.24	0/855
13	1	0.14	0/1569	0.32	0/2137
14	2	0.12	0/1666	0.27	0/2282
15	3	0.13	0/1780	0.33	0/2414
16	4	0.16	0/1604	0.34	0/2187
All	All	0.17	0/26267	0.34	0/35781

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5840	0	5691	37	0
2	B	5864	0	5642	25	0
3	C	605	0	587	0	0
4	D	1124	0	1128	5	0
5	E	533	0	538	0	0
6	H	715	0	715	5	0
7	I	258	0	285	3	0
8	L	1192	0	1196	11	0
9	F	1238	0	1257	8	0
10	G	721	0	713	13	0
11	J	342	0	351	3	0
12	K	628	0	653	6	0
13	1	1519	0	1485	24	0
14	2	1609	0	1554	11	0
15	3	1725	0	1689	28	0
16	4	1555	0	1502	12	0
17	A	65	0	72	0	0
17	H	55	0	49	2	0
18	1	630	0	561	24	0
18	2	565	0	544	6	0
18	3	511	0	432	16	0
18	4	598	0	546	11	0
18	A	2670	0	2645	46	0
18	B	2297	0	2368	30	0
18	F	180	0	183	6	0
18	G	148	0	119	6	0
18	J	45	0	33	0	0
18	K	150	0	125	0	0
18	L	150	0	125	3	0
19	A	33	0	46	0	0
19	B	33	0	46	0	0
20	1	49	0	74	5	0
20	2	43	0	56	2	0
20	A	80	0	106	4	0
20	B	88	0	125	2	0
21	3	40	0	56	4	0
21	4	40	0	56	3	0
21	A	200	0	280	11	0
21	B	200	0	280	4	0
21	F	80	0	111	2	0
21	G	80	0	112	4	0
21	I	40	0	56	0	0
21	J	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	K	80	0	112	2	0
21	L	120	0	168	3	0
22	A	8	0	0	0	0
22	C	16	0	0	0	0
23	4	91	0	128	5	0
23	A	43	0	59	3	0
23	F	30	0	30	2	0
24	1	94	0	127	4	0
24	2	35	0	46	1	0
24	4	82	0	111	2	0
24	A	59	0	81	1	0
24	B	24	0	35	1	0
24	F	140	0	184	6	0
24	G	70	0	92	4	0
24	H	24	0	35	1	0
24	L	20	0	24	2	0
25	4	49	0	56	1	0
25	B	61	0	83	0	0
25	J	58	0	77	3	0
26	1	84	0	112	5	0
26	2	42	0	56	1	0
26	3	84	0	112	4	0
26	4	42	0	56	4	0
26	J	42	0	56	3	0
27	1	112	0	101	5	0
27	2	195	0	136	1	0
27	3	117	0	107	5	0
27	4	209	0	169	2	0
28	1	44	0	56	2	0
28	2	44	0	56	1	0
29	1	42	0	0	0	0
30	4	43	0	0	0	0
31	1	4	0	0	0	0
31	2	4	0	0	0	0
31	3	2	0	0	0	0
31	4	4	0	0	0	0
31	A	199	0	0	2	0
31	B	267	0	0	3	0
31	C	75	0	0	0	0
31	D	58	0	0	0	0
31	E	22	0	0	0	0
31	F	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	G	2	0	0	1	0
31	H	7	0	0	0	0
31	I	5	0	0	0	0
31	J	8	0	0	0	0
31	K	2	0	0	0	0
31	L	12	0	0	0	0
All	All	37485	0	36713	311	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 4.

All (311) 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)
18:4:609:CLA:HAB	26:4:616:LUT:H12	1.60	0.81
13:1:146:ILE:HG22	18:1:309:CLA:HAB	1.66	0.77
13:1:95:VAL:HG11	26:1:316:LUT:H32	1.65	0.76
13:1:87:HIS:HD2	28:1:317:XAT:H35	1.49	0.75
18:A:823:CLA:HAB	18:A:845:CLA:HBB1	1.72	0.72
9:F:163:GLU:HG3	9:F:168:ASP:HB2	1.71	0.72
15:3:260:ASN:HB2	18:3:311:CLA:HED1	1.72	0.72
18:1:310:CLA:HAB	26:1:316:LUT:H12	1.74	0.68
18:B:810:CLA:HAB	24:G:203:LMU:H101	1.75	0.67
13:1:218:LEU:HD12	26:1:316:LUT:H222	1.78	0.65
13:1:153:ARG:NH2	18:1:309:CLA:O1D	2.29	0.65
18:G:205:CLA:HMA3	21:G:206:BCR:H312	1.79	0.63
2:B:203:ARG:NH1	31:B:905:HOH:O	2.29	0.63
9:F:110:PHE:CE1	18:F:802:CLA:NB	2.67	0.63
18:A:816:CLA:H42	15:3:240:ILE:HG23	1.80	0.62
18:A:822:CLA:HAA2	18:A:826:CLA:HAB	1.82	0.62
4:D:109:GLU:O	4:D:139:ARG:NH2	2.31	0.62
18:2:601:CLA:HBC3	20:2:617:LHG:HC42	1.80	0.62
13:1:234:VAL:HG12	13:1:235:ILE:HG13	1.82	0.61
18:B:820:CLA:O1A	24:1:301:LMU:O2'	2.18	0.61
15:3:98:ASN:ND2	18:3:307:CLA:OBD	2.34	0.61
1:A:245:ASP:OD1	1:A:245:ASP:N	2.32	0.61
1:A:244:ARG:HH22	15:3:266:LEU:HD21	1.67	0.60
6:H:72:SER:HB2	8:L:83:SER:HB2	1.84	0.60
15:3:165:ARG:HH12	18:3:307:CLA:HED1	1.66	0.59
15:3:259:ASN:HA	15:3:263:LEU:HD12	1.84	0.59
13:1:150:GLU:OE1	18:1:309:CLA:C4B	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:313:CLA:HBA1	18:1:313:CLA:HBD	1.85	0.59
1:A:13:VAL:HA	15:3:81:GLY:HA3	1.84	0.59
10:G:64:ARG:NH2	10:G:106:ASP:OD1	2.37	0.58
13:1:181:PHE:HZ	18:1:310:CLA:HED3	1.69	0.58
18:B:817:CLA:HAA2	18:B:822:CLA:HAB	1.85	0.57
12:K:84:ARG:HG2	12:K:85:GLU:H	1.69	0.57
2:B:301:ILE:HG21	18:B:822:CLA:HAC1	1.85	0.57
1:A:65:GLU:HG3	1:A:69:LYS:HE2	1.86	0.57
8:L:203:LEU:HD22	8:L:213:LYS:HG3	1.85	0.57
6:H:123:LEU:HD11	24:H:201:LMU:H101	1.87	0.57
1:A:436:SER:HB3	2:B:677:THR:HG22	1.86	0.56
18:A:841:CLA:HAB	18:A:841:CLA:H102	1.88	0.56
21:A:851:BCR:H321	21:A:851:BCR:HC8	1.86	0.56
18:4:609:CLA:HBA1	26:4:616:LUT:H182	1.86	0.56
1:A:33:SER:HB3	1:A:36:LEU:HB2	1.87	0.56
1:A:118:ILE:HG21	26:J:101:LUT:H382	1.86	0.56
18:A:856:CLA:HMA1	23:A:857:LMG:H121	1.88	0.56
1:A:670:PHE:HZ	18:A:829:CLA:H121	1.71	0.56
15:3:61:LEU:HD13	15:3:70:GLY:HA2	1.88	0.55
15:3:195:TYR:HB3	18:3:308:CLA:HED2	1.87	0.55
2:B:180:SER:HB3	18:B:818:CLA:HAC2	1.89	0.55
27:1:302:CHL:HAB	20:1:319:LHG:H131	1.89	0.54
2:B:229:GLN:OE1	10:G:134:SER:OG	2.19	0.54
14:2:100:GLY:HA2	28:2:616:XAT:H181	1.89	0.54
15:3:105:GLY:HA2	26:3:315:LUT:H381	1.89	0.54
1:A:12:ILE:HG21	18:A:811:CLA:HAA2	1.90	0.54
16:4:51:LEU:HD13	18:4:601:CLA:HMA3	1.90	0.54
1:A:22:SER:HA	23:A:857:LMG:HC71	1.90	0.54
12:K:72:ASN:ND2	12:K:95:GLY:O	2.41	0.54
13:1:52:PRO:HG2	13:1:55:LEU:HD12	1.89	0.54
15:3:103:MET:HE1	18:3:308:CLA:HAB	1.90	0.54
18:A:829:CLA:H203	21:J:103:BCR:H12C	1.89	0.53
1:A:29:PRO:HB3	18:A:804:CLA:HAC1	1.89	0.53
18:B:807:CLA:H72	18:B:807:CLA:HBB1	1.89	0.53
18:B:807:CLA:H2	18:B:807:CLA:H71	1.89	0.53
1:A:731:LEU:HD12	20:A:846:LHG:H171	1.90	0.53
2:B:311:PRO:HG2	20:B:846:LHG:HC2	1.89	0.53
13:1:232:ASP:OD1	13:1:232:ASP:N	2.40	0.53
1:A:64:GLU:OE2	1:A:68:ARG:NH2	2.41	0.53
17:H:202:CL0:H15	18:L:303:CLA:HED1	1.90	0.53
1:A:587:TRP:HE1	20:A:846:LHG:HC91	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:309:CLA:H171	18:1:309:CLA:H121	1.91	0.52
18:A:855:CLA:H122	23:F:810:LMG:H152	1.91	0.52
18:A:815:CLA:CHD	18:A:817:CLA:HBB1	2.40	0.52
24:4:623:LMU:H51	24:4:624:LMU:H52	1.91	0.51
4:D:105:GLU:HA	4:D:118:MET:O	2.10	0.51
13:1:45:TRP:HH2	24:1:321:LMU:H42	1.76	0.51
16:4:99:GLY:O	16:4:103:MET:HB2	2.10	0.51
1:A:205:LEU:HD22	21:A:848:BCR:H361	1.93	0.51
2:B:465:SER:O	2:B:479:SER:HB2	2.10	0.51
13:1:125:TYR:OH	26:1:318:LUT:O23	2.28	0.51
16:4:103:MET:HE3	16:4:120:TRP:CE2	2.46	0.51
1:A:518:LYS:NZ	31:A:911:HOH:O	2.41	0.51
18:B:804:CLA:H8	18:B:822:CLA:HBA1	1.92	0.51
18:B:824:CLA:H122	21:B:844:BCR:H20C	1.92	0.51
13:1:187:LYS:HE2	18:1:312:CLA:HBA2	1.92	0.51
1:A:432:ASP:OD1	31:A:901:HOH:O	2.19	0.51
15:3:256:ASP:OD1	15:3:256:ASP:N	2.42	0.51
10:G:94:ARG:NH1	31:G:301:HOH:O	2.39	0.51
10:G:128:TYR:HB2	18:G:201:CLA:H72	1.93	0.51
2:B:187:SER:HB3	2:B:281:ALA:HB2	1.93	0.51
13:1:59:SER:HB2	13:1:62:ASP:HB2	1.94	0.50
18:B:820:CLA:HAA1	24:1:301:LMU:H3'	1.92	0.50
2:B:351:HIS:CE1	18:B:824:CLA:NB	2.79	0.50
18:A:843:CLA:H61	18:A:843:CLA:H112	1.93	0.50
18:B:815:CLA:H61	18:B:815:CLA:H111	1.94	0.49
18:A:817:CLA:HBC2	18:3:305:CLA:HBB2	1.93	0.49
18:1:311:CLA:NC	20:1:319:LHG:HC42	2.26	0.49
16:4:213:LEU:O	16:4:217:ASN:ND2	2.44	0.49
18:A:806:CLA:H151	21:A:848:BCR:H323	1.94	0.49
18:B:820:CLA:H11	24:G:207:LMU:H1'	1.95	0.49
20:1:319:LHG:H191	18:4:614:CLA:HBA1	1.95	0.49
18:3:303:CLA:HBB1	21:3:313:BCR:H383	1.93	0.49
18:3:308:CLA:H2	26:3:314:LUT:H173	1.94	0.49
2:B:80:ASP:OD2	2:B:83:HIS:HB2	2.13	0.49
18:B:833:CLA:HMB1	18:B:833:CLA:HBB1	1.94	0.49
14:2:207:LYS:NZ	18:2:610:CLA:O1D	2.38	0.49
16:4:238:THR:OG1	16:4:241:GLN:OE1	2.26	0.49
21:A:852:BCR:H362	18:A:854:CLA:H2	1.94	0.49
1:A:367:HIS:CE1	18:A:828:CLA:NB	2.81	0.48
18:A:819:CLA:HBC3	18:A:819:CLA:H101	1.94	0.48
2:B:276:HIS:HE1	18:B:815:CLA:ND	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:92:MET:HE2	26:1:316:LUT:H14	1.95	0.48
4:D:185:ARG:NH2	4:D:206:VAL:OXT	2.46	0.48
13:1:154:THR:HG21	18:1:309:CLA:HMA1	1.95	0.48
15:3:85:PHE:HB2	18:3:302:CLA:H43	1.96	0.48
18:A:855:CLA:H142	23:F:810:LMG:H161	1.95	0.48
18:1:308:CLA:HBD	18:1:308:CLA:HBA1	1.95	0.48
18:F:804:CLA:H112	18:F:804:CLA:H62	1.95	0.48
2:B:368:GLN:NE2	31:B:909:HOH:O	2.34	0.48
16:4:103:MET:HE3	16:4:120:TRP:CD2	2.48	0.48
2:B:70:TRP:CD1	24:B:848:LMU:H12	2.48	0.48
9:F:156:TRP:CG	9:F:157:PRO:HD3	2.49	0.47
18:4:602:CLA:HBC1	23:4:619:LMG:H301	1.96	0.47
16:4:111:LYS:NZ	16:4:228:GLN:OE1	2.28	0.47
21:L:306:BCR:H23C	21:L:306:BCR:H392	1.96	0.47
10:G:128:TYR:HD1	18:G:201:CLA:H51	1.80	0.47
15:3:62:ASP:N	15:3:62:ASP:OD1	2.47	0.47
8:L:80:TRP:O	8:L:84:ASN:ND2	2.47	0.47
2:B:311:PRO:HG3	18:B:839:CLA:HBC2	1.95	0.47
14:2:79:ASP:OD1	14:2:79:ASP:N	2.42	0.47
7:I:6:LEU:HD22	7:I:10:PHE:HE2	1.79	0.47
18:1:312:CLA:HBA2	18:1:312:CLA:HBD	1.97	0.47
18:3:304:CLA:HAA2	18:3:304:CLA:HBD	1.97	0.47
18:1:310:CLA:HBA2	18:1:310:CLA:H3A	1.61	0.46
20:A:847:LHG:H281	21:A:850:BCR:H20C	1.96	0.46
18:2:609:CLA:CBB	26:2:615:LUT:H32	2.44	0.46
1:A:173:ALA:HB2	18:A:811:CLA:HBC2	1.97	0.46
18:A:825:CLA:H61	18:A:825:CLA:H41	1.81	0.46
10:G:72:ARG:NH2	10:G:109:GLY:O	2.47	0.46
16:4:147:GLU:HG3	18:4:608:CLA:C4B	2.46	0.46
18:A:815:CLA:H2	18:A:817:CLA:HMB1	1.97	0.46
18:A:818:CLA:H62	12:K:117:LEU:HD12	1.97	0.46
18:A:812:CLA:H41	18:A:812:CLA:H62	1.48	0.46
18:A:818:CLA:HBA1	18:A:818:CLA:HBD	1.97	0.46
18:A:820:CLA:H171	18:A:836:CLA:H41	1.97	0.46
13:1:234:VAL:HG13	18:1:315:CLA:C4B	2.46	0.46
1:A:23:PHE:CD2	23:A:857:LMG:HC72	2.50	0.46
1:A:363:VAL:HG11	18:A:820:CLA:H201	1.98	0.46
1:A:570:ARG:CZ	20:A:846:LHG:HC41	2.46	0.46
12:K:96:PHE:CE2	12:K:101:THR:HG22	2.51	0.46
18:4:609:CLA:H51	18:4:611:CLA:HBA1	1.97	0.46
18:A:827:CLA:H62	18:A:827:CLA:H41	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:84:ASN:HB3	18:L:303:CLA:HAC1	1.98	0.45
18:F:804:CLA:H141	23:4:620:LMG:H322	1.97	0.45
18:G:201:CLA:H62	18:G:201:CLA:H41	1.67	0.45
1:A:223:GLN:HG2	1:A:250:LEU:HD13	1.96	0.45
9:F:156:TRP:CD1	9:F:157:PRO:HD3	2.51	0.45
10:G:111:ASN:HA	18:G:205:CLA:HBA2	1.97	0.45
27:1:302:CHL:C1C	20:1:319:LHG:H242	2.47	0.45
1:A:94:ARG:HG2	1:A:157:TYR:OH	2.16	0.45
14:2:98:MET:HG3	14:2:209:GLY:HA2	1.98	0.45
18:A:855:CLA:H143	11:J:28:TRP:HZ3	1.81	0.45
2:B:3:LEU:HD12	7:I:34:LYS:HE2	1.99	0.45
9:F:158:VAL:HA	18:4:603:CLA:H51	1.98	0.45
13:1:176:LYS:HD3	13:1:176:LYS:H	1.80	0.45
27:1:302:CHL:H11	16:4:145:TYR:HB2	1.99	0.45
18:1:306:CLA:HAB	27:1:307:CHL:OMC	2.17	0.45
18:4:612:CLA:C3B	26:4:616:LUT:H383	2.47	0.45
2:B:498:LEU:HA	2:B:501:VAL:HG22	1.99	0.45
10:G:70:PHE:CG	24:G:207:LMU:H6D	2.51	0.45
17:H:202:CL0:H40	17:H:202:CL0:H35	1.71	0.45
15:3:144:TRP:CE3	15:3:145:ALA:HB2	2.52	0.45
4:D:107:VAL:HG22	4:D:117:ILE:HG12	1.99	0.45
6:H:101:LYS:HA	6:H:101:LYS:HD3	1.84	0.45
13:1:158:ASP:HB3	13:1:161:LYS:HB2	2.00	0.45
18:2:610:CLA:C1B	20:2:617:LHG:HC31	2.47	0.45
18:B:824:CLA:HMB1	18:B:824:CLA:HBB1	1.99	0.44
15:3:232:PHE:CD2	26:3:315:LUT:H34	2.53	0.44
1:A:522:LEU:HD21	1:A:616:VAL:HA	1.99	0.44
18:A:822:CLA:HBB1	18:A:822:CLA:HMB3	1.99	0.44
21:A:849:BCR:H24C	21:A:849:BCR:H371	1.84	0.44
18:1:313:CLA:C4B	18:1:313:CLA:H93	2.48	0.44
18:2:601:CLA:HBC2	21:3:313:BCR:HC31	2.00	0.44
15:3:260:ASN:ND2	15:3:262:ILE:H	2.16	0.44
21:4:618:BCR:H281	25:4:622:DGD:HB31	1.99	0.44
1:A:297:ALA:HB1	18:A:818:CLA:HBC2	1.99	0.44
10:G:62:LEU:HD23	10:G:66:VAL:HG21	1.99	0.44
15:3:232:PHE:CG	26:3:315:LUT:H32	2.52	0.44
18:4:608:CLA:H92	18:4:608:CLA:H61	1.86	0.44
2:B:48:ALA:HB1	20:B:847:LHG:H272	2.00	0.44
18:B:810:CLA:CAD	24:G:203:LMU:H22	2.47	0.44
18:A:843:CLA:H62	18:A:843:CLA:H41	1.85	0.44
24:F:809:LMU:H21	24:F:809:LMU:H1'	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:829:CLA:H62	18:B:829:CLA:H2	1.81	0.44
16:4:66:GLY:HA2	23:4:619:LMG:HC61	1.99	0.44
18:4:609:CLA:H61	18:4:609:CLA:H41	1.66	0.44
9:F:164:TRP:CH2	24:F:809:LMU:H42	2.53	0.44
1:A:118:ILE:CG2	26:J:101:LUT:H382	2.47	0.43
25:J:104:DGD:O5E	25:J:104:DGD:O4E	2.34	0.43
14:2:164:ASP:HB3	14:2:167:PHE:O	2.18	0.43
15:3:242:THR:HG22	15:3:244:VAL:HG23	2.00	0.43
18:A:824:CLA:HAA1	12:K:69:PRO:HG3	1.99	0.43
2:B:4:ARG:NH1	31:B:922:HOH:O	2.48	0.43
2:B:257:LEU:HD13	18:B:815:CLA:HMB3	2.00	0.43
12:K:62:ALA:HA	12:K:67:LEU:HB2	2.00	0.43
8:L:110:VAL:HG21	8:L:199:ALA:HB3	2.00	0.43
10:G:85:LYS:HE3	10:G:85:LYS:HB2	1.84	0.43
11:J:11:MET:HA	11:J:14:ILE:HG22	1.99	0.43
15:3:91:LEU:HD13	27:3:301:CHL:H12	2.01	0.43
1:A:110:PRO:HB3	1:A:142:PHE:CD2	2.53	0.43
18:B:830:CLA:H161	25:J:104:DGD:HB91	1.99	0.43
9:F:98:ARG:NH2	24:F:807:LMU:O4'	2.43	0.43
24:F:807:LMU:H1'	24:F:807:LMU:H21	1.67	0.43
14:2:173:THR:N	14:2:181:GLY:O	2.50	0.43
27:2:606:CHL:HAB	24:2:618:LMU:H112	2.00	0.43
18:A:823:CLA:H61	18:A:823:CLA:H41	1.78	0.43
2:B:399:ASN:O	2:B:403:ASN:ND2	2.45	0.43
18:1:303:CLA:HBC1	20:1:319:LHG:H132	2.00	0.43
27:4:605:CHL:HBB2	27:4:606:CHL:CBB	2.49	0.43
8:L:84:ASN:O	8:L:89:ARG:NH2	2.52	0.43
18:F:804:CLA:H171	23:4:620:LMG:H362	2.00	0.43
1:A:390:HIS:HE1	18:A:829:CLA:ND	2.15	0.43
8:L:120:ARG:NE	24:L:301:LMU:O2'	2.52	0.43
15:3:71:PHE:N	27:3:301:CHL:OBD	2.51	0.43
15:3:221:GLU:HB2	18:3:308:CLA:C1B	2.49	0.43
21:A:849:BCR:H20C	21:A:849:BCR:H361	1.88	0.43
6:H:86:PHE:CD1	8:L:99:ILE:HD13	2.54	0.43
1:A:11:LYS:HD2	1:A:11:LYS:HA	1.78	0.43
18:A:843:CLA:H52	18:B:836:CLA:H43	2.01	0.43
18:A:855:CLA:H61	18:A:855:CLA:H41	1.86	0.43
21:K:202:BCR:H20C	21:K:202:BCR:H361	1.87	0.43
27:3:301:CHL:H61	27:3:301:CHL:H41	1.73	0.43
18:A:838:CLA:H2	18:A:839:CLA:O1A	2.19	0.42
18:B:820:CLA:HAB	21:B:844:BCR:H321	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:20:VAL:HG13	11:J:22:PRO:HD2	2.00	0.42
13:1:225:PRO:O	13:1:229:ASN:ND2	2.46	0.42
18:A:819:CLA:HBA2	18:A:819:CLA:H3A	1.79	0.42
2:B:282:PHE:CZ	18:G:201:CLA:H91	2.54	0.42
13:1:164:TYR:HB3	18:1:310:CLA:HED2	2.01	0.42
8:L:116:THR:HG22	24:L:301:LMU:H11	2.01	0.42
13:1:181:PHE:CZ	18:1:310:CLA:HED3	2.53	0.42
27:4:606:CHL:HMD2	24:4:623:LMU:H22	2.01	0.42
18:A:829:CLA:HBB1	18:A:829:CLA:HMB3	2.00	0.42
18:A:805:CLA:H42	18:A:812:CLA:HMC2	2.00	0.42
2:B:407:VAL:O	2:B:411:MET:HG2	2.19	0.42
13:1:150:GLU:OE1	18:1:309:CLA:C1B	2.43	0.42
18:1:303:CLA:CBB	28:1:317:XAT:H12	2.49	0.42
27:3:301:CHL:H91	18:3:302:CLA:HMB3	2.02	0.42
16:4:100:VAL:HG11	26:4:616:LUT:H32	2.02	0.42
18:A:813:CLA:O1A	15:3:74:LEU:HB3	2.19	0.42
18:B:817:CLA:HMB3	18:B:822:CLA:H61	2.00	0.42
21:L:306:BCR:H20C	21:L:306:BCR:H361	1.92	0.42
10:G:114:ASP:OD1	10:G:118:TRP:HD1	2.03	0.42
16:4:145:TYR:O	16:4:148:ILE:HG13	2.20	0.42
21:B:843:BCR:H24C	21:B:843:BCR:H371	1.86	0.42
21:G:202:BCR:H20C	21:G:202:BCR:H361	1.89	0.42
18:3:304:CLA:HAA1	21:3:313:BCR:H392	2.01	0.42
18:B:829:CLA:NA	21:F:806:BCR:H361	2.34	0.42
4:D:126:LYS:HD3	6:H:55:PHE:HD1	1.84	0.42
8:L:115:LEU:HD12	18:L:305:CLA:HMB1	2.00	0.42
21:K:202:BCR:H392	21:K:202:BCR:H24C	1.80	0.42
1:A:294:HIS:HE2	18:A:820:CLA:C2B	2.32	0.41
18:A:841:CLA:HAA2	18:B:829:CLA:HMB1	2.02	0.41
21:A:851:BCR:H24C	21:A:851:BCR:H371	1.89	0.41
2:B:497:TRP:O	2:B:501:VAL:HG13	2.20	0.41
18:F:805:CLA:HMD1	24:F:808:LMU:H22	2.01	0.41
15:3:144:TRP:NE1	15:3:150:LEU:HD21	2.35	0.41
1:A:327:LYS:HE3	1:A:327:LYS:HB2	1.92	0.41
18:A:855:CLA:H143	18:A:855:CLA:H112	1.96	0.41
21:F:806:BCR:H371	21:F:806:BCR:H24C	1.84	0.41
14:2:197:LYS:HA	14:2:200:GLU:HG2	2.02	0.41
15:3:52:PHE:HB2	15:3:71:PHE:HD1	1.85	0.41
18:3:302:CLA:H93	18:3:307:CLA:H52	2.02	0.41
14:2:182:GLY:O	14:2:186:ASP:N	2.47	0.41
15:3:52:PHE:HB2	15:3:71:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:859:LMU:H22	24:A:859:LMU:H1'	1.78	0.41
18:1:310:CLA:HMB3	18:1:312:CLA:HAA1	2.01	0.41
14:2:228:THR:OG1	14:2:229:GLY:N	2.53	0.41
15:3:106:VAL:HG13	15:3:235:MET:HE2	2.02	0.41
9:F:116:TRP:CD1	9:F:153:GLY:HA3	2.54	0.41
18:F:804:CLA:H143	18:F:804:CLA:H111	1.86	0.41
24:F:803:LMU:H22	24:F:803:LMU:H1'	1.81	0.41
21:A:850:BCR:H24C	21:A:850:BCR:H371	1.88	0.41
18:B:820:CLA:H91	18:B:820:CLA:H112	1.92	0.41
1:A:12:ILE:HD13	18:A:811:CLA:HAA2	2.03	0.41
18:B:819:CLA:HAA2	10:G:70:PHE:CE2	2.56	0.41
21:B:844:BCR:H24C	21:B:844:BCR:H371	1.88	0.41
18:1:306:CLA:HMC3	27:1:307:CHL:C1C	2.51	0.41
14:2:94:CYS:SG	14:2:213:MET:HE2	2.60	0.41
1:A:94:ARG:HD2	1:A:95:PHE:CZ	2.55	0.41
21:A:848:BCR:H371	21:A:848:BCR:H24C	1.85	0.41
18:A:838:CLA:HHC	18:A:838:CLA:HAB	1.93	0.40
2:B:303:ASP:OD2	10:G:78:GLN:HA	2.21	0.40
2:B:684:ARG:HD3	8:L:67:SER:HB2	2.03	0.40
18:B:806:CLA:H12	7:I:14:VAL:HG21	2.02	0.40
25:J:104:DGD:HAE1	25:J:104:DGD:HAF2	1.98	0.40
21:4:618:BCR:H20C	21:4:618:BCR:H361	1.97	0.40
1:A:474:ILE:H	1:A:474:ILE:HG13	1.72	0.40
21:G:202:BCR:H24C	21:G:202:BCR:H371	1.85	0.40
21:G:206:BCR:H24C	21:G:206:BCR:H371	1.92	0.40
18:1:313:CLA:H62	18:1:313:CLA:H41	1.47	0.40
15:3:122:PRO:HA	15:3:123:PRO:HD3	1.97	0.40
18:3:303:CLA:HBB1	21:3:313:BCR:H24C	2.04	0.40
23:4:620:LMG:H382	23:4:620:LMG:H421	2.04	0.40
18:B:823:CLA:H161	18:B:823:CLA:H122	1.97	0.40
13:1:156:GLU:OE2	24:1:320:LMU:O4'	2.39	0.40
14:2:217:MET:HE3	18:2:603:CLA:HAB	2.03	0.40
1:A:93:ALA:HB2	1:A:156:LEU:HB2	2.04	0.40
1:A:118:ILE:HD12	26:J:101:LUT:H383	2.02	0.40
21:A:848:BCR:H361	21:A:848:BCR:H20C	1.88	0.40
21:L:307:BCR:H24C	21:L:307:BCR:H371	1.83	0.40
27:3:301:CHL:H91	18:3:302:CLA:HBB	2.04	0.40
21:4:618:BCR:H331	21:4:618:BCR:C8	2.52	0.40

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	740/750 (99%)	717 (97%)	22 (3%)	1 (0%)	48	57
2	B	731/734 (100%)	715 (98%)	16 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	141/206 (68%)	136 (96%)	5 (4%)	0	100	100
5	E	65/143 (46%)	65 (100%)	0	0	100	100
6	H	92/94 (98%)	92 (100%)	0	0	100	100
7	I	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
8	L	155/213 (73%)	152 (98%)	3 (2%)	0	100	100
9	F	156/178 (88%)	153 (98%)	3 (2%)	0	100	100
10	G	92/144 (64%)	86 (94%)	6 (6%)	0	100	100
11	J	41/52 (79%)	41 (100%)	0	0	100	100
12	K	84/130 (65%)	82 (98%)	2 (2%)	0	100	100
13	1	193/242 (80%)	186 (96%)	7 (4%)	0	100	100
14	2	205/207 (99%)	201 (98%)	4 (2%)	0	100	100
15	3	220/269 (82%)	205 (93%)	15 (7%)	0	100	100
16	4	197/256 (77%)	189 (96%)	8 (4%)	0	100	100
All	All	3221/3735 (86%)	3126 (97%)	94 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	VAL

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	600/608 (99%)	597 (100%)	3 (0%)	81	90
2	B	598/599 (100%)	595 (100%)	3 (0%)	81	90
3	C	70/71 (99%)	70 (100%)	0	100	100
4	D	120/163 (74%)	119 (99%)	1 (1%)	73	85
5	E	59/115 (51%)	58 (98%)	1 (2%)	53	69
6	H	76/76 (100%)	75 (99%)	1 (1%)	61	76
7	I	30/33 (91%)	30 (100%)	0	100	100
8	L	123/168 (73%)	122 (99%)	1 (1%)	73	85
9	F	128/142 (90%)	125 (98%)	3 (2%)	44	59
10	G	77/112 (69%)	76 (99%)	1 (1%)	61	76
11	J	37/44 (84%)	35 (95%)	2 (5%)	20	25
12	K	66/102 (65%)	63 (96%)	3 (4%)	24	33
13	1	155/192 (81%)	150 (97%)	5 (3%)	34	47
14	2	165/165 (100%)	162 (98%)	3 (2%)	51	68
15	3	176/216 (82%)	171 (97%)	5 (3%)	38	52
16	4	160/203 (79%)	160 (100%)	0	100	100
All	All	2640/3009 (88%)	2608 (99%)	32 (1%)	61	78

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ILE
1	A	245	ASP
1	A	749	VAL
2	B	458	ILE
2	B	608	GLN
2	B	684	ARG
4	D	206	VAL
5	E	99	ASN
6	H	60	ILE
8	L	143	VAL
9	F	128	VAL
9	F	137	ARG

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Mol	Chain	Res	Type
9	F	155	ILE
10	G	75	VAL
11	J	11	MET
11	J	20	VAL
12	K	52	MET
12	K	97	THR
12	K	129	ILE
13	1	139	LEU
13	1	141	ILE
13	1	151	GLN
13	1	232	ASP
13	1	234	VAL
14	2	144	ILE
14	2	173	THR
14	2	206	ILE
15	3	86	ILE
15	3	121	VAL
15	3	175	MET
15	3	208	THR
15	3	264	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	A	293	HIS
1	A	439	ASN
1	A	704	ASN
1	A	713	GLN
2	B	10	GLN
2	B	83	HIS
2	B	220	GLN
2	B	333	GLN
2	B	452	GLN
4	D	91	GLN
6	H	66	GLN
8	L	84	ASN
10	G	82	GLN
14	2	233	ASN
15	3	260	ASN
16	4	92	ASN
16	4	174	HIS

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Mol	Chain	Res	Type
16	4	236	HIS
16	4	237	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

224 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	801	2	69,73,73	1.15	4 (5%)	83,113,113	0.88	4 (4%)
24	LMU	F	808	-	36,36,36	0.11	0	47,47,47	0.20	0
18	CLA	L	304	8	64,68,73	1.16	5 (7%)	77,107,113	0.95	5 (6%)
18	CLA	B	821	2	49,53,73	1.42	4 (8%)	59,89,113	1.03	4 (6%)
24	LMU	1	320	-	36,36,36	0.11	0	47,47,47	0.17	0
18	CLA	B	822	31	69,73,73	1.22	4 (5%)	83,113,113	0.91	4 (4%)
18	CLA	1	313	13	69,73,73	1.18	4 (5%)	83,113,113	0.95	4 (4%)
18	CLA	2	613	14	54,58,73	1.32	4 (7%)	65,95,113	1.01	4 (6%)
24	LMU	1	321	-	24,24,36	0.13	0	29,29,47	0.24	0
21	BCR	A	848	-	41,41,41	0.14	0	56,56,56	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	818	2	64,68,73	1.24	4 (6%)	77,107,113	0.90	4 (5%)
18	CLA	B	831	2	69,73,73	1.14	4 (5%)	83,113,113	0.92	4 (4%)
24	LMU	F	803	-	36,36,36	0.12	0	47,47,47	0.41	0
18	CLA	2	603	14	69,73,73	1.17	4 (5%)	83,113,113	0.87	3 (3%)
21	BCR	A	850	-	41,41,41	0.13	0	56,56,56	0.40	0
18	CLA	3	307	15	64,68,73	1.25	4 (6%)	77,107,113	0.93	4 (5%)
18	CLA	4	610	-	49,53,73	1.42	4 (8%)	59,89,113	1.03	4 (6%)
18	CLA	B	830	2	69,73,73	1.15	4 (5%)	83,113,113	0.88	4 (4%)
21	BCR	G	202	-	41,41,41	0.16	0	56,56,56	0.36	0
18	CLA	B	837	2	69,73,73	1.08	4 (5%)	83,113,113	0.88	4 (4%)
17	CL0	A	801	1	69,73,73	1.54	9 (13%)	83,113,113	1.19	6 (7%)
24	LMU	4	624	-	24,24,36	0.13	0	29,29,47	0.26	0
25	DGD	B	845	-	62,62,67	0.17	0	76,76,81	0.29	0
18	CLA	4	614	16	54,58,73	1.29	4 (7%)	65,95,113	0.99	4 (6%)
27	CHL	4	606	31	50,54,74	2.05	9 (18%)	56,90,114	1.24	6 (10%)
18	CLA	A	815	1	58,62,73	1.25	4 (6%)	69,99,113	0.98	4 (5%)
21	BCR	L	307	-	41,41,41	0.13	0	56,56,56	0.31	0
21	BCR	B	841	-	41,41,41	0.15	0	56,56,56	0.34	0
18	CLA	1	304	13	64,68,73	1.21	4 (6%)	77,107,113	0.93	3 (3%)
18	CLA	B	826	2	69,73,73	1.17	4 (5%)	83,113,113	0.88	3 (3%)
18	CLA	1	315	13	49,53,73	1.39	4 (8%)	59,89,113	1.02	4 (6%)
18	CLA	1	308	31	49,53,73	1.42	4 (8%)	59,89,113	1.06	4 (6%)
18	CLA	A	841	1	69,73,73	1.11	4 (5%)	83,113,113	0.89	4 (4%)
18	CLA	A	829	1	69,73,73	1.17	4 (5%)	83,113,113	0.90	3 (3%)
18	CLA	A	840	1	59,63,73	1.25	4 (6%)	71,101,113	1.00	4 (5%)
18	CLA	4	611	16	51,55,73	1.36	4 (7%)	61,91,113	1.05	4 (6%)
24	LMU	F	809	-	36,36,36	0.12	0	47,47,47	0.35	0
18	CLA	1	303	13	69,73,73	1.18	4 (5%)	83,113,113	0.89	4 (4%)
27	CHL	3	301	15	70,74,74	1.72	7 (10%)	80,114,114	1.06	6 (7%)
18	CLA	B	819	2	62,66,73	1.21	4 (6%)	74,104,113	0.99	4 (5%)
18	CLA	A	836	1	69,73,73	1.16	4 (5%)	83,113,113	0.90	4 (4%)
18	CLA	3	311	15	49,53,73	1.43	4 (8%)	59,89,113	1.04	4 (6%)
20	LHG	1	319	-	48,48,48	0.22	0	51,54,54	0.27	0
21	BCR	A	849	-	41,41,41	0.16	0	56,56,56	0.30	0
18	CLA	B	824	2	69,73,73	1.18	4 (5%)	83,113,113	0.88	3 (3%)
18	CLA	1	310	13	59,63,73	1.34	4 (6%)	71,101,113	1.00	2 (2%)
18	CLA	B	828	2	49,53,73	1.33	4 (8%)	59,89,113	1.02	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	827	2	69,73,73	1.14	4 (5%)	83,113,113	0.89	4 (4%)
24	LMU	1	301	-	36,36,36	0.12	0	47,47,47	0.39	0
28	XAT	2	616	-	39,47,47	0.10	0	54,74,74	0.48	0
18	CLA	B	816	2	69,73,73	1.16	4 (5%)	83,113,113	0.88	3 (3%)
18	CLA	2	610	20	64,68,73	1.24	4 (6%)	77,107,113	0.91	4 (5%)
24	LMU	G	207	-	36,36,36	0.12	0	47,47,47	0.25	0
18	CLA	A	823	1	56,60,73	1.31	4 (7%)	67,97,113	1.01	4 (5%)
18	CLA	A	854	31	69,73,73	1.17	4 (5%)	83,113,113	0.88	3 (3%)
21	BCR	J	103	-	41,41,41	0.26	0	56,56,56	0.43	0
18	CLA	3	302	15	59,63,73	1.29	4 (6%)	71,101,113	0.96	4 (5%)
21	BCR	A	851	-	41,41,41	0.17	0	56,56,56	0.33	0
18	CLA	B	804	2	69,73,73	1.12	4 (5%)	83,113,113	0.90	4 (4%)
18	CLA	A	843	31	69,73,73	1.13	4 (5%)	83,113,113	0.93	5 (6%)
18	CLA	A	818	1	64,68,73	1.21	4 (6%)	77,107,113	1.00	5 (6%)
18	CLA	A	831	1	69,73,73	1.14	4 (5%)	83,113,113	0.86	4 (4%)
18	CLA	B	811	2	56,60,73	1.33	4 (7%)	67,97,113	0.98	4 (5%)
18	CLA	3	305	15	65,69,73	1.22	4 (6%)	78,108,113	0.92	4 (5%)
18	CLA	B	810	2	60,64,73	1.24	4 (6%)	72,102,113	0.96	4 (5%)
24	LMU	F	807	-	36,36,36	0.12	0	47,47,47	0.27	0
18	CLA	A	816	1	64,68,73	1.18	4 (6%)	77,107,113	0.94	4 (5%)
18	CLA	A	822	31	69,73,73	1.19	4 (5%)	83,113,113	0.89	3 (3%)
18	CLA	K	203	31	64,68,73	1.24	4 (6%)	77,107,113	0.93	4 (5%)
24	LMU	4	623	-	36,36,36	0.11	0	47,47,47	0.41	0
18	CLA	A	837	1	49,53,73	1.37	4 (8%)	59,89,113	1.07	5 (8%)
18	CLA	J	102	11	49,53,73	1.40	4 (8%)	59,89,113	1.03	4 (6%)
18	CLA	F	804	31	69,73,73	1.18	4 (5%)	83,113,113	0.91	4 (4%)
20	LHG	B	846	18	38,38,48	0.26	0	41,44,54	0.30	0
18	CLA	A	833	1	59,63,73	1.26	4 (6%)	71,101,113	0.94	4 (5%)
18	CLA	A	806	1	69,73,73	1.12	4 (5%)	83,113,113	0.89	3 (3%)
26	LUT	4	616	-	42,43,43	0.22	0	51,60,60	0.34	0
18	CLA	B	806	2	64,68,73	1.19	4 (6%)	77,107,113	0.91	4 (5%)
23	LMG	4	620	-	45,45,55	0.20	0	53,53,63	0.22	0
18	CLA	A	805	1,18	54,58,73	1.29	4 (7%)	65,95,113	1.01	4 (6%)
18	CLA	B	805	2	69,73,73	1.19	4 (5%)	83,113,113	0.84	4 (4%)
27	CHL	4	605	31	70,74,74	1.72	7 (10%)	80,114,114	1.10	7 (8%)
18	CLA	1	309	13	69,73,73	1.17	4 (5%)	83,113,113	0.83	4 (4%)
18	CLA	A	819	1	60,64,73	1.26	4 (6%)	72,102,113	0.95	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	2	604	-	49,53,73	1.41	4 (8%)	59,89,113	1.05	4 (6%)
18	CLA	B	803	2	49,53,73	1.39	4 (8%)	59,89,113	1.00	4 (6%)
18	CLA	B	823	31	69,73,73	1.13	4 (5%)	83,113,113	0.90	4 (4%)
18	CLA	A	808	1	51,55,73	1.32	4 (7%)	61,91,113	1.03	4 (6%)
18	CLA	3	309	15	49,53,73	1.39	4 (8%)	59,89,113	1.06	4 (6%)
18	CLA	B	833	2	65,69,73	1.16	4 (6%)	78,108,113	0.94	3 (3%)
18	CLA	A	811	1	49,53,73	1.35	4 (8%)	59,89,113	1.08	4 (6%)
18	CLA	A	830	1	69,73,73	1.14	4 (5%)	83,113,113	0.87	4 (4%)
18	CLA	2	612	14	69,73,73	1.19	4 (5%)	83,113,113	0.88	4 (4%)
29	C7Z	1	322	-	43,43,43	0.11	0	58,60,60	0.34	0
25	DGD	J	104	-	59,59,67	0.16	0	73,73,81	0.16	0
18	CLA	B	802	-	69,73,73	1.13	4 (5%)	83,113,113	0.82	2 (2%)
18	CLA	4	601	16	54,58,73	1.33	4 (7%)	65,95,113	1.01	4 (6%)
18	CLA	A	828	1	69,73,73	1.18	4 (5%)	83,113,113	0.88	4 (4%)
26	LUT	J	101	-	42,43,43	0.19	0	51,60,60	0.43	0
18	CLA	F	805	9	54,58,73	1.27	4 (7%)	65,95,113	0.98	4 (6%)
18	CLA	A	856	-	49,53,73	1.40	4 (8%)	59,89,113	1.06	3 (5%)
26	LUT	3	315	-	42,43,43	0.19	0	51,60,60	0.32	0
18	CLA	1	305	31	54,58,73	1.35	4 (7%)	65,95,113	1.01	4 (6%)
18	CLA	A	813	1	49,53,73	1.42	4 (8%)	59,89,113	1.05	4 (6%)
24	LMU	4	621	-	23,23,36	0.14	0	28,28,47	0.26	0
27	CHL	2	607	-	55,59,74	1.96	8 (14%)	62,96,114	1.24	7 (11%)
27	CHL	4	615	16	50,54,74	2.02	7 (14%)	56,90,114	1.30	7 (12%)
27	CHL	1	307	13	50,54,74	2.09	8 (16%)	56,90,114	1.29	7 (12%)
18	CLA	2	602	14	69,73,73	1.19	4 (5%)	83,113,113	0.88	4 (4%)
18	CLA	A	839	1	69,73,73	1.13	4 (5%)	83,113,113	0.91	4 (4%)
21	BCR	B	843	-	41,41,41	0.16	0	56,56,56	0.34	0
26	LUT	1	318	-	42,43,43	0.22	0	51,60,60	0.32	0
18	CLA	4	603	16	69,73,73	1.14	4 (5%)	83,113,113	0.90	3 (3%)
27	CHL	3	306	31	55,59,74	1.95	7 (12%)	62,96,114	1.25	7 (11%)
27	CHL	2	606	31	50,54,74	2.04	8 (16%)	56,90,114	1.26	7 (12%)
24	LMU	A	858	-	24,24,36	0.11	0	29,29,47	0.26	0
18	CLA	4	604	31	49,53,73	1.42	4 (8%)	59,89,113	1.06	4 (6%)
18	CLA	4	609	16	64,68,73	1.26	4 (6%)	77,107,113	0.88	3 (3%)
18	CLA	B	817	31	59,63,73	1.25	4 (6%)	71,101,113	0.97	4 (5%)
24	LMU	H	201	-	24,24,36	0.12	0	29,29,47	0.25	0
21	BCR	L	302	-	41,41,41	0.15	0	56,56,56	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	824	1	49,53,73	1.39	4 (8%)	59,89,113	1.06	4 (6%)
18	CLA	B	809	2	69,73,73	1.15	4 (5%)	83,113,113	0.86	3 (3%)
18	CLA	2	608	14	49,53,73	1.39	4 (8%)	59,89,113	1.04	4 (6%)
18	CLA	B	808	2	69,73,73	1.18	4 (5%)	83,113,113	0.89	4 (4%)
18	CLA	G	201	2	61,65,73	1.24	4 (6%)	73,103,113	0.94	4 (5%)
24	LMU	2	618	-	36,36,36	0.10	0	47,47,47	0.15	0
18	CLA	A	804	1	69,73,73	1.16	4 (5%)	83,113,113	0.93	4 (4%)
18	CLA	B	814	2	49,53,73	1.32	4 (8%)	59,89,113	1.05	4 (6%)
18	CLA	B	835	2	54,58,73	1.29	4 (7%)	65,95,113	1.00	4 (6%)
18	CLA	A	803	31	69,73,73	1.18	4 (5%)	83,113,113	0.90	3 (3%)
18	CLA	3	312	15	49,53,73	1.40	4 (8%)	59,89,113	1.04	4 (6%)
18	CLA	K	201	12	49,53,73	1.43	4 (8%)	59,89,113	1.07	4 (6%)
19	PQN	A	844	-	34,34,34	0.35	0	42,45,45	0.34	0
27	CHL	2	614	14	51,55,74	2.02	7 (13%)	57,91,114	1.28	7 (12%)
18	CLA	A	838	1	55,59,73	1.28	4 (7%)	66,96,113	1.01	4 (6%)
18	CLA	A	810	1	54,58,73	1.32	4 (7%)	65,95,113	1.02	4 (6%)
18	CLA	A	814	1	69,73,73	1.16	4 (5%)	83,113,113	0.87	3 (3%)
20	LHG	B	847	-	48,48,48	0.23	0	51,54,54	0.25	0
18	CLA	1	312	13	49,53,73	1.39	4 (8%)	59,89,113	1.05	4 (6%)
18	CLA	A	834	1	69,73,73	1.14	4 (5%)	83,113,113	0.92	4 (4%)
18	CLA	1	311	-	49,53,73	1.40	4 (8%)	59,89,113	1.04	4 (6%)
18	CLA	4	602	16	64,68,73	1.24	4 (6%)	77,107,113	0.93	4 (5%)
21	BCR	B	842	-	41,41,41	0.17	0	56,56,56	0.46	0
18	CLA	2	609	14	64,68,73	1.23	4 (6%)	77,107,113	0.91	4 (5%)
21	BCR	F	806	-	41,41,41	0.24	0	56,56,56	0.39	0
18	CLA	3	310	15	59,63,73	1.26	4 (6%)	71,101,113	0.96	4 (5%)
27	CHL	1	302	13	70,74,74	1.72	8 (11%)	80,114,114	1.09	7 (8%)
26	LUT	3	314	-	42,43,43	0.19	0	51,60,60	0.50	0
19	PQN	B	838	-	34,34,34	0.32	0	42,45,45	0.34	0
21	BCR	B	840	-	41,41,41	0.26	0	56,56,56	0.43	0
21	BCR	4	618	-	41,41,41	0.17	0	56,56,56	0.45	0
24	LMU	B	848	-	24,24,36	0.14	0	29,29,47	0.22	0
18	CLA	A	820	1	69,73,73	1.19	4 (5%)	83,113,113	0.86	3 (3%)
24	LMU	A	859	-	36,36,36	0.11	0	47,47,47	0.21	0
18	CLA	B	834	2	69,73,73	1.10	4 (5%)	83,113,113	0.95	5 (6%)
18	CLA	G	204	10	49,53,73	1.42	4 (8%)	59,89,113	1.06	4 (6%)
18	CLA	3	308	15	59,63,73	1.26	4 (6%)	71,101,113	0.96	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	4	608	16	69,73,73	1.20	4 (5%)	83,113,113	0.97	5 (6%)
18	CLA	A	845	20	49,53,73	1.43	4 (8%)	59,89,113	1.05	4 (6%)
18	CLA	B	812	2	69,73,73	1.16	4 (5%)	83,113,113	0.89	4 (4%)
28	XAT	1	317	-	39,47,47	0.12	0	54,74,74	0.56	0
18	CLA	1	306	-	49,53,73	1.41	4 (8%)	59,89,113	1.06	4 (6%)
18	CLA	K	204	12	49,53,73	1.43	4 (8%)	59,89,113	1.07	3 (5%)
26	LUT	1	316	-	42,43,43	0.20	0	51,60,60	0.33	0
21	BCR	G	206	-	41,41,41	0.14	0	56,56,56	0.37	0
26	LUT	2	615	-	42,43,43	0.26	0	51,60,60	0.35	0
18	CLA	2	611	14	49,53,73	1.39	4 (8%)	59,89,113	1.04	4 (6%)
21	BCR	K	205	-	41,41,41	0.15	0	56,56,56	0.28	0
18	CLA	A	802	-	69,73,73	1.06	4 (5%)	83,113,113	0.83	3 (3%)
18	CLA	F	802	2	69,73,73	1.17	4 (5%)	83,113,113	0.96	4 (4%)
21	BCR	3	313	-	41,41,41	0.14	0	56,56,56	0.40	0
18	CLA	G	205	10	50,54,73	1.40	4 (8%)	60,90,113	1.02	3 (5%)
23	LMG	A	857	-	43,43,55	0.19	0	51,51,63	0.17	0
18	CLA	A	809	1	69,73,73	1.16	4 (5%)	83,113,113	1.04	6 (7%)
18	CLA	A	835	1	69,73,73	1.14	4 (5%)	83,113,113	0.90	3 (3%)
24	LMU	L	301	-	20,20,36	0.14	0	25,25,47	0.32	0
20	LHG	A	846	-	48,48,48	0.25	0	51,54,54	0.28	0
18	CLA	A	825	1	64,68,73	1.22	4 (6%)	77,107,113	0.91	4 (5%)
21	BCR	F	801	-	41,41,41	0.33	0	56,56,56	0.47	0
18	CLA	1	314	13	49,53,73	1.42	4 (8%)	59,89,113	1.04	4 (6%)
23	LMG	F	810	-	30,30,55	0.21	0	38,38,63	0.19	0
25	DGD	4	622	-	50,50,67	0.18	0	64,64,81	0.38	0
21	BCR	B	844	-	41,41,41	0.16	0	56,56,56	0.30	0
21	BCR	L	306	-	41,41,41	0.23	0	56,56,56	0.50	0
18	CLA	B	807	2	69,73,73	1.14	4 (5%)	83,113,113	0.87	4 (4%)
18	CLA	B	839	20	69,73,73	1.19	4 (5%)	83,113,113	0.89	4 (4%)
18	CLA	L	303	8	49,53,73	1.39	4 (8%)	59,89,113	1.07	4 (6%)
21	BCR	K	202	-	41,41,41	0.25	0	56,56,56	0.50	0
18	CLA	4	612	16	69,73,73	1.17	4 (5%)	83,113,113	0.89	4 (4%)
18	CLA	A	832	1	49,53,73	1.34	4 (8%)	59,89,113	1.05	4 (6%)
18	CLA	B	825	2	69,73,73	1.21	4 (5%)	83,113,113	0.94	4 (4%)
20	LHG	2	617	18	42,42,48	0.24	0	45,48,54	0.28	0
18	CLA	A	812	1,18	69,73,73	1.14	5 (7%)	83,113,113	0.89	3 (3%)
22	SF4	C	102	3	0,12,12	-	-	-	-	-
18	CLA	A	821	1	49,53,73	1.39	4 (8%)	59,89,113	1.03	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	815	2	64,68,73	1.22	4 (6%)	77,107,113	0.94	4 (5%)
18	CLA	A	807	1	69,73,73	1.17	4 (5%)	83,113,113	0.86	4 (4%)
18	CLA	A	827	31	59,63,73	1.22	5 (8%)	71,101,113	0.96	3 (4%)
27	CHL	4	607	-	55,59,74	1.98	8 (14%)	62,96,114	1.31	7 (11%)
18	CLA	B	832	31	49,53,73	1.42	4 (8%)	59,89,113	1.06	4 (6%)
18	CLA	B	836	31	69,73,73	1.12	4 (5%)	83,113,113	0.92	4 (4%)
18	CLA	3	304	31	49,53,73	1.43	4 (8%)	59,89,113	1.07	4 (6%)
21	BCR	A	852	-	41,41,41	0.22	0	56,56,56	0.42	0
17	CL0	H	202	6	59,63,73	1.76	9 (15%)	71,101,113	1.36	9 (12%)
18	CLA	A	842	1	69,73,73	1.09	4 (5%)	83,113,113	0.97	3 (3%)
18	CLA	A	855	31	69,73,73	1.11	4 (5%)	83,113,113	0.90	3 (3%)
18	CLA	4	613	16	50,54,73	1.36	4 (8%)	60,90,113	1.03	3 (5%)
27	CHL	2	605	31	55,59,74	1.96	7 (12%)	62,96,114	1.25	7 (11%)
30	QDL	4	617	-	41,45,45	0.14	0	56,67,67	0.75	2 (3%)
18	CLA	B	813	2	69,73,73	1.16	4 (5%)	83,113,113	0.90	4 (4%)
18	CLA	B	829	2	69,73,73	1.19	4 (5%)	83,113,113	0.88	4 (4%)
21	BCR	I	101	-	41,41,41	0.15	0	56,56,56	0.40	0
22	SF4	A	853	1,2	0,12,12	-	-	-	-	-
18	CLA	B	820	2	69,73,73	1.15	4 (5%)	83,113,113	0.92	4 (4%)
23	LMG	4	619	-	46,46,55	0.19	0	54,54,63	0.14	0
24	LMU	G	203	-	36,36,36	0.09	0	47,47,47	0.28	0
22	SF4	C	101	3	0,12,12	-	-	-	-	-
18	CLA	A	826	31	69,73,73	1.17	4 (5%)	83,113,113	0.92	4 (4%)
20	LHG	A	847	18	30,30,48	0.29	0	33,36,54	0.33	0
18	CLA	A	817	31	49,53,73	1.40	4 (8%)	59,89,113	1.04	3 (5%)
18	CLA	2	601	14	69,73,73	1.19	4 (5%)	83,113,113	0.90	4 (4%)
18	CLA	L	305	31	49,53,73	1.40	4 (8%)	59,89,113	1.04	4 (6%)
18	CLA	3	303	-	49,53,73	1.41	4 (8%)	59,89,113	1.05	4 (6%)

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
18	CLA	B	801	2	-	5/39/115/115	-
24	LMU	F	808	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	L	304	8	-	3/33/109/115	-
18	CLA	B	821	2	-	4/15/91/115	-
24	LMU	1	320	-	-	3/21/61/61	0/2/2/2
18	CLA	B	822	31	-	7/39/115/115	-
18	CLA	1	313	13	-	10/39/115/115	-
18	CLA	2	613	14	-	3/21/97/115	-
24	LMU	1	321	-	-	0/15/35/61	0/1/1/2
21	BCR	A	848	-	-	2/29/63/63	0/2/2/2
18	CLA	B	818	2	-	6/33/109/115	-
18	CLA	B	831	2	-	7/39/115/115	-
24	LMU	F	803	-	-	3/21/61/61	0/2/2/2
18	CLA	2	603	14	-	5/39/115/115	-
21	BCR	A	850	-	-	2/29/63/63	0/2/2/2
18	CLA	3	307	15	-	6/33/109/115	-
18	CLA	4	610	-	-	6/15/91/115	-
18	CLA	B	830	2	-	3/39/115/115	-
21	BCR	G	202	-	-	0/29/63/63	0/2/2/2
18	CLA	B	837	2	-	5/39/115/115	-
17	CL0	A	801	1	-	3/39/115/115	-
24	LMU	4	624	-	-	1/15/35/61	0/1/1/2
25	DGD	B	845	-	-	10/50/90/95	0/2/2/2
18	CLA	4	614	16	-	4/21/97/115	-
27	CHL	4	606	31	-	2/17/93/117	-
18	CLA	A	815	1	-	2/26/102/115	-
21	BCR	L	307	-	-	2/29/63/63	0/2/2/2
21	BCR	B	841	-	-	4/29/63/63	0/2/2/2
18	CLA	1	304	13	-	3/33/109/115	-
18	CLA	B	826	2	-	2/39/115/115	-
18	CLA	1	315	13	-	1/15/91/115	-
18	CLA	1	308	31	-	4/15/91/115	-
18	CLA	A	841	1	-	3/39/115/115	-
18	CLA	A	829	1	-	5/39/115/115	-
18	CLA	A	840	1	-	2/27/103/115	-
18	CLA	4	611	16	-	4/18/94/115	-
24	LMU	F	809	-	-	1/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	1	303	13	-	2/39/115/115	-
27	CHL	3	301	15	-	9/41/117/117	-
18	CLA	B	819	2	-	7/31/107/115	-
18	CLA	A	836	1	-	1/39/115/115	-
18	CLA	3	311	15	-	6/15/91/115	-
20	LHG	1	319	-	-	9/53/53/53	-
21	BCR	A	849	-	-	2/29/63/63	0/2/2/2
18	CLA	B	824	2	-	2/39/115/115	-
18	CLA	1	310	13	-	3/27/103/115	-
18	CLA	B	828	2	-	0/15/91/115	-
18	CLA	B	827	2	-	5/39/115/115	-
24	LMU	1	301	-	-	2/21/61/61	0/2/2/2
28	XAT	2	616	-	-	0/31/93/93	0/4/4/4
18	CLA	B	816	2	-	2/39/115/115	-
18	CLA	2	610	20	-	2/33/109/115	-
24	LMU	G	207	-	-	2/21/61/61	0/2/2/2
18	CLA	A	823	1	-	5/24/100/115	-
18	CLA	A	854	31	-	5/39/115/115	-
21	BCR	J	103	-	-	2/29/63/63	0/2/2/2
18	CLA	3	302	15	-	2/27/103/115	-
21	BCR	A	851	-	-	2/29/63/63	0/2/2/2
18	CLA	B	804	2	-	8/39/115/115	-
18	CLA	A	843	31	-	7/39/115/115	-
18	CLA	A	818	1	-	3/33/109/115	-
18	CLA	A	831	1	-	3/39/115/115	-
18	CLA	B	811	2	-	3/24/100/115	-
18	CLA	3	305	15	-	7/35/111/115	-
18	CLA	B	810	2	-	4/29/105/115	-
24	LMU	F	807	-	-	4/21/61/61	0/2/2/2
18	CLA	A	816	1	-	3/33/109/115	-
18	CLA	A	822	31	-	5/39/115/115	-
18	CLA	K	203	31	-	7/33/109/115	-
24	LMU	4	623	-	-	4/21/61/61	0/2/2/2
18	CLA	A	837	1	-	2/15/91/115	-
18	CLA	J	102	11	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	F	804	31	-	7/39/115/115	-
20	LHG	B	846	18	-	8/43/43/53	-
18	CLA	A	833	1	-	1/27/103/115	-
18	CLA	A	806	1	-	3/39/115/115	-
26	LUT	4	616	-	-	2/29/67/67	0/2/2/2
18	CLA	B	806	2	-	3/33/109/115	-
23	LMG	4	620	-	-	5/40/60/70	0/1/1/1
18	CLA	A	805	1,18	-	2/21/97/115	-
18	CLA	B	805	2	-	4/39/115/115	-
27	CHL	4	605	31	-	5/41/117/117	-
18	CLA	1	309	13	-	7/39/115/115	-
18	CLA	A	819	1	-	6/29/105/115	-
18	CLA	2	604	-	-	0/15/91/115	-
18	CLA	B	803	2	-	2/15/91/115	-
18	CLA	B	823	31	-	2/39/115/115	-
18	CLA	A	808	1	-	0/18/94/115	-
18	CLA	3	309	15	-	6/15/91/115	-
18	CLA	B	833	2	-	3/35/111/115	-
18	CLA	A	811	1	-	2/15/91/115	-
18	CLA	A	830	1	-	2/39/115/115	-
18	CLA	2	612	14	-	5/39/115/115	-
29	C7Z	1	322	-	-	4/29/67/67	0/2/2/2
25	DGD	J	104	-	-	5/47/87/95	0/2/2/2
18	CLA	B	802	-	-	1/39/115/115	-
18	CLA	4	601	16	-	6/21/97/115	-
18	CLA	A	828	1	-	2/39/115/115	-
26	LUT	J	101	-	-	4/29/67/67	0/2/2/2
18	CLA	F	805	9	-	4/21/97/115	-
18	CLA	A	856	-	-	5/15/91/115	-
26	LUT	3	315	-	-	0/29/67/67	0/2/2/2
18	CLA	1	305	31	-	4/21/97/115	-
18	CLA	A	813	1	-	3/15/91/115	-
24	LMU	4	621	-	-	2/14/34/61	0/1/1/2
27	CHL	2	607	-	-	6/23/99/117	-
27	CHL	4	615	16	-	4/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CHL	1	307	13	-	5/17/93/117	-
18	CLA	2	602	14	-	3/39/115/115	-
18	CLA	A	839	1	-	4/39/115/115	-
21	BCR	B	843	-	-	2/29/63/63	0/2/2/2
26	LUT	1	318	-	-	1/29/67/67	0/2/2/2
18	CLA	4	603	16	-	5/39/115/115	-
27	CHL	3	306	31	-	6/23/99/117	-
27	CHL	2	606	31	-	5/17/93/117	-
24	LMU	A	858	-	-	2/15/35/61	0/1/1/2
18	CLA	4	604	31	-	7/15/91/115	-
18	CLA	4	609	16	-	4/33/109/115	-
18	CLA	B	817	31	-	2/27/103/115	-
24	LMU	H	201	-	-	3/15/35/61	0/1/1/2
21	BCR	L	302	-	-	4/29/63/63	0/2/2/2
18	CLA	A	824	1	-	5/15/91/115	-
18	CLA	B	809	2	-	3/39/115/115	-
18	CLA	2	608	14	-	0/15/91/115	-
18	CLA	B	808	2	-	4/39/115/115	-
18	CLA	G	201	2	-	6/30/106/115	-
24	LMU	2	618	-	-	2/21/61/61	0/2/2/2
18	CLA	A	804	1	-	5/39/115/115	-
18	CLA	B	814	2	-	2/15/91/115	-
18	CLA	B	835	2	-	0/21/97/115	-
18	CLA	A	803	31	-	2/39/115/115	-
18	CLA	3	312	15	-	2/15/91/115	-
18	CLA	K	201	12	-	6/15/91/115	-
19	PQN	A	844	-	-	0/23/43/43	0/2/2/2
27	CHL	2	614	14	-	2/19/95/117	-
18	CLA	A	838	1	-	1/23/99/115	-
18	CLA	A	810	1	-	2/21/97/115	-
18	CLA	A	814	1	-	7/39/115/115	-
20	LHG	B	847	-	-	14/53/53/53	-
18	CLA	1	312	13	-	7/15/91/115	-
18	CLA	A	834	1	-	5/39/115/115	-
18	CLA	1	311	-	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	4	602	16	-	2/33/109/115	-
21	BCR	B	842	-	-	2/29/63/63	0/2/2/2
18	CLA	2	609	14	-	6/33/109/115	-
21	BCR	F	806	-	-	2/29/63/63	0/2/2/2
18	CLA	3	310	15	-	7/27/103/115	-
27	CHL	1	302	13	-	7/41/117/117	-
26	LUT	3	314	-	-	0/29/67/67	0/2/2/2
19	PQN	B	838	-	-	3/23/43/43	0/2/2/2
21	BCR	B	840	-	-	2/29/63/63	0/2/2/2
21	BCR	4	618	-	-	2/29/63/63	0/2/2/2
24	LMU	B	848	-	-	1/15/35/61	0/1/1/2
18	CLA	A	820	1	-	7/39/115/115	-
24	LMU	A	859	-	-	3/21/61/61	0/2/2/2
18	CLA	B	834	2	-	0/39/115/115	-
18	CLA	G	204	10	-	5/15/91/115	-
18	CLA	3	308	15	-	7/27/103/115	-
18	CLA	4	608	16	-	12/39/115/115	-
18	CLA	A	845	20	-	5/15/91/115	-
18	CLA	B	812	2	-	3/39/115/115	-
28	XAT	1	317	-	-	0/31/93/93	0/4/4/4
18	CLA	1	306	-	-	2/15/91/115	-
18	CLA	K	204	12	-	6/15/91/115	-
26	LUT	1	316	-	-	0/29/67/67	0/2/2/2
21	BCR	G	206	-	-	4/29/63/63	0/2/2/2
26	LUT	2	615	-	-	2/29/67/67	0/2/2/2
18	CLA	2	611	14	-	4/15/91/115	-
21	BCR	K	205	-	-	2/29/63/63	0/2/2/2
18	CLA	A	802	-	-	1/39/115/115	-
18	CLA	F	802	2	-	0/39/115/115	-
21	BCR	3	313	-	-	4/29/63/63	0/2/2/2
18	CLA	G	205	10	-	3/17/93/115	-
23	LMG	A	857	-	-	4/38/58/70	0/1/1/1
18	CLA	A	809	1	-	8/39/115/115	-
18	CLA	A	835	1	-	6/39/115/115	-
24	LMU	L	301	-	-	0/11/31/61	0/1/1/2
20	LHG	A	846	-	-	6/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	825	1	-	6/33/109/115	-
21	BCR	F	801	-	-	0/29/63/63	0/2/2/2
18	CLA	1	314	13	-	6/15/91/115	-
23	LMG	F	810	-	-	2/25/45/70	0/1/1/1
25	DGD	4	622	-	-	5/38/78/95	0/2/2/2
21	BCR	B	844	-	-	2/29/63/63	0/2/2/2
21	BCR	L	306	-	-	2/29/63/63	0/2/2/2
18	CLA	B	807	2	-	10/39/115/115	-
18	CLA	B	839	20	-	8/39/115/115	-
18	CLA	L	303	8	-	6/15/91/115	-
21	BCR	K	202	-	-	0/29/63/63	0/2/2/2
18	CLA	4	612	16	-	7/39/115/115	-
18	CLA	A	832	1	-	3/15/91/115	-
18	CLA	B	825	2	-	5/39/115/115	-
20	LHG	2	617	18	-	15/47/47/53	-
18	CLA	A	812	1,18	-	7/39/115/115	-
22	SF4	C	102	3	-	-	0/6/5/5
18	CLA	A	821	1	-	5/15/91/115	-
18	CLA	B	815	2	-	6/33/109/115	-
18	CLA	A	807	1	-	9/39/115/115	-
18	CLA	A	827	31	-	5/27/103/115	-
27	CHL	4	607	-	-	1/23/99/117	-
18	CLA	B	832	31	-	0/15/91/115	-
18	CLA	B	836	31	-	5/39/115/115	-
18	CLA	3	304	31	-	3/15/91/115	-
21	BCR	A	852	-	-	4/29/63/63	0/2/2/2
17	CL0	H	202	6	-	9/27/103/115	-
18	CLA	A	842	1	-	8/39/115/115	-
18	CLA	A	855	31	-	5/39/115/115	-
18	CLA	4	613	16	-	2/17/93/115	-
27	CHL	2	605	31	-	2/23/99/117	-
30	QDL	4	617	-	-	0/30/80/80	0/3/3/3
18	CLA	B	813	2	-	4/39/115/115	-
18	CLA	B	829	2	-	4/39/115/115	-
21	BCR	I	101	-	-	0/29/63/63	0/2/2/2
22	SF4	A	853	1,2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	820	2	-	6/39/115/115	-
23	LMG	4	619	-	-	1/41/61/70	0/1/1/1
24	LMU	G	203	-	-	3/21/61/61	0/2/2/2
22	SF4	C	101	3	-	-	0/6/5/5
18	CLA	A	826	31	-	7/39/115/115	-
20	LHG	A	847	18	-	12/35/35/53	-
18	CLA	A	817	31	-	5/15/91/115	-
18	CLA	2	601	14	-	7/39/115/115	-
18	CLA	L	305	31	-	1/15/91/115	-
18	CLA	3	303	-	-	4/15/91/115	-

All (672) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	607	CHL	MG-NB	-7.28	1.91	2.05
27	3	306	CHL	MG-NB	-7.28	1.91	2.05
27	2	607	CHL	MG-NB	-7.23	1.91	2.05
27	1	307	CHL	MG-NB	-7.21	1.91	2.05
27	1	302	CHL	MG-NB	-7.18	1.91	2.05
27	4	606	CHL	MG-NB	-7.15	1.91	2.05
27	3	301	CHL	MG-NB	-7.13	1.91	2.05
27	2	614	CHL	MG-NB	-7.09	1.91	2.05
27	2	605	CHL	MG-NB	-7.09	1.91	2.05
27	4	605	CHL	MG-NB	-7.06	1.91	2.05
27	2	606	CHL	MG-NB	-7.05	1.91	2.05
27	4	615	CHL	MG-NB	-6.97	1.92	2.05
27	2	614	CHL	C4B-NB	6.79	1.46	1.37
27	1	307	CHL	C4B-NB	6.71	1.46	1.37
27	2	606	CHL	C4B-NB	6.65	1.46	1.37
27	4	615	CHL	C4B-NB	6.64	1.46	1.37
27	3	306	CHL	C4B-NB	6.63	1.45	1.37
27	3	301	CHL	C4B-NB	6.62	1.45	1.37
27	2	605	CHL	C4B-NB	6.62	1.45	1.37
27	4	605	CHL	C4B-NB	6.59	1.45	1.37
27	2	607	CHL	C4B-NB	6.54	1.45	1.37
27	4	607	CHL	C4B-NB	6.49	1.45	1.37
27	4	606	CHL	C4B-NB	6.43	1.45	1.37
27	1	302	CHL	C4B-NB	6.29	1.45	1.37
18	B	801	CLA	C1D-ND	6.23	1.45	1.37
18	B	825	CLA	C1D-ND	6.19	1.45	1.37
17	A	801	CL0	C4B-NB	6.06	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	807	CLA	C1D-ND	5.97	1.45	1.37
27	1	302	CHL	MG-ND	-5.97	1.94	2.05
18	3	302	CLA	C1D-ND	5.95	1.45	1.37
18	A	831	CLA	C1D-ND	5.93	1.45	1.37
18	4	603	CLA	C1D-ND	5.93	1.45	1.37
18	A	845	CLA	C1D-ND	5.91	1.45	1.37
18	B	826	CLA	C1D-ND	5.91	1.45	1.37
18	A	840	CLA	C1D-ND	5.91	1.45	1.37
18	A	829	CLA	C1D-ND	5.90	1.45	1.37
18	B	822	CLA	C1D-ND	5.89	1.45	1.37
27	1	307	CHL	MG-ND	-5.87	1.94	2.05
27	3	306	CHL	MG-ND	-5.87	1.94	2.05
18	3	309	CLA	C1D-ND	5.86	1.45	1.37
18	3	311	CLA	C1D-ND	5.85	1.45	1.37
27	2	607	CHL	MG-ND	-5.84	1.94	2.05
27	4	607	CHL	MG-ND	-5.84	1.94	2.05
18	L	305	CLA	C1D-ND	5.83	1.45	1.37
27	4	606	CHL	MG-ND	-5.81	1.94	2.05
18	B	818	CLA	C1D-ND	5.81	1.44	1.37
27	4	605	CHL	MG-ND	-5.81	1.94	2.05
18	F	802	CLA	C1D-ND	5.80	1.44	1.37
18	A	825	CLA	C1D-ND	5.80	1.44	1.37
27	2	605	CHL	MG-ND	-5.79	1.94	2.05
27	2	606	CHL	MG-ND	-5.76	1.94	2.05
18	B	803	CLA	C1D-ND	5.75	1.44	1.37
27	2	614	CHL	MG-ND	-5.75	1.94	2.05
18	B	833	CLA	C1D-ND	5.75	1.44	1.37
18	1	305	CLA	C1D-ND	5.74	1.44	1.37
27	3	301	CHL	MG-ND	-5.73	1.94	2.05
18	B	805	CLA	C1D-ND	5.73	1.44	1.37
27	4	615	CHL	MG-ND	-5.73	1.94	2.05
18	A	814	CLA	C1D-ND	5.72	1.44	1.37
18	B	815	CLA	C1D-ND	5.72	1.44	1.37
18	B	808	CLA	C1D-ND	5.71	1.44	1.37
18	G	201	CLA	C1D-ND	5.71	1.44	1.37
18	1	315	CLA	C1D-ND	5.71	1.44	1.37
18	A	838	CLA	C1D-ND	5.69	1.44	1.37
18	1	309	CLA	C1D-ND	5.69	1.44	1.37
18	G	205	CLA	C1D-ND	5.69	1.44	1.37
18	4	608	CLA	C1D-ND	5.69	1.44	1.37
18	1	306	CLA	C1D-ND	5.68	1.44	1.37
18	K	204	CLA	C1D-ND	5.68	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	828	CLA	C1D-ND	5.68	1.44	1.37
18	4	611	CLA	C1D-ND	5.68	1.44	1.37
18	4	614	CLA	C1D-ND	5.67	1.44	1.37
18	F	804	CLA	C1D-ND	5.67	1.44	1.37
18	2	611	CLA	C1D-ND	5.67	1.44	1.37
18	L	303	CLA	C1D-ND	5.67	1.44	1.37
18	A	839	CLA	C1D-ND	5.67	1.44	1.37
18	A	854	CLA	C1D-ND	5.66	1.44	1.37
18	1	304	CLA	C1D-ND	5.66	1.44	1.37
18	1	312	CLA	C1D-ND	5.66	1.44	1.37
18	B	829	CLA	C1D-ND	5.65	1.44	1.37
18	A	820	CLA	C1D-ND	5.65	1.44	1.37
18	A	805	CLA	C1D-ND	5.65	1.44	1.37
18	A	819	CLA	C1D-ND	5.64	1.44	1.37
18	2	610	CLA	C1D-ND	5.64	1.44	1.37
18	B	812	CLA	C1D-ND	5.63	1.44	1.37
18	1	310	CLA	MG-NB	-5.63	1.94	2.05
18	3	303	CLA	C1D-ND	5.63	1.44	1.37
18	A	813	CLA	C1D-ND	5.62	1.44	1.37
18	3	305	CLA	C1D-ND	5.61	1.44	1.37
18	G	204	CLA	C1D-ND	5.61	1.44	1.37
18	A	830	CLA	C1D-ND	5.61	1.44	1.37
18	A	842	CLA	C1D-ND	5.61	1.44	1.37
18	B	821	CLA	C1D-ND	5.60	1.44	1.37
18	B	823	CLA	C1D-ND	5.59	1.44	1.37
18	4	601	CLA	C1D-ND	5.58	1.44	1.37
18	A	823	CLA	C1D-ND	5.57	1.44	1.37
18	3	304	CLA	C1D-ND	5.57	1.44	1.37
18	2	603	CLA	C1D-ND	5.56	1.44	1.37
18	A	807	CLA	C1D-ND	5.56	1.44	1.37
18	1	314	CLA	C1D-ND	5.55	1.44	1.37
18	A	834	CLA	C1D-ND	5.54	1.44	1.37
18	2	613	CLA	C1D-ND	5.53	1.44	1.37
18	A	804	CLA	C1D-ND	5.53	1.44	1.37
18	B	810	CLA	C1D-ND	5.53	1.44	1.37
18	2	602	CLA	C1D-ND	5.53	1.44	1.37
18	4	610	CLA	C1D-ND	5.53	1.44	1.37
18	A	821	CLA	C1D-ND	5.53	1.44	1.37
18	A	803	CLA	C1D-ND	5.53	1.44	1.37
18	4	613	CLA	C1D-ND	5.52	1.44	1.37
18	A	809	CLA	C1D-ND	5.52	1.44	1.37
18	2	601	CLA	C1D-ND	5.52	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	832	CLA	C1D-ND	5.52	1.44	1.37
18	J	102	CLA	C1D-ND	5.50	1.44	1.37
18	4	602	CLA	C1D-ND	5.48	1.44	1.37
18	A	826	CLA	C1D-ND	5.48	1.44	1.37
18	A	843	CLA	C1D-ND	5.48	1.44	1.37
17	H	202	CL0	C4B-NB	5.47	1.44	1.37
18	A	808	CLA	C1D-ND	5.47	1.44	1.37
18	4	609	CLA	C1D-ND	5.46	1.44	1.37
18	A	818	CLA	C1D-ND	5.46	1.44	1.37
18	2	604	CLA	C1D-ND	5.46	1.44	1.37
18	B	809	CLA	C1D-ND	5.46	1.44	1.37
18	B	824	CLA	C1D-ND	5.45	1.44	1.37
18	A	833	CLA	C1D-ND	5.45	1.44	1.37
18	B	835	CLA	C1D-ND	5.45	1.44	1.37
18	3	312	CLA	C1D-ND	5.44	1.44	1.37
18	1	308	CLA	C1D-ND	5.43	1.44	1.37
18	B	811	CLA	C1D-ND	5.43	1.44	1.37
18	B	839	CLA	C1D-ND	5.43	1.44	1.37
18	4	604	CLA	C1D-ND	5.43	1.44	1.37
18	1	303	CLA	C1D-ND	5.42	1.44	1.37
18	3	308	CLA	C1D-ND	5.42	1.44	1.37
18	A	855	CLA	C1D-ND	5.42	1.44	1.37
18	B	813	CLA	C1D-ND	5.41	1.44	1.37
18	1	313	CLA	C1D-ND	5.40	1.44	1.37
18	4	609	CLA	MG-NB	-5.40	1.95	2.05
18	B	816	CLA	C1D-ND	5.40	1.44	1.37
18	B	834	CLA	C1D-ND	5.39	1.44	1.37
18	2	609	CLA	C1D-ND	5.38	1.44	1.37
17	H	202	CL0	MG-NB	-5.38	1.95	2.05
27	4	607	CHL	MG-NA	-5.38	1.93	2.06
18	A	815	CLA	C1D-ND	5.37	1.44	1.37
18	A	817	CLA	C1D-ND	5.37	1.44	1.37
18	B	831	CLA	C1D-ND	5.37	1.44	1.37
18	3	310	CLA	C1D-ND	5.37	1.44	1.37
18	B	802	CLA	C1D-ND	5.36	1.44	1.37
18	A	811	CLA	C1D-ND	5.34	1.44	1.37
18	2	612	CLA	C1D-ND	5.34	1.44	1.37
27	1	307	CHL	MG-NA	-5.34	1.93	2.06
18	A	835	CLA	C1D-ND	5.33	1.44	1.37
18	3	307	CLA	MG-NB	-5.33	1.95	2.05
18	A	822	CLA	MG-NB	-5.33	1.95	2.05
18	A	856	CLA	C1D-ND	5.33	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	612	CLA	C1D-ND	5.33	1.44	1.37
18	3	307	CLA	C1D-ND	5.31	1.44	1.37
18	A	832	CLA	C1D-ND	5.31	1.44	1.37
18	B	828	CLA	C1D-ND	5.31	1.44	1.37
18	B	822	CLA	MG-NB	-5.30	1.95	2.05
18	B	827	CLA	C1D-ND	5.29	1.44	1.37
18	K	201	CLA	MG-NB	-5.28	1.95	2.05
18	A	806	CLA	C1D-ND	5.28	1.44	1.37
18	B	837	CLA	C1D-ND	5.27	1.44	1.37
18	B	820	CLA	C1D-ND	5.27	1.44	1.37
18	1	311	CLA	C1D-ND	5.26	1.44	1.37
18	B	830	CLA	C1D-ND	5.26	1.44	1.37
18	K	203	CLA	MG-NB	-5.26	1.95	2.05
18	2	608	CLA	C1D-ND	5.25	1.44	1.37
18	F	805	CLA	C1D-ND	5.24	1.44	1.37
18	K	201	CLA	C1D-ND	5.24	1.44	1.37
18	A	822	CLA	C1D-ND	5.24	1.44	1.37
18	A	816	CLA	C1D-ND	5.23	1.44	1.37
18	B	804	CLA	C1D-ND	5.22	1.44	1.37
18	3	304	CLA	MG-NB	-5.22	1.95	2.05
18	A	841	CLA	C1D-ND	5.20	1.44	1.37
18	A	837	CLA	C1D-ND	5.20	1.44	1.37
18	A	812	CLA	C1D-ND	5.20	1.44	1.37
18	B	832	CLA	MG-NB	-5.20	1.95	2.05
18	A	836	CLA	C1D-ND	5.19	1.44	1.37
18	4	610	CLA	MG-NB	-5.19	1.95	2.05
18	A	856	CLA	MG-NB	-5.18	1.95	2.05
18	K	203	CLA	C1D-ND	5.17	1.44	1.37
18	2	601	CLA	MG-NB	-5.16	1.95	2.05
18	A	826	CLA	MG-NB	-5.16	1.95	2.05
18	1	310	CLA	C1D-ND	5.16	1.44	1.37
18	B	829	CLA	MG-NB	-5.16	1.95	2.05
18	1	311	CLA	MG-NB	-5.15	1.95	2.05
18	B	806	CLA	C1D-ND	5.15	1.44	1.37
18	A	824	CLA	MG-NB	-5.13	1.95	2.05
18	G	204	CLA	MG-NB	-5.13	1.95	2.05
18	4	604	CLA	MG-NB	-5.13	1.95	2.05
17	A	801	CL0	C1D-ND	5.12	1.44	1.37
27	4	606	CHL	MG-NA	-5.12	1.94	2.06
18	A	845	CLA	MG-NB	-5.11	1.95	2.05
18	A	823	CLA	MG-NB	-5.11	1.95	2.05
18	G	205	CLA	MG-NB	-5.11	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	810	CLA	C1D-ND	5.11	1.44	1.37
18	B	817	CLA	MG-NB	-5.10	1.95	2.05
18	A	817	CLA	MG-NB	-5.10	1.95	2.05
18	2	609	CLA	MG-NB	-5.09	1.95	2.05
18	B	819	CLA	C1D-ND	5.08	1.44	1.37
18	B	839	CLA	MG-NB	-5.08	1.95	2.05
18	2	610	CLA	MG-NB	-5.07	1.95	2.05
18	A	854	CLA	MG-NB	-5.07	1.95	2.05
18	2	612	CLA	MG-NB	-5.07	1.95	2.05
18	B	814	CLA	C1D-ND	5.06	1.44	1.37
18	L	304	CLA	C1D-ND	5.06	1.44	1.37
18	3	311	CLA	MG-NB	-5.06	1.95	2.05
18	A	813	CLA	MG-NB	-5.06	1.95	2.05
18	B	817	CLA	C1D-ND	5.05	1.44	1.37
18	2	602	CLA	MG-NB	-5.05	1.95	2.05
18	K	204	CLA	MG-NB	-5.05	1.95	2.05
18	2	604	CLA	MG-NB	-5.05	1.95	2.05
18	J	102	CLA	MG-NB	-5.05	1.95	2.05
18	1	308	CLA	MG-NB	-5.04	1.95	2.05
18	A	827	CLA	C1D-ND	5.04	1.44	1.37
27	2	607	CHL	MG-NA	-5.03	1.94	2.06
18	1	313	CLA	MG-NB	-5.03	1.95	2.05
18	2	608	CLA	MG-NB	-5.03	1.95	2.05
27	2	605	CHL	MG-NA	-5.02	1.94	2.06
18	A	803	CLA	MG-NB	-5.02	1.95	2.05
18	A	819	CLA	MG-NB	-5.02	1.95	2.05
18	3	305	CLA	MG-NB	-5.02	1.95	2.05
27	1	302	CHL	MG-NA	-5.00	1.94	2.06
18	1	305	CLA	MG-NB	-4.99	1.95	2.05
18	4	602	CLA	MG-NB	-4.99	1.95	2.05
18	1	314	CLA	MG-NB	-4.99	1.95	2.05
18	A	821	CLA	MG-NB	-4.98	1.95	2.05
18	B	825	CLA	MG-NB	-4.98	1.95	2.05
18	B	836	CLA	C1D-ND	4.98	1.43	1.37
18	1	303	CLA	MG-NB	-4.97	1.95	2.05
18	A	833	CLA	MG-NB	-4.97	1.95	2.05
18	B	824	CLA	MG-NB	-4.96	1.95	2.05
18	3	303	CLA	MG-NB	-4.96	1.95	2.05
18	B	808	CLA	MG-NB	-4.96	1.96	2.05
18	B	818	CLA	MG-NB	-4.95	1.96	2.05
18	1	306	CLA	MG-NB	-4.94	1.96	2.05
18	4	612	CLA	MG-NB	-4.94	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	608	CLA	MG-NB	-4.94	1.96	2.05
18	A	824	CLA	C1D-ND	4.94	1.43	1.37
18	B	819	CLA	MG-NB	-4.94	1.96	2.05
18	3	312	CLA	MG-NB	-4.93	1.96	2.05
18	B	813	CLA	MG-NB	-4.91	1.96	2.05
18	3	310	CLA	MG-NB	-4.91	1.96	2.05
18	A	810	CLA	MG-NB	-4.91	1.96	2.05
17	H	202	CL0	MG-ND	-4.89	1.96	2.05
18	B	810	CLA	MG-NB	-4.89	1.96	2.05
18	B	816	CLA	MG-NB	-4.88	1.96	2.05
18	B	815	CLA	MG-NB	-4.88	1.96	2.05
18	B	806	CLA	MG-NB	-4.88	1.96	2.05
18	A	837	CLA	MG-NB	-4.88	1.96	2.05
18	3	308	CLA	MG-NB	-4.88	1.96	2.05
18	B	812	CLA	MG-NB	-4.87	1.96	2.05
18	A	815	CLA	MG-NB	-4.87	1.96	2.05
18	B	821	CLA	MG-NB	-4.87	1.96	2.05
18	B	811	CLA	MG-NB	-4.86	1.96	2.05
18	B	820	CLA	MG-NB	-4.85	1.96	2.05
18	F	804	CLA	MG-NB	-4.83	1.96	2.05
27	4	605	CHL	MG-NA	-4.83	1.94	2.06
18	4	601	CLA	MG-NB	-4.82	1.96	2.05
18	A	828	CLA	MG-NB	-4.82	1.96	2.05
18	A	836	CLA	MG-NB	-4.81	1.96	2.05
18	L	305	CLA	MG-NB	-4.81	1.96	2.05
17	H	202	CL0	C1D-ND	4.81	1.43	1.37
18	2	613	CLA	MG-NB	-4.80	1.96	2.05
17	A	801	CL0	MG-NB	-4.80	1.96	2.05
18	L	303	CLA	MG-NB	-4.80	1.96	2.05
18	2	611	CLA	MG-NB	-4.79	1.96	2.05
18	A	809	CLA	MG-NB	-4.79	1.96	2.05
18	B	809	CLA	MG-NB	-4.79	1.96	2.05
18	F	802	CLA	MG-NB	-4.77	1.96	2.05
27	3	306	CHL	MG-NA	-4.76	1.95	2.06
18	4	613	CLA	MG-NB	-4.76	1.96	2.05
18	1	315	CLA	MG-NB	-4.75	1.96	2.05
17	H	202	CL0	MG-NA	-4.74	1.95	2.06
18	B	804	CLA	MG-NB	-4.74	1.96	2.05
27	3	301	CHL	MG-NA	-4.74	1.95	2.06
18	A	827	CLA	MG-NB	-4.73	1.96	2.05
18	A	814	CLA	MG-NB	-4.72	1.96	2.05
18	3	302	CLA	MG-NB	-4.72	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	606	CHL	MG-NA	-4.72	1.95	2.06
18	4	611	CLA	MG-NB	-4.71	1.96	2.05
18	A	806	CLA	MG-NB	-4.70	1.96	2.05
18	B	831	CLA	MG-NB	-4.70	1.96	2.05
18	A	807	CLA	MG-NB	-4.70	1.96	2.05
27	4	615	CHL	MG-NA	-4.69	1.95	2.06
18	A	804	CLA	MG-NB	-4.69	1.96	2.05
18	B	803	CLA	MG-NB	-4.68	1.96	2.05
18	1	312	CLA	MG-NB	-4.68	1.96	2.05
18	B	830	CLA	MG-NB	-4.68	1.96	2.05
18	B	827	CLA	MG-NB	-4.68	1.96	2.05
18	A	829	CLA	MG-NB	-4.67	1.96	2.05
18	A	812	CLA	MG-NB	-4.67	1.96	2.05
18	L	304	CLA	MG-NB	-4.67	1.96	2.05
27	2	614	CHL	MG-NA	-4.66	1.95	2.06
18	1	304	CLA	MG-NB	-4.66	1.96	2.05
18	1	309	CLA	MG-NB	-4.66	1.96	2.05
18	A	825	CLA	MG-NB	-4.66	1.96	2.05
18	B	805	CLA	MG-NB	-4.66	1.96	2.05
18	A	808	CLA	MG-NB	-4.65	1.96	2.05
18	A	820	CLA	MG-NB	-4.64	1.96	2.05
18	3	309	CLA	MG-NB	-4.63	1.96	2.05
18	A	816	CLA	MG-NB	-4.60	1.96	2.05
18	B	811	CLA	MG-ND	-4.58	1.96	2.05
18	B	836	CLA	MG-NB	-4.58	1.96	2.05
18	A	811	CLA	MG-NB	-4.57	1.96	2.05
18	A	835	CLA	MG-NB	-4.57	1.96	2.05
18	A	843	CLA	MG-NB	-4.56	1.96	2.05
18	B	802	CLA	MG-NB	-4.56	1.96	2.05
18	B	835	CLA	MG-NB	-4.56	1.96	2.05
18	K	201	CLA	MG-ND	-4.55	1.96	2.05
18	2	603	CLA	MG-NB	-4.55	1.96	2.05
18	B	823	CLA	MG-NB	-4.53	1.96	2.05
18	A	805	CLA	MG-NB	-4.52	1.96	2.05
18	4	614	CLA	MG-NB	-4.51	1.96	2.05
18	A	818	CLA	MG-NB	-4.50	1.96	2.05
18	A	834	CLA	MG-NB	-4.50	1.96	2.05
18	G	201	CLA	MG-NB	-4.50	1.96	2.05
18	F	805	CLA	MG-NB	-4.46	1.96	2.05
18	A	832	CLA	MG-NB	-4.46	1.97	2.05
18	A	838	CLA	MG-NB	-4.46	1.97	2.05
18	A	840	CLA	MG-NB	-4.45	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	612	CLA	MG-ND	-4.42	1.97	2.05
18	B	814	CLA	MG-NB	-4.42	1.97	2.05
18	A	810	CLA	MG-ND	-4.38	1.97	2.05
18	1	308	CLA	MG-ND	-4.38	1.97	2.05
18	K	203	CLA	MG-ND	-4.36	1.97	2.05
18	A	841	CLA	MG-NB	-4.36	1.97	2.05
18	A	802	CLA	C1D-ND	4.34	1.43	1.37
18	A	820	CLA	MG-ND	-4.33	1.97	2.05
18	B	826	CLA	MG-NB	-4.32	1.97	2.05
18	A	839	CLA	MG-NB	-4.32	1.97	2.05
18	B	834	CLA	MG-NB	-4.28	1.97	2.05
18	B	833	CLA	MG-NB	-4.28	1.97	2.05
18	A	802	CLA	MG-NB	-4.28	1.97	2.05
18	B	801	CLA	MG-NB	-4.27	1.97	2.05
18	A	824	CLA	MG-ND	-4.26	1.97	2.05
18	B	805	CLA	MG-ND	-4.26	1.97	2.05
18	4	602	CLA	MG-ND	-4.26	1.97	2.05
18	4	604	CLA	MG-ND	-4.25	1.97	2.05
18	A	836	CLA	MG-ND	-4.25	1.97	2.05
18	A	855	CLA	MG-NB	-4.23	1.97	2.05
18	B	837	CLA	MG-NB	-4.22	1.97	2.05
18	B	839	CLA	MG-ND	-4.22	1.97	2.05
18	4	608	CLA	MG-ND	-4.21	1.97	2.05
18	4	612	CLA	MG-ND	-4.21	1.97	2.05
18	3	310	CLA	MG-ND	-4.21	1.97	2.05
17	A	801	CL0	MG-NA	-4.19	1.96	2.06
18	3	307	CLA	MG-ND	-4.18	1.97	2.05
18	3	304	CLA	MG-ND	-4.18	1.97	2.05
18	A	842	CLA	MG-NB	-4.16	1.97	2.05
18	K	204	CLA	MG-ND	-4.16	1.97	2.05
18	2	602	CLA	MG-ND	-4.15	1.97	2.05
18	B	832	CLA	MG-ND	-4.15	1.97	2.05
18	1	310	CLA	MG-ND	-4.15	1.97	2.05
18	2	604	CLA	MG-ND	-4.15	1.97	2.05
18	1	314	CLA	MG-ND	-4.15	1.97	2.05
18	2	601	CLA	MG-ND	-4.15	1.97	2.05
18	B	828	CLA	MG-NB	-4.14	1.97	2.05
18	A	831	CLA	MG-NB	-4.13	1.97	2.05
17	H	202	CL0	MG-NC	-4.13	1.96	2.06
18	B	821	CLA	MG-ND	-4.13	1.97	2.05
18	2	610	CLA	MG-ND	-4.12	1.97	2.05
18	4	609	CLA	MG-ND	-4.11	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	303	CLA	MG-ND	-4.11	1.97	2.05
18	1	309	CLA	MG-ND	-4.10	1.97	2.05
18	4	601	CLA	MG-ND	-4.10	1.97	2.05
18	A	830	CLA	MG-ND	-4.10	1.97	2.05
18	2	603	CLA	MG-ND	-4.09	1.97	2.05
18	3	312	CLA	MG-ND	-4.09	1.97	2.05
18	3	303	CLA	MG-ND	-4.09	1.97	2.05
18	A	830	CLA	MG-NB	-4.09	1.97	2.05
18	1	313	CLA	MG-ND	-4.09	1.97	2.05
18	A	822	CLA	MG-ND	-4.08	1.97	2.05
18	B	828	CLA	MG-ND	-4.08	1.97	2.05
18	A	813	CLA	MG-ND	-4.07	1.97	2.05
18	A	856	CLA	MG-ND	-4.07	1.97	2.05
18	2	613	CLA	MG-ND	-4.07	1.97	2.05
18	2	608	CLA	MG-ND	-4.06	1.97	2.05
18	B	807	CLA	MG-NB	-4.06	1.97	2.05
18	1	305	CLA	MG-ND	-4.06	1.97	2.05
18	A	817	CLA	MG-ND	-4.06	1.97	2.05
18	1	306	CLA	MG-ND	-4.05	1.97	2.05
18	2	609	CLA	MG-ND	-4.05	1.97	2.05
18	A	825	CLA	MG-ND	-4.05	1.97	2.05
18	1	311	CLA	MG-ND	-4.05	1.97	2.05
18	3	305	CLA	MG-ND	-4.05	1.97	2.05
18	G	204	CLA	MG-ND	-4.04	1.97	2.05
18	B	816	CLA	MG-ND	-4.04	1.97	2.05
18	1	312	CLA	MG-ND	-4.04	1.97	2.05
18	4	610	CLA	MG-ND	-4.04	1.97	2.05
18	B	824	CLA	MG-ND	-4.03	1.97	2.05
18	4	603	CLA	MG-NB	-4.03	1.97	2.05
18	3	302	CLA	MG-ND	-4.03	1.97	2.05
18	A	818	CLA	MG-ND	-4.02	1.97	2.05
18	A	807	CLA	MG-ND	-4.02	1.97	2.05
18	3	308	CLA	MG-ND	-4.02	1.97	2.05
18	B	830	CLA	MG-ND	-4.01	1.97	2.05
18	B	836	CLA	MG-ND	-4.01	1.97	2.05
18	4	611	CLA	MG-ND	-4.00	1.97	2.05
18	A	835	CLA	MG-ND	-3.99	1.97	2.05
18	3	311	CLA	MG-ND	-3.99	1.97	2.05
18	L	303	CLA	MG-ND	-3.99	1.97	2.05
18	B	819	CLA	MG-ND	-3.99	1.97	2.05
18	G	201	CLA	MG-ND	-3.98	1.97	2.05
18	A	837	CLA	MG-ND	-3.97	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	817	CLA	MG-ND	-3.97	1.97	2.05
18	A	833	CLA	MG-ND	-3.96	1.97	2.05
18	A	823	CLA	MG-ND	-3.95	1.98	2.05
18	4	613	CLA	MG-ND	-3.95	1.98	2.05
18	B	813	CLA	MG-ND	-3.94	1.98	2.05
18	B	818	CLA	MG-ND	-3.94	1.98	2.05
18	F	804	CLA	MG-ND	-3.94	1.98	2.05
18	G	205	CLA	MG-ND	-3.94	1.98	2.05
18	A	821	CLA	MG-ND	-3.93	1.98	2.05
18	1	315	CLA	MG-ND	-3.93	1.98	2.05
18	B	808	CLA	MG-ND	-3.93	1.98	2.05
18	B	829	CLA	MG-ND	-3.92	1.98	2.05
18	A	845	CLA	MG-ND	-3.92	1.98	2.05
18	B	822	CLA	MG-ND	-3.92	1.98	2.05
18	B	814	CLA	MG-ND	-3.91	1.98	2.05
18	A	812	CLA	MG-ND	-3.90	1.98	2.05
18	A	828	CLA	MG-ND	-3.89	1.98	2.05
18	A	834	CLA	MG-ND	-3.89	1.98	2.05
18	A	816	CLA	MG-ND	-3.89	1.98	2.05
18	L	305	CLA	MG-ND	-3.89	1.98	2.05
18	B	831	CLA	MG-ND	-3.87	1.98	2.05
18	B	806	CLA	MG-ND	-3.87	1.98	2.05
18	F	805	CLA	MG-ND	-3.86	1.98	2.05
18	J	102	CLA	MG-ND	-3.86	1.98	2.05
18	B	826	CLA	MG-ND	-3.85	1.98	2.05
18	L	304	CLA	MG-ND	-3.85	1.98	2.05
18	A	832	CLA	MG-ND	-3.84	1.98	2.05
18	2	611	CLA	MG-ND	-3.84	1.98	2.05
18	B	835	CLA	MG-ND	-3.83	1.98	2.05
18	A	811	CLA	MG-ND	-3.82	1.98	2.05
18	A	804	CLA	MG-ND	-3.82	1.98	2.05
18	1	304	CLA	MG-ND	-3.82	1.98	2.05
27	2	606	CHL	C1D-ND	3.82	1.42	1.37
18	A	802	CLA	MG-ND	-3.82	1.98	2.05
18	B	815	CLA	MG-ND	-3.81	1.98	2.05
18	A	809	CLA	MG-ND	-3.81	1.98	2.05
18	A	803	CLA	MG-ND	-3.81	1.98	2.05
18	A	827	CLA	MG-ND	-3.81	1.98	2.05
18	A	843	CLA	MG-ND	-3.80	1.98	2.05
18	A	814	CLA	MG-ND	-3.80	1.98	2.05
18	B	802	CLA	MG-ND	-3.79	1.98	2.05
18	B	827	CLA	MG-ND	-3.79	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	803	CLA	MG-ND	-3.78	1.98	2.05
18	A	819	CLA	MG-ND	-3.77	1.98	2.05
18	B	820	CLA	MG-ND	-3.75	1.98	2.05
18	A	826	CLA	MG-ND	-3.75	1.98	2.05
18	A	841	CLA	MG-ND	-3.74	1.98	2.05
18	B	809	CLA	MG-ND	-3.74	1.98	2.05
17	A	801	CL0	MG-ND	-3.74	1.98	2.05
18	B	810	CLA	MG-ND	-3.73	1.98	2.05
18	3	309	CLA	MG-ND	-3.73	1.98	2.05
18	B	825	CLA	MG-ND	-3.72	1.98	2.05
18	A	815	CLA	MG-ND	-3.72	1.98	2.05
18	A	808	CLA	MG-ND	-3.71	1.98	2.05
27	4	615	CHL	C1D-ND	3.69	1.42	1.37
27	2	605	CHL	C1D-ND	3.69	1.42	1.37
18	F	802	CLA	MG-ND	-3.68	1.98	2.05
27	4	605	CHL	C1D-ND	3.68	1.42	1.37
18	A	855	CLA	MG-ND	-3.67	1.98	2.05
27	2	614	CHL	C1D-ND	3.67	1.42	1.37
18	A	805	CLA	MG-ND	-3.67	1.98	2.05
18	B	812	CLA	MG-ND	-3.66	1.98	2.05
27	3	301	CHL	C1D-ND	3.66	1.42	1.37
18	A	831	CLA	MG-ND	-3.65	1.98	2.05
18	A	854	CLA	MG-ND	-3.63	1.98	2.05
18	A	838	CLA	MG-ND	-3.63	1.98	2.05
18	4	614	CLA	MG-ND	-3.59	1.98	2.05
18	A	829	CLA	MG-ND	-3.58	1.98	2.05
18	A	839	CLA	MG-ND	-3.58	1.98	2.05
18	4	603	CLA	MG-ND	-3.55	1.98	2.05
18	A	806	CLA	MG-ND	-3.53	1.98	2.05
18	B	804	CLA	MG-ND	-3.50	1.98	2.05
18	A	840	CLA	MG-ND	-3.49	1.98	2.05
18	B	833	CLA	MG-ND	-3.47	1.98	2.05
18	B	823	CLA	MG-ND	-3.47	1.98	2.05
27	3	306	CHL	C1D-ND	3.46	1.42	1.37
18	B	837	CLA	MG-ND	-3.46	1.98	2.05
18	B	807	CLA	MG-ND	-3.44	1.99	2.05
27	4	606	CHL	C1D-ND	3.44	1.42	1.37
18	B	834	CLA	MG-ND	-3.40	1.99	2.05
27	4	607	CHL	C1D-ND	3.40	1.42	1.37
27	1	307	CHL	C1D-ND	3.37	1.41	1.37
27	2	607	CHL	C1D-ND	3.35	1.41	1.37
17	H	202	CL0	C1B-NB	3.34	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1	302	CHL	C1D-ND	3.30	1.41	1.37
27	4	607	CHL	MG-NC	-3.25	1.98	2.06
27	1	307	CHL	MG-NC	-3.15	1.98	2.06
27	2	605	CHL	MG-NC	-3.13	1.98	2.06
27	4	606	CHL	MG-NC	-3.08	1.98	2.06
18	B	801	CLA	MG-ND	-3.08	1.99	2.05
27	2	607	CHL	MG-NC	-3.08	1.99	2.06
18	A	842	CLA	MG-ND	-3.04	1.99	2.05
17	A	801	CL0	MG-NC	-3.03	1.99	2.06
27	2	606	CHL	MG-NC	-2.98	1.99	2.06
27	1	302	CHL	MG-NC	-2.97	1.99	2.06
17	A	801	CL0	C1B-NB	2.94	1.41	1.37
27	4	605	CHL	MG-NC	-2.94	1.99	2.06
27	3	301	CHL	MG-NC	-2.91	1.99	2.06
27	4	615	CHL	MG-NC	-2.86	1.99	2.06
27	3	306	CHL	MG-NC	-2.78	1.99	2.06
27	2	614	CHL	MG-NC	-2.74	1.99	2.06
18	G	201	CLA	C1D-C2D	-2.51	1.40	1.45
18	B	803	CLA	C1D-C2D	-2.51	1.40	1.45
18	B	822	CLA	C1D-C2D	-2.47	1.40	1.45
18	B	815	CLA	C1D-C2D	-2.47	1.40	1.45
18	B	801	CLA	C1D-C2D	-2.46	1.40	1.45
18	B	821	CLA	C1D-C2D	-2.46	1.40	1.45
18	F	802	CLA	C1D-C2D	-2.46	1.40	1.45
18	A	818	CLA	C1D-C2D	-2.46	1.40	1.45
18	4	603	CLA	C1D-C2D	-2.45	1.40	1.45
18	A	807	CLA	C1D-C2D	-2.44	1.40	1.45
18	A	813	CLA	C1D-C2D	-2.44	1.40	1.45
18	A	825	CLA	C1D-C2D	-2.44	1.40	1.45
18	1	309	CLA	C1D-C2D	-2.44	1.40	1.45
18	B	805	CLA	C1D-C2D	-2.44	1.40	1.45
18	B	825	CLA	C1D-C2D	-2.43	1.40	1.45
18	F	805	CLA	C1D-C2D	-2.43	1.40	1.45
18	B	807	CLA	C1D-C2D	-2.43	1.40	1.45
18	B	811	CLA	C1D-C2D	-2.43	1.40	1.45
18	4	608	CLA	C1D-C2D	-2.42	1.40	1.45
18	A	833	CLA	C1D-C2D	-2.42	1.40	1.45
18	A	826	CLA	C1D-C2D	-2.41	1.40	1.45
18	1	315	CLA	C1D-C2D	-2.41	1.40	1.45
18	4	612	CLA	C1D-C2D	-2.40	1.40	1.45
18	A	827	CLA	C1D-C2D	-2.40	1.40	1.45
18	A	830	CLA	C1D-C2D	-2.40	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	829	CLA	C1D-C2D	-2.39	1.40	1.45
18	2	608	CLA	C1D-C2D	-2.39	1.40	1.45
18	F	804	CLA	C1D-C2D	-2.39	1.40	1.45
18	3	302	CLA	C1D-C2D	-2.39	1.40	1.45
18	4	611	CLA	C1D-C2D	-2.39	1.40	1.45
18	A	802	CLA	C1D-C2D	-2.39	1.40	1.45
18	B	827	CLA	C1D-C2D	-2.39	1.40	1.45
18	4	609	CLA	C1D-C2D	-2.39	1.40	1.45
18	A	817	CLA	C1D-C2D	-2.39	1.40	1.45
18	3	304	CLA	C1D-C2D	-2.38	1.40	1.45
18	A	839	CLA	C1D-C2D	-2.38	1.40	1.45
18	A	836	CLA	C1D-C2D	-2.38	1.40	1.45
18	B	818	CLA	C1D-C2D	-2.38	1.40	1.45
18	A	843	CLA	C1D-C2D	-2.38	1.40	1.45
18	A	831	CLA	C1D-C2D	-2.38	1.40	1.45
18	2	601	CLA	C1D-C2D	-2.38	1.40	1.45
18	4	614	CLA	C1D-C2D	-2.38	1.40	1.45
18	B	836	CLA	C1D-C2D	-2.37	1.40	1.45
18	2	603	CLA	C1D-C2D	-2.37	1.40	1.45
18	3	308	CLA	C1D-C2D	-2.37	1.40	1.45
18	A	814	CLA	C1D-C2D	-2.37	1.40	1.45
18	2	612	CLA	C1D-C2D	-2.37	1.40	1.45
18	4	602	CLA	C1D-C2D	-2.37	1.40	1.45
18	L	305	CLA	C1D-C2D	-2.37	1.40	1.45
18	B	802	CLA	C1D-C2D	-2.37	1.40	1.45
18	3	305	CLA	C1D-C2D	-2.37	1.40	1.45
18	B	824	CLA	C1D-C2D	-2.37	1.40	1.45
18	B	826	CLA	C1D-C2D	-2.37	1.40	1.45
18	1	310	CLA	C1D-C2D	-2.37	1.40	1.45
18	A	820	CLA	C1D-C2D	-2.37	1.40	1.45
18	A	840	CLA	C1D-C2D	-2.37	1.40	1.45
18	3	312	CLA	C1D-C2D	-2.36	1.40	1.45
18	3	307	CLA	C1D-C2D	-2.36	1.40	1.45
18	A	809	CLA	C1D-C2D	-2.36	1.40	1.45
18	1	306	CLA	C1D-C2D	-2.36	1.40	1.45
18	4	601	CLA	C1D-C2D	-2.36	1.40	1.45
18	B	835	CLA	C1D-C2D	-2.36	1.40	1.45
18	4	613	CLA	C1D-C2D	-2.36	1.40	1.45
18	B	806	CLA	C1D-C2D	-2.35	1.40	1.45
18	1	308	CLA	C1D-C2D	-2.35	1.40	1.45
18	A	805	CLA	C1D-C2D	-2.35	1.40	1.45
18	A	821	CLA	C1D-C2D	-2.35	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	808	CLA	C1D-C2D	-2.35	1.40	1.45
18	2	602	CLA	C1D-C2D	-2.35	1.40	1.45
18	1	314	CLA	C1D-C2D	-2.35	1.40	1.45
18	A	855	CLA	C1D-C2D	-2.35	1.40	1.45
18	A	812	CLA	C1D-C2D	-2.35	1.40	1.45
18	G	205	CLA	C1D-C2D	-2.34	1.40	1.45
18	A	819	CLA	C1D-C2D	-2.34	1.40	1.45
18	B	831	CLA	C1D-C2D	-2.34	1.40	1.45
18	1	313	CLA	C1D-C2D	-2.34	1.40	1.45
18	A	816	CLA	C1D-C2D	-2.34	1.40	1.45
18	B	832	CLA	C1D-C2D	-2.34	1.40	1.45
18	A	834	CLA	C1D-C2D	-2.34	1.40	1.45
18	B	808	CLA	C1D-C2D	-2.34	1.40	1.45
18	B	829	CLA	C1D-C2D	-2.34	1.40	1.45
18	2	604	CLA	C1D-C2D	-2.34	1.40	1.45
18	B	813	CLA	C1D-C2D	-2.34	1.40	1.45
18	L	304	CLA	C1D-C2D	-2.34	1.40	1.45
18	A	841	CLA	C1D-C2D	-2.34	1.40	1.45
27	2	614	CHL	C1D-C2D	-2.34	1.40	1.45
18	4	610	CLA	C1D-C2D	-2.33	1.40	1.45
18	A	837	CLA	C1D-C2D	-2.33	1.40	1.45
18	A	804	CLA	C1D-C2D	-2.33	1.40	1.45
18	B	833	CLA	C1D-C2D	-2.33	1.40	1.45
18	K	204	CLA	C1D-C2D	-2.33	1.40	1.45
18	A	854	CLA	C1D-C2D	-2.33	1.40	1.45
18	1	311	CLA	C1D-C2D	-2.33	1.40	1.45
18	1	305	CLA	C1D-C2D	-2.33	1.40	1.45
18	2	609	CLA	C1D-C2D	-2.33	1.40	1.45
18	A	835	CLA	C1D-C2D	-2.33	1.40	1.45
27	2	607	CHL	C1D-C2D	-2.33	1.40	1.45
18	A	806	CLA	C1D-C2D	-2.33	1.40	1.45
18	A	828	CLA	C1D-C2D	-2.33	1.40	1.45
18	1	304	CLA	C1D-C2D	-2.32	1.40	1.45
18	A	811	CLA	C1D-C2D	-2.32	1.40	1.45
18	2	610	CLA	C1D-C2D	-2.32	1.40	1.45
18	B	839	CLA	C1D-C2D	-2.32	1.40	1.45
18	A	832	CLA	C1D-C2D	-2.32	1.40	1.45
18	K	203	CLA	C1D-C2D	-2.32	1.40	1.45
18	B	812	CLA	C1D-C2D	-2.32	1.40	1.45
18	A	842	CLA	C1D-C2D	-2.32	1.40	1.45
18	2	611	CLA	C1D-C2D	-2.32	1.40	1.45
18	B	814	CLA	C1D-C2D	-2.32	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	834	CLA	C1D-C2D	-2.32	1.40	1.45
18	1	303	CLA	C1D-C2D	-2.32	1.40	1.45
27	4	605	CHL	C1D-C2D	-2.31	1.40	1.45
27	3	301	CHL	C1D-C2D	-2.31	1.40	1.45
18	B	816	CLA	C1D-C2D	-2.31	1.40	1.45
18	4	604	CLA	C1D-C2D	-2.31	1.40	1.45
18	A	822	CLA	C1D-C2D	-2.31	1.40	1.45
18	A	856	CLA	C1D-C2D	-2.31	1.40	1.45
18	3	311	CLA	C1D-C2D	-2.31	1.40	1.45
18	B	810	CLA	C1D-C2D	-2.31	1.40	1.45
18	3	309	CLA	C1D-C2D	-2.31	1.40	1.45
18	A	845	CLA	C1D-C2D	-2.30	1.40	1.45
18	3	303	CLA	C1D-C2D	-2.30	1.40	1.45
18	A	838	CLA	C1D-C2D	-2.30	1.40	1.45
18	3	310	CLA	C1D-C2D	-2.30	1.40	1.45
18	J	102	CLA	C1D-C2D	-2.30	1.40	1.45
18	B	837	CLA	C1D-C2D	-2.30	1.40	1.45
18	G	204	CLA	C1D-C2D	-2.30	1.40	1.45
18	2	613	CLA	C1D-C2D	-2.30	1.40	1.45
18	1	312	CLA	C1D-C2D	-2.30	1.40	1.45
27	4	615	CHL	C1D-C2D	-2.29	1.40	1.45
18	B	828	CLA	C1D-C2D	-2.29	1.40	1.45
18	B	809	CLA	C1D-C2D	-2.29	1.40	1.45
27	2	606	CHL	C1D-C2D	-2.29	1.40	1.45
18	B	820	CLA	C1D-C2D	-2.28	1.40	1.45
17	A	801	CL0	C1D-C2D	-2.28	1.40	1.45
18	B	823	CLA	C1D-C2D	-2.28	1.40	1.45
27	1	302	CHL	C1D-C2D	-2.28	1.40	1.45
18	A	803	CLA	C1D-C2D	-2.28	1.40	1.45
18	A	824	CLA	C1D-C2D	-2.27	1.40	1.45
18	K	201	CLA	C1D-C2D	-2.27	1.40	1.45
27	3	306	CHL	C1D-C2D	-2.27	1.40	1.45
27	4	607	CHL	C1D-C2D	-2.27	1.40	1.45
18	A	810	CLA	C1D-C2D	-2.27	1.40	1.45
18	A	823	CLA	C1D-C2D	-2.26	1.40	1.45
18	L	303	CLA	C1D-C2D	-2.26	1.40	1.45
18	B	830	CLA	C1D-C2D	-2.26	1.40	1.45
18	B	817	CLA	C1D-C2D	-2.26	1.40	1.45
18	A	815	CLA	C1D-C2D	-2.25	1.40	1.45
27	1	307	CHL	C1D-C2D	-2.24	1.40	1.45
18	B	804	CLA	C1D-C2D	-2.23	1.40	1.45
27	4	606	CHL	C1D-C2D	-2.23	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	605	CHL	C1D-C2D	-2.22	1.40	1.45
18	B	819	CLA	C1D-C2D	-2.16	1.41	1.45
17	H	202	CL0	C1D-C2D	-2.15	1.41	1.45
17	A	801	CL0	C1C-C2C	2.13	1.48	1.44
27	1	307	CHL	C2C-C1C	2.12	1.49	1.44
27	4	607	CHL	C3D-C4D	-2.09	1.39	1.44
27	2	606	CHL	C2C-C1C	2.07	1.49	1.44
27	4	606	CHL	C3D-C4D	-2.06	1.39	1.44
18	A	827	CLA	C3D-C4D	-2.05	1.39	1.44
17	H	202	CL0	C3D-C4D	-2.05	1.39	1.44
27	4	606	CHL	C2C-C1C	2.04	1.48	1.44
27	1	302	CHL	C3D-C4D	-2.02	1.39	1.44
18	A	812	CLA	C3D-C4D	-2.01	1.39	1.44
27	2	607	CHL	C3D-C4D	-2.01	1.39	1.44
18	L	304	CLA	C3D-C4D	-2.00	1.39	1.44

All (634) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	801	CL0	CHB-C1B-NB	-4.60	119.39	124.26
18	4	603	CLA	C1D-ND-C4D	-4.45	103.18	106.33
18	B	833	CLA	C1D-ND-C4D	-4.39	103.22	106.33
27	4	607	CHL	CHD-C1D-ND	-4.39	120.42	124.45
17	H	202	CL0	CHD-C1D-ND	-4.37	120.44	124.45
18	A	842	CLA	C1D-ND-C4D	-4.34	103.25	106.33
18	1	306	CLA	C1D-ND-C4D	-4.32	103.26	106.33
27	1	307	CHL	CHD-C1D-ND	-4.31	120.50	124.45
18	1	304	CLA	C1D-ND-C4D	-4.30	103.28	106.33
18	3	309	CLA	C1D-ND-C4D	-4.29	103.29	106.33
27	2	607	CHL	CHD-C1D-ND	-4.28	120.52	124.45
27	4	606	CHL	CHD-C1D-ND	-4.28	120.52	124.45
18	G	205	CLA	C1D-ND-C4D	-4.28	103.30	106.33
18	A	811	CLA	C1D-ND-C4D	-4.27	103.30	106.33
18	B	807	CLA	C1D-ND-C4D	-4.27	103.30	106.33
27	1	302	CHL	CHD-C1D-ND	-4.26	120.54	124.45
18	2	611	CLA	C1D-ND-C4D	-4.25	103.32	106.33
18	L	304	CLA	C1D-ND-C4D	-4.22	103.34	106.33
18	G	204	CLA	C1D-ND-C4D	-4.21	103.35	106.33
18	4	611	CLA	C1D-ND-C4D	-4.21	103.35	106.33
18	4	613	CLA	C1D-ND-C4D	-4.21	103.35	106.33
18	3	308	CLA	C1D-ND-C4D	-4.19	103.36	106.33
18	1	312	CLA	C1D-ND-C4D	-4.19	103.36	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	837	CLA	C1D-ND-C4D	-4.19	103.36	106.33
18	B	820	CLA	C1D-ND-C4D	-4.18	103.37	106.33
18	4	608	CLA	C1D-ND-C4D	-4.18	103.37	106.33
18	A	822	CLA	C1D-ND-C4D	-4.17	103.37	106.33
27	2	605	CHL	CHD-C1D-ND	-4.17	120.62	124.45
18	A	839	CLA	C1D-ND-C4D	-4.17	103.38	106.33
18	A	809	CLA	C1-C2-C3	4.16	133.24	126.04
18	A	845	CLA	C1D-ND-C4D	-4.16	103.38	106.33
18	L	303	CLA	C1D-ND-C4D	-4.16	103.38	106.33
18	4	614	CLA	C1D-ND-C4D	-4.16	103.38	106.33
18	A	804	CLA	C1D-ND-C4D	-4.15	103.39	106.33
27	4	615	CHL	CHD-C1D-ND	-4.14	120.64	124.45
18	2	613	CLA	C1D-ND-C4D	-4.14	103.39	106.33
18	B	823	CLA	C1D-ND-C4D	-4.14	103.39	106.33
18	1	303	CLA	C1D-ND-C4D	-4.14	103.39	106.33
18	3	302	CLA	C1D-ND-C4D	-4.13	103.40	106.33
18	A	823	CLA	C1D-ND-C4D	-4.13	103.40	106.33
27	4	605	CHL	CHD-C1D-ND	-4.12	120.67	124.45
18	A	806	CLA	C1D-ND-C4D	-4.12	103.41	106.33
18	2	610	CLA	C1D-ND-C4D	-4.12	103.41	106.33
18	A	818	CLA	C1D-ND-C4D	-4.12	103.41	106.33
17	A	801	CL0	C1D-ND-C4D	-4.11	103.41	106.33
18	B	819	CLA	C1D-ND-C4D	-4.11	103.41	106.33
27	3	306	CHL	CHD-C1D-ND	-4.11	120.68	124.45
18	A	840	CLA	C1D-ND-C4D	-4.11	103.42	106.33
18	A	816	CLA	C1D-ND-C4D	-4.11	103.42	106.33
18	A	812	CLA	C1D-ND-C4D	-4.10	103.42	106.33
18	K	204	CLA	C1D-ND-C4D	-4.10	103.42	106.33
18	1	314	CLA	C1D-ND-C4D	-4.09	103.43	106.33
18	3	311	CLA	C1D-ND-C4D	-4.09	103.43	106.33
18	A	838	CLA	C1D-ND-C4D	-4.09	103.43	106.33
18	L	305	CLA	C1D-ND-C4D	-4.09	103.43	106.33
18	2	602	CLA	C1D-ND-C4D	-4.09	103.43	106.33
18	1	308	CLA	C1D-ND-C4D	-4.09	103.43	106.33
17	H	202	CL0	CHB-C1B-NB	-4.08	119.94	124.26
17	H	202	CL0	C1D-ND-C4D	-4.08	103.44	106.33
18	J	102	CLA	C1D-ND-C4D	-4.07	103.45	106.33
18	B	814	CLA	C1D-ND-C4D	-4.07	103.45	106.33
18	B	834	CLA	C1D-ND-C4D	-4.06	103.45	106.33
18	3	303	CLA	C1D-ND-C4D	-4.06	103.45	106.33
18	B	810	CLA	C1D-ND-C4D	-4.06	103.45	106.33
18	G	201	CLA	C1D-ND-C4D	-4.05	103.45	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	837	CLA	C1D-ND-C4D	-4.05	103.46	106.33
18	B	826	CLA	C1D-ND-C4D	-4.05	103.46	106.33
18	A	815	CLA	C1D-ND-C4D	-4.05	103.46	106.33
18	B	809	CLA	C1D-ND-C4D	-4.05	103.46	106.33
18	3	312	CLA	C1D-ND-C4D	-4.04	103.46	106.33
17	H	202	CL0	CHC-C1C-NC	4.04	130.34	124.20
18	A	819	CLA	C1D-ND-C4D	-4.04	103.46	106.33
18	4	610	CLA	C1D-ND-C4D	-4.04	103.47	106.33
18	B	801	CLA	C1D-ND-C4D	-4.04	103.47	106.33
18	2	604	CLA	C1D-ND-C4D	-4.03	103.47	106.33
18	3	305	CLA	C1D-ND-C4D	-4.03	103.47	106.33
18	A	835	CLA	C1D-ND-C4D	-4.03	103.47	106.33
27	2	614	CHL	CHD-C1D-ND	-4.03	120.75	124.45
18	A	827	CLA	C1D-ND-C4D	-4.02	103.48	106.33
18	B	817	CLA	C1D-ND-C4D	-4.02	103.48	106.33
18	A	825	CLA	C1D-ND-C4D	-4.01	103.48	106.33
18	B	806	CLA	C1D-ND-C4D	-4.01	103.48	106.33
18	1	305	CLA	C1D-ND-C4D	-4.01	103.48	106.33
18	B	804	CLA	C1D-ND-C4D	-4.01	103.49	106.33
18	A	834	CLA	C1D-ND-C4D	-4.00	103.49	106.33
18	4	602	CLA	C1D-ND-C4D	-4.00	103.49	106.33
27	2	606	CHL	CHD-C1D-ND	-4.00	120.78	124.45
18	2	608	CLA	C1D-ND-C4D	-3.99	103.50	106.33
18	A	809	CLA	C1D-ND-C4D	-3.99	103.50	106.33
18	A	824	CLA	C1D-ND-C4D	-3.99	103.50	106.33
18	A	828	CLA	C1D-ND-C4D	-3.99	103.50	106.33
18	B	812	CLA	C1D-ND-C4D	-3.99	103.50	106.33
18	4	601	CLA	C1D-ND-C4D	-3.99	103.50	106.33
18	4	604	CLA	C1D-ND-C4D	-3.98	103.51	106.33
18	A	831	CLA	C1D-ND-C4D	-3.98	103.51	106.33
18	1	310	CLA	C1D-ND-C4D	-3.98	103.51	106.33
18	A	805	CLA	C1D-ND-C4D	-3.97	103.51	106.33
18	2	609	CLA	C1D-ND-C4D	-3.97	103.51	106.33
18	B	813	CLA	C1D-ND-C4D	-3.97	103.51	106.33
27	3	301	CHL	CHD-C1D-ND	-3.96	120.82	124.45
18	B	818	CLA	C1D-ND-C4D	-3.95	103.53	106.33
18	A	814	CLA	C1D-ND-C4D	-3.94	103.53	106.33
18	A	808	CLA	C1D-ND-C4D	-3.94	103.53	106.33
18	1	311	CLA	C1D-ND-C4D	-3.94	103.53	106.33
18	B	829	CLA	C1D-ND-C4D	-3.94	103.54	106.33
18	F	804	CLA	C1D-ND-C4D	-3.94	103.54	106.33
18	3	310	CLA	C1D-ND-C4D	-3.94	103.54	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	307	CLA	C1D-ND-C4D	-3.94	103.54	106.33
18	B	832	CLA	C1D-ND-C4D	-3.93	103.54	106.33
18	1	315	CLA	C1D-ND-C4D	-3.93	103.54	106.33
18	B	816	CLA	C1D-ND-C4D	-3.93	103.54	106.33
18	B	803	CLA	C1D-ND-C4D	-3.93	103.54	106.33
18	2	601	CLA	C1D-ND-C4D	-3.93	103.54	106.33
18	A	820	CLA	C1D-ND-C4D	-3.92	103.55	106.33
18	A	817	CLA	C1D-ND-C4D	-3.92	103.55	106.33
18	B	836	CLA	C1D-ND-C4D	-3.92	103.55	106.33
18	4	612	CLA	C1D-ND-C4D	-3.92	103.55	106.33
18	B	831	CLA	C1D-ND-C4D	-3.90	103.56	106.33
18	K	203	CLA	C1D-ND-C4D	-3.90	103.56	106.33
18	A	856	CLA	C1D-ND-C4D	-3.90	103.57	106.33
18	A	813	CLA	C1D-ND-C4D	-3.89	103.57	106.33
18	1	313	CLA	C1D-ND-C4D	-3.89	103.57	106.33
18	3	304	CLA	C1D-ND-C4D	-3.89	103.57	106.33
17	A	801	CL0	CHD-C1D-ND	-3.87	120.90	124.45
18	A	833	CLA	C1D-ND-C4D	-3.87	103.59	106.33
18	A	832	CLA	C1D-ND-C4D	-3.87	103.59	106.33
18	2	612	CLA	C1D-ND-C4D	-3.86	103.59	106.33
18	A	836	CLA	C1D-ND-C4D	-3.85	103.60	106.33
18	B	839	CLA	C1D-ND-C4D	-3.84	103.61	106.33
18	F	802	CLA	C1D-ND-C4D	-3.84	103.61	106.33
18	B	830	CLA	C1D-ND-C4D	-3.83	103.61	106.33
18	F	805	CLA	C1D-ND-C4D	-3.83	103.62	106.33
18	B	827	CLA	C1D-ND-C4D	-3.82	103.62	106.33
18	B	824	CLA	C1D-ND-C4D	-3.82	103.62	106.33
18	B	811	CLA	C1D-ND-C4D	-3.82	103.62	106.33
18	K	201	CLA	C1D-ND-C4D	-3.82	103.62	106.33
18	B	821	CLA	C1D-ND-C4D	-3.81	103.63	106.33
18	A	841	CLA	C1D-ND-C4D	-3.81	103.63	106.33
18	B	808	CLA	C1D-ND-C4D	-3.80	103.63	106.33
18	A	829	CLA	C1D-ND-C4D	-3.80	103.63	106.33
18	4	609	CLA	C1D-ND-C4D	-3.80	103.63	106.33
18	A	826	CLA	C1D-ND-C4D	-3.80	103.64	106.33
18	A	855	CLA	C1D-ND-C4D	-3.80	103.64	106.33
18	2	603	CLA	C1D-ND-C4D	-3.80	103.64	106.33
18	A	807	CLA	C1D-ND-C4D	-3.76	103.66	106.33
18	B	835	CLA	C1D-ND-C4D	-3.76	103.66	106.33
18	A	803	CLA	C1D-ND-C4D	-3.76	103.67	106.33
18	A	821	CLA	C1D-ND-C4D	-3.74	103.68	106.33
18	A	843	CLA	C1D-ND-C4D	-3.74	103.68	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	828	CLA	C1D-ND-C4D	-3.73	103.68	106.33
18	B	815	CLA	C1D-ND-C4D	-3.70	103.71	106.33
18	B	825	CLA	C1D-ND-C4D	-3.70	103.71	106.33
18	1	309	CLA	C1D-ND-C4D	-3.69	103.71	106.33
18	B	822	CLA	C1D-ND-C4D	-3.66	103.73	106.33
18	A	854	CLA	C1D-ND-C4D	-3.64	103.75	106.33
18	B	819	CLA	CHD-C1D-ND	-3.59	121.16	124.45
18	A	830	CLA	C1D-ND-C4D	-3.59	103.79	106.33
18	A	837	CLA	CHD-C1D-ND	-3.58	121.16	124.45
18	L	304	CLA	CHD-C1D-ND	-3.57	121.17	124.45
17	A	801	CL0	CHC-C1C-NC	3.56	129.61	124.20
18	F	802	CLA	CHD-C1D-ND	-3.56	121.18	124.45
27	4	606	CHL	C1D-ND-C4D	-3.55	103.81	106.33
18	B	817	CLA	CHD-C1D-ND	-3.52	121.22	124.45
18	A	804	CLA	CHD-C1D-ND	-3.50	121.24	124.45
18	B	816	CLA	CHD-C1D-ND	-3.50	121.24	124.45
18	A	812	CLA	CHD-C1D-ND	-3.49	121.24	124.45
18	B	805	CLA	C1D-ND-C4D	-3.48	103.86	106.33
18	A	842	CLA	CHD-C1D-ND	-3.48	121.25	124.45
18	B	823	CLA	CHD-C1D-ND	-3.46	121.27	124.45
27	2	605	CHL	C1D-ND-C4D	-3.46	103.88	106.33
27	3	301	CHL	C1D-ND-C4D	-3.46	103.88	106.33
18	B	828	CLA	CHD-C1D-ND	-3.45	121.28	124.45
18	B	806	CLA	CHD-C1D-ND	-3.45	121.29	124.45
18	B	830	CLA	CHD-C1D-ND	-3.44	121.29	124.45
18	A	810	CLA	C1D-ND-C4D	-3.43	103.90	106.33
18	A	835	CLA	CHD-C1D-ND	-3.42	121.31	124.45
27	4	605	CHL	C1D-ND-C4D	-3.42	103.90	106.33
27	4	615	CHL	C1D-ND-C4D	-3.42	103.90	106.33
18	2	613	CLA	CHD-C1D-ND	-3.41	121.32	124.45
18	B	831	CLA	CHD-C1D-ND	-3.41	121.32	124.45
18	G	204	CLA	CHD-C1D-ND	-3.41	121.32	124.45
18	A	824	CLA	CHD-C1D-ND	-3.40	121.33	124.45
18	1	310	CLA	CHD-C1D-ND	-3.40	121.33	124.45
18	A	855	CLA	CHD-C1D-ND	-3.40	121.33	124.45
18	K	203	CLA	CHD-C1D-ND	-3.40	121.33	124.45
18	B	802	CLA	CHD-C1D-ND	-3.39	121.34	124.45
18	A	827	CLA	CHD-C1D-ND	-3.39	121.34	124.45
18	1	303	CLA	CHD-C1D-ND	-3.39	121.34	124.45
18	B	804	CLA	CHD-C1D-ND	-3.38	121.34	124.45
18	A	822	CLA	CHD-C1D-ND	-3.38	121.34	124.45
18	A	856	CLA	CHD-C1D-ND	-3.37	121.35	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	834	CLA	CHD-C1D-ND	-3.37	121.35	124.45
18	K	201	CLA	CHD-C1D-ND	-3.37	121.36	124.45
27	3	306	CHL	C1D-ND-C4D	-3.37	103.94	106.33
17	H	202	CL0	CHC-C1C-C2C	-3.36	117.39	126.73
27	4	607	CHL	C1D-ND-C4D	-3.36	103.95	106.33
18	B	813	CLA	CHD-C1D-ND	-3.36	121.37	124.45
18	3	308	CLA	CHD-C1D-ND	-3.36	121.37	124.45
18	A	823	CLA	CHD-C1D-ND	-3.36	121.37	124.45
18	L	303	CLA	CHD-C1D-ND	-3.34	121.38	124.45
18	B	837	CLA	CHD-C1D-ND	-3.34	121.38	124.45
18	1	304	CLA	CHD-C1D-ND	-3.34	121.39	124.45
18	4	608	CLA	CHD-C1D-ND	-3.34	121.39	124.45
18	B	820	CLA	CHD-C1D-ND	-3.34	121.39	124.45
18	B	836	CLA	CHD-C1D-ND	-3.33	121.39	124.45
18	2	604	CLA	CHD-C1D-ND	-3.33	121.39	124.45
18	4	613	CLA	CHD-C1D-ND	-3.33	121.40	124.45
18	A	820	CLA	CHD-C1D-ND	-3.33	121.40	124.45
18	K	204	CLA	CHD-C1D-ND	-3.33	121.40	124.45
18	2	609	CLA	CHD-C1D-ND	-3.32	121.40	124.45
18	B	810	CLA	CHD-C1D-ND	-3.32	121.40	124.45
18	A	842	CLA	O2A-C1-C2	3.32	117.37	108.64
27	2	614	CHL	C1D-ND-C4D	-3.32	103.97	106.33
18	B	809	CLA	CHD-C1D-ND	-3.32	121.41	124.45
18	B	833	CLA	CHD-C1D-ND	-3.32	121.41	124.45
18	A	836	CLA	CHD-C1D-ND	-3.32	121.41	124.45
18	1	308	CLA	CHD-C1D-ND	-3.32	121.41	124.45
18	A	815	CLA	CHD-C1D-ND	-3.31	121.41	124.45
27	1	307	CHL	C1D-ND-C4D	-3.31	103.98	106.33
18	A	802	CLA	CHD-C1D-ND	-3.31	121.41	124.45
18	A	816	CLA	CHD-C1D-ND	-3.31	121.41	124.45
18	A	811	CLA	CHD-C1D-ND	-3.30	121.42	124.45
18	3	307	CLA	CHD-C1D-ND	-3.30	121.42	124.45
18	B	829	CLA	CHD-C1D-ND	-3.30	121.42	124.45
18	3	310	CLA	CHD-C1D-ND	-3.30	121.42	124.45
18	4	604	CLA	CHD-C1D-ND	-3.29	121.43	124.45
27	2	606	CHL	C1D-ND-C4D	-3.29	104.00	106.33
18	A	808	CLA	CHD-C1D-ND	-3.29	121.43	124.45
27	1	302	CHL	C1D-ND-C4D	-3.29	104.00	106.33
18	1	313	CLA	CHD-C1D-ND	-3.29	121.43	124.45
18	A	834	CLA	CHD-C1D-ND	-3.29	121.44	124.45
18	2	601	CLA	CHD-C1D-ND	-3.29	121.44	124.45
18	A	817	CLA	CHD-C1D-ND	-3.28	121.44	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	833	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	A	803	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	A	814	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	A	854	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	B	814	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	3	312	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	4	602	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	A	829	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	3	311	CLA	CHD-C1D-ND	-3.27	121.45	124.45
18	A	841	CLA	CHD-C1D-ND	-3.27	121.45	124.45
18	G	205	CLA	CHD-C1D-ND	-3.26	121.46	124.45
18	A	830	CLA	CHD-C1D-ND	-3.26	121.46	124.45
18	B	811	CLA	CHD-C1D-ND	-3.26	121.46	124.45
18	1	305	CLA	CHD-C1D-ND	-3.26	121.46	124.45
18	B	808	CLA	CHD-C1D-ND	-3.26	121.46	124.45
18	2	602	CLA	CHD-C1D-ND	-3.26	121.46	124.45
18	1	306	CLA	CHD-C1D-ND	-3.26	121.46	124.45
18	A	805	CLA	CHD-C1D-ND	-3.25	121.47	124.45
18	B	821	CLA	CHD-C1D-ND	-3.24	121.47	124.45
18	B	826	CLA	CHD-C1D-ND	-3.24	121.47	124.45
18	1	311	CLA	CHD-C1D-ND	-3.24	121.48	124.45
18	A	826	CLA	CHD-C1D-ND	-3.23	121.48	124.45
18	B	832	CLA	CHD-C1D-ND	-3.23	121.48	124.45
18	B	827	CLA	CHD-C1D-ND	-3.23	121.49	124.45
18	3	303	CLA	CHD-C1D-ND	-3.23	121.49	124.45
18	A	832	CLA	CHD-C1D-ND	-3.22	121.49	124.45
18	A	839	CLA	CHD-C1D-ND	-3.22	121.49	124.45
18	F	805	CLA	CHD-C1D-ND	-3.22	121.49	124.45
18	L	305	CLA	CHD-C1D-ND	-3.22	121.49	124.45
18	4	609	CLA	CHD-C1D-ND	-3.22	121.50	124.45
18	A	809	CLA	O2A-C1-C2	3.22	117.09	108.64
18	A	806	CLA	CHD-C1D-ND	-3.22	121.50	124.45
18	J	102	CLA	CHD-C1D-ND	-3.22	121.50	124.45
18	A	843	CLA	CHD-C1D-ND	-3.21	121.50	124.45
18	2	603	CLA	CHD-C1D-ND	-3.21	121.50	124.45
18	B	824	CLA	CHD-C1D-ND	-3.20	121.51	124.45
18	2	612	CLA	CHD-C1D-ND	-3.20	121.51	124.45
27	2	607	CHL	C1D-ND-C4D	-3.20	104.06	106.33
18	A	802	CLA	C1D-ND-C4D	-3.20	104.06	106.33
18	3	309	CLA	CHD-C1D-ND	-3.20	121.52	124.45
18	2	611	CLA	CHD-C1D-ND	-3.19	121.52	124.45
18	2	608	CLA	CHD-C1D-ND	-3.19	121.52	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	840	CLA	CHD-C1D-ND	-3.19	121.53	124.45
18	A	838	CLA	CHD-C1D-ND	-3.18	121.53	124.45
18	B	803	CLA	CHD-C1D-ND	-3.18	121.53	124.45
18	A	813	CLA	CHD-C1D-ND	-3.18	121.53	124.45
18	1	314	CLA	CHD-C1D-ND	-3.18	121.53	124.45
18	A	810	CLA	CHD-C1D-ND	-3.17	121.54	124.45
18	B	812	CLA	CHD-C1D-ND	-3.17	121.54	124.45
18	3	305	CLA	CHD-C1D-ND	-3.17	121.55	124.45
18	4	601	CLA	CHD-C1D-ND	-3.16	121.55	124.45
18	A	828	CLA	CHD-C1D-ND	-3.16	121.55	124.45
18	2	610	CLA	CHD-C1D-ND	-3.15	121.56	124.45
18	4	614	CLA	CHD-C1D-ND	-3.14	121.56	124.45
18	A	831	CLA	CHD-C1D-ND	-3.14	121.57	124.45
18	F	804	CLA	CHD-C1D-ND	-3.14	121.57	124.45
18	4	612	CLA	CHD-C1D-ND	-3.14	121.57	124.45
18	A	825	CLA	CHD-C1D-ND	-3.13	121.58	124.45
18	A	845	CLA	CHD-C1D-ND	-3.13	121.58	124.45
18	4	611	CLA	CHD-C1D-ND	-3.13	121.58	124.45
18	A	819	CLA	CHD-C1D-ND	-3.12	121.58	124.45
18	A	809	CLA	CHD-C1D-ND	-3.11	121.59	124.45
17	A	801	CL0	CHC-C1C-C2C	-3.10	118.11	126.73
18	A	818	CLA	CHD-C1D-ND	-3.10	121.61	124.45
18	3	302	CLA	CHD-C1D-ND	-3.09	121.61	124.45
18	3	304	CLA	CHD-C1D-ND	-3.09	121.61	124.45
18	1	312	CLA	CHD-C1D-ND	-3.09	121.62	124.45
18	B	802	CLA	C1D-ND-C4D	-3.08	104.15	106.33
30	4	617	QDL	C8-C13-C14	3.08	130.31	125.53
18	B	835	CLA	CHD-C1D-ND	-3.07	121.64	124.45
18	4	610	CLA	CHD-C1D-ND	-3.06	121.64	124.45
18	B	815	CLA	CHD-C1D-ND	-3.06	121.64	124.45
18	1	309	CLA	CHD-C1D-ND	-3.05	121.65	124.45
18	A	807	CLA	CHD-C1D-ND	-3.05	121.65	124.45
18	B	839	CLA	CHD-C1D-ND	-3.04	121.66	124.45
18	A	821	CLA	CHD-C1D-ND	-3.02	121.68	124.45
18	B	818	CLA	CHD-C1D-ND	-3.01	121.69	124.45
18	B	807	CLA	CHD-C1D-ND	-2.99	121.71	124.45
30	4	617	QDL	O7-C4-C3	2.96	115.61	113.38
18	G	201	CLA	CHD-C1D-ND	-2.94	121.75	124.45
18	B	801	CLA	CHD-C1D-ND	-2.92	121.77	124.45
18	1	315	CLA	CHD-C1D-ND	-2.91	121.78	124.45
18	4	608	CLA	C1-C2-C3	2.89	131.05	126.04
18	B	825	CLA	CHD-C1D-ND	-2.88	121.81	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	615	CHL	CHC-C1C-NC	2.84	128.51	124.20
27	2	605	CHL	CHC-C1C-NC	2.84	128.51	124.20
18	B	822	CLA	CHD-C1D-ND	-2.83	121.85	124.45
18	4	603	CLA	CHD-C1D-ND	-2.81	121.87	124.45
18	F	802	CLA	C4A-NA-C1A	2.76	107.95	106.71
27	1	302	CHL	CHA-C1A-NA	-2.76	120.08	126.40
27	4	605	CHL	CHC-C1C-NC	2.75	128.38	124.20
18	B	805	CLA	CHD-C1D-ND	-2.73	121.94	124.45
18	4	603	CLA	CHC-C4B-NB	2.70	127.11	124.26
27	2	607	CHL	C1-C2-C3	-2.67	122.44	126.75
18	A	829	CLA	CHB-C1B-NB	-2.65	121.45	124.26
18	A	818	CLA	CHC-C4B-NB	2.65	127.06	124.26
18	A	839	CLA	CHC-C4B-NB	2.64	127.05	124.26
18	B	826	CLA	CHC-C4B-NB	2.63	127.05	124.26
18	B	825	CLA	CHB-C1B-NB	-2.62	121.48	124.26
27	2	614	CHL	CHB-C4A-NA	2.62	128.13	124.51
18	A	826	CLA	CHB-C1B-NB	-2.61	121.49	124.26
27	1	307	CHL	CHA-C1A-NA	-2.61	120.42	126.40
27	3	306	CHL	CHB-C4A-NA	2.59	128.09	124.51
27	4	607	CHL	CHA-C1A-NA	-2.58	120.49	126.40
18	B	822	CLA	CHB-C1B-NB	-2.57	121.54	124.26
18	A	807	CLA	CHC-C4B-NB	2.55	126.96	124.26
18	4	611	CLA	CHC-C4B-NB	2.55	126.95	124.26
27	4	607	CHL	C2A-C1A-CHA	2.54	128.31	123.86
18	B	801	CLA	CHB-C1B-NB	-2.54	121.57	124.26
27	3	306	CHL	CHC-C1C-NC	2.54	128.06	124.20
18	G	201	CLA	CHC-C4B-NB	2.53	126.94	124.26
18	A	804	CLA	CHC-C4B-NB	2.51	126.91	124.26
27	3	306	CHL	CHA-C1A-NA	-2.50	120.67	126.40
27	2	606	CHL	CHA-C1A-NA	-2.50	120.67	126.40
18	B	834	CLA	C1-C2-C3	2.50	130.37	126.04
27	4	615	CHL	CHB-C4A-NA	2.50	127.97	124.51
27	2	614	CHL	CHC-C1C-NC	2.50	127.99	124.20
27	2	606	CHL	CHC-C1C-NC	2.49	127.98	124.20
27	4	607	CHL	CHC-C1C-NC	2.48	127.97	124.20
18	A	825	CLA	CHC-C4B-NB	2.47	126.88	124.26
27	3	301	CHL	CHA-C1A-NA	-2.47	120.74	126.40
18	B	818	CLA	CHC-C4B-NB	2.47	126.87	124.26
27	4	605	CHL	CHA-C1A-NA	-2.47	120.74	126.40
27	2	614	CHL	CHA-C1A-NA	-2.47	120.75	126.40
18	F	802	CLA	CHB-C1B-NB	-2.47	121.65	124.26
18	A	809	CLA	CHC-C4B-NB	2.46	126.86	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	302	CLA	CHC-C4B-NB	2.46	126.86	124.26
27	3	301	CHL	CHC-C1C-NC	2.46	127.93	124.20
18	1	312	CLA	CHC-C4B-NB	2.45	126.85	124.26
18	3	309	CLA	CHC-C4B-NB	2.45	126.85	124.26
18	4	608	CLA	CHC-C4B-NB	2.45	126.85	124.26
18	F	804	CLA	CHC-C4B-NB	2.45	126.85	124.26
18	A	843	CLA	CHB-C1B-NB	-2.44	121.67	124.26
18	A	806	CLA	CHB-C1B-NB	-2.44	121.67	124.26
18	B	836	CLA	CHB-C1B-NB	-2.44	121.67	124.26
18	A	816	CLA	CHC-C4B-NB	2.44	126.84	124.26
27	2	607	CHL	CHC-C1C-NC	2.44	127.90	124.20
18	A	854	CLA	CHB-C1B-NB	-2.43	121.69	124.26
18	4	608	CLA	CHB-C1B-NB	-2.42	121.69	124.26
18	A	836	CLA	CHC-C4B-NB	2.42	126.82	124.26
27	1	307	CHL	CHC-C1C-NC	2.42	127.87	124.20
18	A	841	CLA	CHB-C1B-NB	-2.42	121.70	124.26
18	B	836	CLA	CHC-C4B-NB	2.42	126.81	124.26
27	4	606	CHL	CHC-C1C-NC	2.41	127.86	124.20
18	A	821	CLA	CHC-C4B-NB	2.41	126.81	124.26
27	1	302	CHL	CHC-C1C-NC	2.41	127.86	124.20
18	B	805	CLA	CHC-C4B-NB	2.41	126.81	124.26
18	4	614	CLA	CHC-C4B-NB	2.40	126.80	124.26
18	3	312	CLA	CHC-C4B-NB	2.40	126.80	124.26
27	2	606	CHL	CHB-C4A-NA	2.40	127.83	124.51
18	A	805	CLA	CHB-C1B-NB	-2.40	121.72	124.26
27	4	615	CHL	CHA-C1A-NA	-2.40	120.91	126.40
27	2	607	CHL	CHB-C4A-NA	2.39	127.82	124.51
18	L	303	CLA	CHC-C4B-NB	2.39	126.79	124.26
27	3	301	CHL	CHB-C4A-NA	2.39	127.82	124.51
18	B	814	CLA	CHC-C4B-NB	2.39	126.79	124.26
18	B	834	CLA	CHB-C1B-NB	-2.38	121.74	124.26
18	1	315	CLA	CHC-C4B-NB	2.38	126.77	124.26
18	A	855	CLA	CHB-C1B-NB	-2.37	121.75	124.26
18	F	804	CLA	CHB-C1B-NB	-2.37	121.75	124.26
18	3	303	CLA	CHC-C4B-NB	2.37	126.76	124.26
18	A	821	CLA	CHB-C1B-NB	-2.36	121.75	124.26
18	A	834	CLA	CHB-C1B-NB	-2.36	121.75	124.26
18	1	313	CLA	CHB-C1B-NB	-2.36	121.76	124.26
18	B	822	CLA	CHC-C4B-NB	2.36	126.76	124.26
18	4	613	CLA	CHC-C4B-NB	2.36	126.75	124.26
18	A	811	CLA	CHC-C4B-NB	2.35	126.75	124.26
18	B	813	CLA	CHC-C4B-NB	2.35	126.75	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	606	CHL	CHA-C1A-NA	-2.35	121.02	126.40
17	A	801	CL0	C2C-C1C-NC	2.35	112.17	109.97
18	F	805	CLA	CHC-C4B-NB	2.35	126.74	124.26
18	2	601	CLA	CHB-C1B-NB	-2.35	121.77	124.26
18	B	815	CLA	CHB-C1B-NB	-2.35	121.77	124.26
18	1	308	CLA	CHC-C4B-NB	2.35	126.74	124.26
18	B	839	CLA	CHC-C4B-NB	2.35	126.74	124.26
27	4	615	CHL	C4B-CHC-C1C	-2.35	120.77	126.34
18	B	810	CLA	CHB-C1B-NB	-2.34	121.78	124.26
27	2	607	CHL	CHA-C1A-NA	-2.34	121.04	126.40
18	A	826	CLA	CHC-C4B-NB	2.34	126.73	124.26
18	A	856	CLA	CHB-C1B-NB	-2.34	121.78	124.26
18	B	835	CLA	CHC-C4B-NB	2.34	126.73	124.26
18	B	821	CLA	CHB-C1B-NB	-2.33	121.79	124.26
18	A	840	CLA	CHC-C4B-NB	2.33	126.73	124.26
18	B	808	CLA	CHB-C1B-NB	-2.33	121.79	124.26
18	A	831	CLA	CHC-C4B-NB	2.33	126.72	124.26
18	4	601	CLA	CHC-C4B-NB	2.33	126.72	124.26
27	2	605	CHL	CHA-C1A-NA	-2.33	121.06	126.40
18	A	813	CLA	CHB-C1B-NB	-2.33	121.79	124.26
18	3	305	CLA	CHC-C4B-NB	2.33	126.72	124.26
18	3	310	CLA	CHC-C4B-NB	2.33	126.72	124.26
18	1	306	CLA	CHC-C4B-NB	2.32	126.72	124.26
18	B	823	CLA	CHC-C4B-NB	2.32	126.72	124.26
18	4	610	CLA	CHB-C1B-NB	-2.32	121.80	124.26
18	1	314	CLA	CHC-C4B-NB	2.32	126.72	124.26
18	3	304	CLA	CHB-C1B-NB	-2.32	121.80	124.26
18	3	302	CLA	CHB-C1B-NB	-2.32	121.80	124.26
18	1	313	CLA	CHC-C4B-NB	2.32	126.71	124.26
18	B	818	CLA	CHB-C1B-NB	-2.31	121.81	124.26
18	4	602	CLA	CHC-C4B-NB	2.31	126.71	124.26
27	4	605	CHL	C4B-CHC-C1C	-2.31	120.85	126.34
18	A	838	CLA	CHB-C1B-NB	-2.31	121.81	124.26
18	1	305	CLA	CHC-C4B-NB	2.31	126.70	124.26
18	4	611	CLA	CHB-C1B-NB	-2.30	121.82	124.26
18	4	602	CLA	CHB-C1B-NB	-2.30	121.82	124.26
18	4	612	CLA	CHB-C1B-NB	-2.30	121.82	124.26
27	2	605	CHL	C4B-CHC-C1C	-2.30	120.88	126.34
18	B	832	CLA	CHC-C4B-NB	2.30	126.69	124.26
18	K	201	CLA	CHB-C1B-NB	-2.30	121.83	124.26
18	B	830	CLA	CHB-C1B-NB	-2.29	121.83	124.26
18	A	823	CLA	CHB-C1B-NB	-2.29	121.83	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	807	CLA	CHB-C1B-NB	-2.29	121.83	124.26
18	B	835	CLA	CHB-C1B-NB	-2.29	121.83	124.26
18	K	204	CLA	CHB-C1B-NB	-2.29	121.84	124.26
18	F	805	CLA	CHB-C1B-NB	-2.28	121.84	124.26
18	B	804	CLA	CHC-C4B-NB	2.28	126.67	124.26
18	B	811	CLA	CHB-C1B-NB	-2.28	121.84	124.26
17	H	202	CL0	CHA-C1A-NA	-2.28	121.17	126.40
27	3	306	CHL	C4B-CHC-C1C	-2.28	120.93	126.34
27	4	605	CHL	CHB-C4A-NA	2.28	127.67	124.51
18	A	808	CLA	CHC-C4B-NB	2.28	126.67	124.26
27	1	307	CHL	C2A-C1A-CHA	2.28	127.84	123.86
18	2	610	CLA	CHC-C4B-NB	2.28	126.67	124.26
18	2	613	CLA	CHC-C4B-NB	2.28	126.67	124.26
18	4	601	CLA	CHB-C1B-NB	-2.27	121.85	124.26
27	4	615	CHL	CHC-C1C-C2C	-2.27	117.87	126.11
18	3	307	CLA	CHB-C1B-NB	-2.27	121.85	124.26
27	2	605	CHL	CHB-C4A-NA	2.27	127.65	124.51
18	2	612	CLA	CHC-C4B-NB	2.27	126.66	124.26
18	A	837	CLA	CHC-C4B-NB	2.27	126.66	124.26
18	3	307	CLA	CHC-C4B-NB	2.27	126.66	124.26
18	B	823	CLA	CHB-C1B-NB	-2.26	121.86	124.26
18	1	304	CLA	CHC-C4B-NB	2.26	126.65	124.26
18	4	604	CLA	CHC-C4B-NB	2.26	126.65	124.26
18	A	840	CLA	CHB-C1B-NB	-2.26	121.86	124.26
18	A	813	CLA	CHC-C4B-NB	2.26	126.65	124.26
18	A	838	CLA	CHC-C4B-NB	2.26	126.65	124.26
18	A	841	CLA	CHC-C4B-NB	2.26	126.65	124.26
18	B	811	CLA	CHC-C4B-NB	2.26	126.65	124.26
27	2	614	CHL	C4B-CHC-C1C	-2.26	120.99	126.34
27	3	301	CHL	C4B-CHC-C1C	-2.26	120.99	126.34
18	A	837	CLA	CHB-C1B-NB	-2.25	121.87	124.26
18	B	830	CLA	CHC-C4B-NB	2.25	126.64	124.26
18	3	304	CLA	CHC-C4B-NB	2.25	126.64	124.26
18	2	612	CLA	CHB-C1B-NB	-2.25	121.87	124.26
18	3	310	CLA	CHB-C1B-NB	-2.25	121.87	124.26
18	B	819	CLA	CHB-C1B-NB	-2.25	121.87	124.26
18	A	825	CLA	CHB-C1B-NB	-2.25	121.88	124.26
18	B	831	CLA	CHB-C1B-NB	-2.25	121.88	124.26
18	3	305	CLA	CHB-C1B-NB	-2.25	121.88	124.26
18	K	203	CLA	CHB-C1B-NB	-2.25	121.88	124.26
18	2	602	CLA	CHC-C4B-NB	2.25	126.64	124.26
18	2	608	CLA	CHB-C1B-NB	-2.25	121.88	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	611	CLA	CHC-C4B-NB	2.24	126.63	124.26
18	B	834	CLA	CHC-C4B-NB	2.24	126.63	124.26
18	A	845	CLA	CHC-C4B-NB	2.24	126.63	124.26
18	2	608	CLA	CHC-C4B-NB	2.24	126.63	124.26
18	4	604	CLA	CHB-C1B-NB	-2.24	121.89	124.26
18	4	610	CLA	CHC-C4B-NB	2.23	126.62	124.26
18	A	819	CLA	CHC-C4B-NB	2.23	126.62	124.26
18	A	832	CLA	CHB-C1B-NB	-2.23	121.89	124.26
17	H	202	CL0	C2C-C1C-NC	2.23	112.06	109.97
27	1	302	CHL	C2A-C1A-CHA	2.23	127.76	123.86
18	3	311	CLA	CHB-C1B-NB	-2.23	121.90	124.26
18	2	604	CLA	CHC-C4B-NB	2.23	126.61	124.26
18	A	811	CLA	CHB-C1B-NB	-2.23	121.90	124.26
18	B	805	CLA	CHB-C1B-NB	-2.22	121.91	124.26
18	B	813	CLA	CHB-C1B-NB	-2.22	121.91	124.26
18	A	809	CLA	CHB-C1B-NB	-2.22	121.91	124.26
27	1	307	CHL	C4B-CHC-C1C	-2.22	121.08	126.34
18	1	305	CLA	CHB-C1B-NB	-2.22	121.91	124.26
18	A	808	CLA	CHB-C1B-NB	-2.21	121.91	124.26
18	K	203	CLA	CHC-C4B-NB	2.21	126.60	124.26
18	B	804	CLA	CHB-C1B-NB	-2.21	121.92	124.26
18	A	803	CLA	CHB-C1B-NB	-2.21	121.92	124.26
27	4	607	CHL	C4B-CHC-C1C	-2.21	121.10	126.34
18	B	832	CLA	CHB-C1B-NB	-2.21	121.92	124.26
18	B	803	CLA	CHC-C4B-NB	2.21	126.59	124.26
18	B	808	CLA	CHC-C4B-NB	2.21	126.59	124.26
18	2	604	CLA	CHB-C1B-NB	-2.20	121.92	124.26
27	2	607	CHL	C4B-CHC-C1C	-2.20	121.11	126.34
18	1	311	CLA	CHB-C1B-NB	-2.20	121.93	124.26
18	B	820	CLA	CHC-C4B-NB	2.20	126.58	124.26
18	2	603	CLA	CHC-C4B-NB	2.20	126.58	124.26
18	2	601	CLA	CHC-C4B-NB	2.19	126.58	124.26
27	2	605	CHL	CHC-C1C-C2C	-2.19	118.17	126.11
18	4	614	CLA	CHB-C1B-NB	-2.19	121.94	124.26
18	B	820	CLA	CHB-C1B-NB	-2.19	121.94	124.26
18	2	602	CLA	CHB-C1B-NB	-2.19	121.94	124.26
27	2	606	CHL	C4B-CHC-C1C	-2.19	121.15	126.34
18	J	102	CLA	CHB-C1B-NB	-2.19	121.94	124.26
18	A	810	CLA	CHB-C1B-NB	-2.18	121.94	124.26
18	3	303	CLA	CHB-C1B-NB	-2.18	121.94	124.26
18	B	810	CLA	CHC-C4B-NB	2.18	126.57	124.26
27	4	605	CHL	CHC-C1C-C2C	-2.18	118.19	126.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	303	CLA	CHC-C4B-NB	2.18	126.57	124.26
27	1	302	CHL	C4B-CHC-C1C	-2.18	121.16	126.34
18	A	839	CLA	CHB-C1B-NB	-2.18	121.95	124.26
18	A	819	CLA	CHB-C1B-NB	-2.18	121.95	124.26
18	A	827	CLA	CHB-C1B-NB	-2.18	121.95	124.26
18	A	810	CLA	CHC-C4B-NB	2.18	126.56	124.26
18	3	308	CLA	CHC-C4B-NB	2.17	126.56	124.26
18	B	833	CLA	CHB-C1B-NB	-2.17	121.96	124.26
18	A	830	CLA	CHC-C4B-NB	2.17	126.55	124.26
18	A	812	CLA	CHC-C4B-NB	2.17	126.55	124.26
18	A	824	CLA	CHC-C4B-NB	2.17	126.55	124.26
18	2	610	CLA	CHB-C1B-NB	-2.16	121.97	124.26
18	B	827	CLA	CHC-C4B-NB	2.16	126.55	124.26
18	B	831	CLA	CHC-C4B-NB	2.16	126.55	124.26
18	A	828	CLA	CHB-C1B-NB	-2.16	121.97	124.26
18	A	832	CLA	CHC-C4B-NB	2.16	126.54	124.26
18	1	315	CLA	CHB-C1B-NB	-2.16	121.97	124.26
18	A	831	CLA	CHB-C1B-NB	-2.16	121.97	124.26
18	B	806	CLA	CHB-C1B-NB	-2.16	121.97	124.26
18	L	305	CLA	CHB-C1B-NB	-2.15	121.98	124.26
18	A	804	CLA	CHB-C1B-NB	-2.15	121.98	124.26
18	A	814	CLA	CHB-C1B-NB	-2.15	121.98	124.26
18	A	815	CLA	CHB-C1B-NB	-2.15	121.98	124.26
18	A	818	CLA	O2A-C1-C2	2.15	114.29	108.64
18	3	311	CLA	CHC-C4B-NB	2.15	126.53	124.26
18	A	822	CLA	CHC-C4B-NB	2.15	126.53	124.26
17	H	202	CL0	C3D-C4D-ND	2.15	113.71	110.24
18	L	303	CLA	CHB-C1B-NB	-2.14	121.99	124.26
18	A	843	CLA	C4A-NA-C1A	2.14	107.67	106.71
18	B	801	CLA	CHC-C4B-NB	2.14	126.53	124.26
18	1	311	CLA	CHC-C4B-NB	2.14	126.52	124.26
18	B	821	CLA	CHC-C4B-NB	2.14	126.52	124.26
18	2	609	CLA	CHC-C4B-NB	2.14	126.52	124.26
18	A	845	CLA	CHB-C1B-NB	-2.14	121.99	124.26
18	A	836	CLA	CHB-C1B-NB	-2.14	121.99	124.26
18	A	805	CLA	CHC-C4B-NB	2.14	126.52	124.26
18	1	308	CLA	CHB-C1B-NB	-2.13	122.00	124.26
27	1	307	CHL	CHB-C4A-NA	2.13	127.46	124.51
18	A	843	CLA	CHC-C4B-NB	2.13	126.51	124.26
18	B	803	CLA	CHB-C1B-NB	-2.13	122.00	124.26
18	A	817	CLA	CHB-C1B-NB	-2.13	122.00	124.26
18	B	817	CLA	CHB-C1B-NB	-2.13	122.00	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	201	CLA	CHB-C1B-NB	-2.13	122.00	124.26
18	A	807	CLA	CHB-C1B-NB	-2.12	122.01	124.26
18	A	815	CLA	CHC-C4B-NB	2.12	126.51	124.26
18	L	305	CLA	CHC-C4B-NB	2.12	126.50	124.26
27	4	606	CHL	C4B-CHC-C1C	-2.12	121.32	126.34
18	3	309	CLA	CHB-C1B-NB	-2.12	122.02	124.26
18	4	609	CLA	CHC-C4B-NB	2.12	126.50	124.26
27	1	302	CHL	CHB-C4A-NA	2.12	127.44	124.51
18	B	824	CLA	CHB-C1B-NB	-2.11	122.02	124.26
18	A	820	CLA	CHC-C4B-NB	2.11	126.49	124.26
18	B	816	CLA	CHB-C1B-NB	-2.11	122.02	124.26
18	1	309	CLA	CHB-C1B-NB	-2.11	122.02	124.26
27	4	606	CHL	CHB-C4A-NA	2.11	127.43	124.51
18	B	829	CLA	CHB-C1B-NB	-2.11	122.03	124.26
18	B	812	CLA	CHB-C1B-NB	-2.10	122.03	124.26
18	2	611	CLA	CHB-C1B-NB	-2.10	122.03	124.26
18	1	309	CLA	CHC-C4B-NB	2.10	126.48	124.26
18	A	816	CLA	CHB-C1B-NB	-2.09	122.05	124.26
18	L	304	CLA	CHB-C1B-NB	-2.09	122.05	124.26
27	4	607	CHL	CHB-C4A-NA	2.09	127.40	124.51
18	B	819	CLA	C3D-C4D-ND	2.09	113.61	110.24
18	4	612	CLA	CHC-C4B-NB	2.08	126.46	124.26
18	A	835	CLA	CHC-C4B-NB	2.08	126.46	124.26
18	1	303	CLA	CHB-C1B-NB	-2.08	122.05	124.26
18	A	824	CLA	CHB-C1B-NB	-2.08	122.05	124.26
18	2	613	CLA	CHB-C1B-NB	-2.08	122.06	124.26
18	A	802	CLA	CHC-C4B-NB	2.08	126.45	124.26
18	A	834	CLA	CHC-C4B-NB	2.08	126.45	124.26
18	A	830	CLA	CHB-C1B-NB	-2.07	122.06	124.26
18	B	807	CLA	CHC-C4B-NB	2.07	126.45	124.26
18	A	818	CLA	CHB-C1B-NB	-2.07	122.07	124.26
18	A	833	CLA	CHB-C1B-NB	-2.07	122.07	124.26
18	B	828	CLA	CHC-C4B-NB	2.06	126.44	124.26
18	1	314	CLA	CHB-C1B-NB	-2.06	122.07	124.26
18	L	304	CLA	CHC-C4B-NB	2.06	126.44	124.26
18	2	609	CLA	CHB-C1B-NB	-2.06	122.08	124.26
18	B	839	CLA	CHB-C1B-NB	-2.06	122.08	124.26
18	B	806	CLA	CHC-C4B-NB	2.06	126.44	124.26
18	1	306	CLA	CHB-C1B-NB	-2.06	122.08	124.26
18	B	809	CLA	CHB-C1B-NB	-2.06	122.08	124.26
18	B	837	CLA	CHB-C1B-NB	-2.05	122.08	124.26
18	A	828	CLA	CHC-C4B-NB	2.05	126.43	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	823	CLA	CHC-C4B-NB	2.05	126.43	124.26
18	J	102	CLA	CHC-C4B-NB	2.05	126.43	124.26
18	G	204	CLA	CHC-C4B-NB	2.05	126.43	124.26
27	3	306	CHL	CHC-C1C-C2C	-2.05	118.69	126.11
18	B	829	CLA	CHC-C4B-NB	2.05	126.42	124.26
18	B	837	CLA	CHC-C4B-NB	2.05	126.42	124.26
18	B	814	CLA	CHB-C1B-NB	-2.05	122.09	124.26
18	G	205	CLA	CHB-C1B-NB	-2.04	122.09	124.26
18	G	204	CLA	CHB-C1B-NB	-2.04	122.10	124.26
17	H	202	CL0	C1-C2-C3	-2.03	122.52	126.04
18	K	201	CLA	C3B-C4B-NB	-2.03	108.63	110.52
18	B	825	CLA	CAA-C2A-C1A	2.03	118.64	111.97
18	B	815	CLA	CHC-C4B-NB	2.02	126.39	124.26
18	B	827	CLA	CHB-C1B-NB	-2.02	122.12	124.26
27	2	614	CHL	CHC-C1C-C2C	-2.02	118.80	126.11
18	3	312	CLA	CHB-C1B-NB	-2.01	122.12	124.26
18	L	304	CLA	C3D-C4D-ND	2.01	113.50	110.24
27	2	606	CHL	CAA-C2A-C1A	2.01	118.56	111.97
18	B	812	CLA	CHC-C4B-NB	2.01	126.38	124.26
18	1	312	CLA	CHB-C1B-NB	-2.01	122.13	124.26
18	B	817	CLA	CHC-C4B-NB	2.00	126.38	124.26
18	A	837	CLA	C3D-C4D-ND	2.00	113.48	110.24
18	A	833	CLA	CHC-C4B-NB	2.00	126.38	124.26

There are no chirality outliers.

All (858) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	202	CL0	C2-C3-C5-C6
17	H	202	CL0	C4-C3-C5-C6
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	809	CLA	O2A-C1-C2-C3
18	A	812	CLA	C4B-C3B-CAB-CBB
18	A	812	CLA	C4-C3-C5-C6
18	A	819	CLA	C1A-C2A-CAA-CBA
18	A	819	CLA	C3A-C2A-CAA-CBA
18	A	823	CLA	C2B-C3B-CAB-CBB
18	A	823	CLA	C4B-C3B-CAB-CBB
18	A	825	CLA	CHA-CBD-CGD-O1D
18	A	825	CLA	CHA-CBD-CGD-O2D
18	A	834	CLA	C2B-C3B-CAB-CBB
18	A	834	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	A	835	CLA	C2B-C3B-CAB-CBB
18	A	835	CLA	C4B-C3B-CAB-CBB
18	A	835	CLA	CHA-CBD-CGD-O1D
18	A	835	CLA	CHA-CBD-CGD-O2D
18	A	837	CLA	CHA-CBD-CGD-O1D
18	A	837	CLA	CHA-CBD-CGD-O2D
18	A	840	CLA	CHA-CBD-CGD-O1D
18	A	840	CLA	CHA-CBD-CGD-O2D
18	A	841	CLA	CHA-CBD-CGD-O1D
18	A	841	CLA	CHA-CBD-CGD-O2D
18	A	843	CLA	C2B-C3B-CAB-CBB
18	A	843	CLA	C4B-C3B-CAB-CBB
18	A	845	CLA	C2B-C3B-CAB-CBB
18	A	845	CLA	C4B-C3B-CAB-CBB
18	A	856	CLA	C1A-C2A-CAA-CBA
18	A	856	CLA	C2B-C3B-CAB-CBB
18	A	856	CLA	C4B-C3B-CAB-CBB
18	B	804	CLA	C1A-C2A-CAA-CBA
18	B	807	CLA	CHA-CBD-CGD-O1D
18	B	807	CLA	CHA-CBD-CGD-O2D
18	B	808	CLA	C2-C3-C5-C6
18	B	808	CLA	C4-C3-C5-C6
18	B	817	CLA	C2B-C3B-CAB-CBB
18	B	818	CLA	C2B-C3B-CAB-CBB
18	B	818	CLA	C4B-C3B-CAB-CBB
18	B	820	CLA	CHA-CBD-CGD-O1D
18	B	820	CLA	CHA-CBD-CGD-O2D
18	B	820	CLA	CAD-CBD-CGD-O1D
18	B	821	CLA	C1A-C2A-CAA-CBA
18	B	821	CLA	CHA-CBD-CGD-O1D
18	B	821	CLA	CHA-CBD-CGD-O2D
18	B	822	CLA	CHA-CBD-CGD-O1D
18	B	822	CLA	CHA-CBD-CGD-O2D
18	B	836	CLA	C4B-C3B-CAB-CBB
18	L	303	CLA	CHA-CBD-CGD-O1D
18	G	204	CLA	C2B-C3B-CAB-CBB
18	K	203	CLA	C1A-C2A-CAA-CBA
18	K	204	CLA	C2B-C3B-CAB-CBB
18	K	204	CLA	C4B-C3B-CAB-CBB
18	1	305	CLA	C2B-C3B-CAB-CBB
18	1	305	CLA	C4B-C3B-CAB-CBB
18	1	308	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	1	312	CLA	CHA-CBD-CGD-O1D
18	1	312	CLA	CHA-CBD-CGD-O2D
18	1	312	CLA	CAD-CBD-CGD-O1D
18	1	313	CLA	C1A-C2A-CAA-CBA
18	1	313	CLA	C2-C3-C5-C6
18	1	313	CLA	C4-C3-C5-C6
18	1	314	CLA	CHA-CBD-CGD-O1D
18	1	314	CLA	CHA-CBD-CGD-O2D
18	2	601	CLA	C2B-C3B-CAB-CBB
18	2	601	CLA	C4B-C3B-CAB-CBB
18	2	602	CLA	C2B-C3B-CAB-CBB
18	2	602	CLA	C4B-C3B-CAB-CBB
18	2	603	CLA	C1A-C2A-CAA-CBA
18	2	603	CLA	C4-C3-C5-C6
18	2	612	CLA	CHA-CBD-CGD-O1D
18	2	612	CLA	CHA-CBD-CGD-O2D
18	3	303	CLA	C2B-C3B-CAB-CBB
18	3	303	CLA	C4B-C3B-CAB-CBB
18	3	308	CLA	O2A-C1-C2-C3
18	3	309	CLA	C2B-C3B-CAB-CBB
18	3	309	CLA	C4B-C3B-CAB-CBB
18	3	310	CLA	C4B-C3B-CAB-CBB
18	3	311	CLA	C2B-C3B-CAB-CBB
18	3	311	CLA	C4B-C3B-CAB-CBB
18	3	312	CLA	C2B-C3B-CAB-CBB
18	3	312	CLA	C4B-C3B-CAB-CBB
18	4	601	CLA	C2B-C3B-CAB-CBB
18	4	601	CLA	C4B-C3B-CAB-CBB
18	4	603	CLA	C2B-C3B-CAB-CBB
18	4	603	CLA	C4B-C3B-CAB-CBB
18	4	608	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	O2A-C1-C2-C3
18	4	609	CLA	C2-C3-C5-C6
18	4	609	CLA	C4-C3-C5-C6
18	4	610	CLA	CHA-CBD-CGD-O1D
18	4	610	CLA	CHA-CBD-CGD-O2D
20	A	846	LHG	C3-O3-P-O5
20	A	846	LHG	C3-O3-P-O6
20	A	847	LHG	C3-O3-P-O4
20	B	846	LHG	C3-O3-P-O5
20	B	847	LHG	C4-O6-P-O3
20	B	847	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
20	B	847	LHG	C4-O6-P-O5
20	1	319	LHG	C3-O3-P-O5
21	A	849	BCR	C1-C6-C7-C8
21	A	851	BCR	C1-C6-C7-C8
21	A	851	BCR	C5-C6-C7-C8
21	B	840	BCR	C1-C6-C7-C8
21	L	307	BCR	C23-C24-C25-C30
21	J	103	BCR	C1-C6-C7-C8
21	J	103	BCR	C5-C6-C7-C8
23	4	620	LMG	O7-C8-C9-O8
24	H	201	LMU	C2'-C1'-O1'-C1
24	H	201	LMU	O5'-C1'-O1'-C1
24	F	803	LMU	C2-C1-O1'-C1'
24	F	807	LMU	C2-C1-O1'-C1'
24	F	808	LMU	C2'-C1'-O1'-C1
24	F	808	LMU	O5'-C1'-O1'-C1
24	F	809	LMU	C2-C1-O1'-C1'
24	G	203	LMU	C2'-C1'-O1'-C1
24	G	203	LMU	O5'-C1'-O1'-C1
24	G	203	LMU	C2-C1-O1'-C1'
24	1	320	LMU	C2'-C1'-O1'-C1
24	1	320	LMU	O5'-C1'-O1'-C1
24	1	320	LMU	C2-C1-O1'-C1'
24	2	618	LMU	C2-C1-O1'-C1'
24	4	621	LMU	C2-C1-O1'-C1'
25	B	845	DGD	C2D-C1D-O3G-C3G
25	B	845	DGD	O6D-C1D-O3G-C3G
25	J	104	DGD	O6E-C1E-O5D-C6D
25	4	622	DGD	O6D-C1D-O3G-C3G
26	J	101	LUT	C5-C6-C7-C8
26	J	101	LUT	C21-C26-C27-C28
26	J	101	LUT	C25-C26-C27-C28
26	4	616	LUT	C1-C6-C7-C8
27	2	607	CHL	CHA-CBD-CGD-O1D
27	2	607	CHL	CHA-CBD-CGD-O2D
27	2	614	CHL	C2B-C3B-CAB-CBB
27	2	614	CHL	C4B-C3B-CAB-CBB
27	3	301	CHL	C2-C3-C5-C6
27	3	301	CHL	C4-C3-C5-C6
27	4	615	CHL	C2B-C3B-CAB-CBB
27	4	615	CHL	C4B-C3B-CAB-CBB
18	A	825	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	4	605	CHL	C4-C3-C5-C6
18	A	812	CLA	C2-C3-C5-C6
18	2	603	CLA	C2-C3-C5-C6
18	A	830	CLA	C2A-CAA-CBA-CGA
18	B	813	CLA	C2A-CAA-CBA-CGA
18	B	836	CLA	C2A-CAA-CBA-CGA
18	2	603	CLA	C3-C5-C6-C7
25	4	622	DGD	C4D-C5D-C6D-O5D
17	H	202	CL0	C3-C5-C6-C7
24	A	858	LMU	O5'-C1'-O1'-C1
25	4	622	DGD	O6D-C5D-C6D-O5D
20	B	847	LHG	C1-C2-C3-O3
20	B	847	LHG	O2-C2-C3-O3
20	2	617	LHG	O2-C2-C3-O3
25	J	104	DGD	C2E-C1E-O5D-C6D
25	4	622	DGD	C2D-C1D-O3G-C3G
18	A	843	CLA	C4-C3-C5-C6
18	A	843	CLA	C2-C3-C5-C6
18	A	814	CLA	C6-C7-C8-C9
18	B	807	CLA	C14-C13-C15-C16
18	F	804	CLA	C11-C12-C13-C14
27	4	605	CHL	C11-C12-C13-C14
18	A	807	CLA	C5-C6-C7-C8
18	A	814	CLA	C6-C7-C8-C10
18	A	829	CLA	C11-C10-C8-C7
18	A	829	CLA	C11-C12-C13-C15
18	A	809	CLA	C2A-CAA-CBA-CGA
18	A	836	CLA	C8-C10-C11-C12
18	A	802	CLA	C15-C16-C17-C18
18	A	841	CLA	C10-C11-C12-C13
18	3	305	CLA	C10-C11-C12-C13
20	2	617	LHG	C23-C24-C25-C26
18	A	804	CLA	C15-C16-C17-C18
18	A	829	CLA	C15-C16-C17-C18
18	B	830	CLA	C13-C15-C16-C17
18	F	804	CLA	C10-C11-C12-C13
18	4	609	CLA	C8-C10-C11-C12
18	A	807	CLA	C15-C16-C17-C18
18	A	855	CLA	C5-C6-C7-C8
20	1	319	LHG	C3-O3-P-O6
20	1	319	LHG	C4-O6-P-O3
24	4	623	LMU	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
20	2	617	LHG	C1-C2-C3-O3
18	2	612	CLA	C4-C3-C5-C6
27	3	301	CHL	C2A-CAA-CBA-CGA
17	H	202	CL0	C6-C7-C8-C10
24	F	803	LMU	C2'-C1'-O1'-C1
20	A	847	LHG	O7-C5-C6-O8
20	2	617	LHG	O7-C5-C6-O8
20	2	617	LHG	C9-C10-C11-C12
18	A	807	CLA	C4-C3-C5-C6
18	4	612	CLA	C4-C3-C5-C6
18	A	825	CLA	C2-C3-C5-C6
18	2	612	CLA	C2-C3-C5-C6
27	4	605	CHL	C2-C3-C5-C6
18	A	839	CLA	C11-C12-C13-C14
18	A	839	CLA	C14-C13-C15-C16
18	B	831	CLA	C14-C13-C15-C16
18	4	608	CLA	C14-C13-C15-C16
18	F	805	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C3-C5-C6-C7
17	H	202	CL0	C4B-C3B-CAB-CBB
18	A	817	CLA	C4B-C3B-CAB-CBB
18	B	810	CLA	C4B-C3B-CAB-CBB
18	B	815	CLA	C4B-C3B-CAB-CBB
18	B	817	CLA	C4B-C3B-CAB-CBB
18	G	204	CLA	C4B-C3B-CAB-CBB
18	J	102	CLA	C4B-C3B-CAB-CBB
18	K	201	CLA	C4B-C3B-CAB-CBB
18	K	203	CLA	C4B-C3B-CAB-CBB
18	1	311	CLA	C4B-C3B-CAB-CBB
18	1	313	CLA	C4B-C3B-CAB-CBB
18	1	314	CLA	C4B-C3B-CAB-CBB
18	3	308	CLA	C4B-C3B-CAB-CBB
18	4	612	CLA	C4B-C3B-CAB-CBB
27	2	606	CHL	C4B-C3B-CAB-CBB
27	4	606	CHL	C4B-C3B-CAB-CBB
17	H	202	CL0	C6-C7-C8-C9
20	B	846	LHG	C23-C24-C25-C26
25	B	845	DGD	C2B-C3B-C4B-C5B
18	B	822	CLA	C3A-C2A-CAA-CBA
18	1	304	CLA	C3A-C2A-CAA-CBA
18	1	312	CLA	C3A-C2A-CAA-CBA
18	1	313	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	A	855	CLA	C10-C11-C12-C13
24	A	859	LMU	C2-C1-O1'-C1'
18	B	812	CLA	C3-C5-C6-C7
18	A	828	CLA	C4-C3-C5-C6
18	A	834	CLA	C4-C3-C5-C6
18	B	836	CLA	C4-C3-C5-C6
18	G	201	CLA	C4-C3-C5-C6
18	K	203	CLA	C4-C3-C5-C6
18	A	807	CLA	C2-C3-C5-C6
18	A	822	CLA	C2-C3-C5-C6
18	A	828	CLA	C2-C3-C5-C6
18	A	834	CLA	C2-C3-C5-C6
18	B	836	CLA	C2-C3-C5-C6
18	K	203	CLA	C2-C3-C5-C6
18	3	310	CLA	C2-C3-C5-C6
18	4	612	CLA	C2-C3-C5-C6
24	B	848	LMU	C7-C8-C9-C10
17	H	202	CL0	C2B-C3B-CAB-CBB
18	A	812	CLA	C2B-C3B-CAB-CBB
18	B	810	CLA	C2B-C3B-CAB-CBB
18	B	815	CLA	C2B-C3B-CAB-CBB
18	B	836	CLA	C2B-C3B-CAB-CBB
18	J	102	CLA	C2B-C3B-CAB-CBB
18	K	201	CLA	C2B-C3B-CAB-CBB
18	K	203	CLA	C2B-C3B-CAB-CBB
18	1	311	CLA	C2B-C3B-CAB-CBB
18	1	313	CLA	C2B-C3B-CAB-CBB
18	1	314	CLA	C2B-C3B-CAB-CBB
18	3	308	CLA	C2B-C3B-CAB-CBB
18	3	310	CLA	C2B-C3B-CAB-CBB
18	4	610	CLA	C2B-C3B-CAB-CBB
27	2	606	CHL	C2B-C3B-CAB-CBB
27	4	606	CHL	C2B-C3B-CAB-CBB
24	4	623	LMU	C3'-C4'-O1B-C1B
18	1	313	CLA	C3-C5-C6-C7
21	A	848	BCR	C1-C6-C7-C8
21	A	848	BCR	C5-C6-C7-C8
21	A	849	BCR	C5-C6-C7-C8
21	B	840	BCR	C5-C6-C7-C8
21	B	842	BCR	C23-C24-C25-C26
21	B	842	BCR	C23-C24-C25-C30
21	B	844	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
21	L	307	BCR	C23-C24-C25-C26
21	G	206	BCR	C23-C24-C25-C26
21	G	206	BCR	C23-C24-C25-C30
21	3	313	BCR	C1-C6-C7-C8
21	3	313	BCR	C5-C6-C7-C8
21	3	313	BCR	C23-C24-C25-C26
21	3	313	BCR	C23-C24-C25-C30
21	4	618	BCR	C23-C24-C25-C26
21	4	618	BCR	C23-C24-C25-C30
26	J	101	LUT	C1-C6-C7-C8
26	4	616	LUT	C5-C6-C7-C8
24	A	859	LMU	O5'-C5'-C6'-O6'
18	A	822	CLA	C4-C3-C5-C6
18	B	806	CLA	C4-C3-C5-C6
18	B	818	CLA	C4-C3-C5-C6
18	B	829	CLA	C4-C3-C5-C6
18	2	609	CLA	C4-C3-C5-C6
18	3	308	CLA	C4-C3-C5-C6
18	3	310	CLA	C4-C3-C5-C6
18	A	839	CLA	C11-C12-C13-C15
18	B	806	CLA	C2-C3-C5-C6
18	B	818	CLA	C2-C3-C5-C6
18	B	827	CLA	C11-C10-C8-C7
18	B	829	CLA	C2-C3-C5-C6
18	2	609	CLA	C2-C3-C5-C6
18	3	308	CLA	C2-C3-C5-C6
27	4	605	CHL	C11-C12-C13-C15
20	2	617	LHG	C11-C12-C13-C14
18	A	819	CLA	C2A-CAA-CBA-CGA
18	B	802	CLA	C2A-CAA-CBA-CGA
20	A	847	LHG	C11-C10-C9-C8
18	B	837	CLA	C16-C17-C18-C20
24	4	621	LMU	O5'-C5'-C6'-O6'
18	A	827	CLA	C4-C3-C5-C6
18	B	833	CLA	C2-C3-C5-C6
18	G	201	CLA	C2-C3-C5-C6
18	A	829	CLA	C11-C10-C8-C9
18	A	829	CLA	C11-C12-C13-C14
18	B	806	CLA	C11-C10-C8-C9
24	4	624	LMU	O5'-C5'-C6'-O6'
18	A	818	CLA	C2A-CAA-CBA-CGA
18	A	821	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	4	604	CLA	C2A-CAA-CBA-CGA
24	A	858	LMU	O5'-C5'-C6'-O6'
24	F	808	LMU	O5B-C5B-C6B-O6B
18	B	822	CLA	C1A-C2A-CAA-CBA
18	1	304	CLA	C1A-C2A-CAA-CBA
18	1	310	CLA	C1A-C2A-CAA-CBA
18	1	312	CLA	C1A-C2A-CAA-CBA
18	3	308	CLA	C1A-C2A-CAA-CBA
18	4	604	CLA	C1A-C2A-CAA-CBA
27	3	306	CHL	C1A-C2A-CAA-CBA
20	B	847	LHG	O6-C4-C5-C6
24	2	618	LMU	O5B-C5B-C6B-O6B
18	A	842	CLA	C3-C5-C6-C7
20	2	617	LHG	C4-C5-C6-O8
25	J	104	DGD	C5D-C6D-O5D-C1E
18	A	855	CLA	C13-C15-C16-C17
23	A	857	LMG	O6-C5-C6-O5
24	F	807	LMU	O5B-C5B-C6B-O6B
23	A	857	LMG	C12-C13-C14-C15
20	B	847	LHG	C13-C14-C15-C16
18	4	608	CLA	C5-C6-C7-C8
18	A	854	CLA	C2-C1-O2A-CGA
24	G	207	LMU	O5B-C1B-O1B-C4'
18	A	842	CLA	C5-C6-C7-C8
18	A	820	CLA	C4-C3-C5-C6
18	B	809	CLA	C4-C3-C5-C6
18	B	833	CLA	C4-C3-C5-C6
18	A	826	CLA	C11-C10-C8-C7
18	B	807	CLA	C12-C13-C15-C16
18	B	809	CLA	C2-C3-C5-C6
18	F	804	CLA	C11-C12-C13-C15
18	A	820	CLA	C14-C13-C15-C16
18	B	824	CLA	C11-C10-C8-C9
24	G	207	LMU	C2B-C1B-O1B-C4'
18	A	833	CLA	C3-C5-C6-C7
18	A	819	CLA	C4B-C3B-CAB-CBB
18	A	832	CLA	C4B-C3B-CAB-CBB
18	B	801	CLA	C4B-C3B-CAB-CBB
18	B	807	CLA	C4B-C3B-CAB-CBB
18	B	820	CLA	C4B-C3B-CAB-CBB
18	B	822	CLA	C4B-C3B-CAB-CBB
18	1	312	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	2	613	CLA	C4B-C3B-CAB-CBB
18	3	302	CLA	C4B-C3B-CAB-CBB
18	3	305	CLA	C4B-C3B-CAB-CBB
18	4	604	CLA	C4B-C3B-CAB-CBB
18	4	610	CLA	C4B-C3B-CAB-CBB
18	4	613	CLA	C4B-C3B-CAB-CBB
27	3	301	CHL	C4B-C3B-CAB-CBB
27	3	306	CHL	C4B-C3B-CAB-CBB
18	A	823	CLA	C4-C3-C5-C6
18	A	820	CLA	C2-C3-C5-C6
20	A	847	LHG	O2-C2-C3-O3
18	L	304	CLA	C11-C12-C13-C14
20	B	847	LHG	C5-C4-O6-P
18	B	804	CLA	C3A-C2A-CAA-CBA
18	1	310	CLA	C3A-C2A-CAA-CBA
18	4	608	CLA	C3A-C2A-CAA-CBA
24	F	808	LMU	C2-C1-O1'-C1'
18	B	837	CLA	C16-C17-C18-C19
24	A	859	LMU	O1'-C1-C2-C3
20	A	847	LHG	C4-C5-C6-O8
25	B	845	DGD	O1G-C1G-C2G-C3G
23	4	620	LMG	C38-C39-C40-C41
18	A	843	CLA	O2A-C1-C2-C3
18	3	307	CLA	C4-C3-C5-C6
20	B	847	LHG	O6-C4-C5-O7
18	A	842	CLA	CBA-CGA-O2A-C1
23	4	620	LMG	C40-C41-C42-C43
18	A	817	CLA	C2B-C3B-CAB-CBB
18	A	819	CLA	C2B-C3B-CAB-CBB
18	A	832	CLA	C2B-C3B-CAB-CBB
18	B	801	CLA	C2B-C3B-CAB-CBB
18	3	305	CLA	C2B-C3B-CAB-CBB
18	4	612	CLA	C2B-C3B-CAB-CBB
18	4	613	CLA	C2B-C3B-CAB-CBB
27	3	301	CHL	C2B-C3B-CAB-CBB
25	B	845	DGD	O2G-C2G-C3G-O3G
20	B	847	LHG	C25-C26-C27-C28
18	B	830	CLA	C15-C16-C17-C18
20	B	846	LHG	C1-C2-C3-O3
18	B	819	CLA	C4-C3-C5-C6
18	A	827	CLA	C2-C1-O2A-CGA
18	B	801	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
18	B	825	CLA	C2-C1-O2A-CGA
18	B	819	CLA	C2-C3-C5-C6
18	A	826	CLA	C11-C10-C8-C9
18	A	854	CLA	C11-C10-C8-C9
18	1	309	CLA	C11-C12-C13-C14
27	1	302	CHL	C11-C12-C13-C14
27	4	605	CHL	C11-C10-C8-C9
20	1	319	LHG	C2-C3-O3-P
18	A	803	CLA	C2A-CAA-CBA-CGA
18	1	310	CLA	C2A-CAA-CBA-CGA
18	3	305	CLA	C2A-CAA-CBA-CGA
21	A	850	BCR	C1-C6-C7-C8
21	A	850	BCR	C5-C6-C7-C8
21	B	844	BCR	C23-C24-C25-C26
21	L	302	BCR	C23-C24-C25-C30
21	G	206	BCR	C1-C6-C7-C8
21	G	206	BCR	C5-C6-C7-C8
21	K	205	BCR	C1-C6-C7-C8
21	K	205	BCR	C5-C6-C7-C8
26	2	615	LUT	C1-C6-C7-C8
26	2	615	LUT	C5-C6-C7-C8
29	1	322	C7Z	C1-C6-C7-C8
29	1	322	C7Z	C5-C6-C7-C8
29	1	322	C7Z	C21-C26-C27-C28
29	1	322	C7Z	C25-C26-C27-C28
18	A	820	CLA	C12-C13-C15-C16
18	B	816	CLA	C6-C7-C8-C10
18	A	810	CLA	C2A-CAA-CBA-CGA
25	B	845	DGD	C8B-C9B-CAB-CBB
18	A	813	CLA	CAD-CBD-CGD-O2D
18	A	818	CLA	CAD-CBD-CGD-O2D
18	A	834	CLA	CAD-CBD-CGD-O2D
18	A	838	CLA	CAD-CBD-CGD-O2D
18	A	845	CLA	CAD-CBD-CGD-O2D
18	B	833	CLA	CAD-CBD-CGD-O2D
18	G	205	CLA	CAD-CBD-CGD-O2D
18	1	308	CLA	CAD-CBD-CGD-O2D
18	2	602	CLA	CAD-CBD-CGD-O2D
18	2	613	CLA	CAD-CBD-CGD-O2D
18	3	307	CLA	CAD-CBD-CGD-O2D
18	3	308	CLA	CAD-CBD-CGD-O2D
18	4	602	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	4	604	CLA	CAD-CBD-CGD-O2D
18	4	611	CLA	CAD-CBD-CGD-O2D
24	F	803	LMU	O5'-C1'-O1'-C1
20	B	846	LHG	C4-C5-C6-O8
23	A	857	LMG	O1-C7-C8-C9
23	4	620	LMG	C7-C8-C9-O8
25	B	845	DGD	C1G-C2G-C3G-O3G
20	A	847	LHG	C1-C2-C3-O3
18	A	806	CLA	CHA-CBD-CGD-O1D
18	A	806	CLA	CHA-CBD-CGD-O2D
18	A	809	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O2D
18	A	831	CLA	CHA-CBD-CGD-O1D
18	A	831	CLA	CHA-CBD-CGD-O2D
18	B	823	CLA	CHA-CBD-CGD-O1D
18	B	823	CLA	CHA-CBD-CGD-O2D
18	B	839	CLA	CHA-CBD-CGD-O1D
18	B	839	CLA	CHA-CBD-CGD-O2D
18	L	303	CLA	CHA-CBD-CGD-O2D
18	F	805	CLA	CHA-CBD-CGD-O1D
18	F	805	CLA	CHA-CBD-CGD-O2D
18	G	201	CLA	CHA-CBD-CGD-O1D
18	G	201	CLA	CHA-CBD-CGD-O2D
18	2	601	CLA	CHA-CBD-CGD-O1D
18	2	611	CLA	CHA-CBD-CGD-O1D
18	2	611	CLA	CHA-CBD-CGD-O2D
18	3	303	CLA	CHA-CBD-CGD-O1D
18	3	303	CLA	CHA-CBD-CGD-O2D
18	3	309	CLA	CHA-CBD-CGD-O1D
18	3	309	CLA	CHA-CBD-CGD-O2D
18	3	311	CLA	CHA-CBD-CGD-O1D
18	3	311	CLA	CHA-CBD-CGD-O2D
18	4	601	CLA	CHA-CBD-CGD-O1D
18	4	601	CLA	CHA-CBD-CGD-O2D
27	3	301	CHL	CHA-CBD-CGD-O1D
27	3	301	CHL	CHA-CBD-CGD-O2D
23	4	619	LMG	C14-C15-C16-C17
18	L	304	CLA	C11-C12-C13-C15
18	B	807	CLA	C4-C3-C5-C6
18	A	814	CLA	C3-C5-C6-C7
20	A	847	LHG	C3-O3-P-O6
20	B	847	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
20	A	847	LHG	C5-C4-O6-P
18	A	842	CLA	C4B-C3B-CAB-CBB
18	A	855	CLA	C4B-C3B-CAB-CBB
20	A	847	LHG	C3-O3-P-O5
20	1	319	LHG	C3-O3-P-O4
20	1	319	LHG	C4-O6-P-O5
18	A	820	CLA	C16-C17-C18-C20
18	A	806	CLA	CAD-CBD-CGD-O1D
18	B	804	CLA	CAD-CBD-CGD-O1D
18	B	839	CLA	CAD-CBD-CGD-O1D
18	2	601	CLA	CAD-CBD-CGD-O1D
27	2	607	CHL	CAD-CBD-CGD-O1D
24	4	623	LMU	O5B-C1B-O1B-C4'
18	B	839	CLA	C12-C13-C15-C16
19	B	838	PQN	C16-C17-C18-C20
20	A	847	LHG	O6-C4-C5-O7
18	A	807	CLA	C3-C5-C6-C7
24	H	201	LMU	C2-C1-O1'-C1'
24	F	807	LMU	C5-C6-C7-C8
20	2	617	LHG	C7-C8-C9-C10
25	B	845	DGD	O1G-C1G-C2G-O2G
25	4	622	DGD	C5D-C6D-O5D-C1E
18	A	842	CLA	O1A-CGA-O2A-C1
18	A	815	CLA	C4-C3-C5-C6
18	4	608	CLA	C4-C3-C5-C6
27	1	302	CHL	C4-C3-C5-C6
18	B	807	CLA	C2-C3-C5-C6
18	A	830	CLA	C11-C10-C8-C9
18	B	813	CLA	C6-C7-C8-C9
18	B	816	CLA	C6-C7-C8-C9
18	B	827	CLA	C14-C13-C15-C16
18	B	807	CLA	C3-C5-C6-C7
20	A	847	LHG	O7-C7-C8-C9
18	1	313	CLA	C5-C6-C7-C8
17	A	801	CL0	C2B-C3B-CAB-CBB
18	A	821	CLA	C2B-C3B-CAB-CBB
18	A	855	CLA	C2B-C3B-CAB-CBB
18	B	807	CLA	C2B-C3B-CAB-CBB
18	B	811	CLA	C2B-C3B-CAB-CBB
18	B	819	CLA	C2B-C3B-CAB-CBB
18	B	820	CLA	C2B-C3B-CAB-CBB
18	B	822	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	B	831	CLA	C2B-C3B-CAB-CBB
18	L	303	CLA	C2B-C3B-CAB-CBB
18	1	309	CLA	C2B-C3B-CAB-CBB
18	1	312	CLA	C2B-C3B-CAB-CBB
18	2	613	CLA	C2B-C3B-CAB-CBB
18	3	302	CLA	C2B-C3B-CAB-CBB
18	4	604	CLA	C2B-C3B-CAB-CBB
18	4	608	CLA	C2B-C3B-CAB-CBB
27	3	306	CHL	C2B-C3B-CAB-CBB
18	B	804	CLA	C4-C3-C5-C6
18	B	825	CLA	C4-C3-C5-C6
24	1	301	LMU	O5B-C1B-O1B-C4'
18	A	816	CLA	C2-C1-O2A-CGA
18	A	823	CLA	C2-C1-O2A-CGA
27	2	607	CHL	C2-C1-O2A-CGA
20	A	846	LHG	C15-C16-C17-C18
21	B	843	BCR	C1-C6-C7-C8
21	L	302	BCR	C23-C24-C25-C26
27	2	605	CHL	CAA-CBA-CGA-O2A
18	A	817	CLA	C2A-CAA-CBA-CGA
18	4	608	CLA	C2A-CAA-CBA-CGA
20	B	846	LHG	O7-C5-C6-O8
23	A	857	LMG	O1-C7-C8-O7
19	B	838	PQN	C26-C27-C28-C30
18	A	809	CLA	C8-C10-C11-C12
18	A	822	CLA	C6-C7-C8-C10
18	A	823	CLA	C2-C3-C5-C6
18	A	839	CLA	C12-C13-C15-C16
18	B	825	CLA	C2-C3-C5-C6
18	B	831	CLA	C12-C13-C15-C16
18	A	826	CLA	C4-C3-C5-C6
24	1	301	LMU	C2B-C1B-O1B-C4'
24	4	623	LMU	C2B-C1B-O1B-C4'
17	A	801	CL0	C4B-C3B-CAB-CBB
18	B	811	CLA	C4B-C3B-CAB-CBB
18	B	819	CLA	C4B-C3B-CAB-CBB
18	B	831	CLA	C4B-C3B-CAB-CBB
18	B	837	CLA	C4B-C3B-CAB-CBB
18	1	309	CLA	C4B-C3B-CAB-CBB
18	4	614	CLA	C4B-C3B-CAB-CBB
25	B	845	DGD	C6B-C7B-C8B-C9B
25	B	845	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
18	B	837	CLA	C2-C1-O2A-CGA
18	2	609	CLA	C2-C1-O2A-CGA
18	4	601	CLA	C2-C1-O2A-CGA
18	4	609	CLA	C2-C1-O2A-CGA
20	2	617	LHG	C11-C10-C9-C8
18	A	817	CLA	CAA-CBA-CGA-O1A
18	B	807	CLA	C13-C15-C16-C17
18	A	804	CLA	C3A-C2A-CAA-CBA
18	A	818	CLA	C3A-C2A-CAA-CBA
18	B	821	CLA	C3A-C2A-CAA-CBA
18	2	603	CLA	C3A-C2A-CAA-CBA
18	A	819	CLA	CAA-CBA-CGA-O2A
18	1	308	CLA	CAA-CBA-CGA-O1A
18	2	611	CLA	CAA-CBA-CGA-O2A
18	B	804	CLA	C2-C3-C5-C6
27	1	302	CHL	C2-C3-C5-C6
18	A	816	CLA	C6-C7-C8-C9
18	A	822	CLA	C11-C10-C8-C9
18	L	304	CLA	C6-C7-C8-C9
18	F	804	CLA	C6-C7-C8-C9
18	1	309	CLA	C14-C13-C15-C16
18	4	608	CLA	C11-C12-C13-C14
18	A	820	CLA	C16-C17-C18-C19
20	B	847	LHG	C12-C13-C14-C15
21	A	852	BCR	C11-C10-C9-C34
21	A	852	BCR	C16-C17-C18-C36
21	B	841	BCR	C11-C10-C9-C34
21	B	841	BCR	C20-C21-C22-C37
21	L	302	BCR	C20-C21-C22-C37
21	F	806	BCR	C16-C17-C18-C36
18	1	308	CLA	CAA-CBA-CGA-O2A
27	1	307	CHL	CAA-CBA-CGA-O1A
18	F	804	CLA	C16-C17-C18-C20
18	A	805	CLA	O2A-C1-C2-C3
18	1	309	CLA	O2A-C1-C2-C3
18	A	817	CLA	CAA-CBA-CGA-O2A
18	B	831	CLA	C1A-C2A-CAA-CBA
18	3	307	CLA	C1A-C2A-CAA-CBA
27	1	302	CHL	C1A-C2A-CAA-CBA
27	3	301	CHL	C1A-C2A-CAA-CBA
18	A	815	CLA	C2-C3-C5-C6
18	A	826	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	B	805	CLA	C6-C7-C8-C10
18	B	820	CLA	C12-C13-C15-C16
18	2	609	CLA	C6-C7-C8-C10
18	4	608	CLA	C2-C3-C5-C6
18	A	824	CLA	CAA-CBA-CGA-O2A
18	A	845	CLA	CAA-CBA-CGA-O1A
18	2	611	CLA	CAA-CBA-CGA-O1A
18	A	824	CLA	CAA-CBA-CGA-O1A
18	L	303	CLA	CAA-CBA-CGA-O1A
18	A	804	CLA	CAA-CBA-CGA-O2A
18	G	204	CLA	CAA-CBA-CGA-O1A
20	A	847	LHG	O6-C4-C5-C6
18	B	825	CLA	C3-C5-C6-C7
18	A	845	CLA	CAA-CBA-CGA-O2A
18	G	204	CLA	CAA-CBA-CGA-O2A
27	1	307	CHL	CAA-CBA-CGA-O2A
18	A	814	CLA	C2B-C3B-CAB-CBB
18	A	824	CLA	C2B-C3B-CAB-CBB
18	A	842	CLA	C2B-C3B-CAB-CBB
18	B	803	CLA	C2B-C3B-CAB-CBB
18	4	614	CLA	C2B-C3B-CAB-CBB
27	1	302	CHL	C2B-C3B-CAB-CBB
21	A	852	BCR	C11-C10-C9-C8
21	A	852	BCR	C16-C17-C18-C19
21	B	841	BCR	C11-C10-C9-C8
21	B	841	BCR	C20-C21-C22-C23
21	L	302	BCR	C20-C21-C22-C23
21	F	806	BCR	C16-C17-C18-C19
18	A	821	CLA	CAA-CBA-CGA-O1A
18	A	821	CLA	CAA-CBA-CGA-O2A
20	1	319	LHG	C1-C2-C3-O3
18	K	204	CLA	CAA-CBA-CGA-O2A
18	A	809	CLA	C4-C3-C5-C6
18	A	810	CLA	C2-C1-O2A-CGA
18	B	805	CLA	C2-C1-O2A-CGA
18	F	805	CLA	C2-C1-O2A-CGA
18	3	307	CLA	C2-C1-O2A-CGA
18	A	835	CLA	C2-C3-C5-C6
18	A	813	CLA	CAA-CBA-CGA-O2A
18	3	307	CLA	CAA-CBA-CGA-O2A
18	B	813	CLA	C5-C6-C7-C8
18	L	303	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	1	318	LUT	C1-C6-C7-C8
18	A	820	CLA	C15-C16-C17-C18
20	A	846	LHG	O8-C23-C24-C25
20	A	846	LHG	O7-C7-C8-C9
18	1	311	CLA	CAA-CBA-CGA-O2A
20	2	617	LHG	O6-C4-C5-O7
18	1	314	CLA	CAA-CBA-CGA-O2A
18	3	304	CLA	CAA-CBA-CGA-O2A
18	A	814	CLA	C4B-C3B-CAB-CBB
18	A	821	CLA	C4B-C3B-CAB-CBB
18	A	824	CLA	C4B-C3B-CAB-CBB
18	A	825	CLA	C4B-C3B-CAB-CBB
18	B	803	CLA	C4B-C3B-CAB-CBB
18	L	303	CLA	C4B-C3B-CAB-CBB
18	1	306	CLA	C4B-C3B-CAB-CBB
18	4	608	CLA	C4B-C3B-CAB-CBB
27	1	302	CHL	C4B-C3B-CAB-CBB
27	1	307	CHL	C4B-C3B-CAB-CBB
18	B	815	CLA	C4-C3-C5-C6
18	2	610	CLA	C4-C3-C5-C6
18	A	827	CLA	C2-C3-C5-C6
18	B	813	CLA	C6-C7-C8-C10
18	4	602	CLA	C6-C7-C8-C10
27	2	606	CHL	CAA-CBA-CGA-O1A
18	G	205	CLA	CAA-CBA-CGA-O2A
20	1	319	LHG	C5-C4-O6-P
18	K	204	CLA	CAA-CBA-CGA-O1A
18	1	311	CLA	CAA-CBA-CGA-O1A
27	2	606	CHL	CAA-CBA-CGA-O2A
18	B	819	CLA	CAA-CBA-CGA-O2A
18	4	611	CLA	CAA-CBA-CGA-O2A
18	K	201	CLA	CAA-CBA-CGA-O2A
18	B	839	CLA	C4-C3-C5-C6
18	A	813	CLA	CAA-CBA-CGA-O1A
18	3	307	CLA	C2-C3-C5-C6
18	A	826	CLA	CAA-CBA-CGA-O2A
18	3	305	CLA	CAA-CBA-CGA-O2A
18	B	824	CLA	C14-C13-C15-C16
18	B	827	CLA	C11-C10-C8-C9
18	4	608	CLA	C6-C7-C8-C9
18	3	311	CLA	CAA-CBA-CGA-O1A
18	4	604	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
18	B	831	CLA	C3A-C2A-CAA-CBA
18	B	839	CLA	C3A-C2A-CAA-CBA
27	3	306	CHL	CAA-CBA-CGA-O2A
24	F	807	LMU	O1'-C1-C2-C3
17	H	202	CL0	CAD-CBD-CGD-O2D
18	A	824	CLA	CAD-CBD-CGD-O2D
18	A	826	CLA	CAD-CBD-CGD-O2D
18	A	827	CLA	CAD-CBD-CGD-O2D
18	B	811	CLA	CAD-CBD-CGD-O2D
18	L	305	CLA	CAD-CBD-CGD-O2D
18	G	204	CLA	CAD-CBD-CGD-O2D
18	J	102	CLA	CAD-CBD-CGD-O2D
18	1	304	CLA	CAD-CBD-CGD-O2D
18	1	305	CLA	CAD-CBD-CGD-O2D
18	1	309	CLA	CAD-CBD-CGD-O2D
18	1	315	CLA	CAD-CBD-CGD-O2D
18	3	305	CLA	CAD-CBD-CGD-O2D
18	4	614	CLA	CAD-CBD-CGD-O2D
27	1	302	CHL	CAD-CBD-CGD-O2D
27	1	307	CHL	CAD-CBD-CGD-O2D
18	B	822	CLA	C2-C1-O2A-CGA
18	A	843	CLA	CAA-CBA-CGA-O2A
18	2	601	CLA	CAA-CBA-CGA-O2A
18	B	812	CLA	C4-C3-C5-C6
18	1	314	CLA	CAA-CBA-CGA-O1A
18	B	805	CLA	CAA-CBA-CGA-O2A
18	4	603	CLA	CAA-CBA-CGA-O2A
20	2	617	LHG	O8-C23-C24-C25
23	F	810	LMG	O7-C10-C11-C12
18	3	309	CLA	CAA-CBA-CGA-O2A
17	H	202	CL0	O2A-C1-C2-C3
18	A	825	CLA	O2A-C1-C2-C3
18	A	827	CLA	O2A-C1-C2-C3
18	B	815	CLA	O2A-C1-C2-C3
18	B	829	CLA	O2A-C1-C2-C3
18	1	305	CLA	O2A-C1-C2-C3
18	4	601	CLA	O2A-C1-C2-C3
27	3	306	CHL	O2A-C1-C2-C3
20	B	846	LHG	O2-C2-C3-O3
18	A	805	CLA	CHA-CBD-CGD-O2D
18	A	811	CLA	CHA-CBD-CGD-O1D
18	A	811	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	A	832	CLA	CHA-CBD-CGD-O2D
18	B	801	CLA	CHA-CBD-CGD-O1D
18	B	801	CLA	CHA-CBD-CGD-O2D
18	B	804	CLA	CHA-CBD-CGD-O1D
18	B	804	CLA	CHA-CBD-CGD-O2D
18	B	809	CLA	CHA-CBD-CGD-O2D
18	B	810	CLA	CHA-CBD-CGD-O1D
18	B	810	CLA	CHA-CBD-CGD-O2D
18	B	814	CLA	CHA-CBD-CGD-O1D
18	B	814	CLA	CHA-CBD-CGD-O2D
18	B	818	CLA	CHA-CBD-CGD-O1D
18	B	818	CLA	CHA-CBD-CGD-O2D
18	B	819	CLA	CHA-CBD-CGD-O2D
18	B	830	CLA	CHA-CBD-CGD-O1D
18	K	201	CLA	CHA-CBD-CGD-O1D
18	K	201	CLA	CHA-CBD-CGD-O2D
18	K	203	CLA	CHA-CBD-CGD-O1D
18	K	203	CLA	CHA-CBD-CGD-O2D
18	K	204	CLA	CHA-CBD-CGD-O1D
18	K	204	CLA	CHA-CBD-CGD-O2D
18	1	303	CLA	CHA-CBD-CGD-O1D
18	1	303	CLA	CHA-CBD-CGD-O2D
18	2	601	CLA	CHA-CBD-CGD-O2D
18	3	304	CLA	CHA-CBD-CGD-O1D
18	4	603	CLA	CHA-CBD-CGD-O2D
18	4	612	CLA	CHA-CBD-CGD-O1D
18	4	612	CLA	CHA-CBD-CGD-O2D
27	2	605	CHL	CHA-CBD-CGD-O1D
27	4	615	CHL	CHA-CBD-CGD-O1D
27	4	615	CHL	CHA-CBD-CGD-O2D
18	K	201	CLA	CAA-CBA-CGA-O1A
18	3	304	CLA	CAA-CBA-CGA-O1A
18	3	309	CLA	CAA-CBA-CGA-O1A
18	4	604	CLA	CAA-CBA-CGA-O1A
18	A	835	CLA	C4-C3-C5-C6
18	A	814	CLA	CAA-CBA-CGA-O2A
18	3	311	CLA	CAA-CBA-CGA-O2A
25	J	104	DGD	O2G-C1B-C2B-C3B
18	A	856	CLA	CAA-CBA-CGA-O2A
18	A	807	CLA	CAA-CBA-CGA-O2A
18	A	812	CLA	C11-C10-C8-C7
18	B	829	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	1	313	CLA	C6-C7-C8-C10
18	2	601	CLA	C6-C7-C8-C10
27	3	301	CHL	C11-C12-C13-C15
27	2	607	CHL	CAA-CBA-CGA-O2A
18	A	822	CLA	C6-C7-C8-C9
18	B	815	CLA	C6-C7-C8-C9
18	B	831	CLA	C11-C12-C13-C14
18	B	839	CLA	C14-C13-C15-C16
18	2	609	CLA	C6-C7-C8-C9
18	A	854	CLA	C2B-C3B-CAB-CBB
18	B	837	CLA	C2B-C3B-CAB-CBB
18	1	306	CLA	C2B-C3B-CAB-CBB
20	1	319	LHG	C23-C24-C25-C26
18	B	804	CLA	CAA-CBA-CGA-O2A
18	4	603	CLA	CAA-CBA-CGA-O1A
18	3	305	CLA	CAA-CBA-CGA-O1A
18	A	809	CLA	C2-C3-C5-C6
18	A	854	CLA	C1A-C2A-CAA-CBA
18	B	825	CLA	C1A-C2A-CAA-CBA
18	B	839	CLA	C1A-C2A-CAA-CBA
27	1	307	CHL	C1A-C2A-CAA-CBA
18	B	805	CLA	CAA-CBA-CGA-O1A
18	G	205	CLA	CAA-CBA-CGA-O1A
18	A	826	CLA	CAA-CBA-CGA-O1A
18	4	611	CLA	CAA-CBA-CGA-O1A
23	F	810	LMG	O9-C10-C11-C12
18	A	842	CLA	CAA-CBA-CGA-O2A
18	2	612	CLA	C2A-CAA-CBA-CGA
18	4	612	CLA	C2A-CAA-CBA-CGA
18	A	831	CLA	C16-C17-C18-C20
20	2	617	LHG	O10-C23-C24-C25
18	A	843	CLA	CAA-CBA-CGA-O1A
27	2	607	CHL	CAA-CBA-CGA-O1A
18	B	812	CLA	C2-C3-C5-C6
18	B	826	CLA	C4B-C3B-CAB-CBB
18	2	610	CLA	C4B-C3B-CAB-CBB
20	2	617	LHG	C3-O3-P-O5
20	2	617	LHG	C4-O6-P-O5
18	F	804	CLA	C16-C17-C18-C19
18	B	819	CLA	CAA-CBA-CGA-O1A
23	4	620	LMG	O6-C1-O1-C7
21	B	843	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	L	306	BCR	C23-C24-C25-C26
21	L	306	BCR	C23-C24-C25-C30
18	4	611	CLA	C4C-C3C-CAC-CBC
18	4	610	CLA	CAA-CBA-CGA-O2A
18	A	814	CLA	CAA-CBA-CGA-O1A
20	2	617	LHG	C25-C26-C27-C28
18	A	856	CLA	CAA-CBA-CGA-O1A
18	A	807	CLA	CAD-CBD-CGD-O1D
18	B	827	CLA	CAD-CBD-CGD-O1D
18	1	311	CLA	CAD-CBD-CGD-O1D
18	3	310	CLA	CAD-CBD-CGD-O1D
27	2	606	CHL	CAD-CBD-CGD-O1D
27	3	306	CHL	CAA-CBA-CGA-O1A
18	A	812	CLA	C11-C10-C8-C9
18	1	313	CLA	C11-C10-C8-C9
19	B	838	PQN	C16-C17-C18-C19
18	A	807	CLA	C10-C11-C12-C13
20	A	846	LHG	C23-C24-C25-C26
18	B	808	CLA	CAA-CBA-CGA-O2A
18	G	201	CLA	CAA-CBA-CGA-O2A
20	B	846	LHG	O8-C23-C24-C25
20	B	847	LHG	O7-C7-C8-C9
18	1	309	CLA	C13-C15-C16-C17
20	B	847	LHG	C30-C31-C32-C33
18	A	807	CLA	CAA-CBA-CGA-O1A
18	A	854	CLA	C5-C6-C7-C8
18	4	614	CLA	CAA-CBA-CGA-O2A
18	2	609	CLA	C5-C6-C7-C8
18	A	842	CLA	CAA-CBA-CGA-O1A
18	A	803	CLA	C4-C3-C5-C6
18	A	809	CLA	C11-C10-C8-C7
18	A	816	CLA	C6-C7-C8-C10
18	B	815	CLA	C2-C3-C5-C6
18	B	827	CLA	C3A-C2A-CAA-CBA
18	F	804	CLA	C6-C7-C8-C10
27	4	607	CHL	C3A-C2A-CAA-CBA
25	J	104	DGD	O1B-C1B-C2B-C3B
18	4	610	CLA	CAA-CBA-CGA-O1A
18	3	310	CLA	CAA-CBA-CGA-O2A
18	G	201	CLA	CAA-CBA-CGA-O1A
18	B	808	CLA	CAA-CBA-CGA-O1A
20	B	846	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
17	A	801	CL0	CAA-CBA-CGA-O2A
18	3	310	CLA	C2A-CAA-CBA-CGA
18	A	804	CLA	C8-C10-C11-C12
18	B	826	CLA	C4-C3-C5-C6

There are no ring outliers.

141 monomers are involved in 216 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	F	808	LMU	1	0
24	1	320	LMU	1	0
18	B	822	CLA	4	0
18	1	313	CLA	3	0
24	1	321	LMU	1	0
21	A	848	BCR	4	0
18	B	818	CLA	1	0
24	F	803	LMU	1	0
18	2	603	CLA	1	0
21	A	850	BCR	2	0
18	3	307	CLA	3	0
18	B	830	CLA	1	0
21	G	202	BCR	2	0
24	4	624	LMU	1	0
18	4	614	CLA	1	0
27	4	606	CHL	2	0
18	A	815	CLA	2	0
21	L	307	BCR	1	0
18	1	315	CLA	1	0
18	1	308	CLA	1	0
18	A	841	CLA	2	0
18	A	829	CLA	4	0
18	4	611	CLA	1	0
24	F	809	LMU	2	0
18	1	303	CLA	2	0
27	3	301	CHL	5	0
18	B	819	CLA	1	0
18	A	836	CLA	1	0
18	3	311	CLA	1	0
20	1	319	LHG	5	0
21	A	849	BCR	2	0
18	B	824	CLA	3	0
18	1	310	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	1	301	LMU	2	0
28	2	616	XAT	1	0
18	2	610	CLA	2	0
24	G	207	LMU	2	0
18	A	823	CLA	2	0
18	A	854	CLA	1	0
21	J	103	BCR	1	0
18	3	302	CLA	4	0
21	A	851	BCR	2	0
18	B	804	CLA	1	0
18	A	843	CLA	3	0
18	A	818	CLA	3	0
18	3	305	CLA	1	0
18	B	810	CLA	2	0
24	F	807	LMU	2	0
18	A	816	CLA	1	0
18	A	822	CLA	2	0
24	4	623	LMU	2	0
18	F	804	CLA	4	0
20	B	846	LHG	1	0
18	A	806	CLA	1	0
26	4	616	LUT	4	0
18	B	806	CLA	1	0
23	4	620	LMG	3	0
18	A	805	CLA	1	0
27	4	605	CHL	1	0
18	1	309	CLA	6	0
18	A	819	CLA	2	0
18	B	823	CLA	1	0
18	B	833	CLA	1	0
18	A	811	CLA	3	0
25	J	104	DGD	3	0
18	4	601	CLA	1	0
18	A	828	CLA	1	0
26	J	101	LUT	3	0
18	F	805	CLA	1	0
18	A	856	CLA	1	0
26	3	315	LUT	3	0
18	A	813	CLA	1	0
27	1	307	CHL	2	0
18	A	839	CLA	1	0
21	B	843	BCR	1	0

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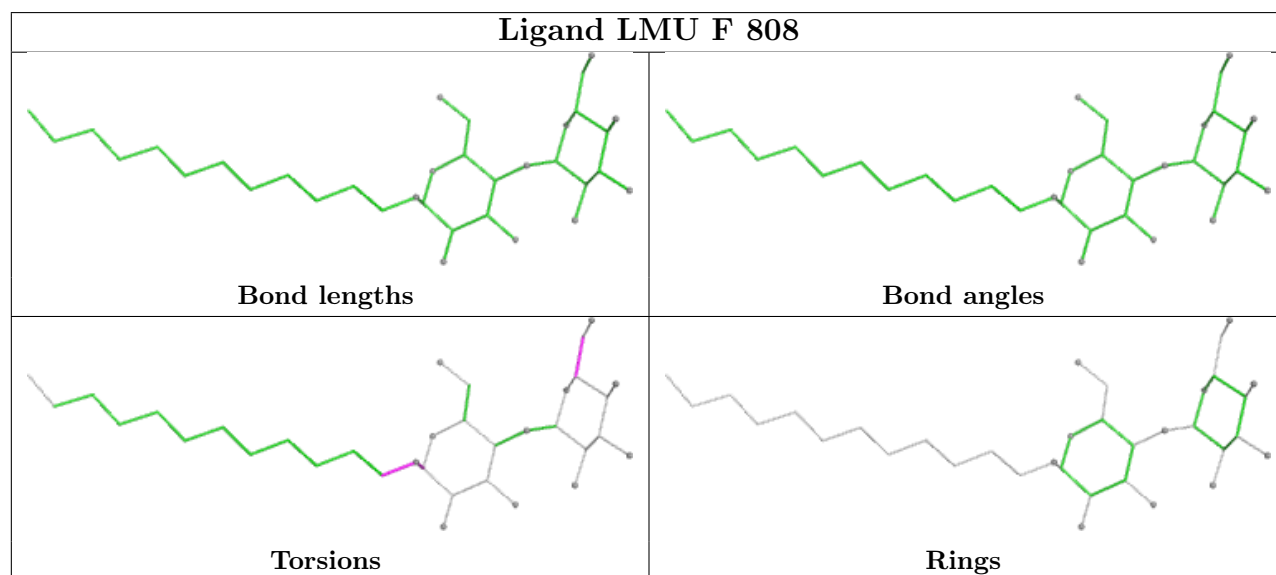
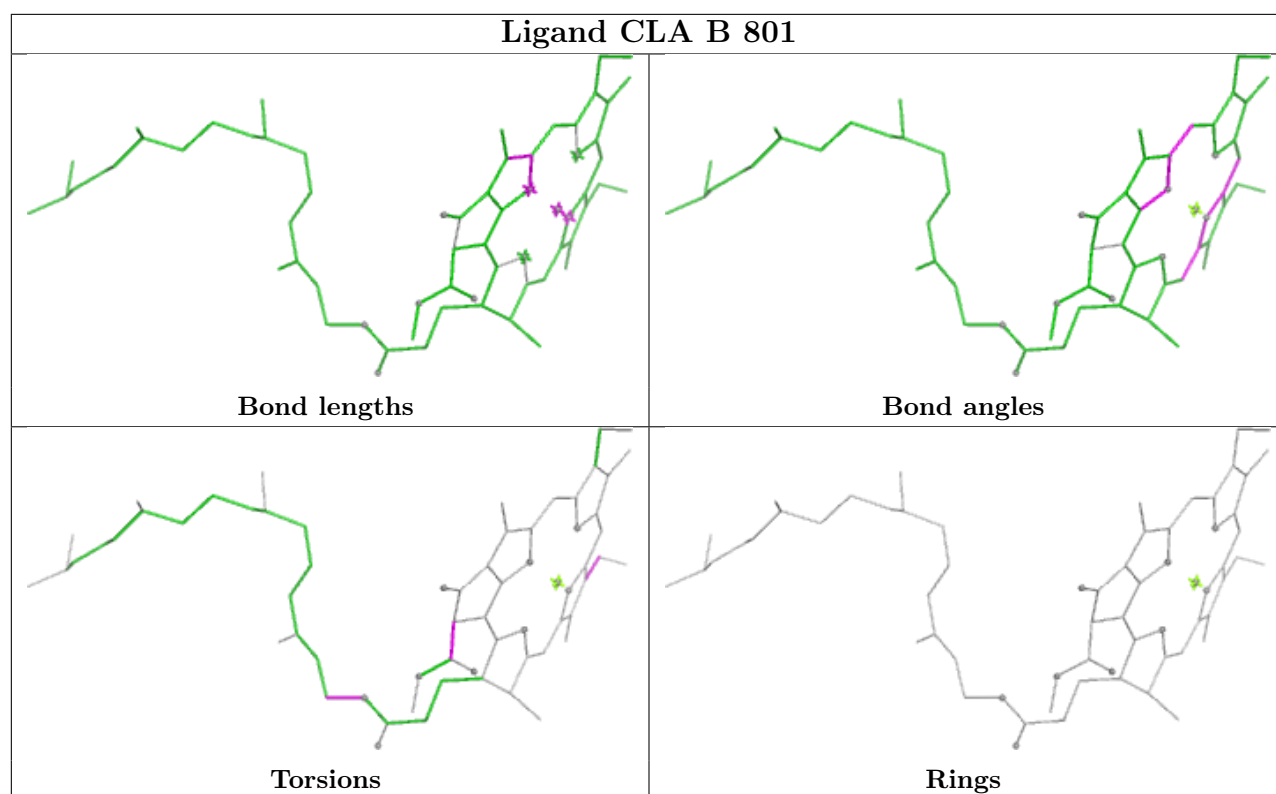
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1	318	LUT	1	0
18	4	603	CLA	1	0
27	2	606	CHL	1	0
18	4	609	CLA	4	0
18	B	817	CLA	2	0
24	H	201	LMU	1	0
18	A	824	CLA	1	0
18	G	201	CLA	4	0
24	2	618	LMU	1	0
18	A	804	CLA	1	0
18	A	838	CLA	2	0
20	B	847	LHG	1	0
18	1	312	CLA	3	0
18	1	311	CLA	1	0
18	4	602	CLA	1	0
18	2	609	CLA	1	0
21	F	806	BCR	2	0
27	1	302	CHL	3	0
26	3	314	LUT	1	0
21	4	618	BCR	3	0
24	B	848	LMU	1	0
18	A	820	CLA	3	0
24	A	859	LMU	1	0
18	3	308	CLA	4	0
18	4	608	CLA	2	0
18	A	845	CLA	1	0
28	1	317	XAT	2	0
18	1	306	CLA	2	0
26	1	316	LUT	4	0
21	G	206	BCR	2	0
26	2	615	LUT	1	0
18	F	802	CLA	1	0
21	3	313	BCR	4	0
18	G	205	CLA	2	0
23	A	857	LMG	3	0
24	L	301	LMU	2	0
20	A	846	LHG	3	0
18	A	825	CLA	1	0
23	F	810	LMG	2	0
25	4	622	DGD	1	0
21	B	844	BCR	3	0
21	L	306	BCR	2	0

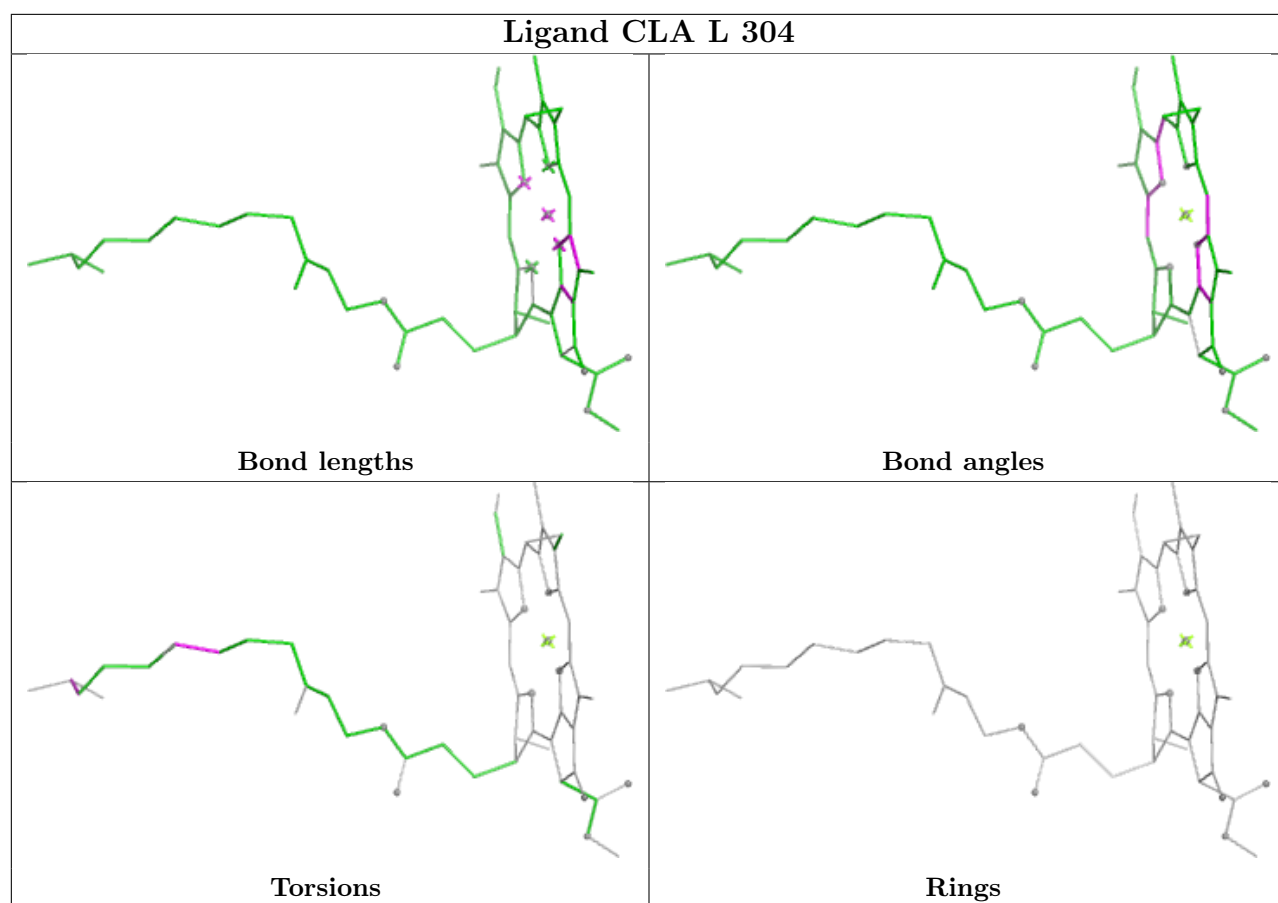
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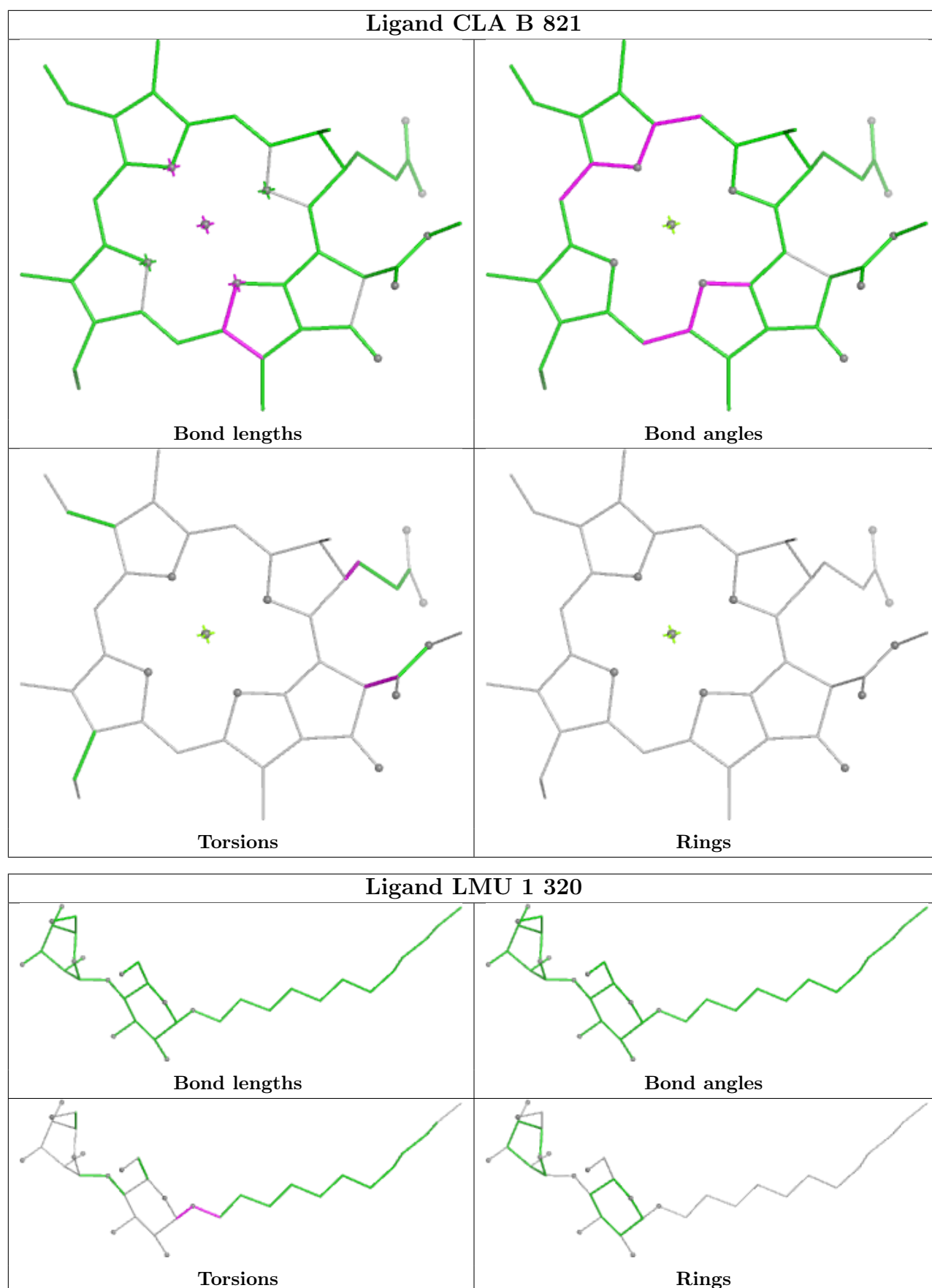
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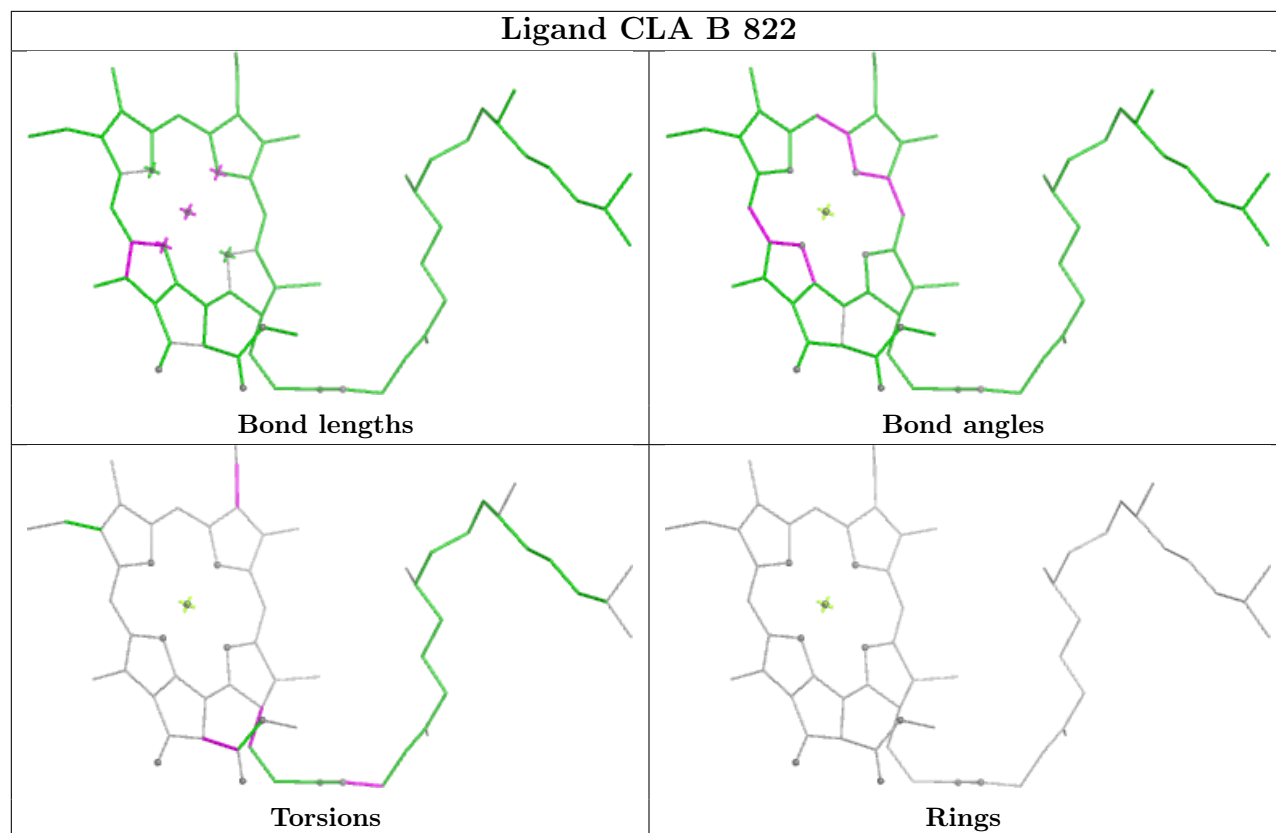
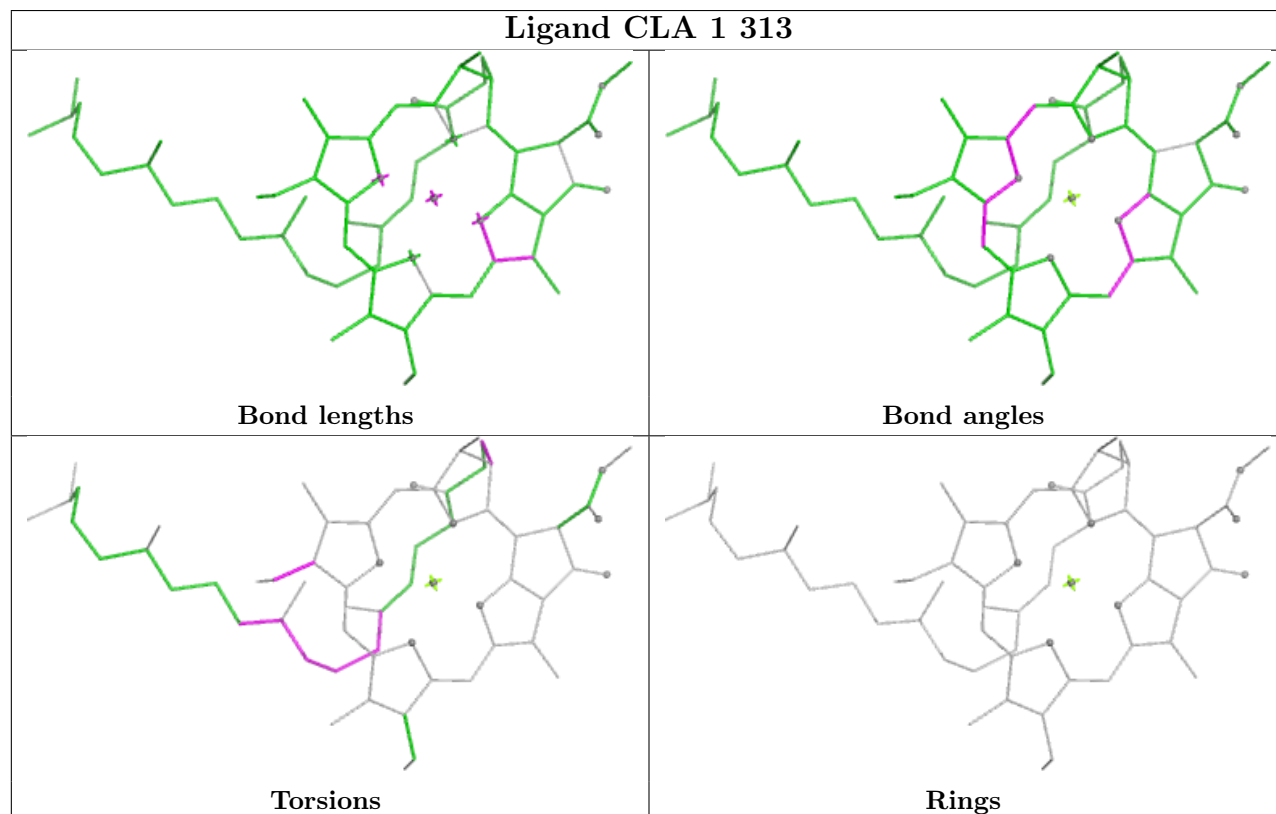
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	807	CLA	2	0
18	B	839	CLA	1	0
18	L	303	CLA	2	0
21	K	202	BCR	2	0
18	4	612	CLA	1	0
20	2	617	LHG	2	0
18	A	812	CLA	2	0
18	B	815	CLA	3	0
18	A	827	CLA	1	0
18	B	836	CLA	1	0
18	3	304	CLA	2	0
21	A	852	BCR	1	0
17	H	202	CL0	2	0
18	A	855	CLA	5	0
18	B	829	CLA	3	0
18	B	820	CLA	5	0
23	4	619	LMG	2	0
24	G	203	LMU	2	0
18	A	826	CLA	1	0
20	A	847	LHG	1	0
18	A	817	CLA	3	0
18	2	601	CLA	2	0
18	L	305	CLA	1	0
18	3	303	CLA	2	0

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

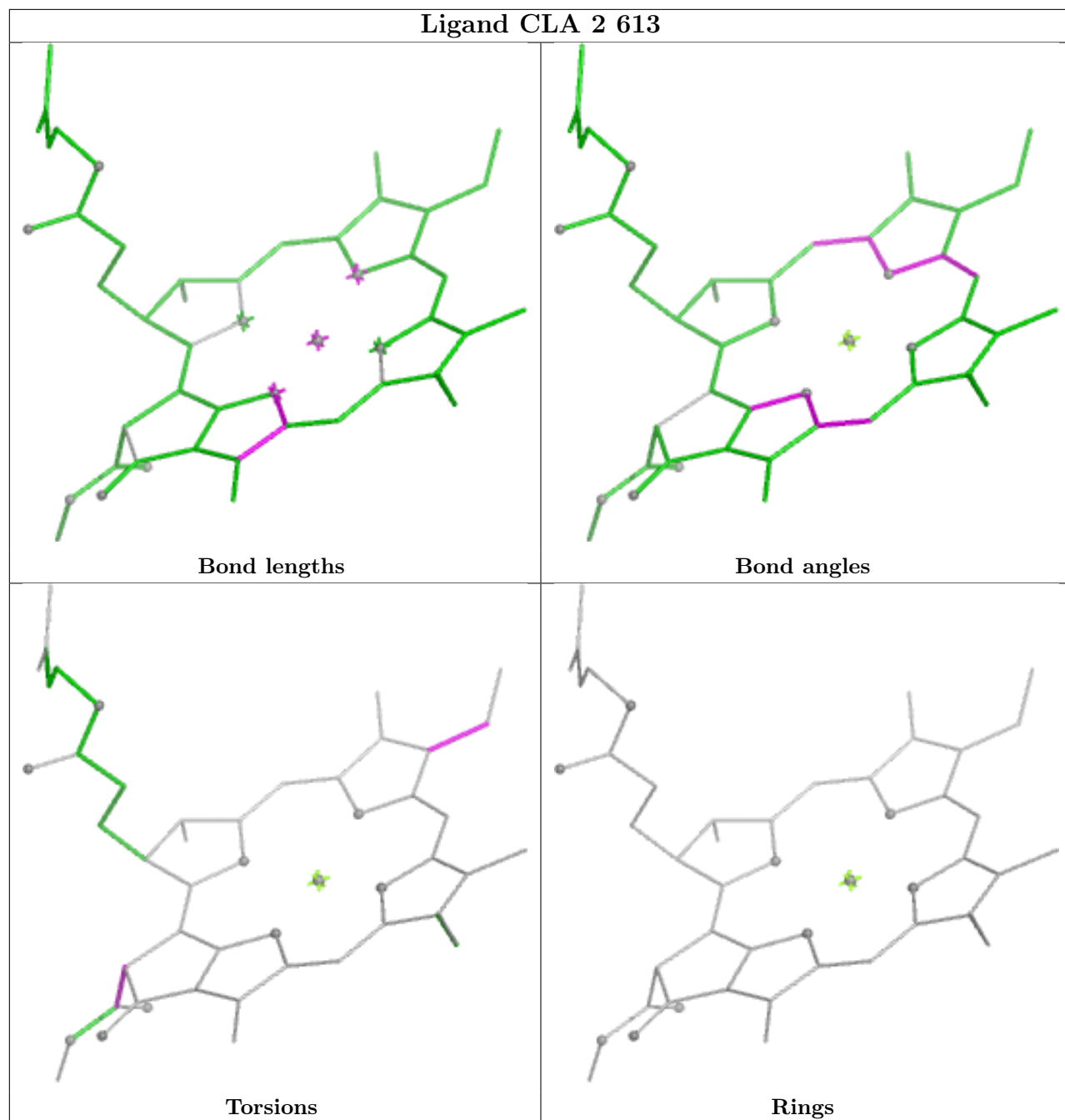


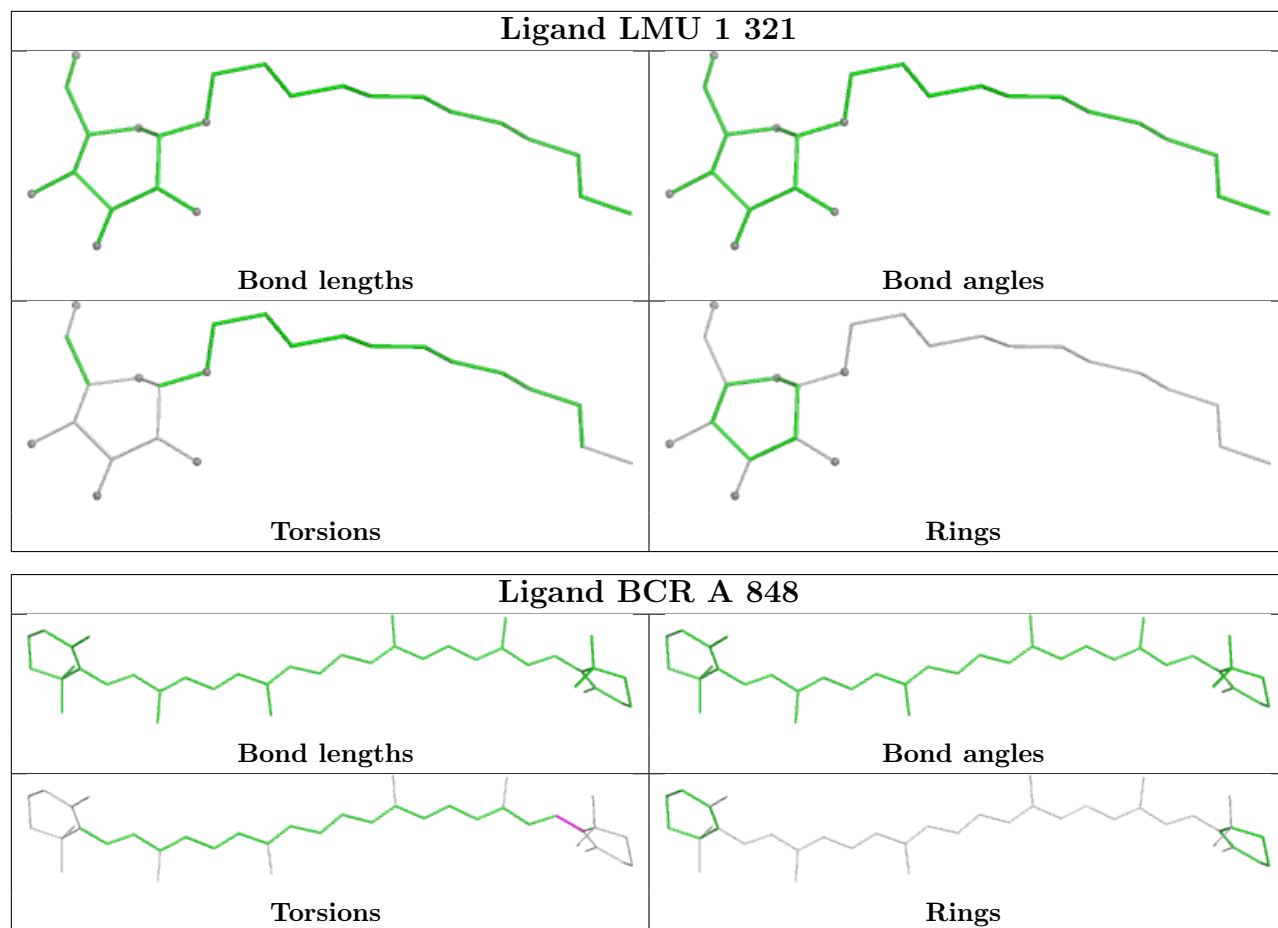


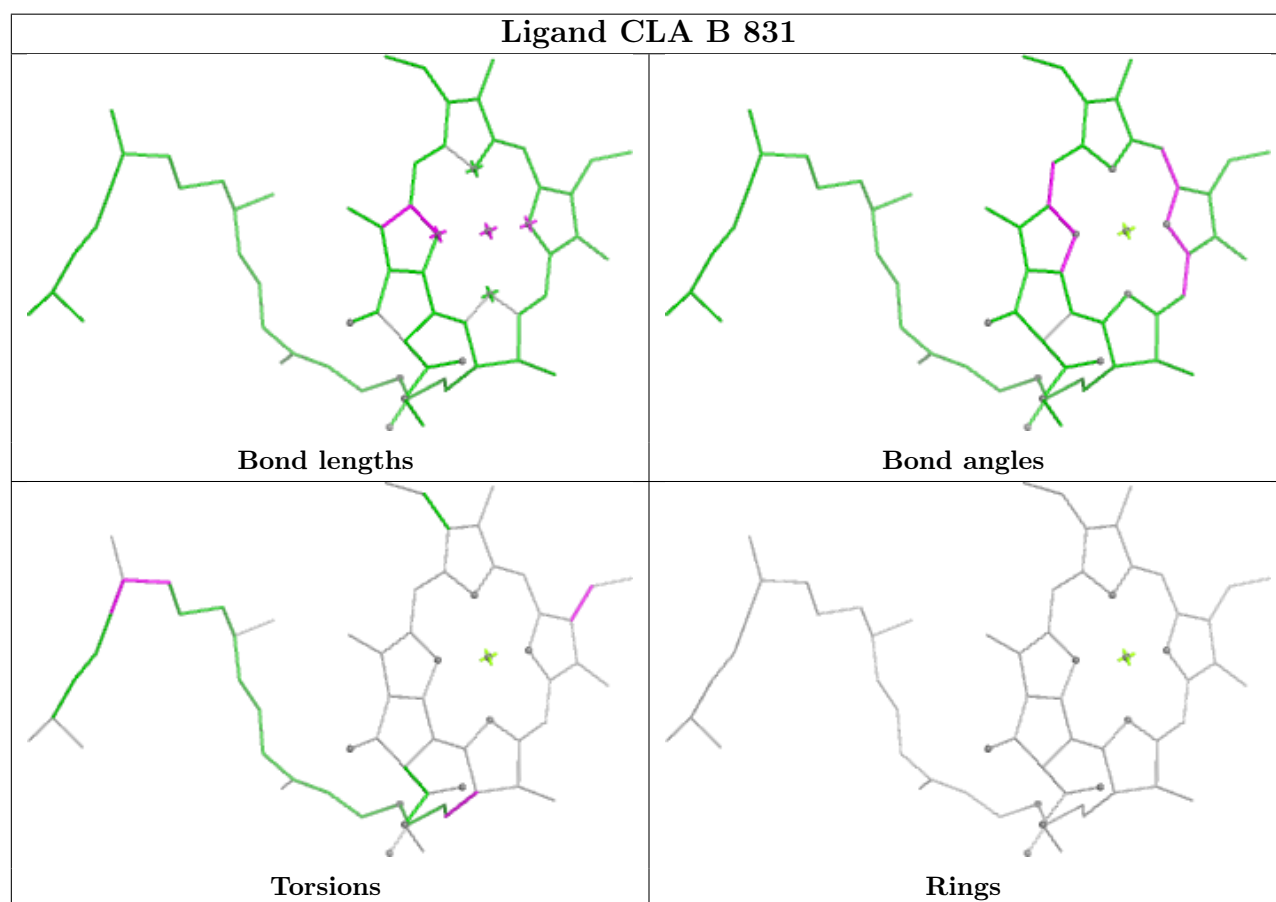
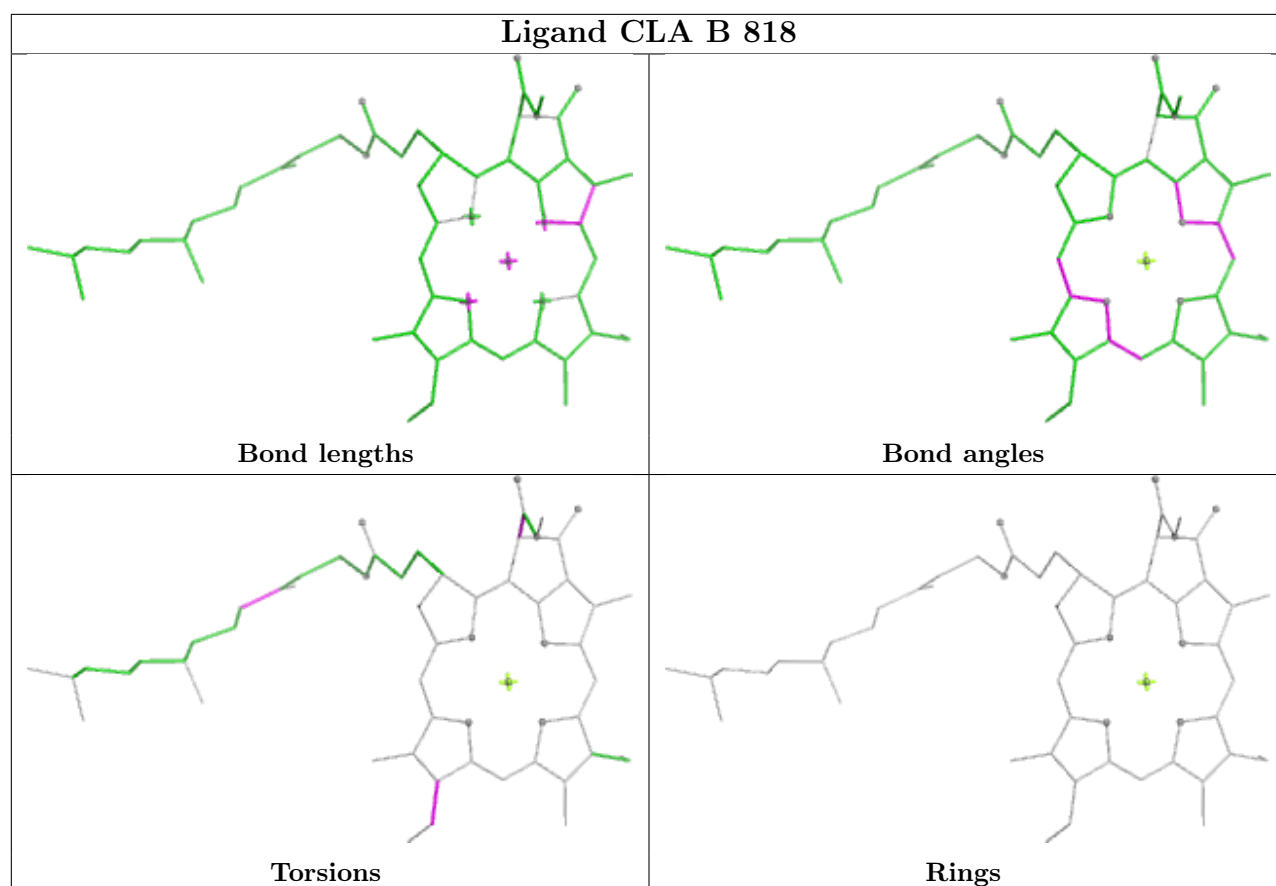


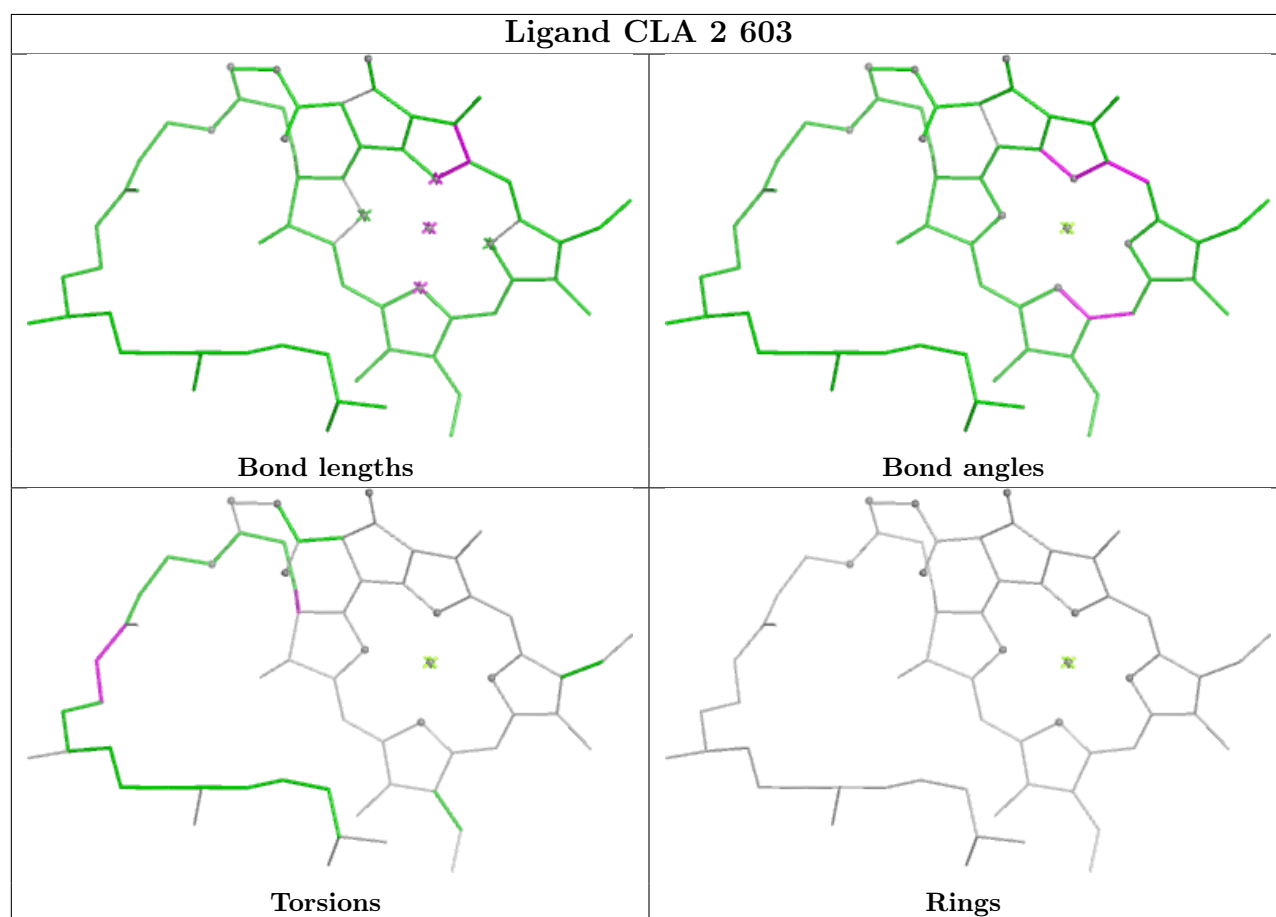
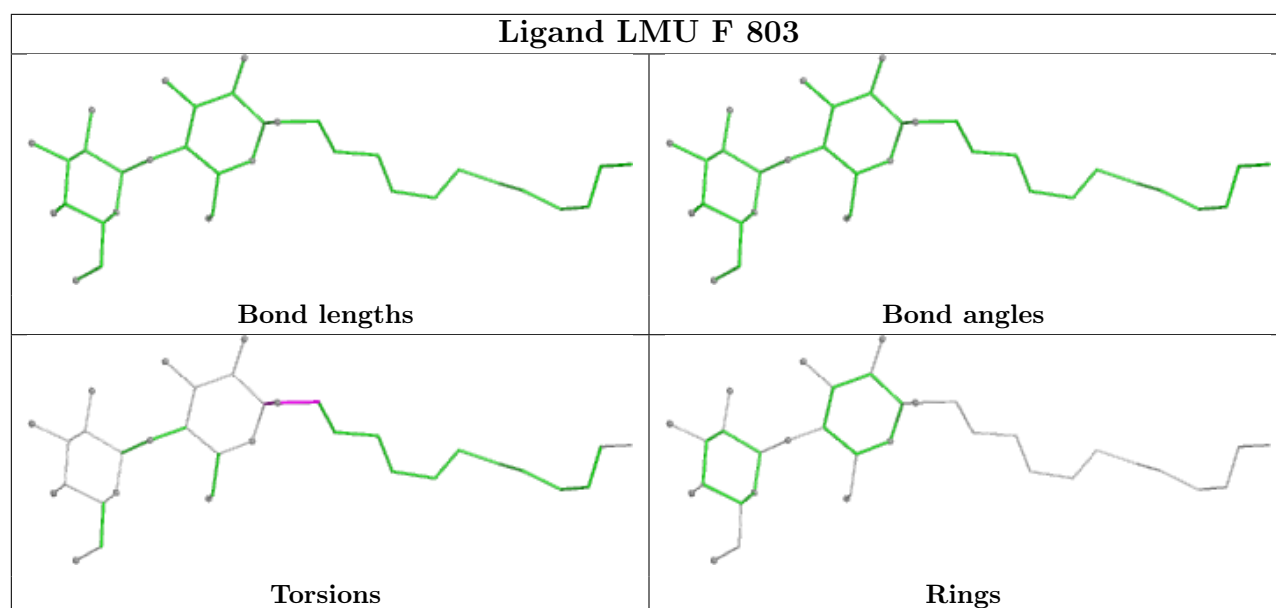
Ligand CLA B 822**Ligand CLA 1 313**

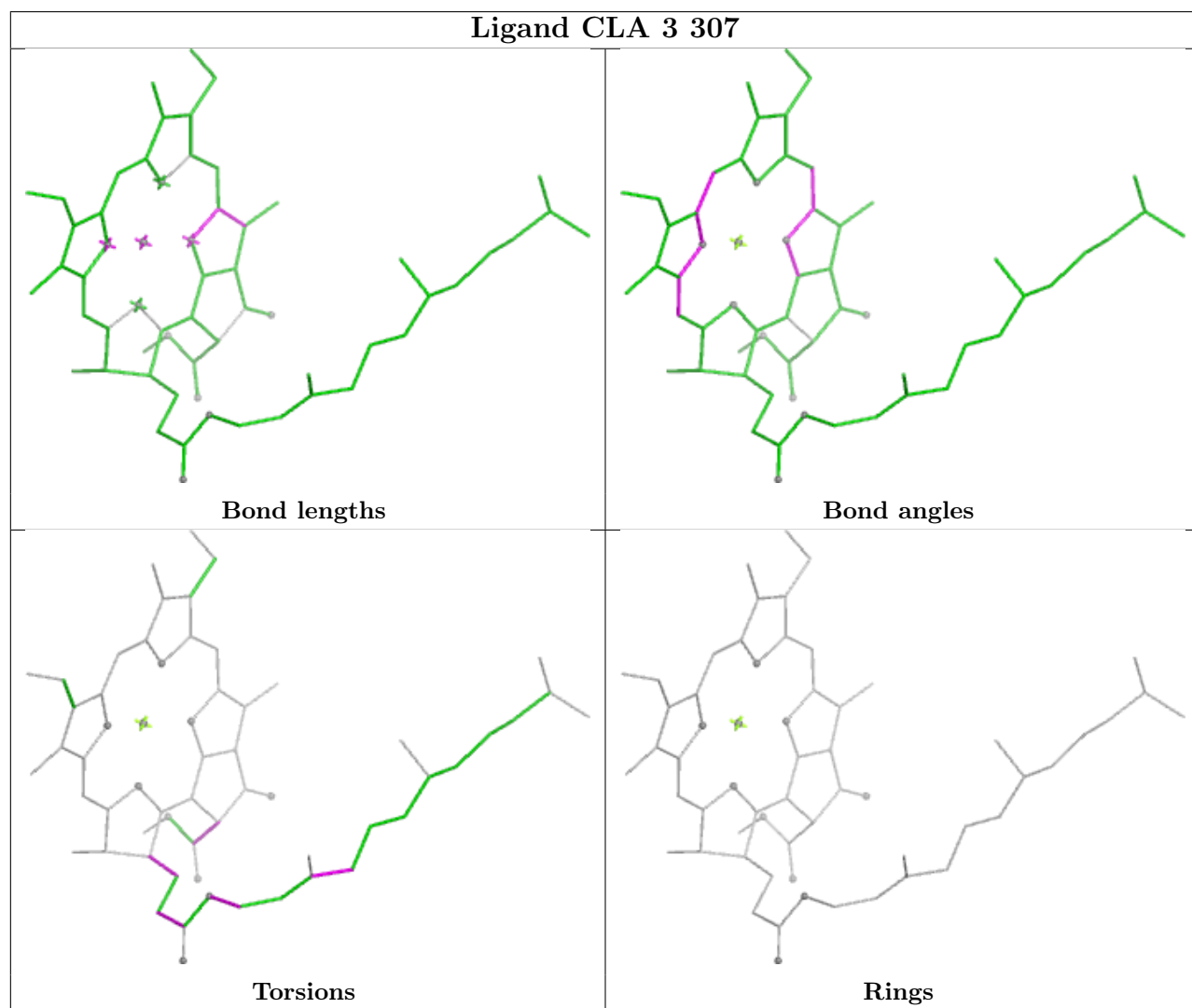
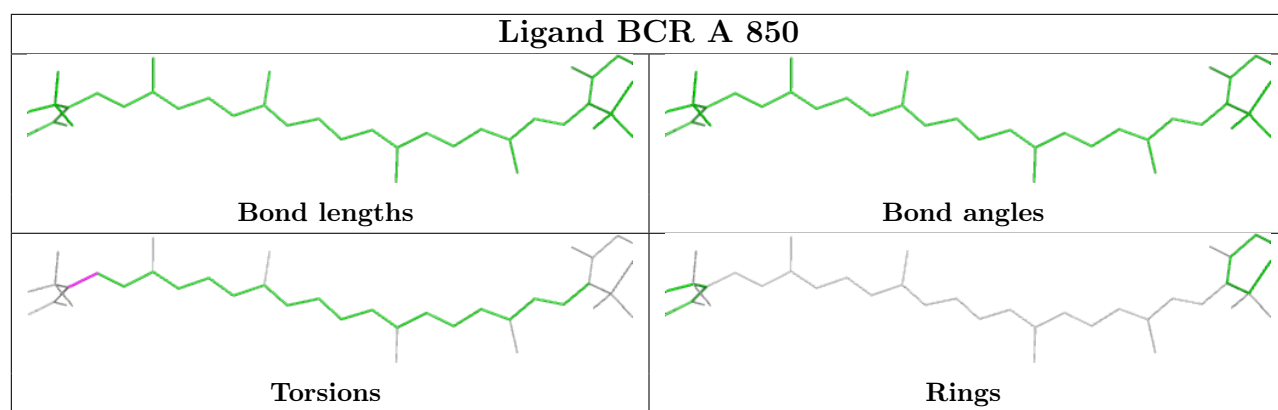
Ligand CLA 2 613



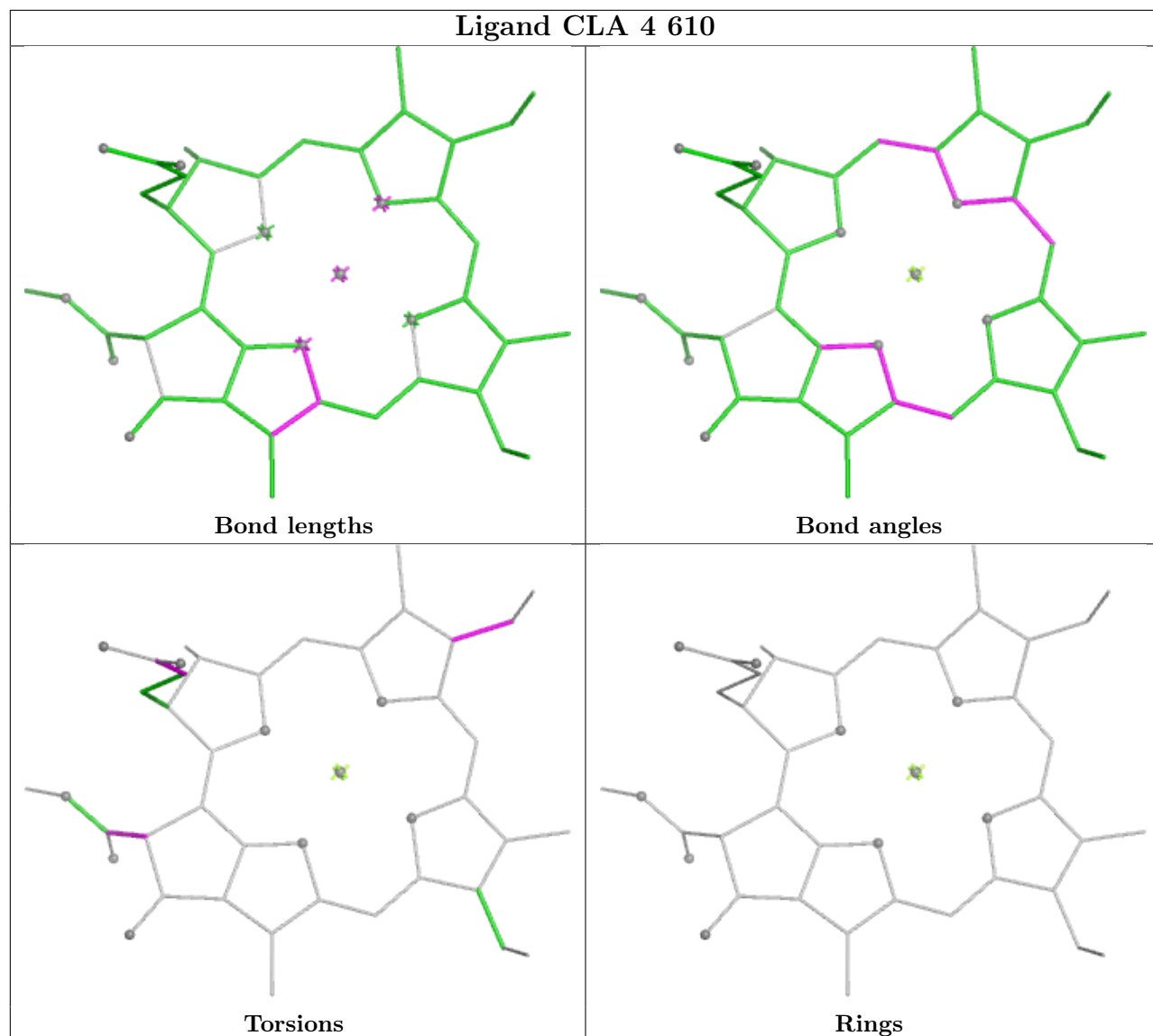


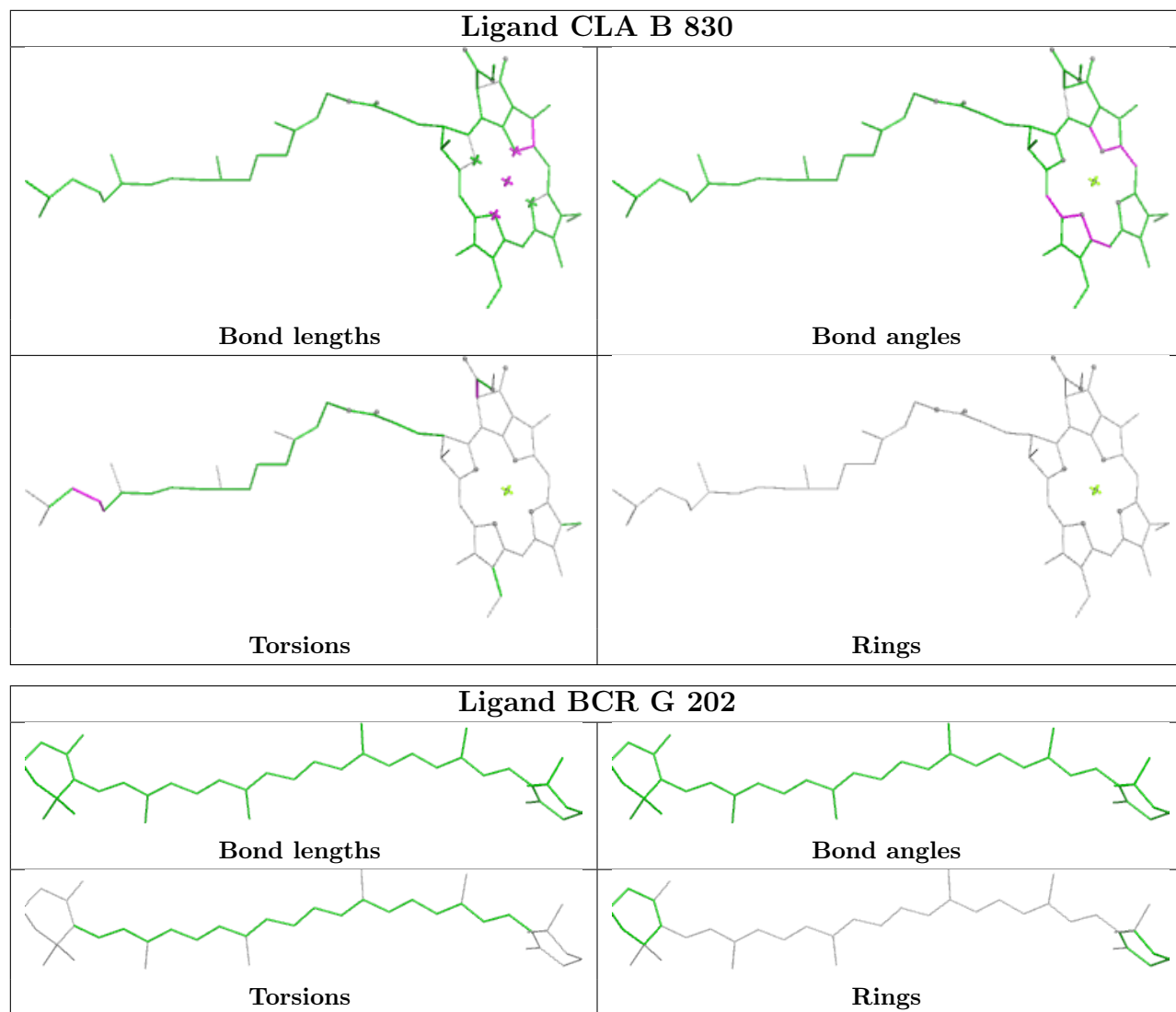


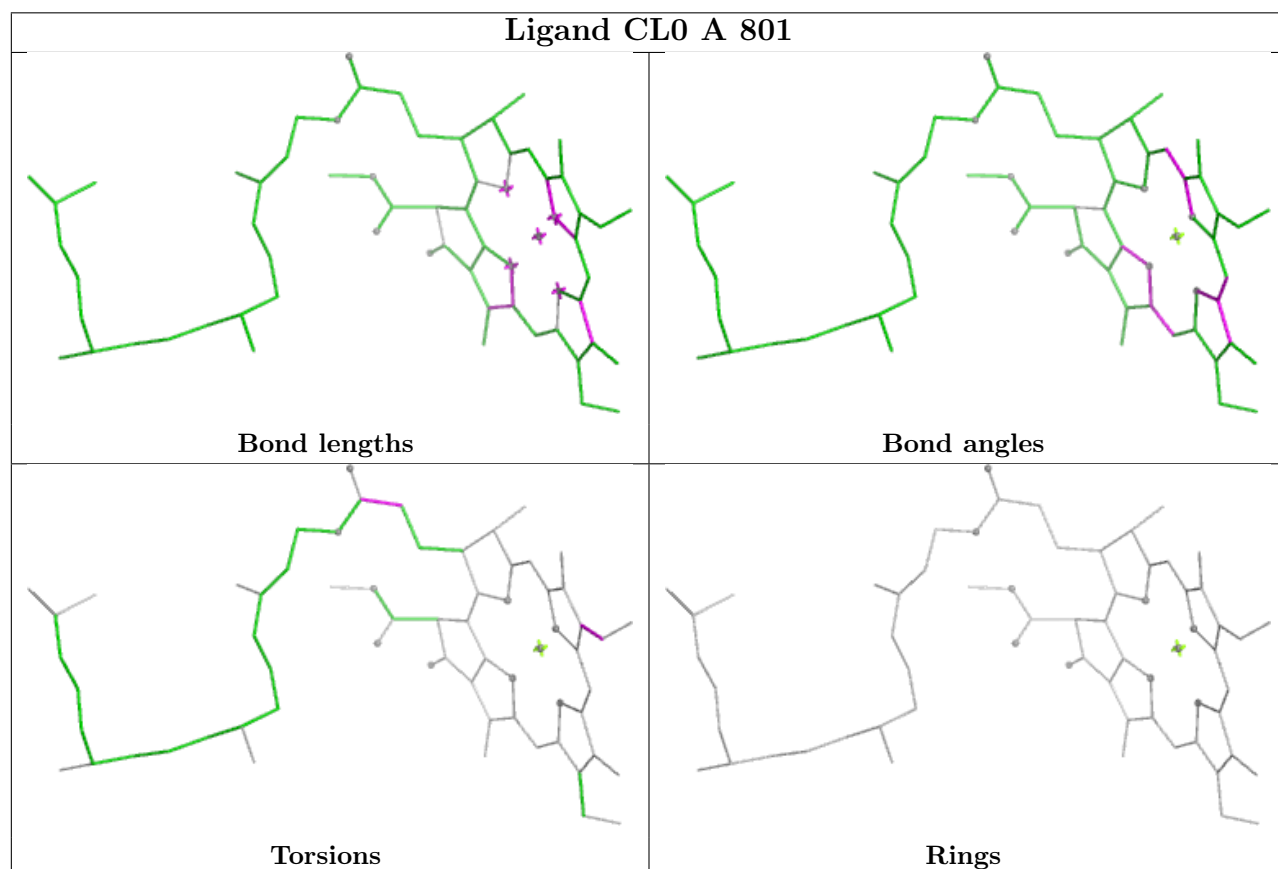
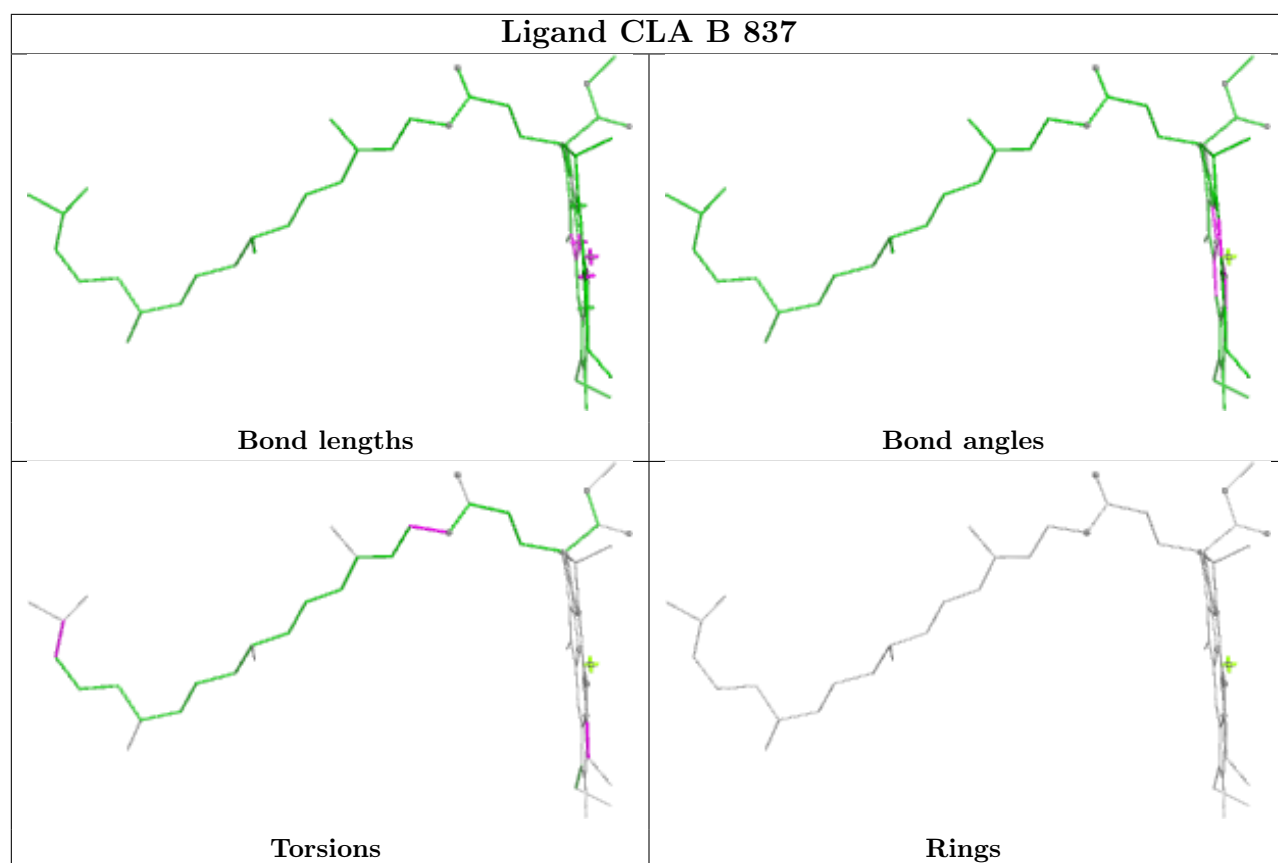


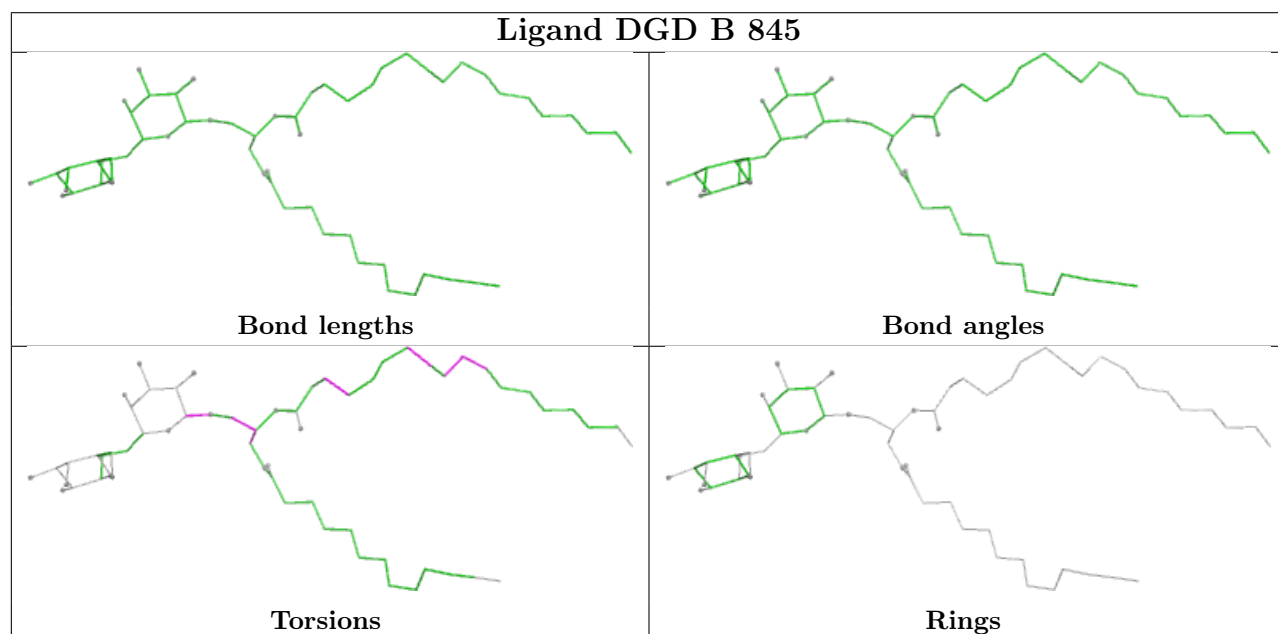
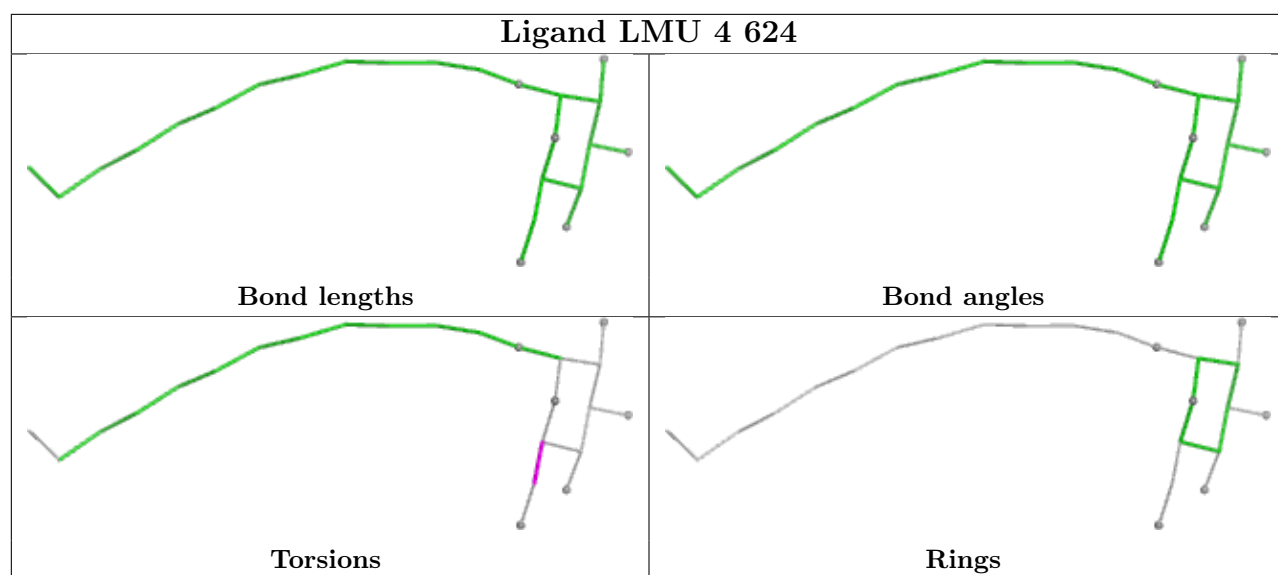


Ligand CLA 4 610

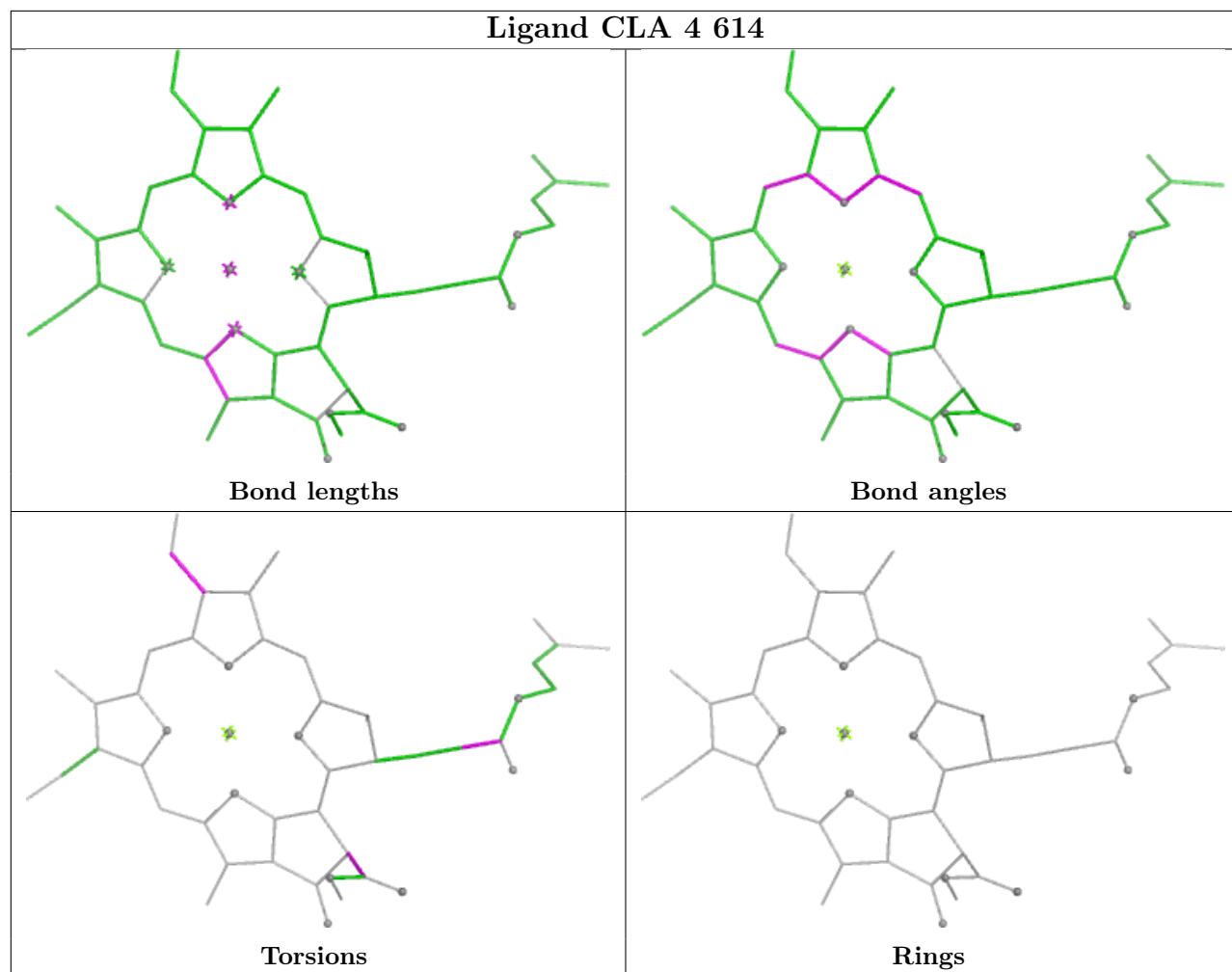




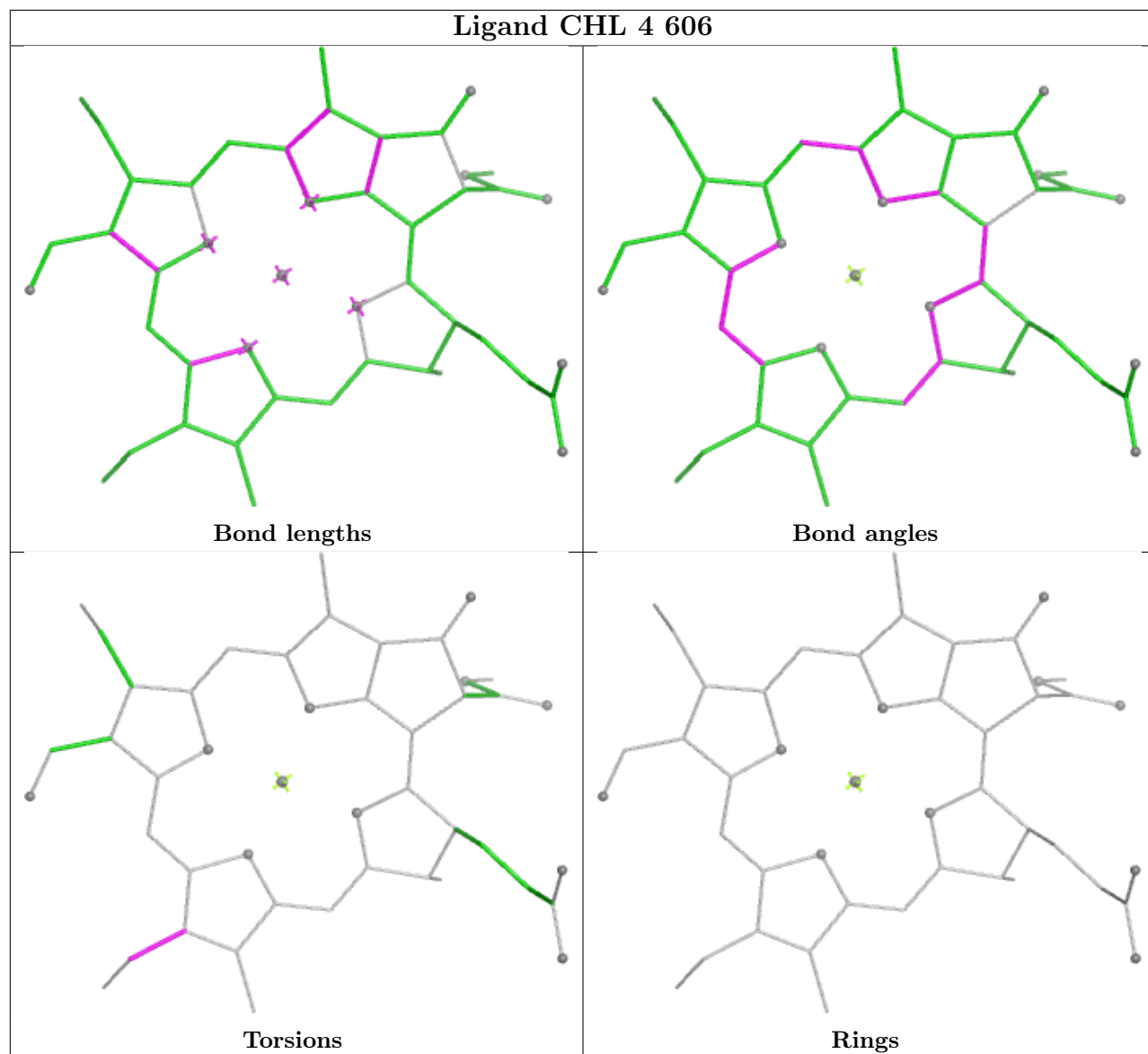


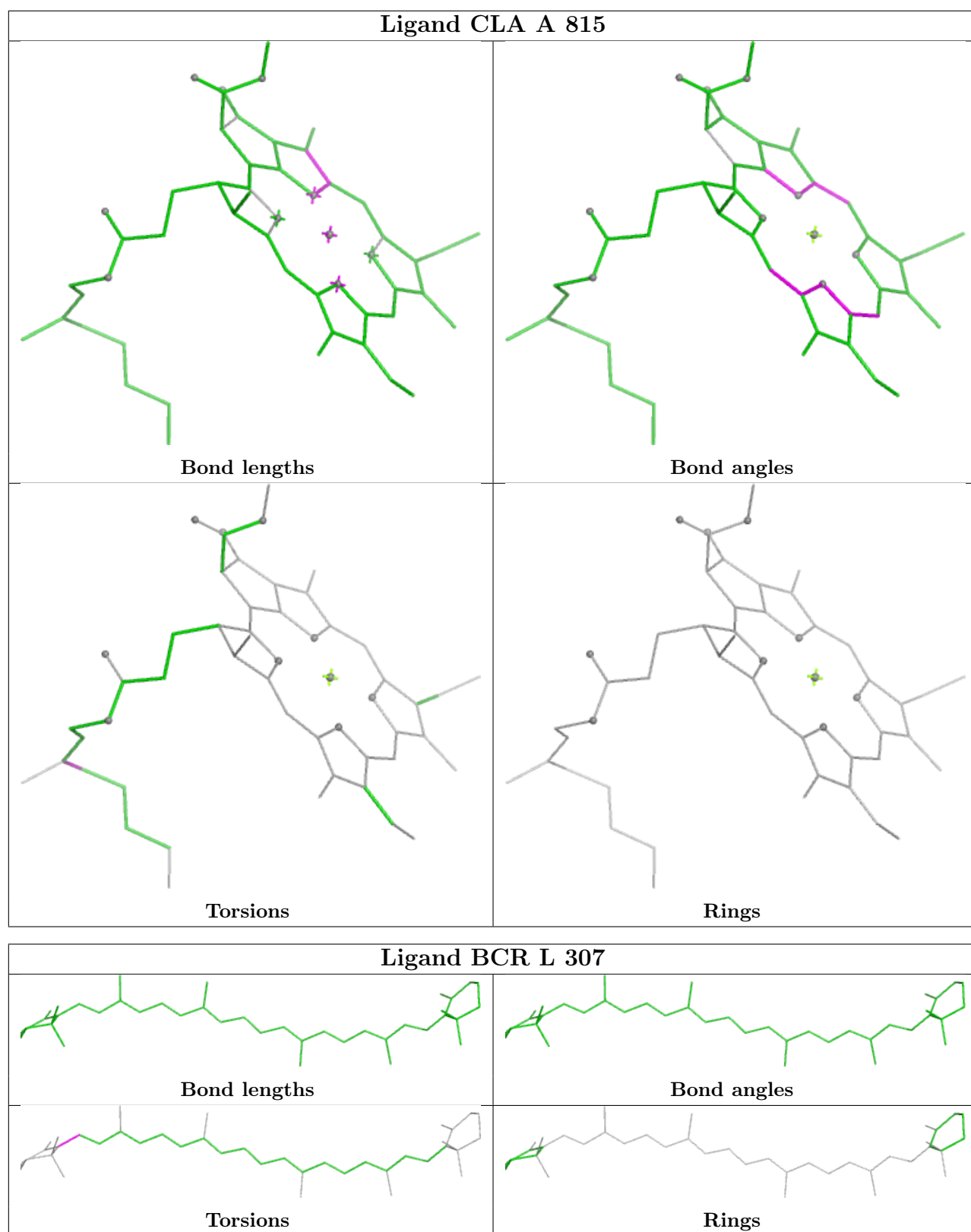


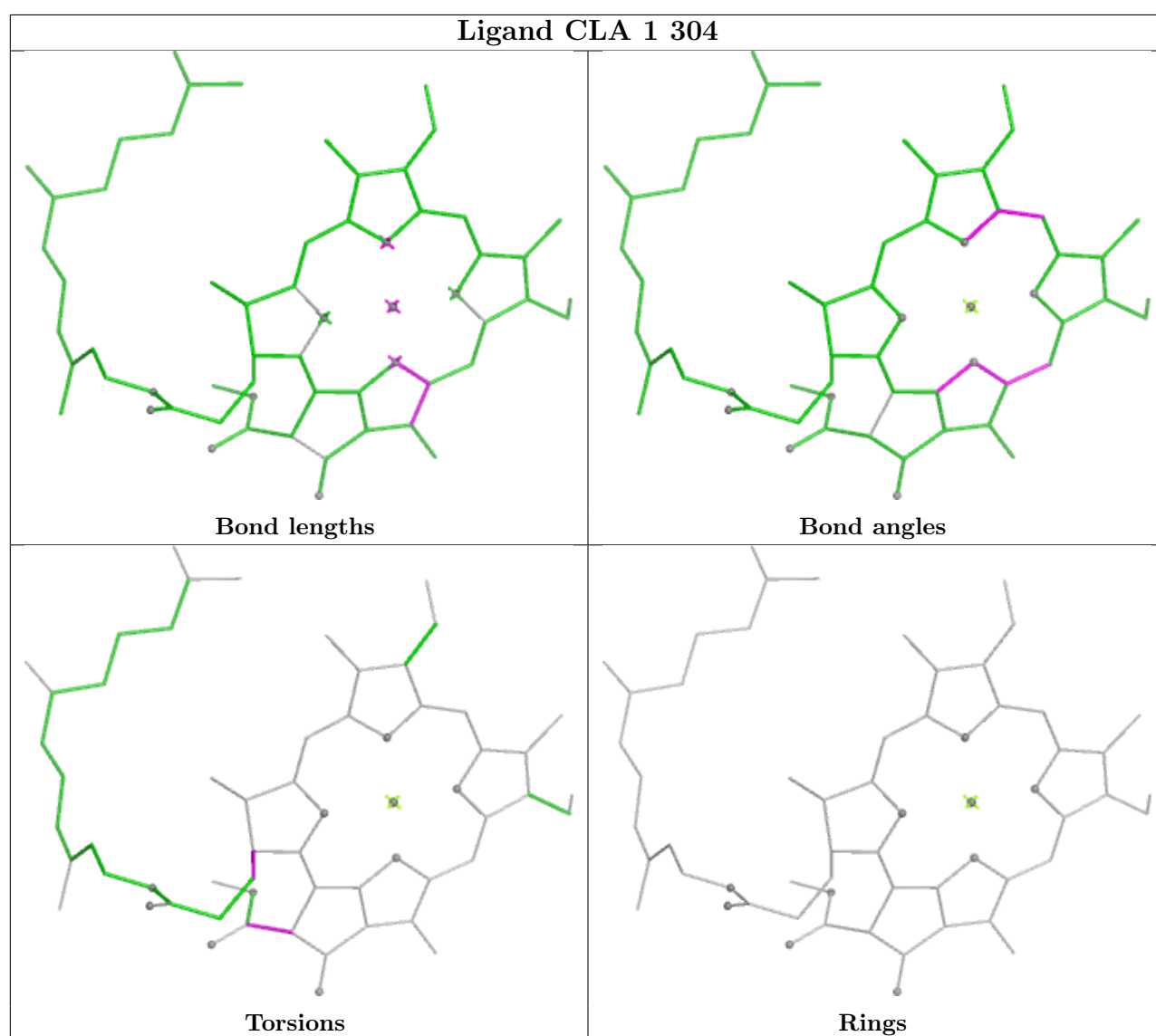
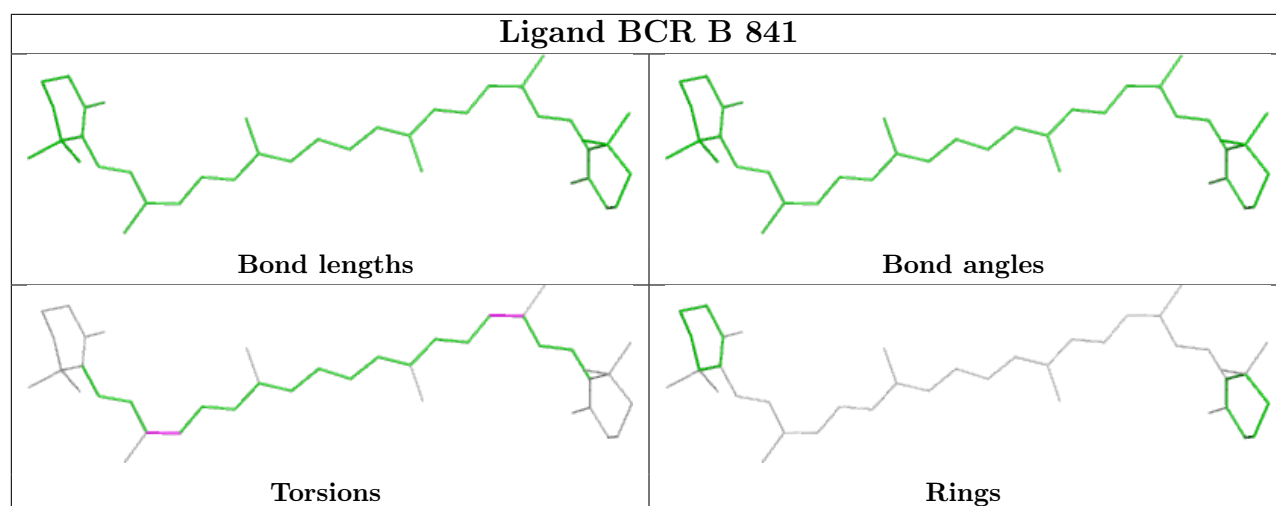
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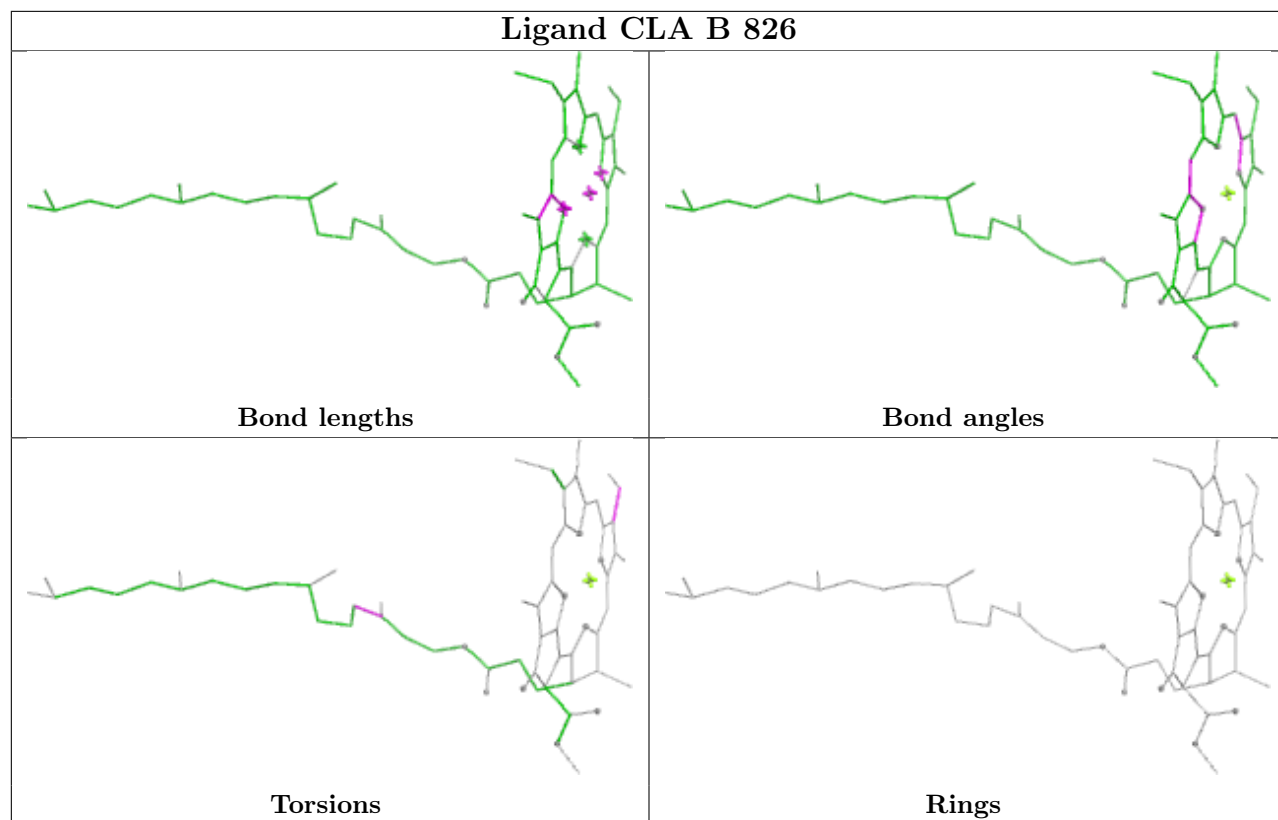


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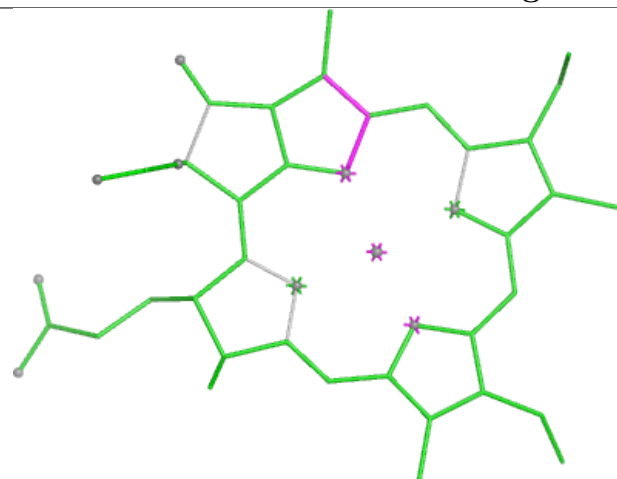




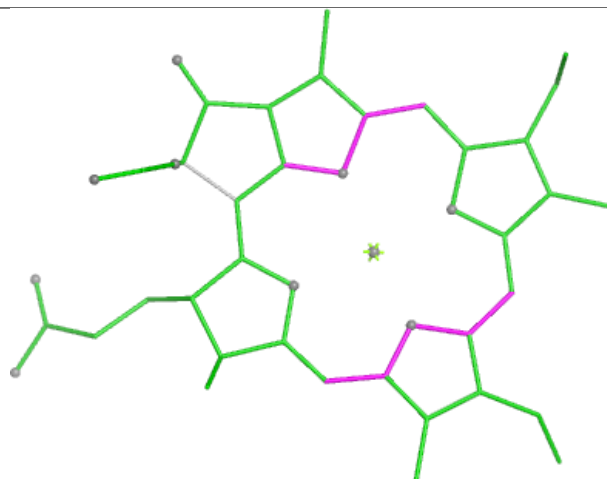




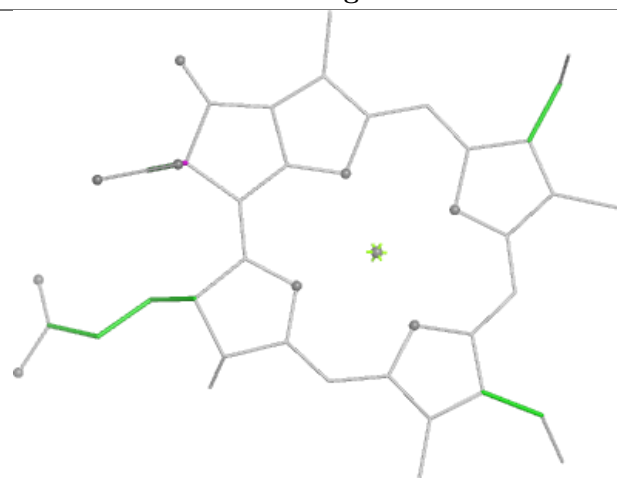
Ligand CLA 1 315



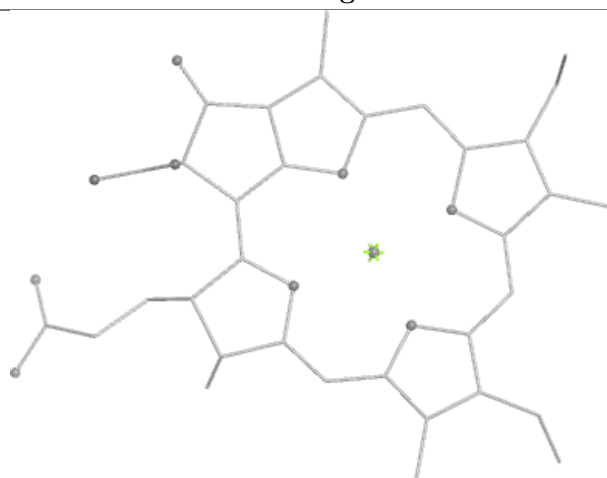
Bond lengths



Bond angles

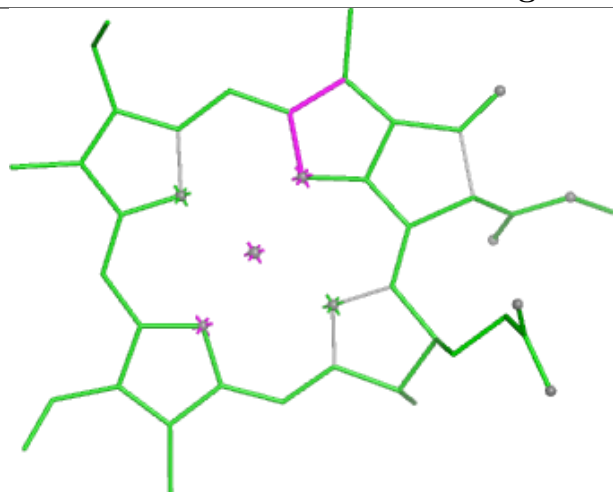


Torsions

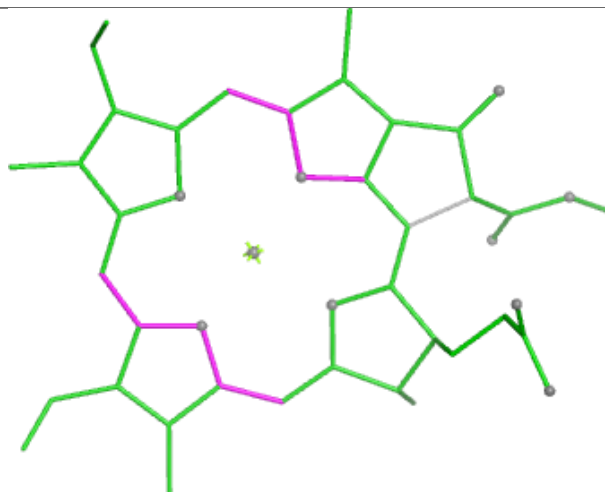


Rings

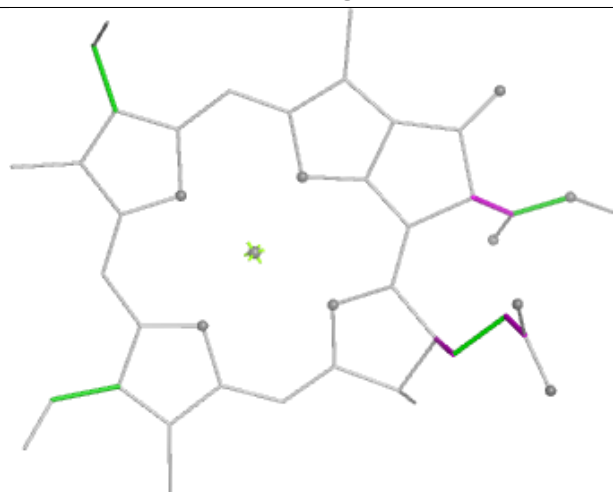
Ligand CLA 1 308



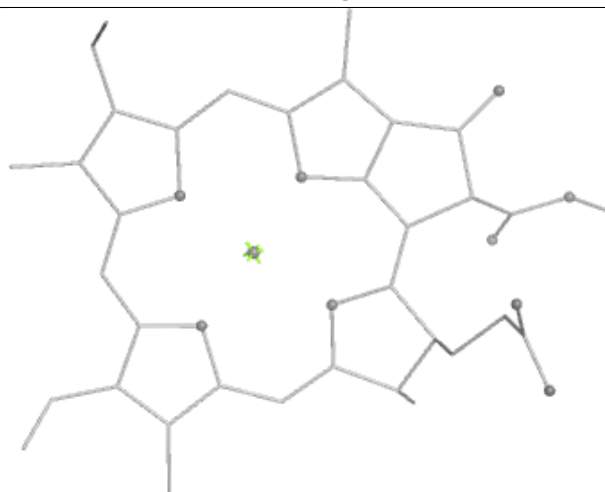
Bond lengths



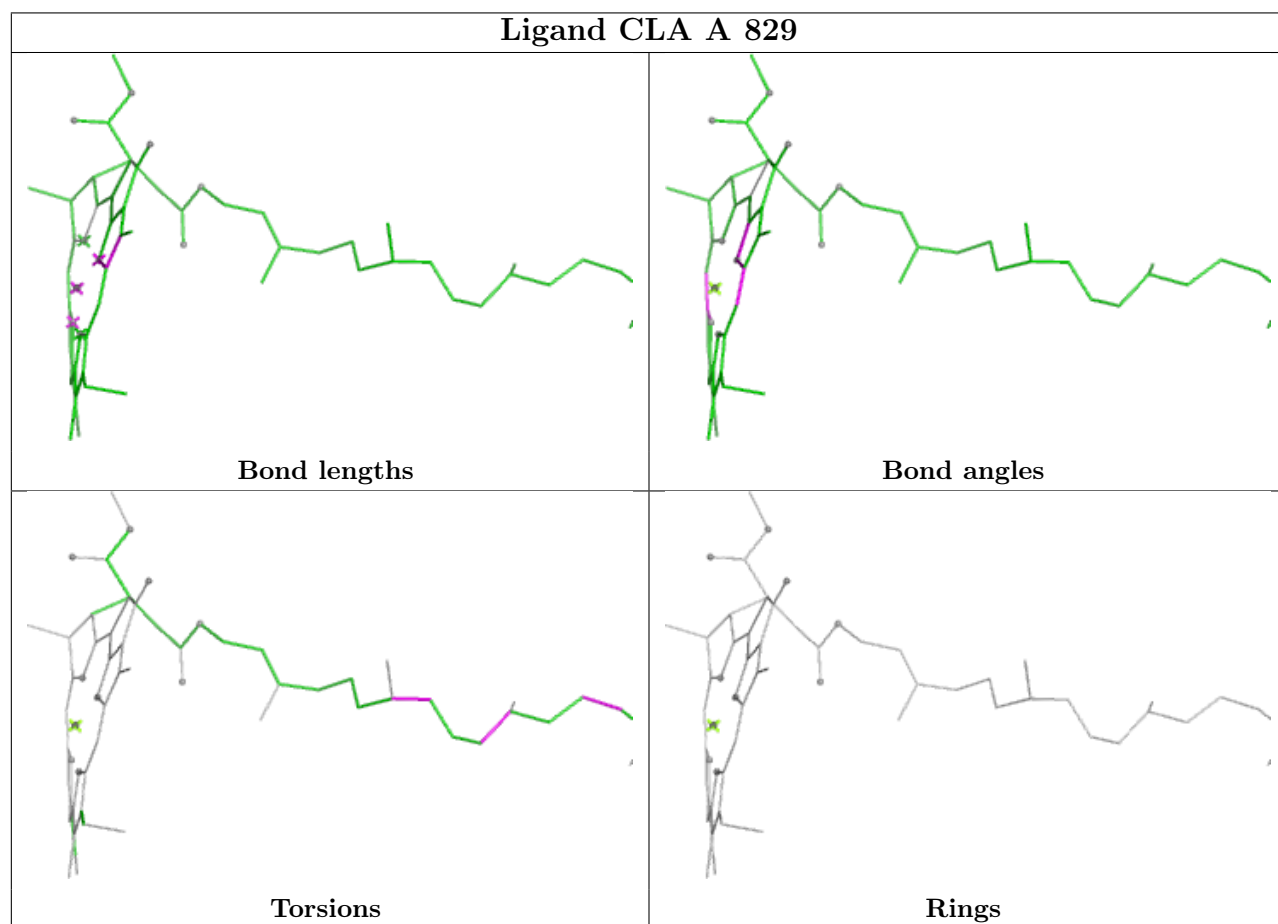
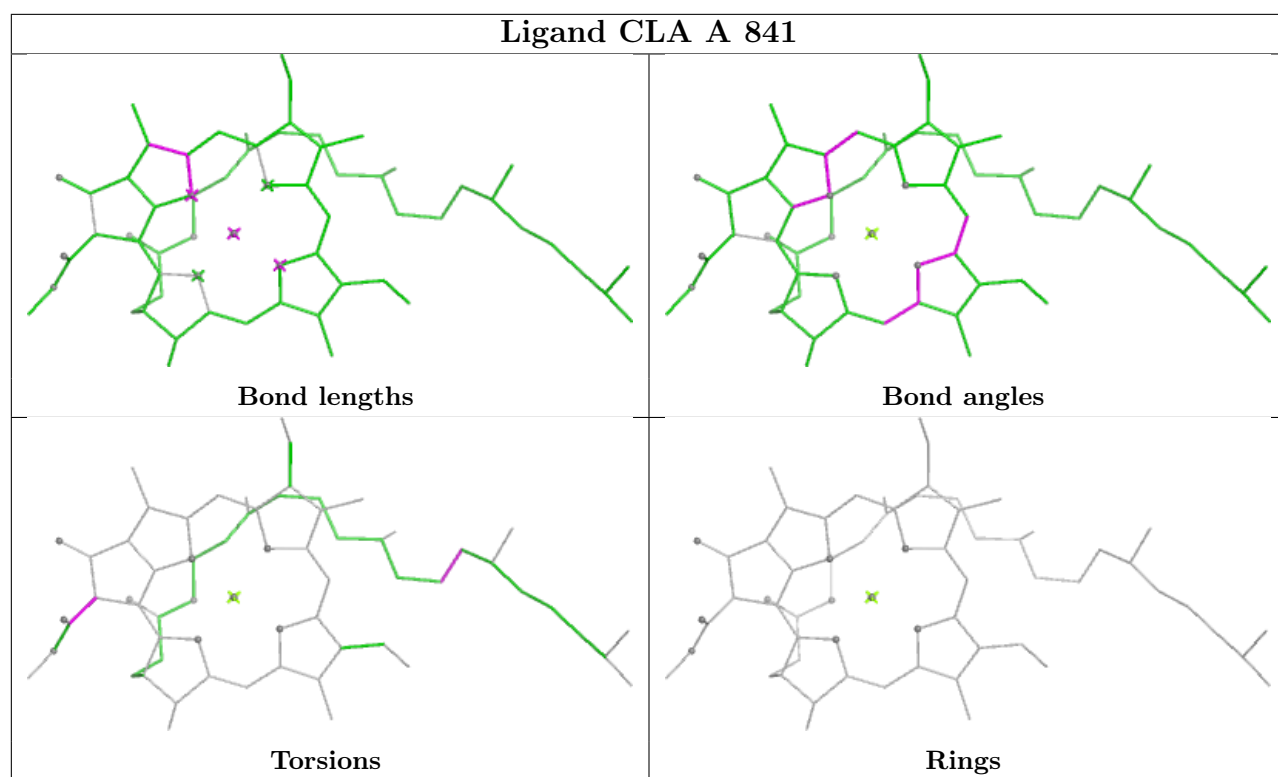
Bond angles

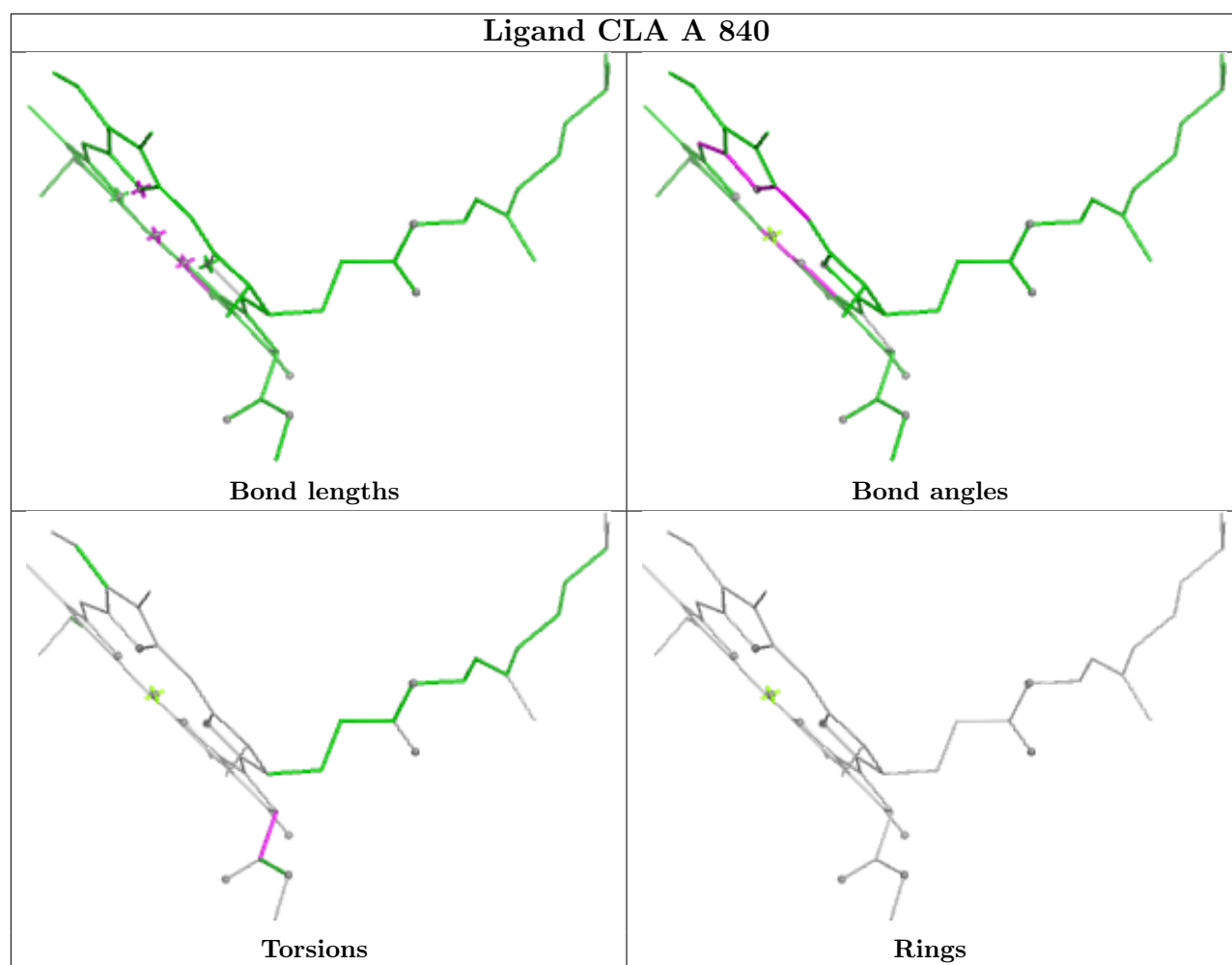


Torsions

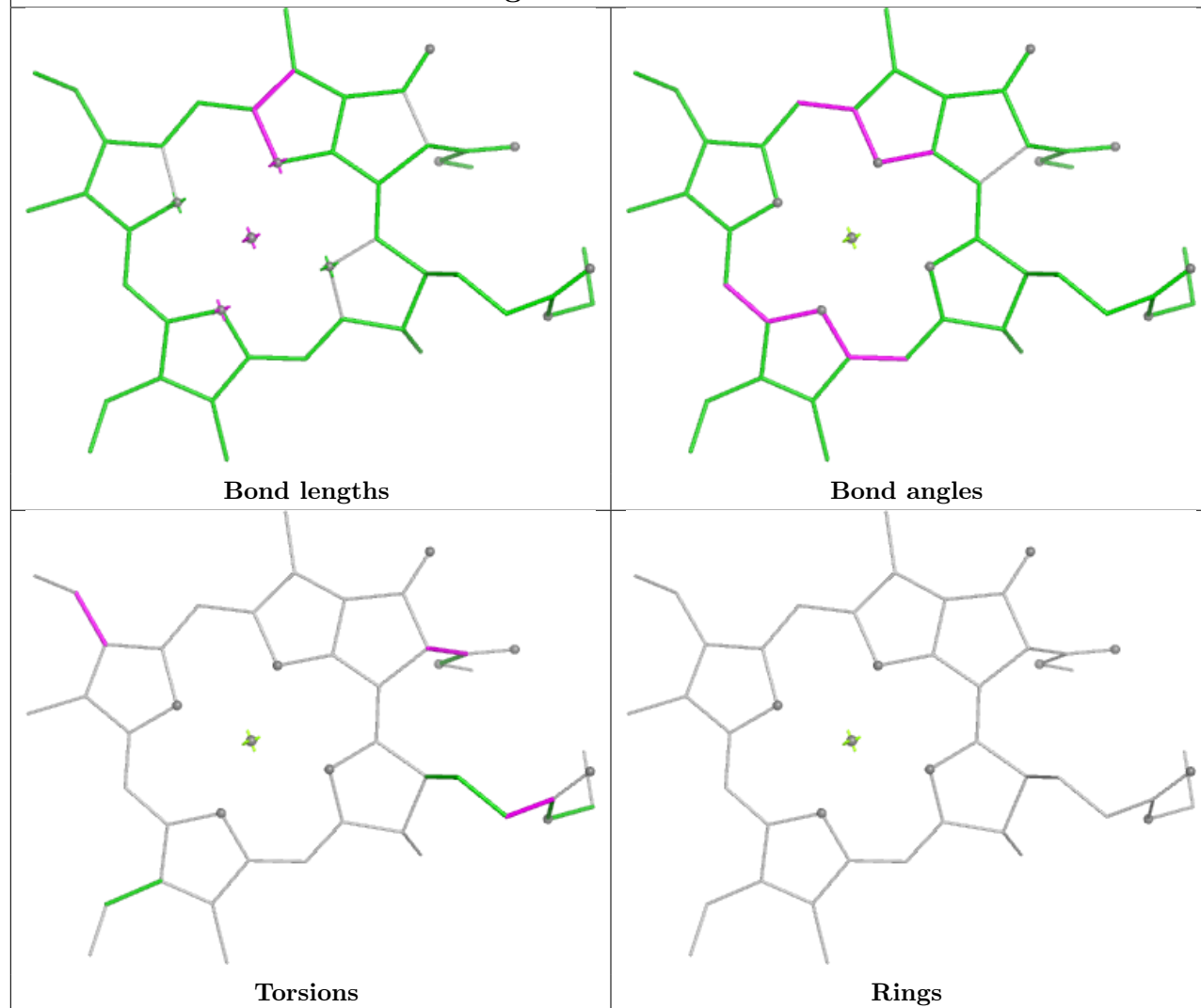


Rings

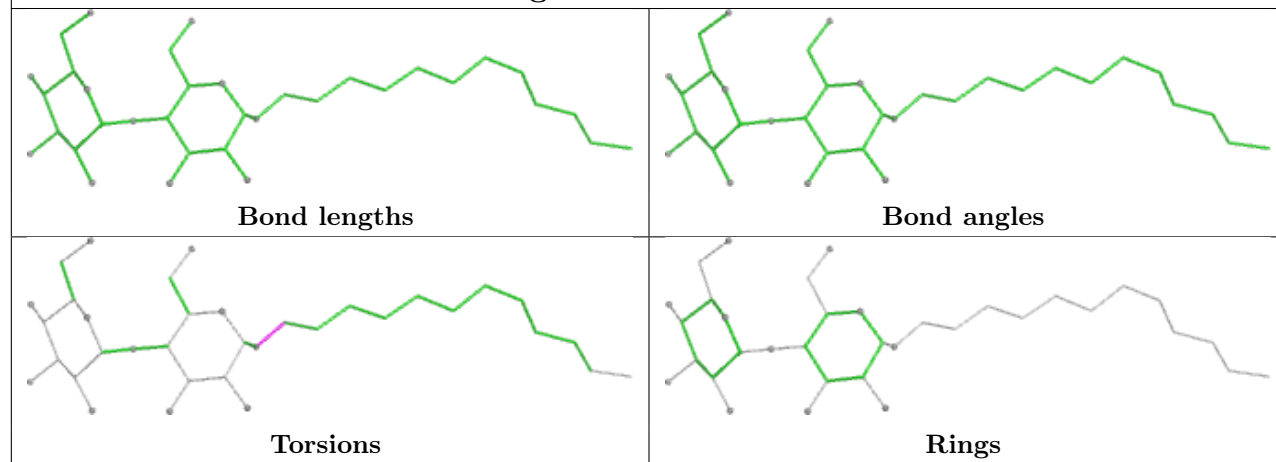




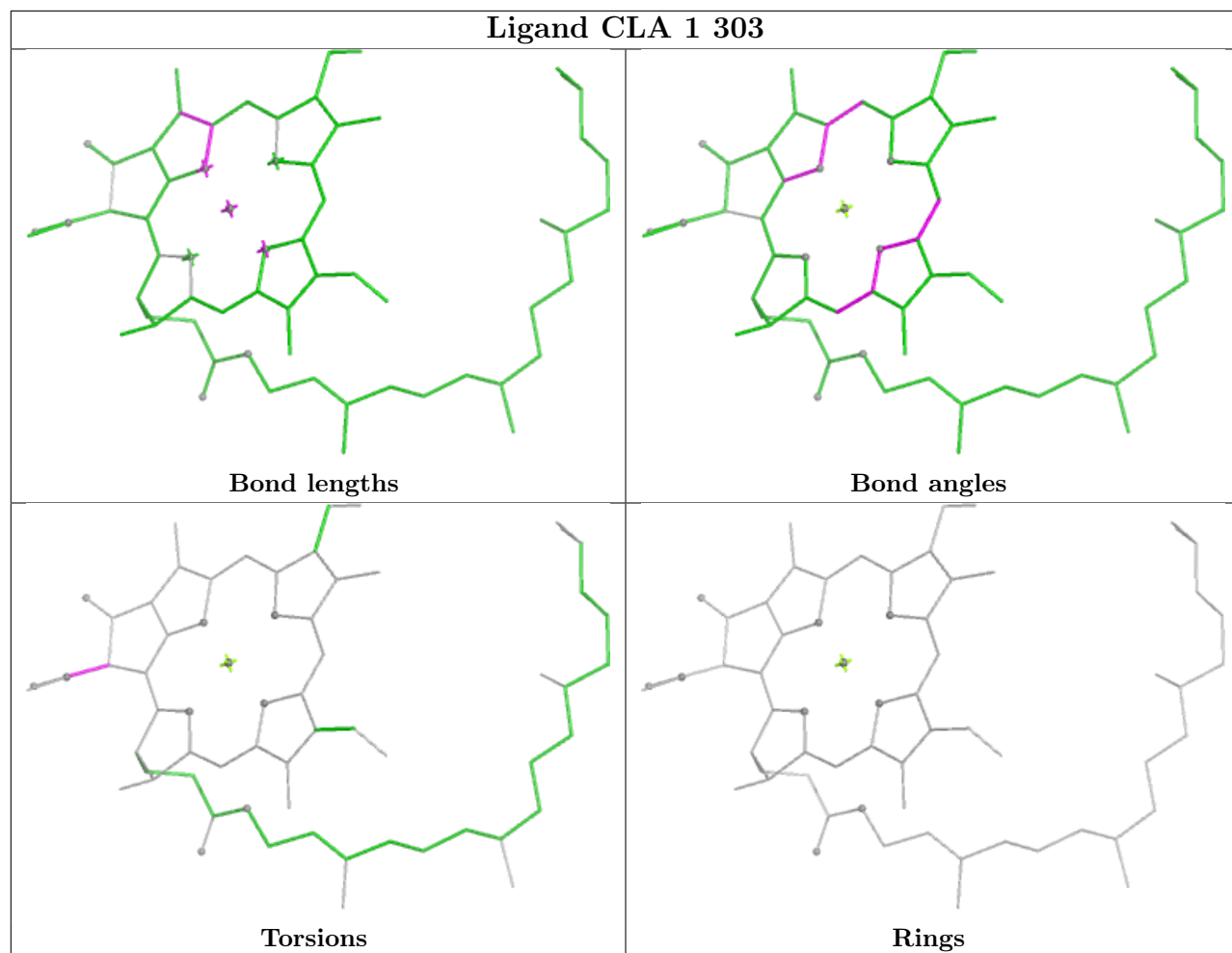
Ligand CLA 4 611

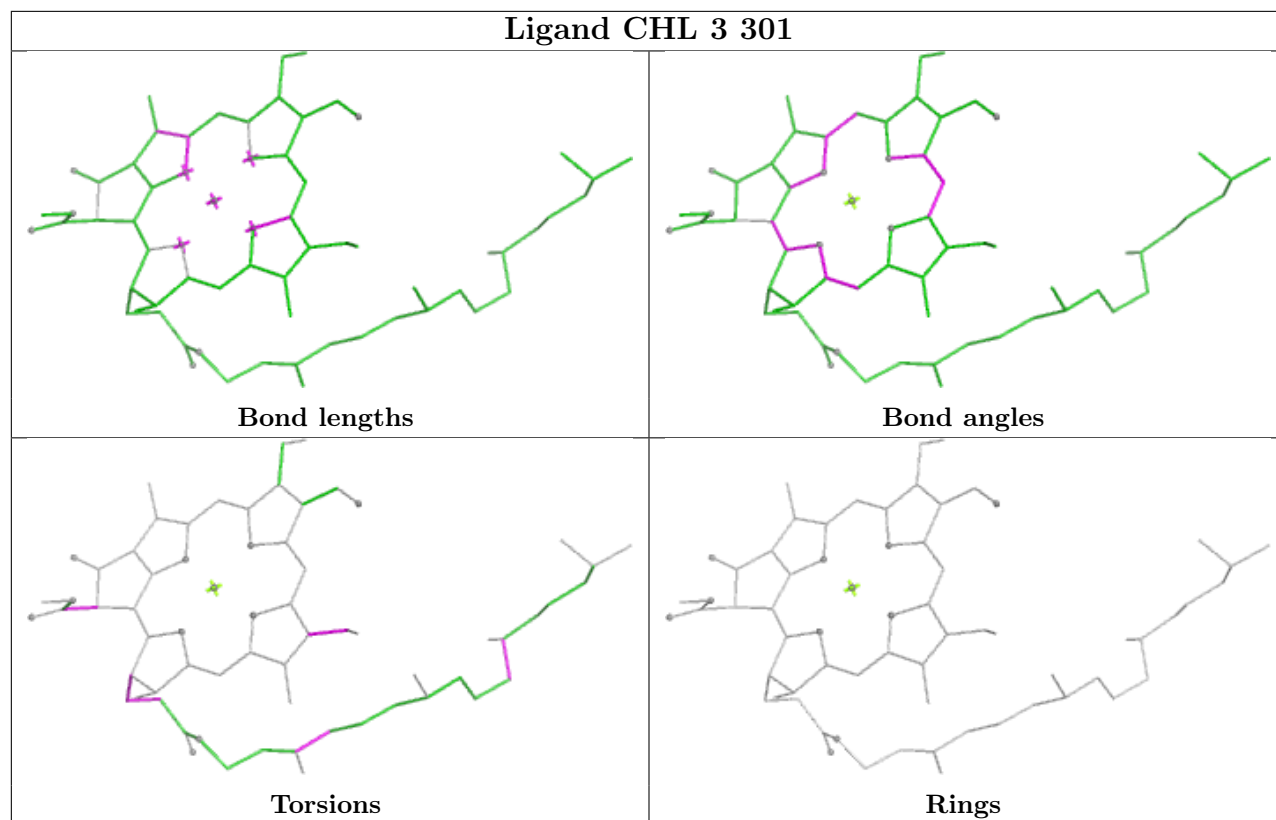


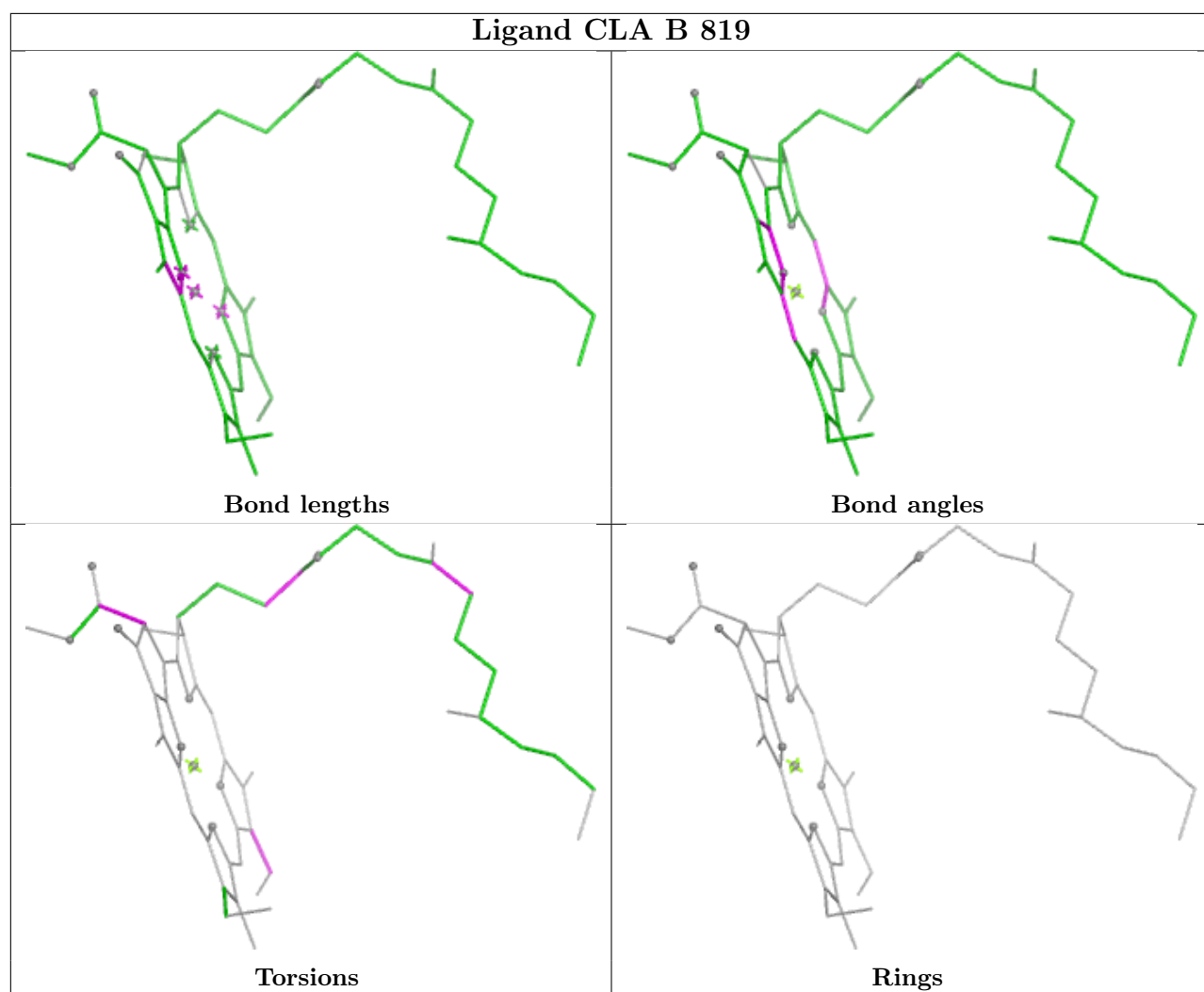
Ligand LMU F 809

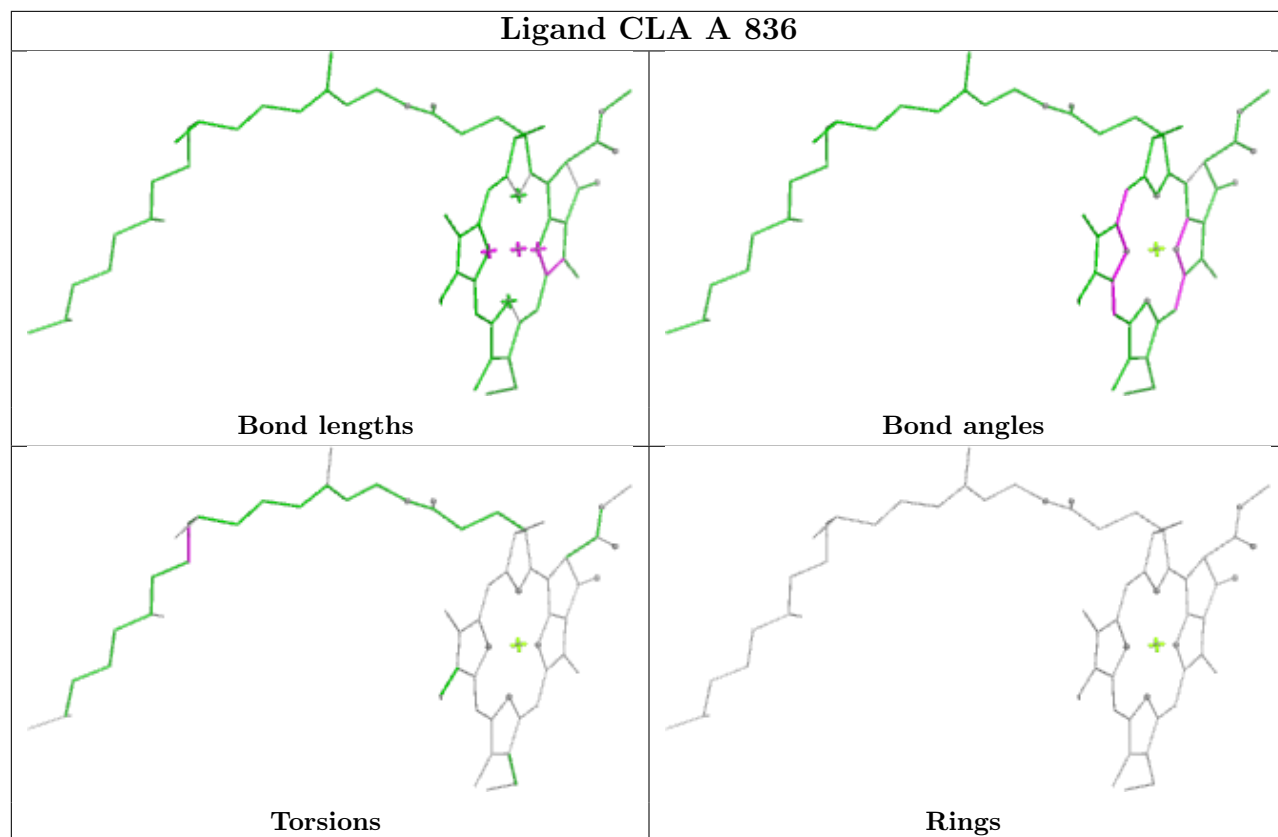


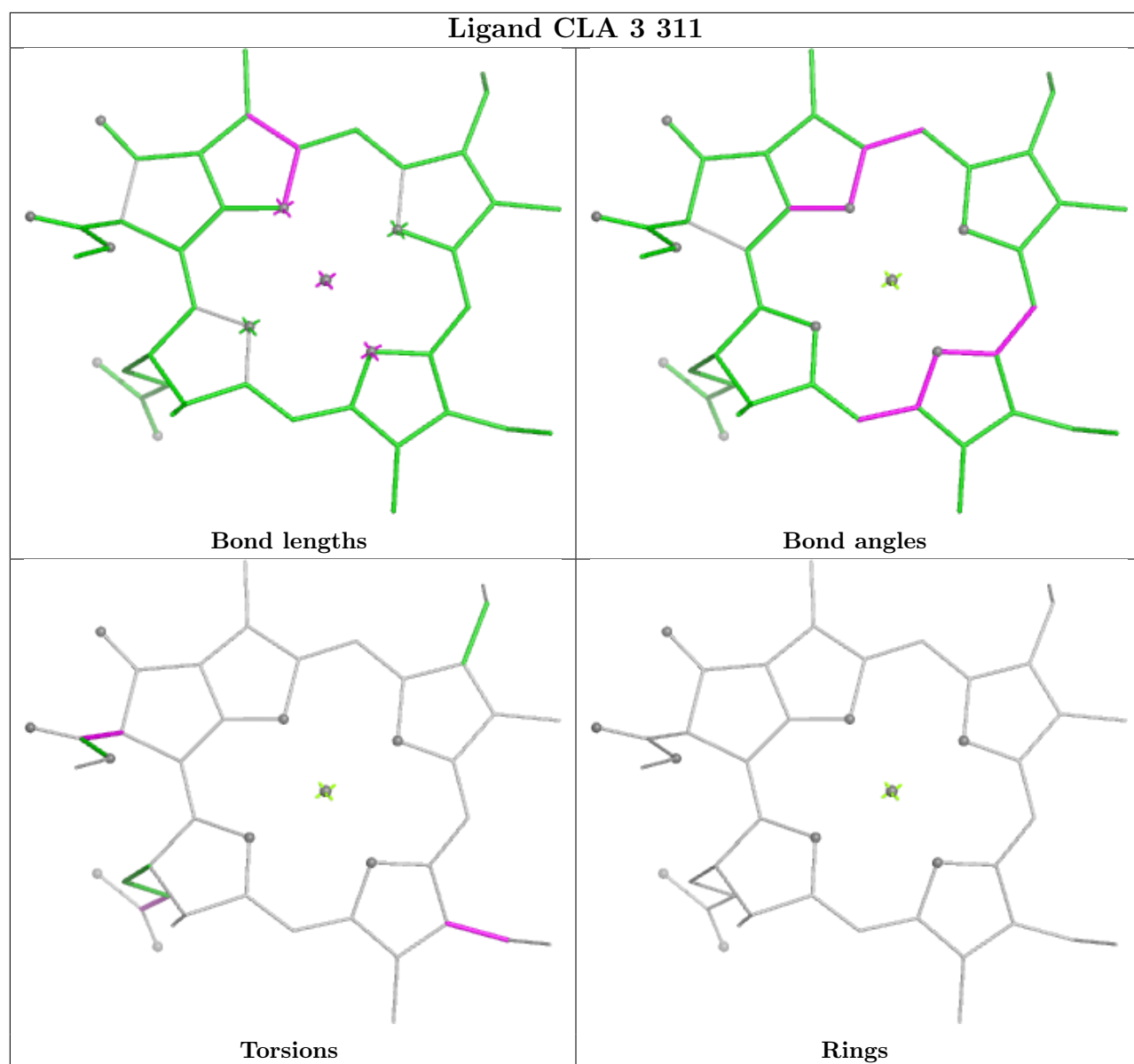
Ligand CLA 1 303

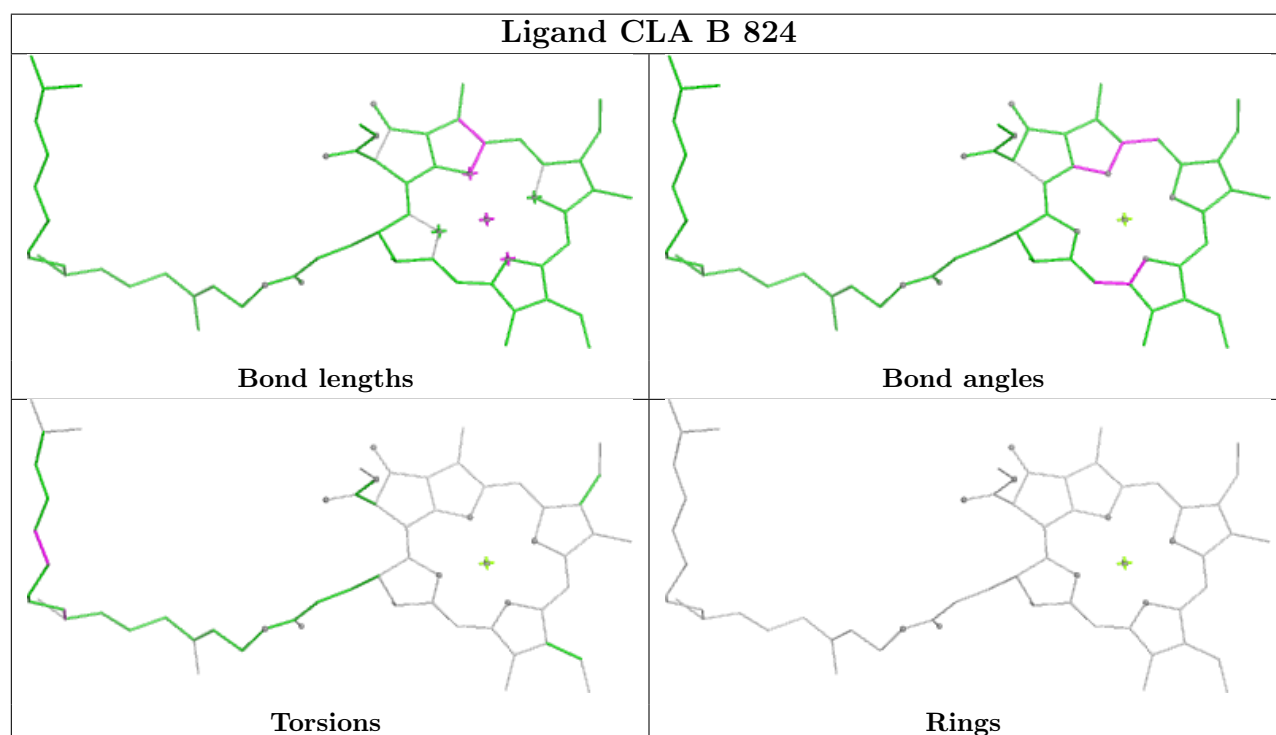
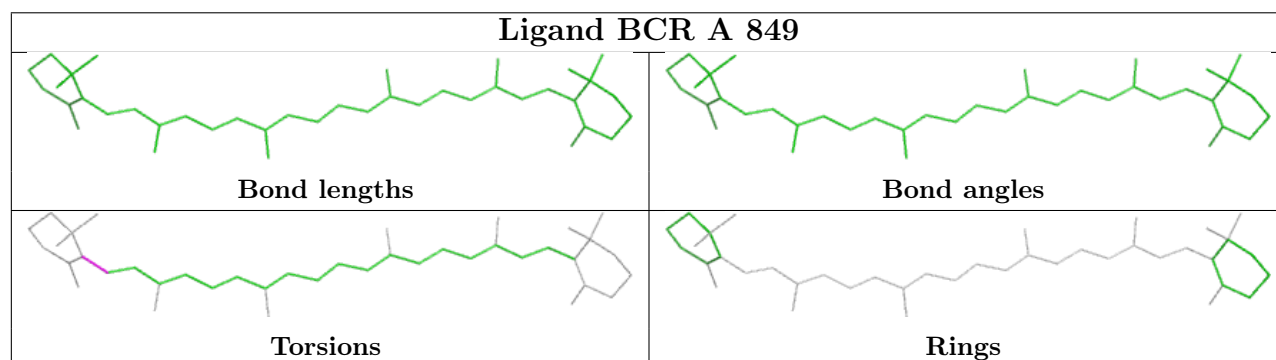
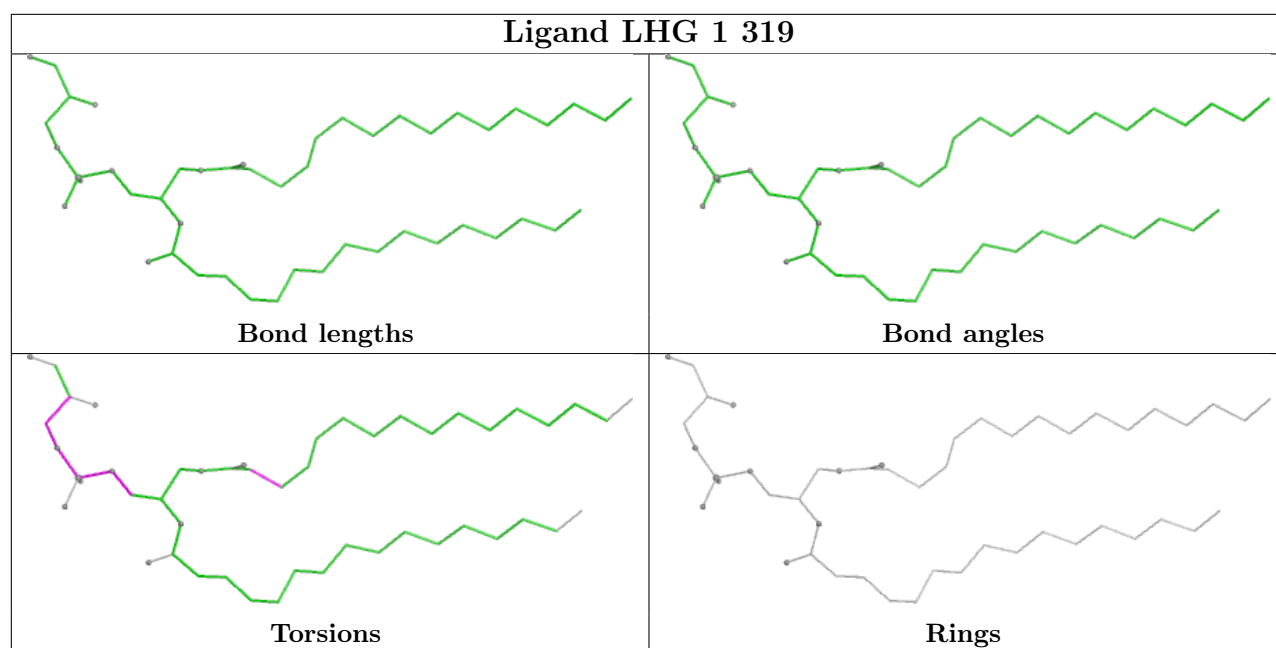


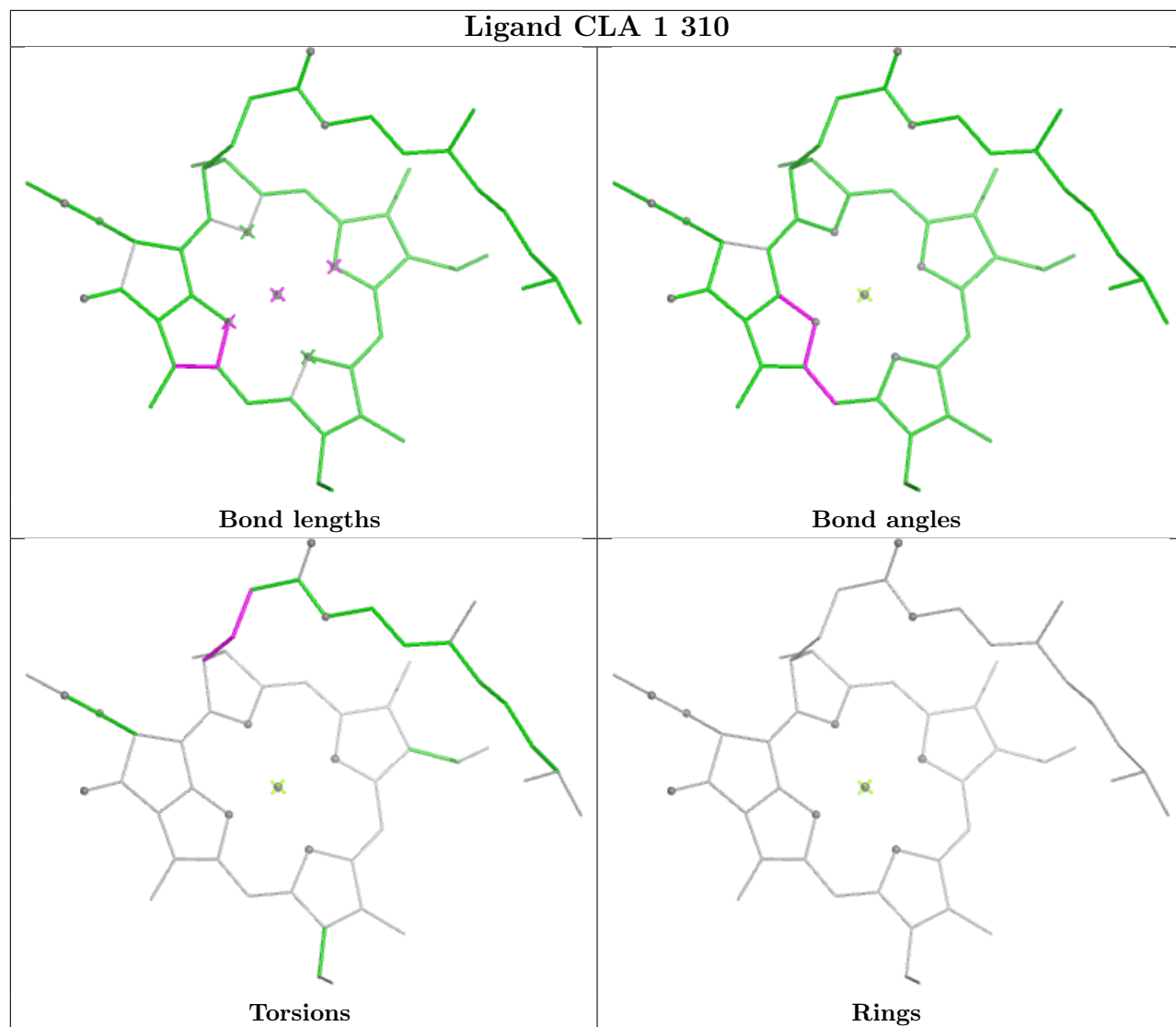


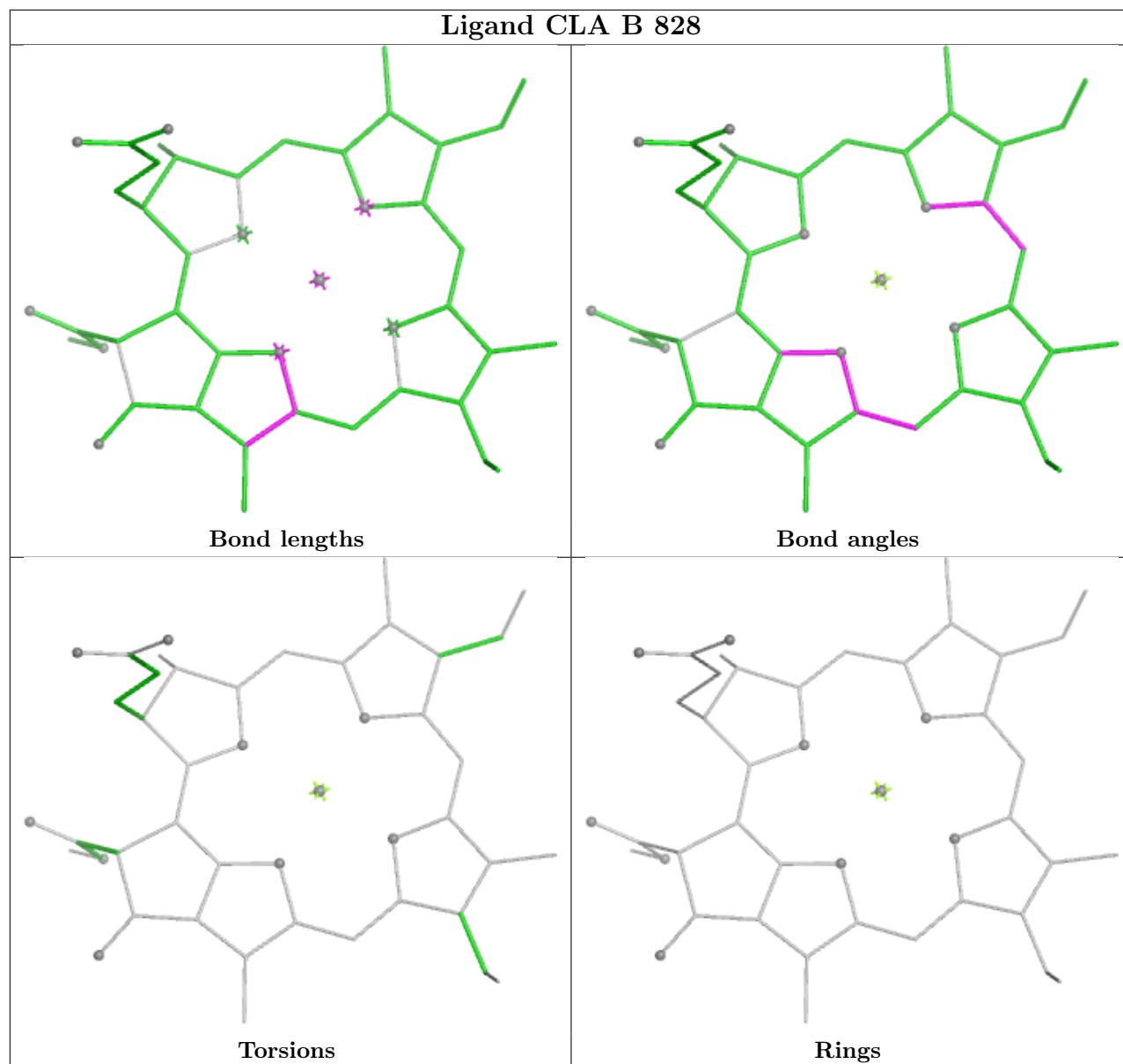


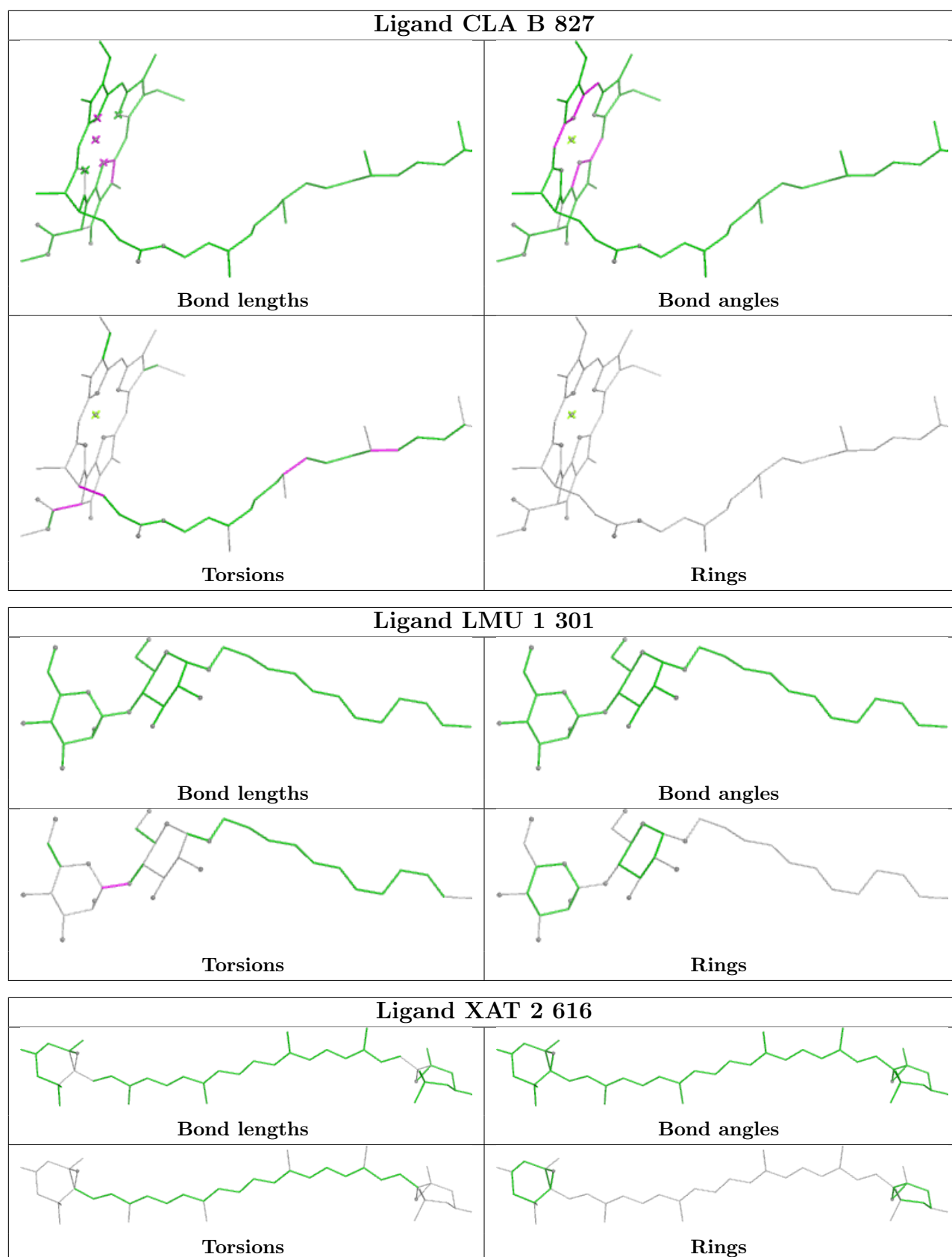


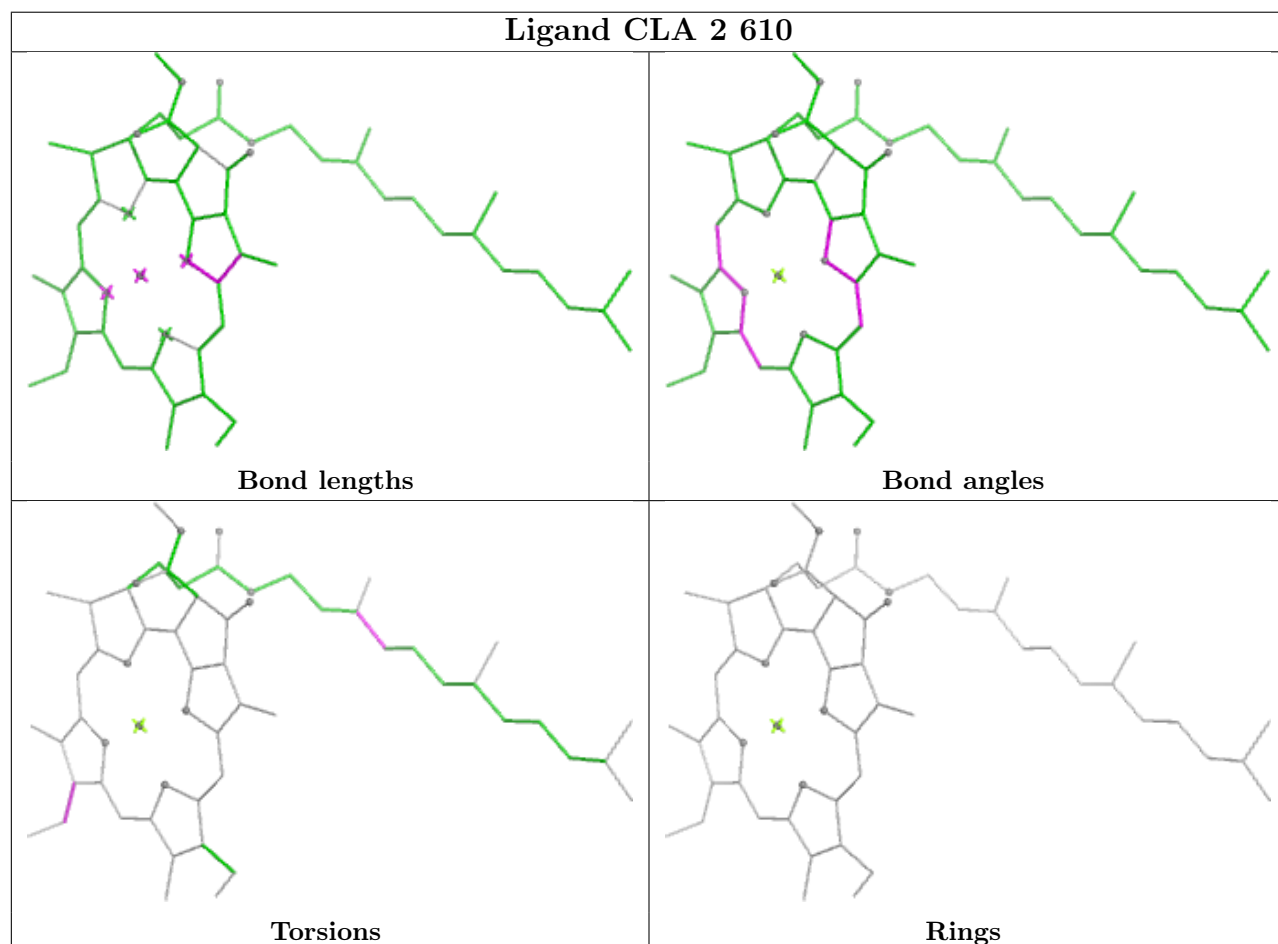
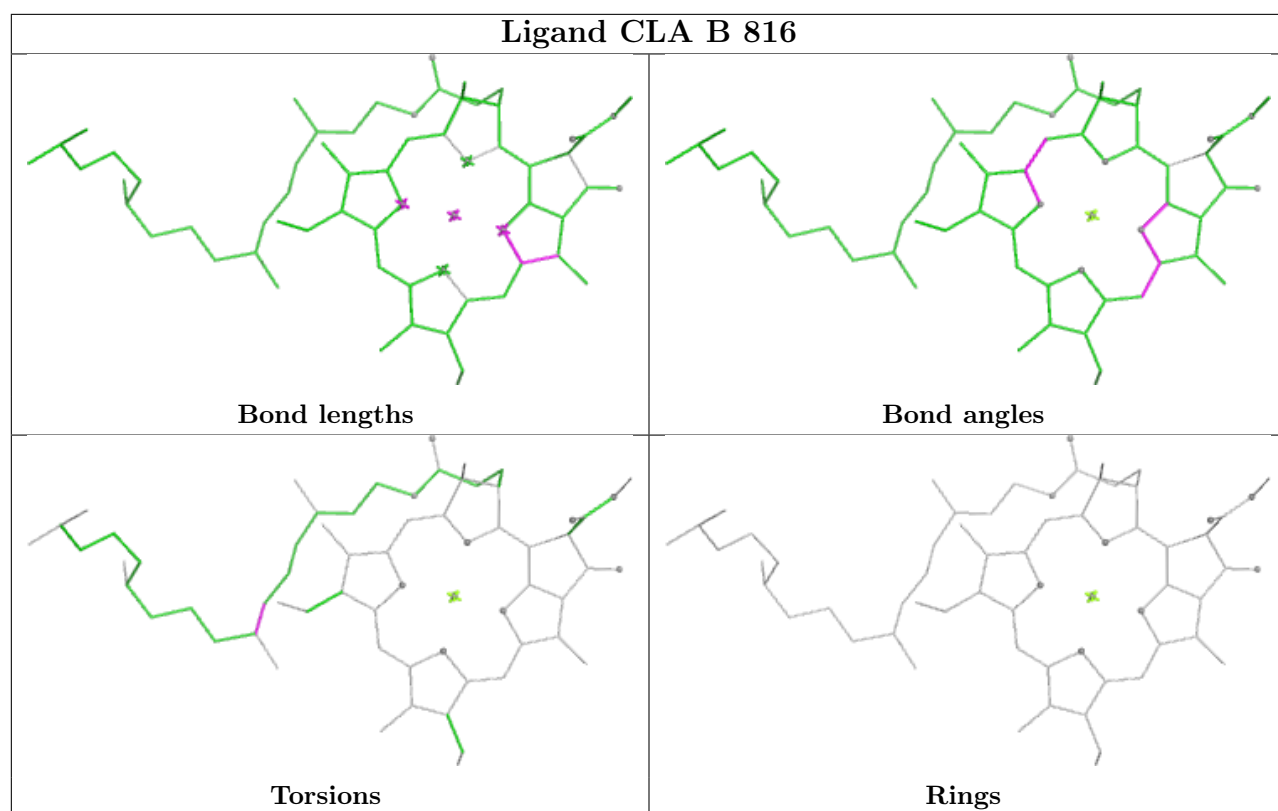


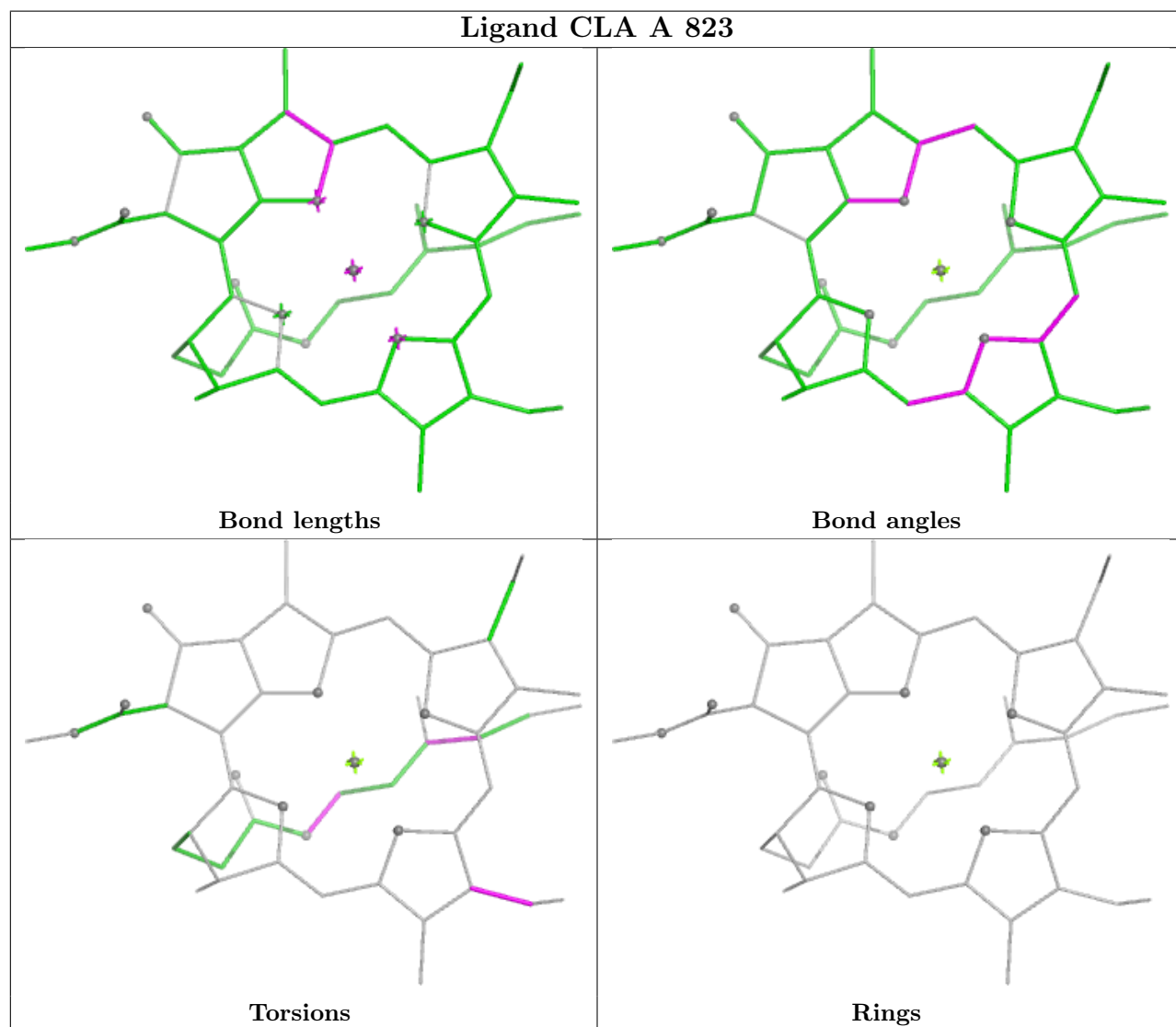
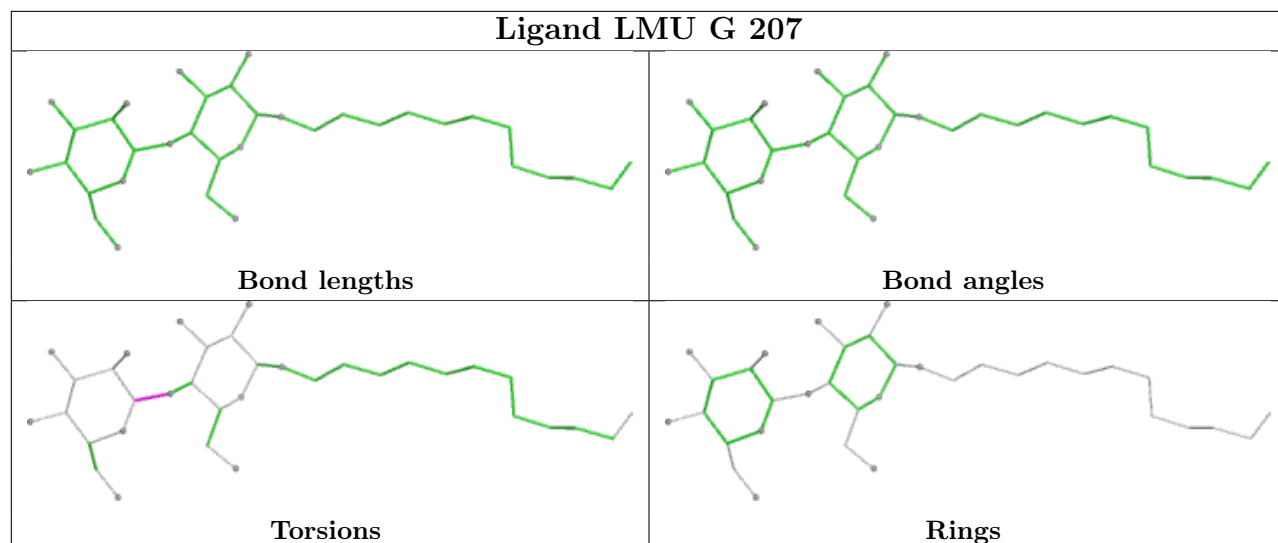


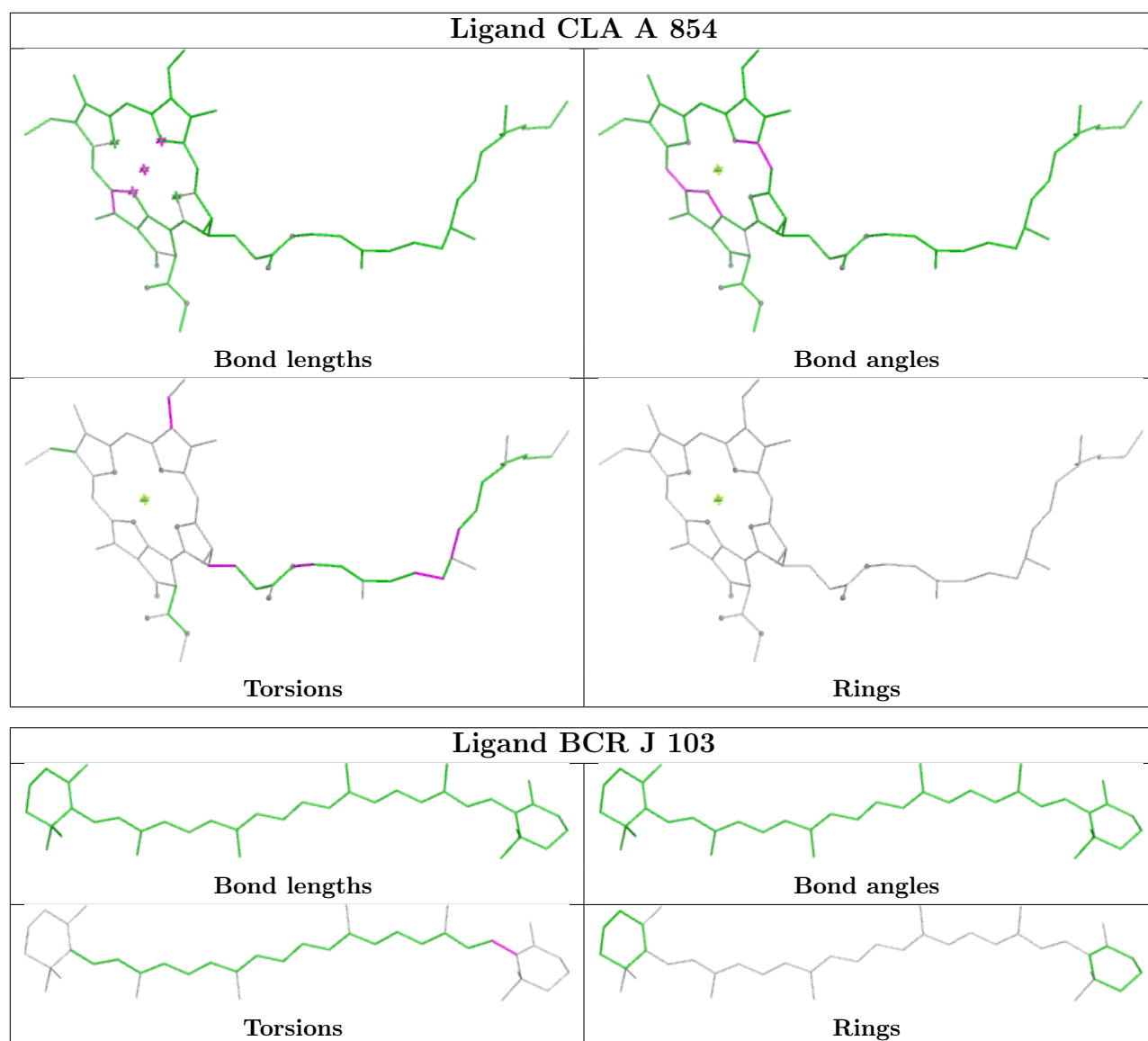


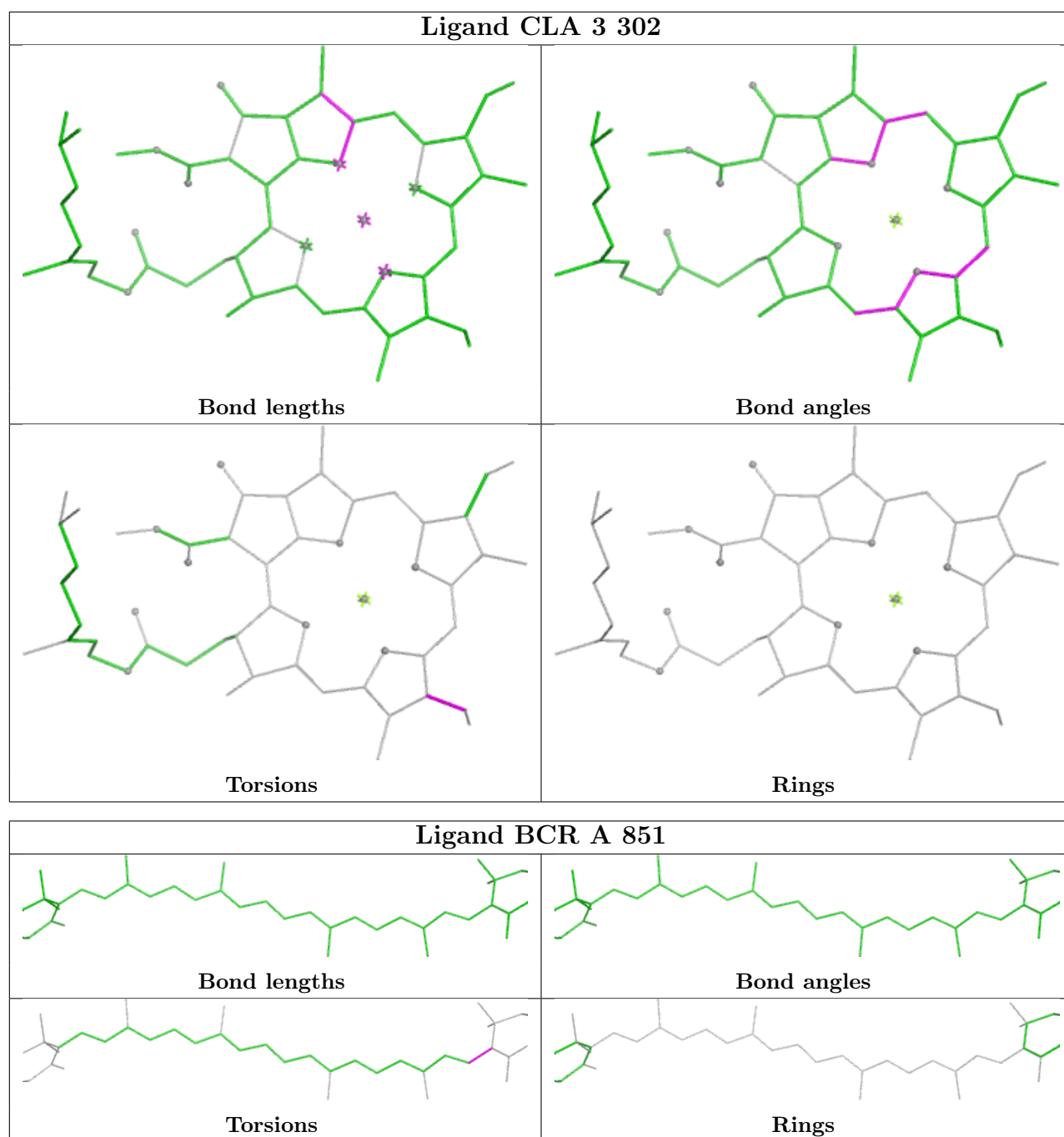




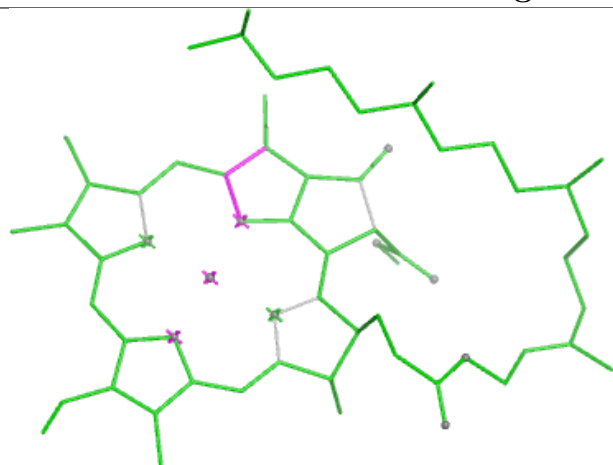




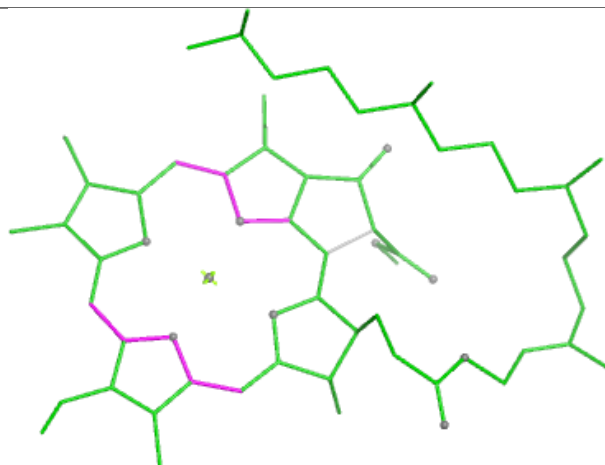




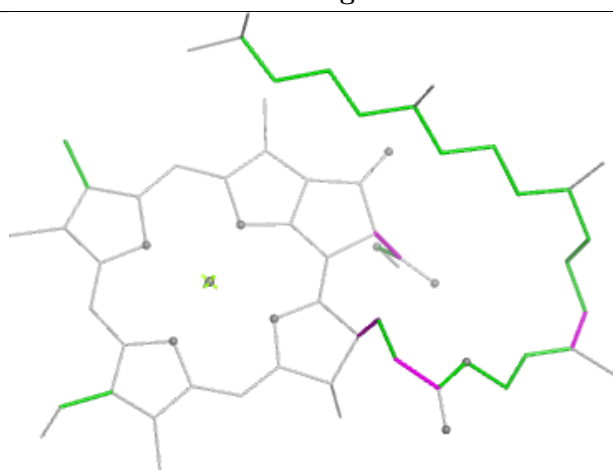
Ligand CLA B 804



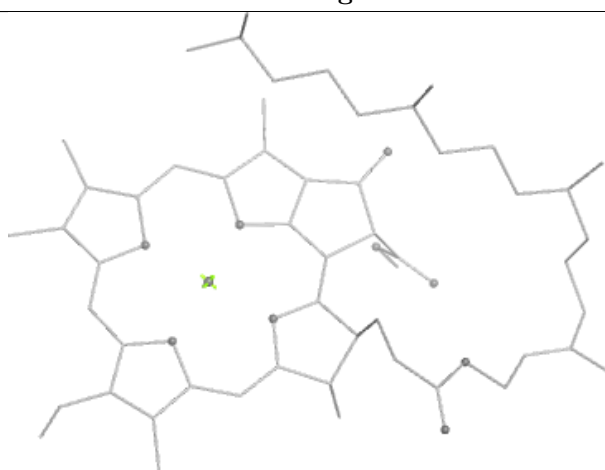
Bond lengths



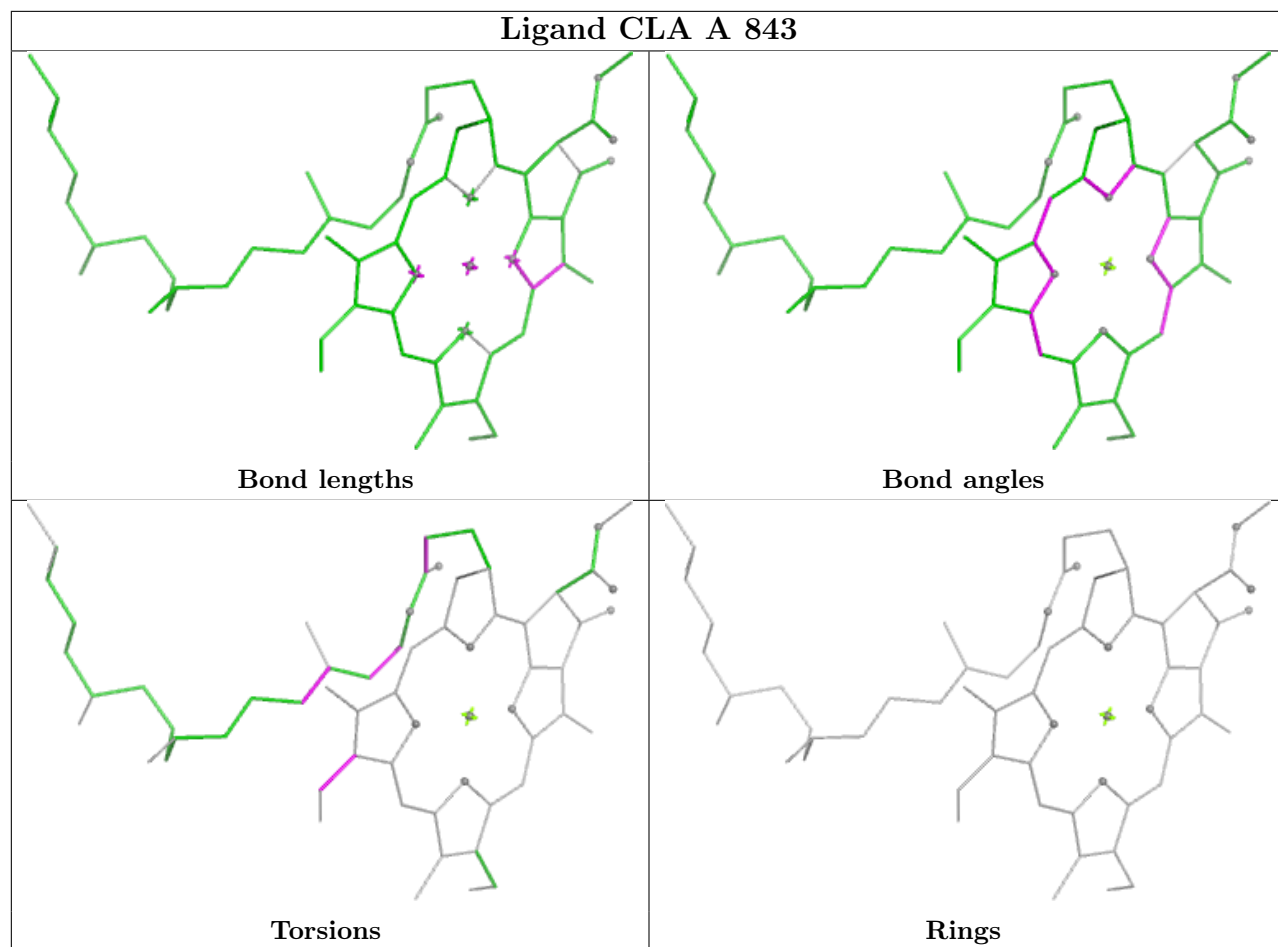
Bond angles

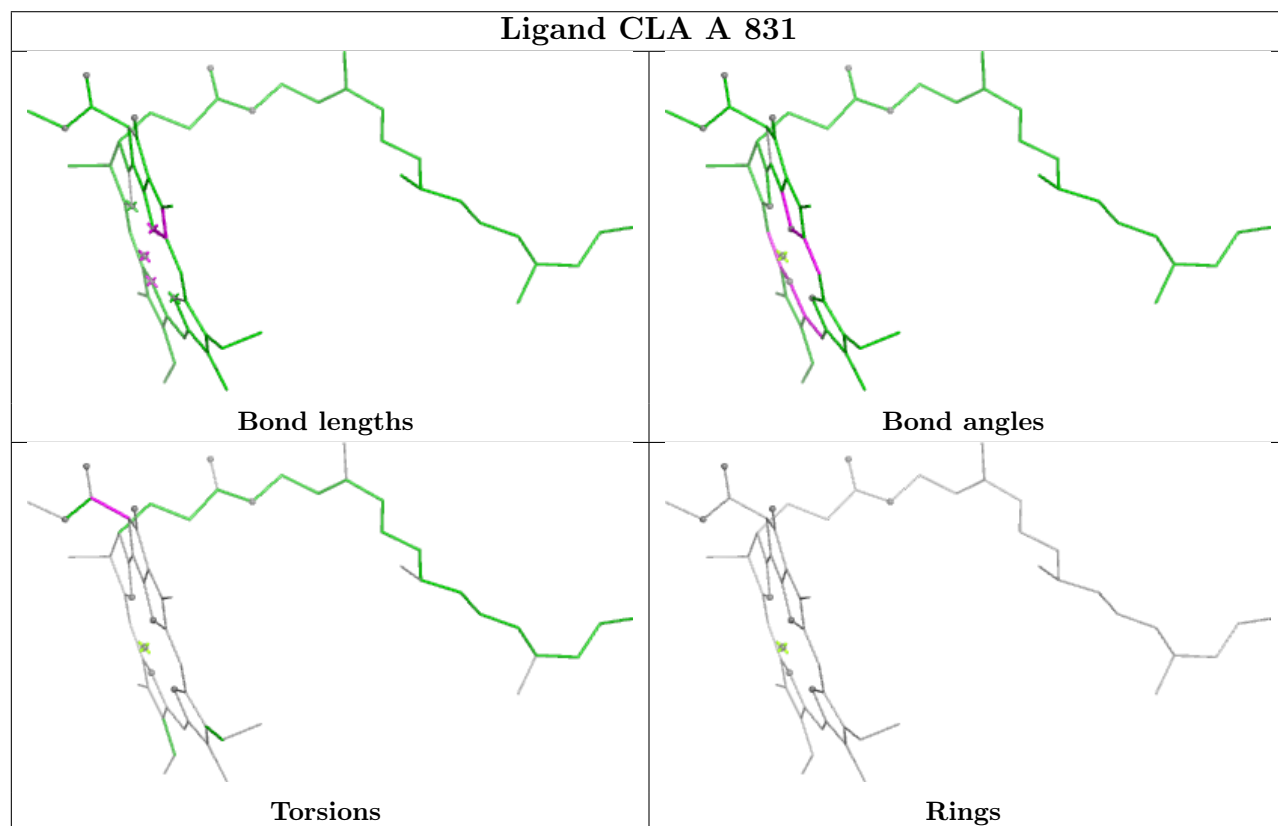
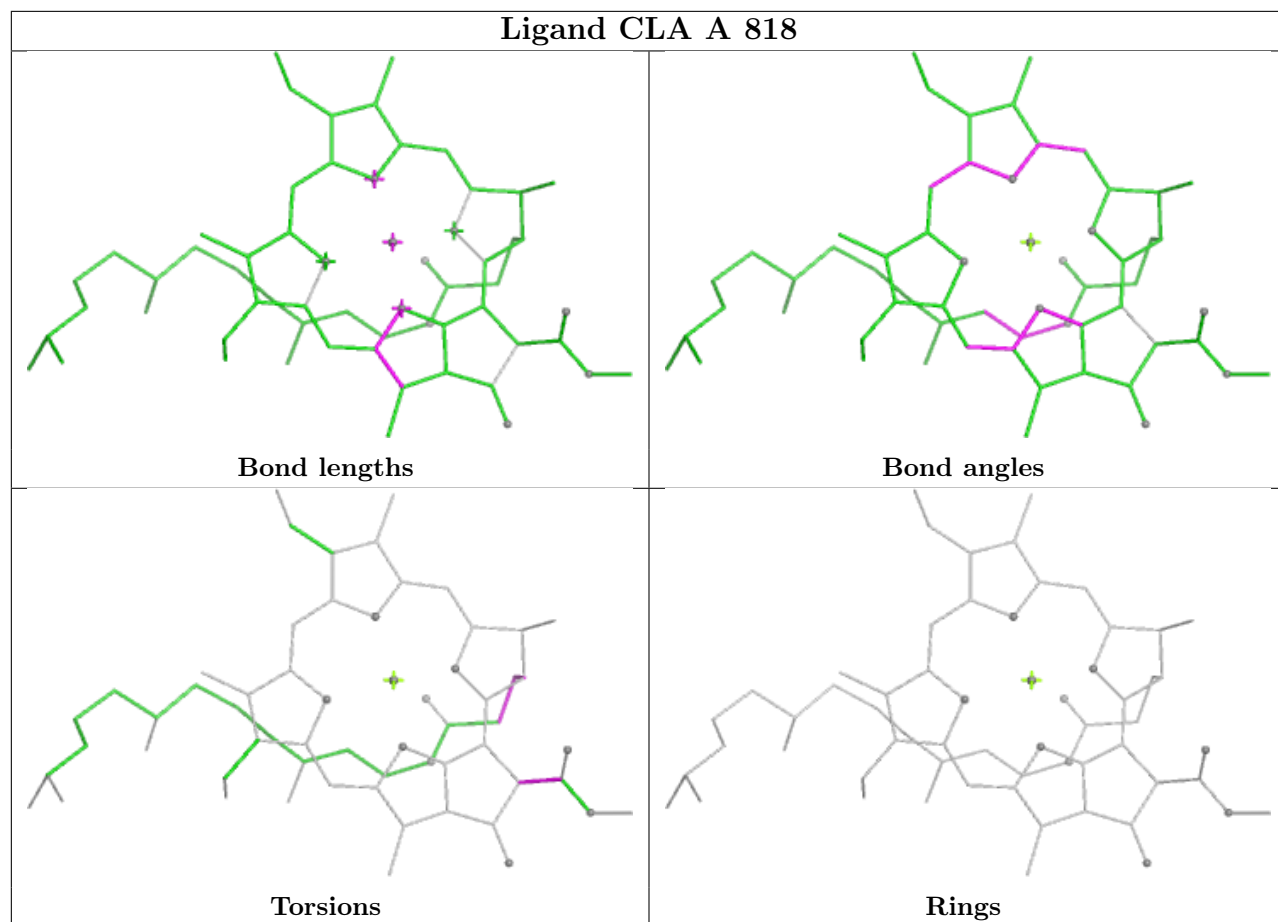


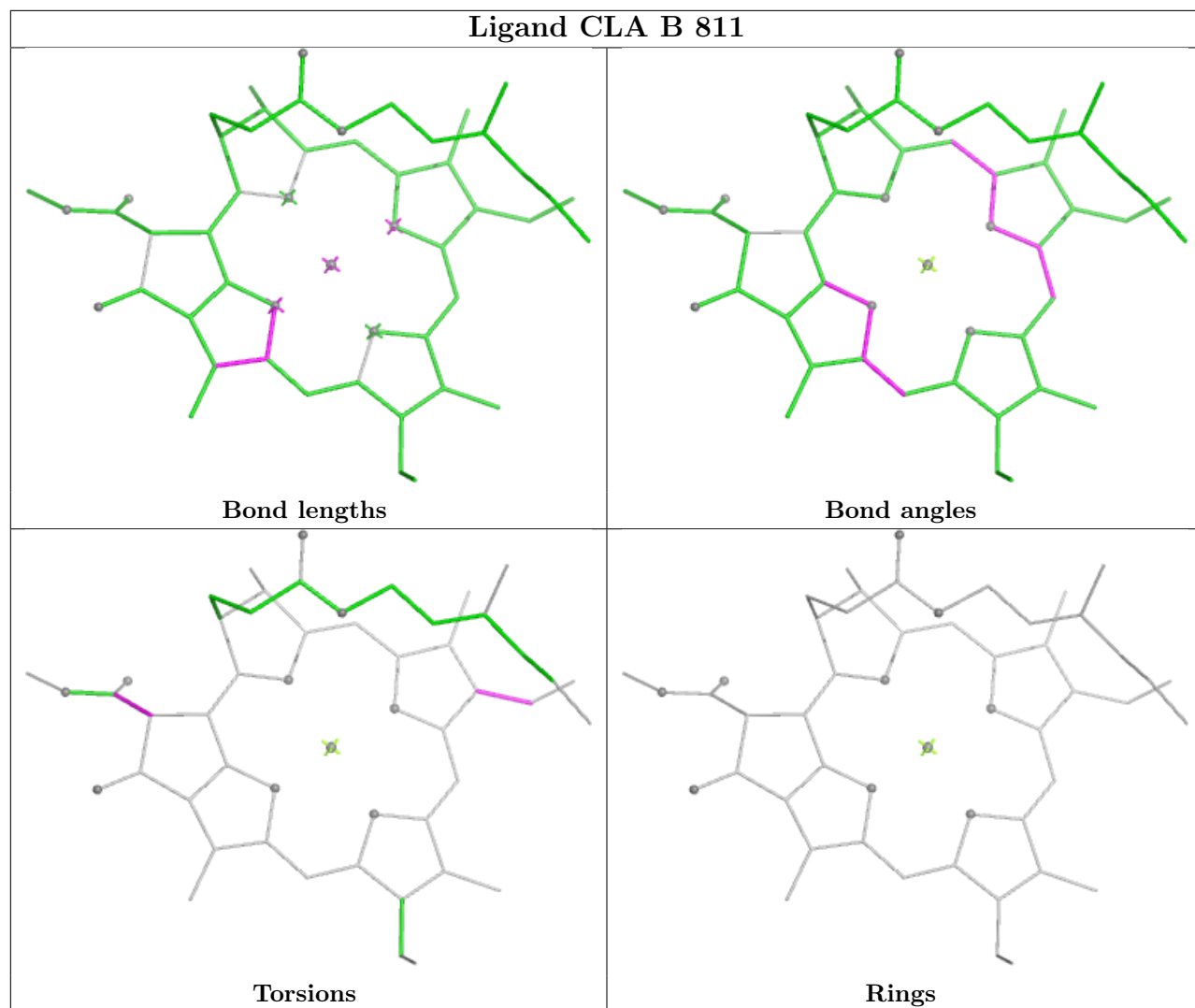
Torsions

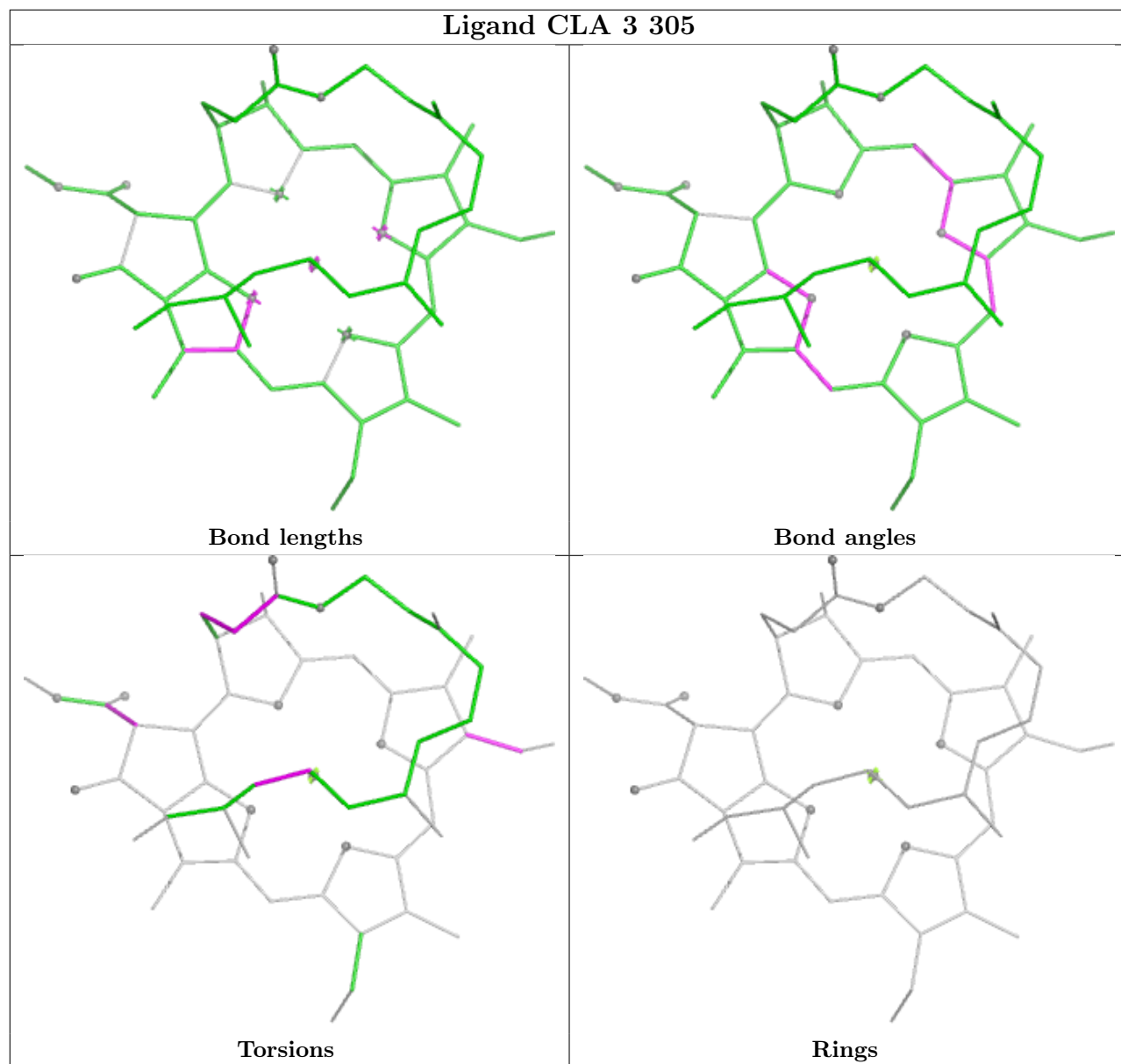


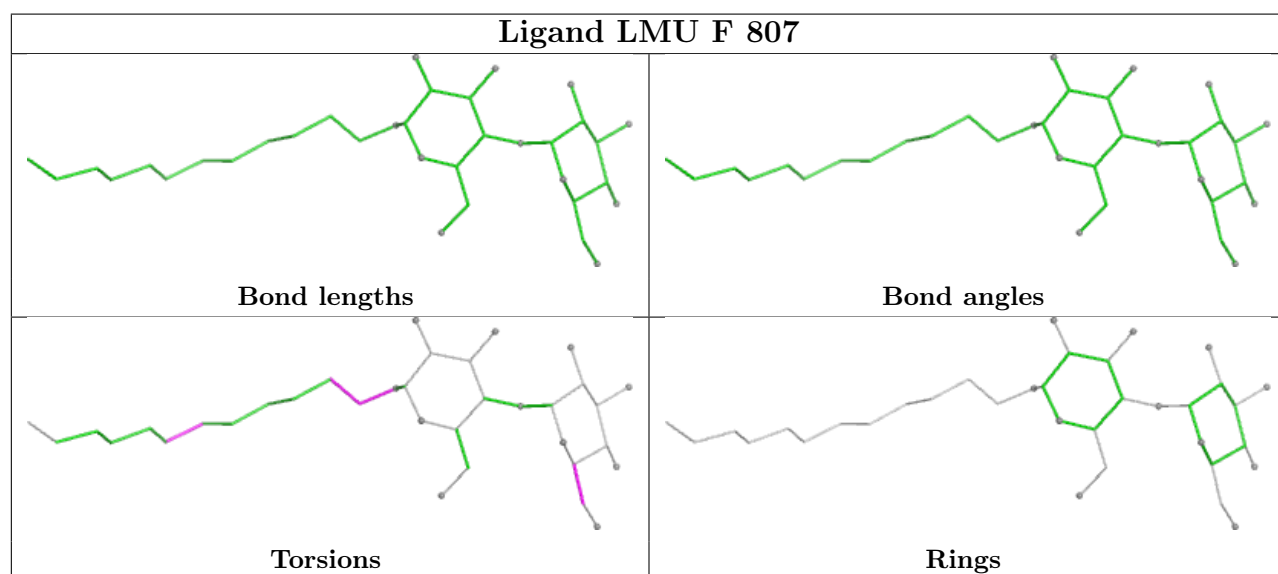
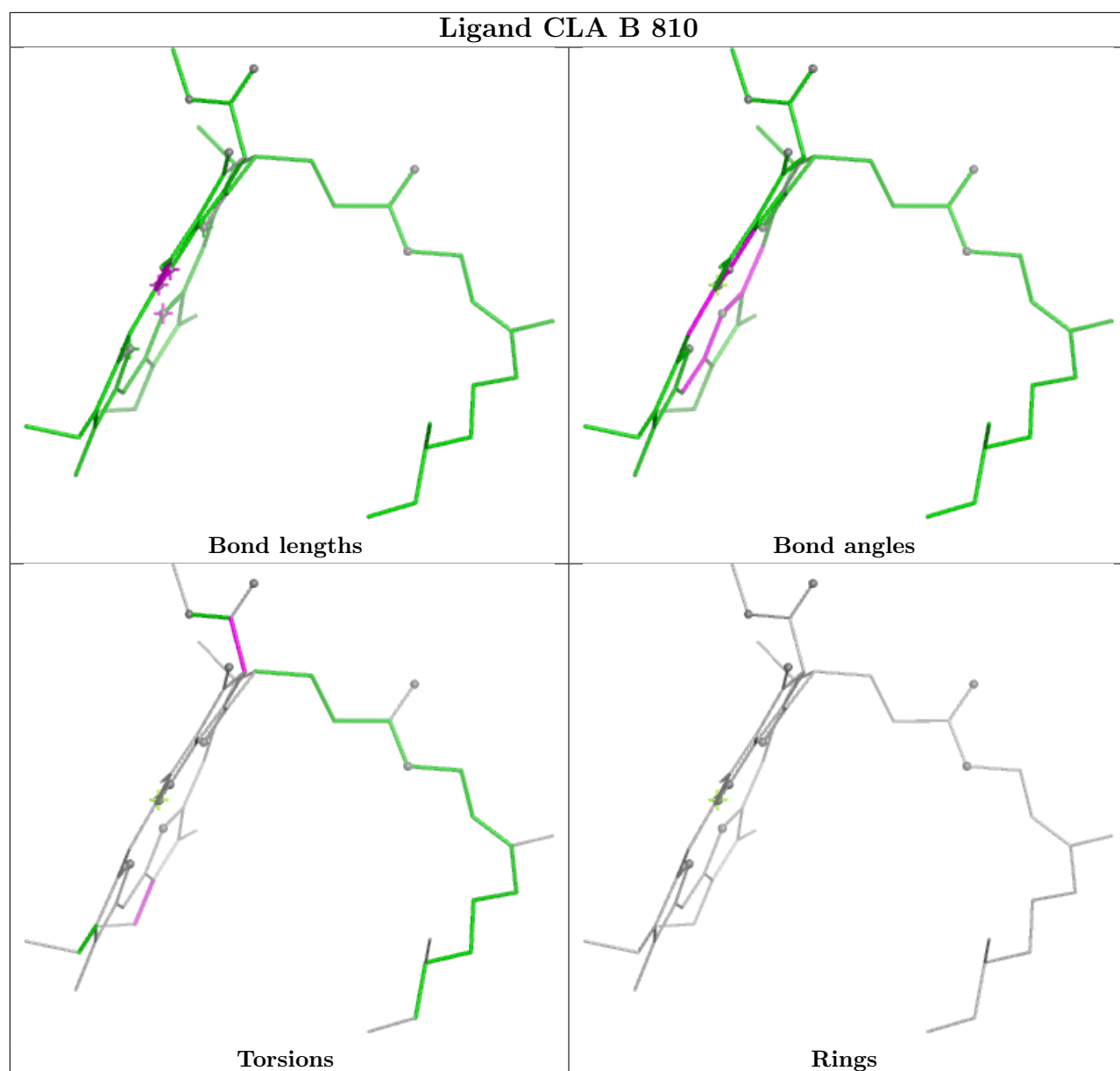
Rings



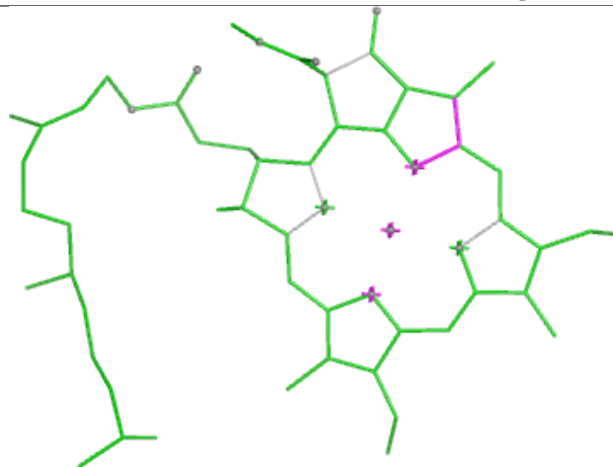




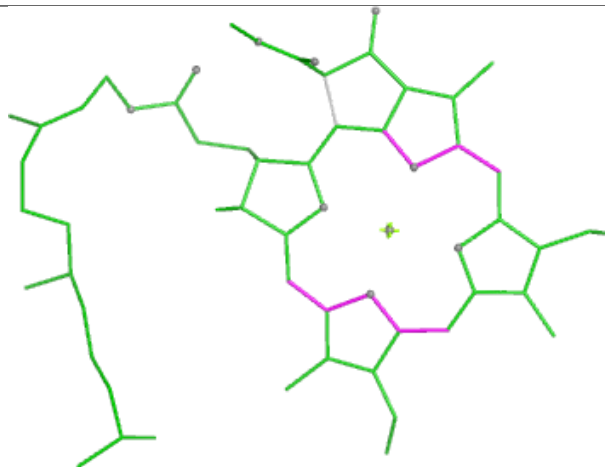




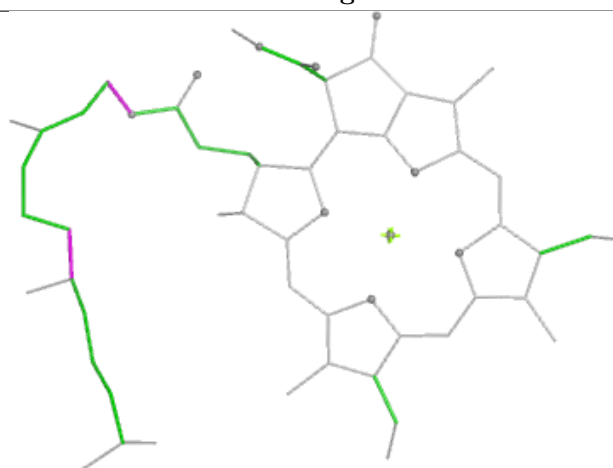
Ligand CLA A 816



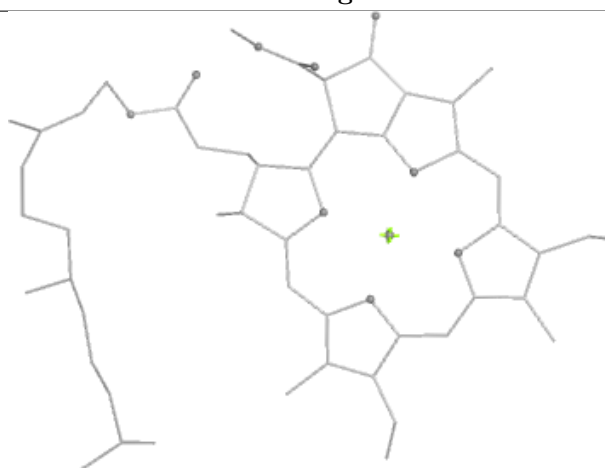
Bond lengths



Bond angles

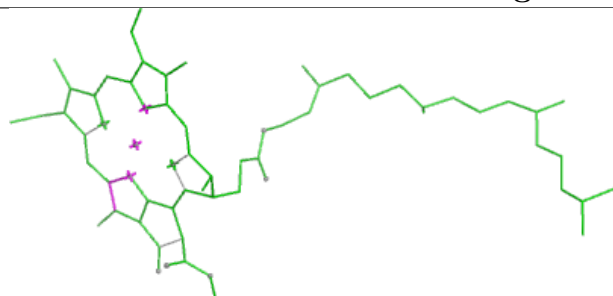


Torsions

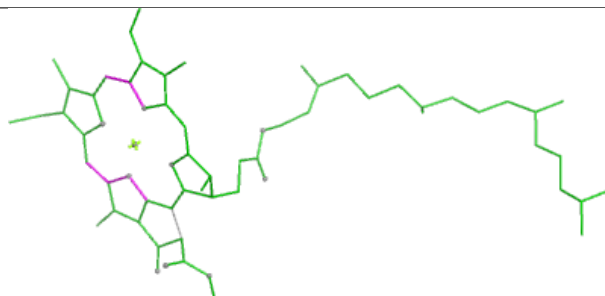


Rings

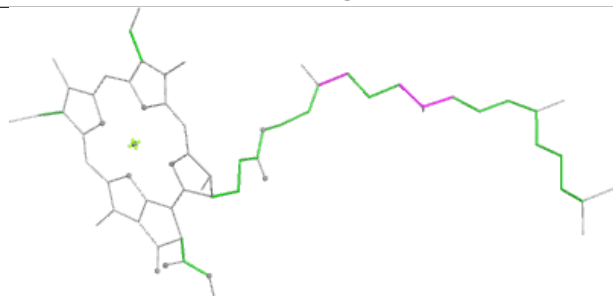
Ligand CLA A 822



Bond lengths



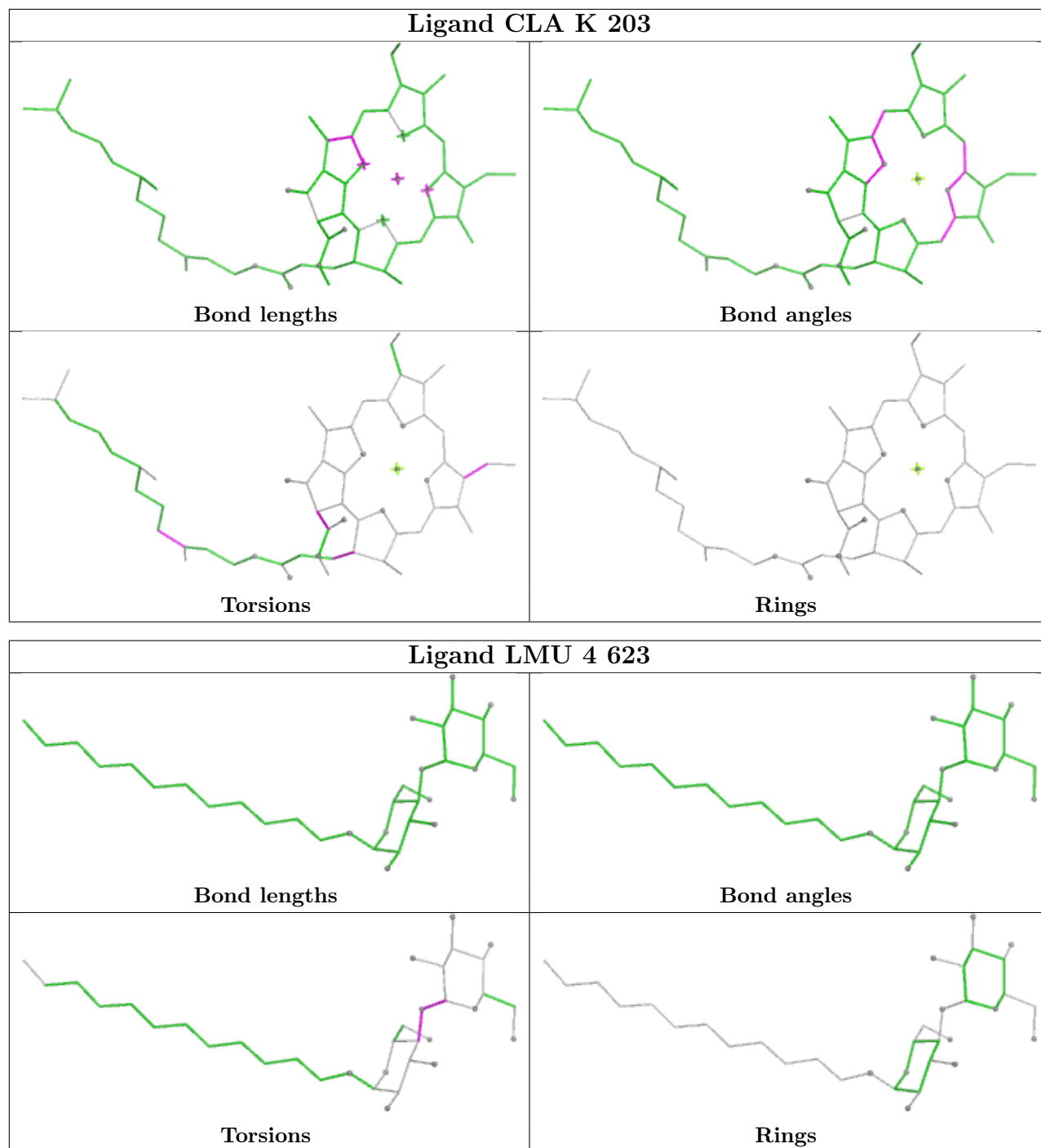
Bond angles

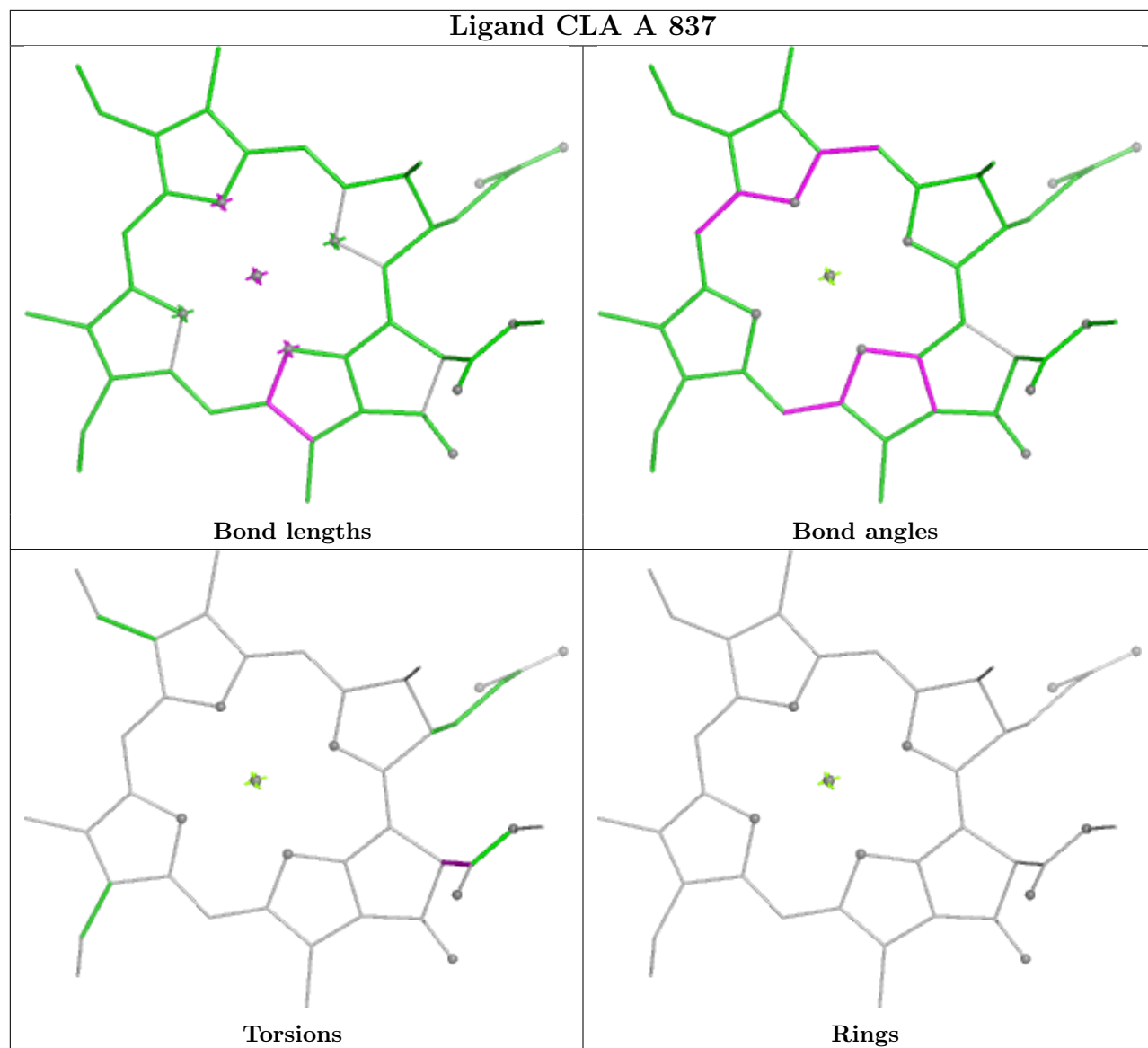


Torsions

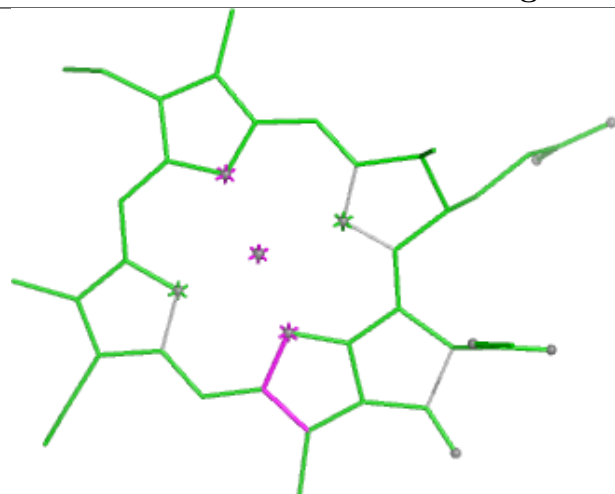


Rings

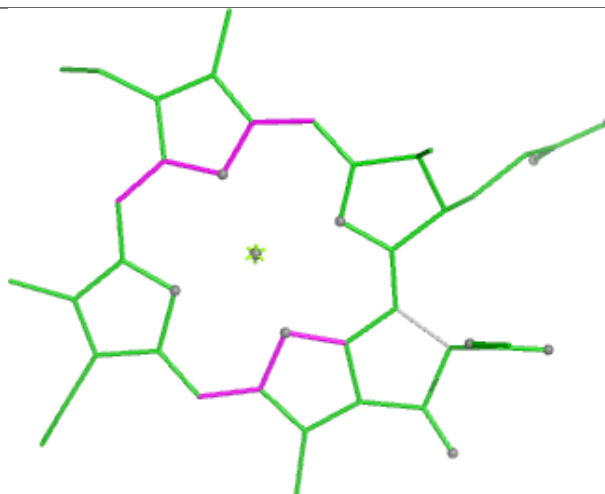




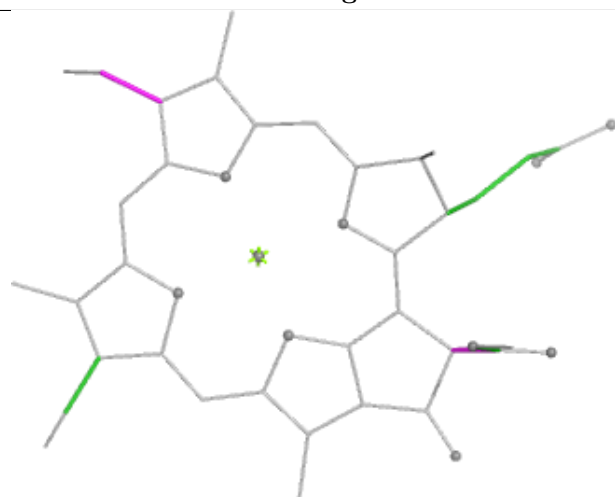
Ligand CLA J 102



Bond lengths



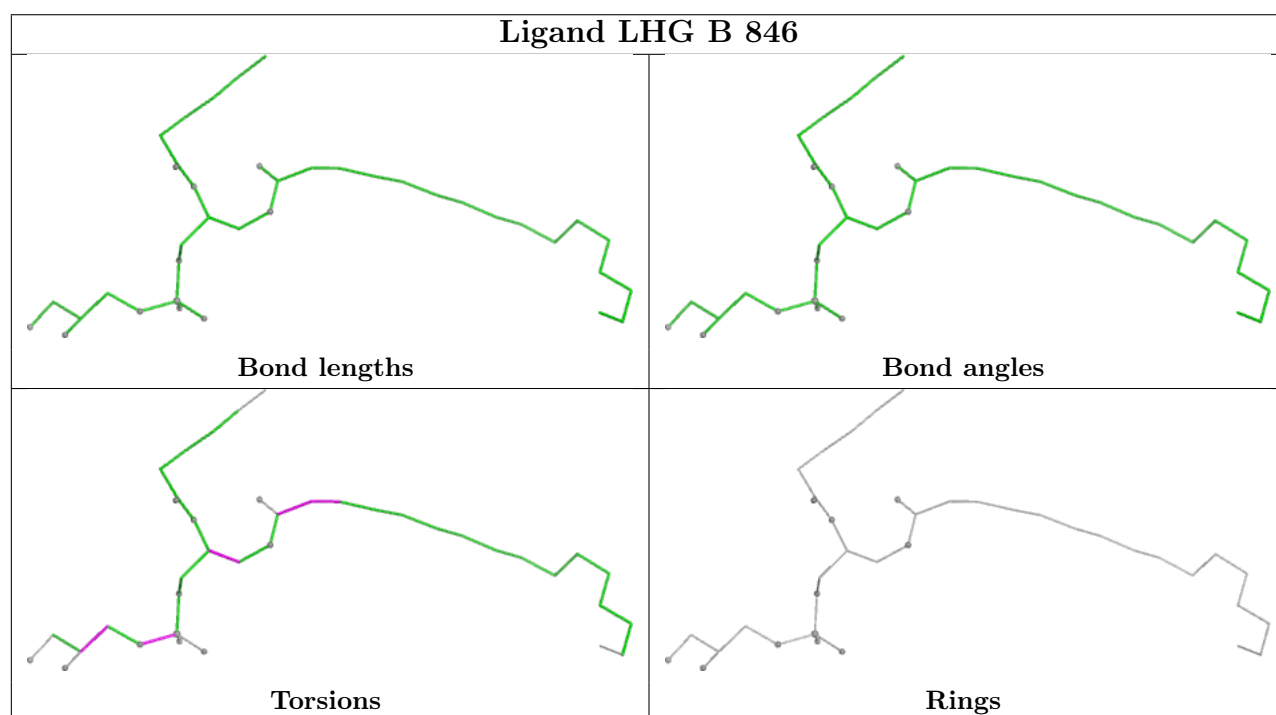
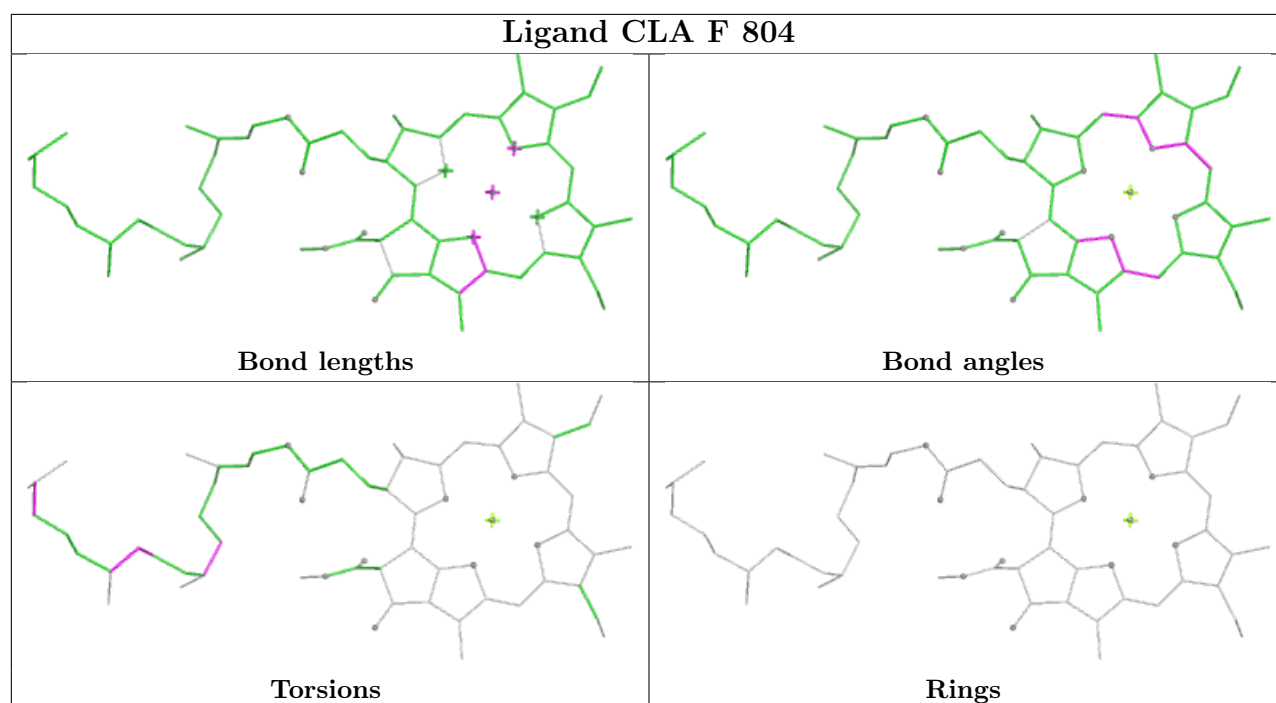
Bond angles

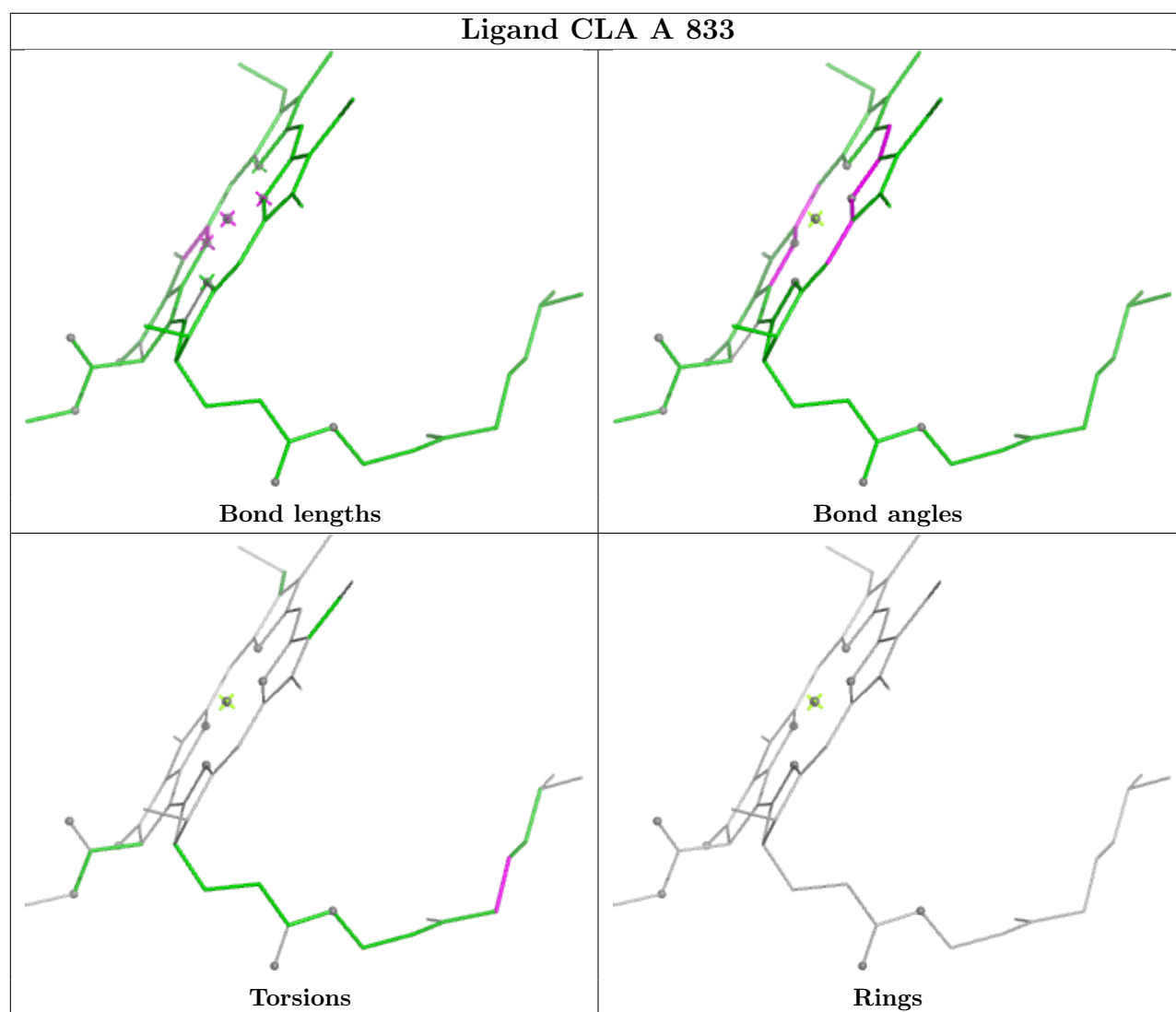


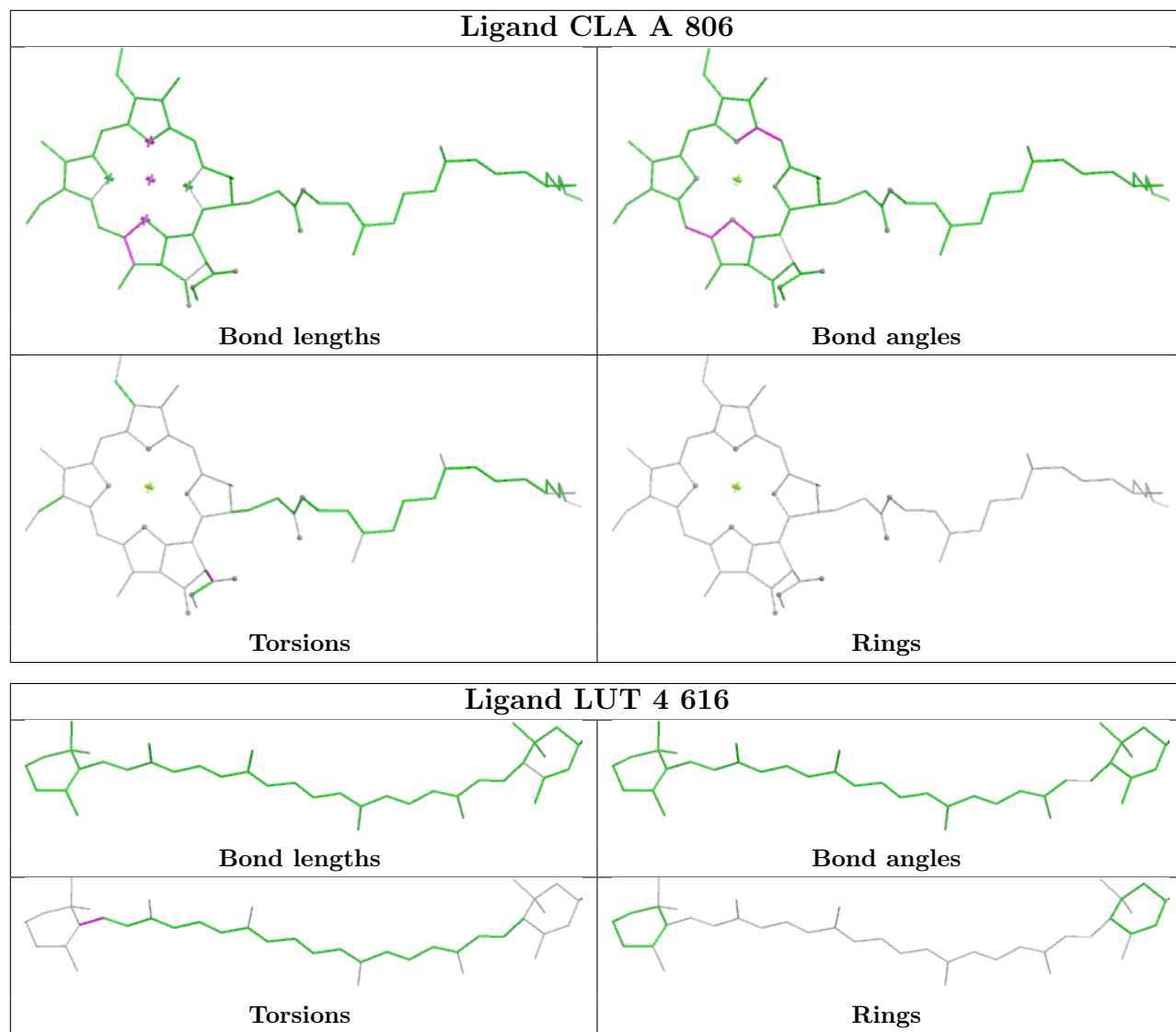
Torsions

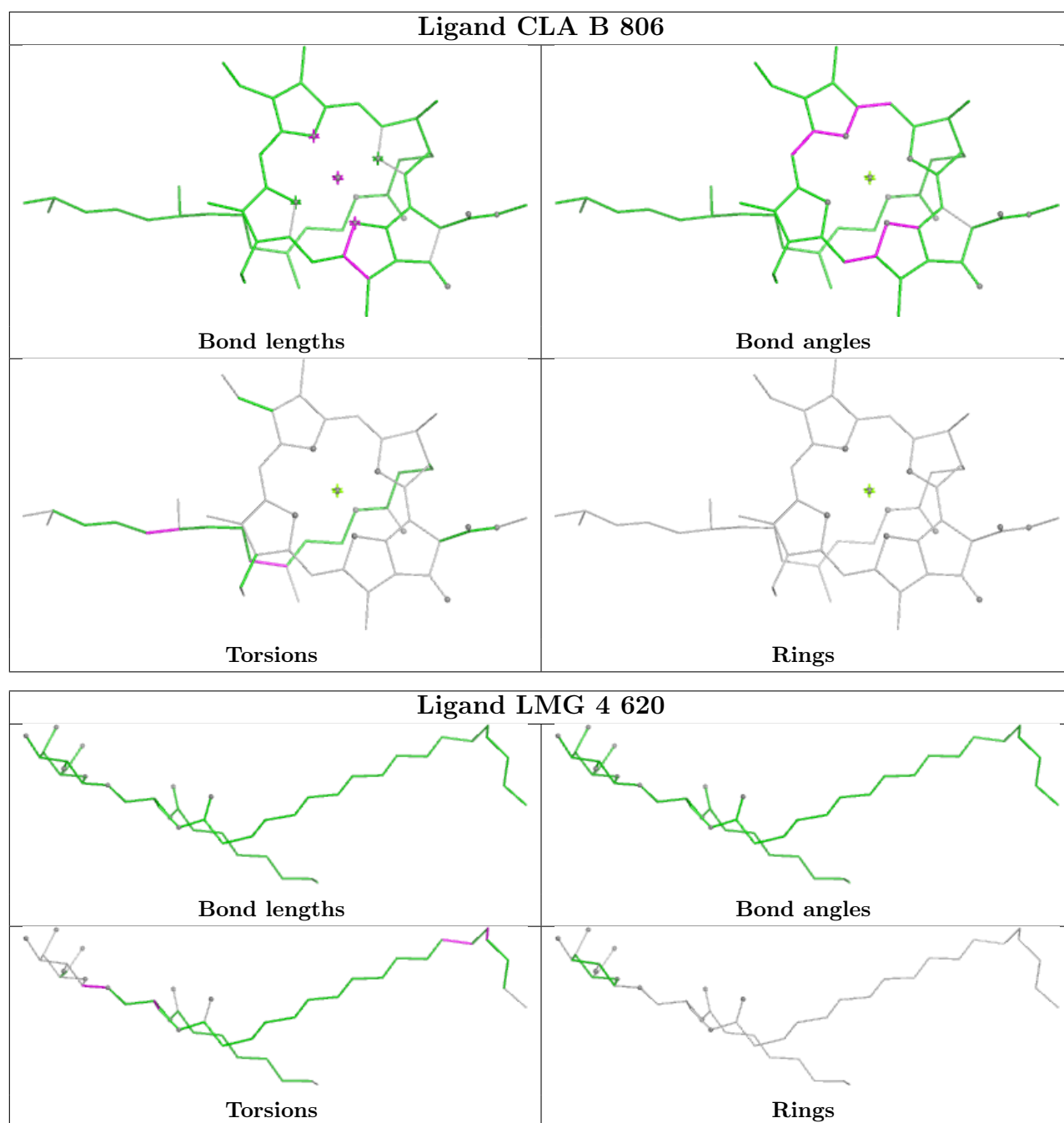


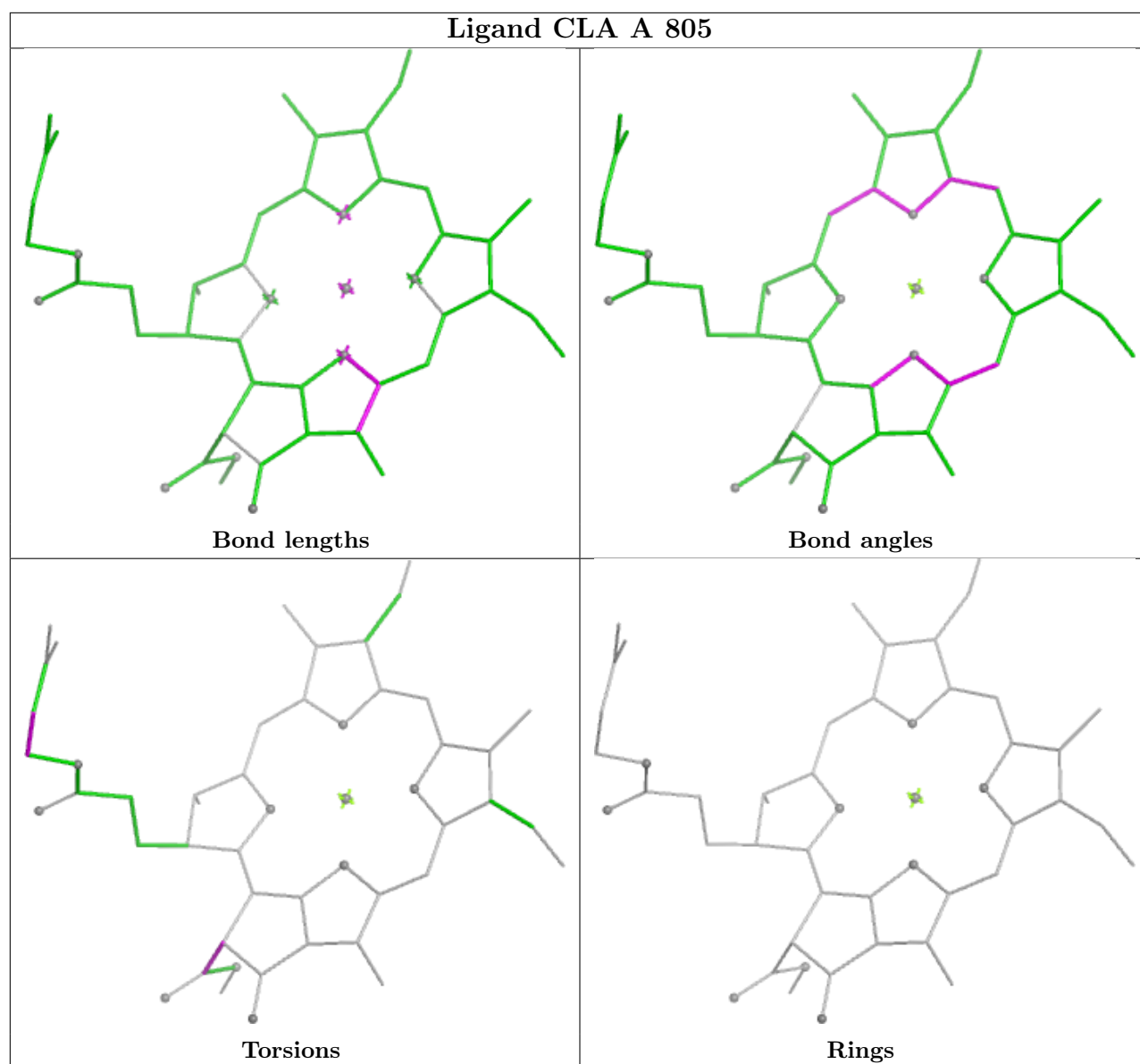
Rings



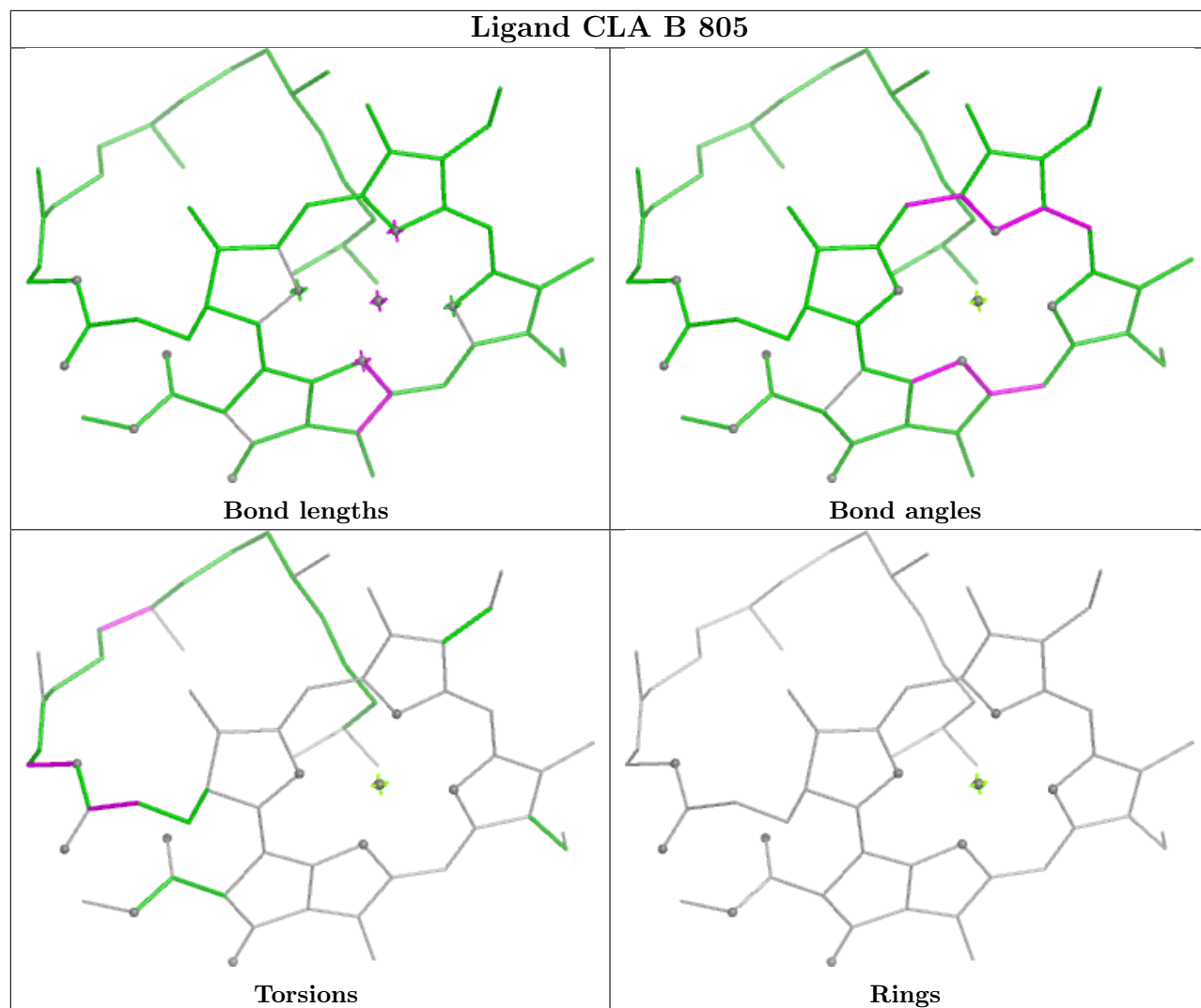


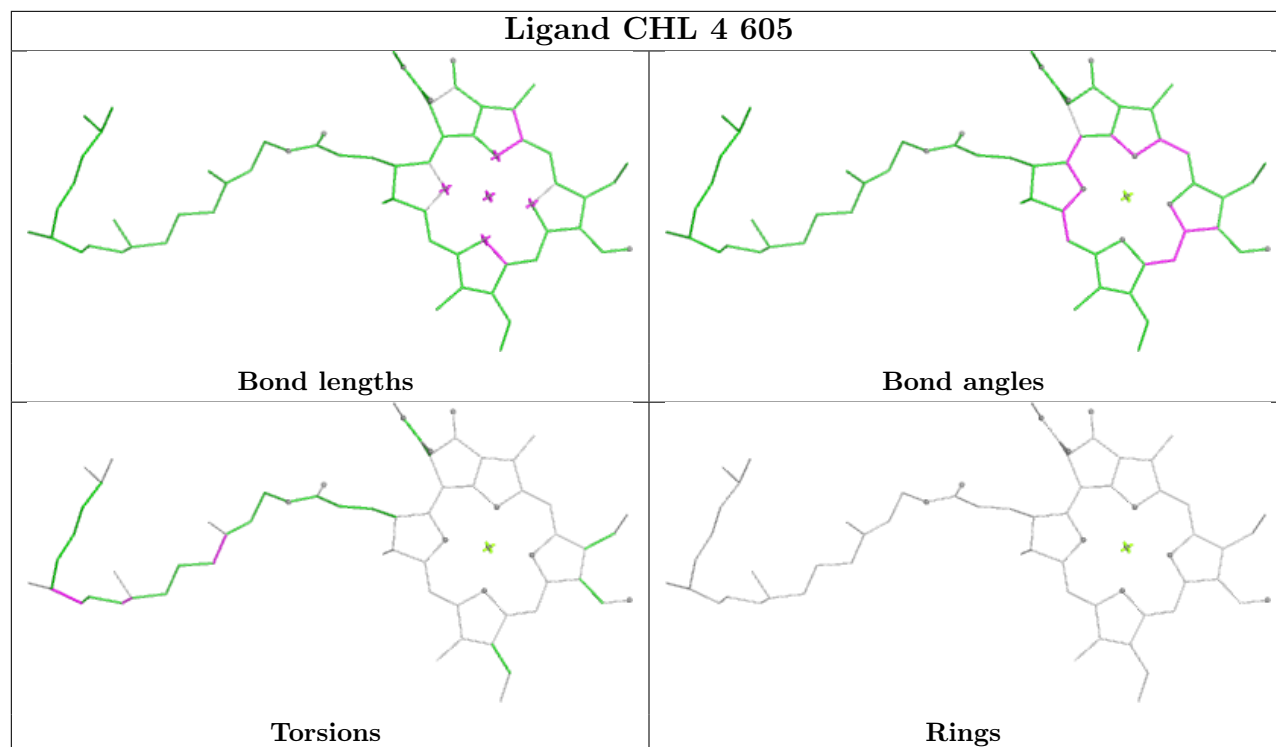
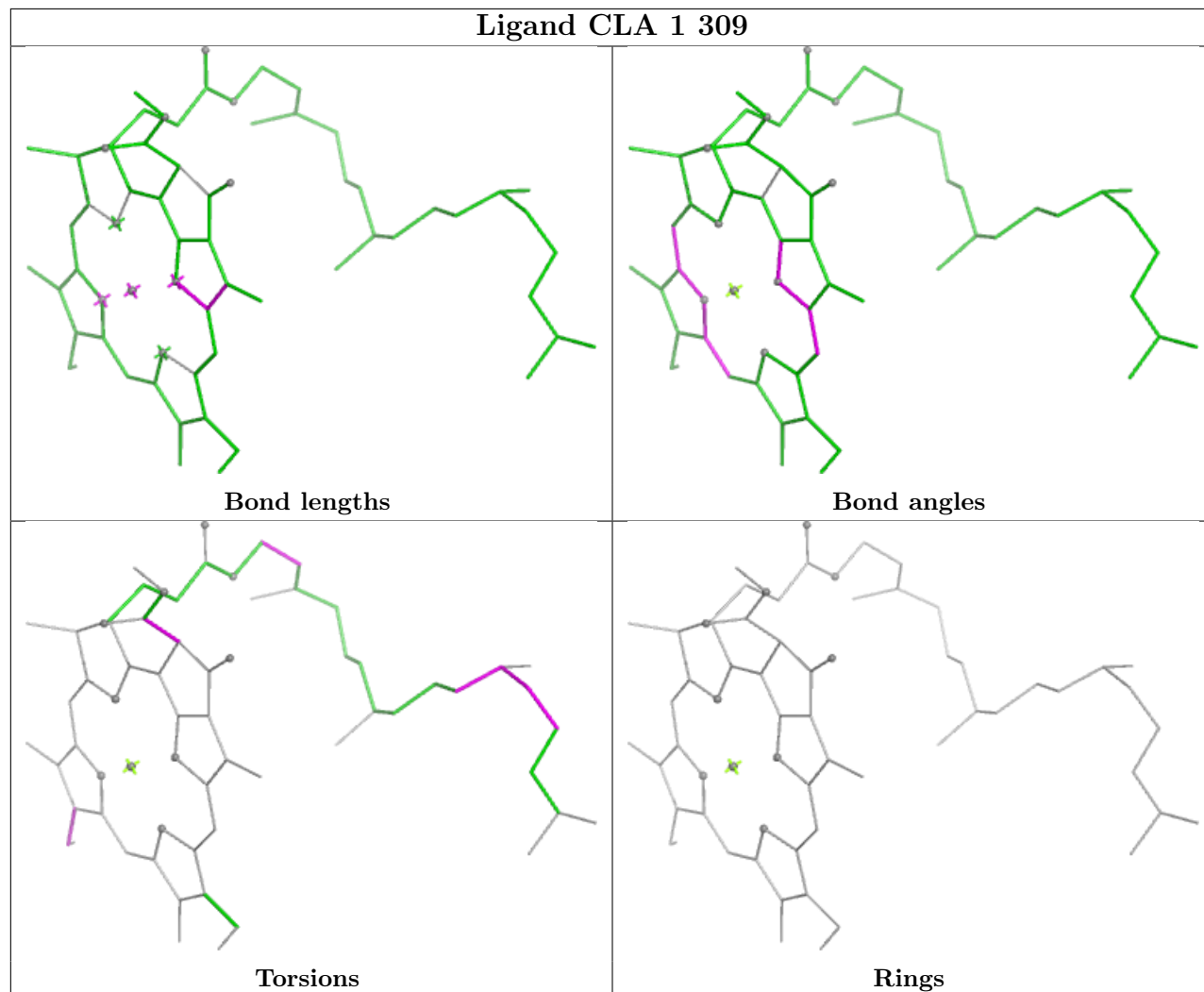


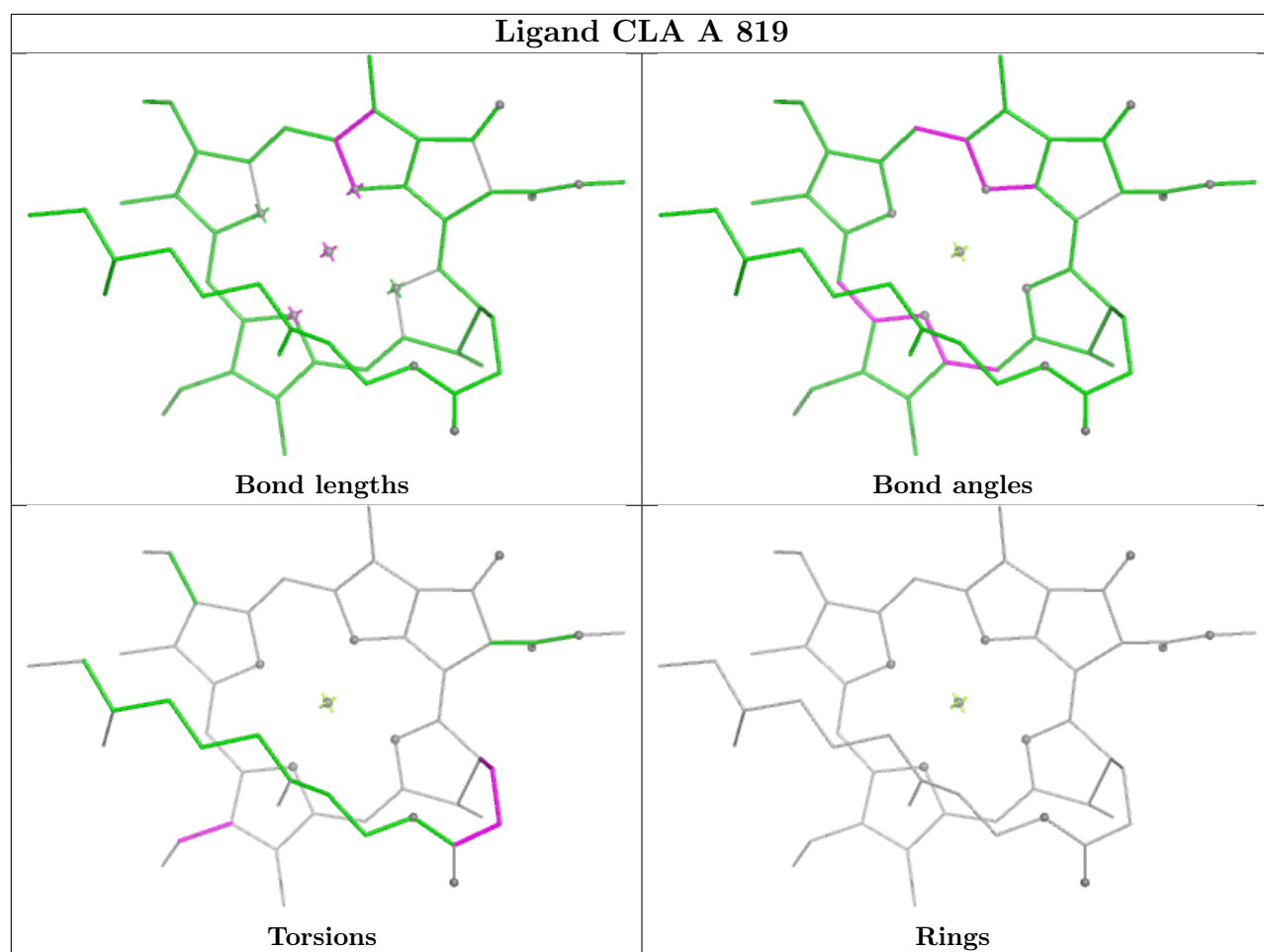




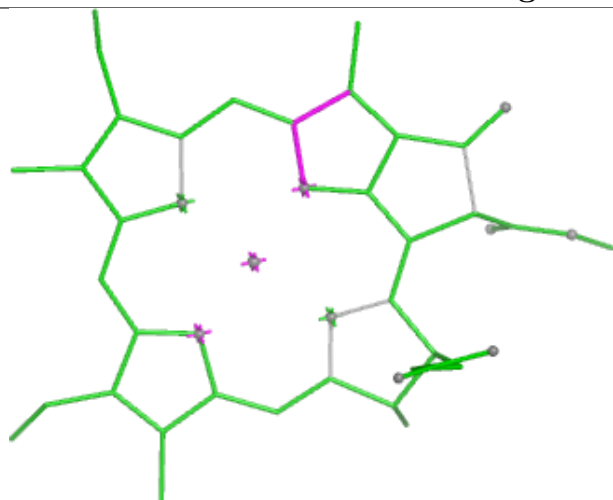
Ligand CLA B 805



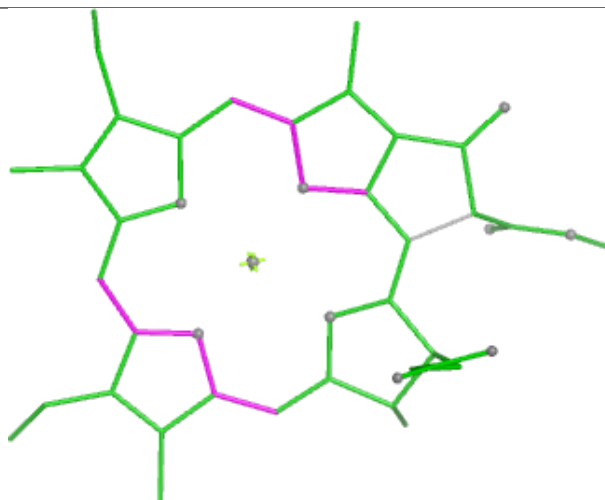
Ligand CHL 4 605**Ligand CLA 1 309**



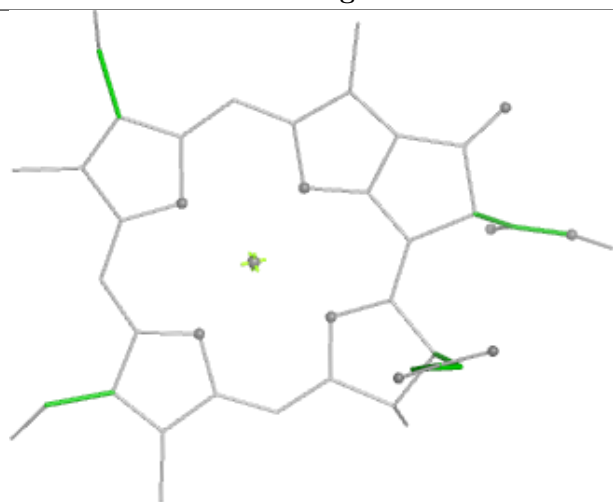
Ligand CLA 2 604



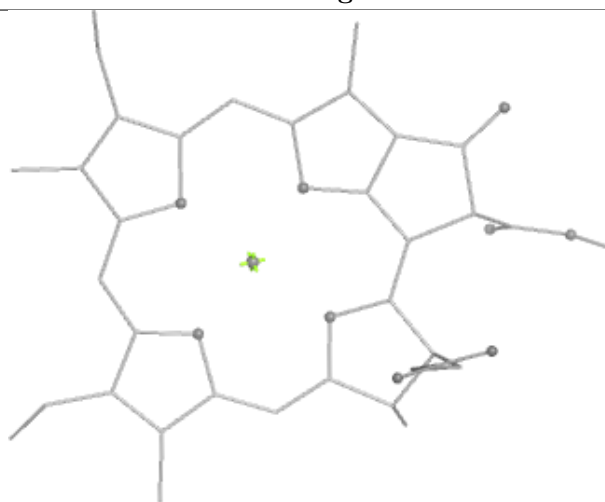
Bond lengths



Bond angles

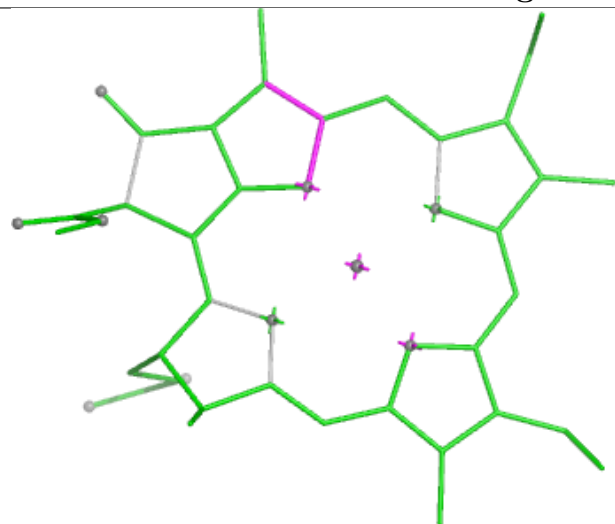


Torsions

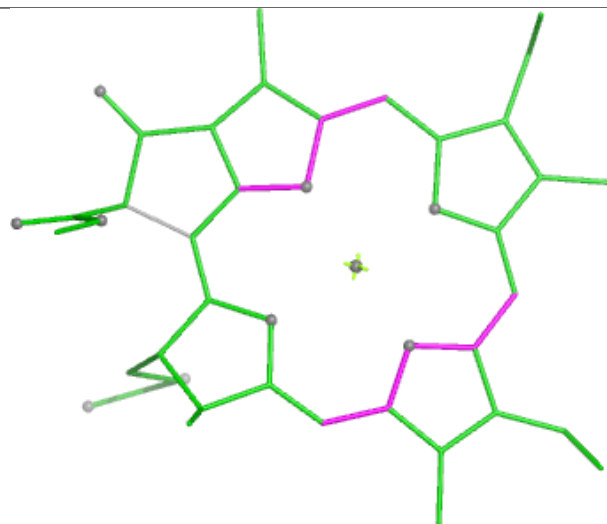


Rings

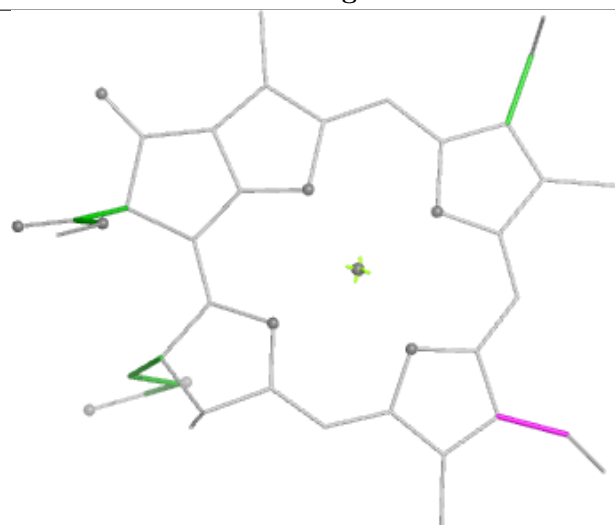
Ligand CLA B 803



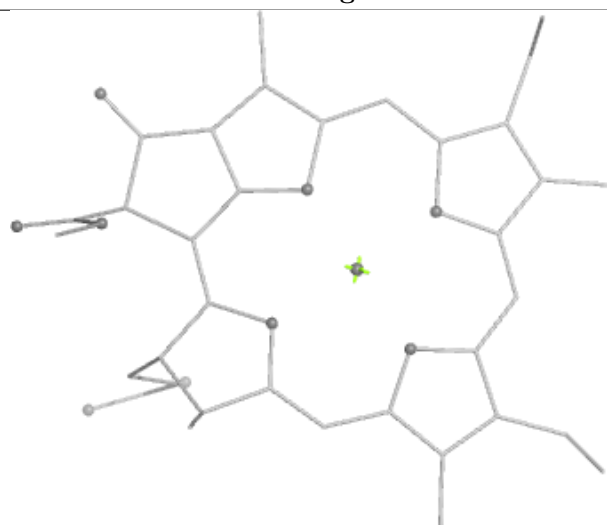
Bond lengths



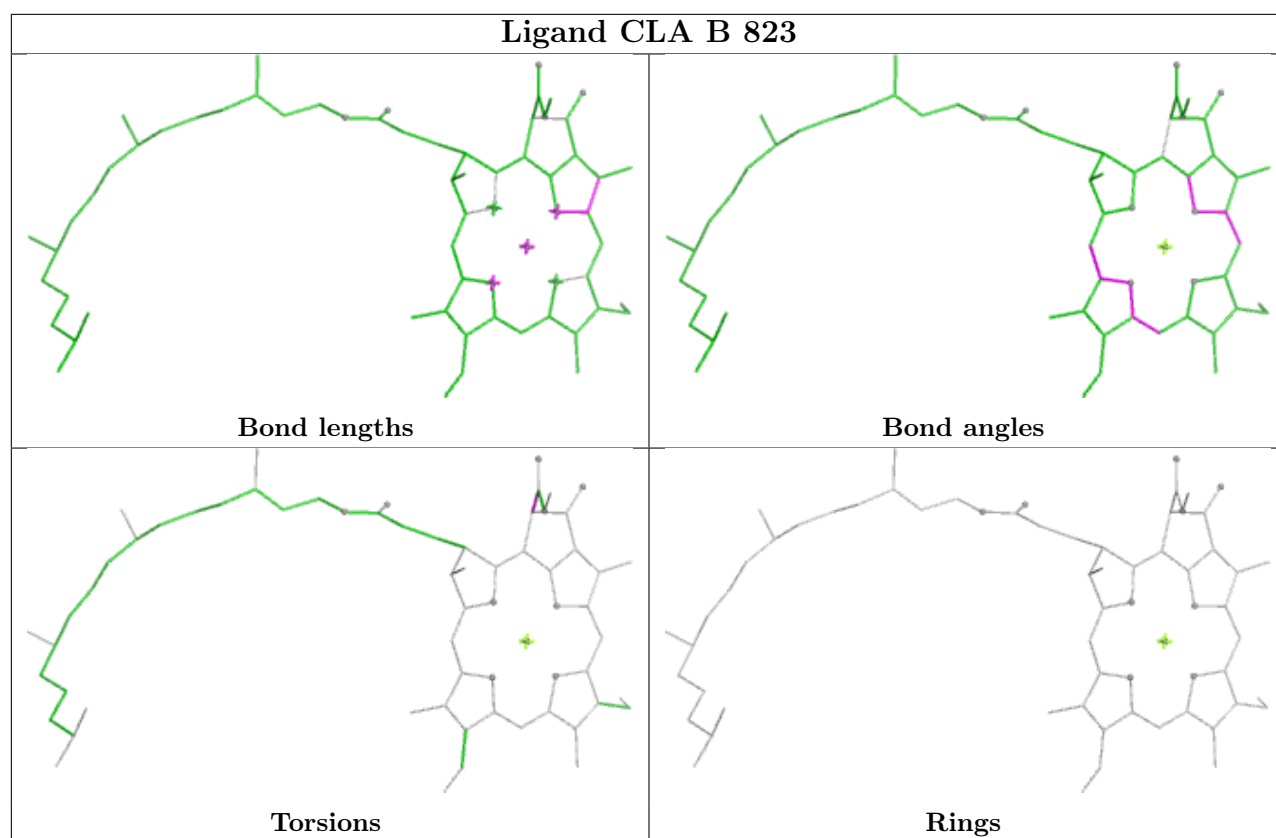
Bond angles



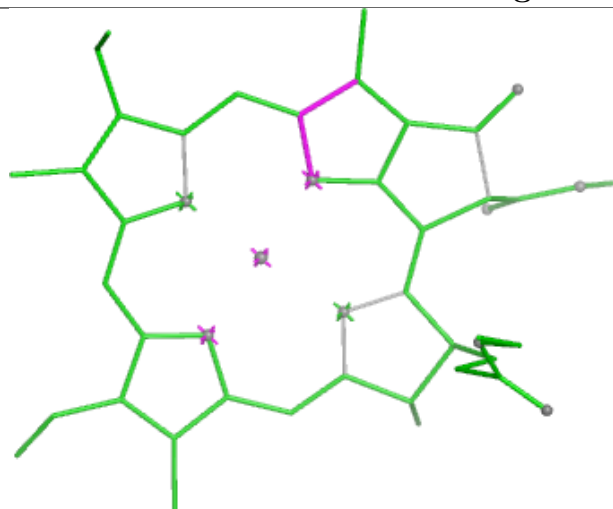
Torsions



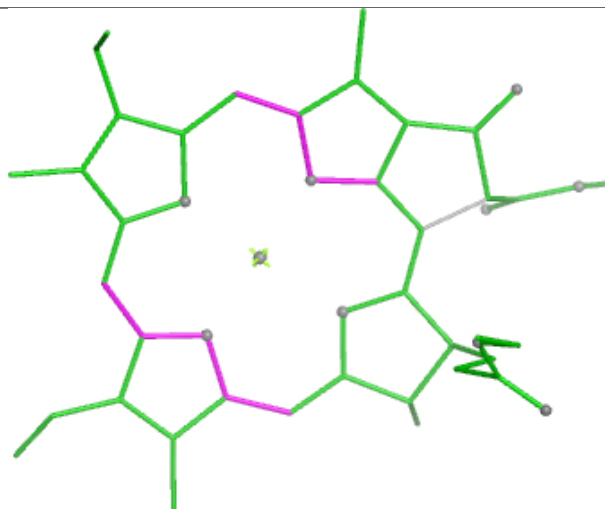
Rings



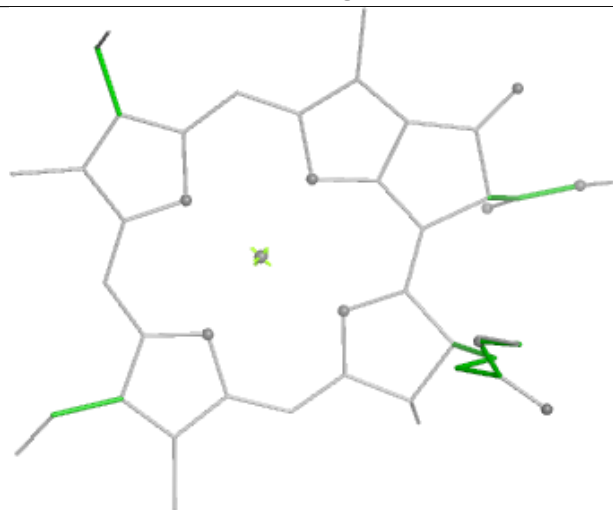
Ligand CLA A 808



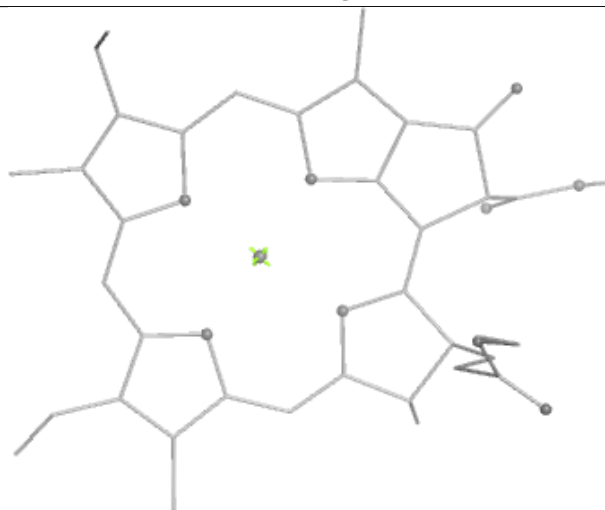
Bond lengths



Bond angles

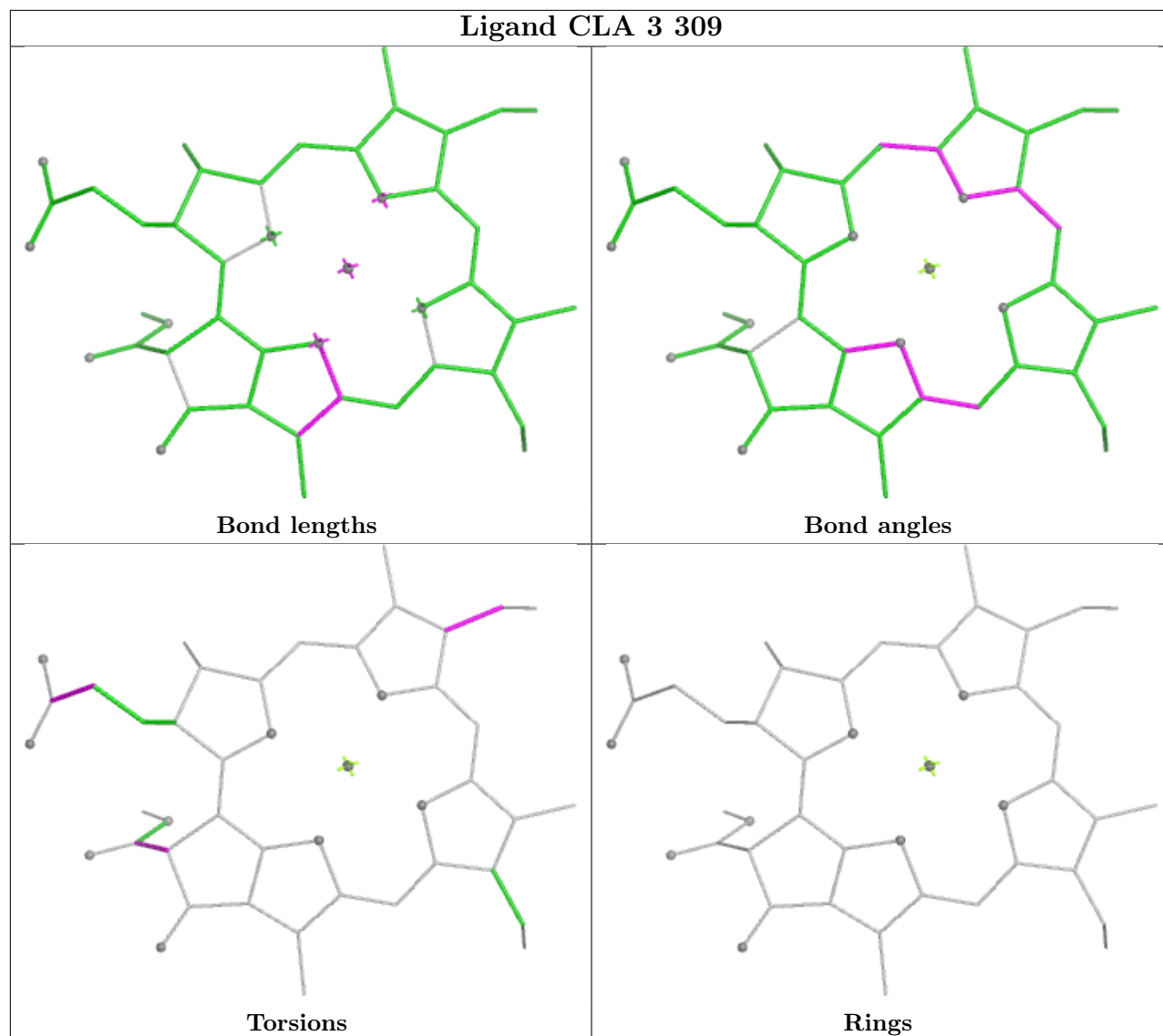


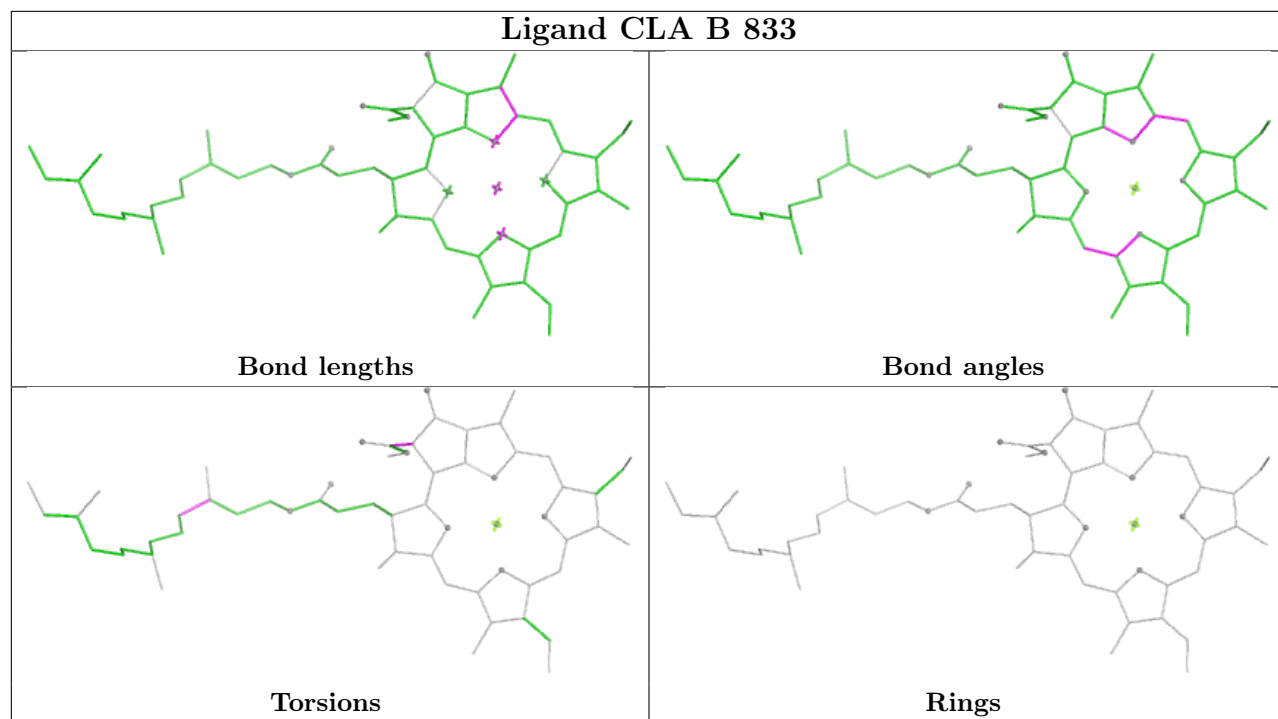
Torsions



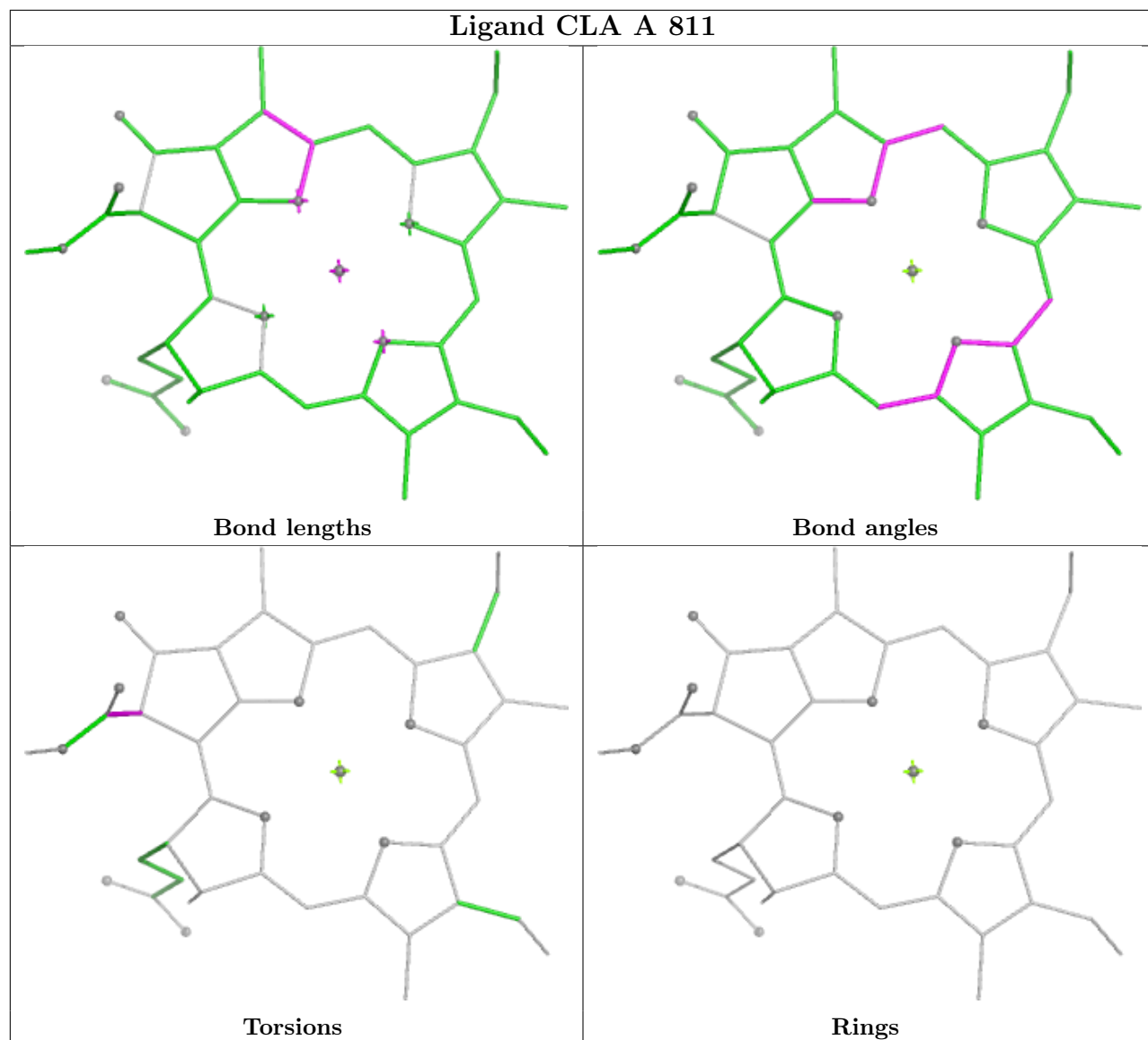
Rings

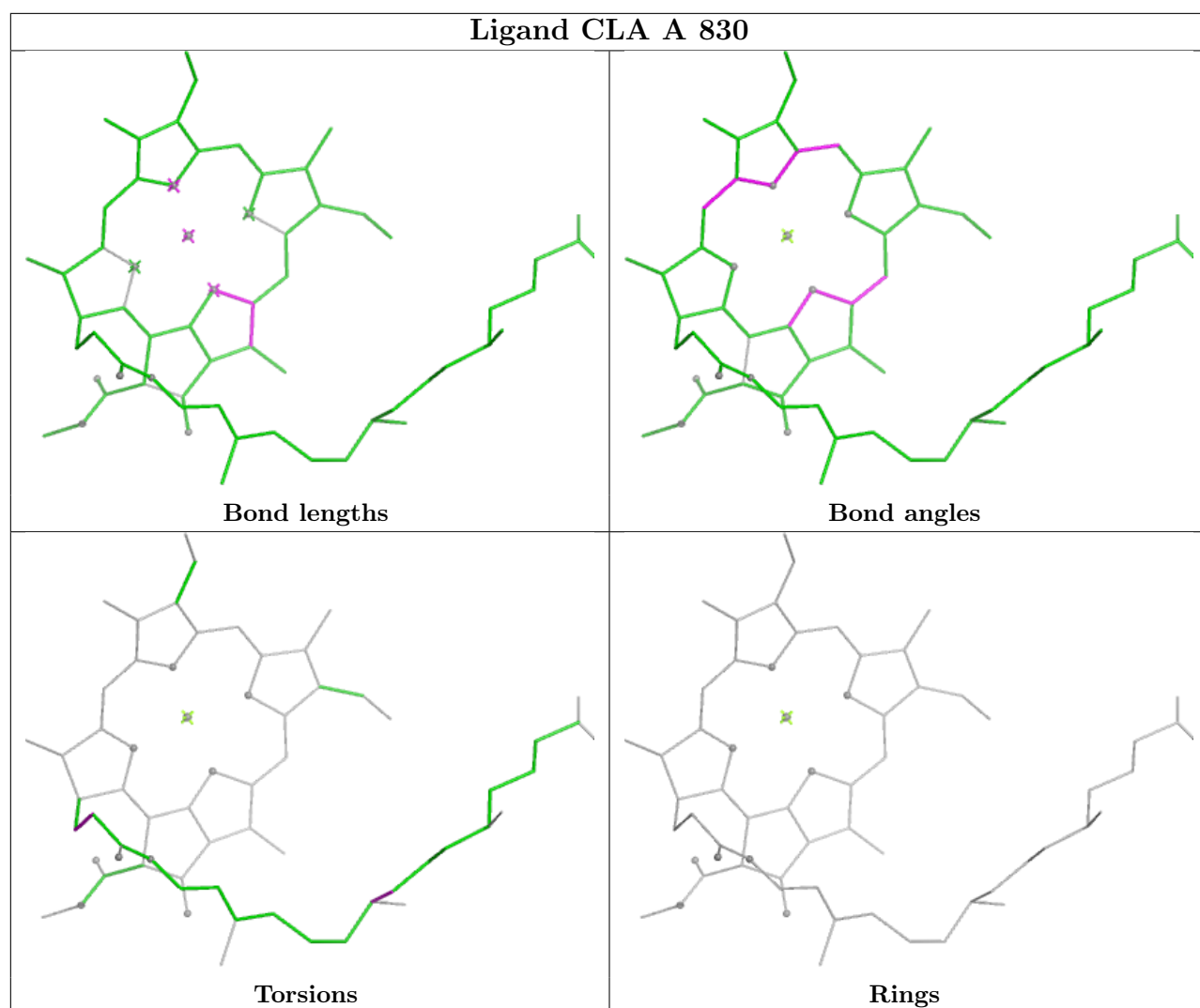
Ligand CLA 3 309

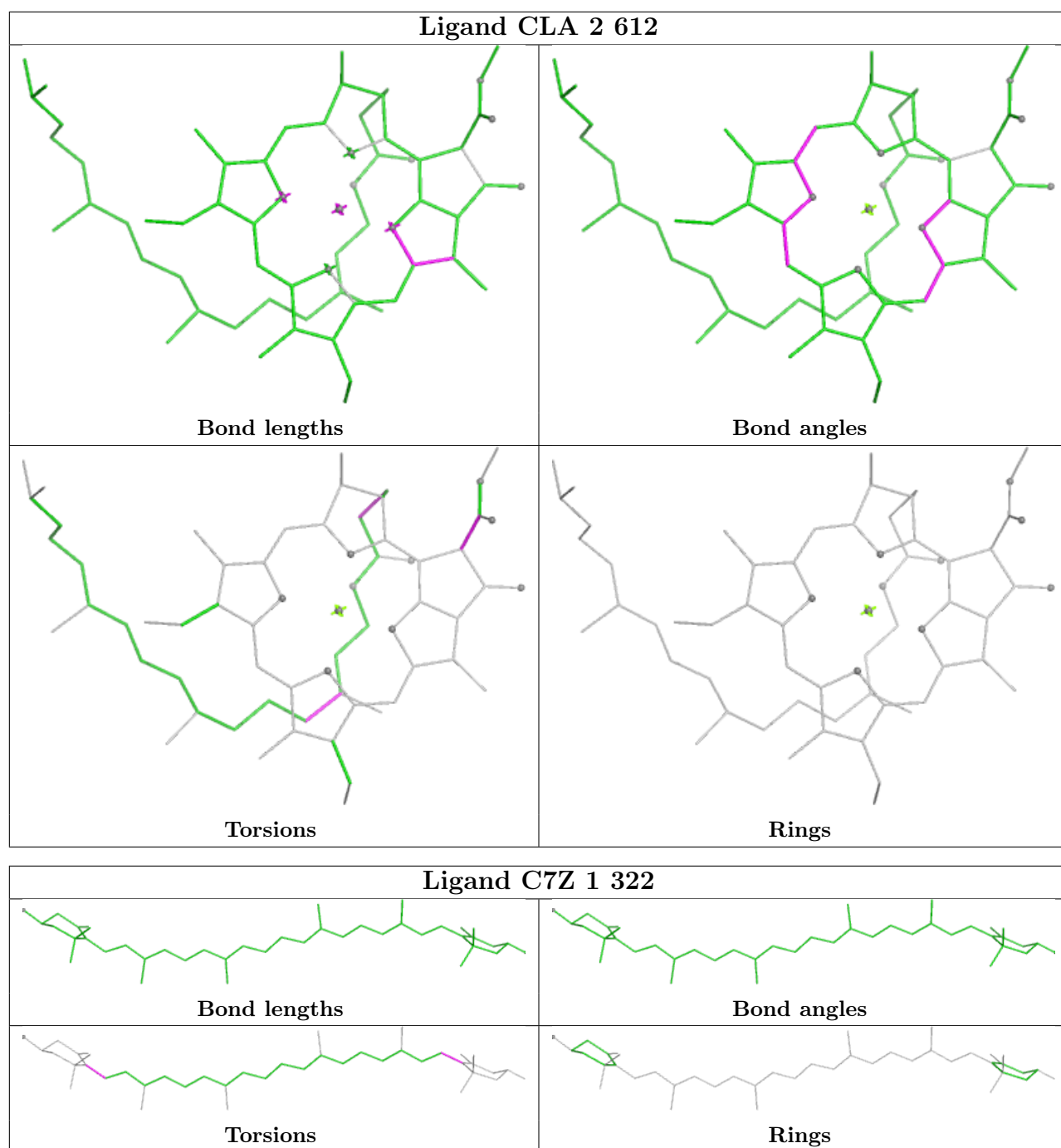


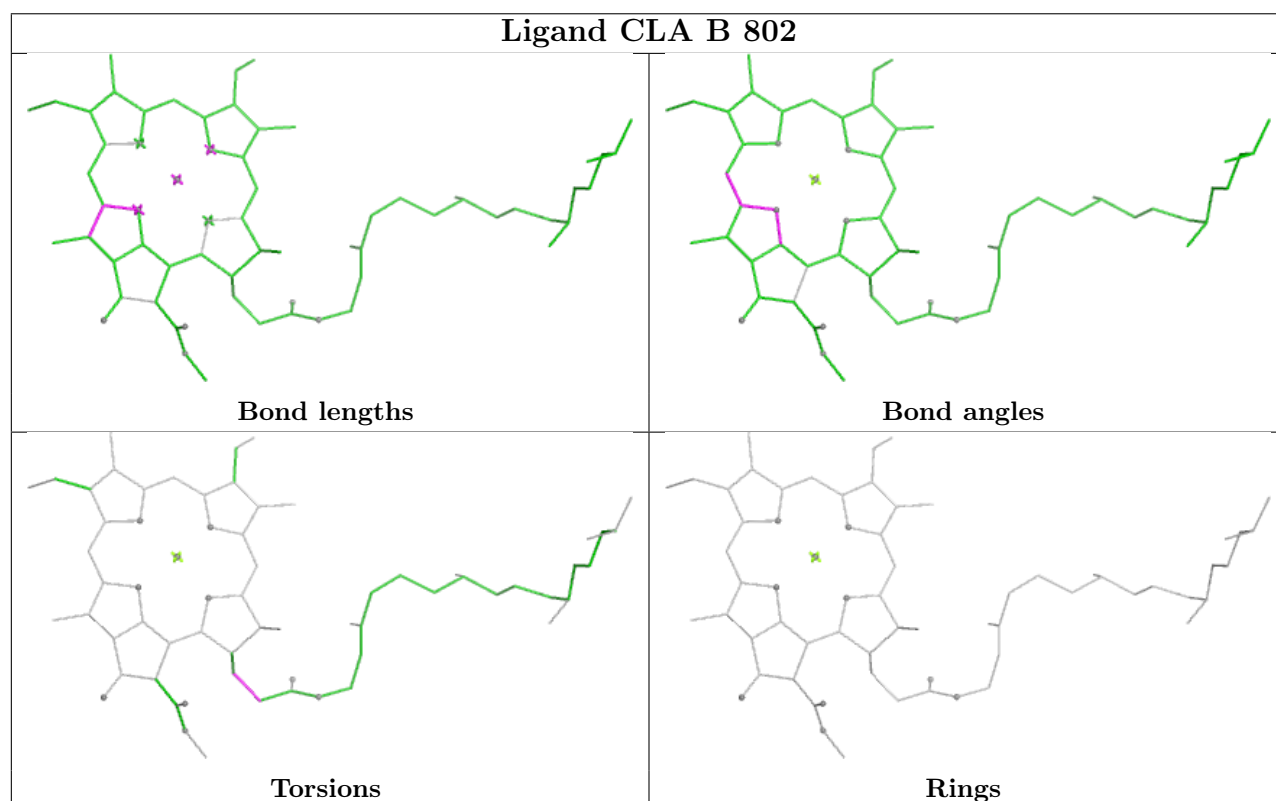
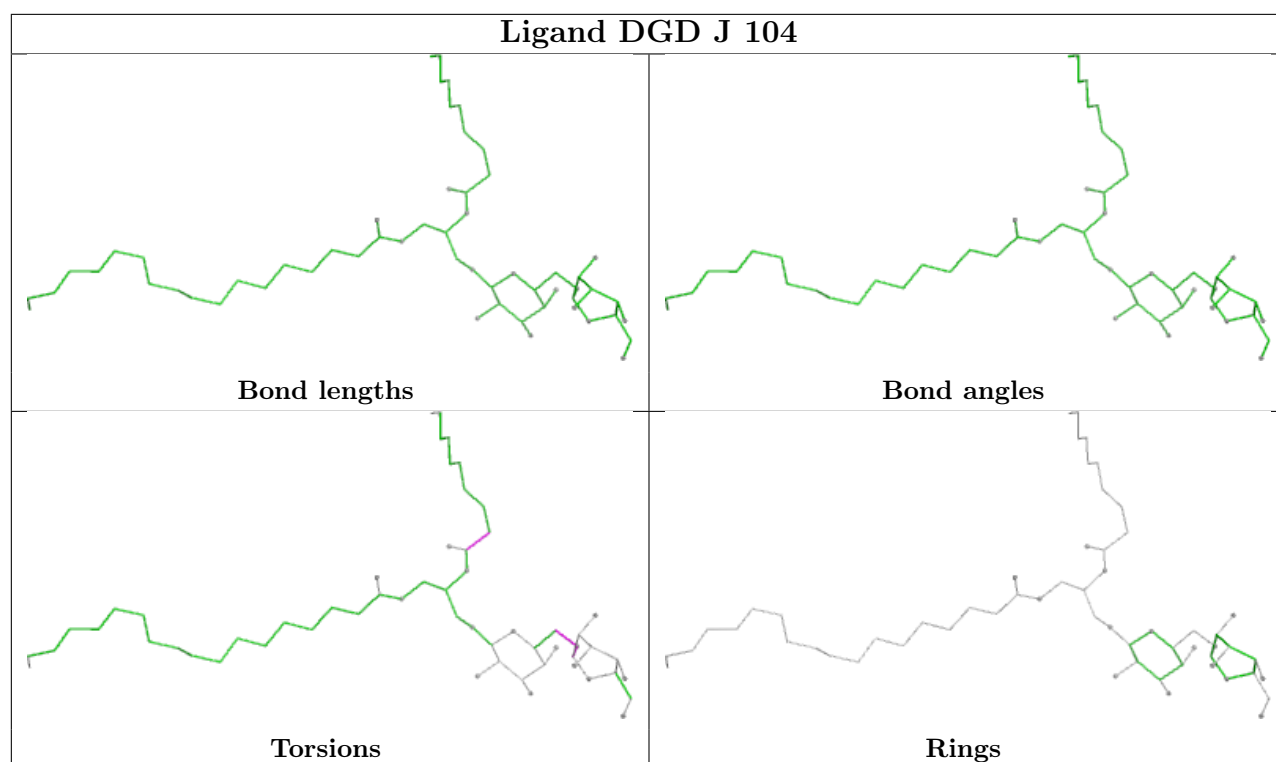


Ligand CLA A 811

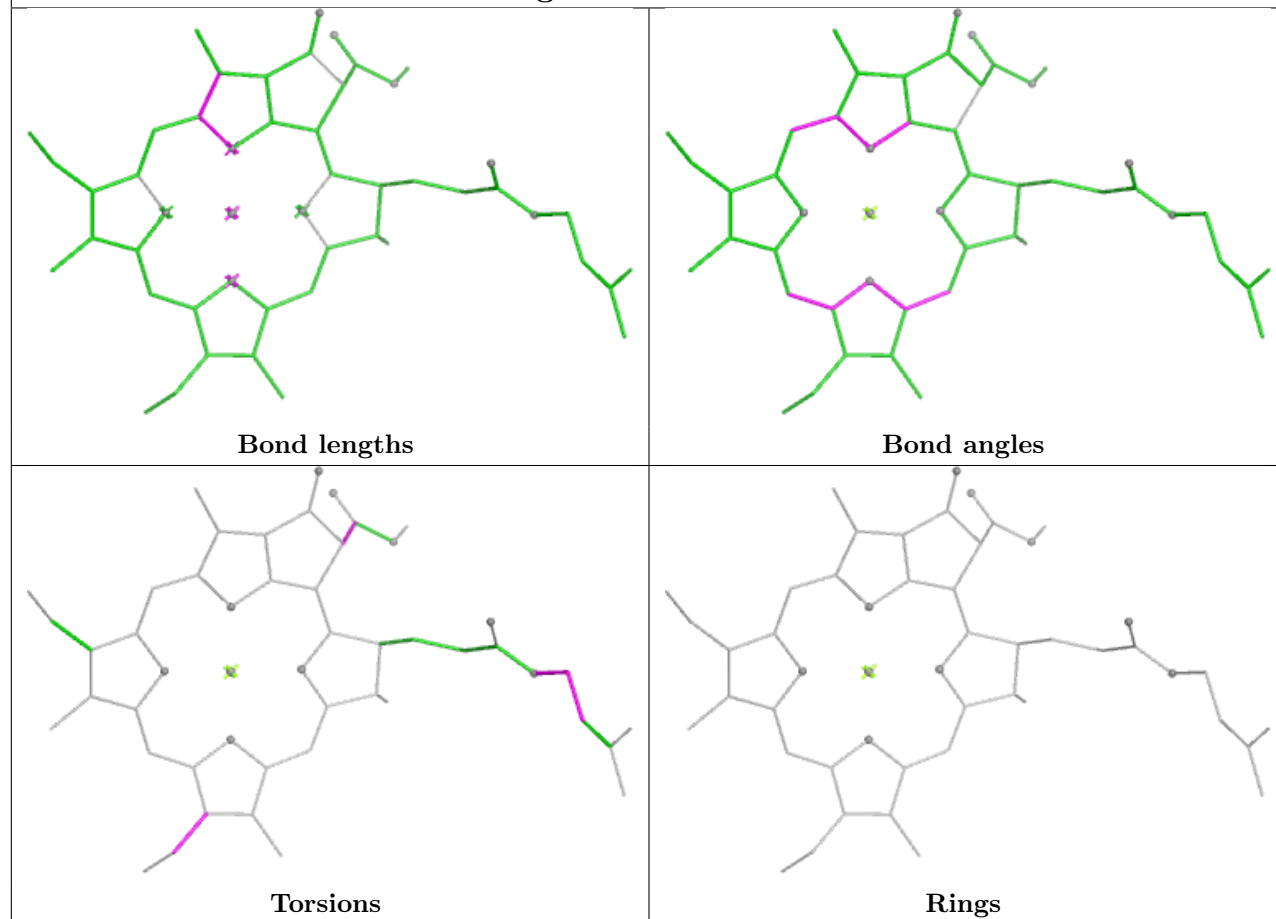




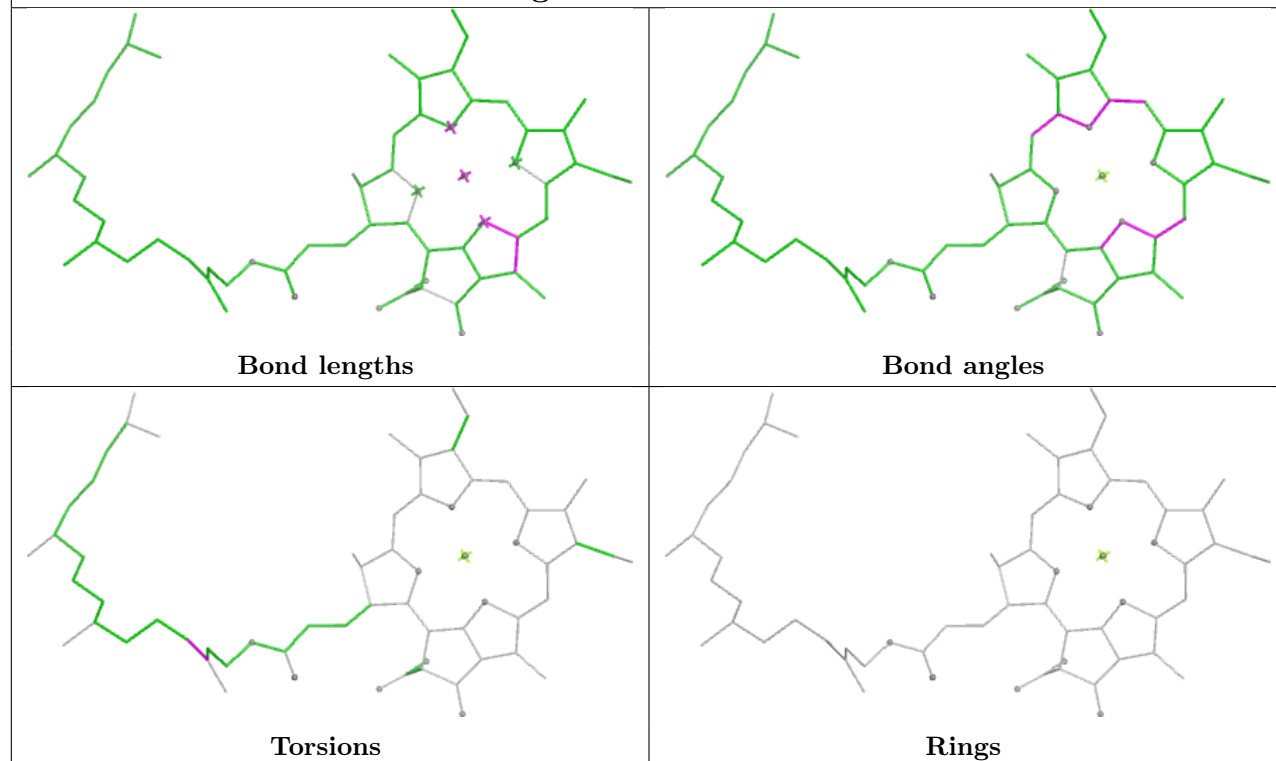


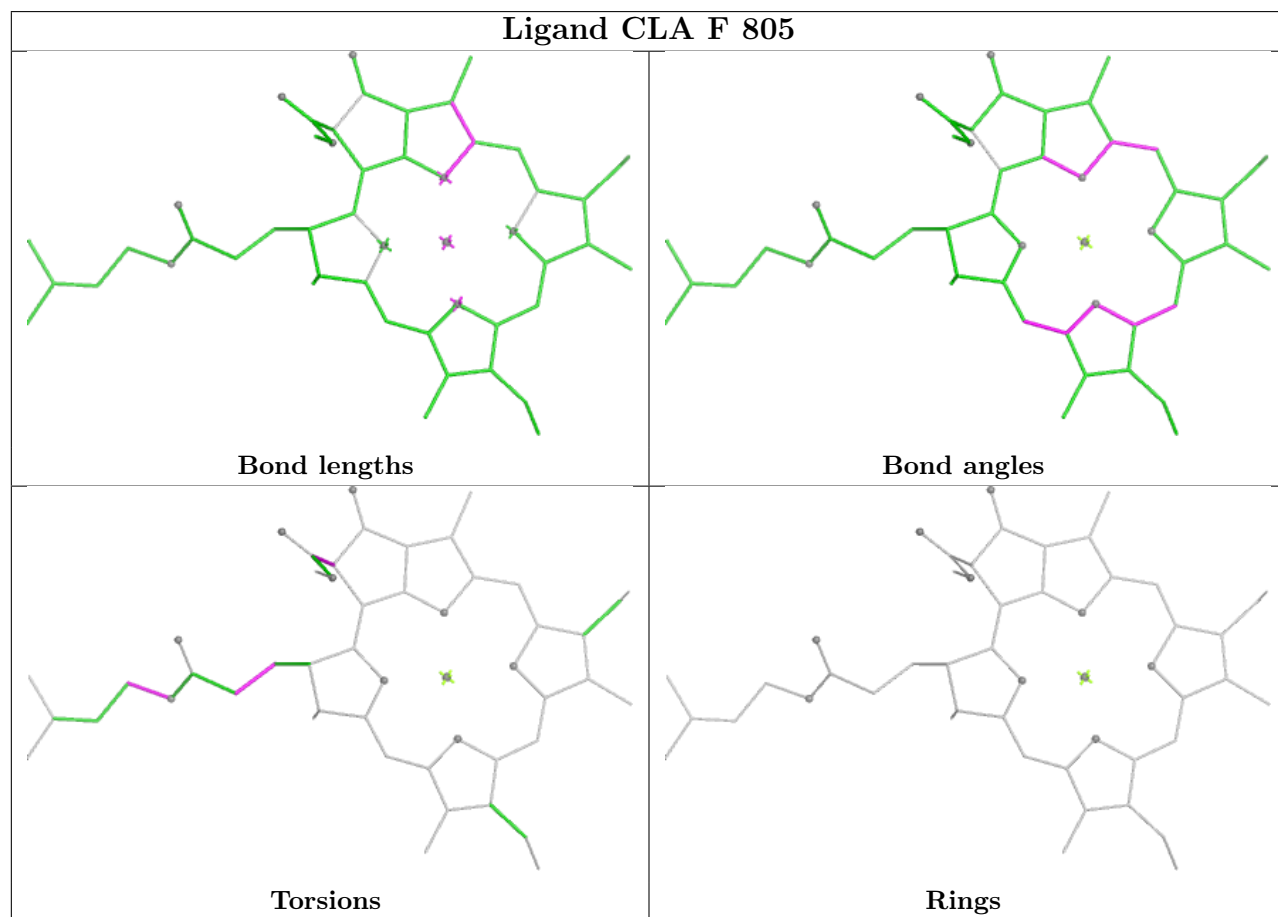
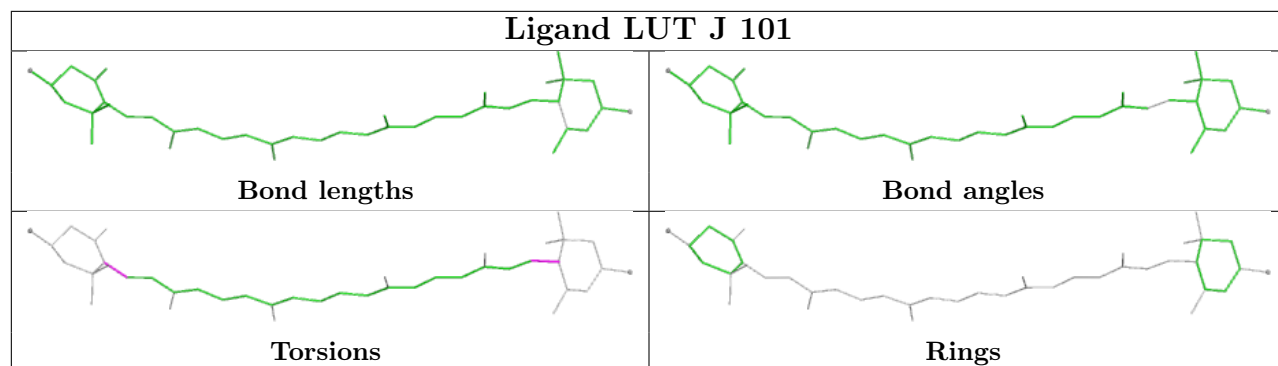


Ligand CLA 4 601

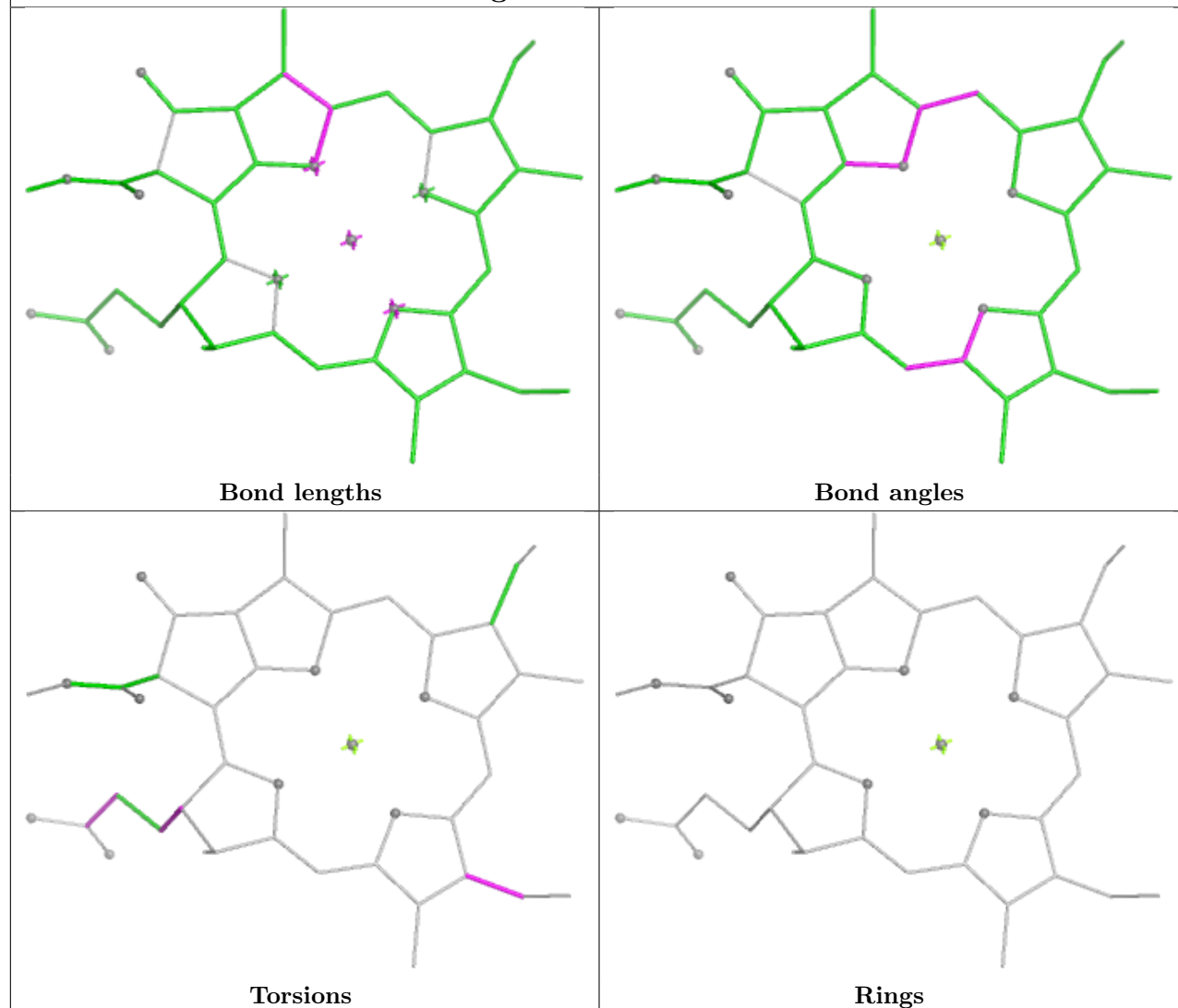


Ligand CLA A 828

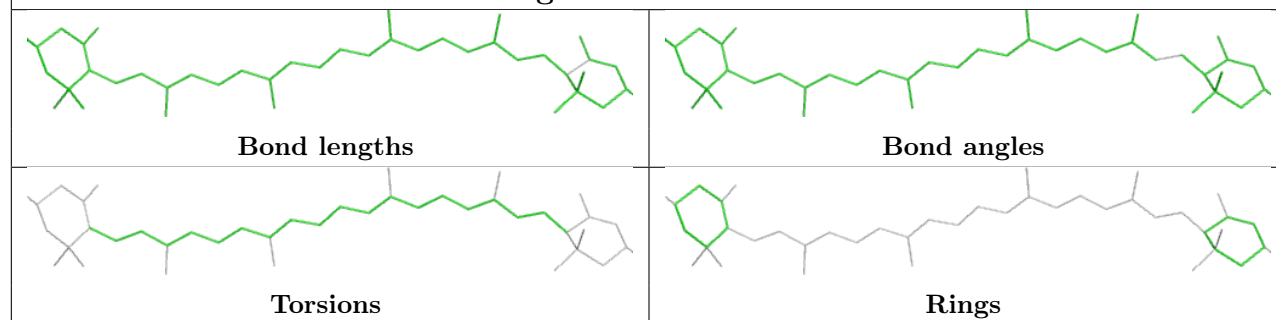




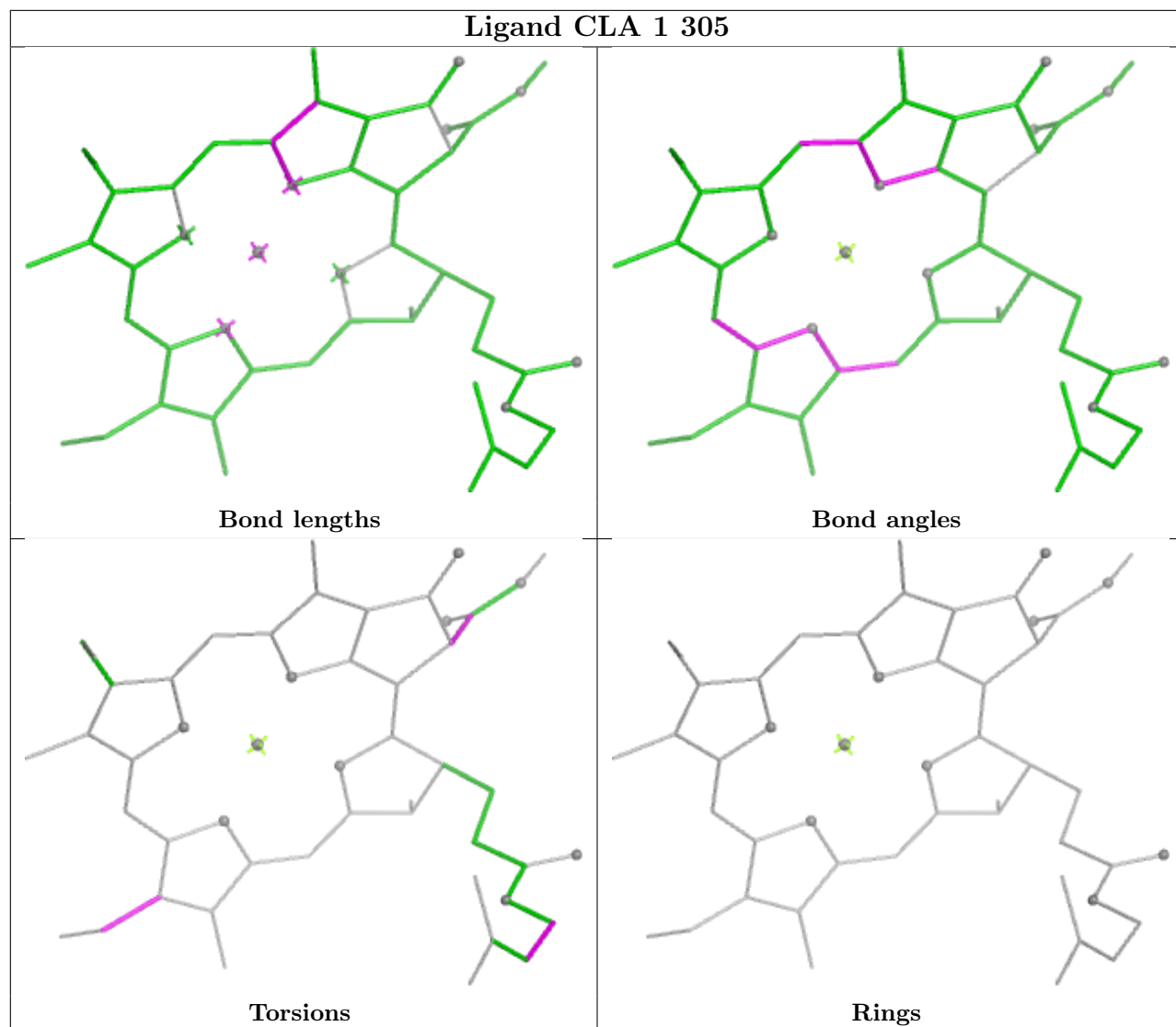
Ligand CLA A 856

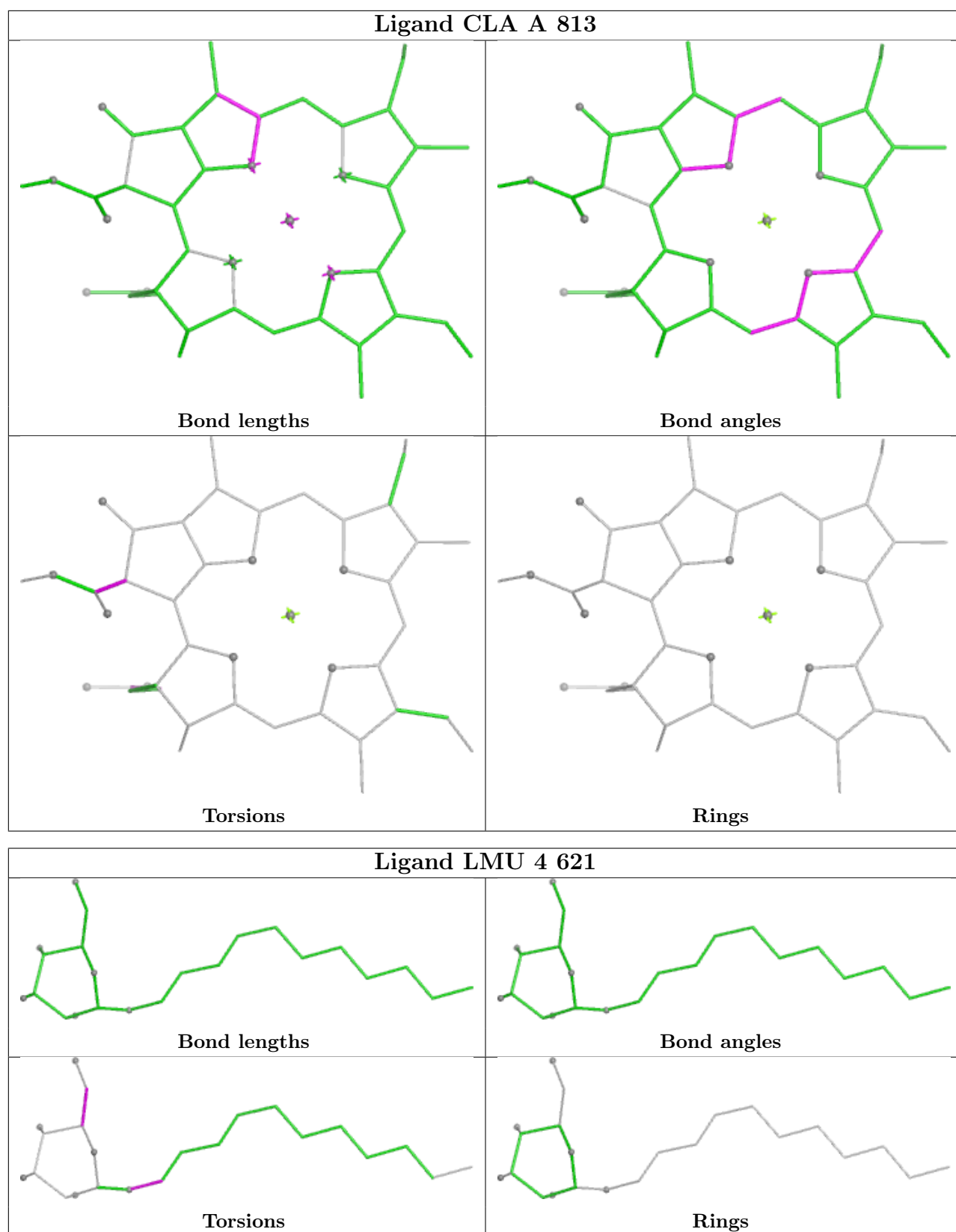


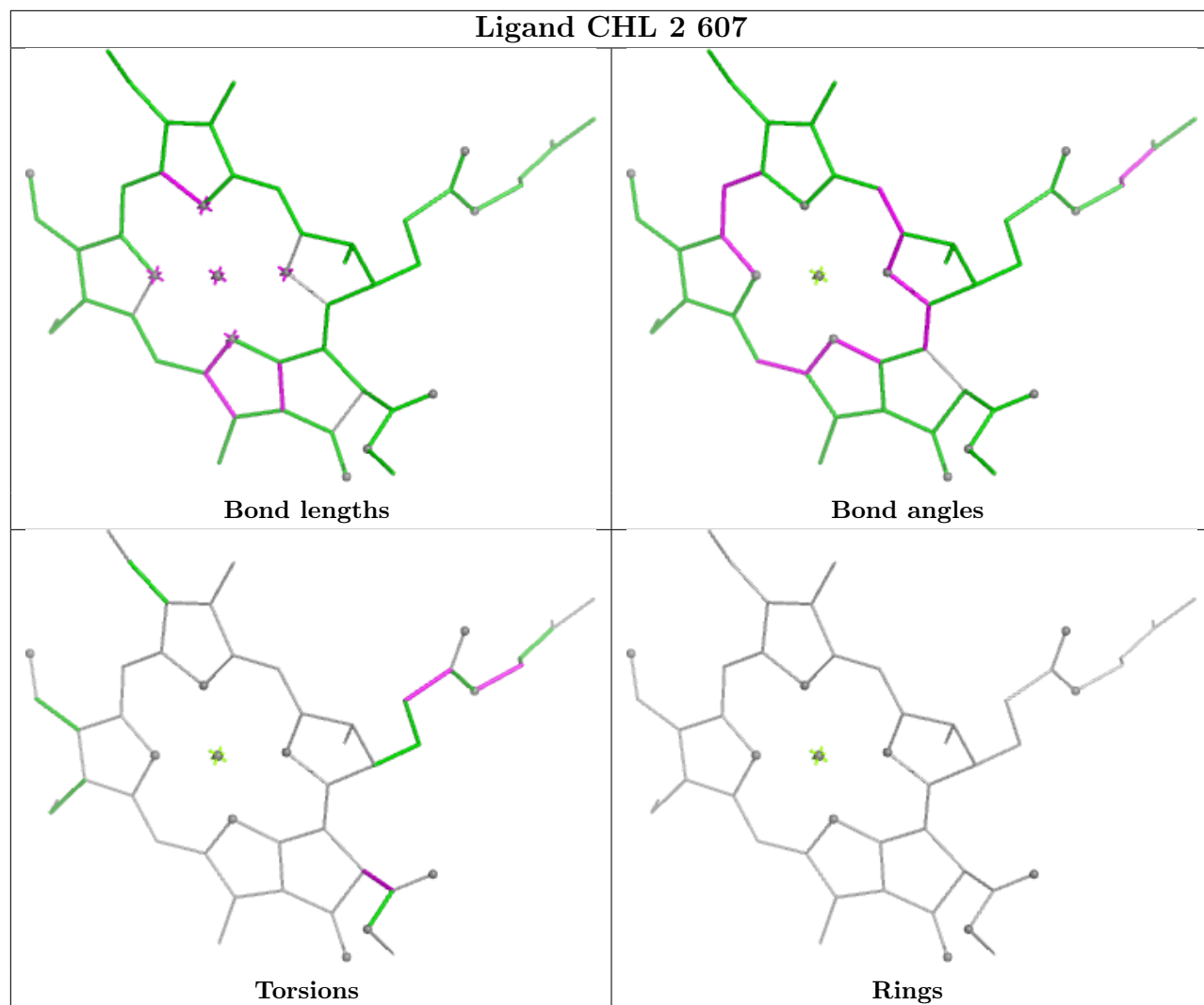
Ligand LUT 3 315

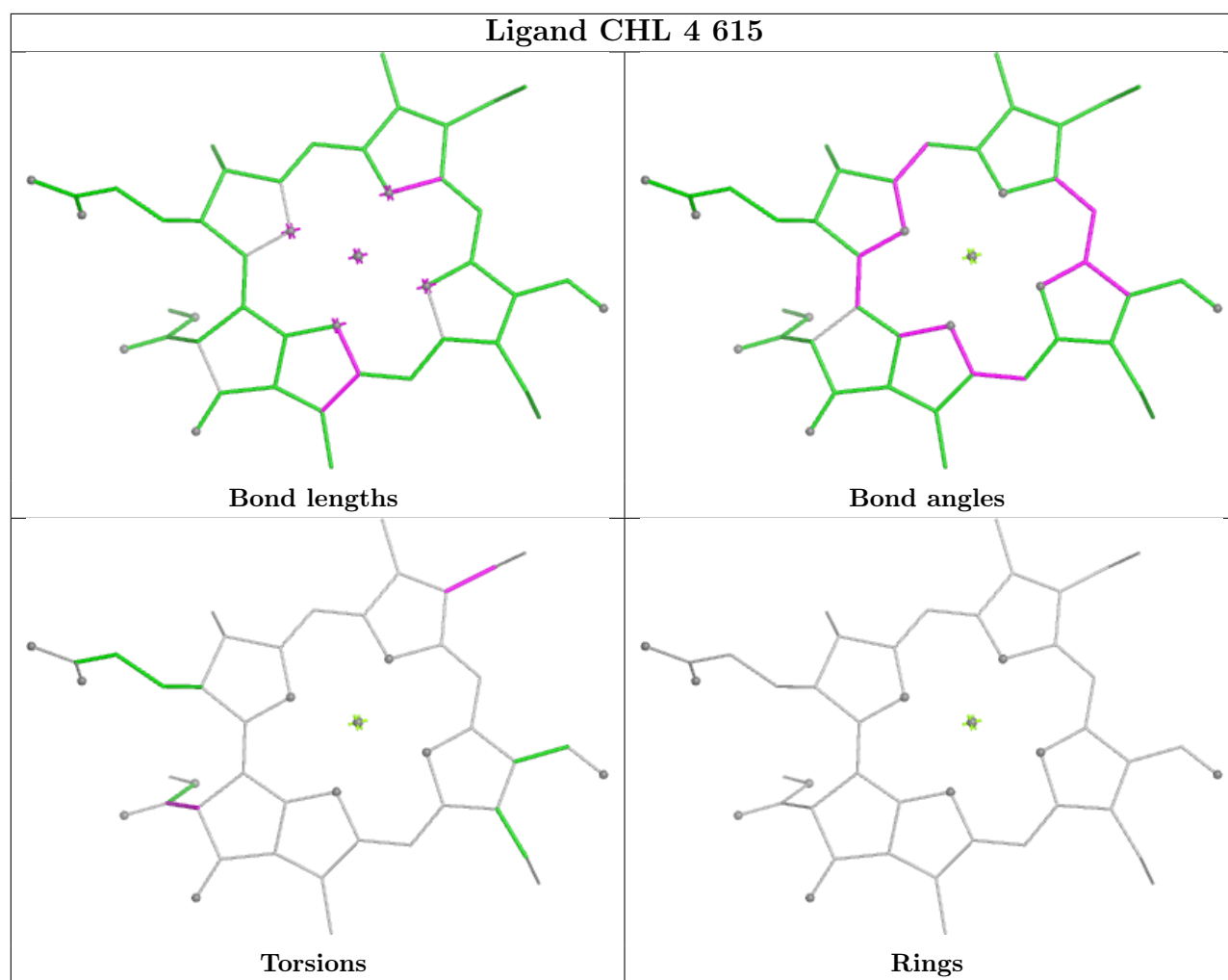


Ligand CLA 1 305

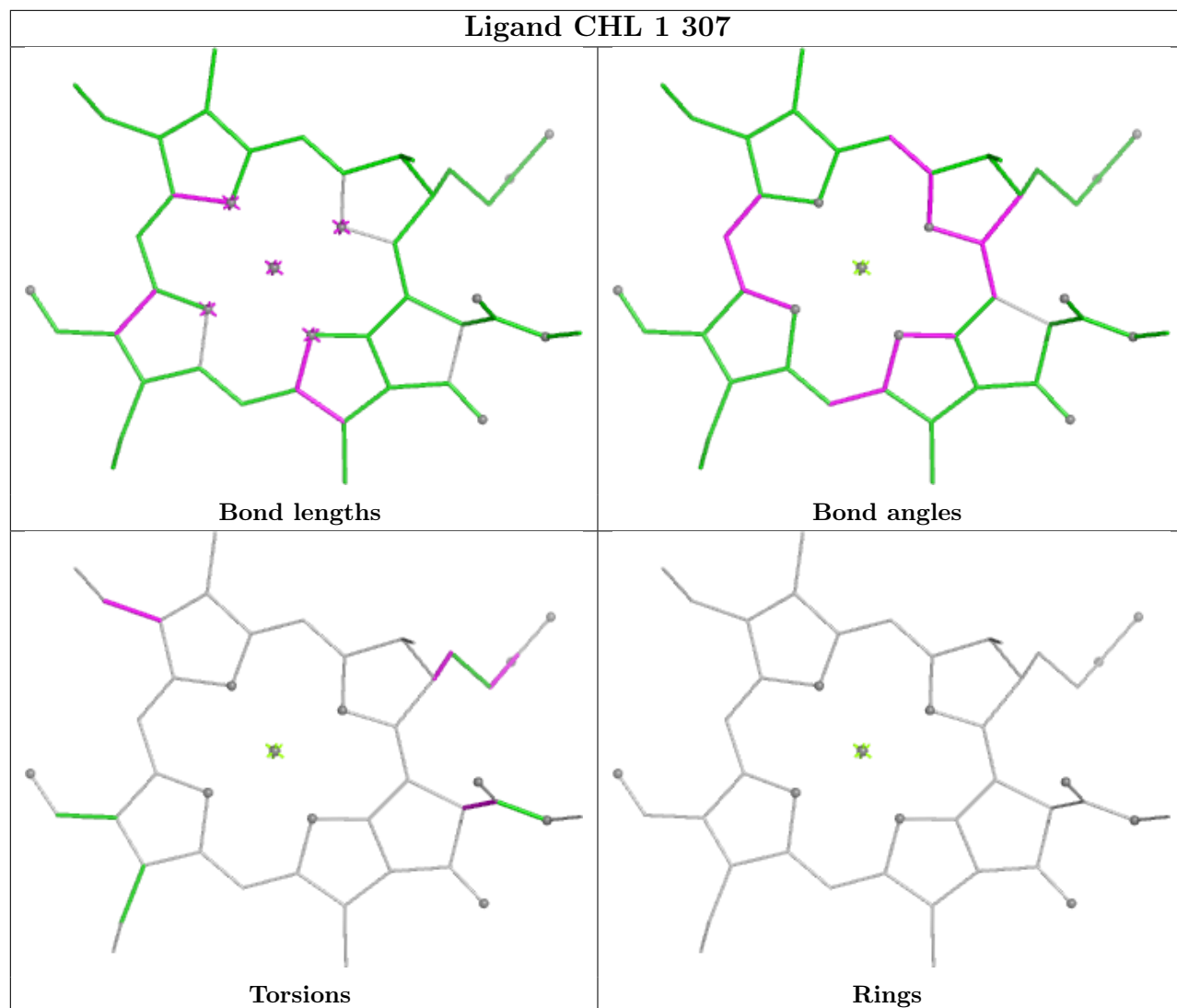




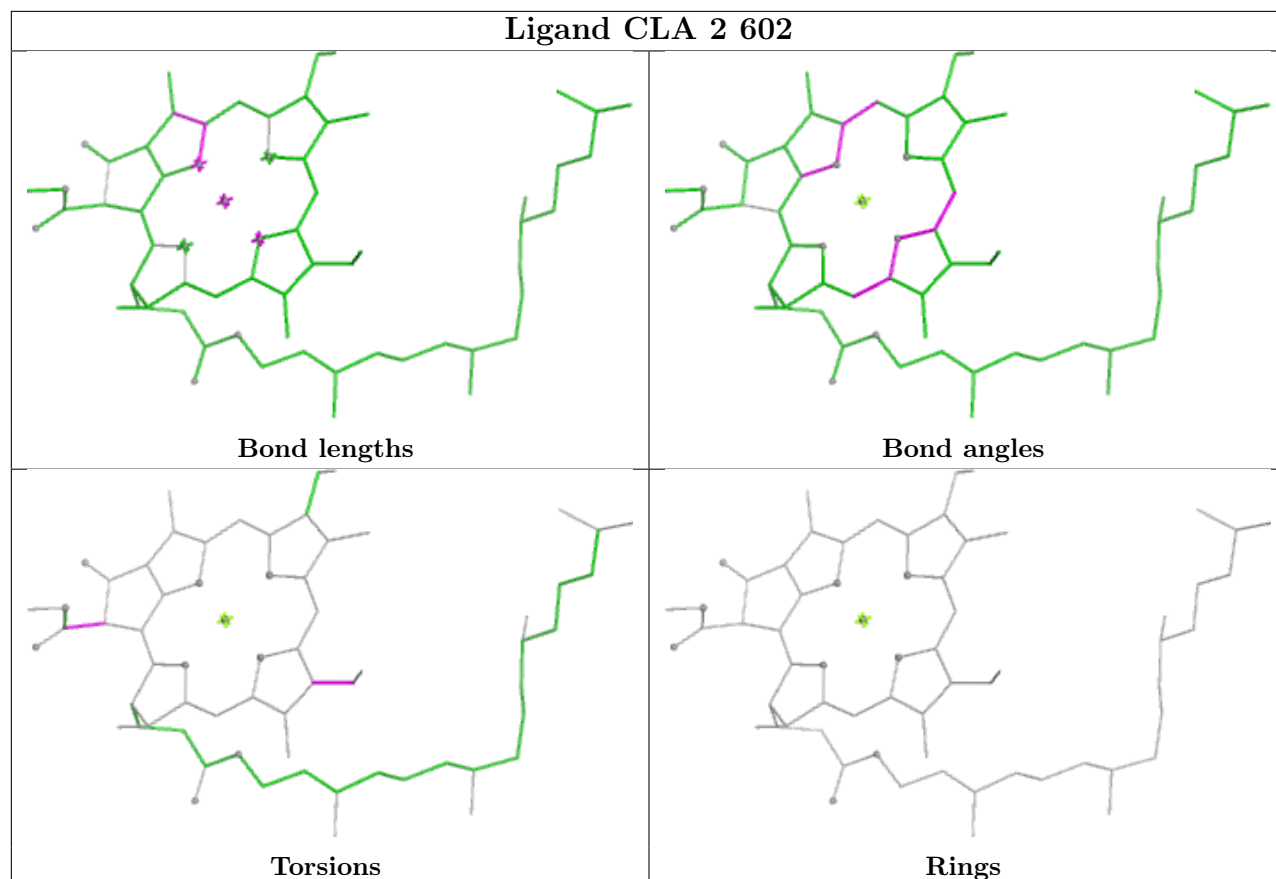




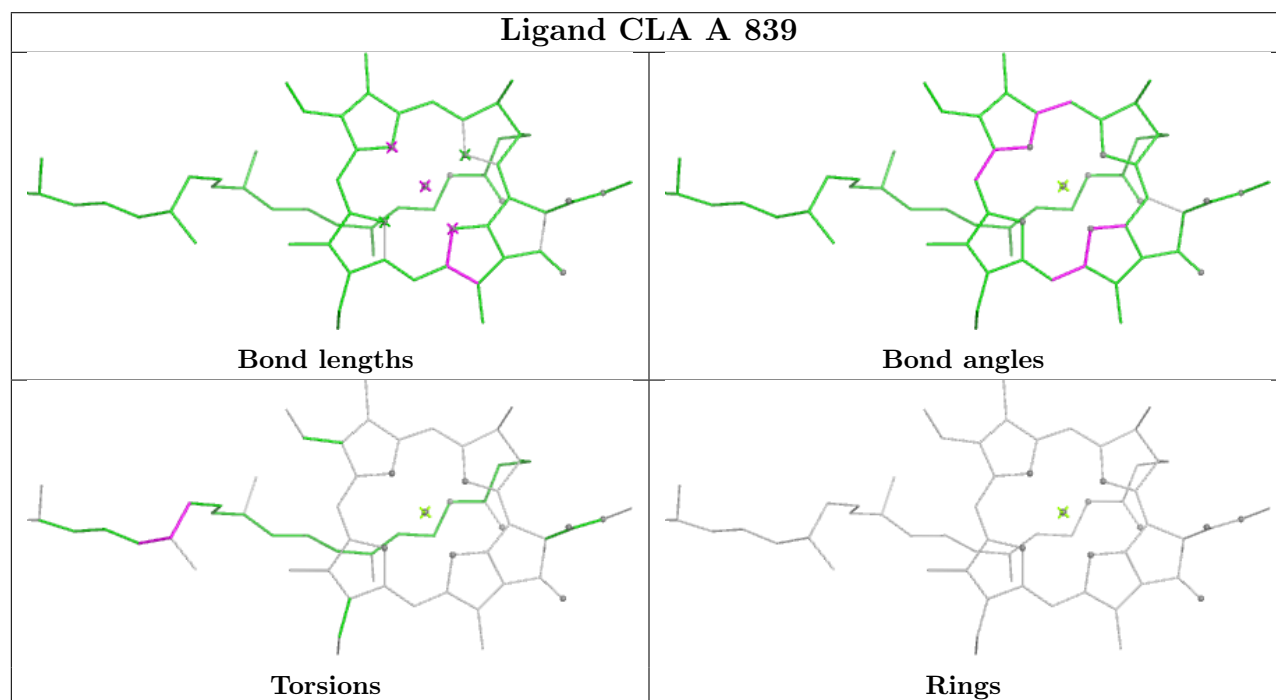
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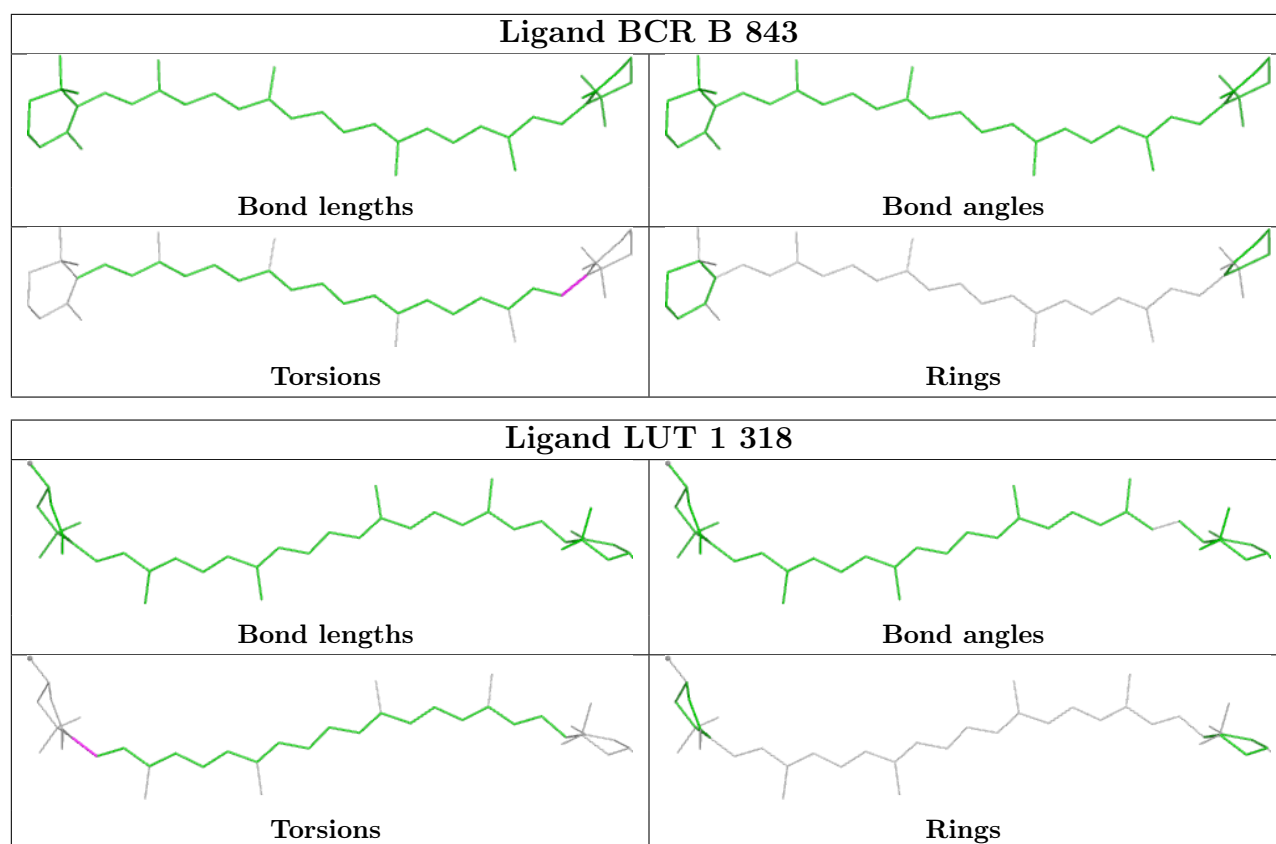


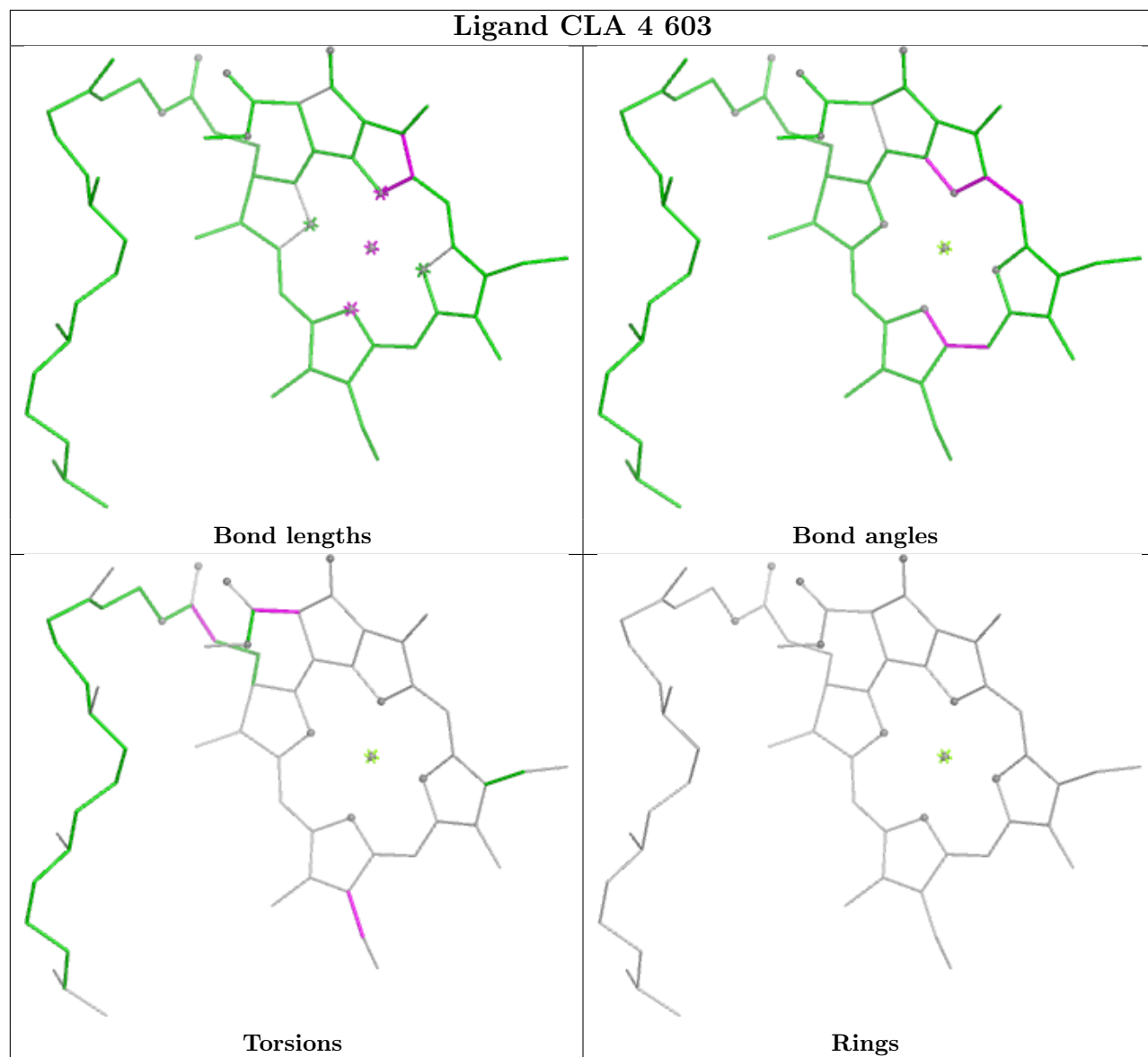
Ligand CLA 2 602

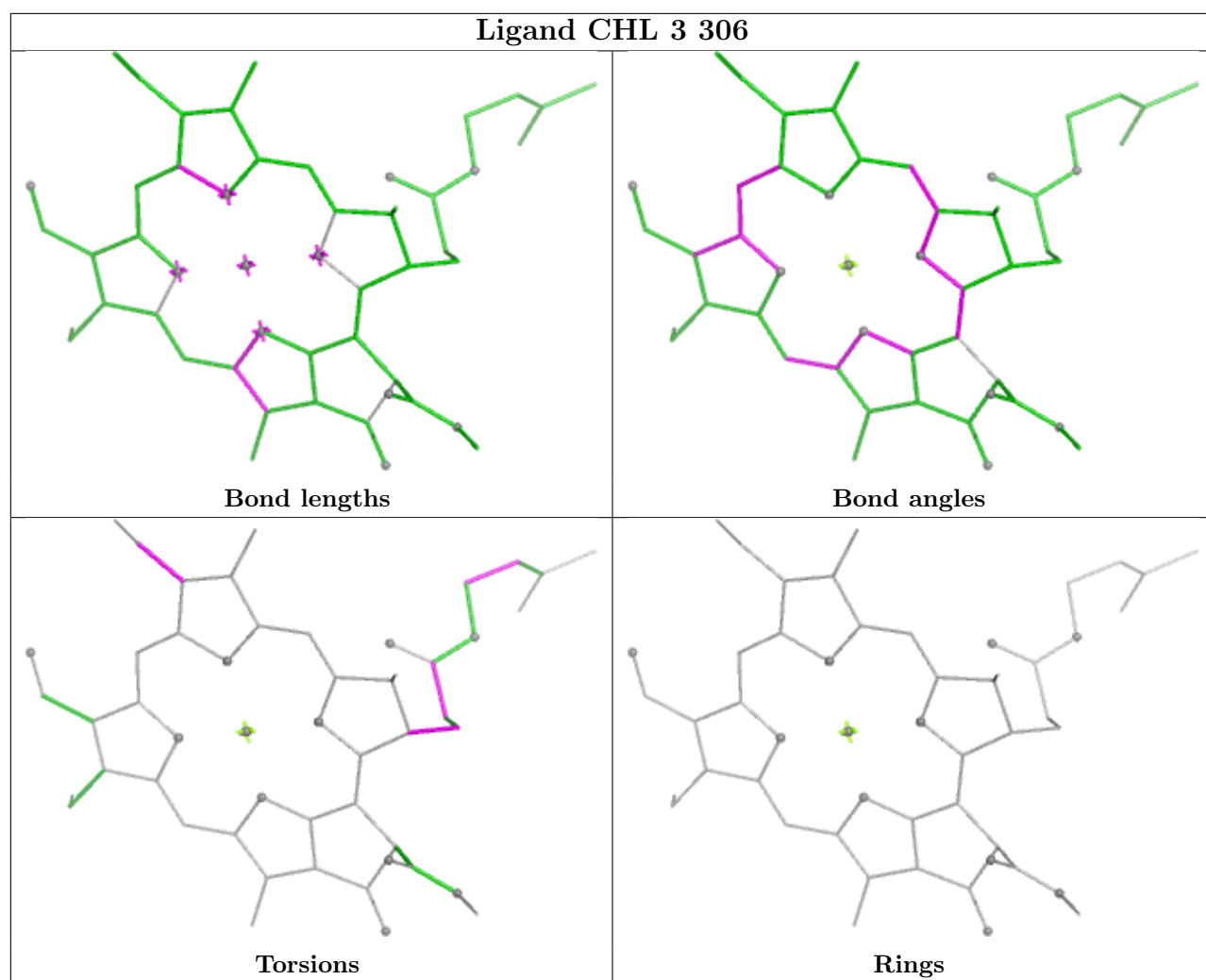


Ligand CLA A 839

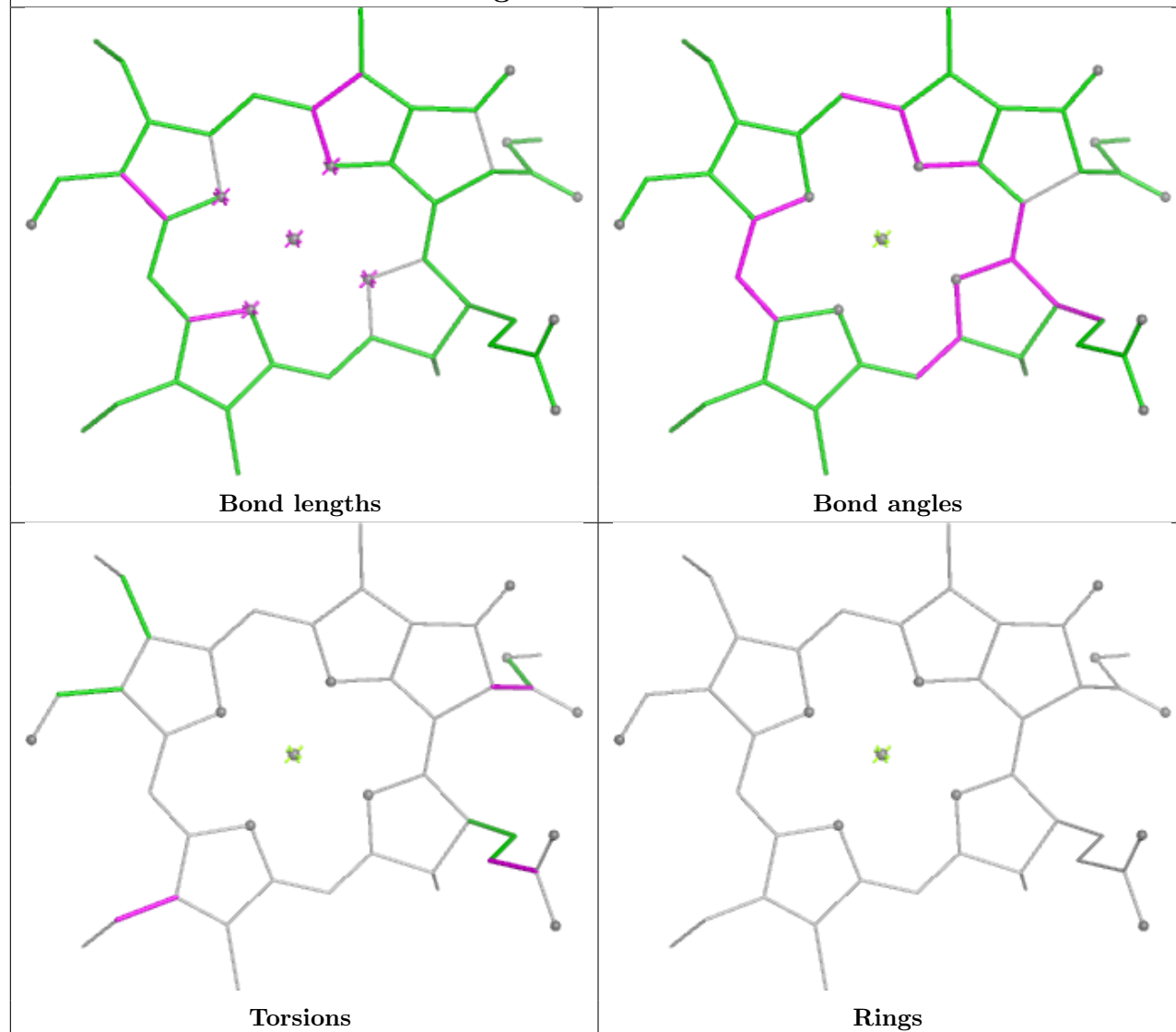




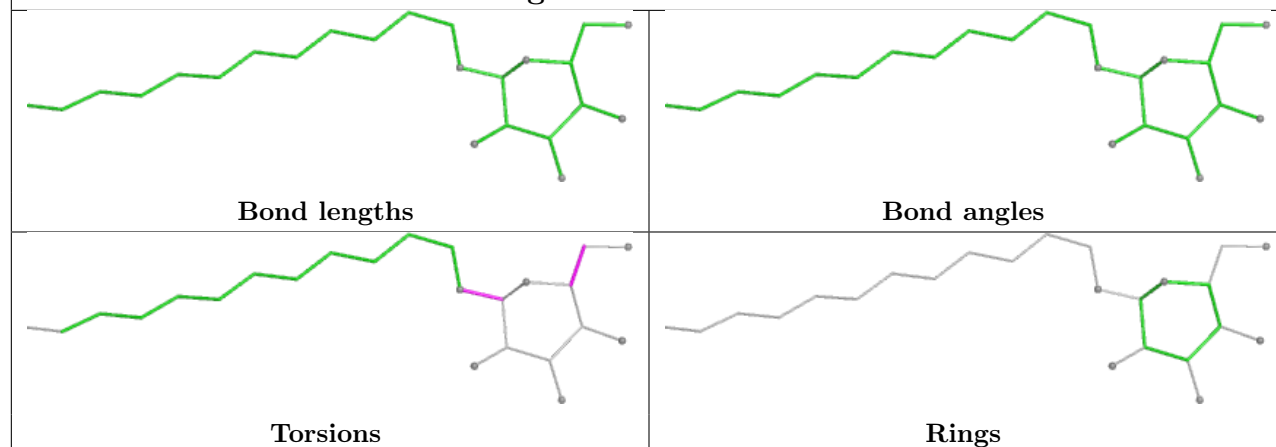




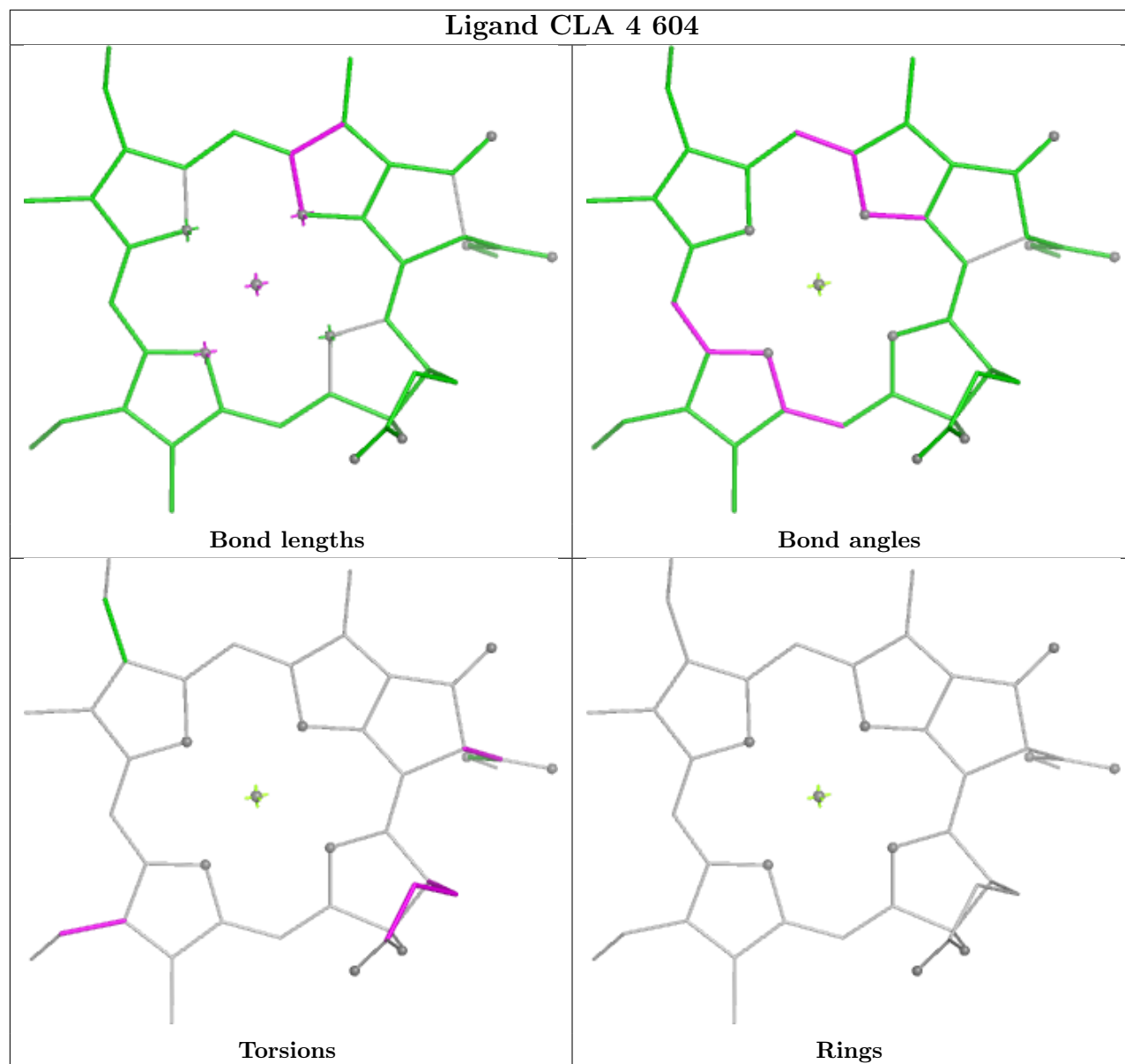
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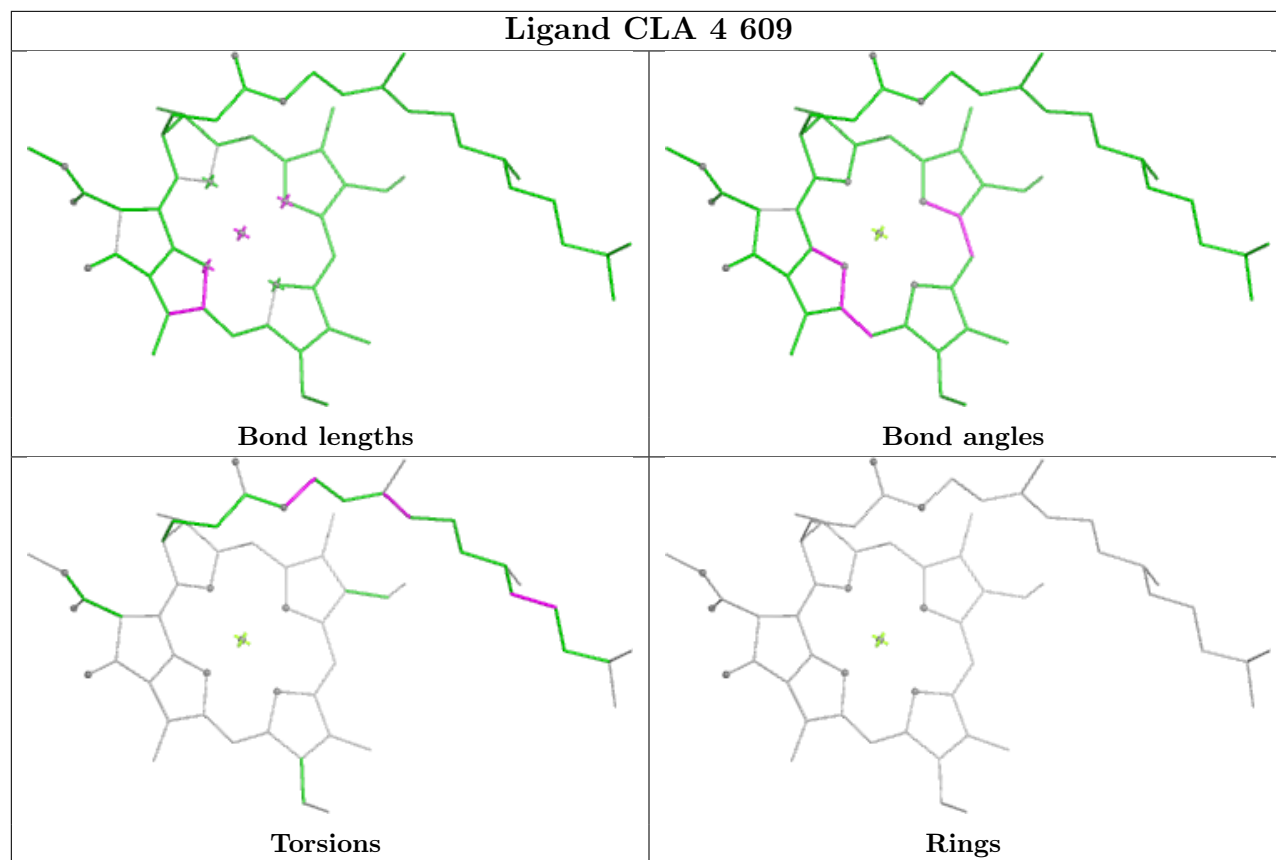


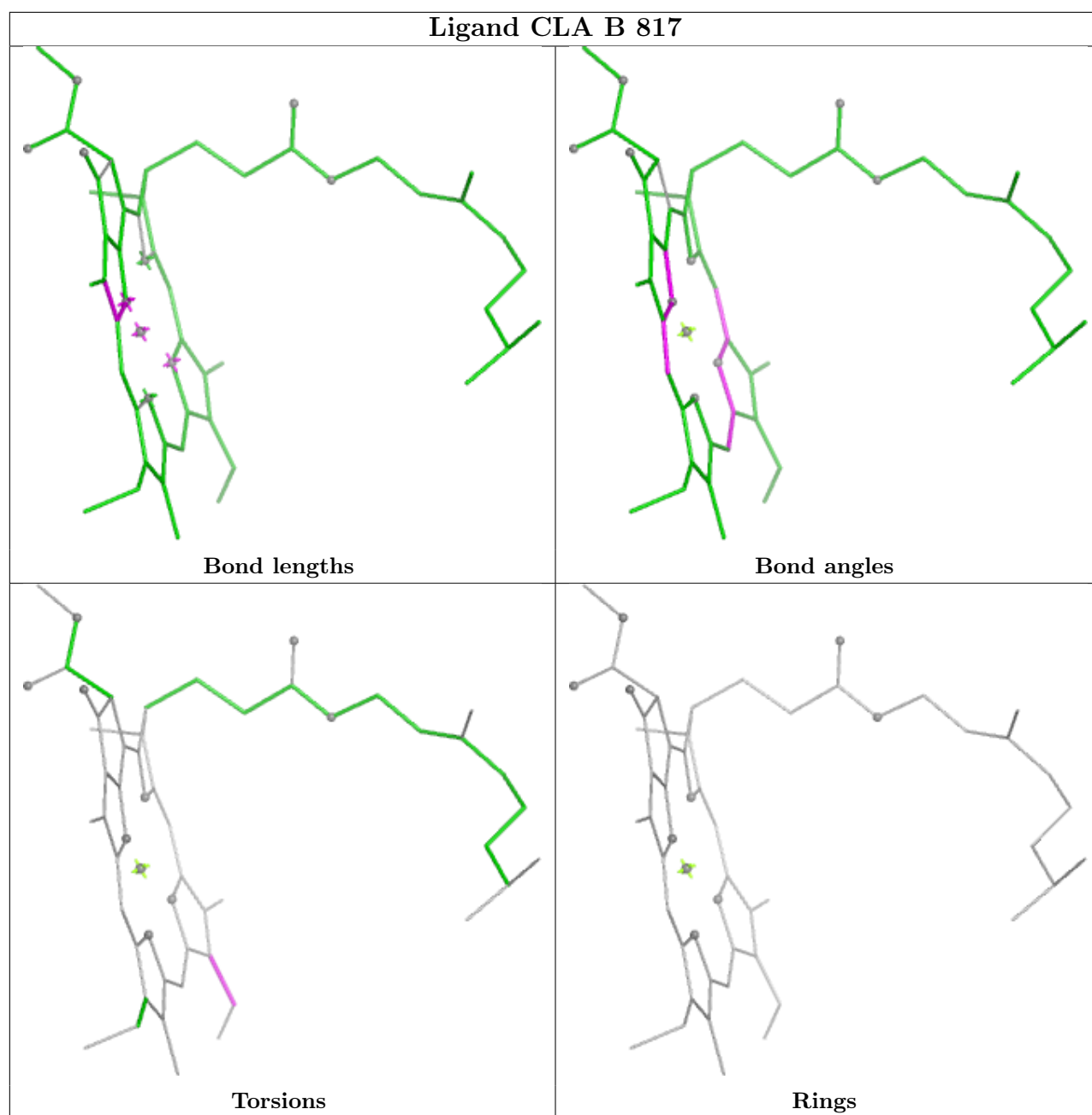
Ligand LMU A 858

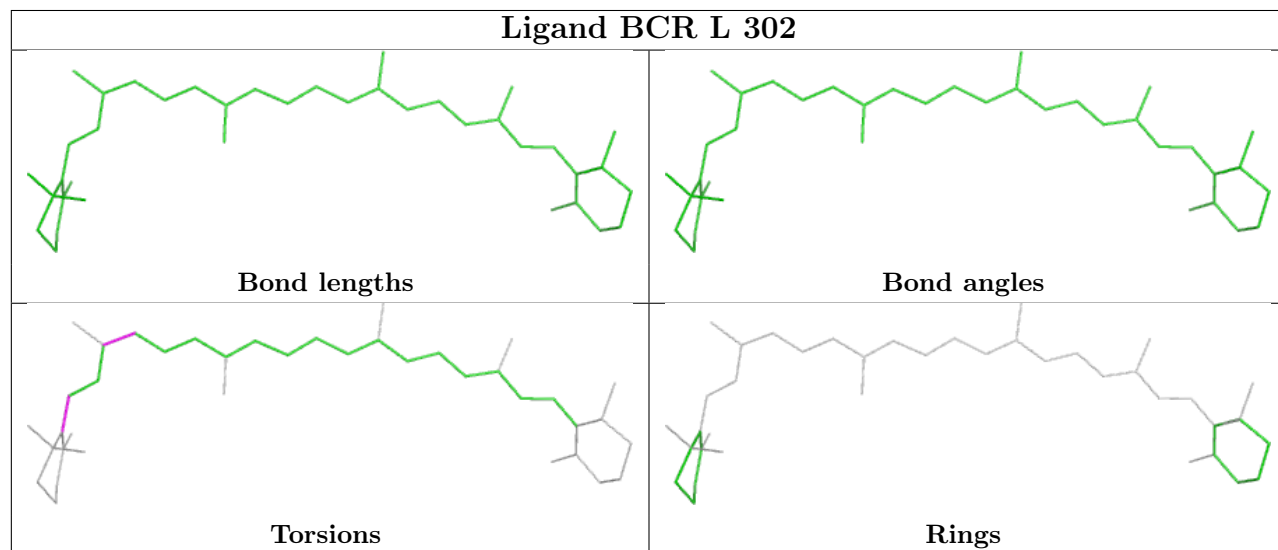
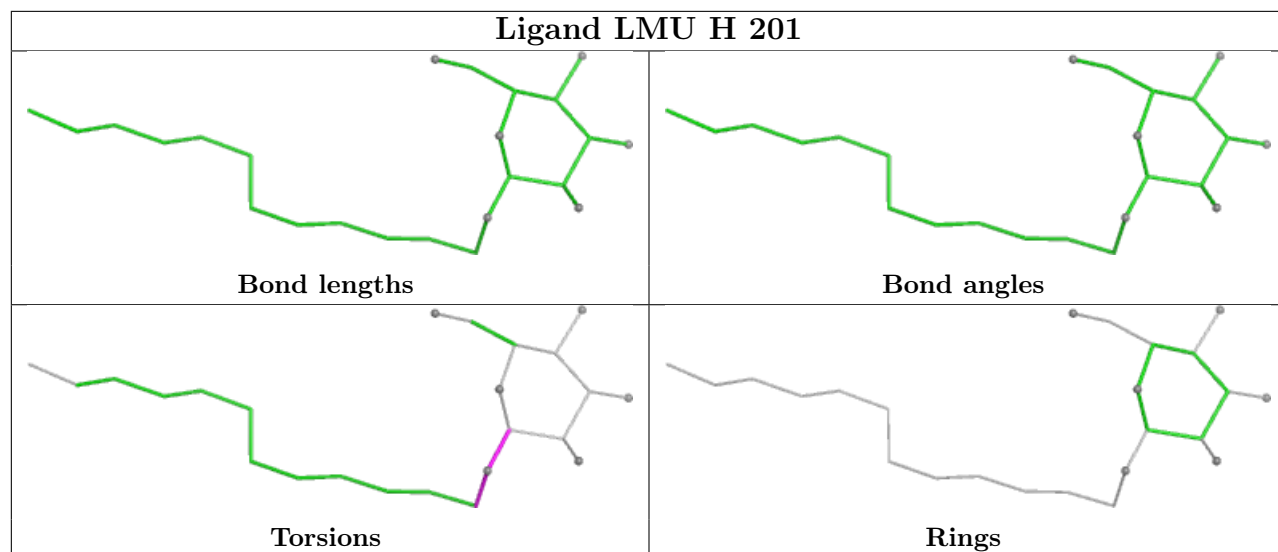


Ligand CLA 4 604

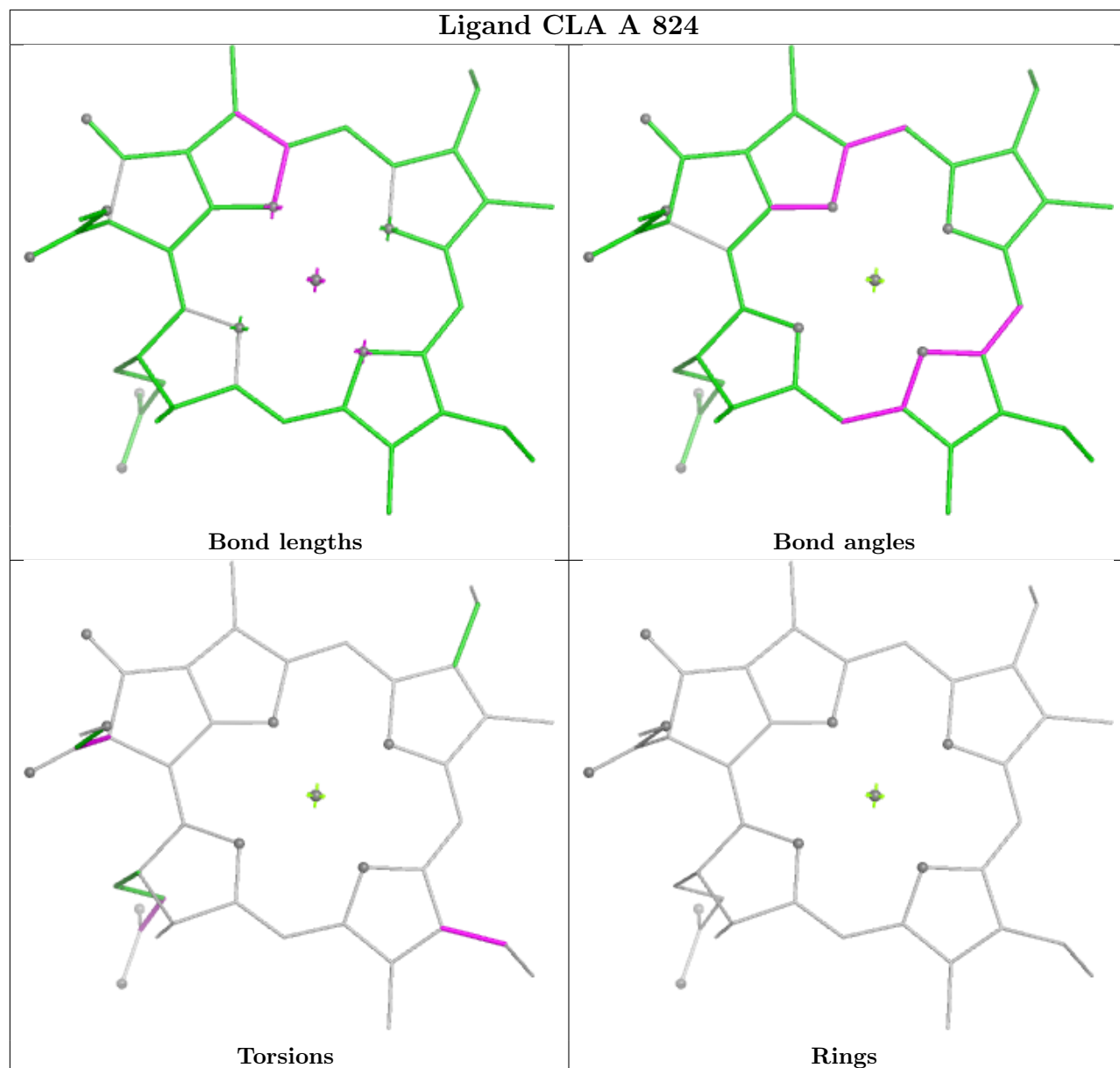


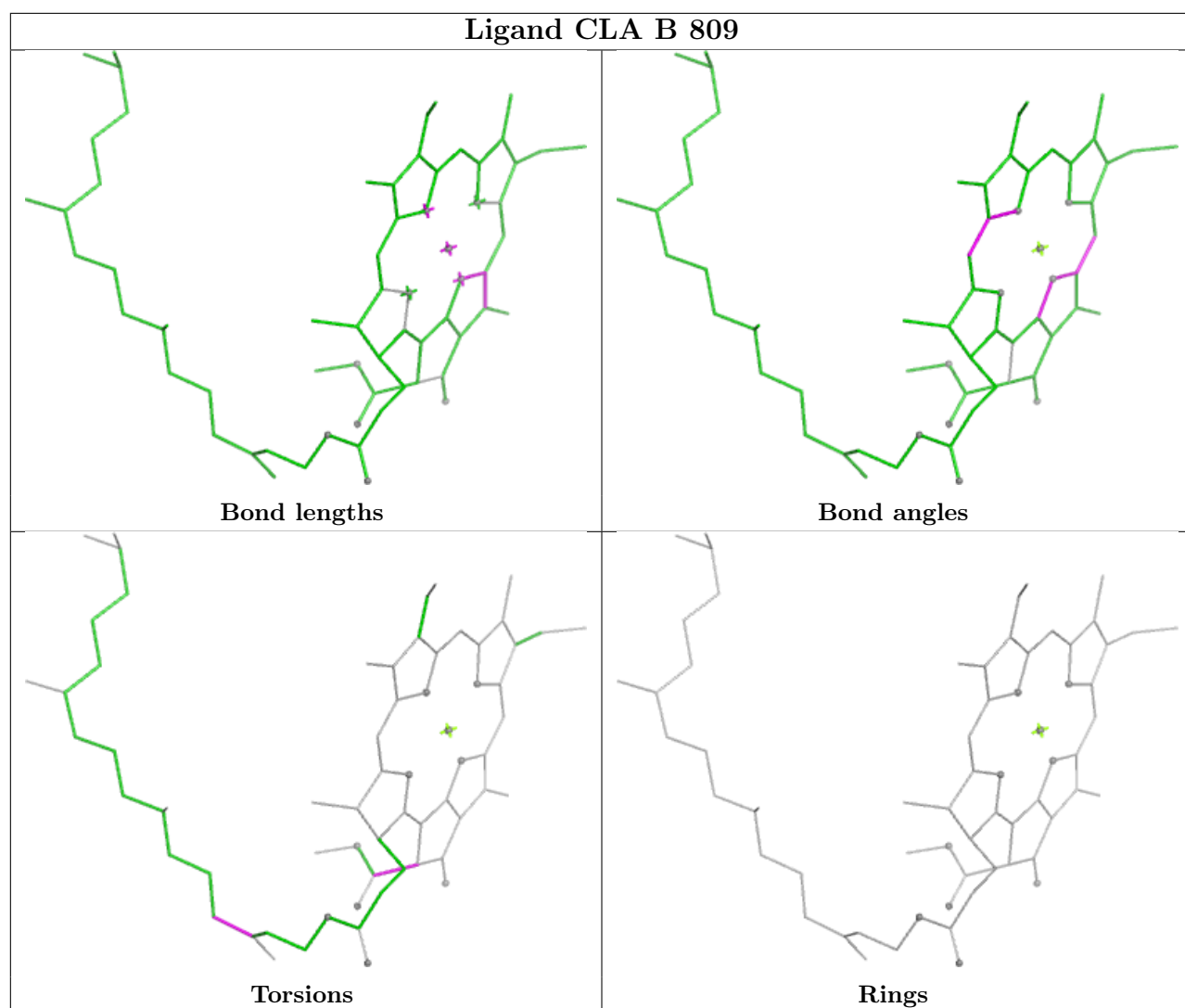




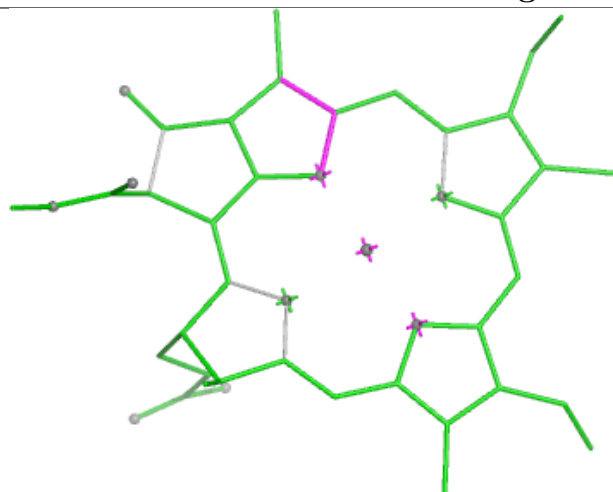


Ligand CLA A 824

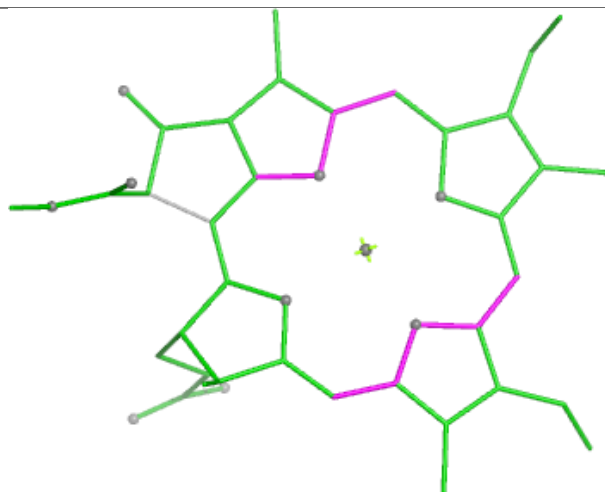




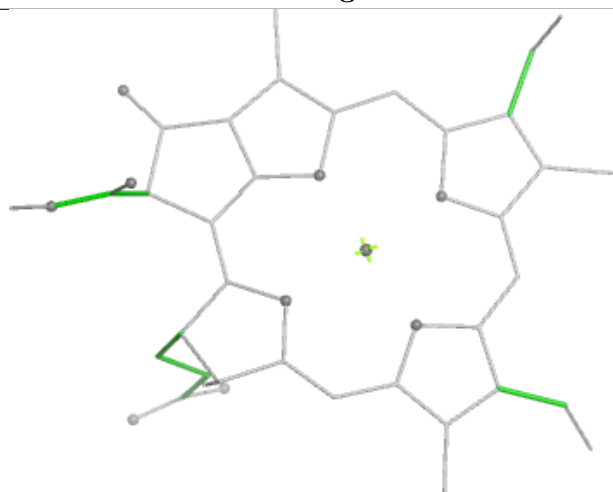
Ligand CLA 2 608



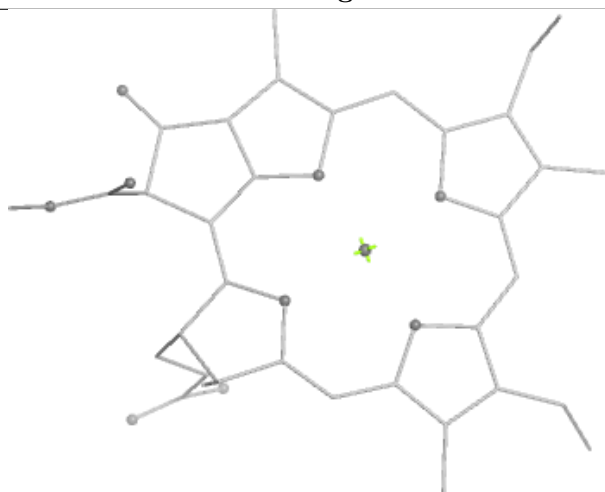
Bond lengths



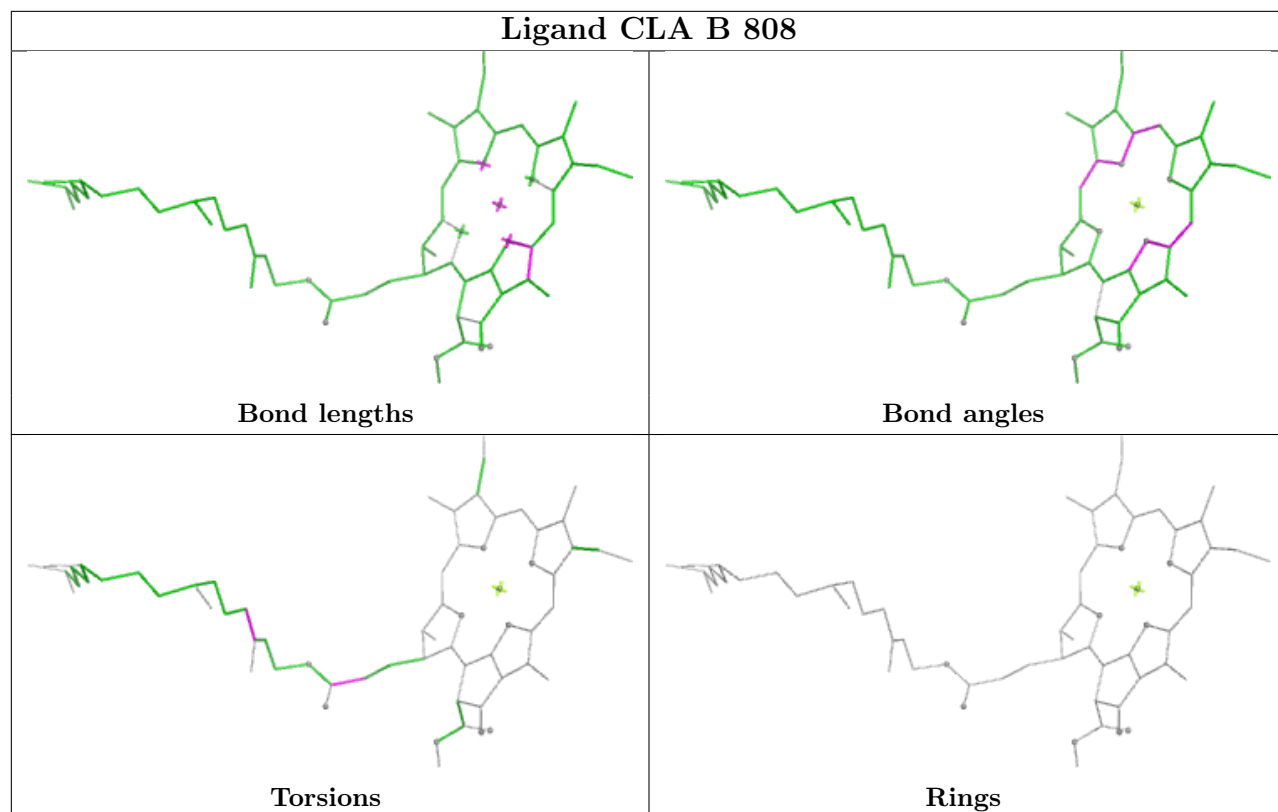
Bond angles

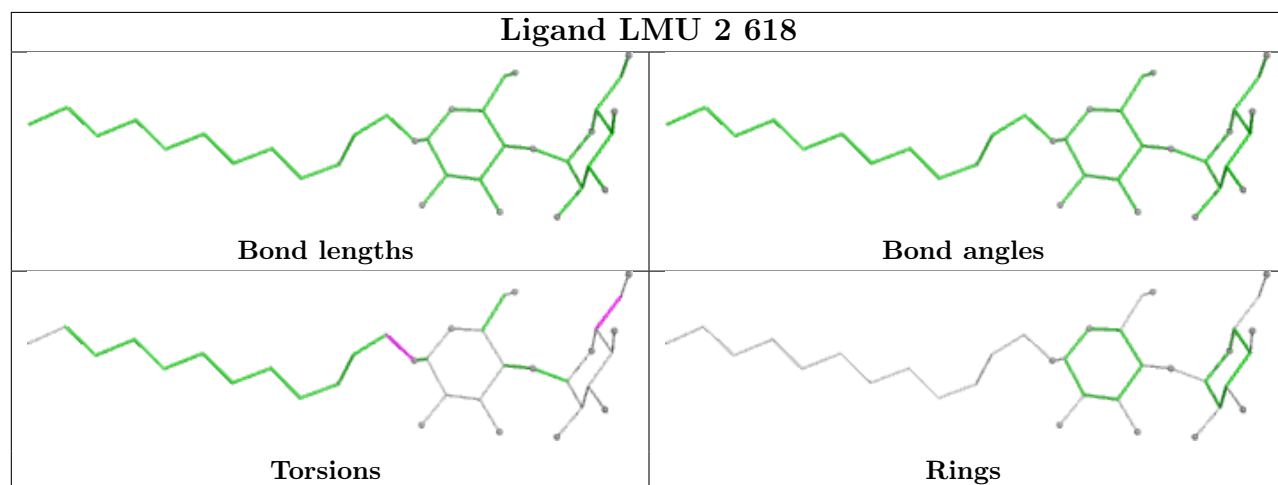
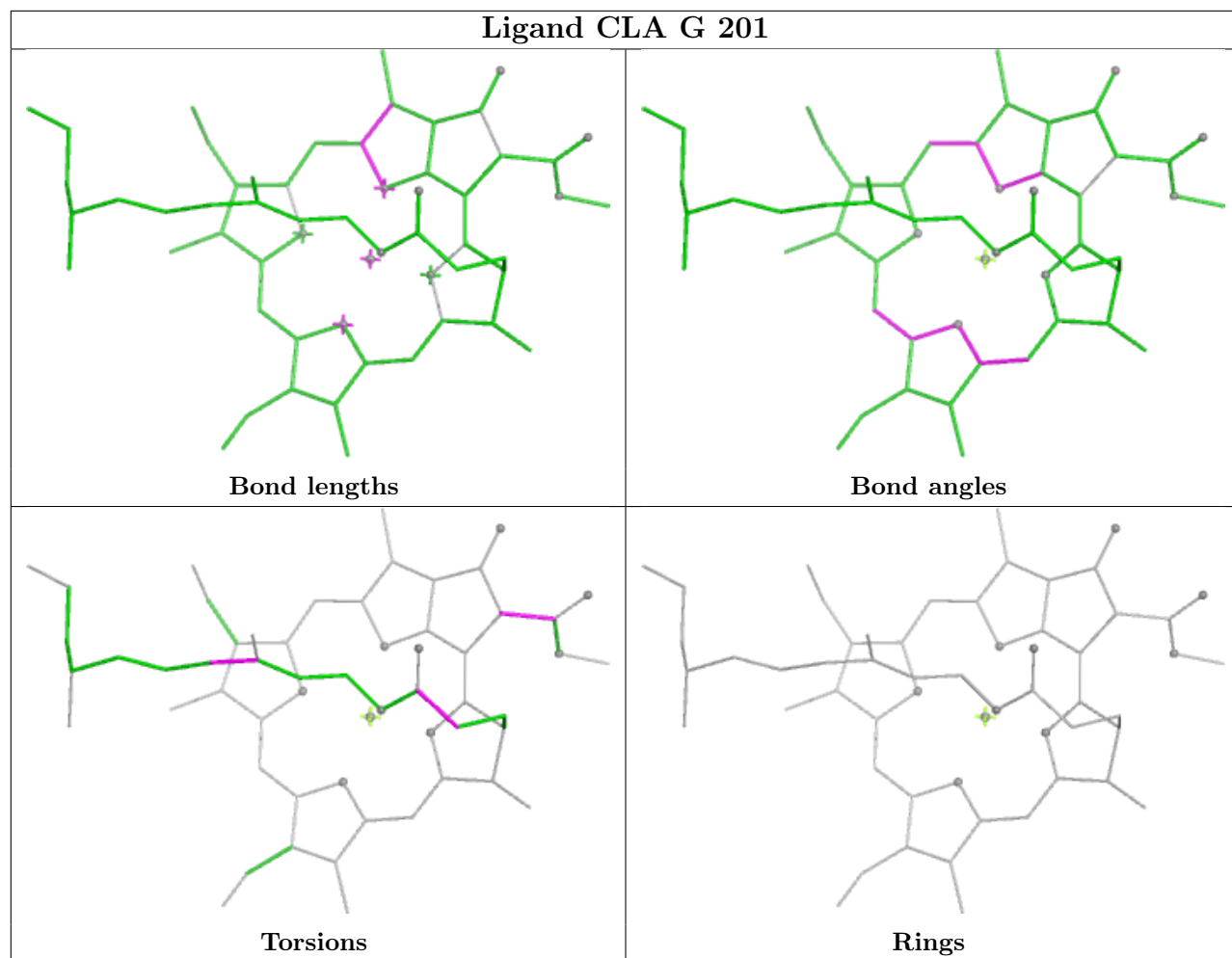


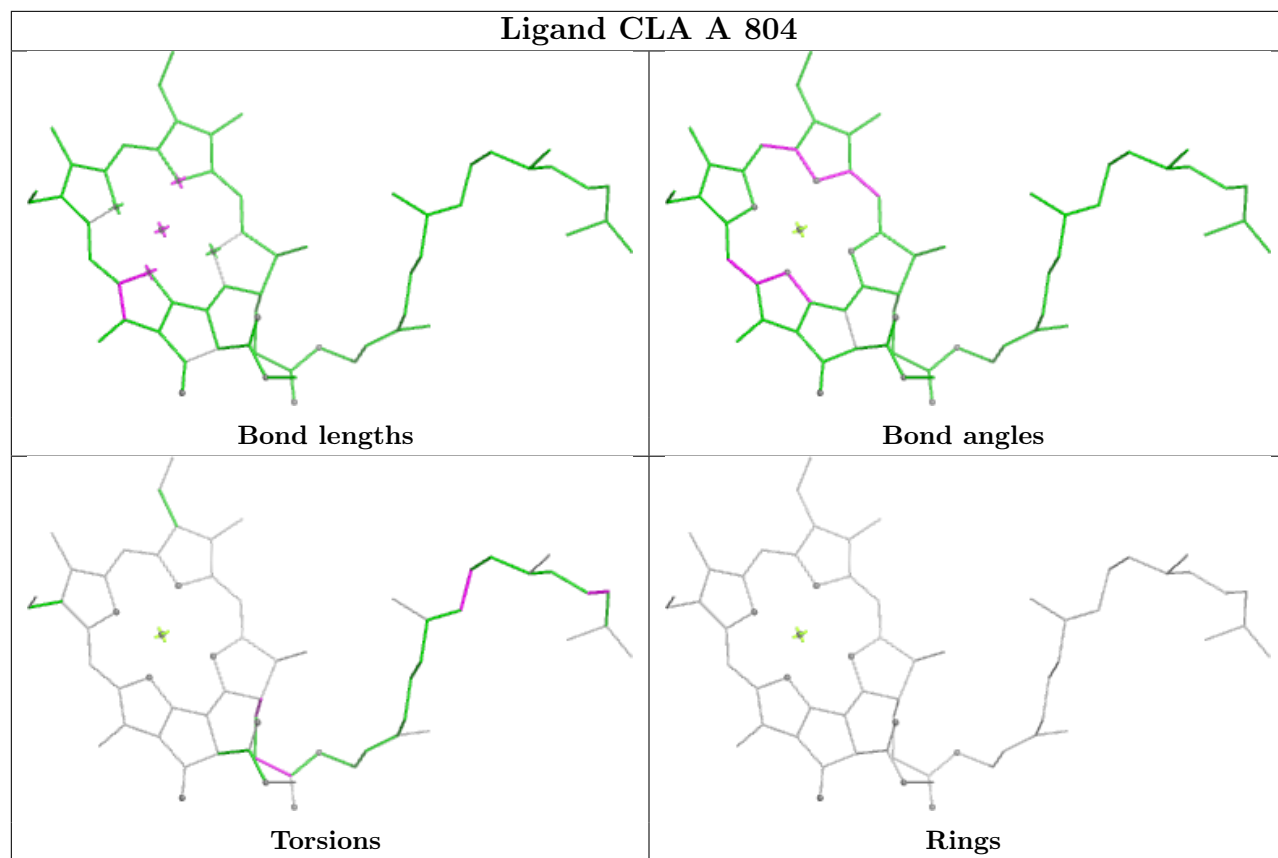
Torsions



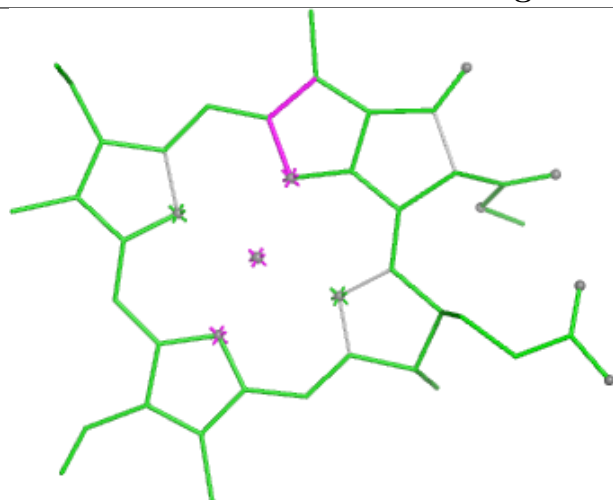
Rings



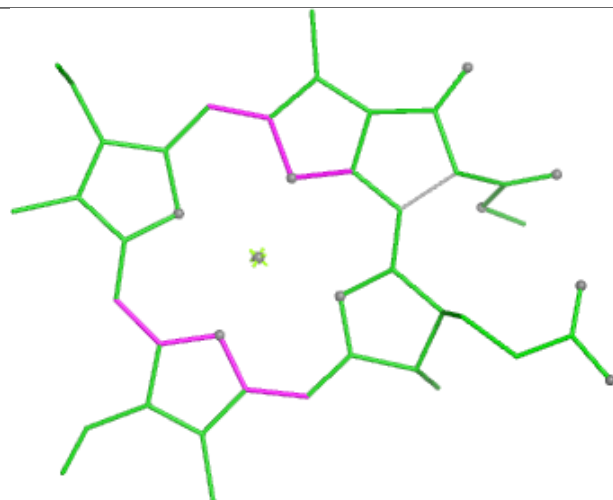




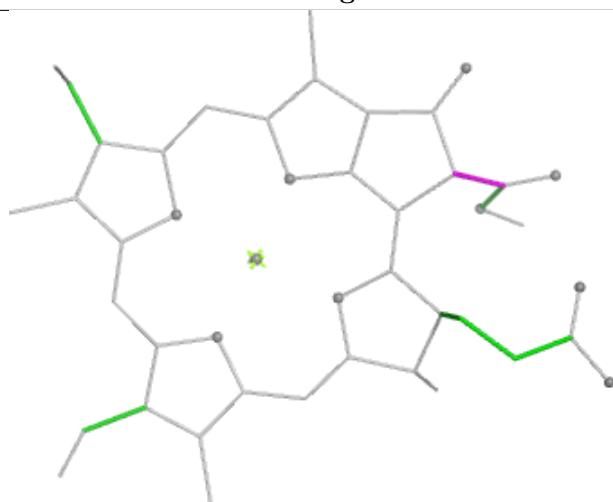
Ligand CLA B 814



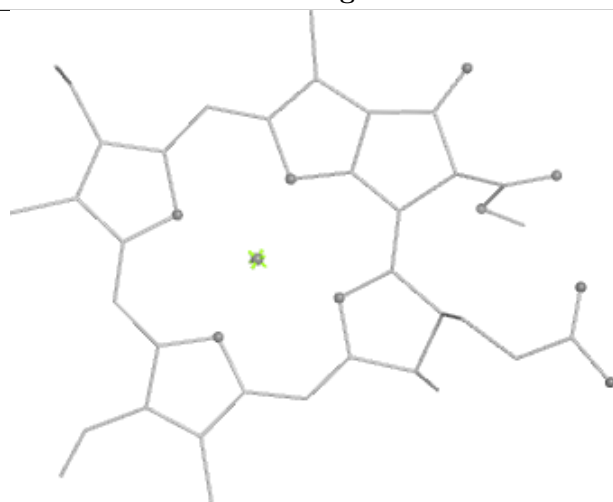
Bond lengths



Bond angles

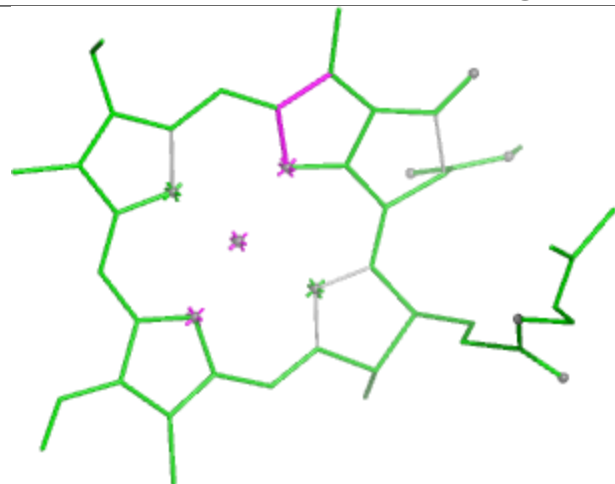


Torsions

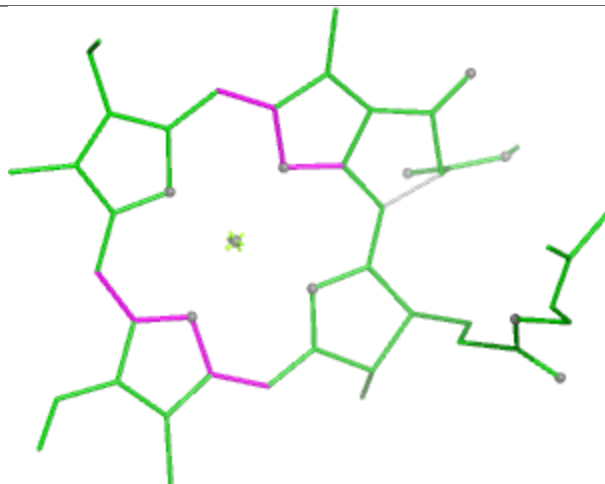


Rings

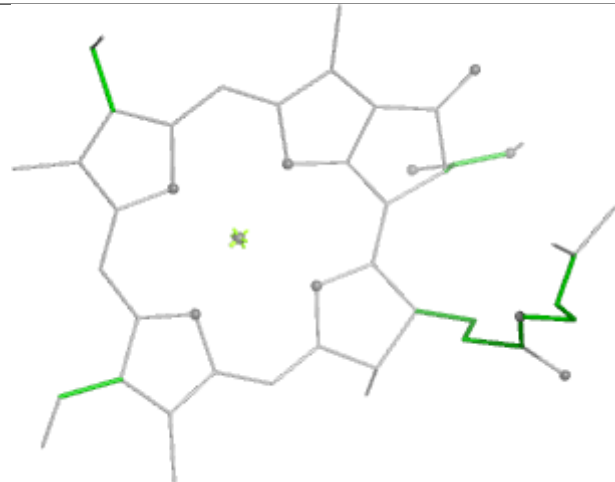
Ligand CLA B 835



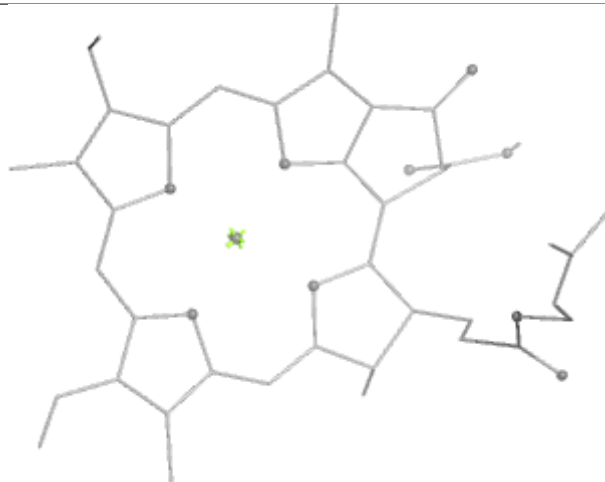
Bond lengths



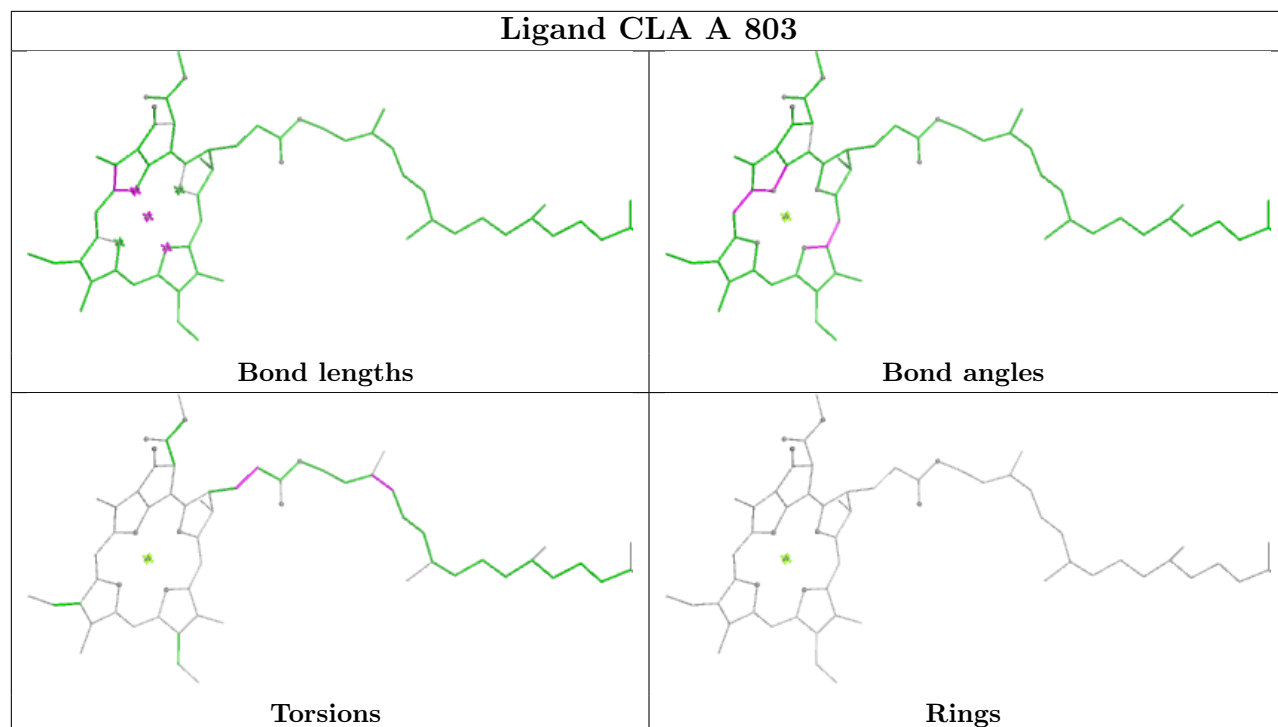
Bond angles



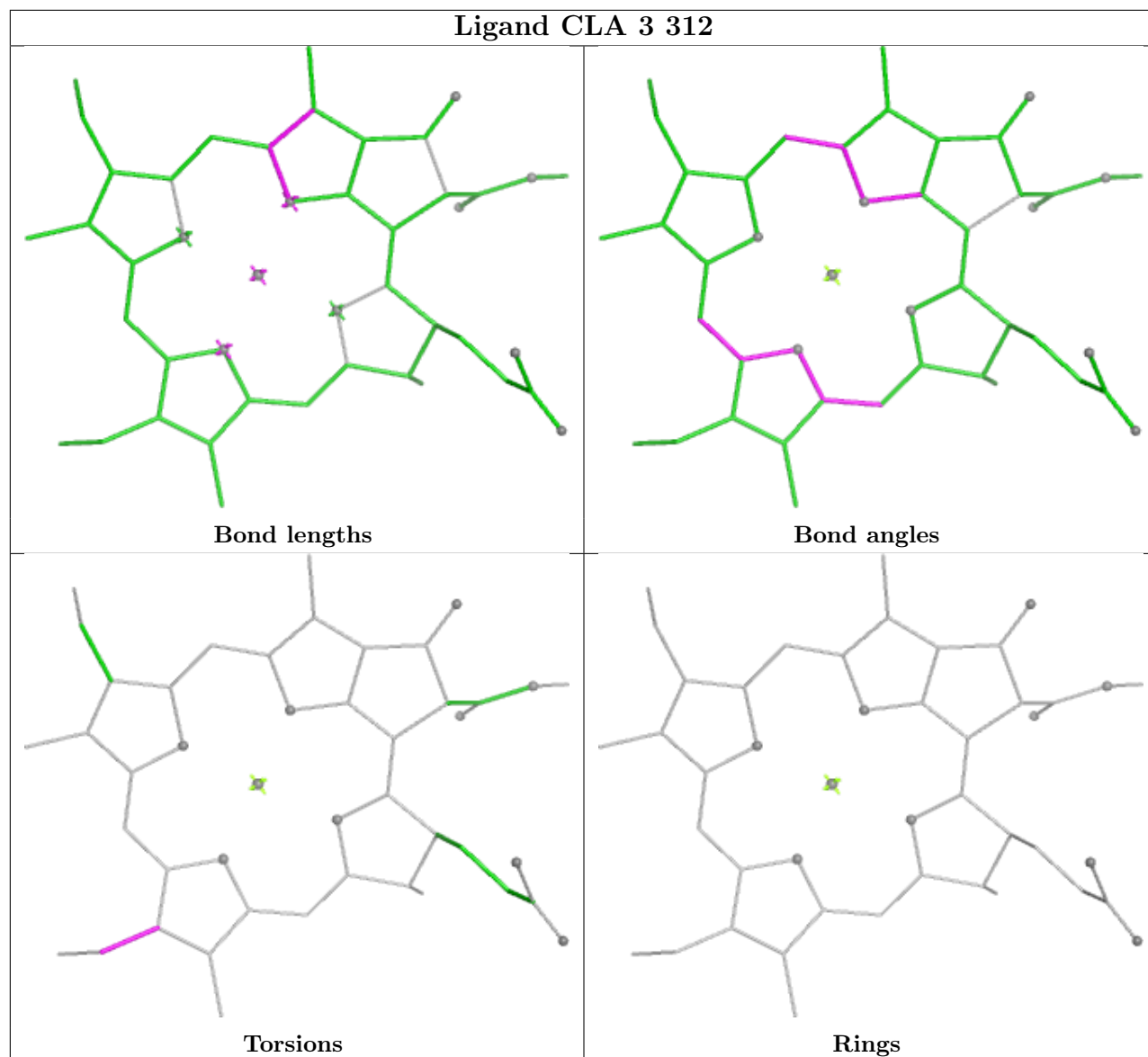
Torsions

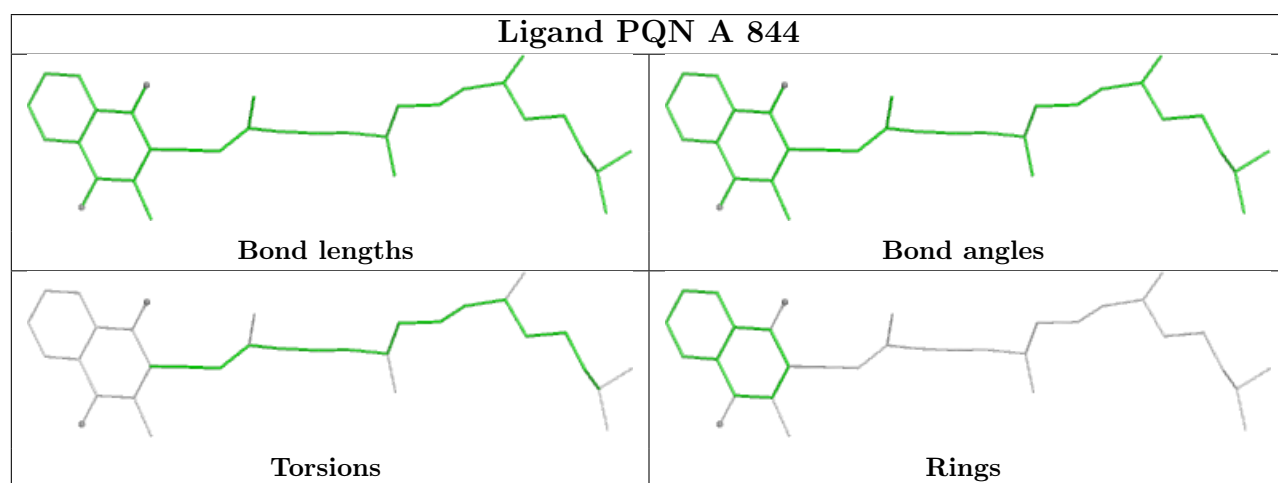
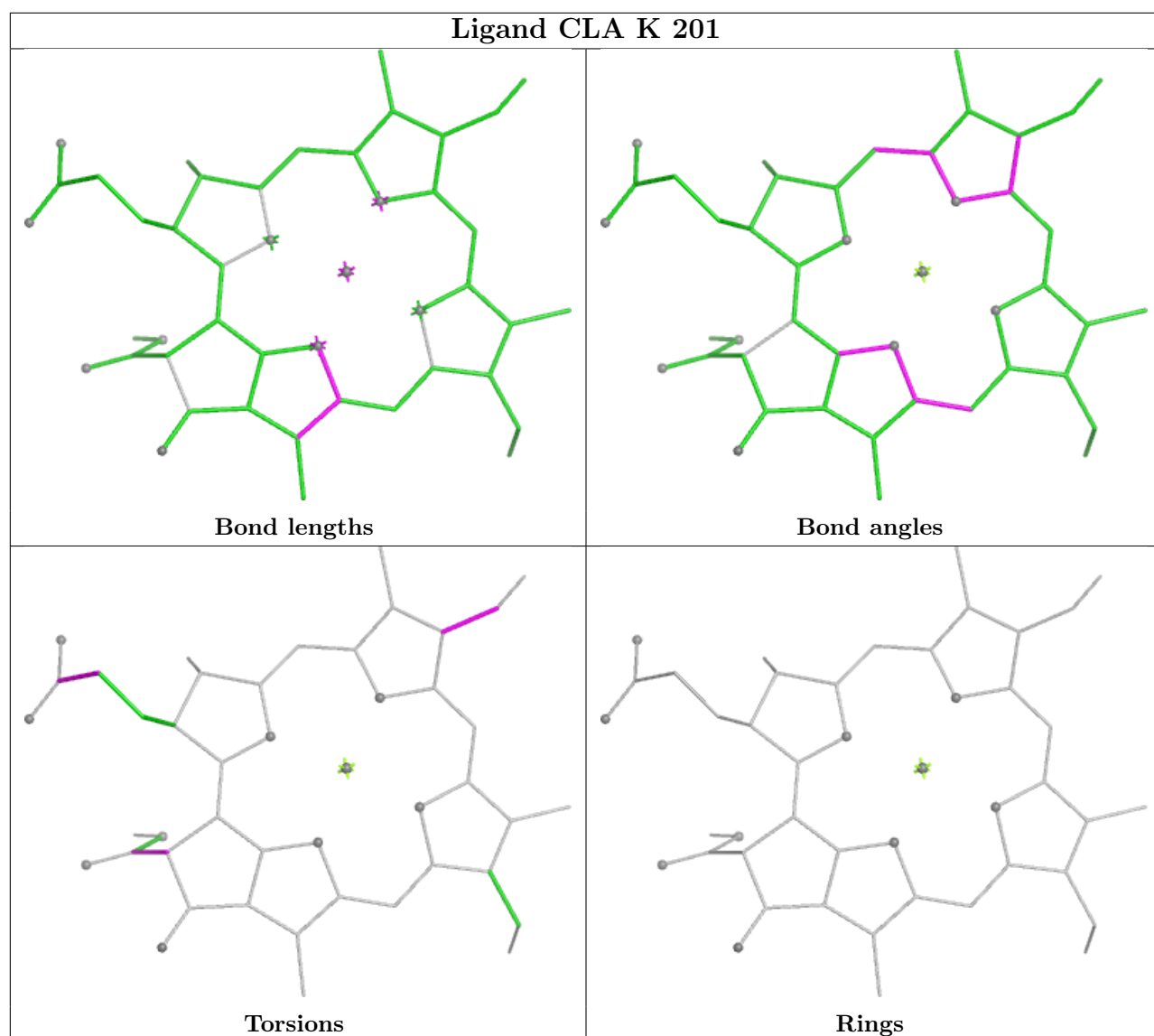


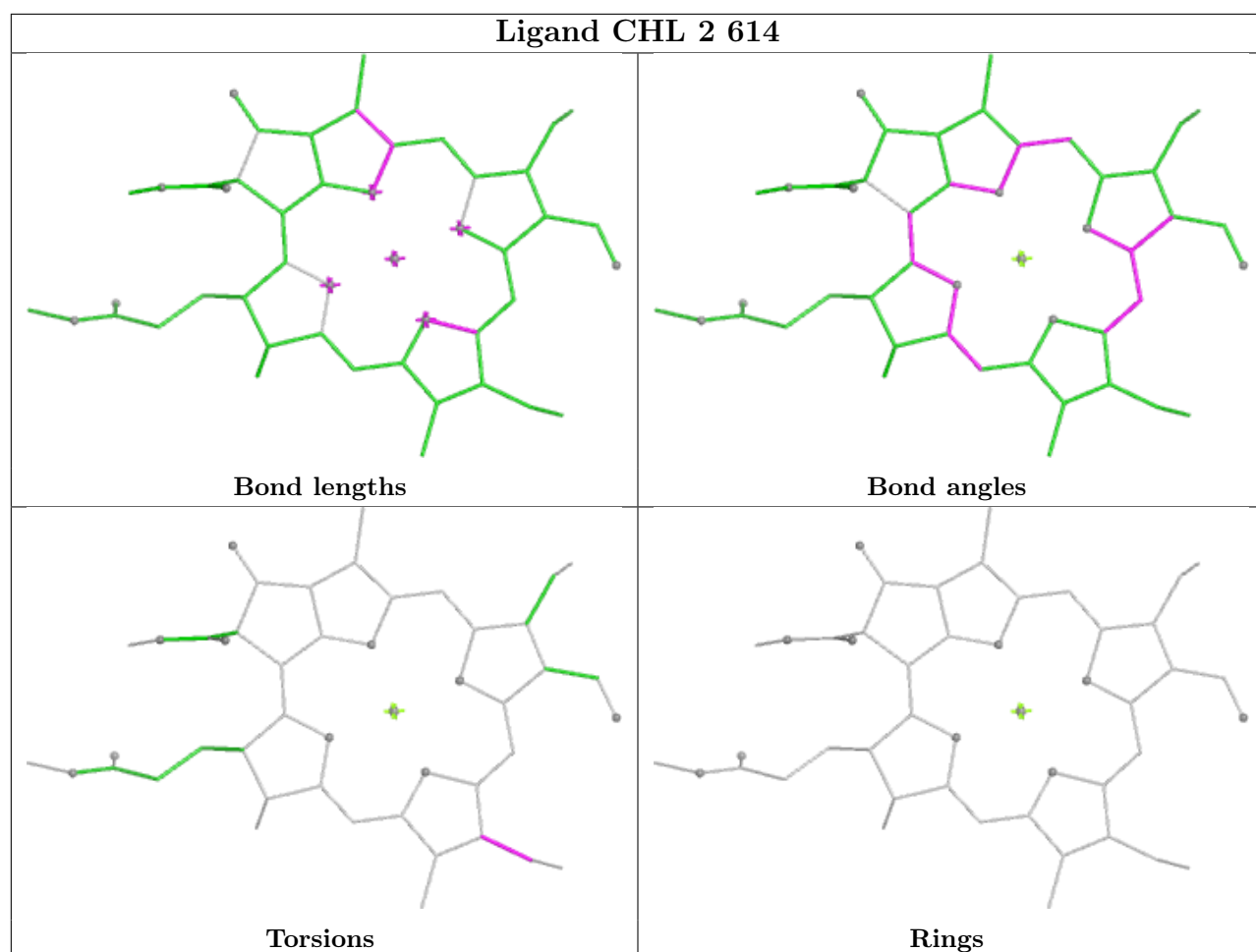
Rings

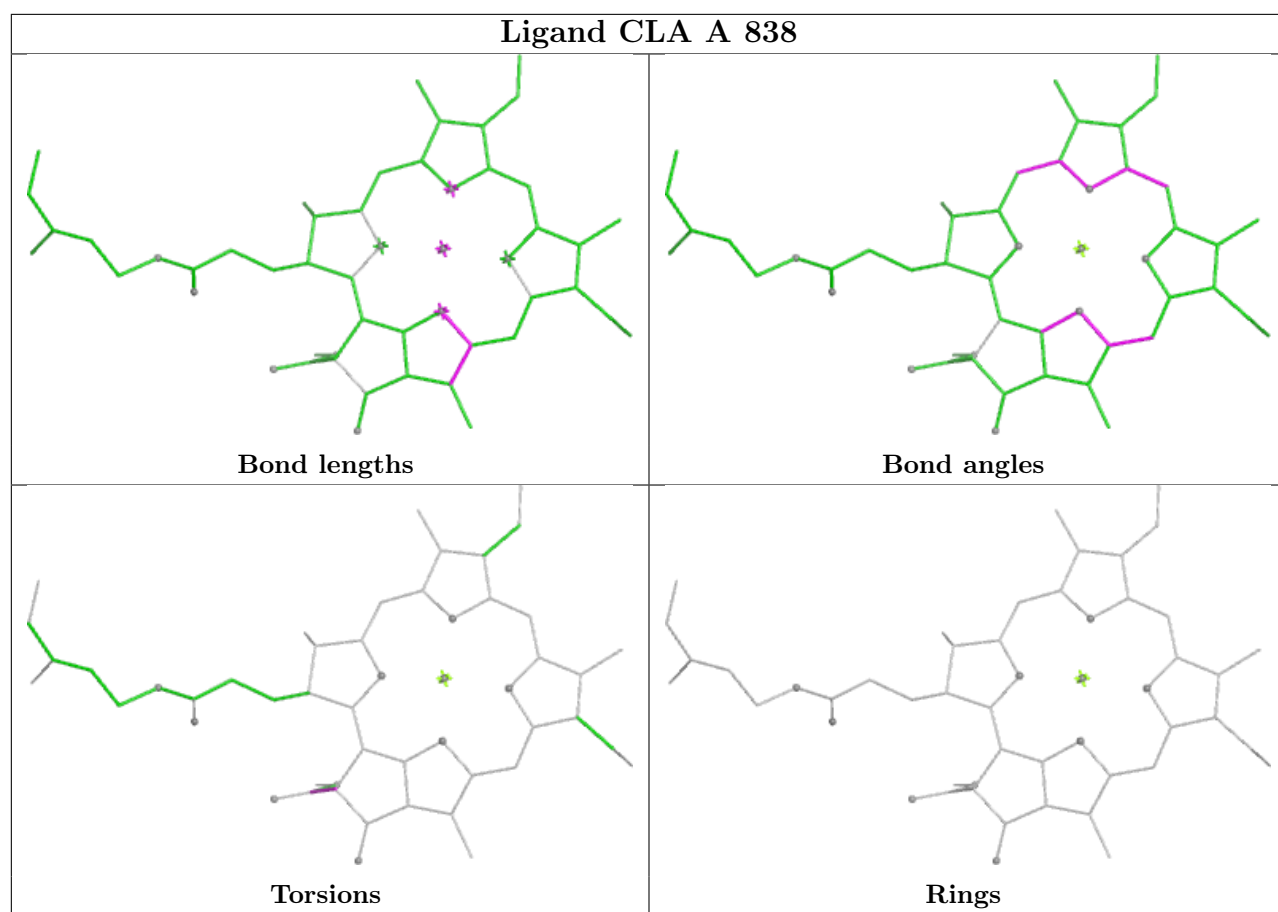


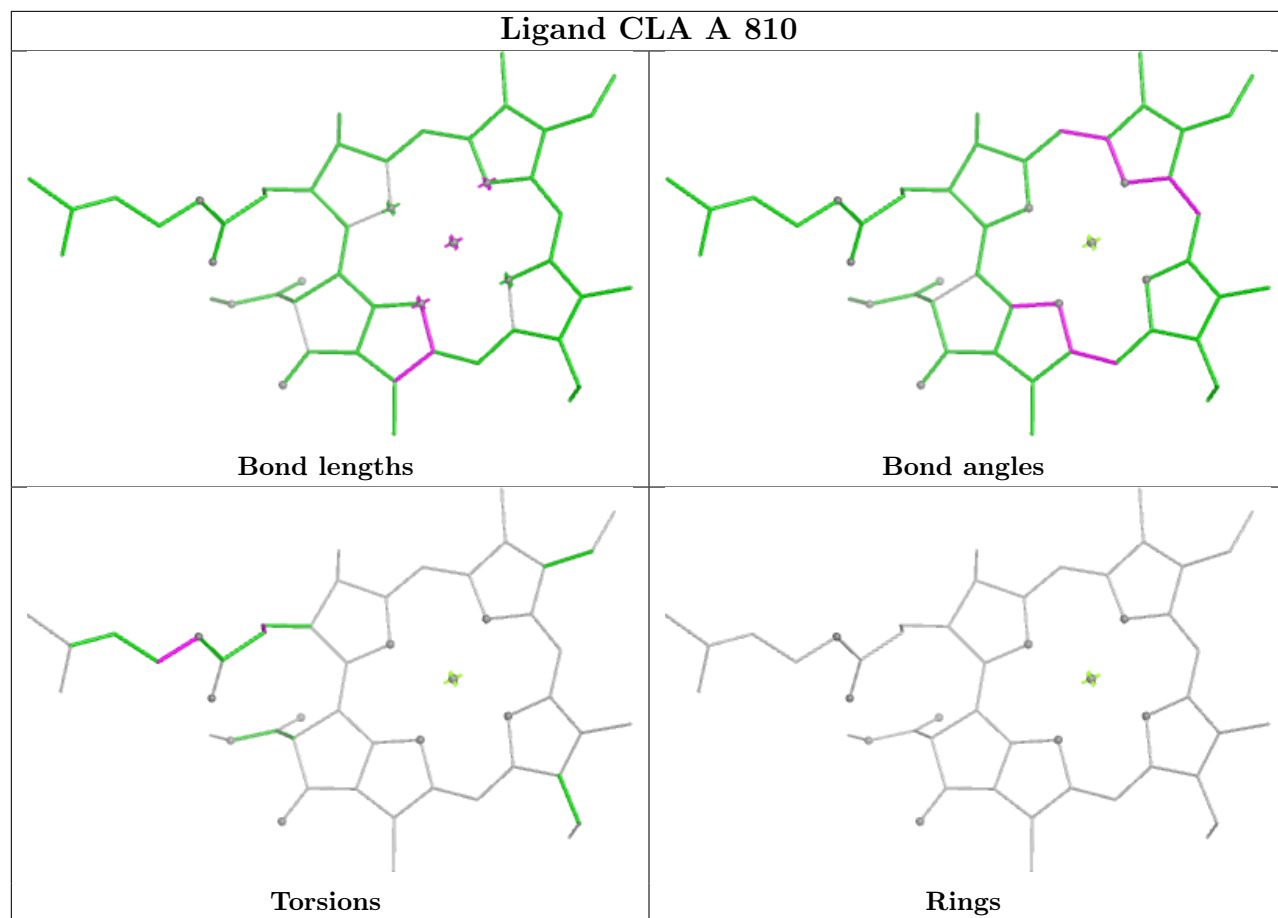
Ligand CLA 3 312

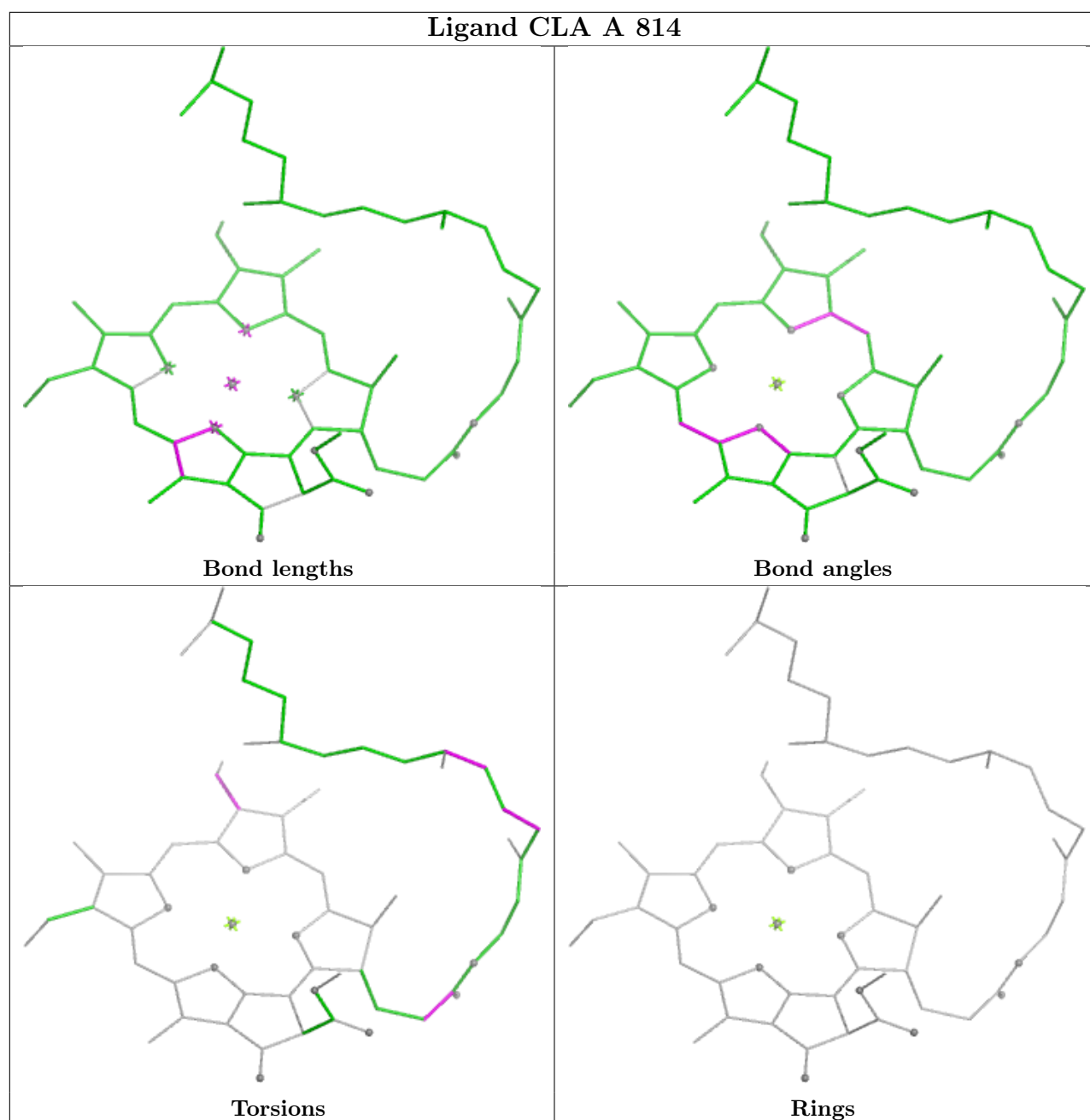


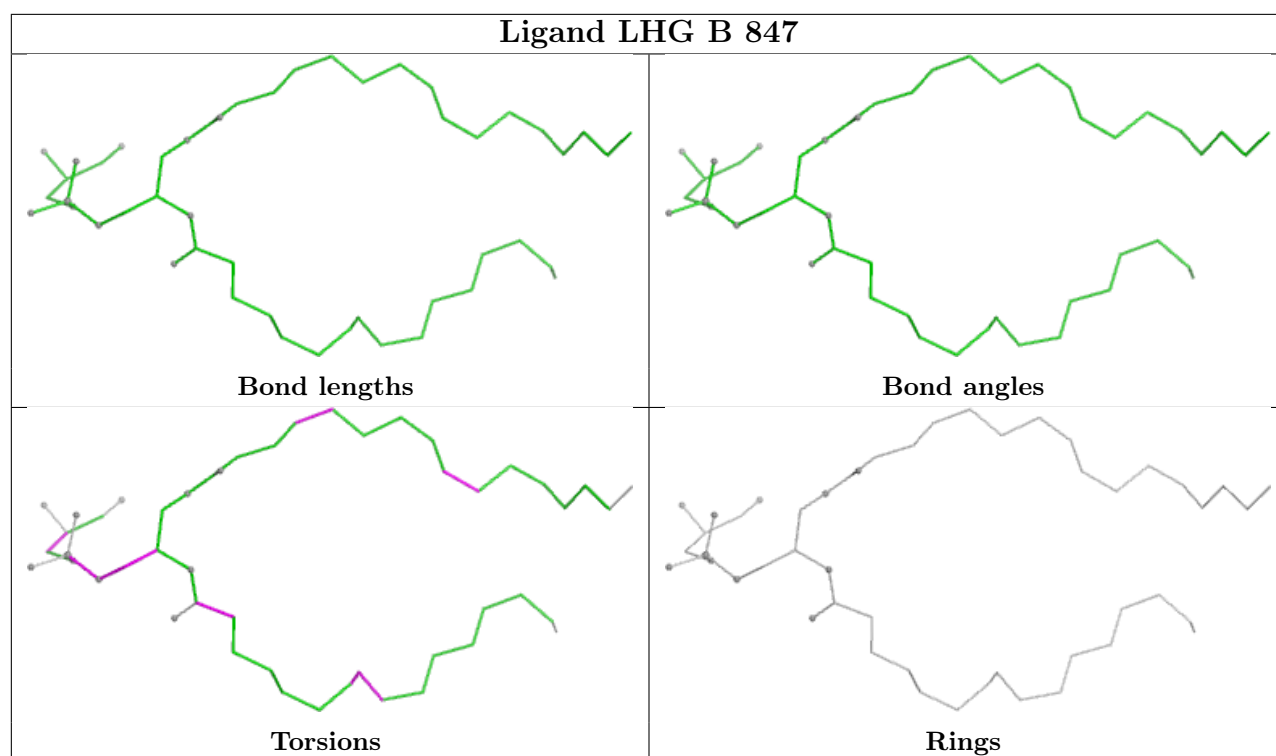




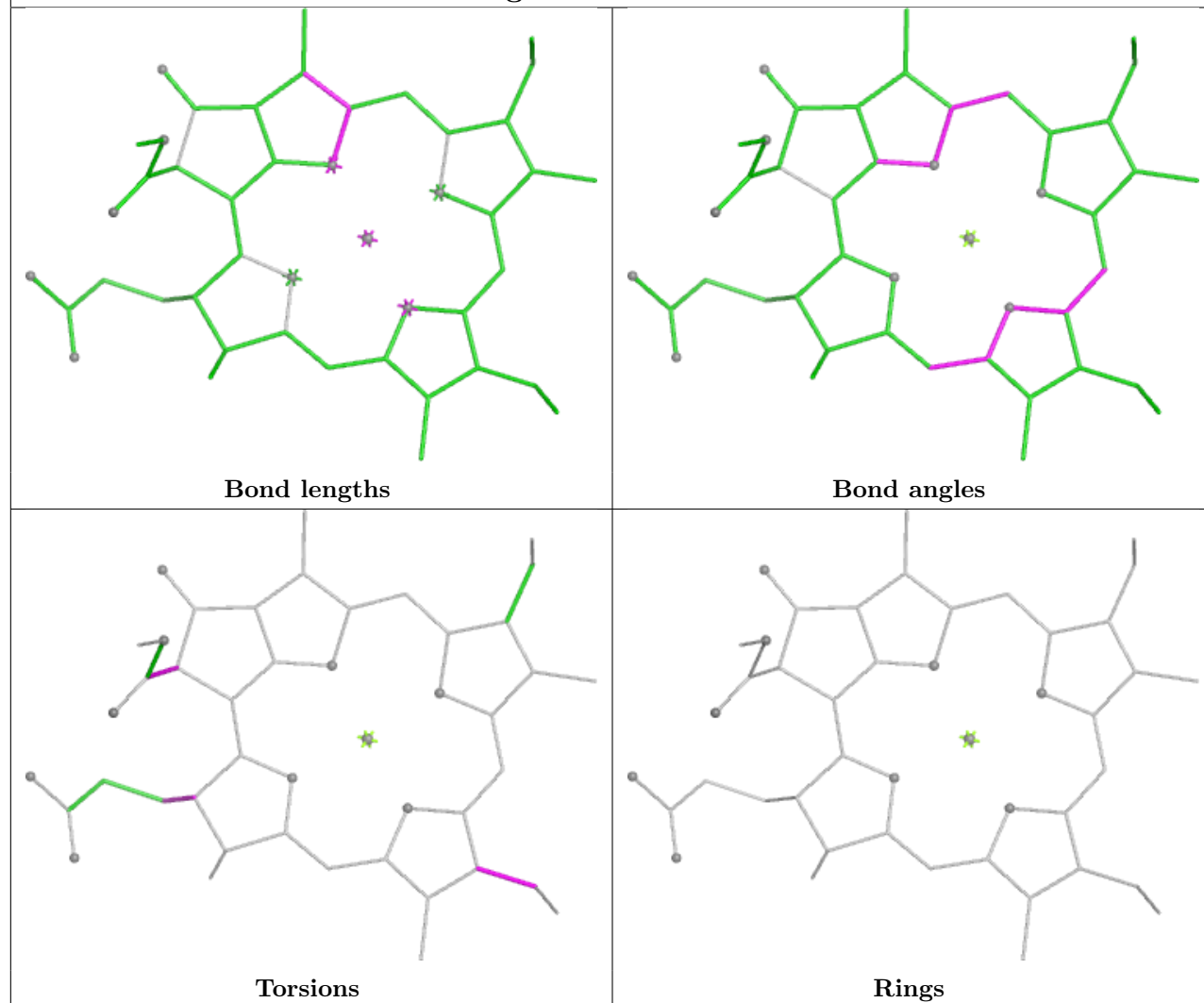




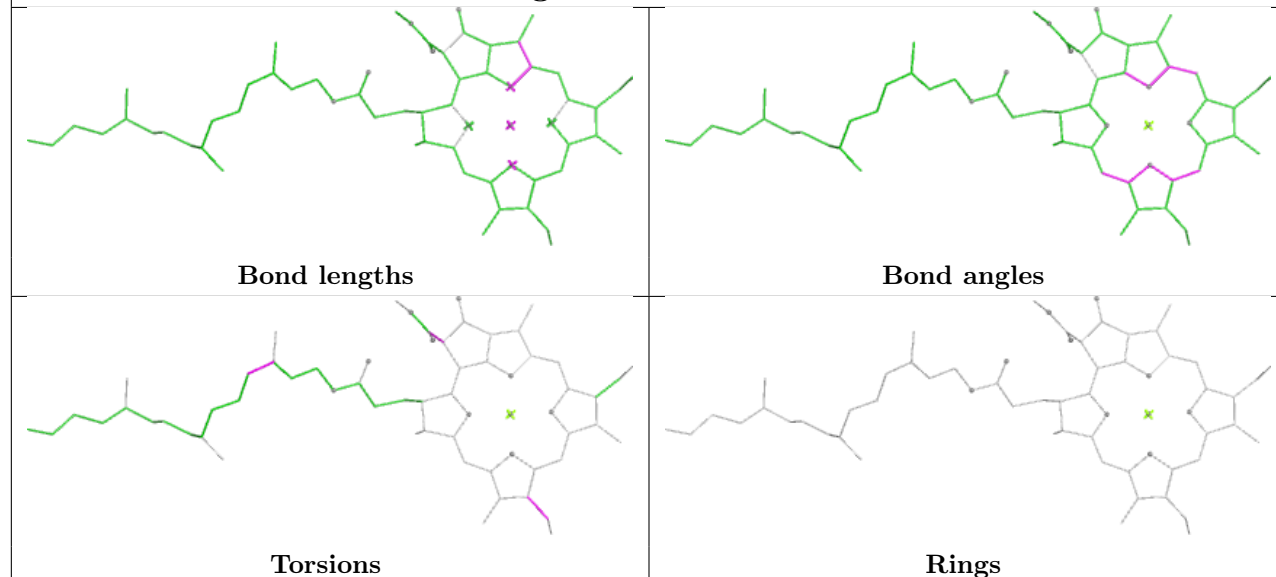


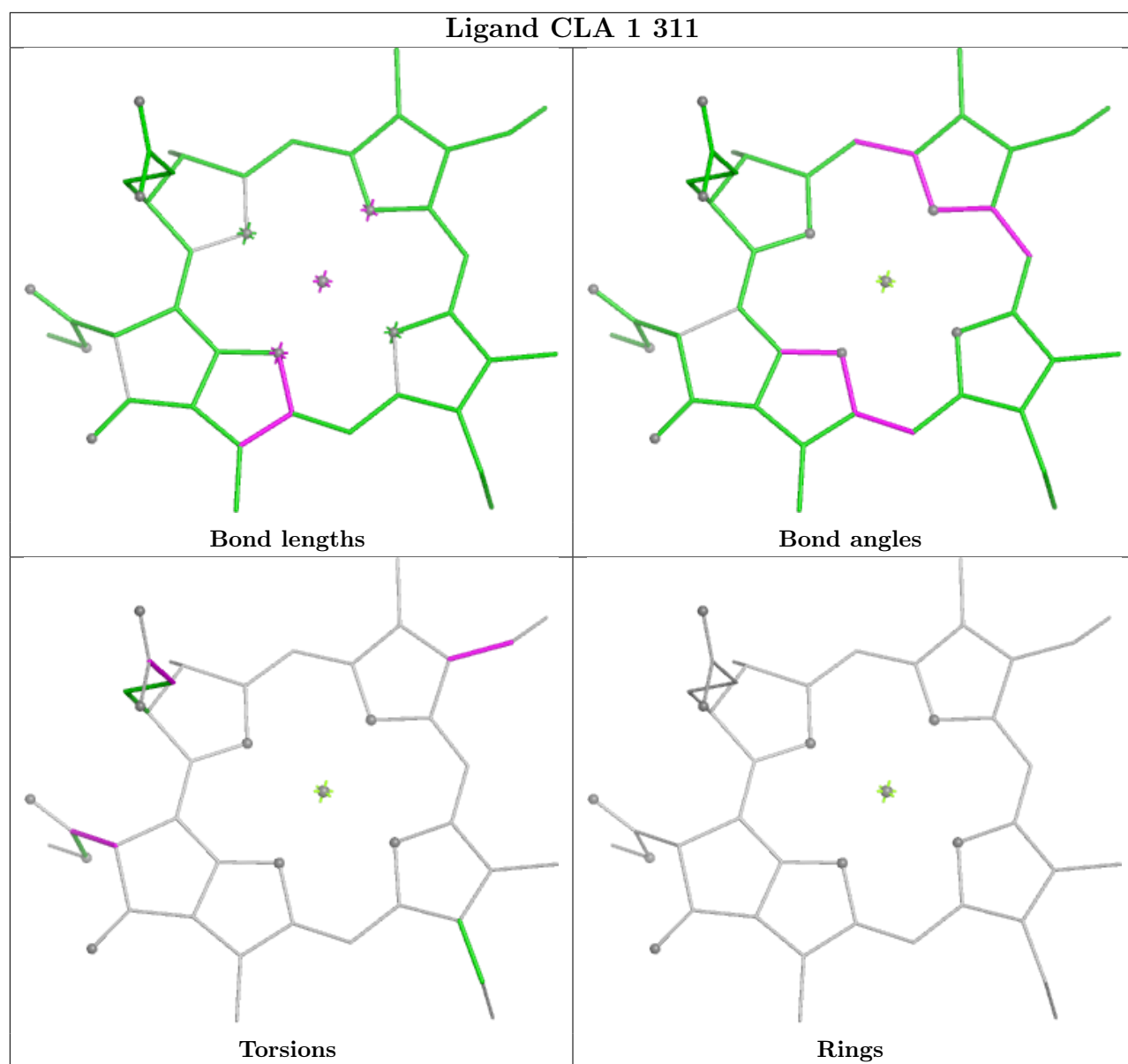


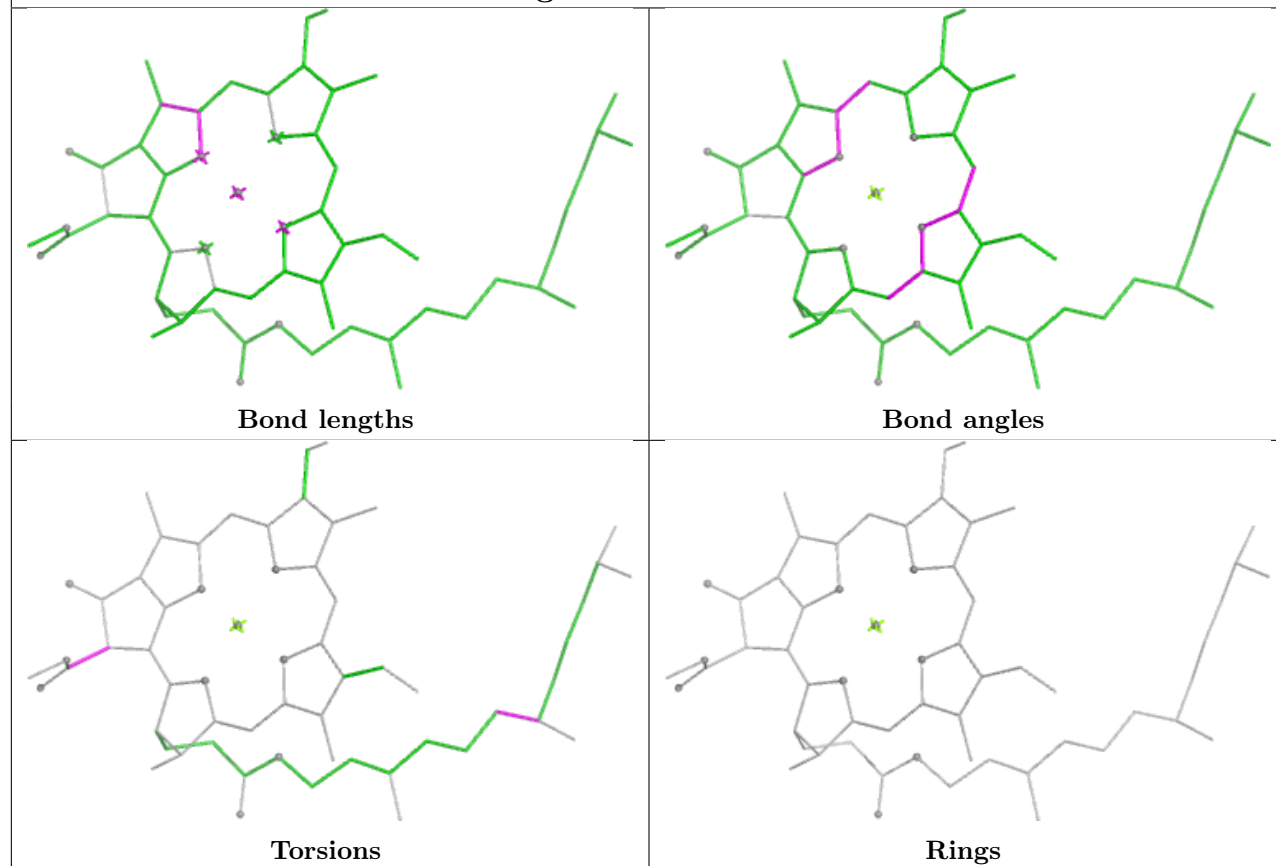
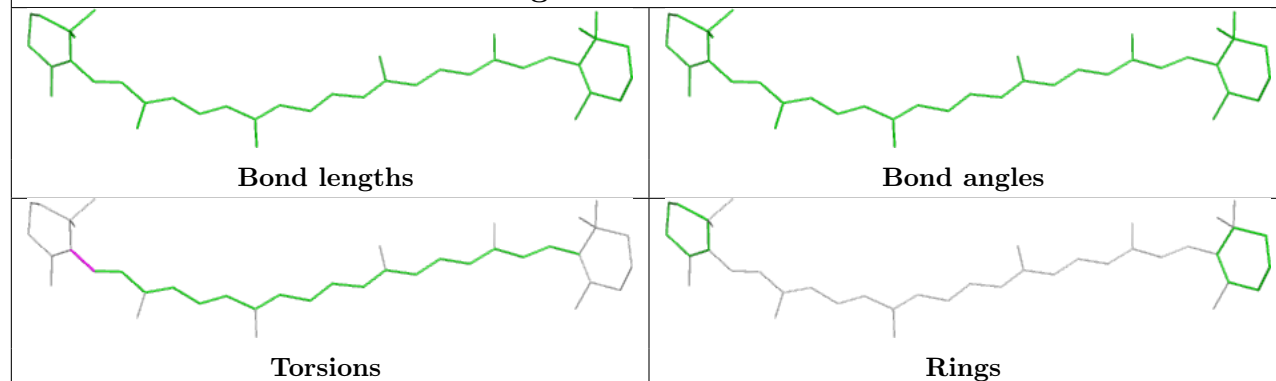
Ligand CLA 1 312



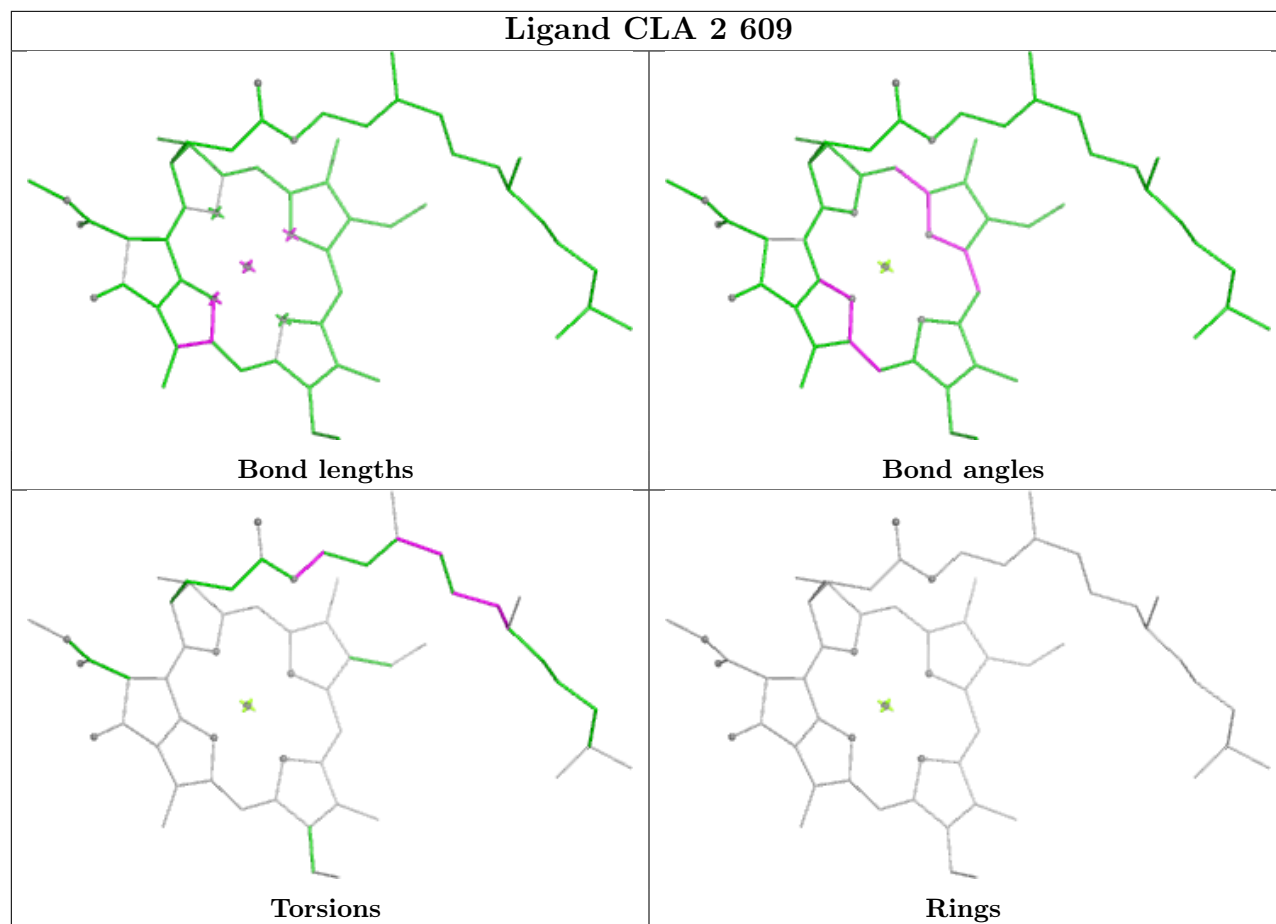
Ligand CLA A 834



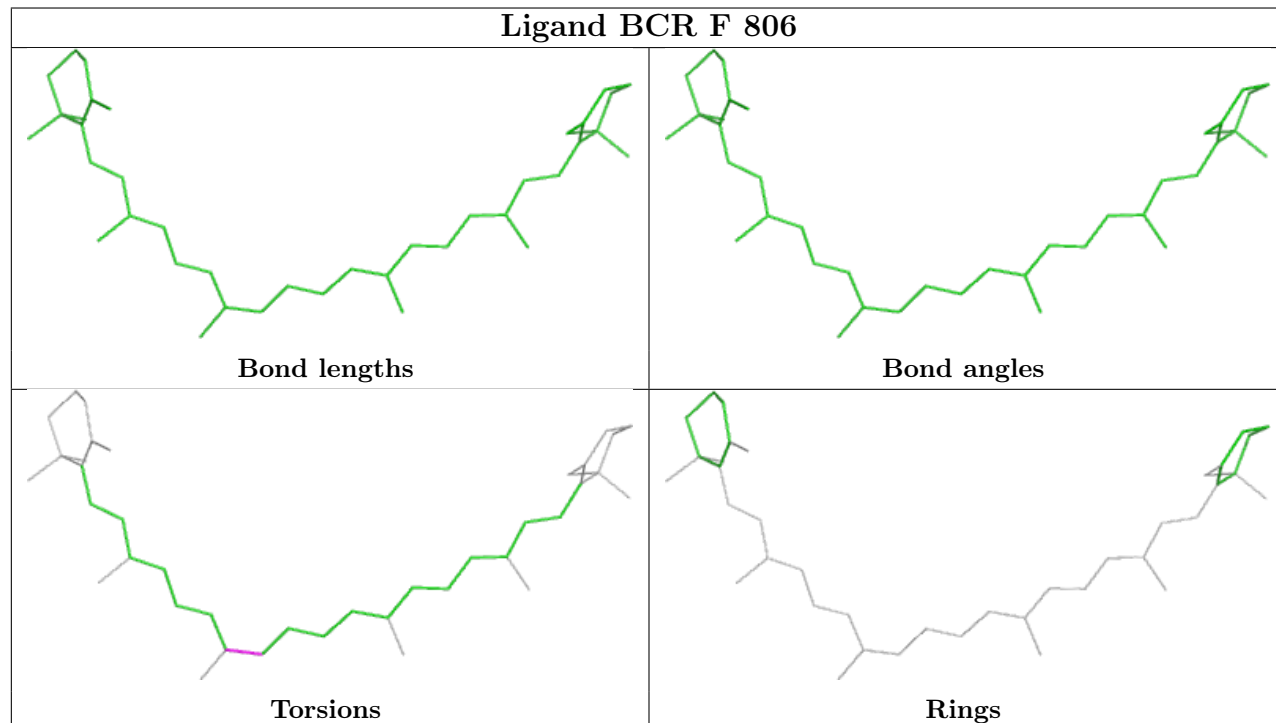


Ligand CLA 4 602**Ligand BCR B 842**

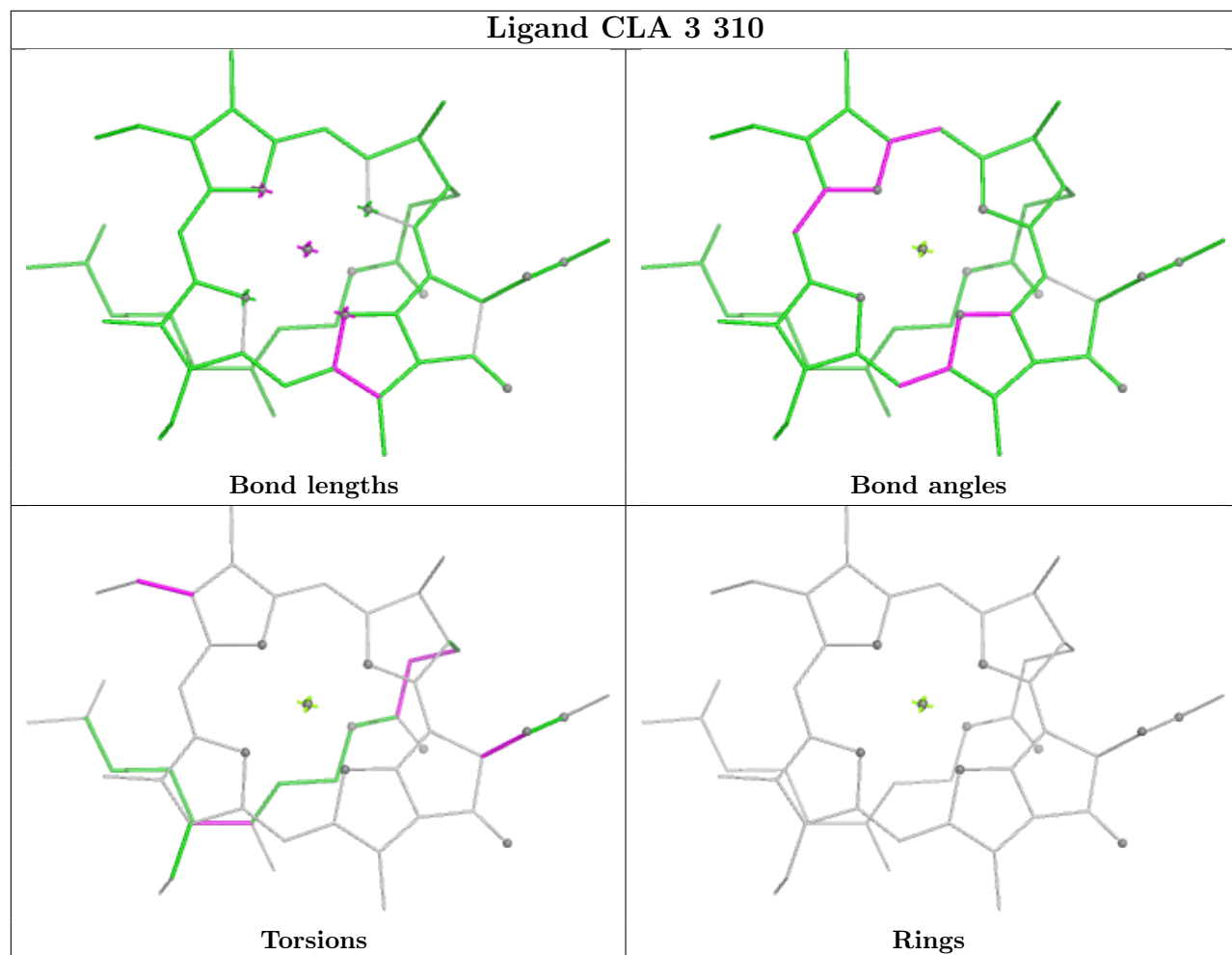
Ligand CLA 2 609

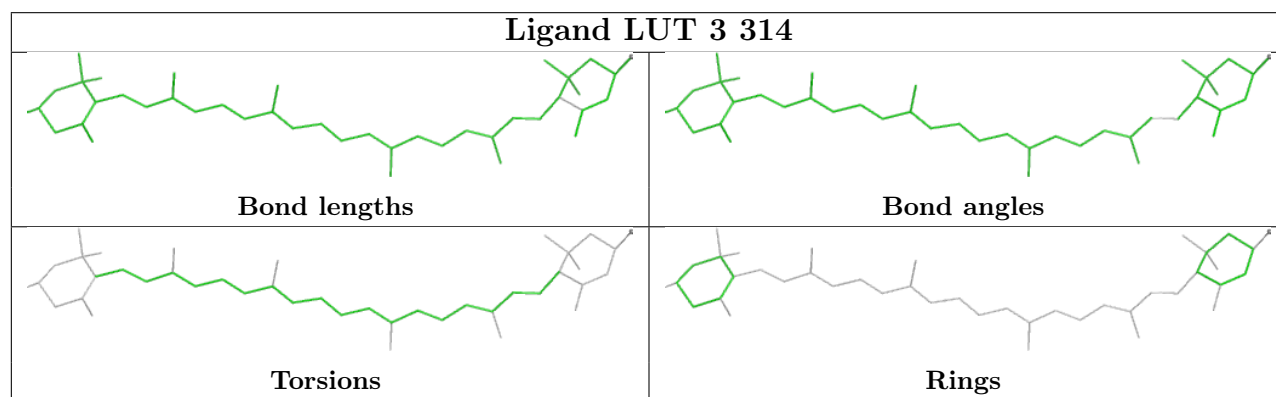
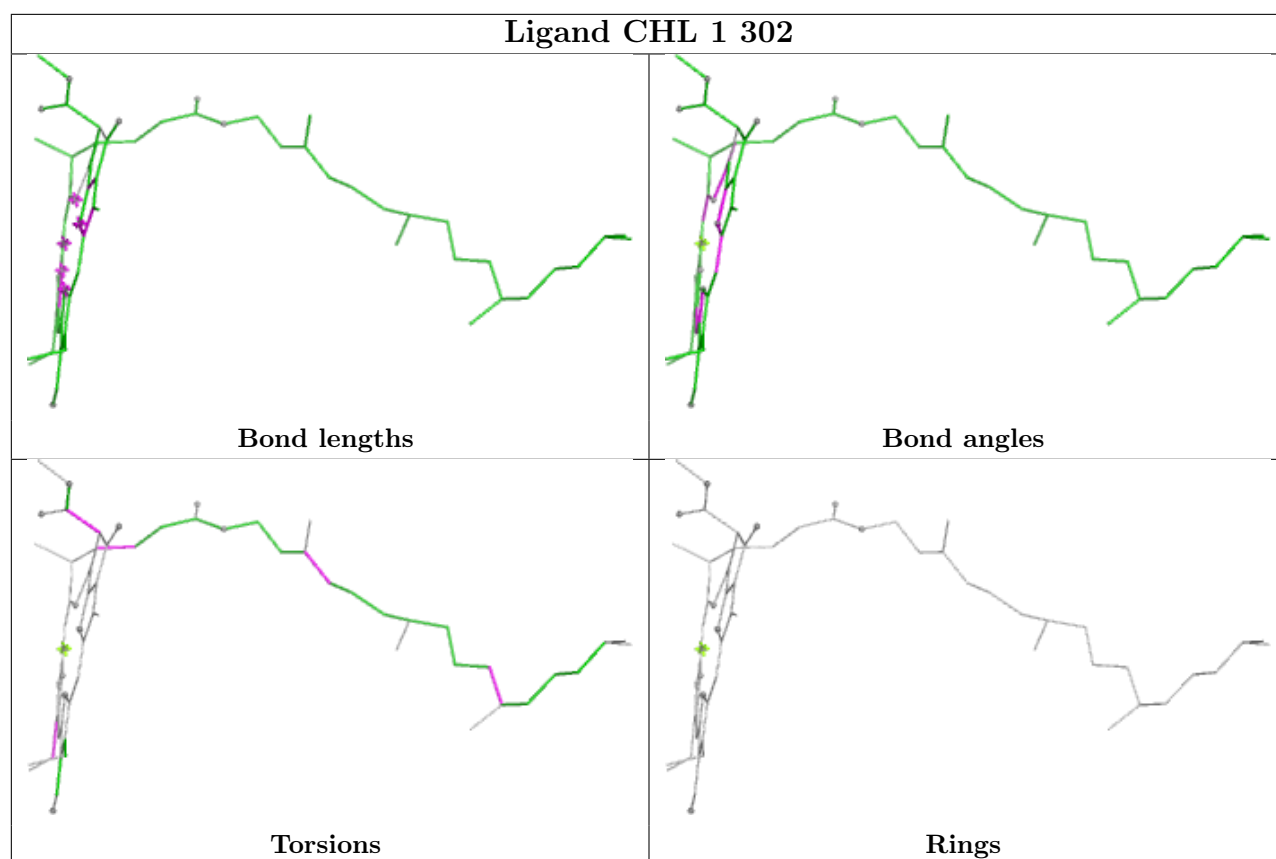


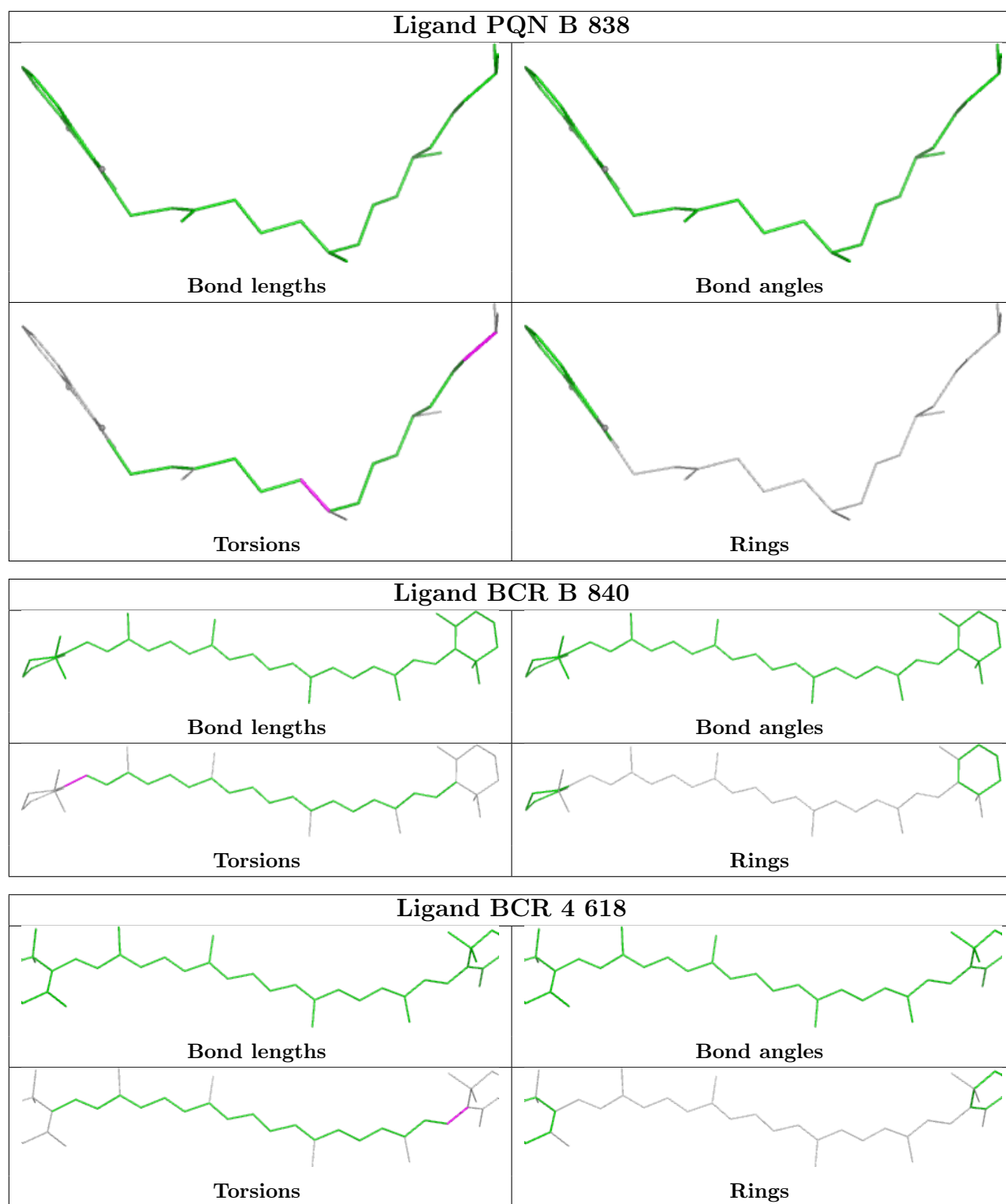
Ligand BCR F 806

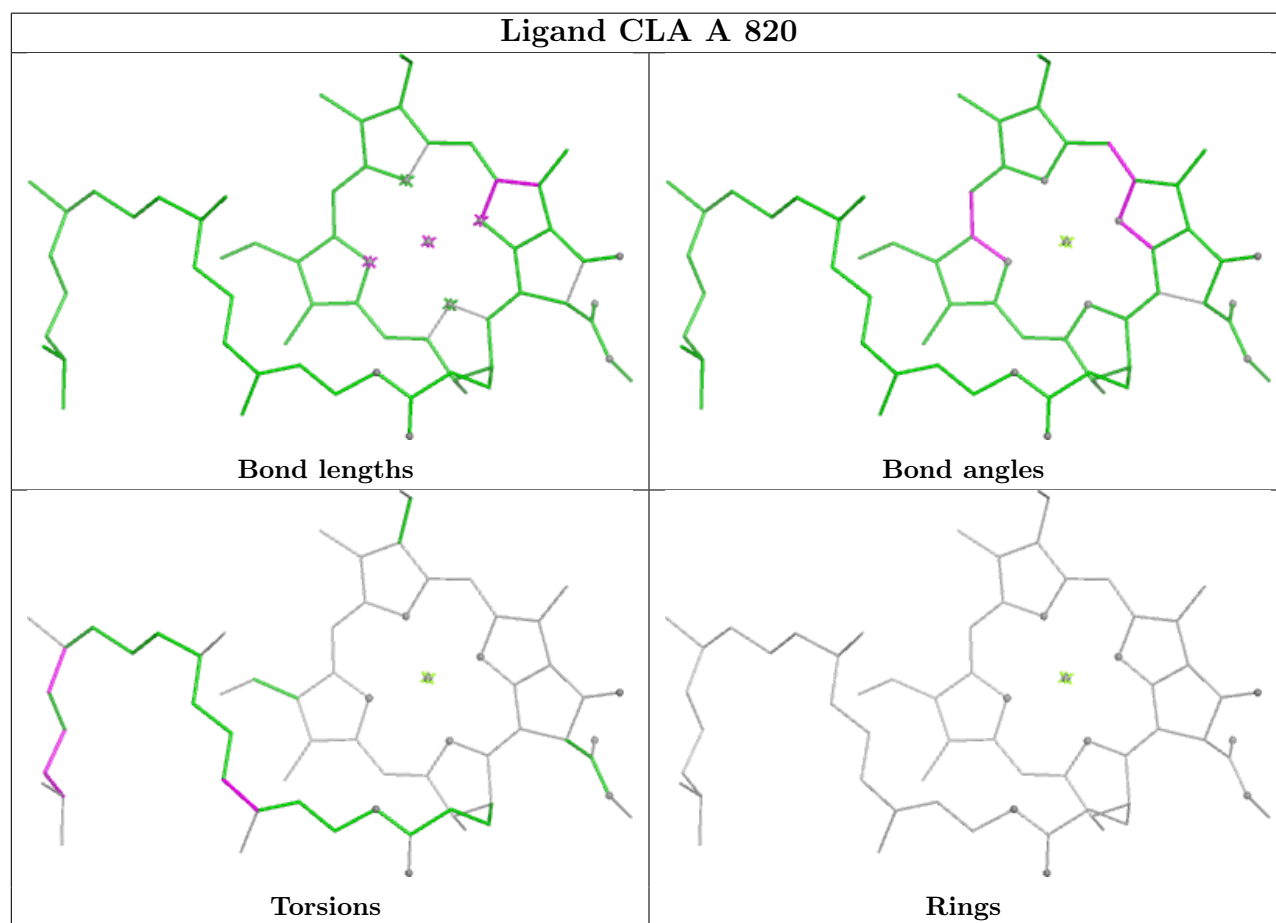
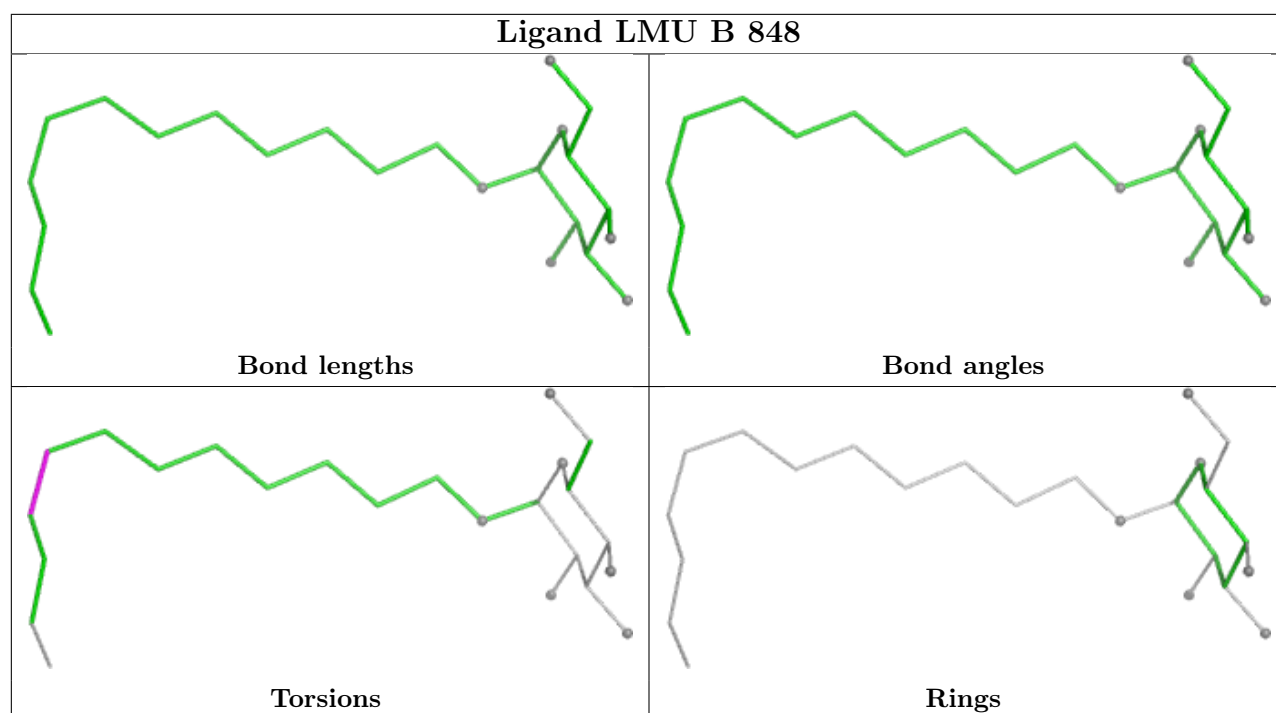


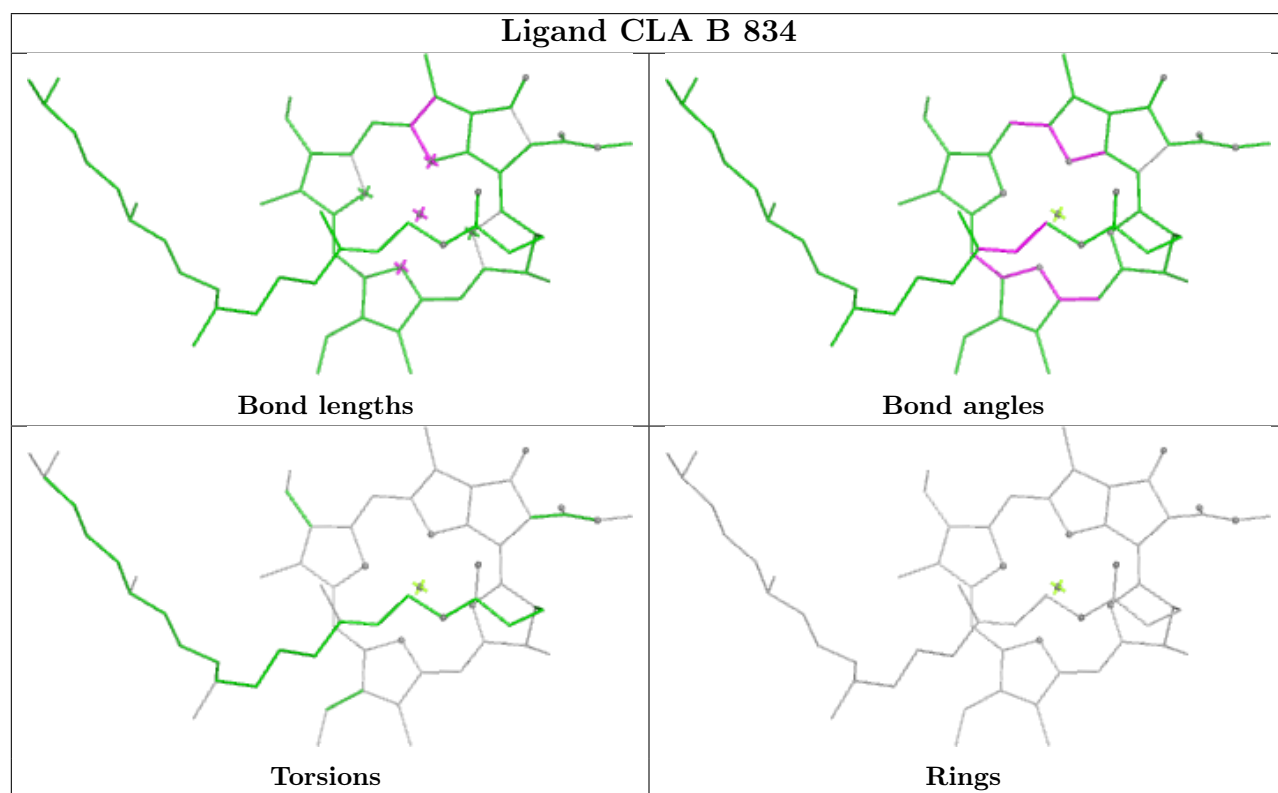
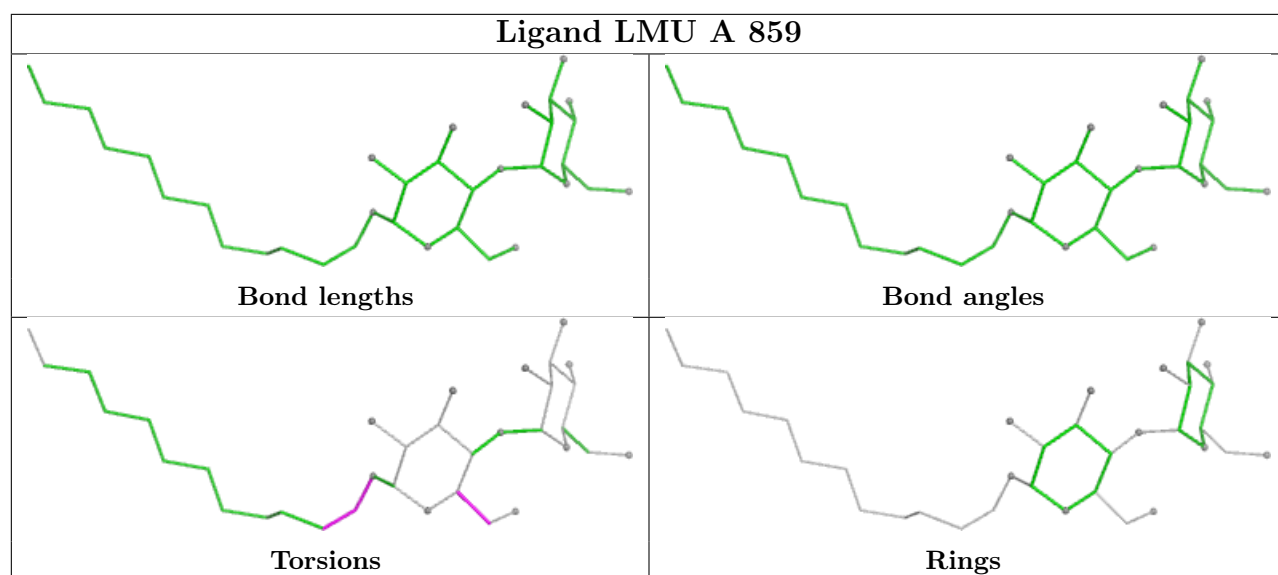
Ligand CLA 3 310

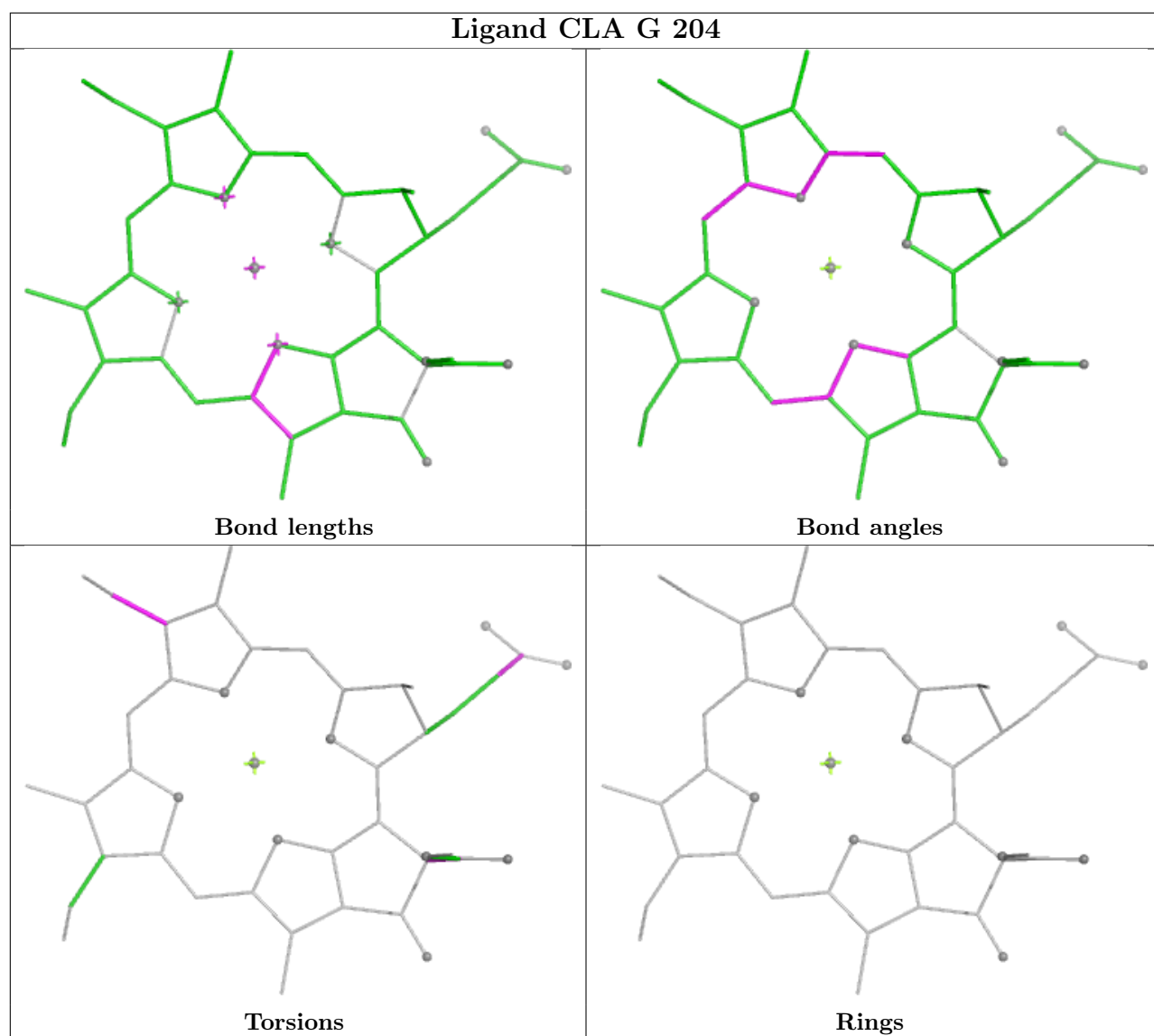


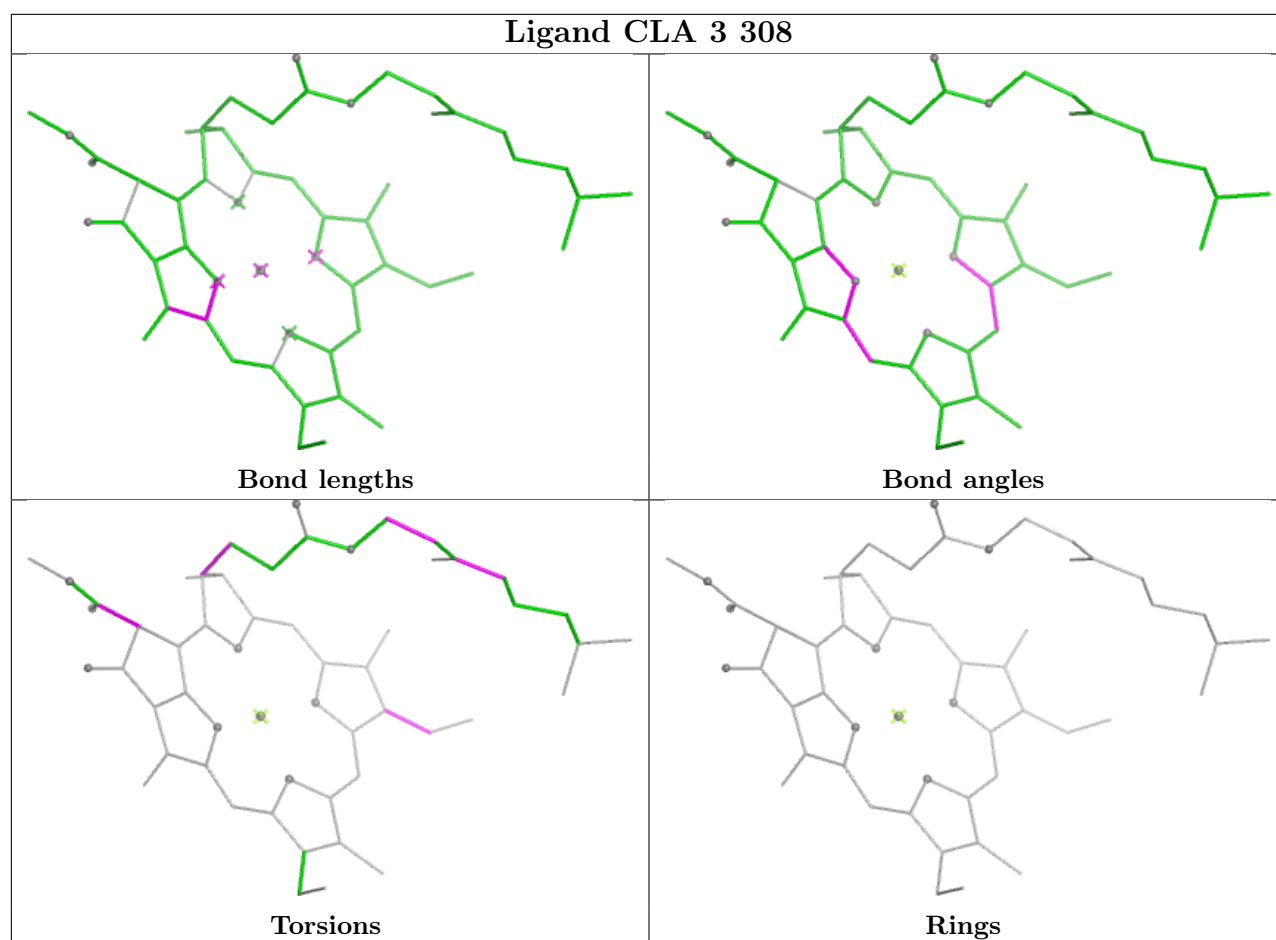


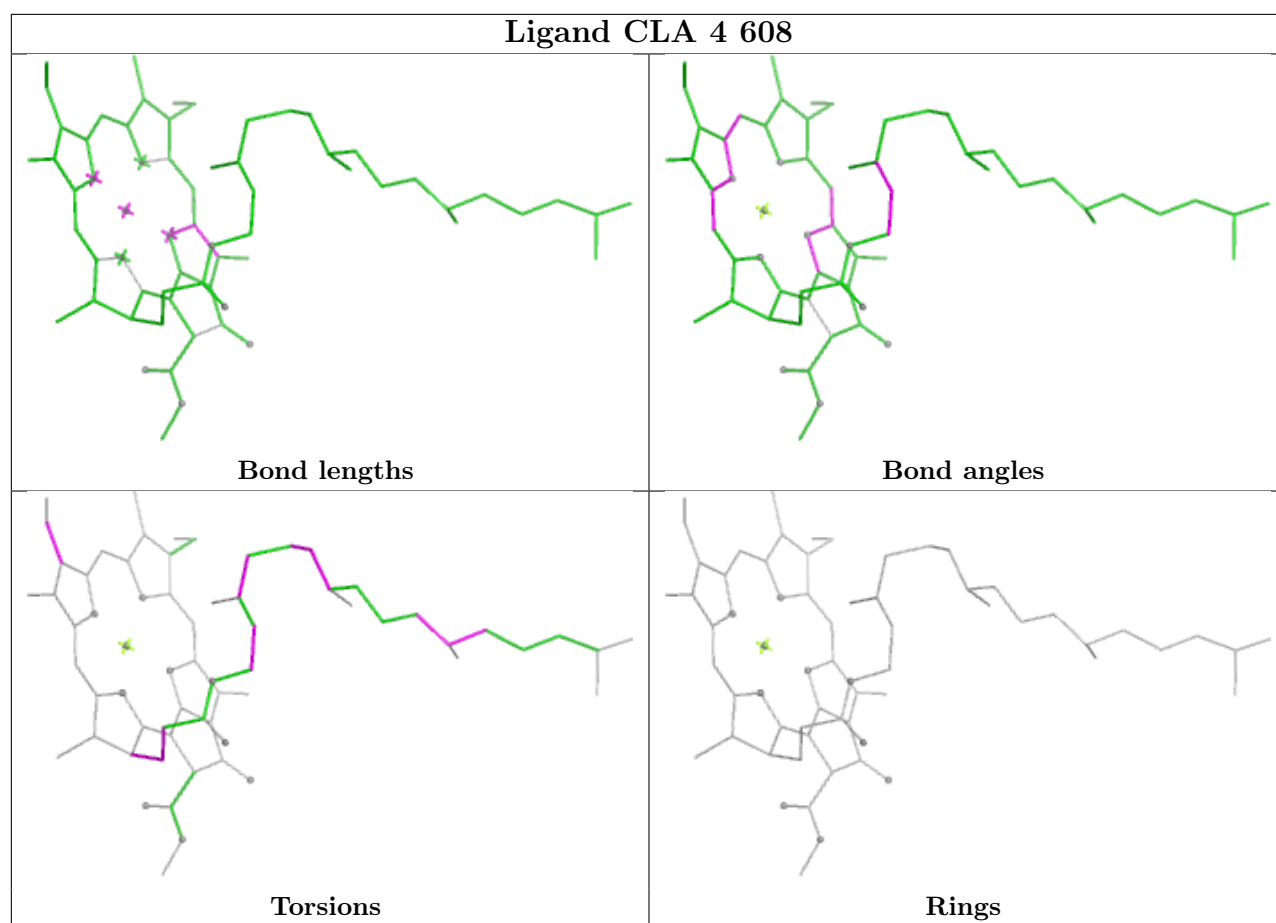


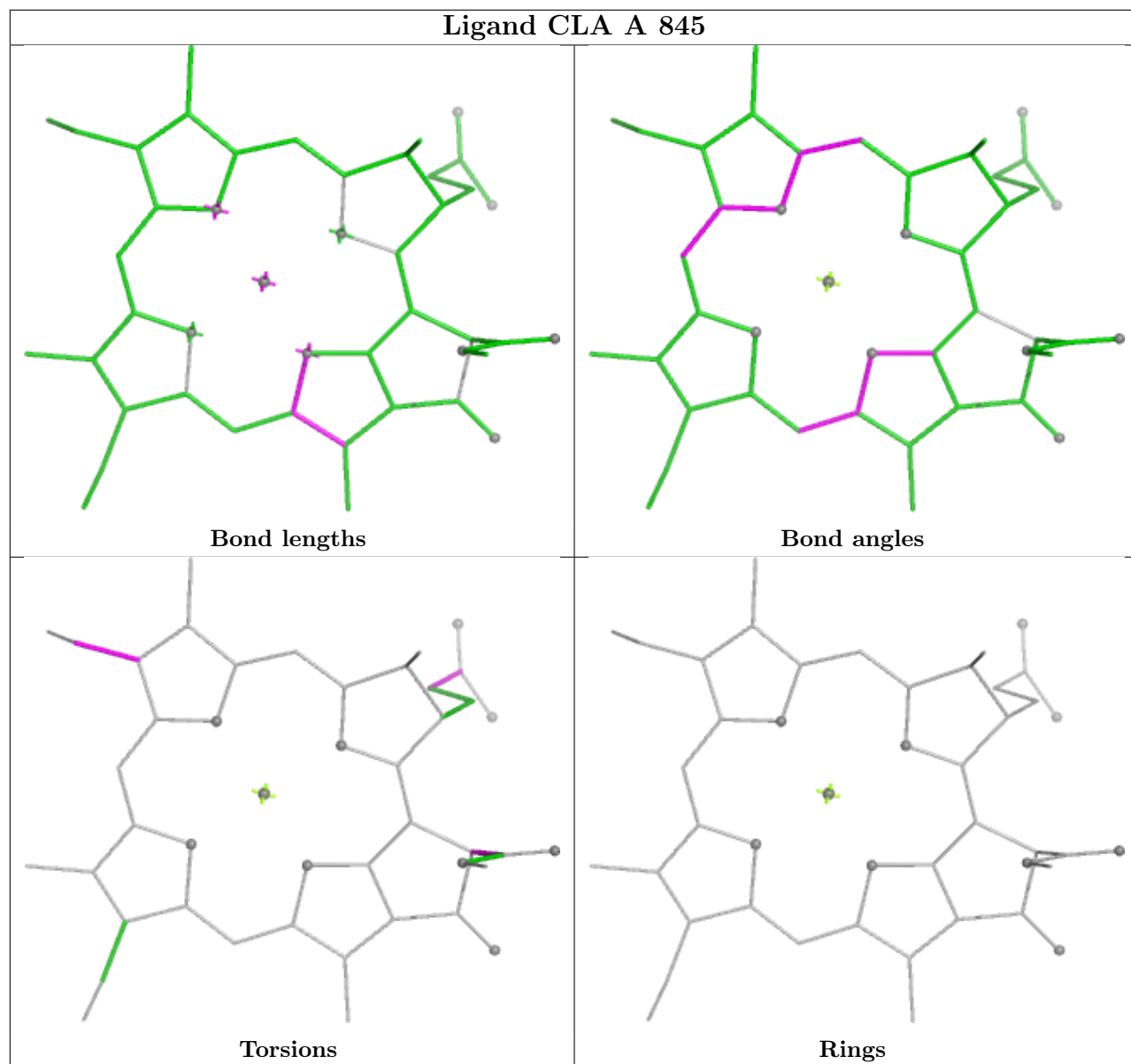


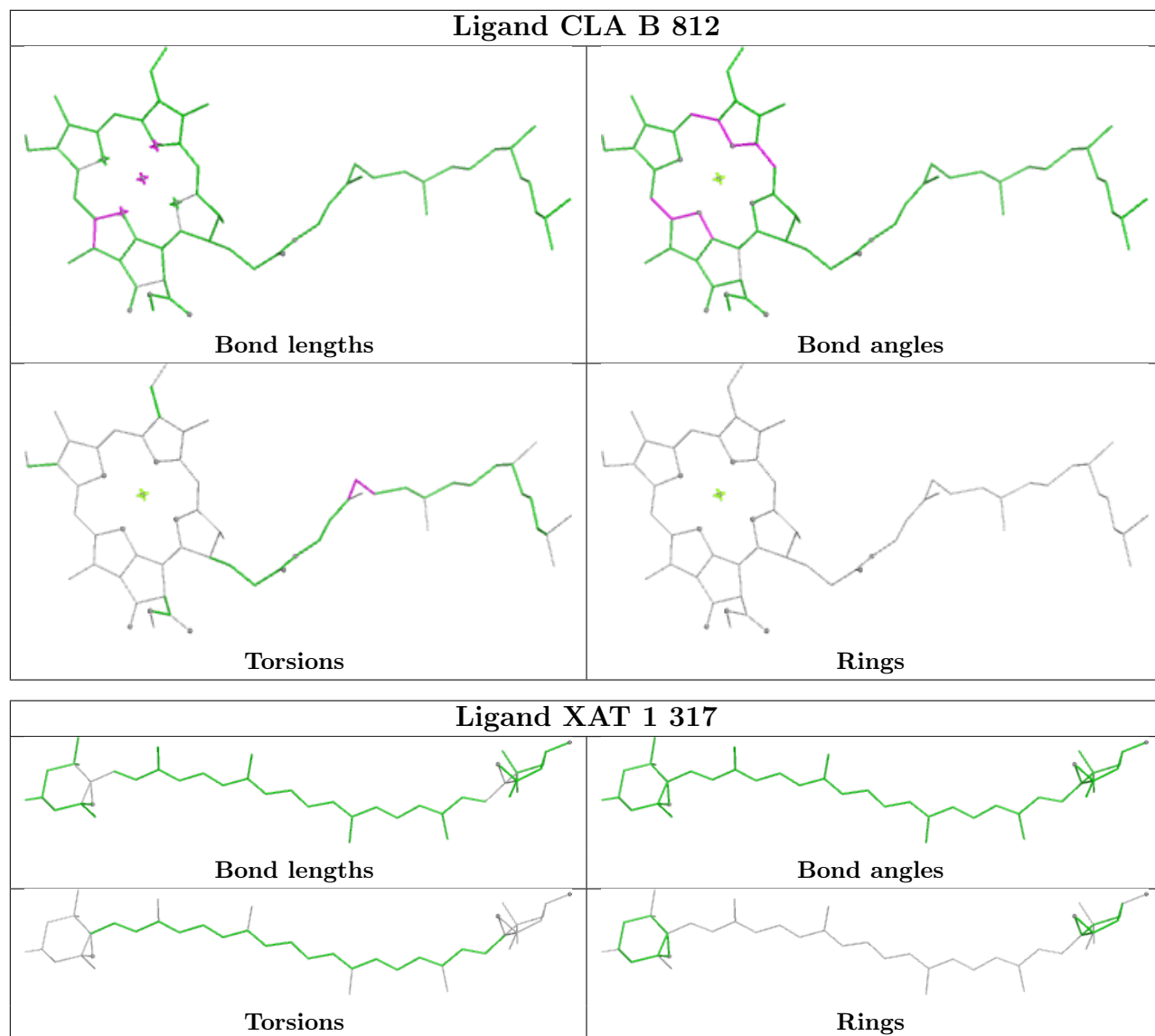


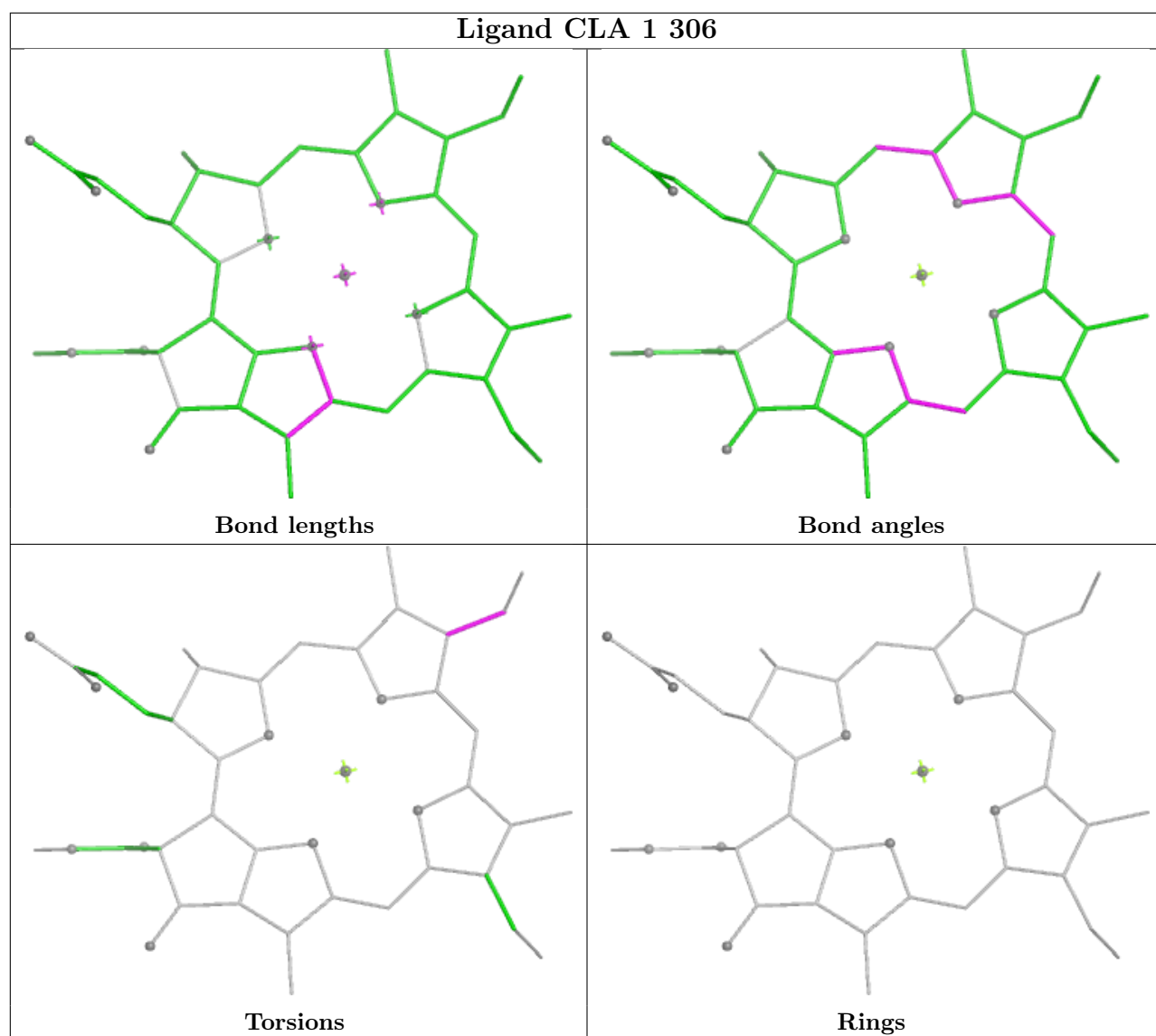


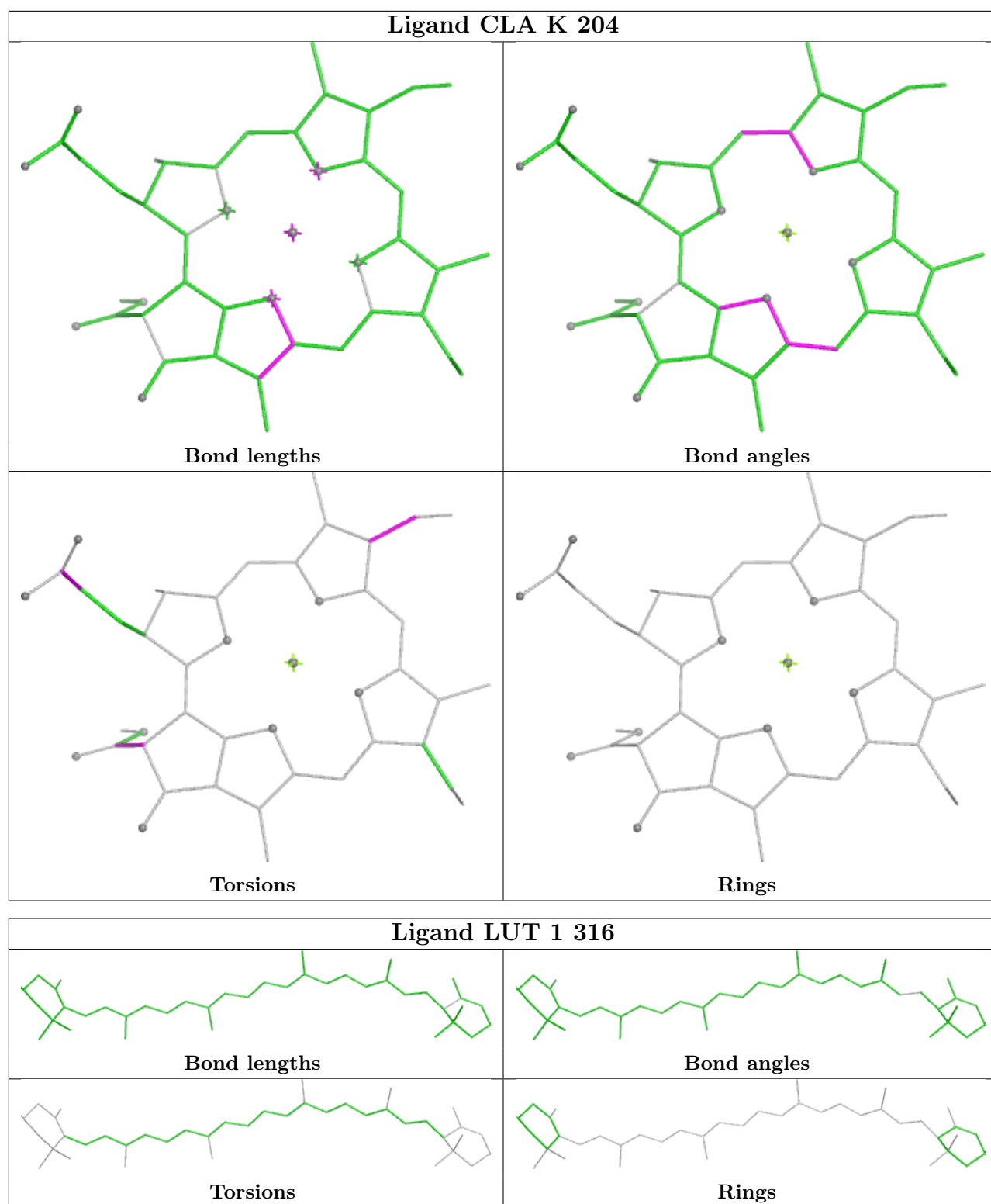


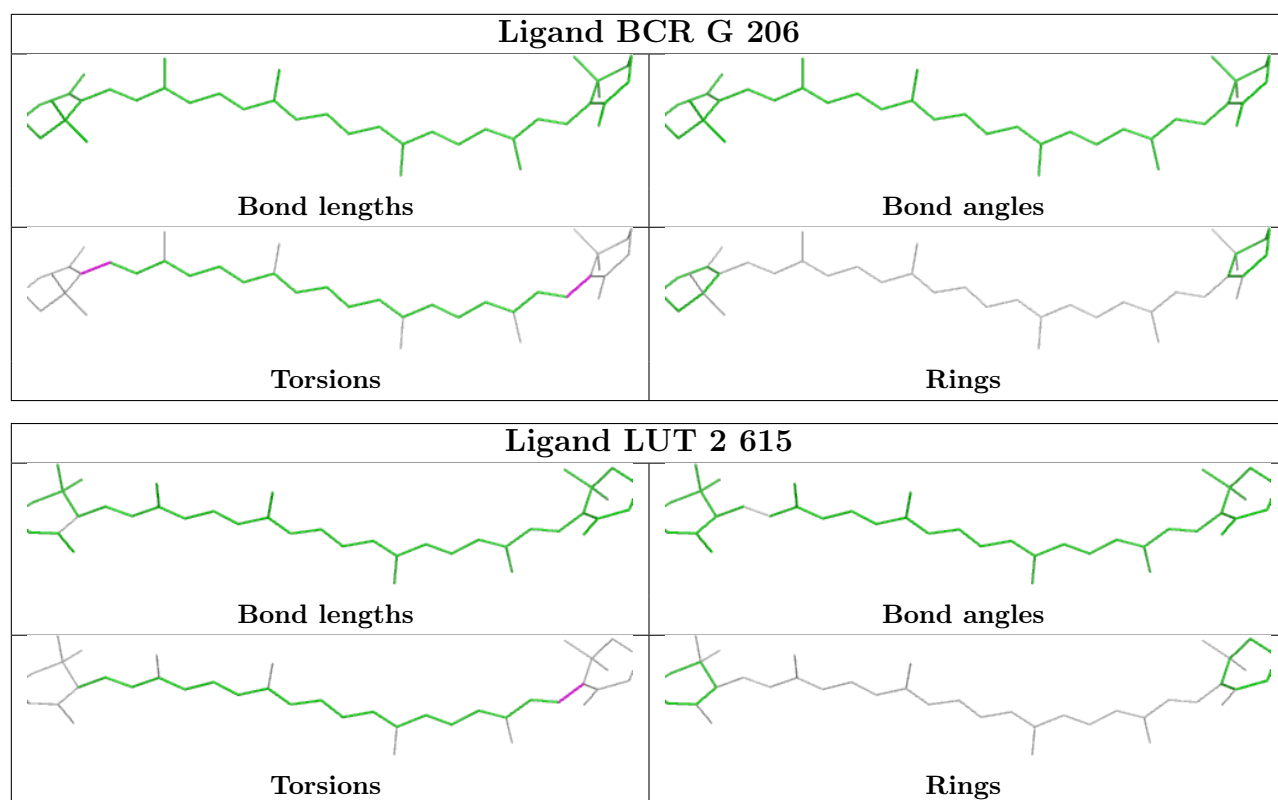


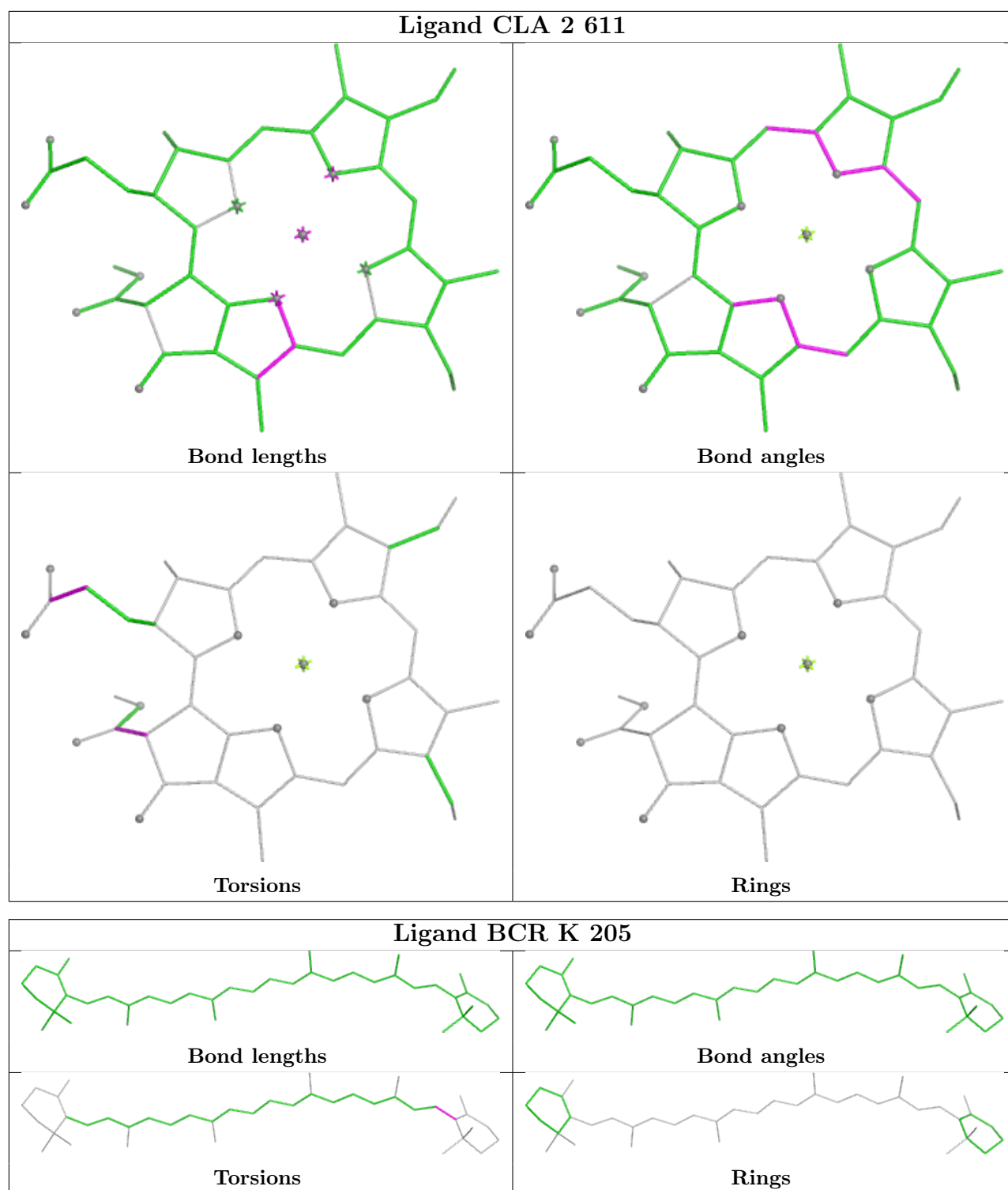


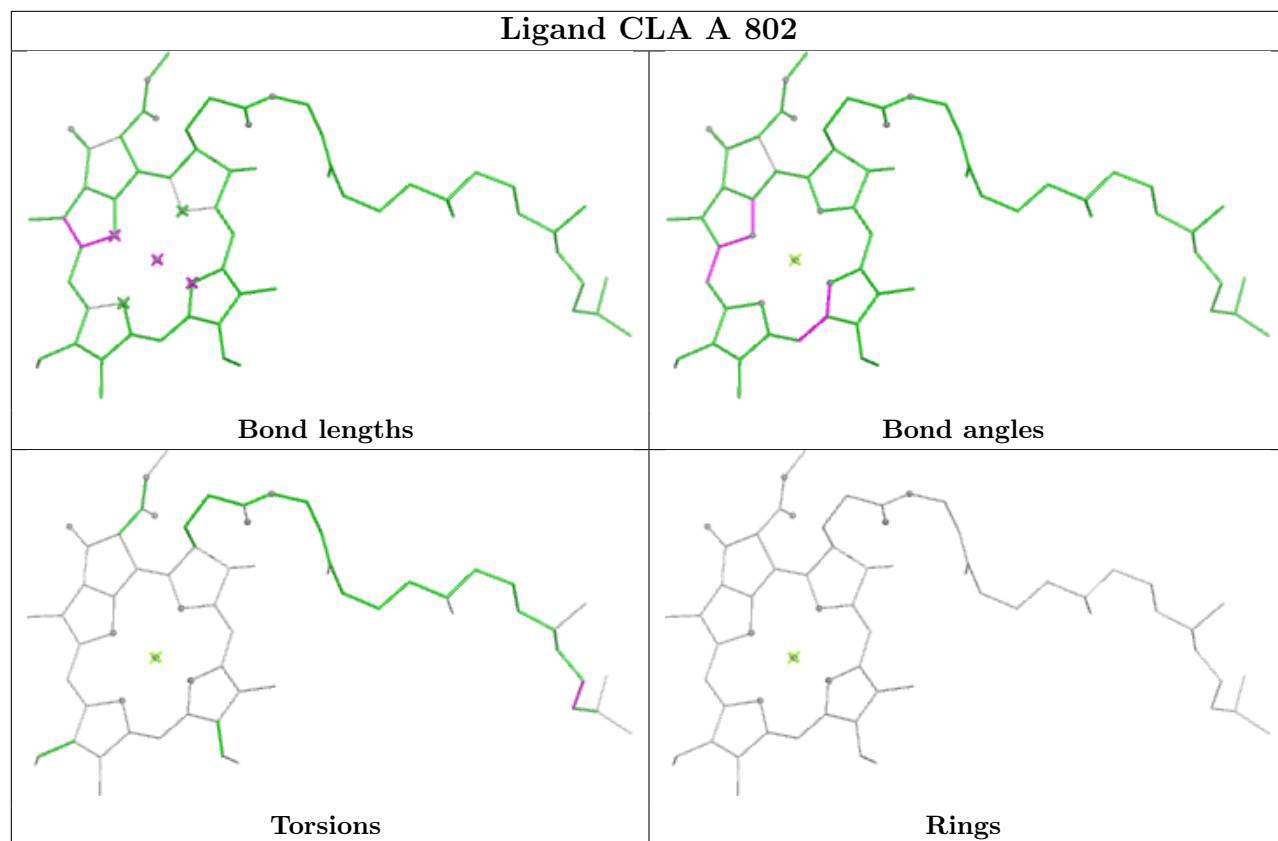


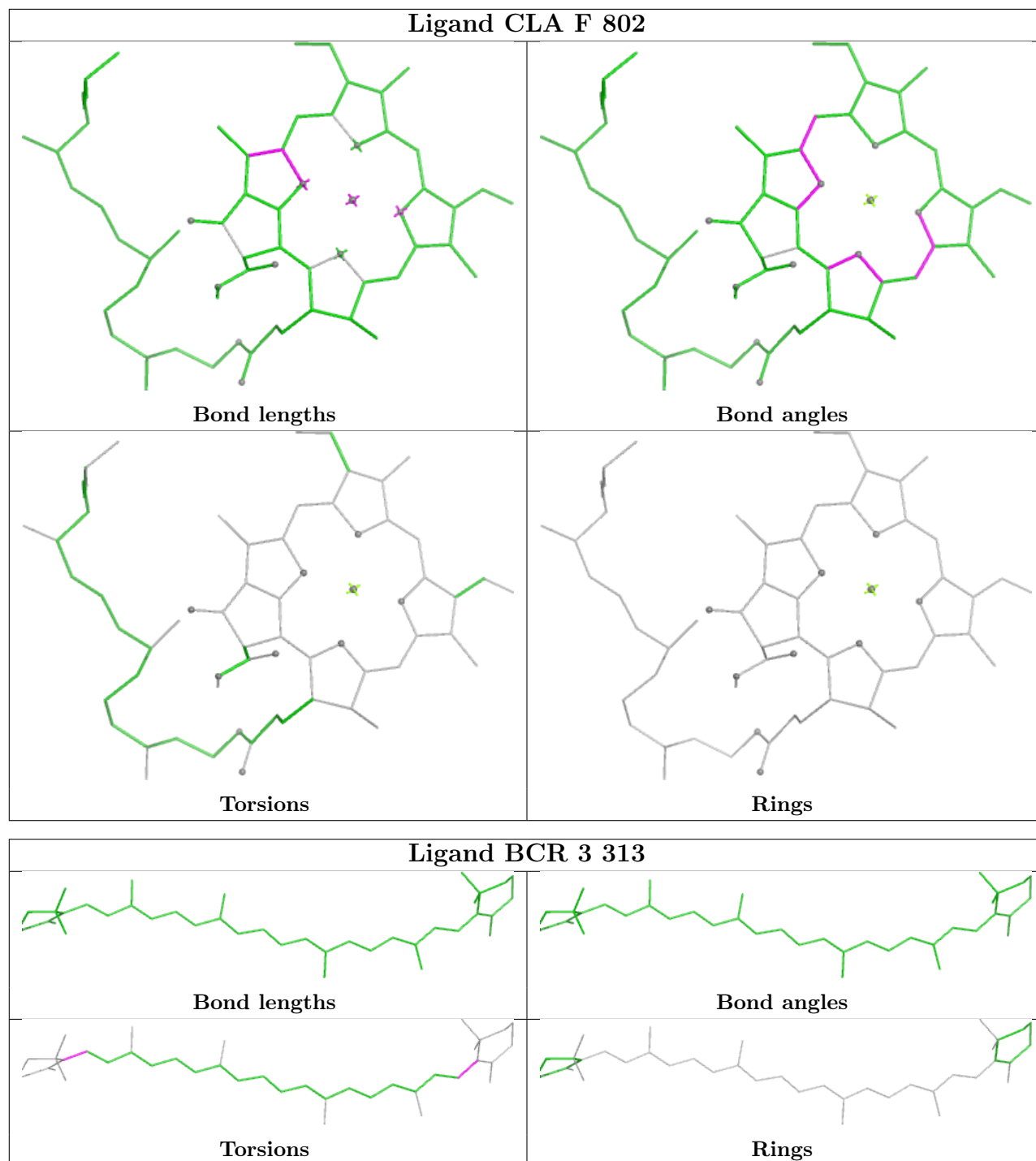




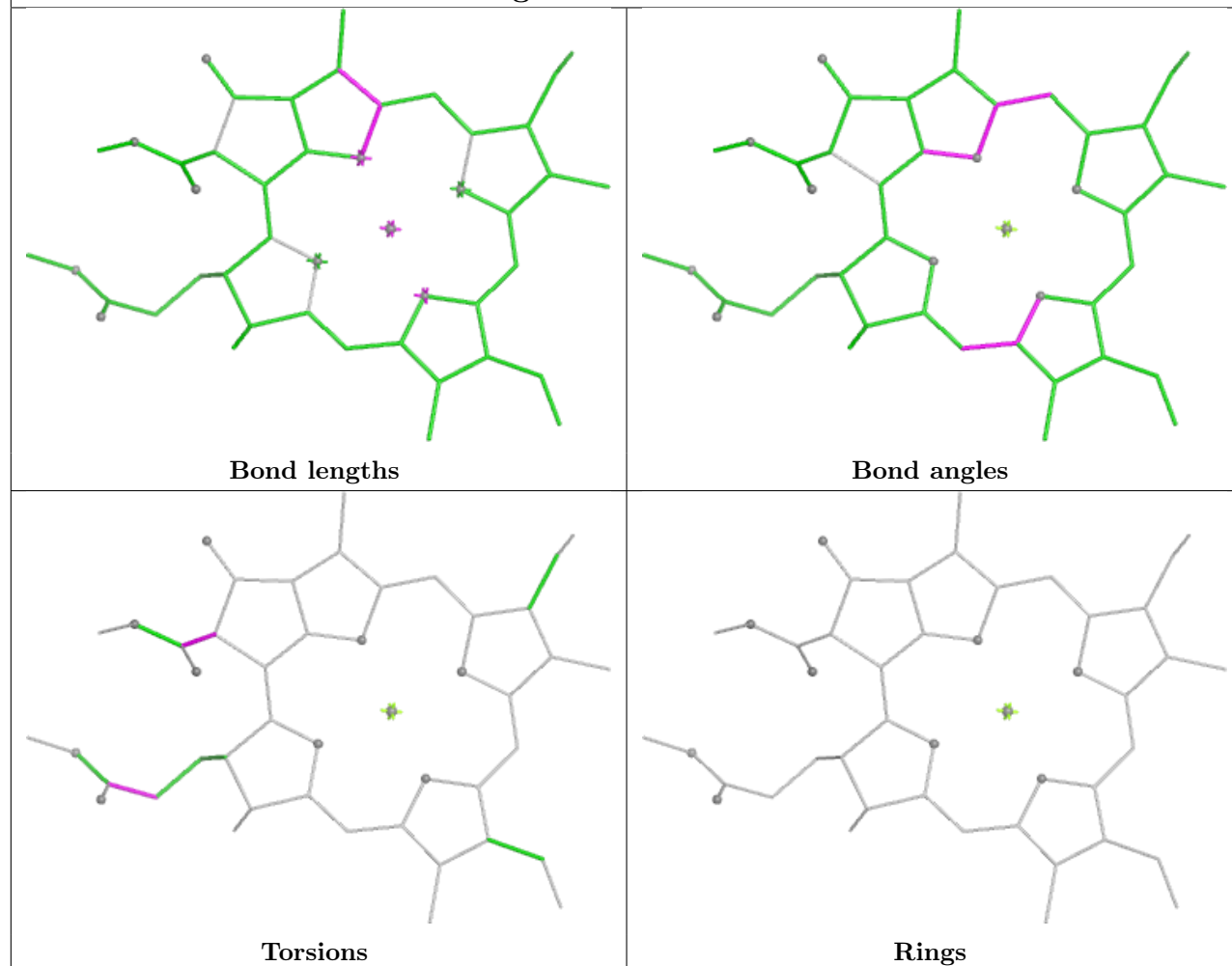




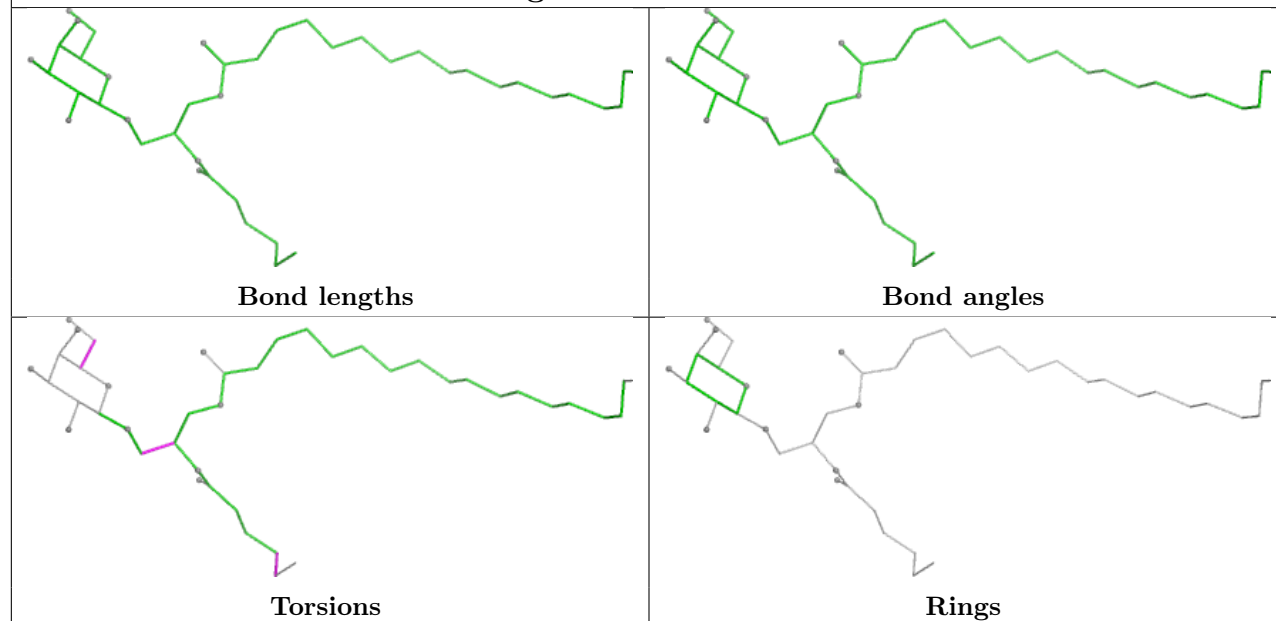


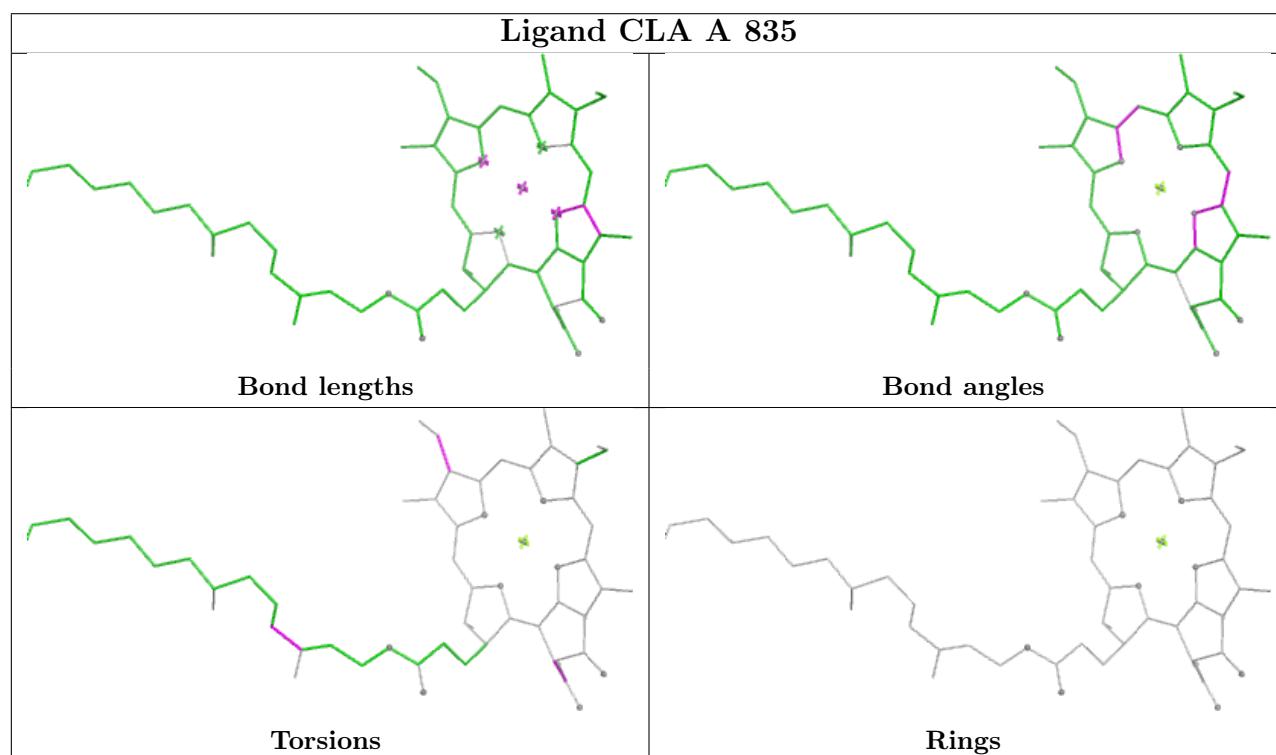
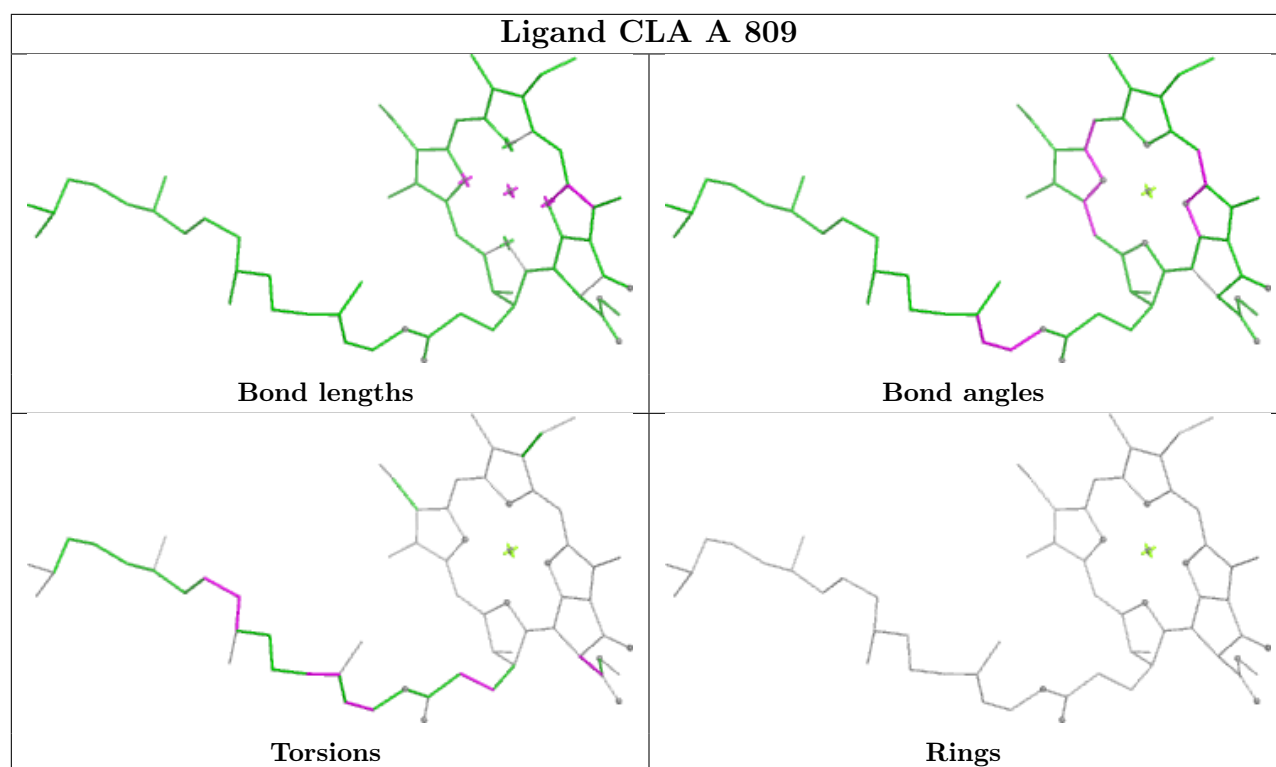


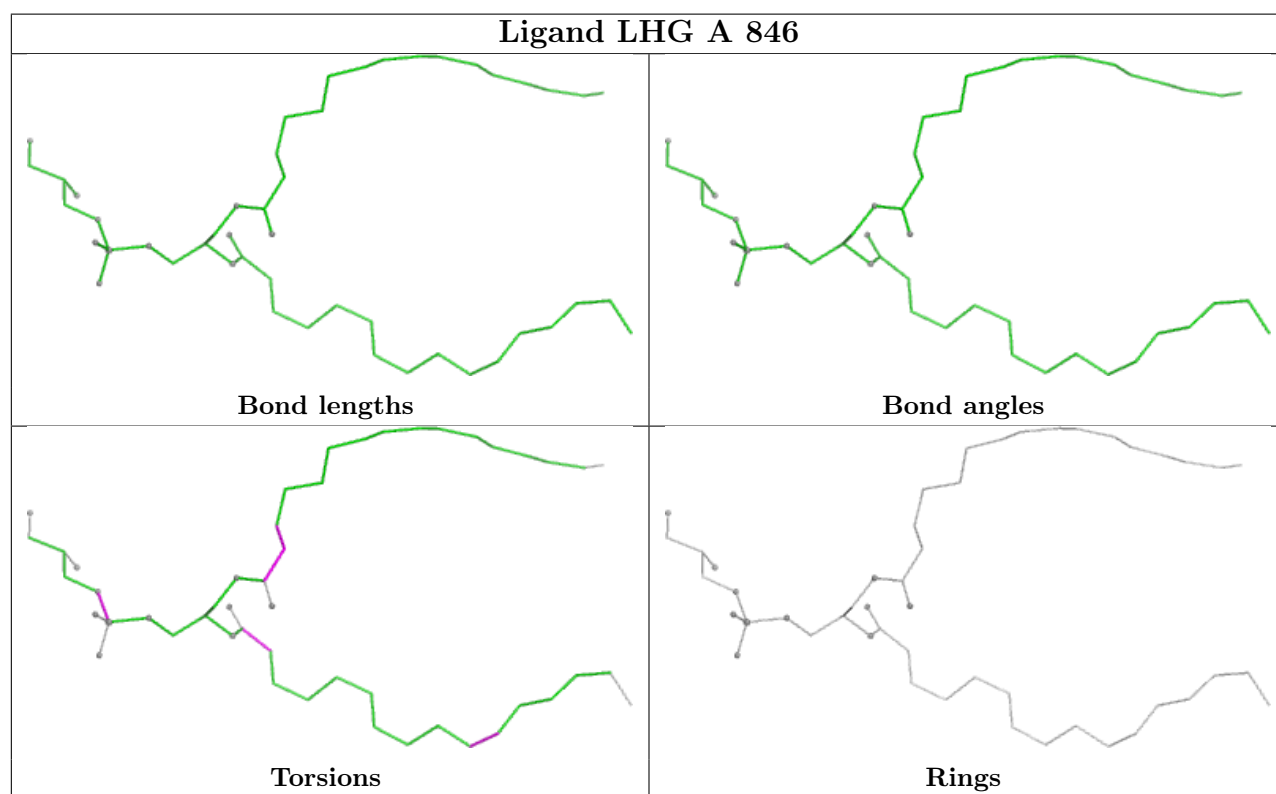
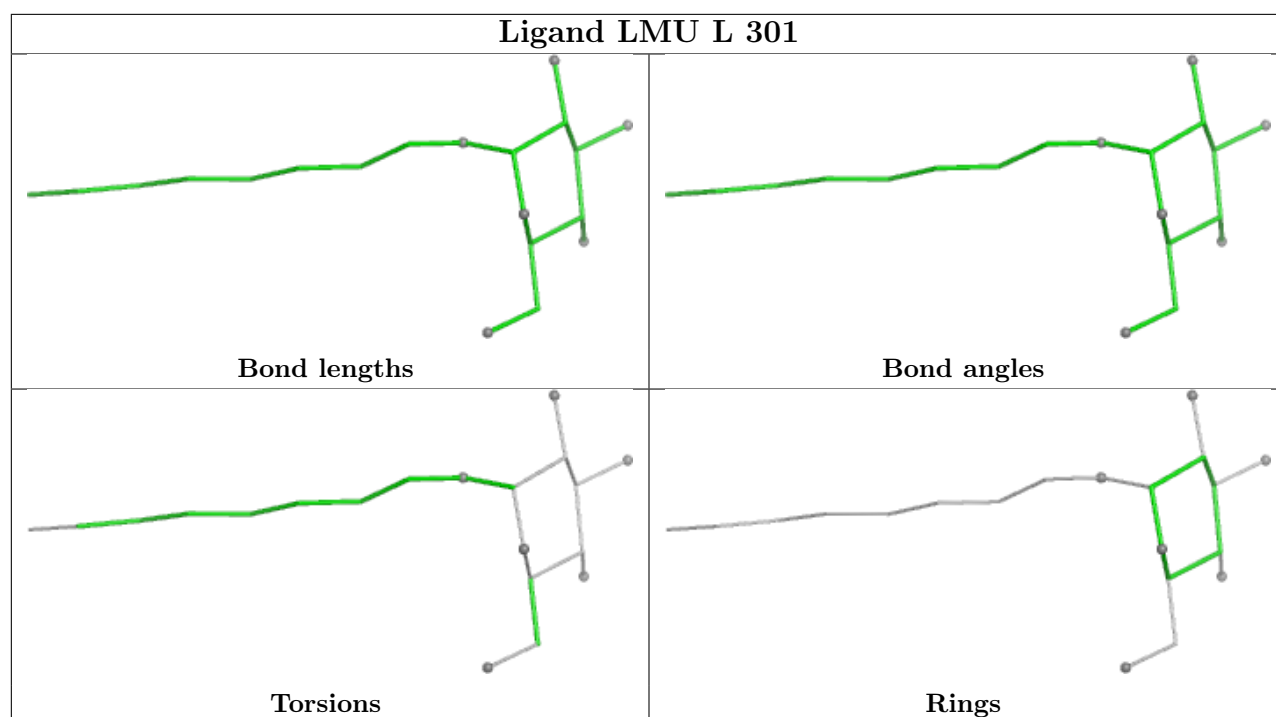
Ligand CLA G 205

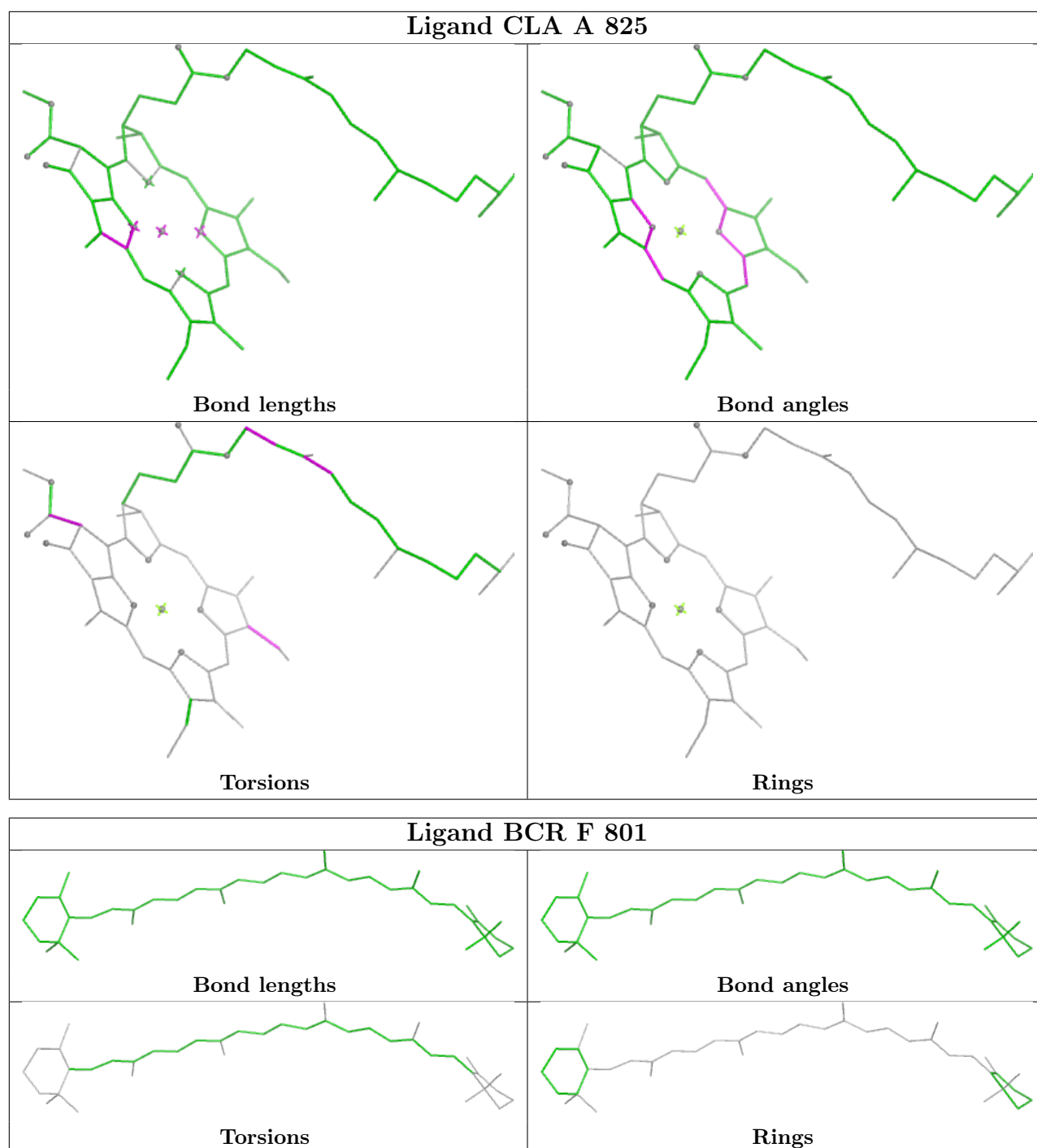


Ligand LMG A 857

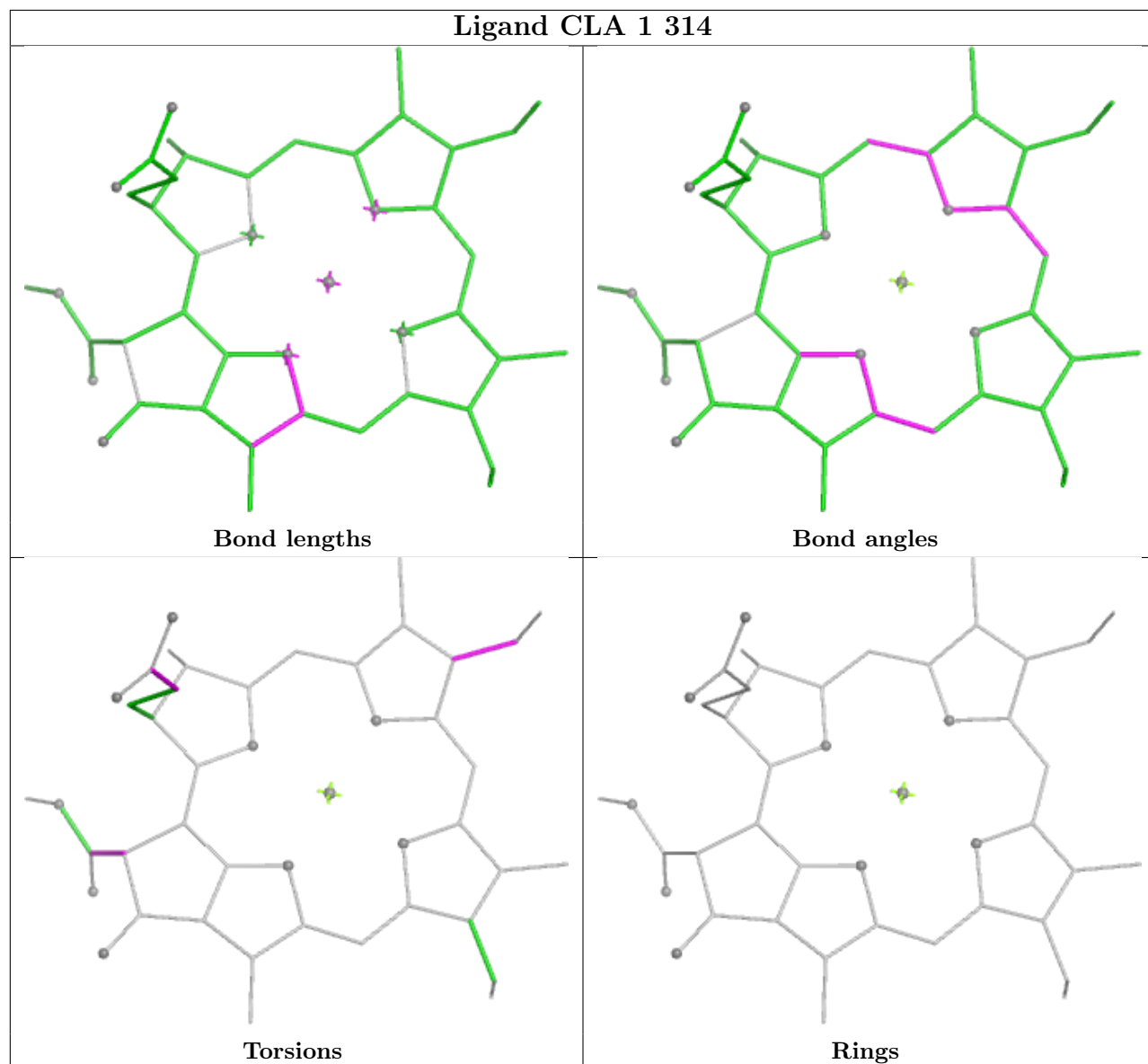


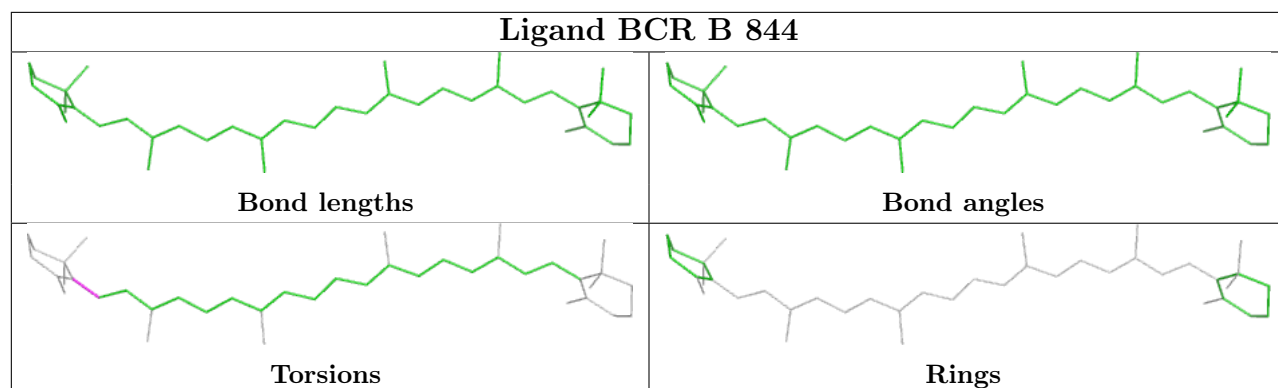
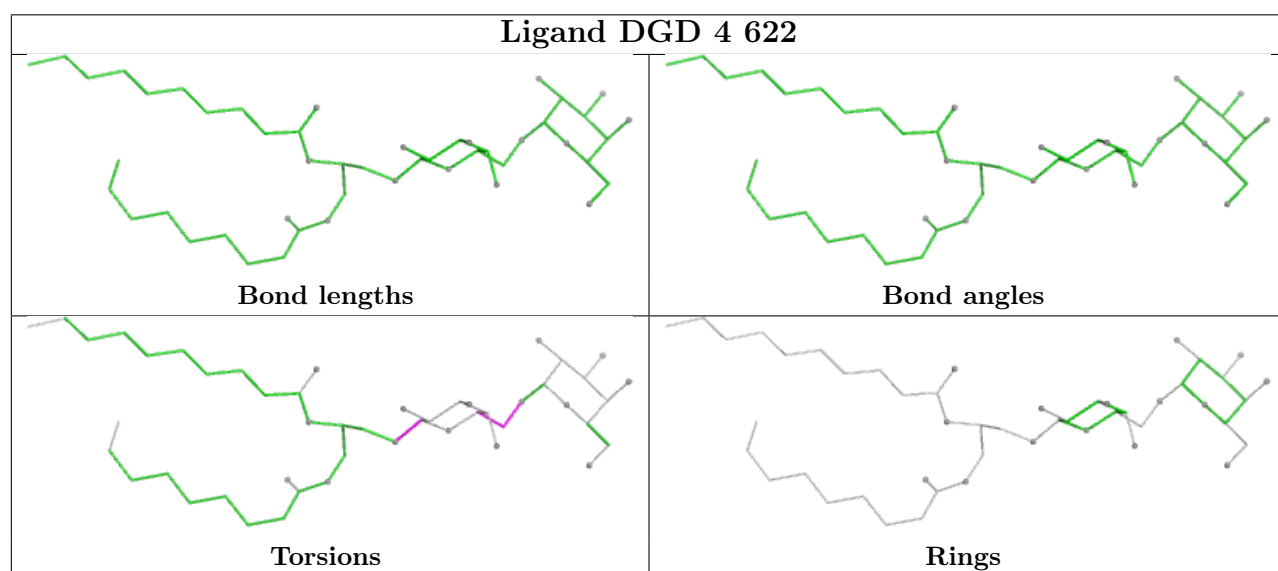
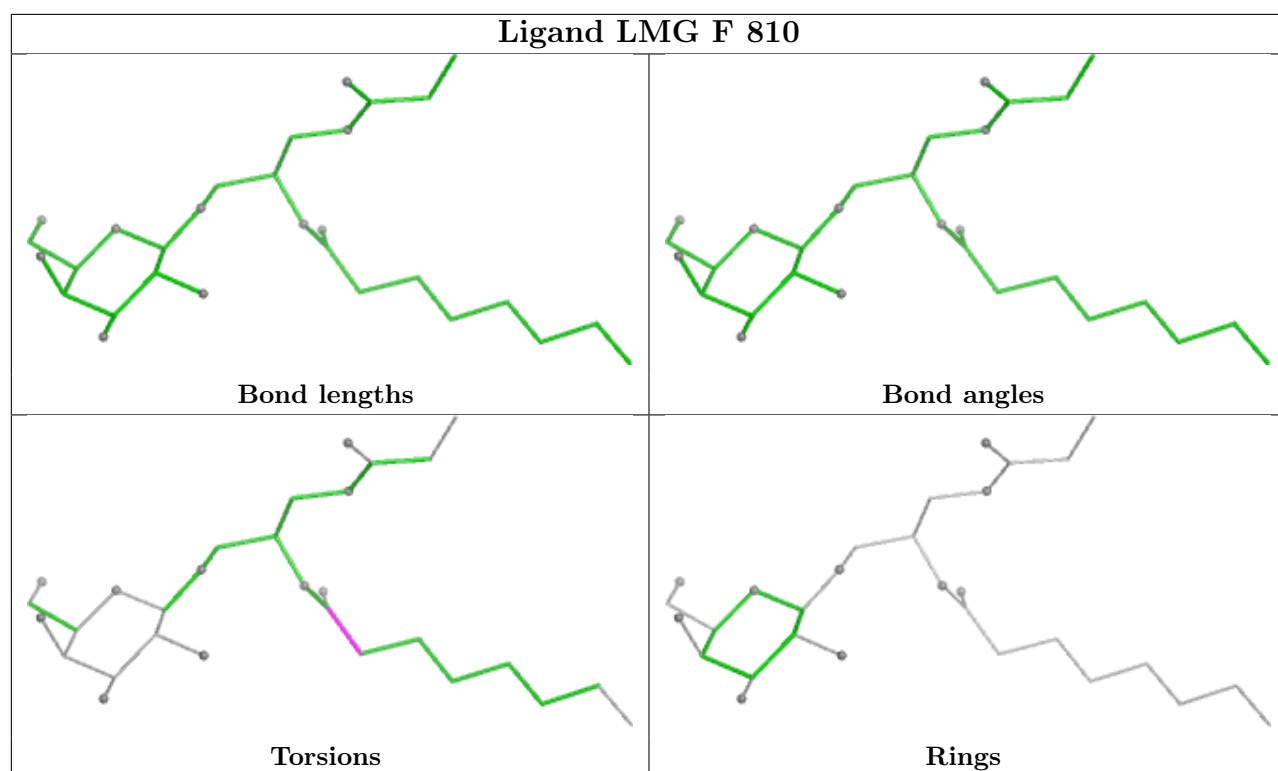


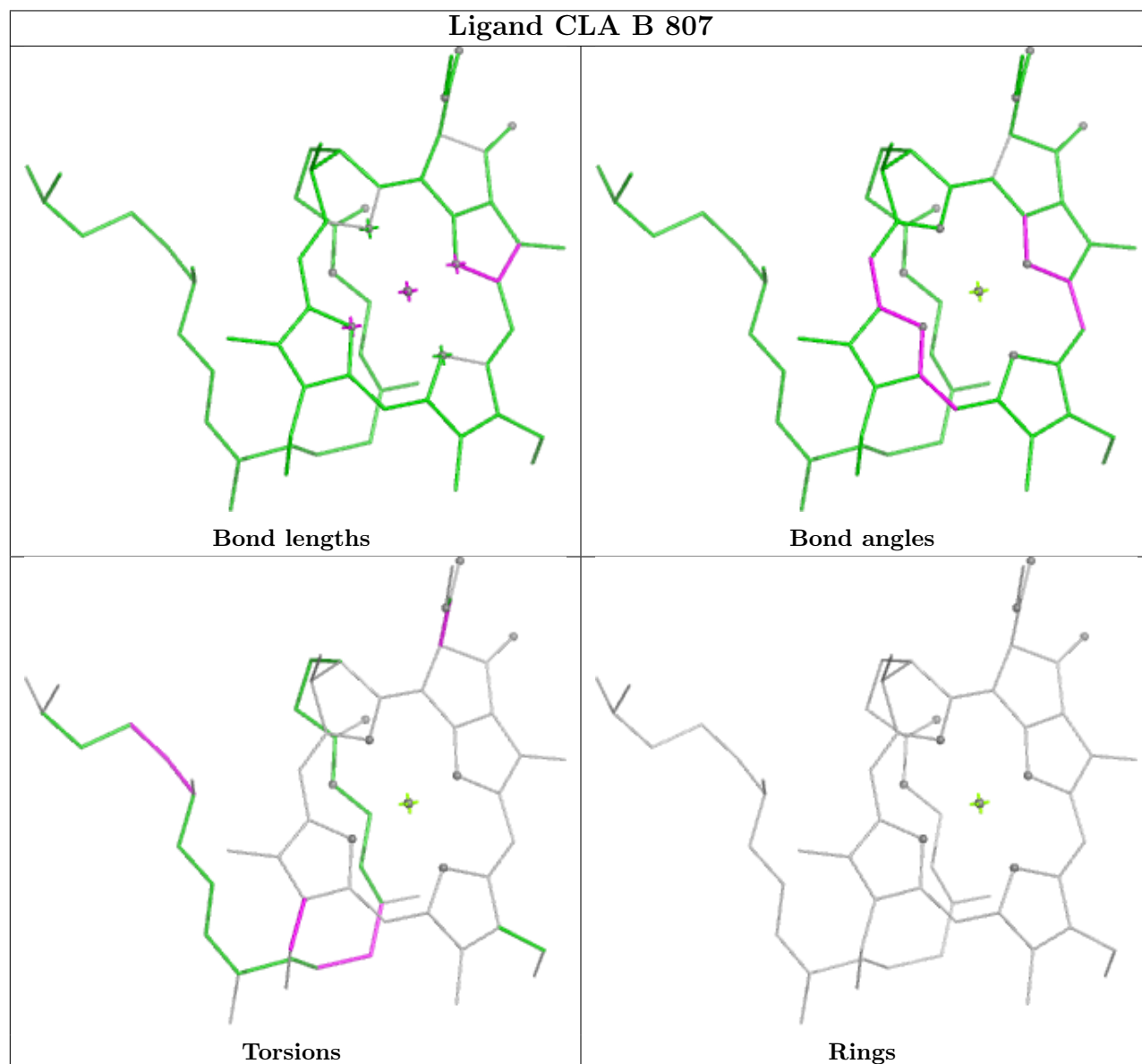
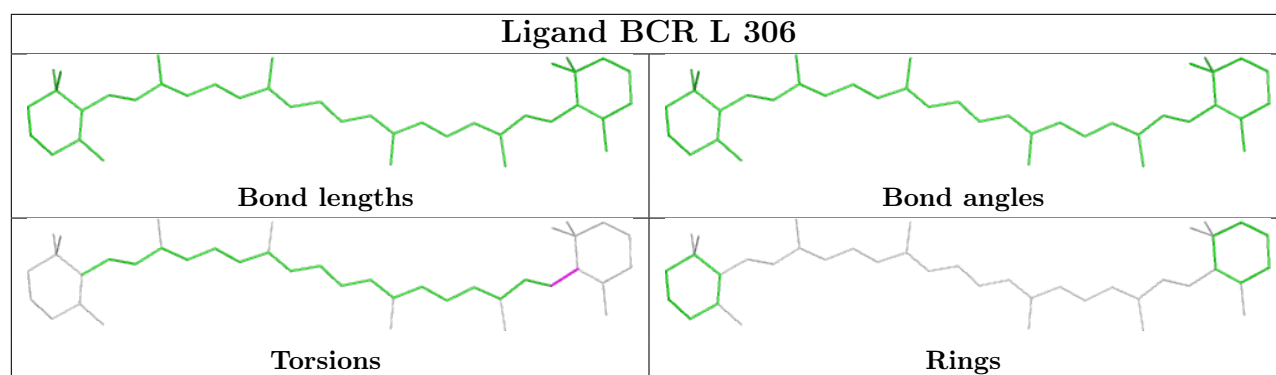


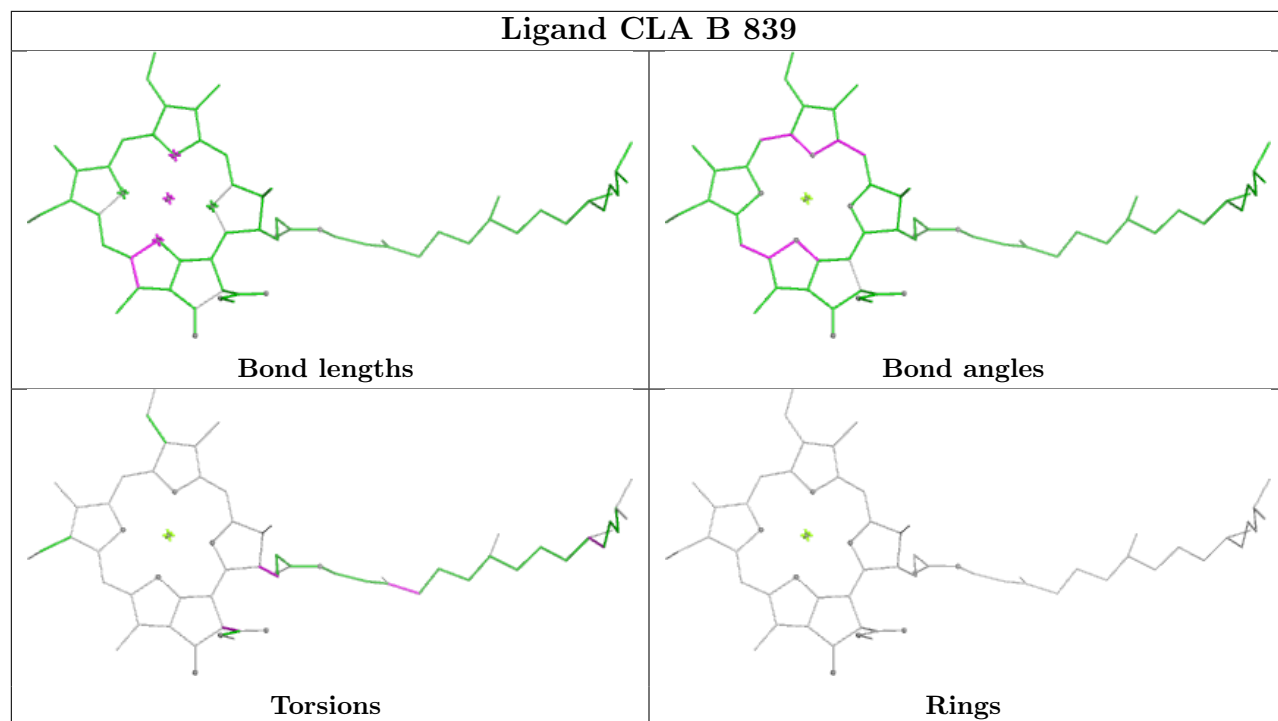


Ligand CLA 1 314

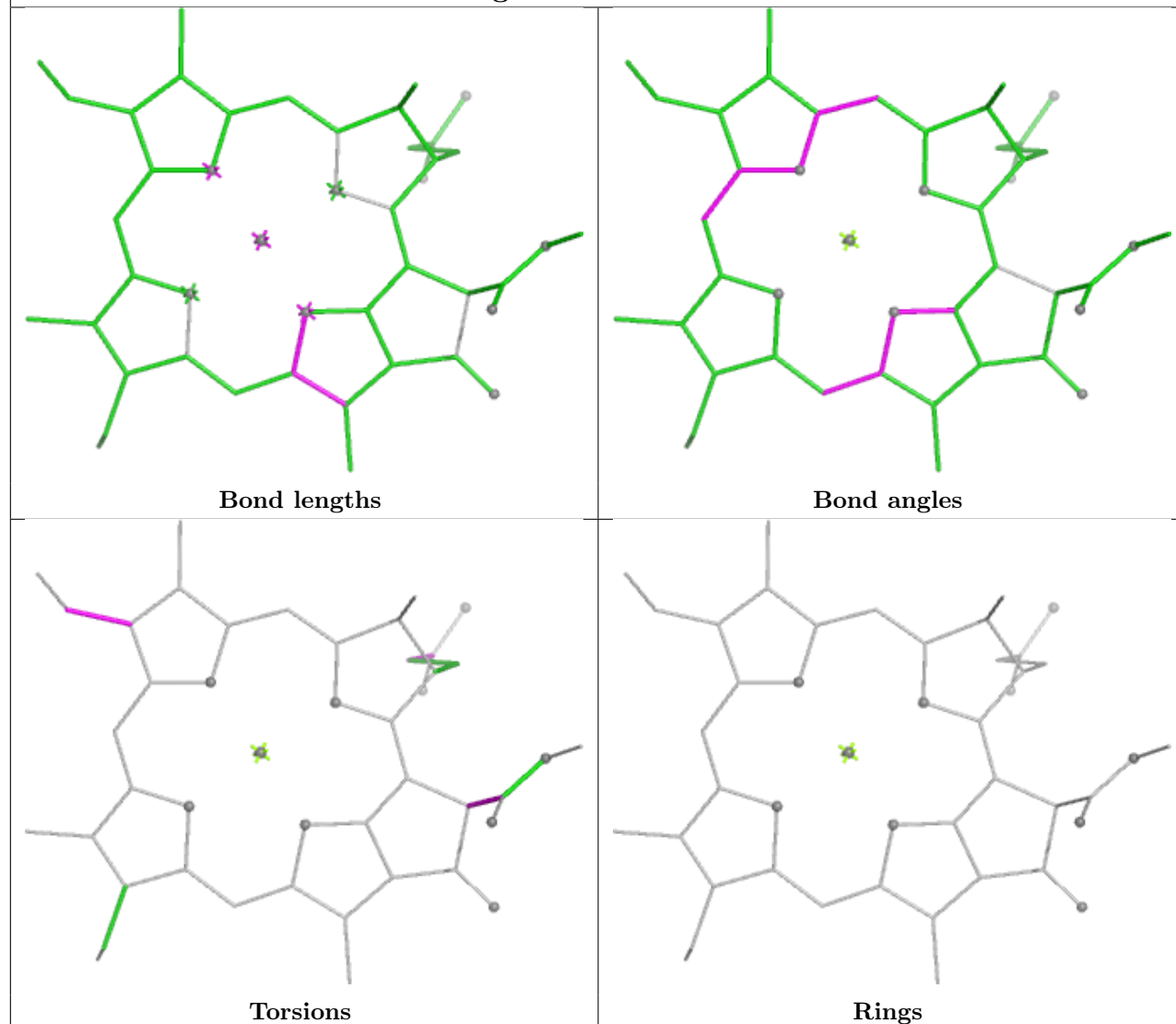




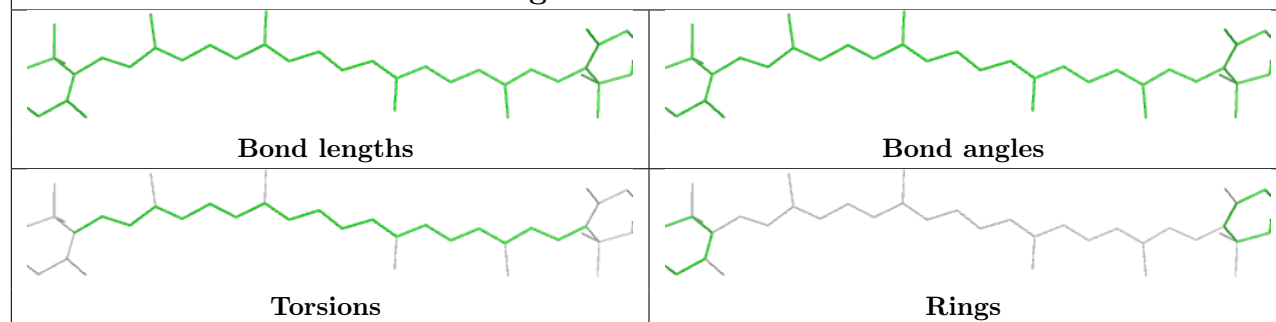


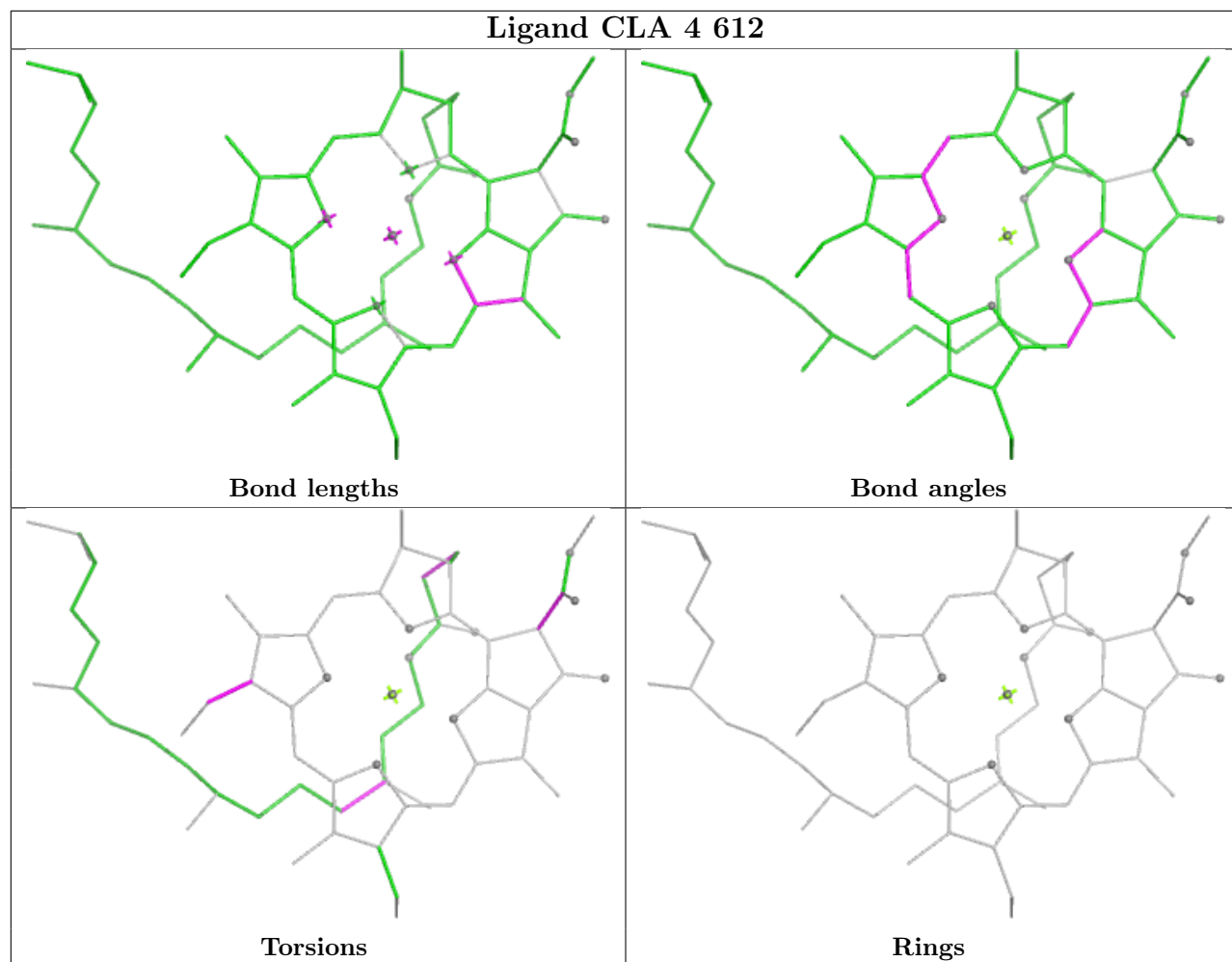


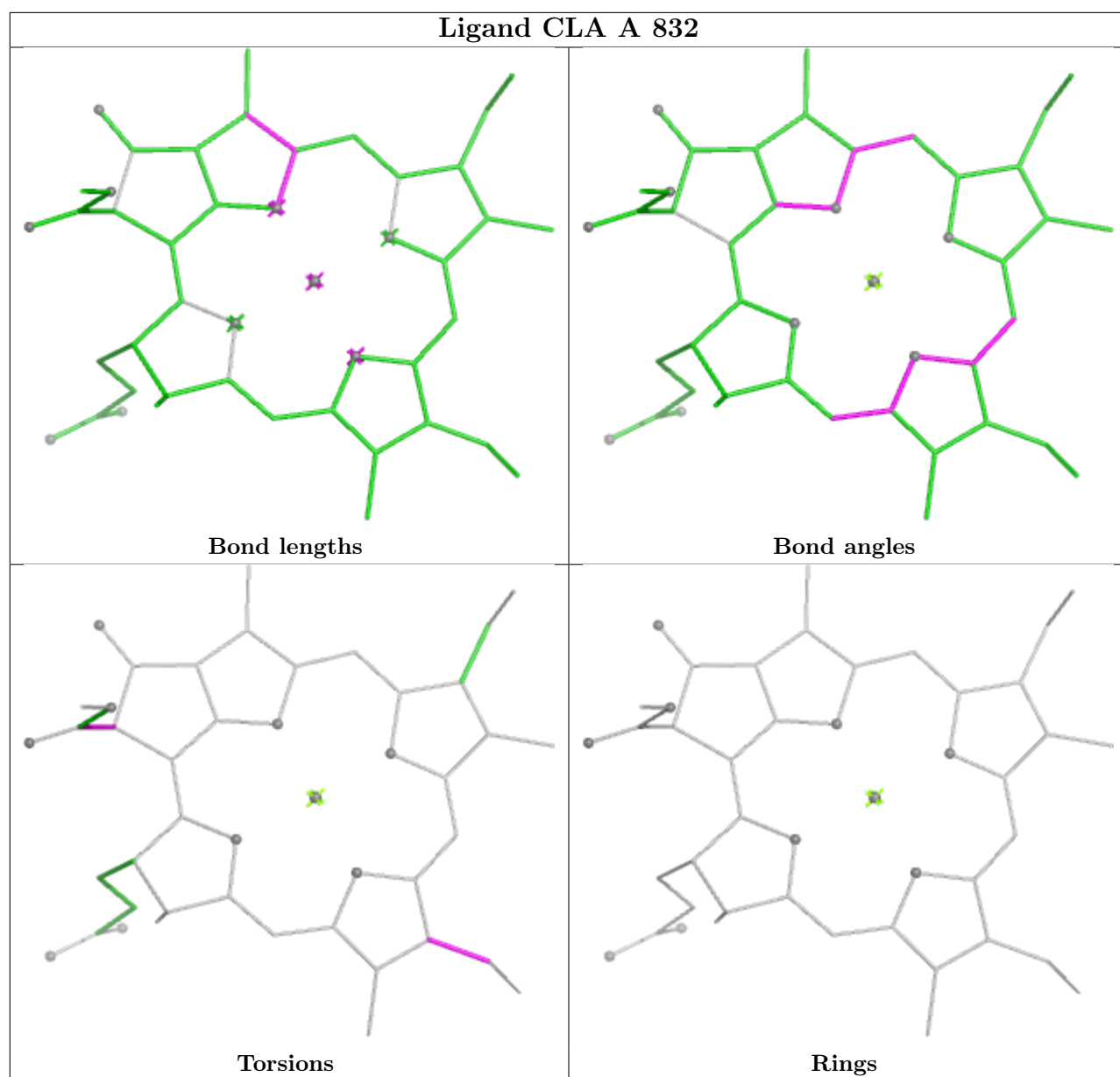
Ligand CLA L 303

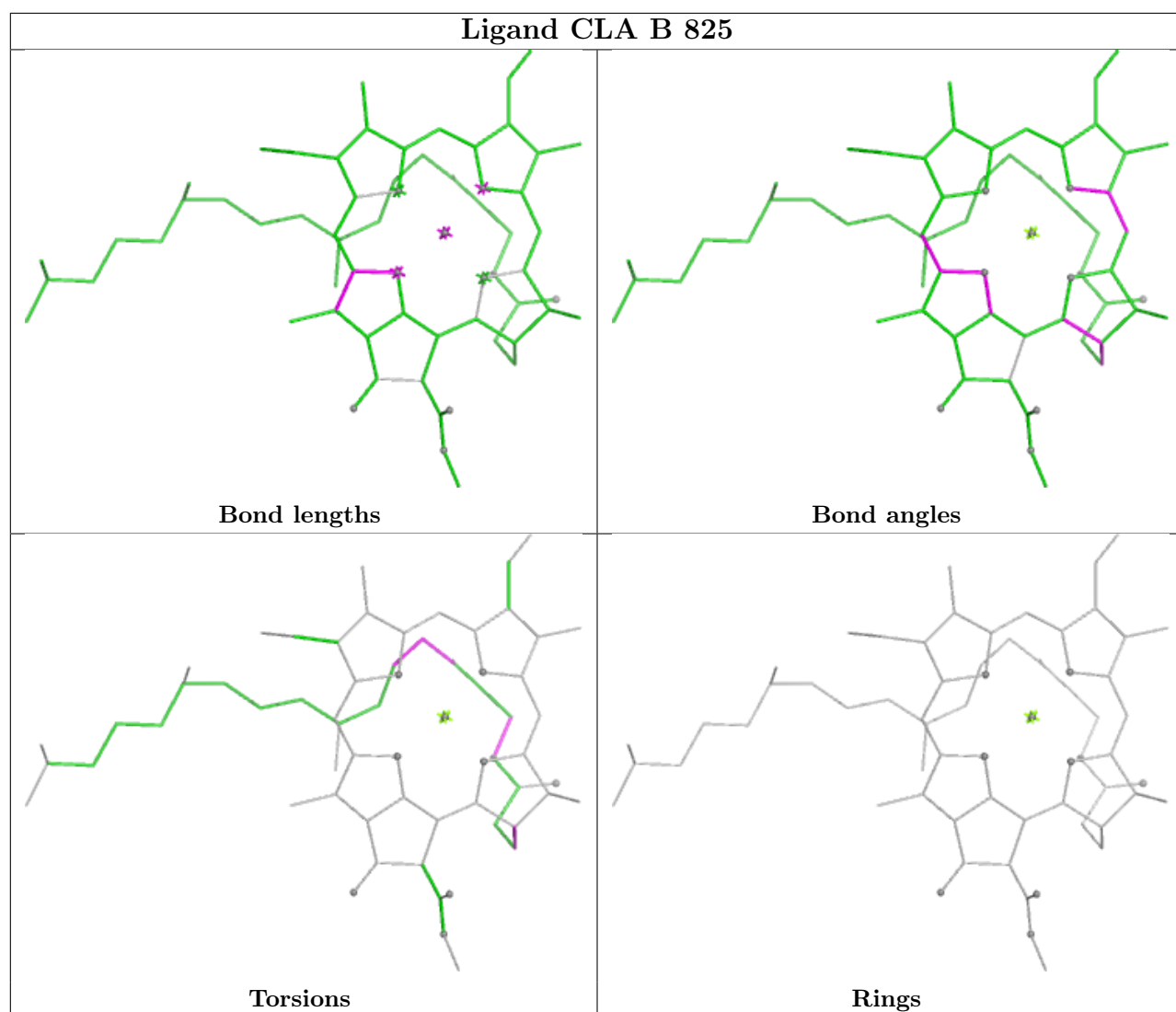


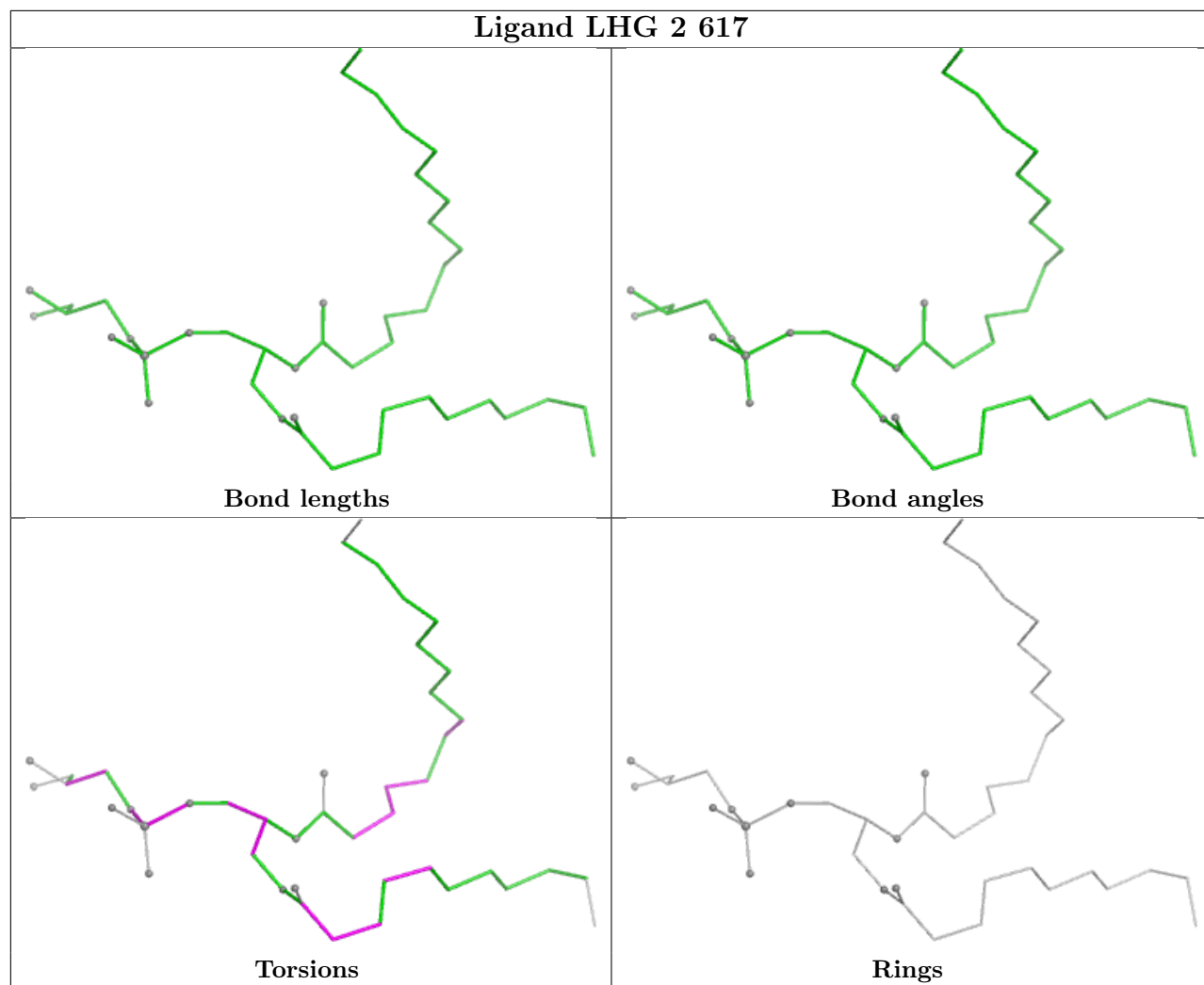
Ligand BCR K 202

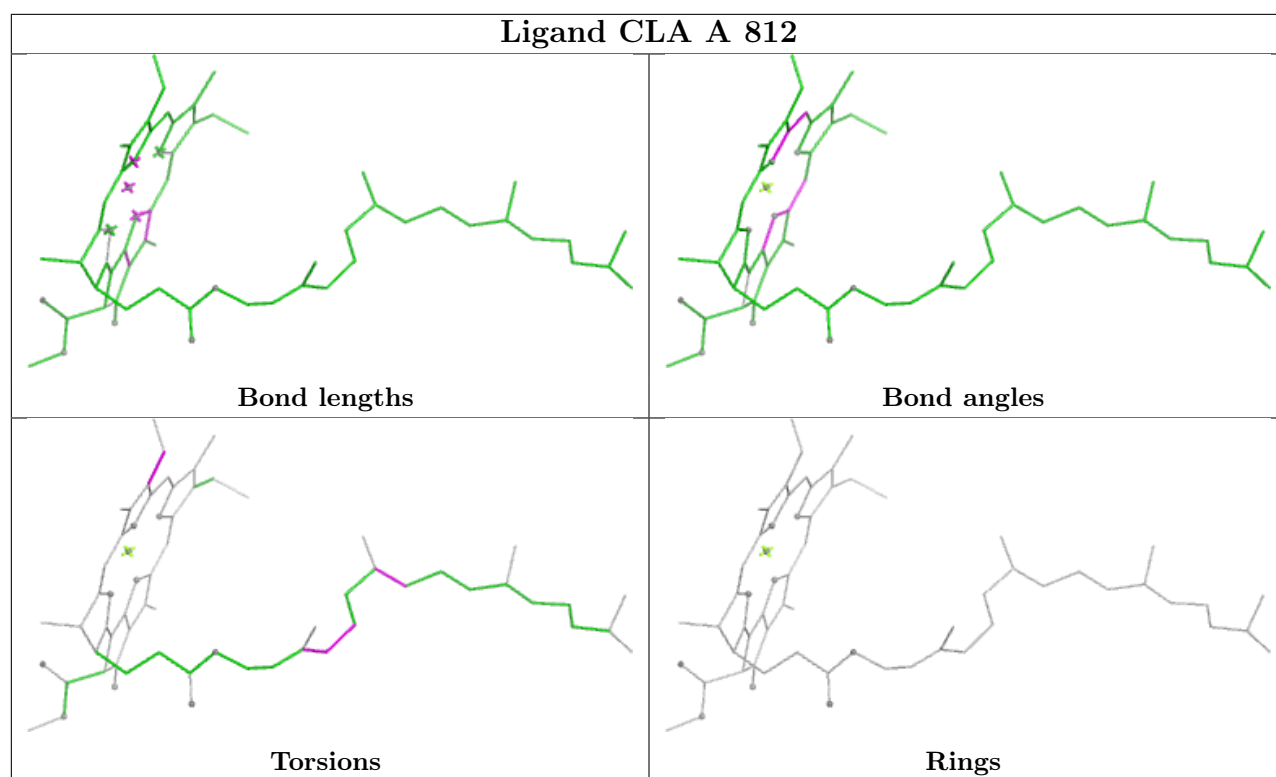


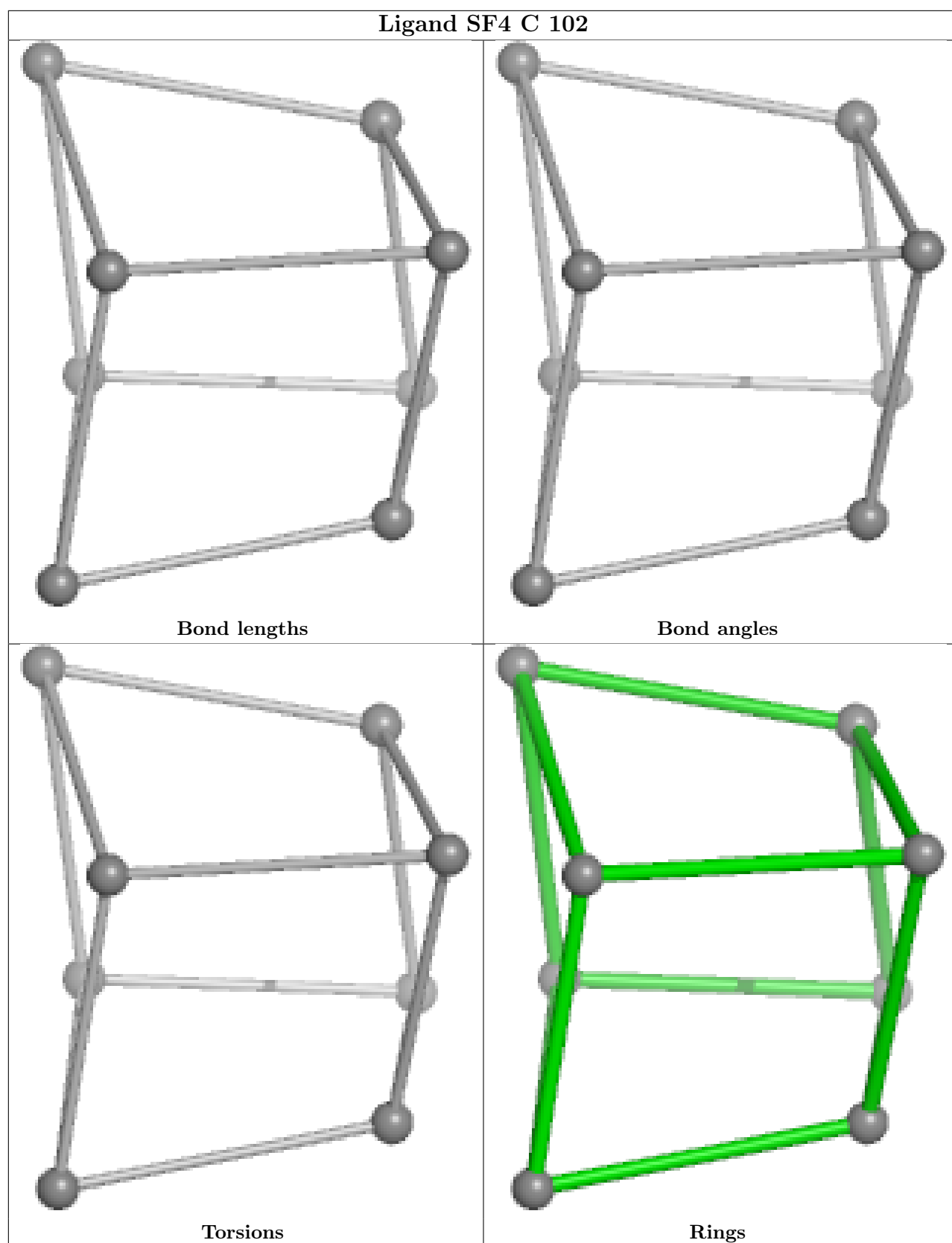




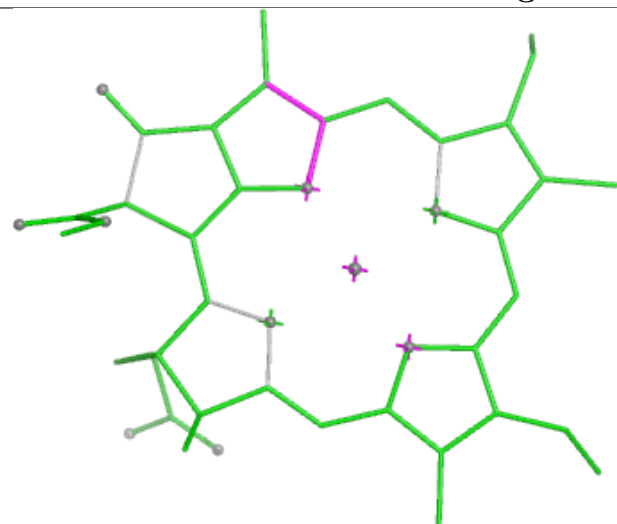




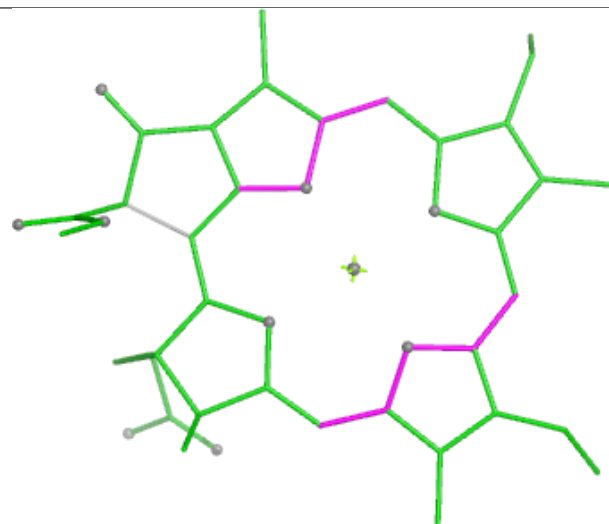




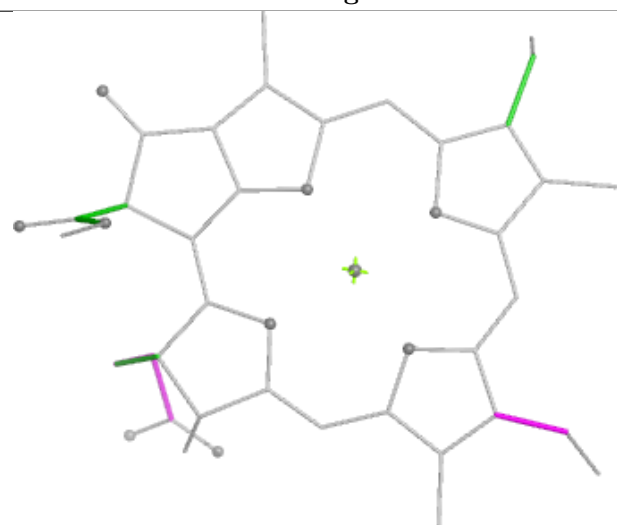
Ligand CLA A 821



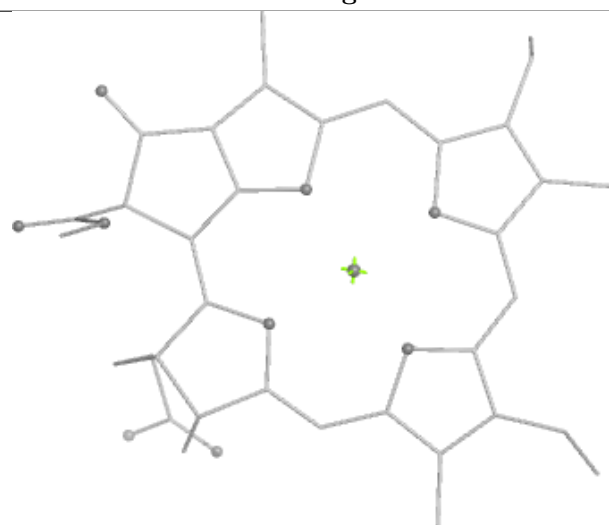
Bond lengths



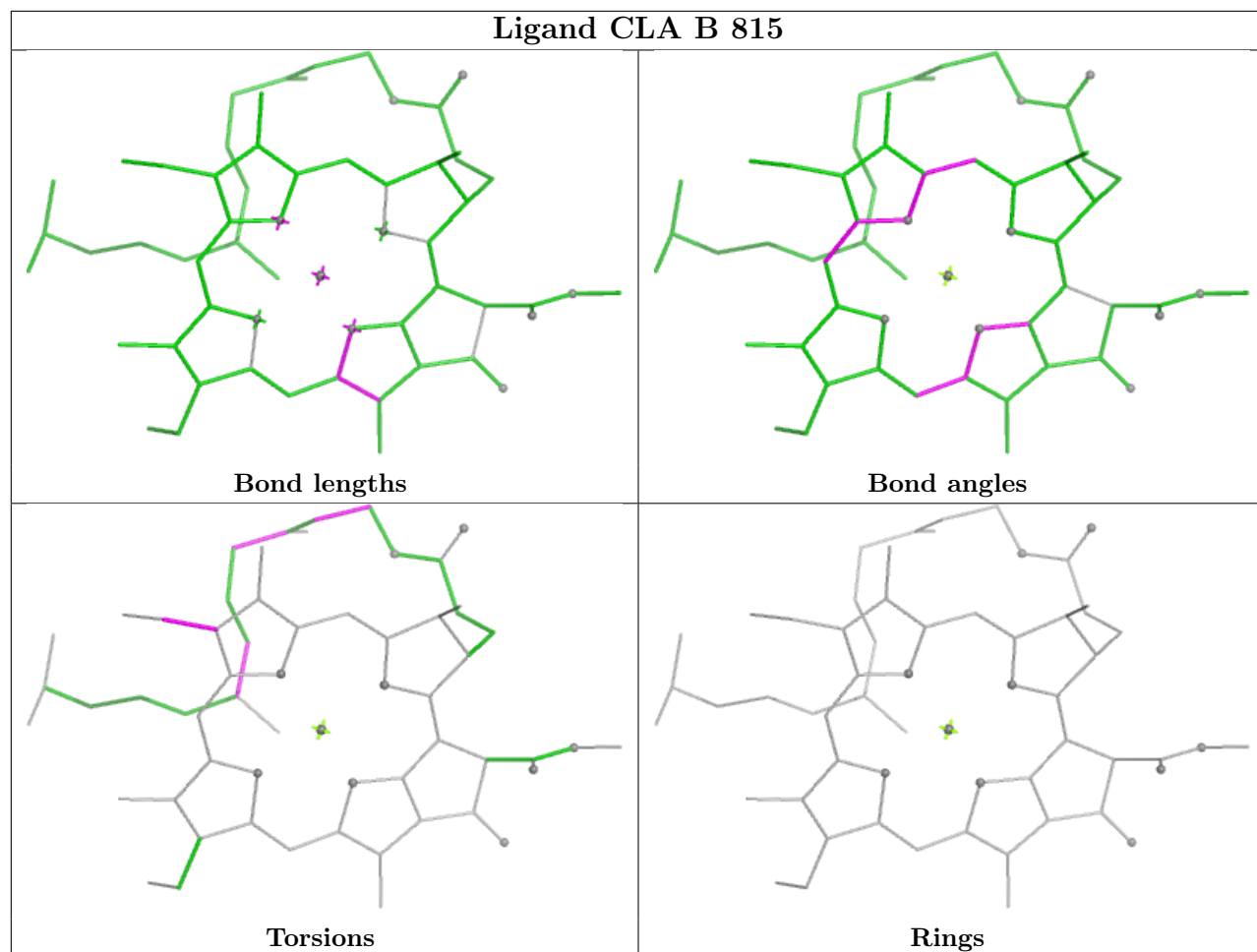
Bond angles

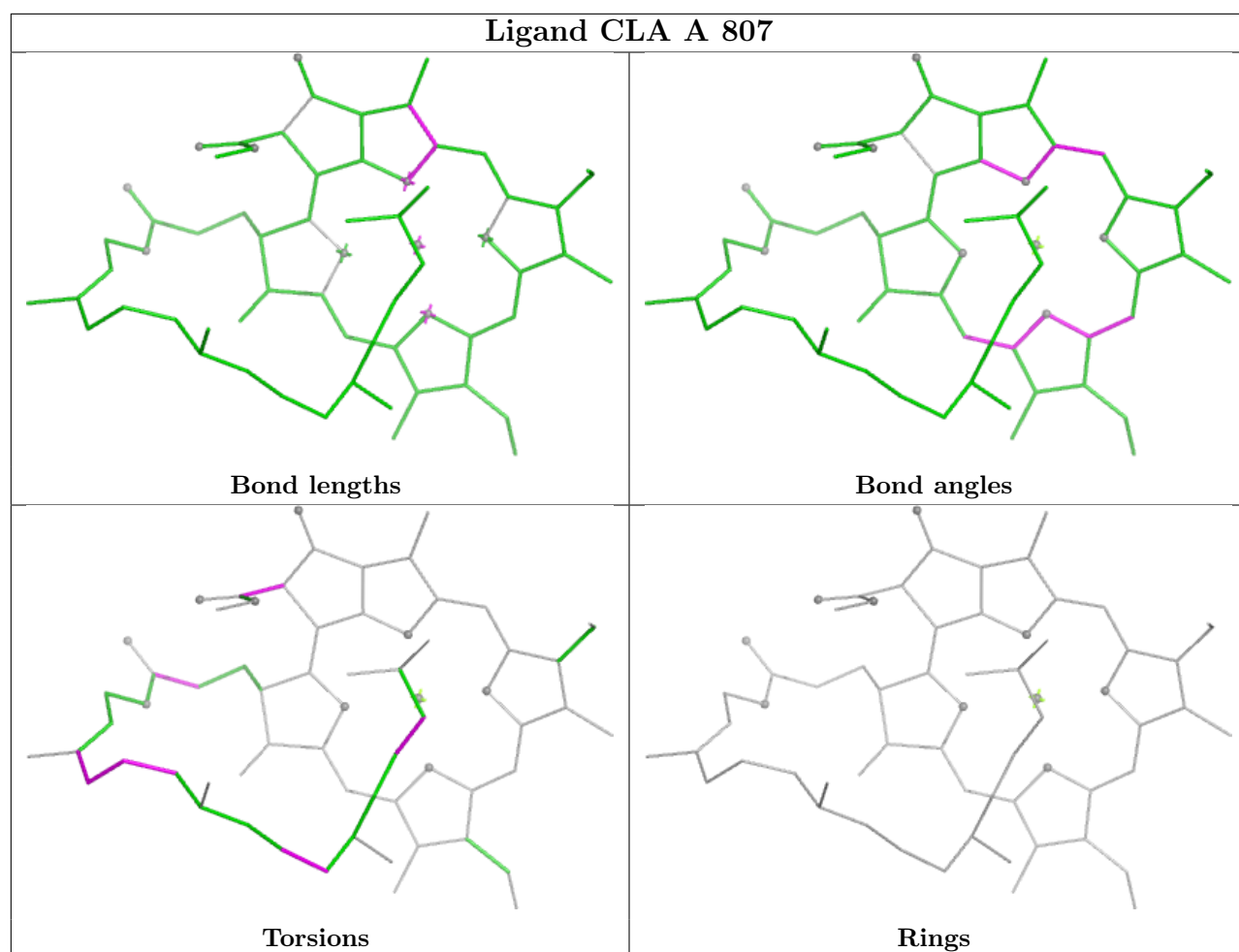


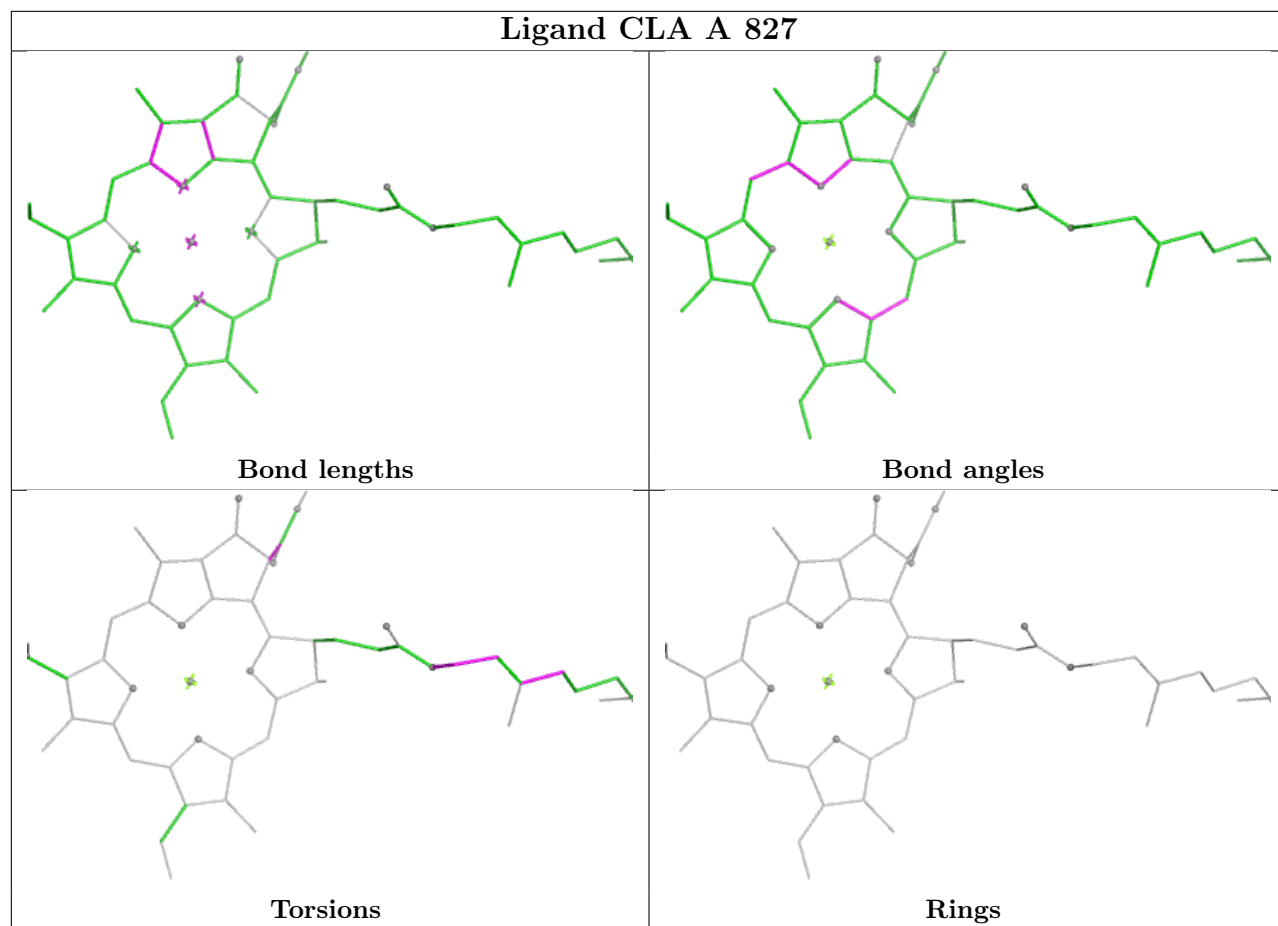
Torsions

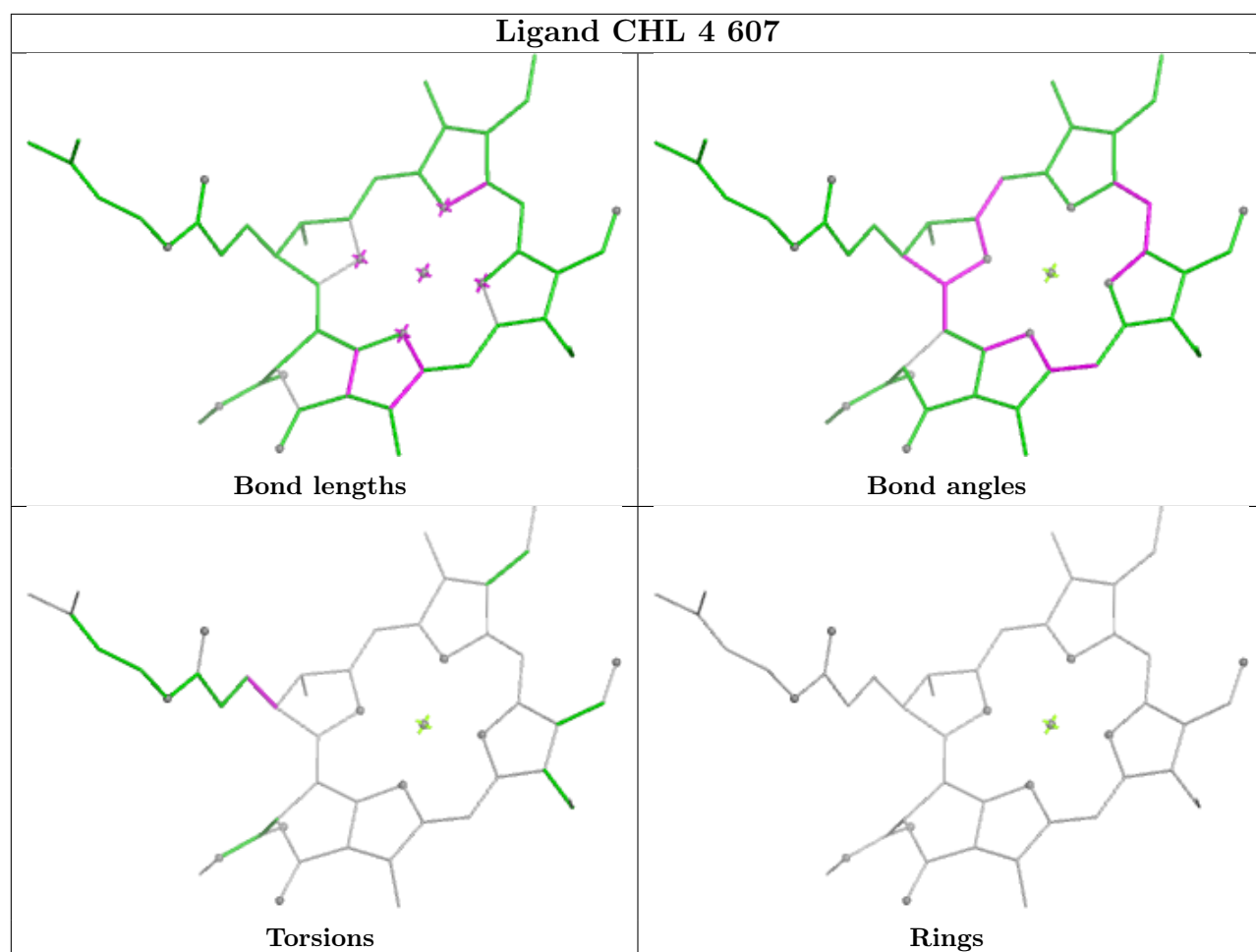


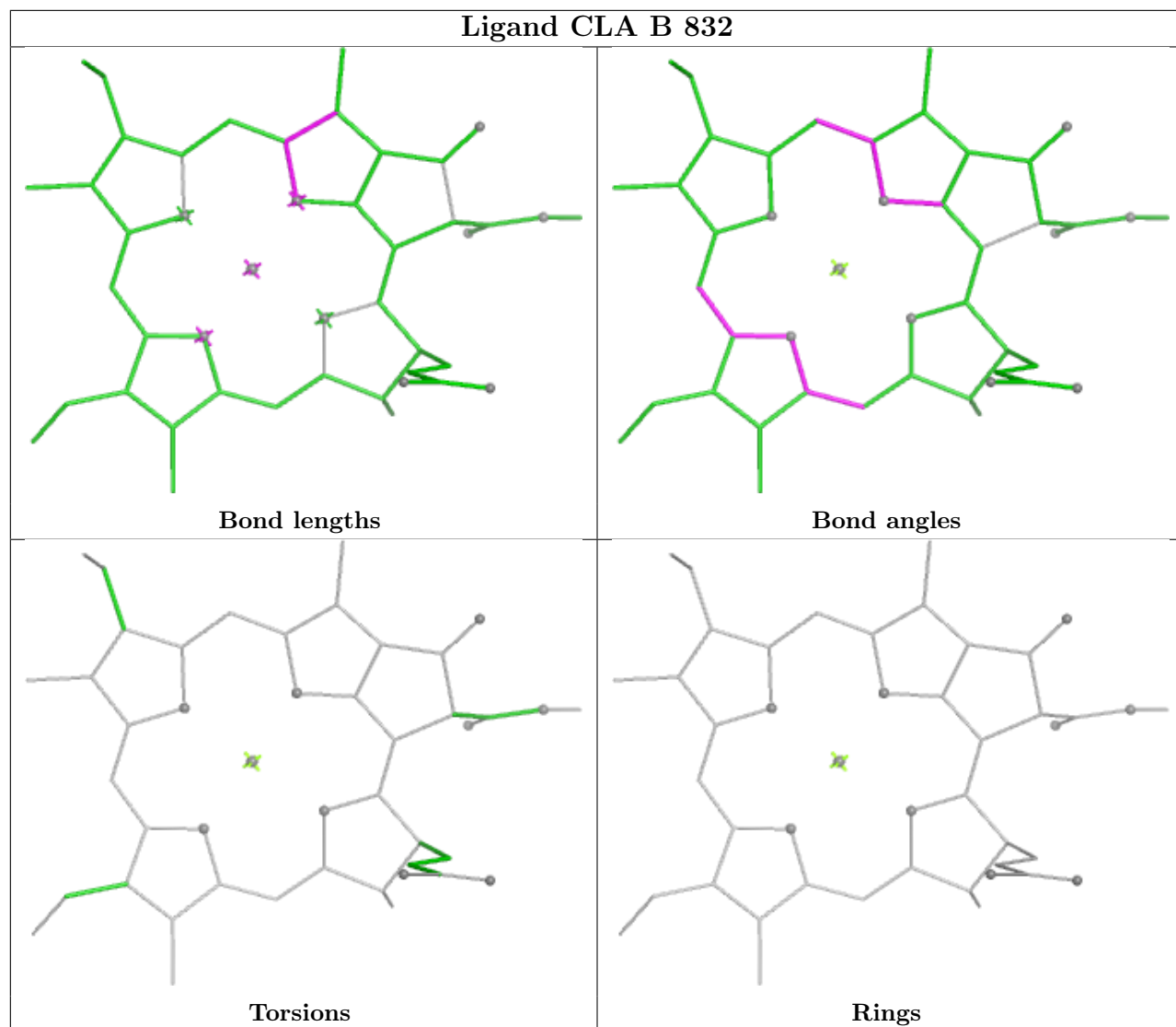
Rings

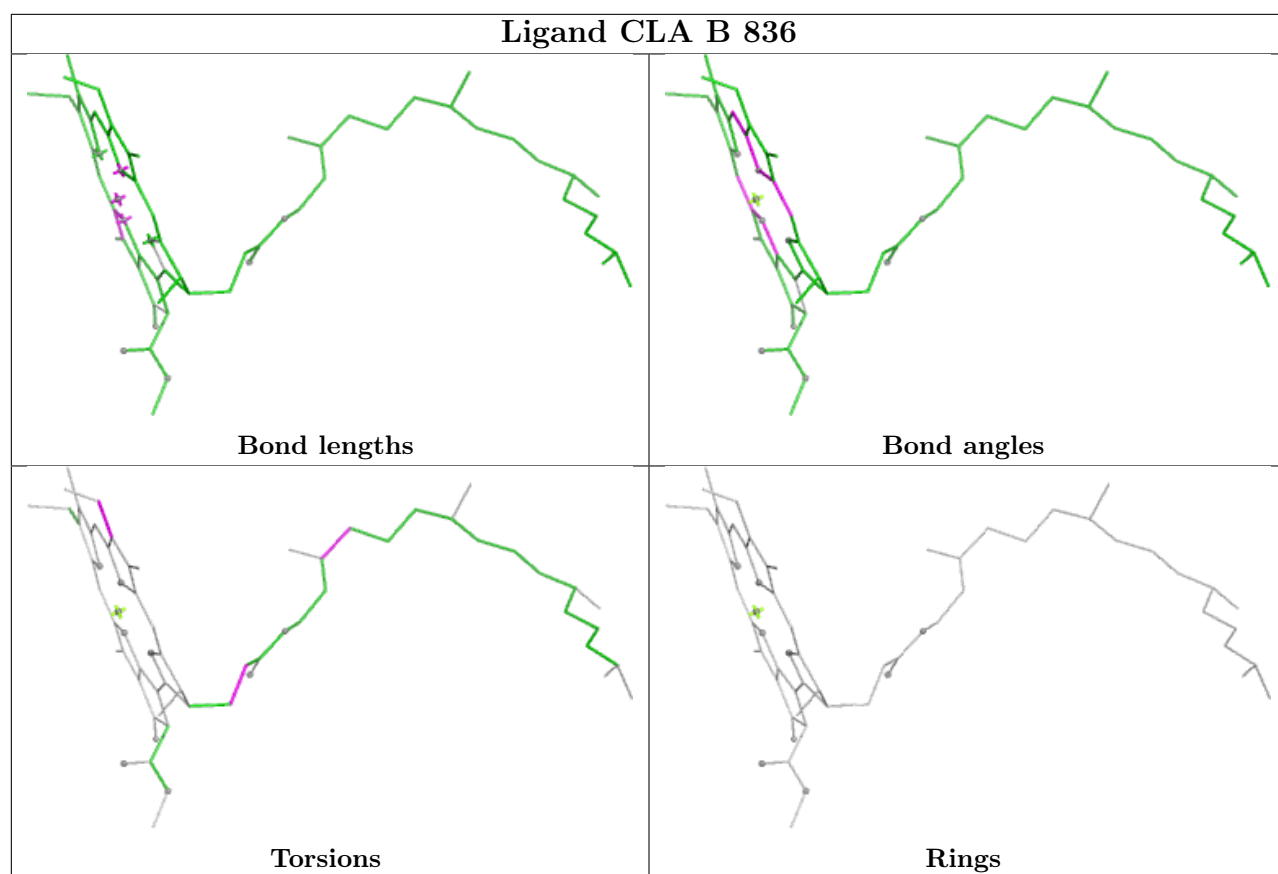




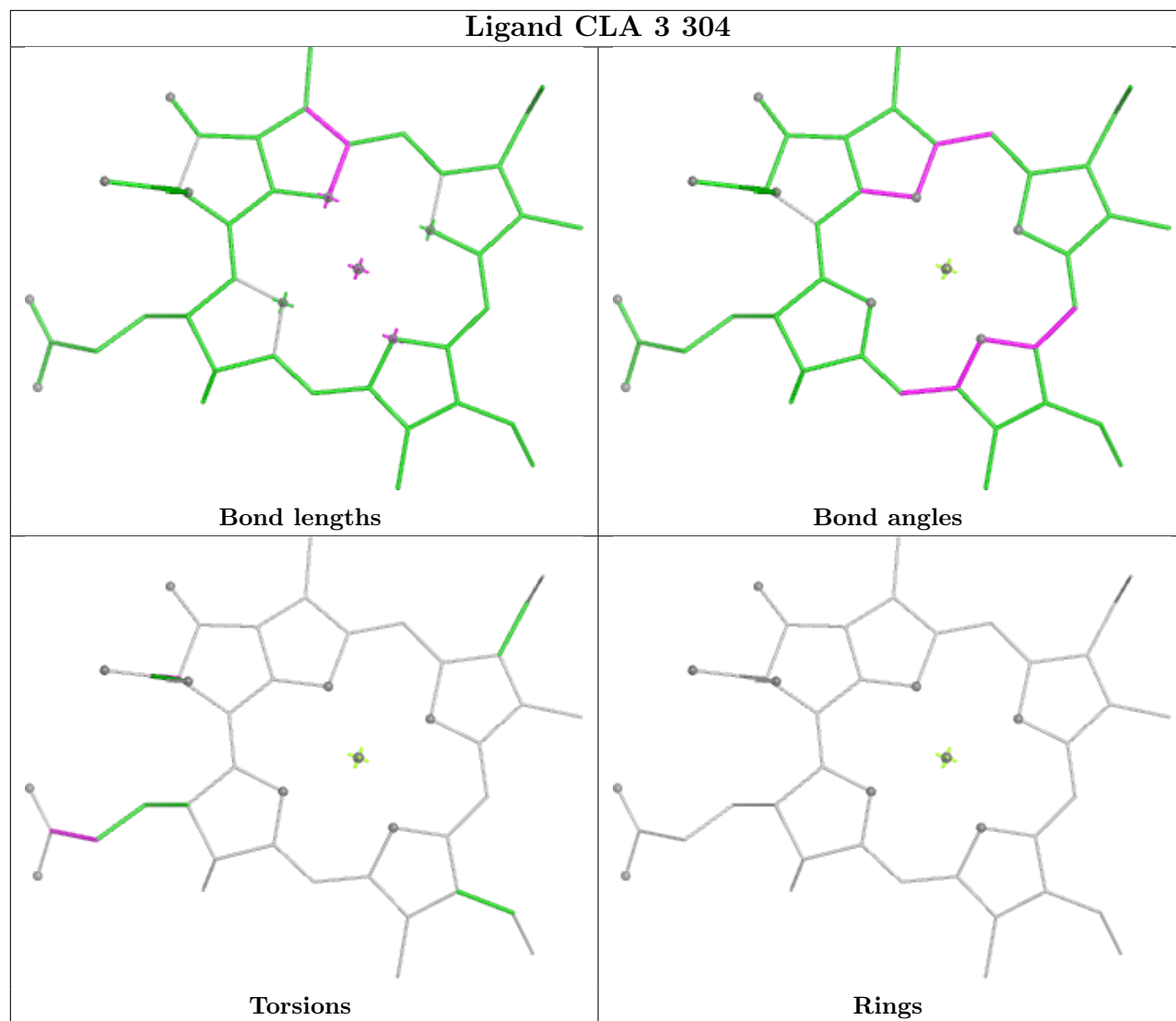




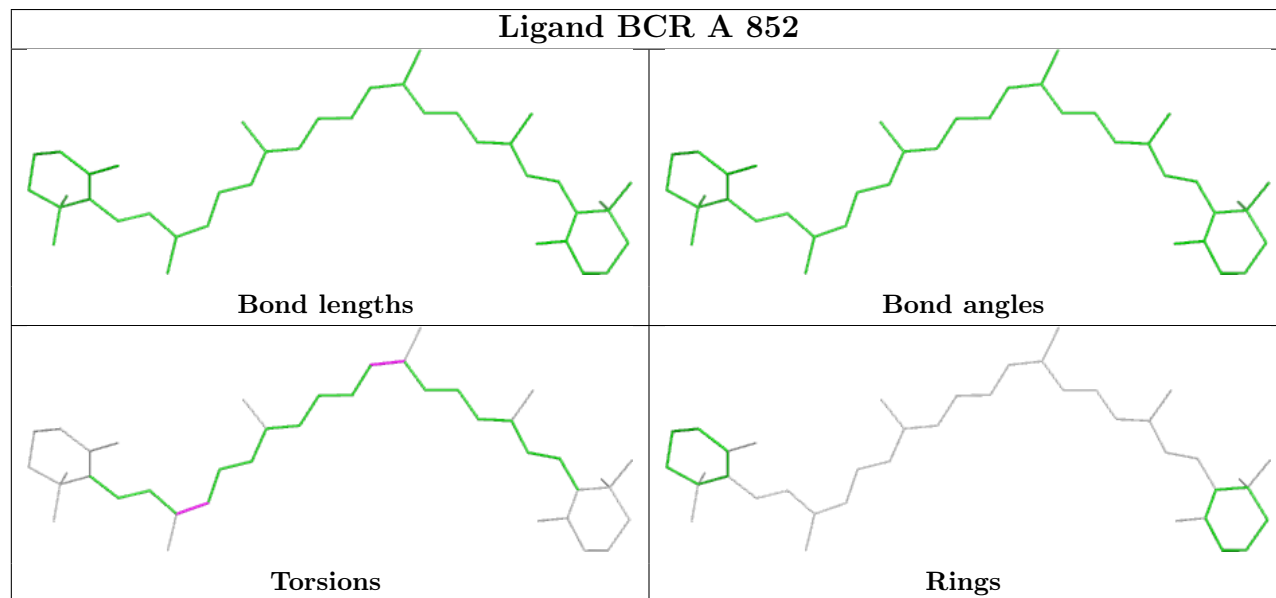




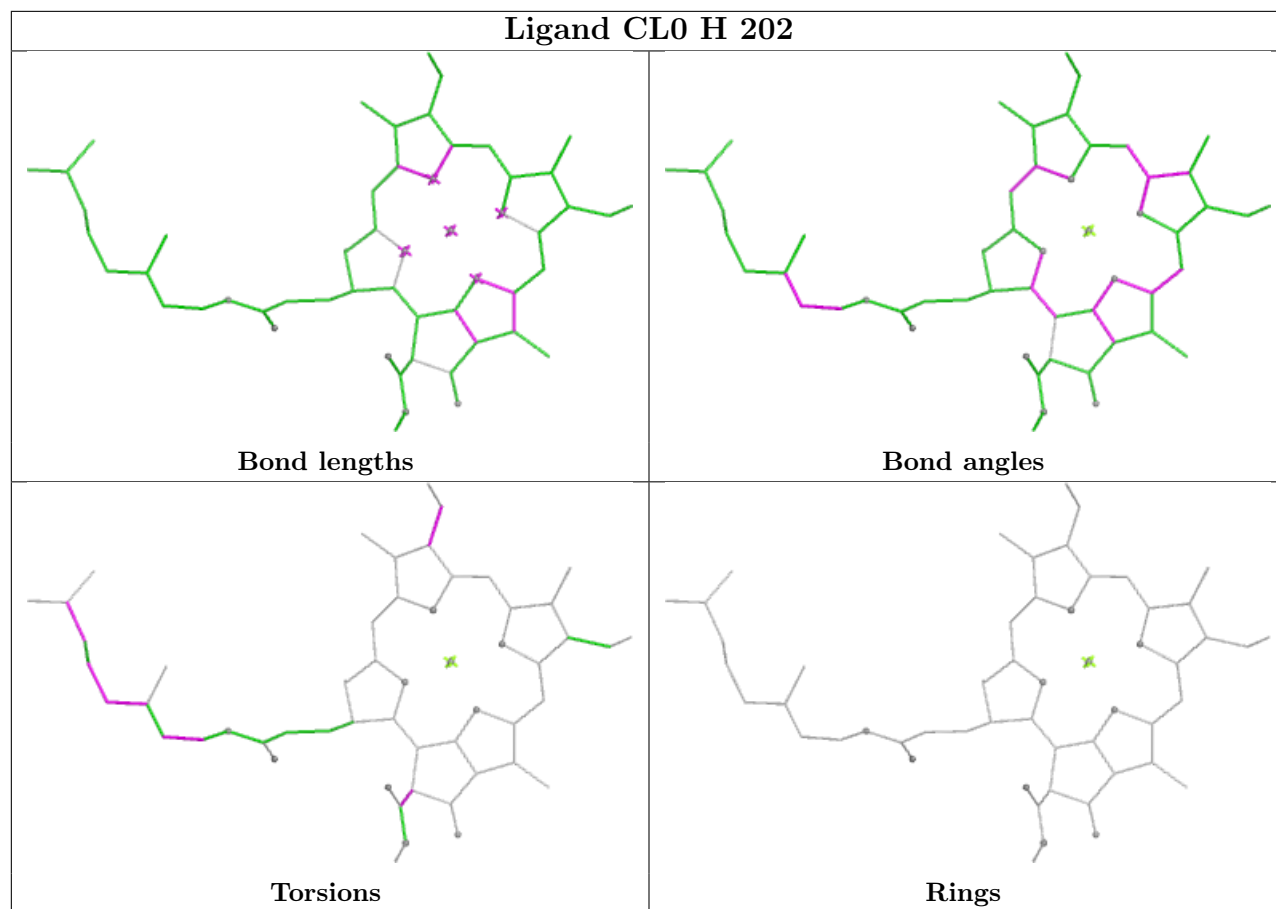
Ligand CLA 3 304



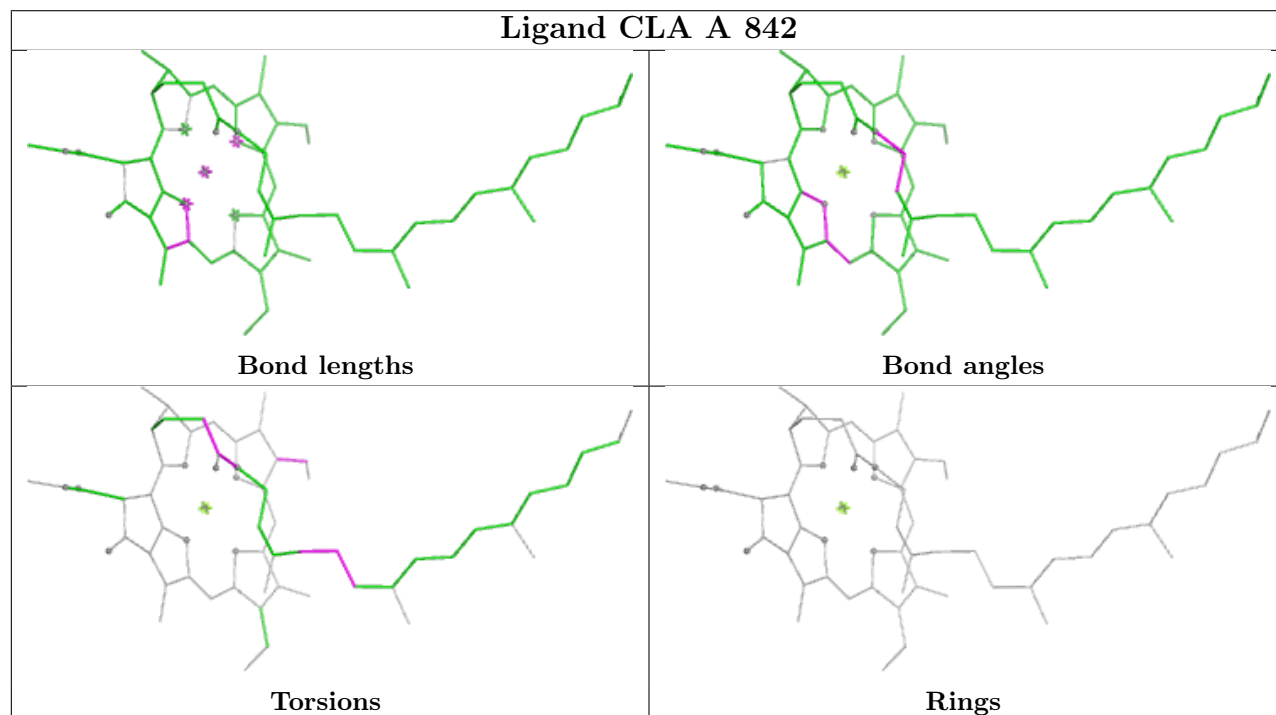
Ligand BCR A 852

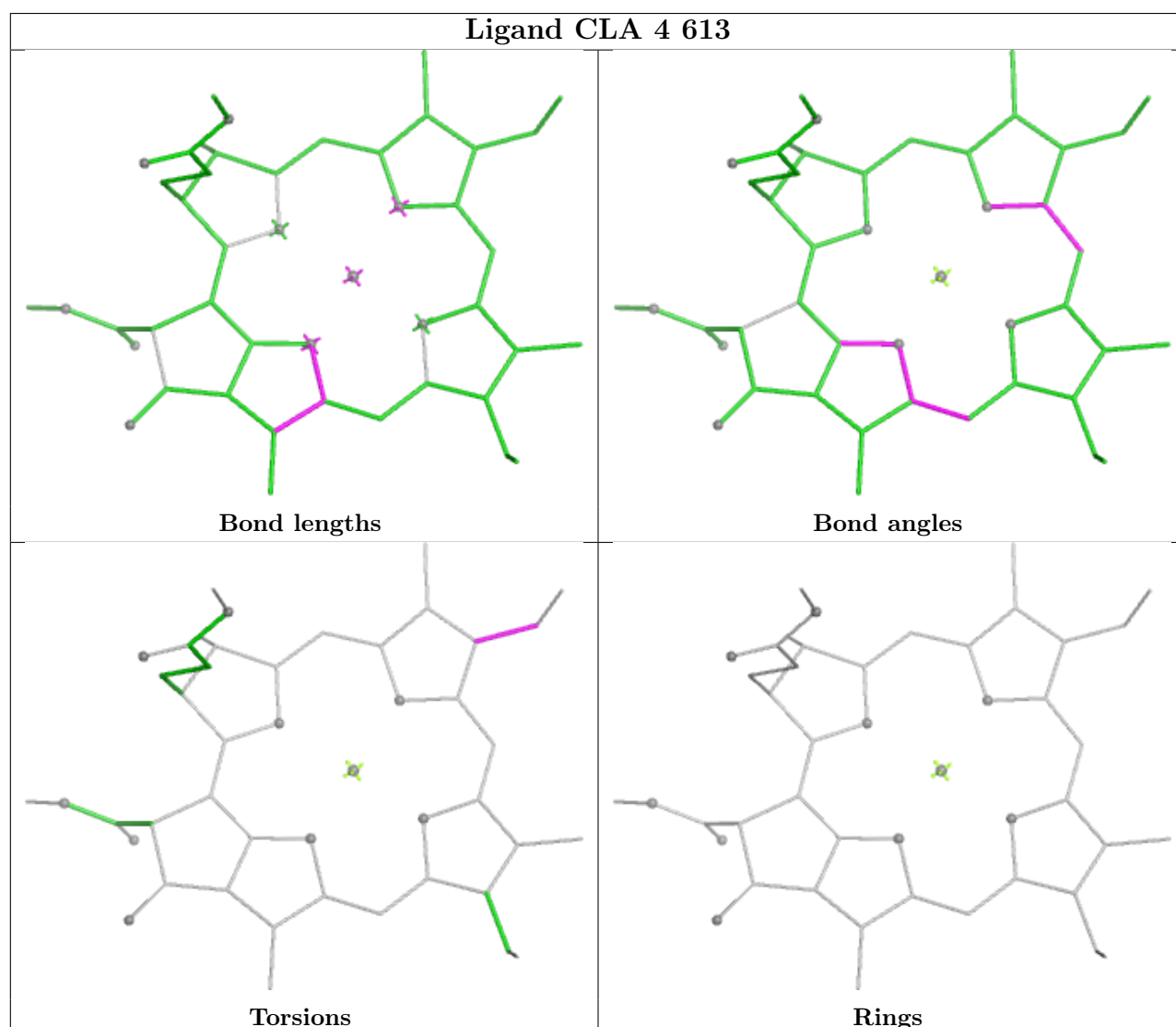
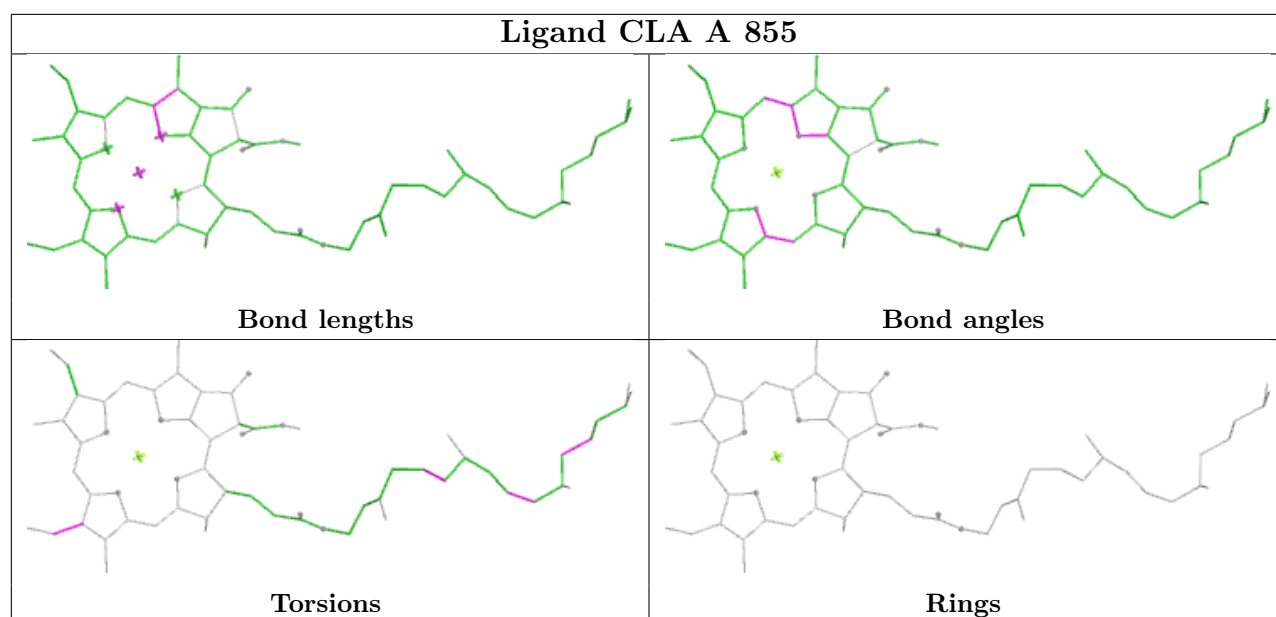


Ligand CL0 H 202

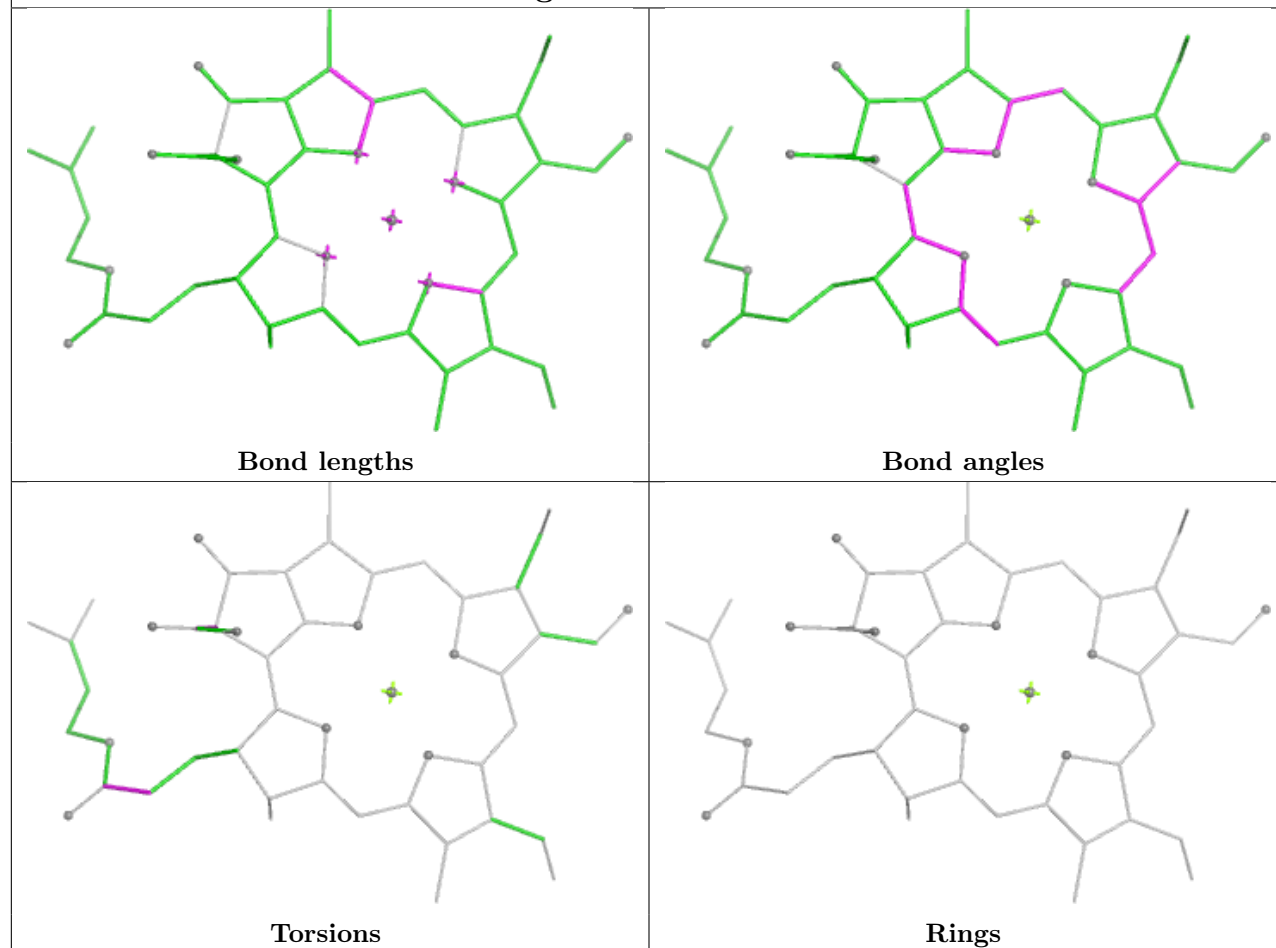


Ligand CLA A 842

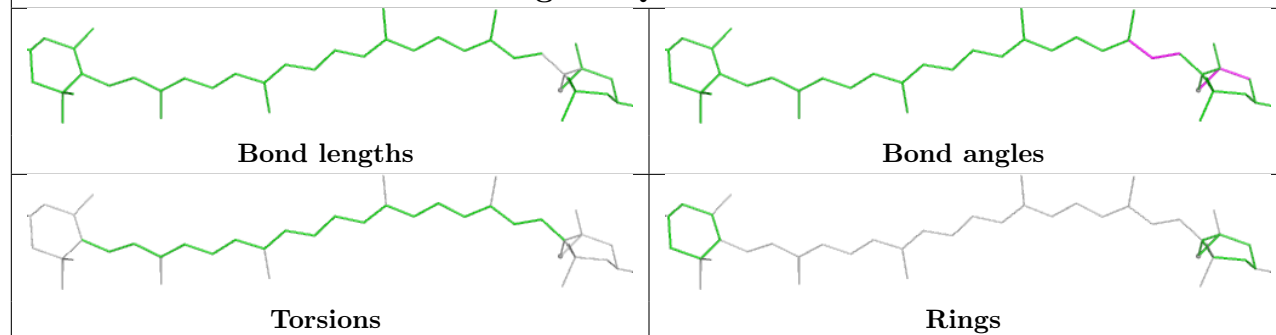


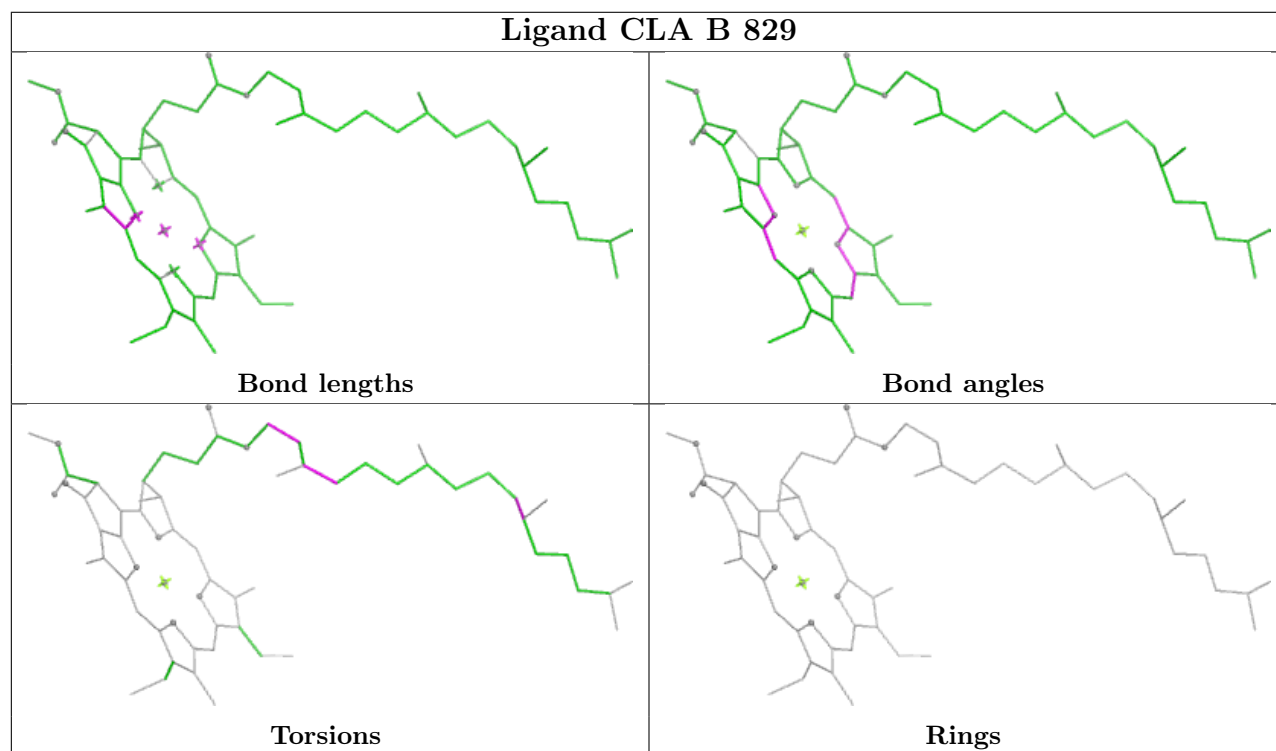
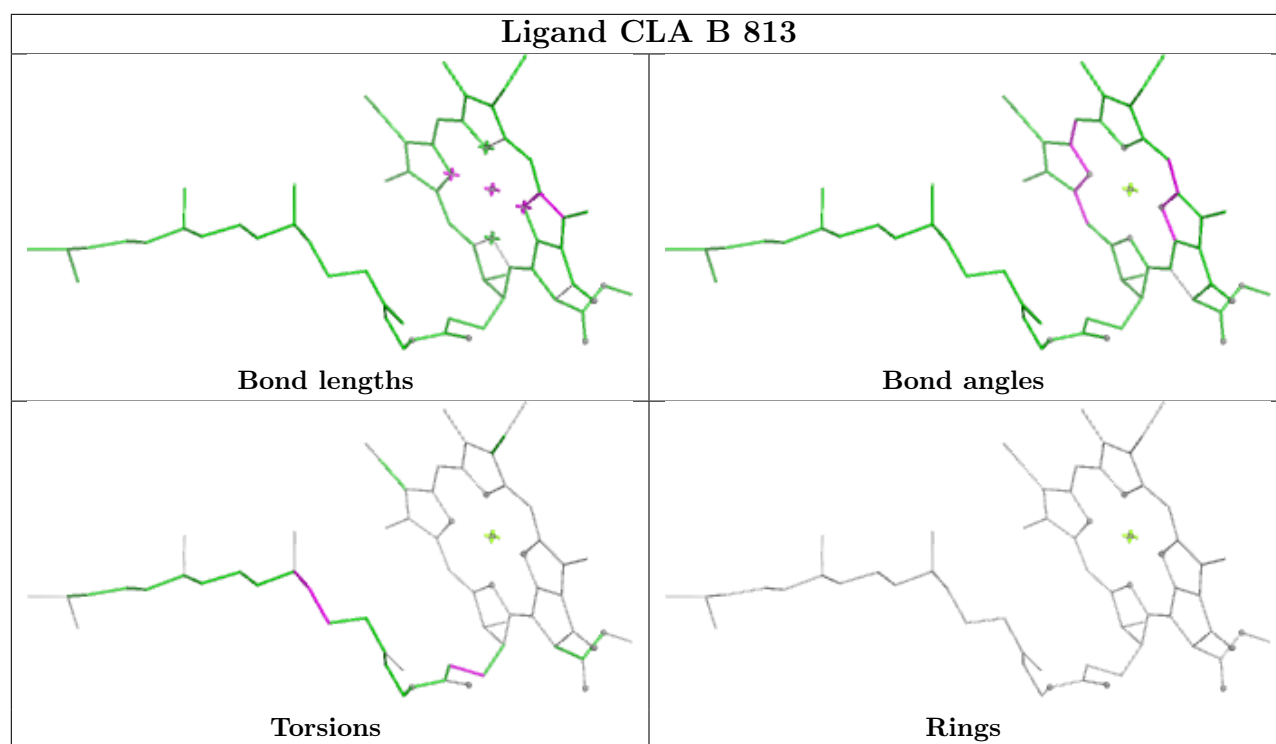


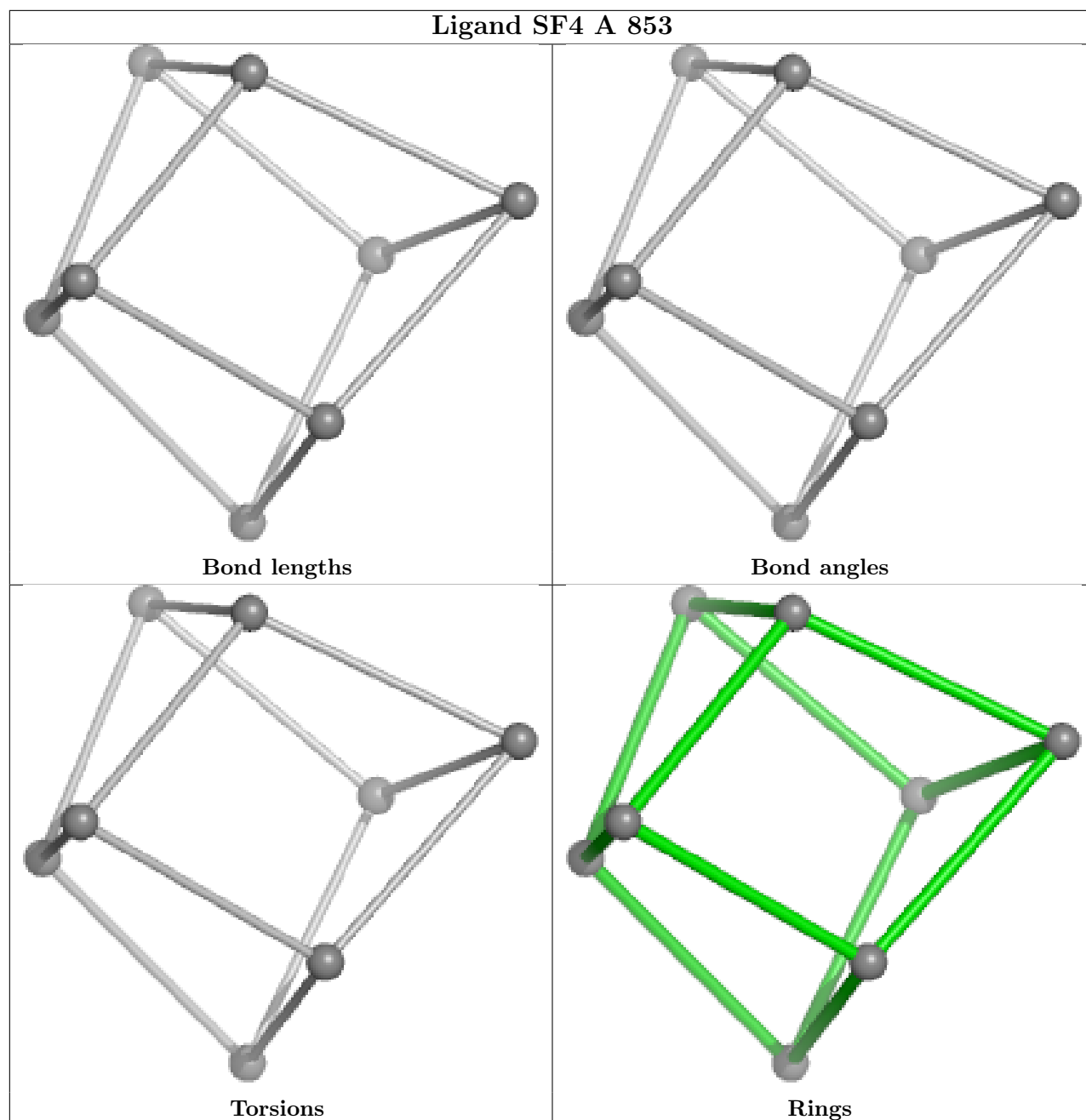
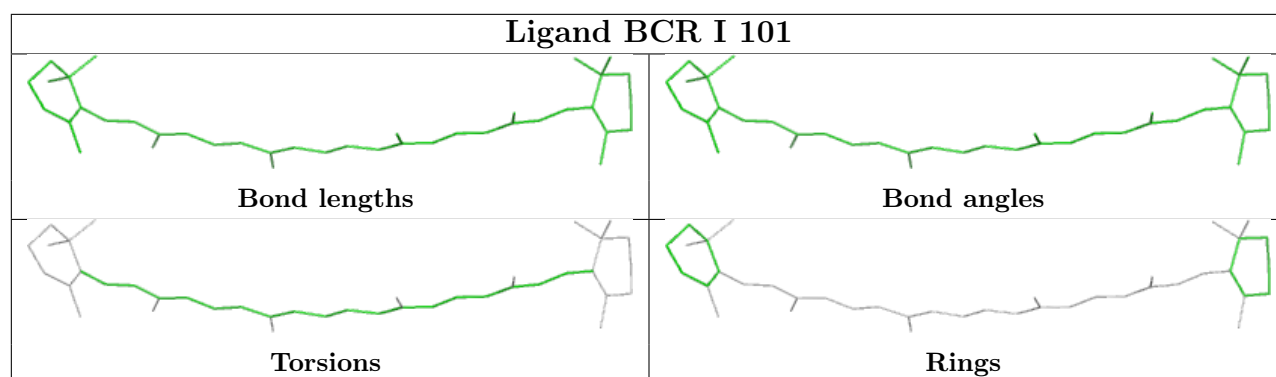
Ligand CHL 2 605

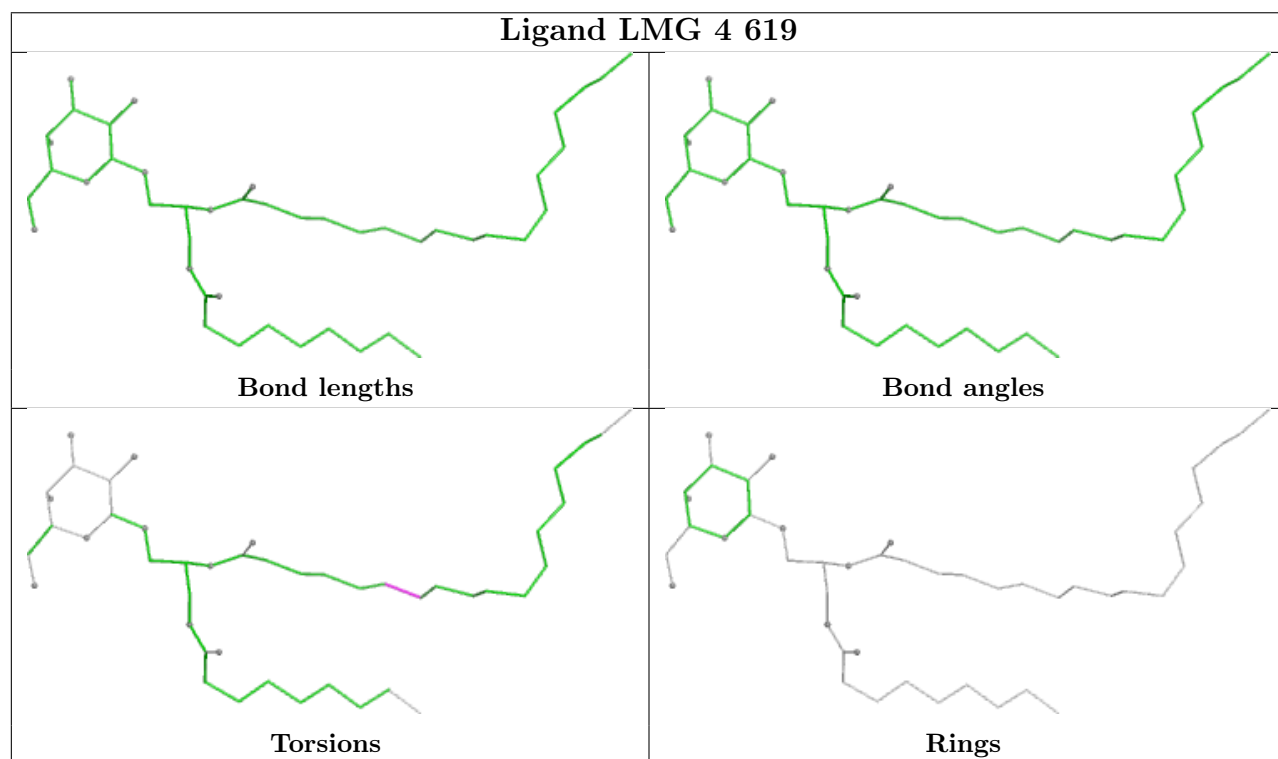
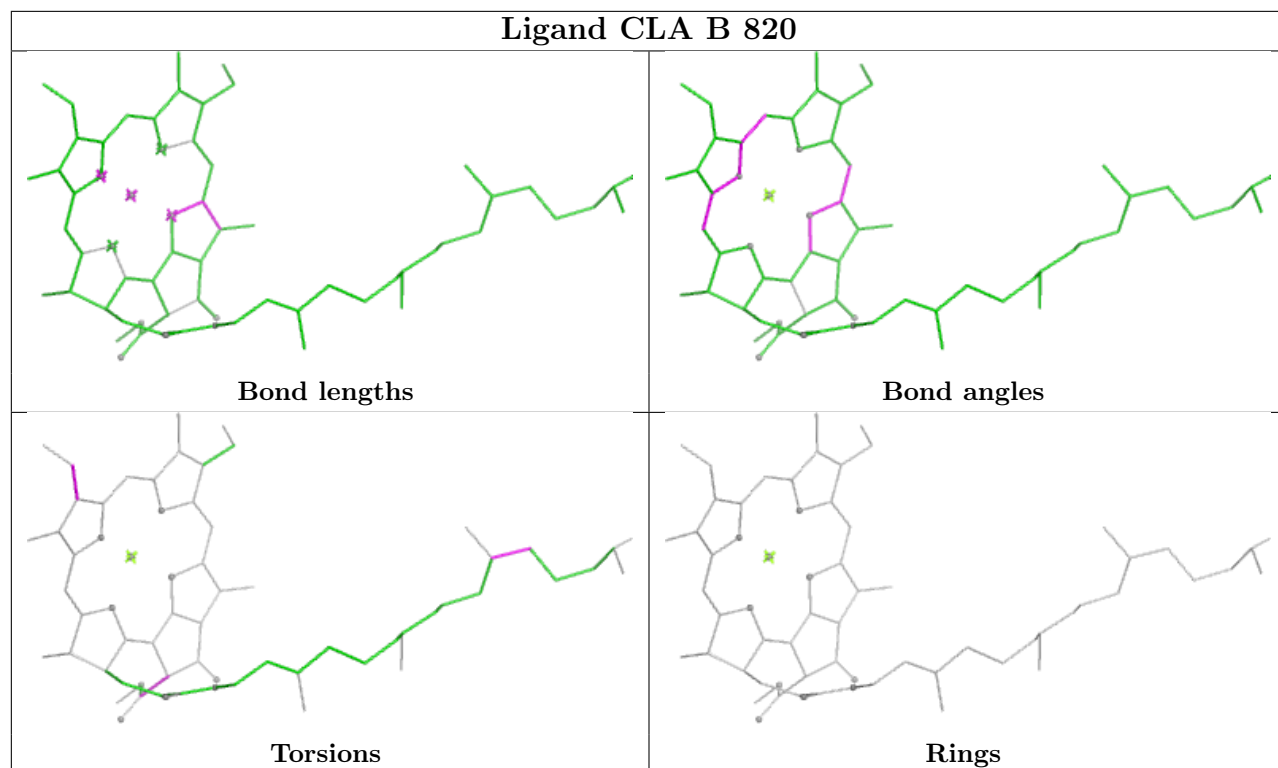


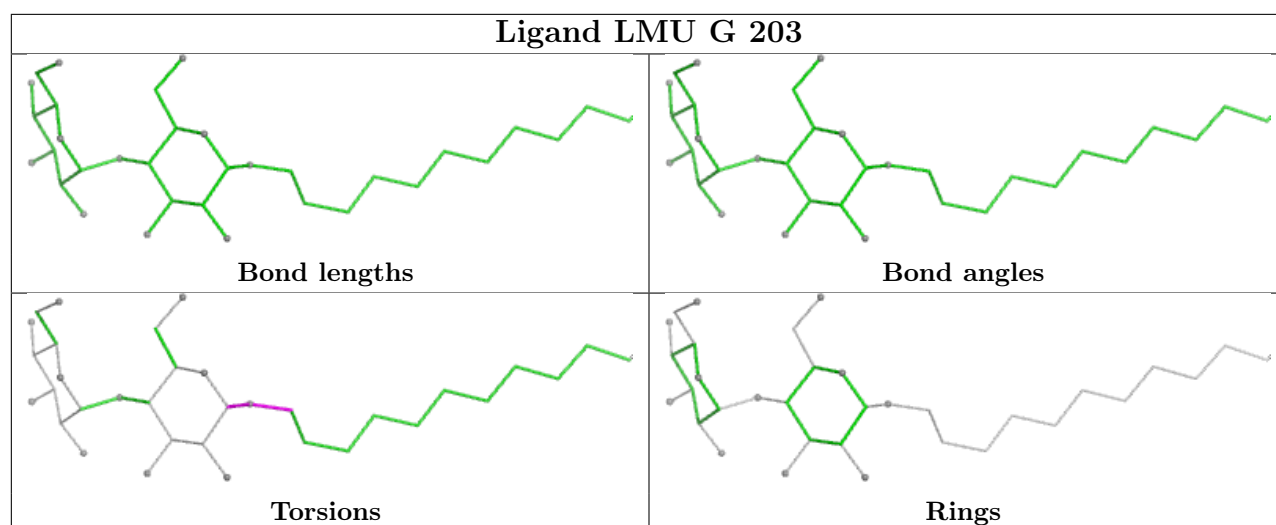
Ligand QDL 4 617

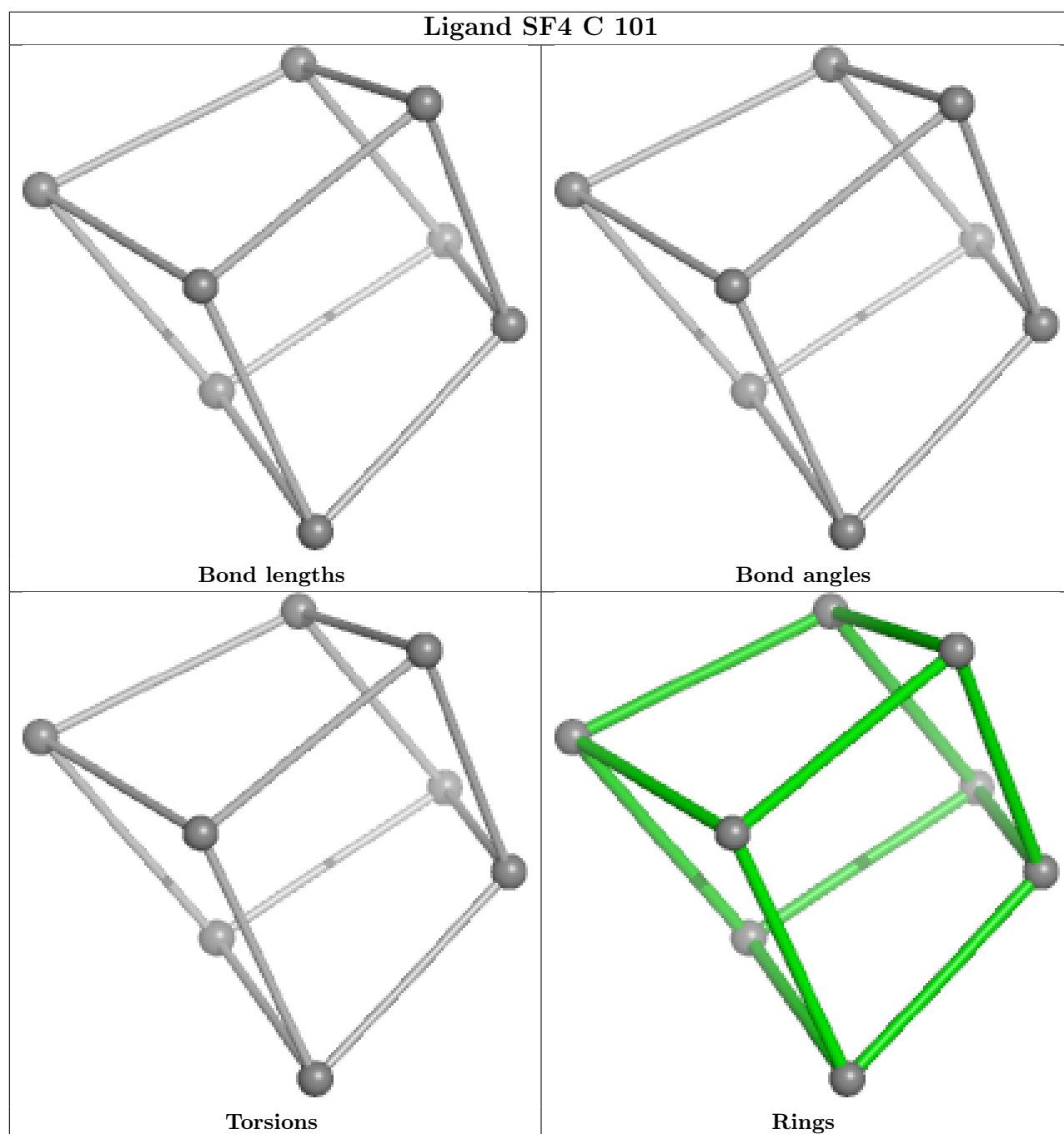


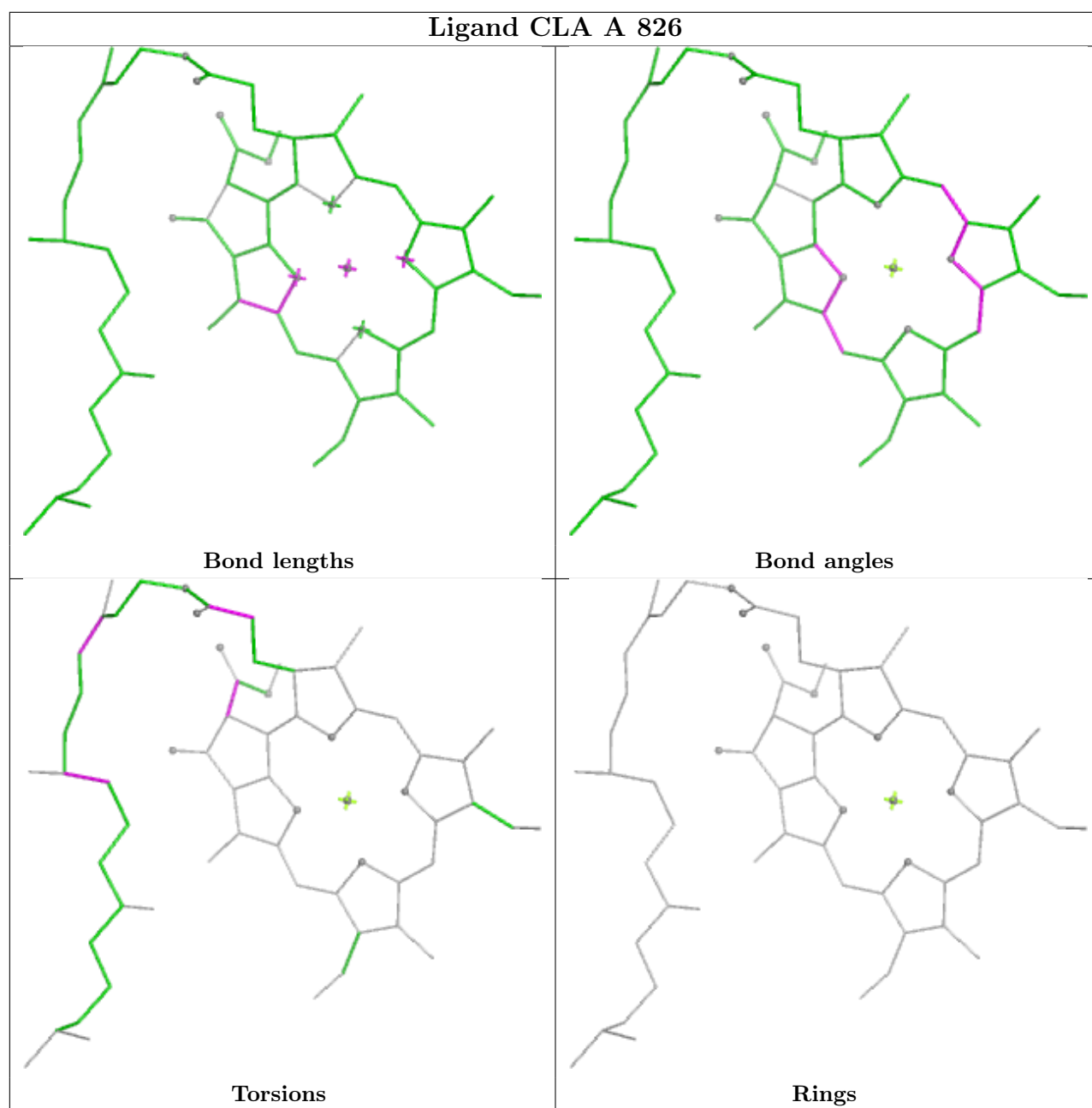


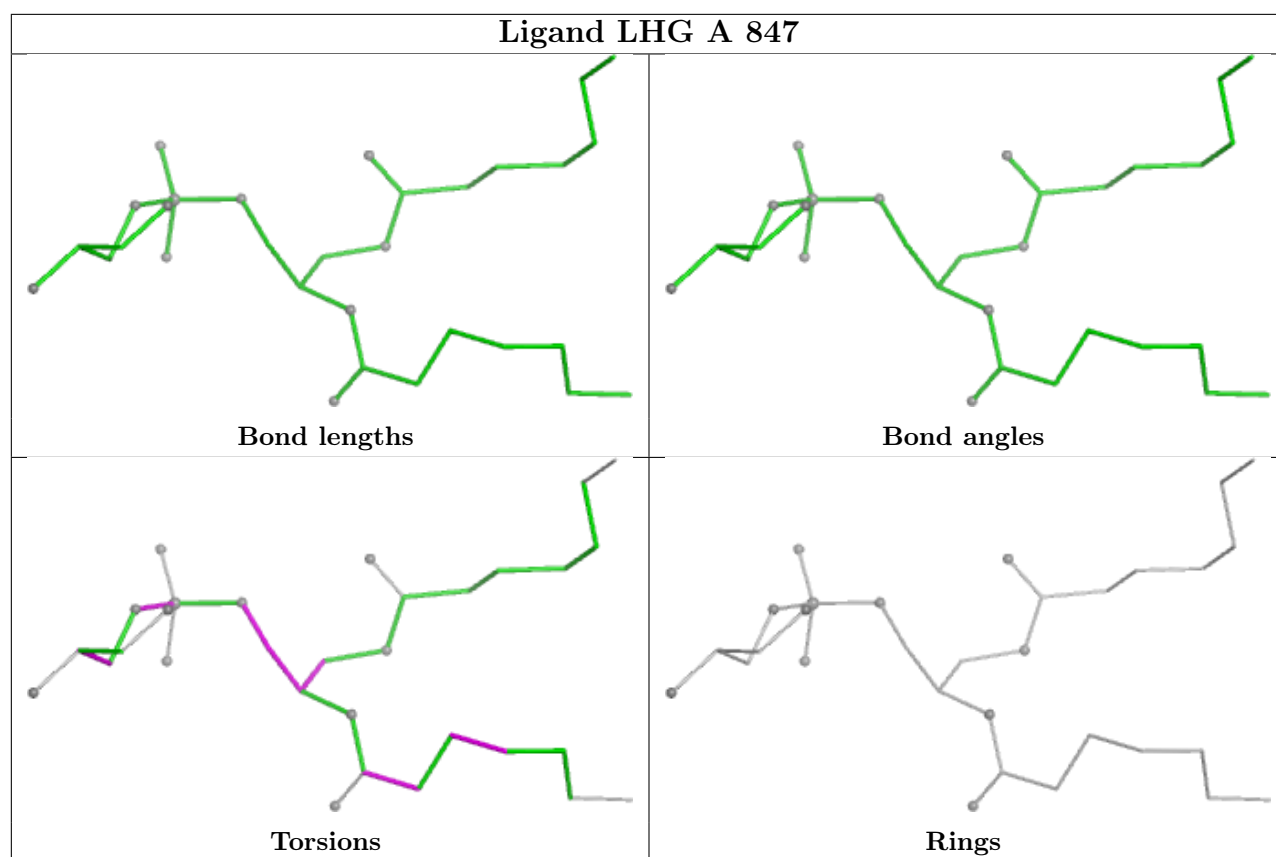


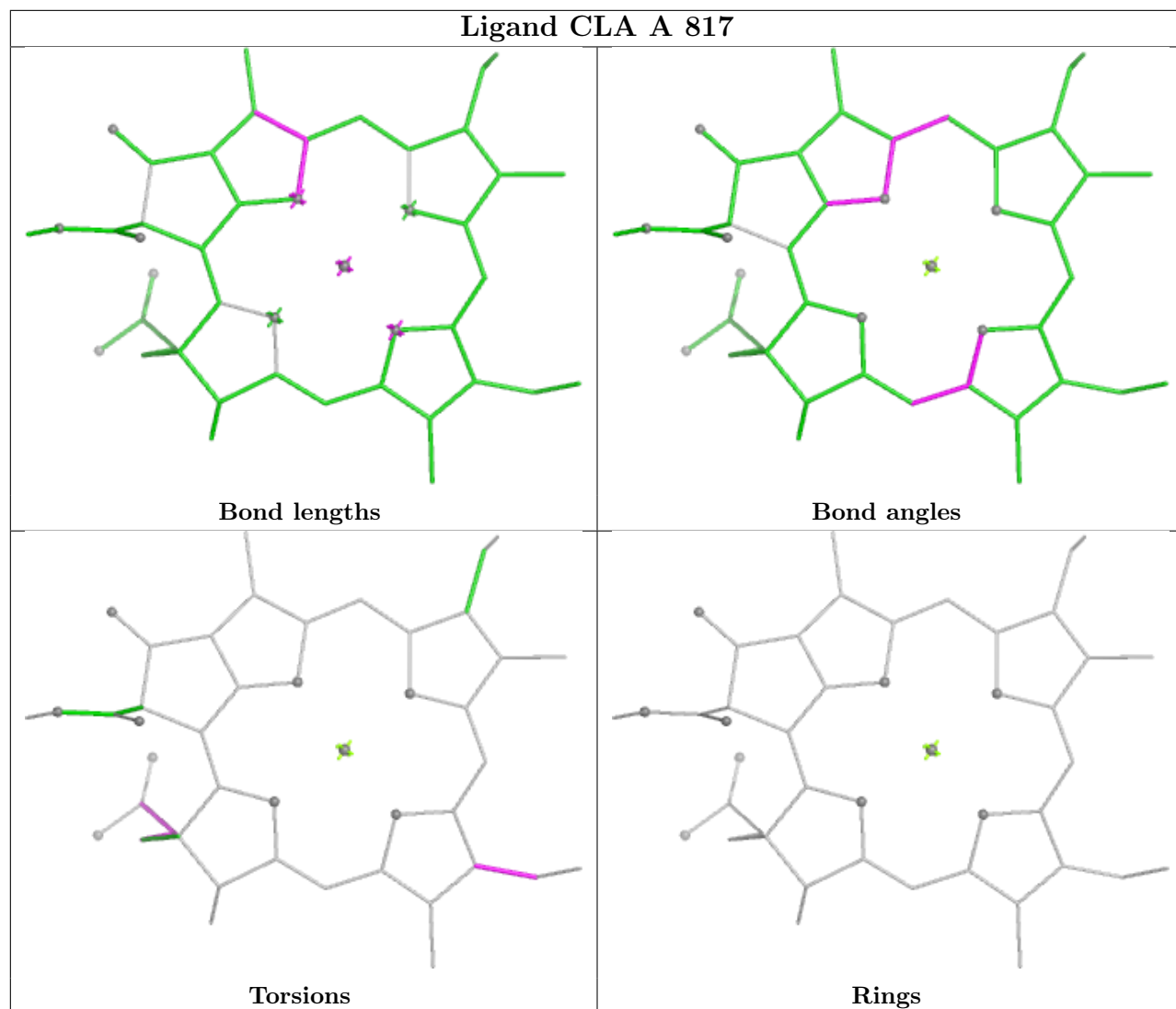


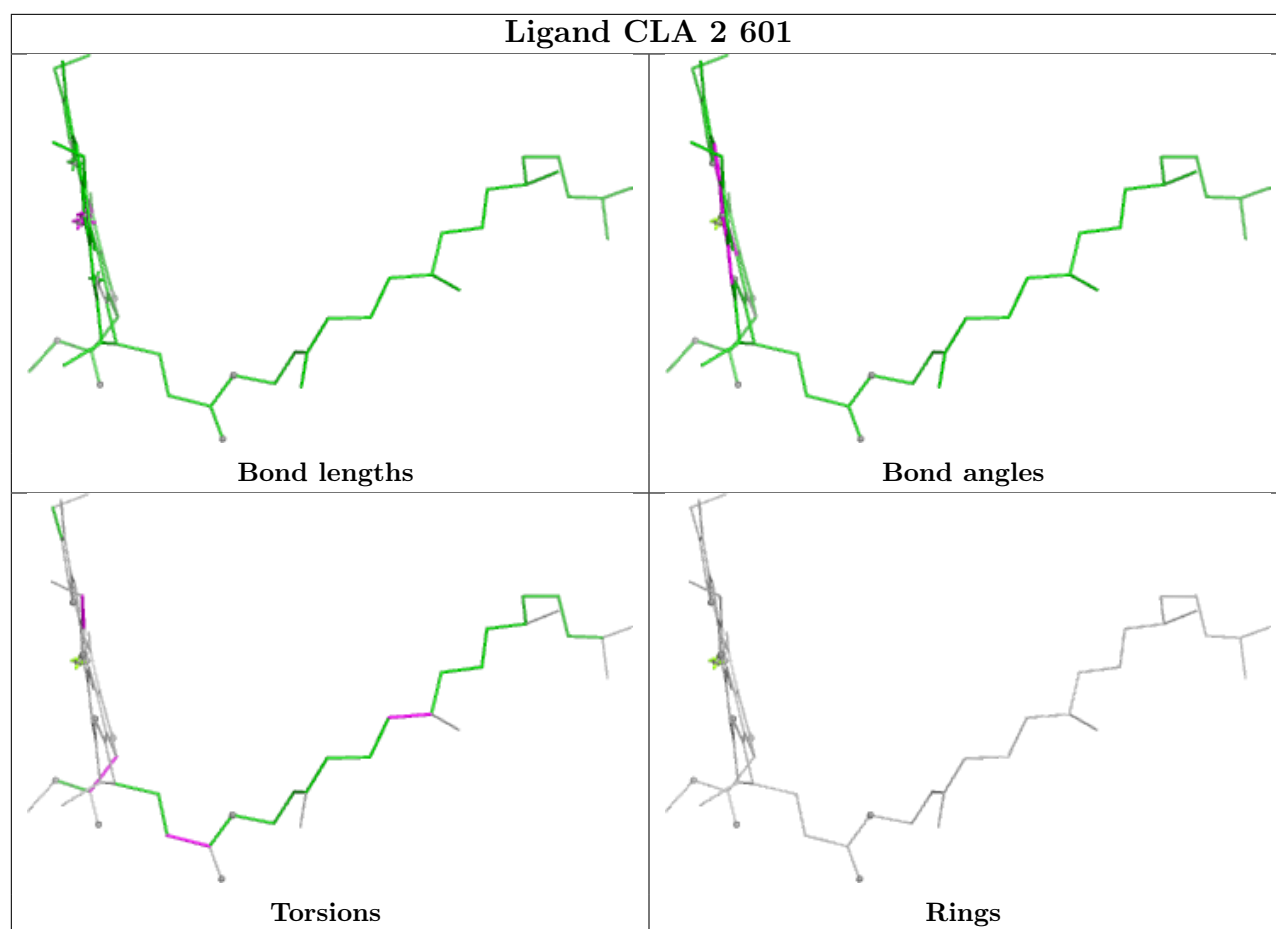




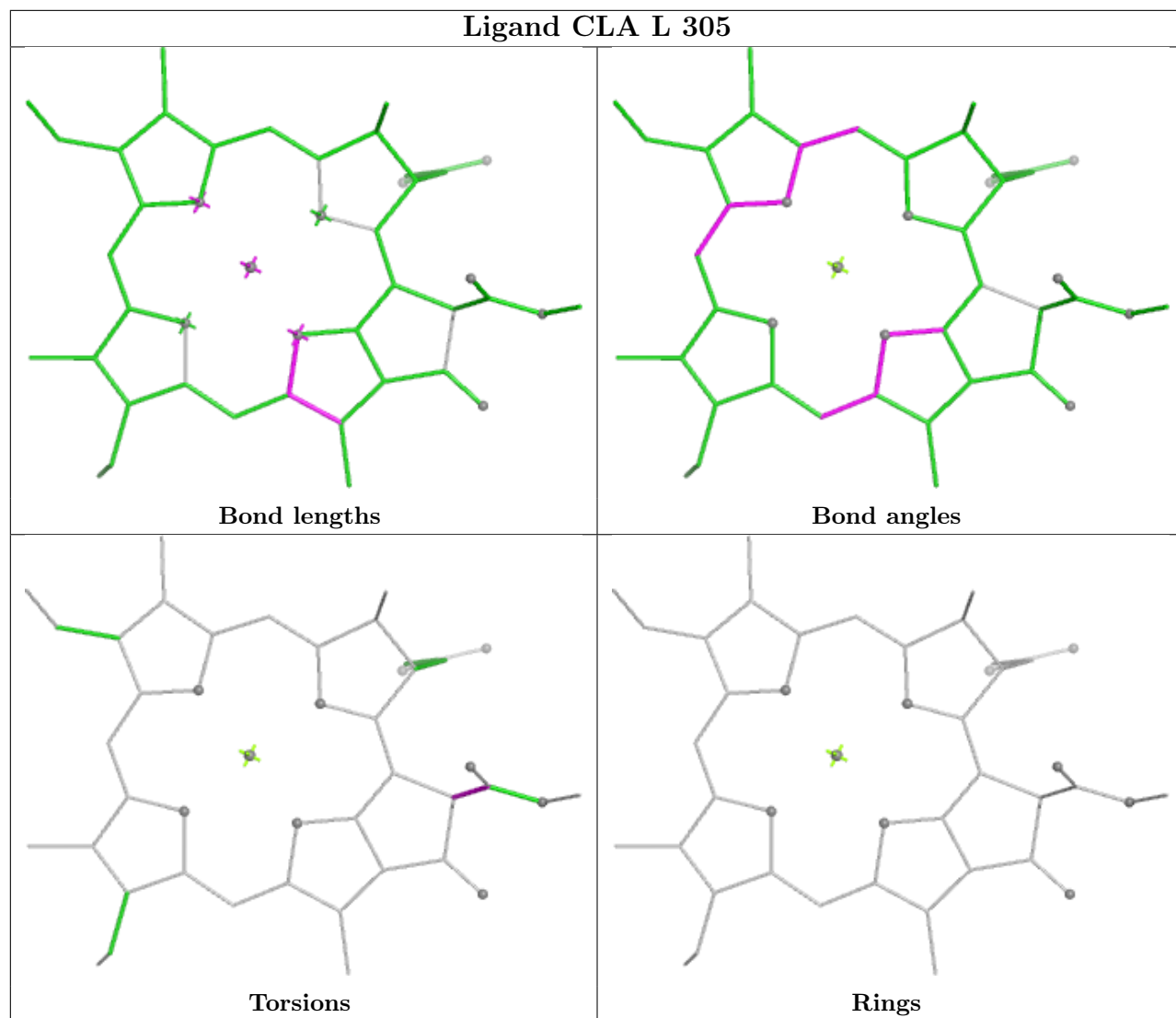


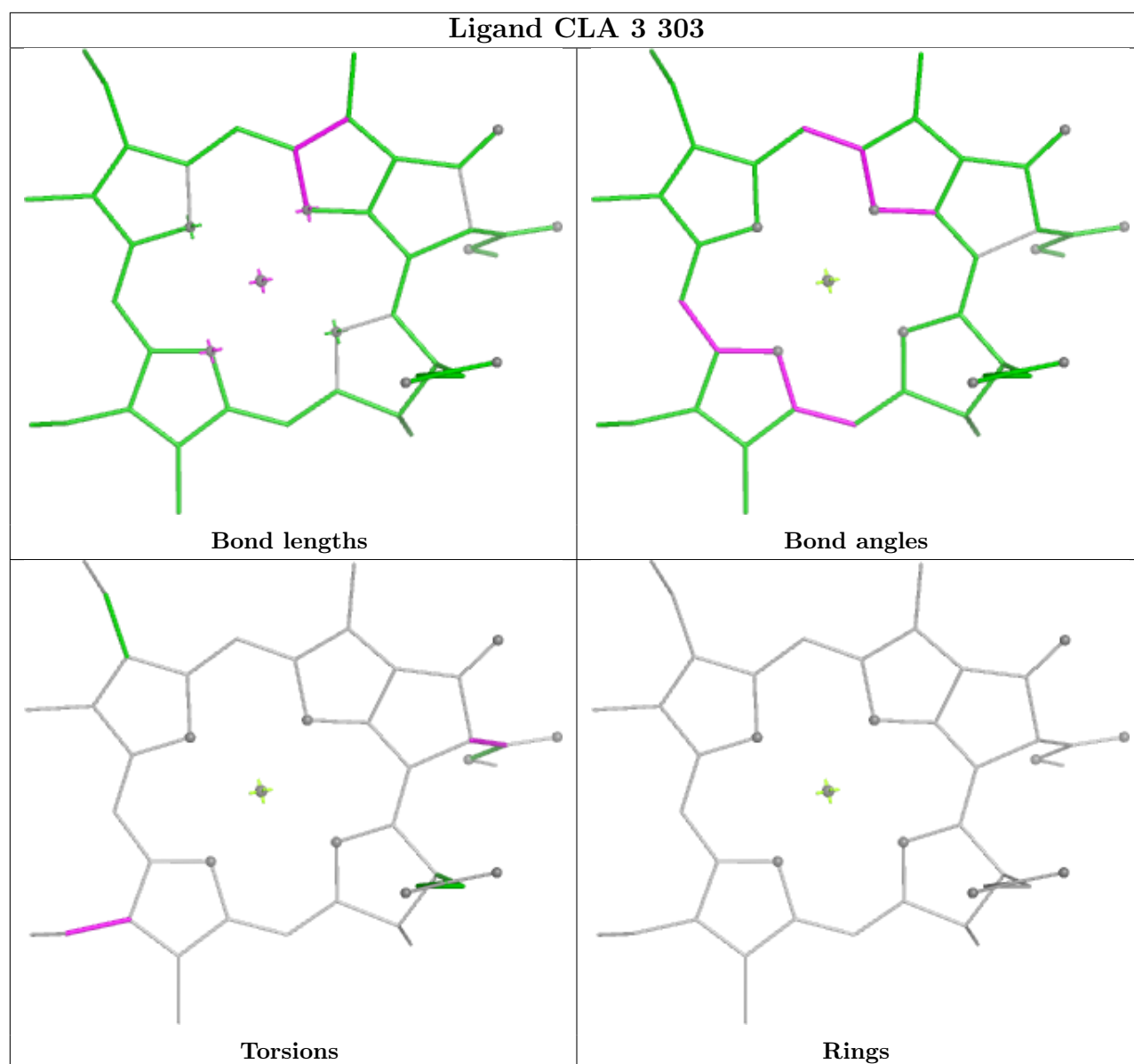






Ligand CLA L 305





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	L	1
12	K	1
13	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	209:PRO	C	210:TYR	N	3.43
1	K	123:GLY	C	124:VAL	N	3.22
1	1	236:PRO	C	237:ARG	N	3.17

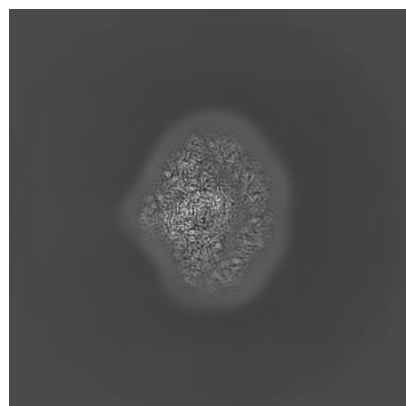
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15969. These allow visual inspection of the internal detail of the map and identification of artifacts.

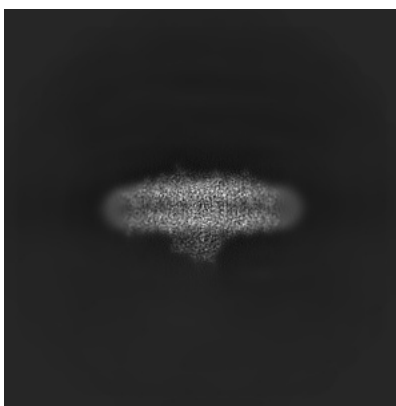
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

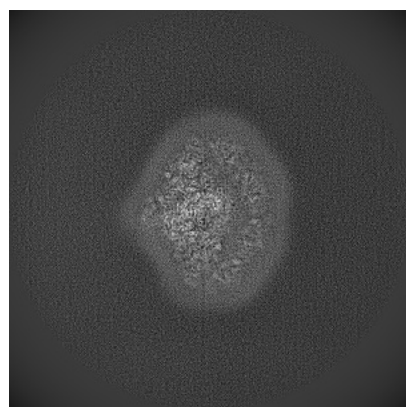


Y



Z

6.1.2 Raw map



X



Y

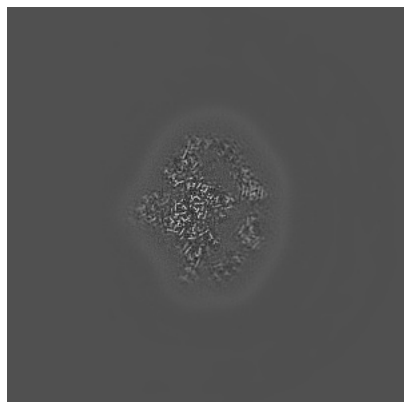


Z

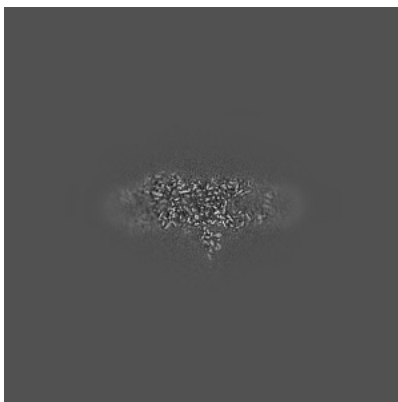
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

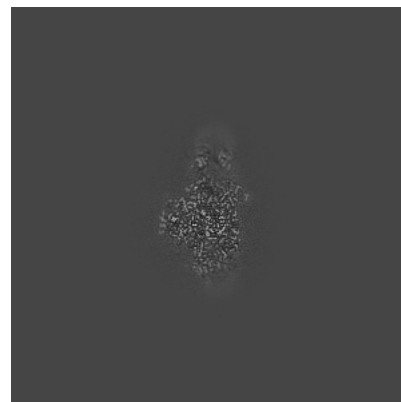
6.2.1 Primary map



X Index: 250

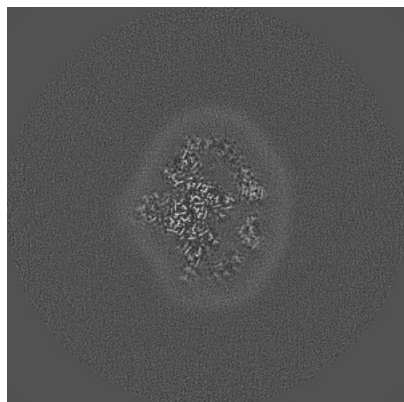


Y Index: 250

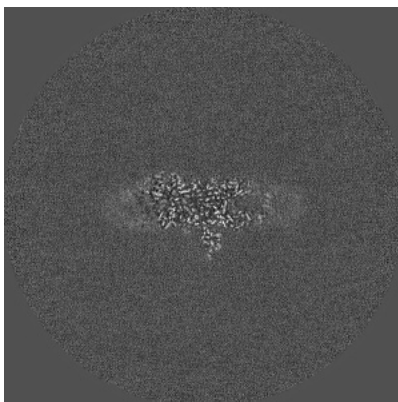


Z Index: 250

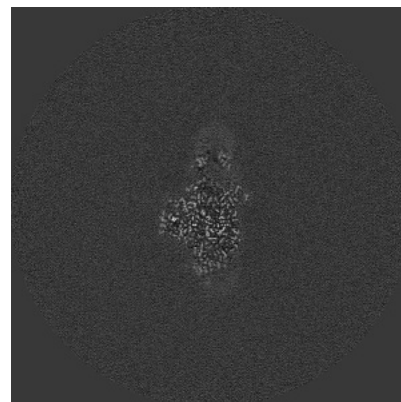
6.2.2 Raw map



X Index: 250



Y Index: 250

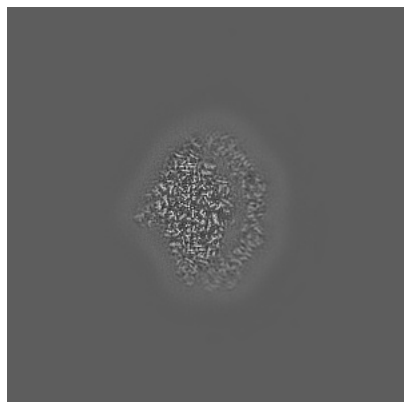


Z Index: 250

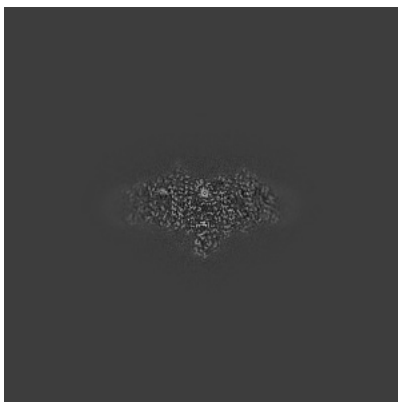
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

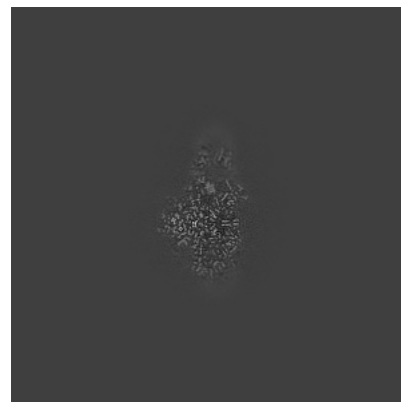
6.3.1 Primary map



X Index: 267

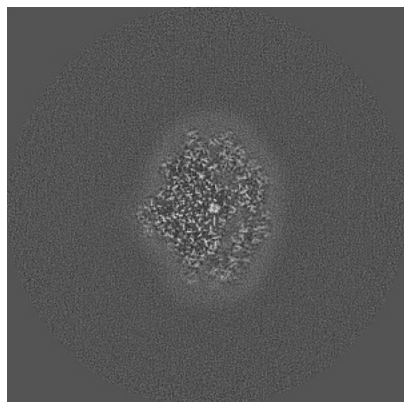


Y Index: 227

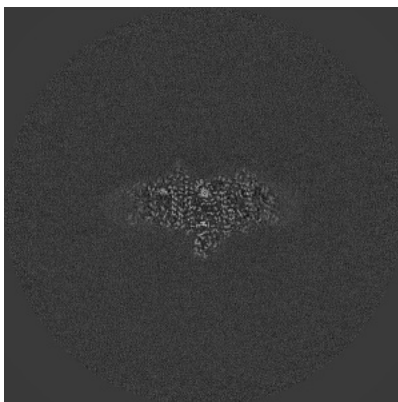


Z Index: 248

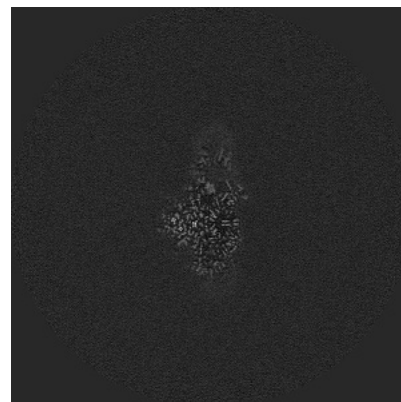
6.3.2 Raw map



X Index: 235



Y Index: 227

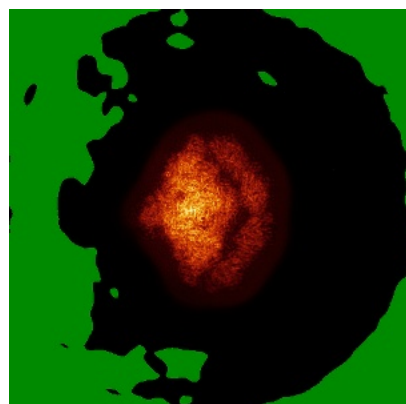


Z Index: 248

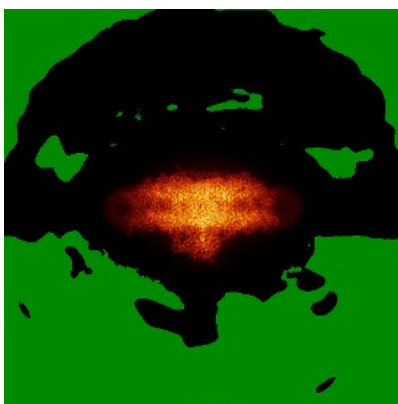
The images above show the largest variance slices of the map in three orthogonal directions.

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

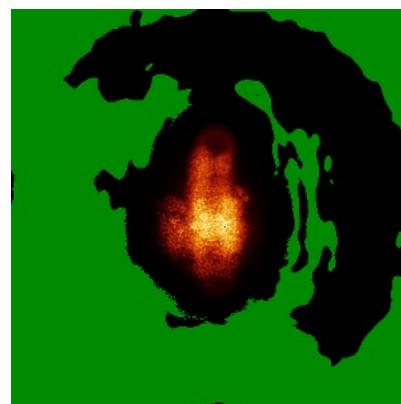
6.4.1 Primary map



X

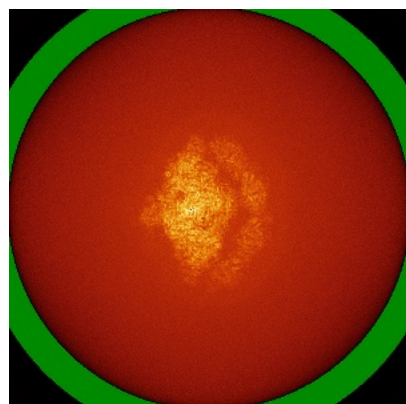


Y

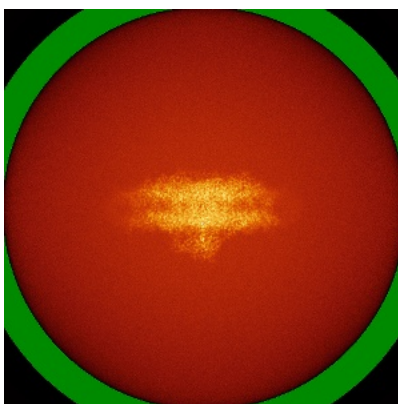


Z

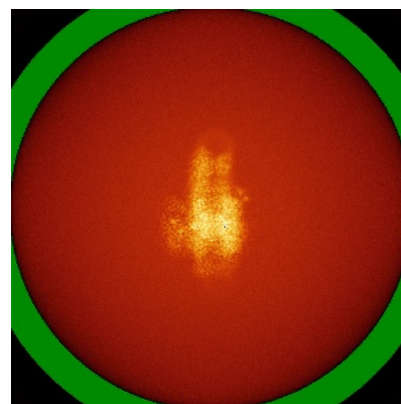
6.4.2 Raw map



X



Y



Z

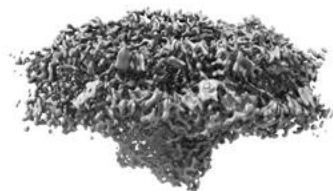
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

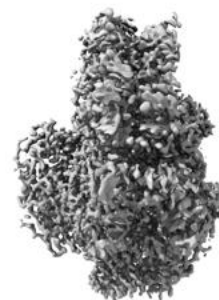
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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



X



Y



Z

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

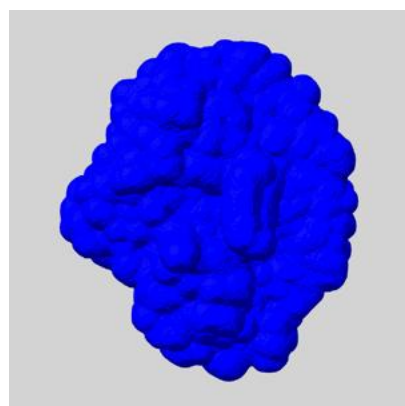
6.6 Mask visualisation [i](#)

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

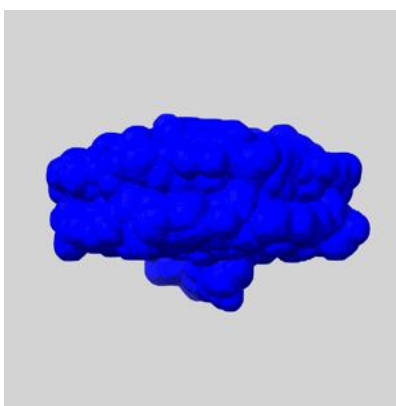
A mask typically either:

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

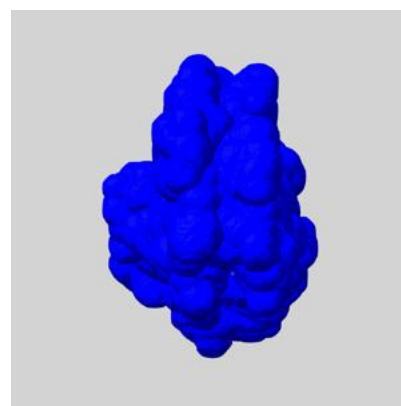
6.6.1 emd_15969_msk_1.map [i](#)



X



Y

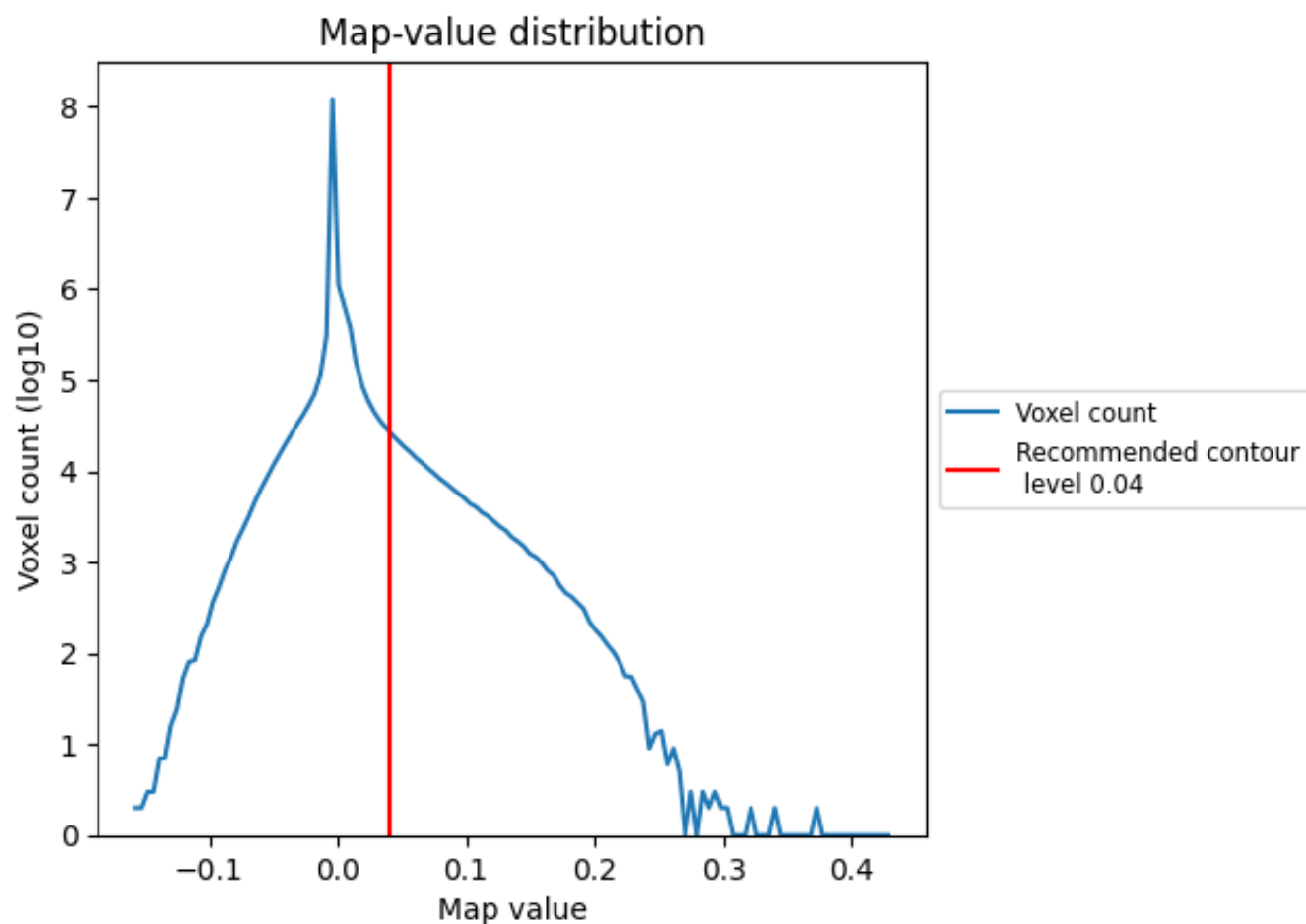


Z

7 Map analysis [i](#)

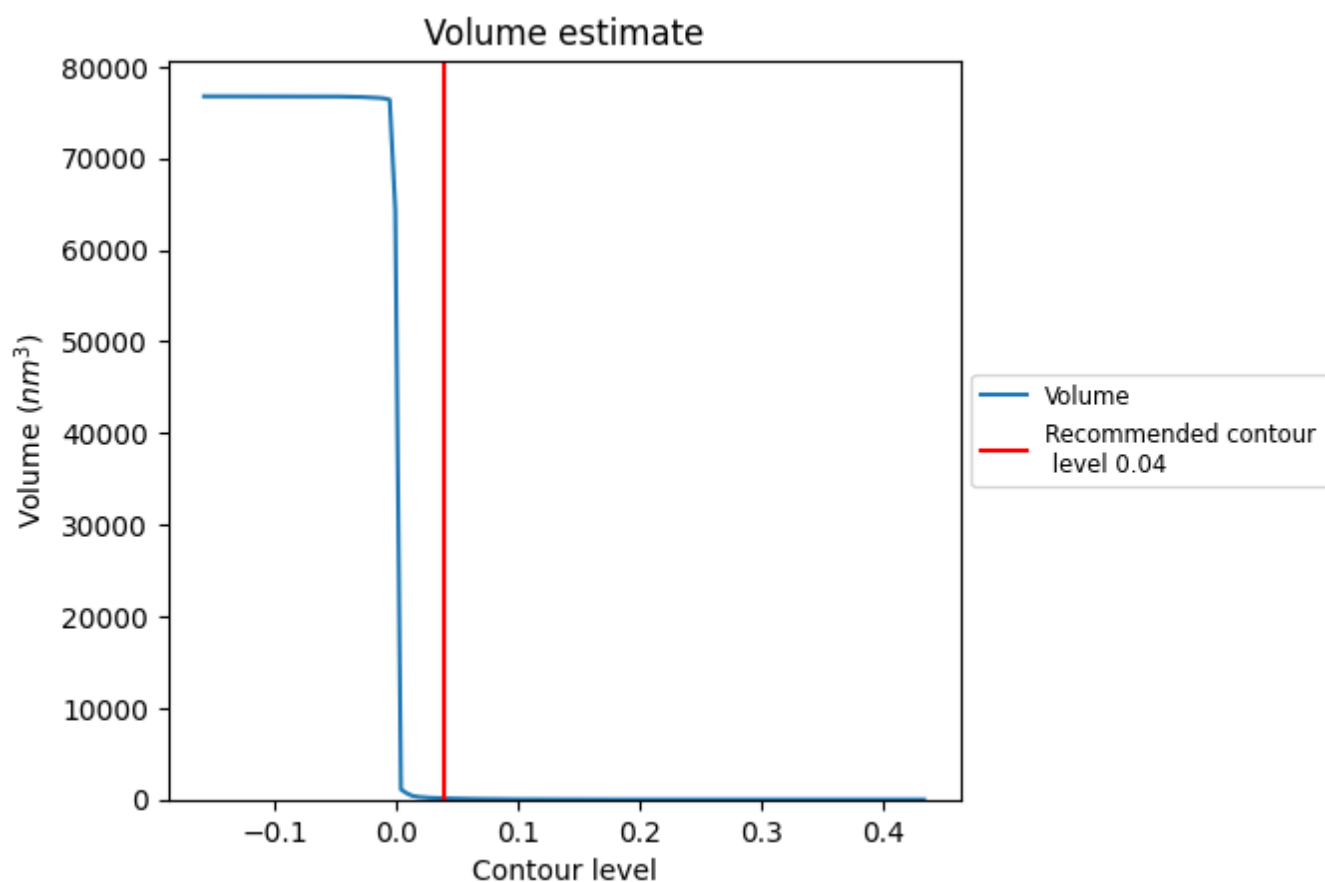
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

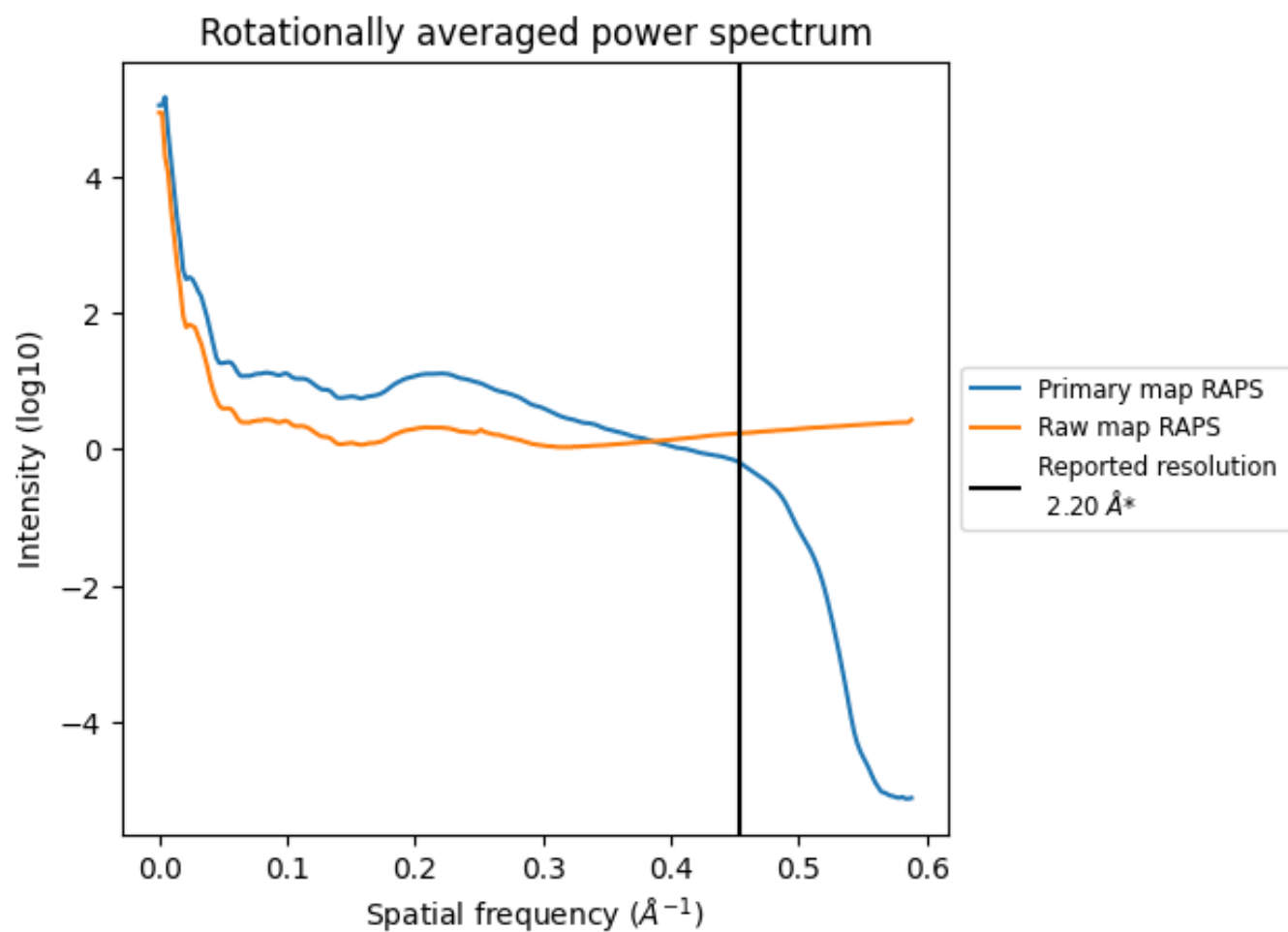
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 130 nm³; this corresponds to an approximate mass of 118 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 [i](#)

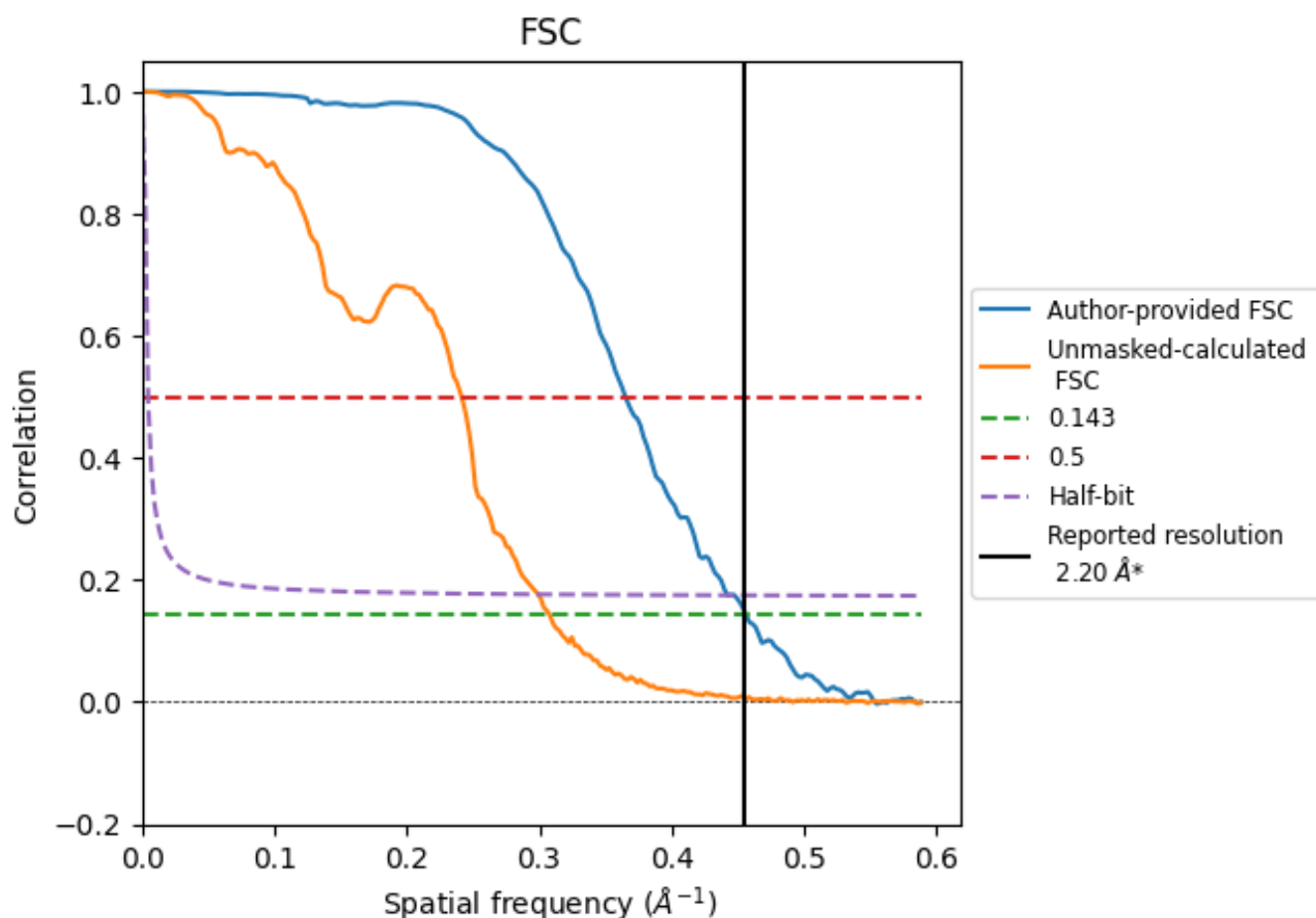


*Reported resolution corresponds to spatial frequency of 0.455 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.455 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

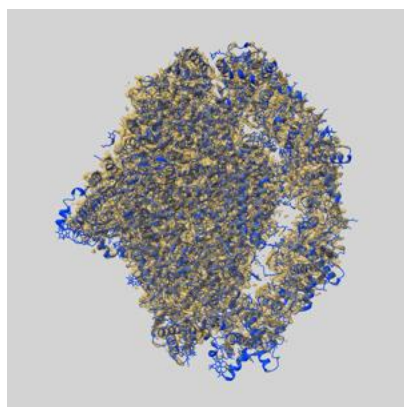
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.19	2.74	2.26
Unmasked-calculated*	3.25	4.14	3.34

*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 3.25 differs from the reported value 2.2 by more than 10 %

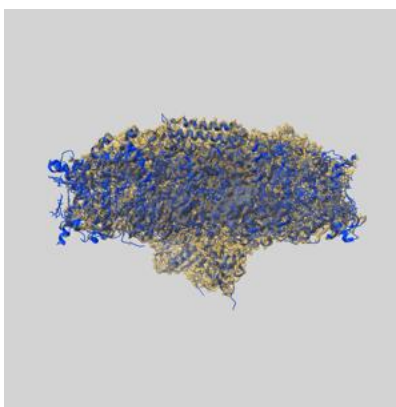
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15969 and PDB model 8BCV. Per-residue inclusion information can be found in section 3 on page 25.

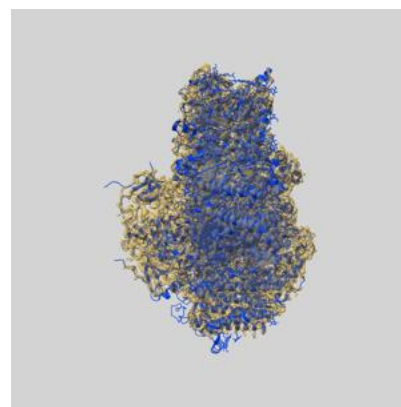
9.1 Map-model overlay [i](#)



X



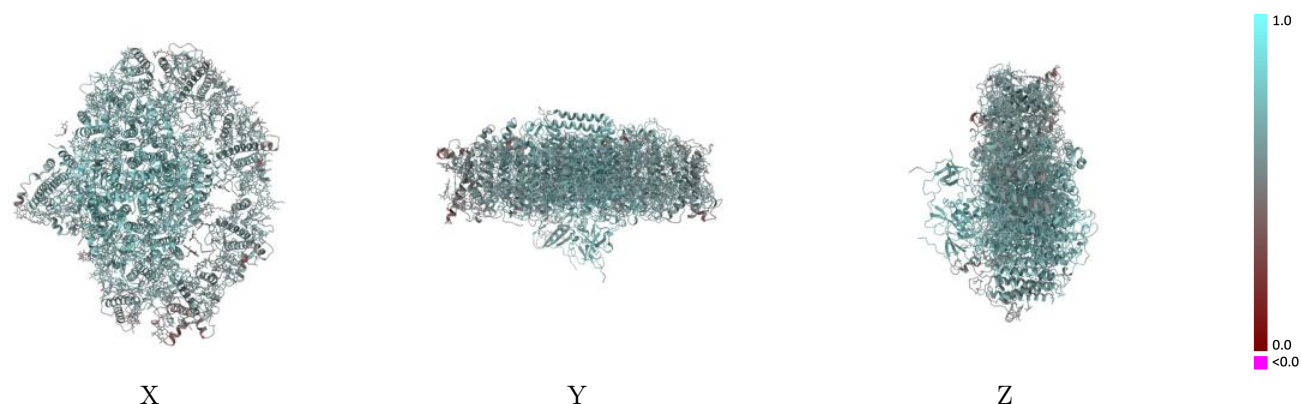
Y



Z

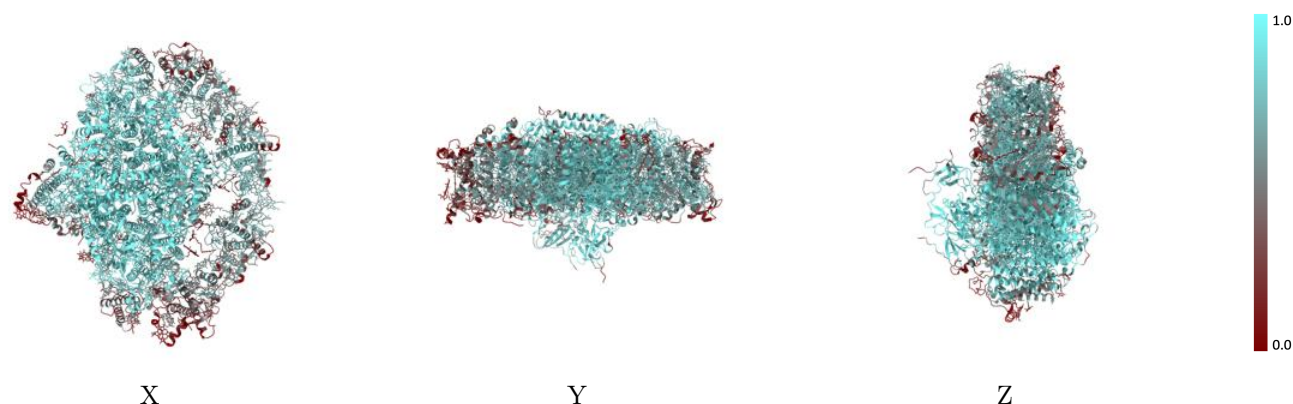
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



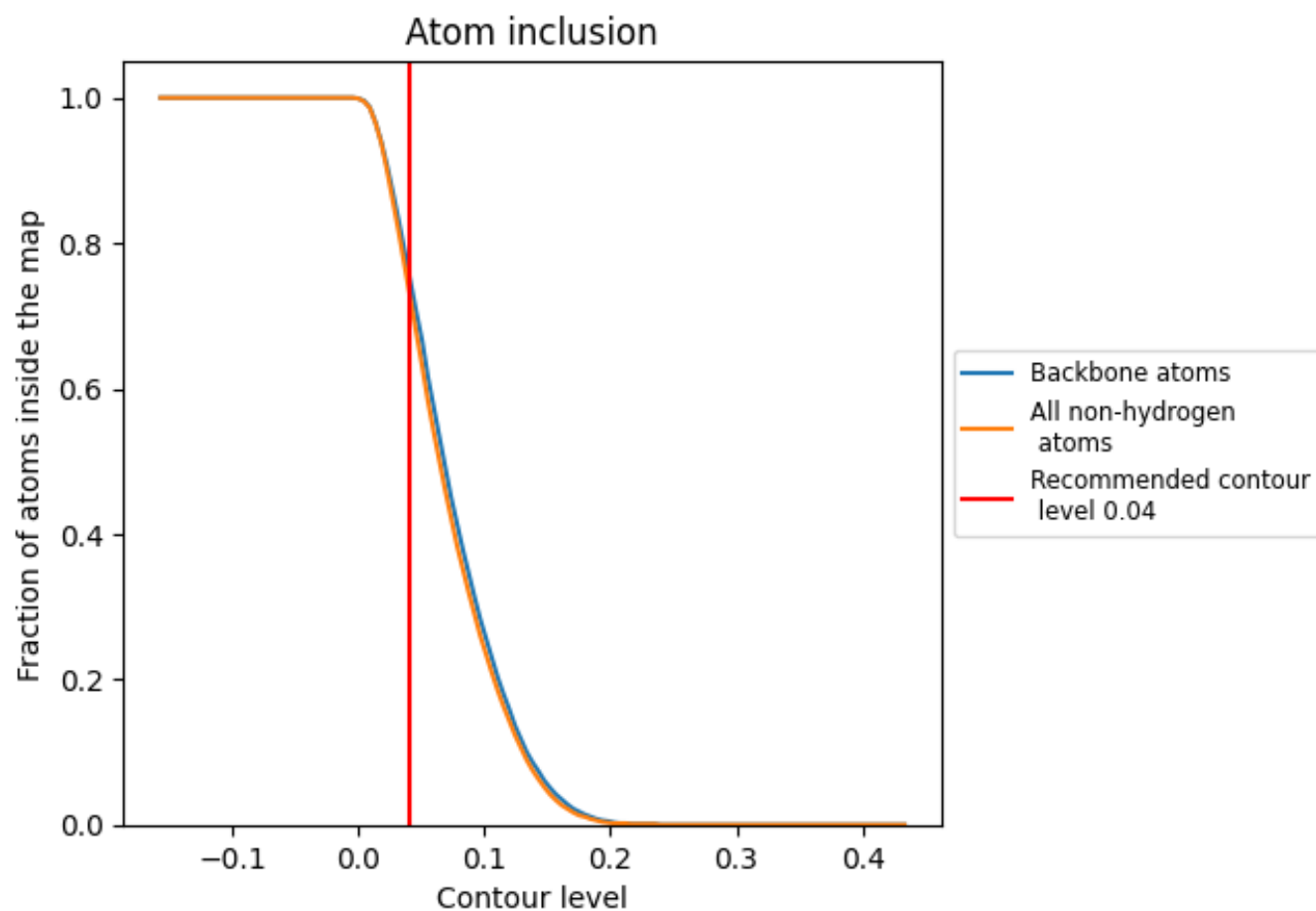
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 73% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7340	 0.6450
1	 0.5320	 0.5570
2	 0.5720	 0.5760
3	 0.3100	 0.5110
4	 0.6350	 0.5870
A	 0.8860	 0.7030
B	 0.9140	 0.7110
C	 0.9770	 0.7440
D	 0.8570	 0.6840
E	 0.7640	 0.6740
F	 0.7910	 0.6720
G	 0.6000	 0.5730
H	 0.2460	 0.5230
I	 0.7910	 0.6630
J	 0.7580	 0.6520
K	 0.2930	 0.4840
L	 0.5770	 0.5950

