



Full wwPDB EM Validation Report ⓘ

Sep 11, 2026 – 05:52 am BST

PDB ID : 9SE6 / pdb_00009se6
EMDB ID : EMD-54803
Title : Structure of Photosystem I from Chlamydomonas reinhardtii at 1.83 Å resolution
Authors : Mahapatra, G.P.; Schuller, J.M.
Deposited on : 2025-08-15
Resolution : 1.83 Å (reported)
Based on initial model : 7ZQC

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

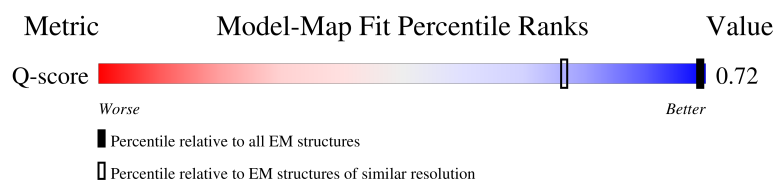
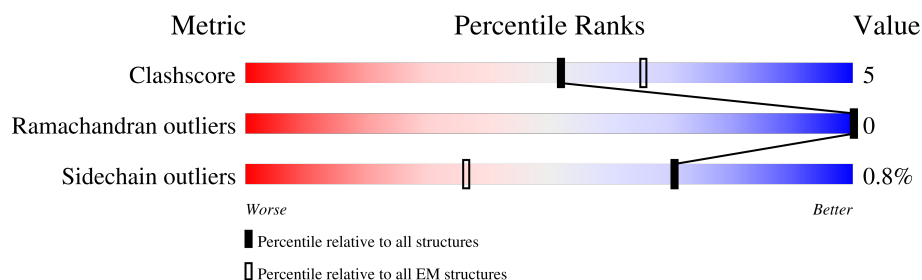
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.83 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	903 (1.33 - 2.33)

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	3	221	 92% 8%
2	4	212	 88% 12%
3	5	227	 89% 10%
4	6	230	 86% 14%

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Mol	Chain	Length	Quality of chain
5	7	213	
6	8	217	
7	A	742	
8	B	733	
9	C	80	
10	D	144	
11	E	64	
12	I	37	
13	J	41	
14	K	86	
15	1	194	
15	Z	194	
16	F	165	
17	G	95	
18	L	124	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	NEX	5	323	X	-	-	-

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 48478 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 Light-harvesting chlorophyll-a/b protein of photosystem I, type III.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	221	Total	C	N	O	S	0	0
			1687	1100	273	306	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	212	Total	C	N	O	S	0	0
			1652	1083	269	295	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	227	Total	C	N	O	S	0	0
			1775	1154	297	316	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	230	Total	C	N	O	S	0	0
			1772	1167	293	306	6		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	213	Total	C	N	O	S	0	0
			1650	1072	274	298	6		

- Molecule 6 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	217	Total	C	N	O	S	0	0
			1650	1073	280	293	4		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	742	Total	C	N	O	S	0	0
			5825	3808	994	1001	22		

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	733	Total	C	N	O	S	0	0
			5824	3824	977	1005	18		

- Molecule 9 is a protein called Photosystem I iron-sulfur center.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	144	Total	C	N	O	S	0	0
			1133	725	200	201	7		

- Molecule 11 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	E	64	Total	C	N	O	0	0
			506	322	89	95		

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

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

- Molecule 13 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	41	Total	C	N	O	S	0	0
			329	224	46	58	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	ACE	-	acetylation	UNP P59777

- Molecule 14 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	86	Total	C	N	O	S	0	0
			583	370	100	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		
15	1	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		

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

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

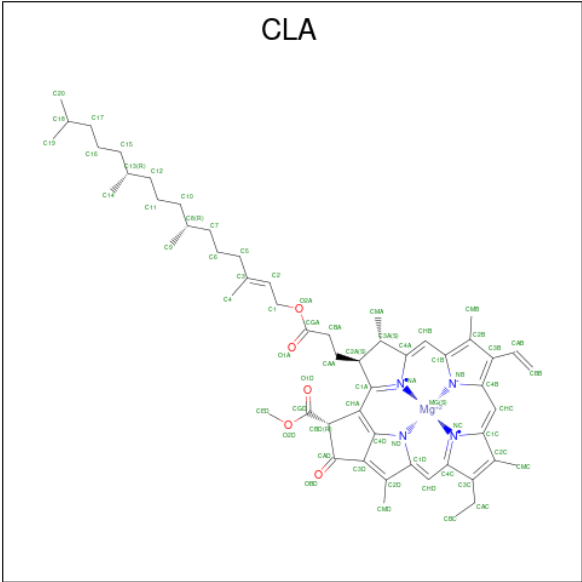
- Molecule 17 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	G	70	Total	C	N	O	0	0
			512	328	90	94		

- Molecule 18 is a protein called Chains: L.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	124	Total	C	N	O	S	0	0
			899	586	146	164	3		

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
19	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	J	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0

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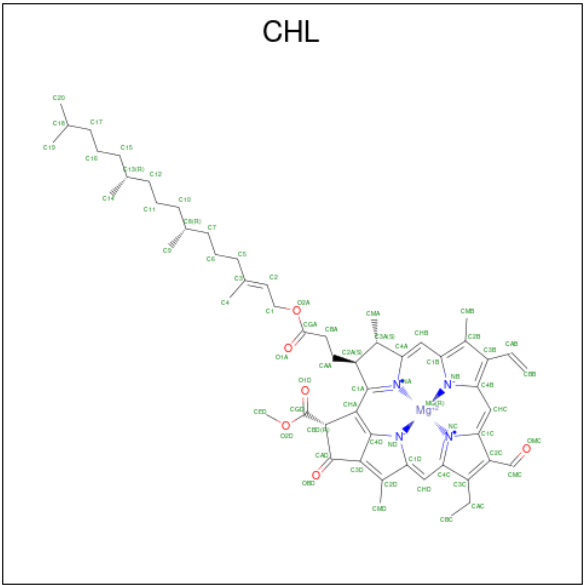
Mol	Chain	Residues	Atoms					AltConf
19	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 20 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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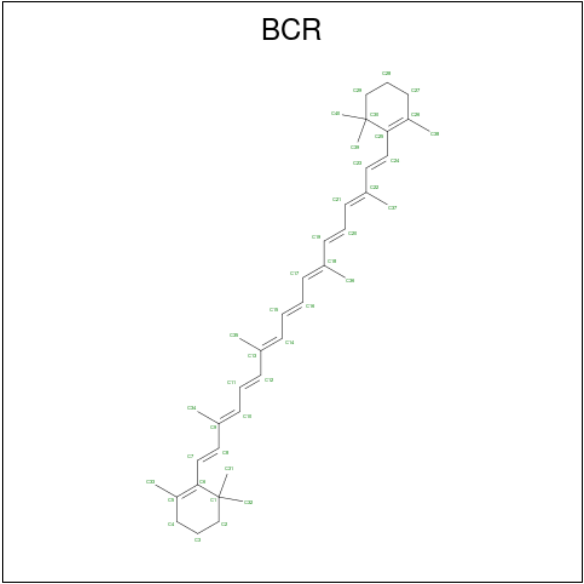
Mol	Chain	Residues	Atoms					AltConf
20	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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



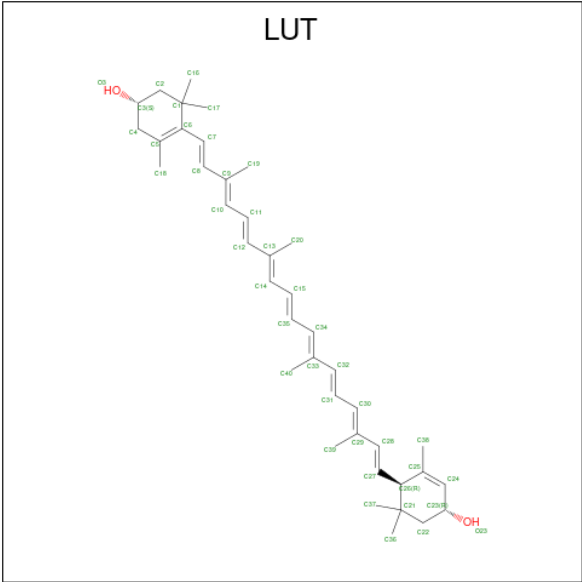
Mol	Chain	Residues	Atoms		AltConf
21	3	1	Total	C	0
			40	40	
21	3	1	Total	C	0
			40	40	
21	3	1	Total	C	0
			40	40	
21	4	1	Total	C	0
			40	40	
21	5	1	Total	C	0
			40	40	
21	6	1	Total	C	0
			40	40	
21	7	1	Total	C	0
			40	40	
21	8	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	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	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	J	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0

- Molecule 22 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).



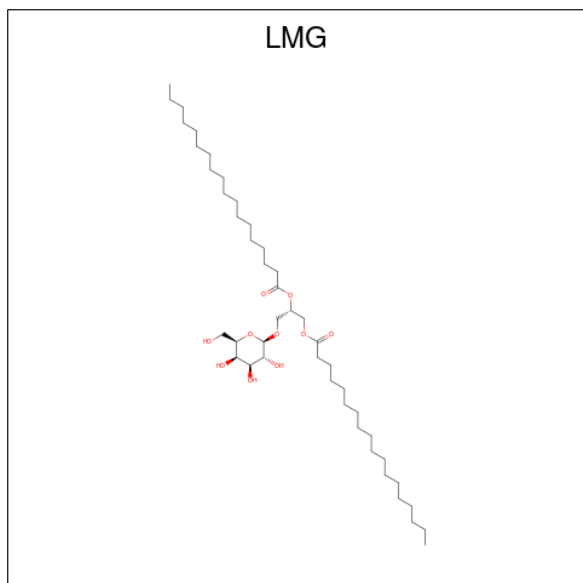
Mol	Chain	Residues	Atoms			AltConf
22	3	1	Total	C	O	0
			42	40	2	
22	3	1	Total	C	O	0
			42	40	2	
22	3	1	Total	C	O	0
			20	19	1	
22	4	1	Total	C	O	0
			42	40	2	
22	5	1	Total	C	O	0
			42	40	2	
22	5	1	Total	C	O	0
			42	40	2	
22	6	1	Total	C	O	0
			42	40	2	
22	7	1	Total	C	O	0
			42	40	2	
22	8	1	Total	C	O	0
			42	40	2	
22	8	1	Total	C	O	0
			42	40	2	
22	J	1	Total	C	O	0
			42	40	2	
22	Z	1	Total	C	O	0
			42	40	2	
22	Z	1	Total	C	O	0
			26	25	1	
22	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			42	40	2	
22	F	1	Total	C	O	0
			42	40	2	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



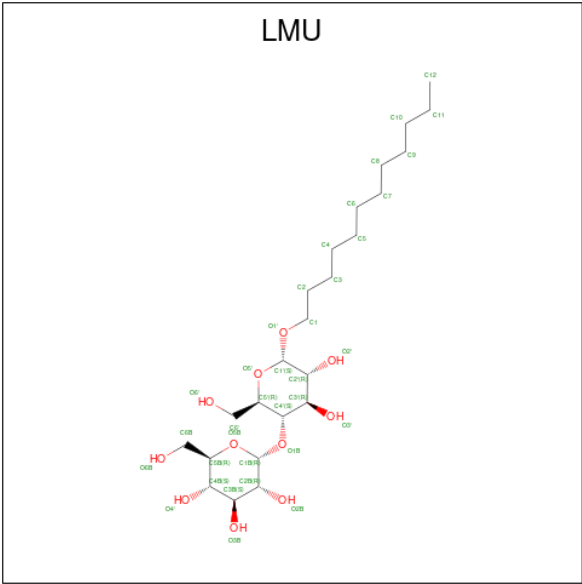
Mol	Chain	Residues	Atoms			AltConf
23	3	1	Total	C	O	0
			37	27	10	
23	4	1	Total	C	O	0
			41	31	10	
23	6	1	Total	C	O	0
			27	22	5	
23	6	1	Total	C	O	0
			20	18	2	
23	7	1	Total	C	O	0
			32	22	10	
23	8	1	Total	C	O	0
			49	39	10	
23	B	1	Total	C	O	0
			43	33	10	
23	J	1	Total	C	O	0
			42	32	10	
23	J	1	Total	C	O	0
			35	25	10	

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Mol	Chain	Residues	Atoms			AltConf
23	F	1	Total	C	O	0
			32	22	10	
23	G	1	Total	C	O	0
			36	26	10	
23	L	1	Total	C	O	0
			40	30	10	

- Molecule 24 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



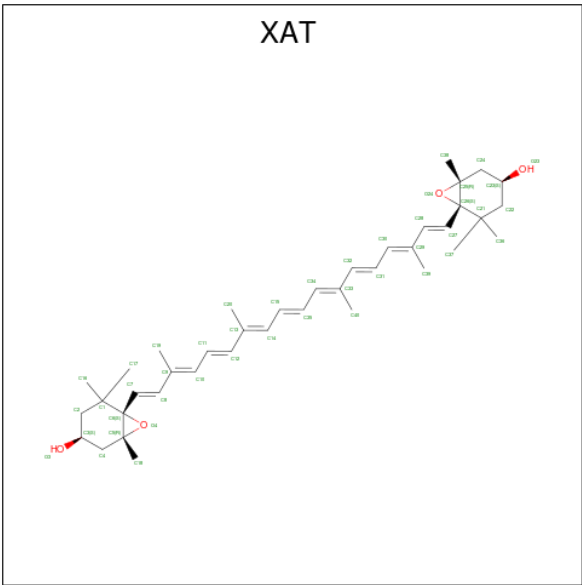
Mol	Chain	Residues	Atoms			AltConf
24	3	1	Total	C	O	0
			34	23	11	
24	3	1	Total	C	O	0
			24	18	6	
24	3	1	Total	C	O	0
			35	24	11	
24	3	1	Total	C	O	0
			24	18	6	
24	4	1	Total	C	O	0
			22	16	6	
24	4	1	Total	C	O	0
			20	14	6	
24	4	1	Total	C	O	0
			24	18	6	
24	4	1	Total	C	O	0
			22	16	6	

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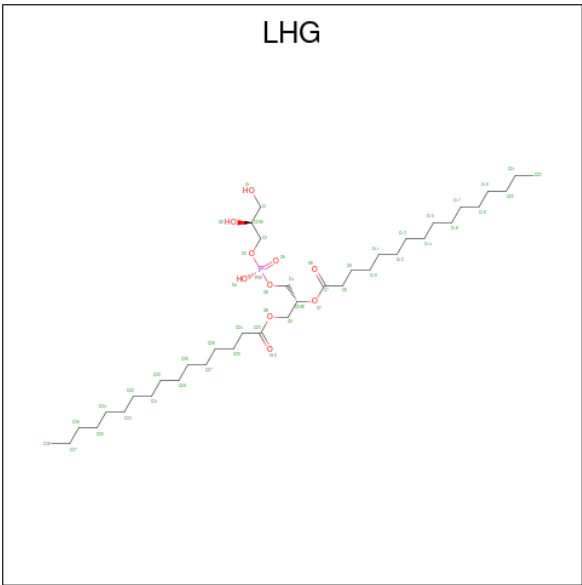
Mol	Chain	Residues	Atoms			AltConf
24	6	1	Total	C	O	0
			24	18	6	
24	6	1	Total	C	O	0
			24	18	6	
24	7	1	Total	C	O	0
			21	15	6	
24	7	1	Total	C	O	0
			22	16	6	
24	8	1	Total	C	O	0
			24	18	6	
24	A	1	Total	C	O	0
			35	24	11	
24	A	1	Total	C	O	0
			20	14	6	
24	A	1	Total	C	O	0
			24	18	6	
24	B	1	Total	C	O	0
			35	24	11	
24	K	1	Total	C	O	0
			24	18	6	
24	Z	1	Total	C	O	0
			31	20	11	
24	Z	1	Total	C	O	0
			24	18	6	
24	Z	1	Total	C	O	0
			24	18	6	
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
			19	13	6	
24	1	1	Total	C	O	0
			24	18	6	
24	1	1	Total	C	O	0
			22	16	6	
24	F	1	Total	C	O	0
			35	24	11	

- Molecule 25 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



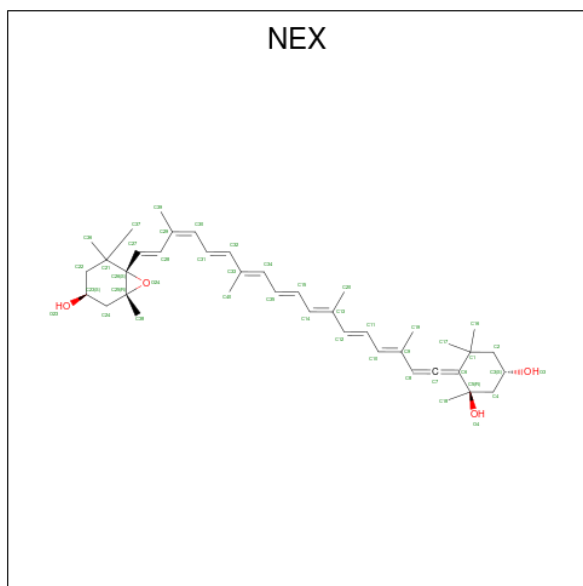
Mol	Chain	Residues	Atoms			AltConf
25	4	1	Total	C	O	0
			44	40	4	
25	5	1	Total	C	O	0
			44	40	4	
25	6	1	Total	C	O	0
			44	40	4	
25	7	1	Total	C	O	0
			44	40	4	
25	8	1	Total	C	O	0
			44	40	4	
25	Z	1	Total	C	O	0
			44	40	4	
25	1	1	Total	C	O	0
			44	40	4	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



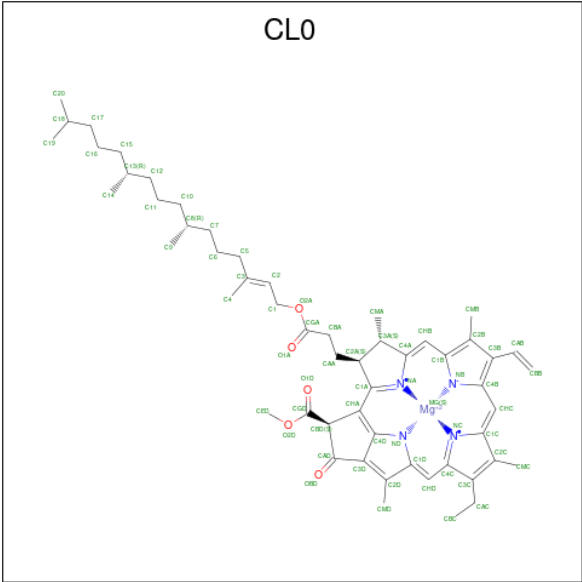
Mol	Chain	Residues	Atoms				AltConf
26	4	1	Total	C	O	P	0
			49	38	10	1	
26	4	1	Total	C	O	P	0
			38	27	10	1	
26	5	1	Total	C	O	P	0
			38	27	10	1	
26	5	1	Total	C	O	P	0
			37	26	10	1	
26	6	1	Total	C	O	P	0
			49	38	10	1	
26	6	1	Total	C	O	P	0
			36	25	10	1	
26	7	1	Total	C	O	P	0
			49	38	10	1	
26	8	1	Total	C	O	P	0
			44	33	10	1	
26	A	1	Total	C	O	P	0
			31	20	10	1	
26	A	1	Total	C	O	P	0
			49	38	10	1	
26	A	1	Total	C	O	P	0
			38	27	10	1	
26	B	1	Total	C	O	P	0
			45	34	10	1	
26	Z	1	Total	C	O	P	0
			39	28	10	1	
26	1	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 27 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



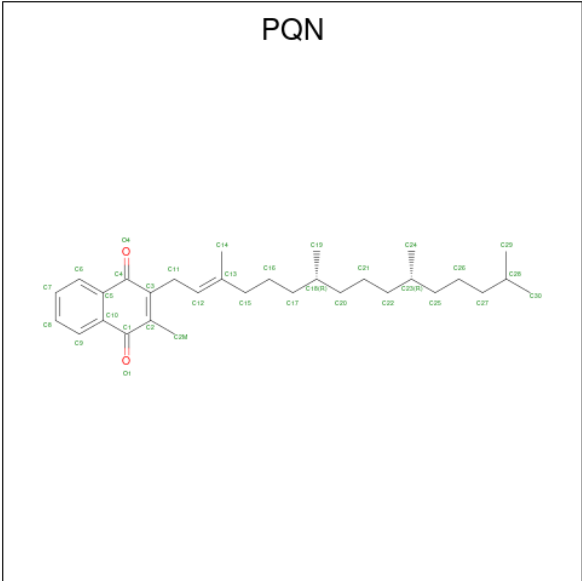
Mol	Chain	Residues	Atoms			AltConf
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	

- Molecule 28 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



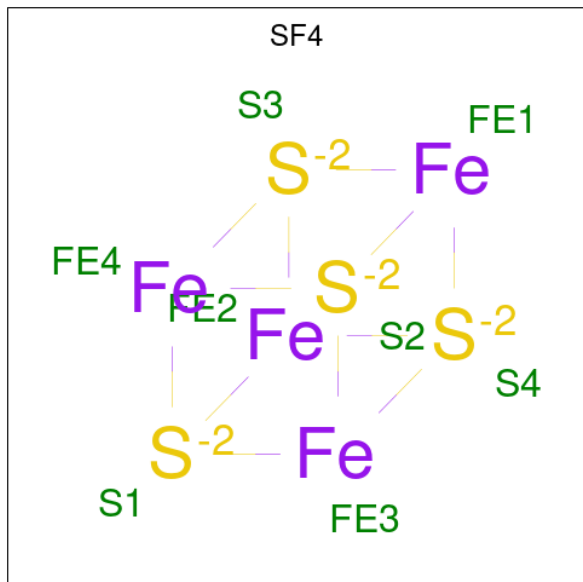
Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 29 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



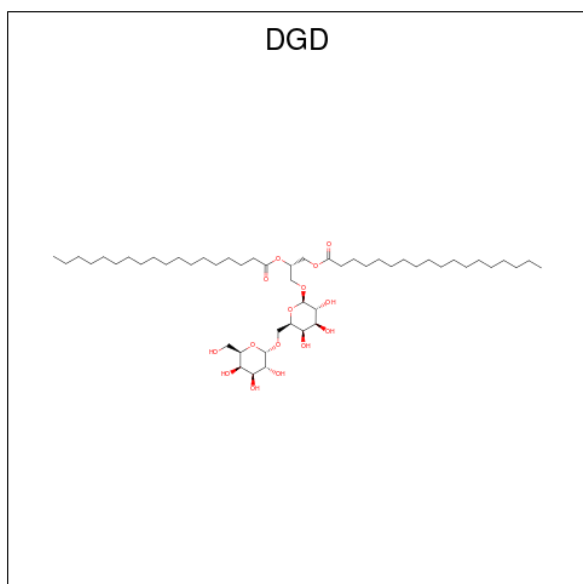
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			33	31	2	
29	B	1	Total	C	O	0
			33	31	2	

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

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



Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			59	44	15	

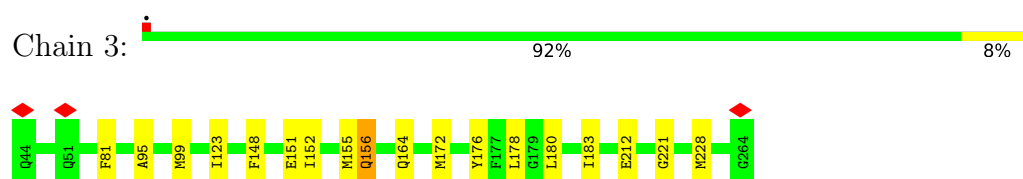
- Molecule 32 is water.

Mol	Chain	Residues	Atoms			AltConf
32	3	55	Total	O		0
			55	55		
32	4	17	Total	O		0
			17	17		
32	5	36	Total	O		0
			36	36		
32	6	21	Total	O		0
			21	21		
32	7	74	Total	O		0
			74	74		
32	8	61	Total	O		0
			61	61		
32	A	288	Total	O		0
			288	288		
32	B	237	Total	O		0
			237	237		
32	C	50	Total	O		0
			50	50		
32	D	49	Total	O		0
			49	49		
32	E	21	Total	O		0
			21	21		
32	I	2	Total	O		0
			2	2		
32	J	9	Total	O		0
			9	9		
32	K	3	Total	O		0
			3	3		
32	Z	11	Total	O		0
			11	11		
32	1	32	Total	O		0
			32	32		
32	F	47	Total	O		0
			47	47		
32	L	6	Total	O		0
			6	6		

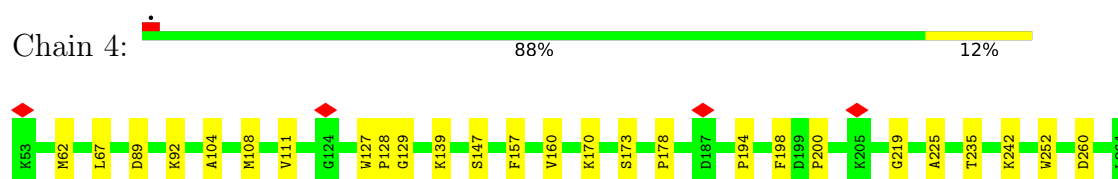
3 Residue-property plots [i](#)

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.

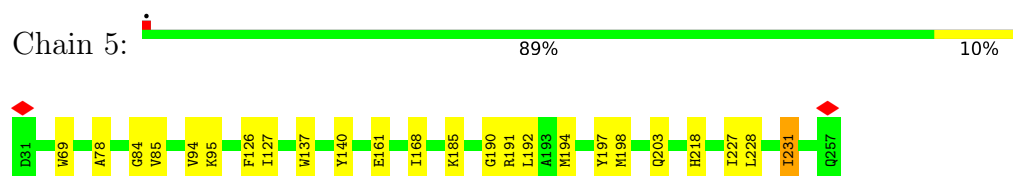
- Molecule 1: Light-harvesting chlorophyll-a/b protein of photosystem I, type III



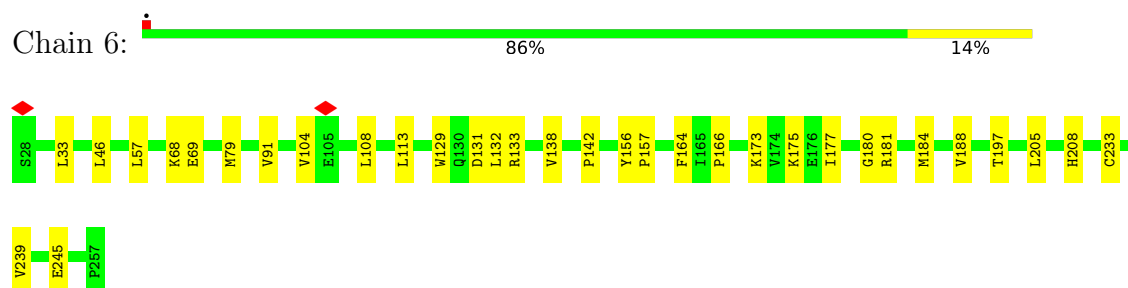
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



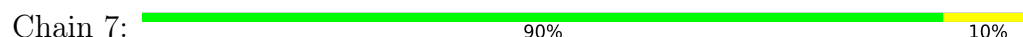
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



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



- Molecule 5: Chlorophyll a-b binding protein, chloroplastic

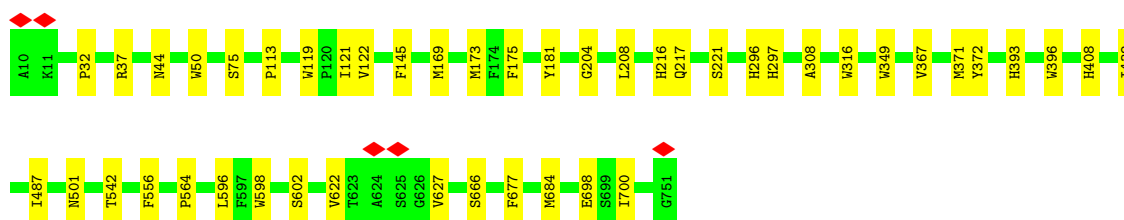




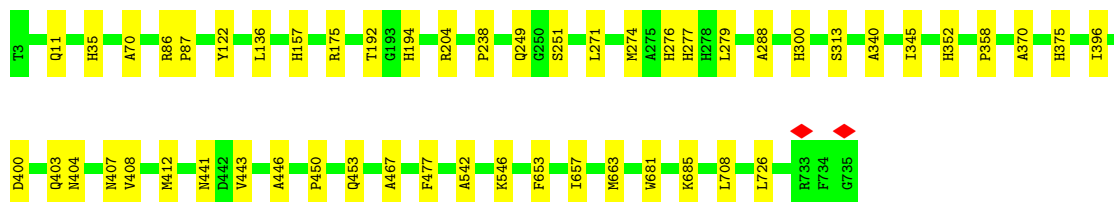
- Molecule 6: Chlorophyll a-b binding protein, chloroplastic



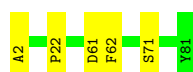
- Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 9: Photosystem I iron-sulfur center

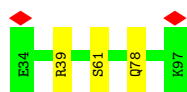


- Molecule 10: Photosystem I reaction center subunit II, chloroplastic

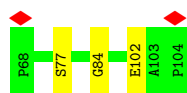
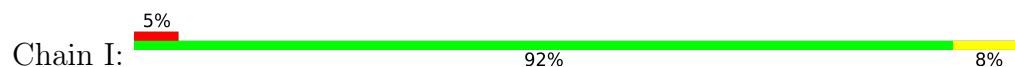


- Molecule 11: Photosystem I reaction center subunit IV, chloroplastic





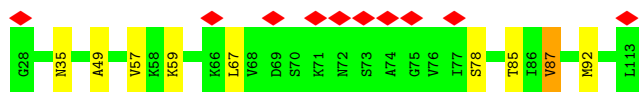
- Molecule 12: Photosystem I reaction center subunit VIII



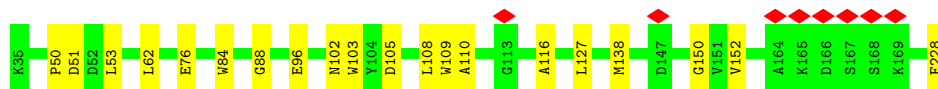
- Molecule 13: Photosystem I reaction center subunit IX



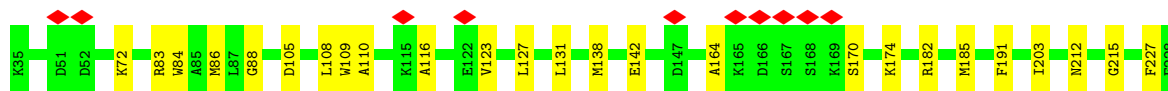
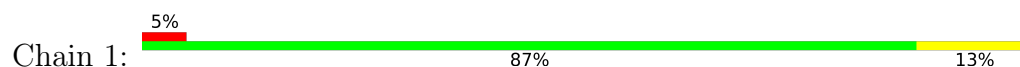
- Molecule 14: Photosystem I reaction center subunit psaK, chloroplastic



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



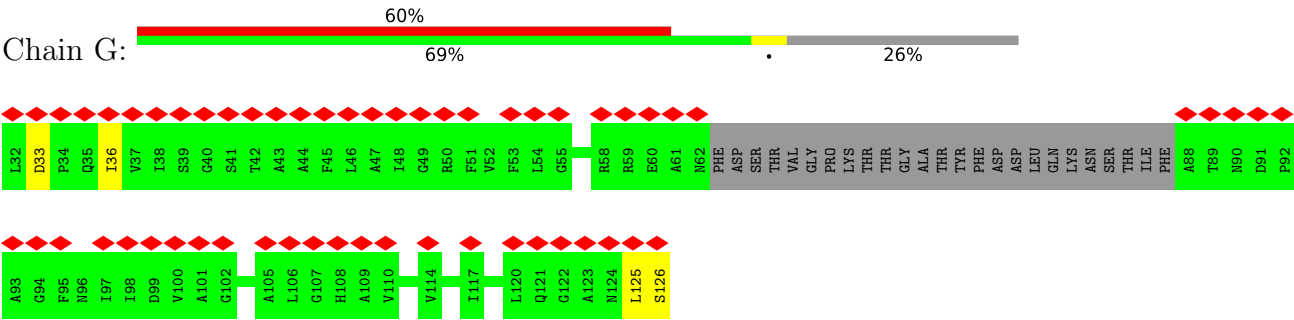
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



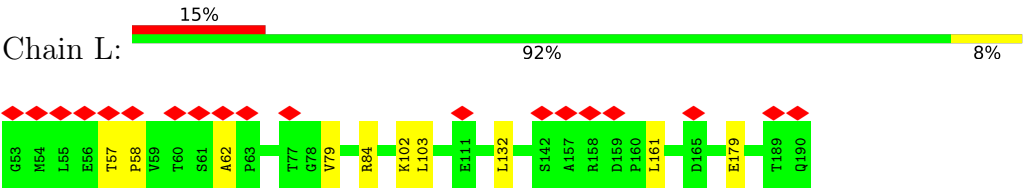
- Molecule 16: Photosystem I reaction center subunit III, chloroplastic



- Molecule 17: Photosystem I reaction center subunit V, chloroplastic



● Molecule 18: Chains: L



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	246159	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.385	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	373.76, 373.76, 373.76	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	Depositor

5 Model quality

5.1 Standard geometry

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

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	3	0.16	0/1735	0.39	1/2355 (0.0%)
2	4	0.13	0/1707	0.28	0/2325
3	5	0.14	0/1830	0.30	0/2492
4	6	0.13	0/1834	0.30	0/2505
5	7	0.14	0/1702	0.30	0/2310
6	8	0.14	0/1701	0.29	0/2315
7	A	0.15	0/6021	0.32	0/8208
8	B	0.15	0/6036	0.34	0/8240
9	C	0.12	0/611	0.34	0/826
10	D	0.12	0/1161	0.34	0/1567
11	E	0.11	0/516	0.29	0/700
12	I	0.13	0/293	0.29	0/406
13	J	0.17	0/338	0.33	0/464
14	K	0.12	0/588	0.26	0/795
15	1	0.15	0/1491	0.32	0/2028
15	Z	0.13	0/1491	0.27	0/2028
16	F	0.13	0/1292	0.31	0/1747
17	G	0.09	0/521	0.20	0/706
18	L	0.13	0/920	0.27	0/1257
All	All	0.14	0/31788	0.32	1/43274 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	156	GLN	CA-CB-CG	7.14	128.39	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	1687	0	1646	16	0
2	4	1652	0	1613	19	0
3	5	1775	0	1746	19	0
4	6	1772	0	1770	29	0
5	7	1650	0	1589	16	0
6	8	1650	0	1629	19	0
7	A	5825	0	5675	40	0
8	B	5824	0	5577	41	0
9	C	601	0	581	3	0
10	D	1133	0	1150	6	0
11	E	506	0	504	2	0
12	I	281	0	292	2	0
13	J	329	0	328	3	0
14	K	583	0	620	7	0
15	1	1445	0	1396	20	0
15	Z	1445	0	1396	14	0
16	F	1266	0	1301	8	0
17	G	512	0	503	3	0
18	L	899	0	905	8	0
19	1	639	0	625	16	0
19	3	720	0	674	22	0
19	4	565	0	534	15	0
19	5	717	0	667	26	0
19	6	667	0	619	19	0
19	7	599	0	553	14	0
19	8	617	0	587	16	0
19	A	2653	0	2784	68	0
19	B	2528	0	2652	79	0
19	F	175	0	177	7	0
19	G	106	0	92	0	0
19	J	55	0	49	1	0
19	K	196	0	158	5	0
19	L	110	0	105	3	0
19	Z	637	0	616	10	0
20	1	92	0	62	2	0
20	3	66	0	70	0	0
20	4	287	0	270	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	5	206	0	167	5	0
20	6	338	0	307	15	0
20	7	224	0	202	3	0
20	8	198	0	210	5	0
20	Z	178	0	171	1	0
21	3	120	0	168	6	0
21	4	40	0	56	1	0
21	5	40	0	56	4	0
21	6	40	0	56	2	0
21	7	40	0	56	3	0
21	8	40	0	56	1	0
21	A	240	0	336	9	0
21	B	280	0	392	10	0
21	G	40	0	56	0	0
21	I	40	0	56	1	0
21	J	40	0	56	1	0
21	K	40	0	56	1	0
21	L	80	0	112	4	0
22	1	84	0	112	3	0
22	3	104	0	138	1	0
22	4	42	0	56	3	0
22	5	84	0	112	4	0
22	6	42	0	56	0	0
22	7	42	0	56	0	0
22	8	84	0	112	0	0
22	F	42	0	56	1	0
22	J	42	0	56	3	0
22	Z	68	0	89	1	0
23	3	37	0	44	4	0
23	4	41	0	55	0	0
23	6	47	0	68	3	0
23	7	32	0	34	0	0
23	8	49	0	71	1	0
23	B	43	0	56	1	0
23	F	32	0	34	1	0
23	G	36	0	42	0	0
23	J	77	0	97	4	0
23	L	40	0	50	2	0
24	1	135	0	177	5	0
24	3	117	0	157	3	0
24	4	88	0	115	2	0
24	6	48	0	70	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	7	43	0	54	1	0
24	8	24	0	35	1	0
24	A	79	0	105	1	0
24	B	35	0	46	2	0
24	F	35	0	46	2	0
24	K	24	0	35	0	0
24	Z	79	0	105	0	0
25	1	44	0	56	1	0
25	4	44	0	56	1	0
25	5	44	0	56	3	0
25	6	44	0	56	2	0
25	7	44	0	56	1	0
25	8	44	0	56	0	0
25	Z	44	0	56	2	0
26	1	44	0	58	0	0
26	4	87	0	123	5	0
26	5	75	0	90	2	0
26	6	85	0	116	7	0
26	7	49	0	74	1	0
26	8	44	0	61	3	0
26	A	118	0	155	3	0
26	B	45	0	63	6	0
26	Z	39	0	48	0	0
27	5	44	0	56	0	0
27	6	44	0	56	2	0
28	A	65	0	72	0	0
29	A	33	0	46	0	0
29	B	33	0	46	0	0
30	A	8	0	0	0	0
30	C	16	0	0	0	0
31	B	59	0	79	2	0
32	1	32	0	0	0	0
32	3	55	0	0	0	0
32	4	17	0	0	0	0
32	5	36	0	0	0	0
32	6	21	0	0	0	0
32	7	74	0	0	0	0
32	8	61	0	0	0	0
32	A	288	0	0	0	0
32	B	237	0	0	1	0
32	C	50	0	0	0	0
32	D	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	E	21	0	0	0	0
32	F	47	0	0	0	0
32	I	2	0	0	0	0
32	J	9	0	0	0	0
32	K	3	0	0	0	0
32	L	6	0	0	0	0
32	Z	11	0	0	0	0
All	All	48478	0	47958	518	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 5.

All (518) 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)
8:B:663:MET:HB2	19:B:804:CLA:C1C	2.07	0.83
20:5:308:CHL:HBB2	20:5:317:CHL:HHC	1.60	0.81
20:4:607:CHL:HBB2	20:4:615:CHL:HHC	1.65	0.77
21:5:320:BCR:HC42	26:6:318:LHG:H102	1.70	0.73
15:1:142:GLU:HG3	19:1:308:CLA:C4B	2.18	0.73
3:5:69:TRP:CG	19:5:319:CLA:HAA1	2.23	0.73
7:A:684:MET:HB2	19:A:803:CLA:C1C	2.17	0.73
19:A:829:CLA:HED1	19:A:837:CLA:HAB	1.72	0.69
3:5:94:VAL:HG12	3:5:95:LYS:HG2	1.73	0.69
1:3:228:MET:HE2	22:3:317:LUT:H10	1.75	0.68
8:B:663:MET:HB2	19:B:804:CLA:C2C	2.23	0.67
19:B:842:CLA:HMB2	26:B:851:LHG:H242	1.75	0.67
15:1:138:MET:O	15:1:142:GLU:HB2	1.95	0.66
4:6:69:GLU:HG2	4:6:132:LEU:HD11	1.78	0.66
19:B:814:CLA:H172	21:B:845:BCR:H271	1.78	0.65
19:B:822:CLA:H201	15:1:131:LEU:HD23	1.78	0.65
19:B:823:CLA:HAA2	24:1:301:LMU:H6D	1.78	0.64
19:6:304:CLA:H2	5:7:173:MET:HE2	1.80	0.64
8:B:708:LEU:HD22	31:B:850:DGD:HB22	1.78	0.64
4:6:129:TRP:CE2	4:6:133:ARG:HD2	2.33	0.64
1:3:156:GLN:NE2	19:3:314:CLA:ND	2.44	0.64
21:7:617:BCR:HC41	26:8:318:LHG:H251	1.80	0.63
15:1:110:ALA:HB1	15:1:127:LEU:HD22	1.80	0.63
8:B:204:ARG:HG2	8:B:251:SER:HB2	1.80	0.62
19:3:305:CLA:HBC1	21:3:319:BCR:H361	1.82	0.62
2:4:194:PRO:HB3	20:4:607:CHL:HBC2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:622:VAL:HG22	7:A:627:VAL:HG22	1.81	0.62
2:4:111:VAL:HG11	22:4:616:LUT:H12	1.81	0.62
26:6:318:LHG:H282	26:6:318:LHG:HC92	1.82	0.62
4:6:181:ARG:HA	4:6:184:MET:HE3	1.81	0.61
19:8:302:CLA:H162	19:8:303:CLA:HBB1	1.83	0.60
19:B:842:CLA:HBC1	24:1:301:LMU:H2'	1.82	0.60
1:3:95:ALA:HB1	1:3:221:GLY:HA3	1.84	0.60
19:B:811:CLA:HBB2	12:I:84:GLY:HA3	1.84	0.59
19:B:817:CLA:HED1	17:G:126:SER:HB2	1.84	0.59
8:B:663:MET:HB2	19:B:804:CLA:NC	2.18	0.59
19:8:302:CLA:H91	19:8:303:CLA:H151	1.83	0.59
4:6:188:VAL:HG11	19:6:303:CLA:H202	1.84	0.59
19:6:327:CLA:HAC2	24:7:620:LMU:H82	1.85	0.59
14:K:59:LYS:HD2	14:K:67:LEU:HB3	1.84	0.59
15:1:227:PHE:HE1	19:1:314:CLA:HAB	1.68	0.58
19:6:313:CLA:H93	26:6:318:LHG:H321	1.86	0.58
21:B:844:BCR:H331	21:B:844:BCR:HC8	1.84	0.57
15:1:88:GLY:HA2	25:1:316:XAT:H181	1.86	0.57
15:1:170:SER:O	15:1:174:LYS:HG3	2.03	0.57
14:K:78:SER:HB2	14:K:85:THR:HG22	1.85	0.57
15:Z:110:ALA:HB1	15:Z:127:LEU:HD22	1.85	0.57
6:8:149:GLU:HG2	6:8:152:SER:HB3	1.85	0.57
8:B:35:HIS:HE1	19:B:805:CLA:HED1	1.70	0.57
2:4:147:SER:HB3	15:Z:228:PHE:HB3	1.87	0.57
19:1:310:CLA:H43	19:1:311:CLA:HMD2	1.86	0.57
15:1:227:PHE:HB3	24:F:306:LMU:H3B	1.87	0.57
6:8:90:PRO:O	6:8:94:THR:HG23	2.03	0.56
23:3:321:LMG:H301	22:5:324:LUT:H371	1.87	0.56
19:A:833:CLA:HMA1	18:L:57:THR:HG21	1.87	0.56
14:K:92:MET:HA	14:K:92:MET:HE2	1.86	0.56
19:B:812:CLA:H42	24:B:853:LMU:H11	1.86	0.56
16:F:142:LYS:HZ3	24:F:306:LMU:H6D	1.70	0.56
19:4:612:CLA:HBA1	19:4:612:CLA:HBD	1.86	0.56
19:A:811:CLA:H142	22:J:101:LUT:H192	1.87	0.56
16:F:95:GLU:HG2	16:F:98:SER:HB3	1.88	0.56
20:8:306:CHL:HHC	24:8:319:LMU:H92	1.87	0.56
21:A:853:BCR:H362	19:B:801:CLA:H2	1.86	0.56
19:B:832:CLA:HBC2	19:B:839:CLA:HMC2	1.87	0.56
4:6:142:PRO:HD2	20:6:317:CHL:HHC	1.87	0.55
7:A:564:PRO:HG2	10:D:119:GLU:HG2	1.88	0.55
3:5:78:ALA:HB1	3:5:190:GLY:HA3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:181:ARG:HD2	19:6:303:CLA:C4C	2.36	0.55
20:4:605:CHL:H203	21:4:618:BCR:H391	1.87	0.55
8:B:175:ARG:HB2	19:B:814:CLA:HBC2	1.88	0.55
19:A:842:CLA:H112	19:A:842:CLA:HAB	1.87	0.55
19:B:837:CLA:H93	19:B:838:CLA:H2	1.89	0.55
19:A:821:CLA:HAB	19:A:821:CLA:H8	1.90	0.54
19:4:603:CLA:HBC3	25:4:617:XAT:H11	1.89	0.54
3:5:85:VAL:HG11	22:5:318:LUT:H12	1.88	0.54
7:A:119:TRP:CD2	19:A:811:CLA:HED3	2.42	0.54
7:A:204:GLY:O	7:A:208:LEU:HB2	2.08	0.54
19:B:801:CLA:HHB	19:B:803:CLA:H202	1.89	0.54
15:Z:138:MET:HG3	19:Z:608:CLA:HMC3	1.90	0.53
10:D:189:ARG:HG3	10:D:189:ARG:HH11	1.73	0.53
2:4:157:PHE:HA	2:4:160:VAL:HG22	1.89	0.53
8:B:408:VAL:O	8:B:412:MET:HG2	2.08	0.53
13:J:0:ACE:H2	13:J:4:PHE:H	1.74	0.53
15:1:203:ILE:HG22	24:1:321:LMU:H1'	1.90	0.53
19:3:303:CLA:H202	19:5:303:CLA:H202	1.90	0.53
6:8:172:PRO:HA	15:Z:62:LEU:HD22	1.89	0.53
8:B:400:ASP:HB3	8:B:403:GLN:HG2	1.90	0.53
19:B:822:CLA:H8	24:1:319:LMU:H42	1.90	0.52
20:5:306:CHL:HHB	21:5:320:BCR:H373	1.92	0.52
7:A:169:MET:HE1	19:A:815:CLA:H92	1.92	0.52
8:B:194:HIS:CE1	19:B:815:CLA:NA	2.78	0.52
4:6:205:LEU:HD11	19:6:314:CLA:HMC2	1.92	0.52
19:B:824:CLA:H71	26:B:851:LHG:H191	1.92	0.52
15:1:182:ARG:HA	15:1:185:MET:HE3	1.92	0.52
18:L:84:ARG:HH21	18:L:161:LEU:HD22	1.75	0.52
23:3:321:LMG:H132	23:3:321:LMG:H322	1.91	0.52
19:5:305:CLA:H2	21:5:320:BCR:H391	1.92	0.52
19:6:305:CLA:H202	19:6:310:CLA:HBC1	1.91	0.52
7:A:367:VAL:O	7:A:371:MET:HG3	2.10	0.52
13:J:33:PHE:HB3	23:J:104:LMG:HC2	1.92	0.52
15:Z:96:GLU:HG3	15:Z:102:ASN:HA	1.92	0.52
7:A:297:HIS:HB2	19:A:820:CLA:C1B	2.40	0.51
20:7:605:CHL:HHB	21:7:617:BCR:H373	1.92	0.51
2:4:139:LYS:HG2	20:4:606:CHL:HED2	1.91	0.51
19:A:820:CLA:H102	19:K:203:CLA:H91	1.91	0.51
20:4:605:CHL:H13	20:4:607:CHL:HBA1	1.92	0.51
4:6:177:ILE:O	4:6:181:ARG:HG3	2.10	0.51
20:6:307:CHL:HBB1	25:6:322:XAT:H193	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:62:MET:HG3	20:4:601:CHL:HMA3	1.93	0.51
4:6:79:MET:SD	19:6:310:CLA:HAB	2.51	0.51
26:6:318:LHG:H302	26:6:318:LHG:H122	1.93	0.51
19:8:304:CLA:H101	19:Z:614:CLA:H3A	1.93	0.51
4:6:57:LEU:HD23	5:7:175:LEU:HD21	1.93	0.51
6:8:109:LYS:O	6:8:113:GLU:HG2	2.11	0.51
19:A:813:CLA:H202	22:J:101:LUT:H193	1.93	0.51
14:K:49:ALA:HB2	14:K:92:MET:SD	2.51	0.51
2:4:200:PRO:HD2	22:4:616:LUT:H23	1.92	0.51
15:Z:76:GLU:HG3	15:Z:152:VAL:HG22	1.92	0.50
3:5:84:GLY:HA2	25:5:322:XAT:H181	1.94	0.50
7:A:75:SER:OG	7:A:181:TYR:HB2	2.10	0.50
19:A:819:CLA:CHD	19:A:820:CLA:HBB2	2.42	0.50
19:B:812:CLA:H93	24:B:853:LMU:H61	1.94	0.50
3:5:218:HIS:CG	19:5:313:CLA:HAA2	2.47	0.50
19:A:811:CLA:H151	21:J:103:BCR:HC41	1.94	0.50
21:A:849:BCR:H362	21:A:850:BCR:H21C	1.94	0.50
15:Z:84:TRP:CE2	19:Z:607:CLA:HED2	2.46	0.49
1:3:164:GLN:HB3	1:3:172:MET:HE3	1.93	0.49
5:7:229:VAL:HG12	19:7:612:CLA:HED1	1.94	0.49
15:Z:50:PRO:HG2	15:Z:53:LEU:HD22	1.93	0.49
15:Z:105:ASP:HA	15:Z:108:LEU:HD23	1.94	0.49
1:3:180:LEU:HD22	21:3:318:BCR:HC31	1.93	0.49
2:4:104:ALA:HB1	2:4:219:GLY:HA3	1.94	0.49
8:B:663:MET:HB2	19:B:804:CLA:C4C	2.42	0.49
19:3:313:CLA:HBB1	21:3:315:BCR:H282	1.93	0.49
8:B:157:HIS:CE1	19:B:812:CLA:NA	2.81	0.49
2:4:170:LYS:HD2	2:4:173:SER:HB3	1.93	0.49
7:A:487:ILE:HD13	19:A:837:CLA:HBB1	1.94	0.49
4:6:33:LEU:HD13	20:6:302:CHL:HMA3	1.95	0.49
19:8:302:CLA:H101	19:8:303:CLA:H172	1.93	0.49
2:4:127:TRP:CD1	2:4:129:GLY:H	2.30	0.49
5:7:82:GLY:HA2	25:7:616:XAT:H181	1.94	0.49
8:B:375:HIS:HB2	19:B:828:CLA:C1B	2.42	0.49
19:B:804:CLA:HBC2	19:B:804:CLA:HHD	1.95	0.49
19:Z:609:CLA:HBB1	19:Z:611:CLA:H3A	1.94	0.49
20:6:315:CHL:HMC	26:6:325:LHG:H151	1.94	0.49
6:8:94:THR:HG21	6:8:101:VAL:H	1.77	0.49
7:A:37:ARG:HA	7:A:37:ARG:NE	2.27	0.49
7:A:50:TRP:HZ2	19:F:302:CLA:HBB1	1.78	0.48
19:B:833:CLA:H121	19:B:838:CLA:H193	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:841:CLA:H101	21:A:852:BCR:H373	1.95	0.48
15:1:105:ASP:HA	15:1:108:LEU:HD13	1.95	0.48
2:4:178:PRO:HG2	20:4:615:CHL:HBB1	1.95	0.48
19:5:304:CLA:HBB1	19:5:304:CLA:HMB1	1.96	0.48
23:3:321:LMG:H302	19:5:319:CLA:CHD	2.44	0.48
20:Z:605:CHL:HBB2	20:Z:606:CHL:CBB	2.44	0.48
7:A:217:GLN:HA	7:A:221:SER:HB2	1.95	0.48
7:A:393:HIS:CE1	19:A:830:CLA:ND	2.82	0.48
19:B:824:CLA:HBB2	19:B:842:CLA:H52	1.95	0.48
18:L:102:LYS:HE2	19:L:204:CLA:HMA2	1.94	0.48
15:1:84:TRP:CE2	19:1:307:CLA:HED3	2.49	0.48
19:3:310:CLA:HBB2	21:3:318:BCR:H392	1.95	0.48
24:A:855:LMU:H22	24:A:855:LMU:H1'	1.69	0.48
19:B:835:CLA:H62	19:B:835:CLA:H102	1.56	0.48
19:3:313:CLA:HBA1	19:3:313:CLA:HBD	1.94	0.48
8:B:443:VAL:HG21	19:B:834:CLA:HAC2	1.96	0.48
1:3:156:GLN:NE2	19:3:314:CLA:NA	2.62	0.47
3:5:227:ILE:HB	19:5:313:CLA:H11	1.96	0.47
19:B:824:CLA:HAB	19:B:831:CLA:HMD2	1.96	0.47
15:1:142:GLU:HG3	19:1:308:CLA:NB	2.29	0.47
21:3:318:BCR:H322	19:5:302:CLA:H101	1.96	0.47
15:1:83:ARG:HA	15:1:86:MET:HE3	1.95	0.47
5:7:95:VAL:HG23	5:7:97:LEU:HG	1.96	0.47
7:A:684:MET:HB2	19:A:803:CLA:NC	2.29	0.47
19:A:810:CLA:H142	22:J:101:LUT:H203	1.97	0.47
8:B:271:LEU:HD23	8:B:274:MET:HE3	1.97	0.47
1:3:151:GLU:O	1:3:155:MET:HB2	2.14	0.47
19:Z:608:CLA:HBA2	19:Z:608:CLA:H3A	1.37	0.47
15:1:116:ALA:HB3	15:1:123:VAL:HB	1.96	0.47
20:5:306:CHL:HBB2	20:5:307:CHL:CBB	2.45	0.47
8:B:87:PRO:HB3	8:B:122:TYR:CD2	2.49	0.47
20:6:307:CHL:H152	23:6:326:LMG:H241	1.96	0.47
5:7:121:MET:HE2	5:7:125:PHE:CE1	2.50	0.47
7:A:50:TRP:CZ2	19:F:302:CLA:HBB1	2.50	0.47
19:A:834:CLA:HMB3	19:A:834:CLA:HBB1	1.97	0.47
8:B:663:MET:HB2	19:B:804:CLA:C3C	2.45	0.47
15:Z:76:GLU:OE2	15:Z:150:GLY:HA2	2.14	0.47
21:B:802:BCR:H321	16:F:156:PHE:HB2	1.97	0.47
19:B:818:CLA:HBC2	19:B:819:CLA:H201	1.96	0.47
2:4:260:ASP:HB3	19:4:614:CLA:C1B	2.45	0.47
4:6:175:LYS:HD3	19:6:312:CLA:HBD	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:802:BCR:H383	21:B:802:BCR:H23C	1.96	0.47
19:5:316:CLA:H62	19:5:316:CLA:H41	1.51	0.46
6:8:81:MET:SD	19:8:309:CLA:HAB	2.55	0.46
2:4:225:ALA:HA	19:4:612:CLA:HBB1	1.97	0.46
19:6:305:CLA:H91	19:6:305:CLA:H111	1.69	0.46
19:A:834:CLA:H52	19:L:203:CLA:H8	1.96	0.46
8:B:277:HIS:HB2	19:B:818:CLA:C1B	2.45	0.46
20:5:307:CHL:H2	20:5:307:CHL:H72	1.98	0.46
19:5:311:CLA:H2	19:5:312:CLA:HMD2	1.96	0.46
6:8:191:LYS:HD3	19:8:311:CLA:HAA2	1.96	0.46
8:B:370:ALA:HB1	8:B:726:LEU:HD11	1.98	0.46
19:1:303:CLA:H61	19:1:303:CLA:H41	1.48	0.46
26:4:620:LHG:HC91	26:4:620:LHG:H122	1.73	0.46
4:6:157:PRO:HB3	20:6:308:CHL:HBC2	1.96	0.46
19:A:844:CLA:H8	19:A:844:CLA:H122	1.72	0.46
3:5:140:TYR:OH	19:5:319:CLA:HBA2	2.16	0.46
19:8:303:CLA:H142	19:8:303:CLA:H112	1.80	0.46
23:J:105:LMG:H141	19:F:302:CLA:H152	1.96	0.46
19:5:310:CLA:HBB1	19:5:310:CLA:HMB3	1.98	0.46
8:B:276:HIS:CE1	19:B:817:CLA:NA	2.83	0.46
19:B:817:CLA:H72	19:B:817:CLA:H111	1.59	0.46
17:G:33:ASP:HB3	17:G:36:ILE:HG12	1.97	0.46
24:3:322:LMU:H102	21:A:850:BCR:H271	1.98	0.46
6:8:183:ASP:OD2	6:8:184:LYS:HG3	2.16	0.46
19:B:815:CLA:H62	19:B:815:CLA:H102	1.65	0.46
19:B:838:CLA:H102	19:B:838:CLA:H62	1.79	0.46
23:J:105:LMG:H142	16:F:193:THR:HG21	1.98	0.46
15:Z:88:GLY:HA2	25:Z:616:XAT:H181	1.98	0.46
19:6:320:CLA:HBB2	19:7:610:CLA:H141	1.98	0.46
8:B:238:PRO:HD2	17:G:125:LEU:HD13	1.98	0.46
19:4:612:CLA:H122	19:4:612:CLA:H161	1.76	0.45
19:8:302:CLA:CGA	19:8:302:CLA:H3A	2.46	0.45
19:A:840:CLA:HBB1	19:A:840:CLA:HMB3	1.97	0.45
15:1:212:ASN:HD21	15:1:215:GLY:HA3	1.81	0.45
3:5:126:PHE:CE2	26:6:318:LHG:H211	2.51	0.45
3:5:191:ARG:HA	3:5:194:MET:HE3	1.98	0.45
4:6:46:LEU:HD22	4:6:68:LYS:HD2	1.98	0.45
19:B:806:CLA:HBA1	19:B:806:CLA:H3A	1.46	0.45
19:B:806:CLA:H122	19:B:806:CLA:HBD	1.97	0.45
23:B:852:LMG:H311	12:I:77:SER:HB2	1.99	0.45
19:B:817:CLA:CHD	19:B:818:CLA:HBB2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:603:CLA:HBC1	19:Z:608:CLA:HAC1	1.98	0.45
19:Z:603:CLA:OBD	19:Z:608:CLA:H2	2.16	0.45
20:5:307:CHL:H42	20:6:315:CHL:HED2	1.97	0.45
20:6:307:CHL:HED2	20:6:307:CHL:HBD	1.68	0.45
6:8:143:LYS:NZ	6:8:143:LYS:HB3	2.31	0.45
19:A:824:CLA:H91	21:A:858:BCR:H401	1.97	0.45
8:B:70:ALA:HB2	8:B:136:LEU:HB2	1.97	0.45
19:1:309:CLA:H51	19:1:311:CLA:HMA2	1.98	0.45
20:4:601:CHL:HAB	26:4:619:LHG:H302	1.98	0.45
5:7:123:ILE:HG12	19:8:313:CLA:HAA2	1.99	0.45
19:A:839:CLA:HBB1	19:A:839:CLA:HMB1	1.96	0.45
19:A:842:CLA:HAA2	19:B:832:CLA:HMB1	1.99	0.45
1:3:212:GLU:OE2	19:3:309:CLA:HED1	2.17	0.45
2:4:252:TRP:CE2	4:6:108:LEU:HD22	2.52	0.45
20:6:307:CHL:HMD2	27:6:323:NEX:H14	1.97	0.45
5:7:225:ASP:OD2	5:7:228:HIS:HB2	2.17	0.45
8:B:340:ALA:HB2	21:B:848:BCR:H372	1.98	0.45
8:B:467:ALA:HB2	8:B:477:PHE:CZ	2.52	0.45
19:B:804:CLA:H202	19:B:804:CLA:H162	1.68	0.45
4:6:239:VAL:HG21	20:6:307:CHL:HED3	1.99	0.45
19:B:804:CLA:H142	21:I:201:BCR:H312	1.98	0.45
19:B:813:CLA:HBC3	19:B:814:CLA:CAB	2.47	0.45
2:4:89:ASP:HB3	2:4:92:LYS:HB2	1.99	0.45
23:6:301:LMG:H172	23:6:301:LMG:H142	1.76	0.45
21:7:617:BCR:HC42	26:8:318:LHG:HC62	1.99	0.45
6:8:175:PRO:HA	15:Z:62:LEU:HD21	1.99	0.45
7:A:216:HIS:CE1	19:A:816:CLA:NA	2.85	0.45
7:A:308:ALA:HB2	19:A:823:CLA:HBC2	1.98	0.45
19:A:814:CLA:HMB1	19:A:814:CLA:HBB1	1.99	0.45
20:8:306:CHL:HBA2	20:8:306:CHL:H3A	1.57	0.45
8:B:288:ALA:HB2	19:B:820:CLA:HBC2	1.98	0.45
19:B:805:CLA:HHC	19:B:807:CLA:OBD	2.17	0.45
19:4:602:CLA:HBC1	26:4:619:LHG:H282	1.97	0.44
20:7:621:CHL:HMA3	6:8:31:LEU:HD13	2.00	0.44
19:8:303:CLA:H41	19:8:303:CLA:H62	1.55	0.44
1:3:156:GLN:HE22	19:3:314:CLA:C4D	2.28	0.44
6:8:95:LYS:HG2	6:8:218:VAL:HG11	1.99	0.44
31:B:850:DGD:HE62	32:B:1024:HOH:O	2.16	0.44
20:1:305:CHL:HBB2	20:1:306:CHL:CBB	2.48	0.44
19:3:309:CLA:HED3	19:3:309:CLA:H2A	1.99	0.44
19:5:316:CLA:H51	19:6:303:CLA:H152	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:104:VAL:HG21	19:6:305:CLA:HAA2	1.99	0.44
6:8:68:TRP:CE3	23:F:301:LMG:HC5	2.51	0.44
7:A:75:SER:HB2	19:A:813:CLA:HMD3	1.99	0.44
21:A:851:BCR:H20C	21:A:851:BCR:H361	1.81	0.44
21:A:853:BCR:H20C	21:A:853:BCR:H361	1.83	0.44
19:B:818:CLA:H3A	19:B:818:CLA:HBA2	1.33	0.44
19:3:302:CLA:H122	7:A:175:PHE:CE2	2.52	0.44
7:A:316:TRP:O	14:K:57:VAL:HG22	2.17	0.44
19:A:827:CLA:H192	19:A:827:CLA:H161	1.83	0.44
19:B:813:CLA:H142	19:B:813:CLA:H111	1.80	0.44
15:1:86:MET:SD	19:1:309:CLA:HAB	2.58	0.44
20:4:607:CHL:H62	20:4:607:CHL:H41	1.75	0.44
19:4:610:CLA:C1C	26:4:619:LHG:HC41	2.48	0.44
19:7:602:CLA:H18	19:7:612:CLA:H161	2.00	0.44
19:A:824:CLA:H91	19:A:824:CLA:H112	1.73	0.44
19:4:614:CLA:HBA2	19:4:614:CLA:H3A	1.43	0.44
19:A:803:CLA:CGA	19:A:803:CLA:H3A	2.48	0.44
19:3:302:CLA:HBB1	19:3:302:CLA:HMB3	1.99	0.44
3:5:137:TRP:CG	19:5:316:CLA:HBC1	2.53	0.44
8:B:681:TRP:CE2	8:B:685:LYS:HG3	2.53	0.44
20:1:305:CHL:HHB	22:1:317:LUT:H192	1.99	0.44
16:F:139:LEU:HD23	19:F:304:CLA:HED2	2.00	0.44
26:5:301:LHG:H251	19:7:613:CLA:H3A	2.00	0.44
19:3:305:CLA:HAC2	19:A:817:CLA:H203	1.98	0.43
19:4:609:CLA:HBA1	22:4:616:LUT:H382	1.99	0.43
19:5:319:CLA:O1A	19:5:319:CLA:H2A	2.17	0.43
20:7:621:CHL:C1C	26:8:318:LHG:H241	2.48	0.43
19:A:810:CLA:H91	19:A:813:CLA:H201	2.00	0.43
19:B:804:CLA:H141	19:B:804:CLA:H161	1.65	0.43
19:B:842:CLA:H192	19:B:842:CLA:H161	1.82	0.43
19:7:609:CLA:HBA2	19:7:609:CLA:H3A	1.42	0.43
19:7:610:CLA:H151	19:7:610:CLA:H18	1.87	0.43
20:8:305:CHL:HBB1	20:8:305:CHL:HMB1	2.00	0.43
7:A:598:TRP:HE1	19:B:804:CLA:C1D	2.32	0.43
19:A:811:CLA:H142	19:A:811:CLA:H111	1.78	0.43
3:5:127:ILE:HG21	20:6:302:CHL:H72	2.00	0.43
19:A:815:CLA:H152	19:A:815:CLA:H112	1.79	0.43
19:A:827:CLA:HBB1	19:A:827:CLA:HMB3	1.99	0.43
10:D:62:THR:HG23	10:D:110:PRO:HB2	2.00	0.43
13:J:2:LYS:HD2	23:J:105:LMG:HC61	2.00	0.43
19:1:307:CLA:H51	19:1:307:CLA:H11	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:123:ILE:HD12	19:3:303:CLA:HED2	2.01	0.43
19:3:303:CLA:H161	19:3:303:CLA:H141	1.71	0.43
19:3:309:CLA:H62	19:3:309:CLA:H41	1.90	0.43
3:5:197:TYR:CZ	25:5:322:XAT:H8	2.54	0.43
19:B:824:CLA:H61	19:B:824:CLA:H2	1.76	0.43
21:B:846:BCR:H24C	21:B:846:BCR:H371	1.77	0.43
21:L:202:BCR:H24C	21:L:202:BCR:H371	1.90	0.43
5:7:188:GLN:O	5:7:192:LYS:HG3	2.19	0.43
21:B:844:BCR:H321	21:B:844:BCR:HC7	1.68	0.43
21:B:845:BCR:H321	21:B:845:BCR:HC8	2.00	0.43
1:3:148:PHE:CE2	1:3:152:ILE:HD11	2.53	0.43
4:6:197:THR:HG21	19:6:313:CLA:HED2	2.00	0.43
5:7:222:HIS:CG	19:7:612:CLA:HAA2	2.54	0.43
6:8:105:TYR:CD2	6:8:210:LYS:HD3	2.53	0.43
20:8:305:CHL:H152	21:8:317:BCR:H372	2.00	0.43
7:A:596:LEU:HD21	19:A:832:CLA:HBC1	2.01	0.43
2:4:198:PHE:HA	20:4:607:CHL:H72	2.01	0.43
4:6:208:HIS:NE2	19:6:314:CLA:NB	2.67	0.43
7:A:44:ASN:OD1	11:E:78:GLN:HG2	2.19	0.43
7:A:438:ILE:HG13	7:A:556:PHE:HE1	1.84	0.43
19:A:821:CLA:H203	19:A:821:CLA:H162	1.83	0.43
15:Z:103:TRP:HB2	25:Z:616:XAT:H3	2.00	0.43
15:1:109:TRP:CZ2	15:1:116:ALA:HB2	2.54	0.43
19:3:302:CLA:H91	19:3:302:CLA:H112	1.73	0.43
24:3:324:LMU:H21	24:3:324:LMU:H1'	1.56	0.43
19:4:603:CLA:HAB	19:4:608:CLA:H143	2.00	0.43
3:5:198:MET:HG3	19:5:304:CLA:HBB2	2.00	0.43
19:5:302:CLA:H152	19:5:302:CLA:H18	1.85	0.43
20:6:307:CHL:HBA2	27:6:323:NEX:H402	2.00	0.43
19:A:810:CLA:HBA1	19:A:810:CLA:C4A	2.49	0.43
8:B:375:HIS:HB2	19:B:828:CLA:CHB	2.49	0.43
19:F:304:CLA:HMC2	22:F:305:LUT:H27	2.00	0.43
18:L:58:PRO:O	18:L:62:ALA:HB2	2.19	0.43
19:6:303:CLA:HBC1	26:6:318:LHG:H292	2.01	0.43
5:7:175:LEU:HB2	19:7:609:CLA:HBA1	2.00	0.43
19:B:809:CLA:CGA	19:B:809:CLA:C1A	2.96	0.43
19:B:823:CLA:HBC2	19:B:824:CLA:HBA1	2.00	0.43
1:3:176:TYR:CZ	1:3:178:LEU:HA	2.54	0.43
23:3:321:LMG:H312	22:5:324:LUT:H30	2.00	0.43
19:7:610:CLA:H61	19:7:610:CLA:H92	1.79	0.43
6:8:224:HIS:CG	19:8:312:CLA:HAA2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:809:CLA:O1A	19:B:828:CLA:HBD	2.18	0.43
9:C:61:ASP:HA	9:C:62:PHE:HA	1.84	0.43
16:F:204:LEU:O	16:F:208:GLN:HG2	2.19	0.42
4:6:184:MET:HB3	25:6:322:XAT:C35	2.49	0.42
6:8:36:ILE:HD12	6:8:53:GLY:HA3	2.02	0.42
19:8:304:CLA:H92	19:8:304:CLA:H62	1.83	0.42
19:8:307:CLA:CGA	19:8:309:CLA:HMD2	2.49	0.42
19:8:309:CLA:HBB1	19:8:311:CLA:H3A	2.01	0.42
19:B:817:CLA:H111	19:B:817:CLA:H142	1.86	0.42
1:3:81:PHE:HE1	26:A:801:LHG:HC82	1.85	0.42
24:3:324:LMU:H62	19:A:818:CLA:ND	2.34	0.42
19:5:304:CLA:H11	19:5:319:CLA:C4B	2.49	0.42
5:7:66:LYS:HG2	5:7:139:PHE:HE1	1.85	0.42
19:A:826:CLA:H12	19:A:837:CLA:H202	1.99	0.42
2:4:108:MET:SD	19:4:609:CLA:HAB	2.60	0.42
7:A:32:PRO:HB3	19:A:805:CLA:HAC1	2.01	0.42
19:B:829:CLA:HBB1	19:B:829:CLA:HMB3	2.01	0.42
9:C:22:PRO:C	10:D:122:LEU:HD23	2.44	0.42
19:Z:608:CLA:H152	19:Z:608:CLA:H112	1.71	0.42
1:3:156:GLN:NE2	19:3:314:CLA:C4D	2.83	0.42
2:4:128:PRO:HG2	24:4:623:LMU:H4'	2.01	0.42
19:4:604:CLA:CAD	24:4:623:LMU:H22	2.49	0.42
19:5:312:CLA:HBC2	19:5:312:CLA:HHD	2.01	0.42
4:6:180:GLY:O	4:6:184:MET:HG3	2.19	0.42
20:6:307:CHL:H52	23:6:326:LMG:H142	2.00	0.42
19:A:840:CLA:C2C	23:L:201:LMG:H191	2.49	0.42
8:B:404:ASN:O	8:B:407:ASN:HB2	2.19	0.42
19:4:603:CLA:H142	19:4:603:CLA:H111	1.77	0.42
21:5:320:BCR:H20C	21:5:320:BCR:H361	1.88	0.42
19:7:609:CLA:H142	19:7:609:CLA:H112	1.79	0.42
7:A:349:TRP:HB3	19:A:807:CLA:HAC1	2.02	0.42
7:A:542:THR:HB	7:A:602:SER:HB2	2.00	0.42
19:B:830:CLA:H71	19:B:841:CLA:HED1	2.01	0.42
9:C:2:ALA:N	9:C:71:SER:HG	2.18	0.42
19:1:314:CLA:HHB	19:F:304:CLA:H143	2.01	0.42
19:5:312:CLA:HBB1	19:5:312:CLA:HMB3	2.02	0.42
7:A:501:ASN:HB2	19:A:838:CLA:HED2	2.02	0.42
19:5:305:CLA:HMB3	25:5:322:XAT:H162	2.02	0.42
4:6:156:TYR:CZ	4:6:173:LYS:HD3	2.55	0.42
4:6:188:VAL:HG13	19:6:320:CLA:H11	2.02	0.42
5:7:200:ALA:HA	19:7:612:CLA:HBB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:408:HIS:CE1	19:A:832:CLA:NA	2.88	0.42
19:A:807:CLA:HBA1	19:A:807:CLA:H3A	1.66	0.42
21:A:849:BCR:H361	21:A:849:BCR:H20C	1.83	0.42
8:B:396:ILE:HD11	8:B:542:ALA:HB1	2.00	0.42
10:D:122:LEU:HD12	10:D:122:LEU:HA	1.89	0.42
15:Z:109:TRP:CZ2	15:Z:116:ALA:HB2	2.55	0.42
19:1:307:CLA:HAA2	19:1:307:CLA:H18	2.01	0.42
20:4:605:CHL:HBB1	20:4:605:CHL:HMB1	2.01	0.42
3:5:192:LEU:HG	22:5:318:LUT:H11	2.02	0.42
19:8:303:CLA:H102	19:8:303:CLA:H61	1.40	0.42
19:A:812:CLA:HBA1	19:A:814:CLA:HMD2	2.02	0.42
19:A:846:CLA:HBB1	19:A:846:CLA:HMB3	2.02	0.42
8:B:352:HIS:CE1	19:B:827:CLA:NB	2.88	0.42
19:B:831:CLA:HMA3	19:B:832:CLA:HED2	2.02	0.42
26:5:321:LHG:HC91	26:5:321:LHG:H282	2.02	0.42
19:6:310:CLA:HBB1	19:6:312:CLA:H3A	2.02	0.42
7:A:216:HIS:HB2	19:A:816:CLA:CHC	2.50	0.42
7:A:296:HIS:CE1	19:A:819:CLA:NA	2.88	0.42
19:B:824:CLA:H101	26:B:851:LHG:H172	2.00	0.42
6:8:138:TRP:CG	23:8:321:LMG:H302	2.55	0.41
7:A:666:SER:HB2	8:B:446:ALA:HB1	2.02	0.41
19:A:829:CLA:H61	19:A:829:CLA:H2	1.82	0.41
19:A:832:CLA:H91	26:A:847:LHG:H332	2.02	0.41
8:B:653:PHE:CZ	8:B:657:ILE:HD11	2.55	0.41
19:Z:602:CLA:CGA	19:Z:602:CLA:H3A	2.49	0.41
18:L:103:LEU:HD11	23:L:201:LMG:H111	2.00	0.41
18:L:179:GLU:OE2	18:L:179:GLU:HA	2.19	0.41
4:6:131:ASP:HB2	4:6:138:VAL:HG11	2.02	0.41
19:7:610:CLA:H111	19:7:610:CLA:H93	1.80	0.41
7:A:700:ILE:HD13	19:A:842:CLA:HMD2	2.03	0.41
8:B:192:THR:HG21	8:B:279:LEU:HB2	2.02	0.41
19:B:814:CLA:H61	19:B:814:CLA:H102	1.90	0.41
19:B:826:CLA:HMA1	21:B:848:BCR:H14C	2.02	0.41
3:5:69:TRP:CB	19:5:319:CLA:HAA1	2.50	0.41
20:6:306:CHL:HBB2	20:6:307:CHL:CBB	2.51	0.41
19:B:811:CLA:H171	19:B:811:CLA:H13	1.75	0.41
19:J:102:CLA:H41	19:J:102:CLA:H61	1.75	0.41
19:1:303:CLA:H12	19:1:303:CLA:HBA1	1.96	0.41
1:3:180:LEU:O	1:3:183:ILE:HG12	2.21	0.41
19:4:613:CLA:H71	21:6:321:BCR:H342	2.03	0.41
6:8:39:HIS:CG	6:8:61:LYS:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:K:206:BCR:H24C	21:K:206:BCR:H371	1.88	0.41
4:6:108:LEU:HD12	4:6:113:LEU:HD21	2.03	0.41
5:7:61:GLU:HA	5:7:62:PRO:HD3	1.97	0.41
5:7:213:LYS:HE2	5:7:213:LYS:HB3	1.68	0.41
19:7:612:CLA:H91	26:7:618:LHG:H302	2.02	0.41
7:A:121:ILE:HG13	7:A:122:VAL:HG13	2.03	0.41
19:A:838:CLA:HBA1	19:K:203:CLA:H92	2.03	0.41
8:B:441:ASN:OD1	8:B:453:GLN:HB2	2.20	0.41
19:B:809:CLA:H8	19:B:809:CLA:HBB1	2.01	0.41
19:B:813:CLA:H3A	19:B:813:CLA:HBA2	1.87	0.41
26:B:851:LHG:H223	26:B:851:LHG:H192	1.97	0.41
15:1:191:PHE:HE1	22:1:315:LUT:H41	1.85	0.41
2:4:242:LYS:HB3	2:4:242:LYS:HE3	1.69	0.41
3:5:185:LYS:HD3	19:5:312:CLA:HBD	2.02	0.41
7:A:173:MET:HE1	19:A:815:CLA:H93	2.03	0.41
7:A:677:PHE:CG	21:A:853:BCR:H363	2.55	0.41
19:A:811:CLA:H2	19:A:811:CLA:H62	1.76	0.41
19:A:811:CLA:H92	19:A:811:CLA:H61	1.83	0.41
19:A:833:CLA:HBA2	26:A:848:LHG:HC91	2.01	0.41
19:B:826:CLA:H3A	19:B:826:CLA:HBA2	1.85	0.41
21:B:845:BCR:H20C	21:B:845:BCR:H361	1.95	0.41
16:F:150:PHE:O	16:F:153:THR:HB	2.21	0.41
19:3:308:CLA:H203	19:3:308:CLA:H161	1.79	0.41
19:A:821:CLA:H172	19:A:837:CLA:H92	2.03	0.41
19:B:837:CLA:H61	19:B:837:CLA:H92	1.68	0.41
19:B:841:CLA:HBA1	19:B:841:CLA:H3A	1.73	0.41
15:1:164:ALA:HB1	15:1:170:SER:HB2	2.02	0.41
19:1:312:CLA:HMA2	22:1:315:LUT:H3	2.03	0.41
18:L:79:VAL:HB	18:L:84:ARG:HD2	2.02	0.41
8:B:277:HIS:HB2	19:B:818:CLA:CHB	2.51	0.41
8:B:313:SER:HB3	26:B:851:LHG:HC32	2.01	0.41
19:B:811:CLA:H71	19:B:811:CLA:H112	1.77	0.41
19:3:308:CLA:HBB1	19:3:308:CLA:HMB3	2.03	0.41
3:5:231:ILE:HD12	3:5:231:ILE:HA	1.90	0.41
19:5:303:CLA:CGA	19:5:303:CLA:H3A	2.50	0.41
4:6:164:PHE:CE2	4:6:166:PRO:HG3	2.56	0.41
7:A:396:TRP:CD1	19:A:830:CLA:HAB	2.56	0.41
19:A:808:CLA:H112	19:A:808:CLA:H152	1.81	0.41
19:A:815:CLA:H161	19:A:815:CLA:H192	1.77	0.41
19:A:836:CLA:H62	19:A:836:CLA:H2	1.84	0.41
8:B:450:PRO:O	8:B:453:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:830:CLA:H92	19:B:830:CLA:H61	1.79	0.41
19:B:837:CLA:H112	19:B:842:CLA:H191	2.01	0.41
14:K:35:ASN:HA	19:K:204:CLA:OBD	2.21	0.41
19:1:310:CLA:H102	19:1:310:CLA:H61	1.38	0.41
19:1:310:CLA:H71	19:1:311:CLA:C4D	2.51	0.41
16:F:202:TRP:CD1	16:F:203:PRO:HD3	2.56	0.41
6:8:112:ILE:HD12	6:8:112:ILE:HA	1.95	0.41
10:D:189:ARG:HG3	10:D:189:ARG:NH1	2.35	0.41
19:1:303:CLA:H102	19:1:303:CLA:H62	1.78	0.41
18:L:132:LEU:HD21	21:L:205:BCR:H24C	2.02	0.41
26:4:620:LHG:HC92	4:6:129:TRP:HH2	1.86	0.40
3:5:203:GLN:HG2	19:5:313:CLA:C4D	2.52	0.40
20:6:306:CHL:HHB	21:6:321:BCR:H373	2.02	0.40
19:A:827:CLA:HBA1	19:A:831:CLA:H193	2.04	0.40
8:B:358:PRO:HG3	19:B:819:CLA:HAA2	2.02	0.40
19:B:810:CLA:H143	19:B:810:CLA:H162	1.86	0.40
19:B:834:CLA:H41	19:B:834:CLA:H101	2.02	0.40
19:Z:612:CLA:HMA2	22:Z:615:LUT:H3	2.02	0.40
19:F:304:CLA:H2	19:F:304:CLA:H111	2.03	0.40
5:7:184:GLN:HA	5:7:187:LYS:HD3	2.03	0.40
19:7:602:CLA:CGA	19:7:602:CLA:H3A	2.51	0.40
7:A:698:GLU:CD	8:B:546:LYS:HB2	2.46	0.40
19:A:837:CLA:H72	19:A:837:CLA:H111	1.80	0.40
19:A:838:CLA:C1B	19:K:203:CLA:H51	2.50	0.40
8:B:35:HIS:CE1	19:B:805:CLA:HED1	2.54	0.40
11:E:39:ARG:HD3	11:E:61:SER:HA	2.03	0.40
21:L:205:BCR:H361	21:L:205:BCR:H20C	1.82	0.40
19:4:603:CLA:H111	19:4:603:CLA:H91	1.75	0.40
7:A:113:PRO:HB3	7:A:145:PHE:CD2	2.56	0.40
8:B:300:HIS:CE1	19:B:822:CLA:NA	2.89	0.40
14:K:57:VAL:HG21	14:K:87:VAL:HG13	2.03	0.40
19:K:203:CLA:HBA1	19:K:203:CLA:HBD	2.04	0.40
19:3:313:CLA:CBB	21:3:315:BCR:H282	2.51	0.40
4:6:91:VAL:HG21	19:6:305:CLA:HMD2	2.04	0.40
19:8:304:CLA:H62	19:8:304:CLA:H2	1.85	0.40
20:8:320:CHL:H142	24:1:322:LMU:H91	2.03	0.40
26:B:851:LHG:H281	26:B:851:LHG:H252	1.90	0.40
21:L:202:BCR:H352	19:L:203:CLA:HAB	2.03	0.40
1:3:99:MET:SD	19:3:308:CLA:HAB	2.61	0.40
19:5:303:CLA:H41	19:5:304:CLA:O1A	2.22	0.40
4:6:177:ILE:HD12	4:6:177:ILE:HA	1.98	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	3	219/221 (99%)	216 (99%)	3 (1%)	0	100	100
2	4	210/212 (99%)	209 (100%)	1 (0%)	0	100	100
3	5	225/227 (99%)	222 (99%)	3 (1%)	0	100	100
4	6	228/230 (99%)	224 (98%)	4 (2%)	0	100	100
5	7	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
6	8	215/217 (99%)	214 (100%)	1 (0%)	0	100	100
7	A	740/742 (100%)	728 (98%)	12 (2%)	0	100	100
8	B	731/733 (100%)	714 (98%)	17 (2%)	0	100	100
9	C	78/80 (98%)	78 (100%)	0	0	100	100
10	D	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
11	E	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
12	I	35/37 (95%)	35 (100%)	0	0	100	100
13	J	39/41 (95%)	39 (100%)	0	0	100	100
14	K	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
15	1	192/194 (99%)	191 (100%)	1 (0%)	0	100	100
15	Z	192/194 (99%)	191 (100%)	1 (0%)	0	100	100
16	F	163/165 (99%)	161 (99%)	2 (1%)	0	100	100
17	G	66/95 (70%)	66 (100%)	0	0	100	100
18	L	120/124 (97%)	120 (100%)	0	0	100	100
All	All	3952/4019 (98%)	3897 (99%)	55 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	168/168 (100%)	168 (100%)	0	100	100
2	4	167/167 (100%)	165 (99%)	2 (1%)	63	51
3	5	184/184 (100%)	180 (98%)	4 (2%)	45	29
4	6	184/184 (100%)	182 (99%)	2 (1%)	65	54
5	7	164/164 (100%)	164 (100%)	0	100	100
6	8	163/163 (100%)	162 (99%)	1 (1%)	78	72
7	A	601/601 (100%)	600 (100%)	1 (0%)	87	84
8	B	596/596 (100%)	592 (99%)	4 (1%)	76	68
9	C	69/69 (100%)	69 (100%)	0	100	100
10	D	121/121 (100%)	117 (97%)	4 (3%)	33	15
11	E	55/55 (100%)	55 (100%)	0	100	100
12	I	31/31 (100%)	30 (97%)	1 (3%)	34	17
13	J	36/36 (100%)	36 (100%)	0	100	100
14	K	59/59 (100%)	58 (98%)	1 (2%)	53	37
15	1	137/137 (100%)	136 (99%)	1 (1%)	76	68
15	Z	137/137 (100%)	136 (99%)	1 (1%)	76	68
16	F	127/127 (100%)	125 (98%)	2 (2%)	55	39
17	G	49/71 (69%)	49 (100%)	0	100	100
18	L	90/90 (100%)	90 (100%)	0	100	100
All	All	3138/3160 (99%)	3114 (99%)	24 (1%)	70	65

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	4	67	LEU
2	4	235	THR
3	5	161	GLU
3	5	168	ILE

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Mol	Chain	Res	Type
3	5	228	LEU
3	5	231	ILE
4	6	233	CYS
4	6	245	GLU
6	8	153	PHE
7	A	372	TYR
8	B	11	GLN
8	B	86	ARG
8	B	249	GLN
8	B	345	ILE
10	D	57	THR
10	D	93	GLU
10	D	175	ILE
10	D	191	MET
12	I	102	GLU
14	K	87	VAL
15	Z	51	ASP
15	1	72	LYS
16	F	63	ASP
16	F	174	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	220	ASN
2	4	103	ASN
2	4	218	ASN
2	4	259	ASN
3	5	76	GLN
3	5	91	GLN
3	5	178	ASN
3	5	189	ASN
4	6	88	GLN
5	7	193	ASN
6	8	28	GLN
6	8	35	GLN
6	8	114	ASN
7	A	296	HIS
7	A	387	GLN
7	A	496	GLN
8	B	77	GLN
8	B	84	HIS

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Mol	Chain	Res	Type
8	B	157	HIS
8	B	159	GLN
8	B	206	GLN
8	B	276	HIS
10	D	130	ASN
15	Z	180	ASN
15	1	128	ASN
15	1	180	ASN
15	1	194	GLN
15	1	212	ASN
18	L	71	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

328 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
30	SF4	C	101	9	0,12,12	-	-	-		
19	CLA	1	304	32	54,58,73	1.41	8 (14%)	65,95,113	1.42	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	7	608	5	49,53,73	1.47	7 (14%)	59,89,113	1.49	5 (8%)
19	CLA	B	812	8	69,73,73	1.26	7 (10%)	83,113,113	1.24	7 (8%)
21	BCR	B	845	-	41,41,41	0.35	0	56,56,56	0.74	0
25	XAT	6	322	-	39,47,47	0.67	2 (5%)	54,74,74	0.82	0
19	CLA	7	603	5	56,60,73	1.39	7 (12%)	67,97,113	1.42	7 (10%)
19	CLA	B	826	32	69,73,73	1.25	7 (10%)	83,113,113	1.28	8 (9%)
19	CLA	A	838	7	61,65,73	1.34	7 (11%)	73,103,113	1.33	7 (9%)
24	LMU	3	322	-	35,35,36	0.48	0	46,46,47	0.64	0
19	CLA	F	303	32	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
19	CLA	A	805	7	69,73,73	1.25	8 (11%)	83,113,113	1.36	8 (9%)
25	XAT	Z	616	-	39,47,47	0.66	2 (5%)	54,74,74	0.82	0
19	CLA	8	309	6	69,73,73	1.24	6 (8%)	83,113,113	1.25	5 (6%)
19	CLA	6	305	4	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
20	CHL	5	317	3	47,51,74	1.11	5 (10%)	52,86,114	1.65	9 (17%)
21	BCR	G	204	-	41,41,41	0.34	0	56,56,56	0.59	0
19	CLA	B	820	32	64,68,73	1.33	7 (10%)	77,107,113	1.30	7 (9%)
19	CLA	A	839	7	55,59,73	1.41	7 (12%)	66,96,113	1.41	7 (10%)
19	CLA	B	836	32	49,53,73	1.49	7 (14%)	59,89,113	1.47	7 (11%)
20	CHL	8	306	32	70,74,74	0.97	4 (5%)	80,114,114	1.33	10 (12%)
20	CHL	6	306	32	50,54,74	1.08	5 (10%)	56,90,114	1.31	8 (14%)
26	LHG	6	318	19	48,48,48	0.51	0	51,54,54	0.51	0
22	LUT	8	315	-	42,43,43	0.28	0	51,60,60	0.63	0
19	CLA	B	807	8	69,73,73	1.27	7 (10%)	83,113,113	1.27	7 (8%)
19	CLA	B	827	8	69,73,73	1.26	8 (11%)	83,113,113	1.28	8 (9%)
19	CLA	4	603	2	69,73,73	1.26	8 (11%)	83,113,113	1.26	4 (4%)
24	LMU	3	323	-	24,24,36	0.37	0	29,29,47	0.67	0
19	CLA	3	309	32	59,63,73	1.35	7 (11%)	71,101,113	1.39	6 (8%)
21	BCR	A	851	-	41,41,41	0.34	0	56,56,56	0.70	0
26	LHG	1	318	19	43,43,48	0.53	0	46,49,54	0.51	0
20	CHL	4	607	32	70,74,74	0.98	5 (7%)	80,114,114	1.17	8 (10%)
20	CHL	7	601	5	70,74,74	0.93	5 (7%)	80,114,114	1.18	10 (12%)
26	LHG	B	851	19	44,44,48	0.53	0	47,50,54	0.53	0
19	CLA	4	602	2	64,68,73	1.31	7 (10%)	77,107,113	1.30	7 (9%)
19	CLA	7	607	32	54,58,73	1.41	6 (11%)	65,95,113	1.47	8 (12%)
30	SF4	C	102	9	0,12,12	-	-	-	-	-
19	CLA	8	308	6	49,53,73	1.47	7 (14%)	59,89,113	1.44	4 (6%)
19	CLA	B	816	8	69,73,73	1.25	8 (11%)	83,113,113	1.30	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LUT	5	318	-	42,43,43	0.30	0	51,60,60	0.74	0
19	CLA	G	202	17	64,68,73	1.31	7 (10%)	77,107,113	1.32	6 (7%)
19	CLA	5	302	3	69,73,73	1.26	7 (10%)	83,113,113	1.28	5 (6%)
19	CLA	8	314	6	49,53,73	1.49	7 (14%)	59,89,113	1.42	7 (11%)
20	CHL	4	606	32	47,51,74	1.11	5 (10%)	52,86,114	1.53	9 (17%)
20	CHL	7	605	32	50,54,74	1.10	5 (10%)	56,90,114	1.48	6 (10%)
25	XAT	4	617	-	39,47,47	0.65	2 (5%)	54,74,74	0.88	1 (1%)
19	CLA	B	803	8	69,73,73	1.25	7 (10%)	83,113,113	1.24	6 (7%)
24	LMU	4	625	-	22,22,36	0.39	0	27,27,47	0.60	0
20	CHL	1	305	32	50,54,74	1.03	4 (8%)	56,90,114	1.48	9 (16%)
30	SF4	A	854	7,8	0,12,12	-	-	-		
19	CLA	A	806	7,19	59,63,73	1.35	6 (10%)	71,101,113	1.35	5 (7%)
19	CLA	7	602	5	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
23	LMG	F	301	-	32,32,55	0.60	0	40,40,63	0.74	0
20	CHL	7	621	6	70,74,74	1.02	5 (7%)	80,114,114	1.29	7 (8%)
19	CLA	5	315	3	49,53,73	1.48	7 (14%)	59,89,113	1.42	6 (10%)
21	BCR	B	849	-	41,41,41	0.31	0	56,56,56	0.70	0
26	LHG	4	620	-	37,37,48	0.57	0	40,43,54	0.52	0
19	CLA	A	828	32	69,73,73	1.26	7 (10%)	83,113,113	1.31	6 (7%)
19	CLA	B	830	8	69,73,73	1.26	8 (11%)	83,113,113	1.23	8 (9%)
19	CLA	B	808	8	59,63,73	1.35	7 (11%)	71,101,113	1.35	6 (8%)
19	CLA	A	807	7	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)
19	CLA	1	311	15	49,53,73	1.48	9 (18%)	59,89,113	1.44	4 (6%)
19	CLA	G	203	17	50,54,73	1.47	6 (12%)	60,90,113	1.42	4 (6%)
19	CLA	K	202	14	49,53,73	1.48	8 (16%)	59,89,113	1.53	6 (10%)
21	BCR	A	852	-	41,41,41	0.31	0	56,56,56	0.56	0
23	LMG	6	301	-	26,26,55	0.45	0	28,28,63	0.48	0
20	CHL	6	307	32	70,74,74	0.93	5 (7%)	80,114,114	1.16	9 (11%)
19	CLA	8	311	6	59,63,73	1.35	6 (10%)	71,101,113	1.35	4 (5%)
19	CLA	3	302	1	69,73,73	1.25	8 (11%)	83,113,113	1.34	6 (7%)
19	CLA	B	833	8	69,73,73	1.27	6 (8%)	83,113,113	1.31	7 (8%)
19	CLA	A	842	7	69,73,73	1.24	7 (10%)	83,113,113	1.28	7 (8%)
19	CLA	A	812	7	69,73,73	1.26	8 (11%)	83,113,113	1.25	7 (8%)
19	CLA	A	824	7	69,73,73	1.27	7 (10%)	83,113,113	1.29	7 (8%)
19	CLA	4	612	2	69,73,73	1.26	8 (11%)	83,113,113	1.41	7 (8%)
19	CLA	A	841	7	69,73,73	1.26	7 (10%)	83,113,113	1.31	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	817	7	69,73,73	1.26	6 (8%)	83,113,113	1.28	6 (7%)
19	CLA	Z	612	32	69,73,73	1.25	7 (10%)	83,113,113	1.30	7 (8%)
19	CLA	6	320	32	59,63,73	1.35	7 (11%)	71,101,113	1.35	7 (9%)
24	LMU	4	622	-	22,22,36	0.41	0	27,27,47	0.70	0
26	LHG	A	847	-	48,48,48	0.51	0	51,54,54	0.47	0
19	CLA	1	302	15	64,68,73	1.31	7 (10%)	77,107,113	1.30	7 (9%)
21	BCR	I	201	-	41,41,41	0.35	0	56,56,56	0.76	0
19	CLA	A	809	7	54,58,73	1.41	8 (14%)	65,95,113	1.43	10 (15%)
19	CLA	A	823	32	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
22	LUT	6	319	-	42,43,43	0.30	0	51,60,60	0.68	0
24	LMU	A	855	-	36,36,36	0.45	0	47,47,47	1.08	2 (4%)
21	BCR	A	850	-	41,41,41	0.31	0	56,56,56	0.62	1 (1%)
19	CLA	B	819	8	69,73,73	1.26	9 (13%)	83,113,113	1.28	10 (12%)
19	CLA	6	316	4	49,53,73	1.49	8 (16%)	59,89,113	1.42	6 (10%)
19	CLA	F	304	16	69,73,73	1.25	8 (11%)	83,113,113	1.19	4 (4%)
19	CLA	4	610	26	64,68,73	1.31	6 (9%)	77,107,113	1.28	5 (6%)
19	CLA	B	821	8	60,64,73	1.35	7 (11%)	72,102,113	1.36	6 (8%)
19	CLA	4	614	2	49,53,73	1.49	6 (12%)	59,89,113	1.44	4 (6%)
27	NEX	5	323	-	38,46,46	0.23	0	50,70,70	1.31	4 (8%)
19	CLA	B	822	8	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
23	LMG	4	621	-	41,41,55	0.54	0	49,49,63	0.69	0
20	CHL	6	308	32	55,59,74	1.04	5 (9%)	62,96,114	1.29	6 (9%)
19	CLA	B	811	8	69,73,73	1.26	8 (11%)	83,113,113	1.30	6 (7%)
26	LHG	A	801	-	30,30,48	0.61	0	33,36,54	0.60	0
25	XAT	7	616	-	39,47,47	0.66	2 (5%)	54,74,74	0.75	0
19	CLA	A	834	7	69,73,73	1.25	6 (8%)	83,113,113	1.31	5 (6%)
19	CLA	A	827	32	69,73,73	1.26	8 (11%)	83,113,113	1.30	6 (7%)
19	CLA	K	204	14	50,54,73	1.46	9 (18%)	60,90,113	1.43	5 (8%)
19	CLA	6	309	4	59,63,73	1.35	6 (10%)	71,101,113	1.33	7 (9%)
19	CLA	B	818	8	69,73,73	1.26	8 (11%)	83,113,113	1.26	7 (8%)
19	CLA	1	314	15	50,54,73	1.46	6 (12%)	60,90,113	1.44	5 (8%)
24	LMU	7	620	-	22,22,36	0.41	0	27,27,47	0.68	0
20	CHL	7	606	32	50,54,74	1.07	5 (10%)	56,90,114	1.50	9 (16%)
23	LMG	L	201	-	40,40,55	0.53	0	48,48,63	0.59	0
20	CHL	3	306	32	70,74,74	0.98	5 (7%)	80,114,114	1.19	7 (8%)
22	LUT	5	324	-	42,43,43	0.29	0	51,60,60	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	843	7	69,73,73	1.27	8 (11%)	83,113,113	1.26	5 (6%)
19	CLA	7	609	5	69,73,73	1.25	8 (11%)	83,113,113	1.26	5 (6%)
21	BCR	B	847	-	41,41,41	0.31	0	56,56,56	0.58	0
19	CLA	3	307	1	65,69,73	1.28	8 (12%)	78,108,113	1.32	6 (7%)
24	LMU	A	857	-	24,24,36	0.37	0	29,29,47	0.61	0
29	PQN	A	845	-	34,34,34	0.34	0	42,45,45	0.52	1 (2%)
24	LMU	1	322	-	22,22,36	0.39	0	27,27,47	0.72	0
19	CLA	Z	610	26	64,68,73	1.29	7 (10%)	77,107,113	1.29	5 (6%)
24	LMU	6	328	-	24,24,36	0.38	0	29,29,47	0.64	0
19	CLA	5	316	3	69,73,73	1.25	9 (13%)	83,113,113	1.27	8 (9%)
22	LUT	7	615	-	42,43,43	0.28	0	51,60,60	0.61	0
19	CLA	B	837	8	64,68,73	1.32	9 (14%)	77,107,113	1.29	8 (10%)
20	CHL	6	317	4	47,51,74	1.11	5 (10%)	52,86,114	1.77	6 (11%)
19	CLA	L	204	32	49,53,73	1.50	6 (12%)	59,89,113	1.43	6 (10%)
19	CLA	8	312	6	69,73,73	1.27	8 (11%)	83,113,113	1.26	7 (8%)
19	CLA	8	303	6	69,73,73	1.26	8 (11%)	83,113,113	1.32	8 (9%)
19	CLA	A	816	7	59,63,73	1.37	7 (11%)	71,101,113	1.33	5 (7%)
19	CLA	1	312	32	69,73,73	1.25	6 (8%)	83,113,113	1.29	8 (9%)
22	LUT	F	305	-	42,43,43	0.28	0	51,60,60	0.78	1 (1%)
28	CL0	A	802	7	69,73,73	0.85	4 (5%)	83,113,113	1.11	5 (6%)
26	LHG	A	848	19	37,37,48	0.58	0	40,43,54	0.52	0
19	CLA	1	303	15	61,65,73	1.34	6 (9%)	73,103,113	1.37	7 (9%)
20	CHL	6	315	4	70,74,74	0.99	5 (7%)	80,114,114	1.25	6 (7%)
24	LMU	8	319	-	24,24,36	0.39	0	29,29,47	0.61	0
19	CLA	A	814	7	69,73,73	1.25	7 (10%)	83,113,113	1.30	7 (8%)
19	CLA	B	831	8	49,53,73	1.49	8 (16%)	59,89,113	1.48	5 (8%)
19	CLA	A	808	7	69,73,73	1.27	8 (11%)	83,113,113	1.28	6 (7%)
19	CLA	7	611	5	56,60,73	1.39	8 (14%)	67,97,113	1.39	5 (7%)
20	CHL	6	302	4	70,74,74	0.96	5 (7%)	80,114,114	1.29	8 (10%)
19	CLA	B	801	32	69,73,73	1.27	8 (11%)	83,113,113	1.21	6 (7%)
21	BCR	B	848	-	41,41,41	0.29	0	56,56,56	0.80	1 (1%)
19	CLA	8	307	32	54,58,73	1.42	7 (12%)	65,95,113	1.43	7 (10%)
26	LHG	5	321	19	36,36,48	0.58	0	39,42,54	0.54	0
19	CLA	8	313	6	61,65,73	1.33	8 (13%)	73,103,113	1.29	7 (9%)
19	CLA	A	819	7	69,73,73	1.24	7 (10%)	83,113,113	1.30	7 (8%)
20	CHL	4	601	2	70,74,74	0.97	5 (7%)	80,114,114	1.28	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	825	32	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
24	LMU	7	619	-	21,21,36	0.40	0	26,26,47	0.71	0
19	CLA	1	310	26	65,69,73	1.28	7 (10%)	78,108,113	1.30	6 (7%)
26	LHG	6	325	-	35,35,48	0.56	0	38,41,54	0.73	1 (2%)
21	BCR	7	617	-	41,41,41	0.31	0	56,56,56	0.65	0
19	CLA	A	803	-	69,73,73	1.24	6 (8%)	83,113,113	1.22	8 (9%)
19	CLA	B	815	8	64,68,73	1.30	7 (10%)	77,107,113	1.31	6 (7%)
21	BCR	3	318	-	41,41,41	0.31	0	56,56,56	0.58	0
22	LUT	Z	615	-	42,43,43	0.30	0	51,60,60	0.70	0
19	CLA	5	304	3	54,58,73	1.41	8 (14%)	65,95,113	1.45	9 (13%)
19	CLA	A	837	7	69,73,73	1.26	8 (11%)	83,113,113	1.27	6 (7%)
24	LMU	B	853	-	36,36,36	0.46	0	47,47,47	0.66	0
21	BCR	L	205	-	41,41,41	0.35	0	56,56,56	0.56	0
19	CLA	A	810	7	69,73,73	1.25	7 (10%)	83,113,113	1.30	5 (6%)
21	BCR	3	319	-	41,41,41	0.30	0	56,56,56	0.61	0
21	BCR	B	844	-	41,41,41	0.36	0	56,56,56	0.89	4 (7%)
19	CLA	B	814	8	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
21	BCR	J	103	-	41,41,41	0.34	0	56,56,56	0.53	0
21	BCR	B	846	-	41,41,41	0.33	0	56,56,56	0.56	0
19	CLA	5	305	32	59,63,73	1.36	9 (15%)	71,101,113	1.35	5 (7%)
19	CLA	A	846	26	49,53,73	1.49	7 (14%)	59,89,113	1.45	6 (10%)
19	CLA	3	305	1	55,59,73	1.41	7 (12%)	66,96,113	1.38	7 (10%)
19	CLA	6	303	4	69,73,73	1.26	6 (8%)	83,113,113	1.28	6 (7%)
19	CLA	Z	614	15	64,68,73	1.31	8 (12%)	77,107,113	1.30	8 (10%)
19	CLA	Z	607	32	54,58,73	1.42	9 (16%)	65,95,113	1.41	7 (10%)
19	CLA	B	817	8	69,73,73	1.25	7 (10%)	83,113,113	1.27	6 (7%)
19	CLA	7	612	5	69,73,73	1.26	7 (10%)	83,113,113	1.28	7 (8%)
24	LMU	3	325	-	24,24,36	0.37	0	29,29,47	0.65	0
22	LUT	3	320	-	19,20,43	0.45	0	20,28,60	0.49	0
19	CLA	4	609	2	64,68,73	1.29	7 (10%)	77,107,113	1.30	6 (7%)
19	CLA	5	311	26	59,63,73	1.35	6 (10%)	71,101,113	1.36	6 (8%)
19	CLA	A	836	7	69,73,73	1.25	8 (11%)	83,113,113	1.29	8 (9%)
19	CLA	Z	603	15	69,73,73	1.26	8 (11%)	83,113,113	1.29	6 (7%)
24	LMU	F	306	-	36,36,36	0.46	0	47,47,47	0.77	1 (2%)
19	CLA	Z	602	15	64,68,73	1.30	7 (10%)	77,107,113	1.33	6 (7%)
24	LMU	Z	619	-	32,32,36	0.47	0	43,43,47	0.85	1 (2%)
19	CLA	3	314	1	49,53,73	1.48	8 (16%)	59,89,113	1.40	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LMG	G	201	-	36,36,55	0.56	0	44,44,63	0.68	0
19	CLA	6	327	32	57,61,73	1.38	8 (14%)	68,98,113	1.37	6 (8%)
24	LMU	4	624	-	24,24,36	0.39	0	29,29,47	0.64	0
19	CLA	B	805	8	49,53,73	1.49	6 (12%)	59,89,113	1.45	7 (11%)
25	XAT	8	316	-	39,47,47	0.66	2 (5%)	54,74,74	0.72	0
19	CLA	B	824	8	69,73,73	1.25	8 (11%)	83,113,113	1.31	9 (10%)
19	CLA	5	313	3	60,64,73	1.33	8 (13%)	72,102,113	1.39	6 (8%)
19	CLA	5	312	3	49,53,73	1.48	7 (14%)	59,89,113	1.48	6 (10%)
20	CHL	4	605	32	70,74,74	0.90	5 (7%)	80,114,114	1.19	9 (11%)
19	CLA	8	310	26	49,53,73	1.48	7 (14%)	59,89,113	1.41	6 (10%)
20	CHL	Z	605	32	50,54,74	1.05	4 (8%)	56,90,114	1.55	10 (17%)
24	LMU	Z	620	-	24,24,36	0.40	0	29,29,47	0.60	0
20	CHL	Z	606	32	70,74,74	0.91	5 (7%)	80,114,114	1.35	7 (8%)
24	LMU	K	201	-	24,24,36	0.39	0	29,29,47	0.71	0
29	PQN	B	843	-	34,34,34	0.35	0	42,45,45	0.59	1 (2%)
19	CLA	A	833	7	59,63,73	1.36	7 (11%)	71,101,113	1.37	4 (5%)
19	CLA	B	828	8	69,73,73	1.25	7 (10%)	83,113,113	1.23	5 (6%)
23	LMG	8	321	-	49,49,55	0.52	0	57,57,63	0.64	0
19	CLA	3	313	32	64,68,73	1.29	7 (10%)	77,107,113	1.46	9 (11%)
22	LUT	4	616	-	42,43,43	0.29	0	51,60,60	0.70	0
19	CLA	J	102	13	59,63,73	1.35	8 (13%)	71,101,113	1.37	7 (9%)
19	CLA	3	303	32	69,73,73	1.25	8 (11%)	83,113,113	1.30	8 (9%)
19	CLA	B	835	8	64,68,73	1.30	8 (12%)	77,107,113	1.34	6 (7%)
24	LMU	3	324	-	36,36,36	0.45	0	47,47,47	1.06	4 (8%)
19	CLA	A	844	32	69,73,73	1.27	8 (11%)	83,113,113	1.30	7 (8%)
19	CLA	L	203	18	69,73,73	1.25	8 (11%)	83,113,113	1.32	9 (10%)
25	XAT	1	316	-	39,47,47	0.66	2 (5%)	54,74,74	0.83	0
22	LUT	3	317	-	42,43,43	0.26	0	51,60,60	0.60	0
19	CLA	8	304	32	64,68,73	1.30	7 (10%)	77,107,113	1.30	5 (6%)
19	CLA	A	830	7	69,73,73	1.26	7 (10%)	83,113,113	1.26	6 (7%)
19	CLA	B	813	8	69,73,73	1.26	7 (10%)	83,113,113	1.28	9 (10%)
20	CHL	5	306	32	50,54,74	1.13	5 (10%)	56,90,114	1.49	7 (12%)
19	CLA	A	831	7	69,73,73	1.27	7 (10%)	83,113,113	1.25	6 (7%)
21	BCR	8	317	-	41,41,41	0.31	0	56,56,56	0.53	0
19	CLA	Z	613	15	54,58,73	1.42	7 (12%)	65,95,113	1.42	6 (9%)
23	LMG	J	104	-	42,42,55	0.53	0	50,50,63	0.64	0
22	LUT	1	317	-	42,43,43	0.28	0	51,60,60	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DGD	B	850	-	60,60,67	0.57	0	74,74,81	0.81	2 (2%)
19	CLA	3	308	1	69,73,73	1.24	7 (10%)	83,113,113	1.27	8 (9%)
21	BCR	6	321	-	41,41,41	0.31	0	56,56,56	0.56	0
19	CLA	Z	611	15	49,53,73	1.50	7 (14%)	59,89,113	1.41	5 (8%)
21	BCR	A	858	-	41,41,41	0.33	0	56,56,56	0.83	2 (3%)
26	LHG	5	301	-	37,37,48	0.57	0	40,43,54	0.56	0
19	CLA	B	823	8	63,67,73	1.32	9 (14%)	75,105,113	1.32	6 (8%)
19	CLA	5	309	3	69,73,73	1.25	7 (10%)	83,113,113	1.29	5 (6%)
19	CLA	B	840	32	69,73,73	1.26	8 (11%)	83,113,113	1.29	8 (9%)
26	LHG	Z	618	19	38,38,48	0.57	0	41,44,54	0.53	0
19	CLA	3	312	1	49,53,73	1.49	7 (14%)	59,89,113	1.41	5 (8%)
19	CLA	Z	604	32	61,65,73	1.33	8 (13%)	73,103,113	1.35	8 (10%)
19	CLA	A	811	7	69,73,73	1.25	7 (10%)	83,113,113	1.32	8 (9%)
20	CHL	4	615	2	50,54,74	1.05	4 (8%)	56,90,114	1.59	9 (16%)
19	CLA	B	832	8	59,63,73	1.35	8 (13%)	71,101,113	1.36	9 (12%)
19	CLA	B	842	26	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
19	CLA	Z	608	15	69,73,73	1.26	7 (10%)	83,113,113	1.24	6 (7%)
19	CLA	5	314	3	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
19	CLA	3	310	1	50,54,73	1.46	8 (16%)	60,90,113	1.40	6 (10%)
22	LUT	Z	617	-	26,26,43	0.42	0	34,35,60	0.61	0
19	CLA	3	301	1	64,68,73	1.30	7 (10%)	77,107,113	1.34	9 (11%)
21	BCR	A	849	-	41,41,41	0.33	0	56,56,56	0.53	0
26	LHG	4	619	19	48,48,48	0.52	0	51,54,54	0.49	0
23	LMG	6	326	-	19,19,55	0.34	0	19,19,63	0.46	0
19	CLA	B	804	-	69,73,73	1.26	9 (13%)	83,113,113	1.28	7 (8%)
19	CLA	4	604	32	54,58,73	1.41	8 (14%)	65,95,113	1.42	7 (10%)
19	CLA	B	829	8	69,73,73	1.24	7 (10%)	83,113,113	1.23	6 (7%)
19	CLA	K	205	14	49,53,73	1.48	9 (18%)	59,89,113	1.47	6 (10%)
20	CHL	5	307	32	70,74,74	0.97	5 (7%)	80,114,114	1.19	7 (8%)
19	CLA	B	841	8	69,73,73	1.26	8 (11%)	83,113,113	1.30	6 (7%)
19	CLA	6	304	4	55,59,73	1.41	6 (10%)	66,96,113	1.41	8 (12%)
21	BCR	3	315	-	41,41,41	0.31	0	56,56,56	0.55	0
19	CLA	B	806	8	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
19	CLA	B	838	8	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
22	LUT	1	315	-	42,43,43	0.30	0	51,60,60	0.68	0
20	CHL	1	306	32	50,54,74	1.08	4 (8%)	56,90,114	1.53	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	826	7	59,63,73	1.37	7 (11%)	71,101,113	1.34	7 (9%)
23	LMG	7	622	-	32,32,55	0.57	0	40,40,63	0.73	0
21	BCR	B	802	-	41,41,41	0.36	0	56,56,56	1.07	4 (7%)
19	CLA	7	614	5	50,54,73	1.46	8 (16%)	60,90,113	1.41	4 (6%)
19	CLA	A	821	7	69,73,73	1.26	9 (13%)	83,113,113	1.27	10 (12%)
19	CLA	4	613	2	59,63,73	1.36	8 (13%)	71,101,113	1.34	6 (8%)
19	CLA	1	308	15	69,73,73	1.25	6 (8%)	83,113,113	1.27	4 (4%)
19	CLA	B	809	8	69,73,73	1.25	8 (11%)	83,113,113	1.31	8 (9%)
26	LHG	8	318	19	43,43,48	0.54	0	46,49,54	0.54	0
19	CLA	6	312	4	49,53,73	1.49	8 (16%)	59,89,113	1.43	4 (6%)
22	LUT	3	316	-	42,43,43	0.26	0	51,60,60	0.58	0
19	CLA	6	314	4	54,58,73	1.42	8 (14%)	65,95,113	1.39	7 (10%)
19	CLA	1	309	15	69,73,73	1.25	6 (8%)	83,113,113	1.27	7 (8%)
21	BCR	A	853	-	41,41,41	0.34	0	56,56,56	0.63	0
19	CLA	B	839	8	54,58,73	1.41	7 (12%)	65,95,113	1.46	8 (12%)
19	CLA	5	319	32	50,54,73	1.47	6 (12%)	60,90,113	1.50	5 (8%)
24	LMU	6	324	-	24,24,36	0.39	0	29,29,47	0.61	0
19	CLA	7	610	26	69,73,73	1.25	7 (10%)	83,113,113	1.28	6 (7%)
20	CHL	Z	601	15	70,74,74	0.96	5 (7%)	80,114,114	1.38	10 (12%)
19	CLA	A	813	7,19	69,73,73	1.23	7 (10%)	83,113,113	1.22	5 (6%)
19	CLA	A	815	7	69,73,73	1.27	7 (10%)	83,113,113	1.29	7 (8%)
19	CLA	4	608	2	64,68,73	1.29	6 (9%)	77,107,113	1.35	6 (7%)
19	CLA	B	834	8	62,66,73	1.31	7 (11%)	74,104,113	1.40	8 (10%)
19	CLA	1	307	32	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)
19	CLA	A	822	7	59,63,73	1.34	7 (11%)	71,101,113	1.34	7 (9%)
19	CLA	A	825	7	49,53,73	1.49	8 (16%)	59,89,113	1.41	5 (8%)
24	LMU	4	623	-	20,20,36	0.40	0	25,25,47	0.78	0
19	CLA	5	310	3	64,68,73	1.29	7 (10%)	77,107,113	1.32	8 (10%)
19	CLA	K	203	32	64,68,73	1.31	7 (10%)	77,107,113	1.38	11 (14%)
19	CLA	A	835	7	69,73,73	1.27	9 (13%)	83,113,113	1.28	6 (7%)
23	LMG	J	105	-	35,35,55	0.60	0	43,43,63	0.72	0
19	CLA	A	832	7	69,73,73	1.25	8 (11%)	83,113,113	1.27	7 (8%)
21	BCR	L	202	-	41,41,41	0.34	0	56,56,56	0.53	0
21	BCR	5	320	-	41,41,41	0.29	0	56,56,56	0.60	0
24	LMU	1	321	-	24,24,36	0.38	0	29,29,47	0.63	0
19	CLA	1	313	15	64,68,73	1.31	8 (12%)	77,107,113	1.30	9 (11%)
24	LMU	1	301	-	36,36,36	0.44	0	47,47,47	1.07	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	3	304	32	46,50,73	1.51	7 (15%)	55,85,113	1.43	5 (9%)
22	LUT	8	301	-	42,43,43	0.30	0	51,60,60	0.62	1 (1%)
19	CLA	A	818	32	59,63,73	1.36	8 (13%)	71,101,113	1.38	6 (8%)
19	CLA	B	810	8	69,73,73	1.27	8 (11%)	83,113,113	1.30	5 (6%)
24	LMU	1	319	-	36,36,36	0.45	0	47,47,47	0.74	1 (2%)
26	LHG	7	618	19	48,48,48	0.51	0	51,54,54	0.49	0
25	XAT	5	322	-	39,47,47	0.66	2 (5%)	54,74,74	0.81	0
19	CLA	4	611	2	49,53,73	1.49	7 (14%)	59,89,113	1.46	5 (8%)
24	LMU	Z	621	-	24,24,36	0.39	0	29,29,47	0.60	0
19	CLA	6	313	32	69,73,73	1.26	8 (11%)	83,113,113	1.26	8 (9%)
19	CLA	A	840	7	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
19	CLA	Z	609	15	64,68,73	1.30	7 (10%)	77,107,113	1.31	8 (10%)
27	NEX	6	323	-	38,46,46	0.21	0	50,70,70	1.29	4 (8%)
19	CLA	F	302	32	69,73,73	1.27	7 (10%)	83,113,113	1.26	5 (6%)
21	BCR	4	618	-	41,41,41	0.31	0	56,56,56	0.58	0
19	CLA	3	311	1	64,68,73	1.31	6 (9%)	77,107,113	1.29	7 (9%)
23	LMG	3	321	-	37,37,55	0.57	0	45,45,63	0.72	0
19	CLA	6	310	4	64,68,73	1.31	8 (12%)	77,107,113	1.28	7 (9%)
19	CLA	A	804	32	69,73,73	1.26	8 (11%)	83,113,113	1.22	5 (6%)
19	CLA	A	829	7	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
22	LUT	J	101	-	42,43,43	0.30	0	51,60,60	0.77	1 (1%)
19	CLA	8	302	6	69,73,73	1.25	6 (8%)	83,113,113	1.30	8 (9%)
19	CLA	7	613	5	47,51,73	1.49	8 (17%)	56,86,113	1.45	6 (10%)
24	LMU	A	856	-	20,20,36	0.41	0	25,25,47	0.70	0
23	LMG	B	852	-	43,43,55	0.53	0	51,51,63	0.68	0
19	CLA	5	303	3	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
20	CHL	8	320	15	70,74,74	1.03	5 (7%)	80,114,114	1.27	7 (8%)
19	CLA	6	311	26	62,66,73	1.33	7 (11%)	74,104,113	1.29	5 (6%)
20	CHL	8	305	32	70,74,74	0.90	5 (7%)	80,114,114	1.24	7 (8%)
19	CLA	A	820	7	64,68,73	1.32	7 (10%)	77,107,113	1.27	6 (7%)
20	CHL	5	308	32	55,59,74	1.13	5 (9%)	62,96,114	1.45	8 (12%)
24	LMU	1	320	-	19,19,36	0.42	0	24,24,47	0.65	0
19	CLA	7	604	32	55,59,73	1.40	8 (14%)	66,96,113	1.40	5 (7%)
21	BCR	K	206	-	41,41,41	0.31	0	56,56,56	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SF4	C	101	9	-	-	0/6/5/5
19	CLA	1	304	32	-	4/21/97/115	-
19	CLA	7	608	5	-	2/15/91/115	-
19	CLA	B	812	8	-	14/39/115/115	-
21	BCR	B	845	-	-	3/29/63/63	0/2/2/2
25	XAT	6	322	-	-	1/31/93/93	0/4/4/4
19	CLA	7	603	5	-	3/24/100/115	-
19	CLA	B	826	32	-	12/39/115/115	-
19	CLA	A	838	7	-	8/30/106/115	-
24	LMU	3	322	-	-	2/20/60/61	0/2/2/2
19	CLA	F	303	32	-	2/15/91/115	-
19	CLA	A	805	7	-	6/39/115/115	-
25	XAT	Z	616	-	-	3/31/93/93	0/4/4/4
19	CLA	8	309	6	-	6/39/115/115	-
19	CLA	6	305	4	-	17/39/115/115	-
20	CHL	5	317	3	-	3/14/90/117	-
21	BCR	G	204	-	-	0/29/63/63	0/2/2/2
19	CLA	B	820	32	-	10/33/109/115	-
19	CLA	A	839	7	-	2/23/99/115	-
19	CLA	B	836	32	-	5/15/91/115	-
20	CHL	8	306	32	-	12/41/117/117	-
20	CHL	6	306	32	-	6/17/93/117	-
26	LHG	6	318	19	-	15/53/53/53	-
22	LUT	8	315	-	-	2/29/67/67	0/2/2/2
19	CLA	B	807	8	-	2/39/115/115	-
19	CLA	B	827	8	-	4/39/115/115	-
19	CLA	4	603	2	-	12/39/115/115	-
24	LMU	3	323	-	-	5/15/35/61	0/1/1/2
19	CLA	3	309	32	-	5/27/103/115	-
21	BCR	A	851	-	-	4/29/63/63	0/2/2/2
26	LHG	1	318	19	-	11/48/48/53	-
20	CHL	4	607	32	-	21/41/117/117	-
20	CHL	7	601	5	-	13/41/117/117	-
26	LHG	B	851	19	-	13/49/49/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	4	602	2	-	3/33/109/115	-
19	CLA	7	607	32	-	1/21/97/115	-
30	SF4	C	102	9	-	-	0/6/5/5
19	CLA	8	308	6	-	4/15/91/115	-
19	CLA	B	816	8	-	13/39/115/115	-
22	LUT	5	318	-	-	4/29/67/67	0/2/2/2
19	CLA	G	202	17	-	9/33/109/115	-
19	CLA	5	302	3	-	8/39/115/115	-
19	CLA	8	314	6	-	1/15/91/115	-
20	CHL	4	606	32	-	4/14/90/117	-
20	CHL	7	605	32	-	0/17/93/117	-
25	XAT	4	617	-	-	0/31/93/93	0/4/4/4
19	CLA	B	803	8	-	8/39/115/115	-
24	LMU	4	625	-	-	0/13/33/61	0/1/1/2
20	CHL	1	305	32	-	2/17/93/117	-
30	SF4	A	854	7,8	-	-	0/6/5/5
19	CLA	A	806	7,19	-	2/27/103/115	-
19	CLA	7	602	5	-	1/39/115/115	-
23	LMG	F	301	-	-	11/27/47/70	0/1/1/1
20	CHL	7	621	6	-	12/41/117/117	-
19	CLA	5	315	3	-	4/15/91/115	-
21	BCR	B	849	-	-	2/29/63/63	0/2/2/2
26	LHG	4	620	-	-	12/42/42/53	-
19	CLA	A	828	32	-	12/39/115/115	-
19	CLA	B	830	8	-	11/39/115/115	-
19	CLA	B	808	8	-	5/27/103/115	-
19	CLA	A	807	7	-	18/39/115/115	-
19	CLA	1	311	15	-	5/15/91/115	-
19	CLA	G	203	17	-	2/17/93/115	-
19	CLA	K	202	14	-	4/15/91/115	-
21	BCR	A	852	-	-	5/29/63/63	0/2/2/2
23	LMG	6	301	-	-	7/28/28/70	-
20	CHL	6	307	32	-	14/41/117/117	-
19	CLA	8	311	6	-	6/27/103/115	-
19	CLA	3	302	1	-	12/39/115/115	-
19	CLA	B	833	8	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	842	7	-	9/39/115/115	-
19	CLA	A	812	7	-	12/39/115/115	-
19	CLA	A	824	7	-	22/39/115/115	-
19	CLA	4	612	2	-	14/39/115/115	-
19	CLA	A	841	7	-	5/39/115/115	-
19	CLA	A	817	7	-	7/39/115/115	-
19	CLA	Z	612	32	-	3/39/115/115	-
19	CLA	6	320	32	-	6/27/103/115	-
24	LMU	4	622	-	-	6/13/33/61	0/1/1/2
26	LHG	A	847	-	-	14/53/53/53	-
19	CLA	1	302	15	-	6/33/109/115	-
21	BCR	I	201	-	-	6/29/63/63	0/2/2/2
19	CLA	A	809	7	-	5/21/97/115	-
19	CLA	A	823	32	-	4/39/115/115	-
22	LUT	6	319	-	-	4/29/67/67	0/2/2/2
24	LMU	A	855	-	-	6/21/61/61	0/2/2/2
21	BCR	A	850	-	-	0/29/63/63	0/2/2/2
19	CLA	B	819	8	-	5/39/115/115	-
19	CLA	6	316	4	-	4/15/91/115	-
19	CLA	F	304	16	-	20/39/115/115	-
19	CLA	4	610	26	-	5/33/109/115	-
19	CLA	B	821	8	-	6/29/105/115	-
19	CLA	4	614	2	-	3/15/91/115	-
27	NEX	5	323	-	1/1/12/25	2/27/83/83	0/3/3/3
19	CLA	B	822	8	-	17/39/115/115	-
23	LMG	4	621	-	-	16/36/56/70	0/1/1/1
20	CHL	6	308	32	-	5/23/99/117	-
19	CLA	B	811	8	-	12/39/115/115	-
26	LHG	A	801	-	-	14/35/35/53	-
25	XAT	7	616	-	-	0/31/93/93	0/4/4/4
19	CLA	A	834	7	-	7/39/115/115	-
19	CLA	A	827	32	-	7/39/115/115	-
19	CLA	K	204	14	-	1/17/93/115	-
19	CLA	6	309	4	-	5/27/103/115	-
19	CLA	B	818	8	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	314	15	-	4/17/93/115	-
24	LMU	7	620	-	-	7/13/33/61	0/1/1/2
20	CHL	7	606	32	-	3/17/93/117	-
23	LMG	L	201	-	-	15/35/55/70	0/1/1/1
20	CHL	3	306	32	-	7/41/117/117	-
22	LUT	5	324	-	-	10/29/67/67	0/2/2/2
19	CLA	A	843	7	-	6/39/115/115	-
19	CLA	7	609	5	-	8/39/115/115	-
21	BCR	B	847	-	-	1/29/63/63	0/2/2/2
19	CLA	3	307	1	-	8/35/111/115	-
24	LMU	A	857	-	-	4/15/35/61	0/1/1/2
29	PQN	A	845	-	-	0/23/43/43	0/2/2/2
24	LMU	1	322	-	-	5/13/33/61	0/1/1/2
19	CLA	Z	610	26	-	7/33/109/115	-
24	LMU	6	328	-	-	7/15/35/61	0/1/1/2
19	CLA	5	316	3	-	16/39/115/115	-
22	LUT	7	615	-	-	2/29/67/67	0/2/2/2
19	CLA	B	837	8	-	6/33/109/115	-
20	CHL	6	317	4	-	0/14/90/117	-
19	CLA	L	204	32	-	3/15/91/115	-
19	CLA	8	312	6	-	5/39/115/115	-
19	CLA	8	303	6	-	18/39/115/115	-
19	CLA	A	816	7	-	6/27/103/115	-
19	CLA	1	312	32	-	10/39/115/115	-
22	LUT	F	305	-	-	10/29/67/67	0/2/2/2
28	CL0	A	802	7	-	3/39/115/115	-
26	LHG	A	848	19	-	11/42/42/53	-
19	CLA	1	303	15	-	8/30/106/115	-
20	CHL	6	315	4	-	17/41/117/117	-
24	LMU	8	319	-	-	6/15/35/61	0/1/1/2
19	CLA	A	814	7	-	8/39/115/115	-
19	CLA	B	831	8	-	0/15/91/115	-
19	CLA	A	808	7	-	10/39/115/115	-
19	CLA	7	611	5	-	5/24/100/115	-
20	CHL	6	302	4	-	14/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	801	32	-	11/39/115/115	-
21	BCR	B	848	-	-	2/29/63/63	0/2/2/2
19	CLA	8	307	32	-	2/21/97/115	-
26	LHG	5	321	19	-	14/41/41/53	-
19	CLA	8	313	6	-	8/30/106/115	-
19	CLA	A	819	7	-	7/39/115/115	-
20	CHL	4	601	2	-	4/41/117/117	-
19	CLA	B	825	32	-	9/39/115/115	-
24	LMU	7	619	-	-	4/12/32/61	0/1/1/2
19	CLA	1	310	26	-	13/35/111/115	-
26	LHG	6	325	-	-	14/40/40/53	-
21	BCR	7	617	-	-	4/29/63/63	0/2/2/2
19	CLA	A	803	-	-	1/39/115/115	-
19	CLA	B	815	8	-	6/33/109/115	-
21	BCR	3	318	-	-	4/29/63/63	0/2/2/2
22	LUT	Z	615	-	-	4/29/67/67	0/2/2/2
19	CLA	5	304	3	-	7/21/97/115	-
19	CLA	A	837	7	-	8/39/115/115	-
24	LMU	B	853	-	-	3/21/61/61	0/2/2/2
21	BCR	L	205	-	-	4/29/63/63	0/2/2/2
19	CLA	A	810	7	-	5/39/115/115	-
21	BCR	3	319	-	-	4/29/63/63	0/2/2/2
21	BCR	B	844	-	-	4/29/63/63	0/2/2/2
19	CLA	B	814	8	-	10/39/115/115	-
21	BCR	J	103	-	-	4/29/63/63	0/2/2/2
21	BCR	B	846	-	-	4/29/63/63	0/2/2/2
19	CLA	5	305	32	-	6/27/103/115	-
19	CLA	A	846	26	-	7/15/91/115	-
19	CLA	3	305	1	-	2/23/99/115	-
19	CLA	6	303	4	-	4/39/115/115	-
19	CLA	Z	614	15	-	10/33/109/115	-
19	CLA	Z	607	32	-	5/21/97/115	-
19	CLA	B	817	8	-	7/39/115/115	-
19	CLA	7	612	5	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMU	3	325	-	-	7/15/35/61	0/1/1/2
22	LUT	3	320	-	-	1/11/30/67	0/1/1/2
19	CLA	4	609	2	-	4/33/109/115	-
19	CLA	5	311	26	-	5/27/103/115	-
19	CLA	A	836	7	-	8/39/115/115	-
19	CLA	Z	603	15	-	9/39/115/115	-
24	LMU	F	306	-	-	8/21/61/61	0/2/2/2
19	CLA	Z	602	15	-	3/33/109/115	-
24	LMU	Z	619	-	-	5/17/57/61	0/2/2/2
19	CLA	3	314	1	-	0/15/91/115	-
23	LMG	G	201	-	-	6/31/51/70	0/1/1/1
19	CLA	6	327	32	-	5/25/101/115	-
24	LMU	4	624	-	-	6/15/35/61	0/1/1/2
19	CLA	B	805	8	-	5/15/91/115	-
25	XAT	8	316	-	-	0/31/93/93	0/4/4/4
19	CLA	B	824	8	-	12/39/115/115	-
19	CLA	5	313	3	-	6/29/105/115	-
19	CLA	5	312	3	-	4/15/91/115	-
20	CHL	4	605	32	-	11/41/117/117	-
19	CLA	8	310	26	-	4/15/91/115	-
20	CHL	Z	605	32	-	4/17/93/117	-
24	LMU	Z	620	-	-	2/15/35/61	0/1/1/2
20	CHL	Z	606	32	-	12/41/117/117	-
24	LMU	K	201	-	-	6/15/35/61	0/1/1/2
29	PQN	B	843	-	-	2/23/43/43	0/2/2/2
19	CLA	A	833	7	-	11/27/103/115	-
19	CLA	B	828	8	-	11/39/115/115	-
23	LMG	8	321	-	-	22/44/64/70	0/1/1/1
19	CLA	3	313	32	-	10/33/109/115	-
22	LUT	4	616	-	-	3/29/67/67	0/2/2/2
19	CLA	J	102	13	-	8/27/103/115	-
19	CLA	3	303	32	-	3/39/115/115	-
19	CLA	B	835	8	-	4/33/109/115	-
24	LMU	3	324	-	-	9/21/61/61	0/2/2/2
19	CLA	A	844	32	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	L	203	18	-	16/39/115/115	-
25	XAT	1	316	-	-	0/31/93/93	0/4/4/4
22	LUT	3	317	-	-	2/29/67/67	0/2/2/2
19	CLA	8	304	32	-	7/33/109/115	-
19	CLA	A	830	7	-	12/39/115/115	-
19	CLA	B	813	8	-	18/39/115/115	-
20	CHL	5	306	32	-	7/17/93/117	-
19	CLA	A	831	7	-	4/39/115/115	-
21	BCR	8	317	-	-	3/29/63/63	0/2/2/2
19	CLA	Z	613	15	-	2/21/97/115	-
23	LMG	J	104	-	-	9/37/57/70	0/1/1/1
22	LUT	1	317	-	-	5/29/67/67	0/2/2/2
31	DGD	B	850	-	-	11/48/88/95	0/2/2/2
19	CLA	3	308	1	-	5/39/115/115	-
21	BCR	6	321	-	-	2/29/63/63	0/2/2/2
19	CLA	Z	611	15	-	5/15/91/115	-
21	BCR	A	858	-	-	5/29/63/63	0/2/2/2
26	LHG	5	301	-	-	12/42/42/53	-
19	CLA	B	823	8	-	5/32/108/115	-
19	CLA	5	309	3	-	12/39/115/115	-
19	CLA	B	840	32	-	11/39/115/115	-
26	LHG	Z	618	19	-	5/43/43/53	-
19	CLA	3	312	1	-	6/15/91/115	-
19	CLA	Z	604	32	-	11/30/106/115	-
19	CLA	A	811	7	-	13/39/115/115	-
20	CHL	4	615	2	-	6/17/93/117	-
19	CLA	B	832	8	-	2/27/103/115	-
19	CLA	B	842	26	-	8/39/115/115	-
19	CLA	Z	608	15	-	19/39/115/115	-
19	CLA	5	314	3	-	6/15/91/115	-
19	CLA	3	310	1	-	7/17/93/115	-
22	LUT	Z	617	-	-	3/18/37/67	0/1/1/2
19	CLA	3	301	1	-	3/33/109/115	-
21	BCR	A	849	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	4	619	19	-	11/53/53/53	-
23	LMG	6	326	-	-	6/17/17/70	-
19	CLA	B	804	-	-	15/39/115/115	-
19	CLA	4	604	32	-	4/21/97/115	-
19	CLA	B	829	8	-	6/39/115/115	-
19	CLA	K	205	14	-	2/15/91/115	-
20	CHL	5	307	32	-	11/41/117/117	-
19	CLA	B	841	8	-	12/39/115/115	-
19	CLA	6	304	4	-	10/23/99/115	-
21	BCR	3	315	-	-	7/29/63/63	0/2/2/2
19	CLA	B	806	8	-	11/39/115/115	-
19	CLA	B	838	8	-	3/39/115/115	-
22	LUT	1	315	-	-	4/29/67/67	0/2/2/2
20	CHL	1	306	32	-	6/17/93/117	-
19	CLA	A	826	7	-	4/27/103/115	-
23	LMG	7	622	-	-	9/27/47/70	0/1/1/1
21	BCR	B	802	-	-	7/29/63/63	0/2/2/2
19	CLA	7	614	5	-	6/17/93/115	-
19	CLA	A	821	7	-	3/39/115/115	-
19	CLA	4	613	2	-	6/27/103/115	-
19	CLA	1	308	15	-	16/39/115/115	-
19	CLA	B	809	8	-	10/39/115/115	-
26	LHG	8	318	19	-	16/48/48/53	-
19	CLA	6	312	4	-	2/15/91/115	-
22	LUT	3	316	-	-	3/29/67/67	0/2/2/2
19	CLA	6	314	4	-	7/21/97/115	-
19	CLA	1	309	15	-	3/39/115/115	-
21	BCR	A	853	-	-	4/29/63/63	0/2/2/2
19	CLA	B	839	8	-	1/21/97/115	-
19	CLA	5	319	32	-	12/17/93/115	-
24	LMU	6	324	-	-	6/15/35/61	0/1/1/2
19	CLA	7	610	26	-	7/39/115/115	-
20	CHL	Z	601	15	-	13/41/117/117	-
19	CLA	A	813	7,19	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	815	7	-	9/39/115/115	-
19	CLA	4	608	2	-	9/33/109/115	-
19	CLA	B	834	8	-	5/31/107/115	-
19	CLA	1	307	32	-	14/39/115/115	-
19	CLA	A	822	7	-	4/27/103/115	-
19	CLA	A	825	7	-	3/15/91/115	-
24	LMU	4	623	-	-	4/11/31/61	0/1/1/2
19	CLA	5	310	3	-	5/33/109/115	-
19	CLA	K	203	32	-	6/33/109/115	-
19	CLA	A	835	7	-	7/39/115/115	-
23	LMG	J	105	-	-	14/30/50/70	0/1/1/1
19	CLA	A	832	7	-	5/39/115/115	-
21	BCR	L	202	-	-	4/29/63/63	0/2/2/2
21	BCR	5	320	-	-	2/29/63/63	0/2/2/2
24	LMU	1	321	-	-	4/15/35/61	0/1/1/2
19	CLA	1	313	15	-	12/33/109/115	-
24	LMU	1	301	-	-	11/21/61/61	0/2/2/2
19	CLA	3	304	32	-	0/12/88/115	-
22	LUT	8	301	-	-	4/29/67/67	0/2/2/2
19	CLA	A	818	32	-	5/27/103/115	-
19	CLA	B	810	8	-	8/39/115/115	-
24	LMU	1	319	-	-	7/21/61/61	0/2/2/2
26	LHG	7	618	19	-	16/53/53/53	-
25	XAT	5	322	-	-	1/31/93/93	0/4/4/4
19	CLA	4	611	2	-	3/15/91/115	-
24	LMU	Z	621	-	-	3/15/35/61	0/1/1/2
19	CLA	6	313	32	-	4/39/115/115	-
19	CLA	A	840	7	-	8/39/115/115	-
19	CLA	Z	609	15	-	2/33/109/115	-
27	NEX	6	323	-	-	3/27/83/83	0/3/3/3
19	CLA	F	302	32	-	10/39/115/115	-
21	BCR	4	618	-	-	5/29/63/63	0/2/2/2
19	CLA	3	311	1	-	5/33/109/115	-
23	LMG	3	321	-	-	12/32/52/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	6	310	4	-	2/33/109/115	-
19	CLA	A	804	32	-	2/39/115/115	-
19	CLA	A	829	7	-	4/39/115/115	-
22	LUT	J	101	-	-	6/29/67/67	0/2/2/2
19	CLA	8	302	6	-	6/39/115/115	-
19	CLA	7	613	5	-	4/13/89/115	-
24	LMU	A	856	-	-	3/11/31/61	0/1/1/2
23	LMG	B	852	-	-	9/38/58/70	0/1/1/1
19	CLA	5	303	3	-	2/39/115/115	-
20	CHL	8	320	15	-	10/41/117/117	-
19	CLA	6	311	26	-	9/31/107/115	-
20	CHL	8	305	32	-	8/41/117/117	-
19	CLA	A	820	7	-	14/33/109/115	-
20	CHL	5	308	32	-	4/23/99/117	-
24	LMU	1	320	-	-	7/10/30/61	0/1/1/2
19	CLA	7	604	32	-	0/23/99/115	-
21	BCR	K	206	-	-	2/29/63/63	0/2/2/2

All (1538) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	601	CHL	MG-NA	4.83	2.17	2.06
20	6	302	CHL	MG-NA	4.81	2.17	2.06
20	7	621	CHL	MG-NA	4.71	2.17	2.06
20	8	320	CHL	MG-NA	4.37	2.16	2.06
20	5	317	CHL	C4D-ND	-4.28	1.31	1.37
20	8	306	CHL	MG-NA	4.28	2.16	2.06
20	7	601	CHL	MG-NA	4.28	2.16	2.06
20	5	307	CHL	C4D-ND	-4.21	1.31	1.37
20	5	308	CHL	C4D-ND	-4.18	1.31	1.37
19	1	308	CLA	C1D-ND	4.17	1.42	1.37
20	Z	605	CHL	C4D-ND	-4.16	1.32	1.37
20	5	306	CHL	MG-NA	4.12	2.16	2.06
20	Z	606	CHL	C4D-ND	-4.11	1.32	1.37
20	7	606	CHL	MG-NA	4.10	2.16	2.06
20	6	317	CHL	C4D-ND	-4.06	1.32	1.37
20	8	306	CHL	C4D-ND	-4.06	1.32	1.37
20	5	306	CHL	C4D-ND	-4.04	1.32	1.37
20	8	305	CHL	MG-NA	4.03	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	607	CHL	MG-NC	4.02	2.15	2.06
20	4	601	CHL	C4D-ND	-4.01	1.32	1.37
19	B	803	CLA	C1D-ND	4.00	1.42	1.37
20	7	605	CHL	MG-NA	3.99	2.15	2.06
20	1	306	CHL	C4D-ND	-3.96	1.32	1.37
19	A	841	CLA	C1D-ND	3.96	1.42	1.37
19	Z	608	CLA	C1D-ND	3.95	1.42	1.37
20	6	315	CHL	MG-NA	3.95	2.15	2.06
20	8	320	CHL	C4D-ND	-3.93	1.32	1.37
20	3	306	CHL	MG-NC	3.92	2.15	2.06
19	G	202	CLA	C1D-ND	3.92	1.42	1.37
20	7	605	CHL	C4D-ND	-3.92	1.32	1.37
19	A	817	CLA	C1D-ND	3.92	1.42	1.37
19	6	314	CLA	C1D-ND	3.92	1.42	1.37
19	A	838	CLA	C1D-ND	3.91	1.42	1.37
20	4	606	CHL	C4D-ND	-3.91	1.32	1.37
19	K	204	CLA	C1D-ND	3.91	1.42	1.37
19	Z	612	CLA	C1D-ND	3.90	1.42	1.37
20	5	308	CHL	MG-NA	3.90	2.15	2.06
19	1	314	CLA	C1D-ND	3.89	1.42	1.37
19	4	608	CLA	C1D-ND	3.89	1.42	1.37
19	B	822	CLA	C1D-ND	3.89	1.42	1.37
20	6	307	CHL	MG-NA	3.88	2.15	2.06
19	Z	613	CLA	C1D-ND	3.88	1.42	1.37
19	6	310	CLA	C1D-ND	3.88	1.42	1.37
19	6	327	CLA	C1D-ND	3.88	1.42	1.37
19	B	807	CLA	C1D-ND	3.87	1.42	1.37
19	G	203	CLA	C1D-ND	3.87	1.42	1.37
19	6	311	CLA	C1D-ND	3.87	1.42	1.37
19	B	837	CLA	C1D-ND	3.87	1.42	1.37
19	B	820	CLA	C1D-ND	3.87	1.42	1.37
20	1	305	CHL	C4D-ND	-3.87	1.32	1.37
19	1	309	CLA	C1D-ND	3.87	1.42	1.37
19	B	833	CLA	C1D-ND	3.87	1.42	1.37
19	B	825	CLA	C1D-ND	3.87	1.42	1.37
19	6	320	CLA	C1D-ND	3.86	1.42	1.37
19	3	303	CLA	C1D-ND	3.86	1.42	1.37
19	1	303	CLA	C1D-ND	3.86	1.42	1.37
19	L	204	CLA	C1D-ND	3.86	1.42	1.37
19	B	815	CLA	C1D-ND	3.86	1.42	1.37
19	8	307	CLA	C1D-ND	3.86	1.42	1.37
19	B	808	CLA	C1D-ND	3.86	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	609	CLA	C1D-ND	3.86	1.42	1.37
19	Z	614	CLA	C1D-ND	3.86	1.42	1.37
20	4	605	CHL	C4D-ND	-3.85	1.32	1.37
19	A	827	CLA	C1D-ND	3.85	1.42	1.37
19	A	843	CLA	C1D-ND	3.85	1.42	1.37
19	B	814	CLA	C1D-ND	3.85	1.42	1.37
19	B	821	CLA	C1D-ND	3.85	1.42	1.37
19	3	311	CLA	C1D-ND	3.84	1.42	1.37
19	Z	611	CLA	C1D-ND	3.84	1.42	1.37
19	5	311	CLA	C1D-ND	3.84	1.42	1.37
19	8	312	CLA	C1D-ND	3.84	1.42	1.37
19	8	309	CLA	C1D-ND	3.84	1.42	1.37
19	A	826	CLA	C1D-ND	3.84	1.42	1.37
19	4	610	CLA	C1D-ND	3.83	1.42	1.37
19	4	613	CLA	C1D-ND	3.83	1.42	1.37
19	6	309	CLA	C1D-ND	3.83	1.42	1.37
19	B	838	CLA	C1D-ND	3.83	1.42	1.37
19	5	319	CLA	C1D-ND	3.83	1.42	1.37
19	B	811	CLA	C1D-ND	3.83	1.42	1.37
19	6	303	CLA	C1D-ND	3.82	1.42	1.37
19	B	832	CLA	C1D-ND	3.82	1.42	1.37
19	7	613	CLA	C1D-ND	3.82	1.42	1.37
19	A	807	CLA	C1D-ND	3.82	1.42	1.37
19	A	831	CLA	C1D-ND	3.82	1.42	1.37
19	A	818	CLA	C1D-ND	3.81	1.42	1.37
19	7	607	CLA	C1D-ND	3.81	1.42	1.37
19	4	614	CLA	C1D-ND	3.81	1.42	1.37
19	B	805	CLA	C1D-ND	3.81	1.42	1.37
20	4	615	CHL	MG-NA	3.81	2.15	2.06
19	F	303	CLA	C1D-ND	3.81	1.42	1.37
20	5	307	CHL	MG-NA	3.81	2.15	2.06
19	7	612	CLA	C1D-ND	3.81	1.42	1.37
19	5	315	CLA	C1D-ND	3.81	1.42	1.37
19	3	313	CLA	C1D-ND	3.80	1.42	1.37
19	Z	607	CLA	C1D-ND	3.80	1.42	1.37
19	1	307	CLA	C1D-ND	3.80	1.42	1.37
19	A	840	CLA	C1D-ND	3.80	1.42	1.37
19	B	829	CLA	C1D-ND	3.80	1.42	1.37
19	4	611	CLA	C1D-ND	3.80	1.42	1.37
19	7	609	CLA	C1D-ND	3.80	1.42	1.37
19	A	806	CLA	C1D-ND	3.80	1.42	1.37
19	Z	603	CLA	C1D-ND	3.80	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	6	312	CLA	C1D-ND	3.80	1.42	1.37
19	B	813	CLA	C1D-ND	3.80	1.42	1.37
19	3	312	CLA	C1D-ND	3.80	1.42	1.37
19	4	602	CLA	C1D-ND	3.80	1.42	1.37
20	3	306	CHL	MG-NA	3.79	2.15	2.06
19	3	307	CLA	C1D-ND	3.79	1.42	1.37
19	3	305	CLA	C1D-ND	3.79	1.42	1.37
19	6	304	CLA	C1D-ND	3.79	1.42	1.37
19	4	604	CLA	C1D-ND	3.79	1.42	1.37
19	5	313	CLA	C1D-ND	3.79	1.42	1.37
19	8	313	CLA	C1D-ND	3.79	1.42	1.37
20	4	615	CHL	C4D-ND	-3.79	1.32	1.37
19	B	810	CLA	C1D-ND	3.79	1.42	1.37
19	K	205	CLA	C1D-ND	3.79	1.42	1.37
19	1	313	CLA	C1D-ND	3.79	1.42	1.37
19	8	314	CLA	C1D-ND	3.79	1.42	1.37
19	A	816	CLA	C1D-ND	3.78	1.42	1.37
19	B	836	CLA	C1D-ND	3.78	1.42	1.37
19	Z	610	CLA	C1D-ND	3.78	1.42	1.37
19	B	817	CLA	C1D-ND	3.78	1.42	1.37
19	A	808	CLA	C1D-ND	3.78	1.42	1.37
19	8	311	CLA	C1D-ND	3.78	1.42	1.37
19	B	841	CLA	C1D-ND	3.78	1.42	1.37
19	5	303	CLA	C1D-ND	3.78	1.42	1.37
19	B	812	CLA	C1D-ND	3.78	1.42	1.37
19	B	819	CLA	C1D-ND	3.78	1.42	1.37
20	6	306	CHL	C4D-ND	-3.78	1.32	1.37
19	5	305	CLA	C1D-ND	3.77	1.42	1.37
19	5	314	CLA	C1D-ND	3.77	1.42	1.37
19	A	814	CLA	C1D-ND	3.77	1.42	1.37
19	1	310	CLA	C1D-ND	3.77	1.42	1.37
19	5	304	CLA	C1D-ND	3.77	1.42	1.37
19	1	304	CLA	C1D-ND	3.77	1.42	1.37
19	7	603	CLA	C1D-ND	3.77	1.42	1.37
19	B	816	CLA	C1D-ND	3.77	1.42	1.37
19	B	828	CLA	C1D-ND	3.77	1.42	1.37
19	B	827	CLA	C1D-ND	3.77	1.42	1.37
19	4	603	CLA	C1D-ND	3.77	1.42	1.37
19	A	837	CLA	C1D-ND	3.76	1.42	1.37
19	Z	604	CLA	C1D-ND	3.76	1.42	1.37
19	5	310	CLA	C1D-ND	3.76	1.42	1.37
19	7	611	CLA	C1D-ND	3.76	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	301	CLA	C1D-ND	3.76	1.42	1.37
19	7	604	CLA	C1D-ND	3.76	1.42	1.37
19	1	302	CLA	C1D-ND	3.76	1.42	1.37
19	B	839	CLA	C1D-ND	3.76	1.42	1.37
19	8	308	CLA	C1D-ND	3.76	1.42	1.37
19	1	312	CLA	C1D-ND	3.76	1.42	1.37
19	8	302	CLA	C1D-ND	3.76	1.42	1.37
19	A	844	CLA	C1D-ND	3.76	1.42	1.37
19	3	308	CLA	C1D-ND	3.76	1.42	1.37
19	6	305	CLA	C1D-ND	3.75	1.42	1.37
19	6	313	CLA	C1D-ND	3.75	1.42	1.37
19	B	835	CLA	C1D-ND	3.75	1.42	1.37
19	A	815	CLA	C1D-ND	3.75	1.42	1.37
19	A	832	CLA	C1D-ND	3.75	1.42	1.37
19	A	842	CLA	C1D-ND	3.75	1.42	1.37
19	3	304	CLA	C1D-ND	3.75	1.42	1.37
19	4	609	CLA	C1D-ND	3.75	1.42	1.37
20	6	315	CHL	MG-NC	3.75	2.15	2.06
19	A	811	CLA	C1D-ND	3.75	1.42	1.37
19	A	824	CLA	C1D-ND	3.75	1.42	1.37
19	A	836	CLA	C1D-ND	3.74	1.42	1.37
19	3	310	CLA	C1D-ND	3.74	1.42	1.37
19	A	829	CLA	C1D-ND	3.74	1.42	1.37
19	7	614	CLA	C1D-ND	3.74	1.42	1.37
19	A	813	CLA	C1D-ND	3.74	1.42	1.37
19	A	823	CLA	C1D-ND	3.74	1.42	1.37
19	8	303	CLA	C1D-ND	3.74	1.42	1.37
19	3	309	CLA	C1D-ND	3.74	1.42	1.37
19	B	823	CLA	C1D-ND	3.74	1.42	1.37
19	K	203	CLA	C1D-ND	3.74	1.42	1.37
19	5	316	CLA	C1D-ND	3.73	1.42	1.37
19	A	810	CLA	C1D-ND	3.73	1.42	1.37
20	1	306	CHL	MG-NA	3.73	2.15	2.06
19	F	302	CLA	C1D-ND	3.73	1.42	1.37
20	8	305	CHL	C4D-ND	-3.73	1.32	1.37
19	Z	602	CLA	C1D-ND	3.73	1.42	1.37
19	5	309	CLA	C1D-ND	3.73	1.42	1.37
19	B	824	CLA	C1D-ND	3.73	1.42	1.37
19	1	311	CLA	C1D-ND	3.73	1.42	1.37
19	A	804	CLA	C1D-ND	3.73	1.42	1.37
20	4	606	CHL	MG-NA	3.72	2.15	2.06
19	3	302	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	831	CLA	C1D-ND	3.72	1.42	1.37
19	A	809	CLA	C1D-ND	3.72	1.42	1.37
19	4	612	CLA	C1D-ND	3.72	1.42	1.37
19	7	602	CLA	C1D-ND	3.72	1.42	1.37
19	B	840	CLA	C1D-ND	3.72	1.42	1.37
19	5	312	CLA	C1D-ND	3.72	1.42	1.37
19	A	839	CLA	C1D-ND	3.72	1.42	1.37
19	B	818	CLA	C1D-ND	3.72	1.42	1.37
19	A	834	CLA	C1D-ND	3.71	1.42	1.37
19	A	803	CLA	C1D-ND	3.71	1.42	1.37
19	J	102	CLA	C1D-ND	3.71	1.42	1.37
19	8	310	CLA	C1D-ND	3.71	1.42	1.37
19	6	316	CLA	C1D-ND	3.71	1.42	1.37
19	A	825	CLA	C1D-ND	3.71	1.42	1.37
19	A	835	CLA	C1D-ND	3.71	1.42	1.37
19	B	806	CLA	C1D-ND	3.71	1.42	1.37
19	A	820	CLA	C1D-ND	3.70	1.42	1.37
20	7	621	CHL	C4D-ND	-3.70	1.32	1.37
20	Z	601	CHL	C4D-ND	-3.70	1.32	1.37
19	5	302	CLA	C1D-ND	3.70	1.42	1.37
20	6	308	CHL	MG-NC	3.70	2.15	2.06
19	A	828	CLA	C1D-ND	3.70	1.42	1.37
19	A	846	CLA	C1D-ND	3.69	1.42	1.37
19	B	809	CLA	C1D-ND	3.69	1.42	1.37
19	7	610	CLA	C1D-ND	3.69	1.42	1.37
19	B	801	CLA	C1D-ND	3.69	1.42	1.37
19	B	826	CLA	C1D-ND	3.69	1.42	1.37
19	A	812	CLA	C1D-ND	3.69	1.42	1.37
19	A	830	CLA	C1D-ND	3.68	1.42	1.37
20	7	606	CHL	C4D-ND	-3.67	1.32	1.37
19	K	202	CLA	C1D-ND	3.67	1.42	1.37
20	4	601	CHL	MG-NA	3.67	2.15	2.06
19	B	834	CLA	C1D-ND	3.66	1.42	1.37
19	7	608	CLA	C1D-ND	3.66	1.42	1.37
19	A	833	CLA	C1D-ND	3.66	1.42	1.37
19	L	203	CLA	C1D-ND	3.66	1.42	1.37
19	A	819	CLA	C1D-ND	3.66	1.42	1.37
20	6	307	CHL	C4D-ND	-3.66	1.32	1.37
19	8	304	CLA	C1D-ND	3.66	1.42	1.37
20	6	302	CHL	C4D-ND	-3.65	1.32	1.37
20	8	320	CHL	MG-NC	3.65	2.14	2.06
19	B	842	CLA	C1D-ND	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	821	CLA	C1D-ND	3.63	1.42	1.37
19	3	314	CLA	C1D-ND	3.63	1.42	1.37
19	A	822	CLA	C1D-ND	3.62	1.42	1.37
20	1	305	CHL	MG-NA	3.61	2.14	2.06
19	B	830	CLA	C1D-ND	3.60	1.42	1.37
20	7	601	CHL	C4D-ND	-3.60	1.32	1.37
19	F	304	CLA	C1D-ND	3.60	1.42	1.37
20	4	607	CHL	MG-NA	3.58	2.14	2.06
19	Z	611	CLA	C4B-NB	3.55	1.42	1.37
19	A	805	CLA	C1D-ND	3.55	1.42	1.37
20	6	306	CHL	MG-NA	3.55	2.14	2.06
20	Z	606	CHL	MG-NA	3.54	2.14	2.06
20	6	308	CHL	C1C-NC	3.53	1.43	1.37
20	7	621	CHL	MG-NC	3.52	2.14	2.06
19	B	804	CLA	C1D-ND	3.51	1.42	1.37
19	B	809	CLA	C4B-NB	3.50	1.42	1.37
20	5	317	CHL	MG-NA	3.48	2.14	2.06
19	A	820	CLA	C4B-NB	3.48	1.42	1.37
19	F	304	CLA	C4B-NB	3.46	1.42	1.37
19	1	308	CLA	C4B-NB	3.45	1.42	1.37
19	4	603	CLA	C4B-NB	3.44	1.42	1.37
19	B	820	CLA	C4B-NB	3.44	1.42	1.37
20	5	308	CHL	MG-NC	3.43	2.14	2.06
19	A	808	CLA	C4B-NB	3.43	1.42	1.37
19	B	830	CLA	C4B-NB	3.43	1.42	1.37
19	3	305	CLA	C4B-NB	3.42	1.42	1.37
19	B	818	CLA	C4B-NB	3.42	1.42	1.37
19	B	822	CLA	C4B-NB	3.42	1.42	1.37
19	B	840	CLA	C4B-NB	3.42	1.42	1.37
19	G	202	CLA	C4B-NB	3.41	1.42	1.37
20	6	315	CHL	C4D-ND	-3.40	1.33	1.37
19	4	610	CLA	C4B-NB	3.40	1.42	1.37
19	A	835	CLA	C4B-NB	3.40	1.42	1.37
19	B	804	CLA	C4B-NB	3.38	1.41	1.37
19	6	313	CLA	C4B-NB	3.38	1.41	1.37
20	6	315	CHL	C1C-NC	3.38	1.42	1.37
19	6	316	CLA	C4B-NB	3.38	1.41	1.37
19	A	812	CLA	C4D-ND	-3.37	1.33	1.37
19	Z	608	CLA	C4B-NB	3.37	1.41	1.37
19	5	302	CLA	C4B-NB	3.37	1.41	1.37
19	A	826	CLA	C4B-NB	3.37	1.41	1.37
19	B	805	CLA	C4B-NB	3.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	607	CHL	C4D-ND	-3.36	1.33	1.37
19	4	612	CLA	C4B-NB	3.36	1.41	1.37
19	8	312	CLA	C4B-NB	3.36	1.41	1.37
19	A	837	CLA	C4B-NB	3.36	1.41	1.37
19	4	613	CLA	C4B-NB	3.36	1.41	1.37
19	3	311	CLA	C4B-NB	3.35	1.41	1.37
19	A	824	CLA	C4B-NB	3.35	1.41	1.37
19	7	614	CLA	C4B-NB	3.34	1.41	1.37
19	Z	614	CLA	C4B-NB	3.34	1.41	1.37
19	3	312	CLA	C4B-NB	3.34	1.41	1.37
19	5	315	CLA	C4B-NB	3.34	1.41	1.37
19	A	821	CLA	C4B-NB	3.34	1.41	1.37
19	G	203	CLA	C4B-NB	3.34	1.41	1.37
19	6	312	CLA	C4B-NB	3.34	1.41	1.37
19	A	803	CLA	C4B-NB	3.34	1.41	1.37
19	Z	613	CLA	C4B-NB	3.33	1.41	1.37
19	1	313	CLA	C4B-NB	3.33	1.41	1.37
20	Z	605	CHL	MG-NA	3.33	2.14	2.06
20	4	601	CHL	C1C-NC	3.32	1.42	1.37
28	A	802	CL0	C4D-ND	-3.32	1.33	1.37
19	A	843	CLA	C4B-NB	3.32	1.41	1.37
19	L	204	CLA	C4B-NB	3.31	1.41	1.37
19	6	314	CLA	C4B-NB	3.31	1.41	1.37
20	4	605	CHL	MG-NA	3.31	2.14	2.06
19	5	314	CLA	C4B-NB	3.31	1.41	1.37
19	6	311	CLA	C4B-NB	3.31	1.41	1.37
19	B	825	CLA	C4B-NB	3.31	1.41	1.37
19	B	813	CLA	C4B-NB	3.31	1.41	1.37
20	3	306	CHL	C4D-ND	-3.31	1.33	1.37
19	4	614	CLA	C4B-NB	3.31	1.41	1.37
19	3	304	CLA	C4B-NB	3.30	1.41	1.37
20	6	317	CHL	MG-NA	3.30	2.14	2.06
19	B	831	CLA	C4D-ND	-3.30	1.33	1.37
19	B	833	CLA	C4B-NB	3.30	1.41	1.37
19	7	612	CLA	C4B-NB	3.30	1.41	1.37
19	5	319	CLA	C4B-NB	3.30	1.41	1.37
19	5	309	CLA	C4B-NB	3.30	1.41	1.37
19	L	203	CLA	C4B-NB	3.29	1.41	1.37
19	A	816	CLA	C4B-NB	3.29	1.41	1.37
19	B	823	CLA	C4B-NB	3.29	1.41	1.37
19	7	602	CLA	C4B-NB	3.28	1.41	1.37
19	Z	607	CLA	C4B-NB	3.28	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	826	CLA	C4B-NB	3.28	1.41	1.37
19	B	841	CLA	C4B-NB	3.28	1.41	1.37
20	6	308	CHL	C4D-ND	-3.28	1.33	1.37
19	A	838	CLA	C4B-NB	3.28	1.41	1.37
19	A	804	CLA	C4D-ND	-3.28	1.33	1.37
19	B	821	CLA	C4B-NB	3.28	1.41	1.37
20	7	621	CHL	C1C-NC	3.27	1.42	1.37
19	6	310	CLA	C4B-NB	3.27	1.41	1.37
19	K	203	CLA	C4B-NB	3.27	1.41	1.37
19	1	303	CLA	C4B-NB	3.27	1.41	1.37
19	A	833	CLA	C4B-NB	3.27	1.41	1.37
19	K	205	CLA	C4B-NB	3.27	1.41	1.37
19	B	819	CLA	C4B-NB	3.27	1.41	1.37
19	1	309	CLA	C4B-NB	3.27	1.41	1.37
19	Z	604	CLA	C4B-NB	3.26	1.41	1.37
19	3	310	CLA	C4B-NB	3.26	1.41	1.37
19	1	307	CLA	C4B-NB	3.26	1.41	1.37
19	A	841	CLA	C4B-NB	3.26	1.41	1.37
19	F	302	CLA	C4B-NB	3.26	1.41	1.37
19	8	303	CLA	C4B-NB	3.26	1.41	1.37
19	A	804	CLA	C4B-NB	3.26	1.41	1.37
19	B	836	CLA	C4B-NB	3.26	1.41	1.37
19	K	202	CLA	C4B-NB	3.26	1.41	1.37
19	4	611	CLA	C4B-NB	3.26	1.41	1.37
19	B	810	CLA	C4B-NB	3.26	1.41	1.37
19	6	303	CLA	C4B-NB	3.25	1.41	1.37
19	8	307	CLA	C4B-NB	3.25	1.41	1.37
19	A	834	CLA	C4B-NB	3.25	1.41	1.37
19	8	311	CLA	C4B-NB	3.25	1.41	1.37
19	A	830	CLA	C4D-ND	-3.25	1.33	1.37
19	A	829	CLA	C4D-ND	-3.25	1.33	1.37
19	8	304	CLA	C4B-NB	3.25	1.41	1.37
19	A	825	CLA	C4B-NB	3.25	1.41	1.37
19	A	831	CLA	C4B-NB	3.25	1.41	1.37
19	1	302	CLA	C4B-NB	3.24	1.41	1.37
19	6	327	CLA	C4B-NB	3.24	1.41	1.37
19	B	812	CLA	C4B-NB	3.24	1.41	1.37
19	5	303	CLA	C4B-NB	3.24	1.41	1.37
19	5	311	CLA	C4B-NB	3.24	1.41	1.37
19	7	611	CLA	C4B-NB	3.24	1.41	1.37
19	5	316	CLA	C4B-NB	3.24	1.41	1.37
19	A	846	CLA	C4B-NB	3.24	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	801	CLA	C4B-NB	3.23	1.41	1.37
19	A	844	CLA	C4B-NB	3.23	1.41	1.37
19	6	304	CLA	C4B-NB	3.23	1.41	1.37
19	B	841	CLA	C4D-ND	-3.23	1.33	1.37
19	8	309	CLA	C4B-NB	3.23	1.41	1.37
19	Z	609	CLA	C4B-NB	3.23	1.41	1.37
19	4	609	CLA	C4B-NB	3.23	1.41	1.37
19	7	613	CLA	C4B-NB	3.23	1.41	1.37
19	B	806	CLA	C4B-NB	3.23	1.41	1.37
19	B	828	CLA	C4B-NB	3.23	1.41	1.37
19	A	819	CLA	C4B-NB	3.23	1.41	1.37
19	8	313	CLA	C4B-NB	3.23	1.41	1.37
19	1	312	CLA	C4B-NB	3.23	1.41	1.37
19	B	842	CLA	C4B-NB	3.22	1.41	1.37
19	1	304	CLA	C4B-NB	3.22	1.41	1.37
20	5	307	CHL	MG-NC	3.22	2.13	2.06
19	B	837	CLA	C4D-ND	-3.22	1.33	1.37
19	B	824	CLA	C4B-NB	3.22	1.41	1.37
19	A	817	CLA	C4B-NB	3.22	1.41	1.37
19	4	602	CLA	C4B-NB	3.22	1.41	1.37
19	A	831	CLA	C4D-ND	-3.22	1.33	1.37
19	5	310	CLA	C4B-NB	3.22	1.41	1.37
19	3	308	CLA	C4B-NB	3.22	1.41	1.37
19	8	310	CLA	C4B-NB	3.21	1.41	1.37
19	4	604	CLA	C4B-NB	3.21	1.41	1.37
19	Z	603	CLA	C4B-NB	3.21	1.41	1.37
19	F	303	CLA	C4B-NB	3.21	1.41	1.37
19	6	309	CLA	C4B-NB	3.21	1.41	1.37
19	B	838	CLA	C4D-ND	-3.21	1.33	1.37
19	Z	602	CLA	C4B-NB	3.21	1.41	1.37
19	A	832	CLA	C4B-NB	3.20	1.41	1.37
19	1	311	CLA	C4B-NB	3.20	1.41	1.37
19	3	309	CLA	C4B-NB	3.20	1.41	1.37
19	A	836	CLA	C4B-NB	3.20	1.41	1.37
19	A	820	CLA	C3B-C4B	3.20	1.50	1.42
19	8	314	CLA	C4B-NB	3.20	1.41	1.37
19	B	830	CLA	C4D-ND	-3.19	1.33	1.37
19	5	305	CLA	C4B-NB	3.19	1.41	1.37
19	B	817	CLA	C4B-NB	3.19	1.41	1.37
20	5	308	CHL	C1C-NC	3.19	1.42	1.37
19	8	302	CLA	C4B-NB	3.19	1.41	1.37
19	B	834	CLA	C4B-NB	3.19	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	302	CLA	C4B-NB	3.19	1.41	1.37
19	B	839	CLA	C4B-NB	3.19	1.41	1.37
19	1	310	CLA	C4B-NB	3.19	1.41	1.37
19	A	813	CLA	C4D-ND	-3.18	1.33	1.37
19	6	305	CLA	C4B-NB	3.18	1.41	1.37
19	A	810	CLA	C4B-NB	3.18	1.41	1.37
19	1	314	CLA	C4B-NB	3.18	1.41	1.37
19	K	204	CLA	C4B-NB	3.18	1.41	1.37
19	F	302	CLA	C4D-ND	-3.18	1.33	1.37
19	B	803	CLA	C4B-NB	3.18	1.41	1.37
19	7	607	CLA	C4D-ND	-3.18	1.33	1.37
19	A	823	CLA	C4B-NB	3.18	1.41	1.37
19	B	831	CLA	C4B-NB	3.18	1.41	1.37
19	B	833	CLA	C4D-ND	-3.18	1.33	1.37
19	B	815	CLA	C4B-NB	3.18	1.41	1.37
19	A	807	CLA	C4D-ND	-3.18	1.33	1.37
19	3	301	CLA	C4B-NB	3.17	1.41	1.37
19	A	805	CLA	C4B-NB	3.17	1.41	1.37
19	A	830	CLA	C4B-NB	3.17	1.41	1.37
19	B	807	CLA	C4B-NB	3.17	1.41	1.37
28	A	802	CL0	C1C-NC	3.17	1.42	1.37
19	6	320	CLA	C4B-NB	3.17	1.41	1.37
19	B	808	CLA	C4B-NB	3.17	1.41	1.37
19	Z	610	CLA	C4B-NB	3.17	1.41	1.37
19	A	813	CLA	C4B-NB	3.17	1.41	1.37
19	A	815	CLA	C4B-NB	3.17	1.41	1.37
19	B	811	CLA	C4B-NB	3.16	1.41	1.37
19	A	815	CLA	C4D-ND	-3.16	1.33	1.37
19	B	811	CLA	C4D-ND	-3.16	1.33	1.37
19	7	610	CLA	C4B-NB	3.16	1.41	1.37
19	A	828	CLA	C4B-NB	3.16	1.41	1.37
19	B	827	CLA	C4D-ND	-3.16	1.33	1.37
19	B	816	CLA	C4B-NB	3.16	1.41	1.37
19	A	839	CLA	C4B-NB	3.16	1.41	1.37
20	8	320	CHL	C1C-NC	3.16	1.42	1.37
19	B	832	CLA	C4B-NB	3.16	1.41	1.37
19	J	102	CLA	C4B-NB	3.16	1.41	1.37
19	8	308	CLA	C4B-NB	3.15	1.41	1.37
19	A	806	CLA	C4B-NB	3.15	1.41	1.37
19	Z	612	CLA	C4B-NB	3.15	1.41	1.37
19	A	818	CLA	C4D-ND	-3.15	1.33	1.37
19	A	809	CLA	C4D-ND	-3.15	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	824	CLA	C4D-ND	-3.15	1.33	1.37
19	B	804	CLA	C4D-ND	-3.15	1.33	1.37
19	B	834	CLA	C4D-ND	-3.15	1.33	1.37
19	Z	611	CLA	C3B-C4B	3.15	1.50	1.42
19	5	304	CLA	C4B-NB	3.15	1.41	1.37
19	A	822	CLA	C4B-NB	3.15	1.41	1.37
19	A	832	CLA	C4D-ND	-3.15	1.33	1.37
19	7	603	CLA	C4B-NB	3.15	1.41	1.37
19	B	838	CLA	C4B-NB	3.14	1.41	1.37
19	B	829	CLA	C4D-ND	-3.14	1.33	1.37
19	3	313	CLA	C4B-NB	3.14	1.41	1.37
19	A	812	CLA	C4B-NB	3.14	1.41	1.37
19	7	607	CLA	C4B-NB	3.14	1.41	1.37
19	B	801	CLA	C4D-ND	-3.14	1.33	1.37
20	3	306	CHL	C1C-NC	3.14	1.42	1.37
19	A	819	CLA	C4D-ND	-3.14	1.33	1.37
19	A	842	CLA	C4D-ND	-3.14	1.33	1.37
19	B	817	CLA	C4D-ND	-3.13	1.33	1.37
19	3	303	CLA	C4B-NB	3.13	1.41	1.37
19	A	818	CLA	C4B-NB	3.13	1.41	1.37
19	B	808	CLA	C4D-ND	-3.13	1.33	1.37
19	A	805	CLA	C4D-ND	-3.13	1.33	1.37
19	B	807	CLA	C4D-ND	-3.13	1.33	1.37
19	7	604	CLA	C4B-NB	3.13	1.41	1.37
19	A	828	CLA	C4D-ND	-3.13	1.33	1.37
19	A	829	CLA	C4B-NB	3.13	1.41	1.37
19	5	312	CLA	C4B-NB	3.12	1.41	1.37
19	4	608	CLA	C4B-NB	3.12	1.41	1.37
19	A	827	CLA	C4B-NB	3.12	1.41	1.37
19	8	302	CLA	C4D-ND	-3.12	1.33	1.37
19	8	304	CLA	C4D-ND	-3.12	1.33	1.37
19	B	839	CLA	C4D-ND	-3.12	1.33	1.37
19	A	837	CLA	C3B-C4B	3.11	1.50	1.42
19	B	835	CLA	C4B-NB	3.11	1.41	1.37
19	B	805	CLA	C4D-ND	-3.11	1.33	1.37
20	4	607	CHL	C1D-C2D	-3.11	1.39	1.45
19	A	843	CLA	C4D-ND	-3.11	1.33	1.37
19	B	818	CLA	C4D-ND	-3.11	1.33	1.37
19	A	809	CLA	C4B-NB	3.11	1.41	1.37
19	A	840	CLA	C4D-ND	-3.10	1.33	1.37
19	A	814	CLA	C4D-ND	-3.10	1.33	1.37
19	A	839	CLA	C4D-ND	-3.10	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	823	CLA	C4D-ND	-3.10	1.33	1.37
19	A	841	CLA	C4D-ND	-3.10	1.33	1.37
19	3	302	CLA	C4D-ND	-3.10	1.33	1.37
19	B	829	CLA	C4B-NB	3.10	1.41	1.37
19	B	824	CLA	C4D-ND	-3.09	1.33	1.37
19	A	811	CLA	C4B-NB	3.09	1.41	1.37
19	8	310	CLA	C4D-ND	-3.09	1.33	1.37
19	8	303	CLA	C4D-ND	-3.09	1.33	1.37
19	B	806	CLA	C4D-ND	-3.09	1.33	1.37
19	A	835	CLA	C4D-ND	-3.09	1.33	1.37
19	A	838	CLA	C4D-ND	-3.09	1.33	1.37
19	7	608	CLA	C4B-NB	3.09	1.41	1.37
19	A	840	CLA	C4B-NB	3.09	1.41	1.37
19	5	316	CLA	C4D-ND	-3.08	1.33	1.37
19	B	837	CLA	C4B-NB	3.08	1.41	1.37
19	B	814	CLA	C4B-NB	3.08	1.41	1.37
19	K	203	CLA	C4D-ND	-3.08	1.33	1.37
19	A	814	CLA	C4B-NB	3.08	1.41	1.37
19	A	822	CLA	C4D-ND	-3.07	1.33	1.37
19	A	833	CLA	C4D-ND	-3.07	1.33	1.37
19	B	820	CLA	C3B-C4B	3.07	1.50	1.42
19	B	827	CLA	C4B-NB	3.07	1.41	1.37
19	A	808	CLA	C4D-ND	-3.07	1.33	1.37
19	B	840	CLA	C3B-C4B	3.07	1.49	1.42
19	A	826	CLA	C4D-ND	-3.07	1.33	1.37
19	B	820	CLA	C4D-ND	-3.07	1.33	1.37
19	3	304	CLA	C4D-ND	-3.07	1.33	1.37
19	5	303	CLA	C4D-ND	-3.07	1.33	1.37
19	B	814	CLA	C4D-ND	-3.07	1.33	1.37
19	F	303	CLA	C4D-ND	-3.06	1.33	1.37
19	A	808	CLA	C3B-C4B	3.06	1.49	1.42
19	B	810	CLA	C4D-ND	-3.06	1.33	1.37
19	1	312	CLA	C4D-ND	-3.06	1.33	1.37
19	3	305	CLA	C3B-C4B	3.06	1.49	1.42
19	5	304	CLA	C4D-ND	-3.06	1.33	1.37
19	7	609	CLA	C4B-NB	3.06	1.41	1.37
19	8	307	CLA	C4D-ND	-3.06	1.33	1.37
20	4	601	CHL	MG-NC	3.06	2.13	2.06
19	1	302	CLA	C4D-ND	-3.06	1.33	1.37
19	B	835	CLA	C4D-ND	-3.06	1.33	1.37
19	L	203	CLA	C4D-ND	-3.06	1.33	1.37
19	B	805	CLA	C3B-C4B	3.06	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	8	312	CLA	C4D-ND	-3.06	1.33	1.37
19	A	836	CLA	C4D-ND	-3.06	1.33	1.37
19	7	602	CLA	C4D-ND	-3.05	1.33	1.37
19	B	826	CLA	C4D-ND	-3.05	1.33	1.37
19	B	836	CLA	C4D-ND	-3.05	1.33	1.37
19	3	307	CLA	C4D-ND	-3.05	1.33	1.37
19	5	313	CLA	C4B-NB	3.05	1.41	1.37
19	B	821	CLA	C4D-ND	-3.05	1.33	1.37
19	7	610	CLA	C4D-ND	-3.05	1.33	1.37
19	B	819	CLA	C4D-ND	-3.05	1.33	1.37
19	A	821	CLA	C4D-ND	-3.05	1.33	1.37
19	3	303	CLA	C4D-ND	-3.04	1.33	1.37
19	B	832	CLA	C4D-ND	-3.04	1.33	1.37
19	B	812	CLA	C4D-ND	-3.04	1.33	1.37
19	B	826	CLA	C3B-C4B	3.04	1.49	1.42
19	6	313	CLA	C3B-C4B	3.04	1.49	1.42
19	B	842	CLA	C4D-ND	-3.04	1.33	1.37
19	6	310	CLA	C3B-C4B	3.04	1.49	1.42
19	B	818	CLA	C3B-C4B	3.04	1.49	1.42
19	4	604	CLA	C4D-ND	-3.04	1.33	1.37
19	4	610	CLA	C3B-C4B	3.03	1.49	1.42
19	7	604	CLA	C4D-ND	-3.03	1.33	1.37
19	7	609	CLA	C4D-ND	-3.03	1.33	1.37
19	A	815	CLA	C3B-C4B	3.03	1.49	1.42
19	A	806	CLA	C4D-ND	-3.03	1.33	1.37
19	B	822	CLA	C3B-C4B	3.03	1.49	1.42
19	3	305	CLA	C4D-ND	-3.03	1.33	1.37
19	A	816	CLA	C4D-ND	-3.03	1.33	1.37
19	A	824	CLA	C3B-C4B	3.03	1.49	1.42
19	A	807	CLA	C4B-NB	3.03	1.41	1.37
19	3	314	CLA	C4D-ND	-3.03	1.33	1.37
19	A	820	CLA	C4D-ND	-3.03	1.33	1.37
19	B	809	CLA	C3B-C4B	3.03	1.49	1.42
19	7	603	CLA	C4D-ND	-3.03	1.33	1.37
19	A	803	CLA	C4D-ND	-3.03	1.33	1.37
19	3	314	CLA	C4B-NB	3.03	1.41	1.37
19	A	810	CLA	C4D-ND	-3.02	1.33	1.37
20	6	306	CHL	MG-NC	3.02	2.13	2.06
19	6	309	CLA	C4D-ND	-3.02	1.33	1.37
19	A	826	CLA	C3B-C4B	3.02	1.49	1.42
19	8	312	CLA	C3B-C4B	3.02	1.49	1.42
19	4	612	CLA	C4D-ND	-3.02	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	8	311	CLA	C4D-ND	-3.02	1.33	1.37
19	A	844	CLA	C4D-ND	-3.02	1.33	1.37
19	6	303	CLA	C4D-ND	-3.01	1.33	1.37
19	5	310	CLA	C3B-C4B	3.01	1.49	1.42
19	B	801	CLA	C3B-C4B	3.01	1.49	1.42
19	A	817	CLA	C4D-ND	-3.01	1.33	1.37
19	A	834	CLA	C4D-ND	-3.01	1.33	1.37
19	5	309	CLA	C4D-ND	-3.01	1.33	1.37
19	5	319	CLA	C3B-C4B	3.01	1.49	1.42
19	A	830	CLA	C3B-C4B	3.01	1.49	1.42
19	7	611	CLA	C4D-ND	-3.01	1.33	1.37
19	F	304	CLA	C4D-ND	-3.01	1.33	1.37
19	5	315	CLA	C3B-C4B	3.01	1.49	1.42
19	6	313	CLA	C4D-ND	-3.01	1.33	1.37
19	3	301	CLA	C4D-ND	-3.00	1.33	1.37
19	8	309	CLA	C4D-ND	-3.00	1.33	1.37
19	A	828	CLA	C3B-C4B	3.00	1.49	1.42
19	6	310	CLA	C4D-ND	-3.00	1.33	1.37
19	8	314	CLA	C4D-ND	-3.00	1.33	1.37
19	1	307	CLA	C4D-ND	-3.00	1.33	1.37
19	3	307	CLA	C4B-NB	3.00	1.41	1.37
19	7	608	CLA	C4D-ND	-3.00	1.33	1.37
20	1	306	CHL	C1C-NC	3.00	1.42	1.37
19	3	301	CLA	C3B-C4B	3.00	1.49	1.42
19	5	309	CLA	C3B-C4B	3.00	1.49	1.42
19	4	602	CLA	C4D-ND	-3.00	1.33	1.37
19	B	828	CLA	C4D-ND	-3.00	1.33	1.37
19	1	313	CLA	C4D-ND	-3.00	1.33	1.37
19	B	816	CLA	C4D-ND	-3.00	1.33	1.37
19	1	304	CLA	C4D-ND	-3.00	1.33	1.37
19	Z	613	CLA	C4D-ND	-2.99	1.33	1.37
19	6	316	CLA	C4D-ND	-2.99	1.33	1.37
19	7	602	CLA	C3B-C4B	2.99	1.49	1.42
19	7	614	CLA	C4D-ND	-2.99	1.33	1.37
19	8	313	CLA	C4D-ND	-2.99	1.33	1.37
19	A	823	CLA	C3B-C4B	2.99	1.49	1.42
20	4	605	CHL	MG-NC	2.99	2.13	2.06
19	7	613	CLA	C4D-ND	-2.99	1.33	1.37
19	A	811	CLA	C4D-ND	-2.99	1.33	1.37
19	Z	604	CLA	C4D-ND	-2.99	1.33	1.37
19	L	203	CLA	C3B-C4B	2.99	1.49	1.42
28	A	802	CL0	MG-NC	2.99	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	J	102	CLA	C4D-ND	-2.99	1.33	1.37
19	A	842	CLA	C4B-NB	2.98	1.41	1.37
20	8	306	CHL	MG-NC	2.98	2.13	2.06
19	3	311	CLA	C4D-ND	-2.98	1.33	1.37
19	3	311	CLA	C3B-C4B	2.98	1.49	1.42
20	6	307	CHL	MG-NC	2.98	2.13	2.06
19	5	302	CLA	C4D-ND	-2.98	1.33	1.37
19	L	204	CLA	C3B-C4B	2.98	1.49	1.42
19	8	310	CLA	C3B-C4B	2.97	1.49	1.42
19	6	304	CLA	C4D-ND	-2.97	1.33	1.37
19	A	846	CLA	C4D-ND	-2.97	1.33	1.37
19	B	813	CLA	C3B-C4B	2.97	1.49	1.42
19	B	833	CLA	C3B-C4B	2.97	1.49	1.42
19	1	303	CLA	C3B-C4B	2.97	1.49	1.42
19	A	807	CLA	C3B-C4B	2.97	1.49	1.42
19	6	311	CLA	C3B-C4B	2.97	1.49	1.42
19	8	308	CLA	C4D-ND	-2.97	1.33	1.37
19	4	609	CLA	C3B-C4B	2.97	1.49	1.42
19	A	821	CLA	C3B-C4B	2.97	1.49	1.42
19	1	310	CLA	C4D-ND	-2.97	1.33	1.37
19	4	603	CLA	C3B-C4B	2.97	1.49	1.42
19	Z	603	CLA	C4D-ND	-2.96	1.33	1.37
19	F	304	CLA	C3B-C4B	2.96	1.49	1.42
19	3	308	CLA	C3B-C4B	2.96	1.49	1.42
19	A	804	CLA	C3B-C4B	2.96	1.49	1.42
19	5	313	CLA	C4D-ND	-2.96	1.33	1.37
19	A	825	CLA	C4D-ND	-2.96	1.33	1.37
19	5	312	CLA	C4D-ND	-2.95	1.33	1.37
19	6	312	CLA	C4D-ND	-2.95	1.33	1.37
19	4	602	CLA	C3B-C4B	2.95	1.49	1.42
19	3	313	CLA	C4D-ND	-2.95	1.33	1.37
19	4	612	CLA	C3B-C4B	2.95	1.49	1.42
19	3	309	CLA	C4D-ND	-2.95	1.33	1.37
19	B	804	CLA	C3B-C4B	2.95	1.49	1.42
19	Z	607	CLA	C4D-ND	-2.95	1.33	1.37
19	A	806	CLA	C3B-C4B	2.95	1.49	1.42
19	Z	602	CLA	C4D-ND	-2.95	1.33	1.37
19	A	827	CLA	C4D-ND	-2.94	1.33	1.37
19	B	841	CLA	C3B-C4B	2.94	1.49	1.42
19	A	829	CLA	C3B-C4B	2.94	1.49	1.42
19	B	825	CLA	C3B-C4B	2.94	1.49	1.42
19	5	315	CLA	C4D-ND	-2.94	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	607	CHL	C1C-NC	2.94	1.42	1.37
19	A	803	CLA	C3B-C4B	2.94	1.49	1.42
19	B	815	CLA	C3B-C4B	2.94	1.49	1.42
19	Z	604	CLA	C3B-C4B	2.94	1.49	1.42
19	A	843	CLA	C3B-C4B	2.94	1.49	1.42
19	7	612	CLA	C4D-ND	-2.94	1.33	1.37
19	8	302	CLA	C3B-C4B	2.94	1.49	1.42
20	6	317	CHL	C1C-NC	2.94	1.42	1.37
19	1	302	CLA	C3B-C4B	2.93	1.49	1.42
19	B	832	CLA	C3B-C4B	2.93	1.49	1.42
19	1	303	CLA	C4D-ND	-2.93	1.33	1.37
19	Z	613	CLA	C3B-C4B	2.93	1.49	1.42
19	3	312	CLA	C4D-ND	-2.93	1.33	1.37
19	8	314	CLA	C3B-C4B	2.93	1.49	1.42
19	B	823	CLA	C4D-ND	-2.93	1.33	1.37
19	A	827	CLA	C3B-C4B	2.93	1.49	1.42
19	7	603	CLA	C3B-C4B	2.93	1.49	1.42
19	A	817	CLA	C3B-C4B	2.93	1.49	1.42
19	B	840	CLA	C4D-ND	-2.93	1.33	1.37
19	A	811	CLA	C3B-C4B	2.93	1.49	1.42
19	3	304	CLA	C3B-C4B	2.93	1.49	1.42
19	F	303	CLA	C3B-C4B	2.93	1.49	1.42
19	3	312	CLA	C3B-C4B	2.93	1.49	1.42
19	B	824	CLA	C3B-C4B	2.93	1.49	1.42
19	Z	609	CLA	C3B-C4B	2.93	1.49	1.42
19	4	608	CLA	C4D-ND	-2.92	1.33	1.37
19	1	309	CLA	C3B-C4B	2.92	1.49	1.42
19	A	816	CLA	C3B-C4B	2.92	1.49	1.42
19	Z	608	CLA	C3B-C4B	2.92	1.49	1.42
19	Z	607	CLA	C3B-C4B	2.92	1.49	1.42
19	B	806	CLA	C3B-C4B	2.92	1.49	1.42
20	Z	606	CHL	C1C-NC	2.92	1.42	1.37
19	A	834	CLA	C3B-C4B	2.92	1.49	1.42
19	A	809	CLA	C3B-C4B	2.92	1.49	1.42
19	4	613	CLA	C4D-ND	-2.92	1.33	1.37
19	4	603	CLA	C4D-ND	-2.92	1.33	1.37
19	5	319	CLA	C4D-ND	-2.92	1.33	1.37
19	Z	610	CLA	C3B-C4B	2.92	1.49	1.42
19	B	815	CLA	C4D-ND	-2.92	1.33	1.37
19	8	309	CLA	C3B-C4B	2.92	1.49	1.42
19	B	828	CLA	C3B-C4B	2.92	1.49	1.42
19	3	310	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	310	CLA	C4D-ND	-2.91	1.33	1.37
19	A	842	CLA	C3B-C4B	2.91	1.49	1.42
19	K	204	CLA	C4D-ND	-2.91	1.33	1.37
19	6	304	CLA	C3B-C4B	2.91	1.49	1.42
19	B	837	CLA	C3B-C4B	2.91	1.49	1.42
19	6	312	CLA	C3B-C4B	2.91	1.49	1.42
19	B	838	CLA	C3B-C4B	2.91	1.49	1.42
19	Z	614	CLA	C3B-C4B	2.91	1.49	1.42
19	5	314	CLA	C3B-C4B	2.91	1.49	1.42
19	B	823	CLA	C3B-C4B	2.91	1.49	1.42
19	1	311	CLA	C4D-ND	-2.91	1.33	1.37
19	A	846	CLA	C3B-C4B	2.91	1.49	1.42
19	4	610	CLA	C4D-ND	-2.91	1.33	1.37
19	B	809	CLA	C4D-ND	-2.91	1.33	1.37
19	A	839	CLA	C3B-C4B	2.91	1.49	1.42
19	7	608	CLA	C3B-C4B	2.91	1.49	1.42
19	B	803	CLA	C4D-ND	-2.91	1.33	1.37
19	B	836	CLA	C3B-C4B	2.91	1.49	1.42
19	A	822	CLA	C3B-C4B	2.90	1.49	1.42
19	1	304	CLA	C3B-C4B	2.90	1.49	1.42
19	7	609	CLA	C3B-C4B	2.90	1.49	1.42
19	A	812	CLA	C3B-C4B	2.90	1.49	1.42
19	3	309	CLA	C3B-C4B	2.90	1.49	1.42
19	5	302	CLA	C3B-C4B	2.90	1.49	1.42
19	G	202	CLA	C3B-C4B	2.90	1.49	1.42
19	6	305	CLA	C4D-ND	-2.90	1.33	1.37
19	5	303	CLA	C3B-C4B	2.90	1.49	1.42
19	Z	602	CLA	C3B-C4B	2.90	1.49	1.42
19	8	308	CLA	C3B-C4B	2.90	1.49	1.42
19	1	313	CLA	C3B-C4B	2.90	1.49	1.42
19	6	327	CLA	C4D-ND	-2.90	1.33	1.37
19	6	320	CLA	C4D-ND	-2.90	1.33	1.37
19	B	825	CLA	C4D-ND	-2.90	1.33	1.37
19	5	304	CLA	C3B-C4B	2.89	1.49	1.42
19	B	813	CLA	C4D-ND	-2.89	1.33	1.37
19	B	807	CLA	C3B-C4B	2.89	1.49	1.42
19	Z	612	CLA	C4D-ND	-2.89	1.33	1.37
19	A	819	CLA	C3B-C4B	2.89	1.49	1.42
19	K	203	CLA	C3B-C4B	2.89	1.49	1.42
19	Z	611	CLA	C4D-ND	-2.89	1.33	1.37
19	7	612	CLA	C3B-C4B	2.89	1.49	1.42
19	6	309	CLA	C3B-C4B	2.89	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	810	CLA	C3B-C4B	2.89	1.49	1.42
19	3	310	CLA	C3B-C4B	2.89	1.49	1.42
19	5	311	CLA	C3B-C4B	2.89	1.49	1.42
19	Z	609	CLA	C4D-ND	-2.89	1.33	1.37
19	7	604	CLA	C3B-C4B	2.88	1.49	1.42
19	8	307	CLA	C3B-C4B	2.88	1.49	1.42
19	4	611	CLA	C4D-ND	-2.88	1.33	1.37
19	G	203	CLA	C3B-C4B	2.88	1.49	1.42
19	B	829	CLA	C3B-C4B	2.88	1.49	1.42
19	3	303	CLA	C3B-C4B	2.88	1.49	1.42
19	Z	614	CLA	C4D-ND	-2.88	1.33	1.37
19	6	303	CLA	C3B-C4B	2.88	1.49	1.42
19	B	821	CLA	C3B-C4B	2.88	1.49	1.42
19	5	314	CLA	C4D-ND	-2.88	1.33	1.37
19	J	102	CLA	C3B-C4B	2.88	1.49	1.42
19	A	837	CLA	C4D-ND	-2.88	1.33	1.37
19	6	314	CLA	C4D-ND	-2.87	1.33	1.37
19	B	839	CLA	C3B-C4B	2.87	1.49	1.42
19	B	803	CLA	C1B-C2B	2.87	1.50	1.43
19	A	805	CLA	C3B-C4B	2.87	1.49	1.42
20	6	308	CHL	C1D-C2D	-2.87	1.39	1.45
19	4	613	CLA	C3B-C4B	2.87	1.49	1.42
19	8	303	CLA	C3B-C4B	2.87	1.49	1.42
19	8	304	CLA	C3B-C4B	2.87	1.49	1.42
19	6	316	CLA	C3B-C4B	2.87	1.49	1.42
19	A	814	CLA	C3B-C4B	2.87	1.49	1.42
19	1	310	CLA	C3B-C4B	2.87	1.49	1.42
19	A	836	CLA	C3B-C4B	2.87	1.49	1.42
19	1	309	CLA	C4D-ND	-2.87	1.33	1.37
19	B	819	CLA	C3B-C4B	2.87	1.49	1.42
19	5	305	CLA	C4D-ND	-2.86	1.33	1.37
19	A	813	CLA	C3B-C4B	2.86	1.49	1.42
19	B	822	CLA	C4D-ND	-2.86	1.33	1.37
19	4	608	CLA	C3B-C4B	2.86	1.49	1.42
19	Z	610	CLA	C4D-ND	-2.86	1.33	1.37
19	F	302	CLA	C3B-C4B	2.86	1.49	1.42
19	B	835	CLA	C3B-C4B	2.86	1.49	1.42
19	5	305	CLA	C3B-C4B	2.86	1.49	1.42
19	B	812	CLA	C3B-C4B	2.86	1.49	1.42
19	3	302	CLA	C3B-C4B	2.86	1.49	1.42
19	G	203	CLA	C4D-ND	-2.86	1.33	1.37
19	Z	608	CLA	C4D-ND	-2.86	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	6	320	CLA	C3B-C4B	2.85	1.49	1.42
19	A	840	CLA	C3B-C4B	2.85	1.49	1.42
19	1	314	CLA	C3B-C4B	2.85	1.49	1.42
19	4	611	CLA	C3B-C4B	2.85	1.49	1.42
19	4	614	CLA	C3B-C4B	2.85	1.49	1.42
19	7	610	CLA	C3B-C4B	2.85	1.49	1.42
19	1	314	CLA	C4D-ND	-2.85	1.33	1.37
19	B	811	CLA	C3B-C4B	2.85	1.49	1.42
19	Z	603	CLA	C3B-C4B	2.85	1.49	1.42
20	5	306	CHL	MG-NC	2.85	2.13	2.06
19	7	614	CLA	C3B-C4B	2.84	1.49	1.42
19	3	314	CLA	C1B-C2B	2.84	1.49	1.43
19	B	827	CLA	C3B-C4B	2.84	1.49	1.42
19	8	311	CLA	C3B-C4B	2.84	1.49	1.42
19	B	831	CLA	C3B-C4B	2.84	1.49	1.42
19	4	609	CLA	C4D-ND	-2.84	1.33	1.37
19	6	311	CLA	C4D-ND	-2.84	1.33	1.37
19	5	312	CLA	C3B-C4B	2.84	1.49	1.42
19	A	832	CLA	C3B-C4B	2.84	1.49	1.42
19	K	202	CLA	C3B-C4B	2.84	1.49	1.42
19	6	327	CLA	C3B-C4B	2.84	1.49	1.42
19	A	833	CLA	C3B-C4B	2.84	1.49	1.42
19	8	313	CLA	C3B-C4B	2.83	1.49	1.42
19	5	311	CLA	C4D-ND	-2.83	1.33	1.37
19	K	202	CLA	C4D-ND	-2.83	1.33	1.37
19	B	830	CLA	C3B-C4B	2.83	1.49	1.42
19	A	831	CLA	C3B-C4B	2.83	1.49	1.42
19	1	307	CLA	C3B-C4B	2.83	1.49	1.42
19	A	825	CLA	C3B-C4B	2.83	1.49	1.42
19	G	202	CLA	C4D-ND	-2.83	1.33	1.37
19	4	604	CLA	C3B-C4B	2.83	1.49	1.42
19	4	614	CLA	C4D-ND	-2.83	1.33	1.37
19	1	308	CLA	C3B-C4B	2.83	1.49	1.42
19	7	611	CLA	C3B-C4B	2.83	1.49	1.42
19	K	204	CLA	C3B-C4B	2.82	1.49	1.42
19	3	308	CLA	C4D-ND	-2.82	1.33	1.37
19	B	842	CLA	C3B-C4B	2.82	1.49	1.42
19	7	607	CLA	C3B-C4B	2.82	1.49	1.42
19	A	838	CLA	C3B-C4B	2.82	1.49	1.42
19	3	314	CLA	C3B-C4B	2.82	1.49	1.42
19	6	314	CLA	C3B-C4B	2.82	1.49	1.42
19	B	834	CLA	C3B-C4B	2.82	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	302	CLA	C1B-C2B	2.81	1.49	1.43
19	K	205	CLA	C4D-ND	-2.81	1.33	1.37
19	L	204	CLA	C4D-ND	-2.81	1.33	1.37
19	K	205	CLA	C1B-C2B	2.80	1.49	1.43
19	A	835	CLA	C3B-C4B	2.80	1.49	1.42
19	Z	612	CLA	C3B-C4B	2.80	1.49	1.42
19	A	818	CLA	C3B-C4B	2.79	1.49	1.42
19	B	817	CLA	C3B-C4B	2.79	1.49	1.42
19	A	819	CLA	C1B-C2B	2.79	1.49	1.43
19	B	810	CLA	C3B-C4B	2.79	1.49	1.42
19	B	814	CLA	C3B-C4B	2.79	1.49	1.42
19	6	305	CLA	C3B-C4B	2.78	1.49	1.42
19	A	841	CLA	C3B-C4B	2.78	1.49	1.42
19	B	816	CLA	C3B-C4B	2.78	1.49	1.42
19	5	316	CLA	C3B-C4B	2.78	1.49	1.42
19	B	808	CLA	C1B-C2B	2.78	1.49	1.43
19	B	801	CLA	C1B-C2B	2.78	1.49	1.43
19	G	203	CLA	C1B-C2B	2.78	1.49	1.43
19	1	308	CLA	C1B-C2B	2.77	1.49	1.43
19	7	607	CLA	C1B-C2B	2.77	1.49	1.43
19	8	311	CLA	C1B-C2B	2.77	1.49	1.43
19	B	838	CLA	C1B-C2B	2.77	1.49	1.43
19	4	614	CLA	C1B-C2B	2.77	1.49	1.43
19	A	813	CLA	C1B-C2B	2.77	1.49	1.43
19	B	839	CLA	C1B-C2B	2.76	1.49	1.43
19	K	205	CLA	C3B-C4B	2.76	1.49	1.42
19	1	311	CLA	C3B-C4B	2.76	1.49	1.42
19	1	312	CLA	C1B-C2B	2.76	1.49	1.43
19	1	314	CLA	C1B-C2B	2.75	1.49	1.43
19	1	312	CLA	C3B-C4B	2.75	1.49	1.42
19	L	204	CLA	C1B-C2B	2.75	1.49	1.43
19	7	614	CLA	C1B-C2B	2.75	1.49	1.43
19	7	613	CLA	C3B-C4B	2.75	1.49	1.42
19	B	803	CLA	C3B-C4B	2.75	1.49	1.42
19	A	806	CLA	C1B-C2B	2.75	1.49	1.43
19	A	814	CLA	C1B-C2B	2.75	1.49	1.43
19	3	313	CLA	C3B-C4B	2.75	1.49	1.42
19	F	303	CLA	C1B-C2B	2.75	1.49	1.43
19	B	842	CLA	C1B-C2B	2.75	1.49	1.43
19	A	846	CLA	C1B-C2B	2.74	1.49	1.43
19	A	844	CLA	C3B-C4B	2.74	1.49	1.42
19	A	815	CLA	C1B-C2B	2.74	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	313	CLA	C1B-C2B	2.74	1.49	1.43
19	B	814	CLA	C1B-C2B	2.74	1.49	1.43
19	B	828	CLA	C1B-C2B	2.74	1.49	1.43
19	Z	612	CLA	C1B-C2B	2.74	1.49	1.43
20	7	601	CHL	C1C-NC	2.74	1.41	1.37
19	4	608	CLA	C1B-C2B	2.73	1.49	1.43
19	A	831	CLA	C1B-C2B	2.73	1.49	1.43
19	5	312	CLA	C1B-C2B	2.73	1.49	1.43
19	A	817	CLA	C1B-C2B	2.73	1.49	1.43
19	B	806	CLA	C1B-C2B	2.73	1.49	1.43
19	6	314	CLA	C1B-C2B	2.73	1.49	1.43
19	6	320	CLA	C1B-C2B	2.73	1.49	1.43
19	A	818	CLA	C1B-C2B	2.73	1.49	1.43
19	1	304	CLA	C1B-C2B	2.73	1.49	1.43
19	8	307	CLA	C1B-C2B	2.72	1.49	1.43
19	A	842	CLA	C1B-C2B	2.72	1.49	1.43
19	8	304	CLA	C1B-C2B	2.72	1.49	1.43
19	7	611	CLA	C1B-C2B	2.72	1.49	1.43
19	6	303	CLA	C1B-C2B	2.72	1.49	1.43
19	Z	602	CLA	C1B-C2B	2.72	1.49	1.43
19	B	808	CLA	C3B-C4B	2.72	1.49	1.42
19	5	313	CLA	C3B-C4B	2.71	1.49	1.42
19	5	311	CLA	C1B-C2B	2.71	1.49	1.43
19	B	813	CLA	C1B-C2B	2.71	1.49	1.43
19	4	613	CLA	C1B-C2B	2.71	1.49	1.43
19	A	811	CLA	C1B-C2B	2.71	1.49	1.43
19	A	841	CLA	C1B-C2B	2.71	1.49	1.43
19	B	821	CLA	C1B-C2B	2.71	1.49	1.43
19	7	612	CLA	C1B-C2B	2.71	1.49	1.43
19	7	608	CLA	C1B-C2B	2.71	1.49	1.43
19	A	843	CLA	C1B-C2B	2.71	1.49	1.43
19	4	611	CLA	C1B-C2B	2.71	1.49	1.43
19	1	302	CLA	C1B-C2B	2.71	1.49	1.43
19	B	807	CLA	C1B-C2B	2.70	1.49	1.43
19	A	805	CLA	C1B-C2B	2.70	1.49	1.43
19	3	302	CLA	C1B-C2B	2.70	1.49	1.43
19	B	824	CLA	C1B-C2B	2.70	1.49	1.43
19	B	817	CLA	C1B-C2B	2.70	1.49	1.43
19	B	833	CLA	C1B-C2B	2.70	1.49	1.43
19	7	613	CLA	C1B-C2B	2.70	1.49	1.43
19	Z	603	CLA	C1B-C2B	2.70	1.49	1.43
19	6	309	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	8	314	CLA	C1B-C2B	2.69	1.49	1.43
19	7	604	CLA	C1B-C2B	2.69	1.49	1.43
19	3	313	CLA	C1B-C2B	2.69	1.49	1.43
19	5	302	CLA	C1B-C2B	2.69	1.49	1.43
19	A	830	CLA	C1B-C2B	2.69	1.49	1.43
19	7	602	CLA	C1B-C2B	2.69	1.49	1.43
19	B	841	CLA	C1B-C2B	2.69	1.49	1.43
19	5	303	CLA	C1B-C2B	2.69	1.49	1.43
20	4	606	CHL	C1C-NC	2.69	1.41	1.37
19	6	304	CLA	C1B-C2B	2.69	1.49	1.43
19	G	202	CLA	C1B-C2B	2.69	1.49	1.43
19	Z	607	CLA	C1B-C2B	2.69	1.49	1.43
19	1	311	CLA	C1B-C2B	2.69	1.49	1.43
19	B	835	CLA	C1B-C2B	2.69	1.49	1.43
19	A	828	CLA	C1B-C2B	2.69	1.49	1.43
19	A	834	CLA	C1B-C2B	2.69	1.49	1.43
19	A	810	CLA	C1B-C2B	2.69	1.49	1.43
19	B	834	CLA	C1B-C2B	2.69	1.49	1.43
19	3	311	CLA	C1B-C2B	2.69	1.49	1.43
19	A	832	CLA	C1B-C2B	2.69	1.49	1.43
19	A	816	CLA	C1B-C2B	2.69	1.49	1.43
19	8	309	CLA	C1B-C2B	2.68	1.49	1.43
19	3	307	CLA	C3B-C4B	2.68	1.49	1.42
19	3	304	CLA	C1B-C2B	2.68	1.49	1.43
19	F	304	CLA	C1B-C2B	2.68	1.49	1.43
19	3	310	CLA	C1B-C2B	2.68	1.49	1.43
19	A	833	CLA	C1B-C2B	2.68	1.49	1.43
19	A	835	CLA	C1B-C2B	2.68	1.49	1.43
19	A	827	CLA	C1B-C2B	2.68	1.49	1.43
19	A	825	CLA	C1B-C2B	2.68	1.49	1.43
19	B	812	CLA	C1B-C2B	2.68	1.49	1.43
19	A	838	CLA	C1B-C2B	2.68	1.49	1.43
19	K	202	CLA	C1B-C2B	2.68	1.49	1.43
19	6	327	CLA	C1B-C2B	2.68	1.49	1.43
19	8	312	CLA	C1B-C2B	2.68	1.49	1.43
19	5	305	CLA	C1B-C2B	2.68	1.49	1.43
19	7	609	CLA	C1B-C2B	2.68	1.49	1.43
19	7	610	CLA	C1B-C2B	2.67	1.49	1.43
19	B	831	CLA	C1B-C2B	2.67	1.49	1.43
19	A	822	CLA	C1B-C2B	2.67	1.49	1.43
19	B	822	CLA	C1B-C2B	2.67	1.49	1.43
19	B	816	CLA	C1B-C2B	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	807	CLA	C1B-C2B	2.67	1.49	1.43
19	Z	608	CLA	C1B-C2B	2.67	1.49	1.43
19	6	305	CLA	C1B-C2B	2.67	1.49	1.43
19	6	312	CLA	C1B-C2B	2.67	1.49	1.43
19	A	836	CLA	C1B-C2B	2.67	1.49	1.43
19	5	316	CLA	C1B-C2B	2.67	1.49	1.43
19	B	811	CLA	C1B-C2B	2.67	1.49	1.43
19	8	308	CLA	C1B-C2B	2.67	1.49	1.43
19	5	315	CLA	C1B-C2B	2.66	1.49	1.43
19	K	204	CLA	C1B-C2B	2.66	1.49	1.43
19	A	840	CLA	C1B-C2B	2.66	1.49	1.43
19	4	610	CLA	C1B-C2B	2.66	1.49	1.43
19	A	812	CLA	C1B-C2B	2.66	1.49	1.43
19	Z	613	CLA	C1B-C2B	2.66	1.49	1.43
19	4	602	CLA	C1B-C2B	2.66	1.49	1.43
19	B	836	CLA	C1B-C2B	2.66	1.49	1.43
19	B	825	CLA	C1B-C2B	2.66	1.49	1.43
19	1	307	CLA	C1B-C2B	2.66	1.49	1.43
19	A	844	CLA	C1B-C2B	2.65	1.49	1.43
19	A	809	CLA	C1B-C2B	2.65	1.49	1.43
19	B	809	CLA	C1B-C2B	2.65	1.49	1.43
19	4	604	CLA	C1B-C2B	2.65	1.49	1.43
19	B	823	CLA	C1B-C2B	2.65	1.49	1.43
19	3	309	CLA	C1B-C2B	2.65	1.49	1.43
19	B	810	CLA	C1B-C2B	2.65	1.49	1.43
19	1	310	CLA	C1B-C2B	2.64	1.49	1.43
19	Z	614	CLA	C1B-C2B	2.64	1.49	1.43
19	B	829	CLA	C1B-C2B	2.64	1.49	1.43
19	A	839	CLA	C1B-C2B	2.64	1.49	1.43
19	7	603	CLA	C1B-C2B	2.64	1.49	1.43
19	5	304	CLA	C1B-C2B	2.64	1.49	1.43
19	4	603	CLA	C1B-C2B	2.64	1.49	1.43
19	Z	611	CLA	C1B-C2B	2.63	1.49	1.43
19	5	314	CLA	C1B-C2B	2.63	1.49	1.43
19	3	312	CLA	C1B-C2B	2.63	1.49	1.43
19	6	311	CLA	C1B-C2B	2.63	1.49	1.43
19	8	303	CLA	C1B-C2B	2.63	1.49	1.43
19	B	830	CLA	C1B-C2B	2.63	1.49	1.43
20	7	605	CHL	MG-NC	2.63	2.12	2.06
19	1	313	CLA	C1B-C2B	2.63	1.49	1.43
19	A	826	CLA	C1B-C2B	2.63	1.49	1.43
19	1	308	CLA	C4D-ND	-2.63	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	832	CLA	C1B-C2B	2.63	1.49	1.43
19	A	804	CLA	C1B-C2B	2.63	1.49	1.43
19	A	824	CLA	C1B-C2B	2.62	1.49	1.43
19	4	609	CLA	C1B-C2B	2.62	1.49	1.43
19	A	820	CLA	C1B-C2B	2.62	1.49	1.43
19	A	829	CLA	C1B-C2B	2.62	1.49	1.43
19	K	203	CLA	C1B-C2B	2.62	1.49	1.43
19	B	818	CLA	C1B-C2B	2.62	1.49	1.43
19	B	837	CLA	C1B-C2B	2.62	1.49	1.43
19	5	309	CLA	C1B-C2B	2.62	1.49	1.43
19	1	303	CLA	C1B-C2B	2.62	1.49	1.43
20	5	307	CHL	C1C-NC	2.62	1.41	1.37
19	8	313	CLA	C1B-C2B	2.62	1.49	1.43
19	8	302	CLA	C1B-C2B	2.61	1.49	1.43
19	3	308	CLA	C1B-C2B	2.61	1.49	1.43
19	B	827	CLA	C1B-C2B	2.61	1.49	1.43
19	L	203	CLA	C1B-C2B	2.61	1.49	1.43
19	Z	610	CLA	C1B-C2B	2.60	1.49	1.43
19	5	319	CLA	C1B-C2B	2.60	1.49	1.43
19	3	303	CLA	C1B-C2B	2.59	1.49	1.43
19	A	803	CLA	C1B-C2B	2.59	1.49	1.43
19	8	310	CLA	C1B-C2B	2.59	1.49	1.43
19	B	826	CLA	C1B-C2B	2.59	1.49	1.43
19	6	316	CLA	C1B-C2B	2.59	1.49	1.43
19	1	309	CLA	C1B-C2B	2.59	1.49	1.43
19	3	307	CLA	C1B-C2B	2.59	1.49	1.43
19	Z	604	CLA	C1B-C2B	2.59	1.49	1.43
20	6	317	CHL	MG-NC	2.58	2.12	2.06
19	3	301	CLA	C1B-C2B	2.58	1.49	1.43
19	6	313	CLA	C1B-C2B	2.58	1.49	1.43
19	Z	609	CLA	C1B-C2B	2.58	1.49	1.43
20	6	302	CHL	C1C-NC	2.58	1.41	1.37
19	3	305	CLA	C1B-C2B	2.57	1.49	1.43
19	J	102	CLA	C1B-C2B	2.57	1.49	1.43
19	A	808	CLA	C1B-C2B	2.57	1.49	1.43
20	5	317	CHL	MG-NC	2.57	2.12	2.06
19	4	612	CLA	C1B-C2B	2.55	1.49	1.43
19	5	310	CLA	C1B-C2B	2.55	1.49	1.43
19	B	804	CLA	C1B-C2B	2.55	1.49	1.43
19	B	815	CLA	C1B-C2B	2.54	1.49	1.43
19	6	310	CLA	C1B-C2B	2.54	1.49	1.43
19	A	837	CLA	C1B-C2B	2.53	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	840	CLA	C1B-C2B	2.52	1.49	1.43
19	B	820	CLA	C1B-C2B	2.52	1.49	1.43
19	A	823	CLA	C1B-C2B	2.51	1.49	1.43
25	6	322	XAT	O4-C5	-2.51	1.42	1.46
19	B	805	CLA	C1B-C2B	2.50	1.49	1.43
19	B	819	CLA	C1B-C2B	2.50	1.49	1.43
20	Z	601	CHL	C1D-C2D	-2.49	1.40	1.45
25	8	316	XAT	O24-C25	-2.49	1.42	1.46
25	7	616	XAT	O24-C25	-2.48	1.42	1.46
20	7	606	CHL	C1C-NC	2.48	1.41	1.37
25	5	322	XAT	O4-C5	-2.48	1.42	1.46
19	A	821	CLA	C1B-C2B	2.48	1.49	1.43
20	8	306	CHL	C1C-NC	2.46	1.41	1.37
25	8	316	XAT	O4-C5	-2.46	1.42	1.46
25	1	316	XAT	O24-C25	-2.45	1.42	1.46
20	Z	605	CHL	C1D-C2D	-2.45	1.40	1.45
25	Z	616	XAT	O24-C25	-2.44	1.42	1.46
25	6	322	XAT	O24-C25	-2.44	1.42	1.46
19	B	805	CLA	CHC-C1C	2.44	1.43	1.38
25	4	617	XAT	O24-C25	-2.43	1.42	1.46
25	4	617	XAT	O4-C5	-2.43	1.42	1.46
25	7	616	XAT	O4-C5	-2.42	1.42	1.46
25	Z	616	XAT	O4-C5	-2.42	1.42	1.46
25	5	322	XAT	O24-C25	-2.41	1.42	1.46
20	7	601	CHL	MG-NC	2.39	2.11	2.06
20	8	305	CHL	C1C-NC	2.38	1.41	1.37
20	4	615	CHL	C1C-NC	2.38	1.41	1.37
20	6	307	CHL	C1C-NC	2.37	1.41	1.37
25	1	316	XAT	O4-C5	-2.36	1.42	1.46
20	4	605	CHL	C1D-C2D	-2.36	1.40	1.45
19	B	820	CLA	CHC-C1C	2.36	1.43	1.38
19	5	303	CLA	CHC-C1C	2.36	1.43	1.38
20	6	308	CHL	MG-NA	2.36	2.11	2.06
19	5	310	CLA	CHC-C1C	2.35	1.43	1.38
19	6	310	CLA	CHC-C1C	2.35	1.43	1.38
20	Z	601	CHL	C1C-NC	2.35	1.41	1.37
19	B	813	CLA	CHC-C1C	2.35	1.43	1.38
19	A	825	CLA	CMD-C2D	-2.35	1.45	1.50
19	4	602	CLA	CHC-C1C	2.35	1.43	1.38
19	A	820	CLA	CHC-C1C	2.34	1.43	1.38
19	B	840	CLA	CHC-C1C	2.34	1.43	1.38
19	A	821	CLA	CHC-C1C	2.34	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	307	CHL	C1D-C2D	-2.33	1.40	1.45
20	7	605	CHL	C1C-NC	2.33	1.41	1.37
19	A	830	CLA	CHC-C1C	2.32	1.43	1.38
20	6	315	CHL	C1D-C2D	-2.31	1.40	1.45
19	3	301	CLA	CHC-C1C	2.31	1.43	1.38
19	A	837	CLA	CHC-C1C	2.31	1.43	1.38
19	5	309	CLA	CHC-C1C	2.31	1.43	1.38
19	1	313	CLA	CHC-C1C	2.30	1.43	1.38
19	A	806	CLA	CHC-C1C	2.30	1.43	1.38
20	4	601	CHL	C1D-C2D	-2.30	1.40	1.45
19	4	609	CLA	CHC-C1C	2.30	1.43	1.38
20	5	317	CHL	C1C-NC	2.30	1.41	1.37
19	B	815	CLA	CHC-C1C	2.30	1.43	1.38
19	3	312	CLA	CHC-C1C	2.30	1.43	1.38
19	B	806	CLA	CHC-C1C	2.30	1.43	1.38
19	B	824	CLA	CHC-C1C	2.29	1.43	1.38
19	A	823	CLA	CHC-C1C	2.29	1.43	1.38
20	1	305	CHL	C1C-NC	2.29	1.41	1.37
20	Z	605	CHL	C1C-NC	2.29	1.41	1.37
19	6	312	CLA	CHC-C1C	2.29	1.43	1.38
19	7	602	CLA	CHC-C1C	2.29	1.43	1.38
19	L	204	CLA	CHC-C1C	2.29	1.43	1.38
19	6	311	CLA	CHC-C1C	2.29	1.43	1.38
20	7	606	CHL	MG-NC	2.29	2.11	2.06
19	8	310	CLA	CHC-C1C	2.29	1.43	1.38
19	Z	604	CLA	CHC-C1C	2.29	1.43	1.38
20	6	306	CHL	C1C-NC	2.28	1.41	1.37
19	8	302	CLA	CHC-C1C	2.28	1.43	1.38
19	3	304	CLA	CHC-C1C	2.27	1.43	1.38
19	A	824	CLA	CHC-C1C	2.27	1.43	1.38
19	B	826	CLA	CHC-C1C	2.27	1.43	1.38
19	A	829	CLA	CHC-C1C	2.27	1.43	1.38
19	A	833	CLA	CMD-C2D	-2.27	1.46	1.50
19	A	812	CLA	CHC-C1C	2.27	1.43	1.38
19	Z	613	CLA	CHC-C1C	2.27	1.43	1.38
19	1	303	CLA	CHC-C1C	2.27	1.43	1.38
19	A	828	CLA	CHC-C1C	2.27	1.43	1.38
19	1	302	CLA	CHC-C1C	2.27	1.43	1.38
19	A	816	CLA	CHC-C1C	2.27	1.43	1.38
19	Z	607	CLA	CHC-C1C	2.26	1.43	1.38
19	1	309	CLA	CHC-C1C	2.26	1.43	1.38
19	B	835	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	302	CLA	CHC-C1C	2.26	1.43	1.38
19	Z	602	CLA	CHC-C1C	2.26	1.43	1.38
19	A	809	CLA	CHC-C1C	2.25	1.43	1.38
19	B	833	CLA	CHC-C1C	2.25	1.43	1.38
19	L	203	CLA	CHC-C1C	2.25	1.43	1.38
19	7	609	CLA	CHC-C1C	2.25	1.43	1.38
19	5	314	CLA	CHC-C1C	2.25	1.43	1.38
19	B	807	CLA	CHC-C1C	2.25	1.43	1.38
19	7	610	CLA	CHC-C1C	2.25	1.43	1.38
19	4	610	CLA	CHC-C1C	2.25	1.43	1.38
19	8	313	CLA	CHC-C1C	2.25	1.43	1.38
19	B	818	CLA	CHC-C1C	2.25	1.43	1.38
19	B	836	CLA	CHC-C1C	2.25	1.43	1.38
19	1	310	CLA	CHC-C1C	2.25	1.43	1.38
19	6	313	CLA	CHC-C1C	2.24	1.43	1.38
19	4	613	CLA	CHC-C1C	2.24	1.43	1.38
19	6	309	CLA	CHC-C1C	2.24	1.43	1.38
20	4	606	CHL	MG-NC	2.24	2.11	2.06
19	A	815	CLA	CHC-C1C	2.24	1.43	1.38
19	B	838	CLA	CHC-C1C	2.24	1.43	1.38
19	4	612	CLA	CHC-C1C	2.24	1.43	1.38
19	8	309	CLA	CHC-C1C	2.24	1.43	1.38
20	6	302	CHL	MG-NC	2.24	2.11	2.06
19	Z	609	CLA	CHC-C1C	2.24	1.43	1.38
19	8	314	CLA	CHC-C1C	2.24	1.43	1.38
19	J	102	CLA	CHC-C1C	2.24	1.43	1.38
19	8	312	CLA	CHC-C1C	2.24	1.43	1.38
19	8	308	CLA	CHC-C1C	2.24	1.43	1.38
19	6	316	CLA	CHC-C1C	2.23	1.43	1.38
19	Z	608	CLA	CHC-C1C	2.23	1.43	1.38
20	1	306	CHL	C1D-C2D	-2.23	1.40	1.45
19	B	825	CLA	CHC-C1C	2.23	1.43	1.38
19	F	302	CLA	CHC-C1C	2.23	1.43	1.38
19	F	303	CLA	CHC-C1C	2.23	1.43	1.38
19	B	812	CLA	CHC-C1C	2.23	1.43	1.38
19	Z	610	CLA	CHC-C1C	2.23	1.43	1.38
19	3	310	CLA	CHC-C1C	2.23	1.43	1.38
19	6	304	CLA	CHC-C1C	2.23	1.43	1.38
19	B	819	CLA	CHC-C1C	2.23	1.43	1.38
19	5	304	CLA	CHC-C1C	2.22	1.43	1.38
19	A	808	CLA	CHC-C1C	2.22	1.43	1.38
19	J	102	CLA	CMD-C2D	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	611	CLA	CHC-C1C	2.22	1.43	1.38
19	8	304	CLA	CHC-C1C	2.22	1.43	1.38
19	6	303	CLA	CHC-C1C	2.22	1.43	1.38
19	A	846	CLA	CHC-C1C	2.22	1.43	1.38
19	A	843	CLA	CHC-C1C	2.21	1.43	1.38
19	A	811	CLA	CHC-C1C	2.21	1.43	1.38
19	Z	614	CLA	CHC-C1C	2.21	1.43	1.38
19	K	203	CLA	CHC-C1C	2.21	1.43	1.38
19	1	304	CLA	CHC-C1C	2.21	1.43	1.38
19	G	202	CLA	CHC-C1C	2.21	1.43	1.38
19	7	603	CLA	CHC-C1C	2.21	1.43	1.38
19	B	830	CLA	CMB-C2B	-2.21	1.46	1.50
19	A	844	CLA	MG-NB	-2.21	2.01	2.05
20	6	302	CHL	C1D-C2D	-2.20	1.41	1.45
19	B	828	CLA	CHC-C1C	2.20	1.43	1.38
19	B	824	CLA	CMC-C2C	-2.20	1.46	1.50
19	3	309	CLA	CHC-C1C	2.20	1.43	1.38
19	3	314	CLA	CMD-C2D	-2.20	1.46	1.50
20	6	317	CHL	C1D-C2D	-2.20	1.41	1.45
19	3	308	CLA	CHC-C1C	2.20	1.43	1.38
19	5	305	CLA	CHC-C1C	2.20	1.43	1.38
19	Z	603	CLA	CHC-C1C	2.20	1.43	1.38
19	3	303	CLA	CHC-C1C	2.20	1.43	1.38
19	4	608	CLA	CHC-C1C	2.20	1.43	1.38
19	B	804	CLA	CHC-C1C	2.20	1.43	1.38
19	B	814	CLA	CHC-C1C	2.20	1.43	1.38
19	B	832	CLA	CHC-C1C	2.20	1.43	1.38
19	B	837	CLA	CHC-C1C	2.20	1.43	1.38
19	B	821	CLA	CHC-C1C	2.20	1.43	1.38
19	B	818	CLA	CMC-C2C	-2.20	1.46	1.50
20	5	308	CHL	C1D-C2D	-2.19	1.41	1.45
19	B	823	CLA	CHC-C1C	2.19	1.43	1.38
19	A	826	CLA	CHC-C1C	2.19	1.43	1.38
19	6	320	CLA	CHC-C1C	2.19	1.43	1.38
19	3	311	CLA	CHC-C1C	2.19	1.43	1.38
19	A	803	CLA	CHC-C1C	2.19	1.43	1.38
19	G	203	CLA	CHC-C1C	2.19	1.43	1.38
20	5	306	CHL	C1C-NC	2.19	1.41	1.37
19	A	817	CLA	CHC-C1C	2.19	1.43	1.38
20	6	306	CHL	C1D-C2D	-2.18	1.41	1.45
19	A	835	CLA	CHC-C1C	2.18	1.43	1.38
19	B	810	CLA	CMB-C2B	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	311	CLA	CHC-C1C	2.18	1.43	1.38
19	6	314	CLA	CHC-C1C	2.18	1.43	1.38
19	A	834	CLA	CHC-C1C	2.18	1.43	1.38
19	7	614	CLA	CHC-C1C	2.18	1.43	1.38
19	4	611	CLA	CHC-C1C	2.18	1.43	1.38
19	5	319	CLA	CHC-C1C	2.18	1.43	1.38
19	B	811	CLA	CHC-C1C	2.18	1.42	1.38
20	4	615	CHL	C1D-C2D	-2.18	1.41	1.45
19	B	827	CLA	CHC-C1C	2.18	1.42	1.38
19	1	308	CLA	CHC-C1C	2.18	1.42	1.38
19	F	304	CLA	CHC-C1C	2.18	1.42	1.38
19	6	327	CLA	CHC-C1C	2.18	1.42	1.38
19	4	614	CLA	CHC-C1C	2.17	1.42	1.38
19	B	822	CLA	CHC-C1C	2.17	1.42	1.38
20	6	307	CHL	C1D-C2D	-2.17	1.41	1.45
19	B	830	CLA	CMD-C2D	-2.17	1.46	1.50
19	7	608	CLA	CHC-C1C	2.17	1.42	1.38
19	7	612	CLA	CHC-C1C	2.17	1.42	1.38
19	B	842	CLA	CHC-C1C	2.17	1.42	1.38
19	1	307	CLA	CHC-C1C	2.17	1.42	1.38
19	A	825	CLA	CHC-C1C	2.16	1.42	1.38
19	A	831	CLA	CHC-C1C	2.16	1.42	1.38
19	A	836	CLA	CHC-C1C	2.16	1.42	1.38
19	B	801	CLA	CHC-C1C	2.16	1.42	1.38
19	A	827	CLA	CHC-C1C	2.16	1.42	1.38
19	4	603	CLA	CMD-C2D	-2.16	1.46	1.50
19	7	613	CLA	CHC-C1C	2.16	1.42	1.38
19	B	829	CLA	CHC-C1C	2.16	1.42	1.38
19	A	814	CLA	CHC-C1C	2.16	1.42	1.38
19	A	819	CLA	CHC-C1C	2.16	1.42	1.38
19	A	804	CLA	CHC-C1C	2.15	1.42	1.38
28	A	802	CL0	MG-NA	2.15	2.11	2.06
19	A	805	CLA	CHC-C1C	2.15	1.42	1.38
19	B	837	CLA	MG-NB	-2.15	2.01	2.05
19	1	311	CLA	CHC-C1C	2.15	1.42	1.38
19	B	803	CLA	CHC-C1C	2.15	1.42	1.38
19	4	604	CLA	CHC-C1C	2.15	1.42	1.38
19	7	604	CLA	CHC-C1C	2.15	1.42	1.38
19	A	812	CLA	CMC-C2C	-2.15	1.46	1.50
19	B	808	CLA	CHC-C1C	2.15	1.42	1.38
19	B	809	CLA	CHC-C1C	2.15	1.42	1.38
20	4	606	CHL	C1D-C2D	-2.15	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	813	CLA	CHC-C1C	2.15	1.42	1.38
19	A	833	CLA	CHC-C1C	2.15	1.42	1.38
19	B	839	CLA	CHC-C1C	2.14	1.42	1.38
19	A	818	CLA	CHC-C1C	2.14	1.42	1.38
19	B	817	CLA	CHC-C1C	2.14	1.42	1.38
19	A	841	CLA	CHC-C1C	2.14	1.42	1.38
19	B	831	CLA	CHC-C1C	2.14	1.42	1.38
19	A	839	CLA	CHC-C1C	2.14	1.42	1.38
20	8	320	CHL	C1D-C2D	-2.14	1.41	1.45
19	7	613	CLA	MG-NB	-2.14	2.01	2.05
19	A	842	CLA	CHC-C1C	2.14	1.42	1.38
20	5	317	CHL	C1D-C2D	-2.14	1.41	1.45
19	8	303	CLA	CHC-C1C	2.14	1.42	1.38
19	K	204	CLA	CHC-C1C	2.14	1.42	1.38
19	B	823	CLA	CMD-C2D	-2.14	1.46	1.50
19	1	314	CLA	CHC-C1C	2.14	1.42	1.38
19	A	840	CLA	CHC-C1C	2.13	1.42	1.38
19	A	838	CLA	CHC-C1C	2.13	1.42	1.38
19	A	844	CLA	CMB-C2B	-2.13	1.46	1.50
19	B	827	CLA	MG-NB	-2.13	2.01	2.05
20	Z	606	CHL	MG-NC	2.13	2.11	2.06
19	K	202	CLA	CHC-C1C	2.13	1.42	1.38
19	B	820	CLA	CMB-C2B	-2.13	1.46	1.50
19	8	307	CLA	CHC-C1C	2.13	1.42	1.38
19	1	312	CLA	CHC-C1C	2.13	1.42	1.38
20	7	621	CHL	C1D-C2D	-2.12	1.41	1.45
19	B	809	CLA	CMD-C2D	-2.12	1.46	1.50
19	A	844	CLA	CHC-C1C	2.12	1.42	1.38
19	A	822	CLA	CHC-C1C	2.12	1.42	1.38
19	3	307	CLA	MG-NB	-2.12	2.01	2.05
19	B	830	CLA	CHC-C1C	2.12	1.42	1.38
19	B	804	CLA	CMC-C2C	-2.12	1.46	1.50
19	7	611	CLA	CHC-C1C	2.12	1.42	1.38
19	K	205	CLA	CHC-C1C	2.12	1.42	1.38
19	B	825	CLA	CMD-C2D	-2.12	1.46	1.50
19	A	807	CLA	CHC-C1C	2.12	1.42	1.38
19	A	810	CLA	CHC-C1C	2.12	1.42	1.38
19	6	305	CLA	CHC-C1C	2.12	1.42	1.38
19	8	313	CLA	MG-NB	-2.12	2.01	2.05
19	5	312	CLA	CHC-C1C	2.11	1.42	1.38
20	1	305	CHL	C1D-C2D	-2.11	1.41	1.45
19	1	311	CLA	MG-NB	-2.11	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	305	CLA	CHC-C1C	2.11	1.42	1.38
19	A	816	CLA	MG-NB	-2.11	2.01	2.05
19	B	817	CLA	MG-NB	-2.11	2.01	2.05
20	Z	601	CHL	MG-NC	2.11	2.11	2.06
19	5	315	CLA	CHC-C1C	2.11	1.42	1.38
19	B	840	CLA	CMD-C2D	-2.10	1.46	1.50
19	B	842	CLA	MG-NB	-2.10	2.01	2.05
19	3	301	CLA	CMD-C2D	-2.09	1.46	1.50
19	A	814	CLA	CMD-C2D	-2.09	1.46	1.50
19	Z	612	CLA	CHC-C1C	2.09	1.42	1.38
20	7	605	CHL	C1D-C2D	-2.09	1.41	1.45
19	4	611	CLA	MG-NB	-2.09	2.01	2.05
19	A	832	CLA	CMB-C2B	-2.09	1.46	1.50
19	4	609	CLA	CMD-C2D	-2.09	1.46	1.50
19	8	303	CLA	MG-NB	-2.09	2.01	2.05
19	F	304	CLA	CMD-C2D	-2.09	1.46	1.50
20	7	601	CHL	C1D-C2D	-2.09	1.41	1.45
19	A	843	CLA	MG-NB	-2.09	2.01	2.05
19	B	807	CLA	MG-NB	-2.09	2.01	2.05
19	A	835	CLA	CMD-C2D	-2.08	1.46	1.50
19	A	818	CLA	MG-NB	-2.08	2.01	2.05
19	B	810	CLA	MG-NB	-2.08	2.01	2.05
19	B	810	CLA	CHC-C1C	2.08	1.42	1.38
19	A	805	CLA	CMD-C2D	-2.08	1.46	1.50
19	3	302	CLA	CHC-C1C	2.08	1.42	1.38
19	B	819	CLA	MG-NB	-2.08	2.01	2.05
19	K	203	CLA	MG-NB	-2.08	2.01	2.05
19	K	204	CLA	MG-NB	-2.08	2.01	2.05
19	A	820	CLA	CMD-C2D	-2.08	1.46	1.50
19	3	313	CLA	CHC-C1C	2.08	1.42	1.38
19	A	832	CLA	CHC-C1C	2.08	1.42	1.38
19	4	604	CLA	MG-NB	-2.08	2.01	2.05
19	K	202	CLA	CMD-C2D	-2.08	1.46	1.50
19	J	102	CLA	MG-NB	-2.08	2.01	2.05
19	Z	614	CLA	CMD-C2D	-2.08	1.46	1.50
19	A	809	CLA	MG-NB	-2.08	2.01	2.05
19	B	816	CLA	CHC-C1C	2.07	1.42	1.38
19	B	831	CLA	MG-NB	-2.07	2.01	2.05
20	8	305	CHL	C1D-C2D	-2.07	1.41	1.45
19	8	311	CLA	CHC-C1C	2.07	1.42	1.38
19	A	839	CLA	MG-NB	-2.07	2.01	2.05
20	3	306	CHL	C1D-C2D	-2.07	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	827	CLA	CMC-C2C	-2.07	1.46	1.50
19	7	609	CLA	CMD-C2D	-2.07	1.46	1.50
19	A	830	CLA	CMD-C2D	-2.07	1.46	1.50
19	A	835	CLA	CMB-C2B	-2.07	1.46	1.50
20	4	605	CHL	C1C-NC	2.07	1.40	1.37
19	B	801	CLA	CMD-C2D	-2.07	1.46	1.50
19	5	309	CLA	CMD-C2D	-2.07	1.46	1.50
19	B	835	CLA	CMD-C2D	-2.07	1.46	1.50
19	A	821	CLA	MG-NB	-2.07	2.01	2.05
19	6	305	CLA	MG-NB	-2.07	2.01	2.05
19	B	801	CLA	MG-NB	-2.07	2.01	2.05
19	6	305	CLA	CMB-C2B	-2.07	1.46	1.50
19	4	612	CLA	CMB-C2B	-2.07	1.46	1.50
19	3	302	CLA	MG-NB	-2.07	2.01	2.05
19	4	603	CLA	CHC-C1C	2.07	1.42	1.38
19	8	303	CLA	CMD-C2D	-2.07	1.46	1.50
19	5	305	CLA	CMB-C2B	-2.06	1.46	1.50
19	B	816	CLA	CMD-C2D	-2.06	1.46	1.50
19	B	841	CLA	CHC-C1C	2.06	1.42	1.38
19	5	314	CLA	MG-NB	-2.06	2.01	2.05
19	5	316	CLA	MG-NB	-2.06	2.01	2.05
19	B	814	CLA	MG-NB	-2.06	2.01	2.05
19	B	835	CLA	MG-NB	-2.06	2.01	2.05
19	A	841	CLA	MG-NB	-2.06	2.01	2.05
19	K	202	CLA	MG-NB	-2.06	2.01	2.05
19	3	310	CLA	MG-NB	-2.06	2.01	2.05
19	6	316	CLA	MG-NB	-2.06	2.01	2.05
19	1	313	CLA	MG-NB	-2.06	2.01	2.05
19	B	834	CLA	CHC-C1C	2.06	1.42	1.38
19	B	823	CLA	MG-NB	-2.06	2.01	2.05
19	B	804	CLA	CMD-C2D	-2.06	1.46	1.50
19	5	316	CLA	CHC-C1C	2.06	1.42	1.38
19	Z	604	CLA	CMD-C2D	-2.06	1.46	1.50
19	A	829	CLA	MG-NB	-2.06	2.01	2.05
20	8	305	CHL	MG-NC	2.05	2.11	2.06
19	4	613	CLA	MG-NB	-2.05	2.01	2.05
19	Z	609	CLA	MG-NB	-2.05	2.01	2.05
19	B	829	CLA	CMD-C2D	-2.05	1.46	1.50
19	F	303	CLA	CMD-C2D	-2.05	1.46	1.50
19	A	825	CLA	MG-NB	-2.05	2.01	2.05
19	6	314	CLA	CMD-C2D	-2.05	1.46	1.50
19	B	811	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	302	CLA	CMD-C2D	-2.05	1.46	1.50
19	A	821	CLA	CMD-C2D	-2.05	1.46	1.50
19	5	313	CLA	CMD-C2D	-2.05	1.46	1.50
19	5	305	CLA	MG-NB	-2.05	2.01	2.05
19	A	809	CLA	CMD-C2D	-2.05	1.46	1.50
19	B	819	CLA	CMB-C2B	-2.05	1.46	1.50
19	A	823	CLA	MG-NB	-2.05	2.01	2.05
19	1	307	CLA	MG-NB	-2.05	2.01	2.05
19	6	310	CLA	MG-NB	-2.05	2.01	2.05
19	6	305	CLA	CMD-C2D	-2.05	1.46	1.50
19	8	308	CLA	CMD-C2D	-2.05	1.46	1.50
19	B	831	CLA	CMD-C2D	-2.05	1.46	1.50
19	5	313	CLA	CHC-C1C	2.05	1.42	1.38
19	8	312	CLA	CMB-C2B	-2.05	1.46	1.50
19	A	819	CLA	CMC-C2C	-2.05	1.46	1.50
19	B	826	CLA	CMD-C2D	-2.05	1.46	1.50
19	3	303	CLA	MG-NB	-2.05	2.01	2.05
19	Z	603	CLA	MG-NB	-2.05	2.01	2.05
19	A	822	CLA	CMD-C2D	-2.05	1.46	1.50
19	7	603	CLA	CMD-C2D	-2.05	1.46	1.50
19	B	806	CLA	CMD-C2D	-2.05	1.46	1.50
20	Z	606	CHL	C1D-C2D	-2.05	1.41	1.45
19	Z	607	CLA	CMD-C2D	-2.05	1.46	1.50
19	4	604	CLA	CMB-C2B	-2.05	1.46	1.50
19	B	804	CLA	CMB-C2B	-2.05	1.46	1.50
19	7	611	CLA	CMD-C2D	-2.04	1.46	1.50
19	8	313	CLA	CMD-C2D	-2.04	1.46	1.50
19	A	840	CLA	CMD-C2D	-2.04	1.46	1.50
19	6	316	CLA	CMD-C2D	-2.04	1.46	1.50
19	8	310	CLA	MG-NB	-2.04	2.01	2.05
19	B	811	CLA	MG-NB	-2.04	2.01	2.05
19	A	837	CLA	CMB-C2B	-2.04	1.46	1.50
19	A	804	CLA	MG-NB	-2.04	2.01	2.05
19	7	608	CLA	CMD-C2D	-2.04	1.46	1.50
19	B	815	CLA	CMD-C2D	-2.04	1.46	1.50
19	6	312	CLA	MG-NB	-2.04	2.01	2.05
19	6	314	CLA	MG-NB	-2.04	2.01	2.05
19	3	307	CLA	CHC-C1C	2.04	1.42	1.38
19	K	204	CLA	CMC-C2C	-2.04	1.46	1.50
19	A	813	CLA	CMD-C2D	-2.04	1.46	1.50
19	A	846	CLA	CMD-C2D	-2.04	1.46	1.50
19	A	831	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	310	CLA	CMD-C2D	-2.04	1.46	1.50
19	A	807	CLA	CMC-C2C	-2.04	1.46	1.50
19	B	819	CLA	CMD-C2D	-2.04	1.46	1.50
19	5	316	CLA	CMB-C2B	-2.04	1.46	1.50
19	3	309	CLA	MG-NB	-2.04	2.01	2.05
19	A	840	CLA	MG-NB	-2.04	2.01	2.05
19	B	838	CLA	CMD-C2D	-2.04	1.46	1.50
19	1	304	CLA	CMD-C2D	-2.04	1.46	1.50
19	Z	607	CLA	MG-NB	-2.04	2.01	2.05
19	B	803	CLA	CMD-C2D	-2.04	1.46	1.50
19	L	203	CLA	CMD-C2D	-2.04	1.46	1.50
19	L	203	CLA	MG-NB	-2.04	2.01	2.05
19	7	602	CLA	MG-NB	-2.04	2.01	2.05
19	A	838	CLA	MG-NB	-2.04	2.01	2.05
19	6	312	CLA	CMD-C2D	-2.04	1.46	1.50
19	5	312	CLA	MG-NB	-2.04	2.01	2.05
19	8	304	CLA	MG-NB	-2.04	2.01	2.05
19	6	313	CLA	CMD-C2D	-2.03	1.46	1.50
19	Z	603	CLA	CMD-C2D	-2.03	1.46	1.50
19	Z	604	CLA	MG-NB	-2.03	2.01	2.05
19	B	813	CLA	CMD-C2D	-2.03	1.46	1.50
19	B	816	CLA	MG-NB	-2.03	2.01	2.05
19	3	305	CLA	CMB-C2B	-2.03	1.46	1.50
19	7	604	CLA	CMD-C2D	-2.03	1.46	1.50
19	A	808	CLA	CMD-C2D	-2.03	1.46	1.50
19	3	307	CLA	CMB-C2B	-2.03	1.46	1.50
19	A	835	CLA	MG-NB	-2.03	2.01	2.05
19	B	821	CLA	MG-NB	-2.03	2.01	2.05
19	G	202	CLA	MG-NB	-2.03	2.01	2.05
19	A	826	CLA	CMD-C2D	-2.03	1.46	1.50
19	A	815	CLA	CMD-C2D	-2.03	1.46	1.50
19	3	314	CLA	CHC-C1C	2.03	1.42	1.38
19	5	310	CLA	CMD-C2D	-2.03	1.46	1.50
19	A	824	CLA	CMD-C2D	-2.03	1.46	1.50
19	8	307	CLA	MG-NB	-2.03	2.01	2.05
19	K	205	CLA	MG-NB	-2.03	2.01	2.05
19	Z	602	CLA	CMD-C2D	-2.03	1.46	1.50
19	1	311	CLA	CMD-C2D	-2.03	1.46	1.50
20	5	306	CHL	C1D-C2D	-2.03	1.41	1.45
19	5	304	CLA	MG-NB	-2.03	2.01	2.05
20	7	606	CHL	C1D-C2D	-2.03	1.41	1.45
19	A	837	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	7	614	CLA	CMD-C2D	-2.03	1.46	1.50
19	7	607	CLA	CHC-C1C	2.03	1.42	1.38
19	F	304	CLA	MG-NB	-2.03	2.01	2.05
19	A	827	CLA	CMD-C2D	-2.03	1.46	1.50
19	6	311	CLA	MG-NB	-2.03	2.01	2.05
19	A	827	CLA	MG-NB	-2.03	2.01	2.05
19	A	836	CLA	MG-NB	-2.02	2.01	2.05
19	5	303	CLA	MG-NB	-2.02	2.01	2.05
19	B	832	CLA	MG-NB	-2.02	2.01	2.05
19	7	613	CLA	CMD-C2D	-2.02	1.46	1.50
19	A	821	CLA	CMB-C2B	-2.02	1.46	1.50
19	A	829	CLA	CMB-C2B	-2.02	1.46	1.50
19	Z	610	CLA	MG-NB	-2.02	2.01	2.05
19	A	805	CLA	MG-NB	-2.02	2.01	2.05
19	A	810	CLA	CMD-C2D	-2.02	1.46	1.50
19	Z	611	CLA	CMD-C2D	-2.02	1.46	1.50
19	Z	614	CLA	MG-NB	-2.02	2.01	2.05
19	B	808	CLA	MG-NB	-2.02	2.01	2.05
19	K	205	CLA	CMB-C2B	-2.02	1.46	1.50
19	6	327	CLA	CMD-C2D	-2.02	1.46	1.50
19	3	314	CLA	CMC-C2C	-2.02	1.46	1.50
19	Z	612	CLA	CMD-C2D	-2.02	1.46	1.50
19	B	812	CLA	MG-NB	-2.02	2.01	2.05
19	B	824	CLA	CMD-C2D	-2.02	1.46	1.50
19	4	602	CLA	MG-NB	-2.02	2.01	2.05
19	A	842	CLA	MG-NB	-2.02	2.01	2.05
19	4	613	CLA	CMD-C2D	-2.02	1.46	1.50
19	5	315	CLA	CMD-C2D	-2.02	1.46	1.50
19	A	808	CLA	CMB-C2B	-2.02	1.46	1.50
19	5	304	CLA	CMD-C2D	-2.02	1.46	1.50
19	Z	607	CLA	CMB-C2B	-2.02	1.46	1.50
19	A	832	CLA	CMD-C2D	-2.02	1.46	1.50
19	B	837	CLA	CMD-C2D	-2.02	1.46	1.50
19	7	614	CLA	MG-NB	-2.02	2.01	2.05
19	B	840	CLA	CMB-C2B	-2.01	1.46	1.50
19	A	823	CLA	CMD-C2D	-2.01	1.46	1.50
19	B	828	CLA	CMD-C2D	-2.01	1.46	1.50
19	5	313	CLA	MG-NB	-2.01	2.01	2.05
19	4	612	CLA	MG-NB	-2.01	2.01	2.05
19	6	313	CLA	MG-NB	-2.01	2.01	2.05
19	7	604	CLA	MG-NB	-2.01	2.01	2.05
19	7	610	CLA	MG-NB	-2.01	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	8	312	CLA	CMD-C2D	-2.01	1.46	1.50
19	8	314	CLA	CMD-C2D	-2.01	1.46	1.50
19	1	307	CLA	CMB-C2B	-2.01	1.46	1.50
19	3	312	CLA	MG-NB	-2.01	2.01	2.05
19	K	204	CLA	CMD-C2D	-2.01	1.46	1.50
19	F	302	CLA	MG-NB	-2.01	2.01	2.05
19	1	313	CLA	CMD-C2D	-2.01	1.46	1.50
19	5	316	CLA	CMD-C2D	-2.01	1.46	1.50
19	A	804	CLA	CMD-C2D	-2.01	1.46	1.50
19	B	839	CLA	CMD-C2D	-2.01	1.46	1.50
19	1	310	CLA	CMD-C2D	-2.01	1.46	1.50
19	1	304	CLA	MG-NB	-2.01	2.01	2.05
19	A	812	CLA	CMD-C2D	-2.01	1.46	1.50
19	A	811	CLA	CMD-C2D	-2.01	1.46	1.50
19	3	313	CLA	MG-NB	-2.01	2.01	2.05
19	A	843	CLA	CMD-C2D	-2.01	1.46	1.50
19	B	841	CLA	CMD-C2D	-2.01	1.46	1.50
19	5	302	CLA	MG-NB	-2.01	2.01	2.05
19	6	327	CLA	MG-NB	-2.01	2.01	2.05
19	B	832	CLA	CMD-C2D	-2.01	1.46	1.50
19	6	320	CLA	MG-NB	-2.01	2.01	2.05
19	Z	613	CLA	MG-NB	-2.01	2.01	2.05
19	1	302	CLA	MG-NB	-2.01	2.01	2.05
19	A	836	CLA	CMD-C2D	-2.01	1.46	1.50
19	B	841	CLA	CMB-C2B	-2.01	1.46	1.50
19	A	818	CLA	CMB-C2B	-2.01	1.46	1.50
19	B	837	CLA	CMB-C2B	-2.01	1.46	1.50
19	3	308	CLA	CMD-C2D	-2.01	1.46	1.50
19	B	809	CLA	CMB-C2B	-2.00	1.46	1.50
19	B	822	CLA	CMD-C2D	-2.00	1.46	1.50
19	B	842	CLA	CMD-C2D	-2.00	1.46	1.50
19	3	303	CLA	CMB-C2B	-2.00	1.46	1.50
19	4	603	CLA	CMB-C2B	-2.00	1.46	1.50
19	B	818	CLA	CMD-C2D	-2.00	1.46	1.50
19	B	836	CLA	CMB-C2B	-2.00	1.46	1.50
19	1	311	CLA	CMB-C2B	-2.00	1.46	1.50
19	5	305	CLA	CMD-C2D	-2.00	1.46	1.50
19	7	609	CLA	MG-NB	-2.00	2.01	2.05
19	B	834	CLA	CMD-C2D	-2.00	1.46	1.50
19	Z	608	CLA	CMD-C2D	-2.00	1.46	1.50
19	7	611	CLA	MG-NB	-2.00	2.01	2.05
19	B	838	CLA	MG-NB	-2.00	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	823	CLA	CMB-C2B	-2.00	1.46	1.50
19	1	307	CLA	CMD-C2D	-2.00	1.46	1.50
19	A	828	CLA	CMD-C2D	-2.00	1.46	1.50
19	K	205	CLA	CMD-C2D	-2.00	1.46	1.50
19	7	612	CLA	CMB-C2B	-2.00	1.46	1.50
19	A	807	CLA	MG-NB	-2.00	2.01	2.05
19	6	310	CLA	CMD-C2D	-2.00	1.46	1.50
19	3	304	CLA	MG-NB	-2.00	2.01	2.05

All (1489) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	601	CHL	C4A-NA-C1A	8.19	110.39	106.71
19	K	202	CLA	C4A-NA-C1A	7.38	110.02	106.71
19	B	841	CLA	C4A-NA-C1A	7.37	110.02	106.71
20	6	317	CHL	C4A-NA-C1A	7.35	110.01	106.71
20	7	621	CHL	C4A-NA-C1A	7.33	110.00	106.71
20	6	315	CHL	C4A-NA-C1A	7.26	109.97	106.71
19	B	839	CLA	C4A-NA-C1A	7.22	109.95	106.71
19	7	607	CLA	C4A-NA-C1A	7.20	109.94	106.71
19	3	302	CLA	C4A-NA-C1A	7.17	109.93	106.71
19	A	810	CLA	C4A-NA-C1A	7.15	109.92	106.71
20	4	615	CHL	C4A-NA-C1A	7.15	109.92	106.71
19	B	803	CLA	C4A-NA-C1A	7.13	109.91	106.71
19	K	205	CLA	C4A-NA-C1A	7.11	109.90	106.71
19	4	608	CLA	C4A-NA-C1A	7.10	109.90	106.71
19	A	819	CLA	C4A-NA-C1A	7.09	109.89	106.71
19	A	841	CLA	C4A-NA-C1A	7.08	109.89	106.71
20	Z	606	CHL	C4A-NA-C1A	7.07	109.88	106.71
20	8	306	CHL	C4A-NA-C1A	7.02	109.86	106.71
19	A	833	CLA	C4A-NA-C1A	6.99	109.85	106.71
19	B	810	CLA	C4A-NA-C1A	6.99	109.85	106.71
19	B	808	CLA	C4A-NA-C1A	6.98	109.84	106.71
20	8	320	CHL	C4A-NA-C1A	6.97	109.84	106.71
19	B	838	CLA	C4A-NA-C1A	6.95	109.83	106.71
19	5	319	CLA	C4A-NA-C1A	6.94	109.83	106.71
19	B	831	CLA	C4A-NA-C1A	6.94	109.83	106.71
19	8	311	CLA	C4A-NA-C1A	6.93	109.82	106.71
19	8	307	CLA	C4A-NA-C1A	6.92	109.82	106.71
19	B	806	CLA	C4A-NA-C1A	6.92	109.82	106.71
19	A	834	CLA	C4A-NA-C1A	6.92	109.81	106.71
19	3	313	CLA	C4A-NA-C1A	6.91	109.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	809	CLA	C4A-NA-C1A	6.91	109.81	106.71
19	A	805	CLA	C4A-NA-C1A	6.90	109.81	106.71
19	5	313	CLA	C4A-NA-C1A	6.90	109.81	106.71
19	1	314	CLA	C4A-NA-C1A	6.89	109.80	106.71
19	G	203	CLA	C4A-NA-C1A	6.89	109.80	106.71
19	8	308	CLA	C4A-NA-C1A	6.88	109.80	106.71
19	A	827	CLA	C4A-NA-C1A	6.87	109.80	106.71
19	A	824	CLA	C4A-NA-C1A	6.85	109.79	106.71
19	Z	612	CLA	C4A-NA-C1A	6.85	109.79	106.71
19	B	835	CLA	C4A-NA-C1A	6.83	109.78	106.71
20	6	302	CHL	C4A-NA-C1A	6.83	109.78	106.71
19	F	303	CLA	C4A-NA-C1A	6.82	109.77	106.71
19	A	830	CLA	C4A-NA-C1A	6.82	109.77	106.71
19	B	842	CLA	C4A-NA-C1A	6.81	109.77	106.71
19	A	817	CLA	C4A-NA-C1A	6.79	109.76	106.71
19	A	806	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	1	308	CLA	C4A-NA-C1A	6.77	109.75	106.71
19	7	608	CLA	C4A-NA-C1A	6.76	109.75	106.71
19	A	846	CLA	C4A-NA-C1A	6.75	109.74	106.71
27	6	323	NEX	C5-C6-C1	6.75	126.39	119.70
19	6	327	CLA	C4A-NA-C1A	6.73	109.73	106.71
19	B	836	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	B	825	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	B	833	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	4	611	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	7	611	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	B	816	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	1	307	CLA	C4A-NA-C1A	6.69	109.72	106.71
19	1	311	CLA	C4A-NA-C1A	6.69	109.71	106.71
19	A	818	CLA	C4A-NA-C1A	6.68	109.71	106.71
19	5	311	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	1	304	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	6	312	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	7	612	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	L	203	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	A	844	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	3	301	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	5	302	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	5	309	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	5	315	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	4	614	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	A	843	CLA	C4A-NA-C1A	6.62	109.68	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	611	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	1	312	CLA	C4A-NA-C1A	6.61	109.68	106.71
20	5	317	CHL	C4A-NA-C1A	6.61	109.68	106.71
19	7	614	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	A	811	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	5	305	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	J	102	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	B	817	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	B	801	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	7	604	CLA	C4A-NA-C1A	6.58	109.67	106.71
19	L	204	CLA	C4A-NA-C1A	6.58	109.67	106.71
19	1	303	CLA	C4A-NA-C1A	6.58	109.66	106.71
19	A	832	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	B	834	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	3	304	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	4	603	CLA	C4A-NA-C1A	6.56	109.66	106.71
19	B	821	CLA	C4A-NA-C1A	6.56	109.66	106.71
19	B	822	CLA	C4A-NA-C1A	6.56	109.66	106.71
19	A	842	CLA	C4A-NA-C1A	6.56	109.65	106.71
19	B	811	CLA	C4A-NA-C1A	6.56	109.65	106.71
19	5	310	CLA	C4A-NA-C1A	6.56	109.65	106.71
19	3	311	CLA	C4A-NA-C1A	6.55	109.65	106.71
19	A	835	CLA	C4A-NA-C1A	6.55	109.65	106.71
19	K	204	CLA	C4A-NA-C1A	6.54	109.64	106.71
19	Z	608	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	A	838	CLA	C4A-NA-C1A	6.52	109.64	106.71
20	7	605	CHL	C4A-NA-C1A	6.52	109.64	106.71
19	A	807	CLA	C4A-NA-C1A	6.51	109.64	106.71
19	5	312	CLA	C4A-NA-C1A	6.51	109.63	106.71
19	4	613	CLA	C4A-NA-C1A	6.51	109.63	106.71
19	G	202	CLA	C4A-NA-C1A	6.51	109.63	106.71
19	Z	613	CLA	C4A-NA-C1A	6.50	109.63	106.71
19	4	602	CLA	C4A-NA-C1A	6.50	109.63	106.71
19	7	609	CLA	C4A-NA-C1A	6.50	109.63	106.71
19	4	609	CLA	C4A-NA-C1A	6.49	109.63	106.71
19	4	610	CLA	C4A-NA-C1A	6.49	109.62	106.71
19	6	303	CLA	C4A-NA-C1A	6.49	109.62	106.71
19	A	808	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	6	304	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	8	303	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	8	309	CLA	C4A-NA-C1A	6.47	109.62	106.71
19	B	823	CLA	C4A-NA-C1A	6.47	109.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	602	CLA	C4A-NA-C1A	6.47	109.61	106.71
19	6	305	CLA	C4A-NA-C1A	6.47	109.61	106.71
19	7	613	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	A	829	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	F	302	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	8	302	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	3	303	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	7	610	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	A	839	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	4	612	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	7	603	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	3	307	CLA	C4A-NA-C1A	6.44	109.60	106.71
19	Z	607	CLA	C4A-NA-C1A	6.44	109.60	106.71
19	3	309	CLA	C4A-NA-C1A	6.43	109.60	106.71
19	8	304	CLA	C4A-NA-C1A	6.43	109.60	106.71
19	B	832	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	B	804	CLA	C4A-NA-C1A	6.41	109.59	106.71
19	4	604	CLA	C4A-NA-C1A	6.41	109.59	106.71
19	A	814	CLA	C4A-NA-C1A	6.41	109.59	106.71
19	A	825	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	A	831	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	A	837	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	Z	609	CLA	C4A-NA-C1A	6.39	109.58	106.71
19	6	309	CLA	C4A-NA-C1A	6.39	109.58	106.71
19	A	816	CLA	C4A-NA-C1A	6.38	109.58	106.71
19	A	840	CLA	C4A-NA-C1A	6.38	109.58	106.71
27	5	323	NEX	C5-C6-C1	6.37	126.02	119.70
19	5	314	CLA	C4A-NA-C1A	6.37	109.57	106.71
19	B	828	CLA	C4A-NA-C1A	6.37	109.57	106.71
20	3	306	CHL	C4A-NA-C1A	6.37	109.57	106.71
19	B	807	CLA	C4A-NA-C1A	6.37	109.57	106.71
19	A	828	CLA	C4A-NA-C1A	6.36	109.57	106.71
19	3	308	CLA	C4A-NA-C1A	6.36	109.56	106.71
19	B	814	CLA	C4A-NA-C1A	6.36	109.56	106.71
19	Z	603	CLA	C4A-NA-C1A	6.36	109.56	106.71
19	5	303	CLA	C4A-NA-C1A	6.35	109.56	106.71
19	Z	614	CLA	C4A-NA-C1A	6.35	109.56	106.71
20	7	606	CHL	C4A-NA-C1A	6.35	109.56	106.71
19	8	314	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	3	305	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	7	602	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	Z	604	CLA	C4A-NA-C1A	6.33	109.55	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	813	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	A	815	CLA	C4A-NA-C1A	6.31	109.54	106.71
19	A	826	CLA	C4A-NA-C1A	6.31	109.54	106.71
19	B	805	CLA	C4A-NA-C1A	6.31	109.54	106.71
19	B	827	CLA	C4A-NA-C1A	6.31	109.54	106.71
20	5	308	CHL	C4A-NA-C1A	6.30	109.54	106.71
19	B	830	CLA	C4A-NA-C1A	6.28	109.53	106.71
19	1	309	CLA	C4A-NA-C1A	6.28	109.53	106.71
19	B	815	CLA	C4A-NA-C1A	6.27	109.53	106.71
19	6	314	CLA	C4A-NA-C1A	6.27	109.53	106.71
20	8	305	CHL	C4A-NA-C1A	6.26	109.52	106.71
19	6	320	CLA	C4A-NA-C1A	6.26	109.52	106.71
19	6	316	CLA	C4A-NA-C1A	6.26	109.52	106.71
19	1	310	CLA	C4A-NA-C1A	6.25	109.52	106.71
19	A	809	CLA	C4A-NA-C1A	6.24	109.51	106.71
20	5	307	CHL	C4A-NA-C1A	6.23	109.51	106.71
19	8	312	CLA	C4A-NA-C1A	6.22	109.50	106.71
19	5	316	CLA	C4A-NA-C1A	6.22	109.50	106.71
19	A	812	CLA	C4A-NA-C1A	6.22	109.50	106.71
19	Z	610	CLA	C4A-NA-C1A	6.21	109.50	106.71
19	6	313	CLA	C4A-NA-C1A	6.21	109.50	106.71
19	6	311	CLA	C4A-NA-C1A	6.20	109.50	106.71
19	B	824	CLA	C4A-NA-C1A	6.18	109.49	106.71
28	A	802	CL0	C4A-NA-C1A	6.18	109.48	106.71
19	1	302	CLA	C4A-NA-C1A	6.17	109.48	106.71
19	1	313	CLA	C4A-NA-C1A	6.15	109.47	106.71
19	3	310	CLA	C4A-NA-C1A	6.14	109.47	106.71
19	B	818	CLA	C4A-NA-C1A	6.14	109.47	106.71
19	3	312	CLA	C4A-NA-C1A	6.13	109.46	106.71
20	1	306	CHL	C4A-NA-C1A	6.13	109.46	106.71
19	8	310	CLA	C4A-NA-C1A	6.12	109.46	106.71
19	B	812	CLA	C4A-NA-C1A	6.11	109.45	106.71
19	5	304	CLA	C4A-NA-C1A	6.10	109.45	106.71
20	4	601	CHL	C4A-NA-C1A	6.10	109.45	106.71
19	F	304	CLA	C4A-NA-C1A	6.07	109.44	106.71
19	A	822	CLA	C4A-NA-C1A	6.07	109.44	106.71
19	A	820	CLA	C4A-NA-C1A	6.07	109.43	106.71
19	A	823	CLA	C4A-NA-C1A	6.07	109.43	106.71
19	6	310	CLA	C4A-NA-C1A	6.06	109.43	106.71
19	A	804	CLA	C4A-NA-C1A	6.05	109.43	106.71
19	A	836	CLA	C4A-NA-C1A	6.02	109.41	106.71
19	B	829	CLA	C4A-NA-C1A	6.01	109.41	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	605	CHL	C4A-NA-C1A	6.01	109.41	106.71
19	B	837	CLA	C4A-NA-C1A	5.97	109.39	106.71
19	A	813	CLA	C4A-NA-C1A	5.97	109.39	106.71
20	4	605	CHL	C4A-NA-C1A	5.96	109.39	106.71
19	K	203	CLA	C4A-NA-C1A	5.96	109.39	106.71
19	B	840	CLA	C4A-NA-C1A	5.96	109.38	106.71
20	5	306	CHL	C4A-NA-C1A	5.96	109.38	106.71
19	8	313	CLA	C4A-NA-C1A	5.95	109.38	106.71
19	B	819	CLA	C4A-NA-C1A	5.94	109.38	106.71
19	B	820	CLA	C4A-NA-C1A	5.93	109.37	106.71
19	B	826	CLA	C4A-NA-C1A	5.85	109.33	106.71
20	7	601	CHL	C4A-NA-C1A	5.83	109.33	106.71
20	1	305	CHL	C4A-NA-C1A	5.82	109.32	106.71
19	A	803	CLA	C4A-NA-C1A	5.79	109.31	106.71
19	A	821	CLA	C4A-NA-C1A	5.77	109.30	106.71
19	3	314	CLA	C4A-NA-C1A	5.77	109.30	106.71
20	4	606	CHL	C4A-NA-C1A	5.63	109.24	106.71
20	4	607	CHL	C4A-NA-C1A	5.54	109.20	106.71
20	6	307	CHL	C4A-NA-C1A	5.34	109.11	106.71
20	5	317	CHL	C1D-ND-C4D	-5.07	102.73	106.33
20	6	306	CHL	C4A-NA-C1A	5.06	108.98	106.71
20	6	317	CHL	C1D-ND-C4D	-5.04	102.76	106.33
20	5	306	CHL	C1D-ND-C4D	-4.85	102.89	106.33
20	8	306	CHL	C1D-ND-C4D	-4.65	103.03	106.33
20	6	308	CHL	C4A-NA-C1A	4.60	108.77	106.71
20	Z	605	CHL	C1D-ND-C4D	-4.31	103.27	106.33
20	7	605	CHL	C1D-ND-C4D	-4.19	103.36	106.33
19	3	313	CLA	CAA-C2A-C3A	-4.16	101.39	112.78
24	1	301	LMU	C1B-O5B-C5B	4.05	121.64	113.69
27	5	323	NEX	O24-C25-C24	-3.98	110.39	113.38
19	4	612	CLA	CAA-C2A-C3A	-3.97	101.89	112.78
20	Z	606	CHL	C1D-ND-C4D	-3.88	103.58	106.33
27	6	323	NEX	C2-C1-C6	3.75	112.86	109.21
20	1	306	CHL	C1D-ND-C4D	-3.70	103.70	106.33
20	6	317	CHL	CHC-C4B-NB	-3.57	120.48	124.26
20	4	615	CHL	C1D-ND-C4D	-3.56	103.80	106.33
20	4	606	CHL	C1D-ND-C4D	-3.53	103.83	106.33
19	A	836	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
19	3	309	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
27	5	323	NEX	C2-C1-C6	3.33	112.45	109.21
19	A	832	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
20	4	601	CHL	C1D-ND-C4D	-3.31	103.98	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	805	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
19	B	825	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
19	A	820	CLA	C3B-C4B-NB	-3.22	107.53	110.52
24	A	855	LMU	C1'-O5'-C5'	3.21	119.99	113.69
19	A	818	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
19	B	805	CLA	C3B-C4B-NB	-3.20	107.54	110.52
20	6	302	CHL	C1D-ND-C4D	-3.17	104.08	106.33
20	8	305	CHL	C1D-ND-C4D	-3.17	104.08	106.33
19	A	827	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
19	B	834	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
19	4	612	CLA	O2A-CGA-O1A	-3.13	115.69	123.59
19	B	839	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
19	5	311	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
19	8	310	CLA	C3B-C4B-NB	-3.09	107.64	110.52
19	K	203	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
19	B	840	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
19	B	809	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
19	7	613	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
19	B	819	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
19	A	844	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
19	B	821	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
24	3	324	LMU	C1'-O5'-C5'	3.07	119.71	113.69
19	3	305	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
19	L	203	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
19	1	313	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
19	B	838	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
19	6	313	CLA	C3B-C4B-NB	-3.05	107.69	110.52
19	B	816	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
19	Z	610	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
19	7	608	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
19	6	320	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
19	3	313	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
19	1	310	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
19	B	805	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
19	A	817	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
19	8	313	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
19	5	304	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
19	B	808	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
19	1	314	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
19	A	808	CLA	C3B-C4B-NB	-3.02	107.72	110.52
19	5	303	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
19	A	814	CLA	O2D-CGD-O1D	-3.02	117.94	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	830	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
19	B	815	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
19	A	821	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
19	A	828	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
19	A	834	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
19	A	840	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
19	B	840	CLA	C3B-C4B-NB	-3.00	107.73	110.52
19	Z	604	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
19	A	824	CLA	C3B-C4B-NB	-3.00	107.73	110.52
19	6	313	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
19	K	205	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	4	611	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	6	309	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
19	A	829	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
19	B	822	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
19	7	603	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
19	A	809	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
19	A	839	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
19	B	807	CLA	C3B-C4B-NB	-2.97	107.76	110.52
19	B	817	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
19	1	304	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
19	4	613	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
19	6	305	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
27	6	323	NEX	O24-C25-C24	-2.95	111.17	113.38
19	A	843	CLA	C3B-C4B-NB	-2.95	107.78	110.52
19	B	812	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
19	6	311	CLA	C3B-C4B-NB	-2.94	107.79	110.52
19	B	818	CLA	C3B-C4B-NB	-2.94	107.79	110.52
19	B	806	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
19	Z	602	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
19	A	820	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
19	3	303	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
19	B	813	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
19	7	604	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
19	6	311	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
19	5	305	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
19	Z	603	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
20	7	606	CHL	C1D-ND-C4D	-2.92	104.26	106.33
19	8	310	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
19	8	304	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
19	B	820	CLA	C3B-C4B-NB	-2.92	107.81	110.52
19	5	303	CLA	C3B-C4B-NB	-2.92	107.81	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	833	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
19	3	312	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
19	A	838	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
19	K	204	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
19	A	837	CLA	C3B-C4B-NB	-2.91	107.81	110.52
19	A	813	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
19	6	304	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
19	Z	611	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
19	Z	613	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
19	4	610	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	5	319	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
19	4	614	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
19	G	202	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
19	B	835	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
19	7	602	CLA	C3B-C4B-NB	-2.89	107.83	110.52
19	7	602	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
19	5	314	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
19	1	308	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
19	4	612	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
19	4	604	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	A	837	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	B	842	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
20	7	621	CHL	C1D-ND-C4D	-2.88	104.29	106.33
19	8	312	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	B	832	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	1	307	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	1	311	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	4	608	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
19	A	829	CLA	C3B-C4B-NB	-2.87	107.85	110.52
19	4	609	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
19	A	828	CLA	C3B-C4B-NB	-2.87	107.85	110.52
19	5	302	CLA	C3B-C4B-NB	-2.87	107.85	110.52
20	6	307	CHL	CHD-C4C-C3C	-2.87	120.63	124.84
19	K	202	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
19	F	304	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
19	B	827	CLA	C3B-C4B-NB	-2.86	107.86	110.52
19	B	827	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
19	3	310	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
19	5	310	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
19	5	309	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
26	6	325	LHG	C5-O7-C7	2.85	124.82	117.79
19	4	602	CLA	O2D-CGD-O1D	-2.85	118.27	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	820	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
19	B	826	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	A	826	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	5	319	CLA	C2A-C1A-CHA	2.84	128.83	123.86
19	L	204	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
19	3	301	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
19	5	302	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
19	Z	608	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
19	B	829	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
19	B	836	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
19	B	818	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
20	5	308	CHL	C1D-ND-C4D	-2.83	104.32	106.33
20	1	305	CHL	C1D-ND-C4D	-2.83	104.33	106.33
19	5	319	CLA	CHB-C4A-NA	2.83	128.42	124.51
19	6	312	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
19	A	819	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
19	A	808	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
19	Z	614	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
20	Z	606	CHL	CHC-C4B-NB	-2.82	121.27	124.26
19	7	611	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
19	5	316	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	7	610	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	G	203	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	B	831	CLA	C3B-C4B-NB	-2.82	107.90	110.52
19	Z	608	CLA	C3B-C4B-NB	-2.82	107.90	110.52
19	B	823	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	4	610	CLA	C3B-C4B-NB	-2.81	107.91	110.52
19	1	302	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
19	K	202	CLA	CHB-C4A-NA	2.81	128.40	124.51
19	3	304	CLA	C3B-C4B-NB	-2.81	107.91	110.52
19	8	314	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
19	1	303	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
19	Z	612	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
19	K	202	CLA	C3B-C4B-NB	-2.80	107.91	110.52
19	6	316	CLA	C3B-C4B-NB	-2.80	107.91	110.52
19	7	612	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	3	307	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	B	801	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
20	7	601	CHL	C1D-ND-C4D	-2.80	104.35	106.33
19	A	807	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
19	3	314	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	Z	609	CLA	O2D-CGD-O1D	-2.79	118.38	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	614	CLA	C3B-C4B-NB	-2.79	107.93	110.52
19	A	816	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
19	A	826	CLA	C3B-C4B-NB	-2.79	107.93	110.52
19	7	610	CLA	C3B-C4B-NB	-2.78	107.94	110.52
19	K	203	CLA	CAA-C2A-C3A	-2.78	105.17	112.78
19	3	307	CLA	C3B-C4B-NB	-2.78	107.94	110.52
19	Z	607	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
19	8	302	CLA	C3B-C4B-NB	-2.77	107.94	110.52
19	A	810	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	1	309	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	B	812	CLA	C3B-C4B-NB	-2.77	107.94	110.52
20	6	308	CHL	CHC-C4B-NB	-2.77	121.32	124.26
31	B	850	DGD	C2G-O2G-C1B	2.77	124.61	117.79
19	8	308	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	3	312	CLA	C3B-C4B-NB	-2.77	107.95	110.52
19	7	614	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
19	7	612	CLA	C3B-C4B-NB	-2.77	107.95	110.52
19	Z	604	CLA	C3B-C4B-NB	-2.77	107.95	110.52
19	A	822	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
19	6	310	CLA	C3B-C4B-NB	-2.76	107.95	110.52
19	3	308	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
19	Z	614	CLA	C3B-C4B-NB	-2.76	107.95	110.52
20	4	615	CHL	C3B-C4B-NB	-2.76	107.95	110.52
19	8	311	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
19	A	806	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
19	A	804	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
19	K	203	CLA	C3B-C4B-NB	-2.76	107.95	110.52
19	1	313	CLA	C3B-C4B-NB	-2.76	107.95	110.52
19	A	809	CLA	C1-C2-C3	-2.76	122.29	126.75
19	Z	607	CLA	C3B-C4B-NB	-2.76	107.96	110.52
19	B	815	CLA	C3B-C4B-NB	-2.76	107.96	110.52
19	1	310	CLA	C3B-C4B-NB	-2.76	107.96	110.52
19	5	313	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
19	3	309	CLA	C3B-C4B-NB	-2.76	107.96	110.52
19	B	831	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
24	3	324	LMU	C1B-O5B-C5B	2.75	119.09	113.69
19	3	311	CLA	C3B-C4B-NB	-2.75	107.96	110.52
19	4	612	CLA	C3B-C4B-NB	-2.75	107.97	110.52
19	A	842	CLA	C3B-C4B-NB	-2.74	107.97	110.52
19	8	303	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
19	F	302	CLA	C3B-C4B-NB	-2.74	107.97	110.52
19	3	304	CLA	O2D-CGD-O1D	-2.74	118.48	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	314	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
19	A	822	CLA	C3B-C4B-NB	-2.74	107.98	110.52
19	A	841	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
19	L	203	CLA	C3B-C4B-NB	-2.73	107.98	110.52
19	3	305	CLA	C3B-C4B-NB	-2.73	107.98	110.52
19	4	603	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
19	A	835	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
19	6	303	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
19	7	613	CLA	C3B-C4B-NB	-2.73	107.98	110.52
19	A	825	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
19	A	809	CLA	C3B-C4B-NB	-2.73	107.98	110.52
19	8	302	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
19	A	842	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
19	A	823	CLA	C3B-C4B-NB	-2.73	107.98	110.52
19	B	824	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
19	B	814	CLA	C3B-C4B-NB	-2.73	107.99	110.52
19	A	816	CLA	C3B-C4B-NB	-2.72	107.99	110.52
19	5	315	CLA	C3B-C4B-NB	-2.72	107.99	110.52
19	8	312	CLA	C3B-C4B-NB	-2.72	107.99	110.52
19	A	823	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
19	B	806	CLA	C3B-C4B-NB	-2.72	107.99	110.52
19	B	811	CLA	C3B-C4B-NB	-2.72	107.99	110.52
19	A	843	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
19	1	307	CLA	C3B-C4B-NB	-2.72	108.00	110.52
19	B	841	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
19	J	102	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
19	A	812	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
19	B	803	CLA	C3B-C4B-NB	-2.71	108.00	110.52
19	5	312	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
19	B	837	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
19	8	309	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
20	5	317	CHL	C1D-CHD-C4C	-2.71	120.22	126.06
19	7	607	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
19	5	304	CLA	C1-C2-C3	-2.70	122.38	126.75
19	7	609	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
19	B	811	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
19	A	846	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
19	5	314	CLA	C3B-C4B-NB	-2.70	108.01	110.52
19	6	310	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
19	A	821	CLA	C3B-C4B-NB	-2.69	108.02	110.52
19	B	809	CLA	C3B-C4B-NB	-2.69	108.02	110.52
19	B	822	CLA	C3B-C4B-NB	-2.69	108.02	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	611	CLA	C3B-C4B-NB	-2.69	108.02	110.52
19	A	833	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
19	B	835	CLA	C3B-C4B-NB	-2.69	108.02	110.52
19	A	835	CLA	C1-C2-C3	-2.68	121.40	126.04
19	6	316	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
19	B	828	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
19	3	301	CLA	C3B-C4B-NB	-2.68	108.03	110.52
19	7	609	CLA	C3B-C4B-NB	-2.68	108.03	110.52
19	B	803	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
19	3	313	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	A	844	CLA	C3B-C4B-NB	-2.68	108.03	110.52
19	A	810	CLA	CHB-C4A-NA	2.68	128.21	124.51
19	A	807	CLA	C3B-C4B-NB	-2.67	108.04	110.52
19	A	835	CLA	C3B-C4B-NB	-2.67	108.04	110.52
20	5	308	CHL	CHC-C4B-NB	-2.66	121.44	124.26
19	8	308	CLA	C3B-C4B-NB	-2.66	108.04	110.52
19	B	825	CLA	C3B-C4B-NB	-2.66	108.05	110.52
19	1	302	CLA	C3B-C4B-NB	-2.65	108.05	110.52
19	6	327	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
19	A	837	CLA	CHB-C4A-NA	2.65	128.17	124.51
19	8	304	CLA	C3B-C4B-NB	-2.65	108.06	110.52
19	8	307	CLA	C3B-C4B-NB	-2.65	108.06	110.52
28	A	802	CL0	C3B-C4B-NB	-2.65	108.06	110.52
19	4	609	CLA	C3B-C4B-NB	-2.64	108.06	110.52
19	5	309	CLA	C3B-C4B-NB	-2.64	108.07	110.52
19	5	315	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
19	A	824	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
19	A	831	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
19	3	311	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
20	4	615	CHL	CHB-C1B-NB	-2.63	121.47	124.26
19	F	303	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
19	8	309	CLA	C3B-C4B-NB	-2.63	108.08	110.52
19	1	312	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
19	7	611	CLA	CHB-C4A-NA	2.63	128.15	124.51
19	B	819	CLA	C3B-C4B-NB	-2.63	108.08	110.52
19	4	612	CLA	CHB-C4A-NA	2.62	128.14	124.51
19	4	602	CLA	C3B-C4B-NB	-2.62	108.08	110.52
19	J	102	CLA	C3B-C4B-NB	-2.62	108.08	110.52
19	G	202	CLA	C3B-C4B-NB	-2.62	108.08	110.52
19	B	826	CLA	C3B-C4B-NB	-2.62	108.08	110.52
19	8	314	CLA	C3B-C4B-NB	-2.62	108.08	110.52
24	A	855	LMU	C3'-C4'-C5'	-2.62	104.92	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	317	CHL	CHB-C1B-NB	-2.62	121.49	124.26
19	B	810	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	A	806	CLA	C3B-C4B-NB	-2.61	108.09	110.52
19	A	812	CLA	C3B-C4B-NB	-2.61	108.09	110.52
19	4	614	CLA	C3B-C4B-NB	-2.61	108.09	110.52
19	7	608	CLA	CHB-C4A-NA	2.60	128.11	124.51
19	1	314	CLA	C3B-C4B-NB	-2.60	108.10	110.52
20	Z	606	CHL	CHB-C1B-NB	-2.60	121.51	124.26
20	5	307	CHL	C3B-C4B-NB	-2.60	108.11	110.52
19	8	307	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
20	Z	601	CHL	CHD-C4C-C3C	-2.60	121.02	124.84
19	6	309	CLA	C3B-C4B-NB	-2.60	108.11	110.52
19	B	813	CLA	C3B-C4B-NB	-2.60	108.11	110.52
19	6	303	CLA	C3B-C4B-NB	-2.59	108.11	110.52
19	B	804	CLA	C3B-C4B-NB	-2.59	108.11	110.52
19	Z	607	CLA	C1-C2-C3	-2.59	122.56	126.75
19	5	309	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	A	834	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	8	311	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	6	305	CLA	C3B-C4B-NB	-2.58	108.12	110.52
20	Z	605	CHL	CHD-C4C-C3C	-2.58	121.04	124.84
19	B	820	CLA	CHB-C1B-NB	2.58	126.99	124.26
31	B	850	DGD	C6D-O5D-C1E	2.58	118.78	113.74
19	A	803	CLA	C3B-C4B-NB	-2.58	108.12	110.52
19	5	313	CLA	CHB-C4A-NA	2.58	128.08	124.51
19	K	204	CLA	C3B-C4B-NB	-2.58	108.13	110.52
19	B	821	CLA	C3B-C4B-NB	-2.57	108.13	110.52
19	1	308	CLA	C3B-C4B-NB	-2.57	108.13	110.52
20	7	606	CHL	C3B-C4B-NB	-2.57	108.13	110.52
19	3	314	CLA	CHD-C1D-ND	-2.57	122.09	124.45
19	5	310	CLA	C3B-C4B-NB	-2.57	108.13	110.52
19	Z	609	CLA	C3B-C4B-NB	-2.57	108.14	110.52
20	6	308	CHL	CHA-C4D-ND	-2.57	127.13	132.50
19	4	608	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	3	308	CLA	C3B-C4B-NB	-2.56	108.14	110.52
19	3	302	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
19	6	314	CLA	C3B-C4B-NB	-2.56	108.14	110.52
19	B	841	CLA	C3B-C4B-NB	-2.56	108.14	110.52
19	1	307	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	Z	601	CHL	C3B-C4B-NB	-2.55	108.15	110.52
19	3	303	CLA	C3B-C4B-NB	-2.55	108.15	110.52
19	A	817	CLA	CHB-C4A-NA	2.55	128.04	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	319	CLA	C3B-C4B-NB	-2.55	108.15	110.52
19	8	313	CLA	C3B-C4B-NB	-2.55	108.15	110.52
19	B	835	CLA	CHB-C4A-NA	2.55	128.03	124.51
19	B	809	CLA	O2A-CGA-O1A	-2.55	117.16	123.59
19	A	833	CLA	CHB-C4A-NA	2.55	128.03	124.51
19	Z	602	CLA	C3B-C4B-NB	-2.54	108.16	110.52
20	6	307	CHL	C3D-C4D-ND	-2.54	106.12	110.24
19	A	834	CLA	C3B-C4B-NB	-2.54	108.16	110.52
20	7	601	CHL	C3B-C4B-NB	-2.54	108.16	110.52
19	4	604	CLA	C3B-C4B-NB	-2.54	108.16	110.52
19	F	304	CLA	C3B-C4B-NB	-2.54	108.16	110.52
19	A	830	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
19	A	839	CLA	C3B-C4B-NB	-2.54	108.16	110.52
19	Z	610	CLA	C3B-C4B-NB	-2.54	108.16	110.52
19	A	815	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
19	L	204	CLA	C3B-C4B-NB	-2.53	108.16	110.52
19	Z	604	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	B	842	CLA	C3B-C4B-NB	-2.53	108.17	110.52
19	3	313	CLA	C1-C2-C3	-2.53	121.66	126.04
19	A	805	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	1	309	CLA	C3B-C4B-NB	-2.53	108.17	110.52
20	5	317	CHL	C3B-C4B-NB	-2.53	108.17	110.52
19	3	314	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	5	316	CLA	C3B-C4B-NB	-2.53	108.17	110.52
19	6	312	CLA	C3B-C4B-NB	-2.53	108.17	110.52
19	4	611	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	B	810	CLA	C3B-C4B-NB	-2.53	108.17	110.52
19	Z	603	CLA	C3B-C4B-NB	-2.53	108.17	110.52
20	Z	605	CHL	C3B-C4B-NB	-2.52	108.17	110.52
19	K	205	CLA	CHB-C4A-NA	2.52	128.00	124.51
20	4	601	CHL	CHC-C4B-NB	-2.52	121.59	124.26
19	L	203	CLA	CHB-C4A-NA	2.52	128.00	124.51
19	A	818	CLA	C3B-C4B-NB	-2.52	108.18	110.52
19	Z	613	CLA	C1-C2-C3	-2.52	122.68	126.75
19	A	827	CLA	C3B-C4B-NB	-2.51	108.18	110.52
20	5	307	CHL	C3D-C4D-ND	-2.51	106.17	110.24
19	G	202	CLA	CHB-C4A-NA	2.51	127.99	124.51
19	6	304	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	8	320	CHL	C1D-ND-C4D	-2.51	104.56	106.33
19	1	310	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	A	811	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
19	5	305	CLA	C3B-C4B-NB	-2.50	108.19	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	810	CLA	C3B-C4B-NB	-2.50	108.19	110.52
19	B	824	CLA	C3B-C4B-NB	-2.50	108.19	110.52
19	8	308	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	A	841	CLA	C3B-C4B-NB	-2.50	108.19	110.52
19	B	834	CLA	C3B-C4B-NB	-2.50	108.19	110.52
19	3	301	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	B	825	CLA	O2D-CGD-CBD	2.50	115.71	111.27
20	8	305	CHL	C1C-C2C-C3C	-2.50	105.13	107.11
19	B	807	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
19	B	838	CLA	C3B-C4B-NB	-2.50	108.20	110.52
19	A	819	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	1	304	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	G	203	CLA	C3B-C4B-NB	-2.49	108.20	110.52
19	K	203	CLA	C1-C2-C3	-2.49	121.74	126.04
19	A	829	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	1	314	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	5	302	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	1	311	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	A	832	CLA	O2D-CGD-CBD	2.49	115.69	111.27
19	A	836	CLA	C3B-C4B-NB	-2.49	108.21	110.52
19	7	608	CLA	C3B-C4B-NB	-2.48	108.21	110.52
19	B	817	CLA	C3B-C4B-NB	-2.48	108.21	110.52
19	A	803	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
20	6	315	CHL	C3B-C4B-NB	-2.48	108.22	110.52
19	F	302	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
19	5	311	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	4	613	CLA	C3B-C4B-NB	-2.47	108.22	110.52
20	8	306	CHL	C3B-C4B-NB	-2.47	108.22	110.52
19	A	811	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	8	302	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	4	614	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	J	102	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	1	312	CLA	C3B-C4B-NB	-2.47	108.22	110.52
19	3	302	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	4	610	CLA	CHB-C4A-NA	2.47	127.92	124.51
19	Z	611	CLA	CHB-C4A-NA	2.47	127.92	124.51
19	4	608	CLA	C3B-C4B-NB	-2.47	108.23	110.52
20	6	315	CHL	CHB-C1B-NB	-2.47	121.64	124.26
19	A	815	CLA	C3B-C4B-NB	-2.47	108.23	110.52
19	3	313	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
19	B	815	CLA	CHB-C4A-NA	2.47	127.92	124.51
19	3	307	CLA	CHB-C4A-NA	2.46	127.92	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	612	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	A	825	CLA	C3B-C4B-NB	-2.46	108.23	110.52
19	Z	613	CLA	C3B-C4B-NB	-2.46	108.23	110.52
19	5	312	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	5	304	CLA	C3B-C4B-NB	-2.46	108.23	110.52
19	1	303	CLA	C3B-C4B-NB	-2.46	108.23	110.52
19	5	312	CLA	CAC-C3C-C4C	2.46	128.00	124.81
19	B	831	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	B	818	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	1	305	CHL	CHD-C4C-C3C	-2.46	121.23	124.84
19	5	310	CLA	CHB-C4A-NA	2.45	127.91	124.51
19	A	822	CLA	CHB-C4A-NA	2.45	127.90	124.51
19	4	612	CLA	C1-C2-C3	-2.45	121.80	126.04
19	7	604	CLA	CHB-C4A-NA	2.45	127.90	124.51
19	B	816	CLA	CHB-C4A-NA	2.45	127.90	124.51
19	B	825	CLA	CHB-C4A-NA	2.45	127.90	124.51
19	B	836	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
19	6	305	CLA	CHB-C4A-NA	2.45	127.90	124.51
20	Z	605	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
19	7	612	CLA	CHB-C4A-NA	2.45	127.90	124.51
20	4	605	CHL	C1D-CHD-C4C	-2.45	120.78	126.06
19	B	816	CLA	C3B-C4B-NB	-2.44	108.25	110.52
19	6	309	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	3	309	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	A	826	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	B	822	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	A	846	CLA	C3B-C4B-NB	-2.44	108.25	110.52
19	B	837	CLA	C3B-C4B-NB	-2.44	108.25	110.52
19	B	829	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	8	303	CLA	C3B-C4B-NB	-2.44	108.25	110.52
19	B	824	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	L	204	CLA	CHB-C4A-NA	2.44	127.88	124.51
19	1	311	CLA	C3B-C4B-NB	-2.44	108.25	110.52
20	5	317	CHL	CHB-C1B-NB	-2.44	121.68	124.26
19	Z	613	CLA	CHB-C4A-NA	2.44	127.88	124.51
19	3	303	CLA	CHB-C4A-NA	2.44	127.88	124.51
19	B	814	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
19	A	804	CLA	CHD-C1D-ND	-2.44	122.22	124.45
19	B	840	CLA	C1-C2-C3	-2.43	121.83	126.04
19	4	603	CLA	CHB-C4A-NA	2.43	127.88	124.51
20	8	306	CHL	C1D-CHD-C4C	-2.43	120.82	126.06
19	5	314	CLA	CHB-C4A-NA	2.43	127.87	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	304	CLA	C3B-C4B-NB	-2.43	108.26	110.52
19	6	310	CLA	CHB-C1B-NB	2.43	126.83	124.26
19	Z	614	CLA	C1-C2-C3	-2.43	121.84	126.04
19	Z	602	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	1	313	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	L	203	CLA	CHD-C1D-ND	-2.43	122.22	124.45
19	A	832	CLA	C3B-C4B-NB	-2.43	108.26	110.52
19	A	840	CLA	C3B-C4B-NB	-2.43	108.26	110.52
19	A	815	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	B	839	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	K	205	CLA	C3B-C4B-NB	-2.42	108.27	110.52
19	6	312	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	7	613	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	A	813	CLA	C3B-C4B-NB	-2.42	108.27	110.52
19	B	804	CLA	CAC-C3C-C4C	2.42	127.95	124.81
19	B	841	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	G	203	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	B	829	CLA	C3B-C4B-NB	-2.42	108.27	110.52
19	K	204	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	B	832	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	6	327	CLA	C3B-C4B-NB	-2.42	108.27	110.52
19	A	811	CLA	C1-C2-C3	-2.42	121.86	126.04
19	6	303	CLA	CHB-C4A-NA	2.42	127.85	124.51
19	B	832	CLA	C3B-C4B-NB	-2.42	108.27	110.52
19	3	310	CLA	CHB-C4A-NA	2.42	127.85	124.51
19	3	301	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
20	6	302	CHL	C2C-C3C-C4C	2.41	108.21	106.49
19	A	811	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
19	B	840	CLA	CHB-C1B-NB	2.41	126.81	124.26
19	B	836	CLA	C3B-C4B-NB	-2.41	108.28	110.52
19	B	813	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	1	308	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	4	604	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	7	607	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	B	823	CLA	C3B-C4B-NB	-2.41	108.28	110.52
19	4	602	CLA	CMB-C2B-C1B	-2.41	121.70	125.37
20	Z	606	CHL	C3B-C4B-NB	-2.41	108.28	110.52
19	Z	614	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	4	606	CHL	CHD-C4C-C3C	-2.40	121.31	124.84
20	4	607	CHL	CHA-C4D-ND	-2.40	127.47	132.50
19	A	833	CLA	C3B-C4B-NB	-2.40	108.29	110.52
19	A	835	CLA	CHB-C4A-NA	2.40	127.83	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	836	CLA	O2D-CGD-CBD	2.40	115.54	111.27
20	7	621	CHL	C2C-C3C-C4C	2.40	108.20	106.49
19	8	307	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	A	812	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	A	840	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	A	846	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	A	823	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
19	Z	609	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	3	308	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	B	834	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	Z	608	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	7	611	CLA	C3B-C4B-NB	-2.40	108.29	110.52
20	4	605	CHL	CHD-C4C-C3C	-2.40	121.32	124.84
19	Z	607	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	7	604	CLA	C3B-C4B-NB	-2.40	108.29	110.52
20	6	306	CHL	CHD-C4C-C3C	-2.40	121.32	124.84
19	A	808	CLA	CHB-C4A-NA	2.40	127.82	124.51
19	6	327	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	1	303	CLA	CHB-C4A-NA	2.39	127.82	124.51
20	Z	601	CHL	CHB-C1B-NB	-2.39	121.72	124.26
20	8	320	CHL	C2C-C3C-C4C	2.39	108.19	106.49
20	8	320	CHL	C3B-C4B-NB	-2.39	108.30	110.52
19	A	814	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	B	805	CLA	CHB-C1B-NB	2.39	126.79	124.26
19	B	837	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
20	5	317	CHL	C2C-C3C-C4C	2.39	108.19	106.49
19	3	308	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
19	B	806	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	B	820	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	B	842	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	4	609	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	B	834	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
19	4	613	CLA	CHB-C4A-NA	2.39	127.81	124.51
19	B	809	CLA	CHB-C4A-NA	2.39	127.81	124.51
19	Z	610	CLA	CHB-C4A-NA	2.39	127.81	124.51
19	7	603	CLA	C3B-C4B-NB	-2.39	108.30	110.52
21	A	858	BCR	C2-C1-C6	2.39	114.16	110.48
19	8	312	CLA	CHB-C4A-NA	2.39	127.81	124.51
19	6	320	CLA	C3B-C4B-NB	-2.38	108.30	110.52
19	B	818	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
20	5	306	CHL	C3B-C4B-NB	-2.38	108.30	110.52
19	3	303	CLA	CHD-C1D-ND	-2.38	122.26	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	304	CLA	CHB-C4A-NA	2.38	127.80	124.51
20	7	605	CHL	C3B-C4B-NB	-2.38	108.31	110.52
19	6	314	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	A	842	CLA	CHB-C4A-NA	2.38	127.80	124.51
20	7	606	CHL	C2C-C3C-C4C	2.38	108.19	106.49
19	A	817	CLA	C3B-C4B-NB	-2.38	108.31	110.52
19	B	814	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	B	830	CLA	C3B-C4B-NB	-2.38	108.31	110.52
19	A	823	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	B	811	CLA	CHB-C4A-NA	2.38	127.80	124.51
20	5	307	CHL	CHD-C4C-C3C	-2.38	121.35	124.84
19	A	807	CLA	CHB-C4A-NA	2.37	127.80	124.51
19	B	826	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	K	203	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	B	828	CLA	C3B-C4B-NB	-2.37	108.31	110.52
19	B	836	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	3	324	LMU	C3'-C4'-C5'	-2.37	105.49	110.93
19	A	844	CLA	C1-C2-C3	-2.37	121.94	126.04
19	7	607	CLA	C1-C2-C3	-2.37	122.92	126.75
19	5	310	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
19	A	836	CLA	CHD-C1D-ND	-2.37	122.28	124.45
19	B	837	CLA	CHB-C1B-NB	2.37	126.76	124.26
19	A	809	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
19	1	309	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
19	B	834	CLA	CHD-C1D-ND	-2.36	122.28	124.45
20	3	306	CHL	C3B-C4B-NB	-2.36	108.32	110.52
19	A	821	CLA	C1-C2-C3	-2.36	121.95	126.04
20	5	306	CHL	CHD-C4C-C3C	-2.36	121.37	124.84
19	1	304	CLA	C1-C2-C3	-2.36	122.93	126.75
20	1	306	CHL	C2B-C1B-NB	-2.36	108.65	110.23
19	3	302	CLA	C1-C2-C3	-2.36	121.97	126.04
20	7	606	CHL	C1C-C2C-C3C	-2.36	105.24	107.11
20	6	315	CHL	CHC-C4B-NB	-2.35	121.76	124.26
21	B	844	BCR	C2-C1-C6	2.35	114.11	110.48
19	5	305	CLA	CHB-C4A-NA	2.35	127.77	124.51
19	B	821	CLA	CHB-C4A-NA	2.35	127.76	124.51
20	1	306	CHL	CHB-C1B-NB	-2.35	121.77	124.26
19	7	610	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	B	840	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
19	A	809	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
19	A	814	CLA	C3B-C4B-NB	-2.35	108.33	110.52
19	5	315	CLA	CHB-C4A-NA	2.35	127.76	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	805	CLA	CHD-C1D-ND	-2.35	122.30	124.45
19	8	307	CLA	C1-C2-C3	-2.35	122.95	126.75
19	3	305	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	F	303	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	B	804	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	J	102	CLA	CMB-C2B-C1B	-2.35	121.79	125.37
19	A	832	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	B	828	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	B	833	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	F	303	CLA	C3B-C4B-NB	-2.35	108.34	110.52
20	4	605	CHL	C3D-C4D-ND	-2.34	106.44	110.24
19	B	804	CLA	CHB-C1B-NB	2.34	126.74	124.26
19	A	839	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	5	310	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
19	7	602	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	B	827	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	Z	603	CLA	CHB-C4A-NA	2.34	127.75	124.51
20	4	607	CHL	CHC-C4B-NB	-2.34	121.78	124.26
19	A	811	CLA	C3B-C4B-NB	-2.34	108.35	110.52
20	6	306	CHL	C1D-CHD-C4C	-2.34	121.01	126.06
19	1	312	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
19	7	614	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	3	310	CLA	C3B-C4B-NB	-2.34	108.35	110.52
19	A	824	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	B	805	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	B	830	CLA	O2D-CGD-CBD	2.34	115.42	111.27
29	B	843	PQN	C11-C3-C4	-2.34	116.00	118.50
21	B	802	BCR	C12-C13-C14	-2.33	115.36	118.94
19	7	609	CLA	CHB-C4A-NA	2.33	127.73	124.51
19	A	818	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	J	101	LUT	C36-C21-C26	2.33	113.07	109.55
19	A	805	CLA	O2D-CGD-CBD	2.33	115.41	111.27
19	8	303	CLA	CHD-C1D-ND	-2.33	122.31	124.45
20	1	306	CHL	C3D-C4D-ND	-2.33	106.47	110.24
19	3	301	CLA	CMB-C2B-C1B	-2.33	121.83	125.37
20	4	601	CHL	C2C-C3C-C4C	2.33	108.15	106.49
19	4	602	CLA	CHB-C4A-NA	2.33	127.73	124.51
19	A	842	CLA	C1-C2-C3	-2.33	122.02	126.04
19	3	312	CLA	CHB-C4A-NA	2.32	127.73	124.51
19	8	311	CLA	C3B-C4B-NB	-2.32	108.36	110.52
19	A	841	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	6	320	CLA	CHB-C4A-NA	2.32	127.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	312	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	A	809	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	B	840	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	B	820	CLA	CHD-C1D-ND	-2.32	122.33	124.45
19	B	810	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	4	603	CLA	C3B-C4B-NB	-2.32	108.37	110.52
19	B	812	CLA	CHB-C4A-NA	2.31	127.71	124.51
19	B	832	CLA	CMB-C2B-C1B	-2.31	121.84	125.37
20	4	607	CHL	C2C-C3C-C4C	2.31	108.14	106.49
19	5	304	CLA	CHD-C1D-ND	-2.31	122.33	124.45
19	5	304	CLA	CHB-C4A-NA	2.31	127.71	124.51
19	A	827	CLA	CHB-C4A-NA	2.31	127.71	124.51
19	5	304	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
19	3	303	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
20	4	601	CHL	C2B-C1B-NB	-2.31	108.68	110.23
19	A	822	CLA	CHD-C1D-ND	-2.31	122.33	124.45
20	1	305	CHL	C3D-C4D-ND	-2.30	106.51	110.24
19	6	311	CLA	CHB-C4A-NA	2.30	127.70	124.51
19	A	836	CLA	CHB-C4A-NA	2.30	127.70	124.51
19	A	817	CLA	CHD-C1D-ND	-2.30	122.34	124.45
19	A	837	CLA	CHD-C1D-ND	-2.30	122.34	124.45
19	B	833	CLA	C3B-C4B-NB	-2.30	108.38	110.52
19	7	607	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
19	7	608	CLA	O2D-CGD-CBD	2.30	115.36	111.27
19	1	313	CLA	CHD-C1D-ND	-2.30	122.34	124.45
19	6	310	CLA	CHB-C4A-NA	2.30	127.69	124.51
19	8	314	CLA	CHB-C4A-NA	2.30	127.69	124.51
19	A	838	CLA	C3B-C4B-NB	-2.30	108.38	110.52
19	3	311	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	4	617	XAT	C11-C10-C9	2.30	130.59	127.31
20	4	601	CHL	CHB-C1B-NB	-2.30	121.83	124.26
19	A	823	CLA	CHB-C1B-NB	2.30	126.69	124.26
20	1	306	CHL	CHC-C4B-NB	-2.30	121.83	124.26
19	1	302	CLA	CHB-C4A-NA	2.29	127.69	124.51
19	B	833	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
19	4	611	CLA	C3B-C4B-NB	-2.29	108.39	110.52
19	B	838	CLA	CHB-C4A-NA	2.29	127.68	124.51
20	4	606	CHL	C3B-C4B-NB	-2.29	108.39	110.52
20	4	606	CHL	C2B-C1B-NB	-2.29	108.70	110.23
19	L	203	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
19	B	808	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	A	828	CLA	CAA-C2A-C1A	-2.29	104.47	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	203	CLA	O2D-CGD-CBD	2.29	115.34	111.27
19	3	301	CLA	CHD-C1D-ND	-2.29	122.35	124.45
19	A	806	CLA	CHB-C4A-NA	2.29	127.67	124.51
19	6	316	CLA	CHB-C4A-NA	2.29	127.67	124.51
19	7	607	CLA	CHD-C1D-ND	-2.29	122.35	124.45
19	A	811	CLA	CHD-C1D-ND	-2.29	122.35	124.45
19	A	806	CLA	CHD-C1D-ND	-2.28	122.36	124.45
19	6	314	CLA	C1-C2-C3	-2.28	123.06	126.75
19	A	818	CLA	O2D-CGD-CBD	2.28	115.32	111.27
19	6	310	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
19	5	303	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	K	203	CLA	O2D-CGD-CBD	2.28	115.32	111.27
19	A	813	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	B	817	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	Z	609	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
19	7	607	CLA	C3B-C4B-NB	-2.27	108.41	110.52
19	3	304	CLA	CHB-C4A-NA	2.27	127.66	124.51
19	6	313	CLA	CHB-C4A-NA	2.27	127.66	124.51
19	A	804	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
19	A	805	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
19	A	839	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
20	4	606	CHL	CHB-C1B-NB	-2.27	121.85	124.26
19	7	603	CLA	CHB-C4A-NA	2.27	127.65	124.51
19	8	303	CLA	CHB-C4A-NA	2.27	127.65	124.51
19	B	819	CLA	C1-C2-C3	-2.27	122.12	126.04
19	A	819	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
20	4	605	CHL	CHB-C1B-NB	-2.27	121.85	124.26
19	A	828	CLA	CHB-C4A-NA	2.27	127.65	124.51
19	B	803	CLA	CHC-C4B-NB	2.27	126.66	124.26
19	5	316	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
19	K	203	CLA	CHD-C1D-ND	-2.27	122.37	124.45
19	Z	610	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
19	1	313	CLA	C1-C2-C3	-2.27	122.12	126.04
19	8	310	CLA	CHB-C4A-NA	2.27	127.65	124.51
19	A	830	CLA	CHB-C4A-NA	2.27	127.65	124.51
19	A	803	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
19	1	309	CLA	CHB-C1B-NB	2.27	126.66	124.26
19	8	302	CLA	CHD-C1D-ND	-2.26	122.37	124.45
20	1	305	CHL	C2B-C1B-NB	-2.26	108.72	110.23
19	B	808	CLA	C3B-C4B-NB	-2.26	108.42	110.52
19	A	807	CLA	C1-C2-C3	-2.26	122.14	126.04
19	6	320	CLA	CMB-C2B-C1B	-2.26	121.93	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	6	302	CHL	C3B-C4B-NB	-2.26	108.42	110.52
22	F	305	LUT	C22-C23-C24	2.26	114.31	111.74
19	K	202	CLA	C2A-C1A-CHA	2.26	127.81	123.86
19	3	305	CLA	CHD-C1D-ND	-2.26	122.38	124.45
19	B	824	CLA	CHD-C1D-ND	-2.26	122.38	124.45
19	A	832	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
21	B	802	BCR	C15-C14-C13	2.26	130.53	127.31
20	6	302	CHL	C2B-C1B-NB	-2.25	108.72	110.23
19	8	309	CLA	CHB-C4A-NA	2.25	127.63	124.51
19	A	814	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
24	3	324	LMU	O5'-C1'-C2'	2.25	115.12	110.35
19	B	819	CLA	CHB-C4A-NA	2.25	127.63	124.51
19	A	838	CLA	CHB-C4A-NA	2.25	127.62	124.51
19	1	309	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
19	A	840	CLA	CHD-C1D-ND	-2.25	122.39	124.45
19	B	826	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
19	5	312	CLA	C3B-C4B-NB	-2.25	108.43	110.52
19	A	805	CLA	C3B-C4B-NB	-2.25	108.43	110.52
20	6	307	CHL	C3B-C4B-NB	-2.25	108.43	110.52
19	4	609	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
19	A	821	CLA	CHB-C4A-NA	2.25	127.62	124.51
20	6	306	CHL	C3B-C4B-NB	-2.25	108.43	110.52
19	A	803	CLA	CHB-C4A-NA	2.24	127.62	124.51
20	6	308	CHL	C2C-C3C-C4C	2.24	108.09	106.49
20	5	308	CHL	C3B-C4B-NB	-2.24	108.43	110.52
20	Z	601	CHL	CHD-C1D-ND	2.24	126.52	124.45
20	4	601	CHL	CHD-C4C-C3C	-2.24	121.54	124.84
19	B	824	CLA	CAA-C2A-C1A	-2.24	104.63	111.97
19	A	808	CLA	CHB-C1B-NB	2.24	126.63	124.26
19	G	202	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
19	1	312	CLA	C1-C2-C3	-2.24	122.17	126.04
19	8	303	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
19	B	804	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
20	5	317	CHL	C3D-C4D-ND	-2.24	106.62	110.24
19	8	313	CLA	CHB-C4A-NA	2.24	127.61	124.51
19	A	834	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
19	6	304	CLA	C3B-C4B-NB	-2.24	108.44	110.52
19	A	825	CLA	CHB-C4A-NA	2.24	127.60	124.51
21	B	802	BCR	C2-C1-C6	2.24	113.92	110.48
19	B	807	CLA	CHB-C4A-NA	2.24	127.60	124.51
19	A	836	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
19	1	302	CLA	CHD-C1D-ND	-2.23	122.40	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	327	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
19	1	309	CLA	CHB-C4A-NA	2.23	127.60	124.51
19	A	827	CLA	O2D-CGD-CBD	2.23	115.23	111.27
19	B	815	CLA	CHD-C1D-ND	-2.23	122.40	124.45
19	B	807	CLA	C1-C2-C3	-2.23	122.19	126.04
20	5	317	CHL	C2B-C1B-NB	-2.23	108.74	110.23
19	A	846	CLA	CMB-C2B-C1B	-2.23	121.98	125.37
19	A	830	CLA	C3B-C4B-NB	-2.23	108.45	110.52
19	A	831	CLA	C3B-C4B-NB	-2.23	108.45	110.52
20	8	306	CHL	C3D-C4D-ND	-2.23	106.63	110.24
19	B	830	CLA	CMB-C2B-C1B	-2.23	121.98	125.37
19	3	308	CLA	CMB-C2B-C1B	-2.23	121.98	125.37
21	B	844	BCR	C1-C6-C7	-2.22	109.48	115.78
19	B	826	CLA	CMB-C2B-C1B	-2.22	121.98	125.37
19	A	821	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
21	B	844	BCR	C7-C8-C9	-2.22	122.88	126.23
19	A	843	CLA	CHB-C4A-NA	2.22	127.58	124.51
20	8	305	CHL	C3D-C4D-ND	-2.22	106.64	110.24
19	Z	612	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
19	Z	613	CLA	CHD-C1D-ND	-2.22	122.41	124.45
20	1	305	CHL	CHB-C1B-NB	-2.22	121.91	124.26
19	7	612	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
19	8	312	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
19	B	823	CLA	CHB-C4A-NA	2.22	127.58	124.51
19	B	830	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
20	8	305	CHL	C3B-C4B-NB	-2.22	108.46	110.52
19	F	302	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
19	3	302	CLA	C3B-C4B-NB	-2.21	108.46	110.52
19	3	302	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
20	3	306	CHL	CHC-C4B-NB	-2.21	121.91	124.26
19	F	303	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
19	A	820	CLA	CHB-C4A-NA	2.21	127.57	124.51
19	B	811	CLA	C1-C2-C3	-2.21	122.22	126.04
20	8	306	CHL	C2B-C1B-NB	-2.21	108.75	110.23
20	7	601	CHL	C3D-C4D-ND	-2.21	106.66	110.24
19	K	203	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
20	4	606	CHL	C2C-C3C-C4C	2.21	108.06	106.49
19	A	819	CLA	CHD-C1D-ND	-2.21	122.42	124.45
20	6	308	CHL	CHB-C1B-NB	-2.21	121.92	124.26
19	B	828	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
19	8	304	CLA	CHD-C1D-ND	-2.21	122.43	124.45
19	3	313	CLA	C3B-C4B-NB	-2.21	108.47	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	841	CLA	C1-C2-C3	-2.21	122.23	126.04
19	B	834	CLA	CAA-C2A-C1A	-2.20	104.75	111.97
19	B	835	CLA	CHD-C1D-ND	-2.20	122.43	124.45
19	B	829	CLA	CHD-C1D-ND	-2.20	122.43	124.45
19	Z	612	CLA	C3B-C4B-NB	-2.20	108.47	110.52
19	B	839	CLA	C3B-C4B-NB	-2.20	108.47	110.52
20	6	315	CHL	C2C-C3C-C4C	2.20	108.06	106.49
19	5	312	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
19	B	832	CLA	C1-C2-C3	-2.20	122.24	126.04
20	6	307	CHL	C2C-C3C-C4C	2.20	108.06	106.49
19	A	819	CLA	C3B-C4B-NB	-2.20	108.48	110.52
20	7	606	CHL	C3D-C4D-ND	-2.20	106.68	110.24
19	B	833	CLA	CHD-C1D-ND	-2.20	122.44	124.45
19	A	816	CLA	CHB-C4A-NA	2.20	127.55	124.51
19	A	828	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
19	6	314	CLA	CHD-C1D-ND	-2.19	122.44	124.45
19	B	842	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
19	1	307	CLA	CHD-C1D-ND	-2.19	122.44	124.45
20	4	601	CHL	C3D-C4D-ND	-2.19	106.69	110.24
19	B	824	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
19	1	307	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
20	8	305	CHL	CHD-C4C-C3C	-2.19	121.62	124.84
19	B	839	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
20	Z	605	CHL	CHD-C1D-ND	2.19	126.47	124.45
20	7	606	CHL	C2B-C1B-NB	-2.19	108.77	110.23
19	3	314	CLA	C3B-C4B-NB	-2.19	108.48	110.52
19	A	805	CLA	CHD-C1D-ND	-2.19	122.44	124.45
19	6	320	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
20	4	607	CHL	C3B-C4B-NB	-2.19	108.49	110.52
20	Z	605	CHL	C3D-C4D-ND	-2.18	106.70	110.24
20	6	317	CHL	CHD-C1D-ND	2.18	126.46	124.45
19	A	811	CLA	CMB-C2B-C1B	-2.18	122.04	125.37
19	6	304	CLA	CHD-C1D-ND	-2.18	122.45	124.45
19	B	819	CLA	CHD-C1D-ND	-2.18	122.45	124.45
19	4	613	CLA	CHD-C1D-ND	-2.18	122.45	124.45
19	8	310	CLA	CHD-C1D-ND	-2.18	122.45	124.45
19	A	816	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
19	8	313	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
19	4	604	CLA	C1-C2-C3	-2.18	123.23	126.75
19	B	821	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
19	Z	609	CLA	CHB-C1B-NB	2.18	126.56	124.26
20	4	607	CHL	CHD-C4C-C3C	-2.18	121.64	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	827	CLA	CMB-C2B-C1B	-2.18	122.06	125.37
19	B	813	CLA	CMB-C2B-C1B	-2.18	122.06	125.37
19	6	304	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
20	7	601	CHL	CHD-C4C-C3C	-2.17	121.64	124.84
19	5	316	CLA	CHB-C1B-NB	2.17	126.56	124.26
19	6	313	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
19	6	313	CLA	CHB-C1B-NB	2.17	126.56	124.26
19	B	834	CLA	O2D-CGD-CBD	2.17	115.13	111.27
19	B	840	CLA	CHD-C1D-ND	-2.17	122.46	124.45
20	Z	606	CHL	C3D-C4D-ND	-2.17	106.73	110.24
19	B	824	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
20	8	320	CHL	CHD-C1D-ND	2.17	126.45	124.45
19	Z	603	CLA	CHD-C1D-ND	-2.17	122.46	124.45
20	Z	601	CHL	CHC-C1C-NC	-2.17	120.91	124.20
19	7	603	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
19	5	316	CLA	CHB-C4A-NA	2.17	127.51	124.51
19	6	327	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
20	5	308	CHL	C2C-C3C-C4C	2.17	108.03	106.49
19	Z	604	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
19	5	315	CLA	CHB-C1B-NB	2.17	126.55	124.26
19	6	303	CLA	CHD-C1D-ND	-2.17	122.46	124.45
19	5	311	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
19	A	840	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
19	B	817	CLA	CHD-C1D-ND	-2.17	122.46	124.45
19	B	801	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
19	5	311	CLA	C3B-C4B-NB	-2.16	108.51	110.52
20	4	605	CHL	C3B-C4B-NB	-2.16	108.51	110.52
19	K	203	CLA	CHB-C1B-NB	2.16	126.55	124.26
19	8	303	CLA	CHB-C1B-NB	2.16	126.55	124.26
19	B	803	CLA	CHB-C4A-NA	2.16	127.50	124.51
19	B	837	CLA	CHB-C4A-NA	2.16	127.50	124.51
19	Z	609	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
20	7	605	CHL	C3D-C4D-ND	-2.16	106.74	110.24
19	5	316	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
19	4	604	CLA	CHD-C1D-ND	-2.16	122.47	124.45
19	A	814	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
19	7	613	CLA	CHC-C4B-NB	2.16	126.54	124.26
20	8	306	CHL	C1C-C2C-C3C	-2.16	105.40	107.11
21	B	844	BCR	C33-C5-C4	-2.16	109.47	113.62
20	6	306	CHL	C2B-C1B-NB	-2.16	108.78	110.23
20	7	621	CHL	C2B-C1B-NB	-2.16	108.78	110.23
19	A	809	CLA	CHB-C1B-NB	2.16	126.54	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	812	CLA	C1-C2-C3	-2.16	122.31	126.04
19	4	613	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
19	5	309	CLA	CHD-C1D-ND	-2.16	122.47	124.45
19	A	821	CLA	CHD-C1D-ND	-2.16	122.47	124.45
19	A	820	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
19	8	309	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
19	B	835	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
19	A	821	CLA	CHB-C1B-NB	2.15	126.53	124.26
19	F	302	CLA	C1-C2-C3	-2.15	122.33	126.04
19	B	842	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
19	3	305	CLA	O2D-CGD-CBD	2.15	115.09	111.27
19	Z	604	CLA	CHD-C1D-ND	-2.15	122.48	124.45
19	1	313	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
19	A	803	CLA	CHB-C1B-NB	2.15	126.53	124.26
19	1	310	CLA	CHD-C1D-ND	-2.15	122.48	124.45
19	B	804	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
19	A	815	CLA	CHD-C1D-ND	-2.14	122.48	124.45
19	5	313	CLA	C3B-C4B-NB	-2.14	108.53	110.52
20	1	306	CHL	C1C-C2C-C3C	-2.14	105.41	107.11
19	A	830	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
19	1	310	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
19	L	204	CLA	CHD-C1D-ND	-2.14	122.48	124.45
19	B	809	CLA	O2D-CGD-CBD	2.14	115.08	111.27
20	7	605	CHL	C2B-C1B-NB	-2.14	108.80	110.23
19	1	303	CLA	CHD-C1D-ND	-2.14	122.49	124.45
20	4	607	CHL	C1D-CHD-C4C	-2.14	121.44	126.06
20	7	606	CHL	CHB-C1B-NB	-2.14	121.99	124.26
19	8	310	CLA	CHB-C1B-NB	2.14	126.52	124.26
19	B	818	CLA	CHD-C1D-ND	-2.14	122.49	124.45
20	7	621	CHL	CHD-C1D-ND	2.14	126.42	124.45
19	3	305	CLA	CHB-C1B-NB	2.14	126.52	124.26
19	B	820	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
19	6	305	CLA	C1-C2-C3	-2.14	122.35	126.04
19	A	822	CLA	C1-C2-C3	-2.14	122.35	126.04
20	4	606	CHL	C3D-C4D-ND	-2.14	106.78	110.24
19	Z	612	CLA	CMB-C2B-C1B	-2.14	122.12	125.37
19	5	304	CLA	CHB-C1B-NB	2.14	126.52	124.26
19	A	841	CLA	CHC-C4B-NB	2.14	126.52	124.26
19	7	609	CLA	CMB-C2B-C1B	-2.14	122.12	125.37
19	8	312	CLA	CHD-C1D-ND	-2.13	122.49	124.45
20	7	601	CHL	C2C-C3C-C4C	2.13	108.01	106.49
19	B	829	CLA	CMB-C2B-C1B	-2.13	122.12	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	802	CL0	C3D-C4D-ND	-2.13	106.79	110.24
19	B	813	CLA	C1-C2-C3	-2.13	122.36	126.04
19	8	312	CLA	CHB-C1B-NB	2.13	126.51	124.26
19	A	844	CLA	CHB-C4A-NA	2.13	127.46	124.51
19	A	835	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
19	L	203	CLA	CHB-C1B-NB	2.13	126.51	124.26
19	5	303	CLA	CHD-C1D-ND	-2.13	122.50	124.45
19	B	813	CLA	CHD-C1D-ND	-2.13	122.50	124.45
19	A	837	CLA	CHB-C1B-NB	2.13	126.51	124.26
19	B	830	CLA	CHB-C1B-NB	2.13	126.51	124.26
19	A	821	CLA	O2D-CGD-CBD	2.13	115.05	111.27
19	A	841	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
19	A	836	CLA	CHB-C1B-NB	2.13	126.51	124.26
19	A	838	CLA	CHD-C1D-ND	-2.13	122.50	124.45
19	B	841	CLA	CHD-C1D-ND	-2.13	122.50	124.45
24	F	306	LMU	C1B-O5B-C5B	2.12	117.86	113.69
20	4	615	CHL	C3D-C4D-ND	-2.12	106.80	110.24
20	4	605	CHL	C1C-C2C-C3C	-2.12	105.43	107.11
19	A	841	CLA	CHD-C1D-ND	-2.12	122.50	124.45
19	A	824	CLA	CHB-C1B-NB	2.12	126.50	124.26
19	A	844	CLA	CHC-C4B-NB	2.12	126.50	124.26
19	A	819	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
21	A	850	BCR	C2-C1-C6	2.12	113.75	110.48
19	B	808	CLA	O2D-CGD-CBD	2.12	115.03	111.27
19	A	826	CLA	CHB-C1B-NB	2.12	126.50	124.26
19	A	820	CLA	CHB-C1B-NB	2.12	126.50	124.26
19	7	612	CLA	CHD-C1D-ND	-2.12	122.51	124.45
19	1	303	CLA	CHB-C1B-NB	2.12	126.50	124.26
19	5	316	CLA	CHD-C1D-ND	-2.12	122.51	124.45
19	3	303	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
19	1	304	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
19	3	308	CLA	CHB-C1B-NB	2.12	126.50	124.26
19	8	302	CLA	CHB-C1B-NB	2.11	126.50	124.26
20	6	306	CHL	C3D-C4D-ND	-2.11	106.82	110.24
19	B	841	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
20	6	317	CHL	C3B-C4B-NB	-2.11	108.55	110.52
19	B	839	CLA	O2D-CGD-CBD	2.11	115.02	111.27
27	5	323	NEX	O24-C25-C26	-2.11	57.21	58.96
20	4	615	CHL	C1C-C2C-C3C	-2.11	105.44	107.11
19	B	825	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	B	807	CLA	CHB-C1B-NB	2.11	126.49	124.26
20	5	306	CHL	C2B-C1B-NB	-2.11	108.82	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	802	CL0	CHB-C1B-NB	-2.11	122.02	124.26
19	B	838	CLA	CHD-C1D-ND	-2.11	122.51	124.45
19	B	815	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	B	827	CLA	CHB-C1B-NB	2.11	126.49	124.26
20	6	307	CHL	C2B-C1B-NB	-2.11	108.82	110.23
19	6	313	CLA	CHD-C1D-ND	-2.11	122.52	124.45
19	5	302	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
19	B	810	CLA	C1-C2-C3	-2.11	122.40	126.04
20	5	307	CHL	C1C-C2C-C3C	-2.11	105.44	107.11
20	8	320	CHL	CHD-C4C-C3C	-2.11	121.74	124.84
19	B	839	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
19	B	819	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
19	4	609	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
24	1	319	LMU	C1B-O5B-C5B	2.10	117.82	113.69
19	A	804	CLA	CMB-C2B-C3B	2.10	131.68	126.59
19	5	310	CLA	CHB-C1B-NB	2.10	126.48	124.26
19	7	610	CLA	CHD-C1D-ND	-2.10	122.52	124.45
19	A	842	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
20	1	305	CHL	CMD-C2D-C1D	2.10	128.42	124.71
19	A	803	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
19	B	836	CLA	CHD-C1D-ND	-2.10	122.52	124.45
20	7	621	CHL	C3B-C4B-NB	-2.10	108.56	110.52
19	B	822	CLA	CHD-C1D-ND	-2.10	122.52	124.45
19	A	803	CLA	CHD-C1D-ND	-2.10	122.52	124.45
19	B	830	CLA	CHB-C4A-NA	2.10	127.42	124.51
19	A	840	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
19	B	826	CLA	CHB-C1B-NB	2.10	126.48	124.26
19	B	819	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
19	A	824	CLA	CHD-C1D-ND	-2.10	122.53	124.45
19	B	812	CLA	CHD-C1D-ND	-2.10	122.53	124.45
19	1	304	CLA	CHD-C1D-ND	-2.10	122.53	124.45
19	A	838	CLA	O2D-CGD-CBD	2.10	115.00	111.27
19	1	303	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
20	Z	601	CHL	C3D-C4D-ND	-2.10	106.84	110.24
20	5	306	CHL	C3D-C4D-ND	-2.10	106.84	110.24
19	3	312	CLA	CHD-C1D-ND	-2.10	122.53	124.45
19	1	314	CLA	CHD-C1D-ND	-2.10	122.53	124.45
19	G	202	CLA	C1-C2-C3	-2.10	122.42	126.04
20	6	307	CHL	CMD-C2D-C1D	2.09	128.41	124.71
20	4	605	CHL	CHC-C1C-NC	-2.09	121.03	124.20
19	5	315	CLA	O2A-CGA-O1A	-2.09	118.08	123.30
19	B	827	CLA	O2A-CGA-O1A	-2.09	118.31	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	808	CLA	CHD-C1D-ND	-2.09	122.53	124.45
19	1	304	CLA	CMB-C2B-C1B	-2.09	122.18	125.37
21	A	858	BCR	C20-C21-C22	-2.09	124.33	127.31
19	7	607	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
19	6	305	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
19	8	313	CLA	CHD-C1D-ND	-2.09	122.53	124.45
27	6	323	NEX	O24-C25-C26	-2.09	57.23	58.96
19	B	822	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
19	3	311	CLA	CHD-C1D-ND	-2.09	122.53	124.45
19	A	821	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
19	6	305	CLA	CHB-C1B-NB	2.09	126.47	124.26
19	B	837	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
19	3	311	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
19	A	823	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
19	6	316	CLA	CHD-C1D-ND	-2.09	122.54	124.45
19	Z	611	CLA	CHB-C1B-NB	2.09	126.47	124.26
19	3	307	CLA	CHB-C1B-NB	2.08	126.46	124.26
19	B	833	CLA	O2D-CGD-CBD	2.08	114.97	111.27
19	4	604	CLA	CHB-C1B-NB	2.08	126.46	124.26
19	Z	604	CLA	CHB-C1B-NB	2.08	126.46	124.26
19	1	313	CLA	O2D-CGD-CBD	2.08	114.97	111.27
19	3	310	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
19	B	819	CLA	O2D-CGD-CBD	2.08	114.97	111.27
19	7	612	CLA	CHB-C1B-NB	2.08	126.46	124.26
19	4	610	CLA	CHD-C1D-ND	-2.08	122.54	124.45
19	5	313	CLA	CHD-C1D-ND	-2.08	122.54	124.45
19	A	843	CLA	CHD-C1D-ND	-2.08	122.54	124.45
19	4	608	CLA	CHD-C1D-ND	-2.08	122.54	124.45
19	A	846	CLA	CHD-C1D-ND	-2.08	122.54	124.45
20	6	308	CHL	C3B-C4B-NB	-2.08	108.59	110.52
20	5	306	CHL	C2C-C3C-C4C	2.08	107.97	106.49
19	K	205	CLA	O2D-CGD-CBD	2.08	114.96	111.27
19	B	803	CLA	O1D-CGD-CBD	2.08	128.74	124.48
19	7	613	CLA	O2D-CGD-CBD	2.08	114.96	111.27
20	8	305	CHL	C2B-C1B-NB	-2.08	108.84	110.23
20	6	306	CHL	CHC-C1C-NC	-2.08	121.05	124.20
19	3	307	CLA	CHC-C4B-NB	2.08	126.46	124.26
19	6	309	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
19	6	310	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
19	8	302	CLA	CMB-C2B-C1B	-2.08	122.21	125.37
19	A	810	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
19	B	813	CLA	O2A-CGA-O1A	-2.08	118.35	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	306	CHL	C2C-C3C-C4C	2.08	107.97	106.49
19	B	816	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
19	B	809	CLA	C1-C2-C3	-2.08	122.45	126.04
20	8	306	CHL	C2C-C3C-C4C	2.07	107.97	106.49
19	Z	603	CLA	CHB-C1B-NB	2.07	126.45	124.26
19	1	312	CLA	CHD-C1D-ND	-2.07	122.55	124.45
20	3	306	CHL	C2B-C1B-NB	-2.07	108.84	110.23
20	6	302	CHL	CHB-C1B-NB	-2.07	122.06	124.26
20	6	306	CHL	CHB-C1B-NB	-2.07	122.06	124.26
19	A	829	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	B	826	CLA	CAA-C2A-C1A	-2.07	105.19	111.97
19	Z	608	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	A	809	CLA	CMB-C2B-C3B	2.07	131.60	126.59
19	B	824	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
19	A	807	CLA	C7-C6-C5	-2.07	107.74	113.36
20	Z	605	CHL	C2B-C1B-NB	-2.07	108.84	110.23
19	B	818	CLA	CHB-C1B-NB	2.07	126.45	124.26
19	1	302	CLA	CHB-C1B-NB	2.07	126.45	124.26
19	A	809	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	B	832	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	B	838	CLA	O2D-CGD-CBD	2.07	114.94	111.27
19	B	801	CLA	C3B-C4B-NB	-2.07	108.60	110.52
19	4	611	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
19	7	603	CLA	CHD-C1D-ND	-2.07	122.56	124.45
19	Z	607	CLA	CHB-C1B-NB	2.07	126.44	124.26
19	A	832	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
19	B	821	CLA	CHD-C1D-ND	-2.07	122.56	124.45
19	B	836	CLA	CMB-C2B-C3B	2.07	131.59	126.59
19	5	314	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	Z	609	CLA	CHD-C1D-ND	-2.06	122.56	124.45
20	6	307	CHL	CHC-C1C-NC	-2.06	121.07	124.20
29	A	845	PQN	C11-C3-C4	-2.06	116.29	118.50
19	7	603	CLA	CHB-C1B-NB	2.06	126.44	124.26
19	Z	604	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
19	5	313	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
19	8	314	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
20	7	605	CHL	C2C-C3C-C4C	2.06	107.96	106.49
20	Z	601	CHL	C2C-C3C-C4C	2.06	107.96	106.49
20	1	305	CHL	C1C-C2C-C3C	-2.06	105.48	107.11
19	A	805	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
19	A	814	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	B	808	CLA	CHD-C1D-ND	-2.06	122.56	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	313	CLA	O2D-CGD-CBD	2.06	114.93	111.27
20	4	605	CHL	C2B-C1B-NB	-2.06	108.85	110.23
19	A	815	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
19	A	831	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
20	5	307	CHL	CHC-C1C-NC	-2.06	121.08	124.20
19	B	811	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	B	814	CLA	CHD-C1D-ND	-2.06	122.56	124.45
20	4	601	CHL	CHD-C1D-ND	2.06	126.34	124.45
20	Z	605	CHL	CHC-C1C-NC	-2.06	121.08	124.20
19	Z	602	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	F	304	CLA	CHB-C4A-NA	2.06	127.35	124.51
20	8	306	CHL	CMD-C2D-C1D	2.05	128.33	124.71
19	B	814	CLA	CHC-C4B-NB	2.05	126.43	124.26
19	A	813	CLA	O2D-CGD-CBD	2.05	114.92	111.27
19	Z	612	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	8	307	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	Z	602	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
20	5	308	CHL	C2B-C1B-NB	-2.05	108.86	110.23
19	B	801	CLA	C1-C2-C3	-2.05	122.50	126.04
20	5	317	CHL	CHC-C1C-NC	-2.05	121.09	124.20
19	B	819	CLA	CHB-C1B-NB	2.05	126.43	124.26
20	1	305	CHL	CHC-C1C-NC	-2.05	121.09	124.20
19	L	203	CLA	C1-C2-C3	-2.05	122.50	126.04
19	1	313	CLA	CHB-C1B-NB	2.05	126.42	124.26
19	6	313	CLA	C1-C2-C3	-2.05	122.50	126.04
19	7	602	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
19	B	807	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
19	A	831	CLA	CHB-C4A-NA	2.05	127.34	124.51
19	B	839	CLA	C1-C2-C3	-2.05	123.44	126.75
19	3	309	CLA	C1-C2-C3	-2.04	122.51	126.04
19	A	825	CLA	C2D-C1D-ND	-2.04	108.60	110.10
19	5	310	CLA	CHD-C1D-ND	-2.04	122.58	124.45
20	7	601	CHL	CMD-C2D-C1D	2.04	128.31	124.71
21	B	802	BCR	C24-C25-C26	2.04	126.41	121.46
20	1	306	CHL	CHD-C4C-C3C	-2.04	121.84	124.84
20	6	302	CHL	C1C-C2C-C3C	-2.04	105.49	107.11
20	7	606	CHL	CMD-C2D-C1D	2.04	128.31	124.71
19	3	314	CLA	CHB-C1B-NB	2.04	126.42	124.26
19	1	307	CLA	C1-C2-C3	-2.04	122.51	126.04
19	A	815	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
19	J	102	CLA	CMB-C2B-C3B	2.04	131.53	126.59
20	Z	606	CHL	CMD-C2D-C1D	2.04	128.31	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	309	CLA	CHB-C1B-NB	2.04	126.42	124.26
19	A	822	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
19	8	314	CLA	CHD-C1D-ND	-2.04	122.58	124.45
20	7	601	CHL	C2B-C1B-NB	-2.04	108.87	110.23
20	4	615	CHL	CHD-C1D-ND	2.04	126.33	124.45
19	7	602	CLA	CHD-C1D-ND	-2.04	122.58	124.45
19	A	826	CLA	CHD-C1D-ND	-2.04	122.58	124.45
19	F	303	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
19	B	827	CLA	CMB-C2B-C1B	-2.03	122.27	125.37
19	B	809	CLA	CHB-C1B-NB	2.03	126.41	124.26
19	B	831	CLA	CHC-C4B-NB	2.03	126.41	124.26
19	K	204	CLA	CHB-C1B-NB	2.03	126.41	124.26
19	Z	614	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
19	A	831	CLA	CHD-C1D-ND	-2.03	122.58	124.45
19	3	301	CLA	CMB-C2B-C3B	2.03	131.51	126.59
19	1	312	CLA	CHB-C1B-NB	2.03	126.41	124.26
19	4	602	CLA	CMB-C2B-C3B	2.03	131.51	126.59
20	4	615	CHL	CHC-C1C-NC	-2.03	121.12	124.20
19	6	304	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
19	J	102	CLA	CHB-C1B-NB	2.03	126.41	124.26
19	1	302	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
19	6	309	CLA	CHD-C1D-ND	-2.03	122.59	124.45
19	A	817	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
20	1	306	CHL	CMD-C2D-C1D	2.03	128.29	124.71
19	6	316	CLA	CHB-C1B-NB	2.03	126.41	124.26
20	4	606	CHL	CHC-C1C-NC	-2.03	121.12	124.20
28	A	802	CL0	C2B-C1B-NB	-2.03	108.87	110.23
19	K	205	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
19	B	832	CLA	CHB-C1B-NB	2.03	126.40	124.26
19	A	812	CLA	CHD-C1D-ND	-2.03	122.59	124.45
19	Z	608	CLA	CHB-C1B-NB	2.03	126.40	124.26
19	3	308	CLA	C1-C2-C3	-2.03	122.54	126.04
19	Z	614	CLA	CHD-C1D-ND	-2.03	122.59	124.45
19	B	812	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
19	A	842	CLA	CHB-C1B-NB	2.02	126.40	124.26
19	B	813	CLA	CHB-C1B-NB	2.02	126.40	124.26
19	8	303	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
19	A	844	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
20	8	306	CHL	CHB-C1B-NB	-2.02	122.11	124.26
19	3	303	CLA	CHB-C1B-NB	2.02	126.40	124.26
20	7	601	CHL	C1C-C2C-C3C	-2.02	105.51	107.11
20	7	621	CHL	C3D-C4D-ND	-2.02	106.97	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	832	CLA	CMB-C2B-C3B	2.02	131.49	126.59
20	Z	601	CHL	C1C-C2C-C3C	-2.02	105.51	107.11
20	5	307	CHL	C2B-C1B-NB	-2.02	108.88	110.23
19	6	309	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
19	B	801	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
20	1	306	CHL	CHC-C1C-NC	-2.02	121.14	124.20
19	8	307	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
19	A	839	CLA	CHD-C1D-ND	-2.02	122.60	124.45
19	8	302	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
19	3	304	CLA	CHD-C1D-ND	-2.02	122.60	124.45
19	B	837	CLA	CHD-C1D-ND	-2.02	122.60	124.45
19	Z	607	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	8	301	LUT	C38-C25-C24	-2.02	119.24	123.56
21	B	848	BCR	C15-C16-C17	-2.02	119.34	123.47
19	A	839	CLA	CHB-C1B-NB	2.02	126.39	124.26
24	Z	619	LMU	O2B-C2B-C1B	2.02	114.95	110.05
19	B	805	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
19	6	303	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
19	A	830	CLA	C1-C2-C3	-2.02	122.55	126.04
19	B	823	CLA	C1-C2-C3	-2.02	122.55	126.04
20	3	306	CHL	CHD-C4C-C3C	-2.02	121.87	124.84
19	6	304	CLA	CHB-C1B-NB	2.02	126.39	124.26
19	B	842	CLA	CHB-C1B-NB	2.02	126.39	124.26
19	6	314	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
19	B	827	CLA	C1-C2-C3	-2.02	122.56	126.04
20	Z	605	CHL	CHB-C1B-NB	-2.02	122.12	124.26
20	7	601	CHL	CHD-C1D-ND	2.02	126.31	124.45
19	5	311	CLA	CHD-C1D-ND	-2.02	122.60	124.45
20	4	615	CHL	C2B-C1B-NB	-2.02	108.88	110.23
19	A	812	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
19	B	817	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
19	6	311	CLA	CHB-C1B-NB	2.01	126.39	124.26
19	7	610	CLA	CHB-C1B-NB	2.01	126.39	124.26
20	3	306	CHL	C1C-C2C-C3C	-2.01	105.52	107.11
19	3	311	CLA	CHB-C1B-NB	2.01	126.39	124.26
19	Z	614	CLA	CHB-C1B-NB	2.01	126.39	124.26
19	5	303	CLA	CHB-C1B-NB	2.01	126.39	124.26
19	5	314	CLA	CHB-C1B-NB	2.01	126.39	124.26
20	5	308	CHL	CHB-C1B-NB	-2.01	122.13	124.26
20	Z	601	CHL	C1D-CHD-C4C	-2.01	121.72	126.06
19	3	313	CLA	CMB-C2B-C1B	-2.01	122.30	125.37
19	A	818	CLA	CMB-C2B-C1B	-2.01	122.30	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	806	CLA	CHD-C1D-ND	-2.01	122.61	124.45
19	A	829	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
19	A	838	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
19	A	829	CLA	CHB-C1B-NB	2.01	126.39	124.26
19	B	823	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
19	3	310	CLA	CHB-C1B-NB	2.01	126.39	124.26
19	A	824	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
19	L	204	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
20	5	308	CHL	CHD-C4C-C3C	-2.01	121.89	124.84
19	4	608	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
20	6	307	CHL	C1D-CHD-C4C	-2.01	121.72	126.06
19	A	807	CLA	CHD-C1D-ND	-2.01	122.61	124.45
20	1	306	CHL	C3B-C4B-NB	-2.01	108.65	110.52
19	3	301	CLA	CHB-C1B-NB	2.01	126.38	124.26
19	3	313	CLA	CHC-C4B-NB	2.01	126.38	124.26
19	B	806	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
19	K	203	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
19	7	611	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
19	4	602	CLA	CHB-C1B-NB	2.00	126.38	124.26
19	A	826	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
20	4	607	CHL	CHC-C1C-NC	-2.00	121.17	124.20
20	8	320	CHL	C2B-C1B-NB	-2.00	108.89	110.23
19	K	202	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
19	5	305	CLA	CHB-C1B-NB	2.00	126.38	124.26
19	8	314	CLA	CHB-C1B-NB	2.00	126.38	124.26
19	B	812	CLA	CHB-C1B-NB	2.00	126.38	124.26
19	7	604	CLA	CHD-C1D-ND	-2.00	122.61	124.45
19	5	304	CLA	CMB-C2B-C3B	2.00	131.43	126.59
20	6	315	CHL	C2B-C1B-NB	-2.00	108.89	110.23
19	6	320	CLA	CMB-C2B-C3B	2.00	131.43	126.59
20	6	302	CHL	CHD-C1D-ND	2.00	126.29	124.45

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	5	323	NEX	C25

All (2193) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	3	302	CLA	C11-C12-C13-C14
19	3	305	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	3	309	CLA	CBD-CGD-O2D-CED
19	3	312	CLA	C2B-C3B-CAB-CBB
19	3	312	CLA	C4B-C3B-CAB-CBB
19	3	313	CLA	CBD-CGD-O2D-CED
19	3	313	CLA	C2-C3-C5-C6
19	3	313	CLA	C4-C3-C5-C6
19	4	614	CLA	C1A-C2A-CAA-CBA
19	4	614	CLA	C3A-C2A-CAA-CBA
19	5	302	CLA	C2B-C3B-CAB-CBB
19	5	302	CLA	C4B-C3B-CAB-CBB
19	5	309	CLA	C6-C7-C8-C9
19	5	314	CLA	CBD-CGD-O2D-CED
19	5	316	CLA	CBD-CGD-O2D-CED
19	6	304	CLA	C2-C3-C5-C6
19	6	304	CLA	C4-C3-C5-C6
19	6	309	CLA	C1A-C2A-CAA-CBA
19	6	316	CLA	C2B-C3B-CAB-CBB
19	6	316	CLA	C4B-C3B-CAB-CBB
19	7	609	CLA	C1A-C2A-CAA-CBA
19	7	609	CLA	C3A-C2A-CAA-CBA
19	7	611	CLA	C3-C5-C6-C7
19	7	613	CLA	CHA-CBD-CGD-O1D
19	7	613	CLA	CHA-CBD-CGD-O2D
19	8	303	CLA	C2-C3-C5-C6
19	8	303	CLA	C4-C3-C5-C6
19	A	807	CLA	C3A-C2A-CAA-CBA
19	A	807	CLA	CHA-CBD-CGD-O1D
19	A	807	CLA	CHA-CBD-CGD-O2D
19	A	820	CLA	C1A-C2A-CAA-CBA
19	A	820	CLA	C3A-C2A-CAA-CBA
19	A	821	CLA	CHA-CBD-CGD-O1D
19	A	821	CLA	CHA-CBD-CGD-O2D
19	A	826	CLA	CHA-CBD-CGD-O1D
19	A	826	CLA	CHA-CBD-CGD-O2D
19	A	832	CLA	CHA-CBD-CGD-O1D
19	A	832	CLA	CHA-CBD-CGD-O2D
19	A	838	CLA	CHA-CBD-CGD-O1D
19	A	838	CLA	CHA-CBD-CGD-O2D
19	A	841	CLA	CHA-CBD-CGD-O1D
19	A	841	CLA	CHA-CBD-CGD-O2D
19	A	842	CLA	CHA-CBD-CGD-O1D
19	A	842	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	A	846	CLA	CHA-CBD-CGD-O1D
19	A	846	CLA	CHA-CBD-CGD-O2D
19	B	803	CLA	CHA-CBD-CGD-O1D
19	B	803	CLA	CHA-CBD-CGD-O2D
19	B	806	CLA	C3A-C2A-CAA-CBA
19	B	813	CLA	C11-C12-C13-C14
19	B	818	CLA	C1A-C2A-CAA-CBA
19	B	818	CLA	C3A-C2A-CAA-CBA
19	B	824	CLA	CHA-CBD-CGD-O1D
19	B	824	CLA	CHA-CBD-CGD-O2D
19	B	836	CLA	C1A-C2A-CAA-CBA
19	B	841	CLA	C1A-C2A-CAA-CBA
19	J	102	CLA	C1A-C2A-CAA-CBA
19	K	203	CLA	C1A-C2A-CAA-CBA
19	K	205	CLA	CHA-CBD-CGD-O2D
19	Z	608	CLA	C1A-C2A-CAA-CBA
19	Z	608	CLA	C3A-C2A-CAA-CBA
19	Z	608	CLA	C4B-C3B-CAB-CBB
19	1	303	CLA	CBA-CGA-O2A-C1
19	1	310	CLA	C6-C7-C8-C10
19	1	312	CLA	CHA-CBD-CGD-O1D
19	1	312	CLA	CHA-CBD-CGD-O2D
19	1	313	CLA	C6-C7-C8-C10
19	F	304	CLA	CHA-CBD-CGD-O1D
19	F	304	CLA	CHA-CBD-CGD-O2D
19	F	304	CLA	CAD-CBD-CGD-O1D
19	G	202	CLA	C2B-C3B-CAB-CBB
19	G	202	CLA	C4B-C3B-CAB-CBB
19	G	203	CLA	C2A-CAA-CBA-CGA
19	L	203	CLA	C2-C3-C5-C6
19	L	203	CLA	C4-C3-C5-C6
20	4	605	CHL	C1-C2-C3-C4
20	4	605	CHL	C6-C7-C8-C10
20	4	606	CHL	C1A-C2A-CAA-CBA
20	4	607	CHL	C1-C2-C3-C4
20	4	607	CHL	C1-C2-C3-C5
20	4	607	CHL	C6-C7-C8-C9
20	4	615	CHL	C1A-C2A-CAA-CBA
20	4	615	CHL	C3A-C2A-CAA-CBA
20	5	307	CHL	C11-C10-C8-C9
20	5	308	CHL	C1-C2-C3-C4
20	5	308	CHL	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
20	6	302	CHL	C1-C2-C3-C4
20	6	302	CHL	C14-C13-C15-C16
20	6	307	CHL	CBD-CGD-O2D-CED
20	6	307	CHL	O1D-CGD-O2D-CED
20	6	307	CHL	C1-C2-C3-C4
20	6	307	CHL	C1-C2-C3-C5
20	6	308	CHL	C1-C2-C3-C4
20	6	308	CHL	C1-C2-C3-C5
20	6	315	CHL	C1A-C2A-CAA-CBA
20	6	315	CHL	CBA-CGA-O2A-C1
20	6	315	CHL	O1A-CGA-O2A-C1
20	6	315	CHL	CHA-CBD-CGD-O1D
20	6	315	CHL	CHA-CBD-CGD-O2D
20	6	315	CHL	C1-C2-C3-C4
20	7	601	CHL	C1-C2-C3-C4
20	7	606	CHL	C1A-C2A-CAA-CBA
20	7	621	CHL	C2B-C3B-CAB-CBB
20	8	305	CHL	C1-C2-C3-C4
20	8	306	CHL	C1A-C2A-CAA-CBA
20	8	306	CHL	C3A-C2A-CAA-CBA
20	8	306	CHL	C1-C2-C3-C4
20	8	306	CHL	C1-C2-C3-C5
20	8	306	CHL	C11-C10-C8-C9
20	8	306	CHL	C14-C13-C15-C16
20	Z	601	CHL	C6-C7-C8-C9
20	Z	601	CHL	C11-C12-C13-C14
21	3	315	BCR	C1-C6-C7-C8
21	3	315	BCR	C5-C6-C7-C8
21	3	315	BCR	C23-C24-C25-C30
21	3	318	BCR	C11-C12-C13-C14
21	3	318	BCR	C11-C12-C13-C35
21	4	618	BCR	C36-C18-C19-C20
21	6	321	BCR	C11-C12-C13-C14
21	6	321	BCR	C11-C12-C13-C35
21	7	617	BCR	C11-C12-C13-C35
21	8	317	BCR	C5-C6-C7-C8
21	A	851	BCR	C1-C6-C7-C8
21	A	851	BCR	C7-C8-C9-C10
21	A	851	BCR	C7-C8-C9-C34
21	A	852	BCR	C21-C22-C23-C24
21	A	852	BCR	C23-C24-C25-C26
21	A	852	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
21	A	858	BCR	C21-C22-C23-C24
21	A	858	BCR	C37-C22-C23-C24
21	A	858	BCR	C23-C24-C25-C26
21	B	802	BCR	C11-C12-C13-C14
21	B	802	BCR	C11-C12-C13-C35
21	B	802	BCR	C17-C18-C19-C20
21	B	802	BCR	C36-C18-C19-C20
21	B	802	BCR	C23-C24-C25-C26
21	B	844	BCR	C7-C8-C9-C34
21	B	845	BCR	C1-C6-C7-C8
21	B	845	BCR	C23-C24-C25-C26
21	B	848	BCR	C21-C22-C23-C24
21	B	848	BCR	C37-C22-C23-C24
21	I	201	BCR	C5-C6-C7-C8
21	I	201	BCR	C7-C8-C9-C10
21	I	201	BCR	C7-C8-C9-C34
21	J	103	BCR	C17-C18-C19-C20
21	J	103	BCR	C36-C18-C19-C20
21	L	205	BCR	C37-C22-C23-C24
21	L	205	BCR	C23-C24-C25-C26
22	3	320	LUT	C31-C32-C33-C40
22	5	324	LUT	C1-C6-C7-C8
22	5	324	LUT	C5-C6-C7-C8
22	5	324	LUT	C11-C12-C13-C20
22	5	324	LUT	C27-C28-C29-C30
22	6	319	LUT	C7-C8-C9-C19
22	J	101	LUT	C5-C6-C7-C8
22	J	101	LUT	C7-C8-C9-C19
22	1	317	LUT	C40-C33-C34-C35
22	F	305	LUT	C14-C15-C35-C34
22	F	305	LUT	C27-C28-C29-C39
23	3	321	LMG	C2-C1-O1-C7
23	3	321	LMG	O6-C1-O1-C7
23	3	321	LMG	C11-C10-O7-C8
23	B	852	LMG	C2-C1-O1-C7
23	B	852	LMG	O6-C1-O1-C7
23	J	105	LMG	C11-C10-O7-C8
23	F	301	LMG	C11-C10-O7-C8
24	3	324	LMU	C2-C1-O1'-C1'
24	3	325	LMU	C2'-C1'-O1'-C1
24	3	325	LMU	O5'-C1'-O1'-C1
24	3	325	LMU	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
24	4	622	LMU	C2'-C1'-O1'-C1
24	4	622	LMU	O5'-C1'-O1'-C1
24	4	623	LMU	C2-C1-O1'-C1'
24	6	328	LMU	C2'-C1'-O1'-C1
24	6	328	LMU	O5'-C1'-O1'-C1
24	A	855	LMU	C2'-C1'-O1'-C1
24	A	855	LMU	O5'-C1'-O1'-C1
24	A	855	LMU	C2-C1-O1'-C1'
24	A	856	LMU	C2'-C1'-O1'-C1
24	A	856	LMU	O5'-C1'-O1'-C1
24	A	857	LMU	C2-C1-O1'-C1'
24	1	301	LMU	O5B-C1B-O1B-C4'
24	1	301	LMU	C2-C1-O1'-C1'
24	F	306	LMU	C2'-C1'-O1'-C1
25	Z	616	XAT	C7-C8-C9-C10
25	Z	616	XAT	C7-C8-C9-C19
26	5	301	LHG	C2-C3-O3-P
26	5	301	LHG	C3-O3-P-O4
26	5	301	LHG	C3-O3-P-O5
26	5	301	LHG	C3-O3-P-O6
26	5	321	LHG	C1-C2-C3-O3
26	5	321	LHG	C4-O6-P-O4
26	5	321	LHG	C4-O6-P-O5
26	6	325	LHG	C3-O3-P-O5
26	7	618	LHG	C3-O3-P-O5
31	B	850	DGD	C2D-C1D-O3G-C3G
31	B	850	DGD	O6D-C1D-O3G-C3G
19	4	612	CLA	CBD-CGD-O2D-CED
19	6	314	CLA	CBD-CGD-O2D-CED
19	8	303	CLA	O1A-CGA-O2A-C1
19	1	303	CLA	O1A-CGA-O2A-C1
19	5	314	CLA	O1D-CGD-O2D-CED
19	3	313	CLA	O1D-CGD-O2D-CED
19	5	316	CLA	O1D-CGD-O2D-CED
19	8	303	CLA	CBA-CGA-O2A-C1
19	3	302	CLA	CBD-CGD-O2D-CED
19	4	603	CLA	CBD-CGD-O2D-CED
19	B	805	CLA	CBD-CGD-O2D-CED
19	B	811	CLA	CBD-CGD-O2D-CED
19	K	202	CLA	CBD-CGD-O2D-CED
19	Z	607	CLA	CBD-CGD-O2D-CED
19	1	307	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	4	608	CLA	O1A-CGA-O2A-C1
19	Z	610	CLA	O1A-CGA-O2A-C1
19	3	309	CLA	O1D-CGD-O2D-CED
19	5	315	CLA	CBD-CGD-O2D-CED
19	B	828	CLA	CBD-CGD-O2D-CED
19	B	836	CLA	CBD-CGD-O2D-CED
23	3	321	LMG	O9-C10-O7-C8
23	J	105	LMG	O9-C10-O7-C8
23	F	301	LMG	O9-C10-O7-C8
26	A	801	LHG	O9-C7-O7-C5
19	1	314	CLA	CBA-CGA-O2A-C1
19	7	614	CLA	O1A-CGA-O2A-C1
19	8	303	CLA	C3-C5-C6-C7
19	A	824	CLA	C3-C5-C6-C7
19	A	844	CLA	C3-C5-C6-C7
19	B	813	CLA	C3-C5-C6-C7
19	B	834	CLA	C3-C5-C6-C7
19	4	608	CLA	CBA-CGA-O2A-C1
26	A	801	LHG	C8-C7-O7-C5
19	6	316	CLA	CBD-CGD-O2D-CED
19	A	808	CLA	CBD-CGD-O2D-CED
19	A	819	CLA	CBD-CGD-O2D-CED
19	7	614	CLA	CBA-CGA-O2A-C1
19	1	308	CLA	CBD-CGD-O2D-CED
19	8	303	CLA	C2A-CAA-CBA-CGA
19	A	844	CLA	C2A-CAA-CBA-CGA
19	B	840	CLA	C2A-CAA-CBA-CGA
20	6	315	CHL	C2A-CAA-CBA-CGA
19	1	314	CLA	O1A-CGA-O2A-C1
19	6	309	CLA	C3-C5-C6-C7
19	7	610	CLA	C3-C5-C6-C7
19	B	807	CLA	C3-C5-C6-C7
19	F	304	CLA	C3-C5-C6-C7
19	B	841	CLA	CBA-CGA-O2A-C1
19	Z	610	CLA	CBA-CGA-O2A-C1
26	6	325	LHG	C24-C23-O8-C6
20	6	315	CHL	C1-C2-C3-C5
19	A	833	CLA	CBD-CGD-O2D-CED
19	B	818	CLA	CBD-CGD-O2D-CED
26	6	325	LHG	O10-C23-O8-C6
19	5	319	CLA	CBD-CGD-O2D-CED
19	6	304	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	835	CLA	CBD-CGD-O2D-CED
19	B	812	CLA	CBD-CGD-O2D-CED
19	B	823	CLA	CBD-CGD-O2D-CED
19	1	307	CLA	C3-C5-C6-C7
19	6	320	CLA	CBA-CGA-O2A-C1
19	7	609	CLA	CBA-CGA-O2A-C1
19	A	824	CLA	CBA-CGA-O2A-C1
19	F	304	CLA	CBA-CGA-O2A-C1
26	B	851	LHG	C24-C23-O8-C6
19	6	314	CLA	O1D-CGD-O2D-CED
19	3	310	CLA	CBD-CGD-O2D-CED
19	5	302	CLA	CBD-CGD-O2D-CED
19	B	841	CLA	CBD-CGD-O2D-CED
19	G	202	CLA	CBD-CGD-O2D-CED
19	4	612	CLA	O1D-CGD-O2D-CED
19	A	836	CLA	CBD-CGD-O2D-CED
19	Z	604	CLA	C3-C5-C6-C7
19	7	609	CLA	O1A-CGA-O2A-C1
19	A	824	CLA	O1A-CGA-O2A-C1
19	B	841	CLA	O1A-CGA-O2A-C1
26	B	851	LHG	O10-C23-O8-C6
19	5	316	CLA	C4-C3-C5-C6
19	1	303	CLA	C4-C3-C5-C6
19	5	316	CLA	C2-C3-C5-C6
19	1	303	CLA	C2-C3-C5-C6
20	4	607	CHL	C2A-CAA-CBA-CGA
19	6	320	CLA	O1A-CGA-O2A-C1
19	F	304	CLA	O1A-CGA-O2A-C1
19	A	834	CLA	CBA-CGA-O2A-C1
19	A	844	CLA	CBA-CGA-O2A-C1
19	B	822	CLA	CBA-CGA-O2A-C1
19	B	832	CLA	CBA-CGA-O2A-C1
19	Z	607	CLA	CBA-CGA-O2A-C1
19	8	311	CLA	CBD-CGD-O2D-CED
23	8	321	LMG	O6-C5-C6-O5
24	Z	619	LMU	O5'-C5'-C6'-O6'
20	4	605	CHL	C1-C2-C3-C5
19	3	302	CLA	O1D-CGD-O2D-CED
19	B	811	CLA	O1D-CGD-O2D-CED
19	Z	607	CLA	O1D-CGD-O2D-CED
19	A	830	CLA	CBD-CGD-O2D-CED
19	A	844	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	Z	607	CLA	O1A-CGA-O2A-C1
19	A	820	CLA	C3-C5-C6-C7
19	4	603	CLA	O1D-CGD-O2D-CED
19	K	202	CLA	O1D-CGD-O2D-CED
19	1	310	CLA	CBA-CGA-O2A-C1
26	1	318	LHG	C27-C28-C29-C30
19	8	303	CLA	C5-C6-C7-C8
19	B	817	CLA	C10-C11-C12-C13
19	B	842	CLA	C8-C10-C11-C12
26	6	318	LHG	C23-C24-C25-C26
19	3	307	CLA	C6-C7-C8-C9
19	3	308	CLA	C14-C13-C15-C16
19	4	603	CLA	C11-C10-C8-C9
19	4	608	CLA	C11-C10-C8-C9
19	6	305	CLA	C11-C10-C8-C9
19	A	807	CLA	C6-C7-C8-C9
19	A	820	CLA	C11-C10-C8-C9
19	B	804	CLA	C14-C13-C15-C16
19	B	812	CLA	C6-C7-C8-C9
19	B	813	CLA	C6-C7-C8-C9
19	B	822	CLA	C6-C7-C8-C9
19	B	825	CLA	C14-C13-C15-C16
19	B	826	CLA	C6-C7-C8-C9
19	B	837	CLA	C6-C7-C8-C9
19	Z	608	CLA	C11-C10-C8-C9
19	1	308	CLA	C11-C10-C8-C9
20	4	605	CHL	C11-C10-C8-C9
20	5	307	CHL	C11-C12-C13-C14
20	6	307	CHL	C11-C10-C8-C9
20	7	601	CHL	C11-C12-C13-C14
20	7	621	CHL	C14-C13-C15-C16
20	Z	606	CHL	C6-C7-C8-C9
19	B	842	CLA	CBD-CGD-O2D-CED
19	B	842	CLA	C10-C11-C12-C13
21	5	320	BCR	C37-C22-C23-C24
21	A	852	BCR	C37-C22-C23-C24
22	5	324	LUT	C27-C28-C29-C39
22	Z	615	LUT	C7-C8-C9-C19
21	B	844	BCR	C7-C8-C9-C10
21	L	205	BCR	C21-C22-C23-C24
24	6	328	LMU	C4'-C5'-C6'-O6'
23	4	621	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	5	316	CLA	C8-C10-C11-C12
19	8	303	CLA	C13-C15-C16-C17
19	A	838	CLA	C5-C6-C7-C8
24	Z	619	LMU	O5B-C1B-O1B-C4'
19	B	804	CLA	C2C-C3C-CAC-CBC
19	5	304	CLA	CBA-CGA-O2A-C1
19	7	610	CLA	C8-C10-C11-C12
19	A	816	CLA	C5-C6-C7-C8
19	A	824	CLA	C8-C10-C11-C12
19	A	824	CLA	C10-C11-C12-C13
19	A	841	CLA	C5-C6-C7-C8
19	B	817	CLA	C5-C6-C7-C8
23	6	301	LMG	C28-C29-C30-C31
26	A	801	LHG	C23-C24-C25-C26
19	3	302	CLA	C8-C10-C11-C12
19	4	608	CLA	C5-C6-C7-C8
19	5	316	CLA	C10-C11-C12-C13
19	5	316	CLA	C13-C15-C16-C17
19	A	805	CLA	C13-C15-C16-C17
19	A	807	CLA	C8-C10-C11-C12
19	A	830	CLA	C10-C11-C12-C13
19	B	818	CLA	C13-C15-C16-C17
19	B	828	CLA	C13-C15-C16-C17
19	J	102	CLA	C5-C6-C7-C8
19	Z	608	CLA	C8-C10-C11-C12
26	7	618	LHG	C33-C34-C35-C36
23	6	301	LMG	C10-C11-C12-C13
23	F	301	LMG	C28-C29-C30-C31
26	4	619	LHG	C7-C8-C9-C10
26	5	301	LHG	C7-C8-C9-C10
26	1	318	LHG	C7-C8-C9-C10
24	K	201	LMU	O1'-C1-C2-C3
19	1	311	CLA	CBD-CGD-O2D-CED
19	3	303	CLA	C15-C16-C17-C18
19	4	603	CLA	C10-C11-C12-C13
19	B	810	CLA	C13-C15-C16-C17
19	7	603	CLA	CBA-CGA-O2A-C1
23	J	105	LMG	C30-C31-C32-C33
19	1	307	CLA	O1D-CGD-O2D-CED
19	A	818	CLA	C5-C6-C7-C8
19	1	307	CLA	C15-C16-C17-C18
19	L	203	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	A	846	CLA	CBD-CGD-O2D-CED
19	Z	602	CLA	CBD-CGD-O2D-CED
24	1	301	LMU	O1'-C1-C2-C3
24	1	319	LMU	O1'-C1-C2-C3
26	7	618	LHG	C31-C32-C33-C34
26	B	851	LHG	C27-C28-C29-C30
19	5	302	CLA	C10-C11-C12-C13
19	A	833	CLA	C5-C6-C7-C8
19	B	837	CLA	C5-C6-C7-C8
19	4	608	CLA	C11-C10-C8-C7
19	8	302	CLA	C12-C13-C15-C16
19	8	303	CLA	C6-C7-C8-C10
19	A	807	CLA	C11-C12-C13-C15
19	A	812	CLA	C12-C13-C15-C16
19	A	828	CLA	C12-C13-C15-C16
19	B	835	CLA	C6-C7-C8-C10
19	1	309	CLA	C12-C13-C15-C16
20	4	605	CHL	C11-C12-C13-C15
20	6	302	CHL	C12-C13-C15-C16
20	Z	601	CHL	C11-C10-C8-C7
19	B	814	CLA	C3-C5-C6-C7
26	A	847	LHG	C23-C24-C25-C26
19	A	831	CLA	C2A-CAA-CBA-CGA
19	G	202	CLA	C2A-CAA-CBA-CGA
20	Z	606	CHL	C2A-CAA-CBA-CGA
19	5	315	CLA	O1D-CGD-O2D-CED
19	B	805	CLA	O1D-CGD-O2D-CED
19	A	834	CLA	C10-C11-C12-C13
19	B	806	CLA	C15-C16-C17-C18
19	1	307	CLA	C13-C15-C16-C17
19	G	202	CLA	C8-C10-C11-C12
22	5	324	LUT	C6-C7-C8-C9
19	B	832	CLA	O1A-CGA-O2A-C1
19	1	310	CLA	O1A-CGA-O2A-C1
19	B	803	CLA	CBD-CGD-O2D-CED
19	Z	612	CLA	CBD-CGD-O2D-CED
23	8	321	LMG	C4-C5-C6-O5
24	7	619	LMU	O5'-C1'-O1'-C1
24	F	306	LMU	O5'-C1'-O1'-C1
19	B	836	CLA	O1D-CGD-O2D-CED
19	5	312	CLA	C2C-C3C-CAC-CBC
23	8	321	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
26	1	318	LHG	C23-C24-C25-C26
22	5	318	LUT	C10-C11-C12-C13
19	A	831	CLA	C5-C6-C7-C8
19	B	804	CLA	C13-C15-C16-C17
20	Z	606	CHL	C8-C10-C11-C12
19	6	311	CLA	CBA-CGA-O2A-C1
19	5	304	CLA	O1A-CGA-O2A-C1
19	A	834	CLA	O1A-CGA-O2A-C1
19	B	822	CLA	O1A-CGA-O2A-C1
19	5	316	CLA	C15-C16-C17-C18
19	A	811	CLA	C10-C11-C12-C13
19	A	835	CLA	C15-C16-C17-C18
19	B	801	CLA	C10-C11-C12-C13
19	B	812	CLA	C13-C15-C16-C17
19	B	821	CLA	C5-C6-C7-C8
19	B	838	CLA	C5-C6-C7-C8
19	A	808	CLA	O1D-CGD-O2D-CED
19	A	819	CLA	O1D-CGD-O2D-CED
24	1	301	LMU	C4B-C5B-C6B-O6B
19	6	316	CLA	O1D-CGD-O2D-CED
19	5	309	CLA	C5-C6-C7-C8
19	F	304	CLA	C5-C6-C7-C8
20	6	315	CHL	C8-C10-C11-C12
20	7	601	CHL	C1-C2-C3-C5
26	5	321	LHG	C4-O6-P-O3
26	7	618	LHG	C3-O3-P-O6
23	L	201	LMG	C28-C29-C30-C31
19	Z	603	CLA	C3-C5-C6-C7
19	1	303	CLA	C3-C5-C6-C7
19	L	203	CLA	C3-C5-C6-C7
26	5	321	LHG	C9-C10-C11-C12
19	6	314	CLA	CBA-CGA-O2A-C1
19	G	202	CLA	CBA-CGA-O2A-C1
23	3	321	LMG	C29-C28-O8-C9
23	8	321	LMG	C29-C28-O8-C9
19	8	303	CLA	C15-C16-C17-C18
26	7	618	LHG	C7-C8-C9-C10
19	B	828	CLA	O1D-CGD-O2D-CED
19	1	303	CLA	C2A-CAA-CBA-CGA
20	4	605	CHL	C2A-CAA-CBA-CGA
19	3	311	CLA	C11-C12-C13-C14
19	A	833	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B	815	CLA	C11-C12-C13-C14
19	1	302	CLA	C11-C12-C13-C15
19	5	305	CLA	CBA-CGA-O2A-C1
19	B	812	CLA	CBA-CGA-O2A-C1
19	1	313	CLA	CBA-CGA-O2A-C1
23	L	201	LMG	C29-C28-O8-C9
24	7	620	LMU	O1'-C1-C2-C3
24	1	301	LMU	C4-C5-C6-C7
26	A	801	LHG	C24-C25-C26-C27
26	1	318	LHG	C29-C30-C31-C32
26	4	620	LHG	C8-C7-O7-C5
22	5	324	LUT	C39-C29-C30-C31
22	8	301	LUT	C39-C29-C30-C31
22	1	317	LUT	C39-C29-C30-C31
24	6	328	LMU	O5'-C5'-C6'-O6'
27	6	323	NEX	C39-C29-C30-C31
23	6	301	LMG	C16-C17-C18-C19
24	3	323	LMU	O1'-C1-C2-C3
24	4	623	LMU	C4-C5-C6-C7
24	7	620	LMU	C3-C4-C5-C6
26	8	318	LHG	C16-C17-C18-C19
19	A	837	CLA	C16-C17-C18-C19
19	B	812	CLA	C16-C17-C18-C19
19	B	822	CLA	C16-C17-C18-C19
19	B	826	CLA	C16-C17-C18-C20
19	L	203	CLA	C16-C17-C18-C20
23	8	321	LMG	C30-C31-C32-C33
26	4	619	LHG	C11-C12-C13-C14
26	6	325	LHG	C14-C15-C16-C17
24	Z	619	LMU	C2B-C1B-O1B-C4'
19	Z	608	CLA	CBD-CGD-O2D-CED
26	A	847	LHG	C11-C10-C9-C8
19	1	308	CLA	O1D-CGD-O2D-CED
19	7	603	CLA	O1A-CGA-O2A-C1
24	1	301	LMU	O5B-C5B-C6B-O6B
26	6	318	LHG	C25-C26-C27-C28
31	B	850	DGD	C9B-CAB-CBB-CCB
26	5	321	LHG	O2-C2-C3-O3
26	7	618	LHG	C26-C27-C28-C29
19	A	833	CLA	O1D-CGD-O2D-CED
19	B	812	CLA	O1D-CGD-O2D-CED
19	B	818	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	1	317	LUT	C32-C33-C34-C35
24	7	619	LMU	C2'-C1'-O1'-C1
24	8	319	LMU	C2'-C1'-O1'-C1
24	K	201	LMU	C2'-C1'-O1'-C1
24	1	301	LMU	C2'-C1'-O1'-C1
24	3	325	LMU	C4'-C5'-C6'-O6'
19	Z	604	CLA	CBA-CGA-O2A-C1
20	6	302	CHL	C1-C2-C3-C5
19	5	305	CLA	O1A-CGA-O2A-C1
19	B	812	CLA	O1A-CGA-O2A-C1
23	3	321	LMG	O10-C28-O8-C9
19	5	302	CLA	C16-C17-C18-C20
19	5	309	CLA	C16-C17-C18-C19
19	6	309	CLA	C6-C7-C8-C9
19	8	309	CLA	C16-C17-C18-C19
19	A	824	CLA	C4-C3-C5-C6
19	A	842	CLA	C4-C3-C5-C6
19	B	801	CLA	C4-C3-C5-C6
19	B	833	CLA	C4-C3-C5-C6
23	8	321	LMG	C40-C41-C42-C43
24	3	322	LMU	C6-C7-C8-C9
24	1	320	LMU	C2-C3-C4-C5
26	A	847	LHG	C29-C30-C31-C32
19	A	822	CLA	C2-C3-C5-C6
19	3	302	CLA	C6-C7-C8-C9
19	A	844	CLA	C11-C10-C8-C9
19	B	820	CLA	C11-C10-C8-C9
19	B	826	CLA	C14-C13-C15-C16
19	B	828	CLA	C14-C13-C15-C16
19	B	833	CLA	C6-C7-C8-C9
20	4	605	CHL	C6-C7-C8-C9
20	4	607	CHL	C14-C13-C15-C16
20	7	621	CHL	C11-C10-C8-C9
20	8	320	CHL	C11-C10-C8-C9
23	8	321	LMG	C34-C35-C36-C37
19	A	815	CLA	C10-C11-C12-C13
19	A	840	CLA	C10-C11-C12-C13
19	B	822	CLA	C15-C16-C17-C18
19	A	810	CLA	C2A-CAA-CBA-CGA
19	6	311	CLA	O1A-CGA-O2A-C1
19	5	319	CLA	C2C-C3C-CAC-CBC
24	3	323	LMU	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	B	851	LHG	C30-C31-C32-C33
26	1	318	LHG	C25-C26-C27-C28
31	B	850	DGD	C4B-C5B-C6B-C7B
26	6	318	LHG	O1-C1-C2-C3
26	8	318	LHG	O1-C1-C2-C3
26	A	801	LHG	O1-C1-C2-C3
22	F	305	LUT	C27-C28-C29-C30
19	A	833	CLA	C3-C5-C6-C7
24	1	319	LMU	O5'-C5'-C6'-O6'
26	4	620	LHG	O9-C7-O7-C5
24	4	622	LMU	C5-C6-C7-C8
24	7	620	LMU	C4-C5-C6-C7
24	8	319	LMU	C2-C3-C4-C5
26	6	318	LHG	C11-C10-C9-C8
26	8	318	LHG	C11-C10-C9-C8
26	A	848	LHG	C11-C10-C9-C8
26	B	851	LHG	C29-C30-C31-C32
26	1	318	LHG	C13-C14-C15-C16
26	1	318	LHG	C32-C33-C34-C35
24	3	324	LMU	O5'-C5'-C6'-O6'
19	4	612	CLA	C4B-C3B-CAB-CBB
19	6	311	CLA	C4B-C3B-CAB-CBB
19	7	614	CLA	C4B-C3B-CAB-CBB
19	8	310	CLA	C4B-C3B-CAB-CBB
19	A	835	CLA	C4B-C3B-CAB-CBB
19	B	820	CLA	C4B-C3B-CAB-CBB
20	4	601	CHL	C4B-C3B-CAB-CBB
20	7	621	CHL	C4B-C3B-CAB-CBB
20	8	320	CHL	C4B-C3B-CAB-CBB
20	Z	601	CHL	C4B-C3B-CAB-CBB
20	Z	605	CHL	C4B-C3B-CAB-CBB
20	Z	606	CHL	C4B-C3B-CAB-CBB
28	A	802	CL0	C4B-C3B-CAB-CBB
19	A	805	CLA	C16-C17-C18-C19
19	A	805	CLA	C16-C17-C18-C20
19	A	814	CLA	C16-C17-C18-C19
19	A	822	CLA	C6-C7-C8-C10
19	A	833	CLA	C6-C7-C8-C10
19	B	830	CLA	C16-C17-C18-C19
19	B	830	CLA	C16-C17-C18-C20
19	1	302	CLA	C11-C12-C13-C14
24	1	301	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
19	4	603	CLA	C15-C16-C17-C18
19	B	822	CLA	C5-C6-C7-C8
26	Z	618	LHG	C29-C30-C31-C32
31	B	850	DGD	CCB-CDB-CEB-CFB
23	3	321	LMG	C13-C14-C15-C16
26	5	301	LHG	C11-C12-C13-C14
19	A	815	CLA	C13-C15-C16-C17
19	5	319	CLA	O1D-CGD-O2D-CED
23	J	105	LMG	O6-C5-C6-O5
19	6	305	CLA	CBA-CGA-O2A-C1
19	7	610	CLA	CBA-CGA-O2A-C1
23	8	321	LMG	C15-C16-C17-C18
19	A	835	CLA	O1D-CGD-O2D-CED
19	5	304	CLA	C3A-C2A-CAA-CBA
19	6	309	CLA	C3A-C2A-CAA-CBA
19	7	614	CLA	C3A-C2A-CAA-CBA
19	B	836	CLA	C3A-C2A-CAA-CBA
19	J	102	CLA	C3A-C2A-CAA-CBA
19	K	203	CLA	C3A-C2A-CAA-CBA
20	5	306	CHL	C3A-C2A-CAA-CBA
20	6	306	CHL	C3A-C2A-CAA-CBA
20	6	315	CHL	C3A-C2A-CAA-CBA
20	8	305	CHL	C3A-C2A-CAA-CBA
20	Z	605	CHL	C3A-C2A-CAA-CBA
23	4	621	LMG	O6-C5-C6-O5
24	4	624	LMU	C2-C1-O1'-C1'
24	7	620	LMU	C5-C6-C7-C8
19	B	823	CLA	O1D-CGD-O2D-CED
19	1	313	CLA	O1A-CGA-O2A-C1
19	G	202	CLA	O1A-CGA-O2A-C1
19	5	310	CLA	C11-C12-C13-C15
19	A	814	CLA	C16-C17-C18-C20
19	A	822	CLA	C6-C7-C8-C9
19	A	837	CLA	C16-C17-C18-C20
19	B	815	CLA	C11-C12-C13-C15
19	L	203	CLA	C16-C17-C18-C19
23	J	104	LMG	C13-C14-C15-C16
24	1	301	LMU	O5'-C5'-C6'-O6'
24	4	624	LMU	C1-C2-C3-C4
24	3	324	LMU	C5-C6-C7-C8
26	7	618	LHG	C10-C11-C12-C13
19	1	310	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	1	321	LMU	O5'-C5'-C6'-O6'
24	Z	621	LMU	C1-C2-C3-C4
19	6	314	CLA	O1A-CGA-O2A-C1
19	4	612	CLA	C5-C6-C7-C8
19	6	305	CLA	C4-C3-C5-C6
19	B	821	CLA	C4-C3-C5-C6
23	F	301	LMG	C29-C28-O8-C9
19	A	824	CLA	C2-C3-C5-C6
19	B	816	CLA	C2-C3-C5-C6
19	B	821	CLA	C2-C3-C5-C6
19	B	824	CLA	C2-C3-C5-C6
19	5	311	CLA	C5-C6-C7-C8
24	Z	621	LMU	C7-C8-C9-C10
31	B	850	DGD	C8B-C9B-CAB-CBB
23	4	621	LMG	C28-C29-C30-C31
23	8	321	LMG	O10-C28-O8-C9
23	L	201	LMG	O10-C28-O8-C9
19	5	305	CLA	C6-C7-C8-C9
19	B	812	CLA	C16-C17-C18-C20
19	B	822	CLA	C16-C17-C18-C20
19	B	826	CLA	C16-C17-C18-C19
19	F	302	CLA	C16-C17-C18-C19
23	4	621	LMG	C23-C24-C25-C26
26	5	321	LHG	C25-C26-C27-C28
19	4	612	CLA	C2B-C3B-CAB-CBB
19	6	311	CLA	C2B-C3B-CAB-CBB
19	7	614	CLA	C2B-C3B-CAB-CBB
19	8	310	CLA	C2B-C3B-CAB-CBB
19	A	835	CLA	C2B-C3B-CAB-CBB
19	B	820	CLA	C2B-C3B-CAB-CBB
19	K	202	CLA	C2B-C3B-CAB-CBB
19	Z	608	CLA	C2B-C3B-CAB-CBB
20	4	601	CHL	C2B-C3B-CAB-CBB
20	8	320	CHL	C2B-C3B-CAB-CBB
20	Z	601	CHL	C2B-C3B-CAB-CBB
20	Z	605	CHL	C2B-C3B-CAB-CBB
20	Z	606	CHL	C2B-C3B-CAB-CBB
28	A	802	CL0	C2B-C3B-CAB-CBB
24	F	306	LMU	C1-C2-C3-C4
19	A	821	CLA	C15-C16-C17-C18
20	6	307	CHL	C15-C16-C17-C18
23	4	621	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
23	7	622	LMG	C12-C13-C14-C15
26	7	618	LHG	C17-C18-C19-C20
24	1	322	LMU	C1-C2-C3-C4
26	4	619	LHG	C16-C17-C18-C19
19	8	304	CLA	C8-C10-C11-C12
19	B	815	CLA	C5-C6-C7-C8
21	3	315	BCR	C23-C24-C25-C26
21	3	318	BCR	C23-C24-C25-C26
21	3	318	BCR	C23-C24-C25-C30
21	8	317	BCR	C1-C6-C7-C8
21	A	851	BCR	C5-C6-C7-C8
21	A	858	BCR	C23-C24-C25-C30
21	B	802	BCR	C23-C24-C25-C30
21	B	844	BCR	C1-C6-C7-C8
21	B	845	BCR	C5-C6-C7-C8
21	I	201	BCR	C1-C6-C7-C8
21	J	103	BCR	C23-C24-C25-C26
21	J	103	BCR	C23-C24-C25-C30
21	K	206	BCR	C23-C24-C25-C26
21	K	206	BCR	C23-C24-C25-C30
21	L	205	BCR	C23-C24-C25-C30
22	4	616	LUT	C5-C6-C7-C8
22	6	319	LUT	C5-C6-C7-C8
22	8	301	LUT	C5-C6-C7-C8
22	J	101	LUT	C1-C6-C7-C8
22	Z	617	LUT	C5-C6-C7-C8
22	1	317	LUT	C5-C6-C7-C8
22	F	305	LUT	C5-C6-C7-C8
23	J	105	LMG	C14-C15-C16-C17
26	4	619	LHG	C27-C28-C29-C30
19	6	304	CLA	O1D-CGD-O2D-CED
19	B	806	CLA	CBA-CGA-O2A-C1
19	B	823	CLA	CBA-CGA-O2A-C1
19	J	102	CLA	CBA-CGA-O2A-C1
23	7	622	LMG	C29-C28-O8-C9
19	6	305	CLA	C8-C10-C11-C12
19	8	303	CLA	C8-C10-C11-C12
19	A	814	CLA	C8-C10-C11-C12
19	B	804	CLA	C15-C16-C17-C18
19	L	203	CLA	C13-C15-C16-C17
26	B	851	LHG	C11-C10-C9-C8
19	5	302	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	Z	604	CLA	O1A-CGA-O2A-C1
19	B	810	CLA	C15-C16-C17-C18
19	A	822	CLA	C4-C3-C5-C6
19	B	816	CLA	C4-C3-C5-C6
19	B	824	CLA	C4-C3-C5-C6
20	4	607	CHL	C4-C3-C5-C6
19	3	302	CLA	C6-C7-C8-C10
19	6	305	CLA	C2-C3-C5-C6
19	A	842	CLA	C2-C3-C5-C6
19	A	844	CLA	C11-C10-C8-C7
19	B	801	CLA	C2-C3-C5-C6
19	B	811	CLA	C12-C13-C15-C16
19	B	813	CLA	C6-C7-C8-C10
19	B	820	CLA	C11-C10-C8-C7
19	B	825	CLA	C12-C13-C15-C16
19	B	826	CLA	C12-C13-C15-C16
19	B	828	CLA	C12-C13-C15-C16
19	B	833	CLA	C2-C3-C5-C6
19	B	833	CLA	C6-C7-C8-C10
19	B	840	CLA	C6-C7-C8-C10
19	Z	603	CLA	C11-C10-C8-C7
19	Z	608	CLA	C11-C10-C8-C7
20	4	601	CHL	C11-C12-C13-C15
20	7	621	CHL	C11-C10-C8-C7
20	8	320	CHL	C11-C10-C8-C7
20	Z	601	CHL	C12-C13-C15-C16
19	5	316	CLA	C3-C5-C6-C7
19	6	305	CLA	O1A-CGA-O2A-C1
19	7	610	CLA	O1A-CGA-O2A-C1
23	F	301	LMG	O10-C28-O8-C9
19	B	840	CLA	C15-C16-C17-C18
19	5	309	CLA	C16-C17-C18-C20
19	6	309	CLA	C6-C7-C8-C10
19	6	320	CLA	C6-C7-C8-C9
19	8	309	CLA	C16-C17-C18-C20
19	3	310	CLA	O1D-CGD-O2D-CED
23	L	201	LMG	O9-C10-O7-C8
26	B	851	LHG	C23-C24-C25-C26
24	1	322	LMU	C3-C4-C5-C6
24	A	857	LMU	C1-C2-C3-C4
19	Z	608	CLA	C2A-CAA-CBA-CGA
20	5	306	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	6	305	CLA	C5-C6-C7-C8
19	A	830	CLA	C5-C6-C7-C8
19	B	841	CLA	C13-C15-C16-C17
23	8	321	LMG	C29-C30-C31-C32
24	Z	621	LMU	C2-C3-C4-C5
26	A	847	LHG	C14-C15-C16-C17
19	J	102	CLA	O1A-CGA-O2A-C1
19	B	841	CLA	O1D-CGD-O2D-CED
26	6	325	LHG	C25-C26-C27-C28
19	B	813	CLA	C10-C11-C12-C13
23	B	852	LMG	C14-C15-C16-C17
26	6	318	LHG	C9-C10-C11-C12
24	K	201	LMU	C5-C6-C7-C8
24	A	855	LMU	O5'-C5'-C6'-O6'
19	B	823	CLA	O1A-CGA-O2A-C1
19	6	303	CLA	C16-C17-C18-C19
19	A	820	CLA	C11-C12-C13-C14
19	B	820	CLA	C11-C12-C13-C14
24	K	201	LMU	O5'-C1'-O1'-C1
19	B	813	CLA	C15-C16-C17-C18
19	8	311	CLA	O1D-CGD-O2D-CED
23	3	321	LMG	C11-C12-C13-C14
26	B	851	LHG	C18-C19-C20-C21
23	L	201	LMG	C11-C10-O7-C8
26	5	301	LHG	C8-C7-O7-C5
26	A	848	LHG	C8-C7-O7-C5
24	A	855	LMU	O5B-C5B-C6B-O6B
20	5	307	CHL	C13-C15-C16-C17
19	5	313	CLA	CBD-CGD-O2D-CED
19	6	305	CLA	CBD-CGD-O2D-CED
23	6	326	LMG	C17-C18-C19-C20
26	A	848	LHG	C11-C12-C13-C14
26	5	301	LHG	O9-C7-O7-C5
19	B	835	CLA	C3-C5-C6-C7
26	5	301	LHG	C11-C10-C9-C8
23	4	621	LMG	O7-C8-C9-O8
26	6	325	LHG	C11-C10-C9-C8
26	1	318	LHG	C14-C15-C16-C17
19	A	812	CLA	C4-C3-C5-C6
19	A	829	CLA	C4-C3-C5-C6
19	1	313	CLA	C4-C3-C5-C6
20	4	607	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	8	319	LMU	C3-C4-C5-C6
19	5	309	CLA	C11-C10-C8-C9
19	8	302	CLA	C14-C13-C15-C16
19	8	303	CLA	C6-C7-C8-C9
19	A	812	CLA	C14-C13-C15-C16
19	A	824	CLA	C11-C12-C13-C14
19	A	828	CLA	C14-C13-C15-C16
19	A	838	CLA	C6-C7-C8-C9
19	B	801	CLA	C11-C10-C8-C9
19	B	811	CLA	C14-C13-C15-C16
19	B	822	CLA	C11-C12-C13-C14
19	B	835	CLA	C6-C7-C8-C9
19	B	840	CLA	C6-C7-C8-C9
19	1	310	CLA	C6-C7-C8-C9
19	1	313	CLA	C6-C7-C8-C9
19	F	302	CLA	C11-C12-C13-C14
20	4	605	CHL	C11-C12-C13-C14
20	Z	601	CHL	C11-C10-C8-C9
20	Z	601	CHL	C14-C13-C15-C16
19	A	836	CLA	O1D-CGD-O2D-CED
19	B	819	CLA	C5-C6-C7-C8
19	8	313	CLA	C3-C5-C6-C7
19	A	808	CLA	C3-C5-C6-C7
19	6	305	CLA	C2A-CAA-CBA-CGA
19	A	804	CLA	C2A-CAA-CBA-CGA
19	A	811	CLA	C2A-CAA-CBA-CGA
19	L	203	CLA	C2A-CAA-CBA-CGA
23	8	321	LMG	C32-C33-C34-C35
26	4	619	LHG	C25-C26-C27-C28
21	7	617	BCR	C37-C22-C23-C24
23	G	201	LMG	C10-C11-C12-C13
19	G	202	CLA	O1D-CGD-O2D-CED
19	5	302	CLA	C15-C16-C17-C18
26	6	318	LHG	C28-C29-C30-C31
21	7	617	BCR	C11-C12-C13-C14
19	B	806	CLA	O1A-CGA-O2A-C1
23	7	622	LMG	O10-C28-O8-C9
19	5	304	CLA	C1A-C2A-CAA-CBA
19	5	314	CLA	C1A-C2A-CAA-CBA
19	6	314	CLA	C1A-C2A-CAA-CBA
19	7	614	CLA	C1A-C2A-CAA-CBA
19	A	807	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	A	811	CLA	C1A-C2A-CAA-CBA
19	A	813	CLA	C1A-C2A-CAA-CBA
19	A	826	CLA	C1A-C2A-CAA-CBA
19	B	806	CLA	C1A-C2A-CAA-CBA
19	B	830	CLA	C1A-C2A-CAA-CBA
19	F	304	CLA	C1A-C2A-CAA-CBA
20	5	306	CHL	C1A-C2A-CAA-CBA
20	6	306	CHL	C1A-C2A-CAA-CBA
20	6	308	CHL	C1A-C2A-CAA-CBA
20	8	305	CHL	C1A-C2A-CAA-CBA
20	Z	605	CHL	C1A-C2A-CAA-CBA
19	3	302	CLA	C16-C17-C18-C20
19	5	302	CLA	C16-C17-C18-C19
19	5	310	CLA	C11-C12-C13-C14
19	6	303	CLA	C16-C17-C18-C20
19	6	320	CLA	C6-C7-C8-C10
19	A	830	CLA	C16-C17-C18-C19
19	B	820	CLA	C11-C12-C13-C15
19	F	302	CLA	C16-C17-C18-C20
24	4	624	LMU	C2-C3-C4-C5
24	B	853	LMU	C7-C8-C9-C10
19	F	304	CLA	C8-C10-C11-C12
19	7	610	CLA	C5-C6-C7-C8
19	8	309	CLA	C15-C16-C17-C18
19	A	833	CLA	CBA-CGA-O2A-C1
19	A	838	CLA	CBA-CGA-O2A-C1
24	4	622	LMU	O5'-C5'-C6'-O6'
19	3	311	CLA	C11-C12-C13-C15
19	4	612	CLA	C15-C16-C17-C18
19	7	609	CLA	C13-C15-C16-C17
19	B	813	CLA	C4-C3-C5-C6
20	4	606	CHL	C3A-C2A-CAA-CBA
26	4	620	LHG	C11-C12-C13-C14
26	6	318	LHG	C17-C18-C19-C20
19	7	602	CLA	C13-C15-C16-C17
19	5	303	CLA	C16-C17-C18-C20
19	A	830	CLA	O1D-CGD-O2D-CED
23	7	622	LMG	O1-C7-C8-C9
23	J	105	LMG	O1-C7-C8-C9
23	L	201	LMG	O1-C7-C8-C9
26	8	318	LHG	C4-C5-C6-O8
26	A	801	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
24	3	324	LMU	O5B-C5B-C6B-O6B
19	3	308	CLA	C15-C16-C17-C18
19	6	313	CLA	C15-C16-C17-C18
26	8	318	LHG	C17-C18-C19-C20
23	7	622	LMG	C8-C7-O1-C1
23	8	321	LMG	C8-C7-O1-C1
19	A	820	CLA	CBD-CGD-O2D-CED
19	B	822	CLA	C13-C15-C16-C17
24	3	323	LMU	C11-C10-C9-C8
19	3	313	CLA	CAA-CBA-CGA-O2A
24	3	323	LMU	O5'-C5'-C6'-O6'
23	6	301	LMG	C13-C14-C15-C16
19	A	820	CLA	C11-C12-C13-C15
23	F	301	LMG	O6-C5-C6-O5
24	3	325	LMU	O5'-C5'-C6'-O6'
26	A	801	LHG	O1-C1-C2-O2
26	5	321	LHG	C27-C28-C29-C30
19	5	319	CLA	C4C-C3C-CAC-CBC
22	Z	615	LUT	C39-C29-C30-C31
24	Z	619	LMU	O5B-C5B-C6B-O6B
19	A	811	CLA	C4-C3-C5-C6
19	5	316	CLA	C16-C17-C18-C20
26	5	321	LHG	C28-C29-C30-C31
26	A	847	LHG	C11-C12-C13-C14
19	B	804	CLA	CBD-CGD-O2D-CED
19	Z	612	CLA	C5-C6-C7-C8
19	B	823	CLA	C11-C12-C13-C14
19	B	834	CLA	C10-C11-C12-C13
23	8	321	LMG	C18-C19-C20-C21
20	8	306	CHL	C8-C10-C11-C12
19	1	313	CLA	C2-C1-O2A-CGA
23	F	301	LMG	C11-C12-C13-C14
24	1	321	LMU	C2-C3-C4-C5
19	B	842	CLA	O1D-CGD-O2D-CED
19	1	311	CLA	O1D-CGD-O2D-CED
24	8	319	LMU	O5'-C5'-C6'-O6'
24	1	320	LMU	O5'-C5'-C6'-O6'
31	B	850	DGD	O6E-C5E-C6E-O5E
26	A	848	LHG	C12-C13-C14-C15
19	Z	612	CLA	O1D-CGD-O2D-CED
23	B	852	LMG	C16-C17-C18-C19
24	4	623	LMU	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	6	328	LMU	C6-C7-C8-C9
19	B	828	CLA	CBA-CGA-O2A-C1
24	6	324	LMU	C3-C4-C5-C6
24	6	324	LMU	C4'-C5'-C6'-O6'
19	Z	602	CLA	O1D-CGD-O2D-CED
19	Z	610	CLA	C3-C5-C6-C7
26	Z	618	LHG	C7-C8-C9-C10
22	F	305	LUT	C28-C29-C30-C31
24	3	324	LMU	C2'-C1'-O1'-C1
24	1	320	LMU	C2'-C1'-O1'-C1
23	4	621	LMG	C24-C25-C26-C27
19	A	820	CLA	CAA-CBA-CGA-O2A
24	3	325	LMU	C1-C2-C3-C4
19	Z	610	CLA	C5-C6-C7-C8
19	A	833	CLA	O1A-CGA-O2A-C1
19	A	838	CLA	O1A-CGA-O2A-C1
19	A	846	CLA	O1D-CGD-O2D-CED
19	K	203	CLA	C4-C3-C5-C6
20	6	302	CHL	C4-C3-C5-C6
19	3	308	CLA	C12-C13-C15-C16
19	5	309	CLA	C11-C10-C8-C7
19	5	310	CLA	C11-C10-C8-C7
19	6	305	CLA	C12-C13-C15-C16
19	7	612	CLA	C12-C13-C15-C16
19	8	312	CLA	C12-C13-C15-C16
19	8	313	CLA	C6-C7-C8-C10
19	A	810	CLA	C12-C13-C15-C16
19	A	812	CLA	C11-C10-C8-C7
19	A	813	CLA	C11-C12-C13-C15
19	A	820	CLA	C6-C7-C8-C10
19	A	824	CLA	C11-C12-C13-C15
19	A	830	CLA	C6-C7-C8-C10
19	A	837	CLA	C12-C13-C15-C16
19	A	838	CLA	C6-C7-C8-C10
19	A	840	CLA	C12-C13-C15-C16
19	B	801	CLA	C11-C10-C8-C7
19	B	815	CLA	C6-C7-C8-C10
19	B	822	CLA	C11-C12-C13-C15
19	B	826	CLA	C6-C7-C8-C10
19	Z	604	CLA	C6-C7-C8-C10
19	Z	608	CLA	C12-C13-C15-C16
19	Z	614	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	Z	614	CLA	C11-C10-C8-C7
19	1	307	CLA	C11-C12-C13-C15
19	1	310	CLA	C11-C10-C8-C7
19	1	310	CLA	C11-C12-C13-C15
19	1	312	CLA	C12-C13-C15-C16
19	F	302	CLA	C11-C12-C13-C15
19	F	304	CLA	C11-C10-C8-C7
19	L	203	CLA	C6-C7-C8-C10
20	4	607	CHL	C11-C10-C8-C7
20	5	307	CHL	C11-C12-C13-C15
20	6	315	CHL	C6-C7-C8-C10
20	7	601	CHL	C11-C12-C13-C15
20	7	601	CHL	C12-C13-C15-C16
19	3	302	CLA	C11-C10-C8-C9
19	5	310	CLA	C11-C10-C8-C9
19	6	305	CLA	C14-C13-C15-C16
19	7	612	CLA	C14-C13-C15-C16
19	8	312	CLA	C14-C13-C15-C16
19	A	811	CLA	C11-C10-C8-C9
19	A	812	CLA	C11-C10-C8-C9
19	A	824	CLA	C6-C7-C8-C9
19	A	830	CLA	C6-C7-C8-C9
19	A	840	CLA	C6-C7-C8-C9
19	A	840	CLA	C14-C13-C15-C16
19	A	841	CLA	C14-C13-C15-C16
19	B	829	CLA	C11-C12-C13-C14
19	K	203	CLA	C11-C10-C8-C9
19	Z	604	CLA	C6-C7-C8-C9
19	Z	608	CLA	C14-C13-C15-C16
19	Z	609	CLA	C11-C10-C8-C9
19	Z	614	CLA	C11-C10-C8-C9
19	1	303	CLA	C11-C10-C8-C9
19	1	307	CLA	C11-C12-C13-C14
19	1	310	CLA	C11-C12-C13-C14
19	1	312	CLA	C14-C13-C15-C16
19	L	203	CLA	C6-C7-C8-C9
19	L	203	CLA	C14-C13-C15-C16
20	4	607	CHL	C11-C10-C8-C9
20	6	307	CHL	C14-C13-C15-C16
20	6	315	CHL	C6-C7-C8-C9
20	7	601	CHL	C11-C10-C8-C9
20	7	601	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	A	817	CLA	CBA-CGA-O2A-C1
19	4	614	CLA	C2A-CAA-CBA-CGA
24	Z	619	LMU	C4'-C5'-C6'-O6'
21	3	315	BCR	C37-C22-C23-C24
19	B	810	CLA	C16-C17-C18-C19
24	1	319	LMU	C9-C10-C11-C12
26	4	620	LHG	C9-C10-C11-C12
21	4	618	BCR	C17-C18-C19-C20
21	5	320	BCR	C21-C22-C23-C24
22	5	324	LUT	C11-C12-C13-C14
26	4	619	LHG	C17-C18-C19-C20
26	A	848	LHG	C16-C17-C18-C19
19	A	811	CLA	C3-C5-C6-C7
26	A	848	LHG	O9-C7-O7-C5
19	4	609	CLA	C8-C10-C11-C12
23	7	622	LMG	C11-C10-O7-C8
24	Z	620	LMU	C7-C8-C9-C10
24	1	322	LMU	C5-C6-C7-C8
26	A	801	LHG	C9-C10-C11-C12
26	A	847	LHG	C19-C20-C21-C22
19	4	604	CLA	CBA-CGA-O2A-C1
19	B	816	CLA	CBA-CGA-O2A-C1
19	B	824	CLA	CBA-CGA-O2A-C1
24	7	620	LMU	C1-C2-C3-C4
23	G	201	LMG	C16-C17-C18-C19
19	5	319	CLA	C4B-C3B-CAB-CBB
19	7	612	CLA	C4B-C3B-CAB-CBB
19	7	613	CLA	C4B-C3B-CAB-CBB
19	K	202	CLA	C4B-C3B-CAB-CBB
19	1	314	CLA	C4B-C3B-CAB-CBB
20	3	306	CHL	C4B-C3B-CAB-CBB
20	5	306	CHL	C4B-C3B-CAB-CBB
20	6	307	CHL	C4B-C3B-CAB-CBB
19	3	303	CLA	C13-C15-C16-C17
19	B	834	CLA	C5-C6-C7-C8
19	B	809	CLA	C3-C5-C6-C7
19	B	814	CLA	C10-C11-C12-C13
20	8	305	CHL	C1-C2-C3-C5
19	4	613	CLA	C4-C3-C5-C6
19	5	309	CLA	C4-C3-C5-C6
20	6	307	CHL	C4-C3-C5-C6
19	5	309	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	812	CLA	C2-C3-C5-C6
19	A	829	CLA	C2-C3-C5-C6
19	K	203	CLA	C2-C3-C5-C6
19	1	313	CLA	C2-C3-C5-C6
20	6	302	CHL	C2-C3-C5-C6
19	L	203	CLA	C15-C16-C17-C18
24	3	325	LMU	C11-C10-C9-C8
19	Z	608	CLA	O1D-CGD-O2D-CED
19	B	810	CLA	C3-C5-C6-C7
19	A	815	CLA	C16-C17-C18-C20
19	B	810	CLA	C16-C17-C18-C20
26	B	851	LHG	C25-C26-C27-C28
19	A	813	CLA	C13-C15-C16-C17
19	5	309	CLA	CBA-CGA-O2A-C1
19	6	304	CLA	CBA-CGA-O2A-C1
19	A	809	CLA	CBA-CGA-O2A-C1
19	5	311	CLA	C3A-C2A-CAA-CBA
19	B	841	CLA	C3A-C2A-CAA-CBA
19	Z	604	CLA	C3A-C2A-CAA-CBA
20	7	606	CHL	C3A-C2A-CAA-CBA
19	B	803	CLA	O1D-CGD-O2D-CED
24	3	322	LMU	C2-C1-O1'-C1'
24	3	323	LMU	C2-C1-O1'-C1'
24	4	622	LMU	C2-C1-O1'-C1'
24	6	324	LMU	C2-C1-O1'-C1'
24	6	328	LMU	C2-C1-O1'-C1'
24	7	620	LMU	C2-C1-O1'-C1'
24	8	319	LMU	C2-C1-O1'-C1'
24	A	856	LMU	C2-C1-O1'-C1'
24	K	201	LMU	C2-C1-O1'-C1'
24	Z	620	LMU	C2-C1-O1'-C1'
24	1	319	LMU	C2-C1-O1'-C1'
24	1	320	LMU	C2-C1-O1'-C1'
24	4	622	LMU	C6-C7-C8-C9
19	B	828	CLA	O1A-CGA-O2A-C1
19	7	611	CLA	CBA-CGA-O2A-C1
23	4	621	LMG	C7-C8-C9-O8
23	J	104	LMG	C7-C8-C9-O8
23	J	105	LMG	C7-C8-C9-O8
19	1	302	CLA	C8-C10-C11-C12
24	B	853	LMU	C1-C2-C3-C4
19	B	840	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	5	303	CLA	C16-C17-C18-C19
19	A	815	CLA	C16-C17-C18-C19
20	6	307	CHL	C2-C3-C5-C6
19	B	836	CLA	C2A-CAA-CBA-CGA
26	8	318	LHG	O1-C1-C2-O2
19	B	814	CLA	C8-C10-C11-C12
23	6	326	LMG	C18-C19-C20-C21
19	A	817	CLA	O1A-CGA-O2A-C1
19	3	302	CLA	C16-C17-C18-C19
19	5	316	CLA	C16-C17-C18-C19
19	A	844	CLA	C8-C10-C11-C12
19	B	816	CLA	C10-C11-C12-C13
19	1	314	CLA	C2B-C3B-CAB-CBB
19	B	813	CLA	C2C-C3C-CAC-CBC
26	5	301	LHG	C12-C13-C14-C15
26	4	620	LHG	C24-C25-C26-C27
26	5	321	LHG	C11-C12-C13-C14
23	J	104	LMG	O7-C8-C9-O8
23	F	301	LMG	O1-C7-C8-O7
26	8	318	LHG	O7-C5-C6-O8
31	B	850	DGD	O1G-C1G-C2G-O2G
23	G	201	LMG	C29-C28-O8-C9
19	A	828	CLA	C5-C6-C7-C8
19	A	830	CLA	C16-C17-C18-C20
19	B	813	CLA	C16-C17-C18-C20
24	1	301	LMU	C2-C3-C4-C5
24	8	319	LMU	O5'-C1'-O1'-C1
19	A	807	CLA	C10-C11-C12-C13
19	1	307	CLA	C5-C6-C7-C8
26	Z	618	LHG	C31-C32-C33-C34
19	B	806	CLA	C4-C3-C5-C6
19	F	304	CLA	C4-C3-C5-C6
19	A	808	CLA	C2-C1-O2A-CGA
19	A	828	CLA	C2-C1-O2A-CGA
19	B	803	CLA	C2-C1-O2A-CGA
19	1	308	CLA	C2-C1-O2A-CGA
20	8	305	CHL	C2-C1-O2A-CGA
19	4	613	CLA	C2-C3-C5-C6
19	A	811	CLA	C2-C3-C5-C6
19	B	813	CLA	C2-C3-C5-C6
19	1	309	CLA	C10-C11-C12-C13
19	F	302	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	4	610	CLA	C11-C10-C8-C9
19	6	311	CLA	C11-C10-C8-C9
19	A	810	CLA	C14-C13-C15-C16
19	A	813	CLA	C14-C13-C15-C16
19	A	814	CLA	C11-C10-C8-C9
19	A	820	CLA	C6-C7-C8-C9
19	B	812	CLA	C11-C10-C8-C9
19	B	820	CLA	C6-C7-C8-C9
19	B	833	CLA	C11-C10-C8-C9
19	Z	614	CLA	C6-C7-C8-C9
19	1	308	CLA	C11-C12-C13-C14
19	1	308	CLA	C14-C13-C15-C16
20	6	302	CHL	C6-C7-C8-C9
20	8	320	CHL	C14-C13-C15-C16
26	4	620	LHG	C13-C14-C15-C16
24	A	855	LMU	C1-C2-C3-C4
19	1	310	CLA	C5-C6-C7-C8
19	B	824	CLA	O1A-CGA-O2A-C1
23	6	326	LMG	C16-C17-C18-C19
24	7	619	LMU	C3-C4-C5-C6
19	5	305	CLA	C6-C7-C8-C10
21	3	319	BCR	C23-C24-C25-C26
21	4	618	BCR	C23-C24-C25-C26
21	4	618	BCR	C23-C24-C25-C30
21	A	849	BCR	C5-C6-C7-C8
21	B	849	BCR	C5-C6-C7-C8
21	L	202	BCR	C1-C6-C7-C8
21	L	202	BCR	C5-C6-C7-C8
22	3	316	LUT	C1-C6-C7-C8
22	3	317	LUT	C1-C6-C7-C8
22	6	319	LUT	C1-C6-C7-C8
22	7	615	LUT	C1-C6-C7-C8
22	7	615	LUT	C5-C6-C7-C8
22	8	315	LUT	C1-C6-C7-C8
22	8	315	LUT	C5-C6-C7-C8
22	1	315	LUT	C1-C6-C7-C8
22	1	317	LUT	C1-C6-C7-C8
19	A	831	CLA	C13-C15-C16-C17
20	8	306	CHL	C15-C16-C17-C18
24	1	319	LMU	O5B-C5B-C6B-O6B
21	3	315	BCR	C21-C22-C23-C24
21	7	617	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	Z	617	LUT	C40-C33-C34-C35
26	8	318	LHG	C7-C8-C9-C10
23	7	622	LMG	O9-C10-O7-C8
19	5	312	CLA	C4C-C3C-CAC-CBC
24	1	320	LMU	O1'-C1-C2-C3
23	6	301	LMG	C14-C15-C16-C17
26	6	318	LHG	C26-C27-C28-C29
26	8	318	LHG	O6-C4-C5-C6
19	A	823	CLA	C4-C3-C5-C6
19	3	302	CLA	C11-C12-C13-C15
19	3	307	CLA	C6-C7-C8-C10
19	3	308	CLA	C11-C12-C13-C15
19	4	608	CLA	C6-C7-C8-C10
19	5	309	CLA	C6-C7-C8-C10
19	8	313	CLA	C11-C10-C8-C7
19	A	807	CLA	C6-C7-C8-C10
19	A	811	CLA	C11-C10-C8-C7
19	A	812	CLA	C11-C12-C13-C15
19	A	814	CLA	C11-C10-C8-C7
19	A	815	CLA	C11-C10-C8-C7
19	A	819	CLA	C12-C13-C15-C16
19	A	823	CLA	C6-C7-C8-C10
19	A	824	CLA	C6-C7-C8-C10
19	A	824	CLA	C12-C13-C15-C16
19	A	840	CLA	C6-C7-C8-C10
19	A	841	CLA	C12-C13-C15-C16
19	B	804	CLA	C11-C10-C8-C7
19	B	806	CLA	C2-C3-C5-C6
19	B	809	CLA	C6-C7-C8-C10
19	B	809	CLA	C11-C12-C13-C15
19	B	810	CLA	C11-C12-C13-C15
19	B	813	CLA	C11-C12-C13-C15
19	B	813	CLA	C12-C13-C15-C16
19	B	816	CLA	C11-C10-C8-C7
19	B	821	CLA	C6-C7-C8-C10
19	B	825	CLA	C11-C12-C13-C15
19	B	833	CLA	C11-C10-C8-C7
19	B	837	CLA	C11-C10-C8-C7
19	B	838	CLA	C11-C12-C13-C15
19	K	203	CLA	C11-C10-C8-C7
19	Z	603	CLA	C6-C7-C8-C10
19	Z	609	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	1	303	CLA	C11-C10-C8-C7
19	1	308	CLA	C11-C10-C8-C7
19	1	308	CLA	C12-C13-C15-C16
19	F	304	CLA	C2-C3-C5-C6
19	L	203	CLA	C12-C13-C15-C16
20	4	607	CHL	C6-C7-C8-C10
20	5	307	CHL	C11-C10-C8-C7
20	5	307	CHL	C12-C13-C15-C16
20	6	307	CHL	C11-C12-C13-C15
20	6	315	CHL	C11-C12-C13-C15
20	7	601	CHL	C6-C7-C8-C10
20	7	601	CHL	C11-C10-C8-C7
20	8	306	CHL	C12-C13-C15-C16
20	Z	601	CHL	C11-C12-C13-C15
19	B	816	CLA	O1A-CGA-O2A-C1
19	3	302	CLA	C13-C15-C16-C17
19	B	808	CLA	C6-C7-C8-C10
26	5	301	LHG	C24-C23-O8-C6
23	L	201	LMG	C29-C30-C31-C32
24	F	306	LMU	C6-C7-C8-C9
26	4	619	LHG	C13-C14-C15-C16
19	A	824	CLA	C2A-CAA-CBA-CGA
24	A	857	LMU	C2-C3-C4-C5
19	A	808	CLA	C5-C6-C7-C8
22	3	316	LUT	C40-C33-C34-C35
22	4	616	LUT	C40-C33-C34-C35
22	1	315	LUT	C40-C33-C34-C35
23	F	301	LMG	C10-C11-C12-C13
26	6	325	LHG	C23-C24-C25-C26
24	3	324	LMU	C4-C5-C6-C7
26	8	318	LHG	C14-C15-C16-C17
19	8	303	CLA	C10-C11-C12-C13
19	A	815	CLA	C15-C16-C17-C18
20	3	306	CHL	C13-C15-C16-C17
19	3	307	CLA	CAD-CBD-CGD-O2D
19	5	319	CLA	CAD-CBD-CGD-O2D
19	6	320	CLA	CAD-CBD-CGD-O2D
19	8	303	CLA	CAD-CBD-CGD-O2D
19	A	809	CLA	CAD-CBD-CGD-O2D
19	A	814	CLA	CAD-CBD-CGD-O2D
19	A	816	CLA	CAD-CBD-CGD-O2D
19	A	824	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	A	839	CLA	CAD-CBD-CGD-O2D
19	A	843	CLA	CAD-CBD-CGD-O2D
19	B	821	CLA	CAD-CBD-CGD-O2D
19	Z	604	CLA	CAD-CBD-CGD-O2D
19	1	304	CLA	CAD-CBD-CGD-O2D
19	1	311	CLA	CAD-CBD-CGD-O2D
19	F	304	CLA	CAD-CBD-CGD-O2D
20	4	601	CHL	CAD-CBD-CGD-O2D
20	Z	606	CHL	CAD-CBD-CGD-O2D
20	1	306	CHL	CAD-CBD-CGD-O2D
23	4	621	LMG	C14-C15-C16-C17
23	6	326	LMG	C12-C13-C14-C15
23	8	321	LMG	C16-C17-C18-C19
19	A	811	CLA	C5-C6-C7-C8
19	B	820	CLA	C5-C6-C7-C8
22	F	305	LUT	C6-C7-C8-C9
19	A	809	CLA	O1A-CGA-O2A-C1
19	F	302	CLA	CBD-CGD-O2D-CED
19	A	816	CLA	CBA-CGA-O2A-C1
19	B	813	CLA	C4C-C3C-CAC-CBC
23	4	621	LMG	C17-C18-C19-C20
23	3	321	LMG	C7-C8-C9-O8
20	Z	601	CHL	C2A-CAA-CBA-CGA
24	F	306	LMU	C5'-C4'-O1B-C1B
26	1	318	LHG	C16-C17-C18-C19
19	5	313	CLA	O1D-CGD-O2D-CED
19	6	305	CLA	O1D-CGD-O2D-CED
26	4	620	LHG	O2-C2-C3-O3
19	3	313	CLA	CHA-CBD-CGD-O1D
19	3	313	CLA	CHA-CBD-CGD-O2D
19	4	612	CLA	CHA-CBD-CGD-O1D
19	5	304	CLA	CHA-CBD-CGD-O1D
19	5	304	CLA	CHA-CBD-CGD-O2D
19	A	805	CLA	CHA-CBD-CGD-O1D
19	A	805	CLA	CHA-CBD-CGD-O2D
19	A	810	CLA	CHA-CBD-CGD-O1D
19	A	810	CLA	CHA-CBD-CGD-O2D
19	A	827	CLA	CHA-CBD-CGD-O1D
19	A	827	CLA	CHA-CBD-CGD-O2D
19	A	833	CLA	CHA-CBD-CGD-O1D
19	A	833	CLA	CHA-CBD-CGD-O2D
19	A	836	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	A	836	CLA	CHA-CBD-CGD-O2D
19	B	809	CLA	CHA-CBD-CGD-O1D
19	B	809	CLA	CHA-CBD-CGD-O2D
19	B	825	CLA	CHA-CBD-CGD-O1D
19	B	825	CLA	CHA-CBD-CGD-O2D
19	B	826	CLA	CHA-CBD-CGD-O1D
19	B	826	CLA	CHA-CBD-CGD-O2D
19	B	830	CLA	CHA-CBD-CGD-O1D
19	B	830	CLA	CHA-CBD-CGD-O2D
19	K	205	CLA	CHA-CBD-CGD-O1D
19	Z	613	CLA	CHA-CBD-CGD-O1D
20	5	317	CHL	CHA-CBD-CGD-O1D
20	5	317	CHL	CHA-CBD-CGD-O2D
20	7	621	CHL	CHA-CBD-CGD-O1D
20	7	621	CHL	CHA-CBD-CGD-O2D
20	8	320	CHL	CHA-CBD-CGD-O1D
19	B	804	CLA	O1D-CGD-O2D-CED
19	A	809	CLA	CBD-CGD-O2D-CED
19	4	604	CLA	O1A-CGA-O2A-C1
19	7	611	CLA	O1A-CGA-O2A-C1
23	J	105	LMG	O7-C8-C9-O8
23	L	201	LMG	O1-C7-C8-O7
26	A	801	LHG	O7-C5-C6-O8
19	A	812	CLA	C15-C16-C17-C18
19	5	309	CLA	O1A-CGA-O2A-C1
23	G	201	LMG	O10-C28-O8-C9
19	8	311	CLA	C6-C7-C8-C10
26	6	318	LHG	O1-C1-C2-O2
23	J	104	LMG	C18-C19-C20-C21
19	6	304	CLA	O1A-CGA-O2A-C1
19	B	840	CLA	C2-C3-C5-C6
24	F	306	LMU	C3'-C4'-O1B-C1B
19	3	307	CLA	C10-C11-C12-C13
19	A	842	CLA	C10-C11-C12-C13
19	4	610	CLA	C6-C7-C8-C9
19	A	812	CLA	C11-C12-C13-C14
19	A	815	CLA	C11-C10-C8-C9
19	B	804	CLA	C11-C10-C8-C9
19	B	809	CLA	C6-C7-C8-C9
19	B	816	CLA	C11-C10-C8-C9
19	B	821	CLA	C6-C7-C8-C9
20	5	307	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	6	307	CHL	C11-C12-C13-C14
19	B	826	CLA	C13-C15-C16-C17
19	B	811	CLA	C2A-CAA-CBA-CGA
22	8	301	LUT	C7-C8-C9-C10
19	6	311	CLA	C1A-C2A-CAA-CBA
19	A	832	CLA	C1A-C2A-CAA-CBA
19	B	801	CLA	C1A-C2A-CAA-CBA
19	B	828	CLA	C1A-C2A-CAA-CBA
19	Z	604	CLA	C1A-C2A-CAA-CBA
20	4	607	CHL	C1A-C2A-CAA-CBA
24	6	324	LMU	C11-C10-C9-C8
19	B	816	CLA	C3-C5-C6-C7
19	B	817	CLA	C3-C5-C6-C7
26	5	301	LHG	O10-C23-O8-C6
19	3	311	CLA	C4B-C3B-CAB-CBB
19	4	603	CLA	C4B-C3B-CAB-CBB
19	4	610	CLA	C4B-C3B-CAB-CBB
19	5	315	CLA	C4B-C3B-CAB-CBB
19	6	313	CLA	C4B-C3B-CAB-CBB
19	8	312	CLA	C4B-C3B-CAB-CBB
19	A	808	CLA	C4B-C3B-CAB-CBB
19	A	824	CLA	C4B-C3B-CAB-CBB
19	A	843	CLA	C4B-C3B-CAB-CBB
19	B	818	CLA	C4B-C3B-CAB-CBB
19	B	840	CLA	C4B-C3B-CAB-CBB
19	B	841	CLA	C4B-C3B-CAB-CBB
19	Z	614	CLA	C4B-C3B-CAB-CBB
19	F	304	CLA	C4B-C3B-CAB-CBB
20	4	615	CHL	C4B-C3B-CAB-CBB
26	6	325	LHG	C3-O3-P-O4
26	7	618	LHG	C3-O3-P-O4
23	7	622	LMG	O6-C1-O1-C7
24	1	320	LMU	O5'-C1'-O1'-C1
23	4	621	LMG	C29-C28-O8-C9
20	7	621	CHL	CAA-CBA-CGA-O2A
20	8	306	CHL	C2A-CAA-CBA-CGA
19	3	302	CLA	C3-C5-C6-C7
19	A	816	CLA	O1A-CGA-O2A-C1
26	6	318	LHG	C12-C13-C14-C15
19	3	305	CLA	C2-C3-C5-C6
19	3	313	CLA	CAD-CBD-CGD-O1D
19	5	304	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	A	805	CLA	CAD-CBD-CGD-O1D
19	A	807	CLA	CAD-CBD-CGD-O1D
19	A	833	CLA	CAD-CBD-CGD-O1D
19	A	846	CLA	CAD-CBD-CGD-O1D
20	7	621	CHL	CAD-CBD-CGD-O1D
20	8	320	CHL	CAD-CBD-CGD-O1D
19	5	319	CLA	CBA-CGA-O2A-C1
20	4	607	CHL	C13-C15-C16-C17
19	B	804	CLA	C4C-C3C-CAC-CBC
23	8	321	LMG	C35-C36-C37-C38
26	4	620	LHG	C1-C2-C3-O3
19	7	612	CLA	C13-C15-C16-C17
19	A	828	CLA	C10-C11-C12-C13
24	A	857	LMU	C5-C6-C7-C8
19	4	603	CLA	C11-C10-C8-C7
19	A	807	CLA	C11-C10-C8-C7
19	A	820	CLA	C11-C10-C8-C7
19	A	823	CLA	C2-C3-C5-C6
19	A	827	CLA	C11-C12-C13-C15
19	A	835	CLA	C12-C13-C15-C16
19	A	836	CLA	C11-C12-C13-C15
19	A	842	CLA	C11-C10-C8-C7
19	B	801	CLA	C12-C13-C15-C16
19	B	804	CLA	C12-C13-C15-C16
19	B	822	CLA	C6-C7-C8-C10
19	B	822	CLA	C12-C13-C15-C16
19	B	829	CLA	C12-C13-C15-C16
19	L	203	CLA	C3A-C2A-CAA-CBA
20	3	306	CHL	C11-C12-C13-C15
20	4	607	CHL	C11-C12-C13-C15
20	8	306	CHL	C11-C10-C8-C7
20	Z	601	CHL	C6-C7-C8-C10
20	Z	606	CHL	C11-C12-C13-C15
26	8	318	LHG	O6-C4-C5-O7
19	A	830	CLA	C3-C5-C6-C7
24	1	321	LMU	C2-C1-O1'-C1'
19	B	813	CLA	C16-C17-C18-C19
19	1	312	CLA	O1A-CGA-O2A-C1
23	7	622	LMG	O1-C7-C8-O7
23	J	104	LMG	O1-C7-C8-O7
23	J	105	LMG	O1-C7-C8-O7
19	4	603	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	B	816	CLA	C8-C10-C11-C12
24	F	306	LMU	C4-C5-C6-C7
19	B	819	CLA	C4-C3-C5-C6
19	1	312	CLA	CBA-CGA-O2A-C1
24	3	324	LMU	C6-C7-C8-C9
19	4	612	CLA	CAA-CBA-CGA-O2A
19	7	612	CLA	C6-C7-C8-C9
19	8	313	CLA	C11-C10-C8-C9
19	A	819	CLA	C14-C13-C15-C16
19	A	823	CLA	C6-C7-C8-C9
19	A	837	CLA	C14-C13-C15-C16
19	B	809	CLA	C11-C12-C13-C14
19	B	810	CLA	C11-C12-C13-C14
19	B	813	CLA	C14-C13-C15-C16
19	B	826	CLA	C11-C10-C8-C9
19	B	837	CLA	C11-C10-C8-C9
19	B	838	CLA	C11-C12-C13-C14
19	Z	603	CLA	C6-C7-C8-C9
19	F	304	CLA	C6-C7-C8-C9
20	7	601	CHL	C6-C7-C8-C9
19	A	843	CLA	CBD-CGD-O2D-CED
24	B	853	LMU	C6-C7-C8-C9
19	8	311	CLA	C6-C7-C8-C9
21	3	319	BCR	C36-C18-C19-C20
19	B	830	CLA	C5-C6-C7-C8
23	4	621	LMG	O10-C28-O8-C9
24	6	324	LMU	O5'-C5'-C6'-O6'
19	A	819	CLA	C16-C17-C18-C19
19	3	307	CLA	C2B-C3B-CAB-CBB
19	5	319	CLA	C2B-C3B-CAB-CBB
19	6	305	CLA	C2B-C3B-CAB-CBB
19	7	612	CLA	C2B-C3B-CAB-CBB
19	7	613	CLA	C2B-C3B-CAB-CBB
19	A	843	CLA	C2B-C3B-CAB-CBB
19	B	840	CLA	C2B-C3B-CAB-CBB
19	Z	614	CLA	C2B-C3B-CAB-CBB
19	1	310	CLA	C2B-C3B-CAB-CBB
19	1	313	CLA	C2B-C3B-CAB-CBB
20	3	306	CHL	C2B-C3B-CAB-CBB
20	4	607	CHL	C2B-C3B-CAB-CBB
20	5	306	CHL	C2B-C3B-CAB-CBB
20	5	308	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	6	302	CHL	C2B-C3B-CAB-CBB
20	6	306	CHL	C2B-C3B-CAB-CBB
20	6	307	CHL	C2B-C3B-CAB-CBB
20	6	308	CHL	C2B-C3B-CAB-CBB
20	6	315	CHL	C2B-C3B-CAB-CBB
20	7	601	CHL	C2B-C3B-CAB-CBB
20	1	305	CHL	C2B-C3B-CAB-CBB
19	B	812	CLA	C8-C10-C11-C12
23	L	201	LMG	C16-C17-C18-C19
26	6	318	LHG	C27-C28-C29-C30
19	1	308	CLA	C4-C3-C5-C6
19	5	310	CLA	C8-C10-C11-C12
19	A	836	CLA	C5-C6-C7-C8
19	B	816	CLA	CBD-CGD-O2D-CED
19	B	842	CLA	C15-C16-C17-C18
23	J	105	LMG	C13-C14-C15-C16
19	A	820	CLA	O1D-CGD-O2D-CED
23	6	301	LMG	O7-C10-C11-C12
24	1	321	LMU	C4-C5-C6-C7
31	B	850	DGD	C1G-C2G-O2G-C1B
26	B	851	LHG	C11-C12-C13-C14
19	6	303	CLA	C15-C16-C17-C18
19	A	813	CLA	C2-C1-O2A-CGA
23	J	104	LMG	C16-C17-C18-C19
19	1	313	CLA	CAA-CBA-CGA-O2A
23	4	621	LMG	C11-C12-C13-C14
19	F	302	CLA	C15-C16-C17-C18
19	F	302	CLA	O1D-CGD-O2D-CED
19	4	613	CLA	CBA-CGA-O2A-C1
21	B	847	BCR	C23-C24-C25-C26
22	3	316	LUT	C5-C6-C7-C8
22	3	317	LUT	C5-C6-C7-C8
22	Z	617	LUT	C1-C6-C7-C8
22	1	315	LUT	C5-C6-C7-C8
24	K	201	LMU	C4-C5-C6-C7
19	Z	614	CLA	O1D-CGD-O2D-CED
19	3	310	CLA	CBA-CGA-O2A-C1
19	8	302	CLA	C15-C16-C17-C18
19	B	811	CLA	C16-C17-C18-C19
19	1	307	CLA	C16-C17-C18-C20
19	B	809	CLA	C8-C10-C11-C12
20	7	606	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	6	319	LUT	C11-C10-C9-C8
23	3	321	LMG	O7-C8-C9-O8
26	4	620	LHG	C3-O3-P-O6
26	5	321	LHG	C3-O3-P-O6
26	6	325	LHG	C3-O3-P-O6
26	6	325	LHG	C4-O6-P-O3
26	A	847	LHG	C3-O3-P-O6
26	A	848	LHG	C3-O3-P-O6
19	A	837	CLA	C15-C16-C17-C18
23	J	104	LMG	O1-C7-C8-C9
19	3	312	CLA	CBD-CGD-O2D-CED
19	4	610	CLA	C11-C10-C8-C7
19	A	828	CLA	C11-C10-C8-C7
19	B	814	CLA	C11-C10-C8-C7
19	B	814	CLA	C12-C13-C15-C16
19	1	308	CLA	C11-C12-C13-C15
19	F	304	CLA	C6-C7-C8-C10
19	L	203	CLA	C11-C12-C13-C15
20	4	607	CHL	C12-C13-C15-C16
20	6	302	CHL	C6-C7-C8-C10
26	1	318	LHG	C12-C13-C14-C15
19	8	313	CLA	C6-C7-C8-C9
19	A	813	CLA	C11-C12-C13-C14
19	A	824	CLA	C14-C13-C15-C16
19	B	822	CLA	C14-C13-C15-C16
19	B	829	CLA	C14-C13-C15-C16
19	1	309	CLA	C14-C13-C15-C16
19	1	310	CLA	C11-C10-C8-C9
19	F	304	CLA	C11-C10-C8-C9
20	6	315	CHL	C11-C12-C13-C14
19	B	824	CLA	C16-C17-C18-C19
19	A	826	CLA	C2A-CAA-CBA-CGA
19	1	307	CLA	C2A-CAA-CBA-CGA
23	B	852	LMG	C17-C18-C19-C20
23	8	321	LMG	C41-C42-C43-C44
19	4	613	CLA	O1A-CGA-O2A-C1
19	B	841	CLA	C15-C16-C17-C18
19	A	830	CLA	C8-C10-C11-C12
23	G	201	LMG	C30-C31-C32-C33
24	6	324	LMU	C4-C5-C6-C7
24	1	322	LMU	O1'-C1-C2-C3
19	1	310	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	1	307	CLA	C10-C11-C12-C13
19	J	102	CLA	C4-C3-C5-C6
20	5	307	CHL	C4-C3-C5-C6
19	B	819	CLA	C2-C3-C5-C6
23	J	105	LMG	C15-C16-C17-C18
19	4	603	CLA	C16-C17-C18-C20
19	7	612	CLA	C16-C17-C18-C19
19	8	304	CLA	CBA-CGA-O2A-C1
19	A	837	CLA	CBA-CGA-O2A-C1
19	B	829	CLA	CBA-CGA-O2A-C1
19	B	830	CLA	CBA-CGA-O2A-C1
26	6	318	LHG	C10-C11-C12-C13
19	4	609	CLA	C10-C11-C12-C13
19	A	809	CLA	O1D-CGD-O2D-CED
24	3	324	LMU	C4'-C5'-C6'-O6'
24	1	322	LMU	C2-C3-C4-C5
19	A	828	CLA	CBD-CGD-O2D-CED
19	Z	614	CLA	CBD-CGD-O2D-CED
19	3	307	CLA	C4B-C3B-CAB-CBB
19	6	305	CLA	C4B-C3B-CAB-CBB
19	B	809	CLA	C4B-C3B-CAB-CBB
19	1	310	CLA	C4B-C3B-CAB-CBB
19	1	313	CLA	C4B-C3B-CAB-CBB
20	4	607	CHL	C4B-C3B-CAB-CBB
20	5	308	CHL	C4B-C3B-CAB-CBB
20	6	306	CHL	C4B-C3B-CAB-CBB
20	6	308	CHL	C4B-C3B-CAB-CBB
20	6	315	CHL	C4B-C3B-CAB-CBB
20	7	601	CHL	C4B-C3B-CAB-CBB
20	1	305	CHL	C4B-C3B-CAB-CBB
20	1	306	CHL	C4B-C3B-CAB-CBB
19	B	804	CLA	C2A-CAA-CBA-CGA
23	6	326	LMG	O7-C10-C11-C12
21	B	844	BCR	C9-C10-C11-C12
21	I	201	BCR	C15-C16-C17-C18
19	8	307	CLA	CBD-CGD-O2D-CED
26	A	847	LHG	C13-C14-C15-C16
19	8	304	CLA	O1A-CGA-O2A-C1
19	B	829	CLA	O1A-CGA-O2A-C1
19	7	609	CLA	C16-C17-C18-C19
19	B	812	CLA	C4-C3-C5-C6
26	7	618	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
26	A	847	LHG	C24-C25-C26-C27
26	B	851	LHG	C15-C16-C17-C18
19	B	812	CLA	C2-C3-C5-C6
19	1	308	CLA	C2-C3-C5-C6
19	A	837	CLA	O1A-CGA-O2A-C1
19	4	612	CLA	C8-C10-C11-C12
19	6	312	CLA	CAA-CBA-CGA-O2A
19	B	805	CLA	CAA-CBA-CGA-O1A
19	6	311	CLA	C2-C1-O2A-CGA
19	7	607	CLA	C2-C1-O2A-CGA
19	8	304	CLA	C2-C1-O2A-CGA
19	A	834	CLA	C2-C1-O2A-CGA
19	A	837	CLA	C2-C1-O2A-CGA
19	B	839	CLA	C2-C1-O2A-CGA
19	Z	604	CLA	C2-C1-O2A-CGA
19	4	613	CLA	CBD-CGD-O2D-CED
19	6	313	CLA	C13-C15-C16-C17
19	B	835	CLA	C5-C6-C7-C8
19	5	312	CLA	CAA-CBA-CGA-O2A
20	5	306	CHL	CAA-CBA-CGA-O1A
19	4	612	CLA	C2A-CAA-CBA-CGA
19	5	313	CLA	C2A-CAA-CBA-CGA
19	F	303	CLA	C2A-CAA-CBA-CGA
19	B	825	CLA	C13-C15-C16-C17
26	5	321	LHG	C5-C4-O6-P
26	A	801	LHG	C2-C3-O3-P
19	3	313	CLA	CAA-CBA-CGA-O1A
19	B	801	CLA	C3A-C2A-CAA-CBA
19	1	304	CLA	C3A-C2A-CAA-CBA
20	4	607	CHL	C3A-C2A-CAA-CBA
19	A	846	CLA	CAA-CBA-CGA-O2A
20	1	306	CHL	CAA-CBA-CGA-O1A
19	4	609	CLA	C11-C12-C13-C14
19	B	808	CLA	C6-C7-C8-C9
19	5	316	CLA	C5-C6-C7-C8
19	A	825	CLA	CAA-CBA-CGA-O1A
23	6	326	LMG	O9-C10-C11-C12
23	L	201	LMG	C10-C11-C12-C13
26	6	325	LHG	C7-C8-C9-C10
19	7	609	CLA	C11-C12-C13-C14
19	8	309	CLA	C14-C13-C15-C16
19	B	830	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	Z	610	CLA	C11-C10-C8-C9
20	3	306	CHL	C14-C13-C15-C16
24	7	620	LMU	C2-C3-C4-C5
26	A	848	LHG	C9-C10-C11-C12
19	1	312	CLA	C10-C11-C12-C13
21	A	853	BCR	C11-C10-C9-C34
21	A	853	BCR	C16-C17-C18-C36
21	B	846	BCR	C11-C10-C9-C34
21	B	846	BCR	C20-C21-C22-C37
21	L	202	BCR	C11-C10-C9-C34
22	5	318	LUT	C11-C10-C9-C19
22	F	305	LUT	C20-C13-C14-C15
22	F	305	LUT	C40-C33-C34-C35
23	4	621	LMG	O1-C7-C8-C9
27	5	323	NEX	C39-C29-C30-C31
31	B	850	DGD	O1G-C1G-C2G-C3G
26	7	618	LHG	C25-C26-C27-C28
19	A	846	CLA	CAA-CBA-CGA-O1A
19	A	820	CLA	CAA-CBA-CGA-O1A
19	B	816	CLA	O1D-CGD-O2D-CED
19	7	609	CLA	C16-C17-C18-C20
19	B	804	CLA	C16-C17-C18-C20
19	B	811	CLA	C16-C17-C18-C20
19	1	307	CLA	C16-C17-C18-C19
20	4	607	CHL	O2A-C1-C2-C3
20	Z	601	CHL	O2A-C1-C2-C3
19	A	828	CLA	CBA-CGA-O2A-C1
19	3	312	CLA	O1D-CGD-O2D-CED
19	8	307	CLA	O1D-CGD-O2D-CED
26	8	318	LHG	C9-C10-C11-C12
19	3	309	CLA	C4-C3-C5-C6
19	1	312	CLA	C4-C3-C5-C6
19	5	311	CLA	C1A-C2A-CAA-CBA
19	6	310	CLA	C1A-C2A-CAA-CBA
19	A	836	CLA	C1A-C2A-CAA-CBA
19	A	839	CLA	C1A-C2A-CAA-CBA
19	B	814	CLA	C1A-C2A-CAA-CBA
20	Z	606	CHL	C1A-C2A-CAA-CBA
19	B	842	CLA	C16-C17-C18-C19
19	Z	610	CLA	C11-C12-C13-C15
19	5	316	CLA	C6-C7-C8-C10
19	8	303	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	A	840	CLA	C11-C10-C8-C7
19	B	811	CLA	C11-C10-C8-C7
19	B	812	CLA	C12-C13-C15-C16
19	B	819	CLA	C6-C7-C8-C10
19	B	824	CLA	C11-C12-C13-C15
19	B	837	CLA	C6-C7-C8-C10
19	Z	608	CLA	C11-C12-C13-C15
19	1	308	CLA	C6-C7-C8-C10
20	7	621	CHL	C12-C13-C15-C16
20	8	305	CHL	C6-C7-C8-C10
20	8	320	CHL	C12-C13-C15-C16
29	B	843	PQN	C16-C17-C18-C20
23	8	321	LMG	C37-C38-C39-C40
19	B	801	CLA	C3-C5-C6-C7
19	A	825	CLA	CAA-CBA-CGA-O2A
20	5	306	CHL	CAA-CBA-CGA-O2A
19	A	818	CLA	C6-C7-C8-C9
19	A	814	CLA	C2A-CAA-CBA-CGA
19	A	820	CLA	C2A-CAA-CBA-CGA
19	A	843	CLA	C2A-CAA-CBA-CGA
19	B	808	CLA	C2A-CAA-CBA-CGA
19	1	304	CLA	C2A-CAA-CBA-CGA
26	6	318	LHG	C24-C25-C26-C27
26	7	618	LHG	O6-C4-C5-O7
19	4	611	CLA	CAA-CBA-CGA-O1A
19	4	611	CLA	CAA-CBA-CGA-O2A
19	B	805	CLA	CAA-CBA-CGA-O2A
20	6	306	CHL	CAA-CBA-CGA-O2A
20	1	306	CHL	CAA-CBA-CGA-O2A
23	J	105	LMG	C12-C13-C14-C15
24	4	623	LMU	C3-C4-C5-C6
19	8	302	CLA	C13-C15-C16-C17
19	A	818	CLA	CBA-CGA-O2A-C1
19	Z	603	CLA	CBA-CGA-O2A-C1
23	J	104	LMG	C21-C22-C23-C24
19	3	301	CLA	C11-C12-C13-C14
20	6	306	CHL	CAA-CBA-CGA-O1A
24	4	624	LMU	O1'-C1-C2-C3
19	5	309	CLA	C8-C10-C11-C12
19	8	304	CLA	C5-C6-C7-C8
19	A	824	CLA	C15-C16-C17-C18
19	B	822	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	4	619	LHG	C23-C24-C25-C26
19	A	807	CLA	C2-C3-C5-C6
19	3	311	CLA	C2B-C3B-CAB-CBB
19	4	610	CLA	C2B-C3B-CAB-CBB
19	5	315	CLA	C2B-C3B-CAB-CBB
19	6	313	CLA	C2B-C3B-CAB-CBB
19	6	314	CLA	C2B-C3B-CAB-CBB
19	8	312	CLA	C2B-C3B-CAB-CBB
19	A	808	CLA	C2B-C3B-CAB-CBB
19	A	824	CLA	C2B-C3B-CAB-CBB
19	B	818	CLA	C2B-C3B-CAB-CBB
19	B	841	CLA	C2B-C3B-CAB-CBB
19	F	304	CLA	C2B-C3B-CAB-CBB
20	4	606	CHL	C2B-C3B-CAB-CBB
20	4	615	CHL	C2B-C3B-CAB-CBB
20	1	306	CHL	C2B-C3B-CAB-CBB
19	A	827	CLA	C15-C16-C17-C18
19	B	815	CLA	C8-C10-C11-C12
19	B	840	CLA	C13-C15-C16-C17
19	4	613	CLA	O1D-CGD-O2D-CED
24	7	619	LMU	O1'-C1-C2-C3
23	G	201	LMG	C15-C16-C17-C18
21	A	853	BCR	C11-C10-C9-C8
21	A	853	BCR	C16-C17-C18-C19
21	B	846	BCR	C11-C10-C9-C8
21	B	846	BCR	C20-C21-C22-C23
21	L	202	BCR	C11-C10-C9-C8
22	F	305	LUT	C12-C13-C14-C15
22	F	305	LUT	C32-C33-C34-C35
27	5	323	NEX	C28-C29-C30-C31
24	1	301	LMU	C4'-C5'-C6'-O6'
19	Z	608	CLA	C5-C6-C7-C8
19	5	312	CLA	CAA-CBA-CGA-O1A
19	7	612	CLA	C16-C17-C18-C20
23	B	852	LMG	O7-C10-C11-C12
19	A	828	CLA	O1A-CGA-O2A-C1
19	A	843	CLA	O1D-CGD-O2D-CED
19	B	808	CLA	C4-C3-C5-C6
19	4	604	CLA	C2-C1-O2A-CGA
19	A	811	CLA	C2-C1-O2A-CGA
19	B	824	CLA	C2-C1-O2A-CGA
19	B	841	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	Z	610	CLA	C2-C1-O2A-CGA
19	Z	603	CLA	O1A-CGA-O2A-C1
19	6	312	CLA	CAA-CBA-CGA-O1A
19	Z	611	CLA	CAA-CBA-CGA-O2A
23	J	105	LMG	O8-C28-C29-C30
19	4	612	CLA	C16-C17-C18-C20
19	8	304	CLA	C11-C10-C8-C9
19	A	807	CLA	C11-C10-C8-C9
19	A	834	CLA	C14-C13-C15-C16
19	B	803	CLA	C14-C13-C15-C16
19	B	830	CLA	O1A-CGA-O2A-C1
19	Z	608	CLA	O1A-CGA-O2A-C1
24	4	624	LMU	C3-C4-C5-C6
19	B	813	CLA	C8-C10-C11-C12
26	4	619	LHG	C30-C31-C32-C33
26	4	620	LHG	C10-C11-C12-C13
19	B	811	CLA	C13-C15-C16-C17
19	3	313	CLA	C2A-CAA-CBA-CGA
19	A	819	CLA	C2A-CAA-CBA-CGA
19	B	828	CLA	C2A-CAA-CBA-CGA
19	Z	614	CLA	C2A-CAA-CBA-CGA
20	4	615	CHL	C2A-CAA-CBA-CGA
19	5	311	CLA	C6-C7-C8-C9
19	A	818	CLA	O1A-CGA-O2A-C1
21	3	319	BCR	C23-C24-C25-C30
21	A	849	BCR	C1-C6-C7-C8
21	A	858	BCR	C5-C6-C7-C8
21	B	849	BCR	C1-C6-C7-C8
22	4	616	LUT	C1-C6-C7-C8
22	5	318	LUT	C1-C6-C7-C8
22	Z	615	LUT	C1-C6-C7-C8
28	A	802	CL0	CAA-CBA-CGA-O2A
31	B	850	DGD	O2G-C1B-C2B-C3B
23	F	301	LMG	O1-C7-C8-C9
19	3	312	CLA	CAA-CBA-CGA-O2A
23	6	301	LMG	C12-C13-C14-C15
26	7	618	LHG	C24-C25-C26-C27
24	1	319	LMU	C4'-C5'-C6'-O6'
21	I	201	BCR	C13-C14-C15-C16
25	6	322	XAT	C29-C30-C31-C32
25	Z	616	XAT	C29-C30-C31-C32
27	6	323	NEX	C13-C14-C15-C35

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Mol	Chain	Res	Type	Atoms
19	A	807	CLA	C4-C3-C5-C6
19	B	820	CLA	C4-C3-C5-C6
20	7	621	CHL	C4-C3-C5-C6
19	A	816	CLA	C2-C3-C5-C6
23	J	105	LMG	C28-C29-C30-C31
20	5	307	CHL	C3-C5-C6-C7
23	4	621	LMG	C8-C7-O1-C1
26	1	318	LHG	C30-C31-C32-C33
24	3	324	LMU	C1-C2-C3-C4
19	6	305	CLA	C16-C17-C18-C19
19	8	302	CLA	C16-C17-C18-C19
19	1	312	CLA	C16-C17-C18-C19
19	B	811	CLA	C5-C6-C7-C8
19	3	312	CLA	CAA-CBA-CGA-O1A
19	1	311	CLA	CAA-CBA-CGA-O2A
19	Z	608	CLA	CBA-CGA-O2A-C1
19	J	102	CLA	C3-C5-C6-C7
19	Z	611	CLA	CAA-CBA-CGA-O1A
19	6	314	CLA	C4B-C3B-CAB-CBB
19	B	803	CLA	C4B-C3B-CAB-CBB
19	1	307	CLA	C4B-C3B-CAB-CBB
20	4	606	CHL	C4B-C3B-CAB-CBB
20	6	302	CHL	C4B-C3B-CAB-CBB
19	6	311	CLA	C4-C3-C5-C6
19	A	844	CLA	C4-C3-C5-C6
19	A	844	CLA	C6-C7-C8-C10
19	B	808	CLA	C2-C3-C5-C6
20	5	307	CHL	C2-C3-C5-C6
19	5	314	CLA	CAA-CBA-CGA-O2A
19	A	807	CLA	CBA-CGA-O2A-C1
19	1	302	CLA	O1A-CGA-O2A-C1
20	5	307	CHL	C1-C2-C3-C4
20	8	320	CHL	C1-C2-C3-C4
26	7	618	LHG	O8-C23-C24-C25
23	3	321	LMG	O1-C7-C8-O7
19	B	801	CLA	CBD-CGD-O2D-CED
19	1	311	CLA	CAA-CBA-CGA-O1A
23	F	301	LMG	C30-C31-C32-C33
19	4	604	CLA	C2A-CAA-CBA-CGA
19	A	842	CLA	C8-C10-C11-C12
23	B	852	LMG	C34-C35-C36-C37
26	4	619	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
19	5	305	CLA	O1D-CGD-O2D-CED
19	B	817	CLA	CBA-CGA-O2A-C1
19	1	302	CLA	CBA-CGA-O2A-C1
22	5	324	LUT	C20-C13-C14-C15
22	J	101	LUT	C11-C10-C9-C19
19	A	828	CLA	O1D-CGD-O2D-CED
19	3	303	CLA	C4-C3-C5-C6
19	6	327	CLA	C4-C3-C5-C6
19	A	830	CLA	C4-C3-C5-C6
19	B	811	CLA	C4-C3-C5-C6
19	Z	608	CLA	C4-C3-C5-C6
19	A	807	CLA	O1A-CGA-O2A-C1
19	1	312	CLA	C2-C3-C5-C6
19	5	319	CLA	O1A-CGA-O2A-C1
23	B	852	LMG	C12-C13-C14-C15
19	7	612	CLA	C11-C10-C8-C9
19	A	824	CLA	C11-C10-C8-C9
19	A	827	CLA	C11-C12-C13-C14
19	A	835	CLA	C14-C13-C15-C16
19	A	836	CLA	C11-C12-C13-C14
19	A	840	CLA	C11-C10-C8-C9
19	B	801	CLA	C14-C13-C15-C16
19	B	814	CLA	C11-C10-C8-C9
19	B	824	CLA	C11-C12-C13-C14
19	B	825	CLA	C11-C12-C13-C14
19	Z	603	CLA	C11-C10-C8-C9
19	F	302	CLA	C14-C13-C15-C16
20	4	605	CHL	C14-C13-C15-C16
20	Z	606	CHL	C11-C12-C13-C14
19	3	307	CLA	C3A-C2A-CAA-CBA
19	8	308	CLA	C3A-C2A-CAA-CBA
19	B	814	CLA	C3A-C2A-CAA-CBA
19	B	817	CLA	O1A-CGA-O2A-C1
26	8	318	LHG	O7-C7-C8-C9
19	6	327	CLA	CBD-CGD-O2D-CED
19	3	310	CLA	CAD-CBD-CGD-O2D
19	4	611	CLA	CAD-CBD-CGD-O2D
19	6	303	CLA	CAD-CBD-CGD-O2D
19	6	304	CLA	CAD-CBD-CGD-O2D
19	A	808	CLA	CAD-CBD-CGD-O2D
19	A	815	CLA	CAD-CBD-CGD-O2D
19	A	828	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	A	829	CLA	CAD-CBD-CGD-O2D
19	B	805	CLA	CAD-CBD-CGD-O2D
19	B	806	CLA	CAD-CBD-CGD-O2D
19	B	811	CLA	CAD-CBD-CGD-O2D
19	B	813	CLA	CAD-CBD-CGD-O2D
19	B	814	CLA	CAD-CBD-CGD-O2D
19	B	837	CLA	CAD-CBD-CGD-O2D
19	B	840	CLA	CAD-CBD-CGD-O2D
19	K	204	CLA	CAD-CBD-CGD-O2D
19	Z	602	CLA	CAD-CBD-CGD-O2D
19	Z	607	CLA	CAD-CBD-CGD-O2D
19	F	303	CLA	CAD-CBD-CGD-O2D
19	G	202	CLA	CAD-CBD-CGD-O2D
19	G	203	CLA	CAD-CBD-CGD-O2D
20	4	615	CHL	CAD-CBD-CGD-O2D
20	Z	601	CHL	CAD-CBD-CGD-O2D
26	6	325	LHG	C6-C5-O7-C7
19	A	818	CLA	C6-C7-C8-C10
19	Z	604	CLA	C8-C10-C11-C12
19	A	831	CLA	C10-C11-C12-C13
20	7	621	CHL	C10-C11-C12-C13
19	B	826	CLA	C2-C1-O2A-CGA
19	3	310	CLA	CAA-CBA-CGA-O2A
23	8	321	LMG	O7-C10-C11-C12
26	Z	618	LHG	O8-C23-C24-C25
24	F	306	LMU	C11-C10-C9-C8
19	A	828	CLA	C4-C3-C5-C6
20	4	605	CHL	C4-C3-C5-C6
19	Z	611	CLA	O1D-CGD-O2D-CED
19	6	311	CLA	C2-C3-C5-C6
23	J	104	LMG	C15-C16-C17-C18
21	3	319	BCR	C17-C18-C19-C20
21	8	317	BCR	C21-C22-C23-C24
22	5	324	LUT	C7-C8-C9-C10
19	8	310	CLA	CAA-CBA-CGA-O1A
19	8	310	CLA	CAA-CBA-CGA-O2A
19	7	610	CLA	O2A-C1-C2-C3
19	A	817	CLA	O2A-C1-C2-C3
19	A	824	CLA	O2A-C1-C2-C3
19	A	830	CLA	O2A-C1-C2-C3
19	B	825	CLA	O2A-C1-C2-C3
20	6	307	CHL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	6	328	LMU	C7-C8-C9-C10
19	3	309	CLA	C2A-CAA-CBA-CGA
19	A	842	CLA	C2A-CAA-CBA-CGA
19	B	825	CLA	C2A-CAA-CBA-CGA
19	Z	604	CLA	C2A-CAA-CBA-CGA
19	A	834	CLA	C5-C6-C7-C8
26	B	851	LHG	C19-C20-C21-C22
19	5	319	CLA	CAA-CBA-CGA-O2A
19	Z	608	CLA	CAA-CBA-CGA-O2A
19	4	609	CLA	C11-C12-C13-C15
19	4	612	CLA	C16-C17-C18-C19
19	3	301	CLA	CHA-CBD-CGD-O1D
19	4	602	CLA	CHA-CBD-CGD-O2D
19	4	612	CLA	CHA-CBD-CGD-O2D
19	5	316	CLA	CHA-CBD-CGD-O1D
19	6	320	CLA	CHA-CBD-CGD-O2D
19	6	327	CLA	CHA-CBD-CGD-O1D
19	8	311	CLA	CHA-CBD-CGD-O2D
19	8	313	CLA	CHA-CBD-CGD-O1D
19	8	313	CLA	CHA-CBD-CGD-O2D
19	A	803	CLA	CHA-CBD-CGD-O2D
19	A	813	CLA	CHA-CBD-CGD-O1D
19	A	813	CLA	CHA-CBD-CGD-O2D
19	A	817	CLA	CHA-CBD-CGD-O1D
19	A	817	CLA	CHA-CBD-CGD-O2D
19	A	829	CLA	CHA-CBD-CGD-O1D
19	B	804	CLA	CHA-CBD-CGD-O1D
19	B	804	CLA	CHA-CBD-CGD-O2D
19	B	816	CLA	CHA-CBD-CGD-O1D
19	B	827	CLA	CHA-CBD-CGD-O1D
19	B	827	CLA	CHA-CBD-CGD-O2D
19	B	834	CLA	CHA-CBD-CGD-O1D
19	B	834	CLA	CHA-CBD-CGD-O2D
19	B	842	CLA	CHA-CBD-CGD-O1D
19	Z	611	CLA	CHA-CBD-CGD-O2D
19	Z	613	CLA	CHA-CBD-CGD-O2D
19	1	313	CLA	CHA-CBD-CGD-O1D
19	1	313	CLA	CHA-CBD-CGD-O2D
19	L	204	CLA	CHA-CBD-CGD-O1D
20	8	320	CHL	CHA-CBD-CGD-O2D
21	3	315	BCR	C9-C10-C11-C12
19	A	816	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	844	CLA	CAA-CBA-CGA-O2A
20	4	607	CHL	CAA-CBA-CGA-O2A
19	B	824	CLA	C3-C5-C6-C7
26	7	618	LHG	O6-C4-C5-C6
27	6	323	NEX	C28-C29-C30-C31
19	5	314	CLA	CAA-CBA-CGA-O1A
19	A	808	CLA	CAA-CBA-CGA-O2A
26	A	801	LHG	O8-C23-C24-C25
19	1	308	CLA	O1A-CGA-O2A-C1
26	6	318	LHG	C29-C30-C31-C32
19	A	817	CLA	CAA-CBA-CGA-O2A
19	A	825	CLA	C2A-CAA-CBA-CGA
20	4	605	CHL	C5-C6-C7-C8
23	L	201	LMG	C17-C18-C19-C20
26	A	848	LHG	C24-C23-O8-C6
23	L	201	LMG	C14-C15-C16-C17
19	4	603	CLA	CAA-CBA-CGA-O2A
19	B	827	CLA	O1A-CGA-O2A-C1
19	5	313	CLA	C4C-C3C-CAC-CBC
19	8	304	CLA	C11-C10-C8-C7
19	A	844	CLA	C2-C3-C5-C6
19	B	820	CLA	C6-C7-C8-C10
19	3	301	CLA	C11-C12-C13-C15
19	8	303	CLA	C16-C17-C18-C19
23	3	321	LMG	C16-C17-C18-C19
26	4	619	LHG	C10-C11-C12-C13
23	L	201	LMG	O8-C28-C29-C30
26	B	851	LHG	O7-C7-C8-C9
19	3	308	CLA	C11-C12-C13-C14
19	4	608	CLA	C6-C7-C8-C9
19	5	316	CLA	C6-C7-C8-C9
19	8	303	CLA	C11-C10-C8-C9
19	8	309	CLA	C11-C10-C8-C9
19	A	807	CLA	C11-C12-C13-C14
19	A	812	CLA	C6-C7-C8-C9
19	A	842	CLA	C11-C10-C8-C9
19	A	844	CLA	C6-C7-C8-C9
19	B	812	CLA	C14-C13-C15-C16
19	B	814	CLA	C14-C13-C15-C16
19	B	819	CLA	C6-C7-C8-C9
20	3	306	CHL	C11-C12-C13-C14
20	4	607	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	8	305	CHL	C6-C7-C8-C9
20	Z	606	CHL	C14-C13-C15-C16
19	B	809	CLA	C2B-C3B-CAB-CBB
19	1	307	CLA	C2B-C3B-CAB-CBB
19	5	313	CLA	C2C-C3C-CAC-CBC
23	8	321	LMG	C38-C39-C40-C41
24	4	624	LMU	C11-C10-C9-C8
26	A	801	LHG	O7-C7-C8-C9
26	A	847	LHG	O8-C23-C24-C25
26	5	321	LHG	C26-C27-C28-C29
19	5	305	CLA	CBD-CGD-O2D-CED
26	A	847	LHG	O7-C7-C8-C9
26	8	318	LHG	C24-C25-C26-C27
19	B	827	CLA	CBA-CGA-O2A-C1
19	1	308	CLA	CBA-CGA-O2A-C1
19	L	204	CLA	CAA-CBA-CGA-O2A
26	6	325	LHG	C13-C14-C15-C16
19	J	102	CLA	C2-C3-C5-C6
23	B	852	LMG	C31-C32-C33-C34
25	5	322	XAT	C7-C8-C9-C10
19	3	307	CLA	C1A-C2A-CAA-CBA
19	5	319	CLA	C1A-C2A-CAA-CBA
19	8	308	CLA	C1A-C2A-CAA-CBA
19	8	313	CLA	C1A-C2A-CAA-CBA
19	A	804	CLA	C1A-C2A-CAA-CBA
19	Z	614	CLA	C1A-C2A-CAA-CBA
19	1	304	CLA	C1A-C2A-CAA-CBA
19	L	203	CLA	C1A-C2A-CAA-CBA
20	6	302	CHL	C1A-C2A-CAA-CBA
20	1	306	CHL	C1A-C2A-CAA-CBA
26	5	321	LHG	C23-C24-C25-C26
19	3	309	CLA	C6-C7-C8-C10
19	A	844	CLA	CAA-CBA-CGA-O1A
26	Z	618	LHG	O10-C23-C24-C25
19	B	824	CLA	C13-C15-C16-C17
26	A	848	LHG	O10-C23-O8-C6
24	1	319	LMU	C4-C5-C6-C7
19	3	311	CLA	C2A-CAA-CBA-CGA
19	6	310	CLA	C2A-CAA-CBA-CGA
19	B	813	CLA	C2A-CAA-CBA-CGA
19	B	817	CLA	C2A-CAA-CBA-CGA
19	1	302	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	8	321	LMG	C31-C32-C33-C34
19	3	310	CLA	O1A-CGA-O2A-C1
19	6	327	CLA	O1D-CGD-O2D-CED
19	A	827	CLA	CAA-CBA-CGA-O2A
19	Z	603	CLA	C13-C15-C16-C17
19	3	310	CLA	CAA-CBA-CGA-O1A
19	5	319	CLA	CAA-CBA-CGA-O1A
22	5	318	LUT	C6-C7-C8-C9
19	B	822	CLA	C4B-C3B-CAB-CBB
20	5	317	CHL	C4B-C3B-CAB-CBB
26	4	620	LHG	C3-O3-P-O5
26	A	847	LHG	C3-O3-P-O5
26	A	848	LHG	C3-O3-P-O5
19	5	311	CLA	C6-C7-C8-C10
19	B	816	CLA	C16-C17-C18-C19
26	6	318	LHG	C7-C8-C9-C10
19	Z	608	CLA	CAA-CBA-CGA-O1A
20	4	607	CHL	CAA-CBA-CGA-O1A
23	8	321	LMG	O9-C10-C11-C12
26	A	847	LHG	O9-C7-C8-C9
19	1	308	CLA	C13-C15-C16-C17
20	6	302	CHL	C13-C15-C16-C17
19	A	811	CLA	O1A-CGA-O2A-C1
22	1	315	LUT	C11-C10-C9-C19
19	8	308	CLA	CAA-CBA-CGA-O2A
19	B	828	CLA	C3-C5-C6-C7
22	Z	615	LUT	C5-C6-C7-C8
19	A	808	CLA	CAA-CBA-CGA-O1A
23	L	201	LMG	O10-C28-C29-C30
26	A	801	LHG	O9-C7-C8-C9
26	A	801	LHG	O10-C23-C24-C25
19	7	603	CLA	CAA-CBA-CGA-O2A
26	8	318	LHG	O8-C23-C24-C25
23	L	201	LMG	C30-C31-C32-C33
26	8	318	LHG	O9-C7-C8-C9
19	B	828	CLA	C15-C16-C17-C18
19	Z	603	CLA	CAA-CBA-CGA-O2A
19	8	303	CLA	C16-C17-C18-C20
23	4	621	LMG	C15-C16-C17-C18
19	5	316	CLA	CAD-CBD-CGD-O1D
19	6	304	CLA	CAD-CBD-CGD-O1D
19	6	327	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	7	610	CLA	CAD-CBD-CGD-O1D
19	8	314	CLA	CAD-CBD-CGD-O1D
19	A	812	CLA	CAD-CBD-CGD-O1D
19	B	842	CLA	CAD-CBD-CGD-O1D
20	6	302	CHL	CAD-CBD-CGD-O1D
20	7	601	CHL	CAD-CBD-CGD-O1D
26	6	325	LHG	C4-C5-O7-C7
19	4	603	CLA	CAA-CBA-CGA-O1A
19	6	305	CLA	C6-C7-C8-C9
19	8	302	CLA	C11-C10-C8-C9
19	A	819	CLA	C11-C10-C8-C9
19	A	832	CLA	C11-C10-C8-C9
19	B	806	CLA	C6-C7-C8-C9
19	B	830	CLA	C14-C13-C15-C16
19	1	308	CLA	C6-C7-C8-C9
29	B	843	PQN	C16-C17-C18-C19
19	Z	611	CLA	CBD-CGD-O2D-CED
19	B	840	CLA	CBA-CGA-O2A-C1
19	6	304	CLA	CAA-CBA-CGA-O2A
19	A	814	CLA	CAA-CBA-CGA-O2A
19	B	807	CLA	CAA-CBA-CGA-O2A
19	F	304	CLA	CAA-CBA-CGA-O2A
20	8	306	CHL	CAA-CBA-CGA-O2A
19	7	608	CLA	CAA-CBA-CGA-O2A
19	A	806	CLA	O1A-CGA-O2A-C1
19	A	817	CLA	CAA-CBA-CGA-O1A
19	A	840	CLA	C8-C10-C11-C12
19	4	602	CLA	C10-C11-C12-C13
26	7	618	LHG	C30-C31-C32-C33
19	B	804	CLA	C16-C17-C18-C19
19	8	312	CLA	C4-C3-C5-C6
19	4	612	CLA	C3A-C2A-CAA-CBA
19	6	305	CLA	C6-C7-C8-C10
19	7	612	CLA	C11-C10-C8-C7
19	8	309	CLA	C11-C10-C8-C7
19	A	812	CLA	C6-C7-C8-C10
19	A	834	CLA	C12-C13-C15-C16
19	B	803	CLA	C12-C13-C15-C16
19	B	815	CLA	C11-C10-C8-C7
19	B	822	CLA	C11-C10-C8-C7
19	B	826	CLA	C11-C10-C8-C7
19	B	830	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	6	302	CHL	C11-C10-C8-C7
20	Z	606	CHL	C3A-C2A-CAA-CBA
20	Z	606	CHL	C6-C7-C8-C10
22	8	301	LUT	C25-C26-C27-C28
22	J	101	LUT	C25-C26-C27-C28
19	8	308	CLA	CAA-CBA-CGA-O1A
19	L	204	CLA	CAA-CBA-CGA-O1A
19	4	608	CLA	CAA-CBA-CGA-O2A
19	7	611	CLA	CAA-CBA-CGA-O2A
19	8	311	CLA	CAA-CBA-CGA-O2A
19	A	815	CLA	CAA-CBA-CGA-O2A
19	A	824	CLA	CAA-CBA-CGA-O2A
20	8	305	CHL	CAA-CBA-CGA-O2A
21	4	618	BCR	C11-C12-C13-C14
21	A	852	BCR	C17-C18-C19-C20
21	B	802	BCR	C21-C22-C23-C24
22	J	101	LUT	C7-C8-C9-C10
19	A	824	CLA	CAA-CBA-CGA-O1A
19	A	827	CLA	CAA-CBA-CGA-O1A
24	1	320	LMU	C1-C2-C3-C4
19	A	811	CLA	CAA-CBA-CGA-O2A
19	B	810	CLA	CAA-CBA-CGA-O2A
23	8	321	LMG	O8-C28-C29-C30
19	4	603	CLA	C8-C10-C11-C12
19	B	806	CLA	C13-C15-C16-C17
19	4	608	CLA	CAA-CBA-CGA-O1A
19	6	304	CLA	CAA-CBA-CGA-O1A
19	F	304	CLA	CAA-CBA-CGA-O1A
19	F	302	CLA	C8-C10-C11-C12
19	B	806	CLA	CAA-CBA-CGA-O2A
19	B	829	CLA	C5-C6-C7-C8
20	6	315	CHL	C5-C6-C7-C8
19	7	611	CLA	CAA-CBA-CGA-O1A
26	A	847	LHG	O10-C23-C24-C25
19	4	602	CLA	C2A-CAA-CBA-CGA
19	5	314	CLA	C2A-CAA-CBA-CGA
20	3	306	CHL	C2A-CAA-CBA-CGA
19	A	832	CLA	C5-C6-C7-C8
19	B	817	CLA	C8-C10-C11-C12
19	A	806	CLA	CBA-CGA-O2A-C1
19	A	811	CLA	CBA-CGA-O2A-C1
19	5	313	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	B	833	CLA	CBD-CGD-O2D-CED
19	A	838	CLA	C4-C3-C5-C6
19	B	822	CLA	C4-C3-C5-C6
19	A	807	CLA	CAA-CBA-CGA-O2A
19	B	841	CLA	CAA-CBA-CGA-O2A
26	4	620	LHG	O7-C7-C8-C9
19	7	608	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

240 monomers are involved in 396 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	812	CLA	3	0
21	B	845	BCR	3	0
25	6	322	XAT	2	0
19	B	826	CLA	2	0
19	A	838	CLA	3	0
24	3	322	LMU	1	0
19	A	805	CLA	1	0
25	Z	616	XAT	2	0
19	8	309	CLA	3	0
19	6	305	CLA	4	0
20	5	317	CHL	1	0
19	B	820	CLA	1	0
19	A	839	CLA	1	0
20	8	306	CHL	2	0
20	6	306	CHL	2	0
26	6	318	LHG	6	0
19	B	807	CLA	1	0
19	B	827	CLA	1	0
19	4	603	CLA	4	0
19	3	309	CLA	3	0
21	A	851	BCR	1	0
20	4	607	CHL	5	0
26	B	851	LHG	6	0
19	4	602	CLA	1	0
22	5	318	LUT	2	0
19	5	302	CLA	2	0
20	4	606	CHL	1	0
20	7	605	CHL	1	0
25	4	617	XAT	1	0
19	B	803	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	305	CHL	2	0
19	7	602	CLA	2	0
23	F	301	LMG	1	0
20	7	621	CHL	2	0
26	4	620	LHG	2	0
19	B	830	CLA	2	0
19	A	807	CLA	2	0
19	1	311	CLA	3	0
21	A	852	BCR	1	0
23	6	301	LMG	1	0
20	6	307	CHL	8	0
19	8	311	CLA	2	0
19	3	302	CLA	3	0
19	B	833	CLA	1	0
19	A	842	CLA	3	0
19	A	812	CLA	1	0
19	A	824	CLA	2	0
19	4	612	CLA	3	0
19	A	841	CLA	1	0
19	A	817	CLA	1	0
19	Z	612	CLA	1	0
19	6	320	CLA	2	0
26	A	847	LHG	1	0
21	I	201	BCR	1	0
19	A	823	CLA	1	0
24	A	855	LMU	1	0
21	A	850	BCR	2	0
19	B	819	CLA	2	0
19	F	304	CLA	4	0
19	4	610	CLA	1	0
19	4	614	CLA	2	0
19	B	822	CLA	3	0
20	6	308	CHL	1	0
19	B	811	CLA	3	0
26	A	801	LHG	1	0
25	7	616	XAT	1	0
19	A	834	CLA	2	0
19	A	827	CLA	3	0
19	K	204	CLA	1	0
19	B	818	CLA	5	0
19	1	314	CLA	2	0
24	7	620	LMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	L	201	LMG	2	0
22	5	324	LUT	2	0
19	7	609	CLA	3	0
24	1	322	LMU	1	0
19	5	316	CLA	3	0
19	B	837	CLA	3	0
20	6	317	CHL	1	0
19	L	204	CLA	1	0
19	8	312	CLA	1	0
19	8	303	CLA	6	0
19	A	816	CLA	2	0
19	1	312	CLA	1	0
22	F	305	LUT	1	0
26	A	848	LHG	1	0
19	1	303	CLA	3	0
20	6	315	CHL	2	0
24	8	319	LMU	1	0
19	A	814	CLA	2	0
19	B	831	CLA	2	0
19	A	808	CLA	1	0
20	6	302	CHL	2	0
19	B	801	CLA	2	0
21	B	848	BCR	2	0
19	8	307	CLA	1	0
26	5	321	LHG	1	0
19	8	313	CLA	1	0
19	A	819	CLA	2	0
20	4	601	CHL	2	0
19	1	310	CLA	3	0
26	6	325	LHG	1	0
21	7	617	BCR	3	0
19	A	803	CLA	3	0
19	B	815	CLA	2	0
21	3	318	BCR	3	0
22	Z	615	LUT	1	0
19	5	304	CLA	4	0
19	A	837	CLA	5	0
24	B	853	LMU	2	0
21	L	205	BCR	2	0
19	A	810	CLA	3	0
21	3	319	BCR	1	0
21	B	844	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	814	CLA	4	0
21	J	103	BCR	1	0
21	B	846	BCR	1	0
19	5	305	CLA	2	0
19	A	846	CLA	1	0
19	3	305	CLA	2	0
19	6	303	CLA	4	0
19	Z	614	CLA	1	0
19	Z	607	CLA	1	0
19	B	817	CLA	5	0
19	7	612	CLA	5	0
19	4	609	CLA	2	0
19	5	311	CLA	1	0
19	A	836	CLA	1	0
19	Z	603	CLA	2	0
24	F	306	LMU	2	0
19	Z	602	CLA	1	0
19	3	314	CLA	4	0
19	6	327	CLA	1	0
19	B	805	CLA	3	0
19	B	824	CLA	6	0
19	5	313	CLA	3	0
19	5	312	CLA	4	0
20	4	605	CHL	3	0
20	Z	605	CHL	1	0
20	Z	606	CHL	1	0
19	A	833	CLA	2	0
19	B	828	CLA	3	0
23	8	321	LMG	1	0
19	3	313	CLA	3	0
22	4	616	LUT	3	0
19	J	102	CLA	1	0
19	3	303	CLA	3	0
19	B	835	CLA	1	0
24	3	324	LMU	2	0
19	A	844	CLA	1	0
19	L	203	CLA	2	0
25	1	316	XAT	1	0
22	3	317	LUT	1	0
19	8	304	CLA	3	0
19	A	830	CLA	2	0
19	B	813	CLA	3	0

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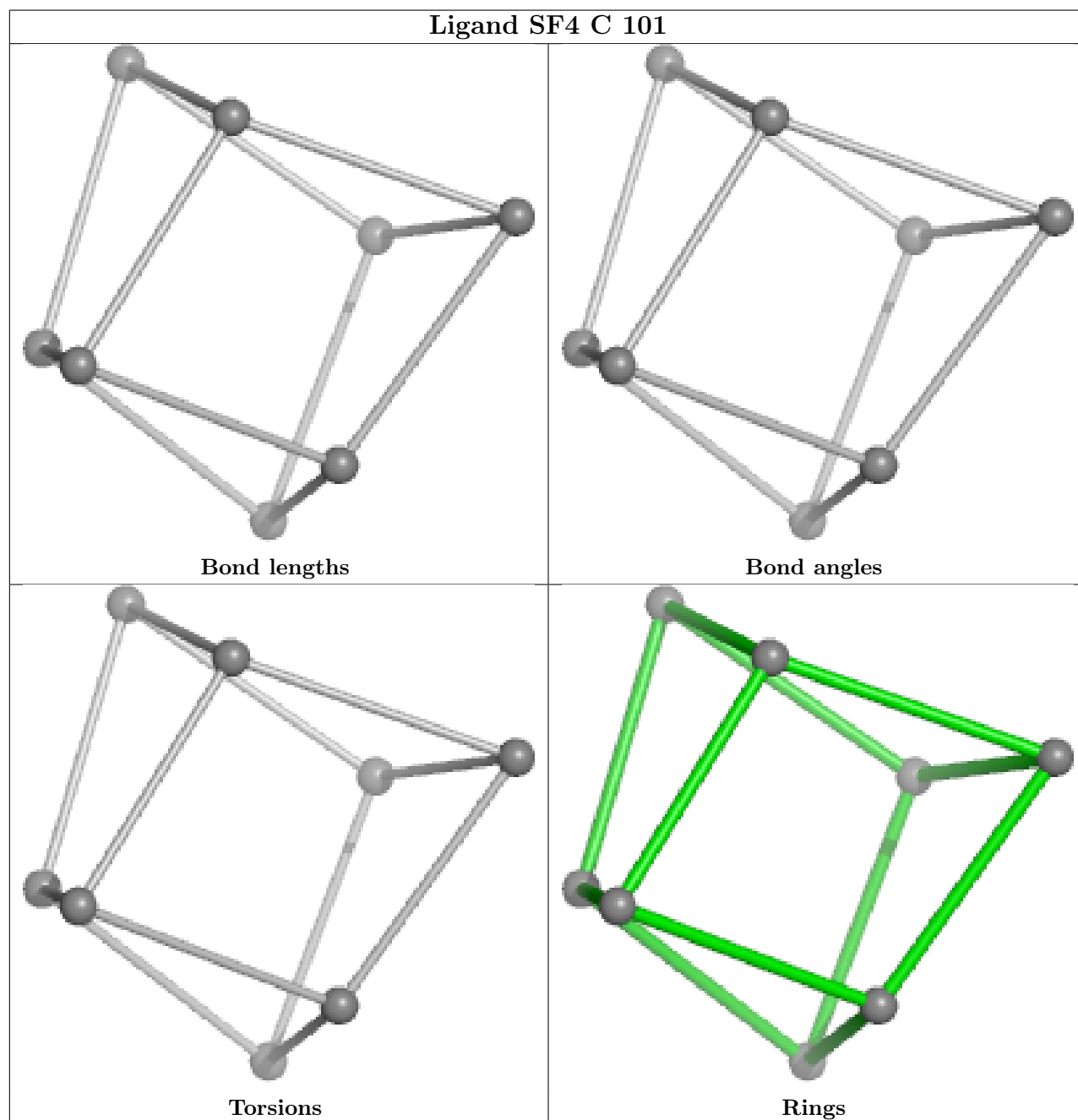
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	5	306	CHL	2	0
19	A	831	CLA	1	0
21	8	317	BCR	1	0
23	J	104	LMG	1	0
22	1	317	LUT	1	0
31	B	850	DGD	2	0
19	3	308	CLA	3	0
21	6	321	BCR	2	0
19	Z	611	CLA	1	0
21	A	858	BCR	1	0
26	5	301	LHG	1	0
19	B	823	CLA	2	0
19	A	811	CLA	6	0
20	4	615	CHL	2	0
19	B	832	CLA	3	0
19	B	842	CLA	5	0
19	Z	608	CLA	5	0
19	3	310	CLA	1	0
21	A	849	BCR	2	0
26	4	619	LHG	3	0
23	6	326	LMG	2	0
19	B	804	CLA	10	0
19	4	604	CLA	1	0
19	B	829	CLA	1	0
20	5	307	CHL	3	0
19	B	841	CLA	2	0
19	6	304	CLA	1	0
21	3	315	BCR	2	0
19	B	806	CLA	2	0
19	B	838	CLA	3	0
22	1	315	LUT	2	0
20	1	306	CHL	1	0
19	A	826	CLA	1	0
21	B	802	BCR	2	0
19	A	821	CLA	3	0
19	4	613	CLA	1	0
19	1	308	CLA	2	0
19	B	809	CLA	3	0
26	8	318	LHG	3	0
19	6	312	CLA	2	0
19	6	314	CLA	2	0
19	1	309	CLA	2	0

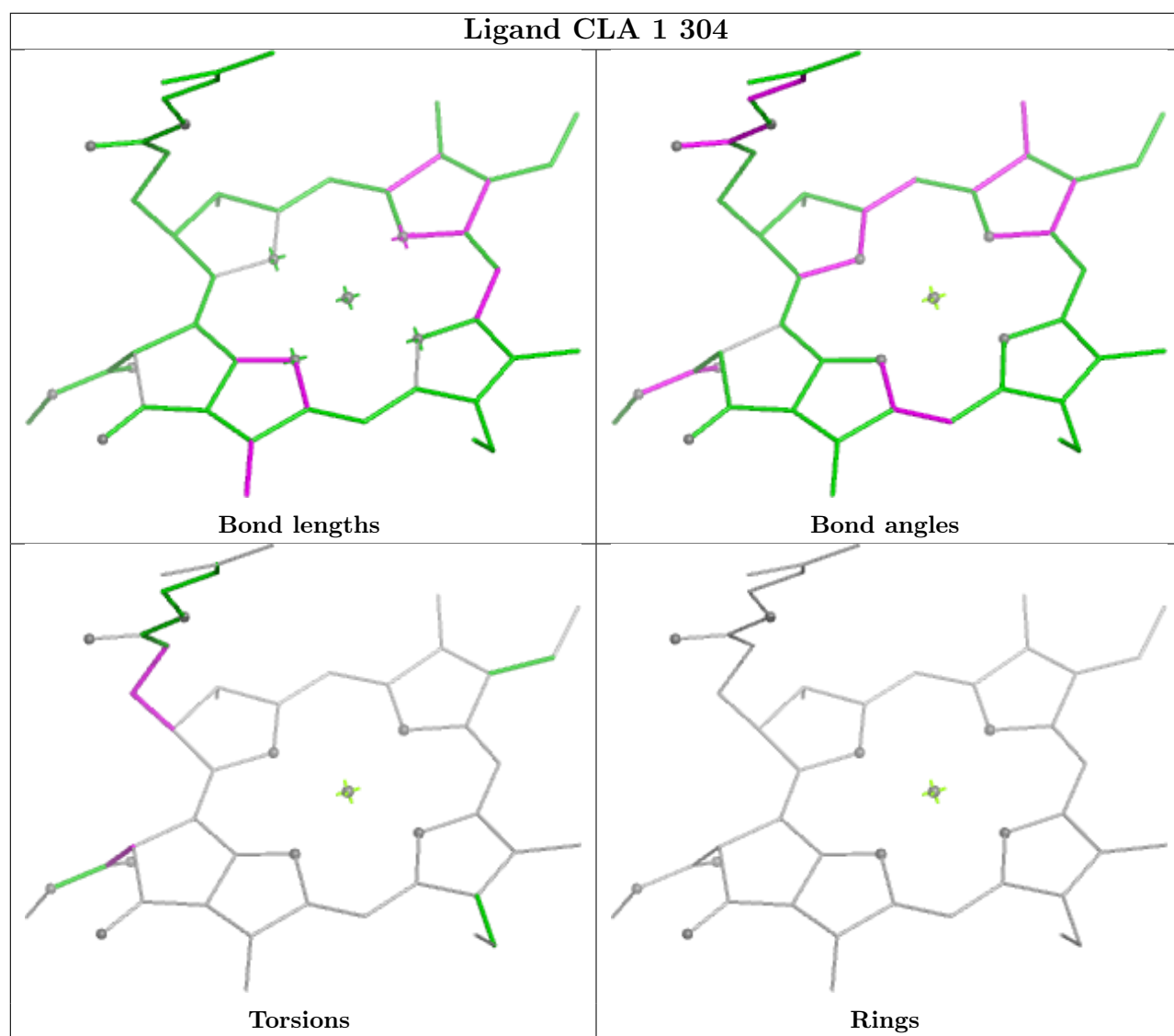
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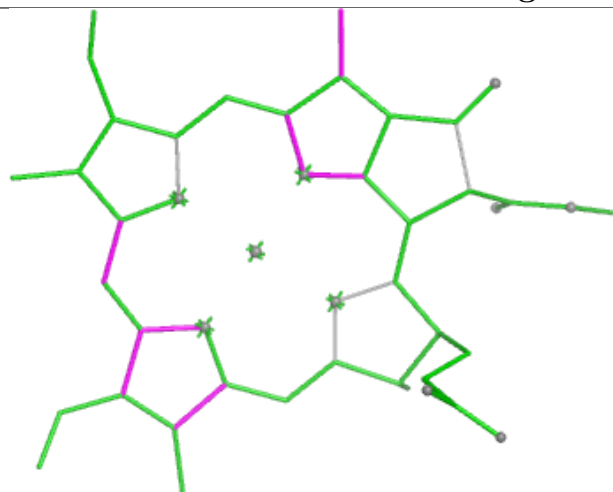
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	853	BCR	3	0
19	B	839	CLA	1	0
19	5	319	CLA	6	0
19	7	610	CLA	4	0
19	A	813	CLA	3	0
19	A	815	CLA	4	0
19	4	608	CLA	1	0
19	B	834	CLA	2	0
19	1	307	CLA	3	0
24	4	623	LMU	2	0
19	5	310	CLA	1	0
19	K	203	CLA	4	0
23	J	105	LMG	3	0
19	A	832	CLA	3	0
21	L	202	BCR	2	0
21	5	320	BCR	4	0
24	1	321	LMU	1	0
24	1	301	LMU	2	0
19	A	818	CLA	1	0
19	B	810	CLA	1	0
24	1	319	LMU	1	0
26	7	618	LHG	1	0
25	5	322	XAT	3	0
19	6	313	CLA	2	0
19	A	840	CLA	2	0
19	Z	609	CLA	1	0
27	6	323	NEX	2	0
19	F	302	CLA	3	0
21	4	618	BCR	1	0
23	3	321	LMG	4	0
19	6	310	CLA	3	0
19	A	829	CLA	2	0
22	J	101	LUT	3	0
19	8	302	CLA	4	0
19	7	613	CLA	1	0
23	B	852	LMG	1	0
19	5	303	CLA	3	0
20	8	320	CHL	1	0
20	8	305	CHL	2	0
19	A	820	CLA	3	0
20	5	308	CHL	1	0
21	K	206	BCR	1	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.

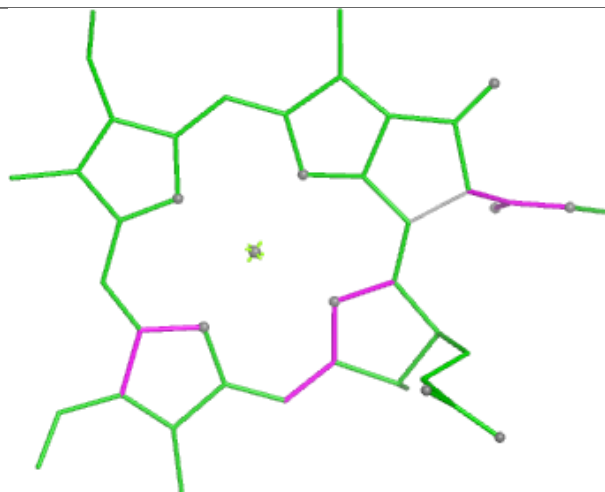




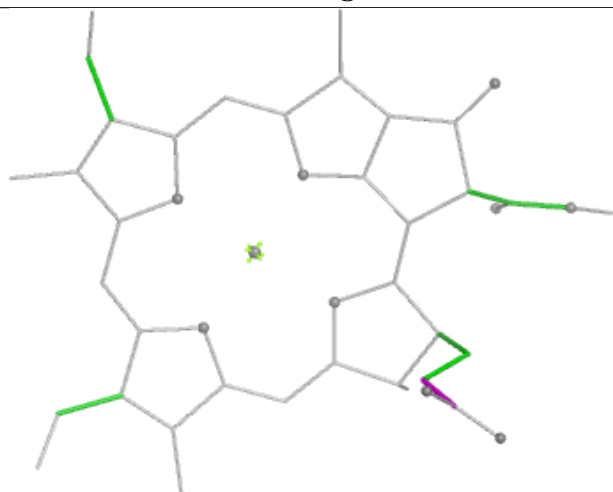
Ligand CLA 7 608



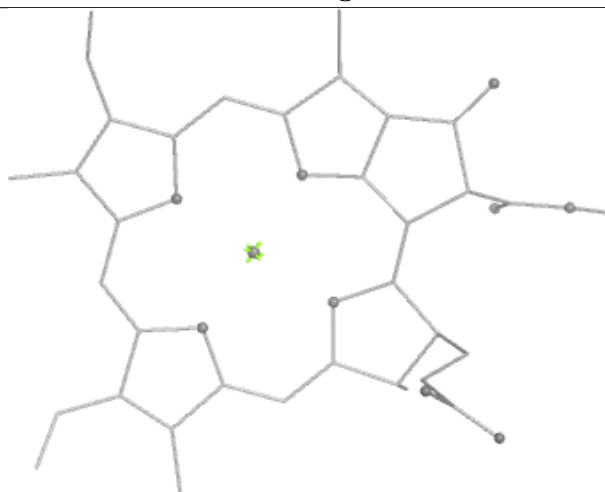
Bond lengths



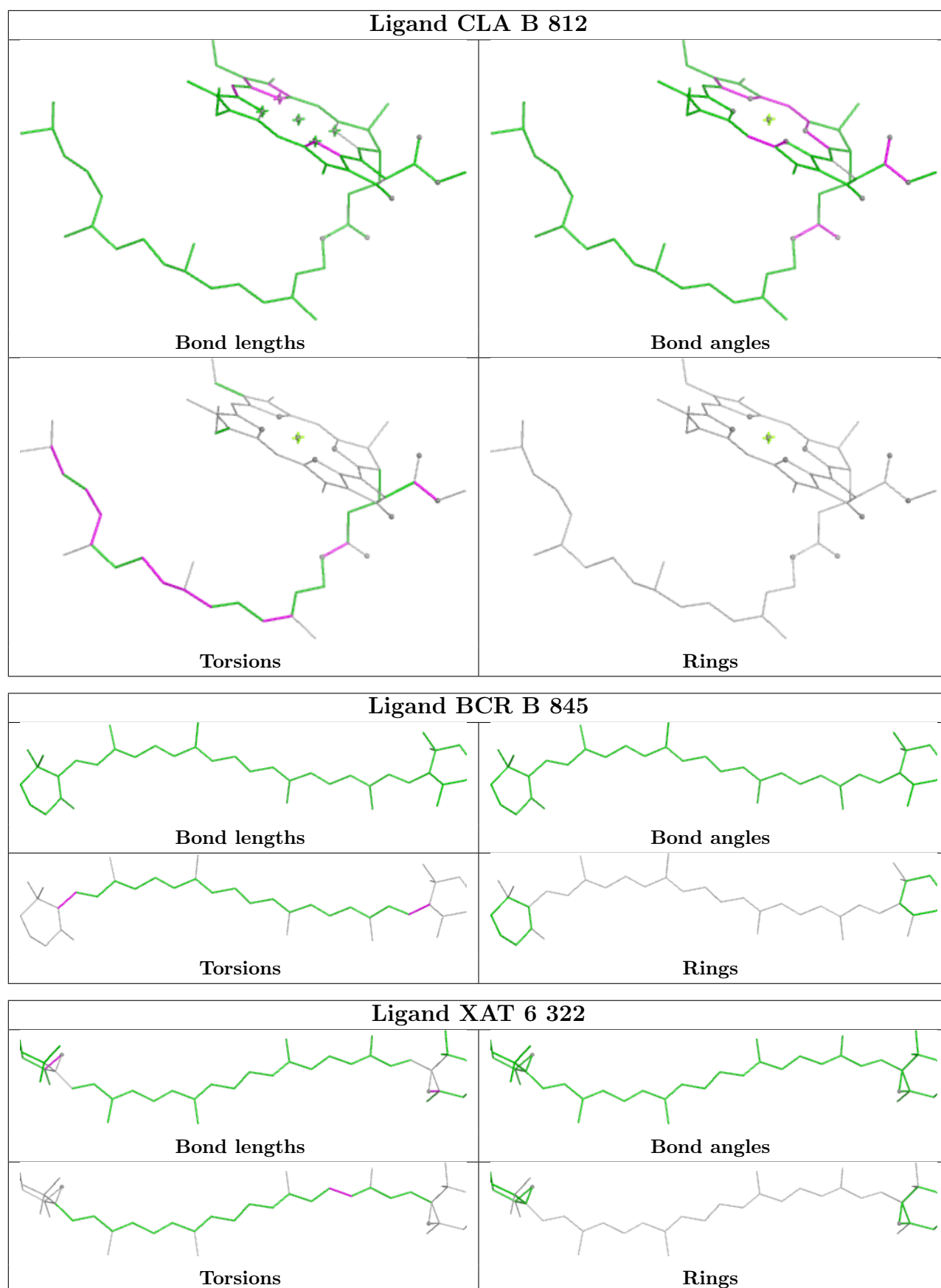
Bond angles



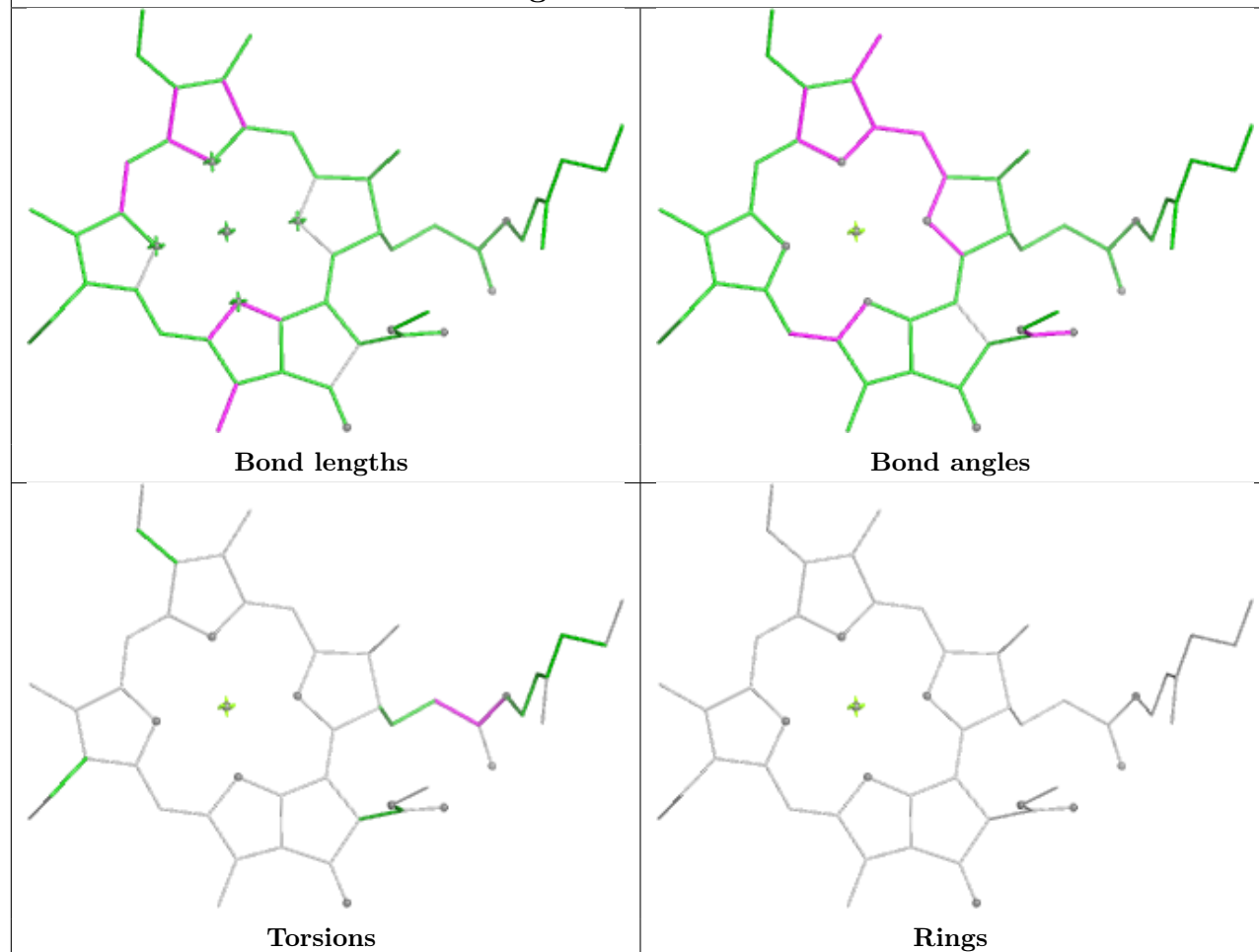
Torsions



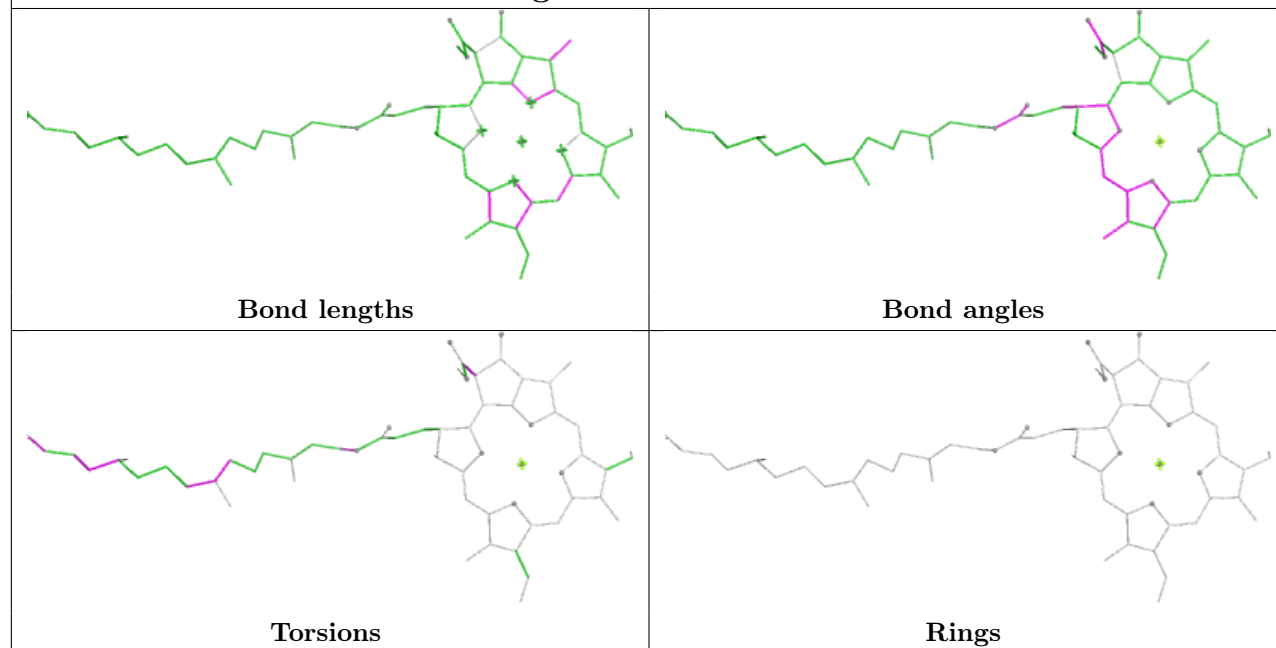
Rings



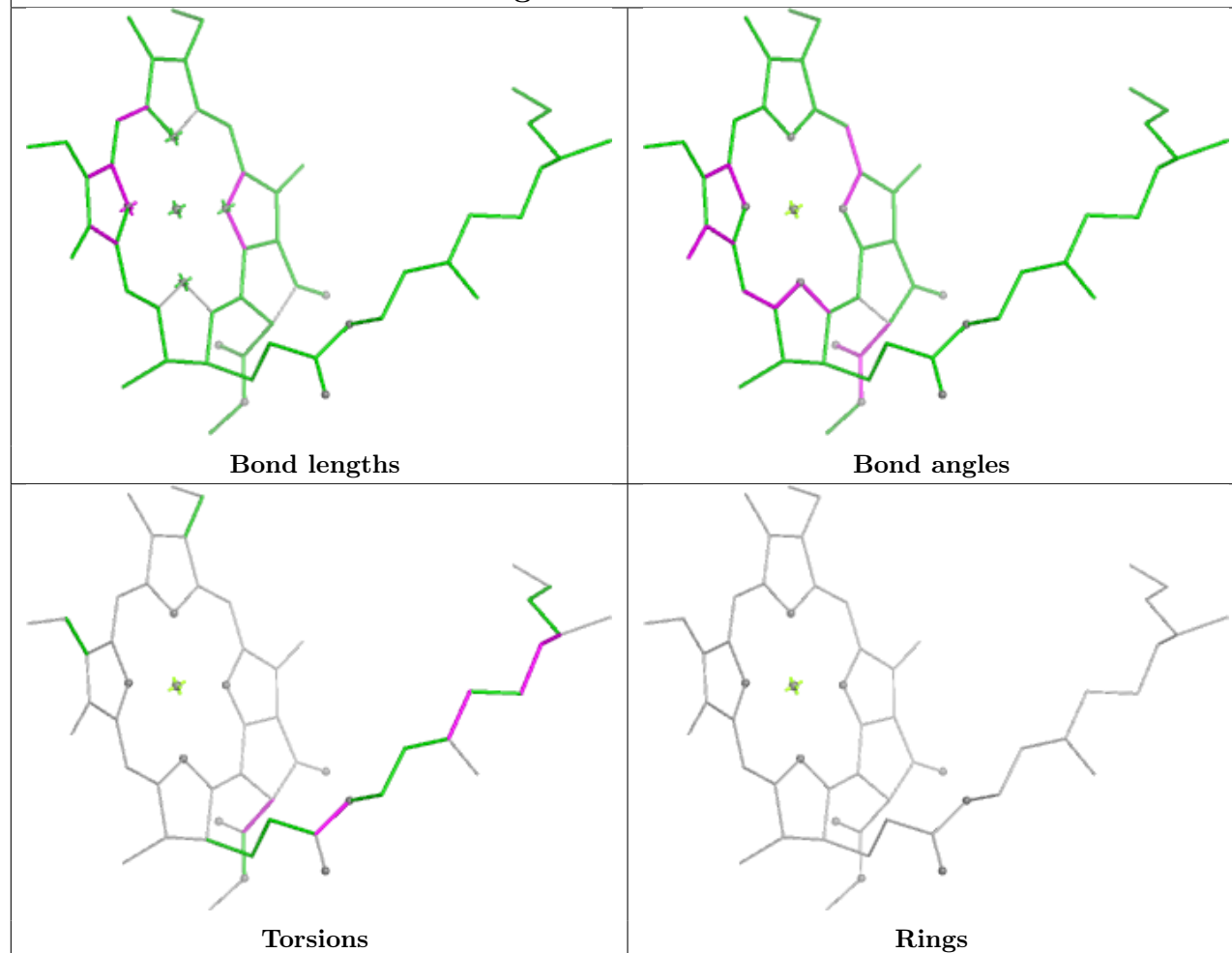
Ligand CLA 7 603



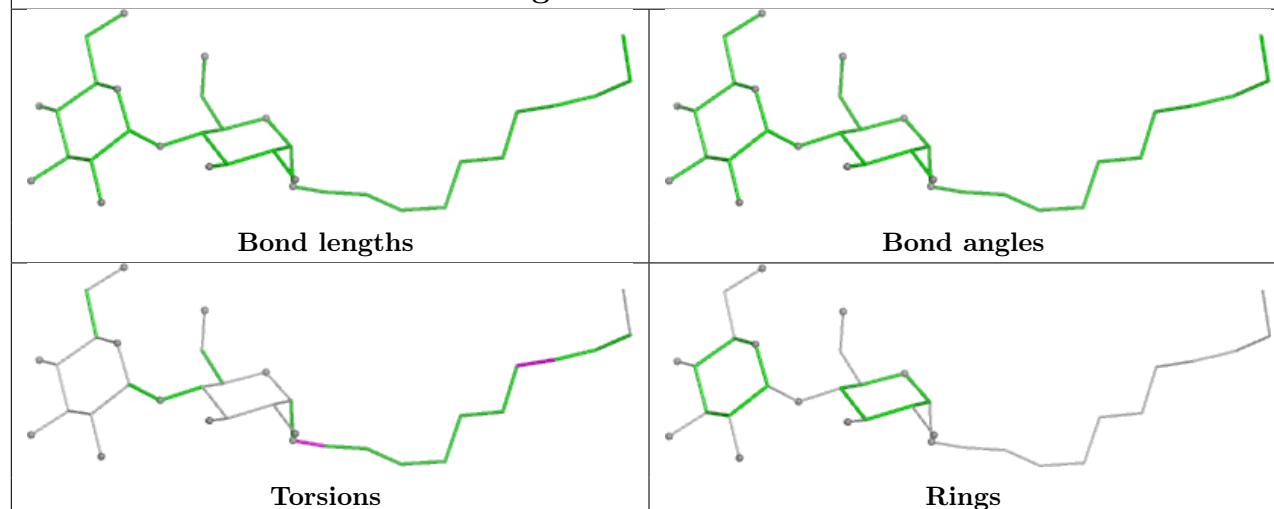
Ligand CLA B 826



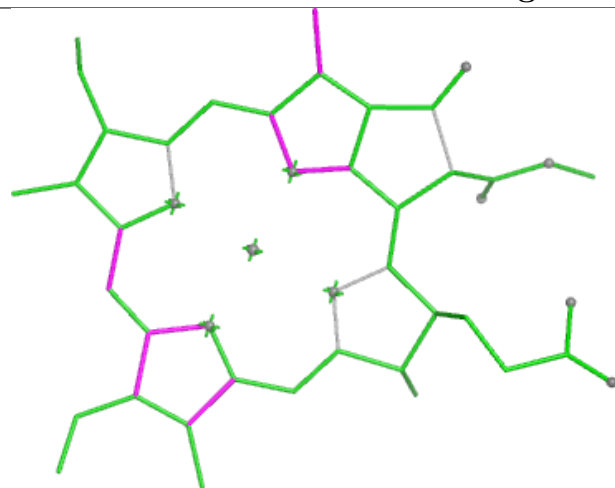
Ligand CLA A 838



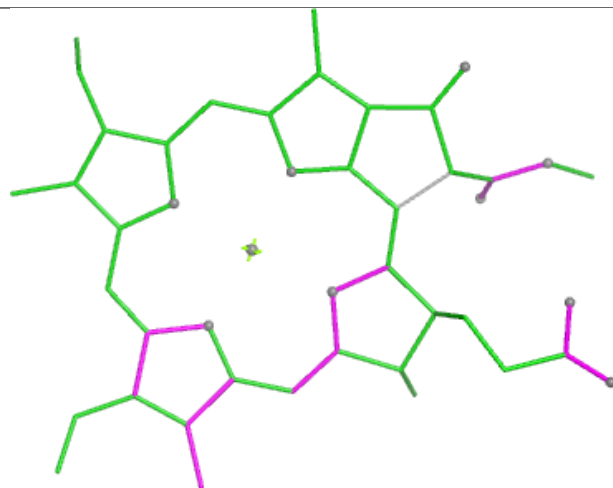
Ligand LMU 3 322



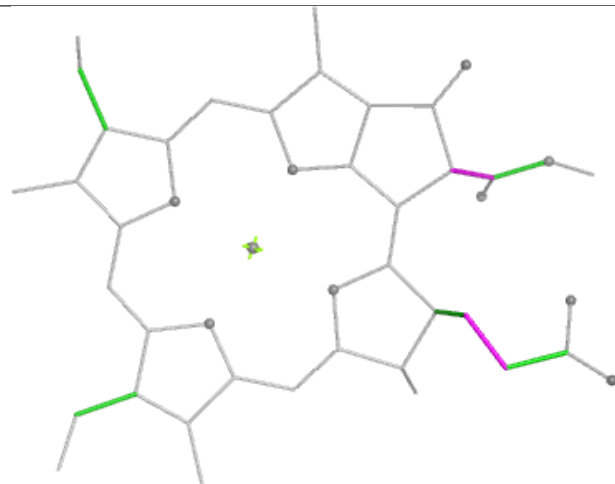
Ligand CLA F 303



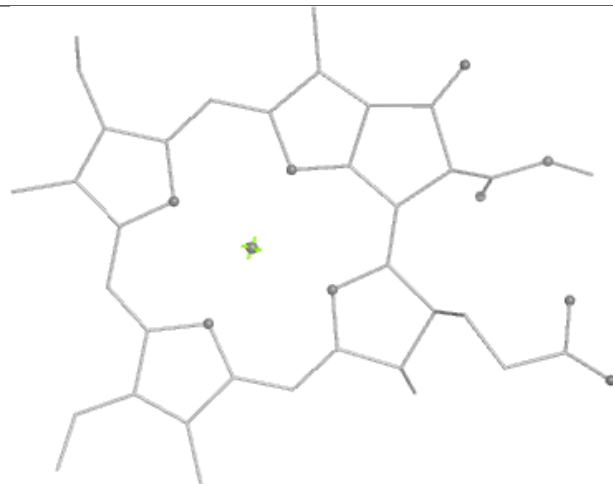
Bond lengths



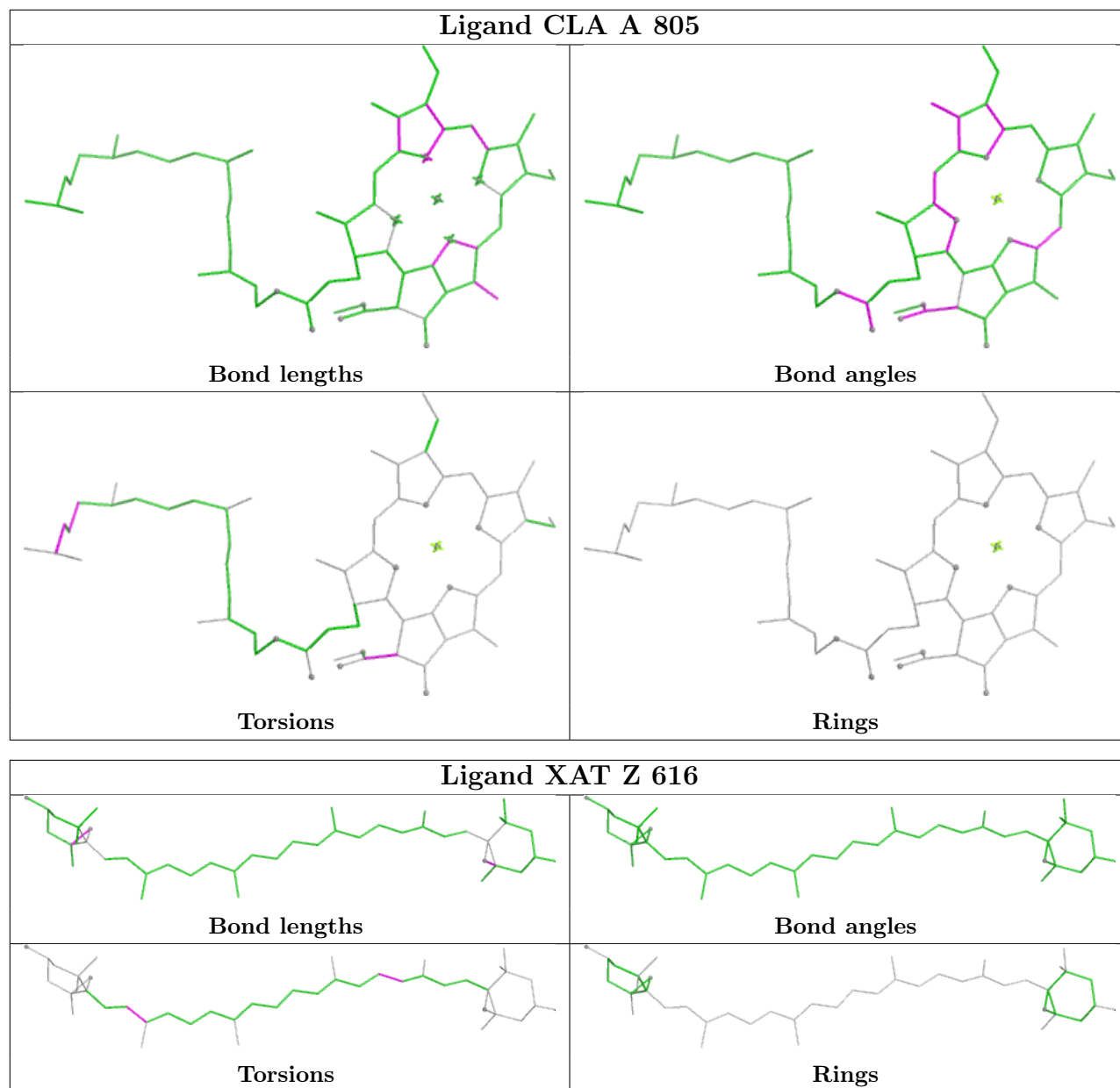
Bond angles



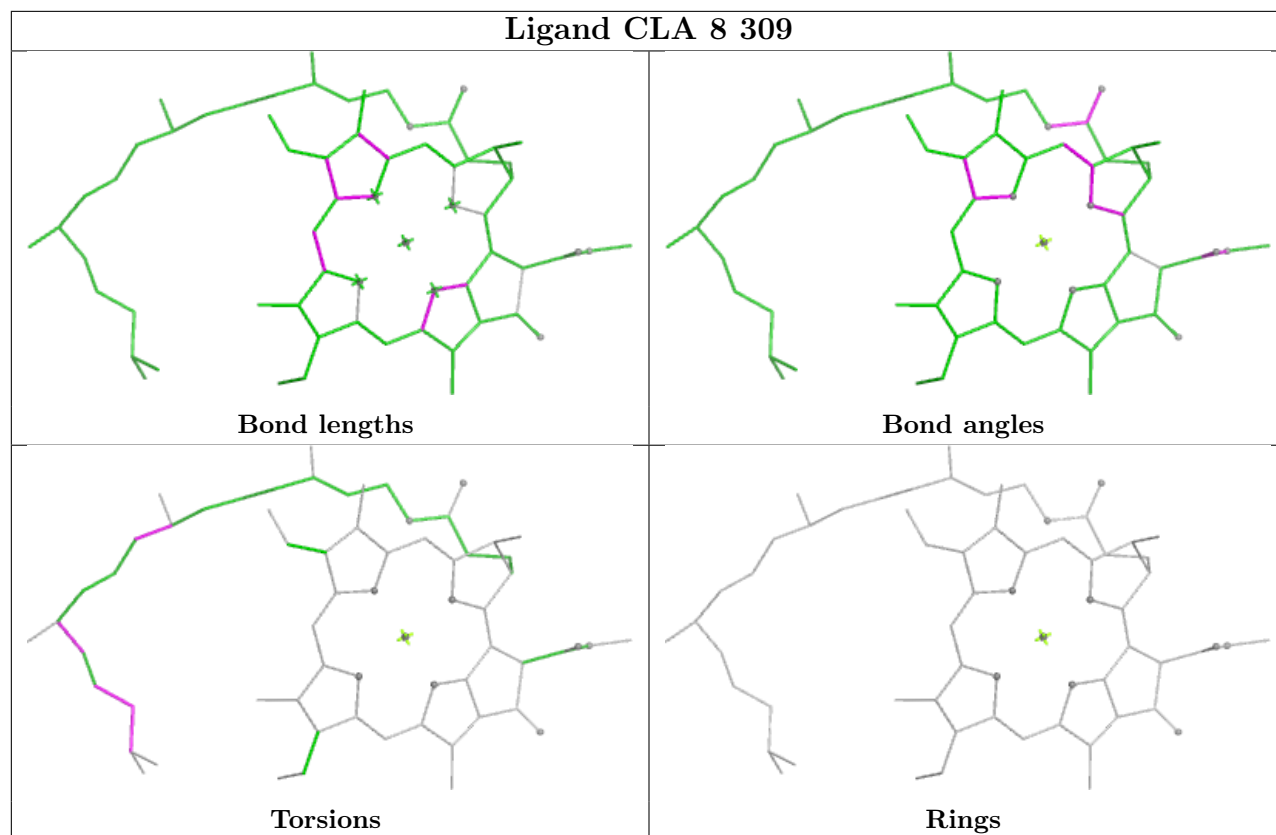
Torsions



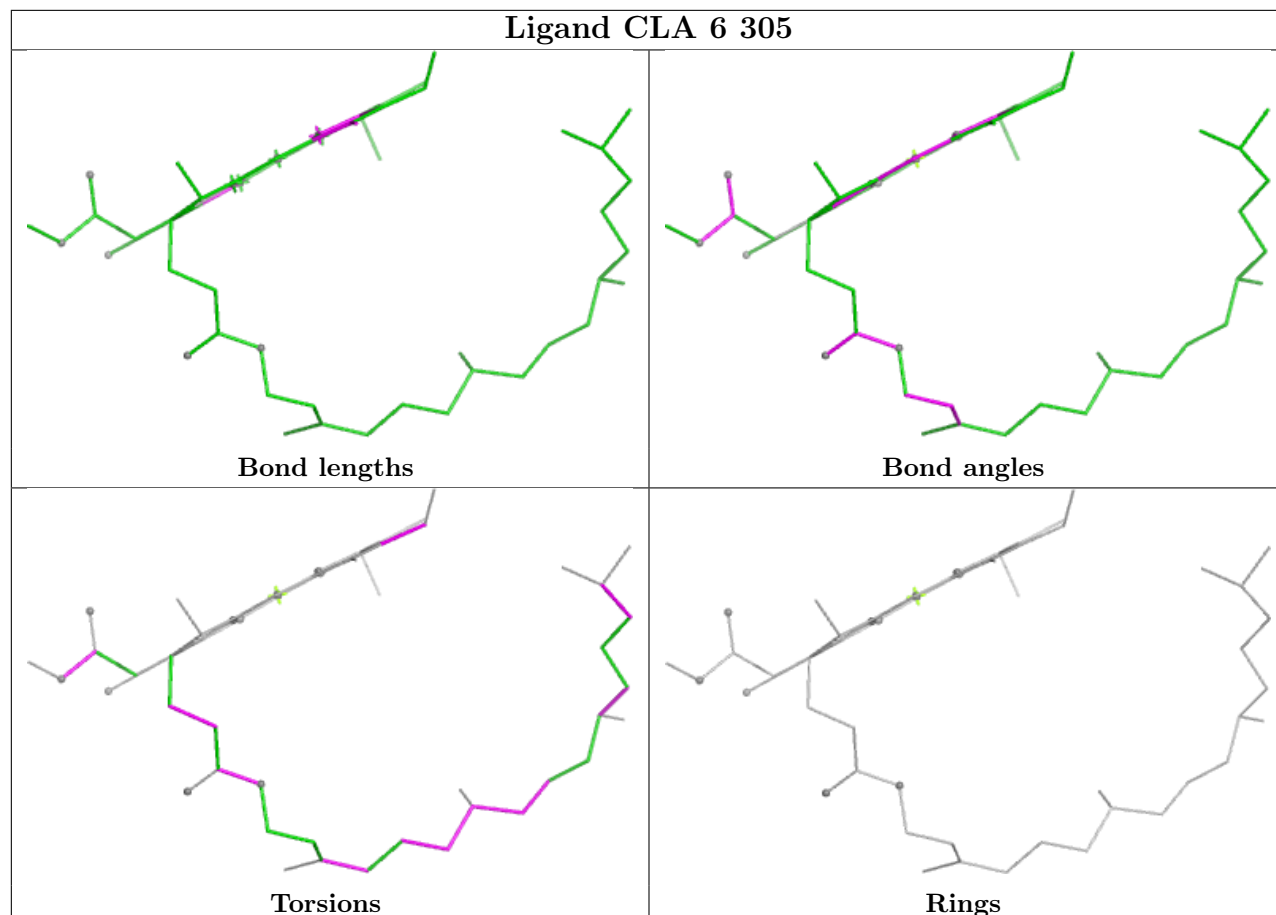
Rings

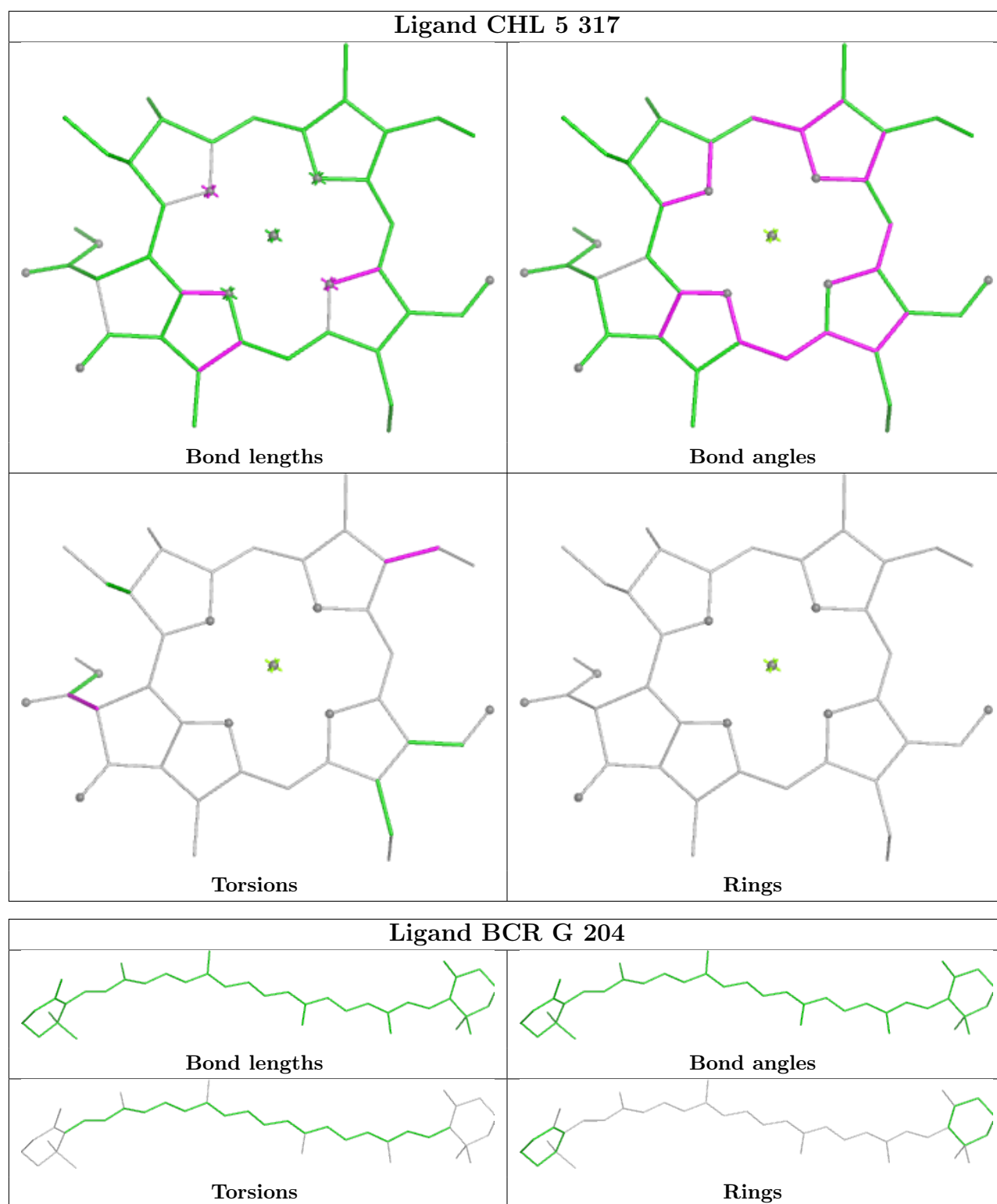


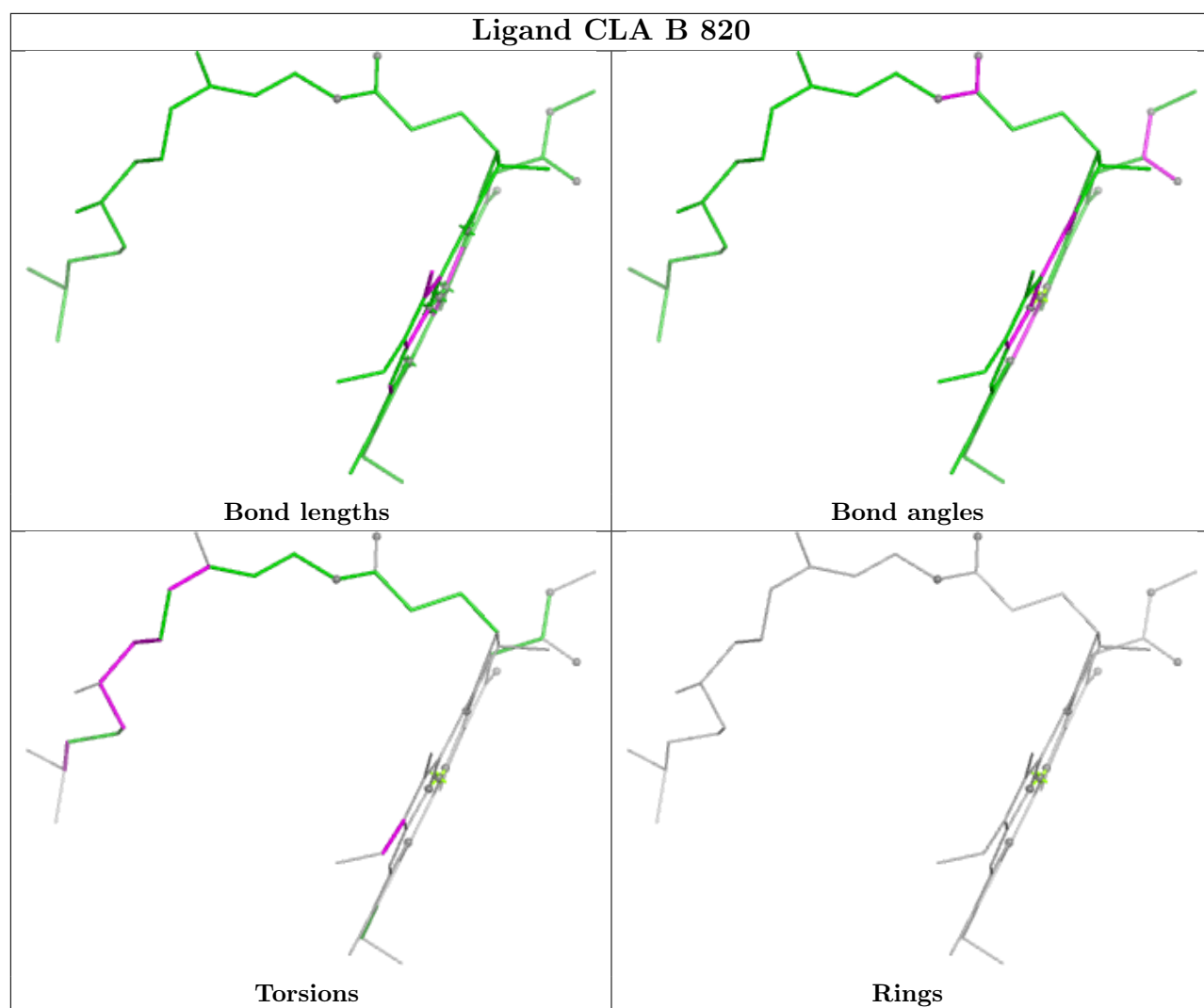
Ligand CLA 8 309

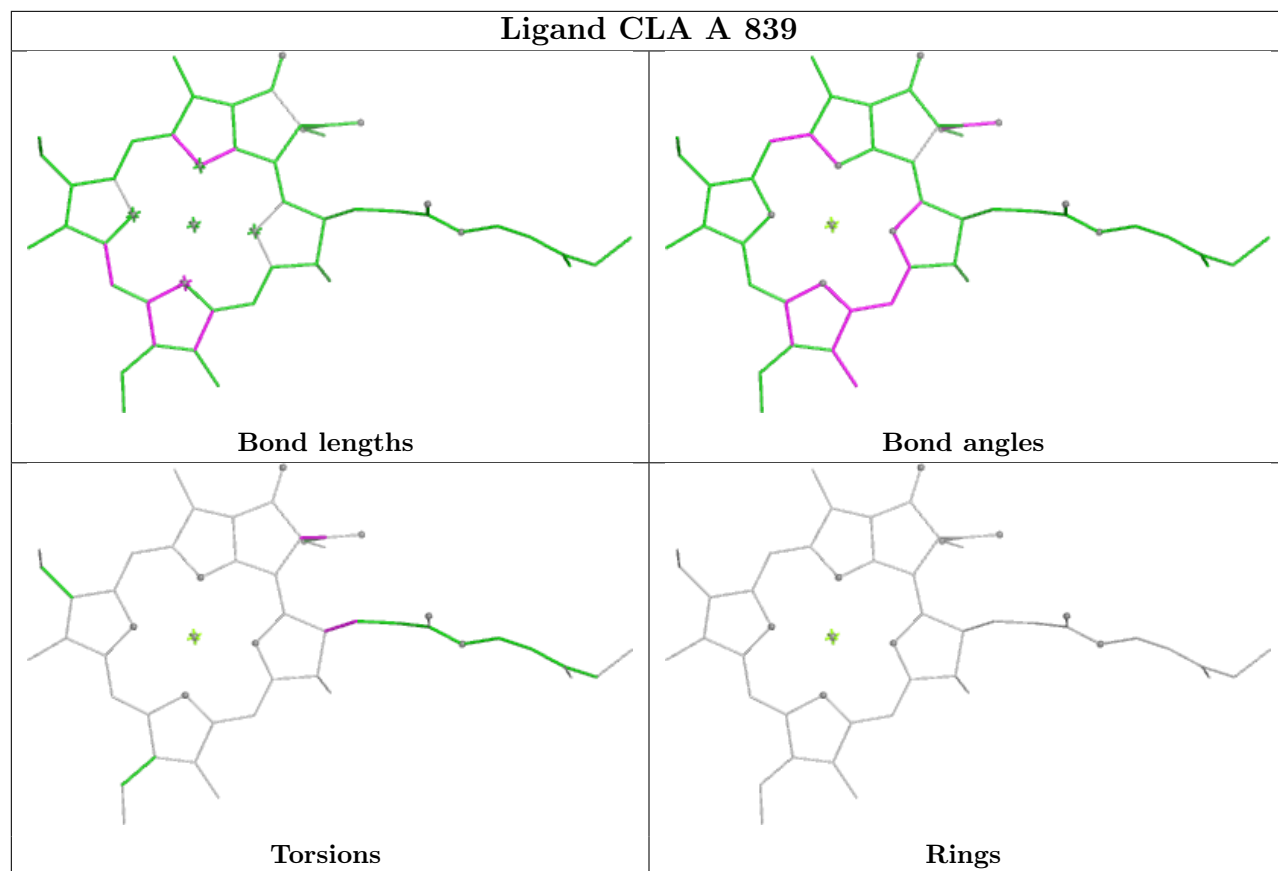


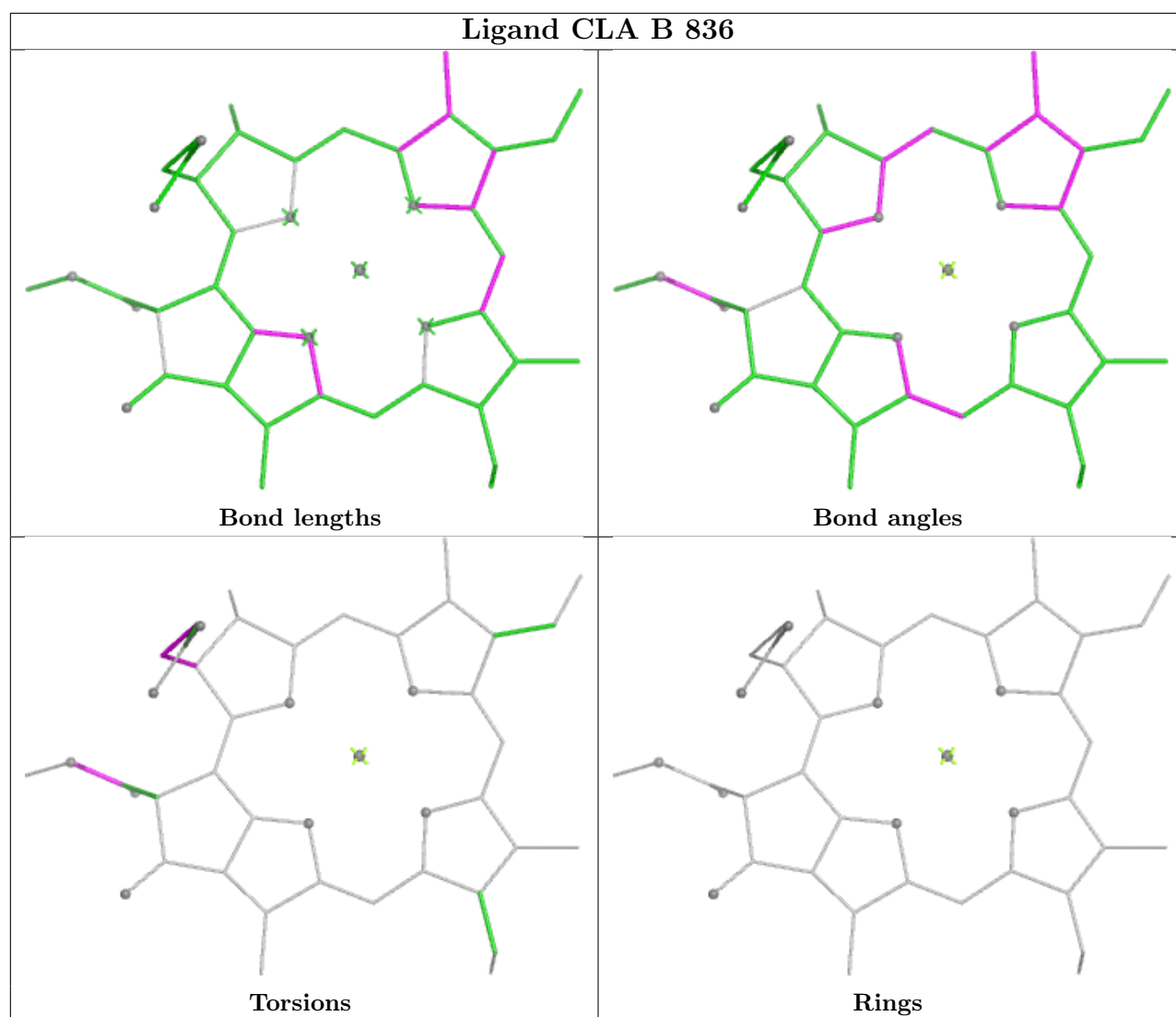
Ligand CLA 6 305

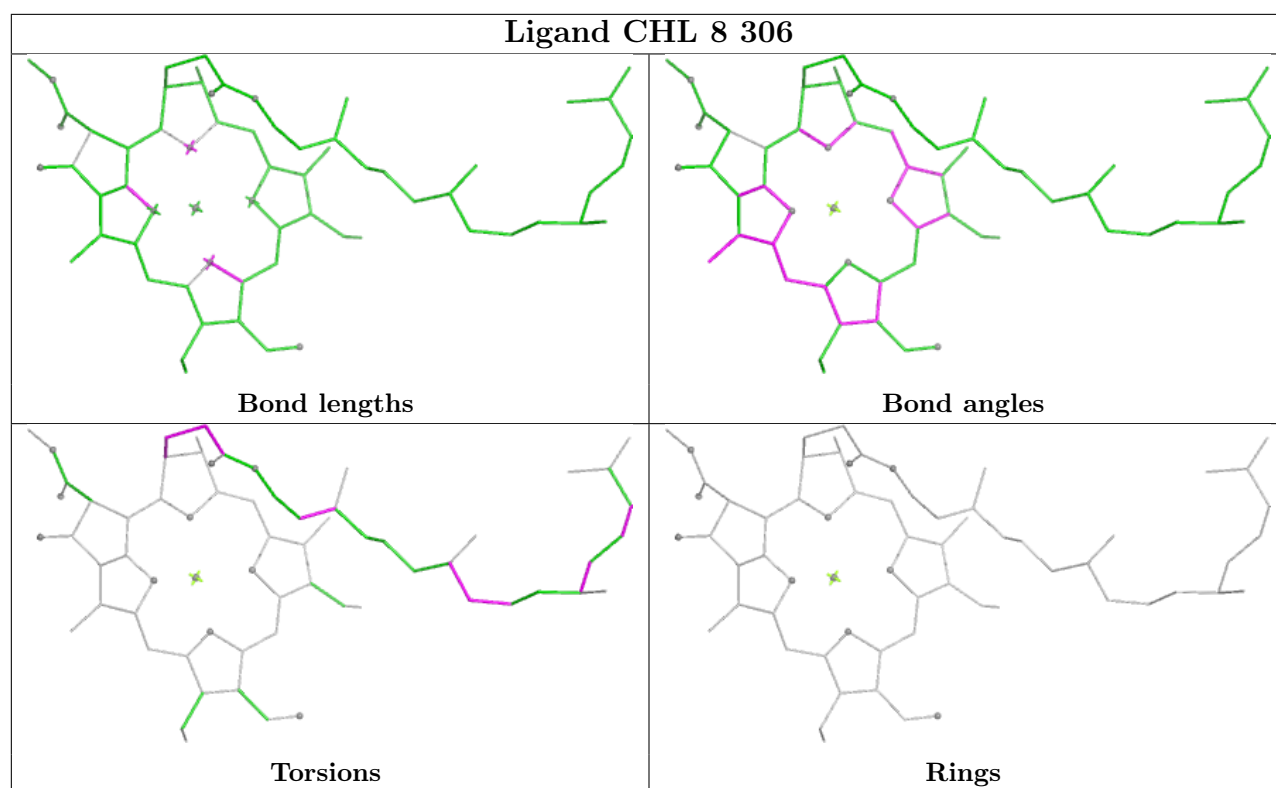




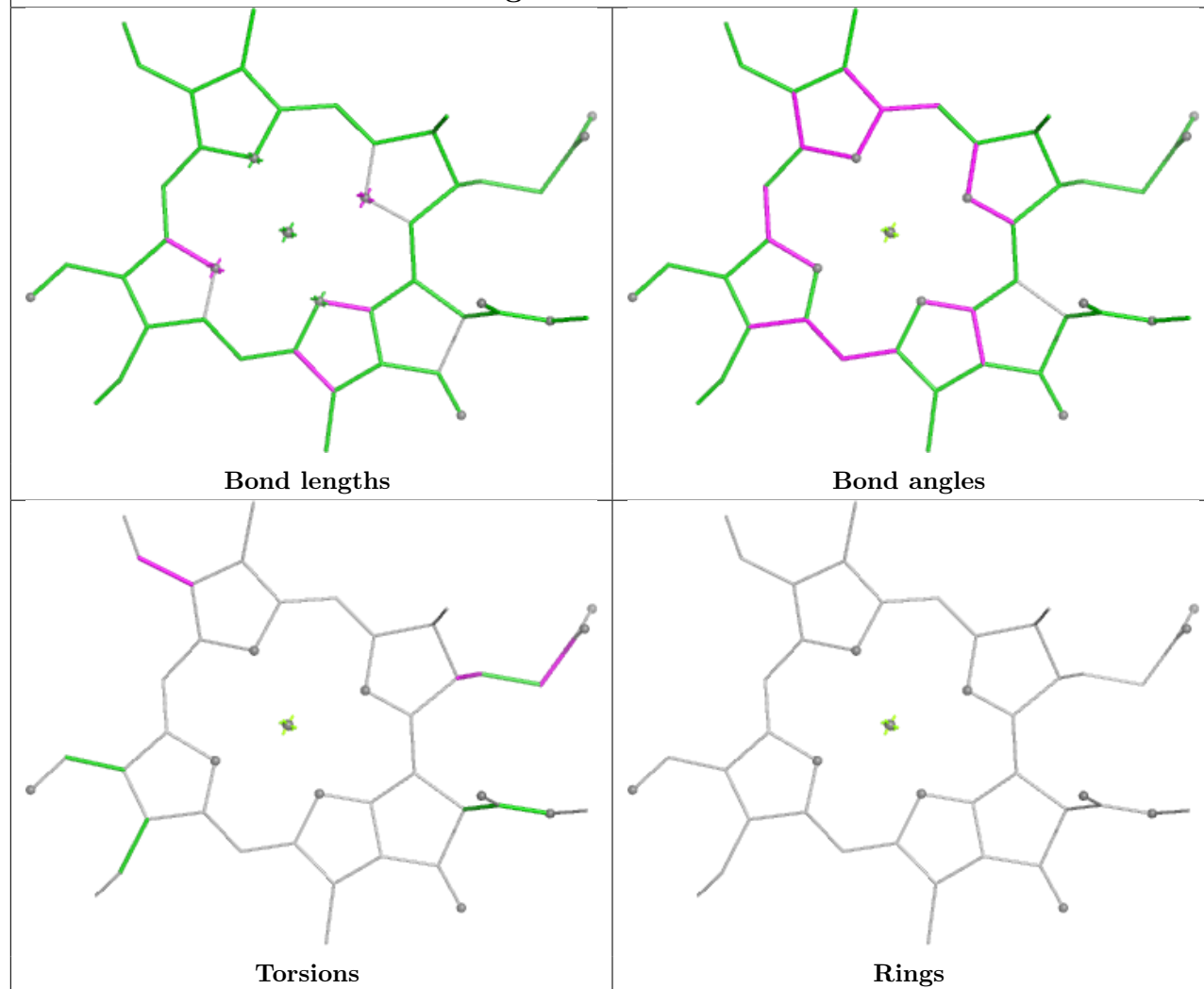




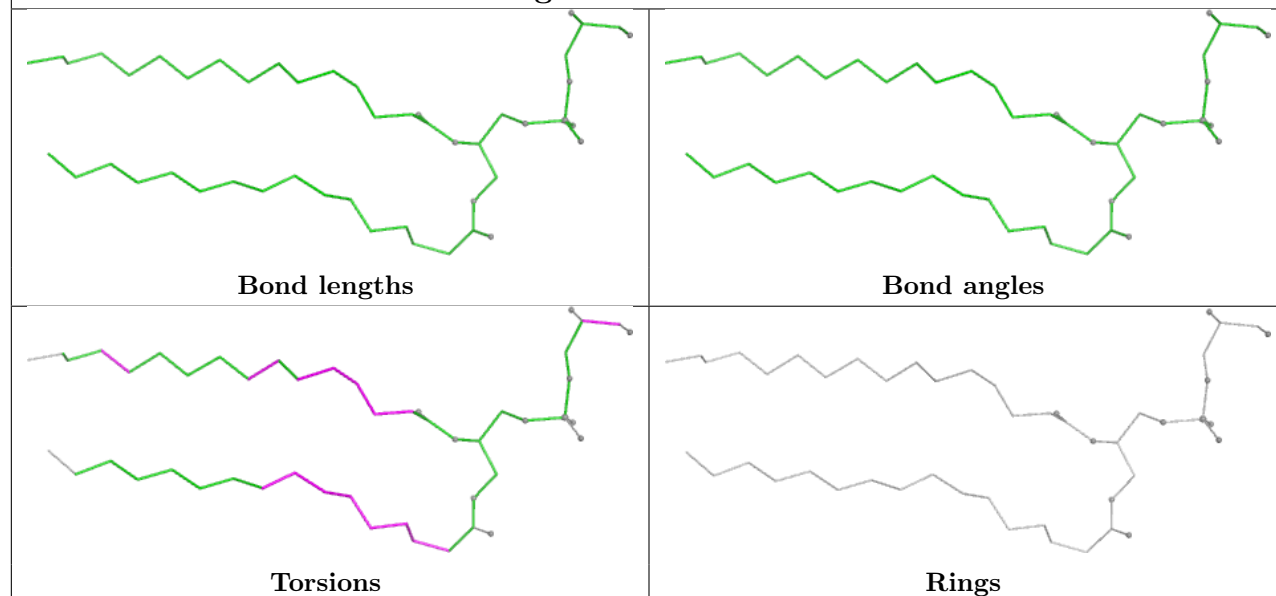


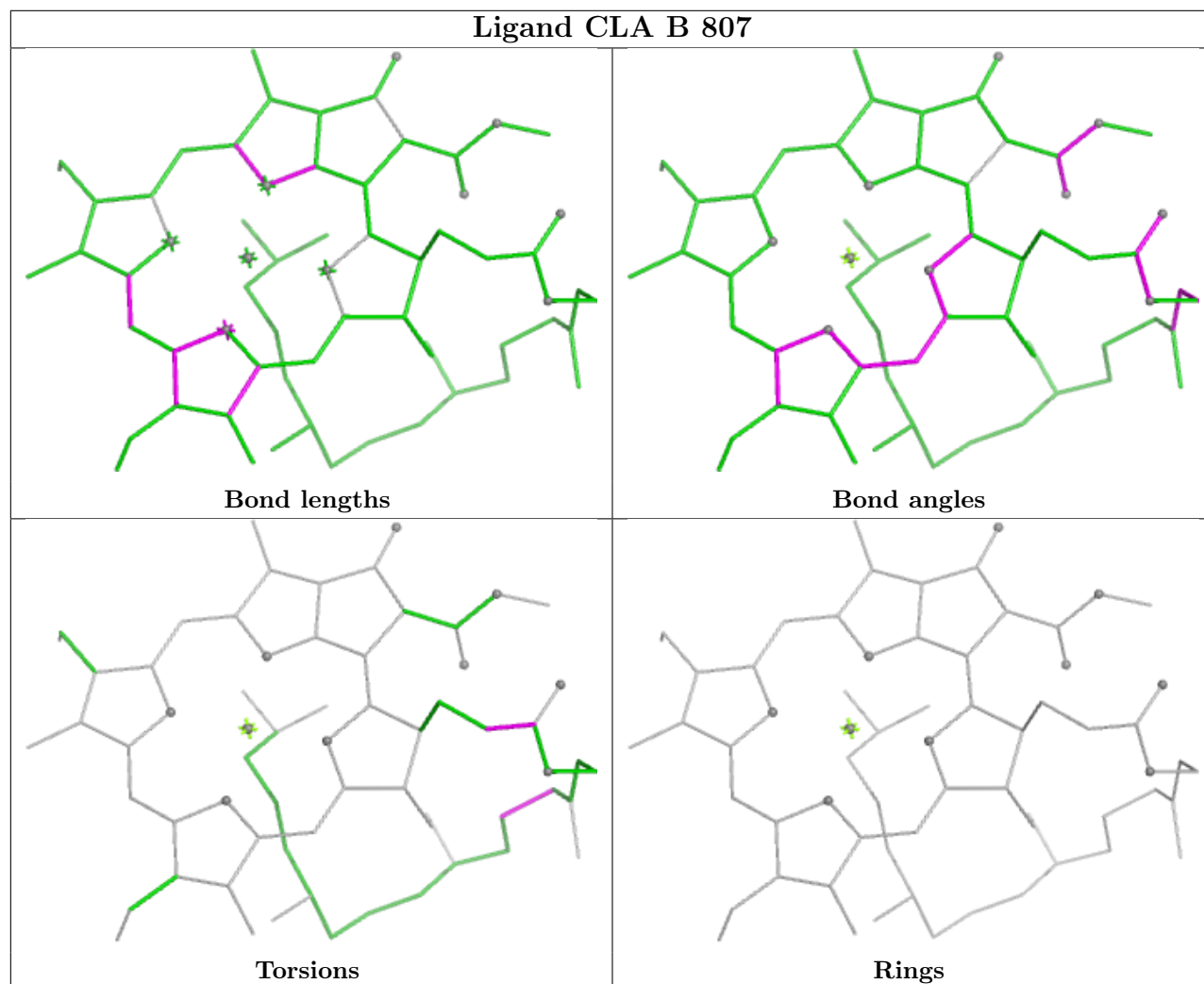
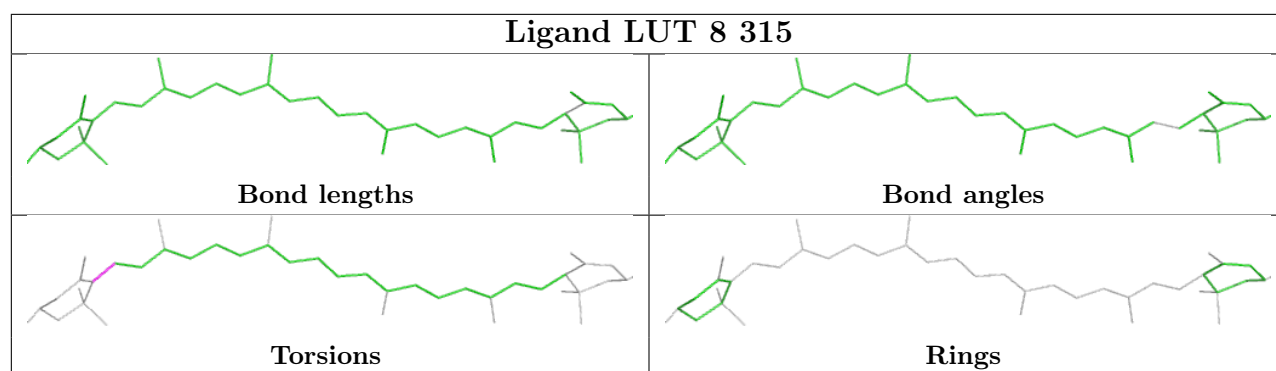


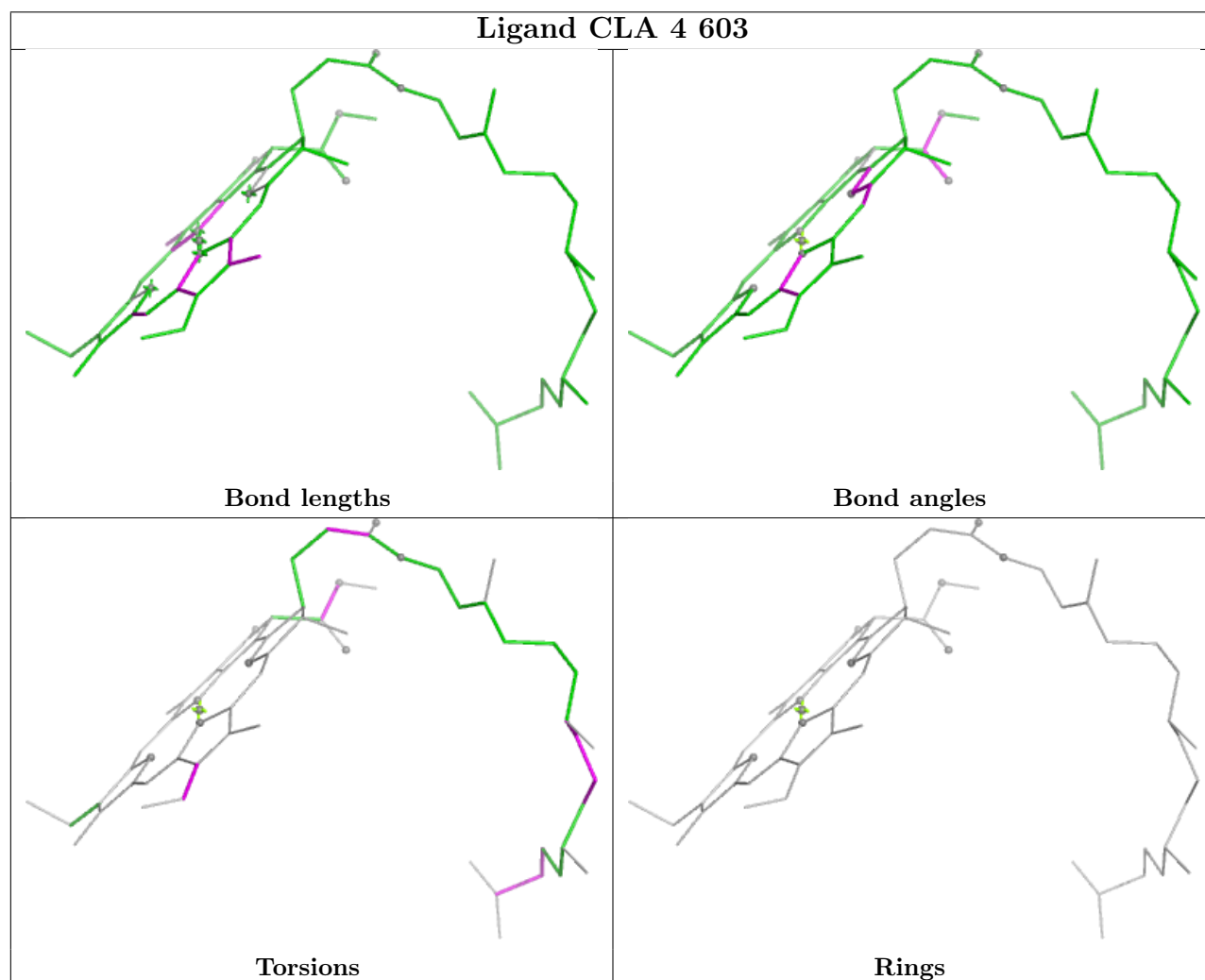
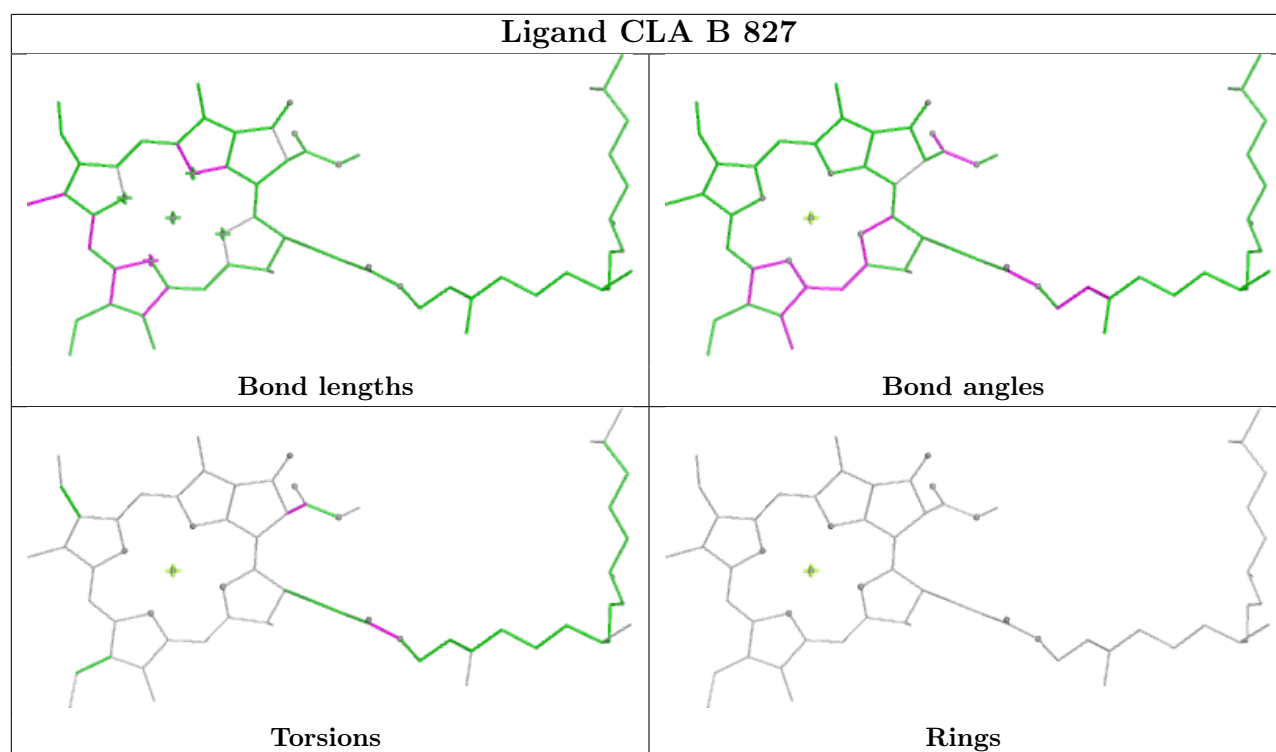
Ligand CHL 6 306

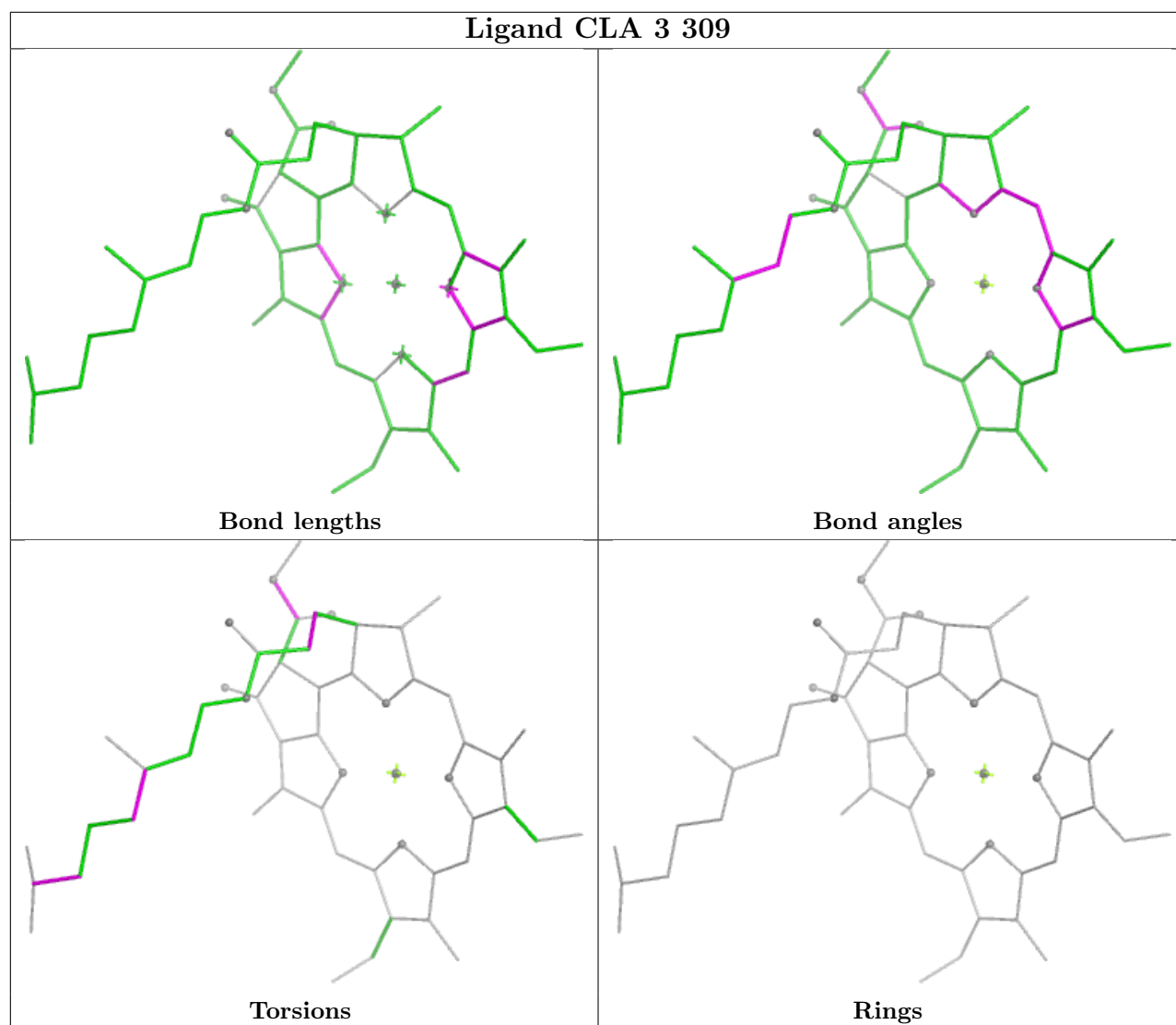
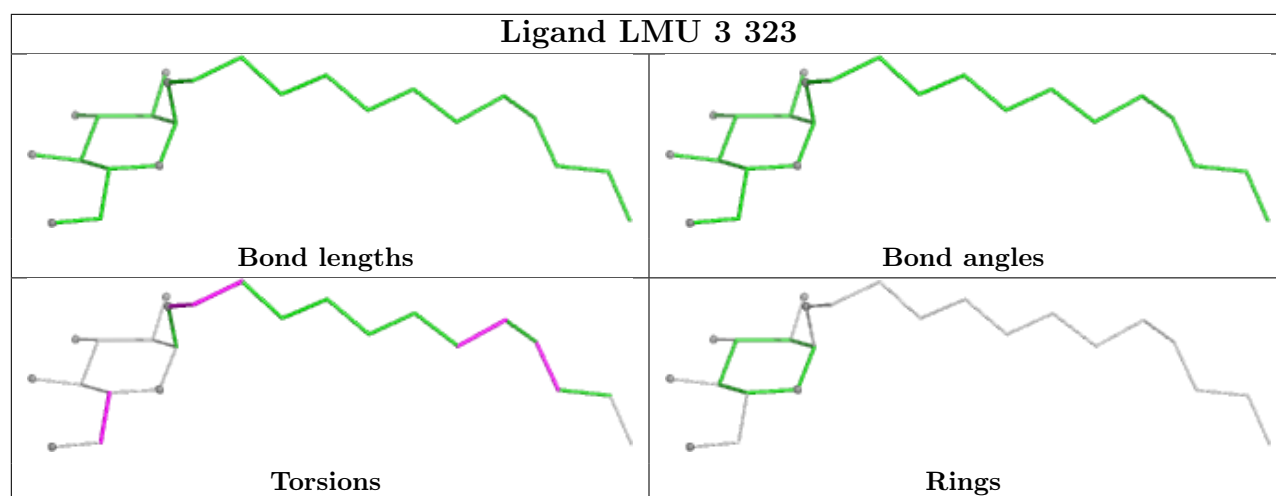


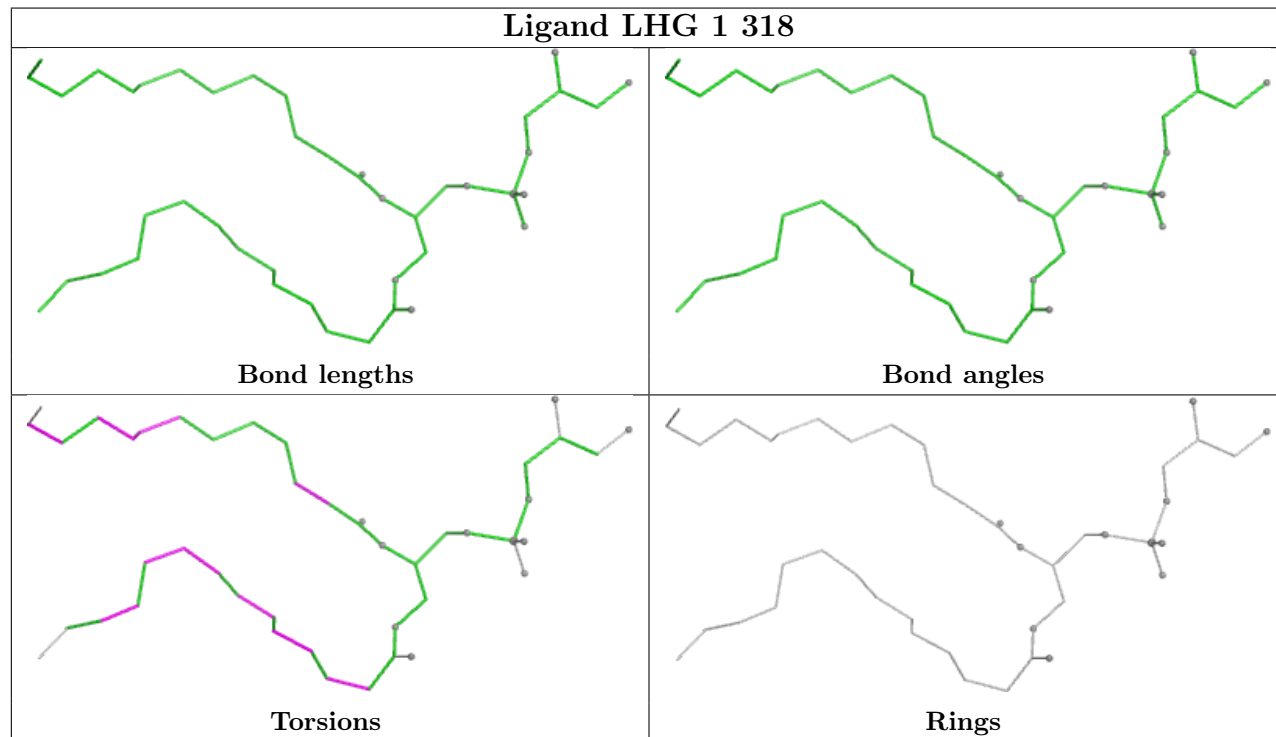
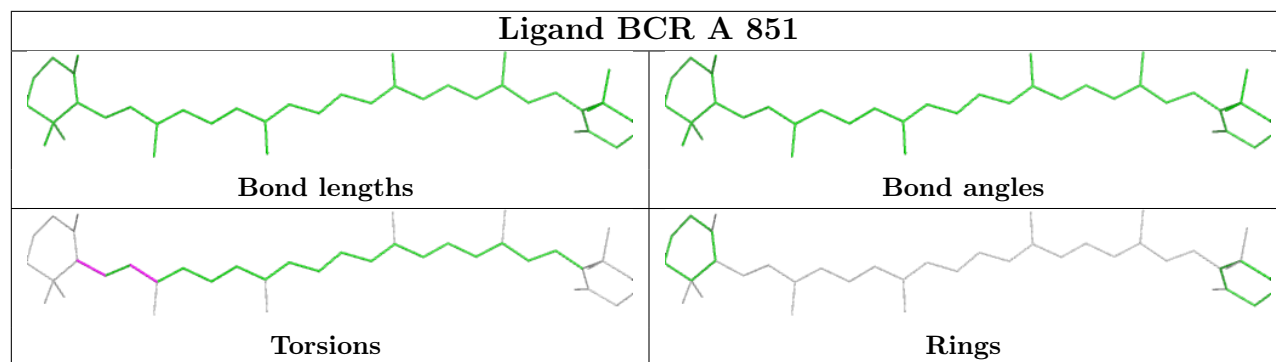
Ligand LHG 6 318

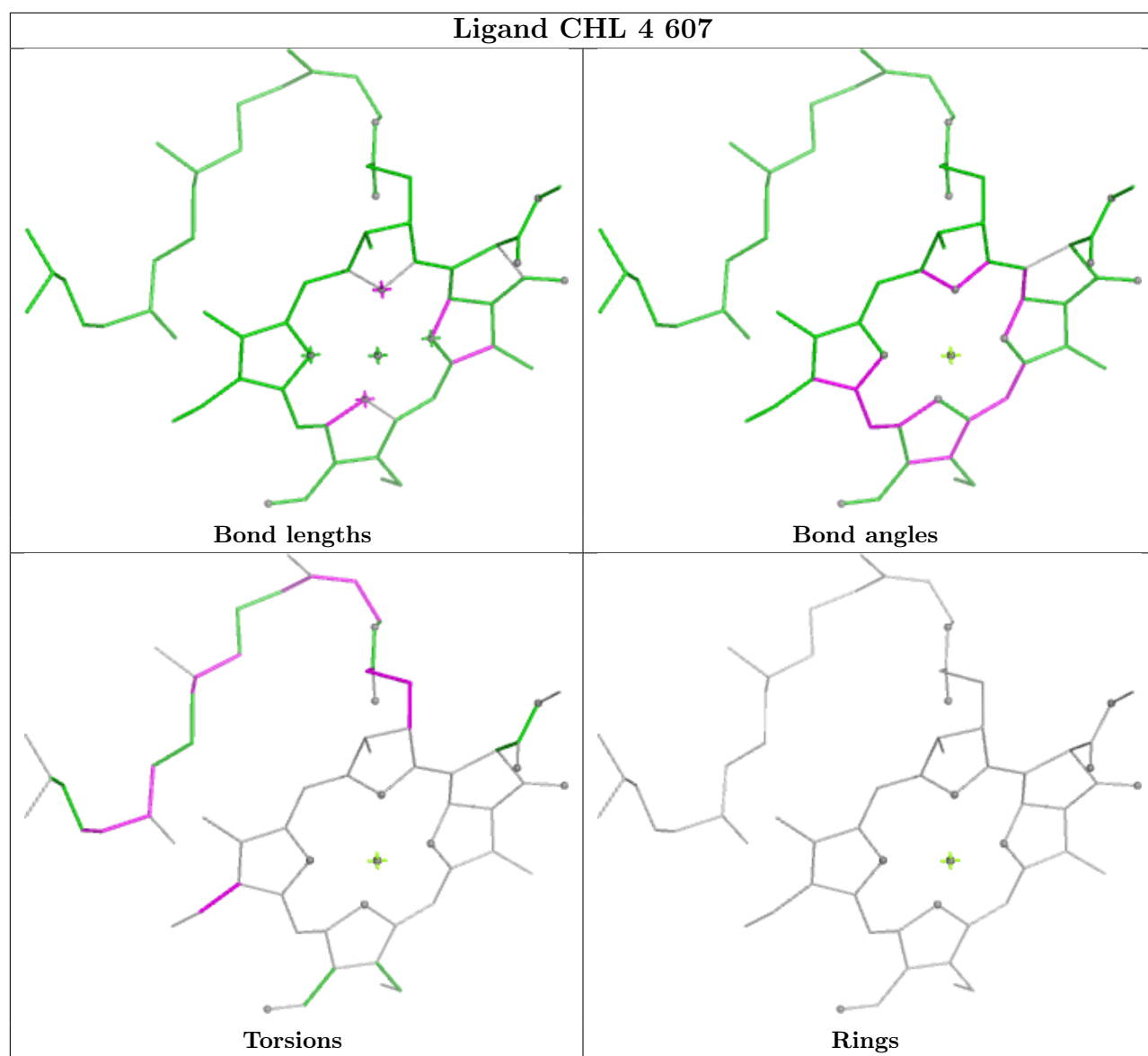


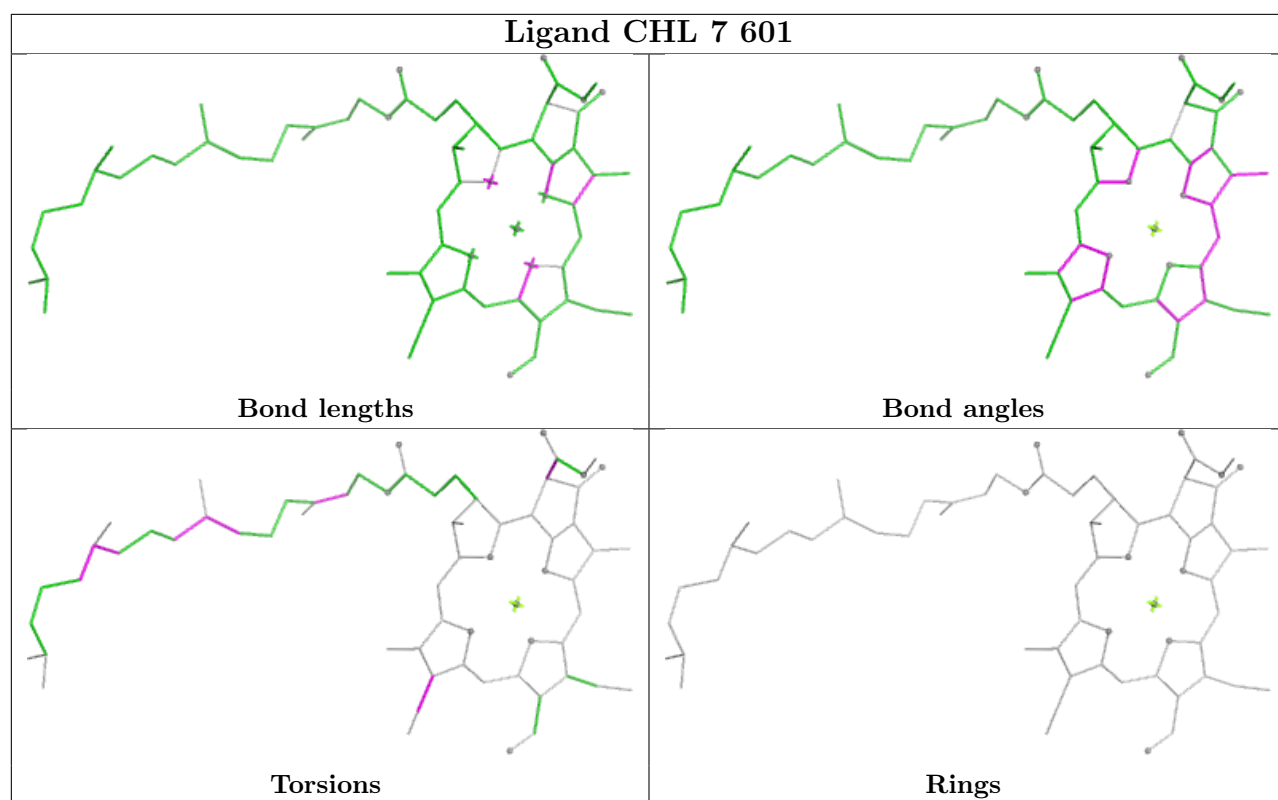


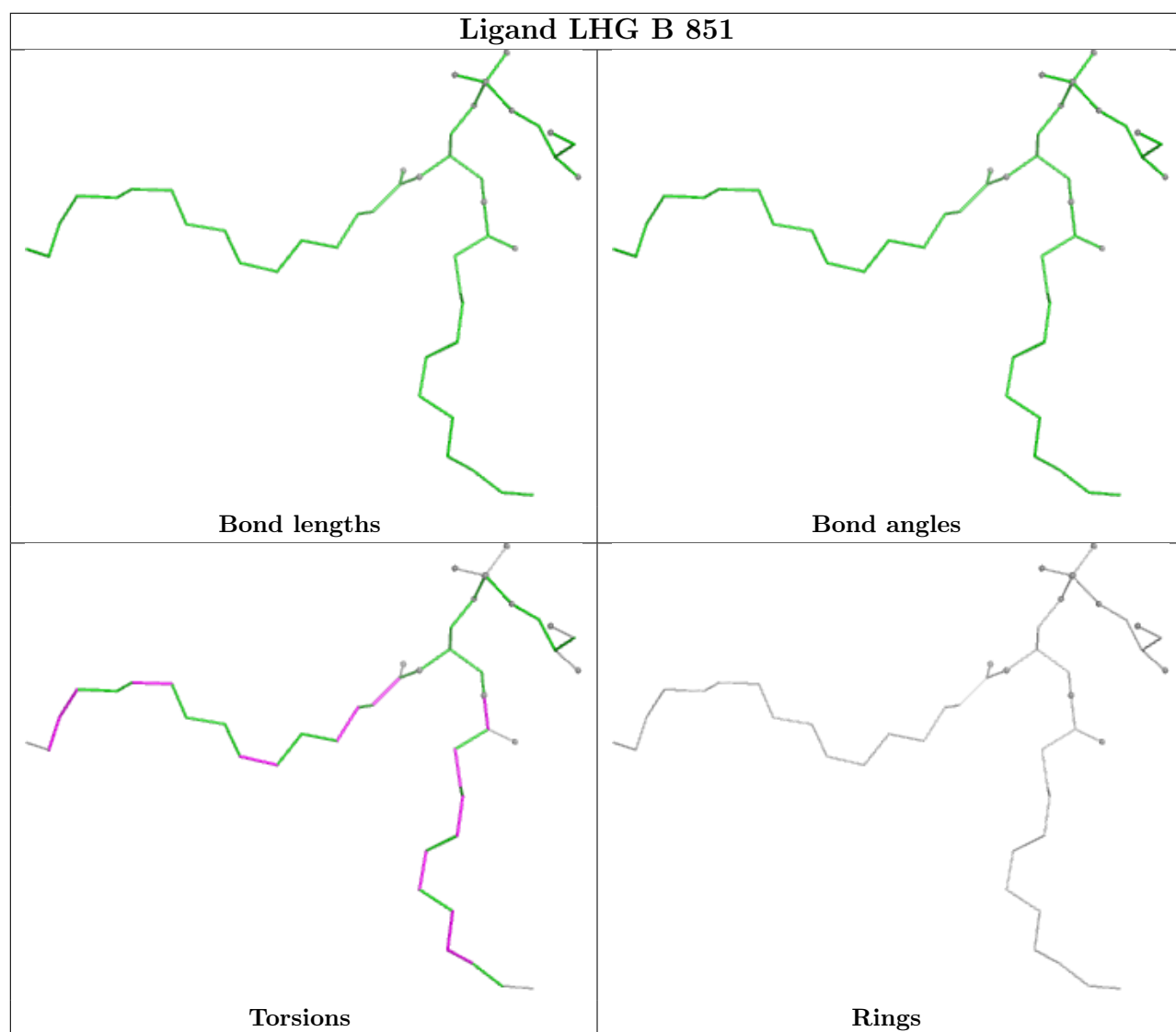


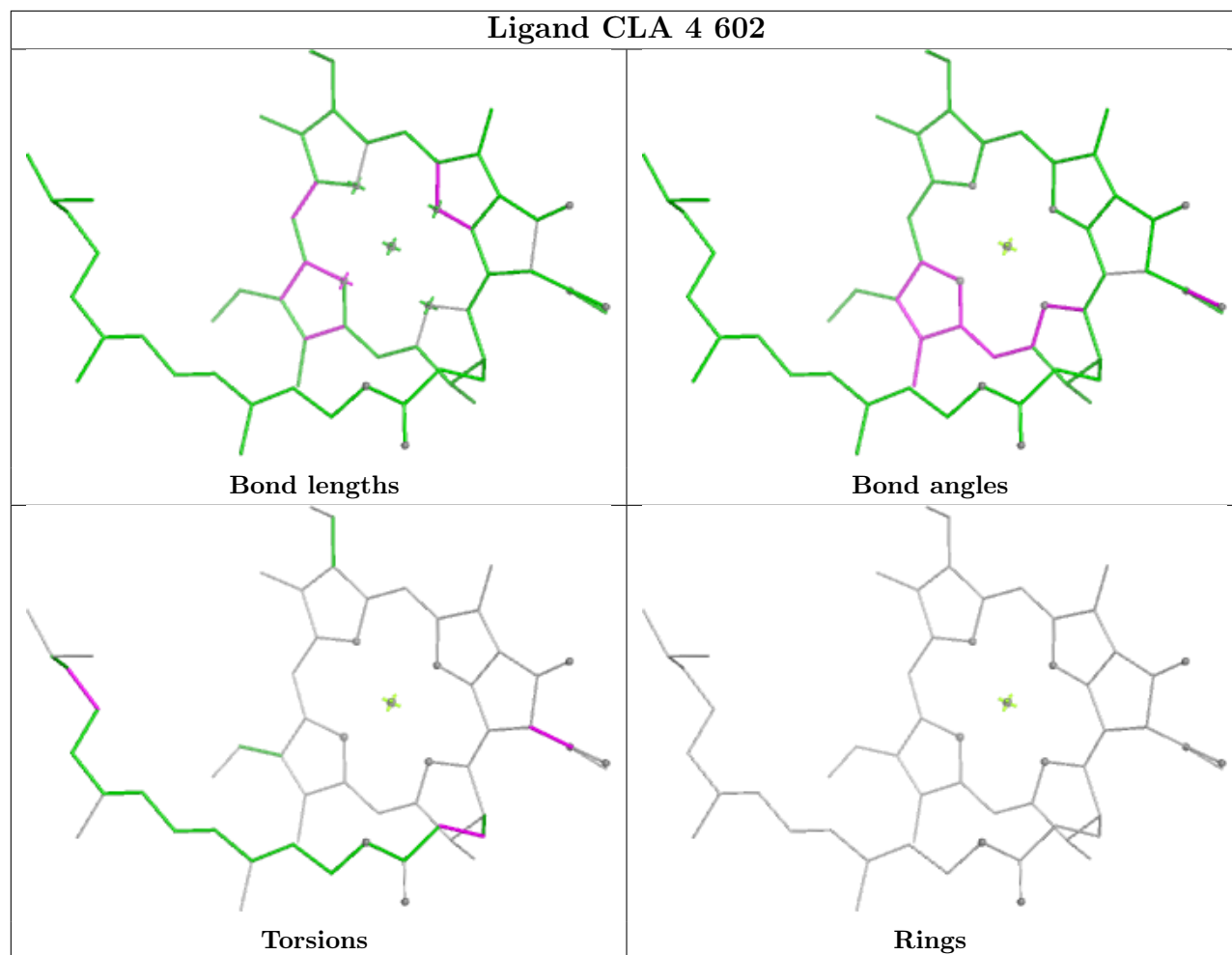




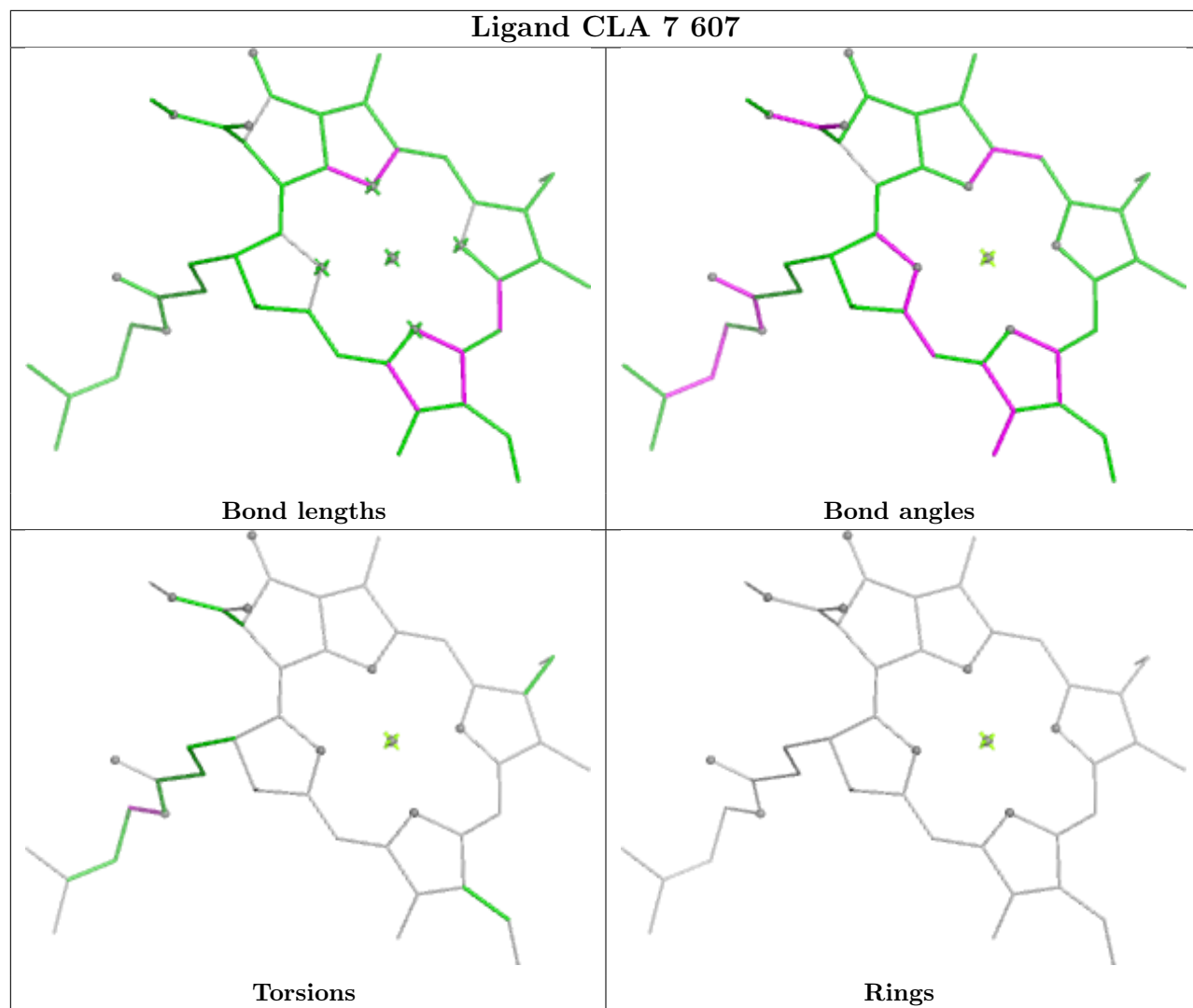


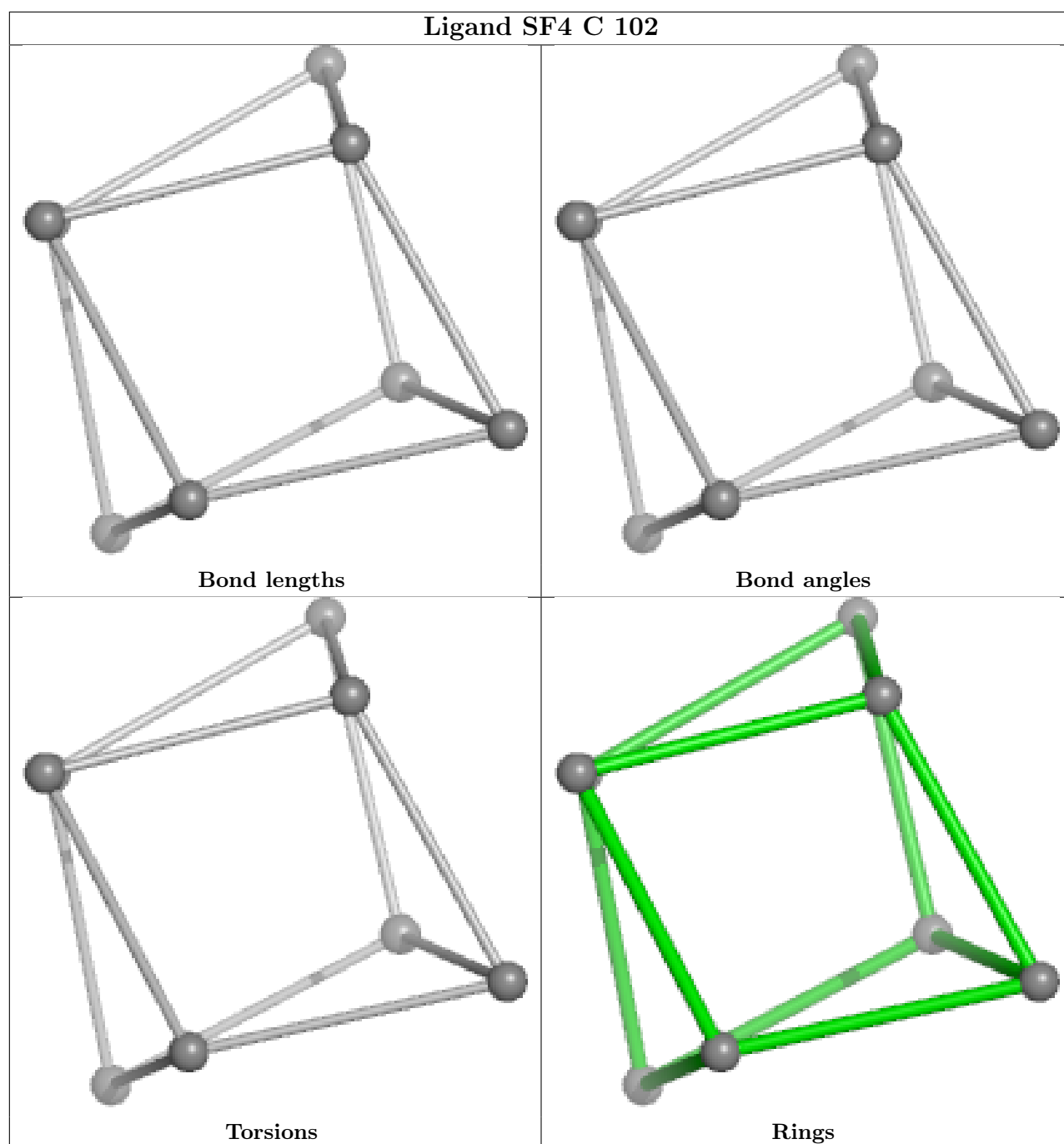




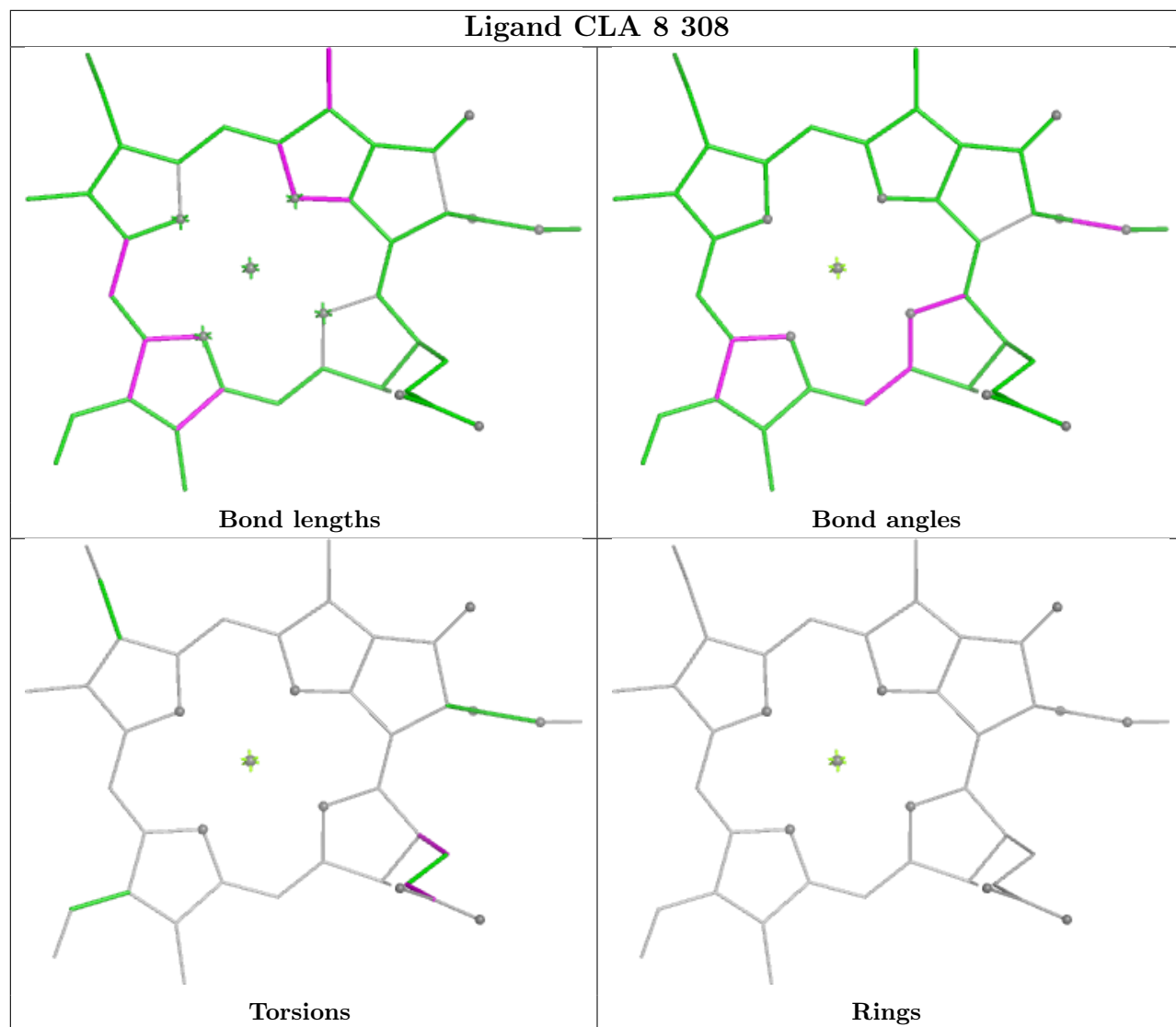


Ligand CLA 7 607

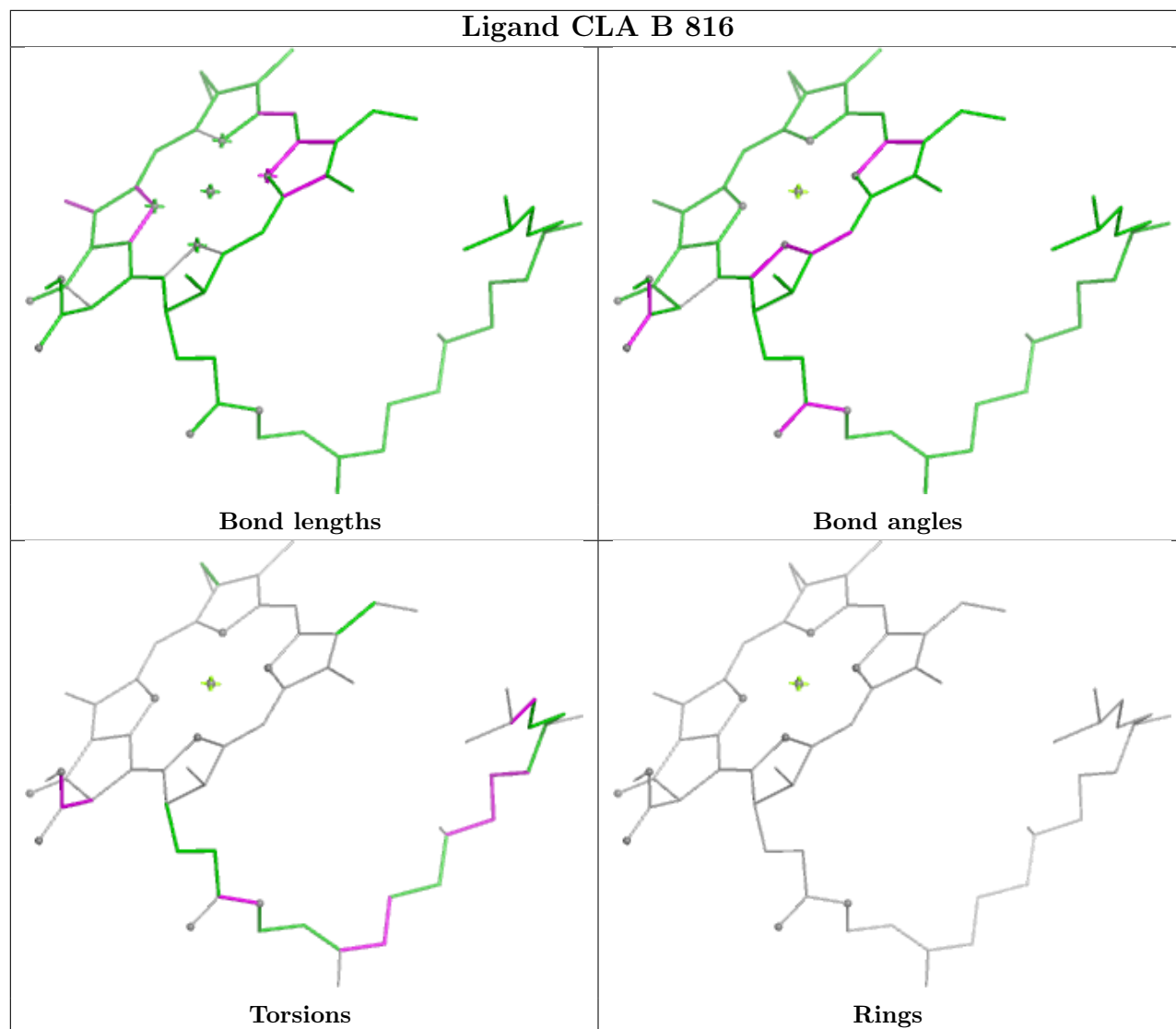




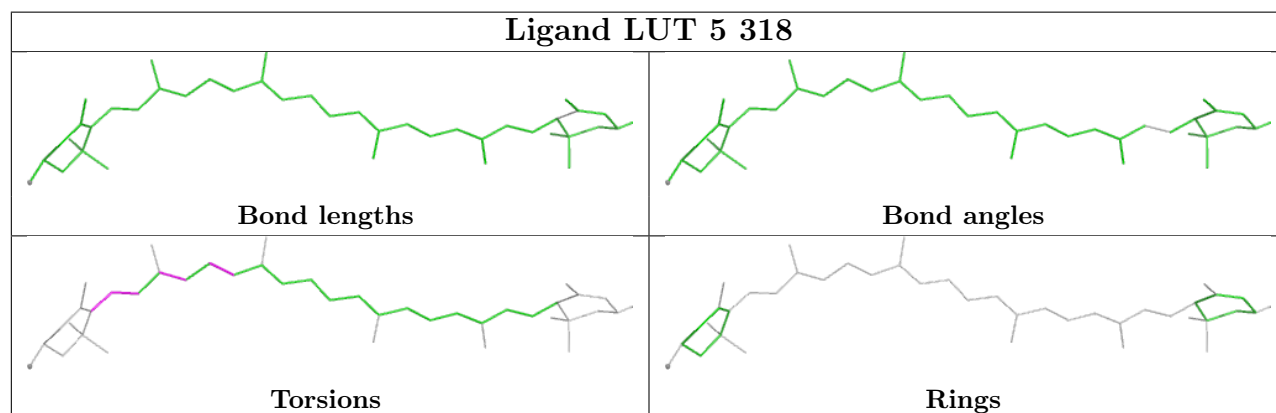
Ligand CLA 8 308

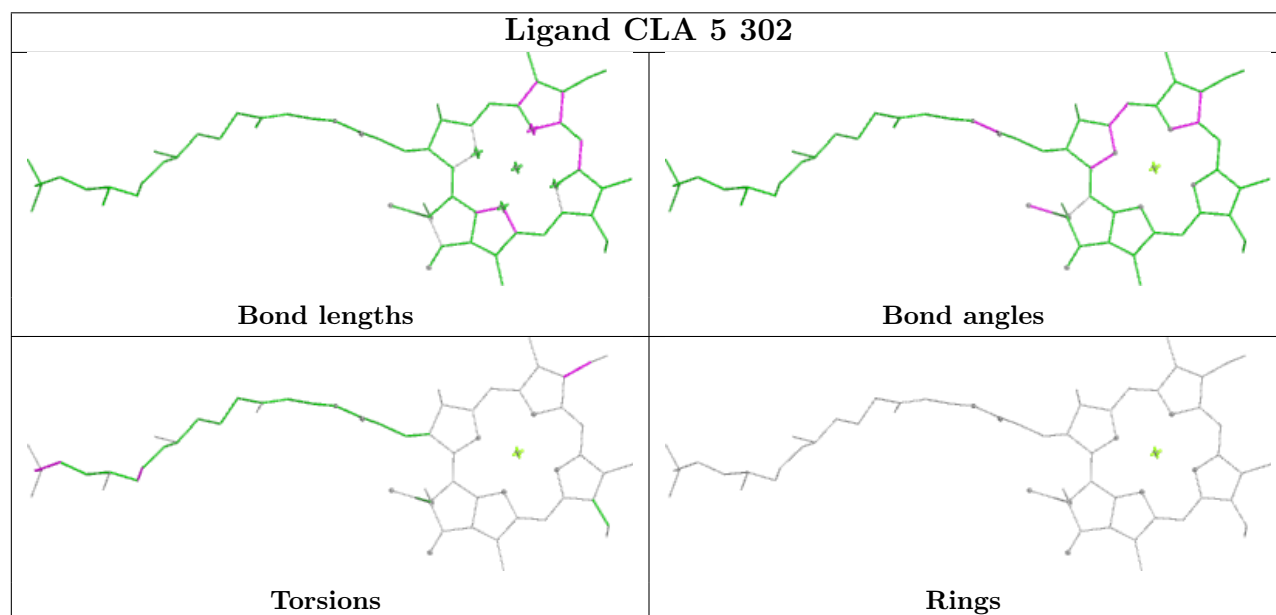
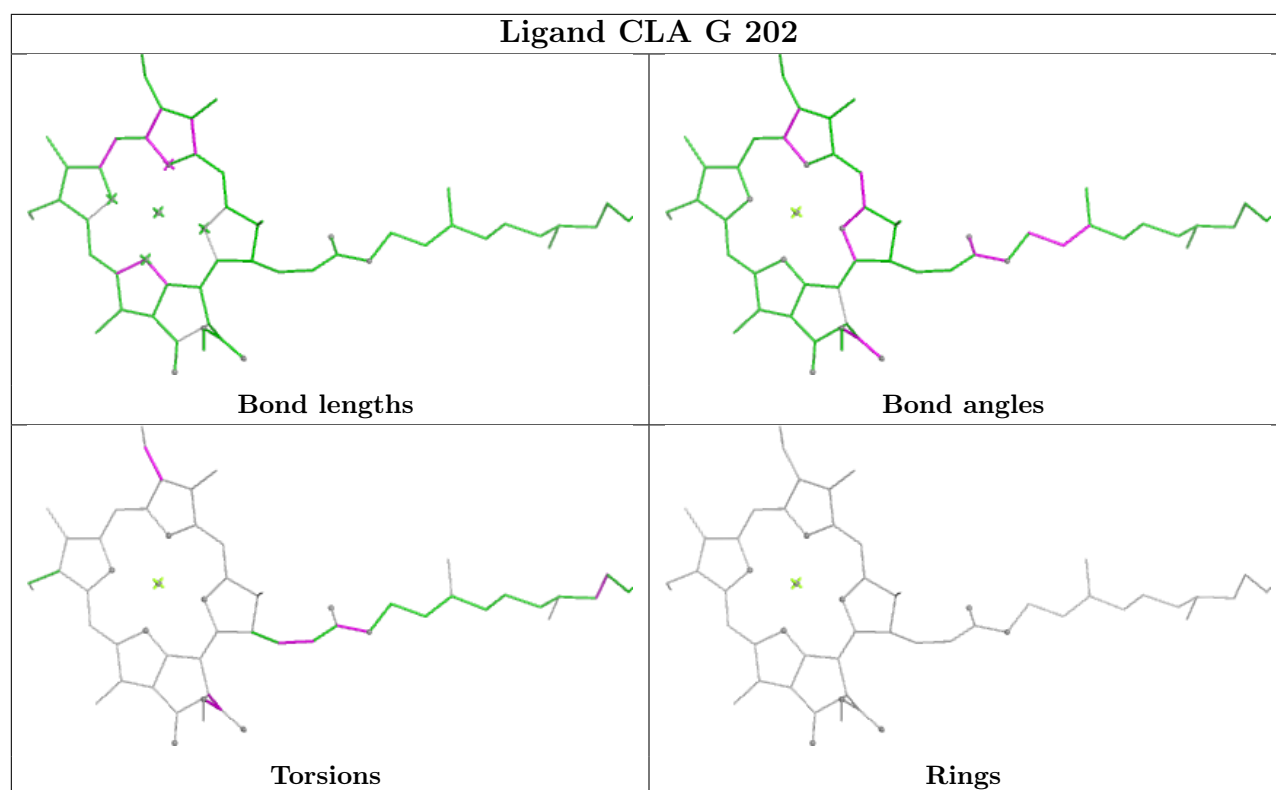


Ligand CLA B 816

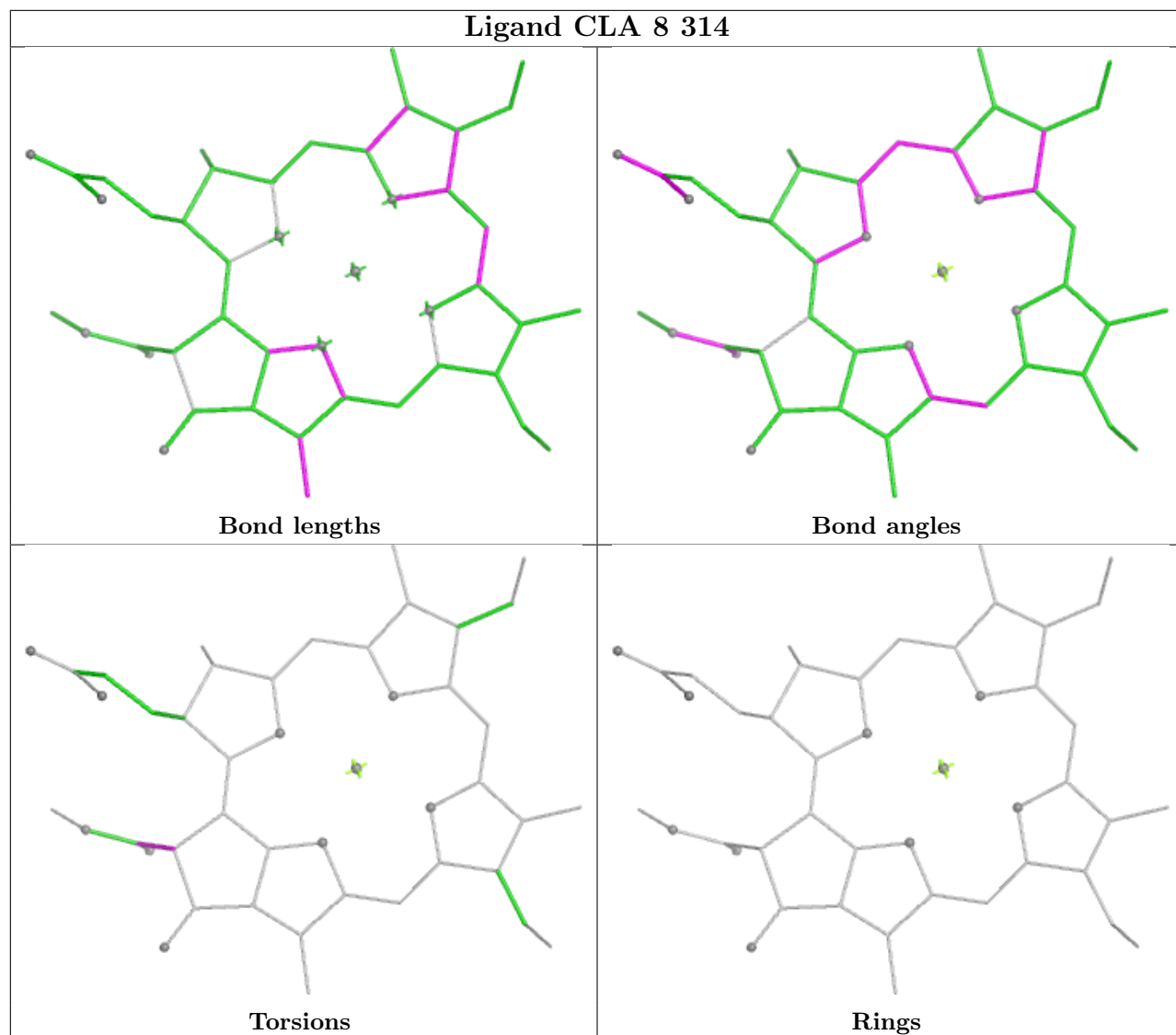


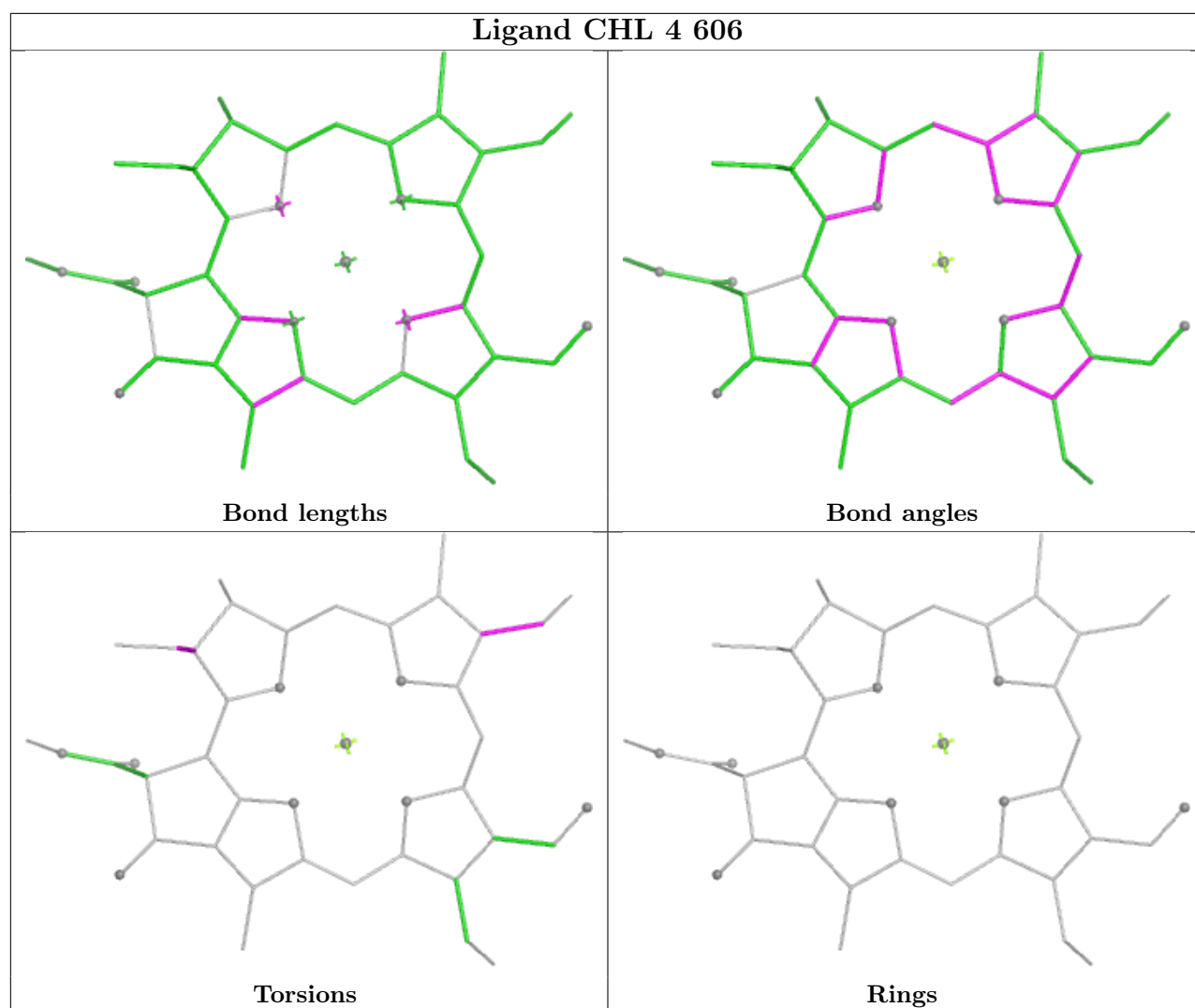
Ligand LUT 5 318



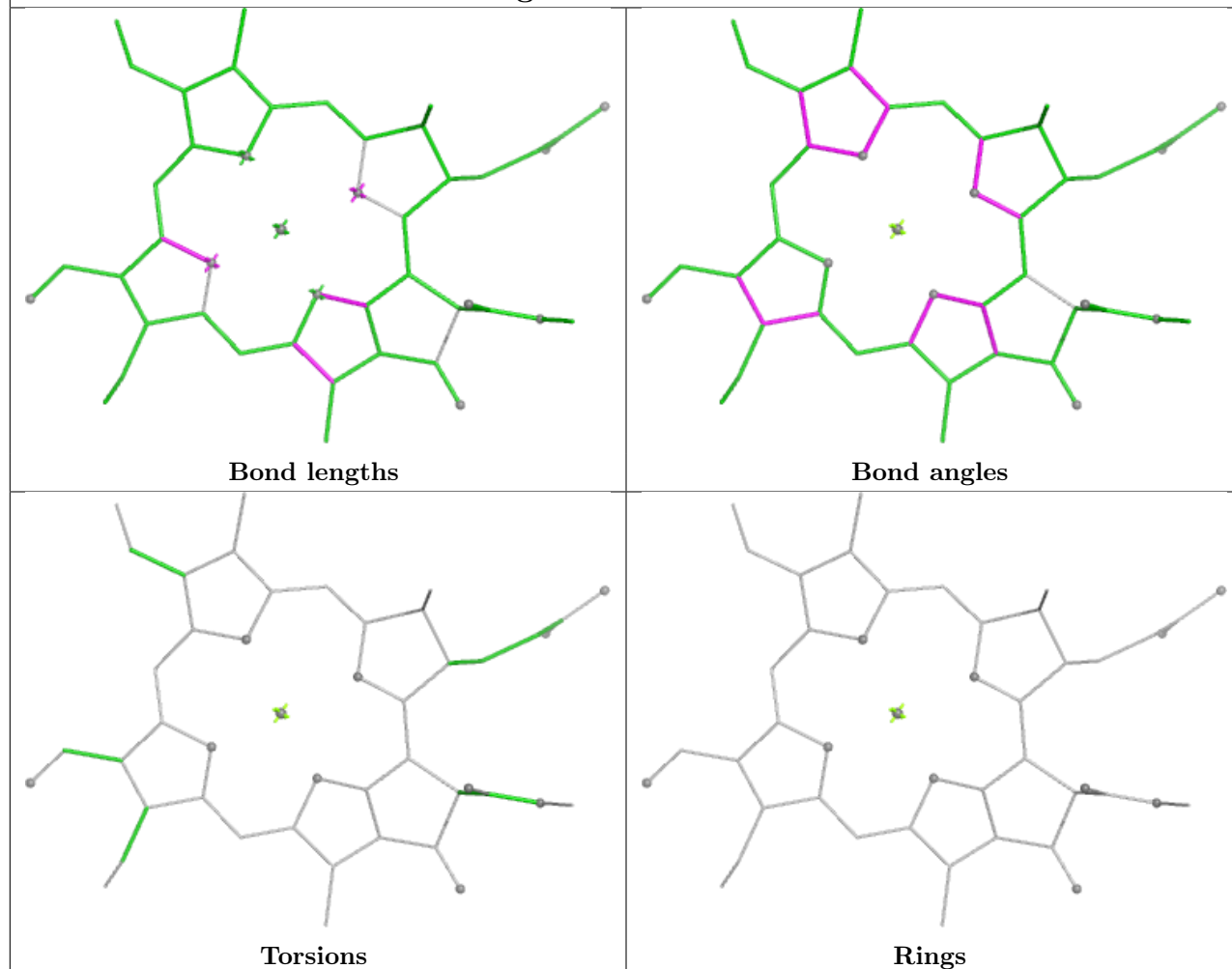


Ligand CLA 8 314

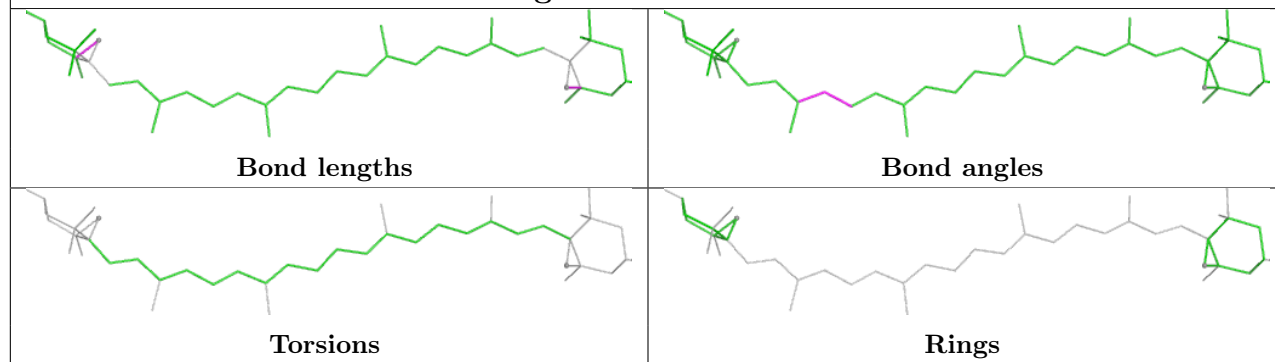


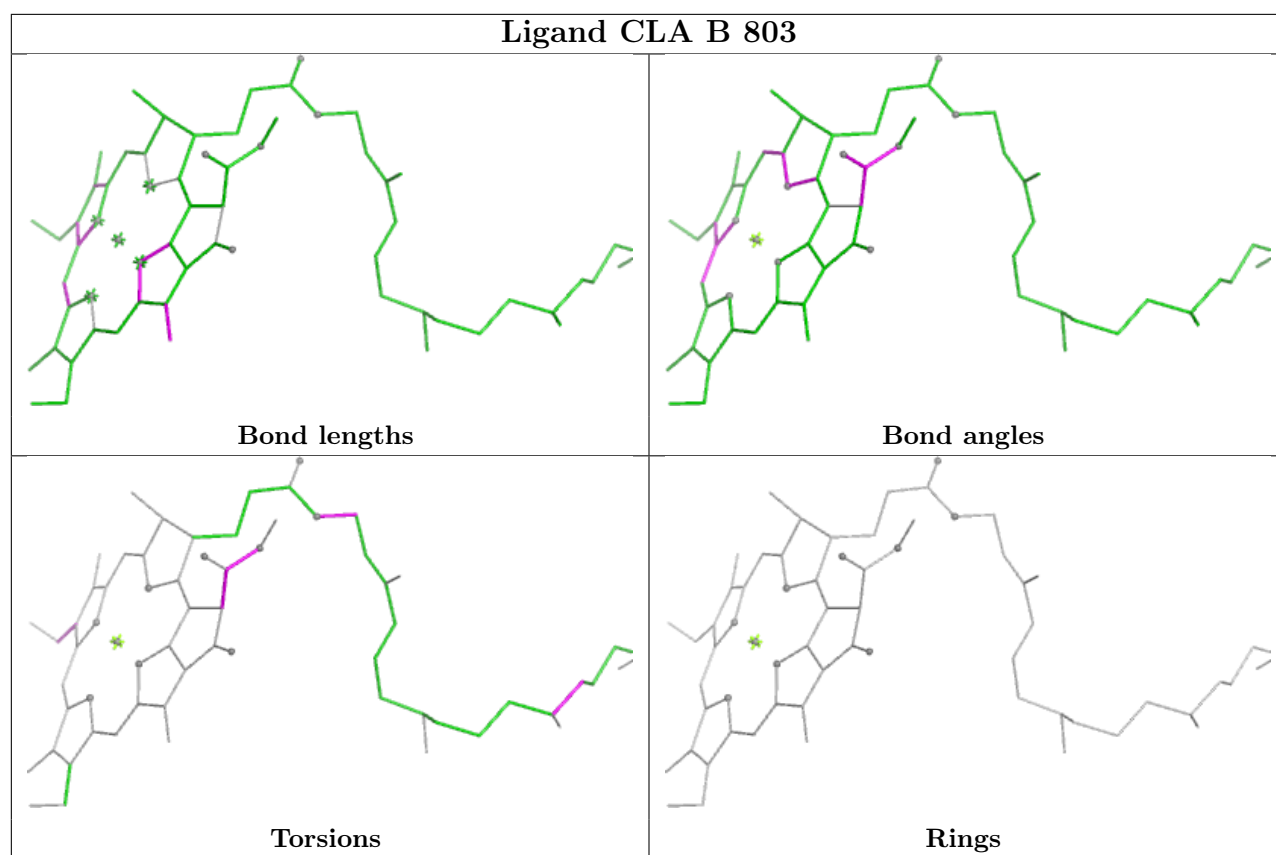


Ligand CHL 7 605

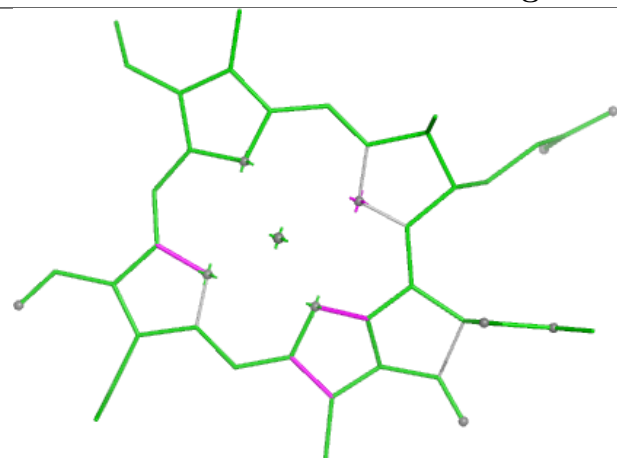


Ligand XAT 4 617

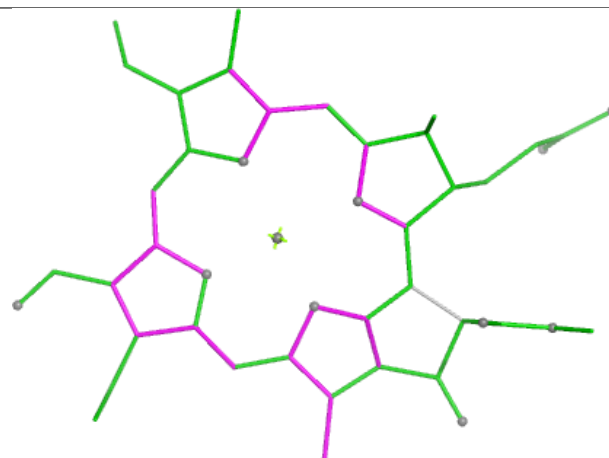




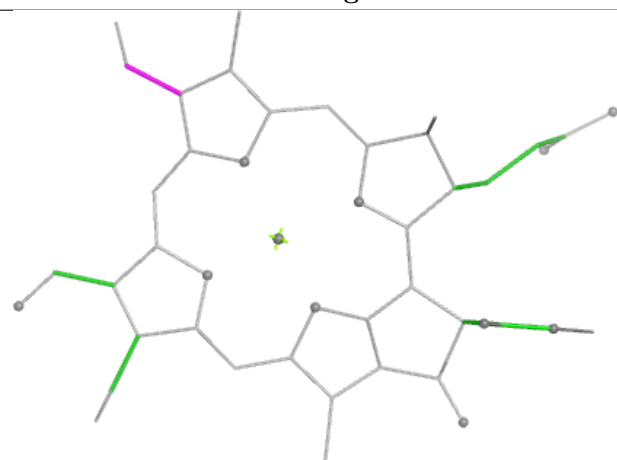
Ligand CHL 1 305



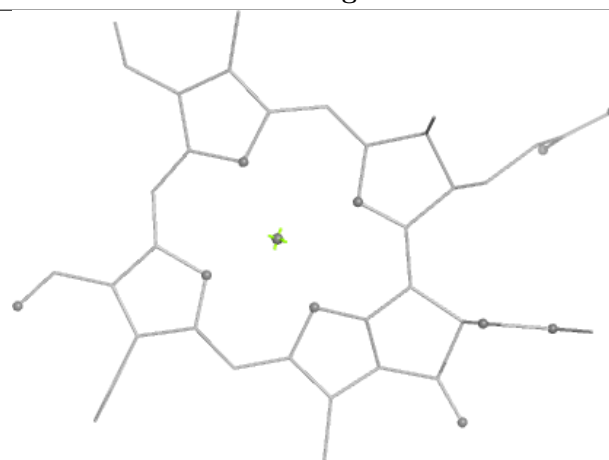
Bond lengths



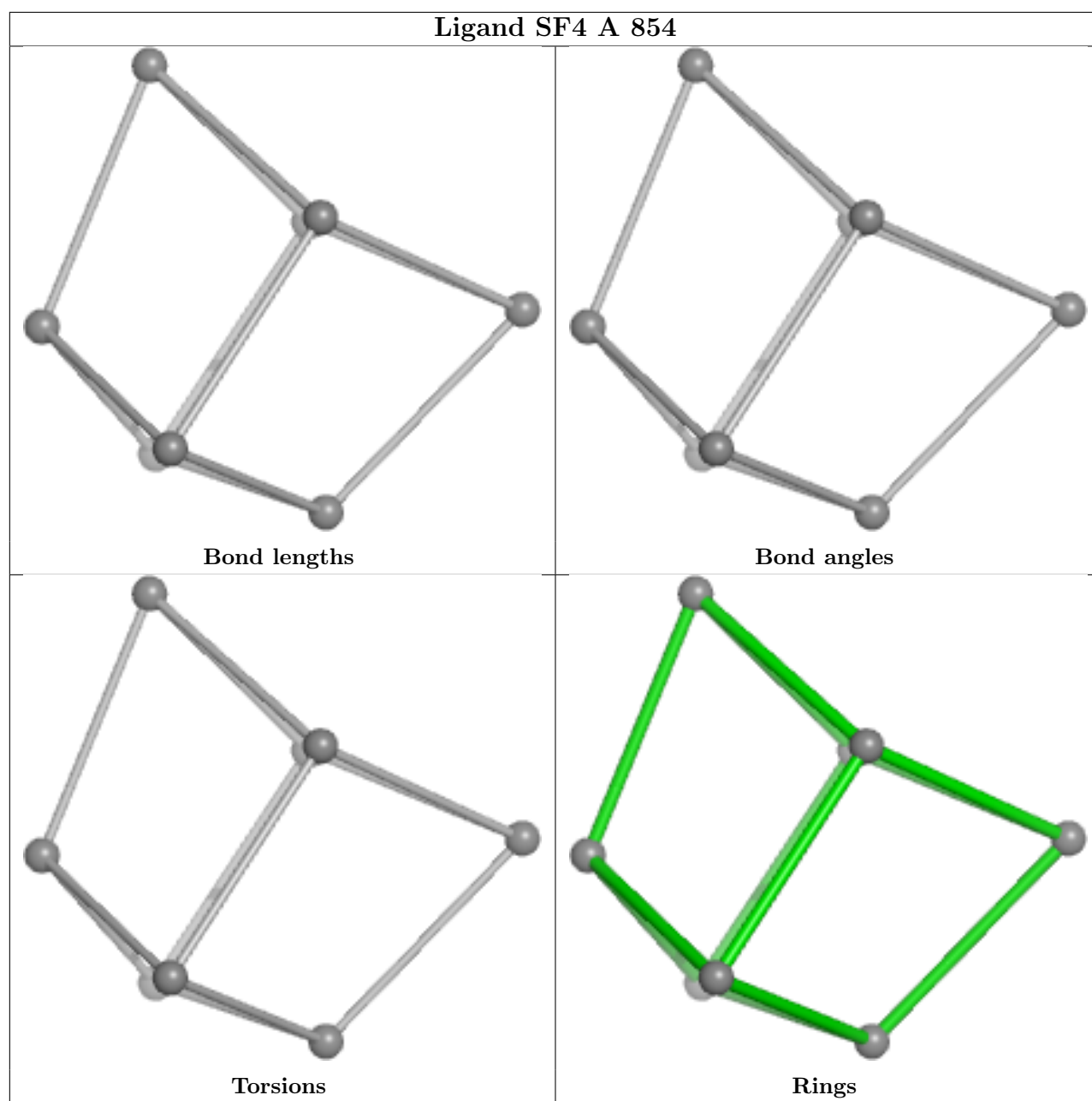
Bond angles

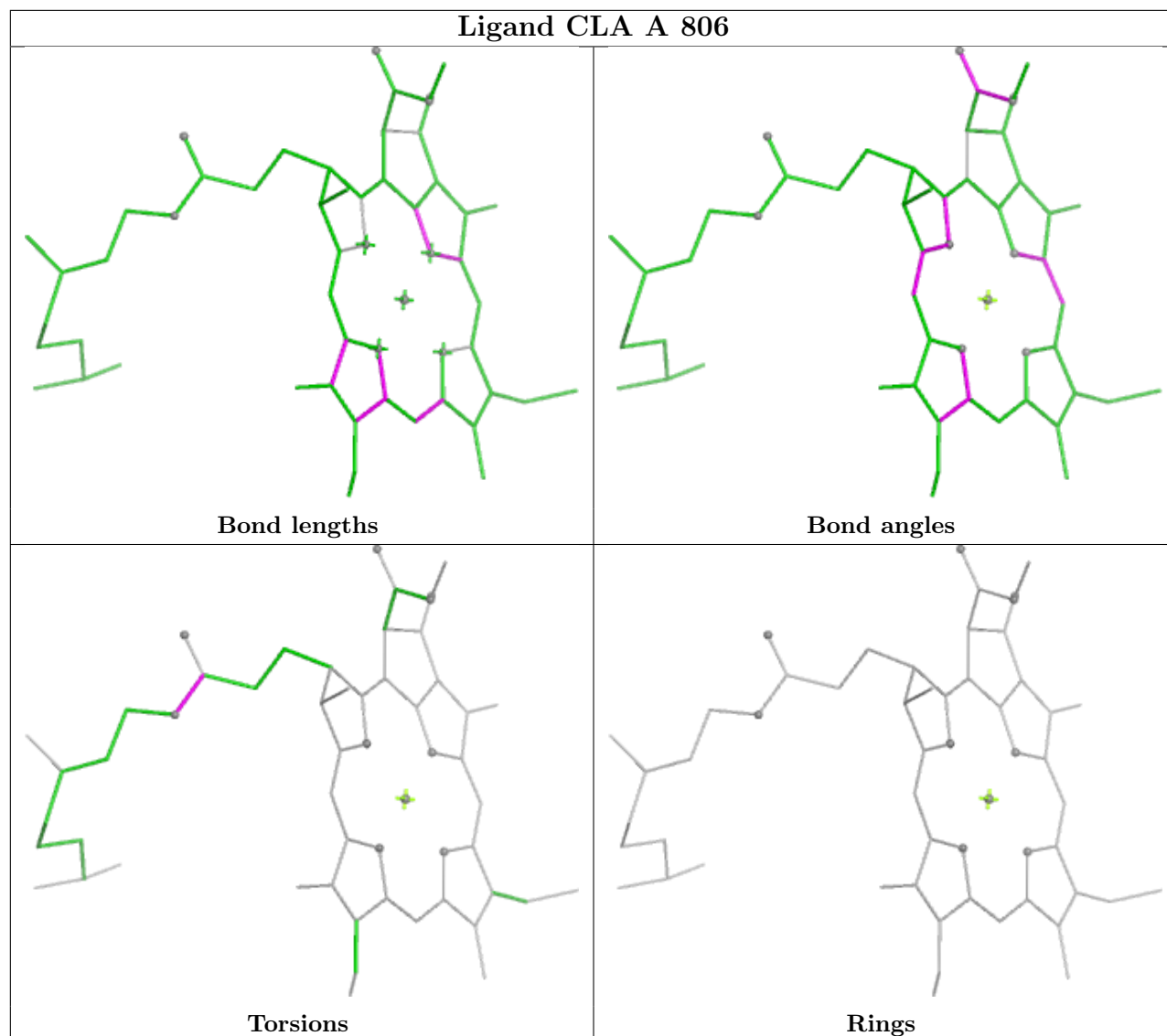


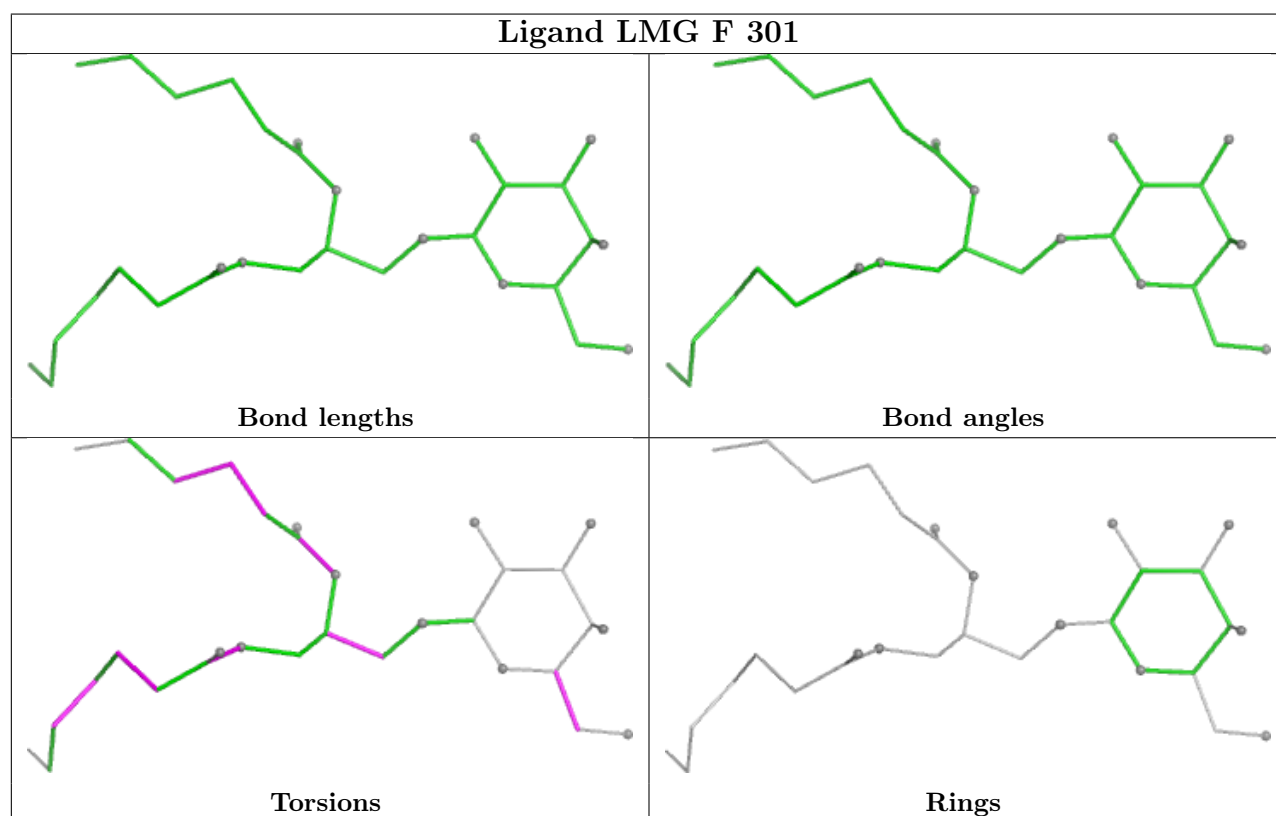
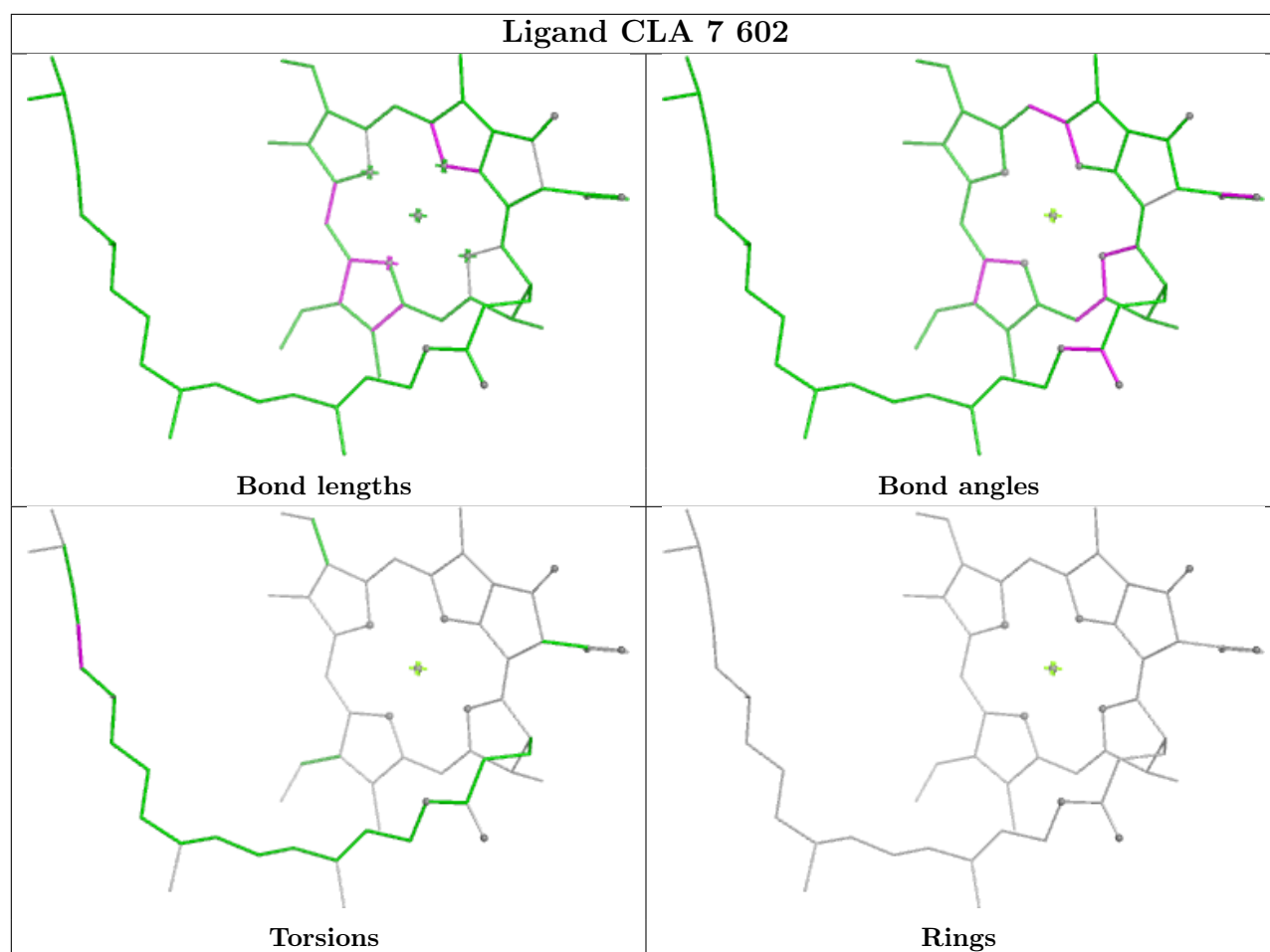
Torsions

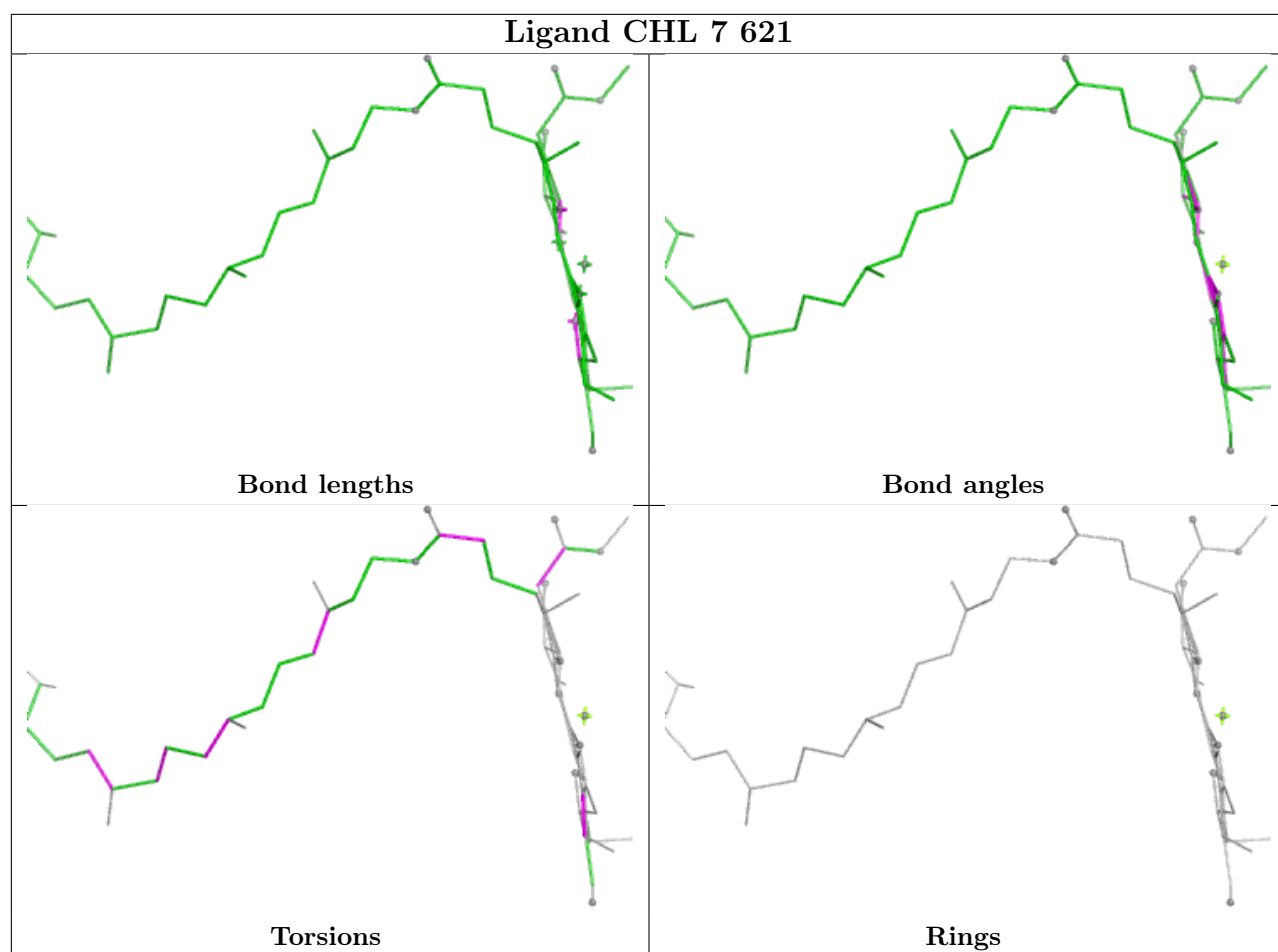


Rings

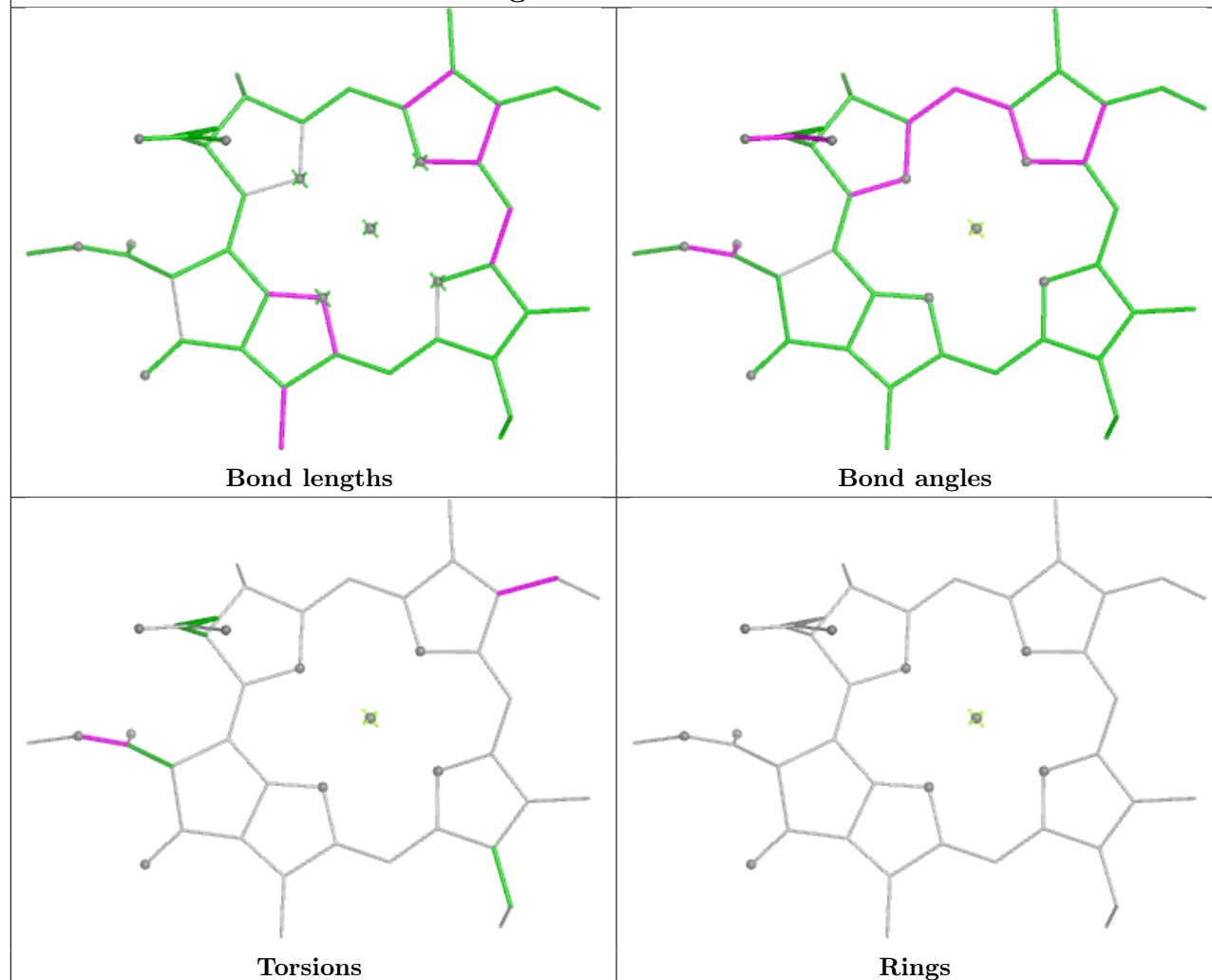




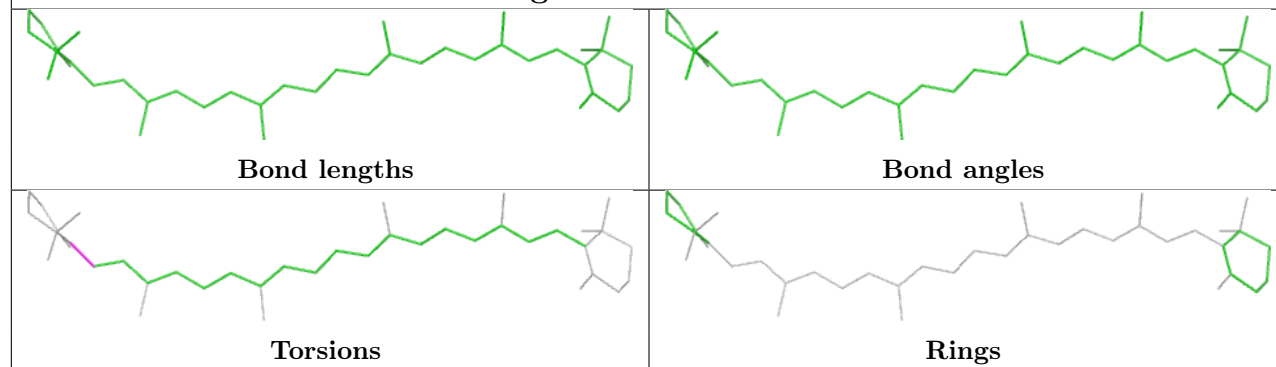


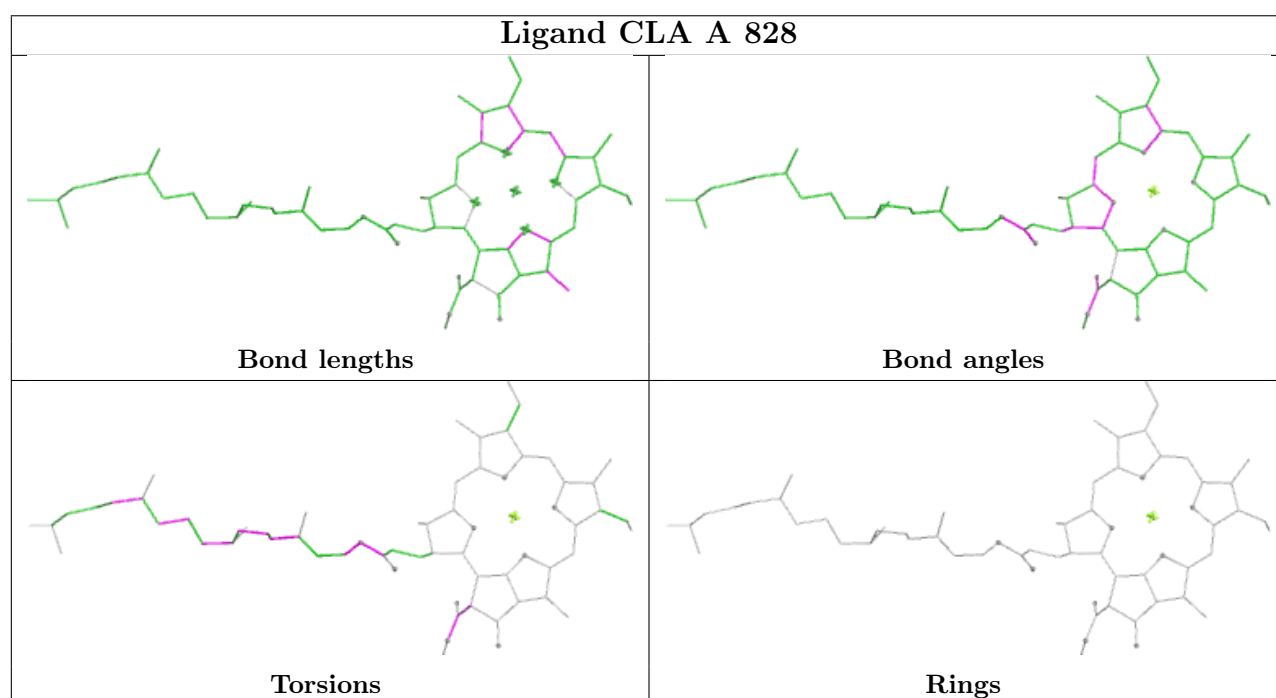
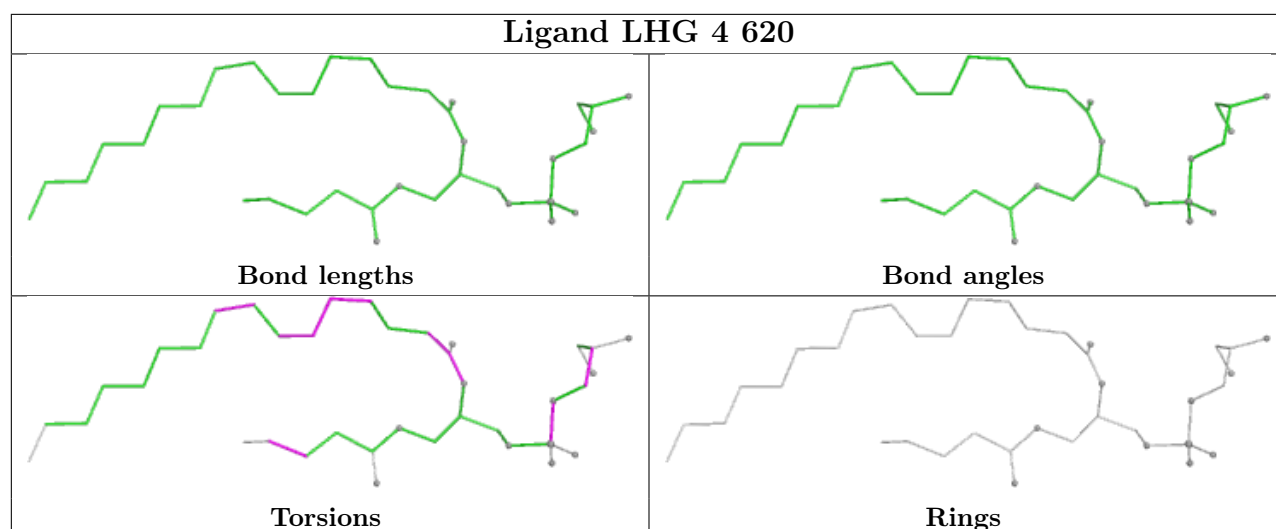


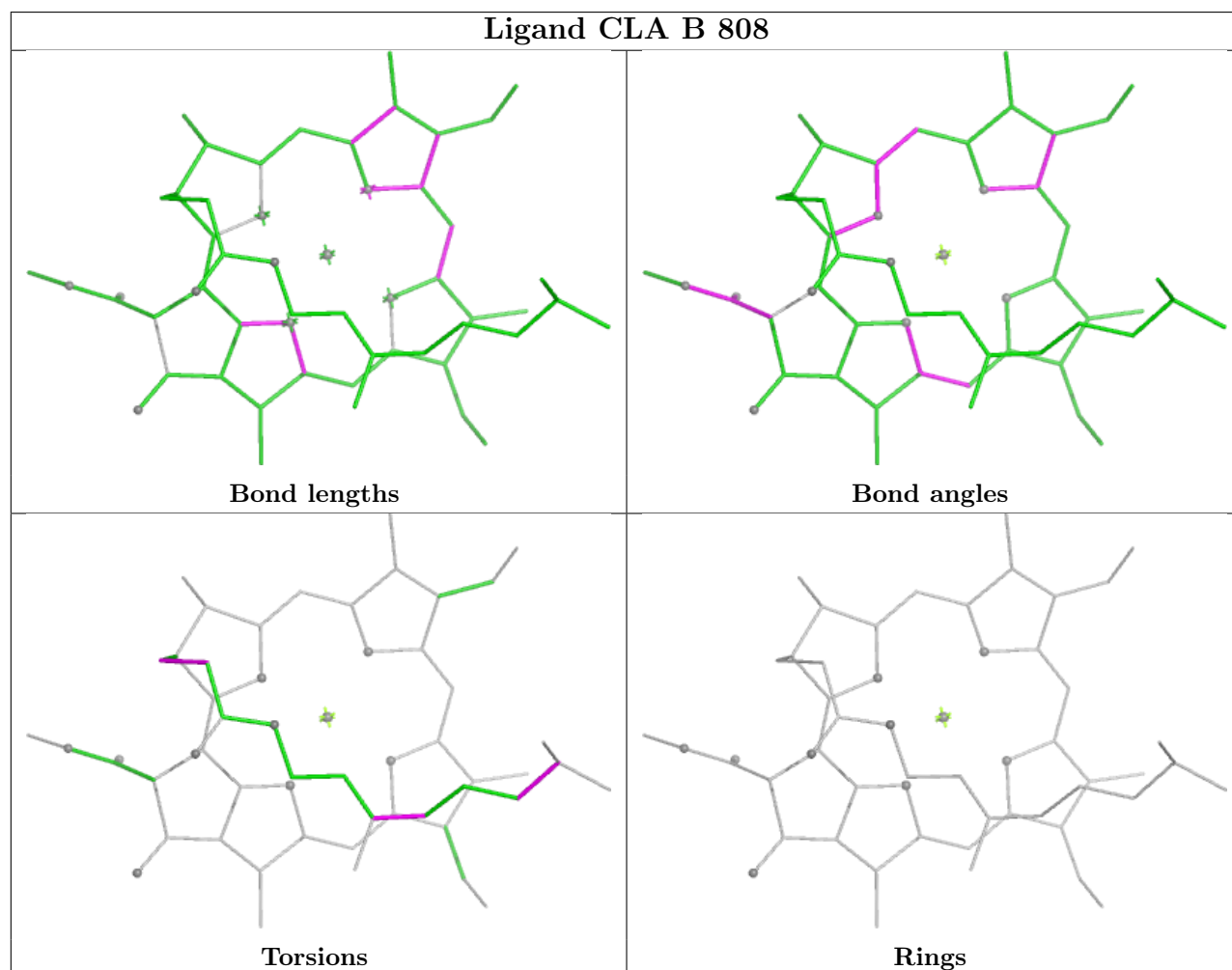
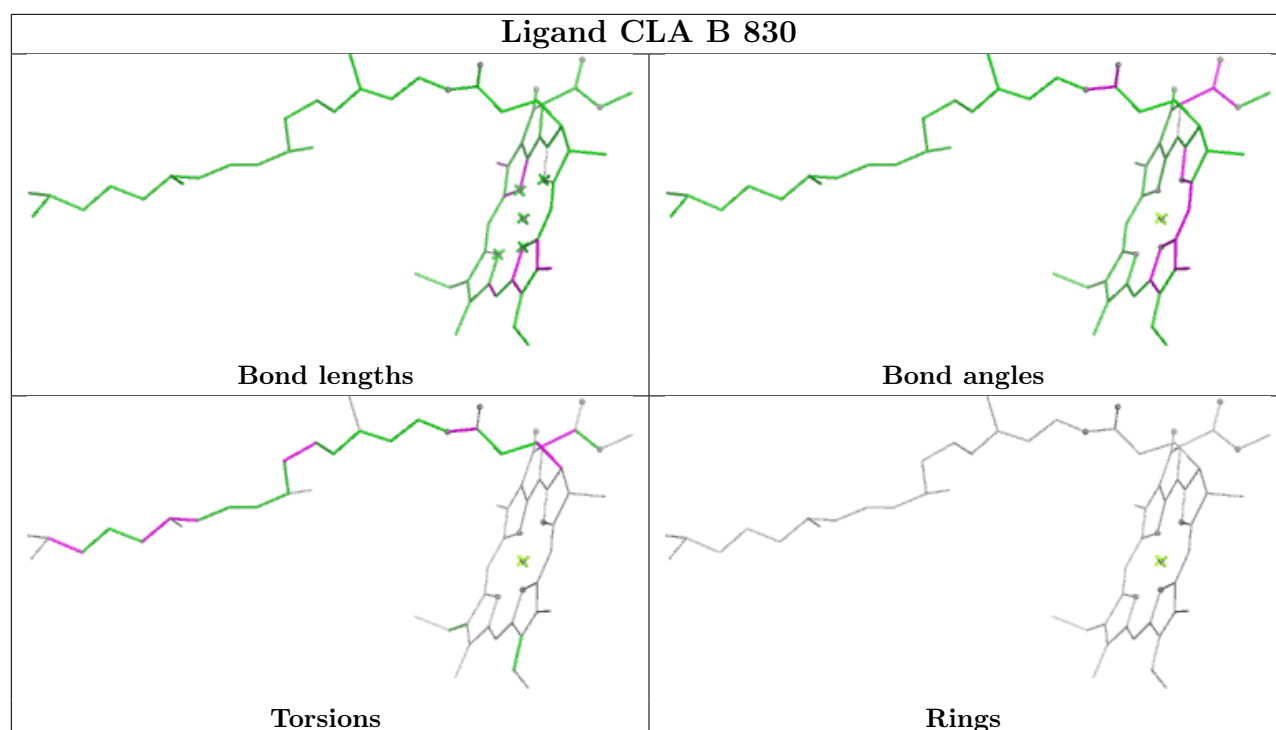
Ligand CLA 5 315

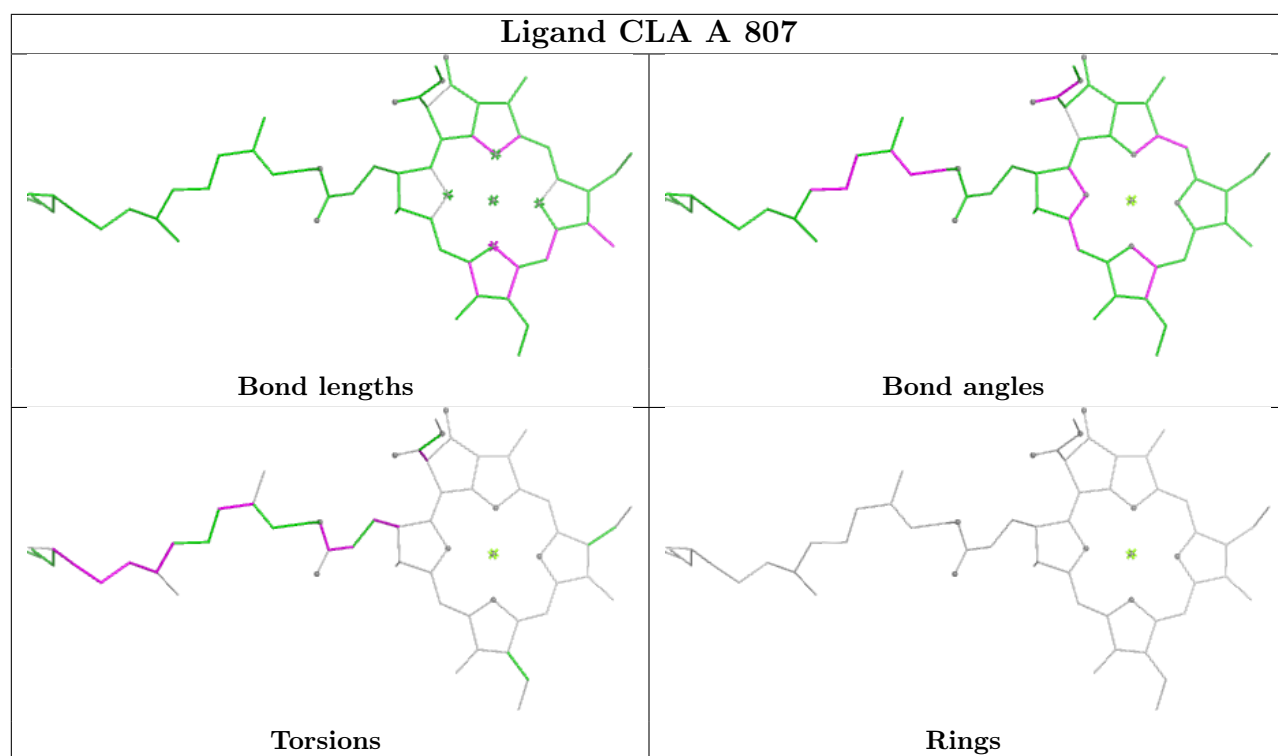


Ligand BCR B 849

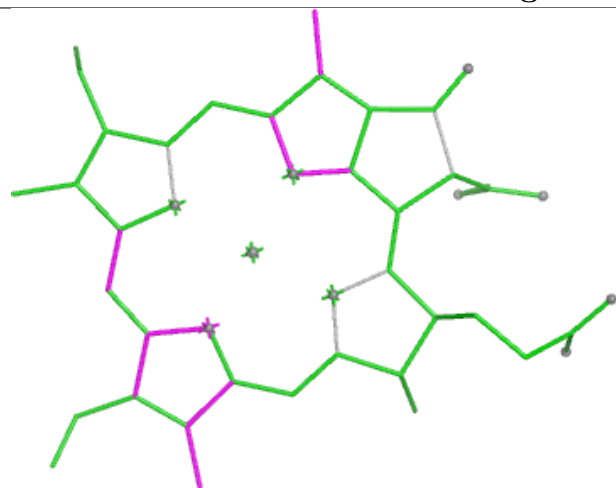




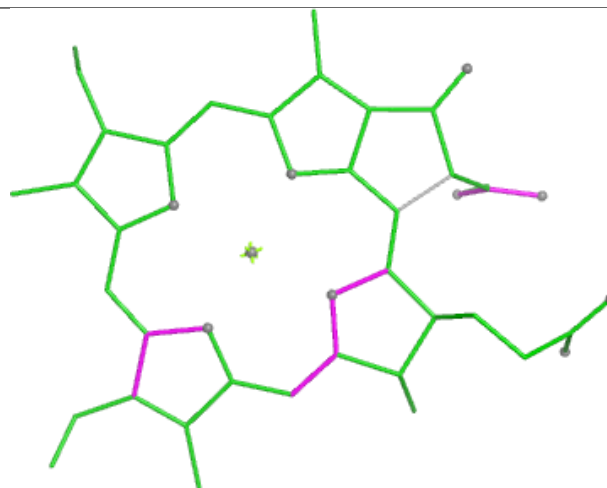




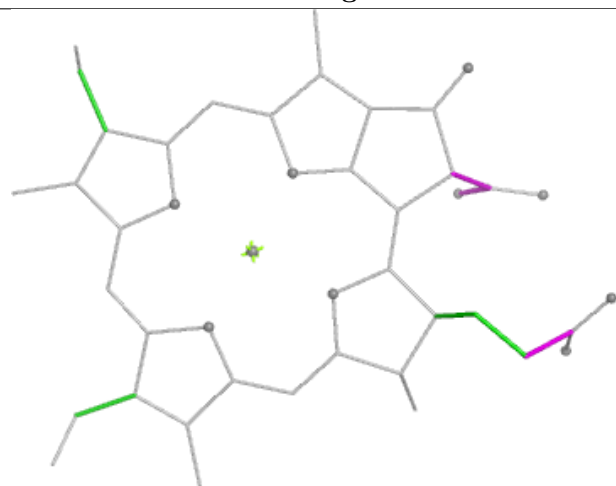
Ligand CLA 1 311



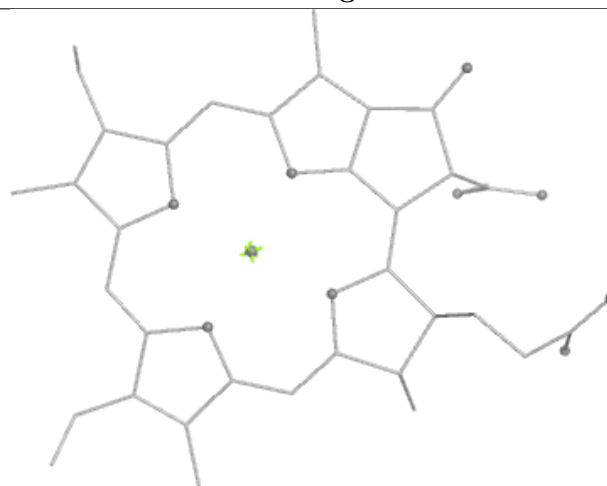
Bond lengths



Bond angles

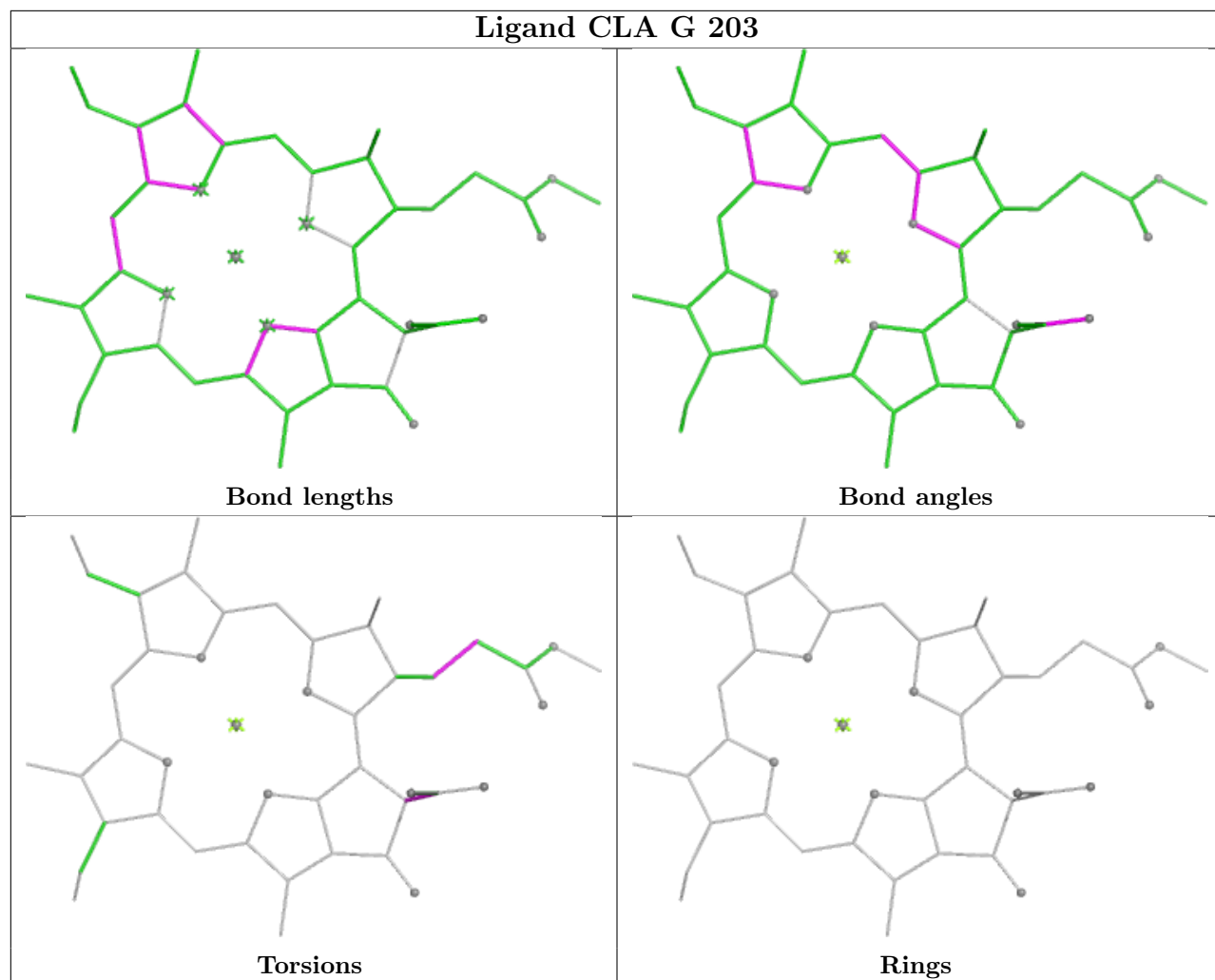


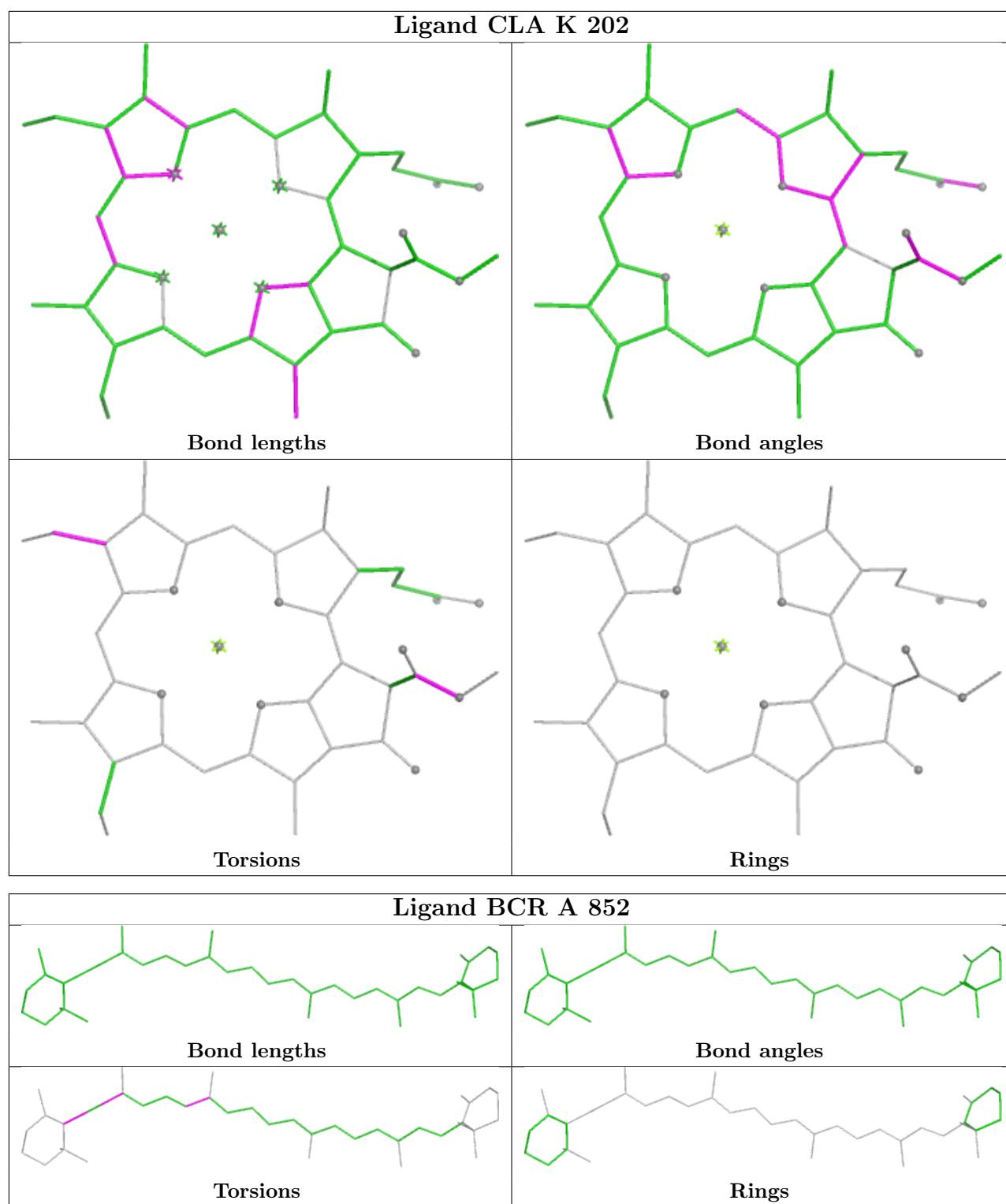
Torsions

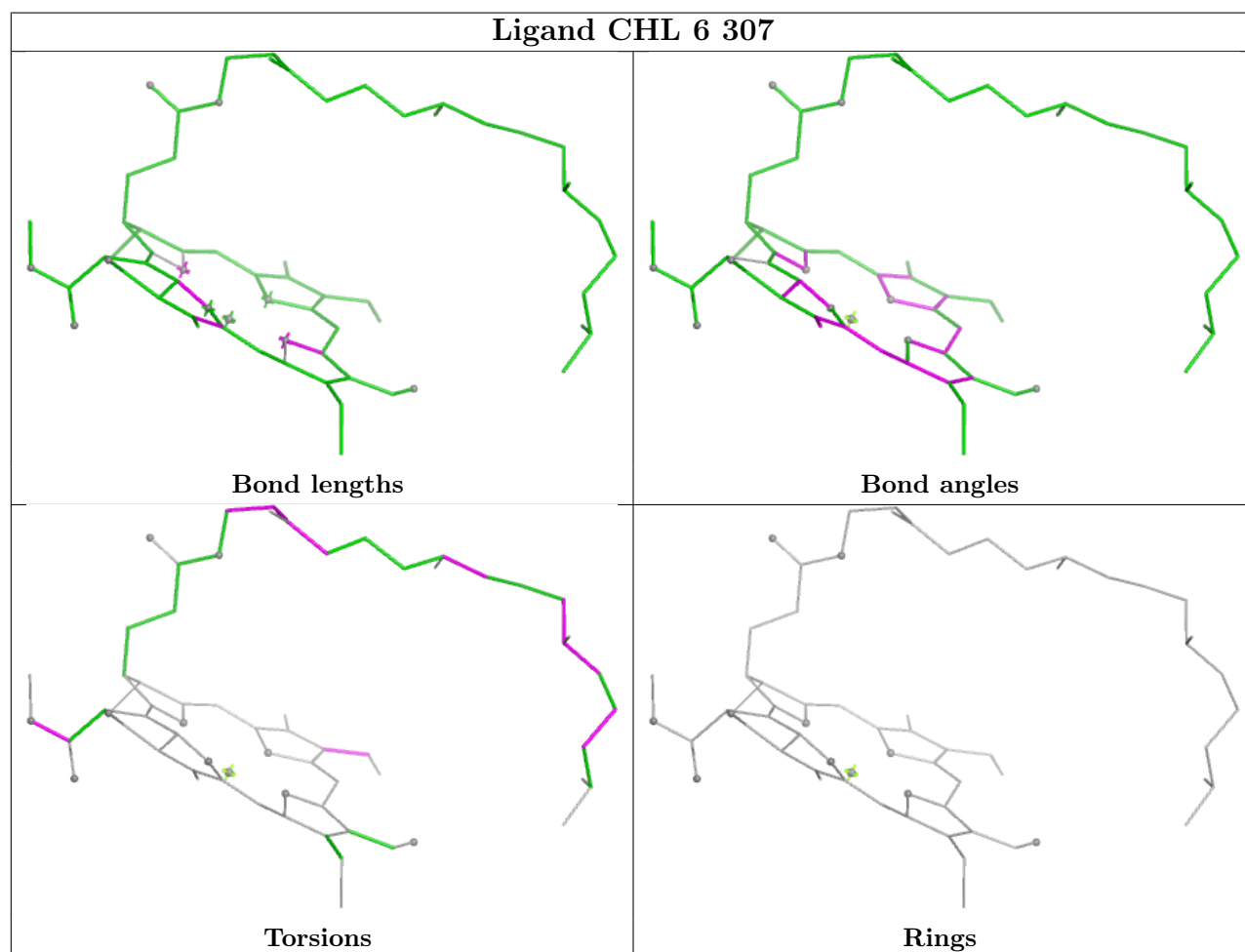
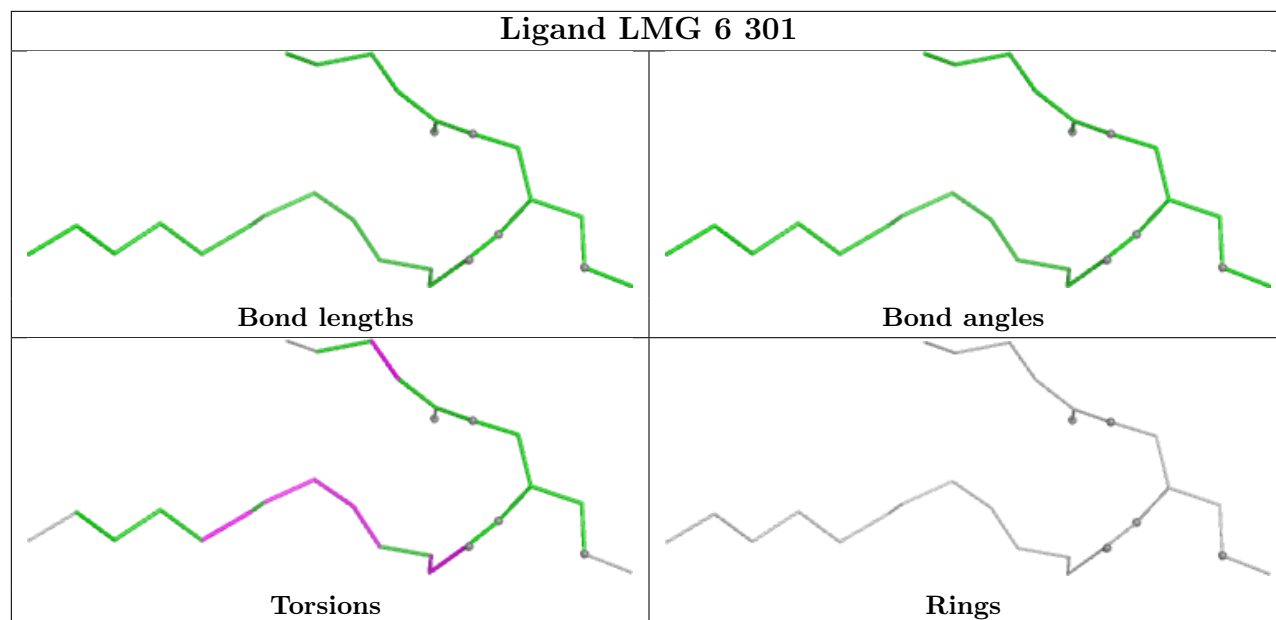


Rings

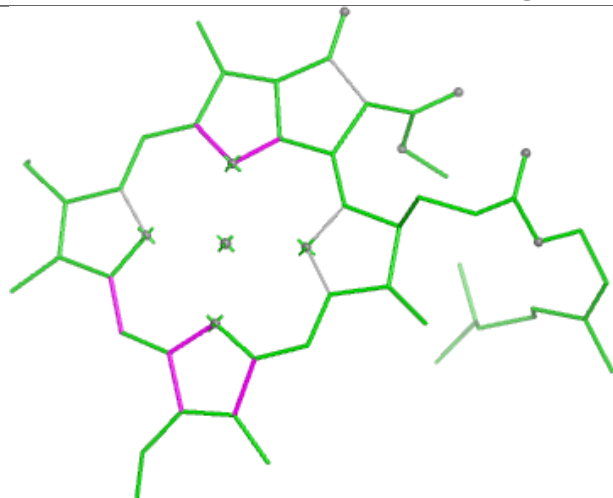
Ligand CLA G 203



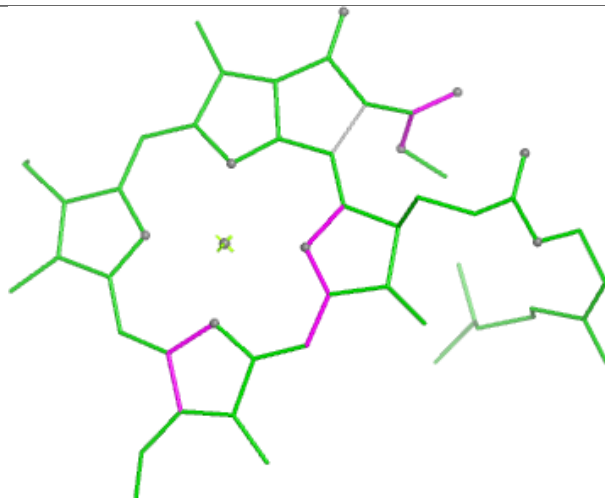




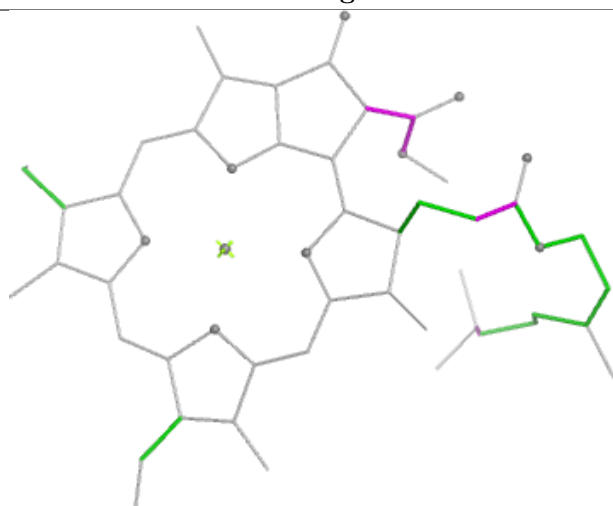
Ligand CLA 8 311



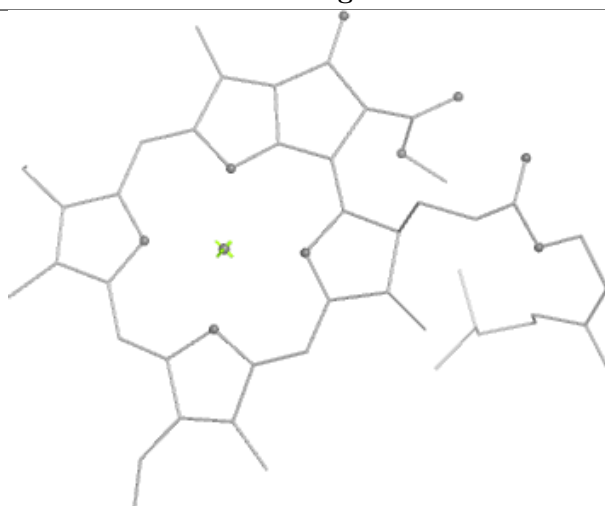
Bond lengths



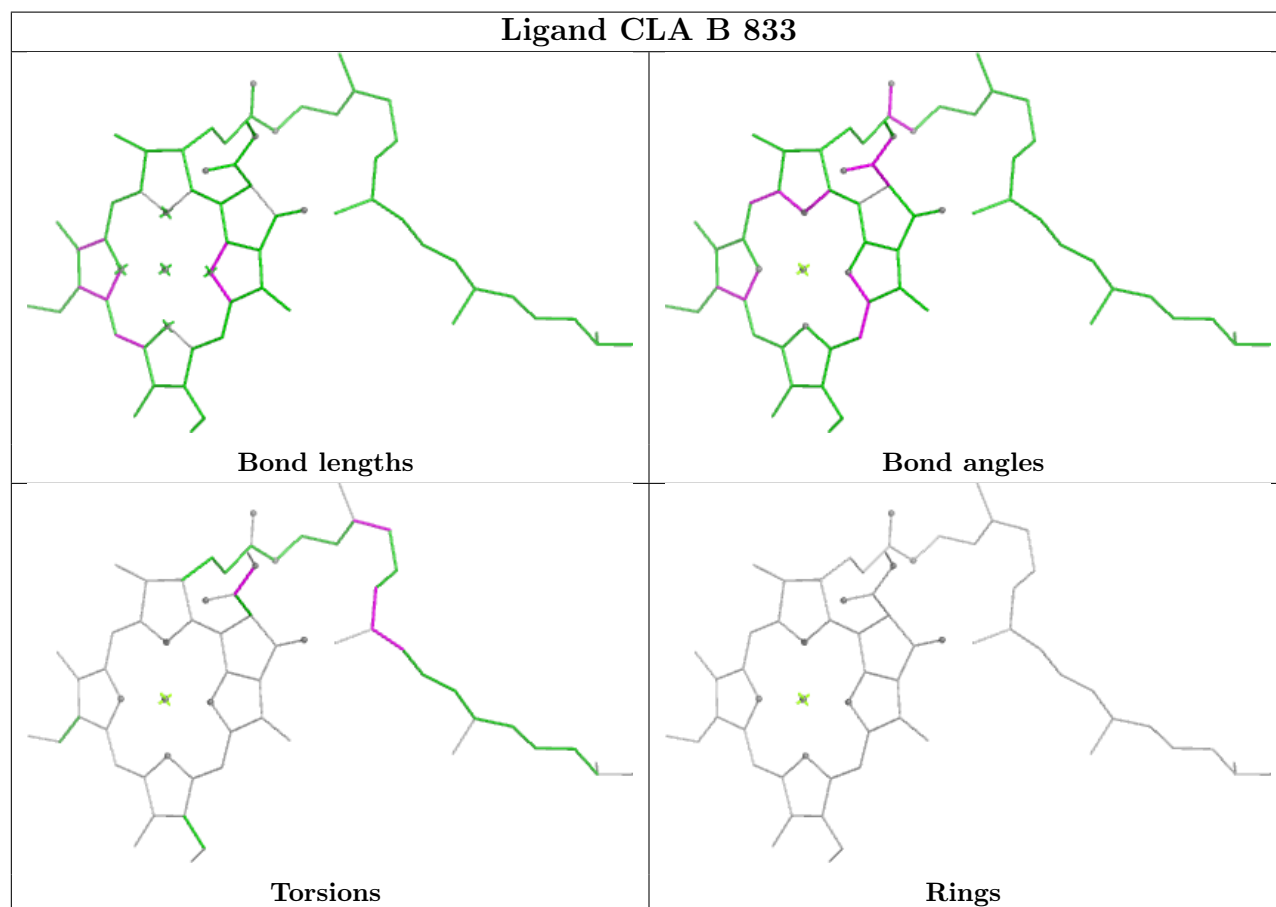
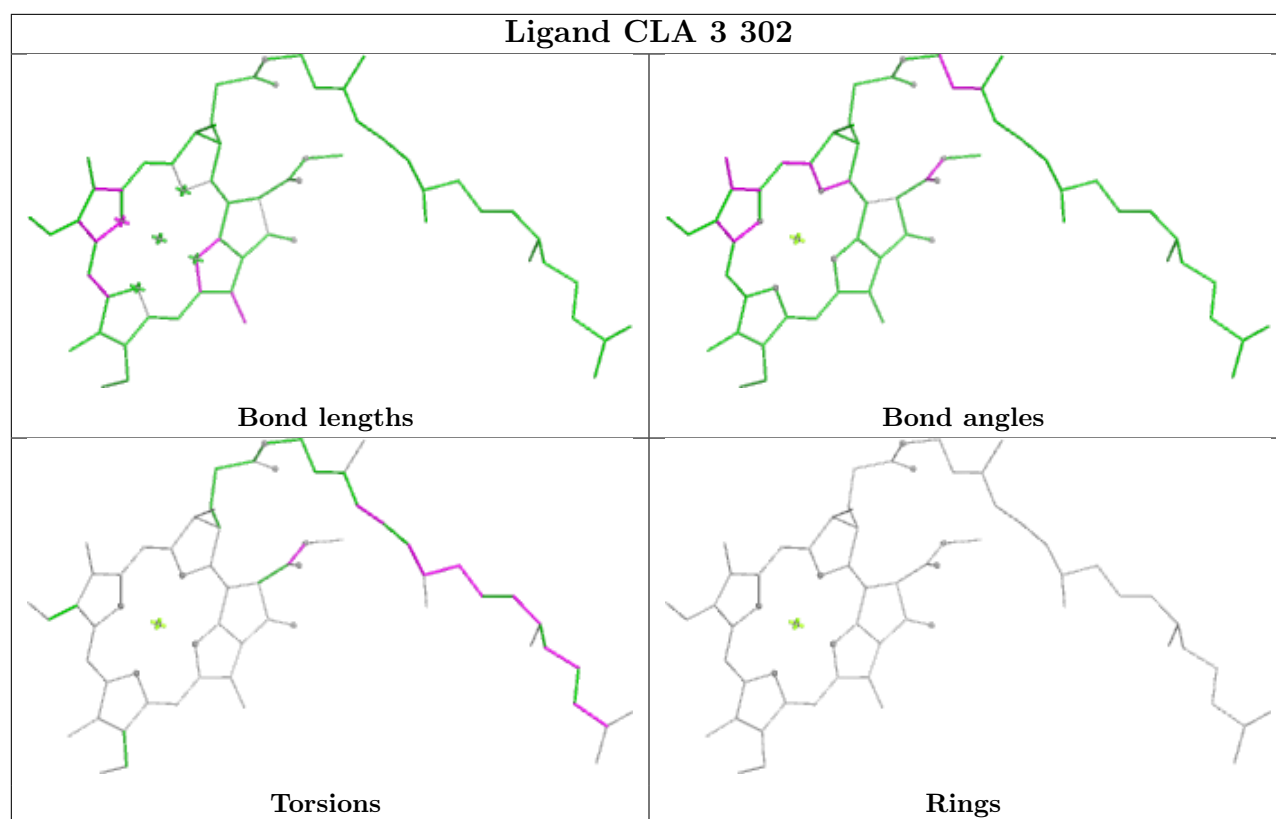
Bond angles



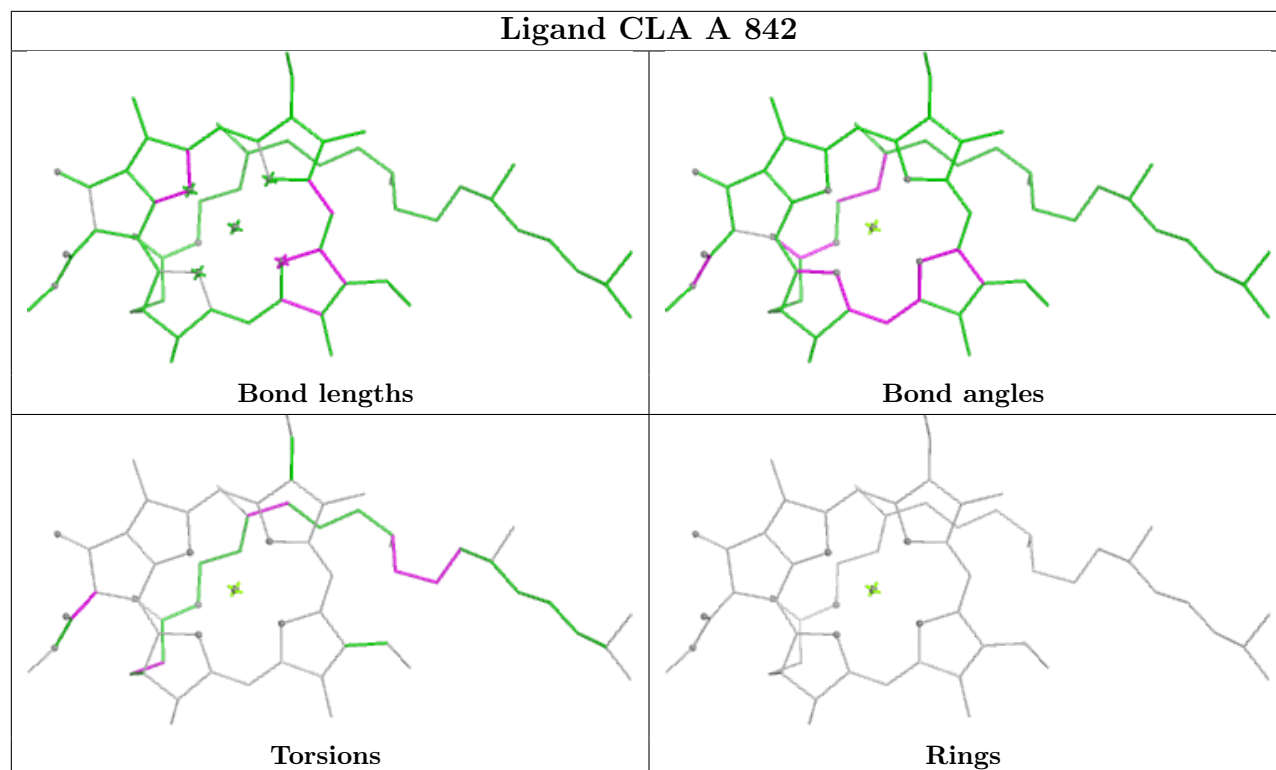
Torsions



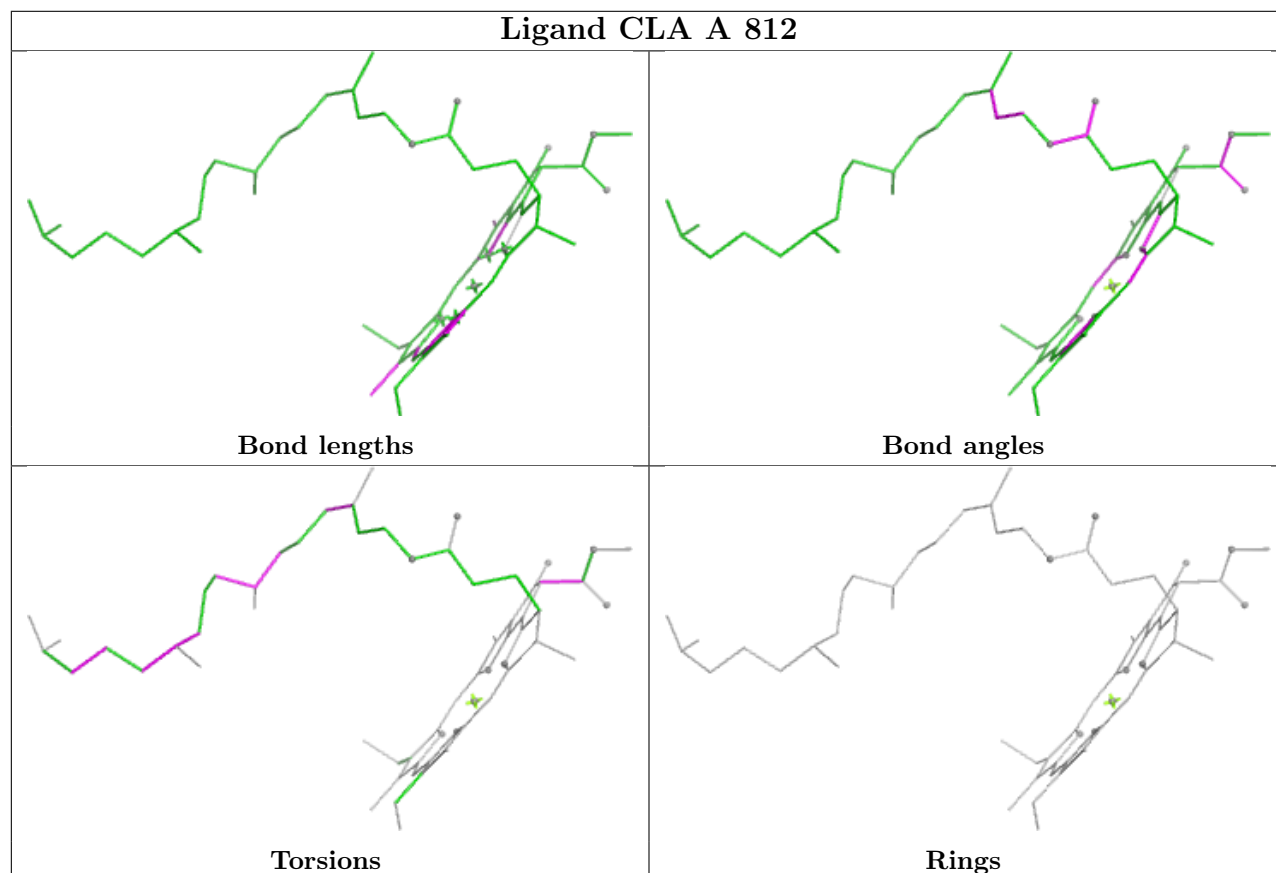
Rings

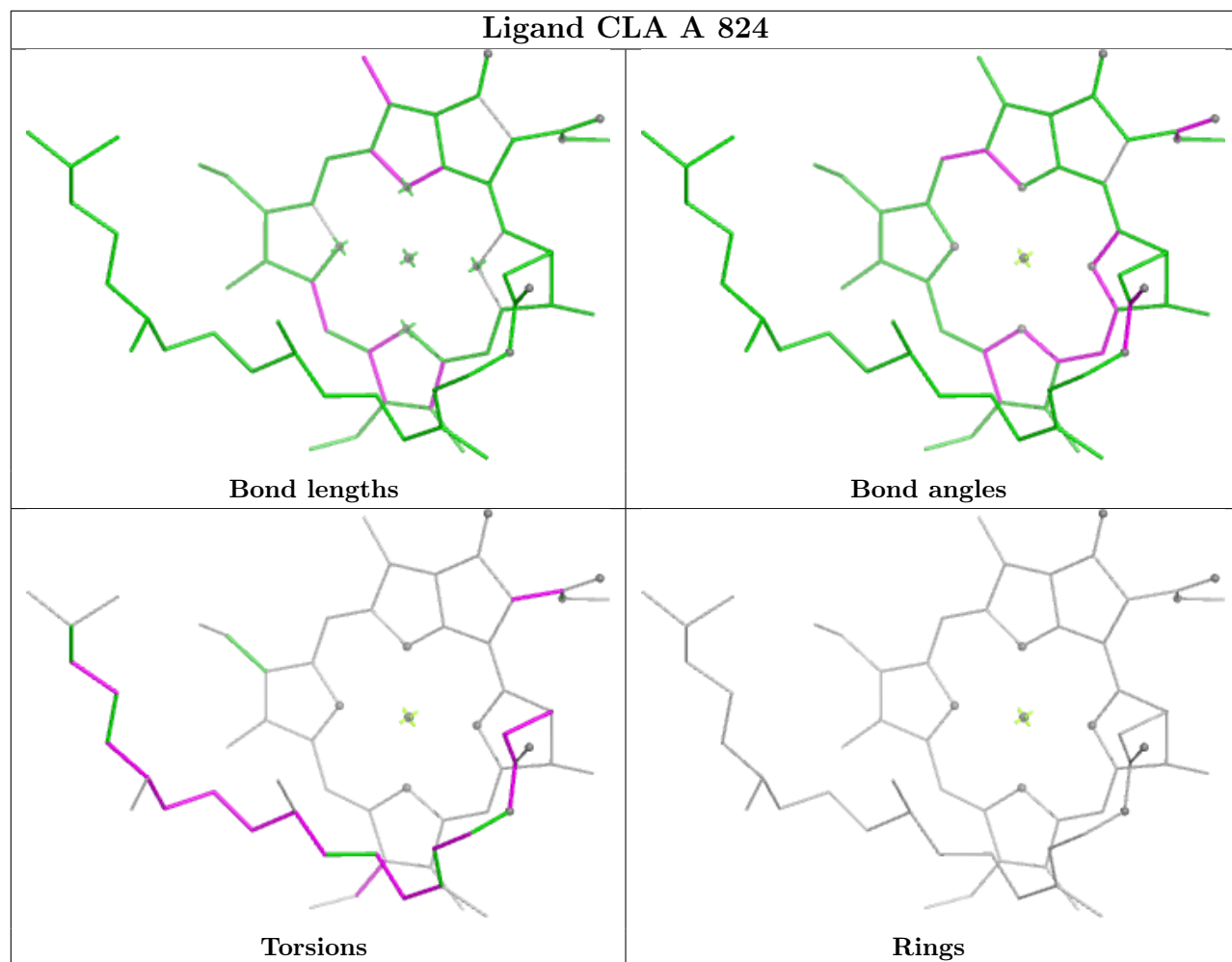


Ligand CLA A 842

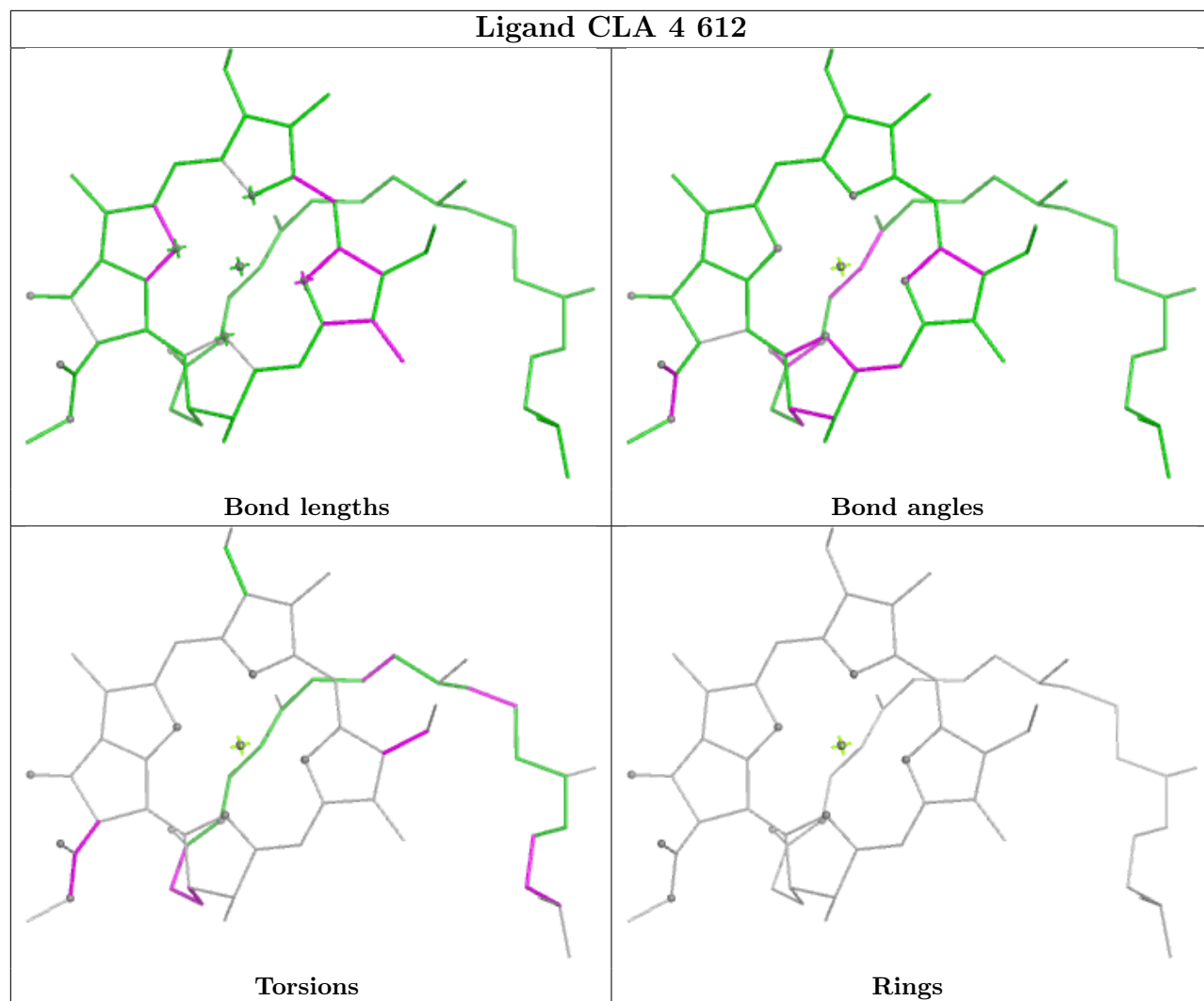


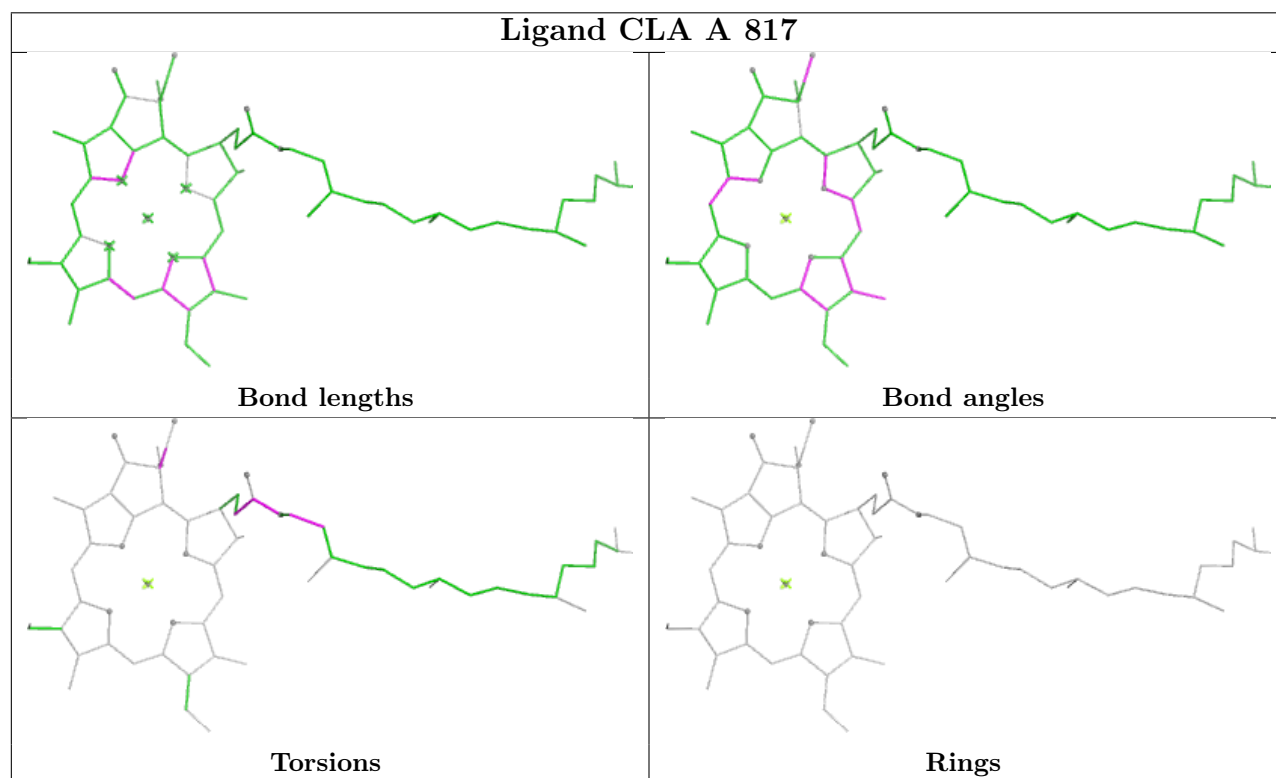
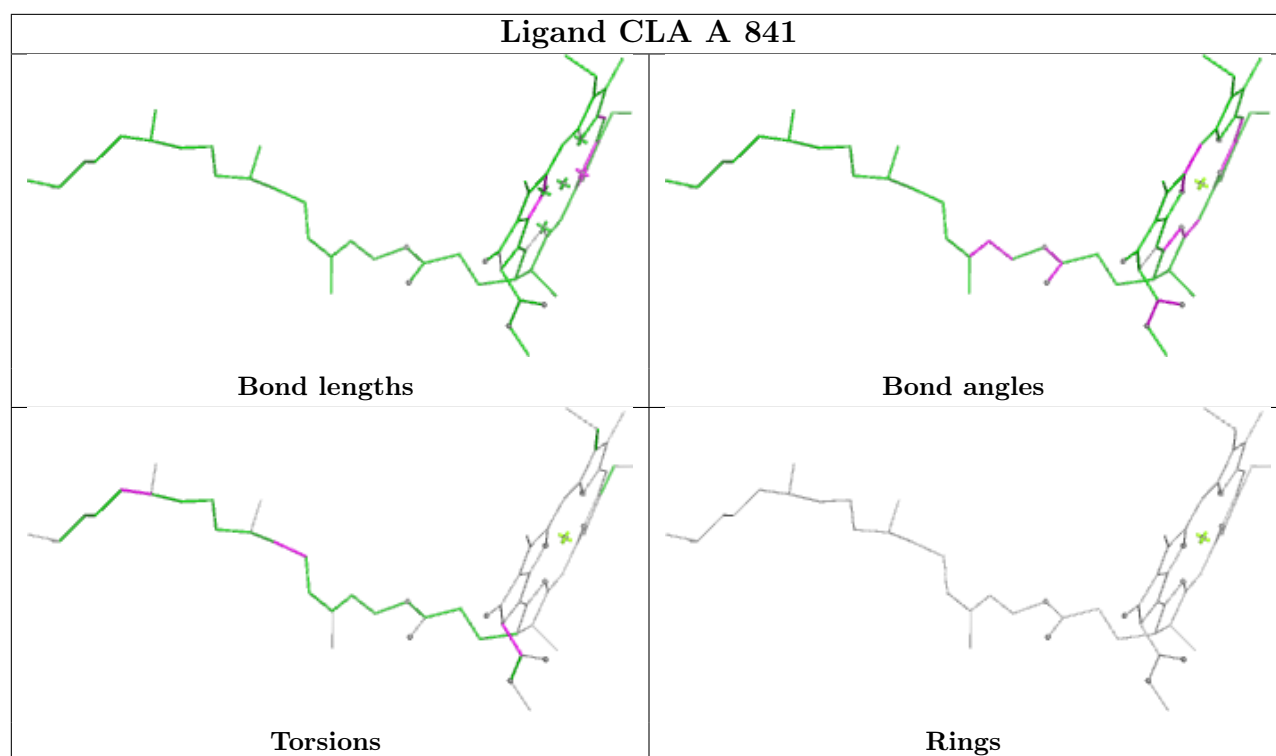
Ligand CLA A 812

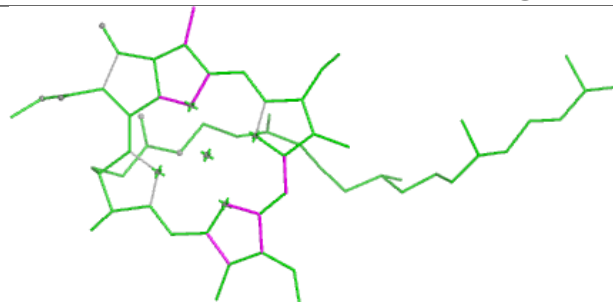
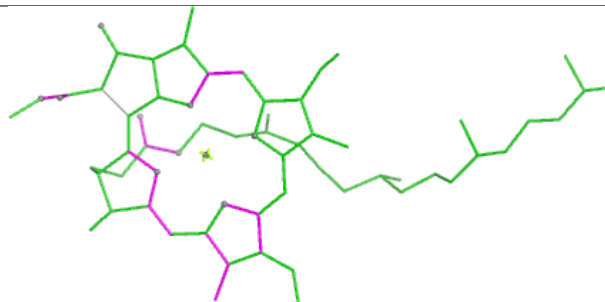
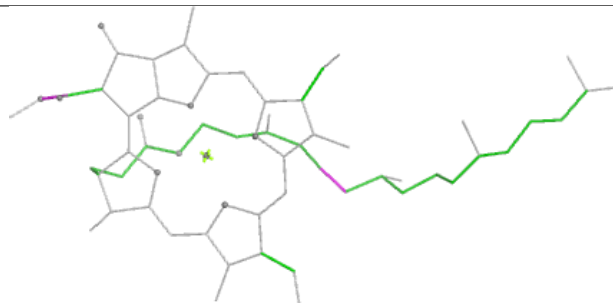
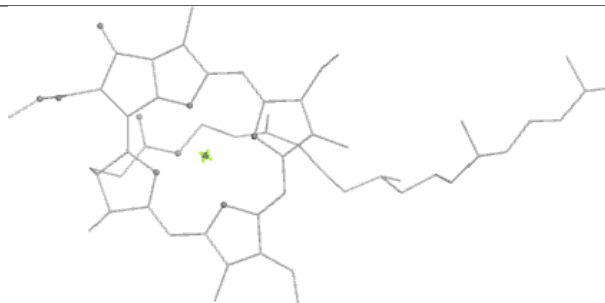
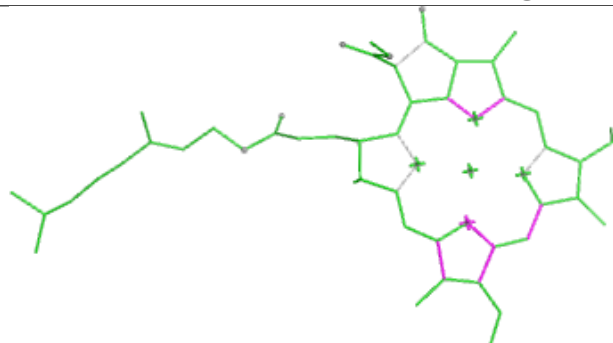
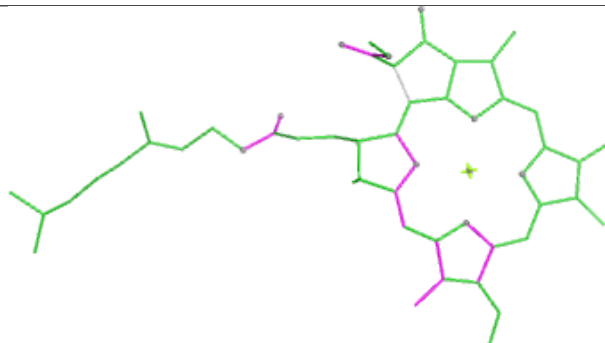
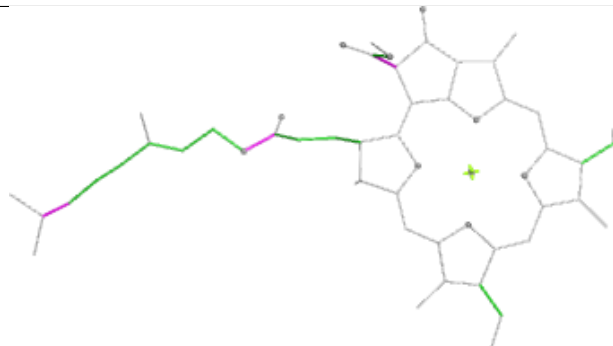
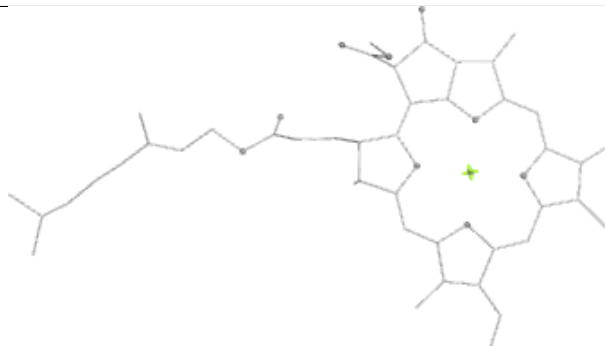


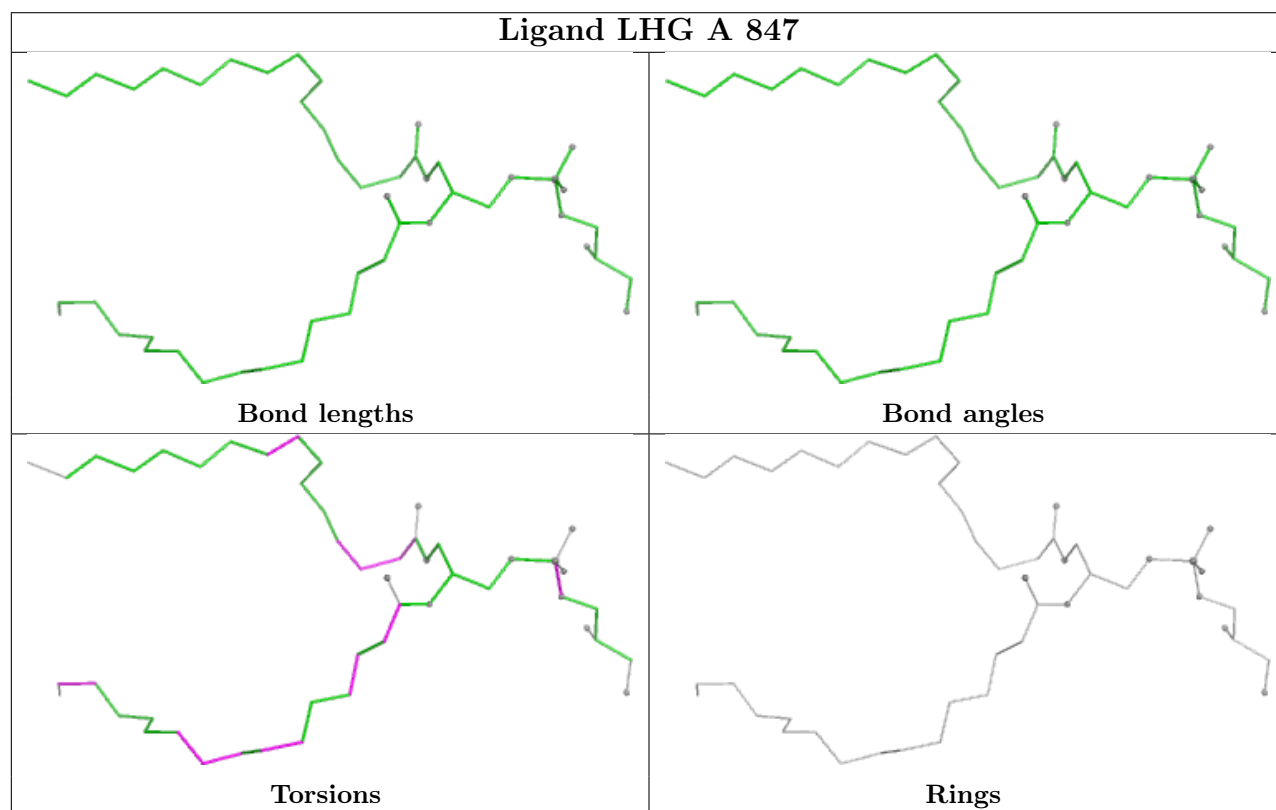
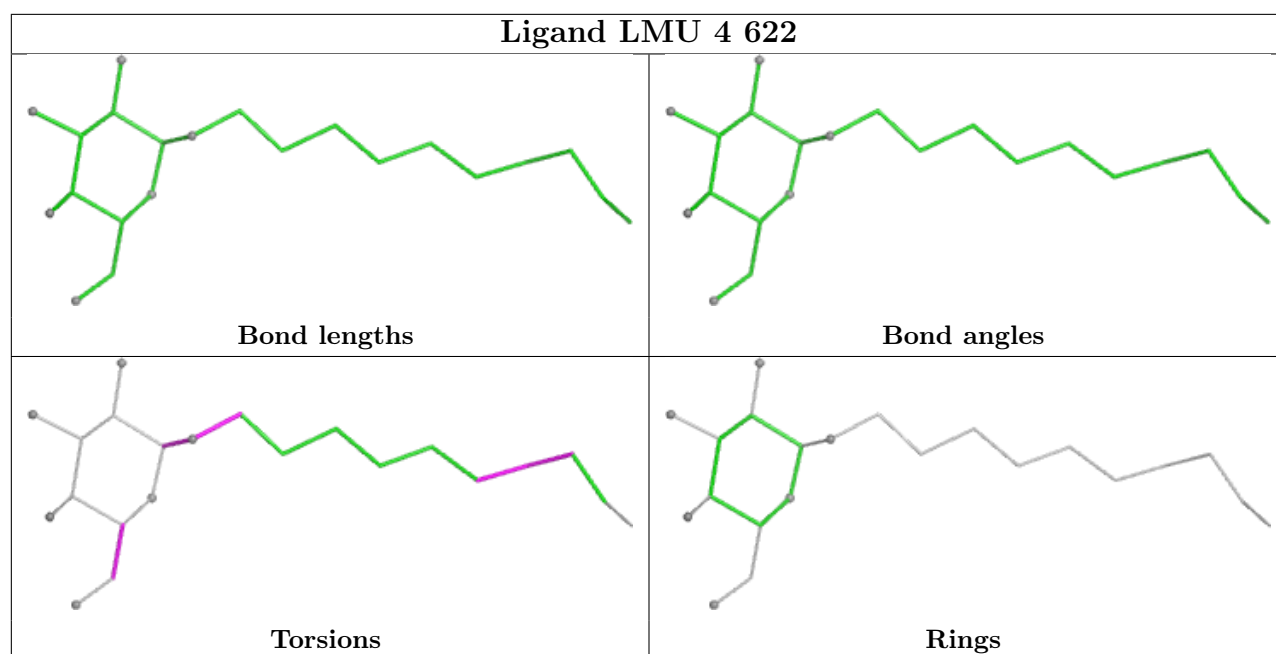


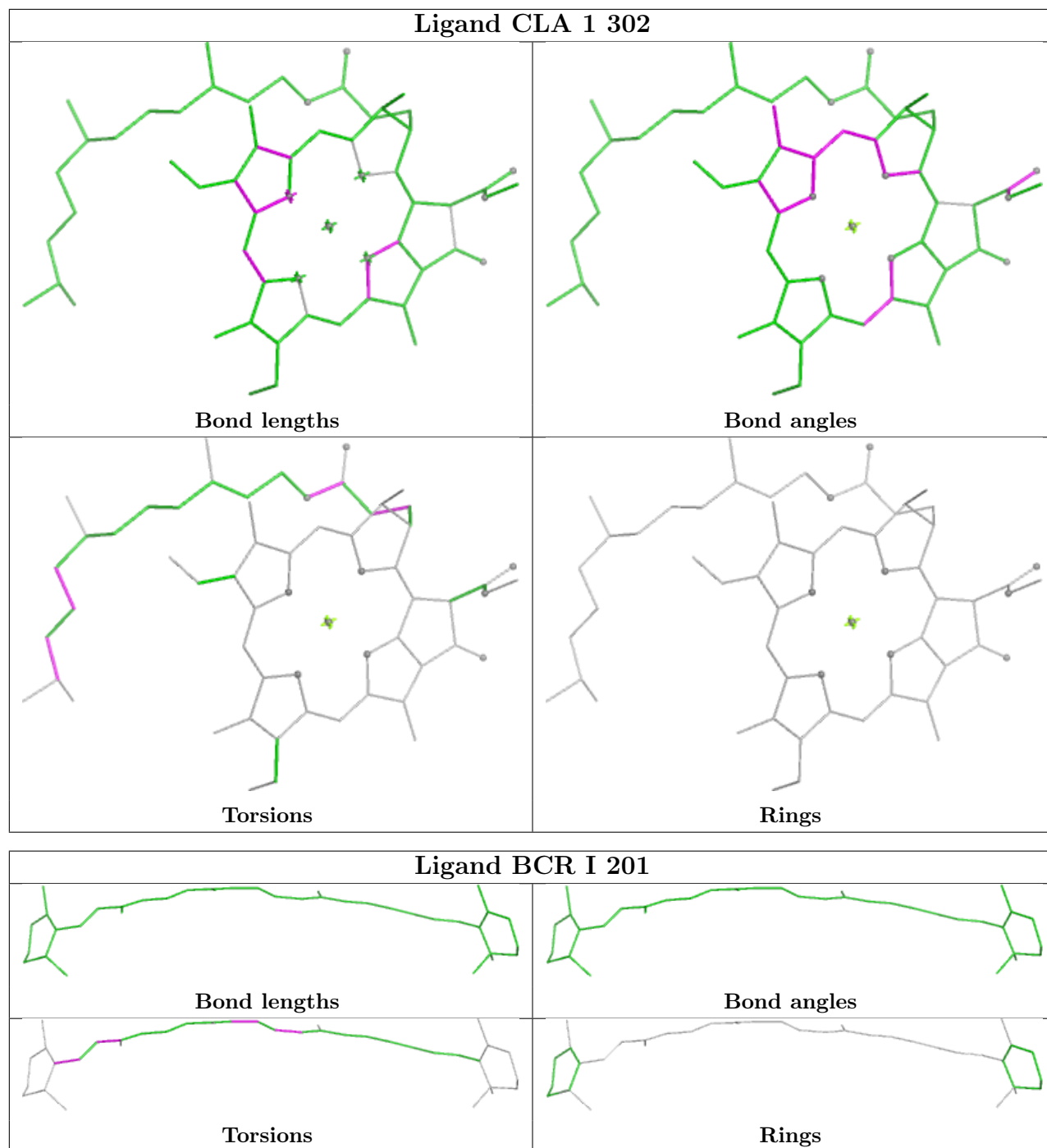
Ligand CLA 4 612

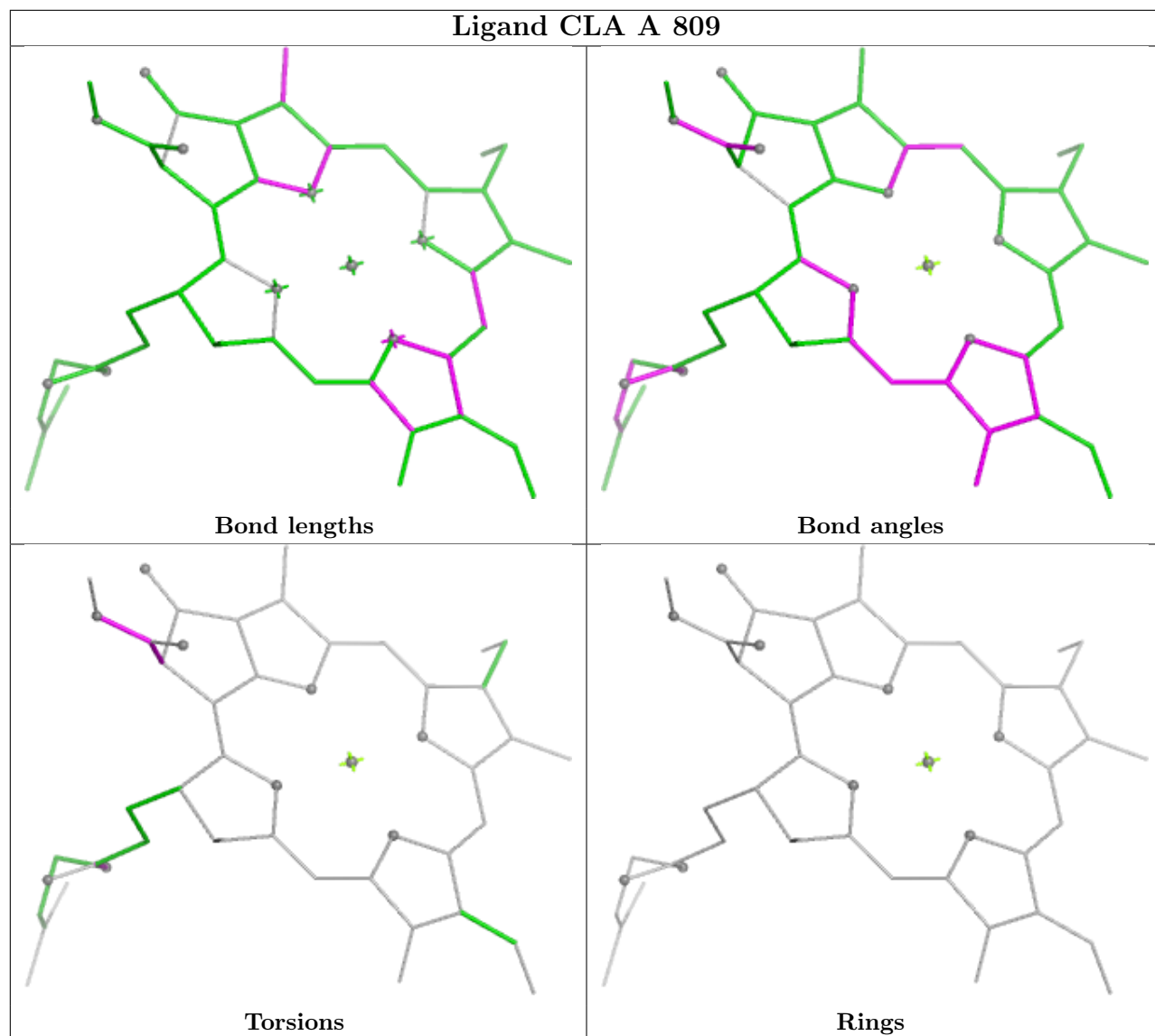


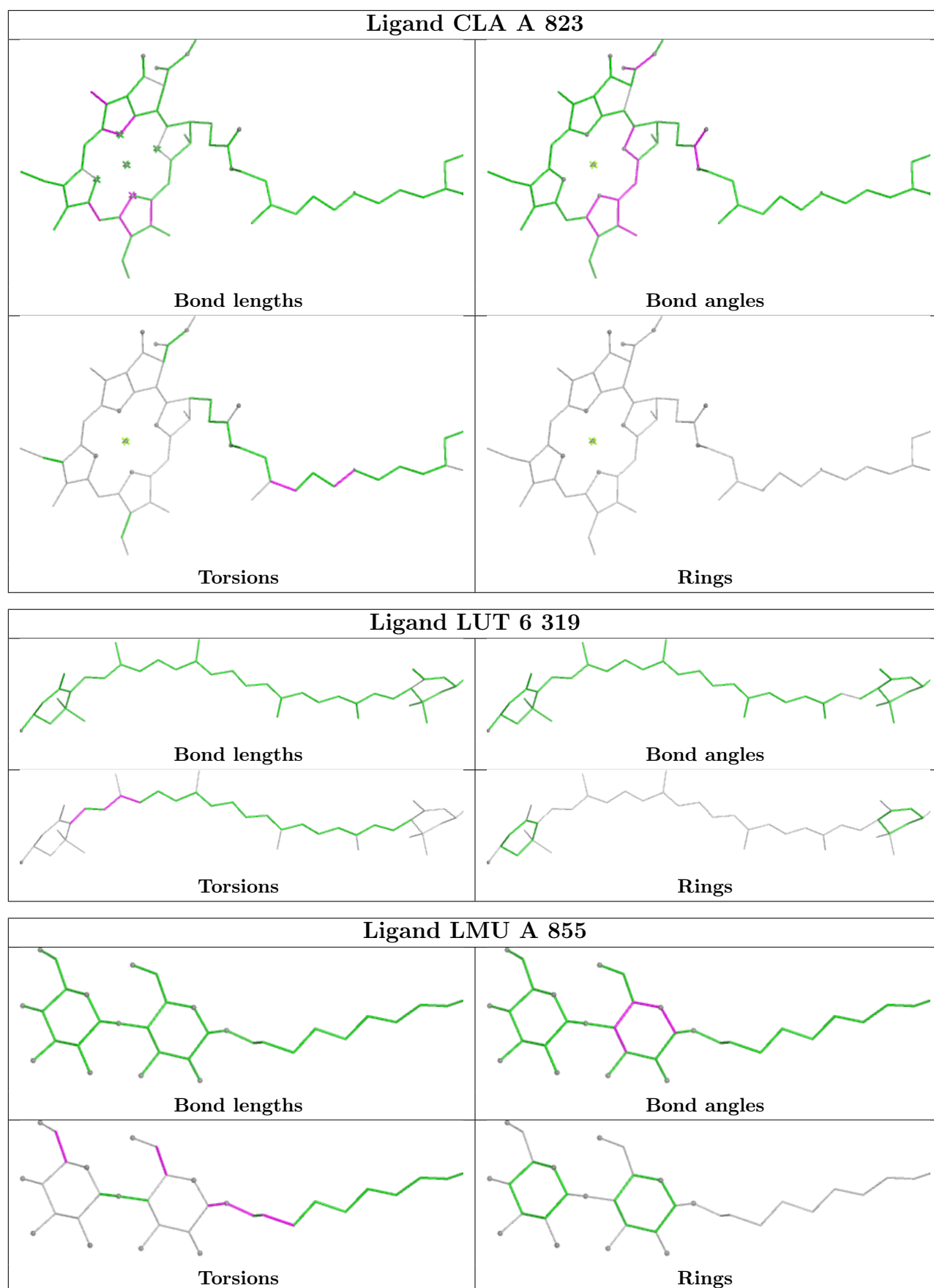


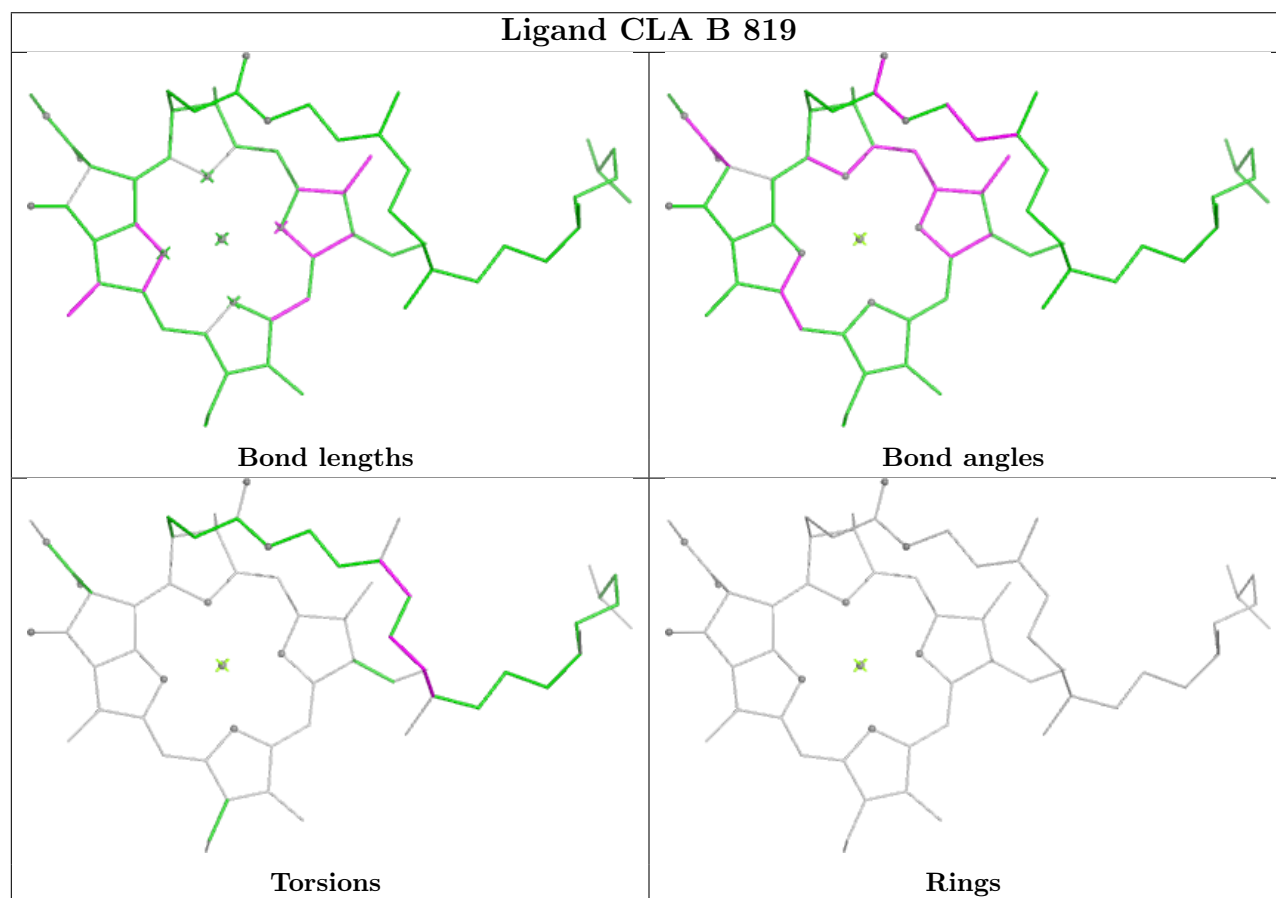
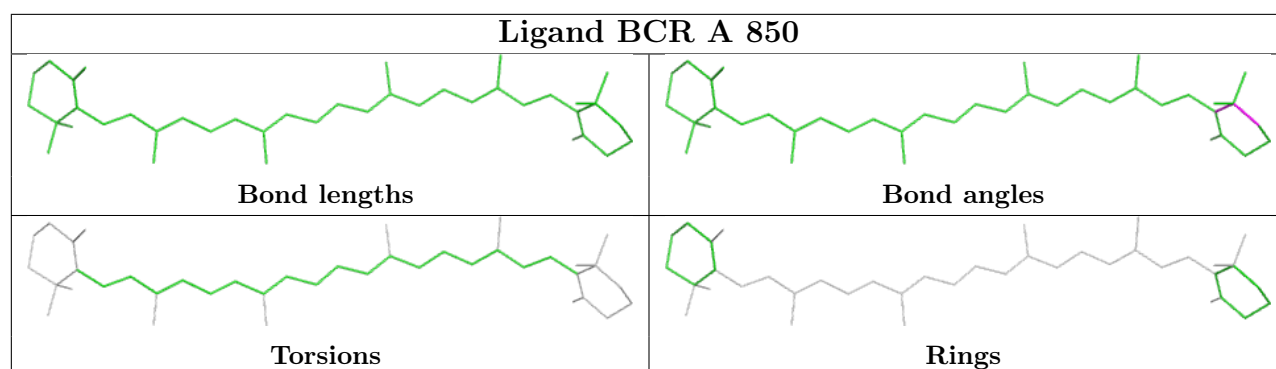
Ligand CLA Z 612**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 6 320****Bond lengths****Bond angles****Torsions****Rings**



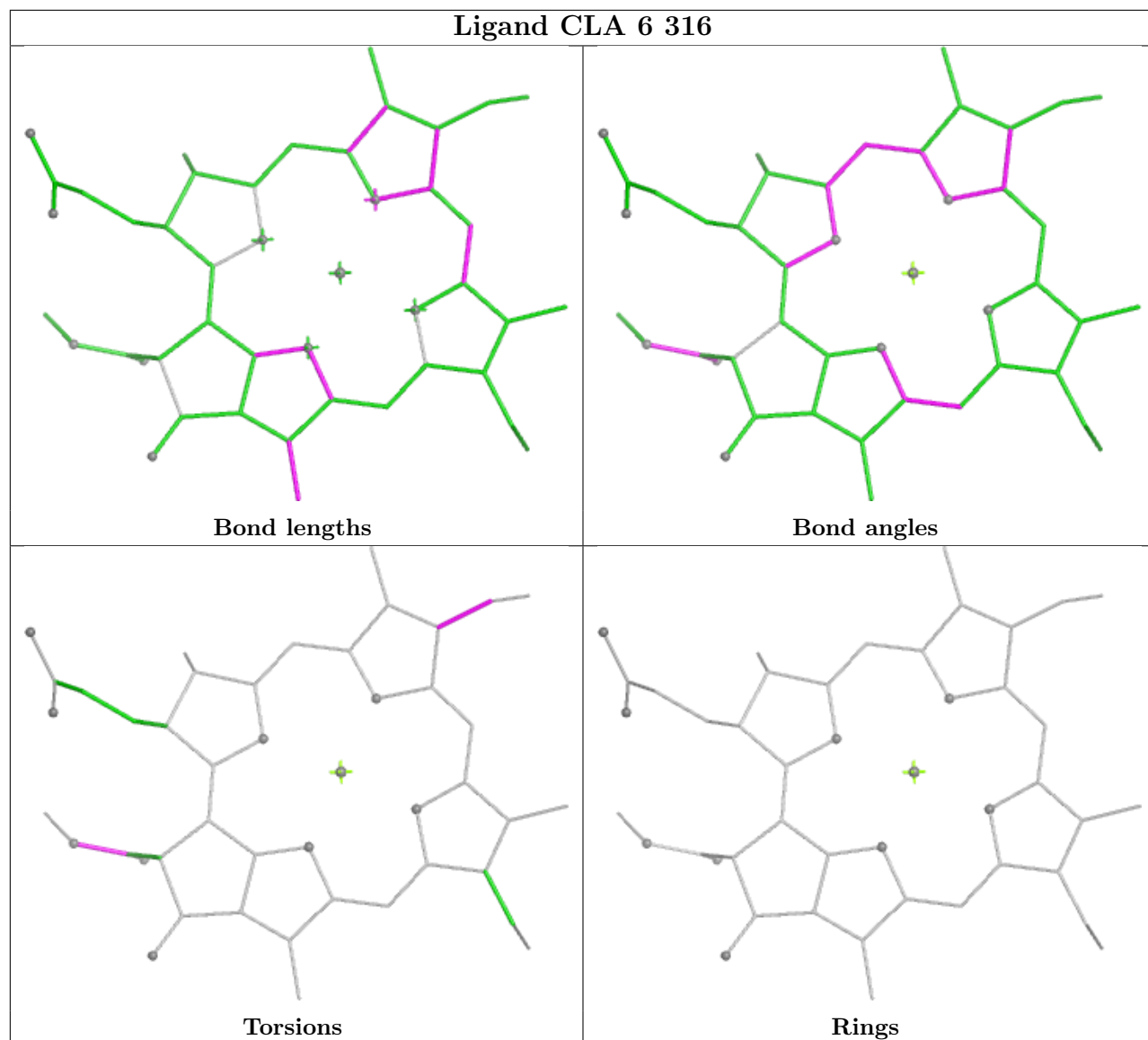


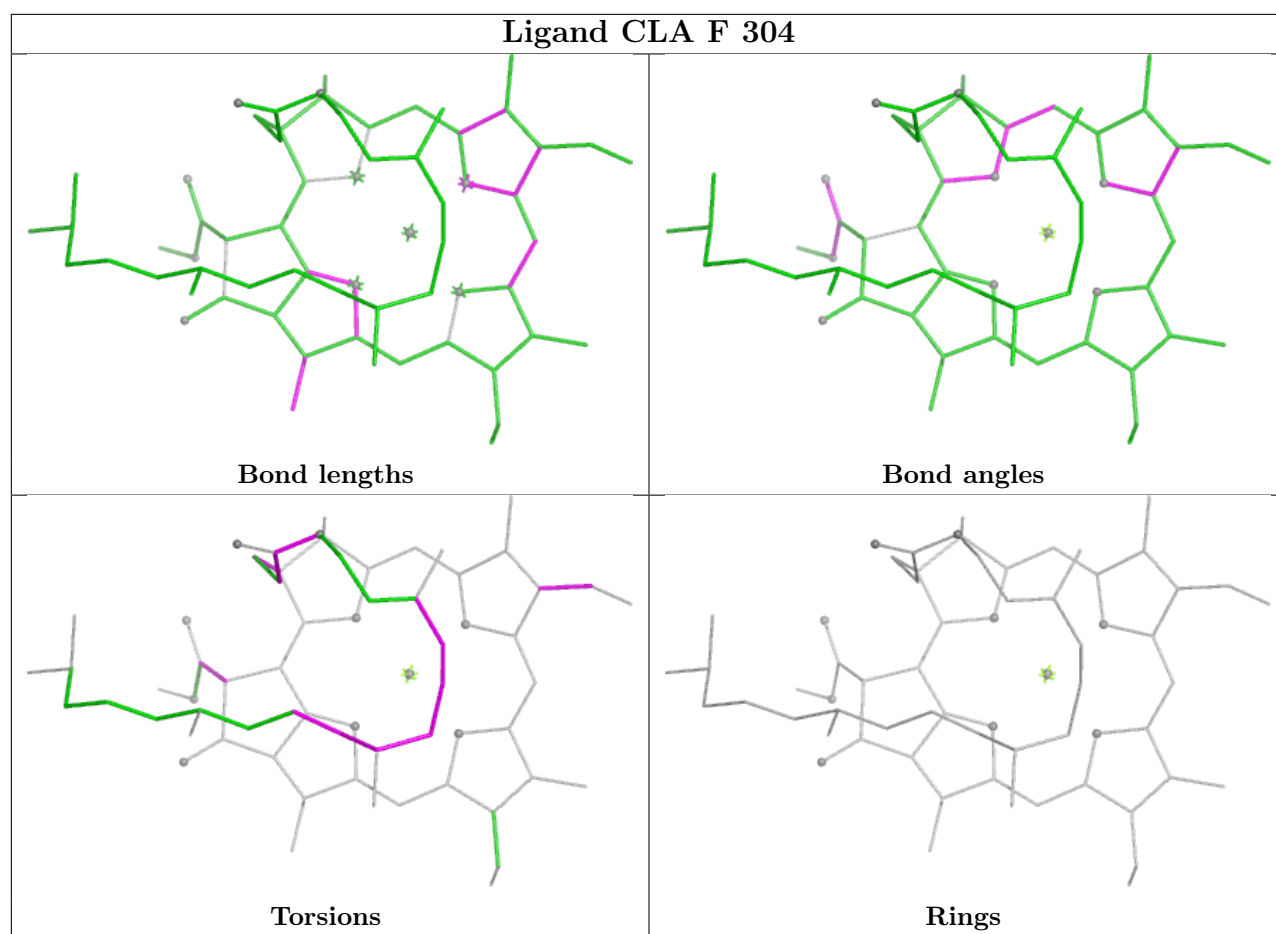


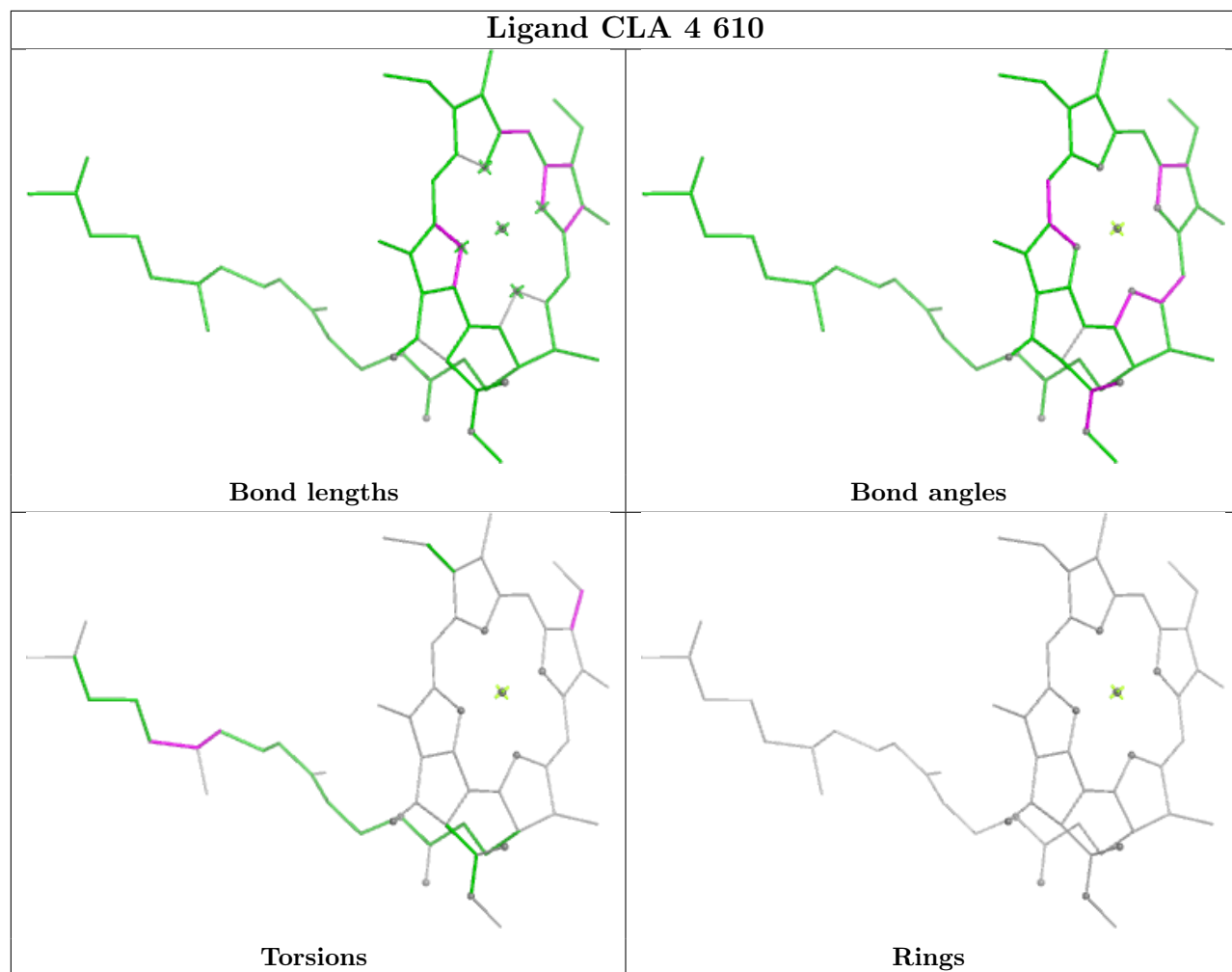




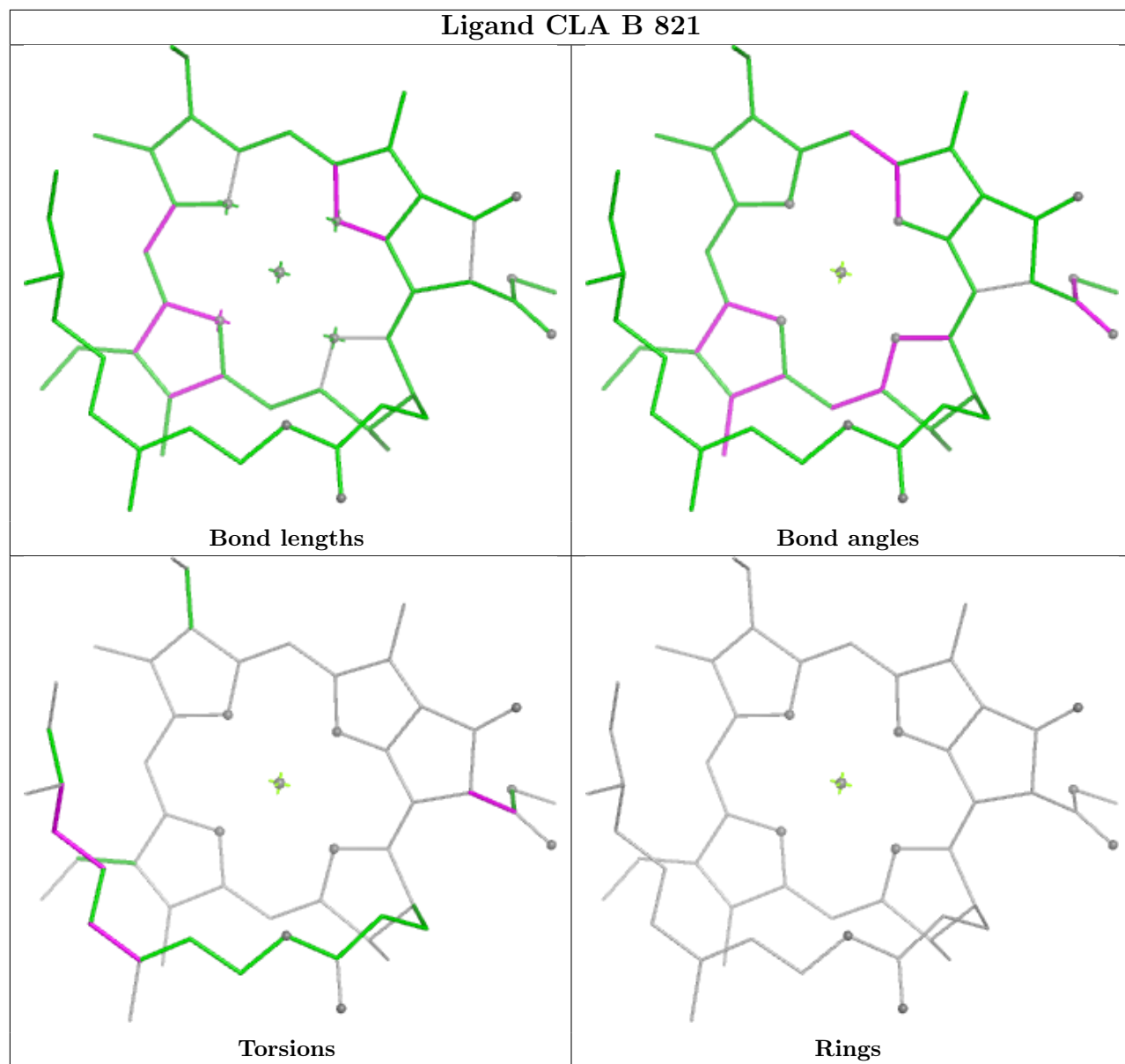
Ligand CLA 6 316



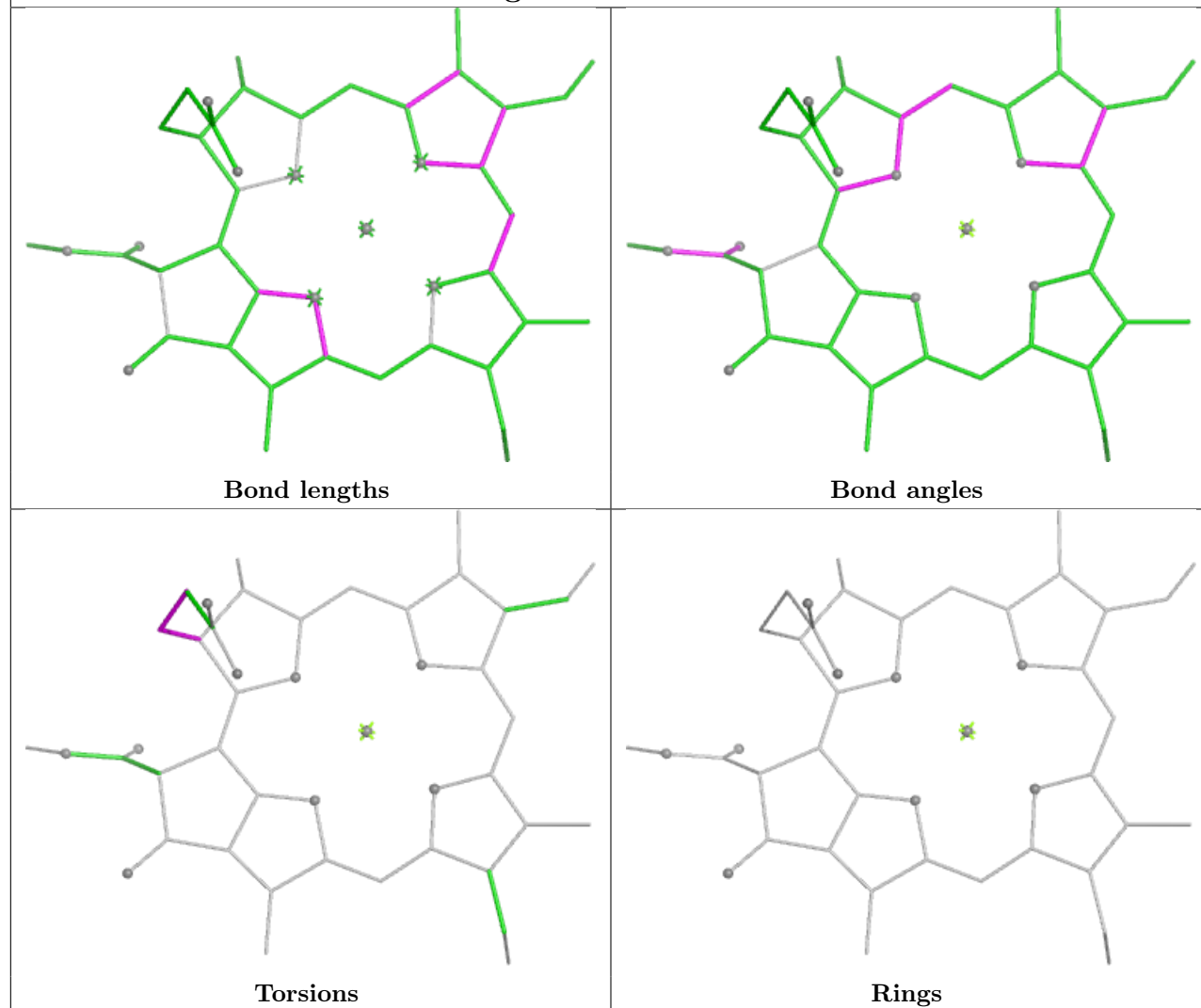




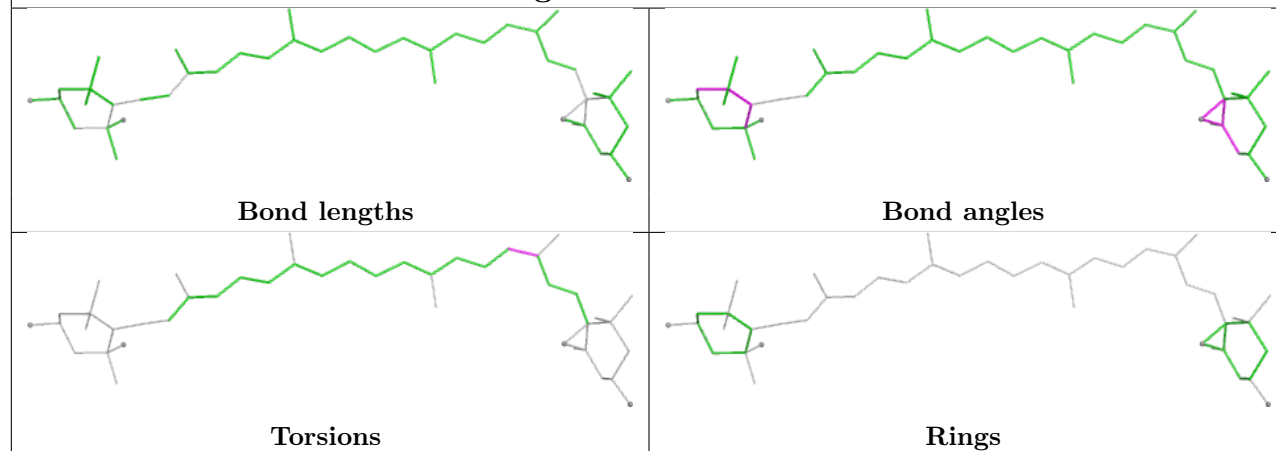
Ligand CLA B 821

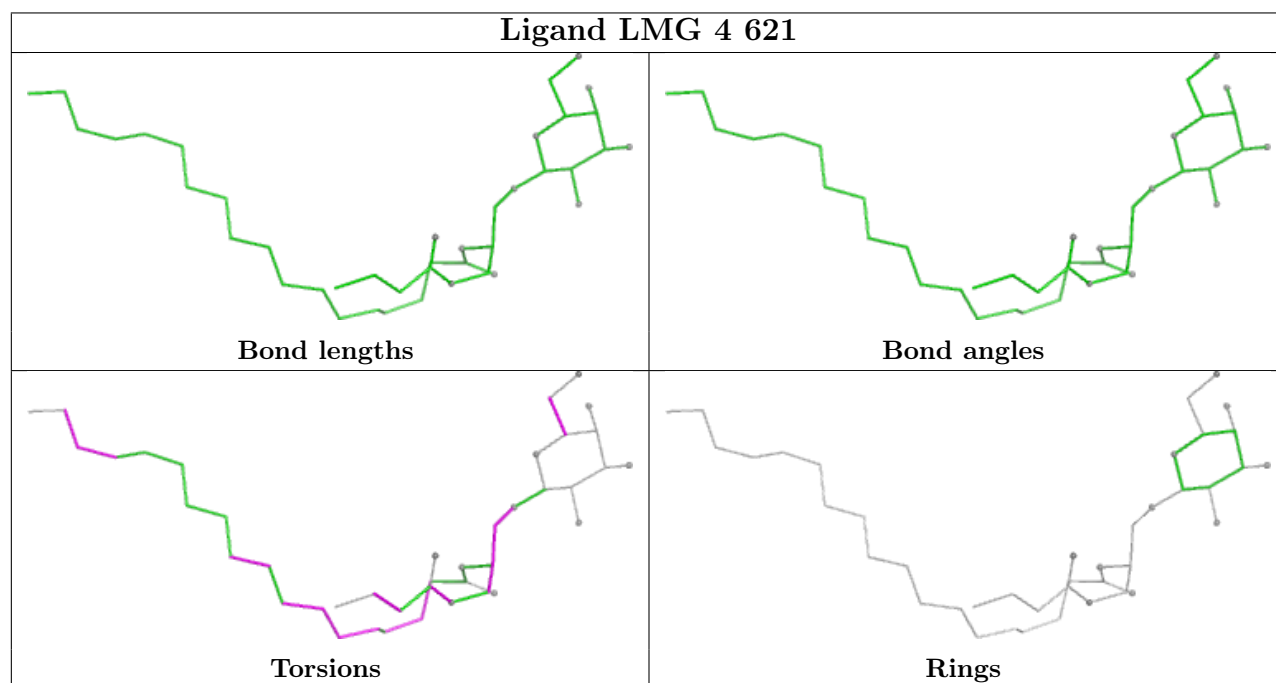
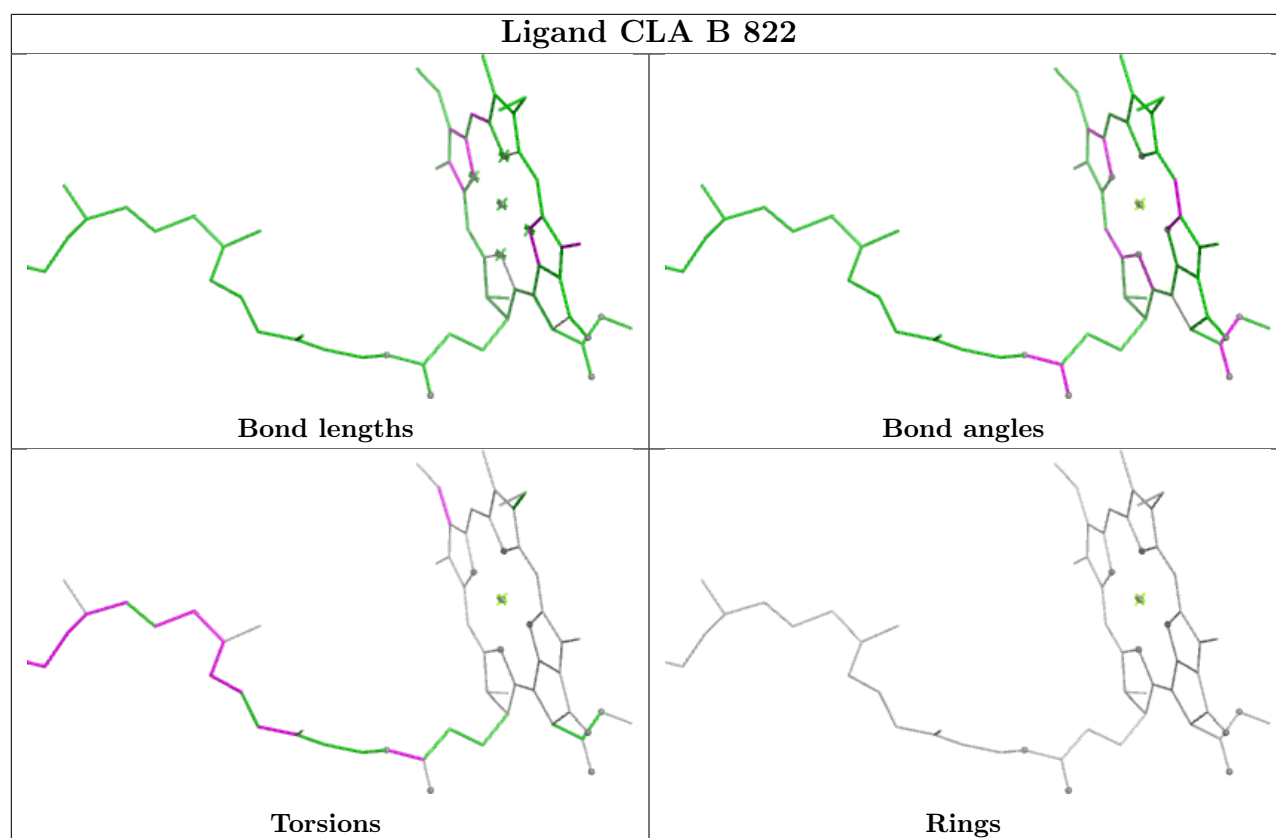


Ligand CLA 4 614

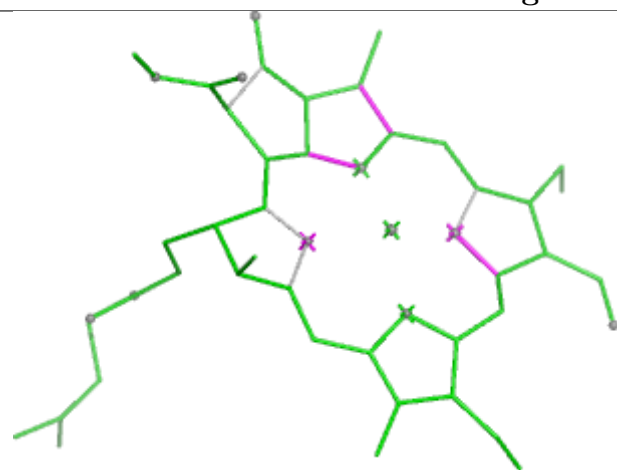


Ligand NEX 5 323

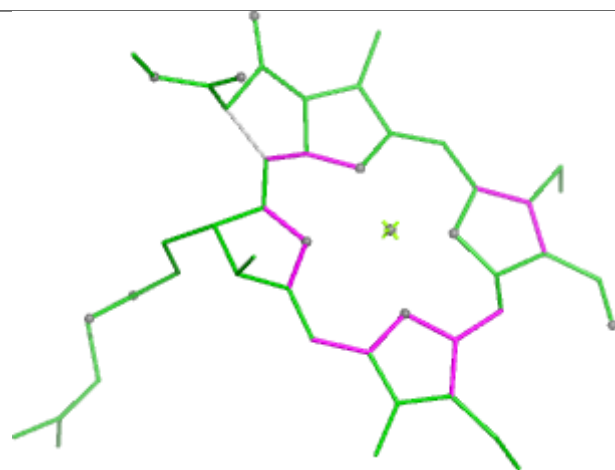




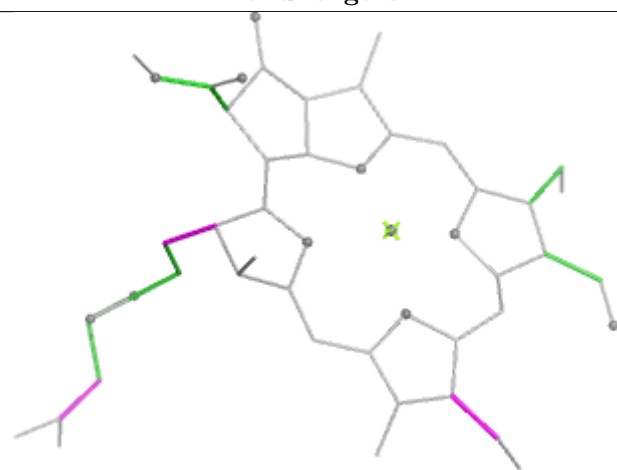
Ligand CHL 6 308



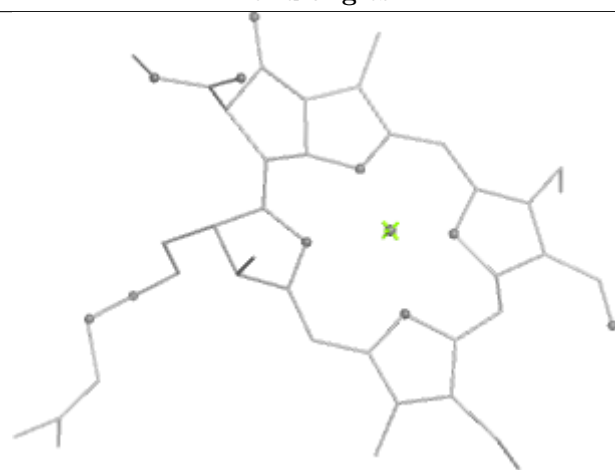
Bond lengths



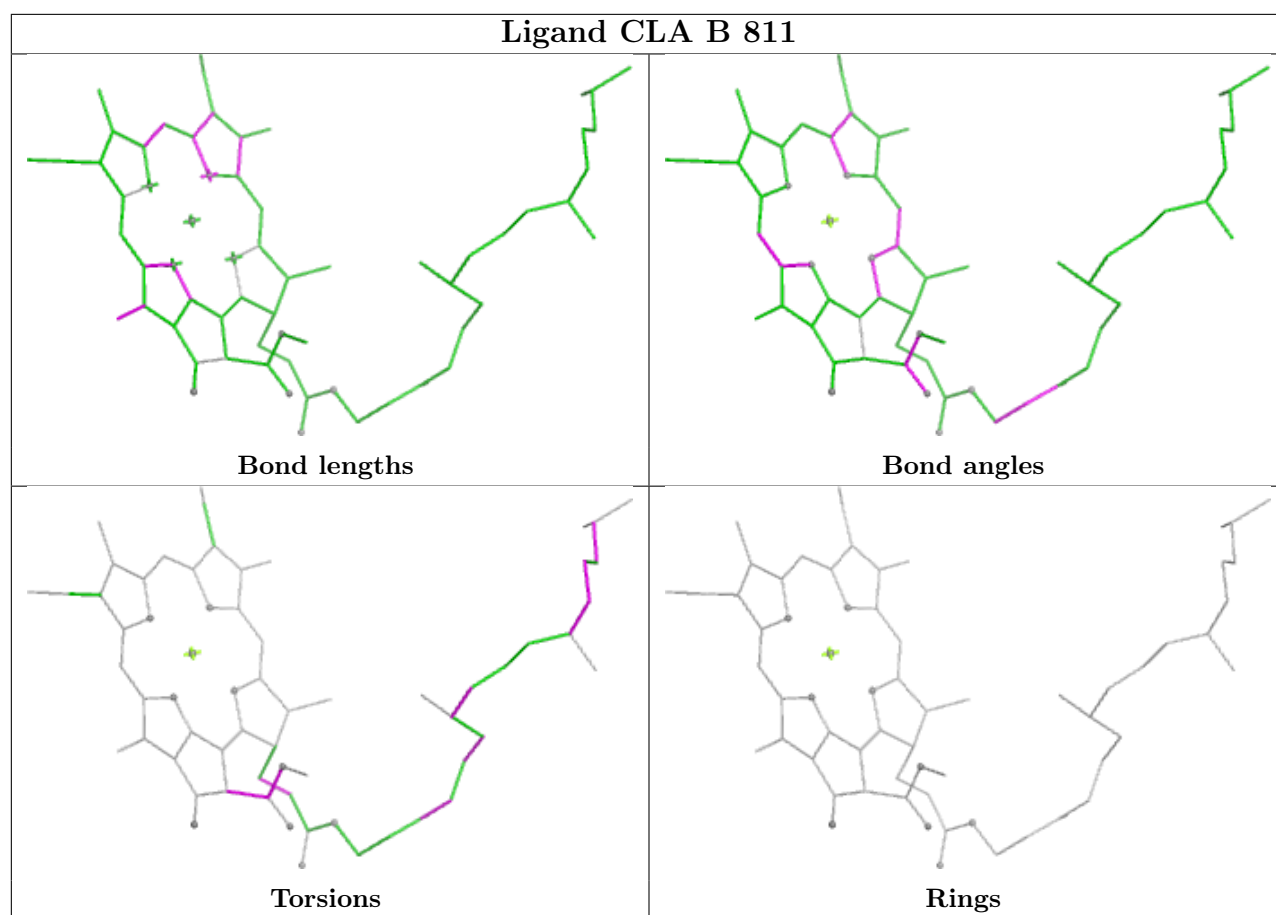
Bond angles

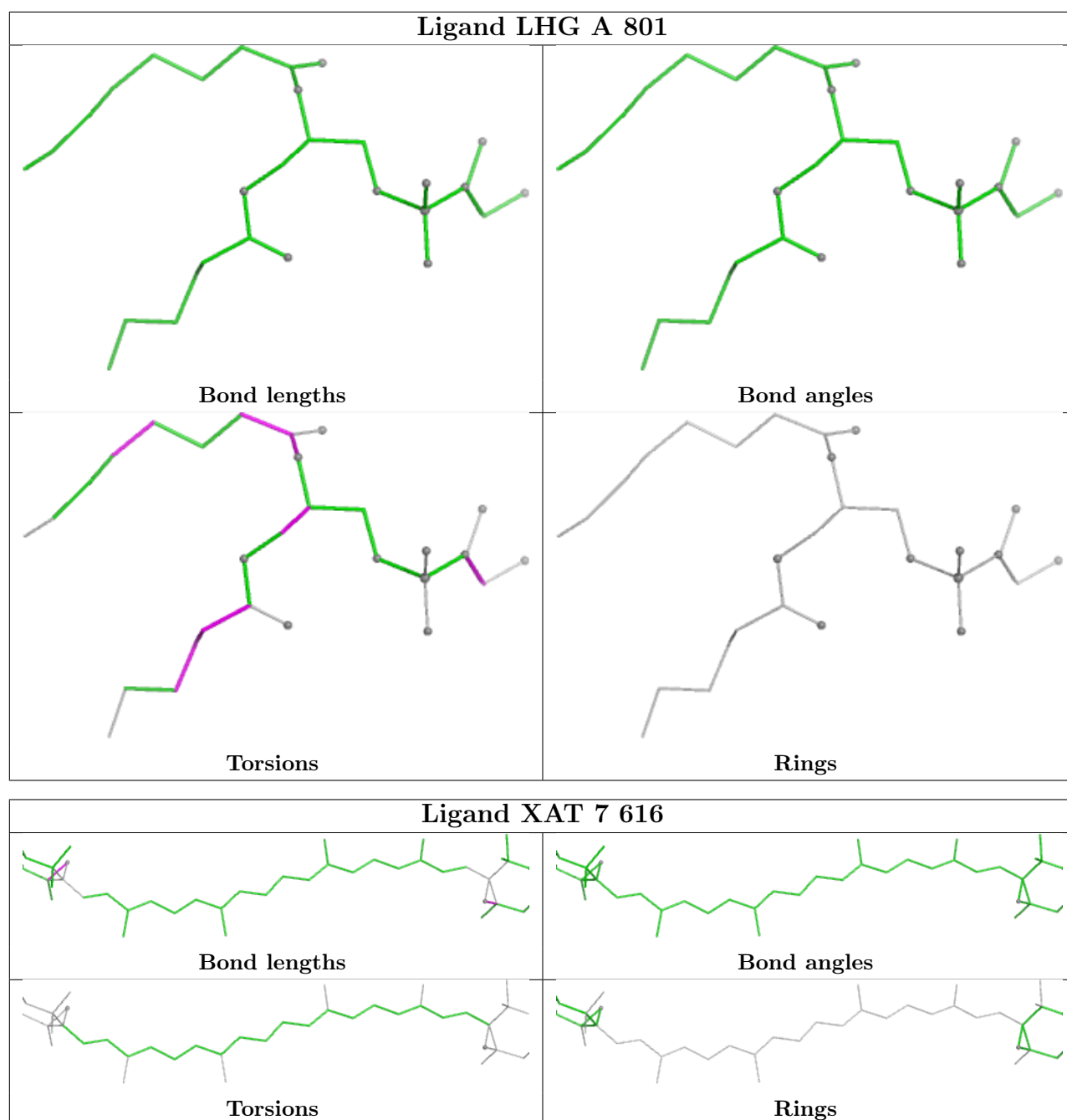


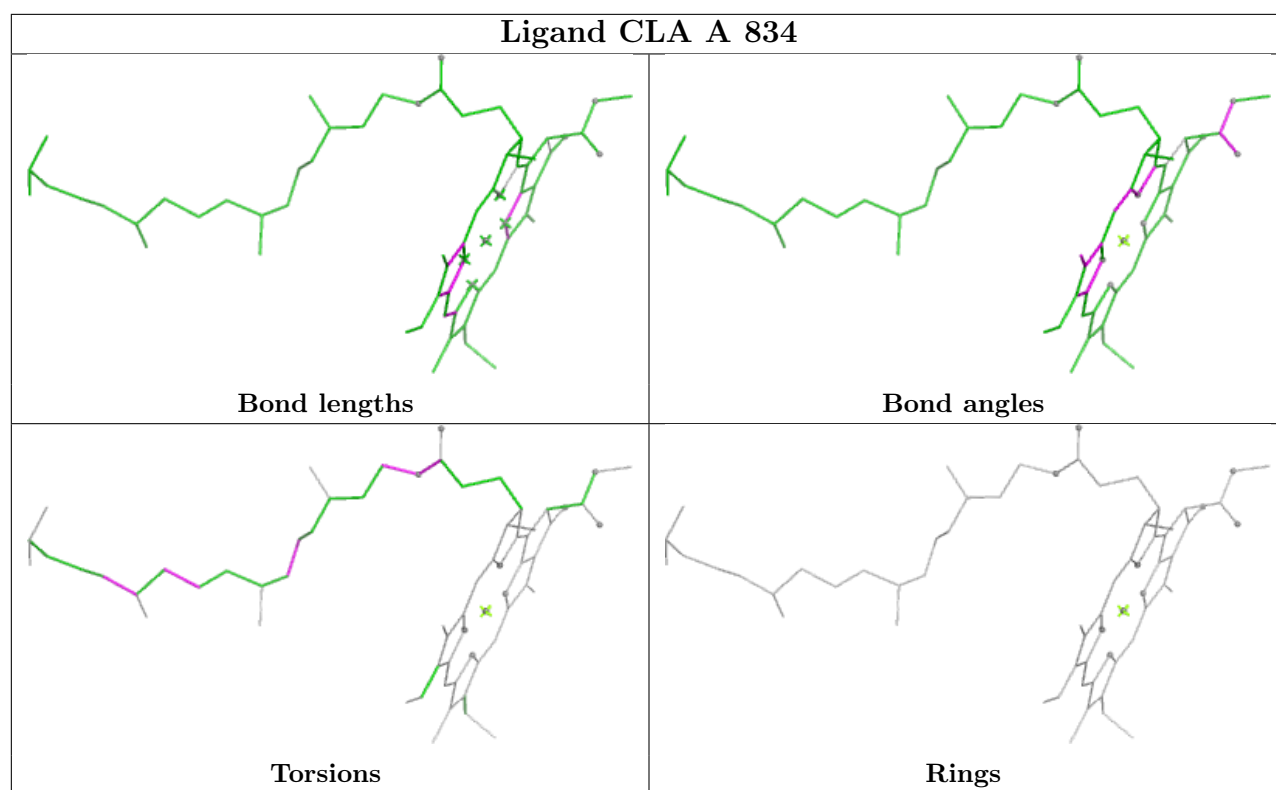
Torsions

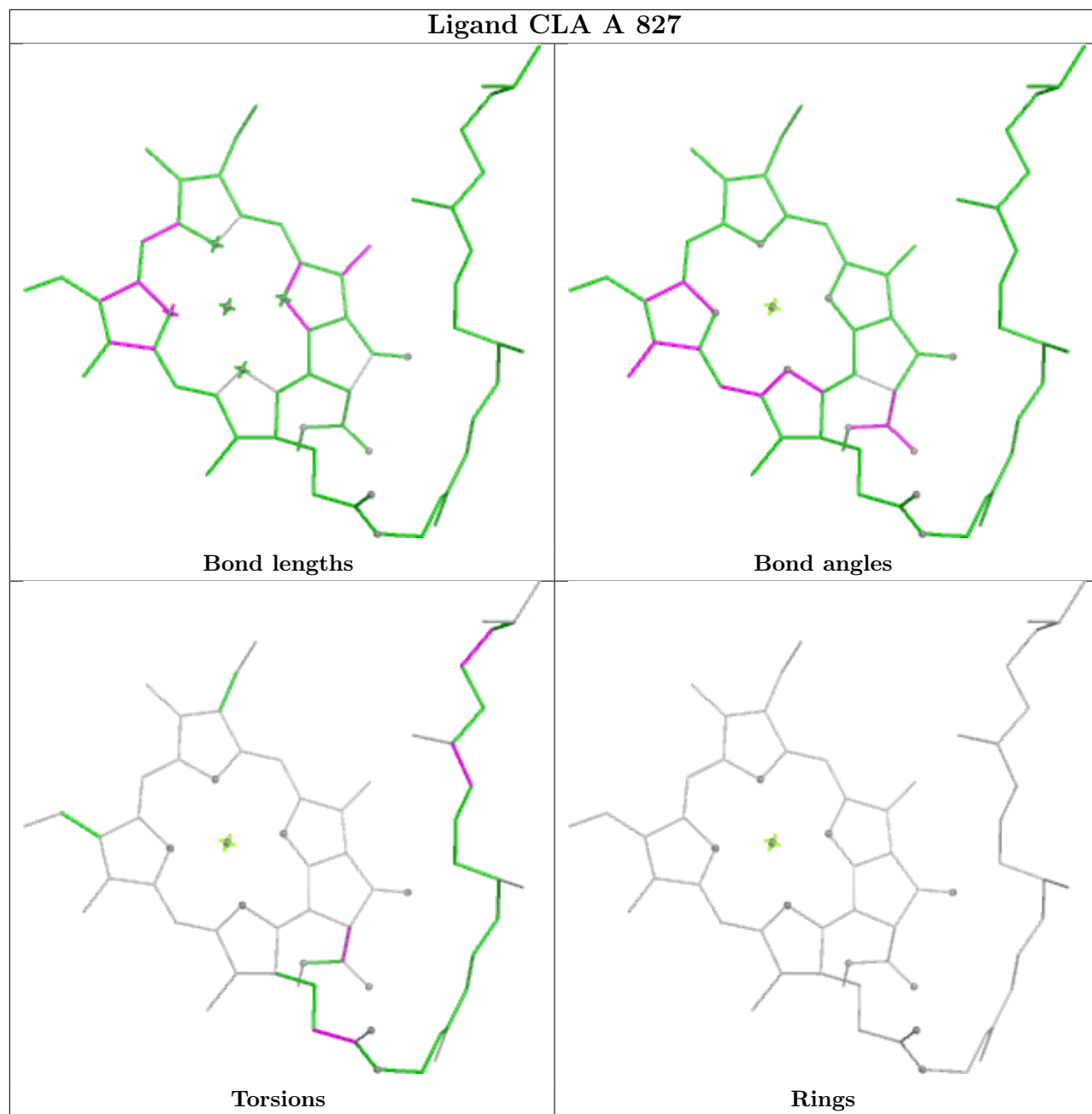


Rings

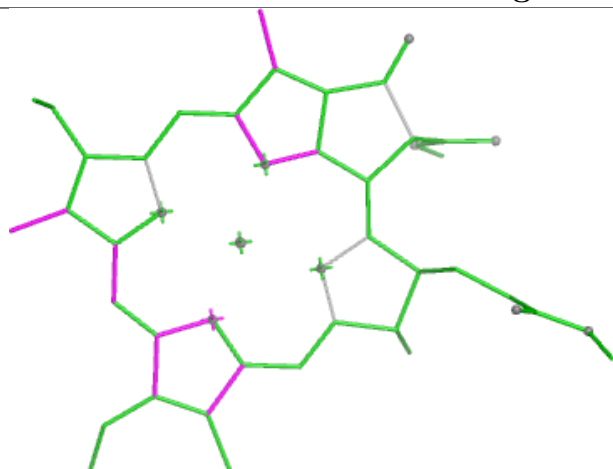




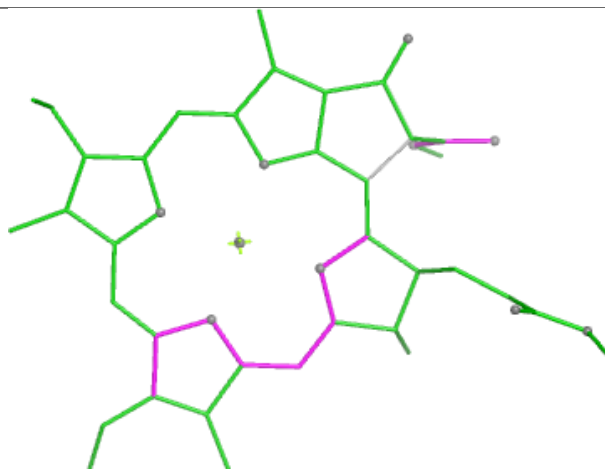




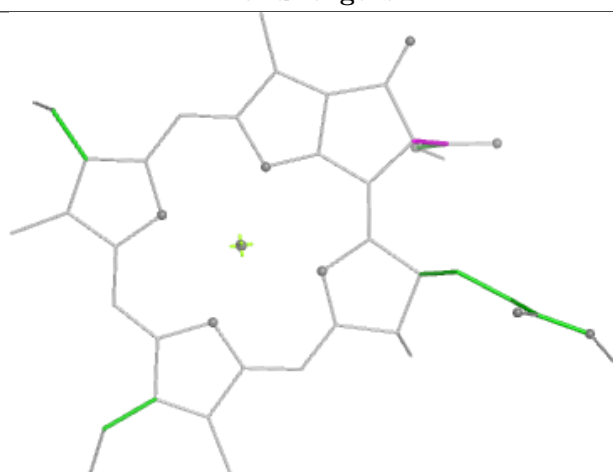
Ligand CLA K 204



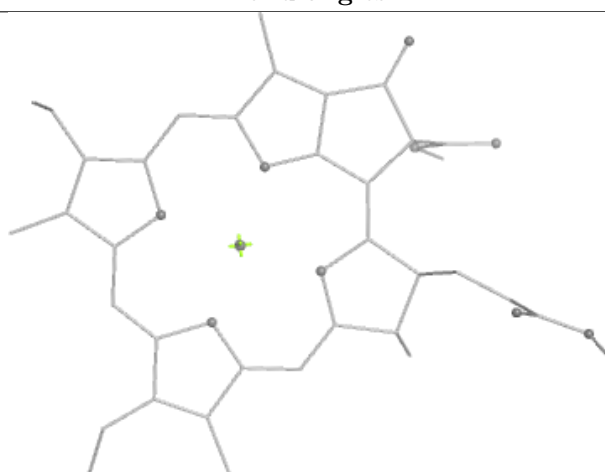
Bond lengths



Bond angles

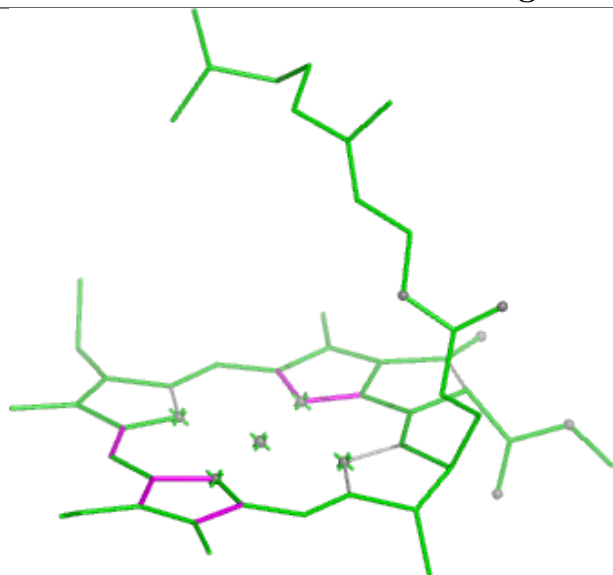


Torsions

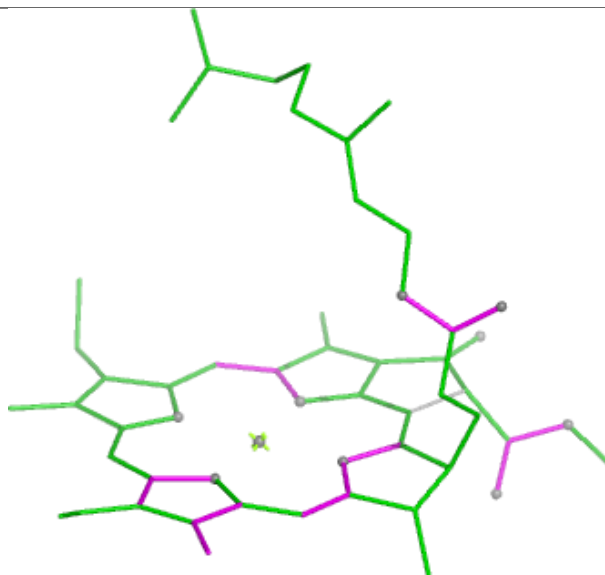


Rings

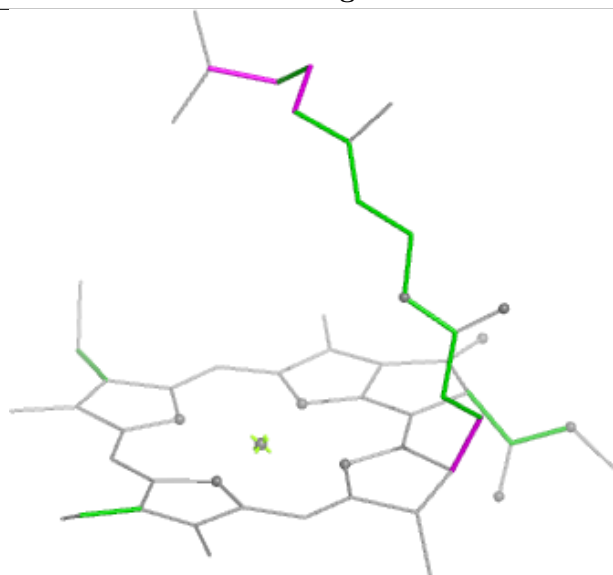
Ligand CLA 6 309



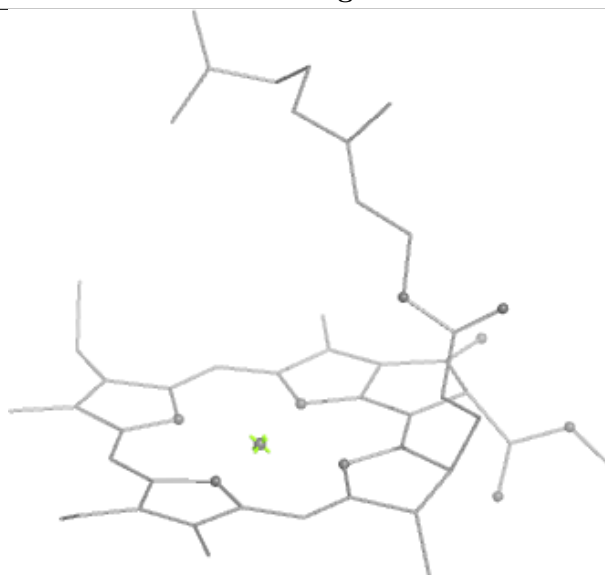
Bond lengths



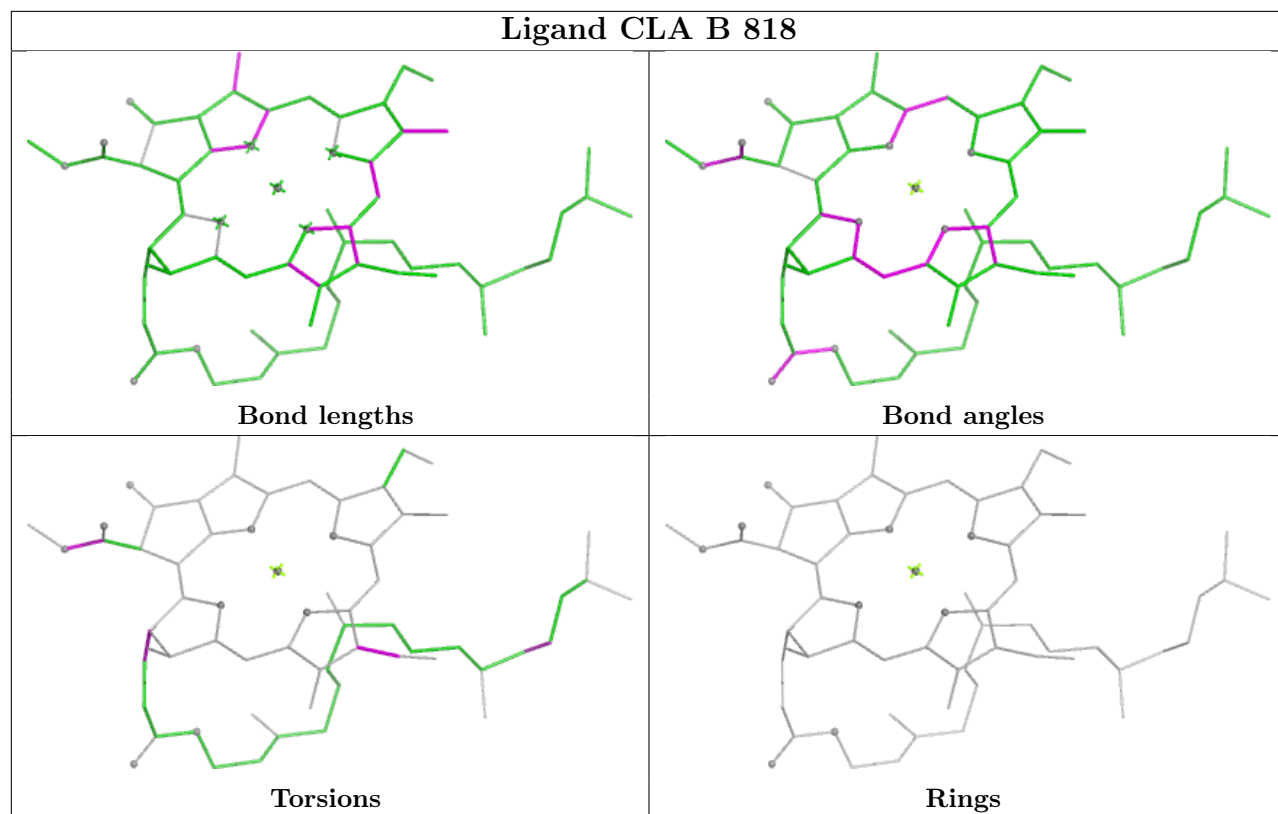
Bond angles



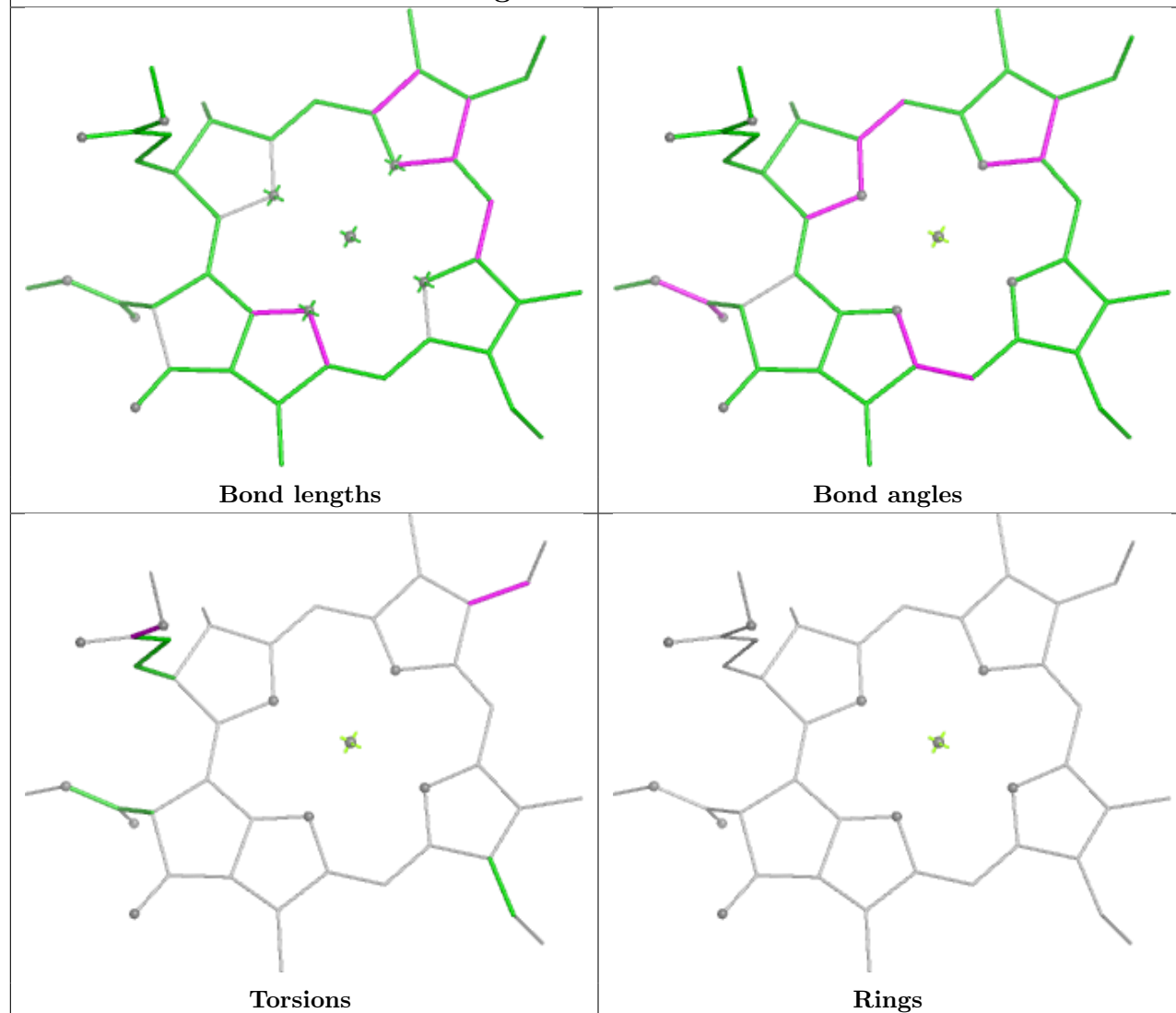
Torsions



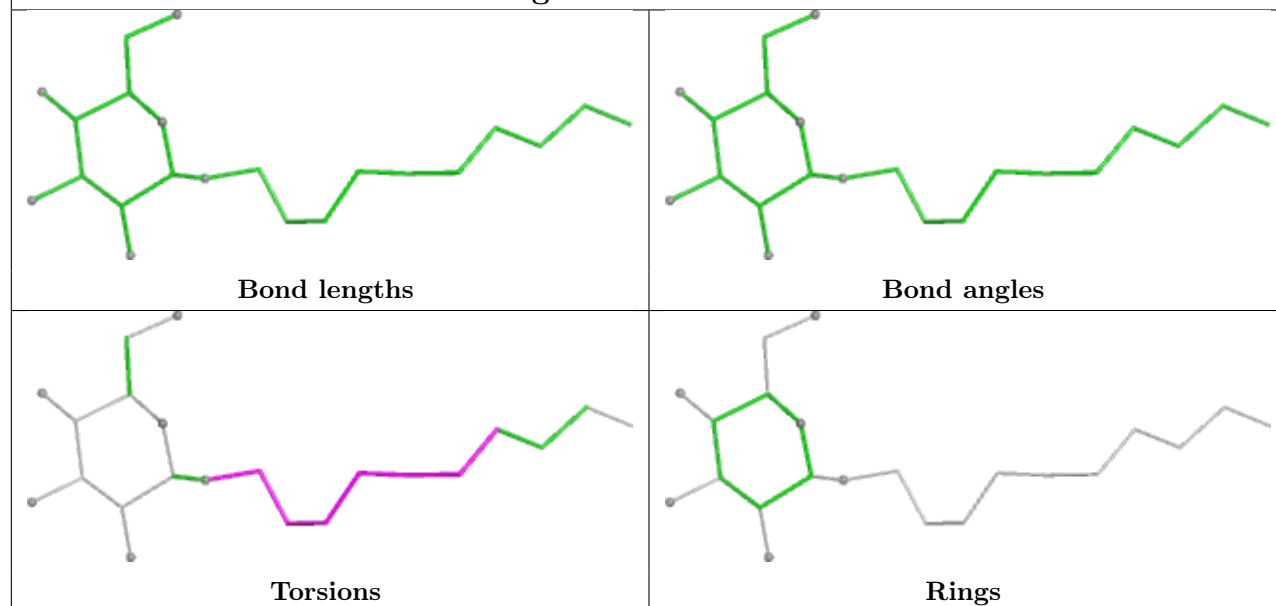
Rings



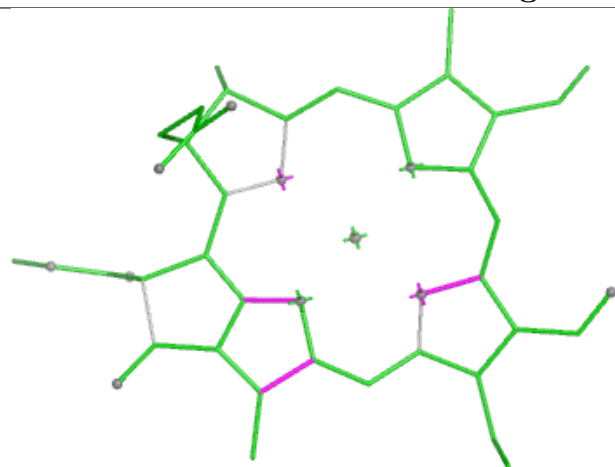
Ligand CLA 1 314



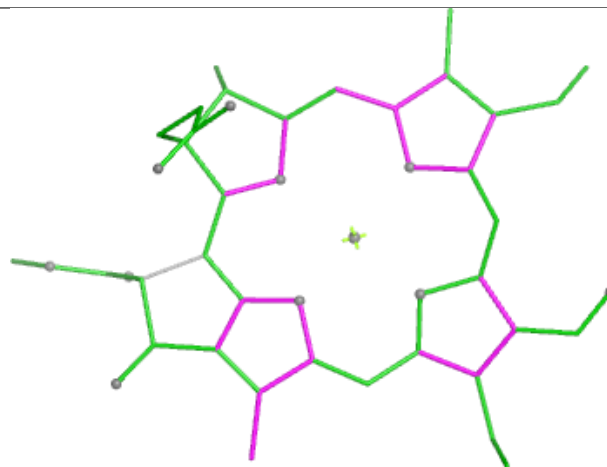
Ligand LMU 7 620



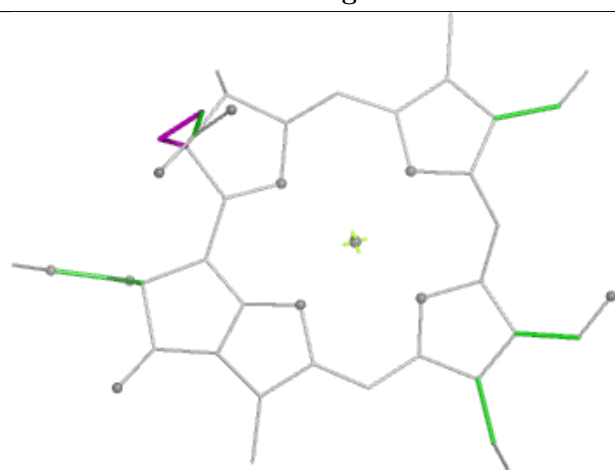
Ligand CHL 7 606



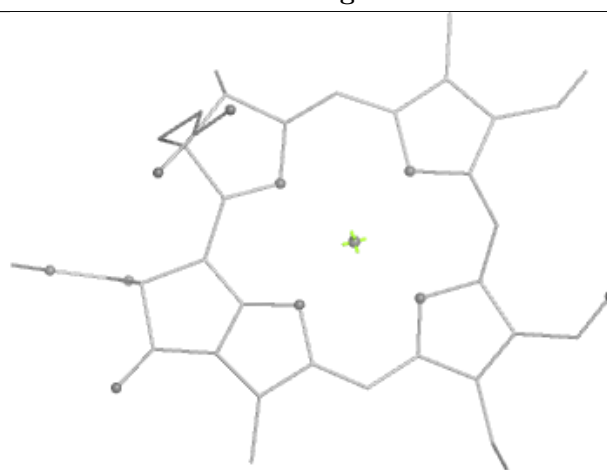
Bond lengths



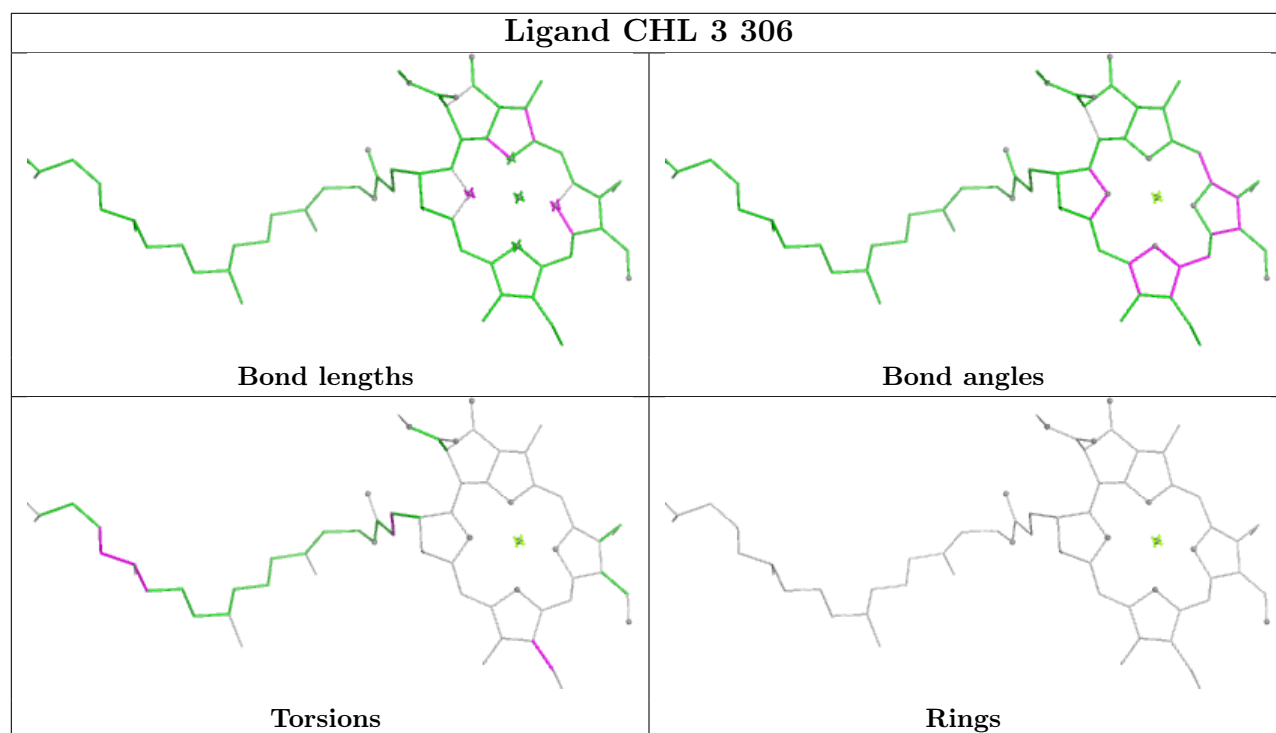
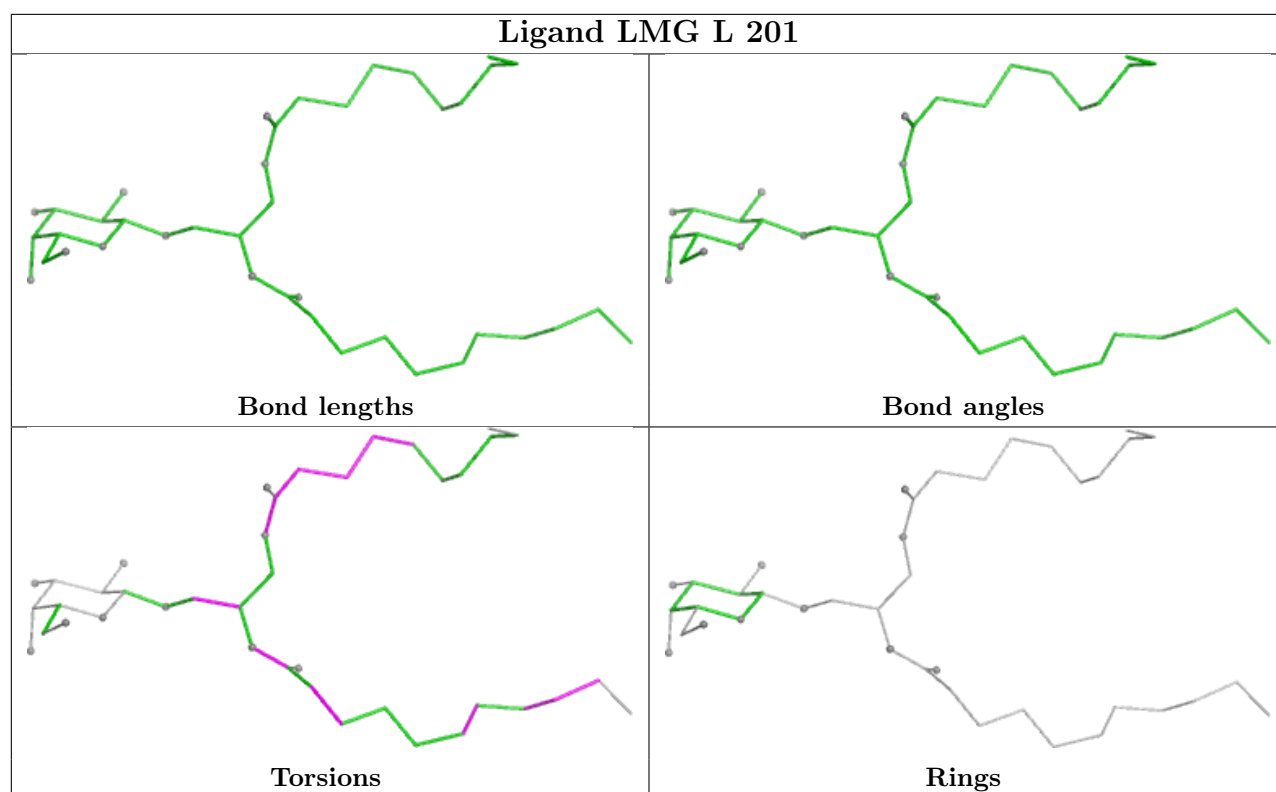
Bond angles

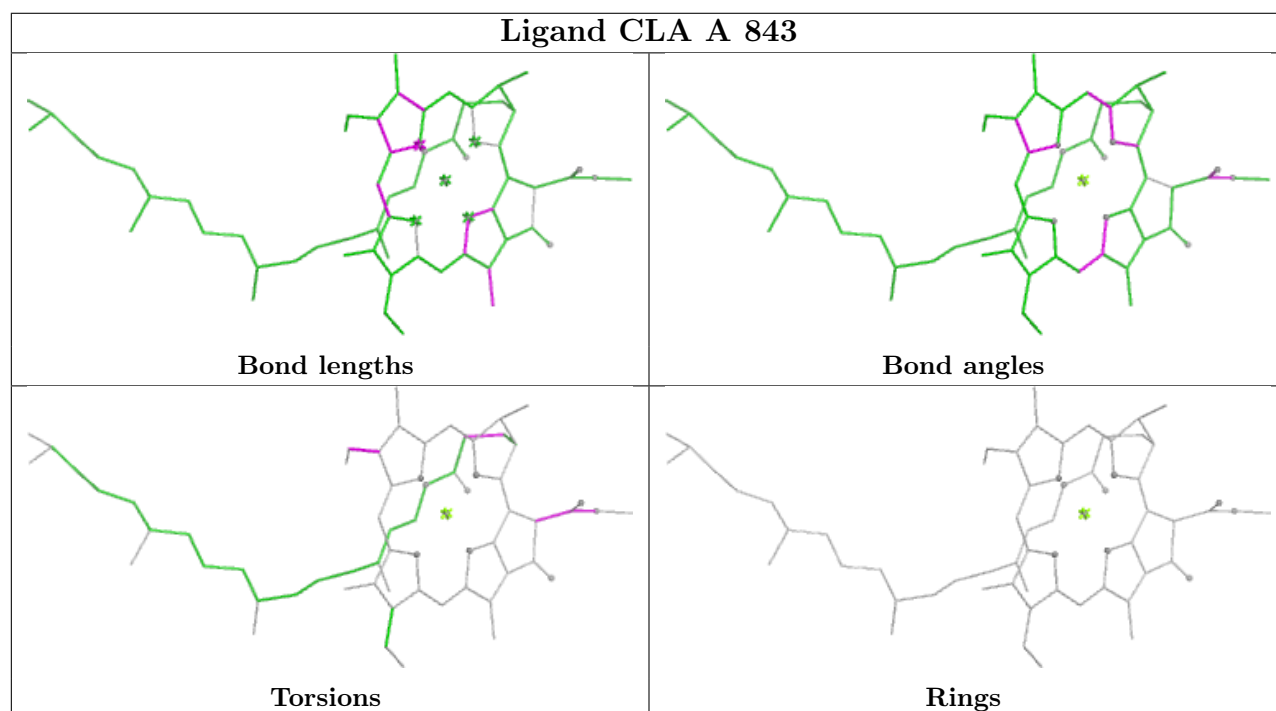
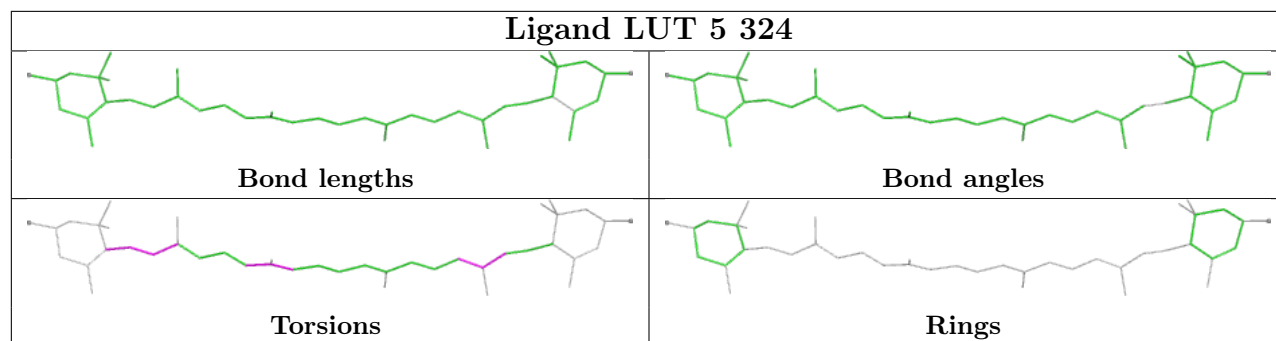


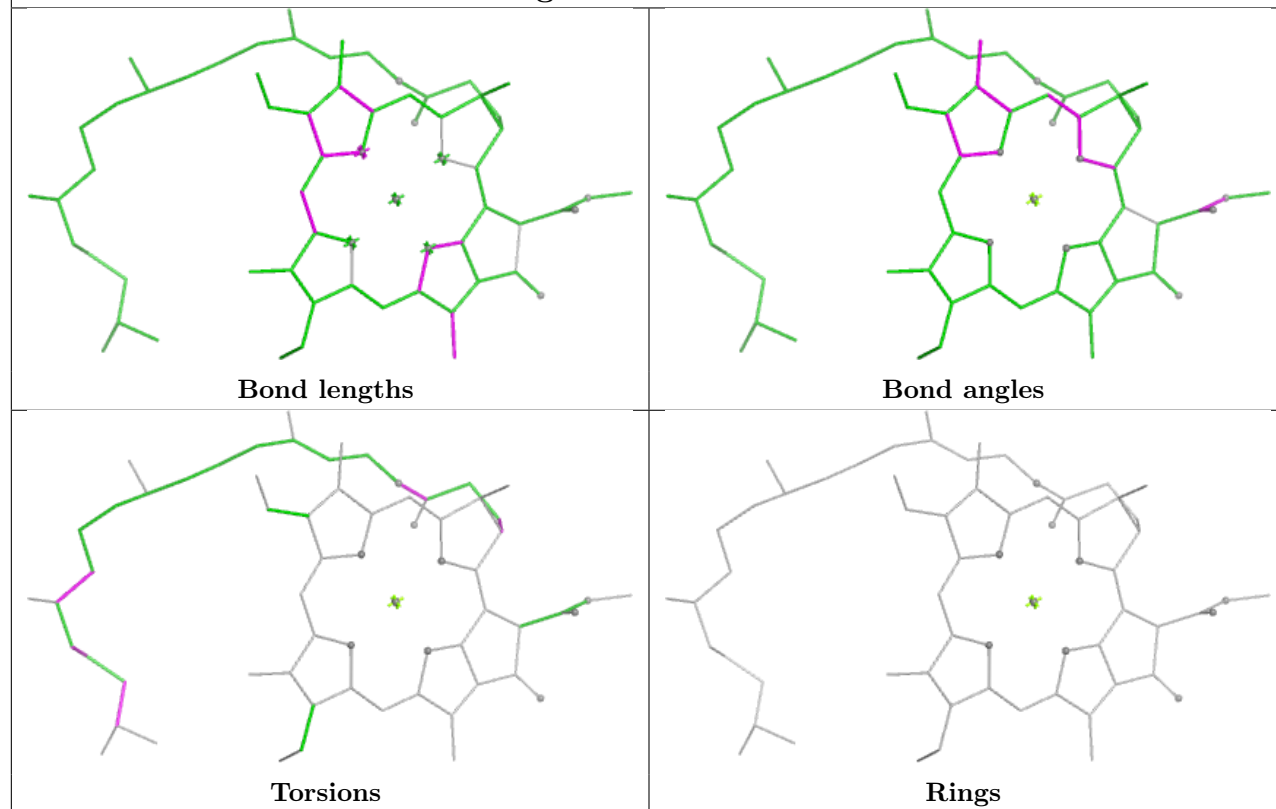
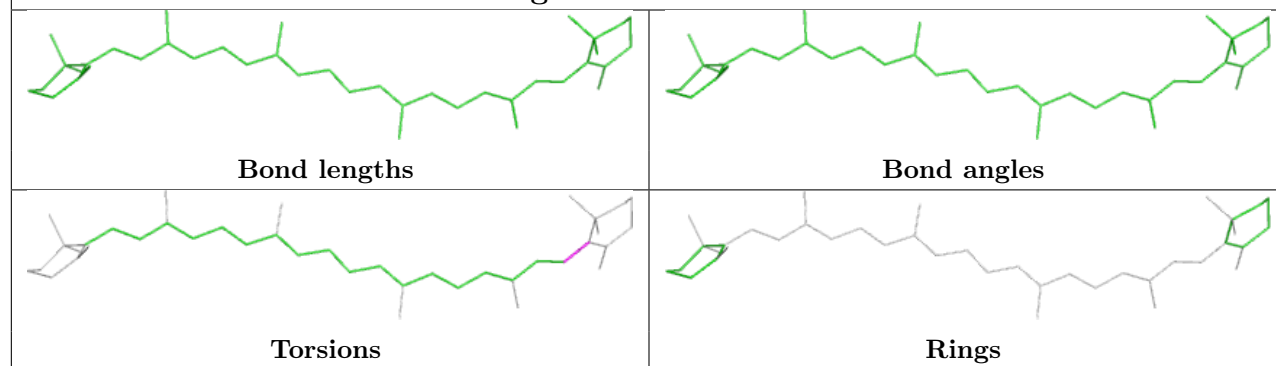
Torsions



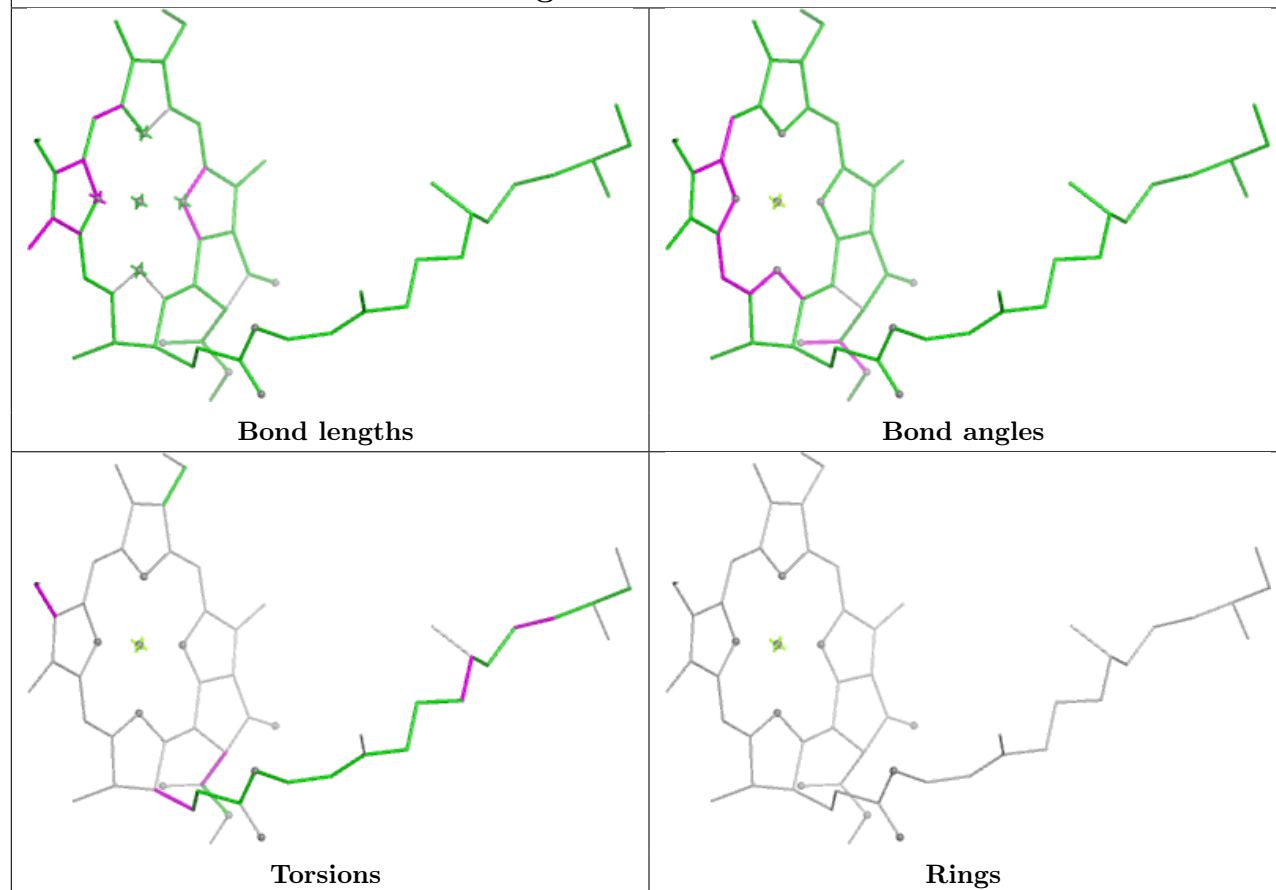
Rings



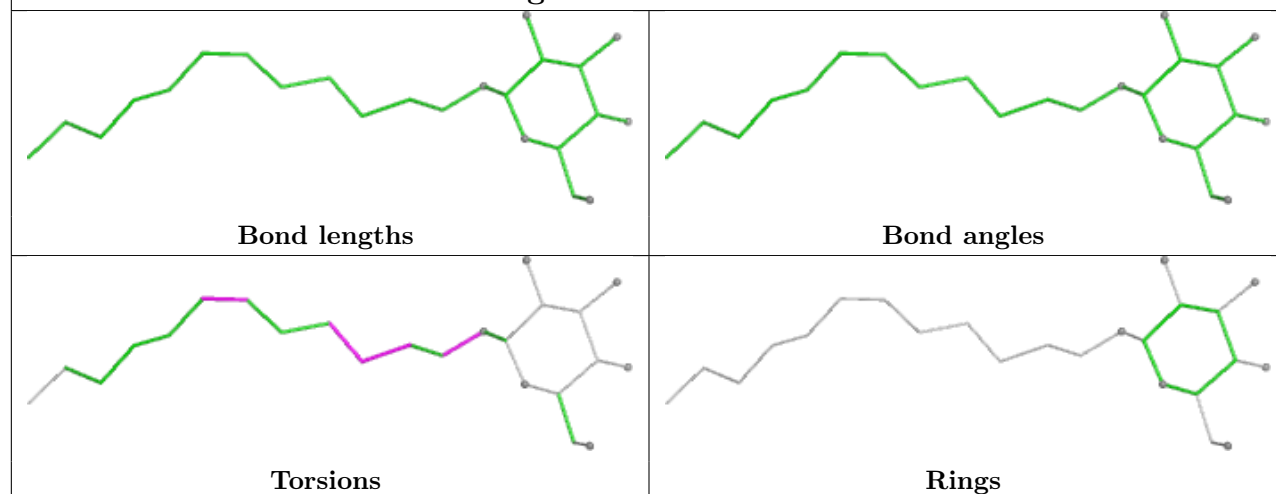


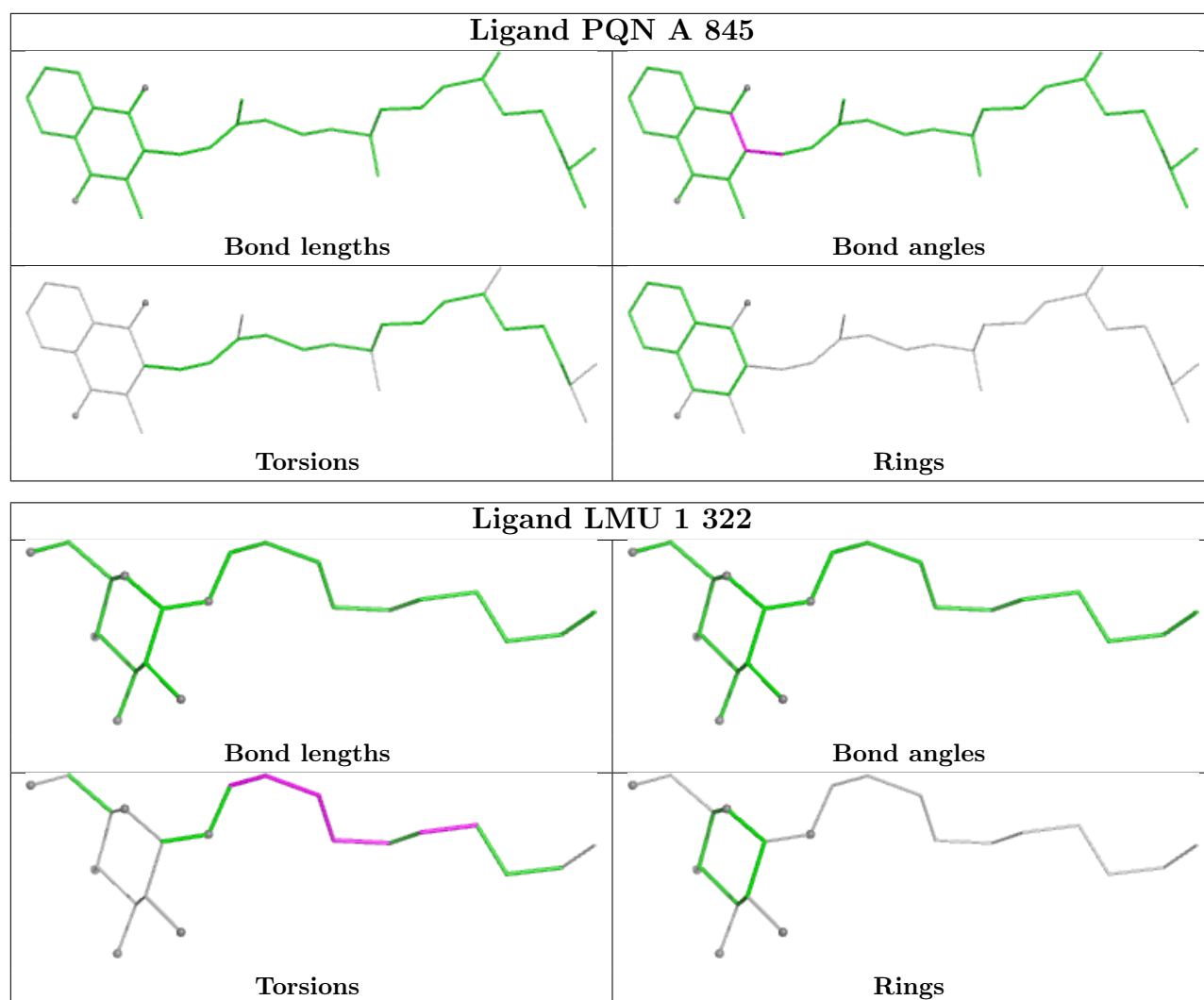
Ligand CLA 7 609**Ligand BCR B 847**

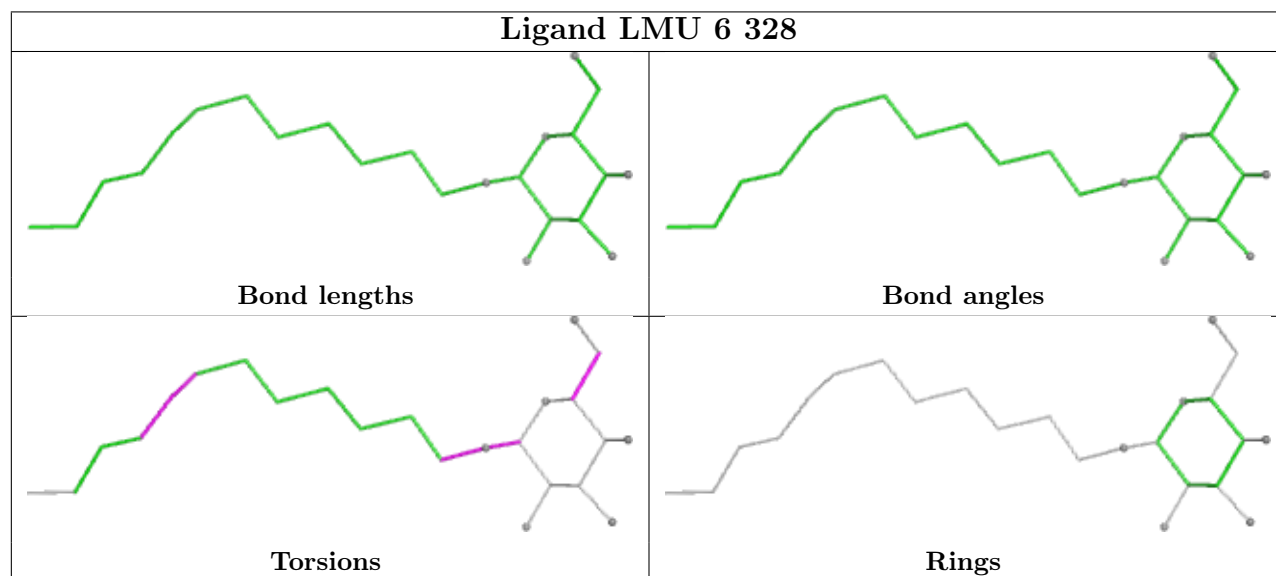
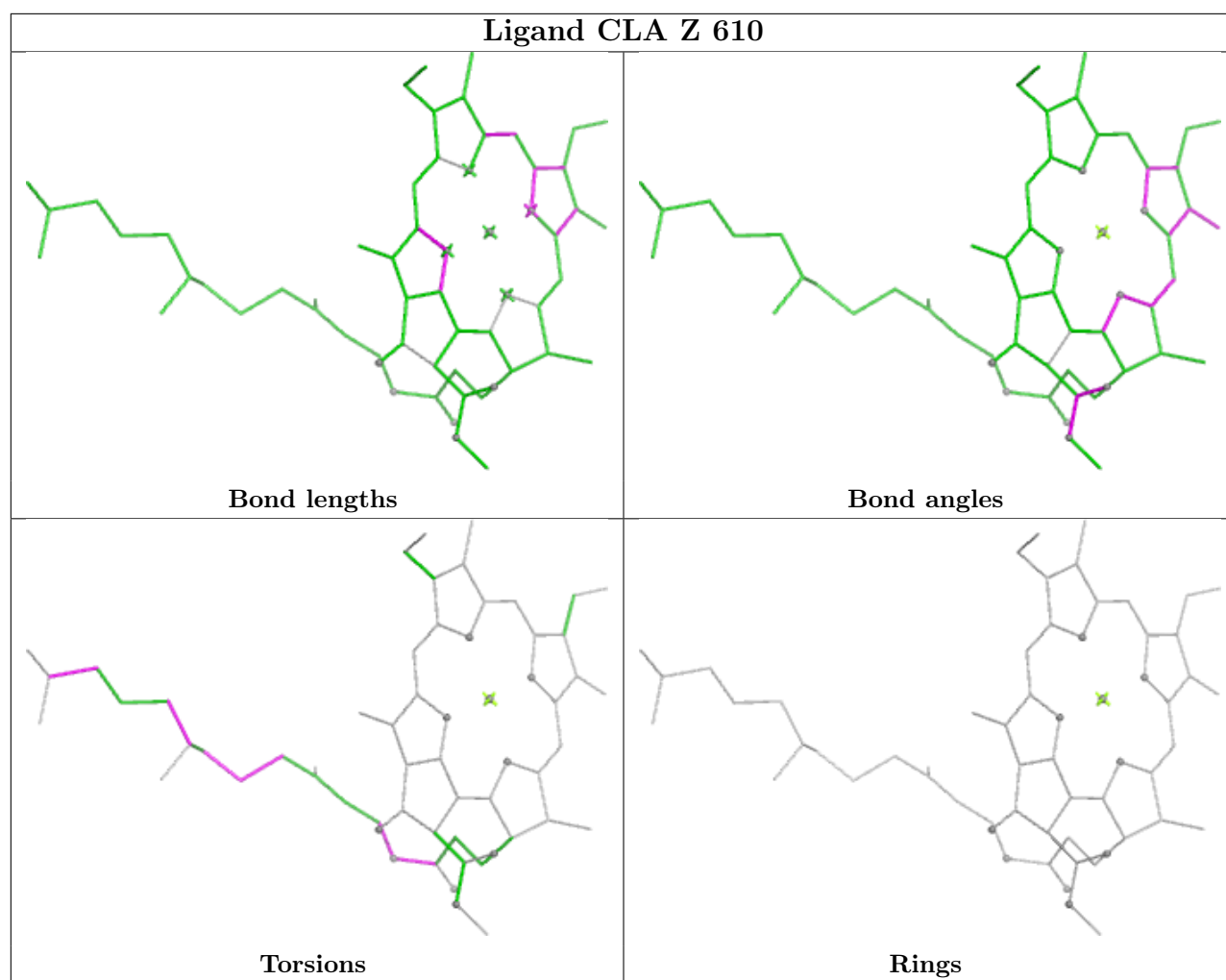
Ligand CLA 3 307

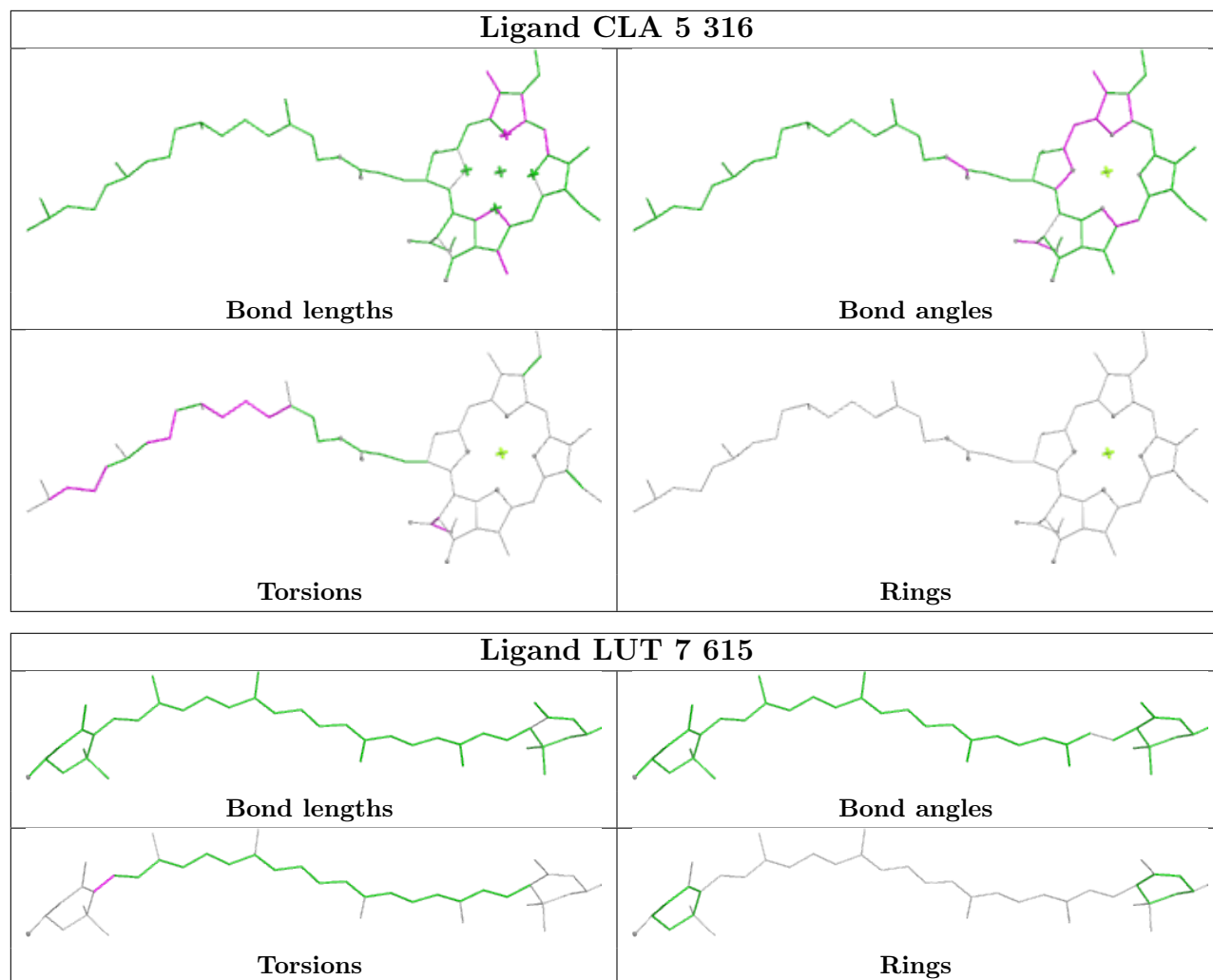


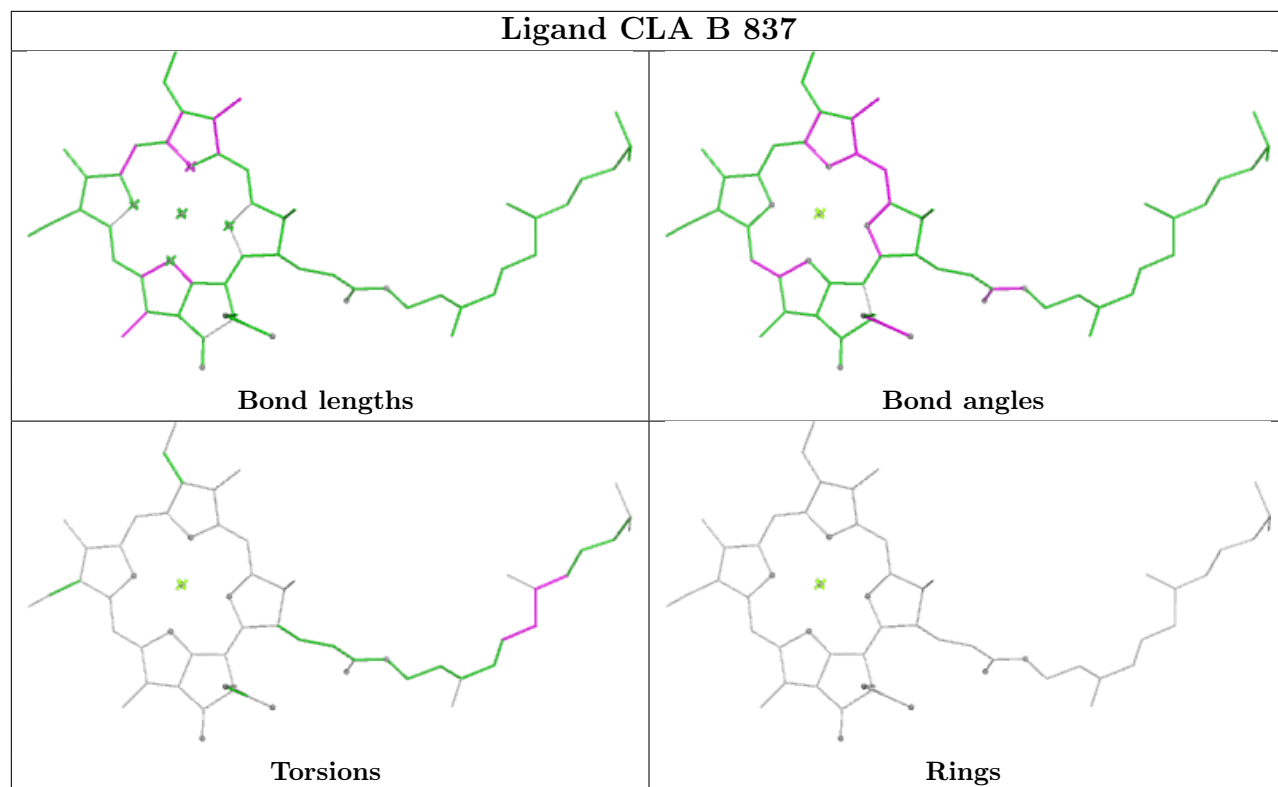
Ligand LMU A 857



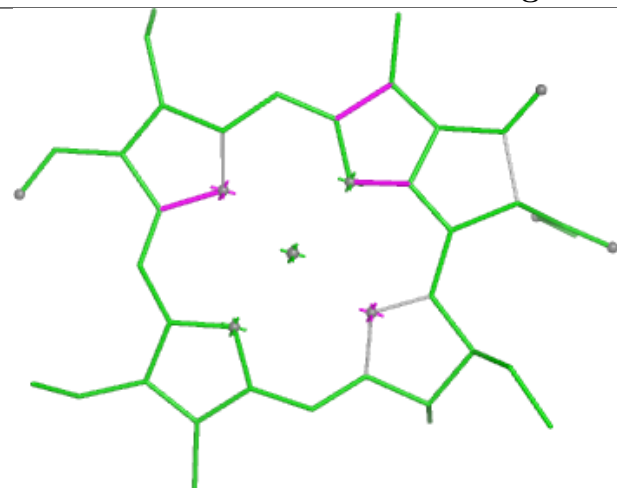




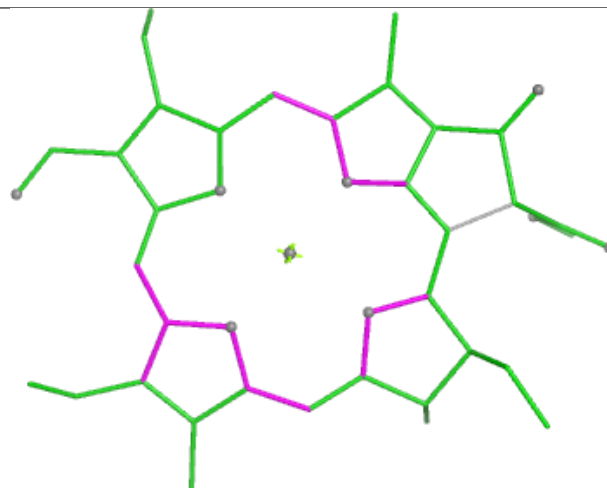




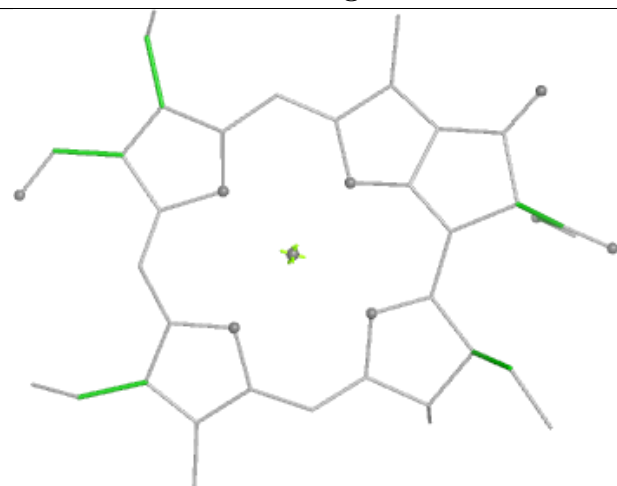
Ligand CHL 6 317



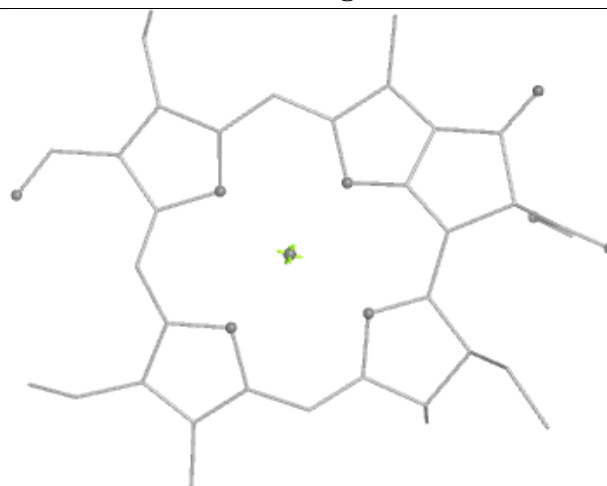
Bond lengths



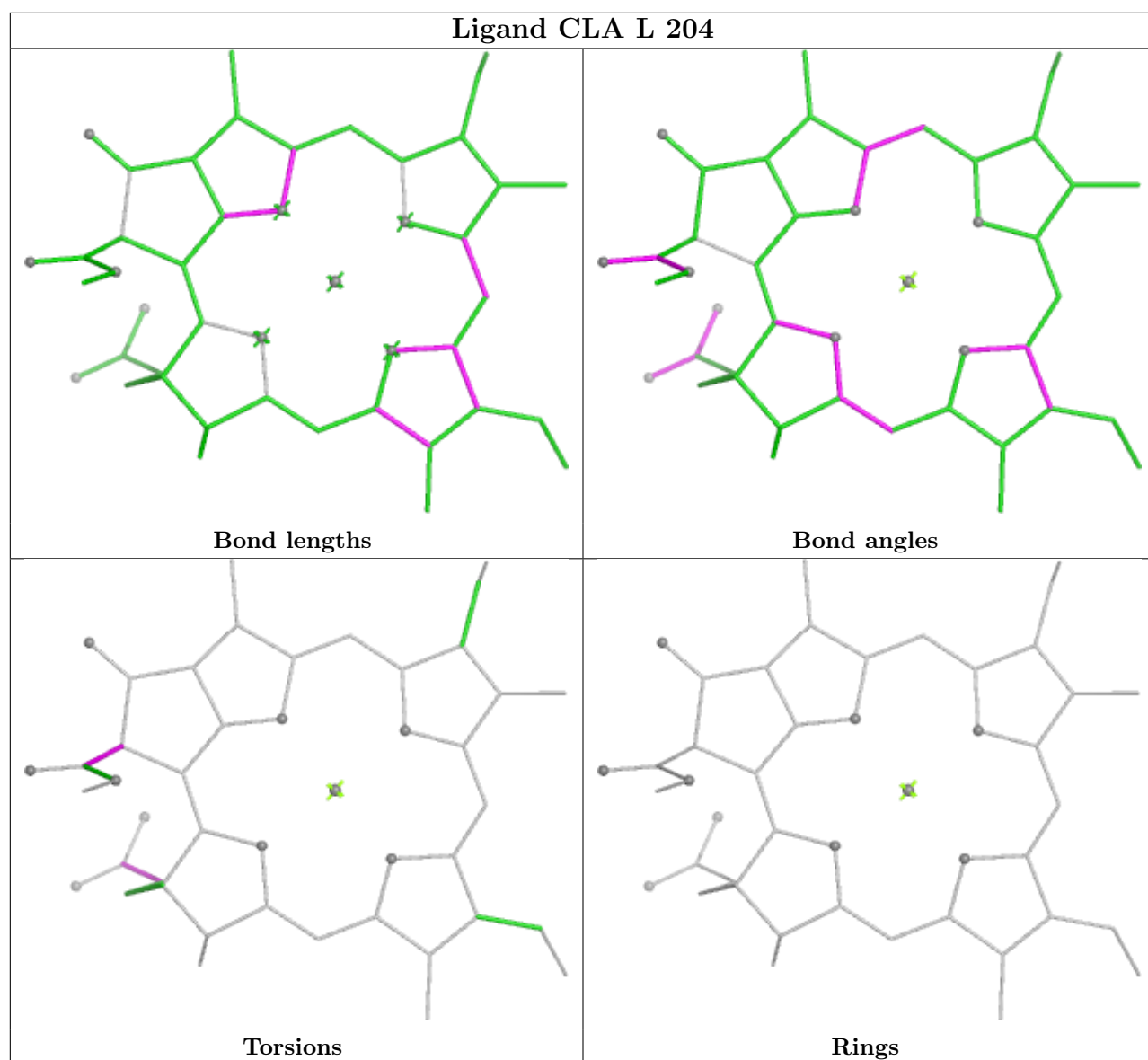
Bond angles



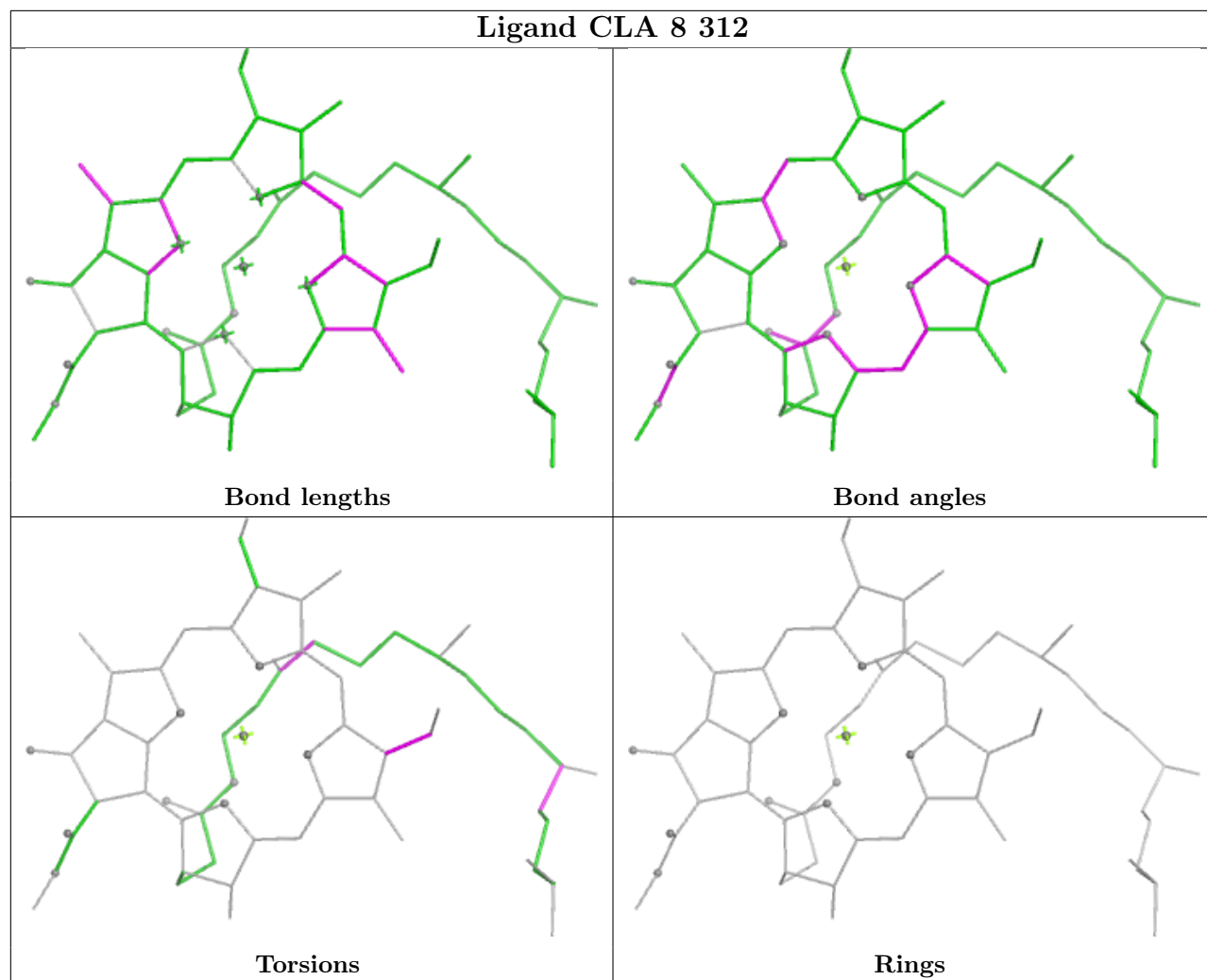
Torsions

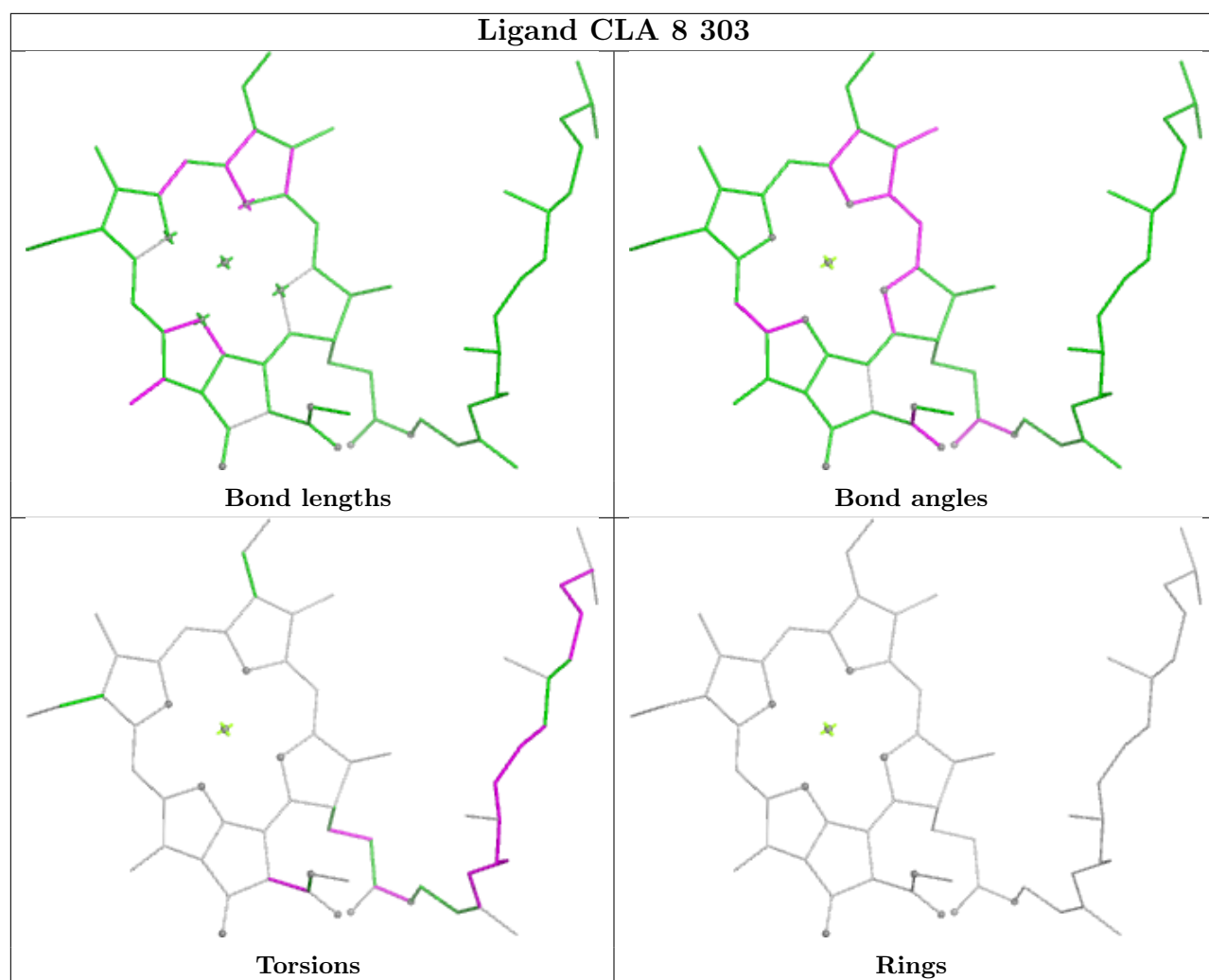


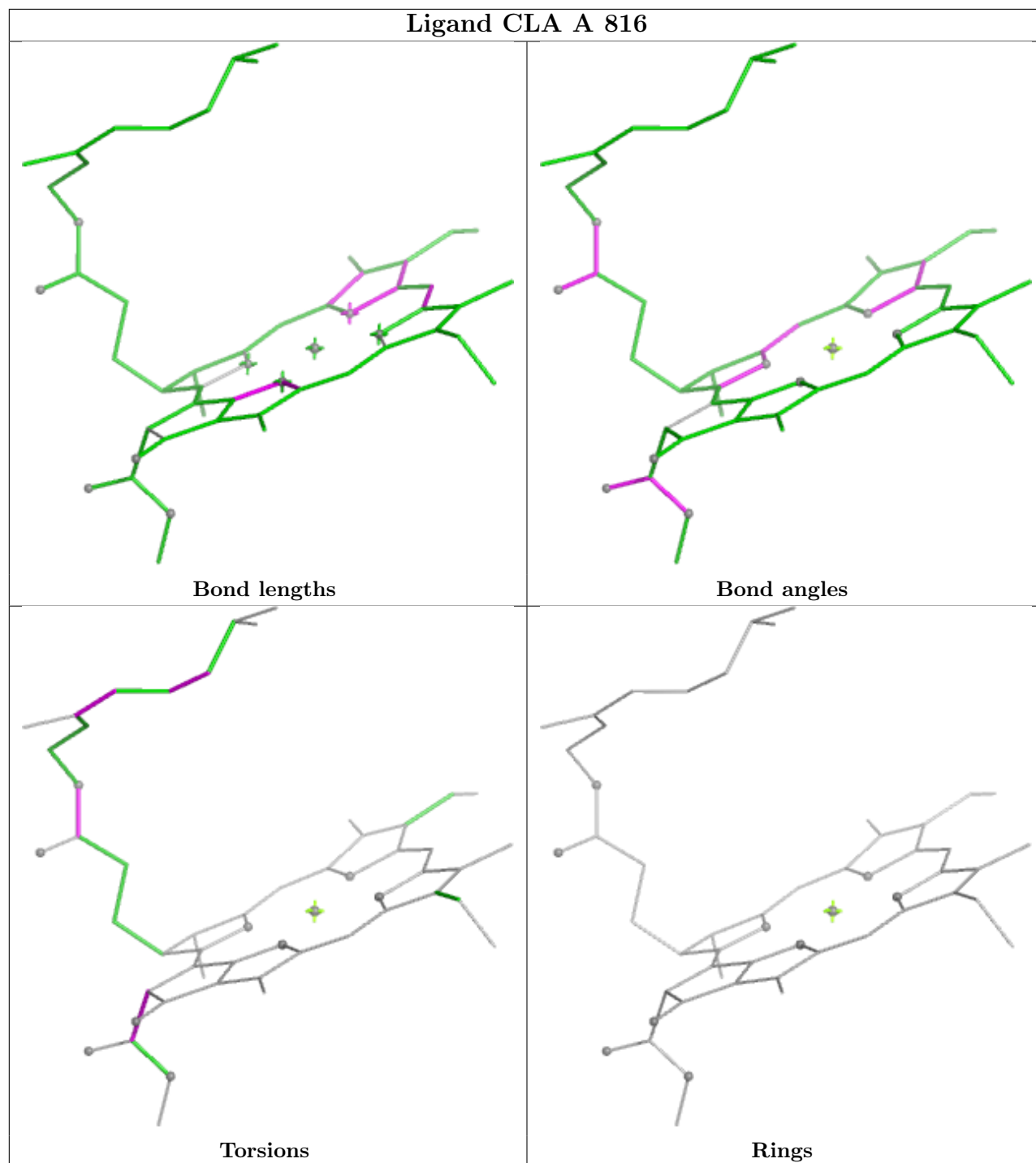
Rings

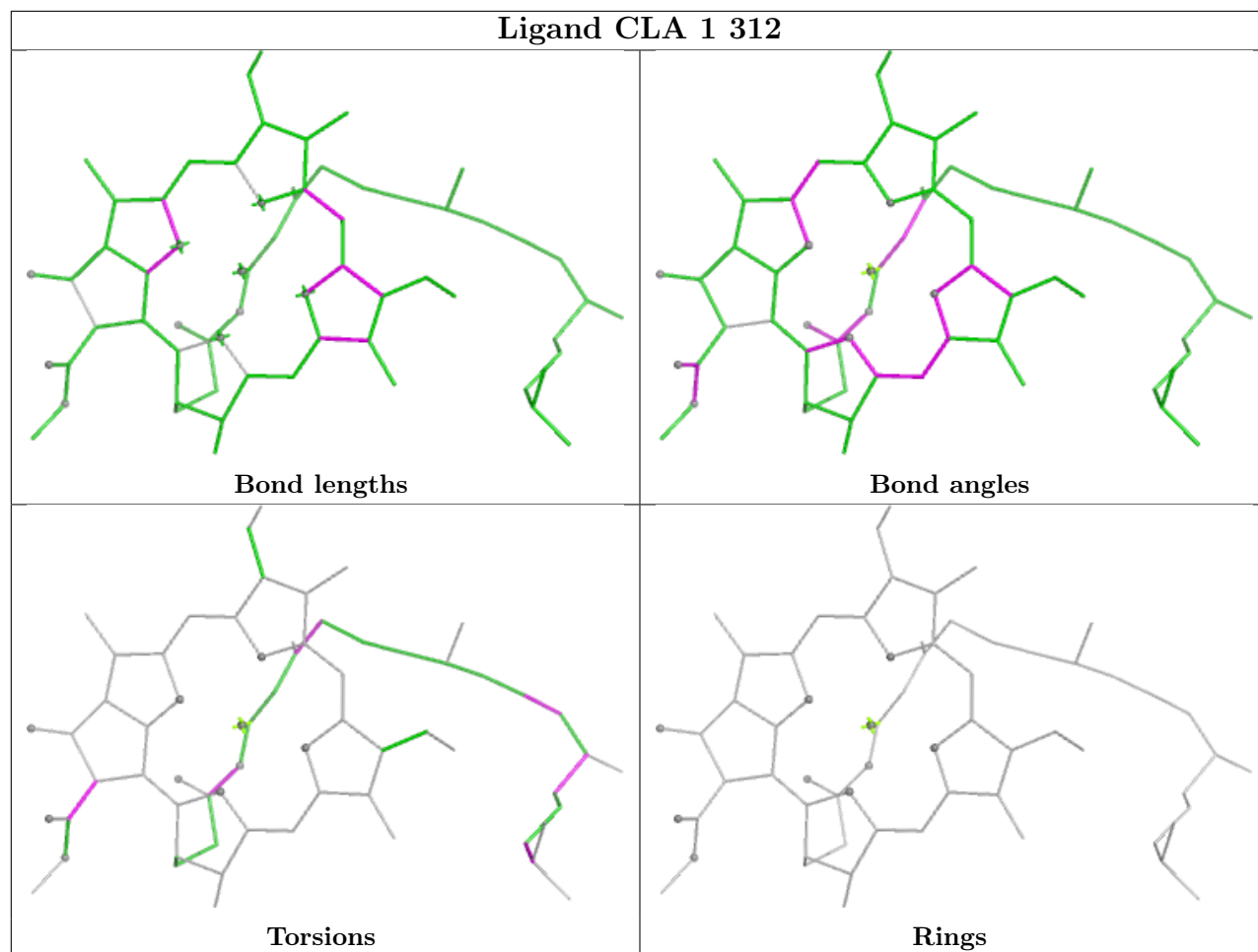
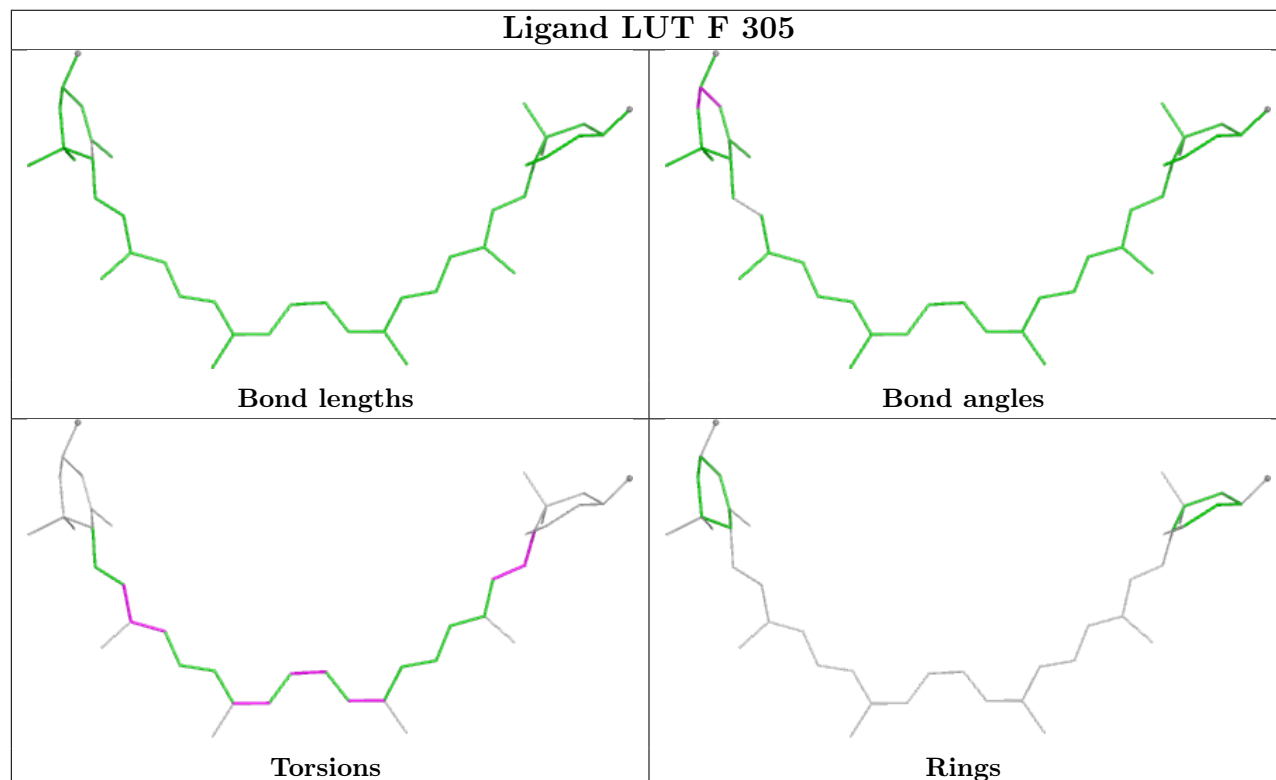


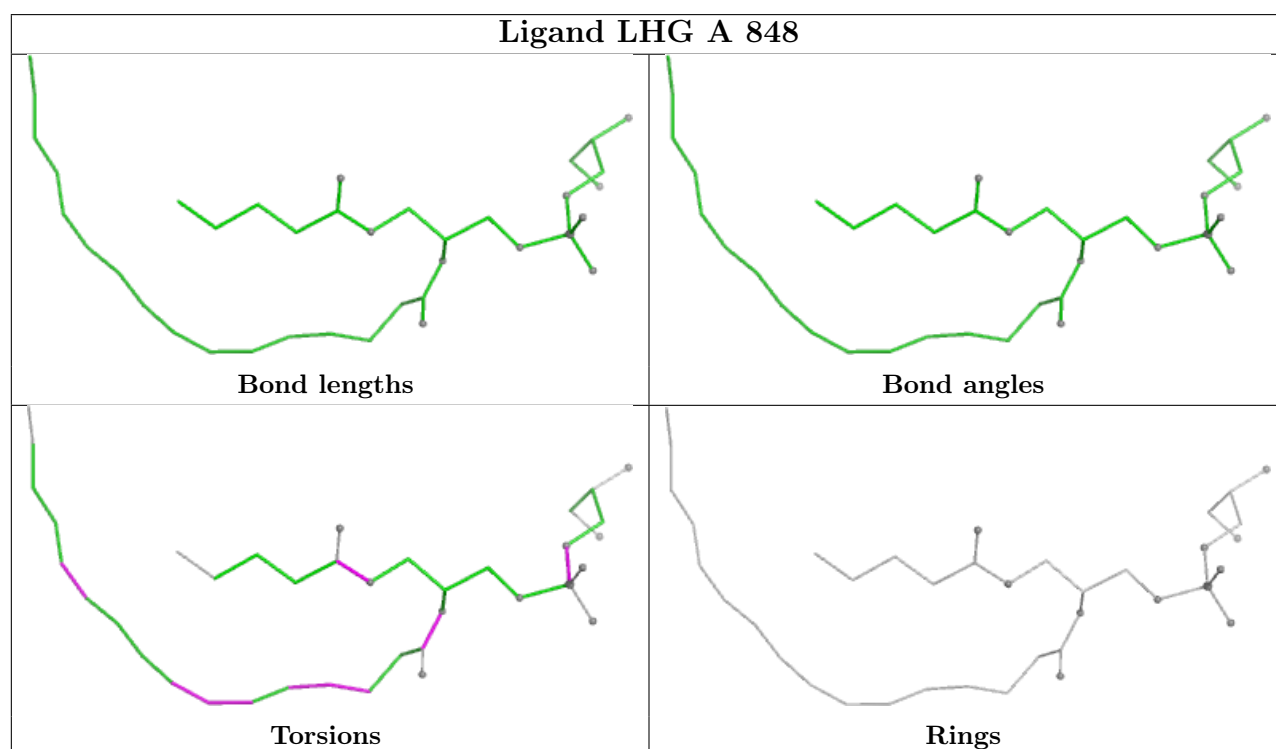
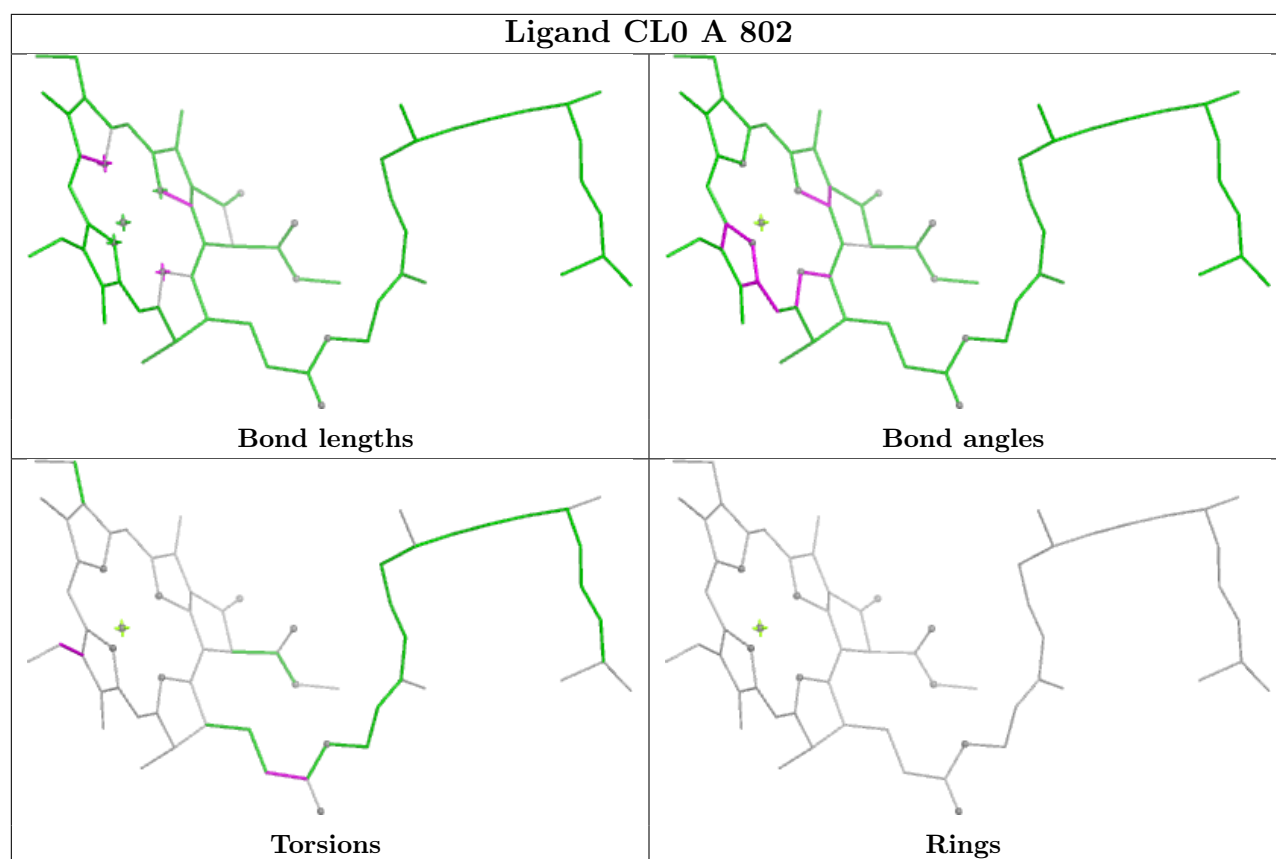
Ligand CLA 8 312

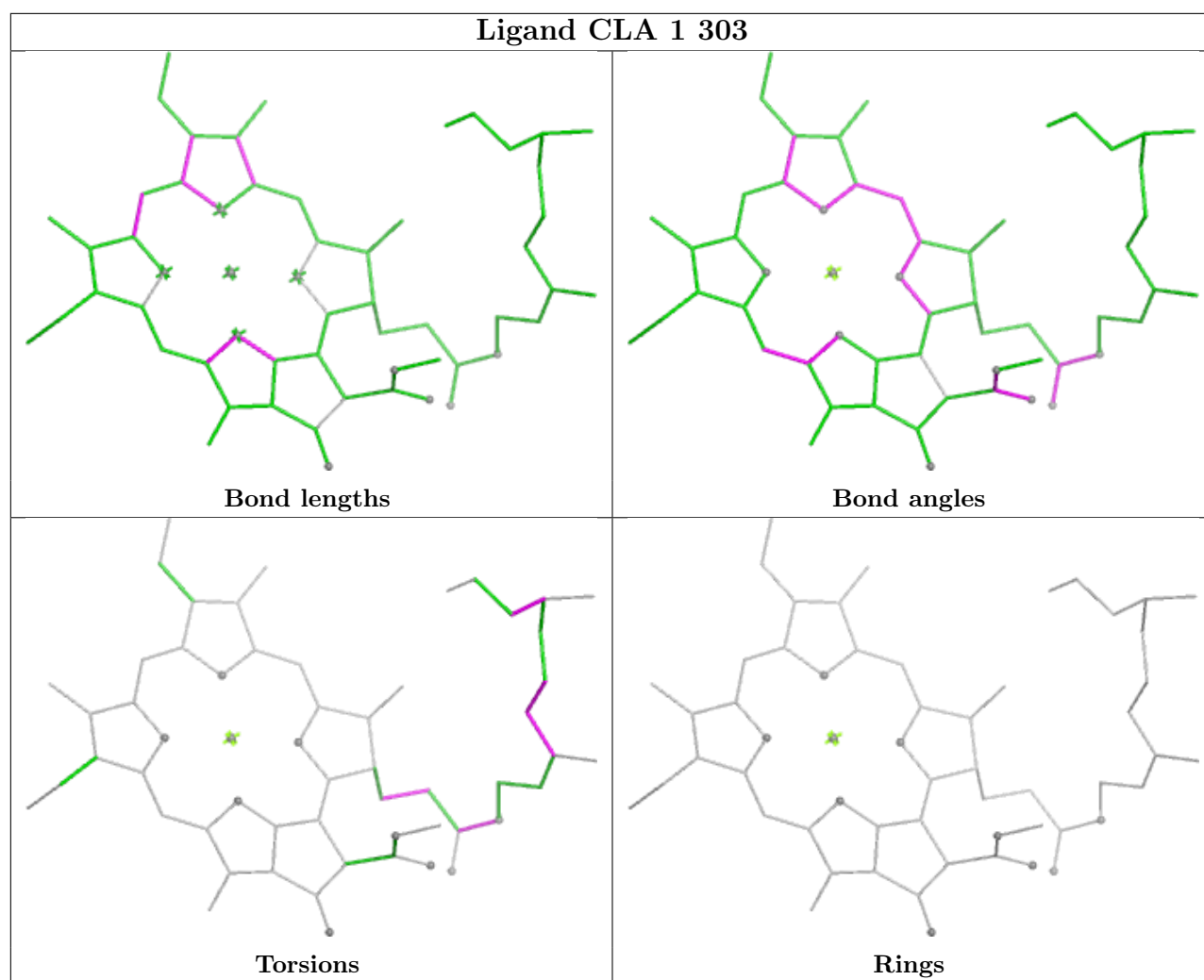


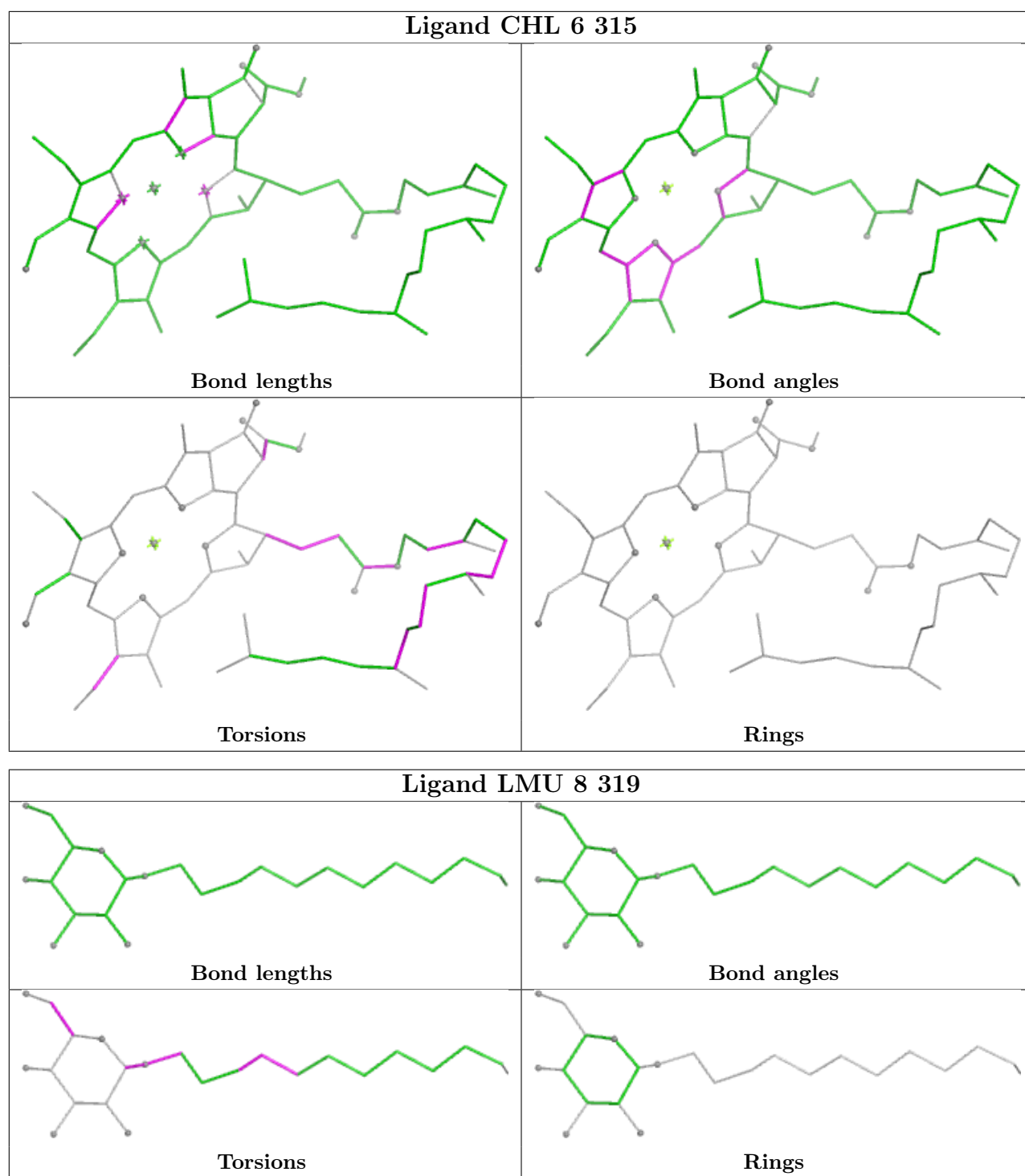


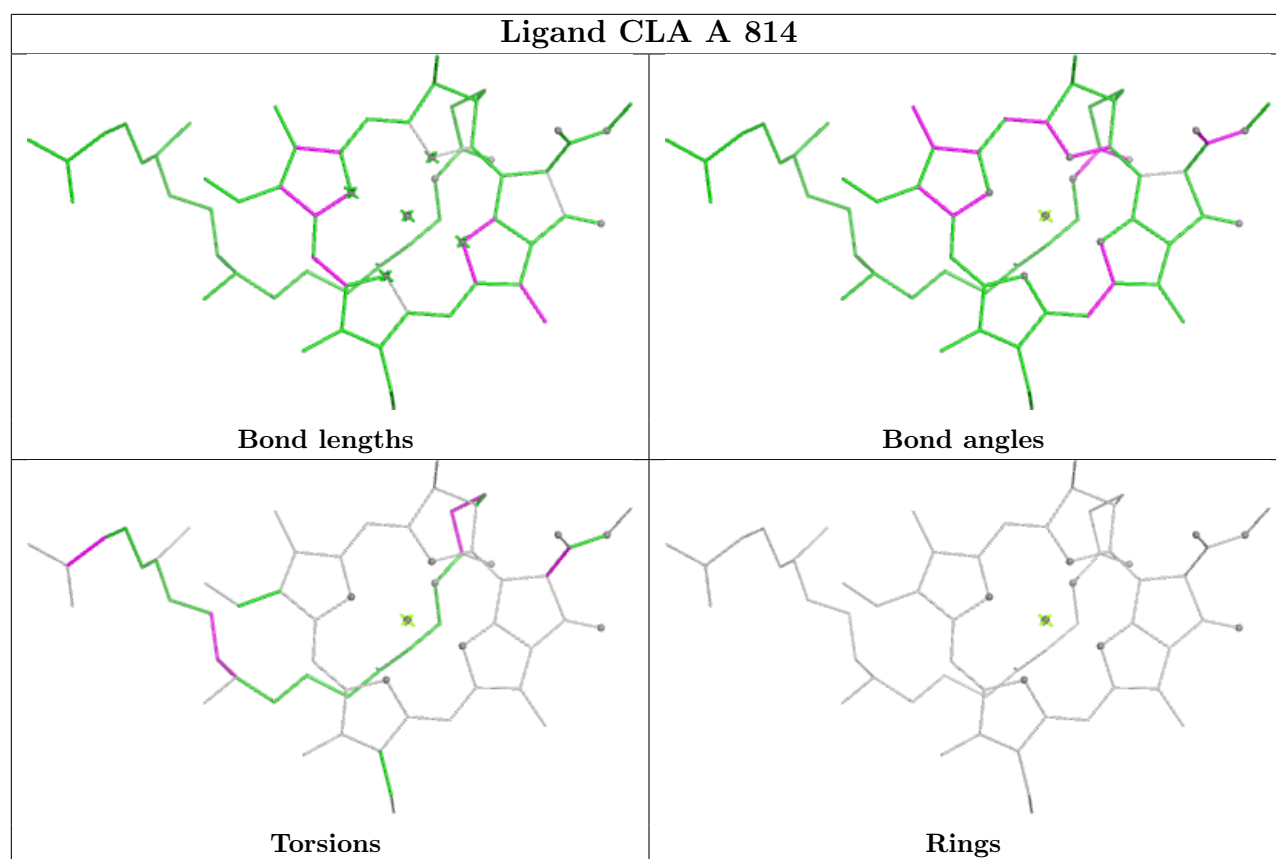


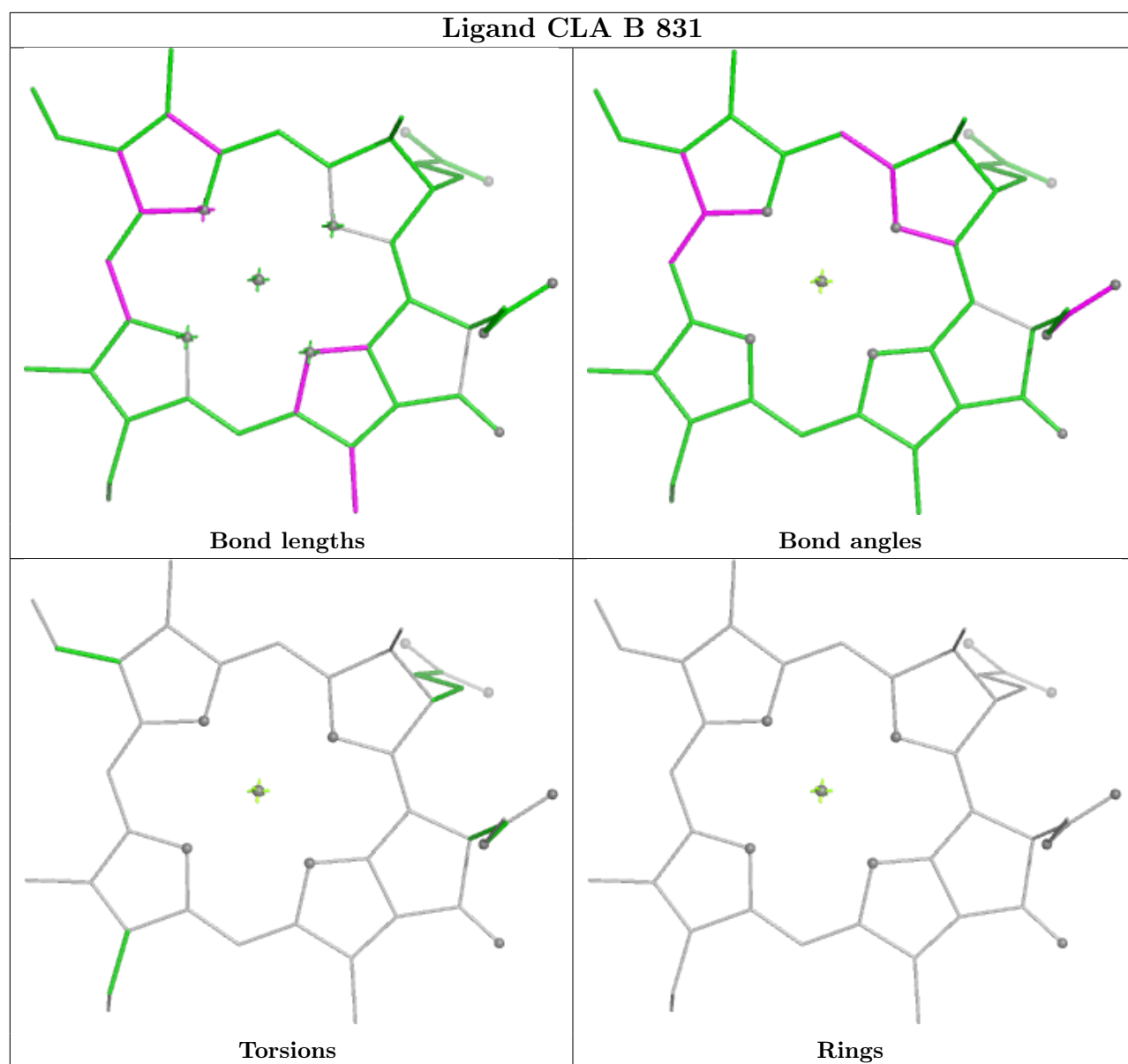
Ligand CLA 1 312**Ligand LUT F 305**

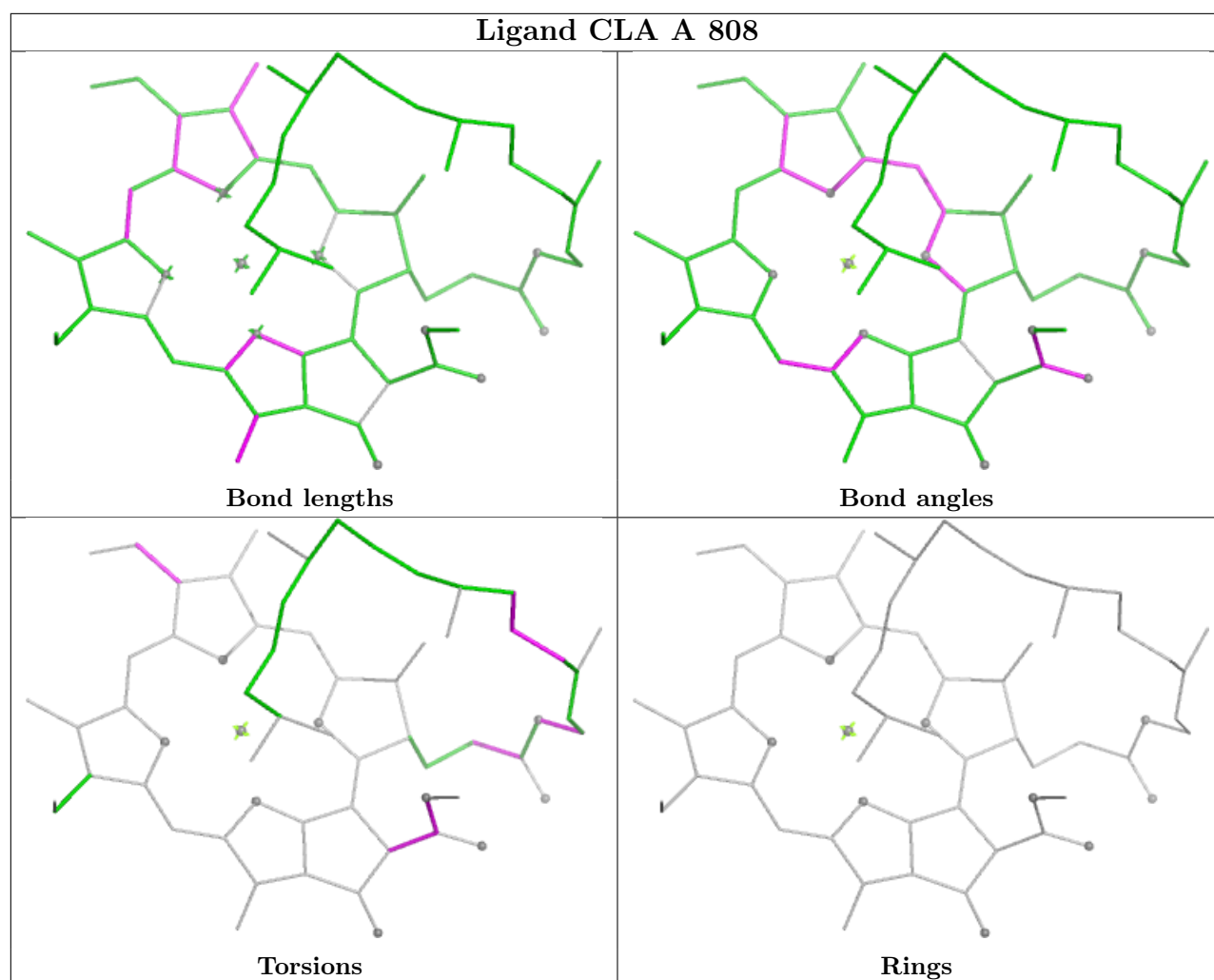


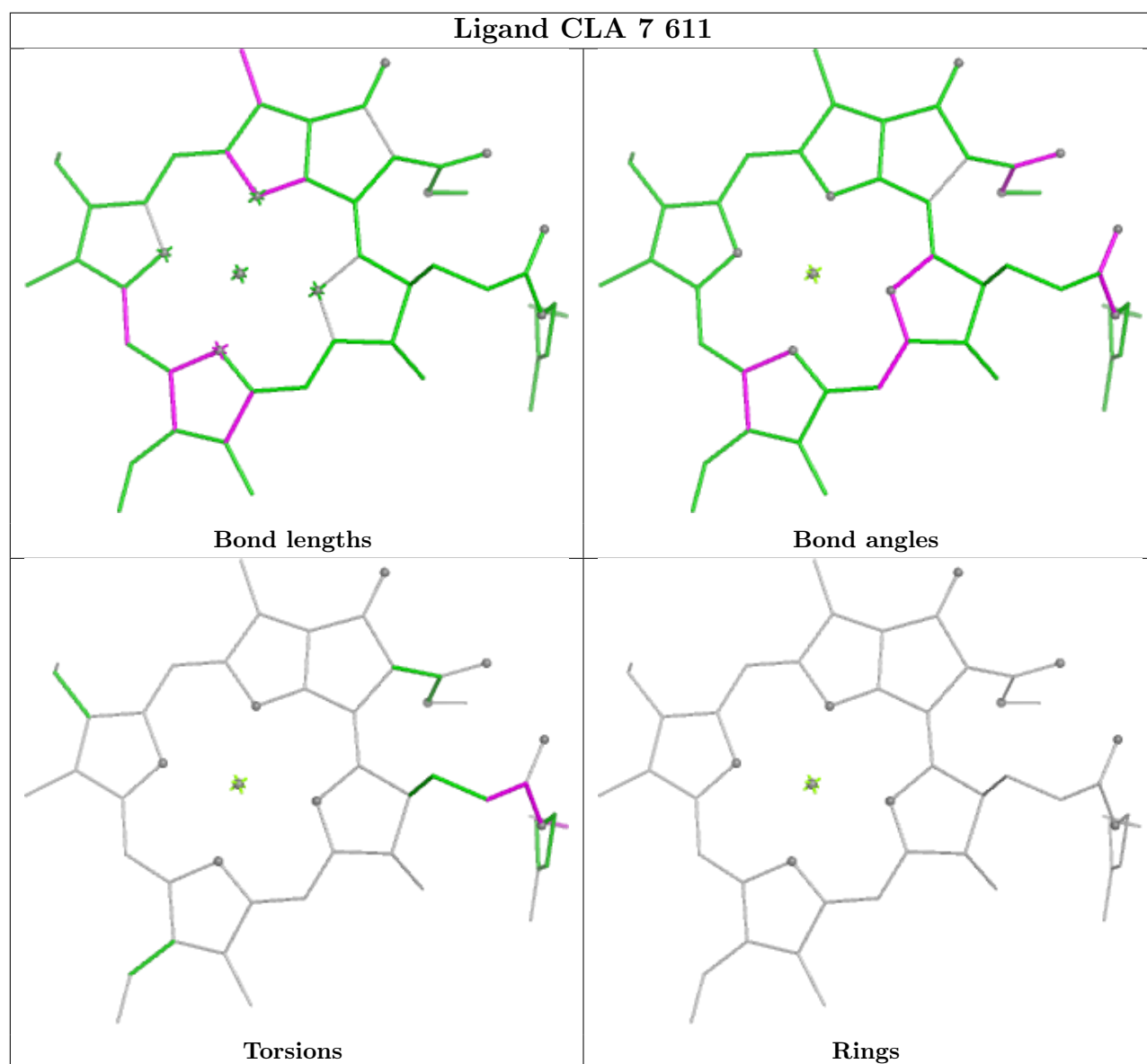


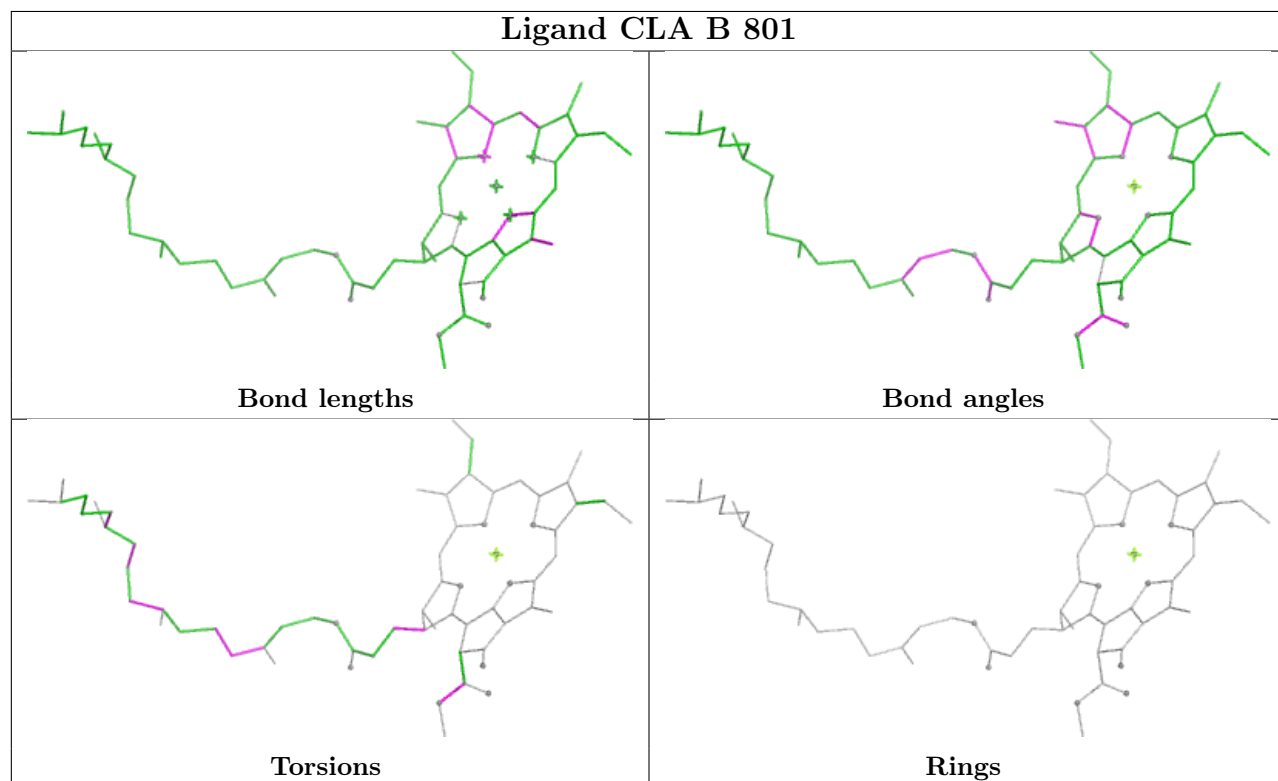
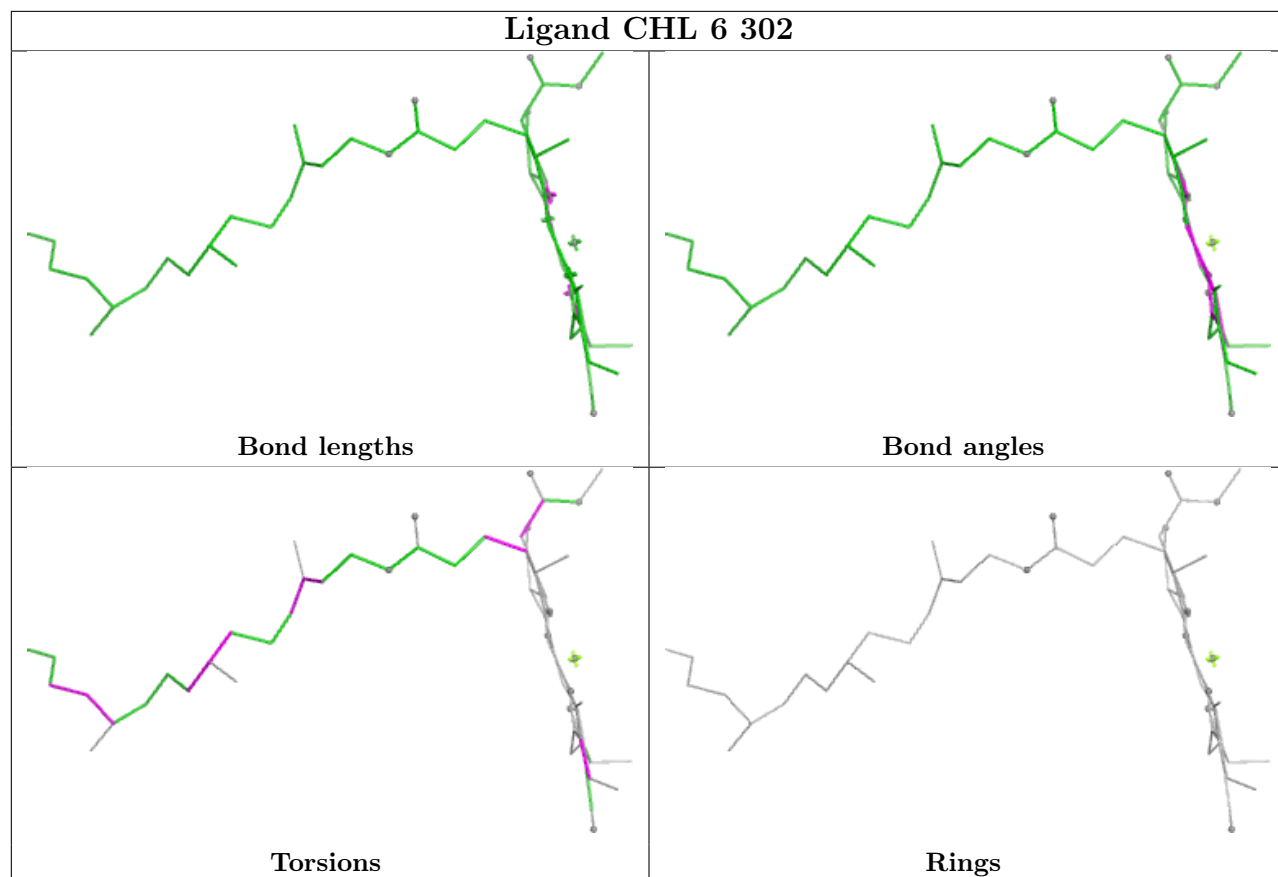


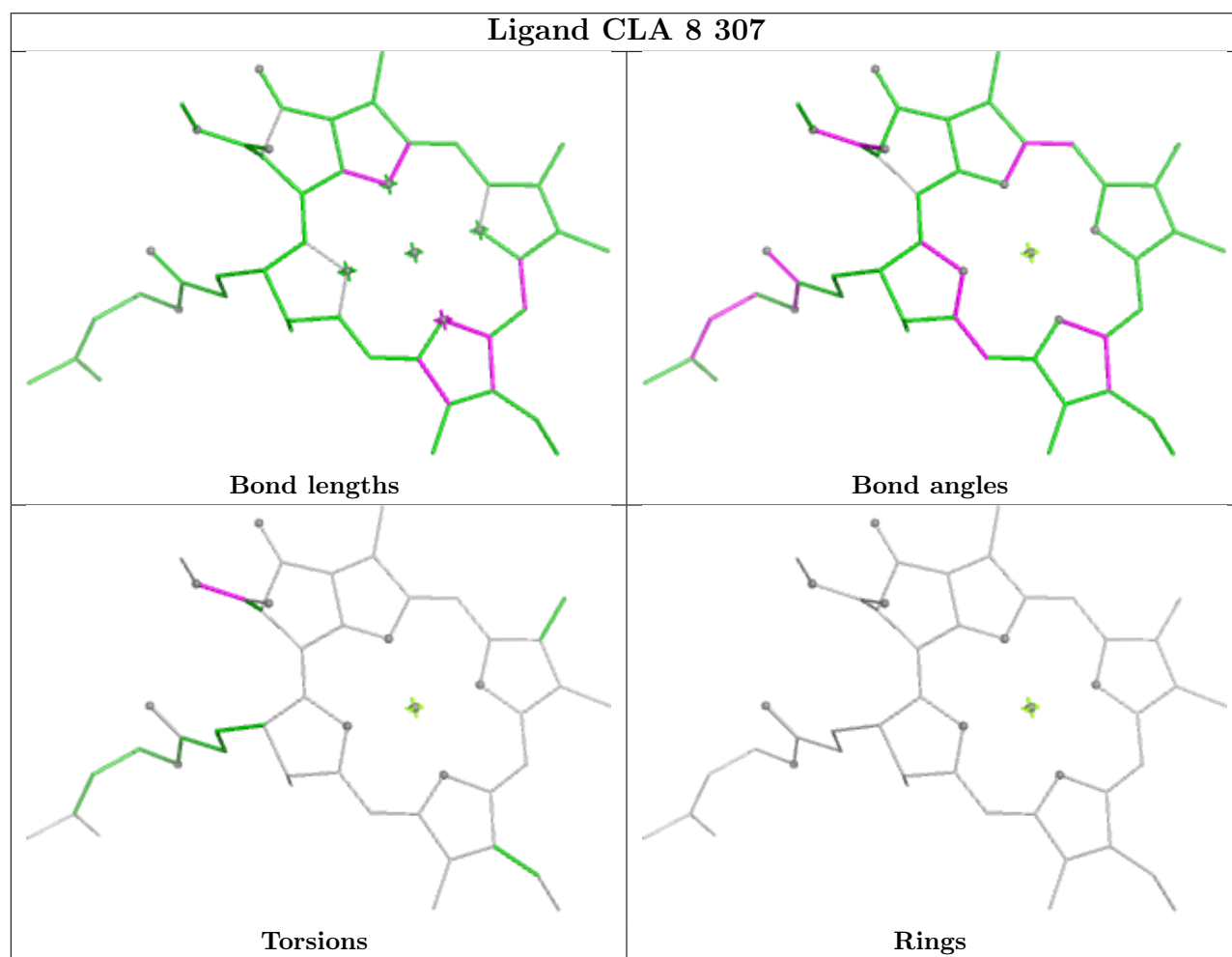
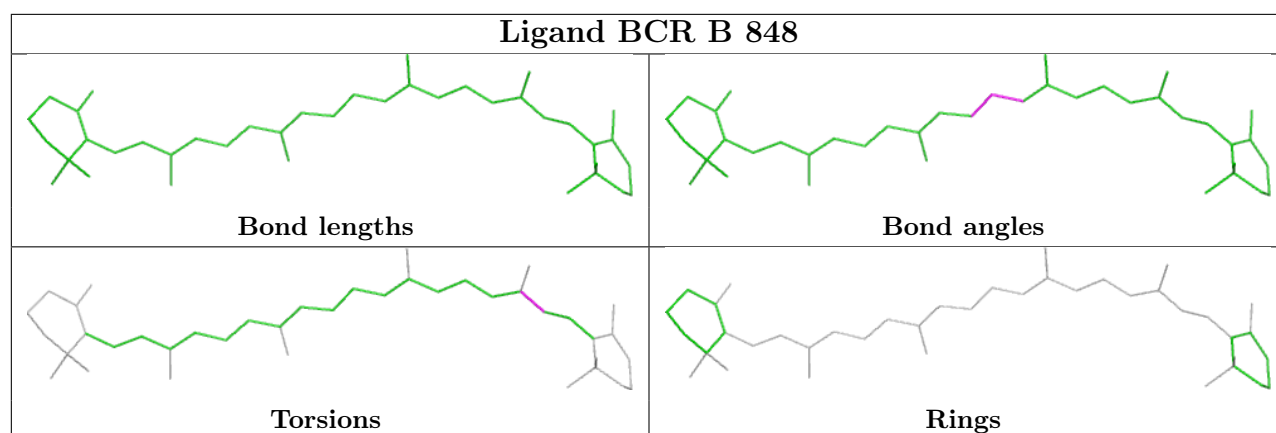


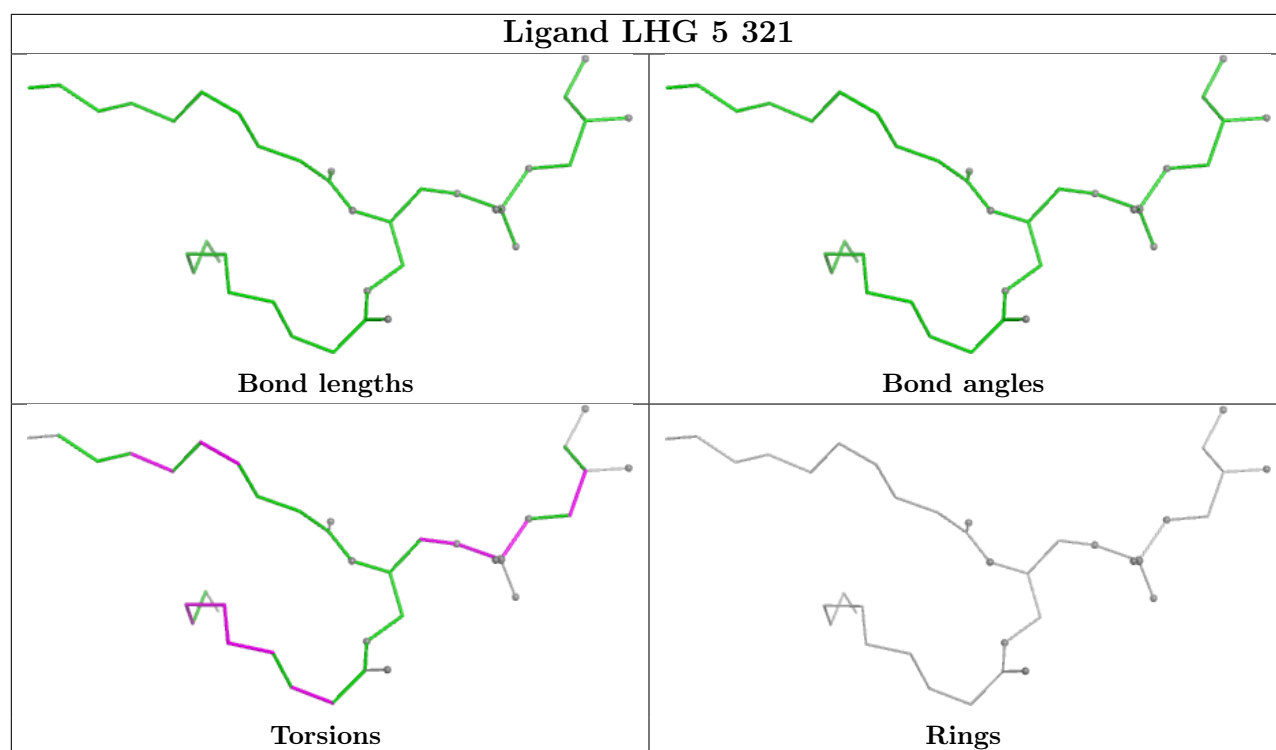


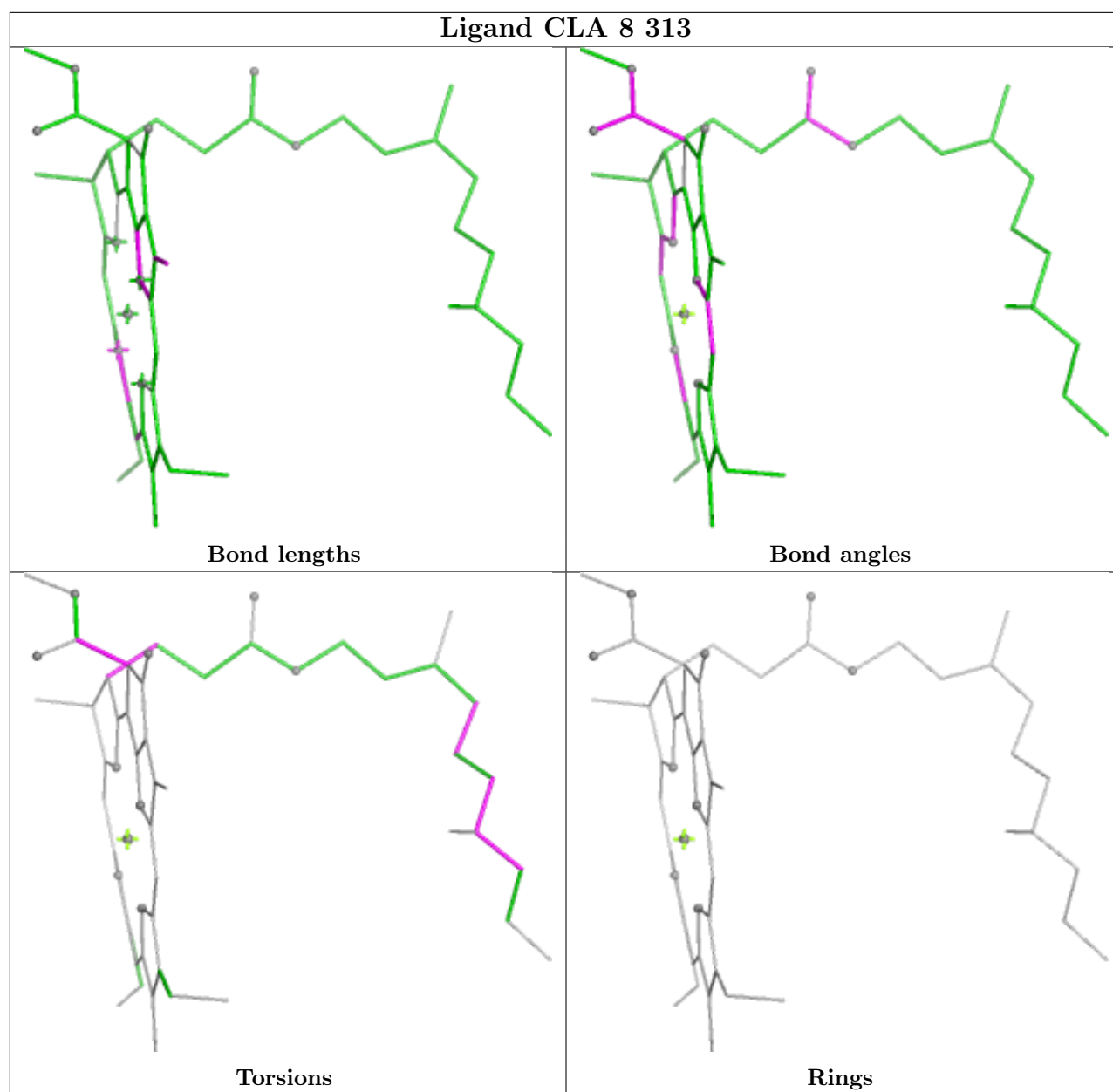


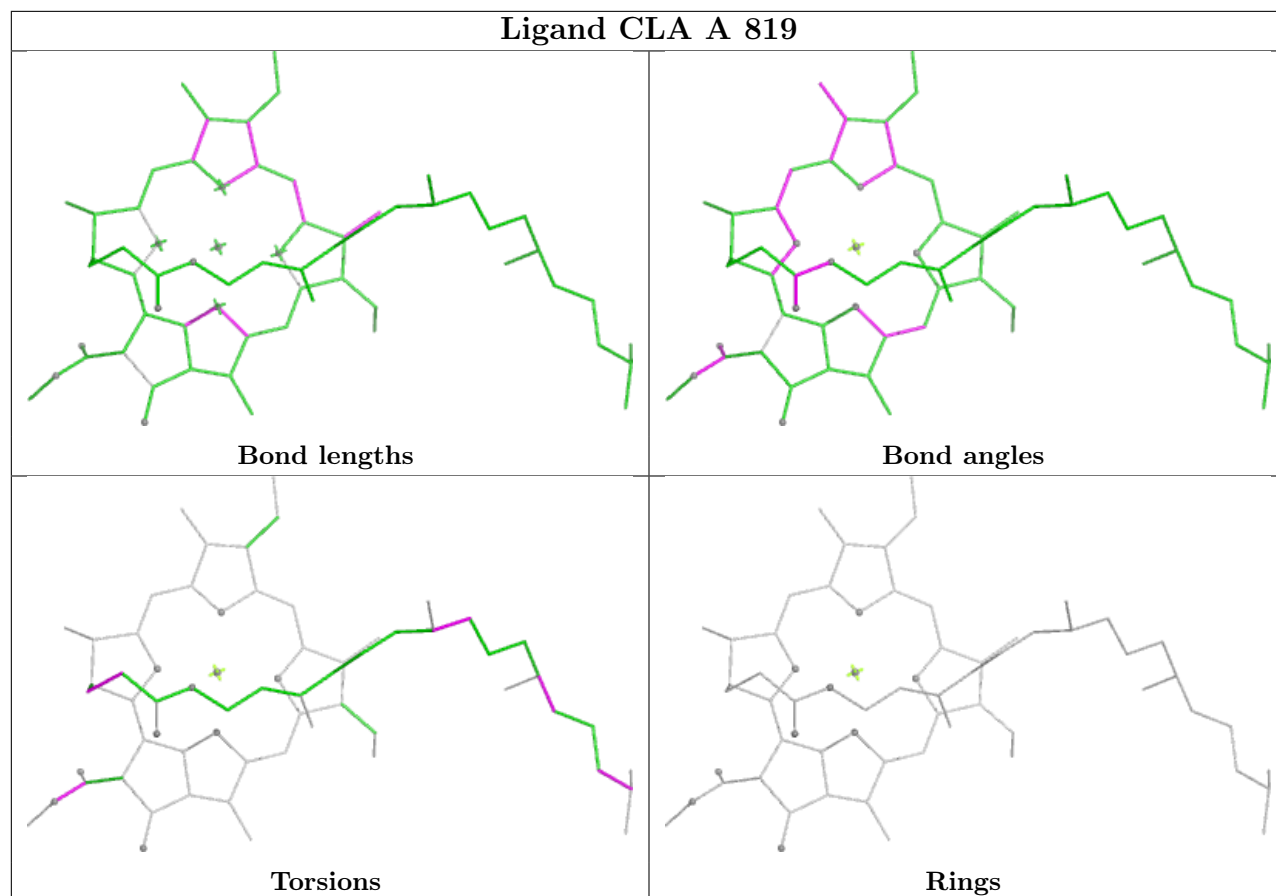


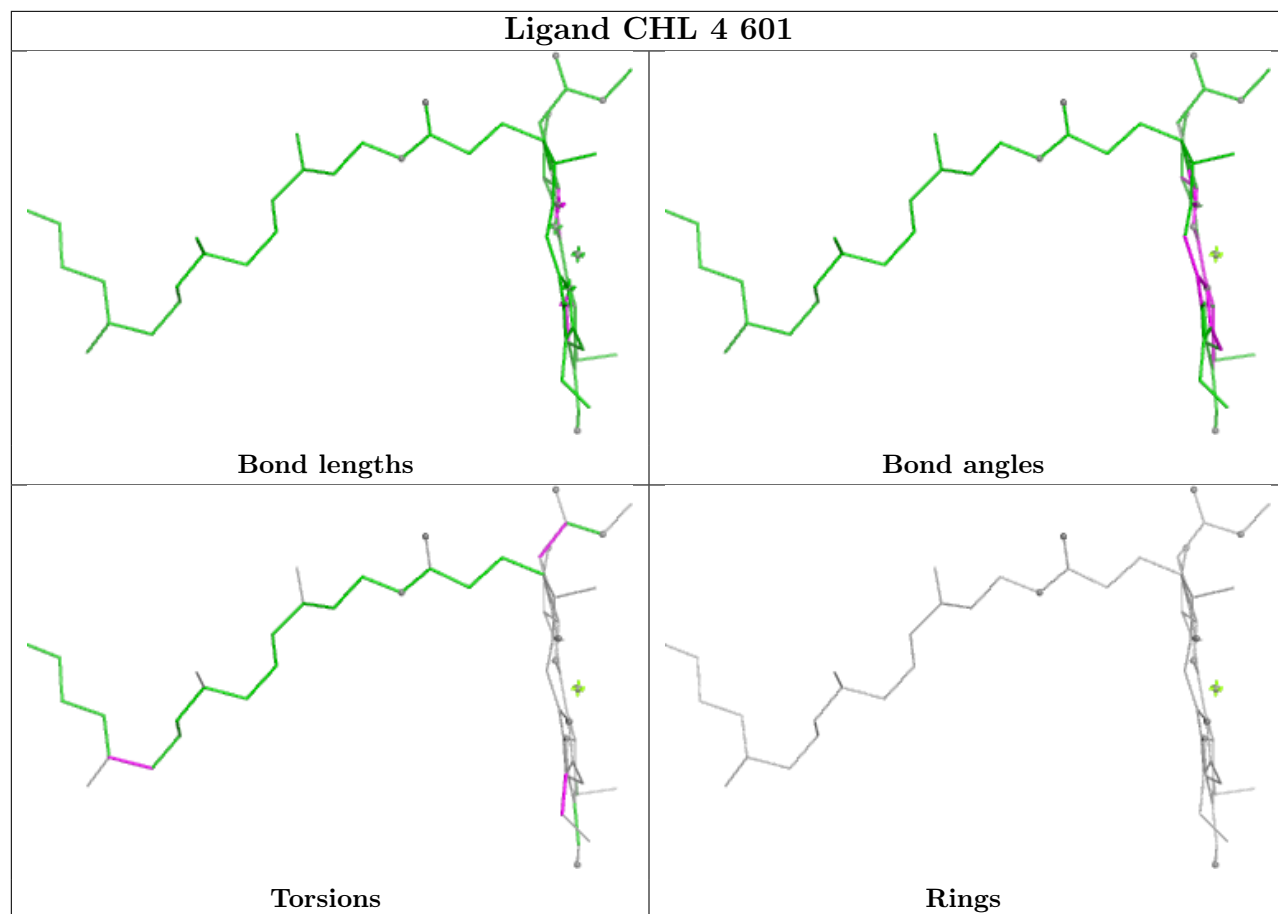




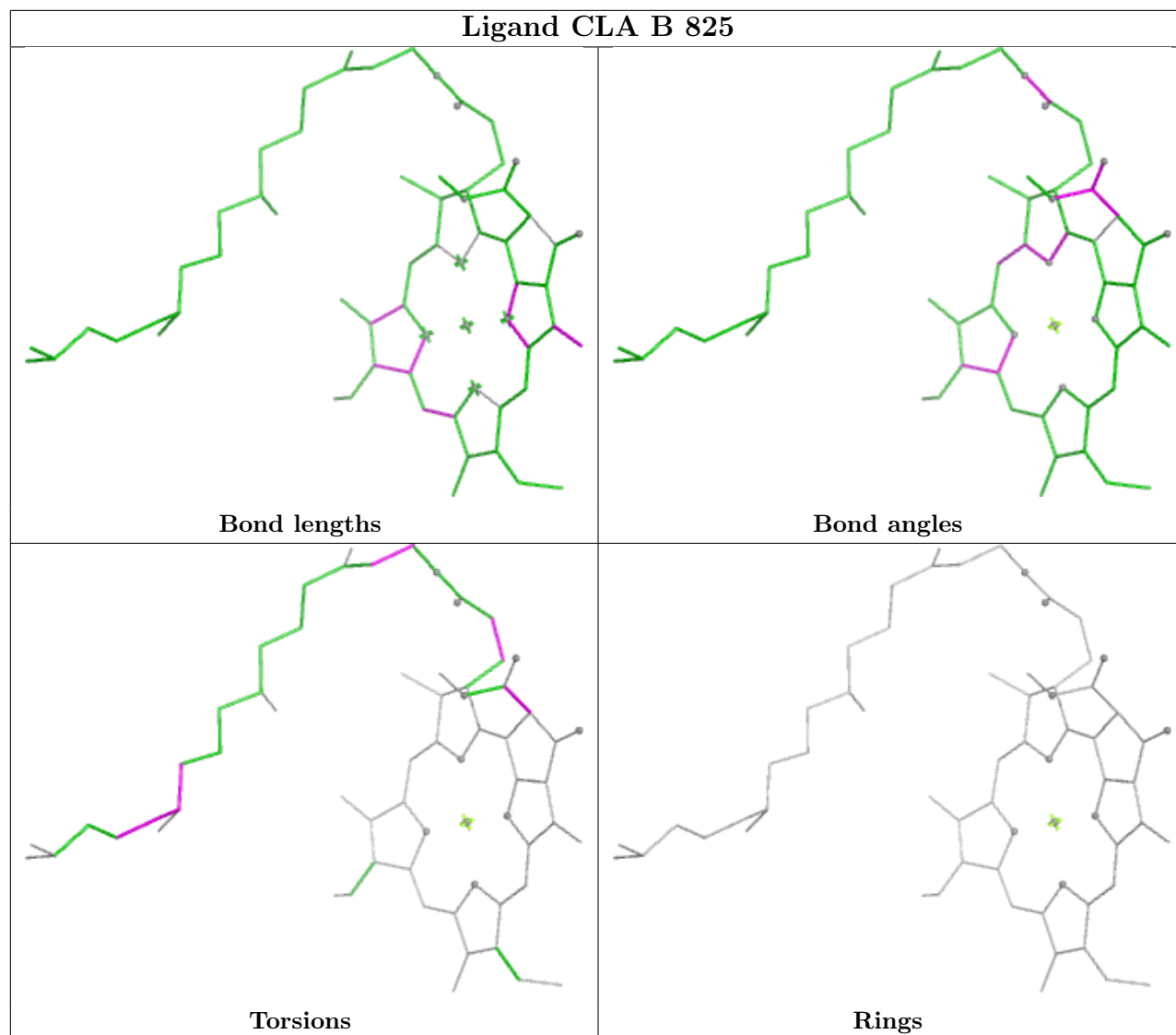




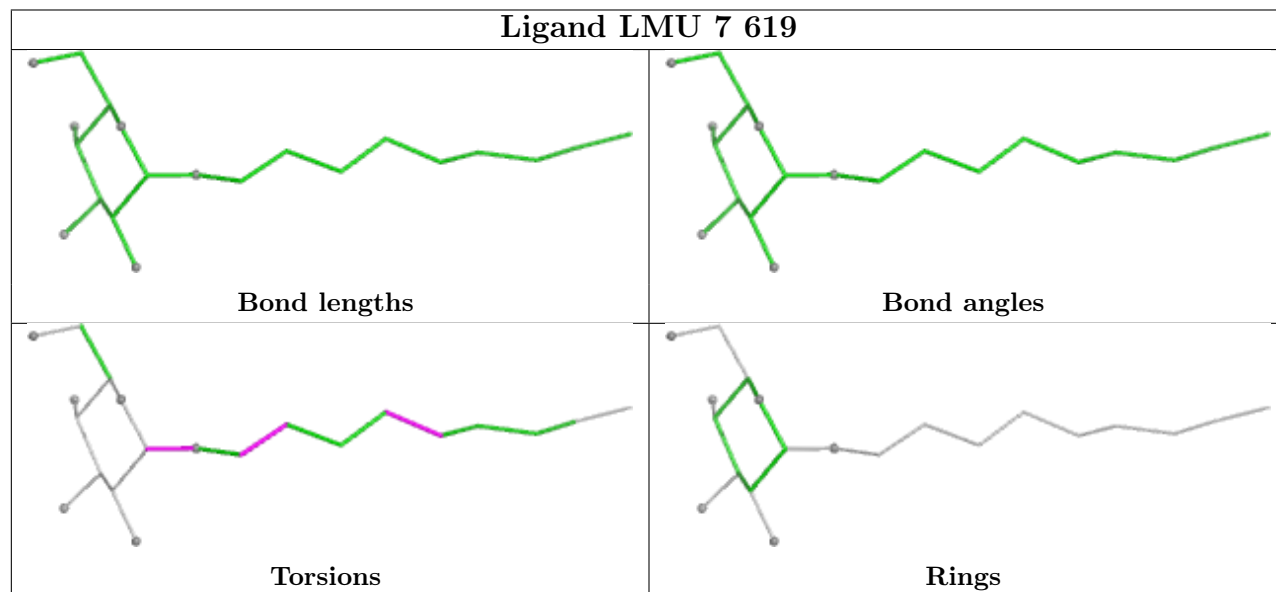


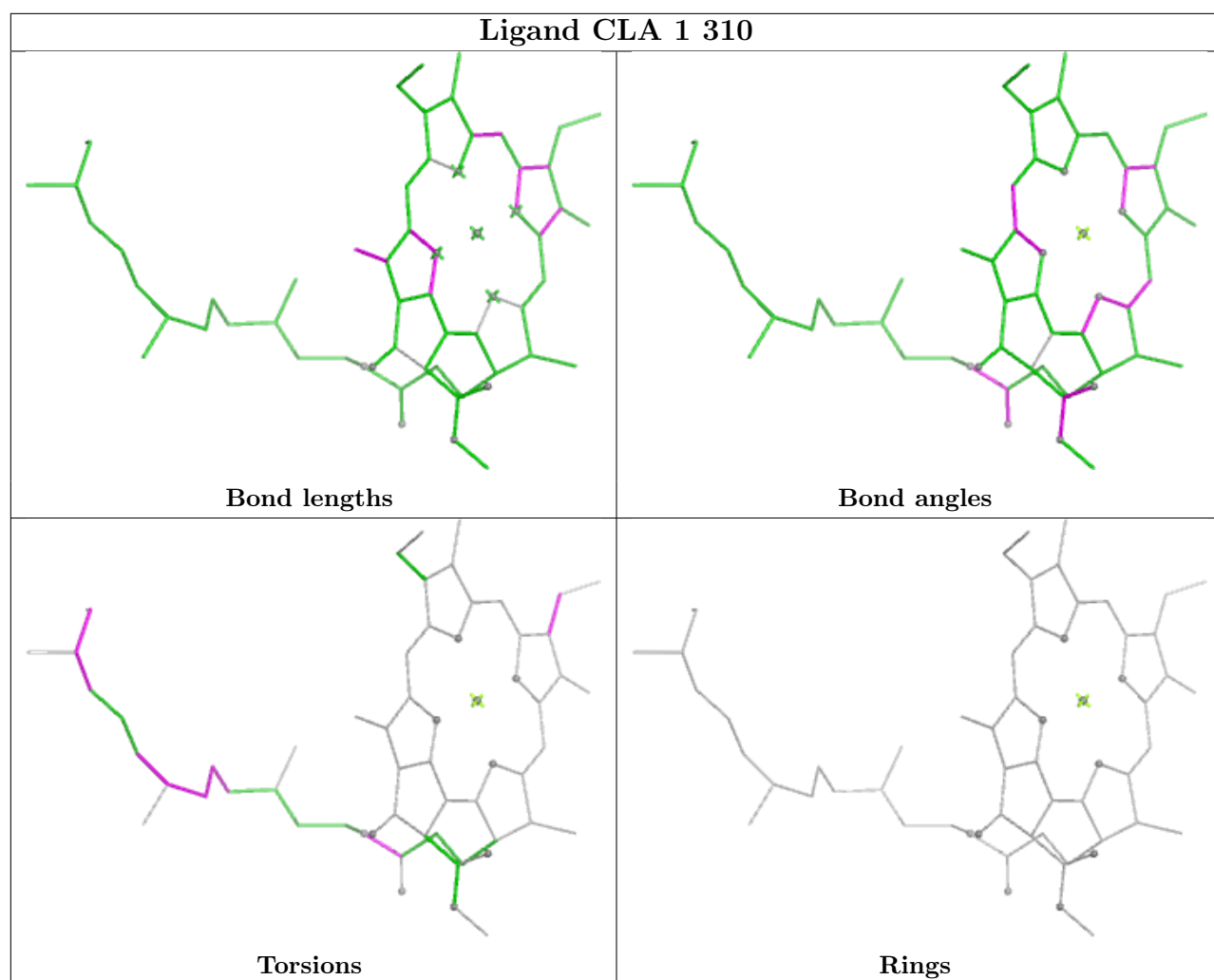


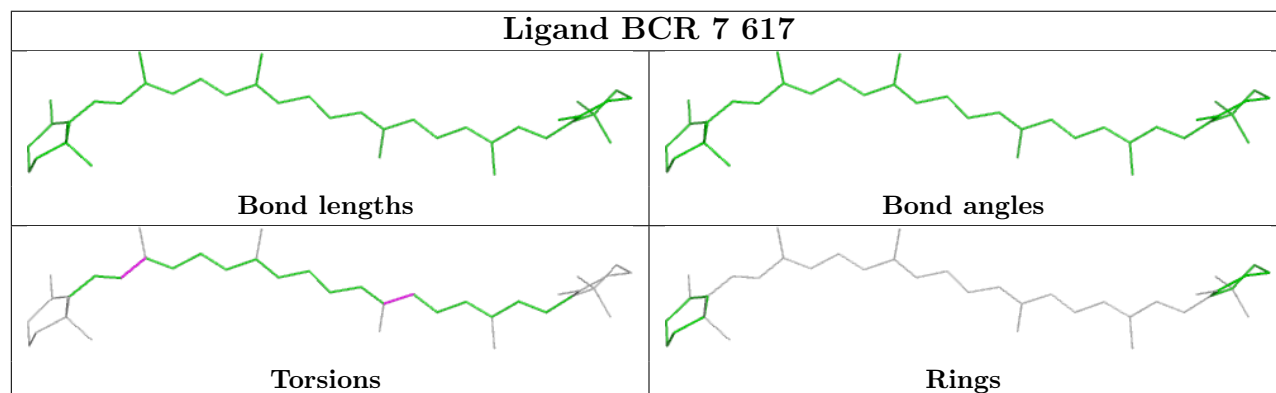
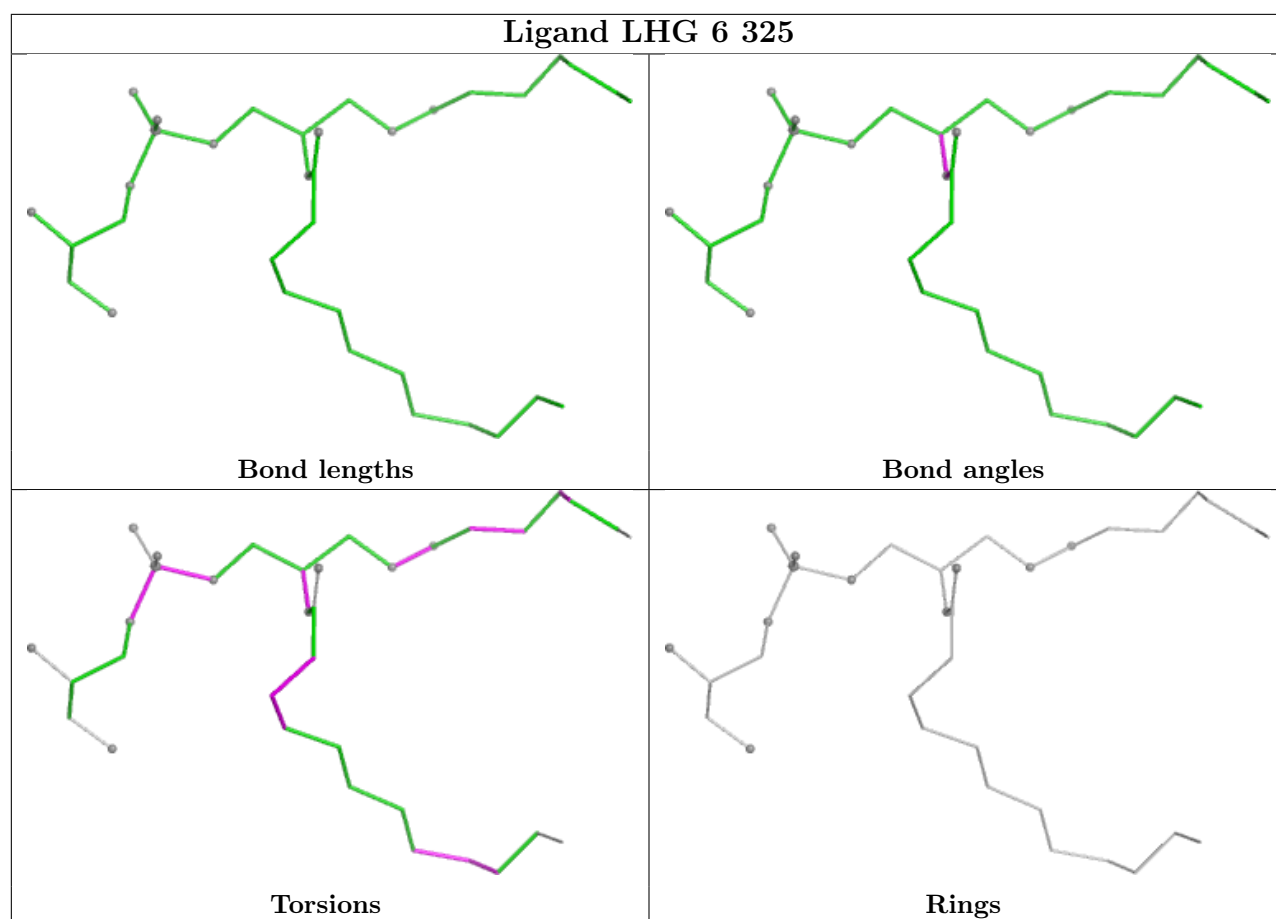
Ligand CLA B 825

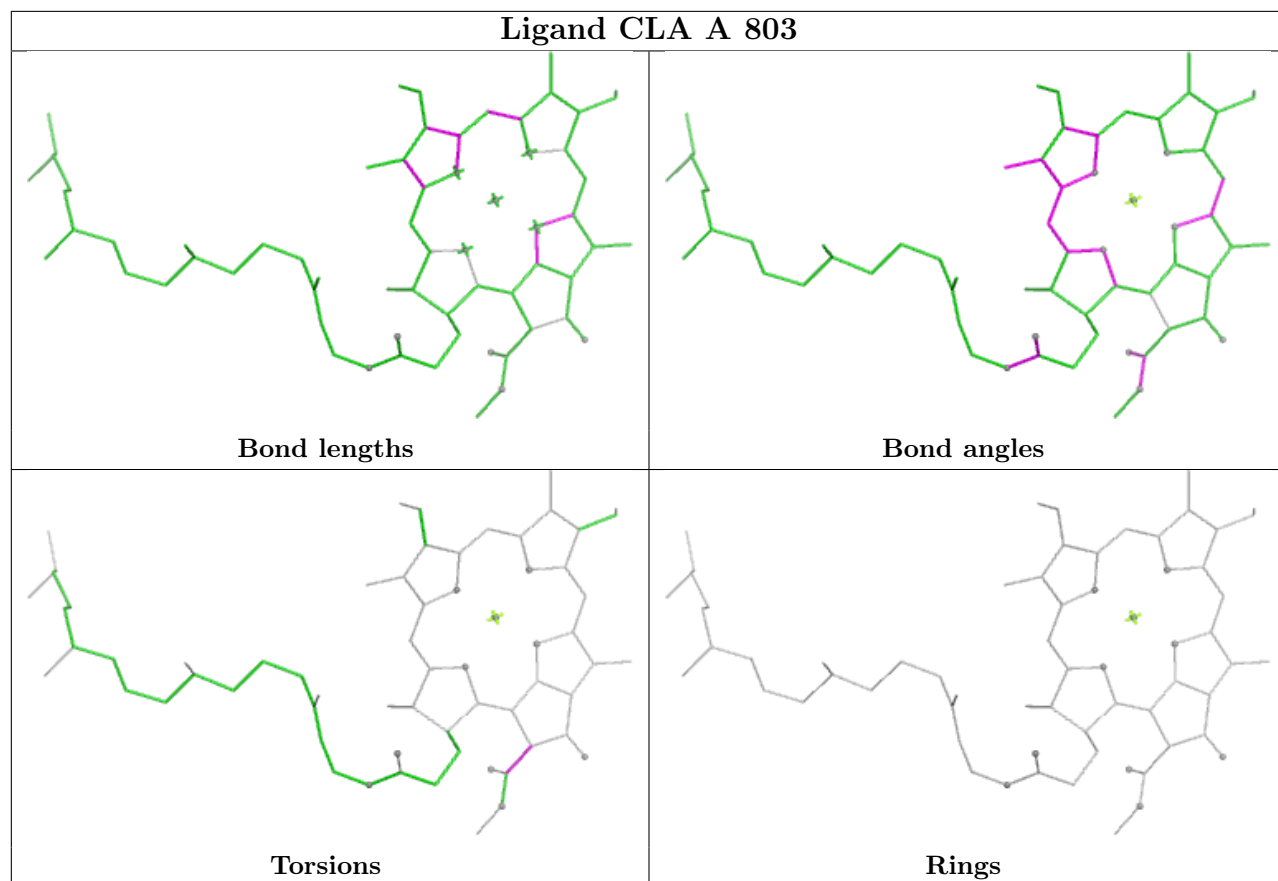


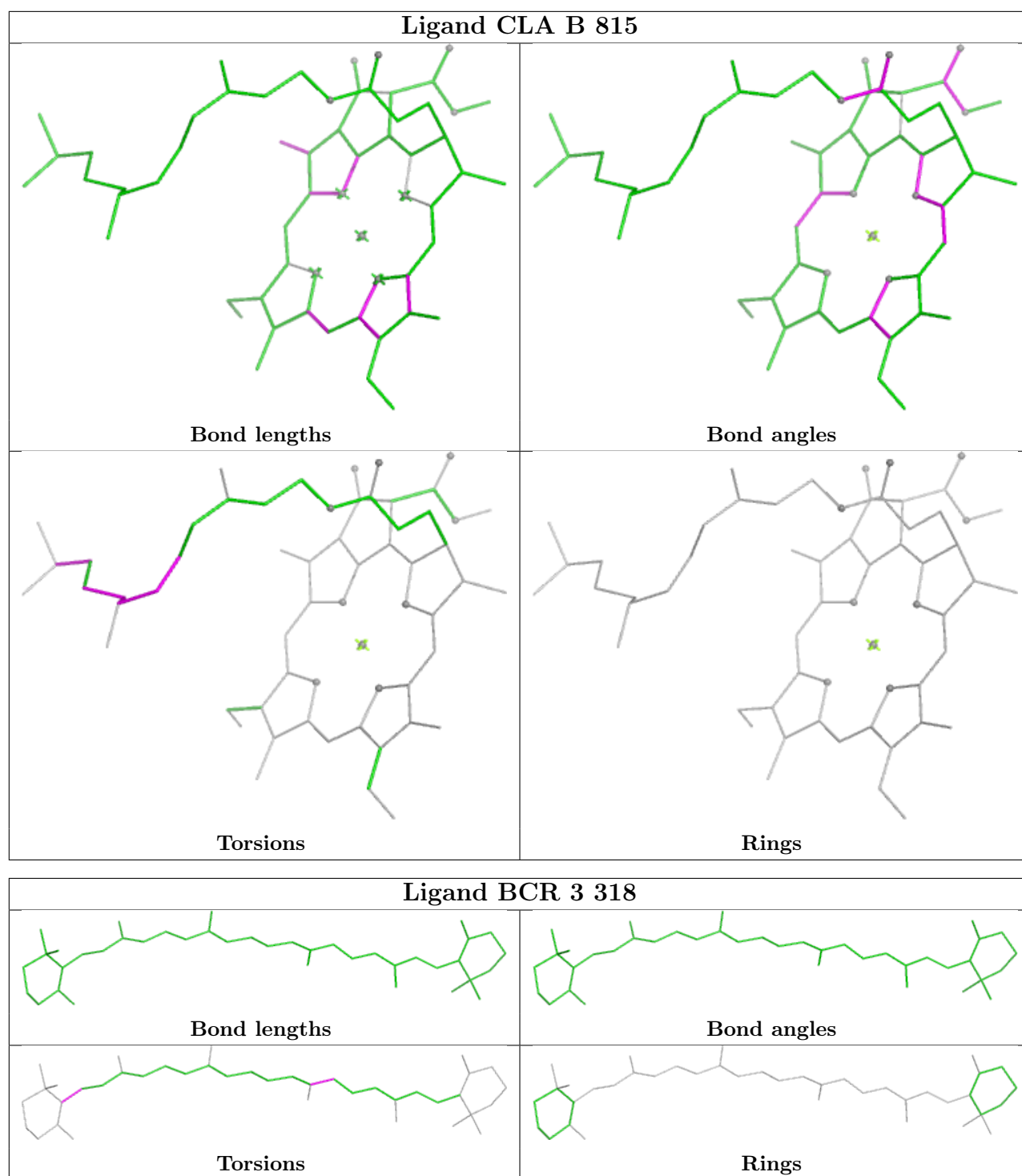
Ligand LMU 7 619

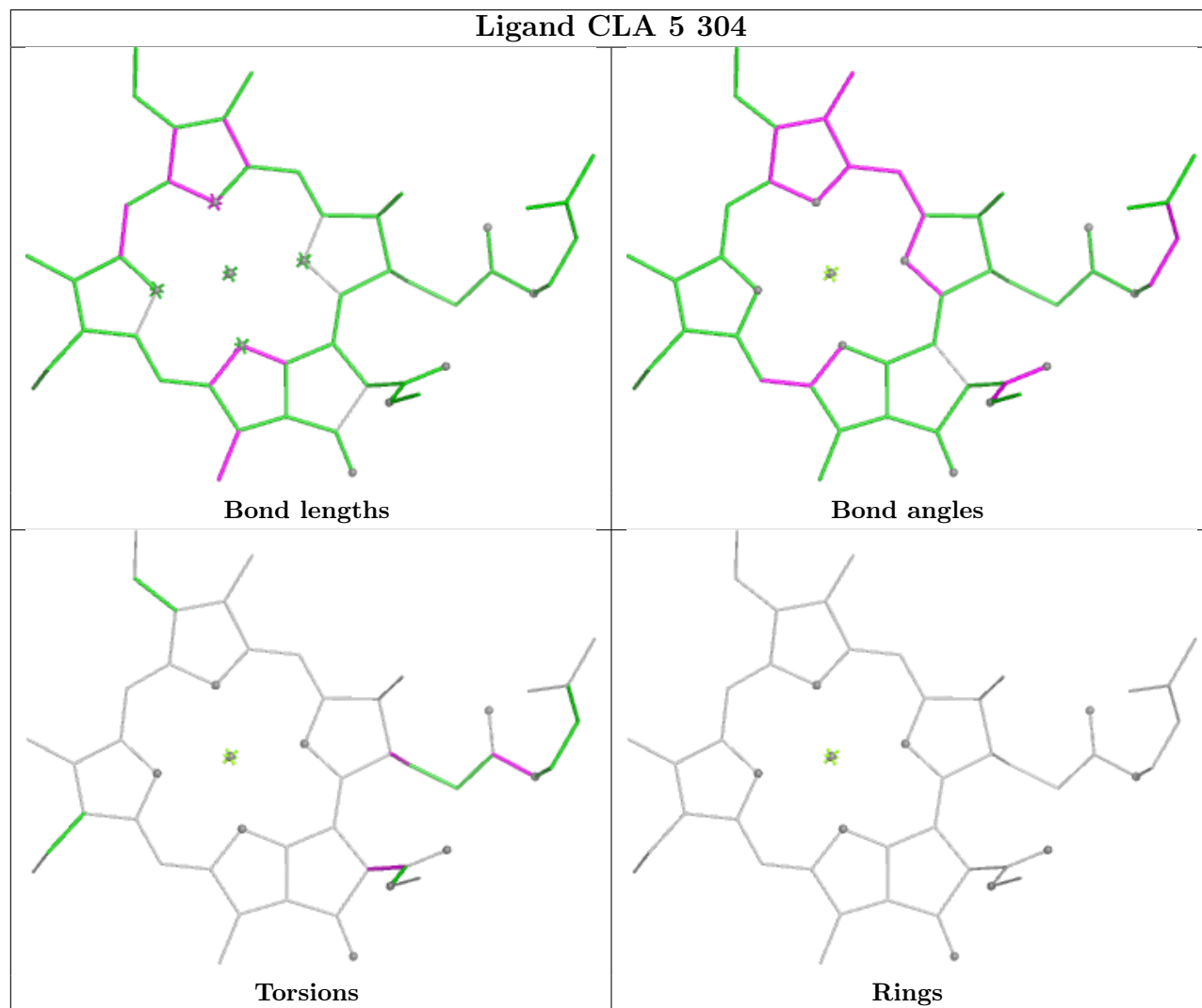
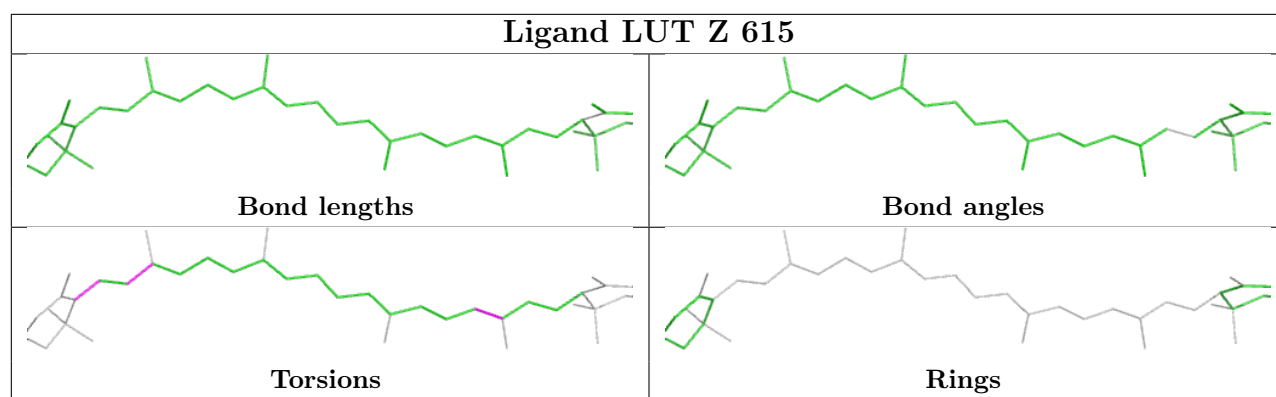


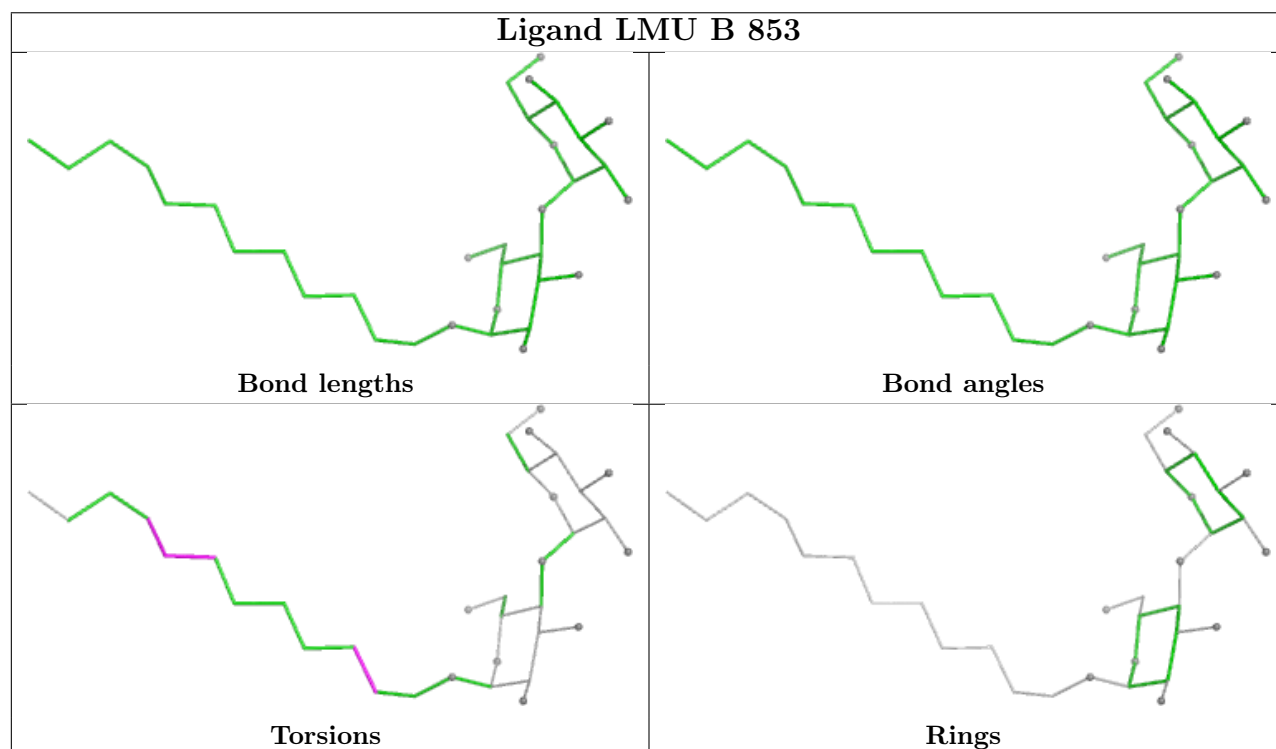
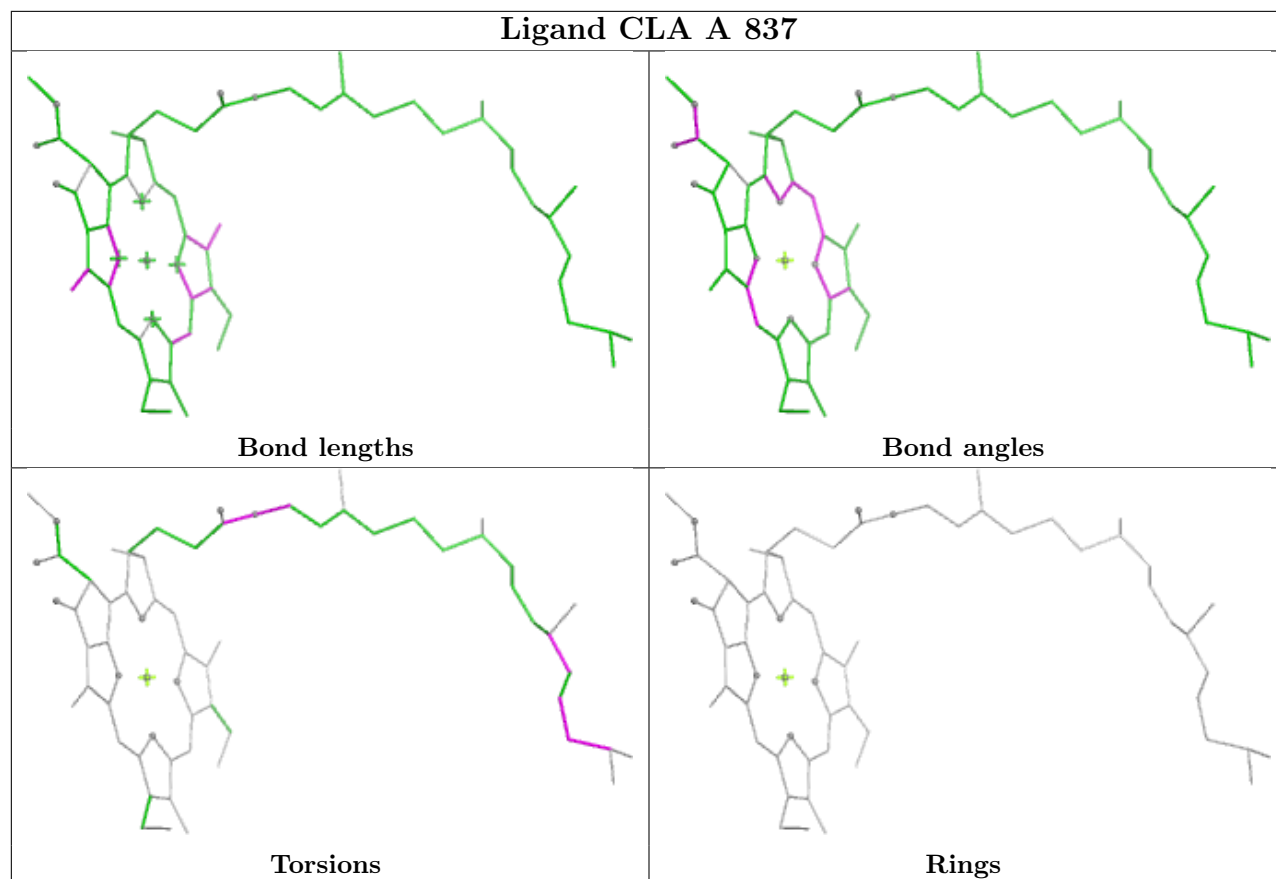


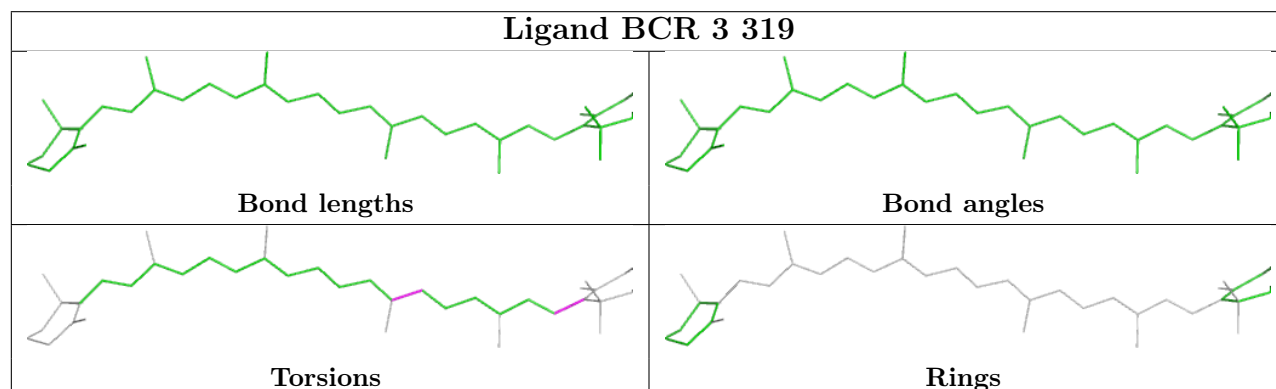
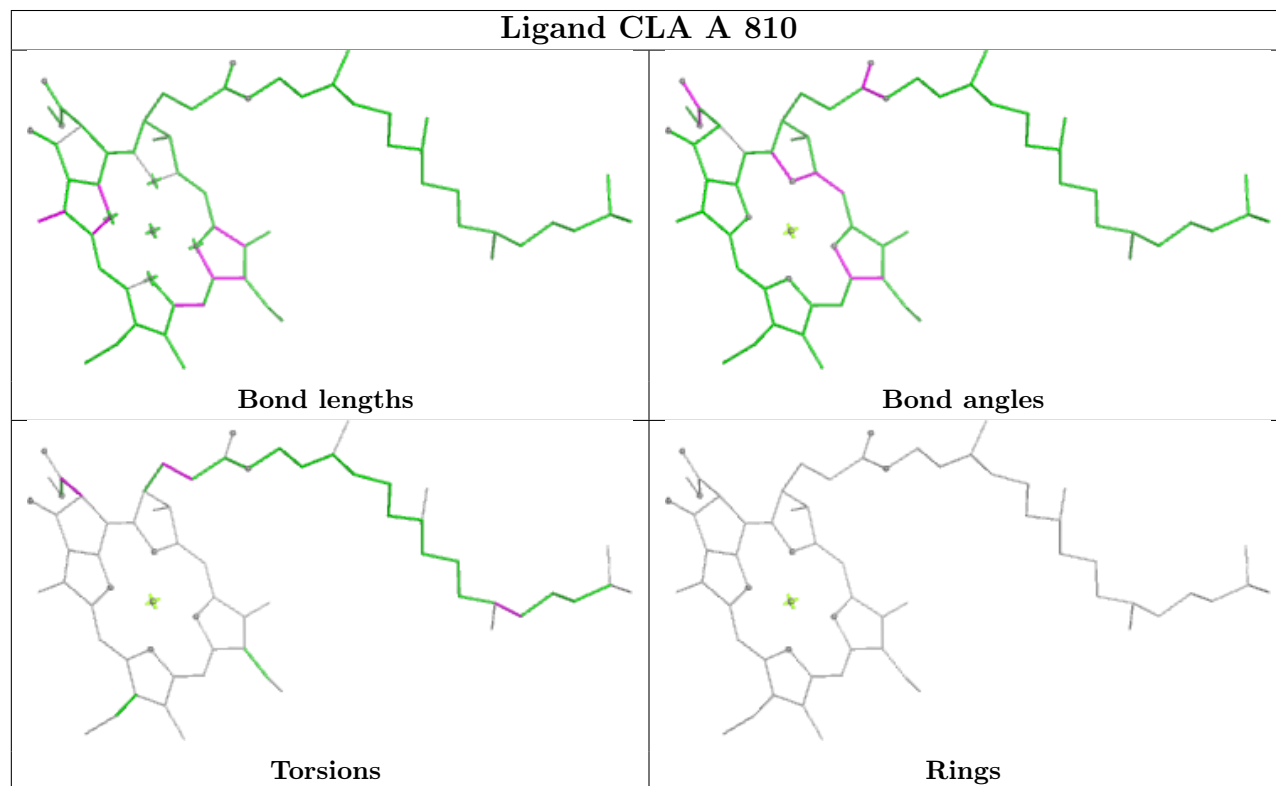
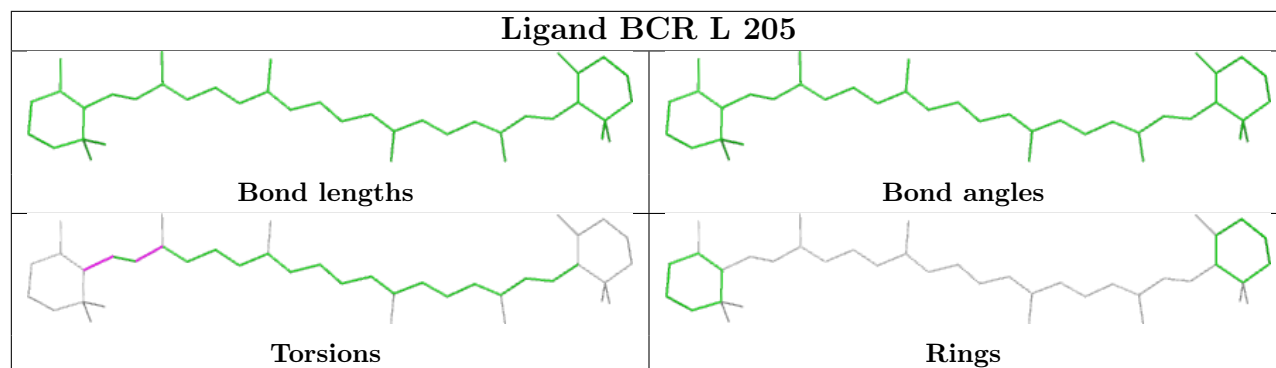


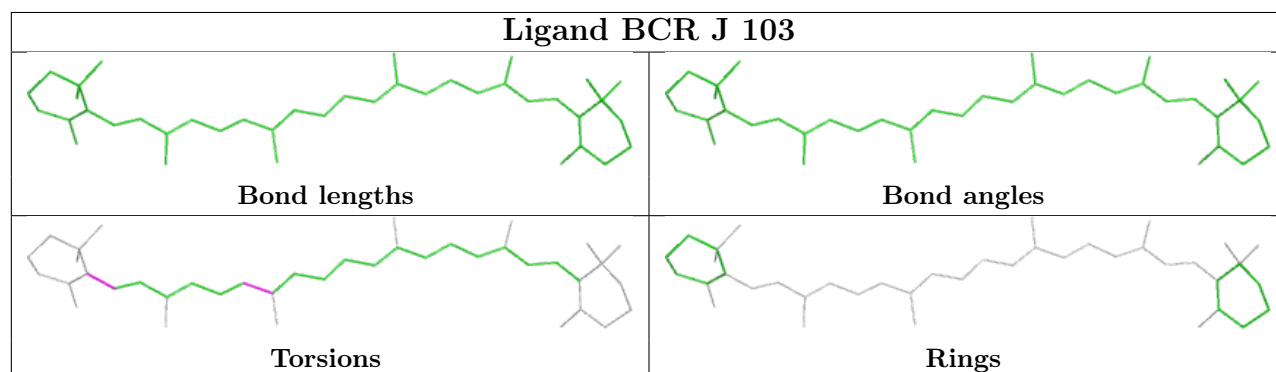
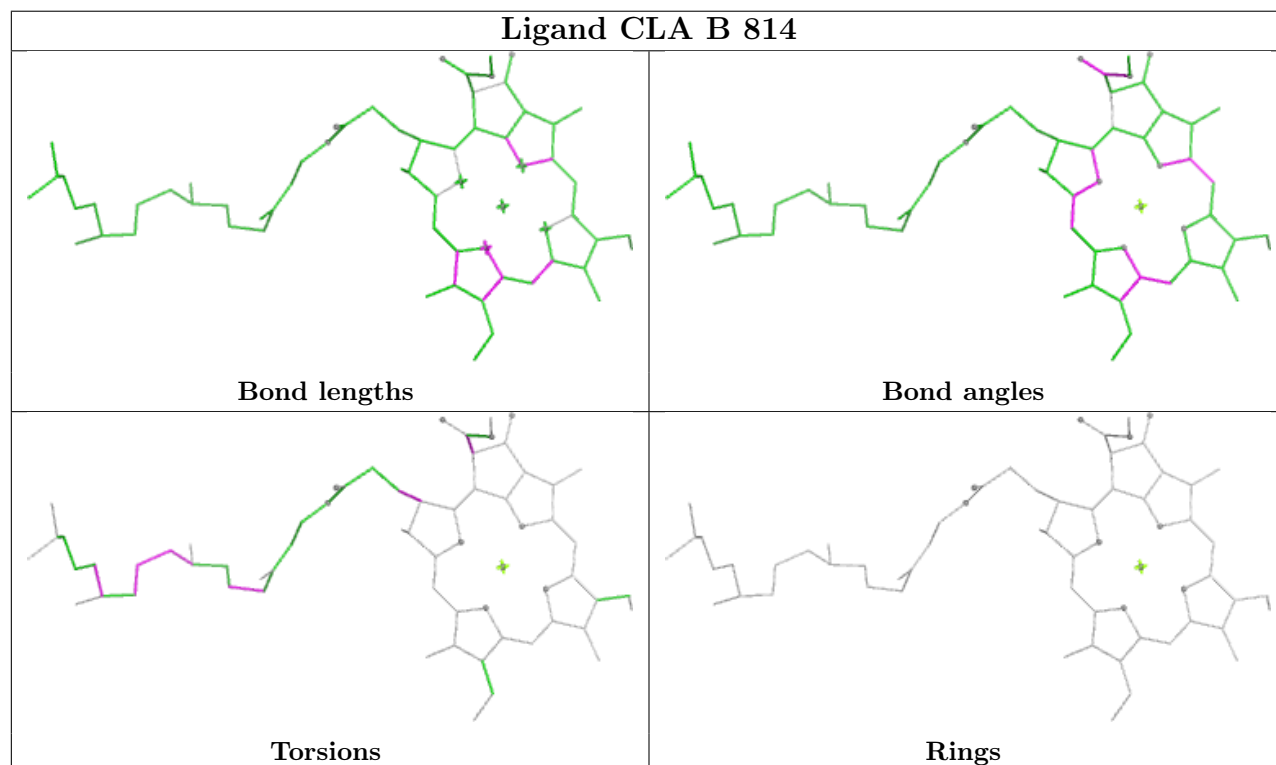
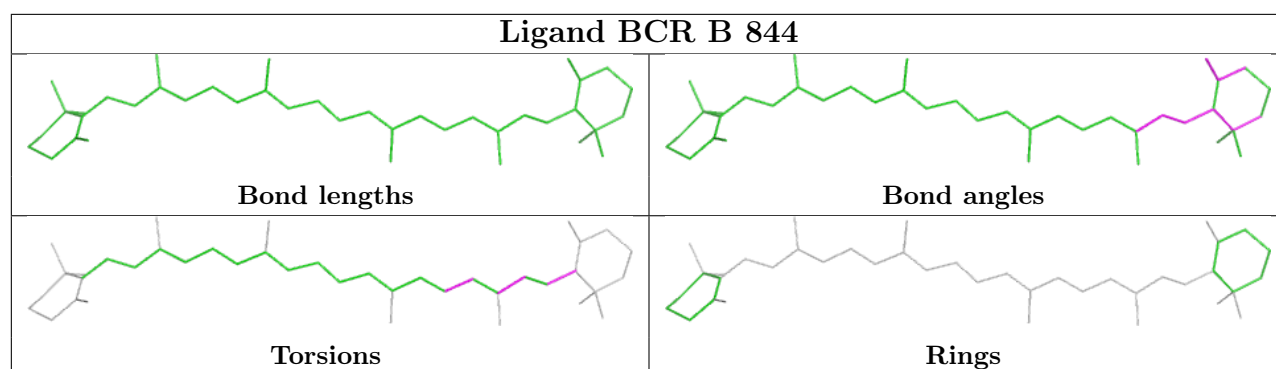


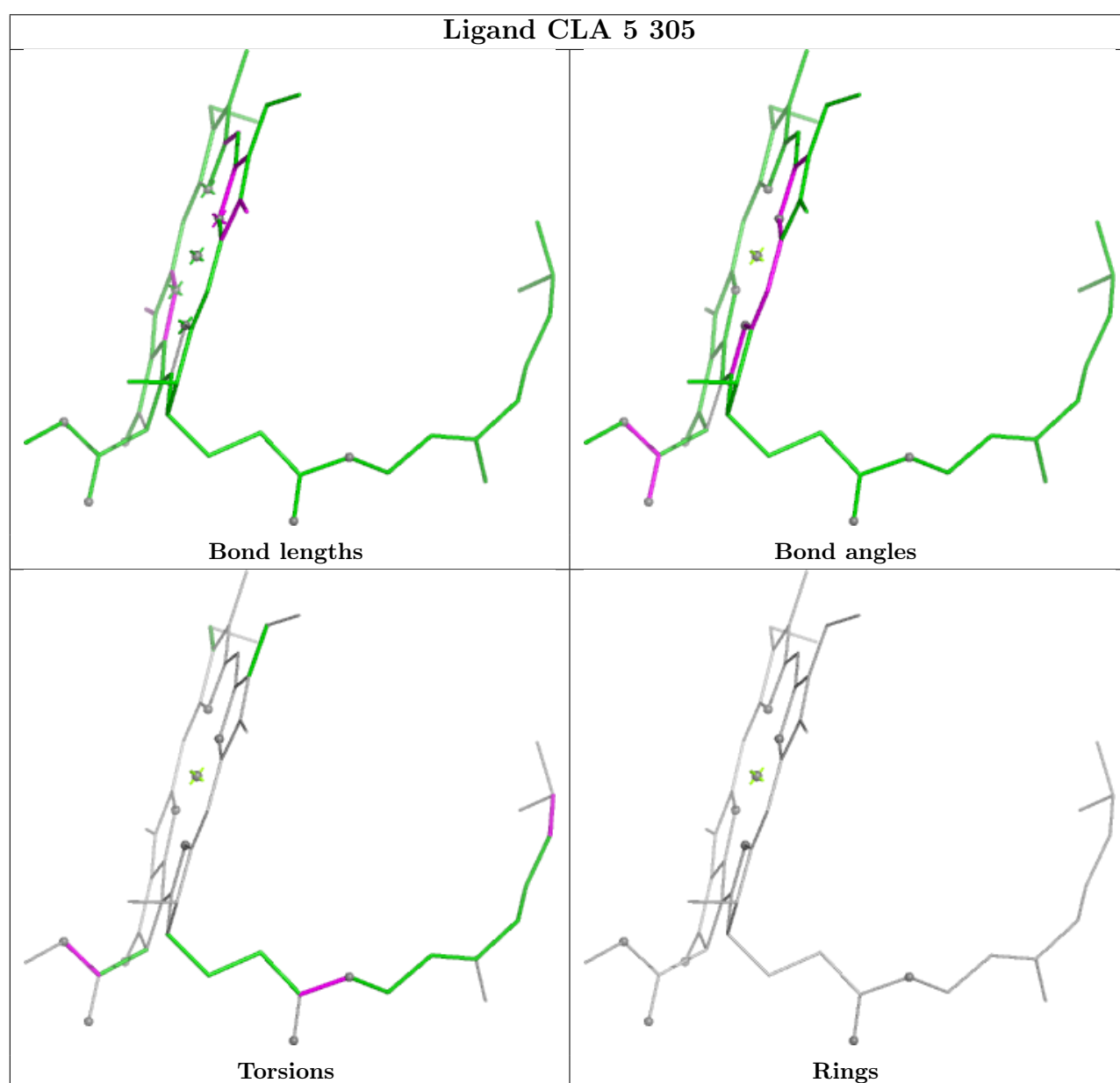
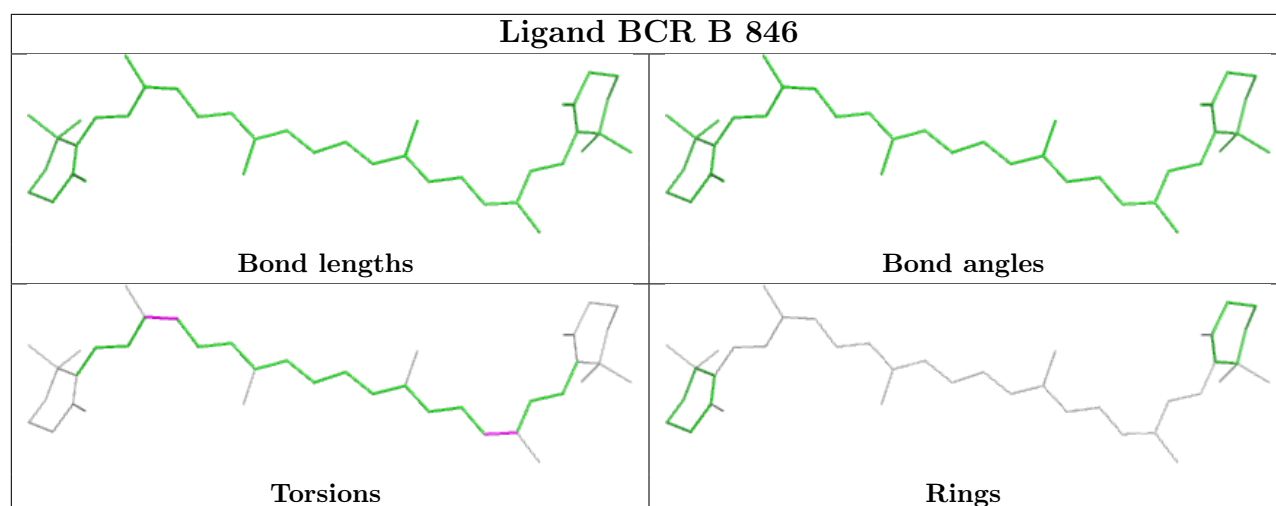


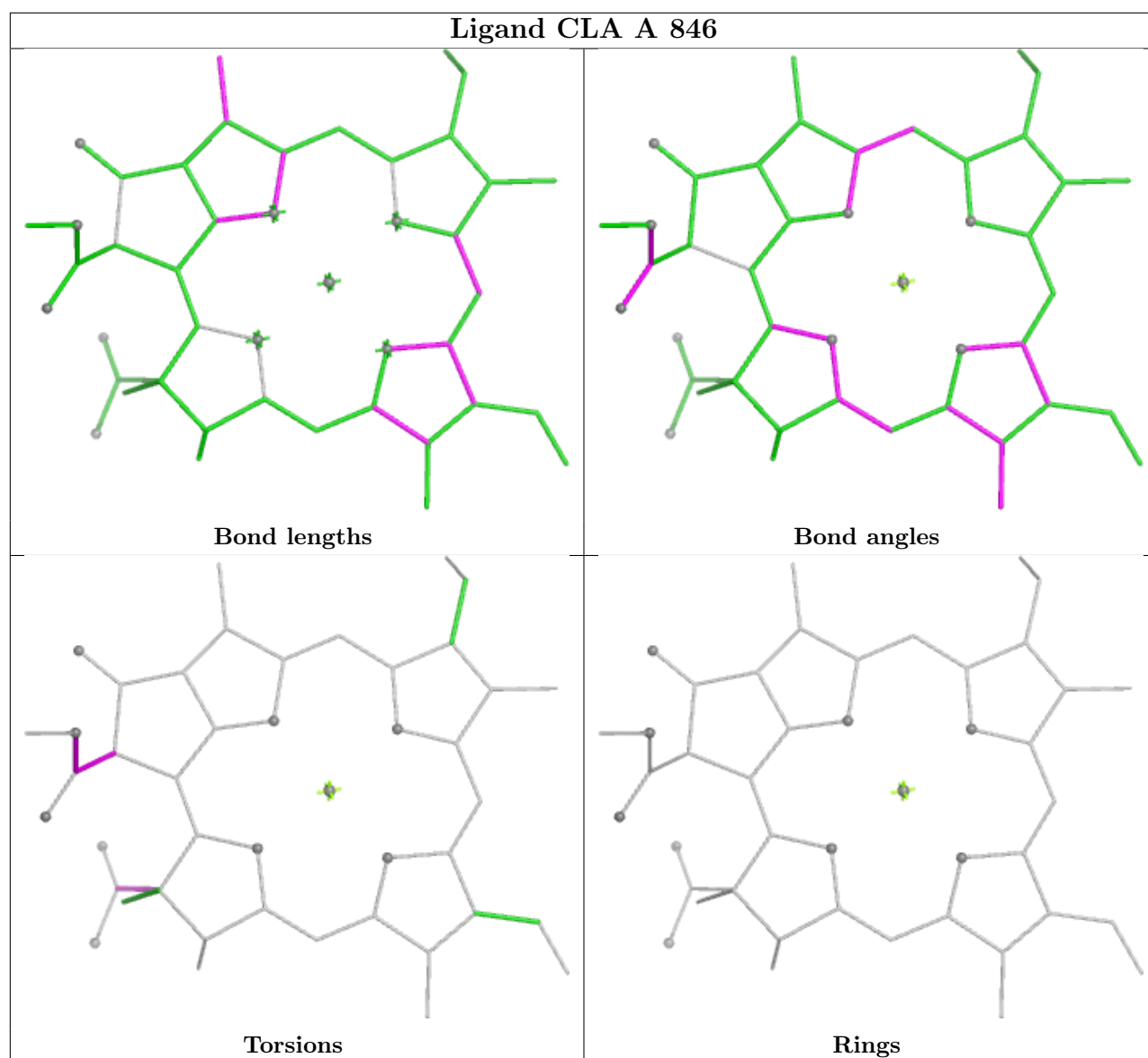


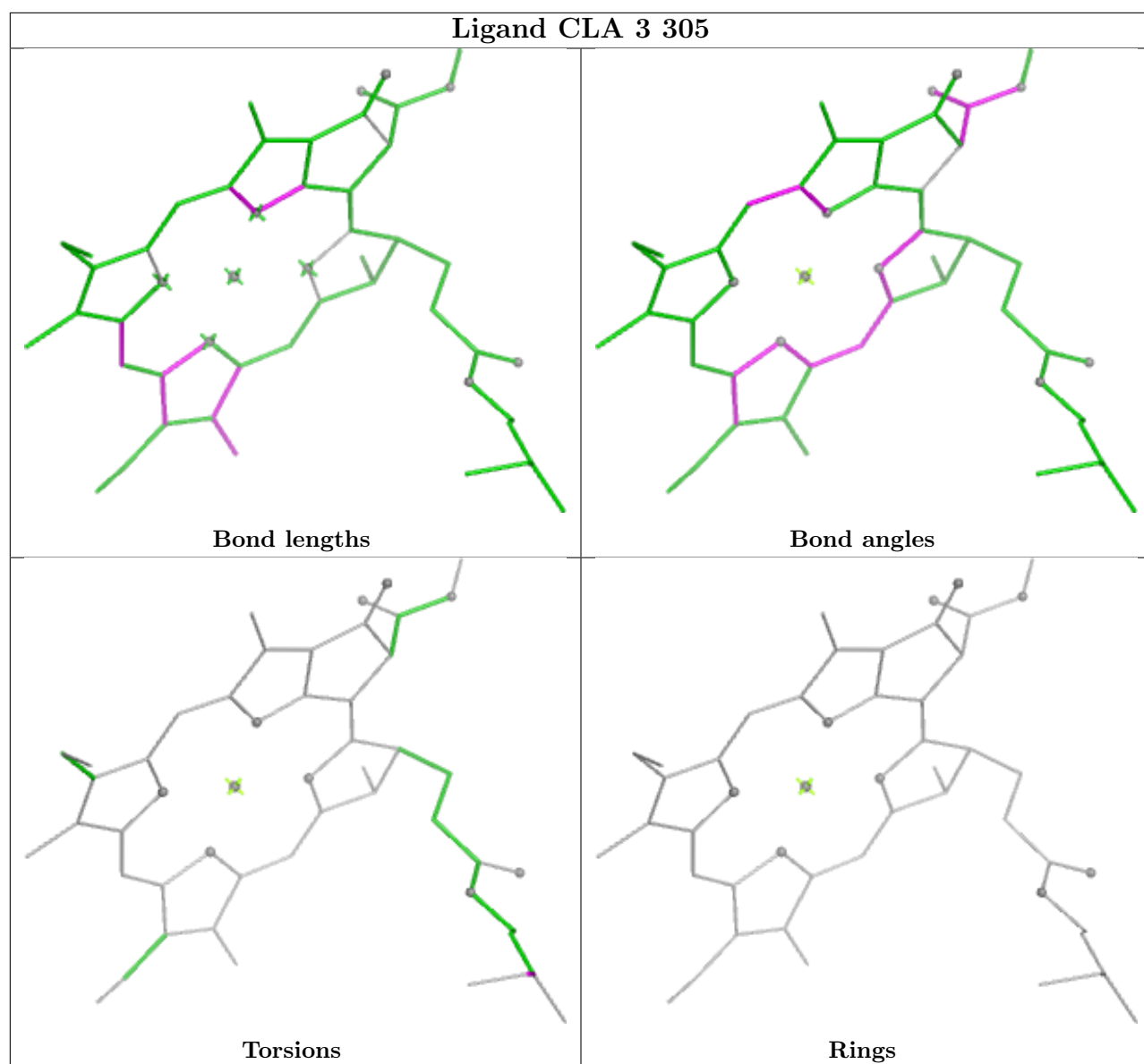


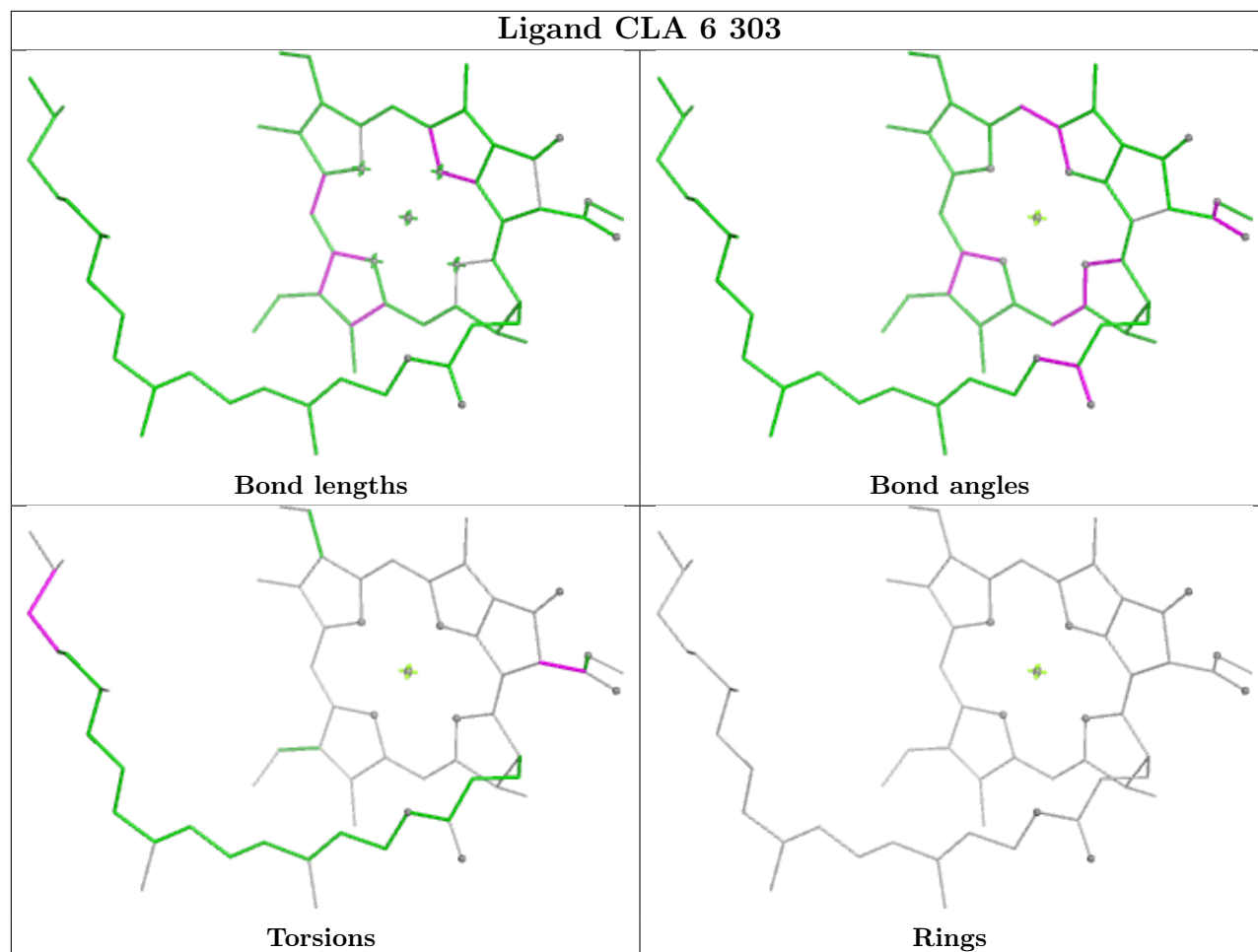


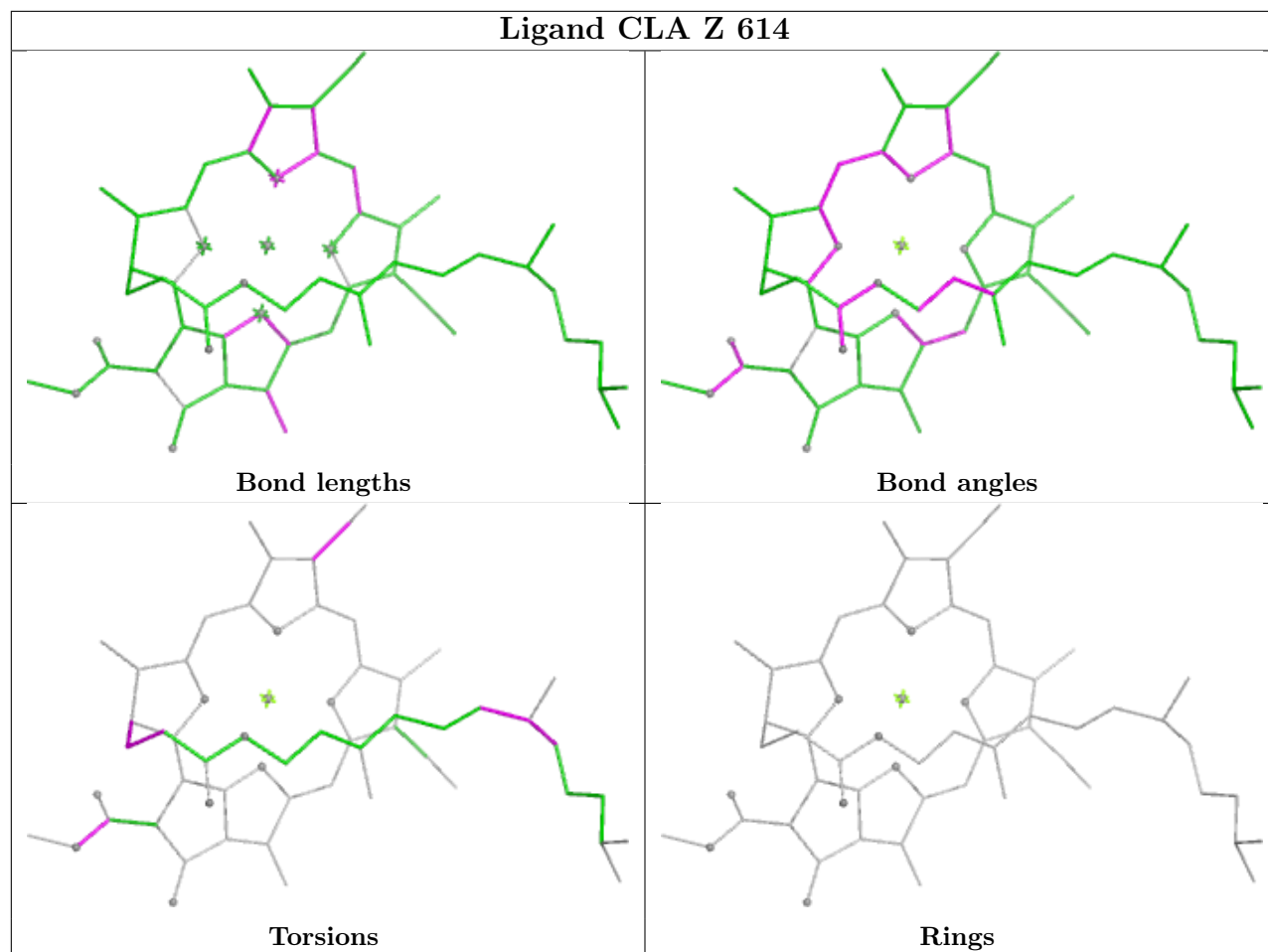




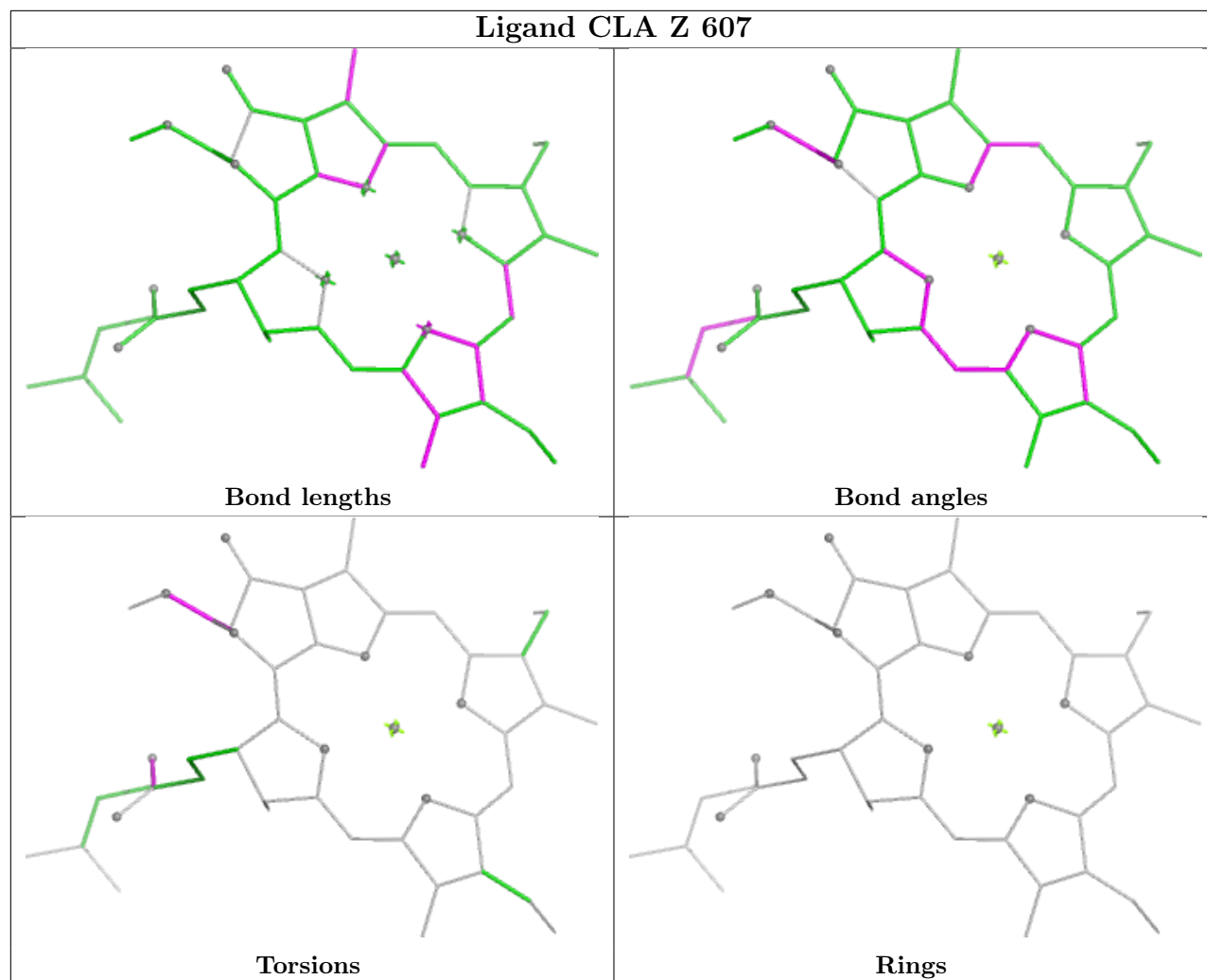


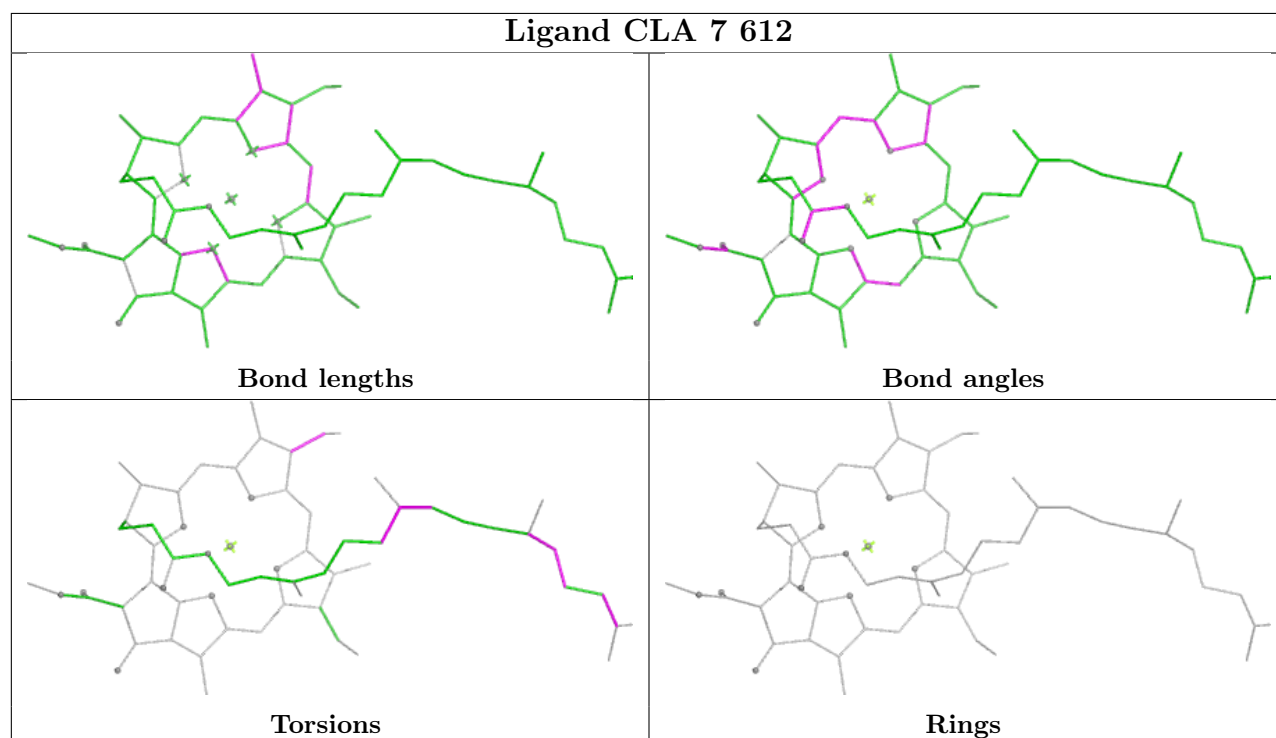
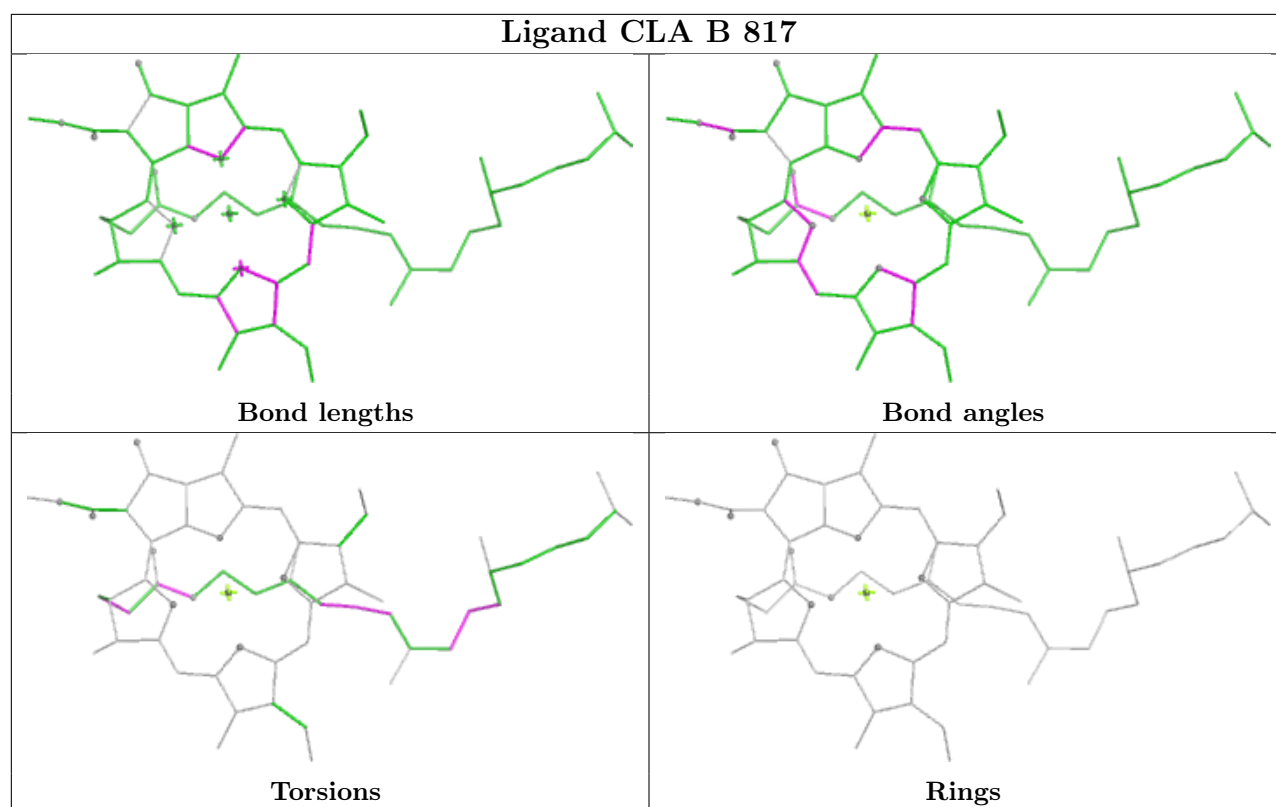


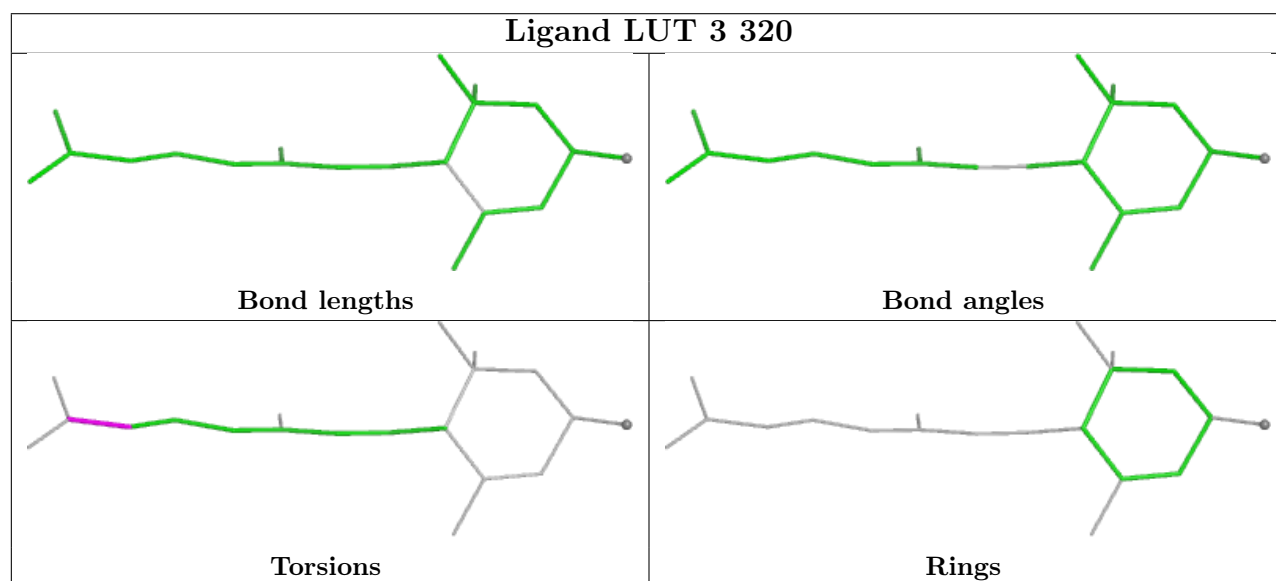
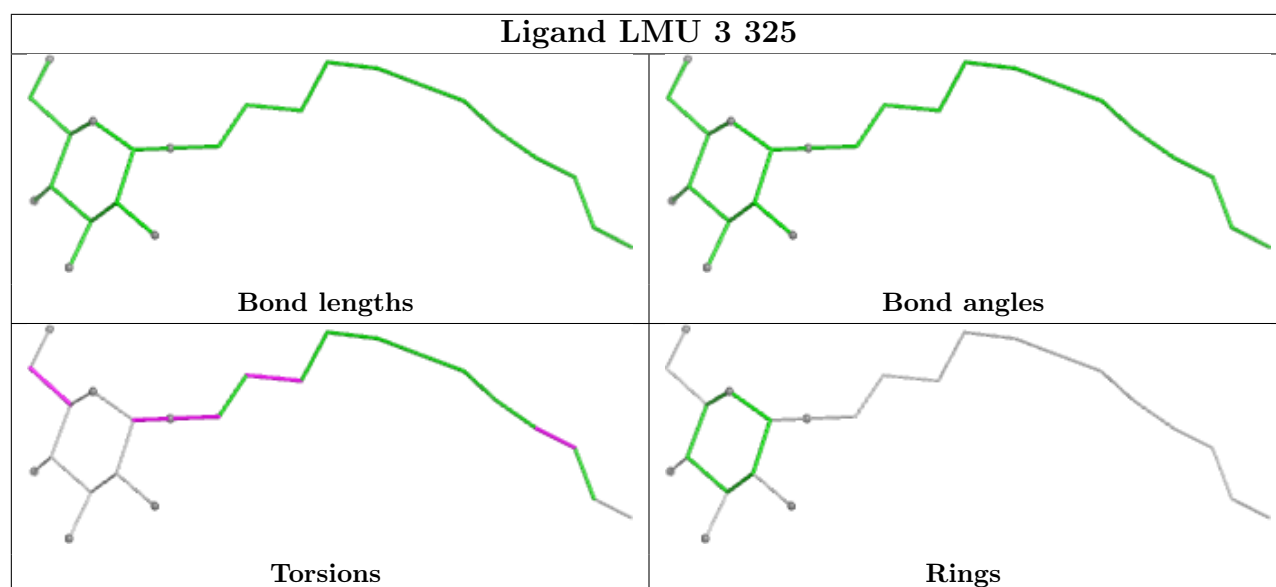


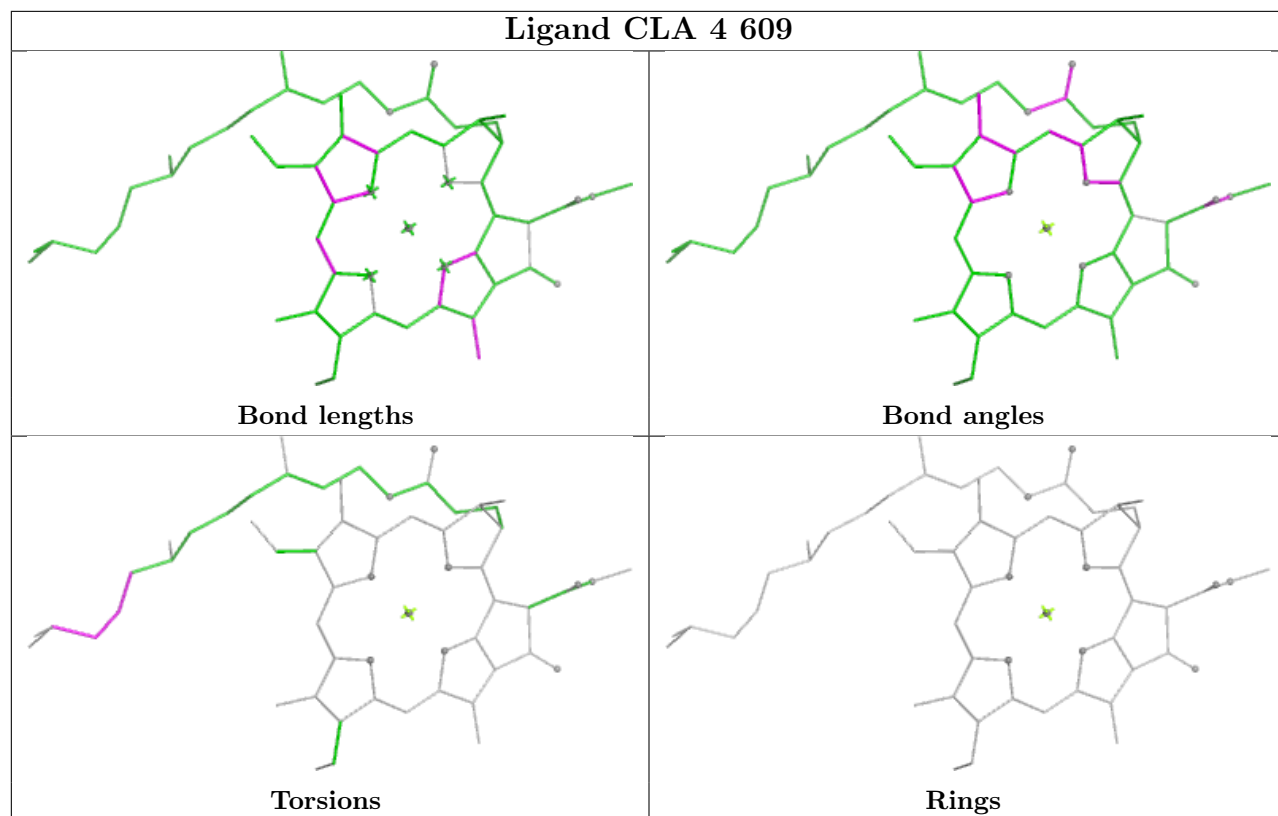


Ligand CLA Z 607

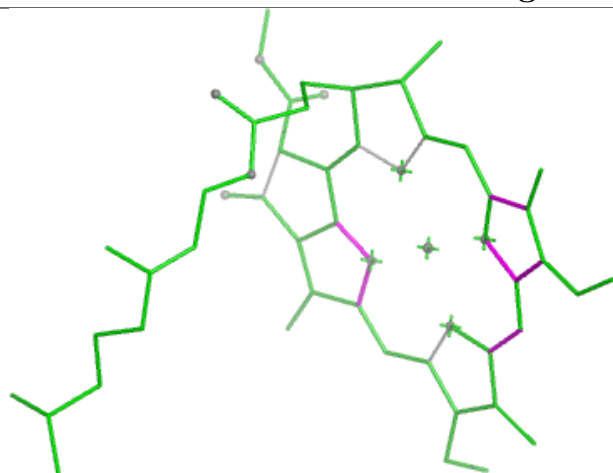




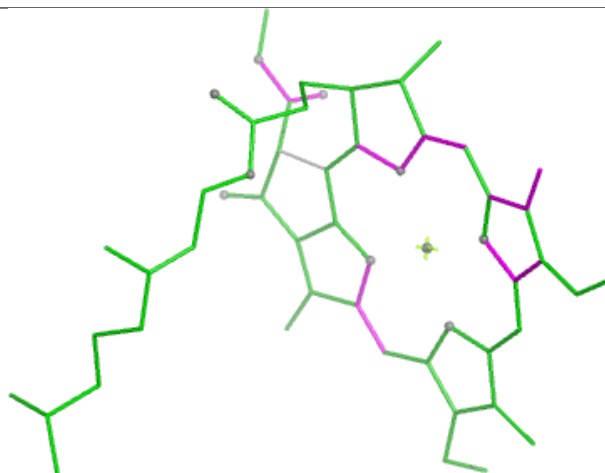




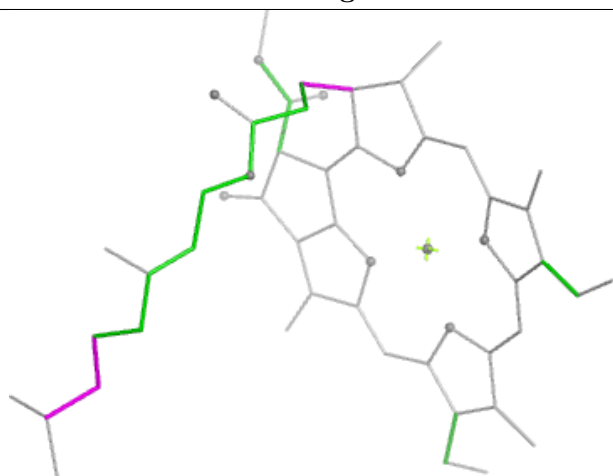
Ligand CLA 5 311



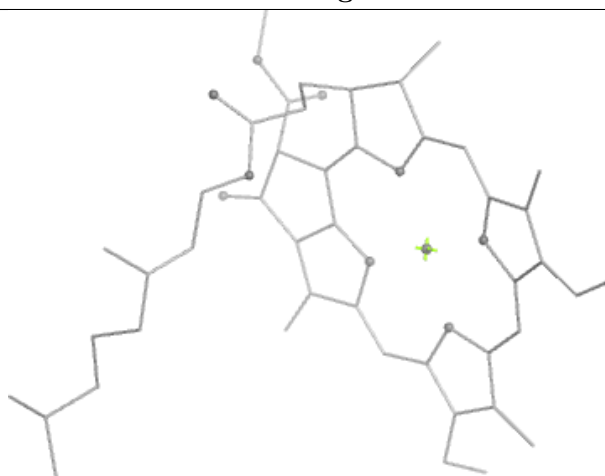
Bond lengths



Bond angles

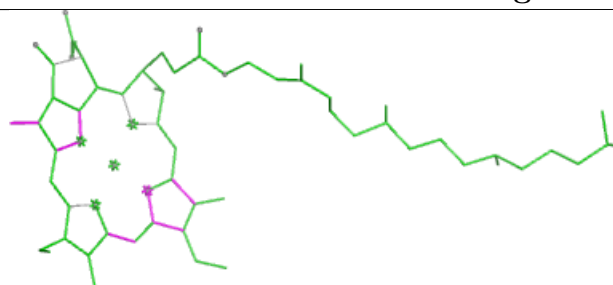


Torsions

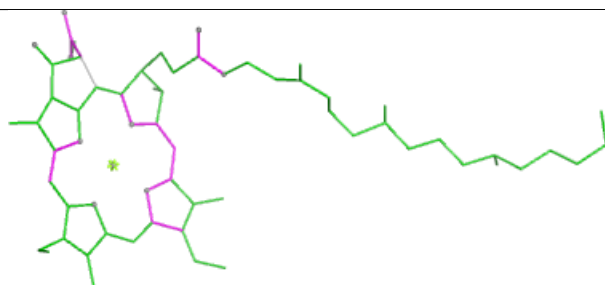


Rings

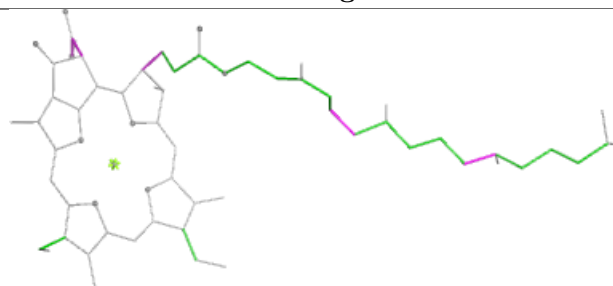
Ligand CLA A 836



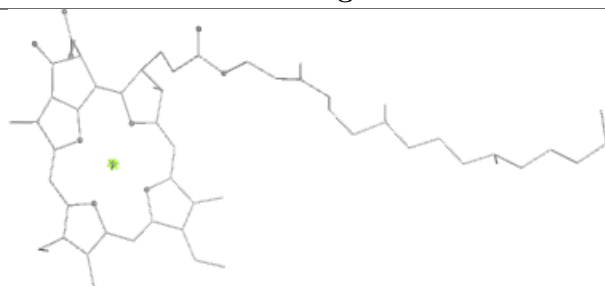
Bond lengths



Bond angles

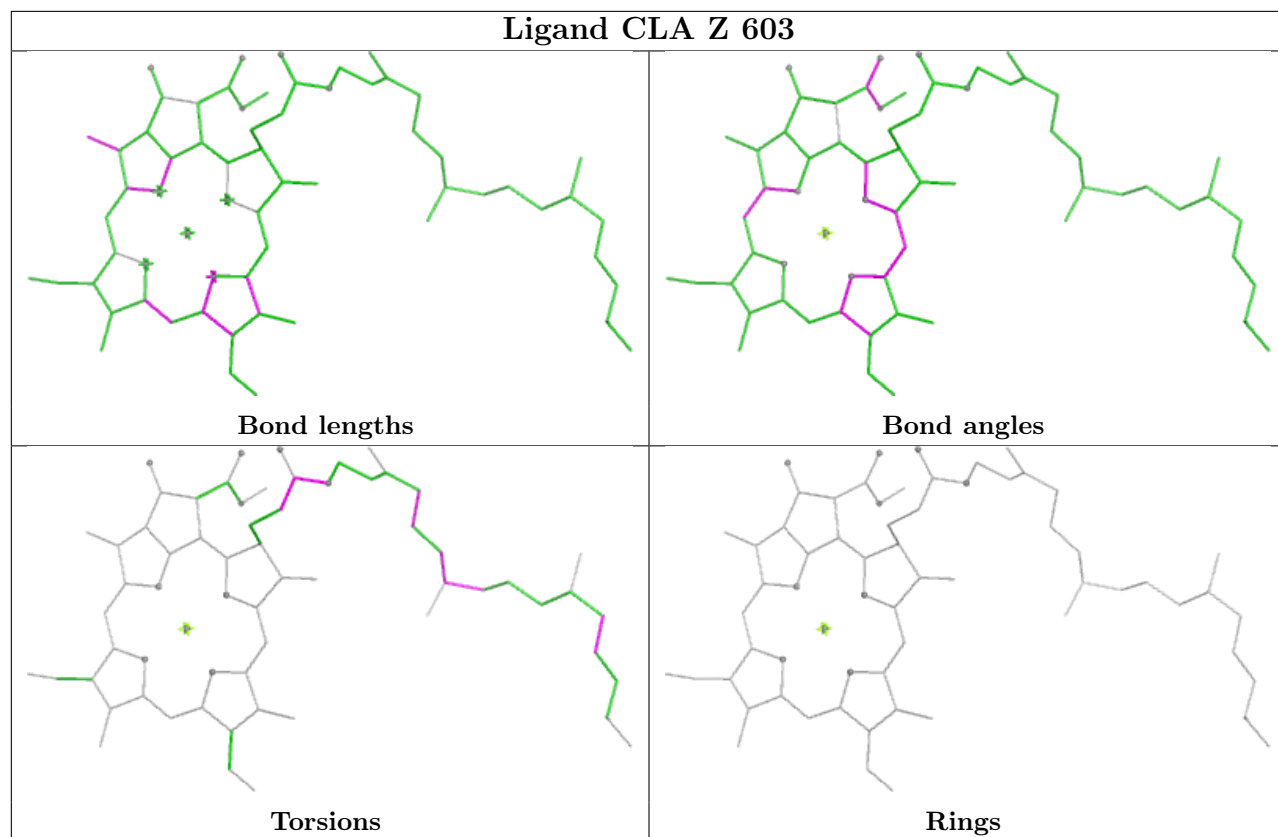


Torsions

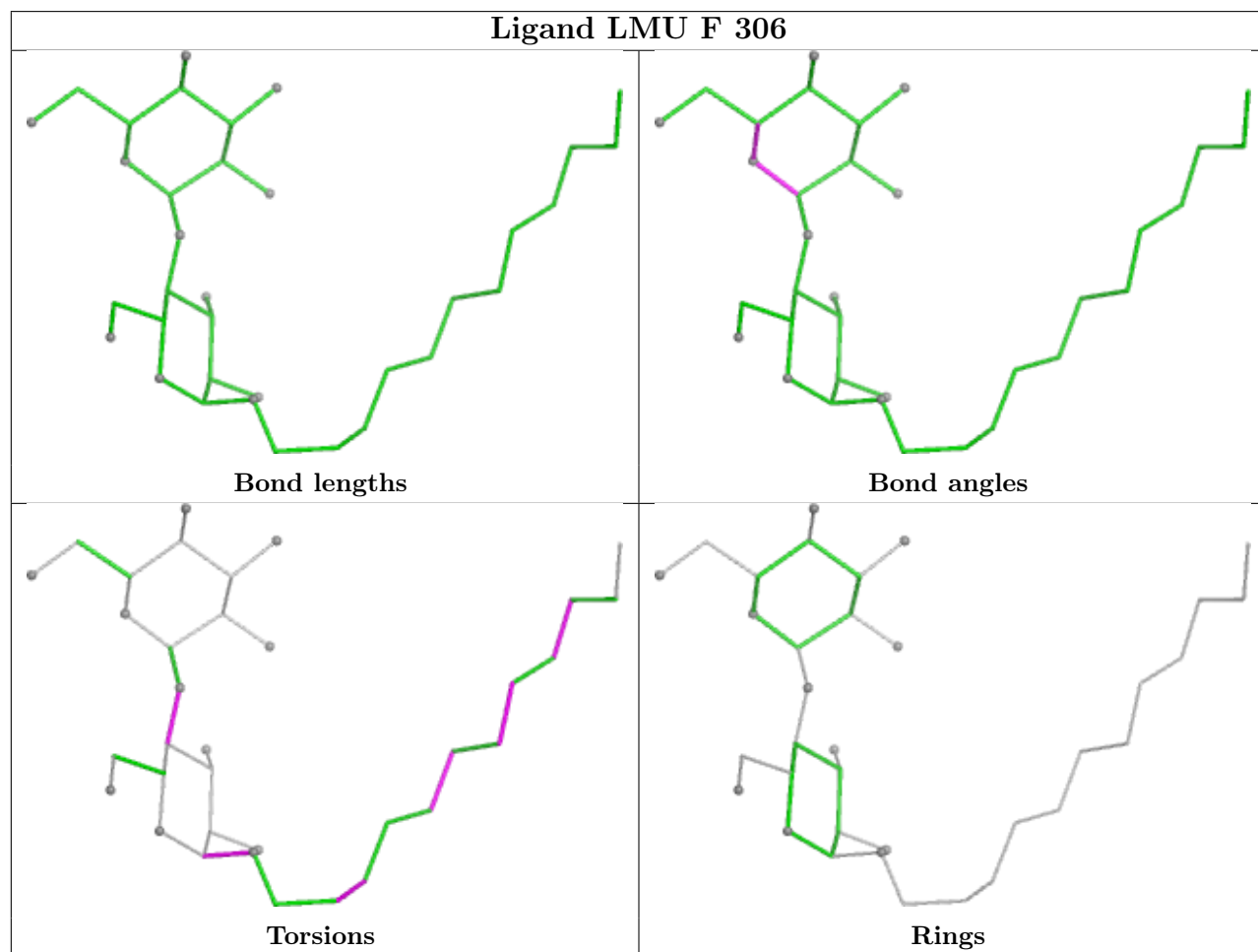


Rings

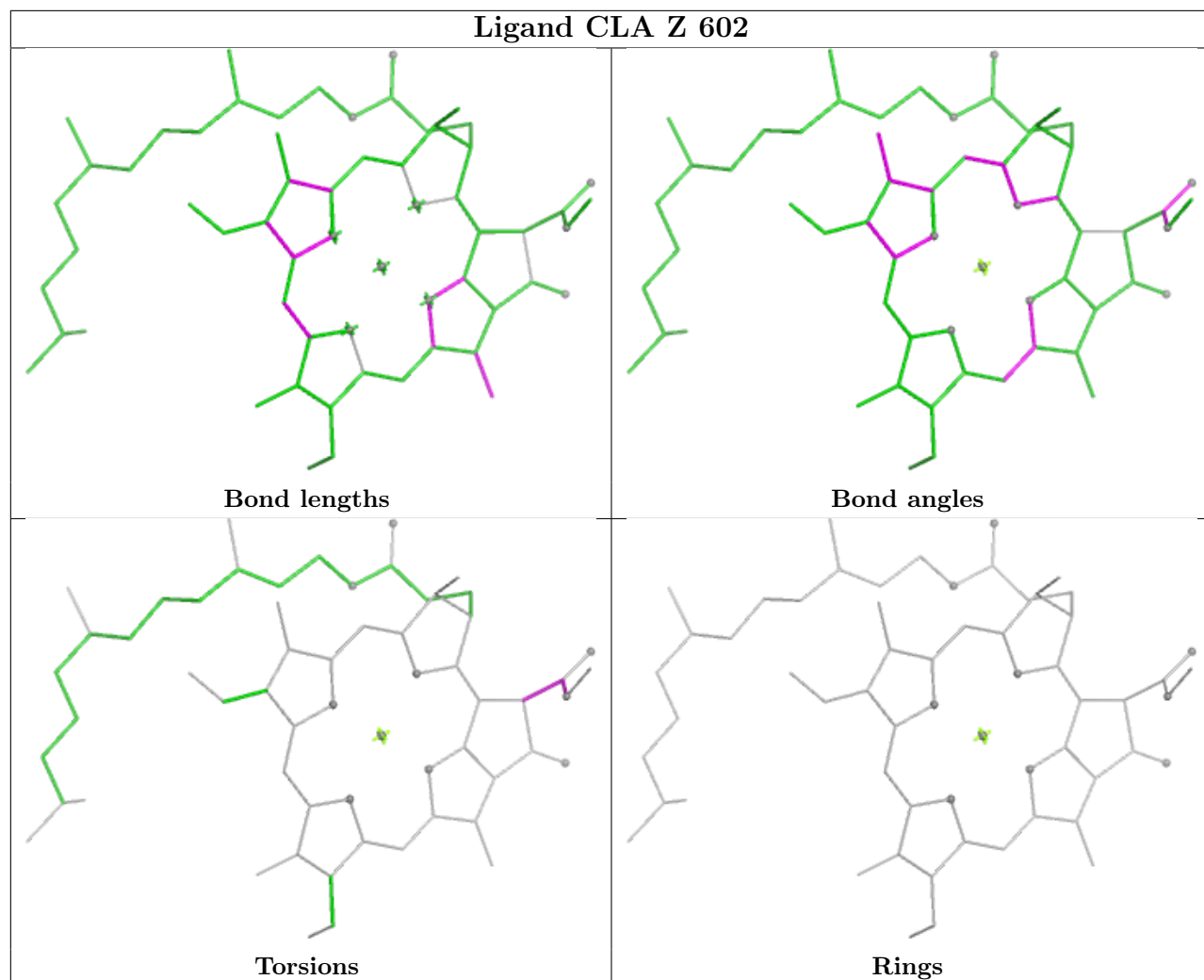
Ligand CLA Z 603

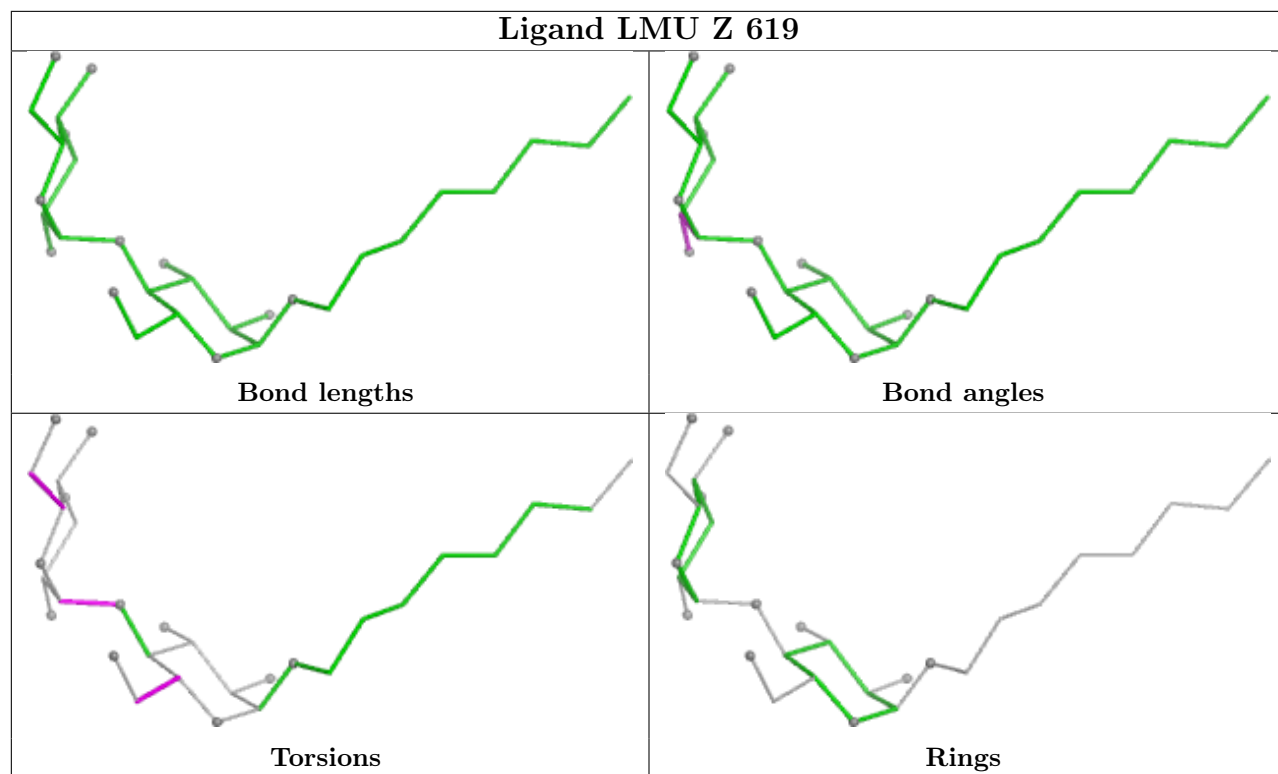


Ligand LMU F 306

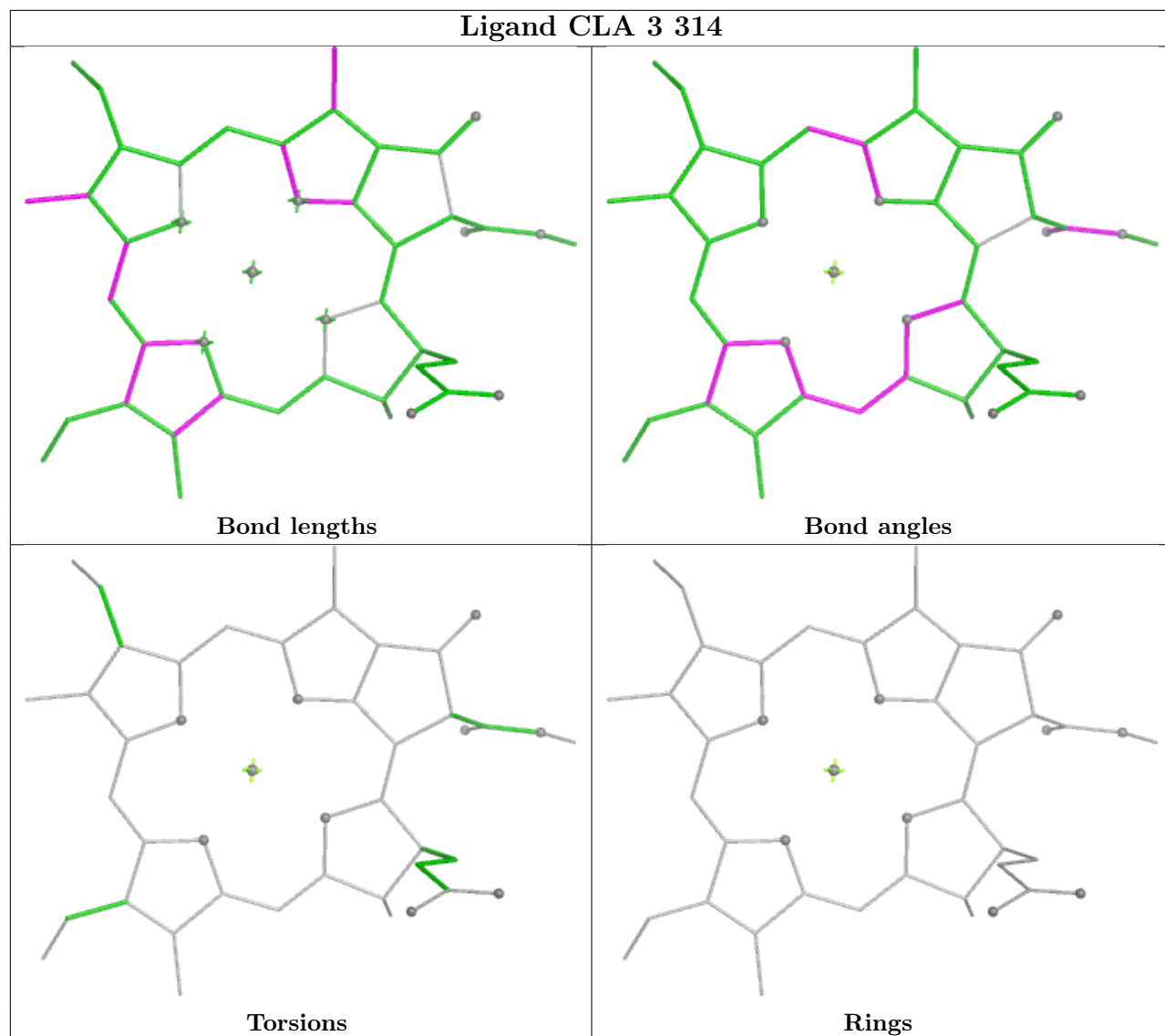


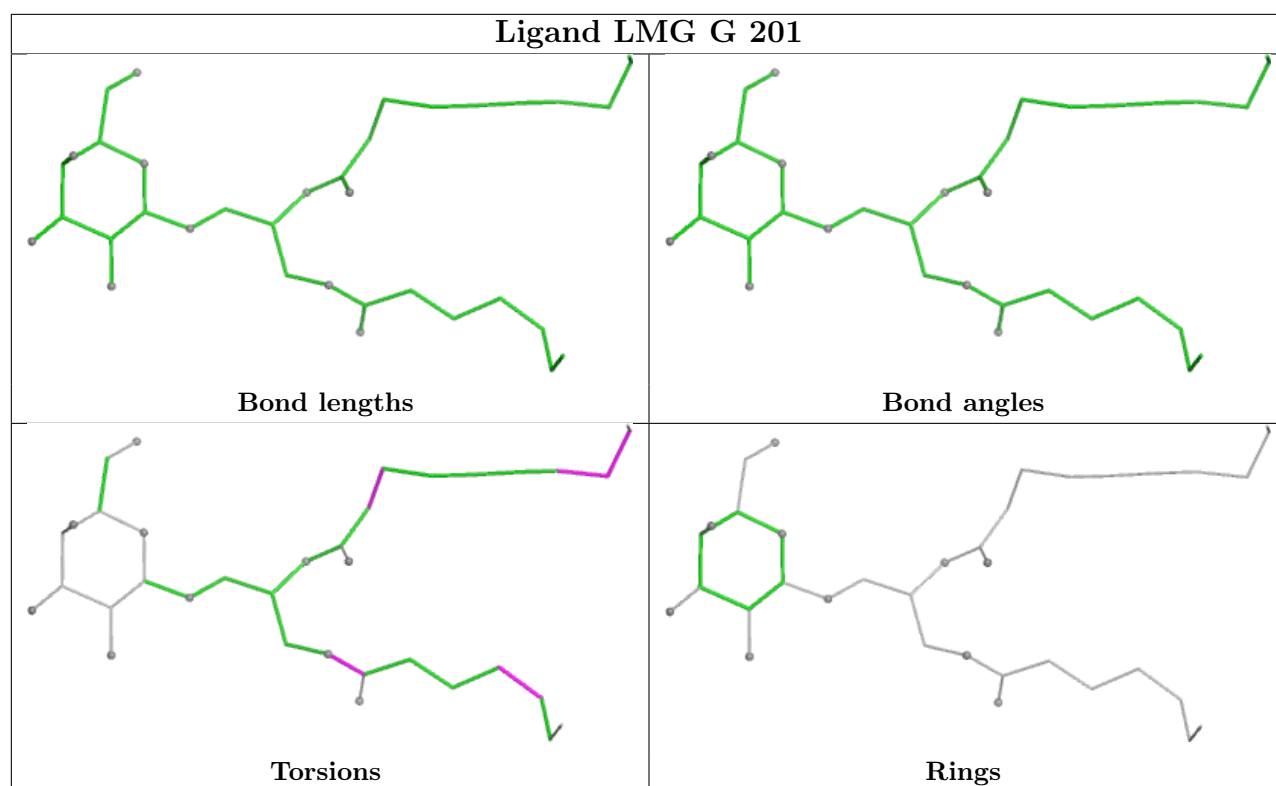
Ligand CLA Z 602



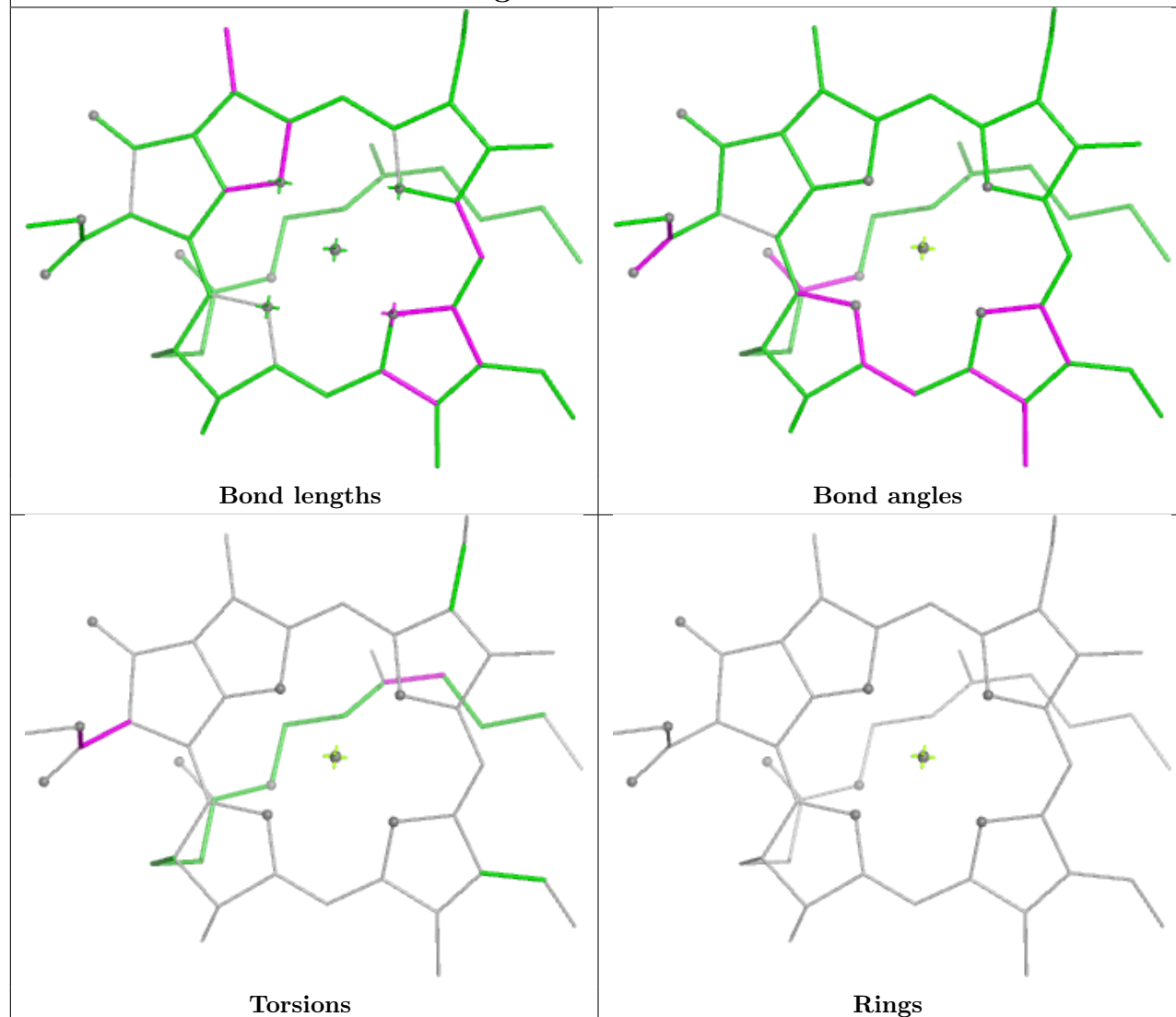


Ligand CLA 3 314

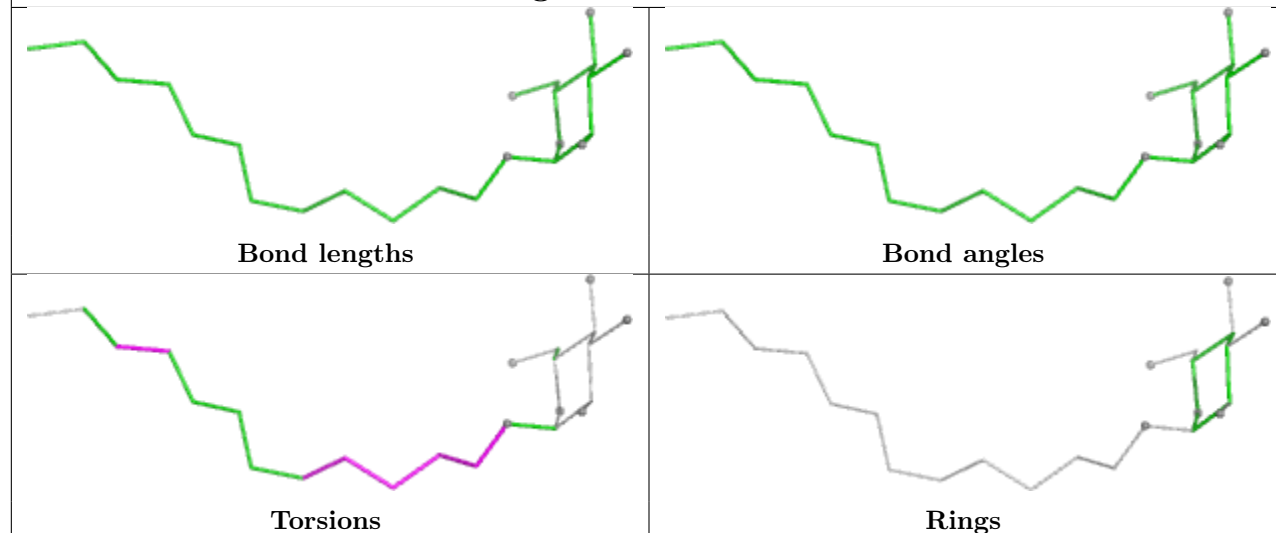


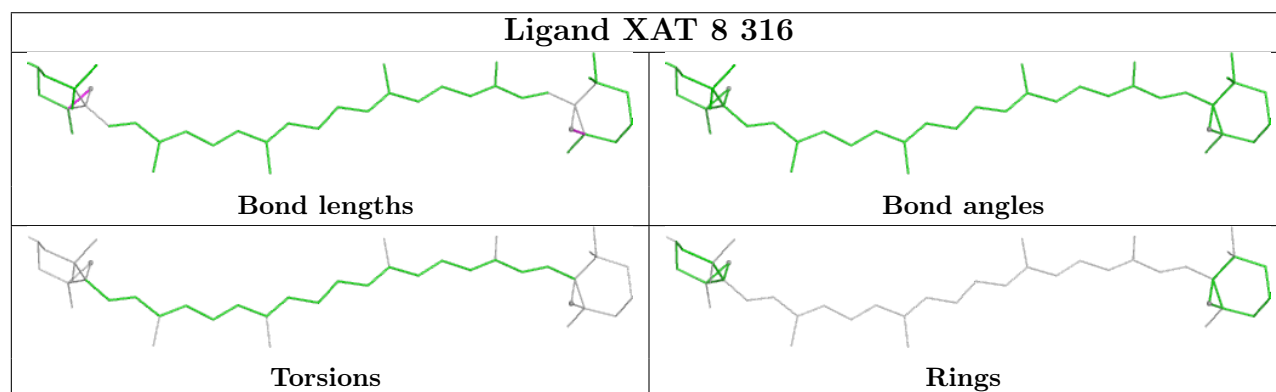
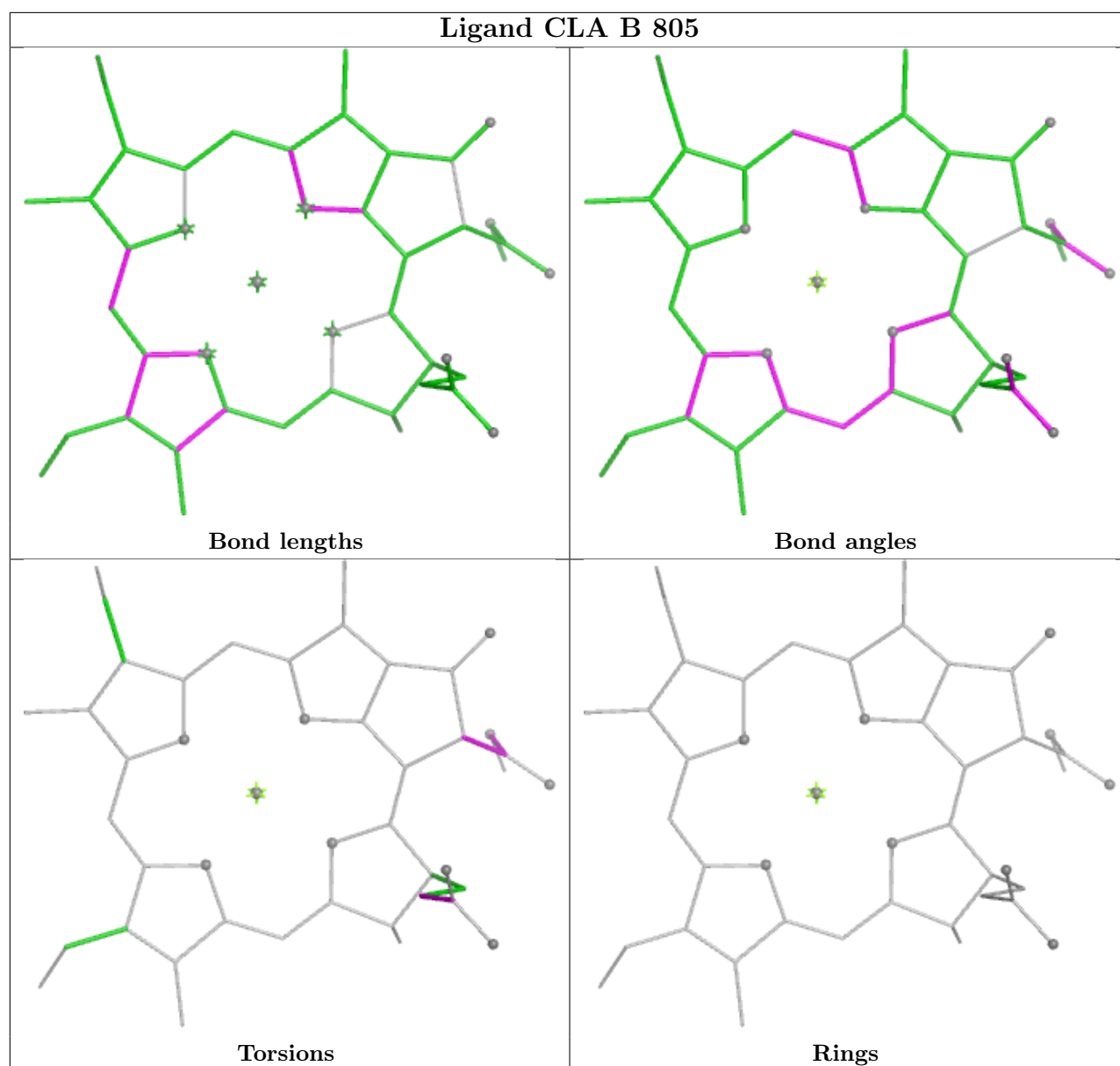


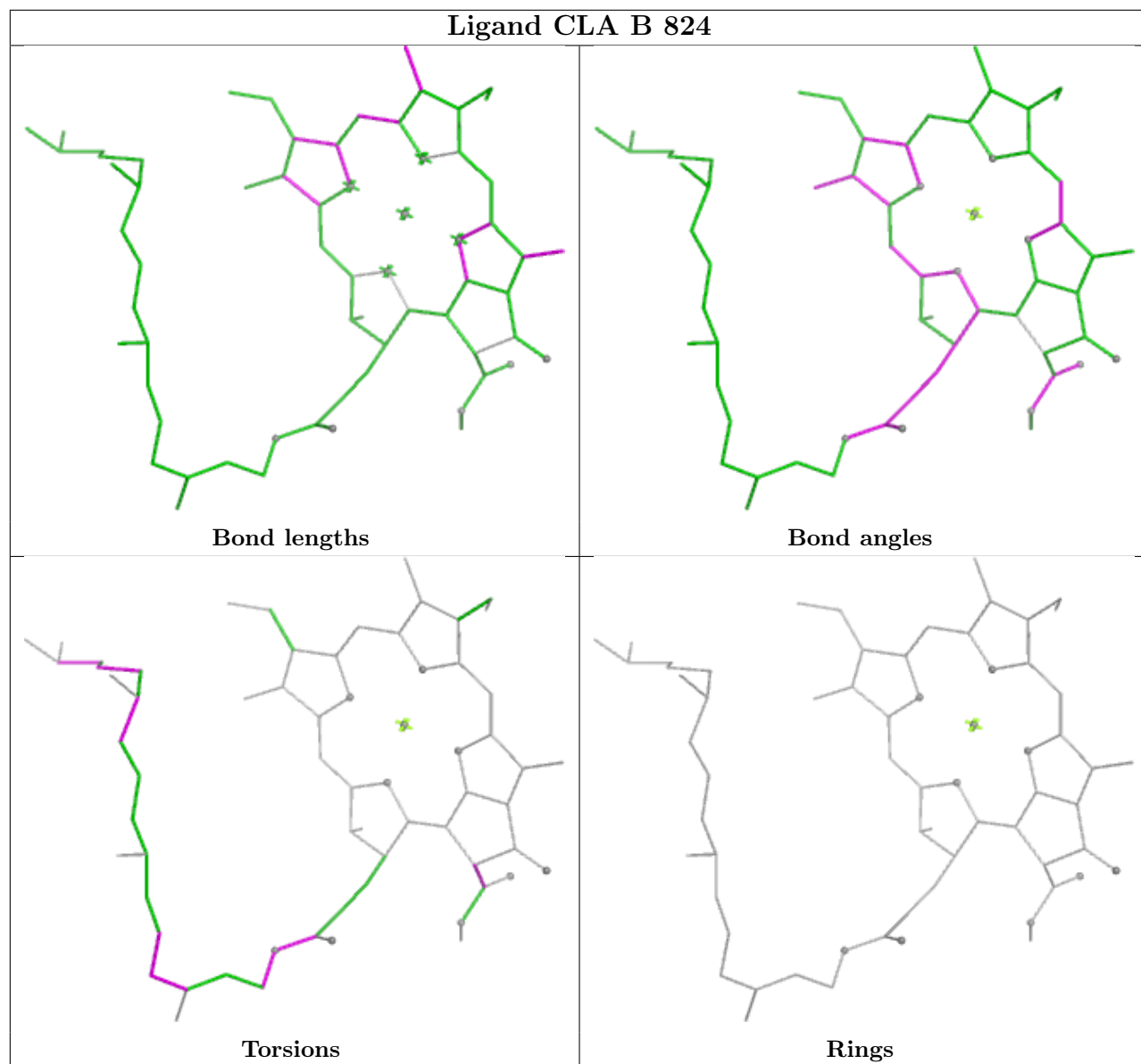
Ligand CLA 6 327

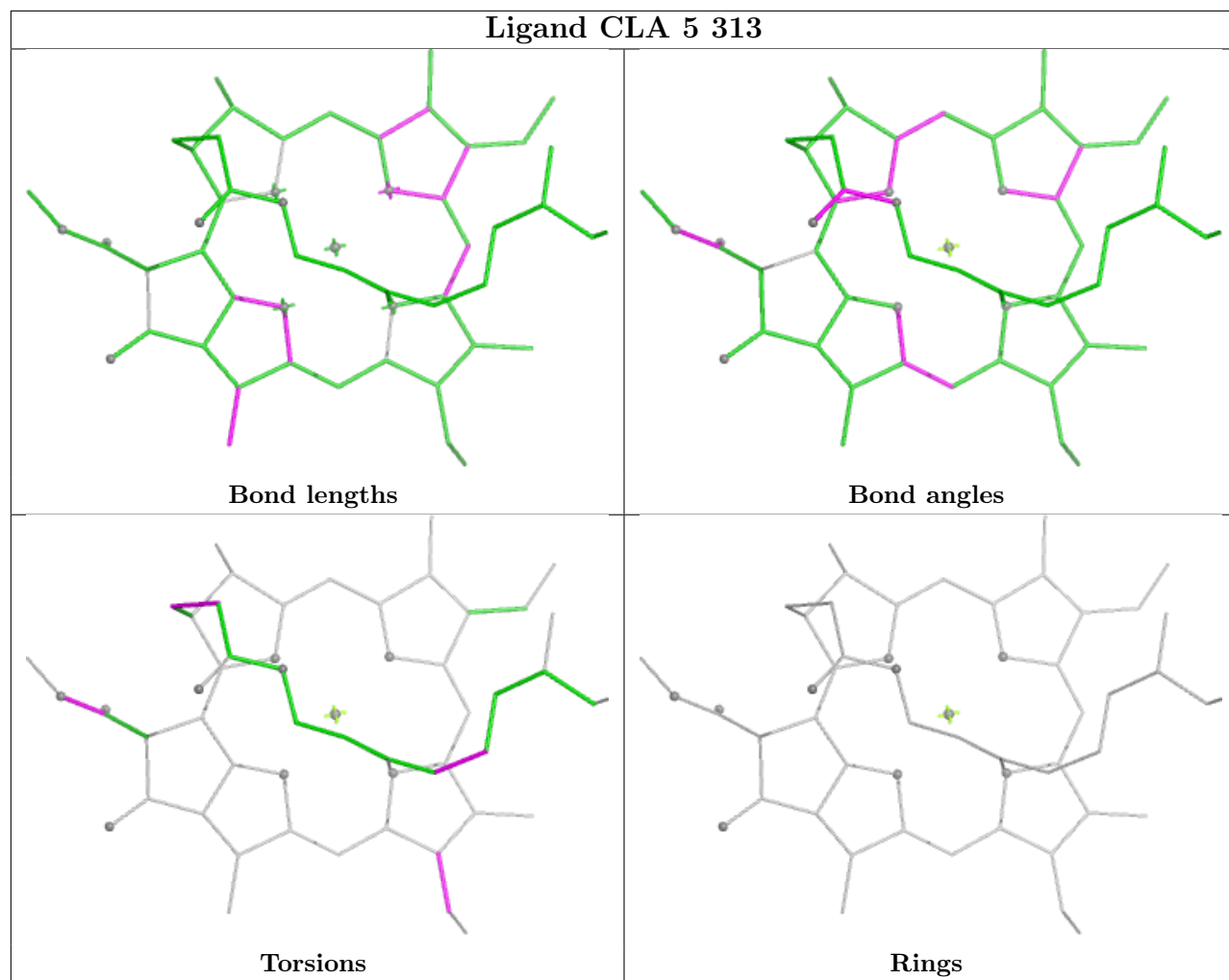


Ligand LMU 4 624

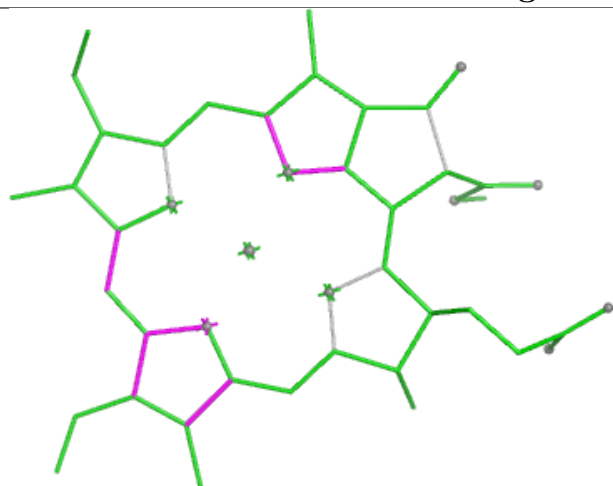




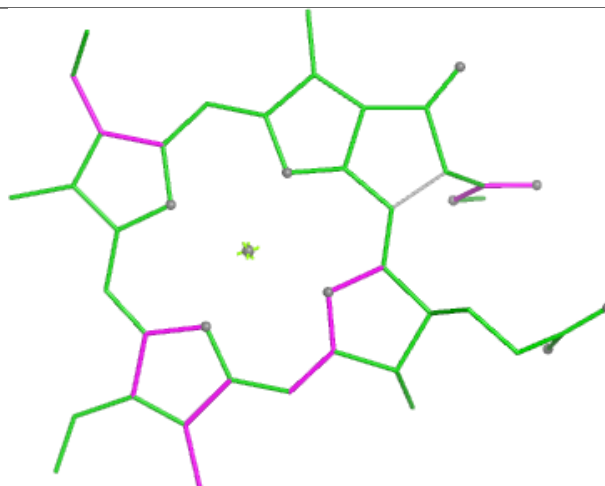




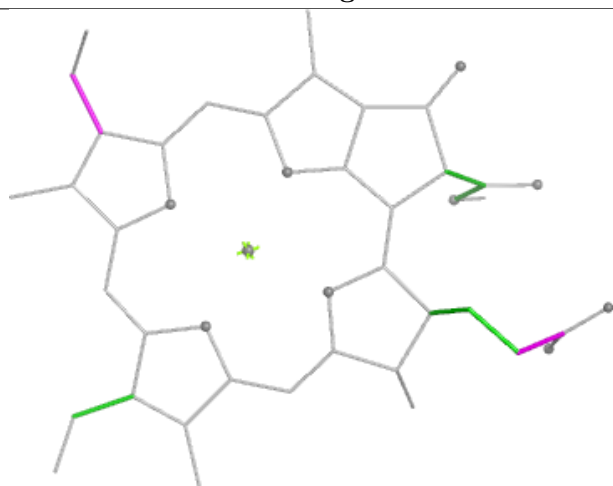
Ligand CLA 5 312



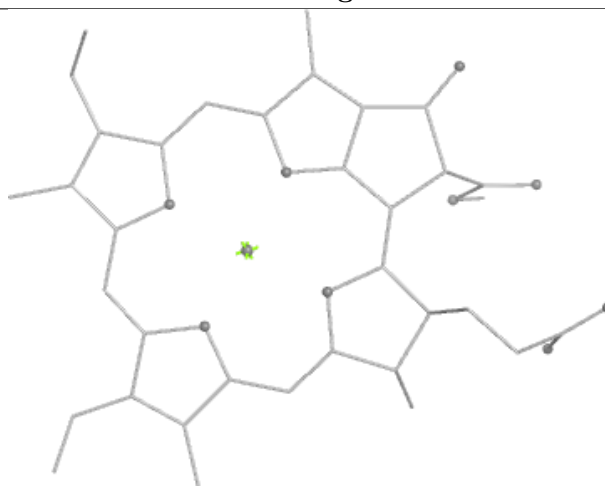
Bond lengths



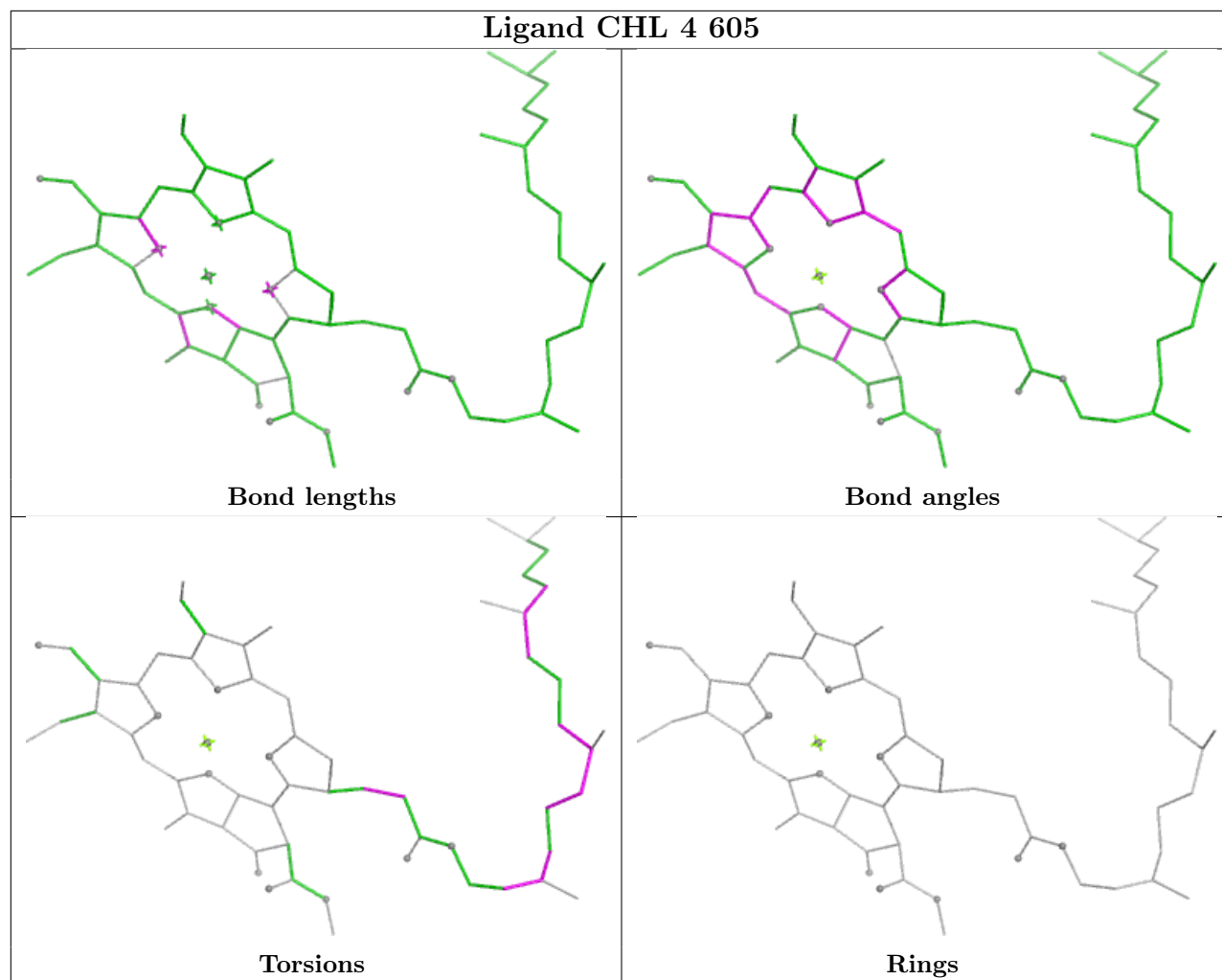
Bond angles



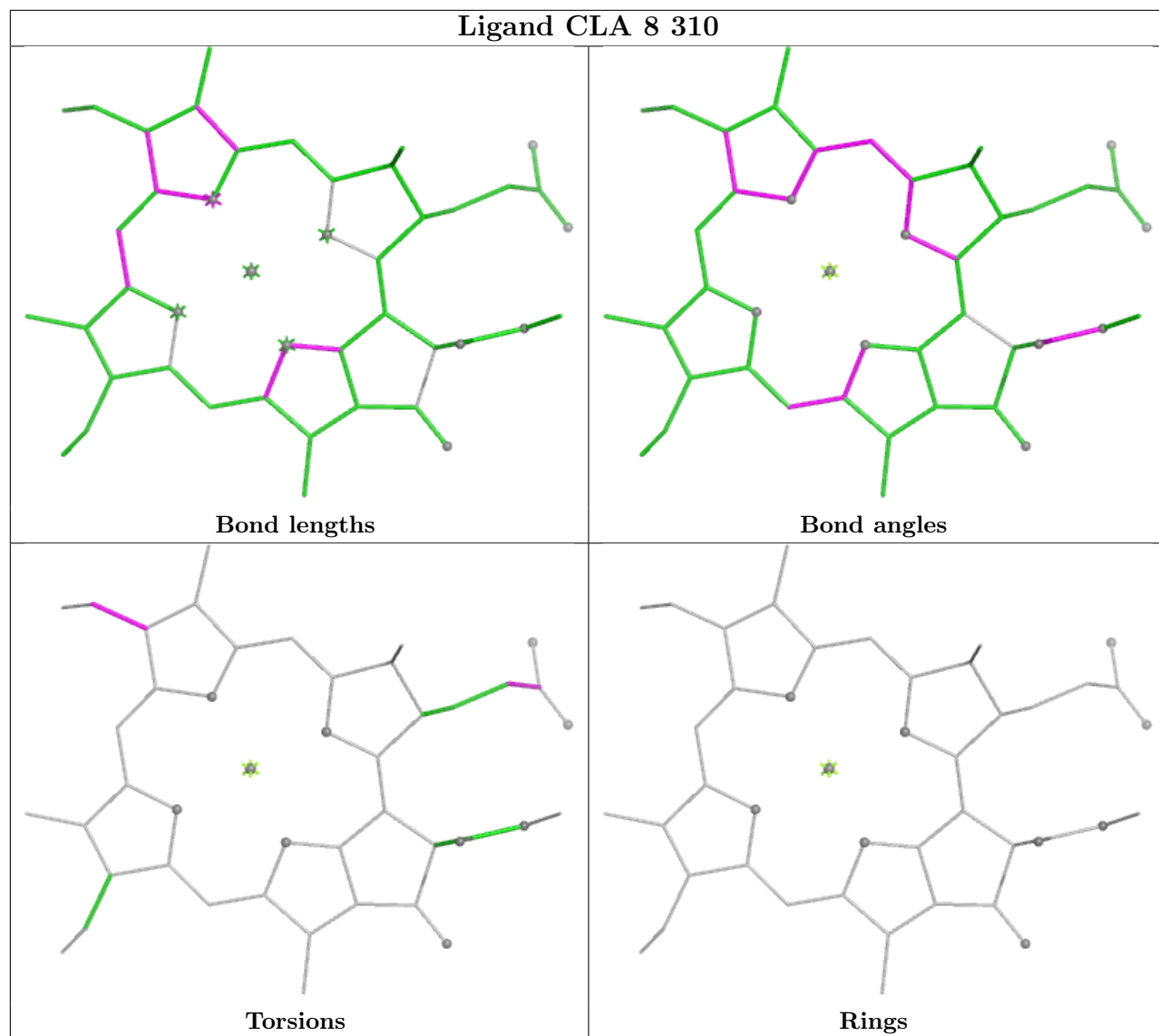
Torsions



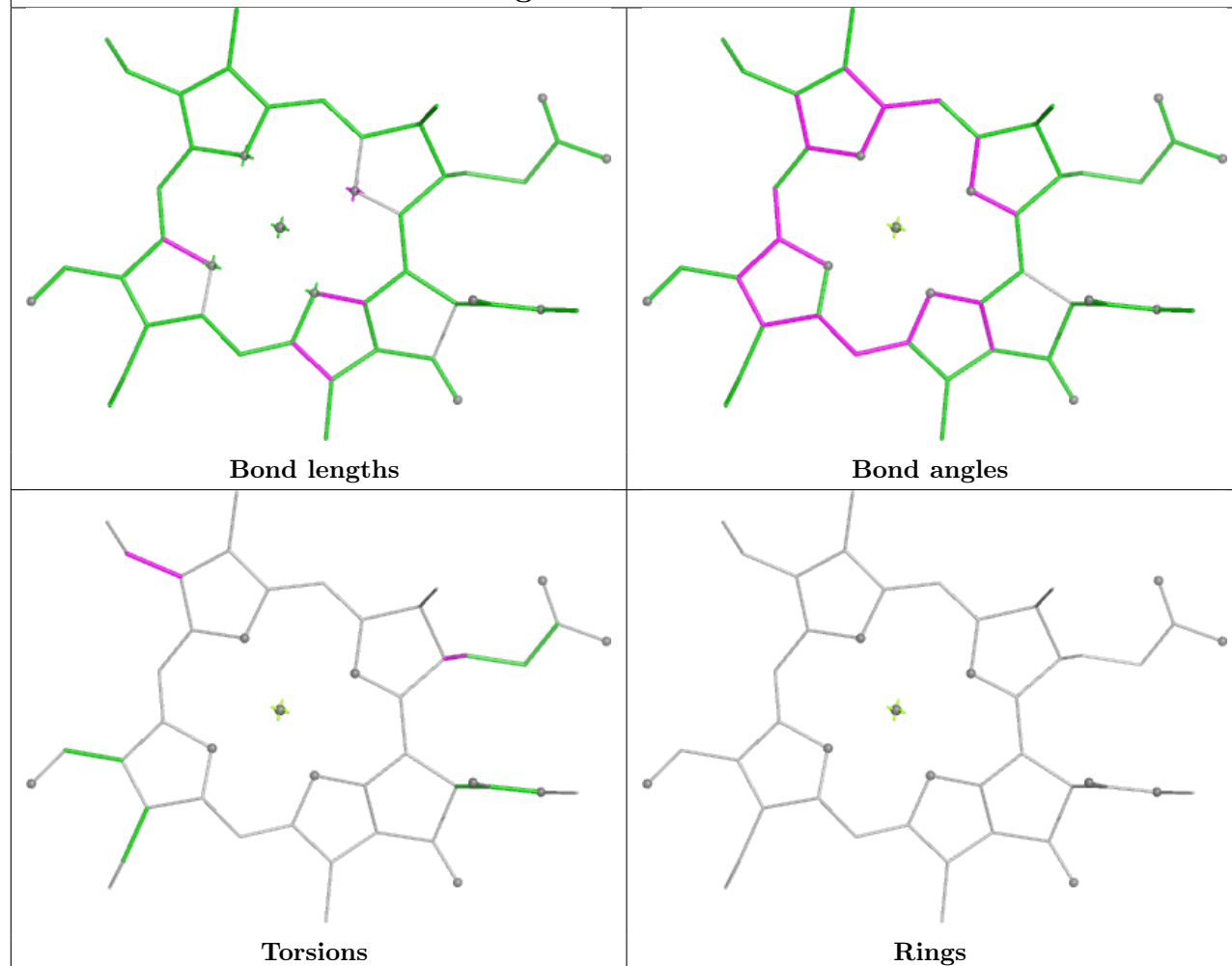
Rings



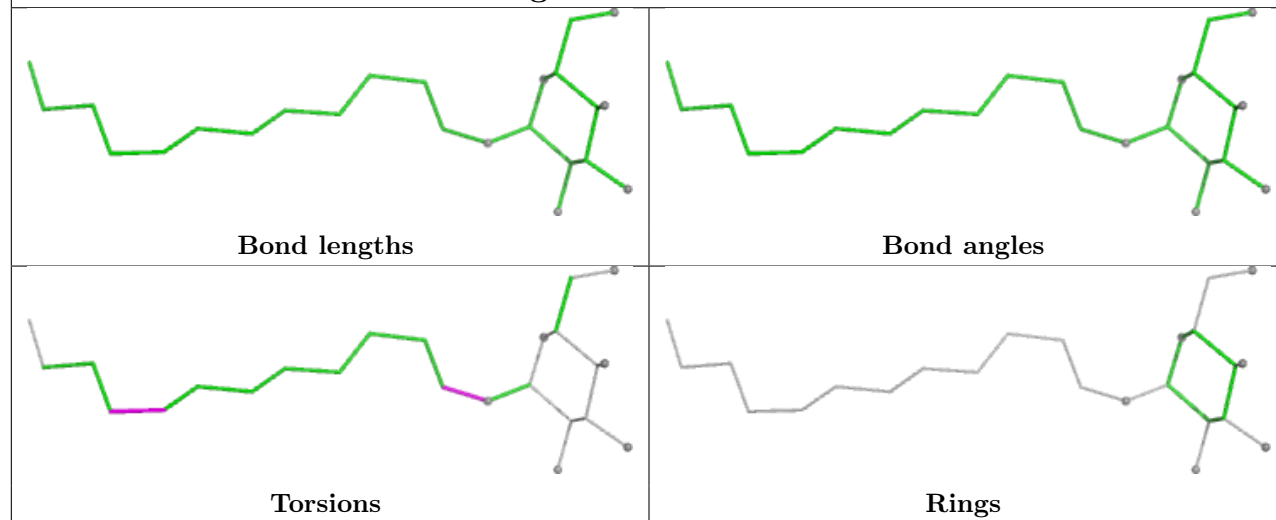
Ligand CLA 8 310

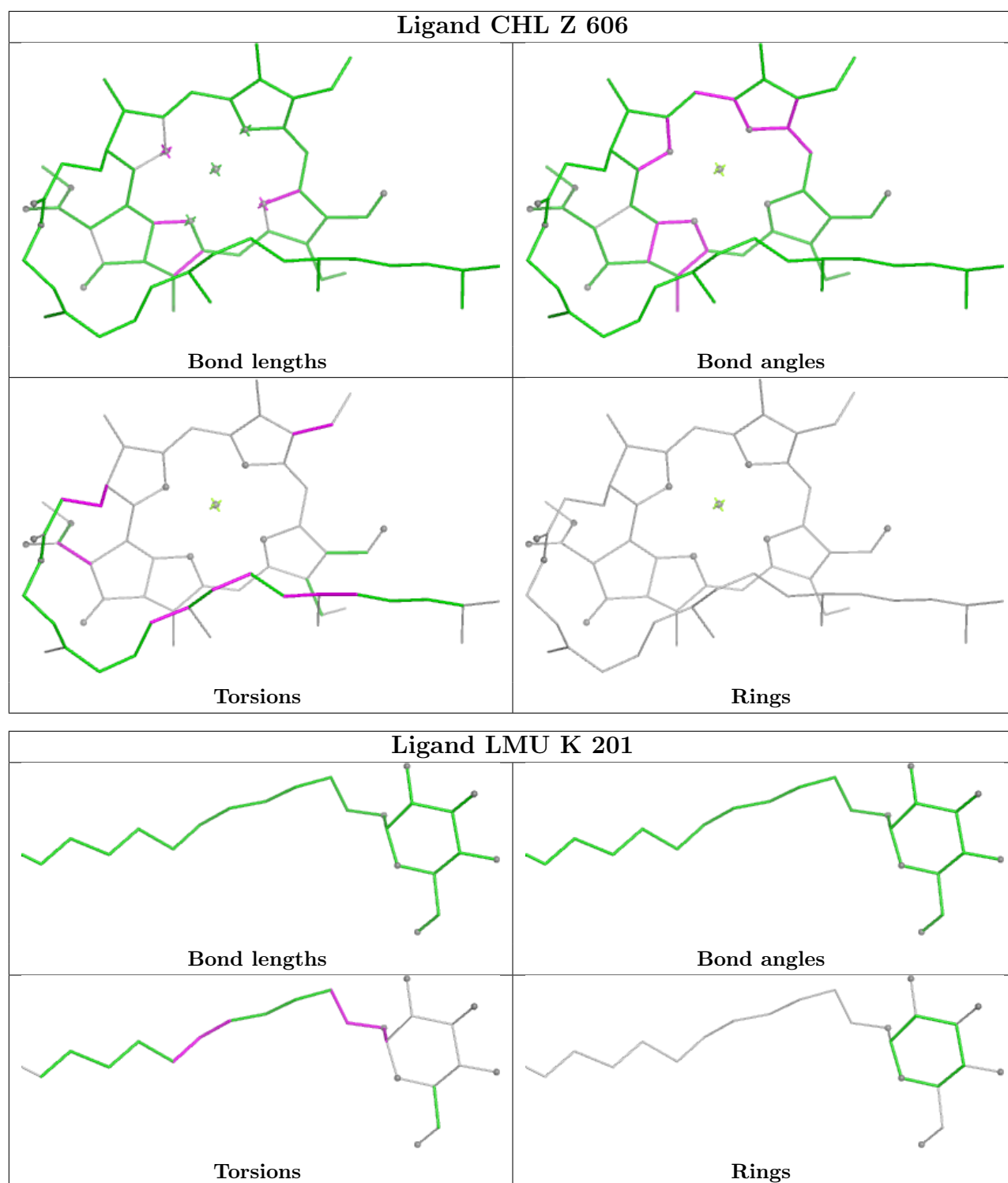


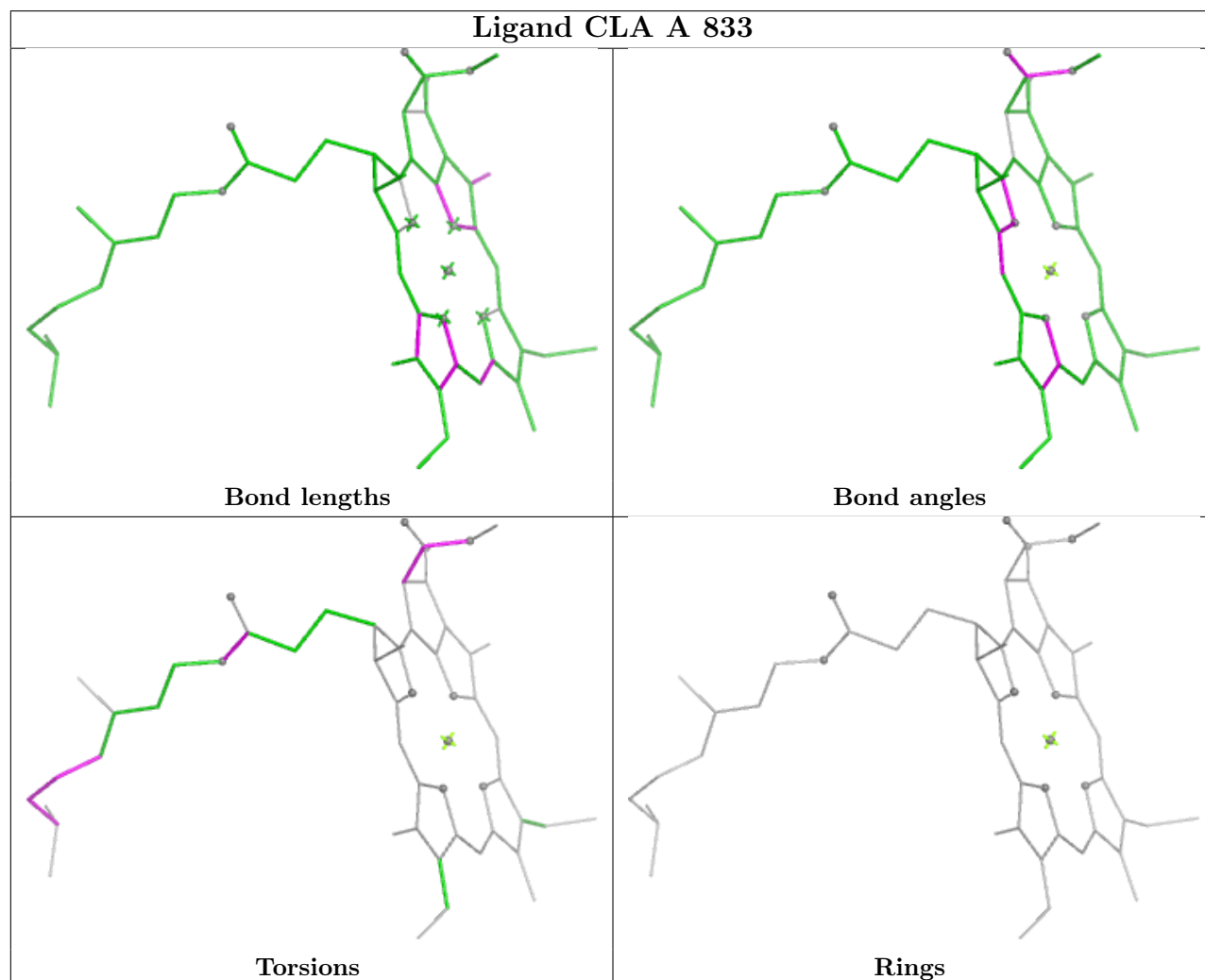
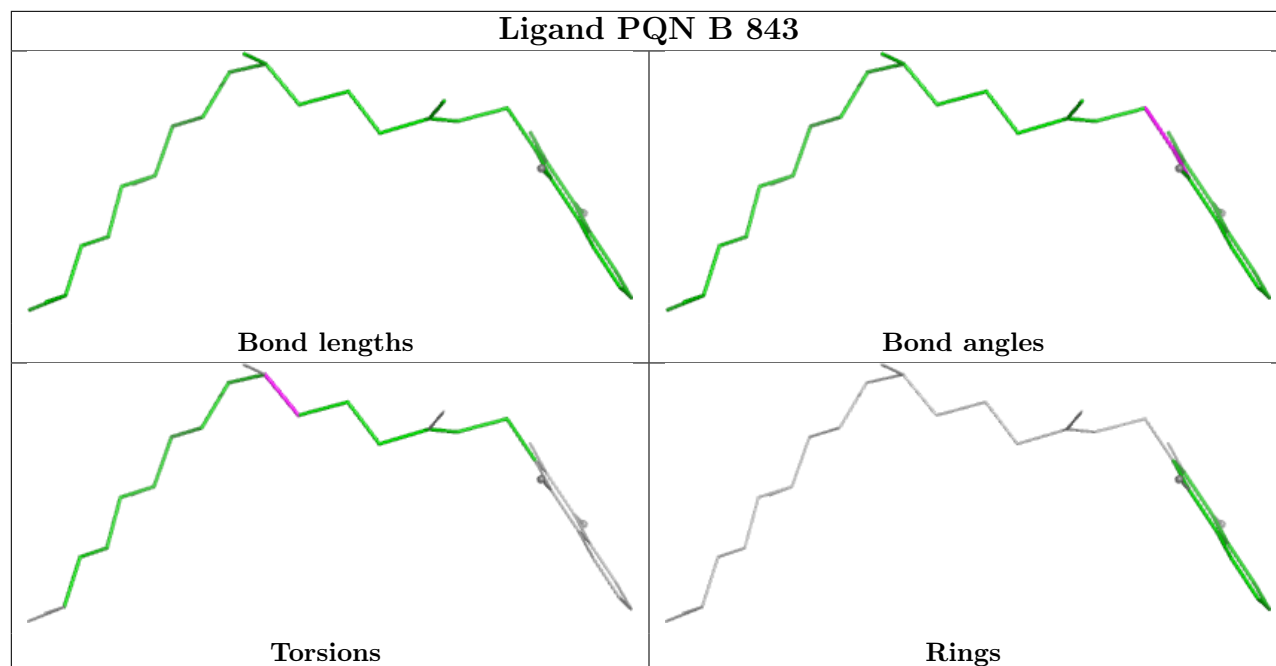
Ligand CHL Z 605

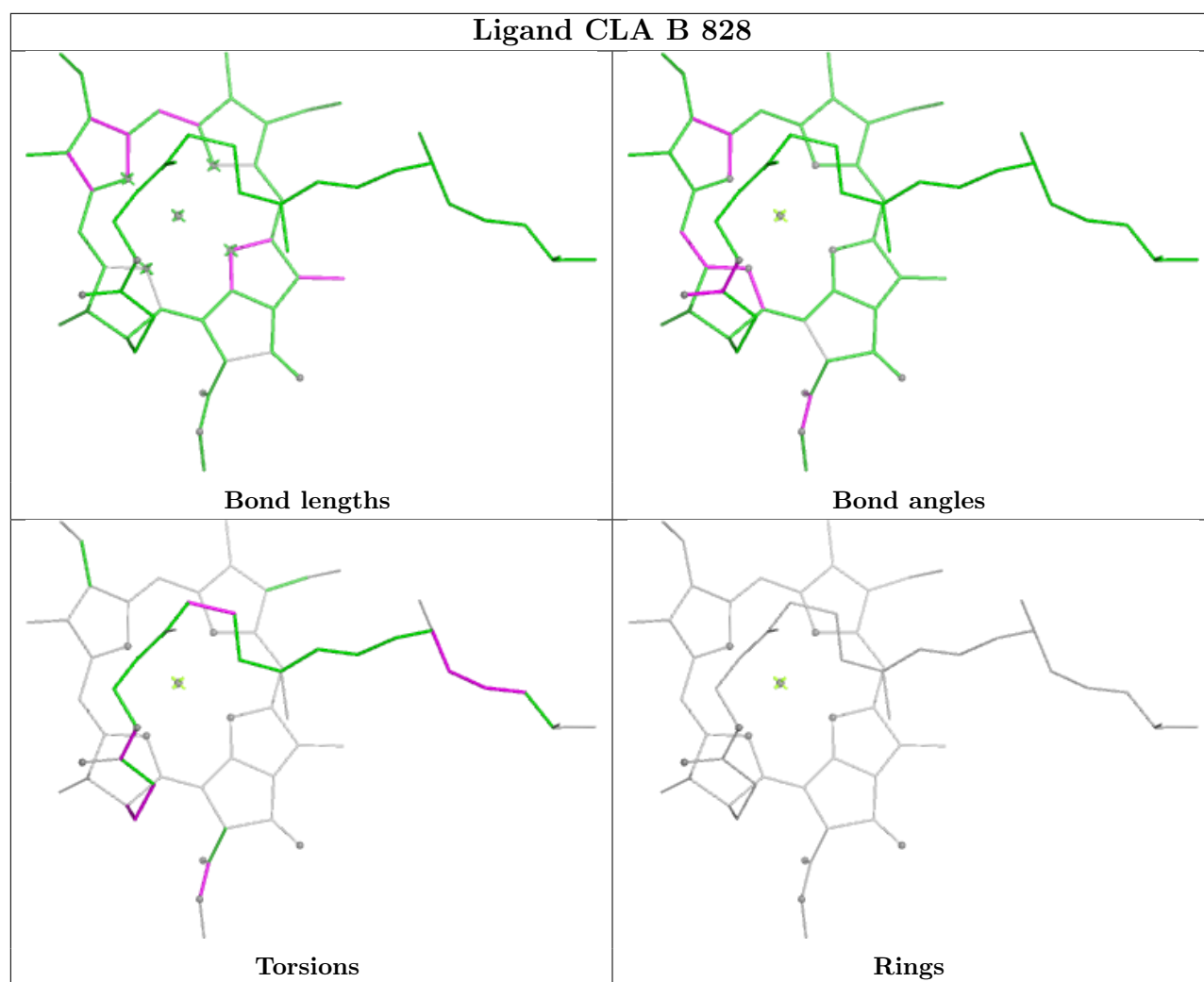


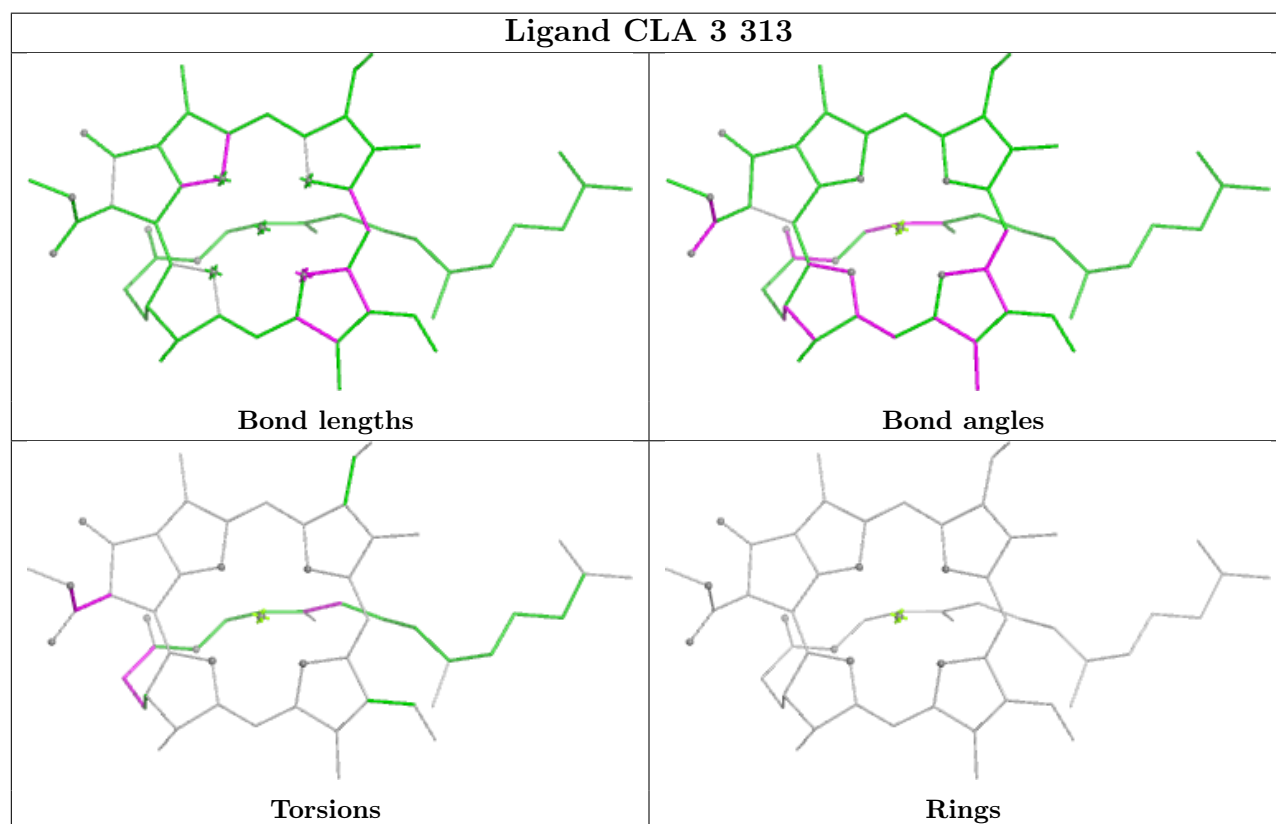
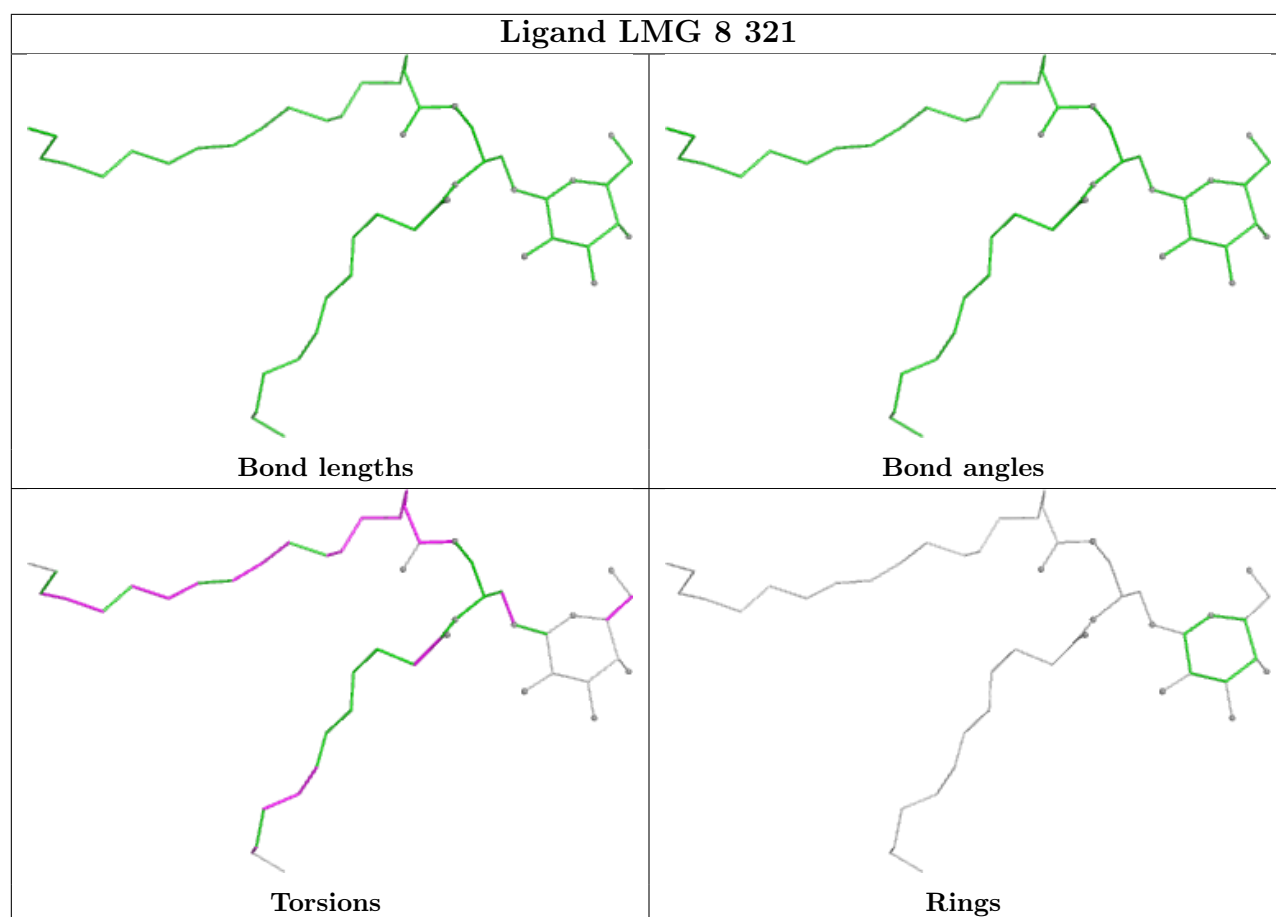
Ligand LMU Z 620

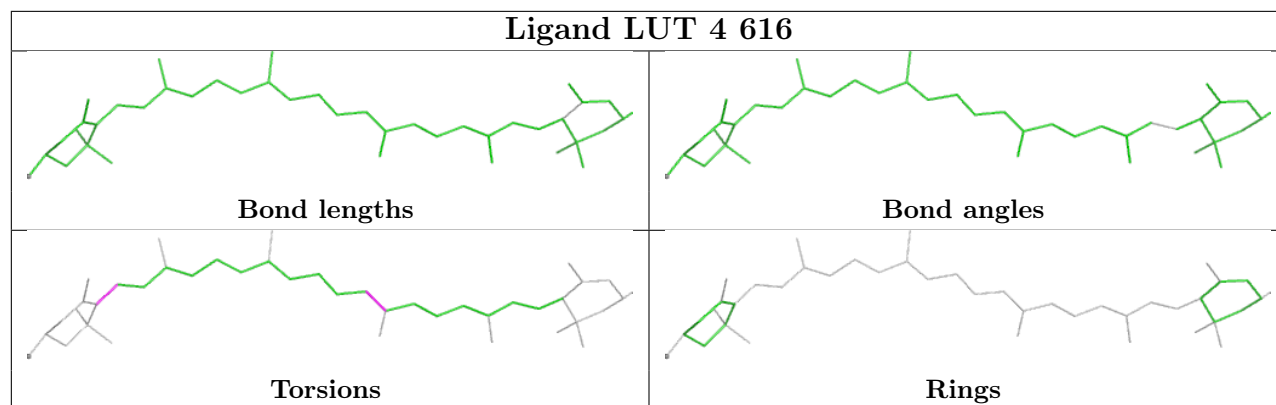
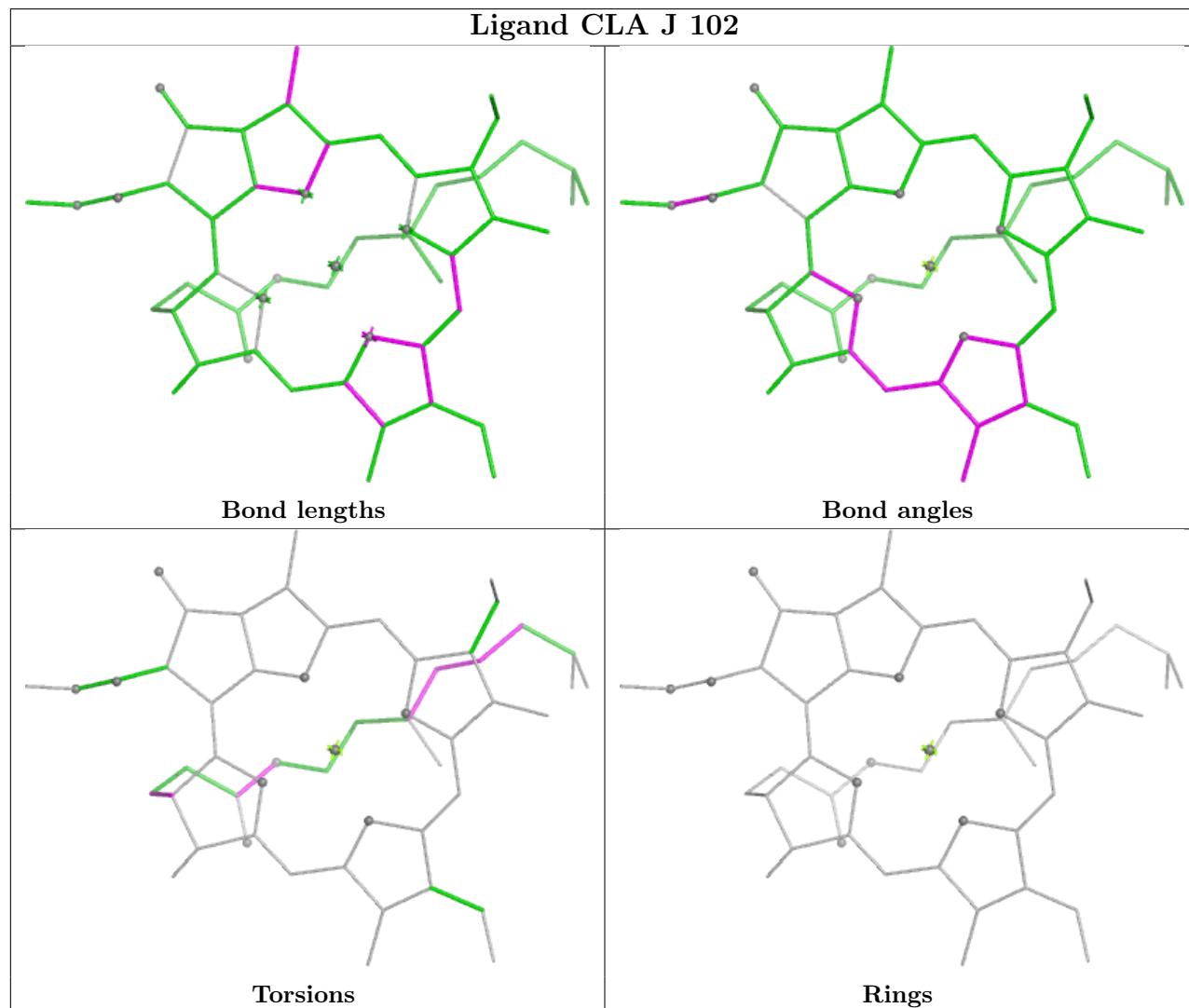


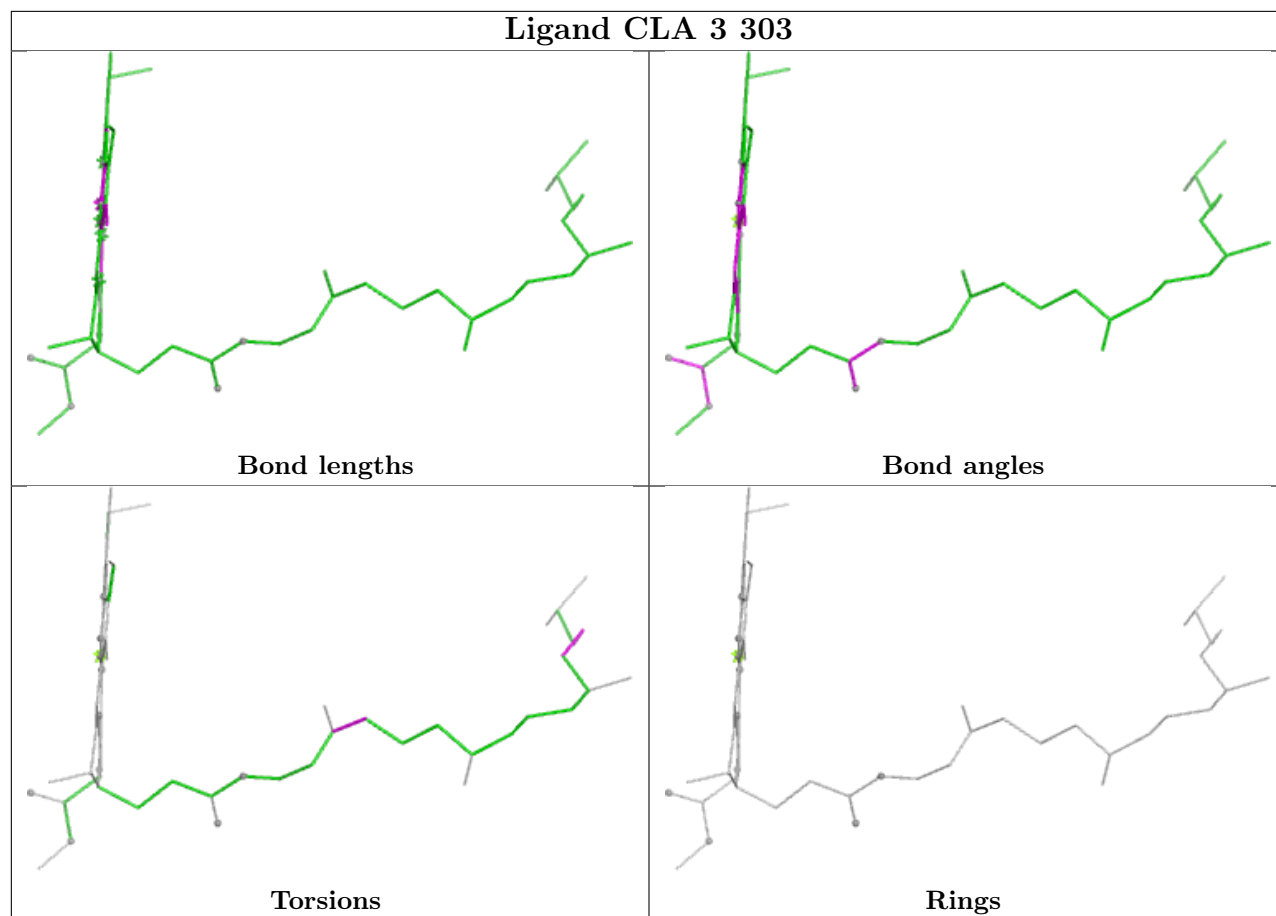




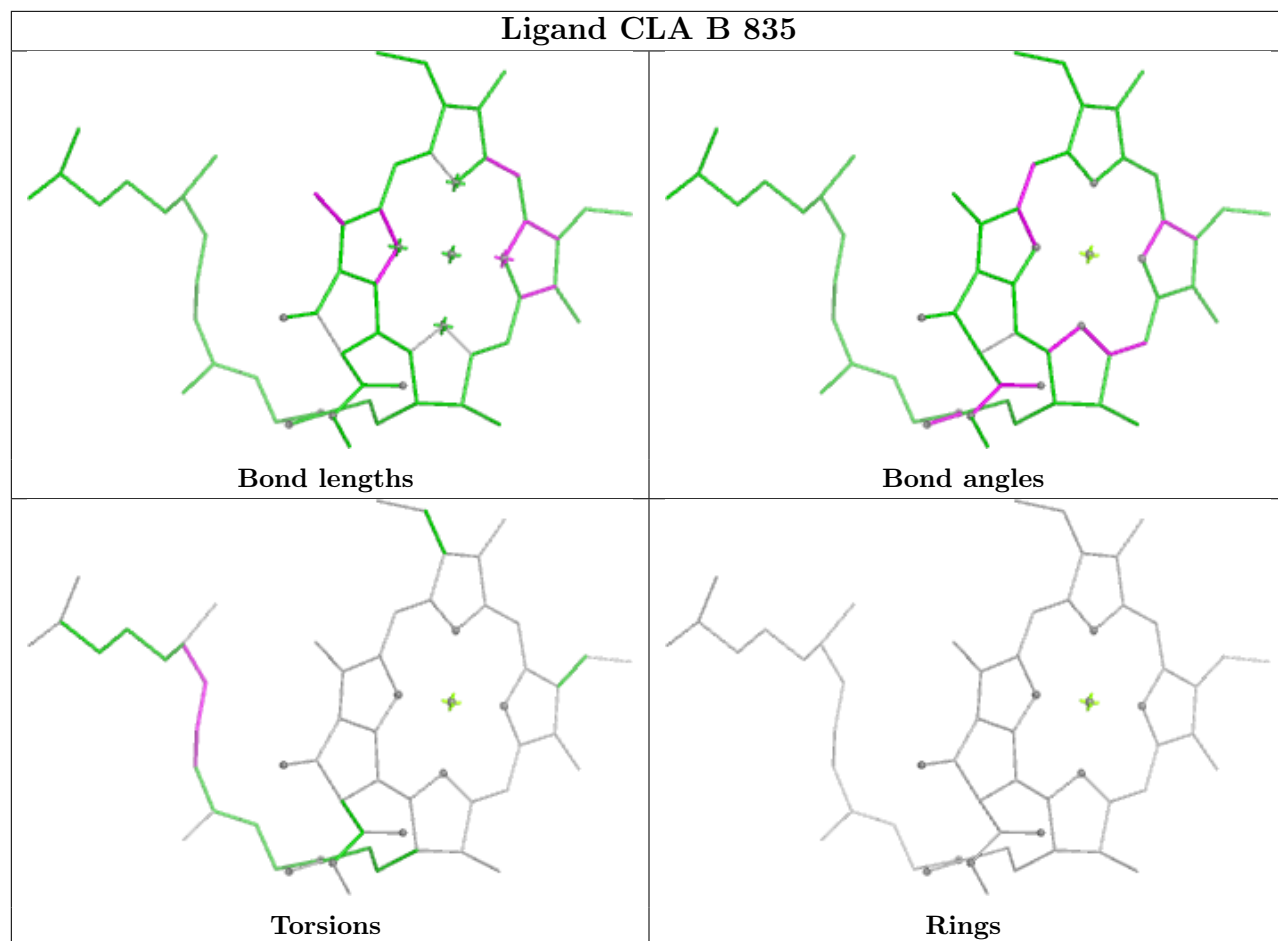




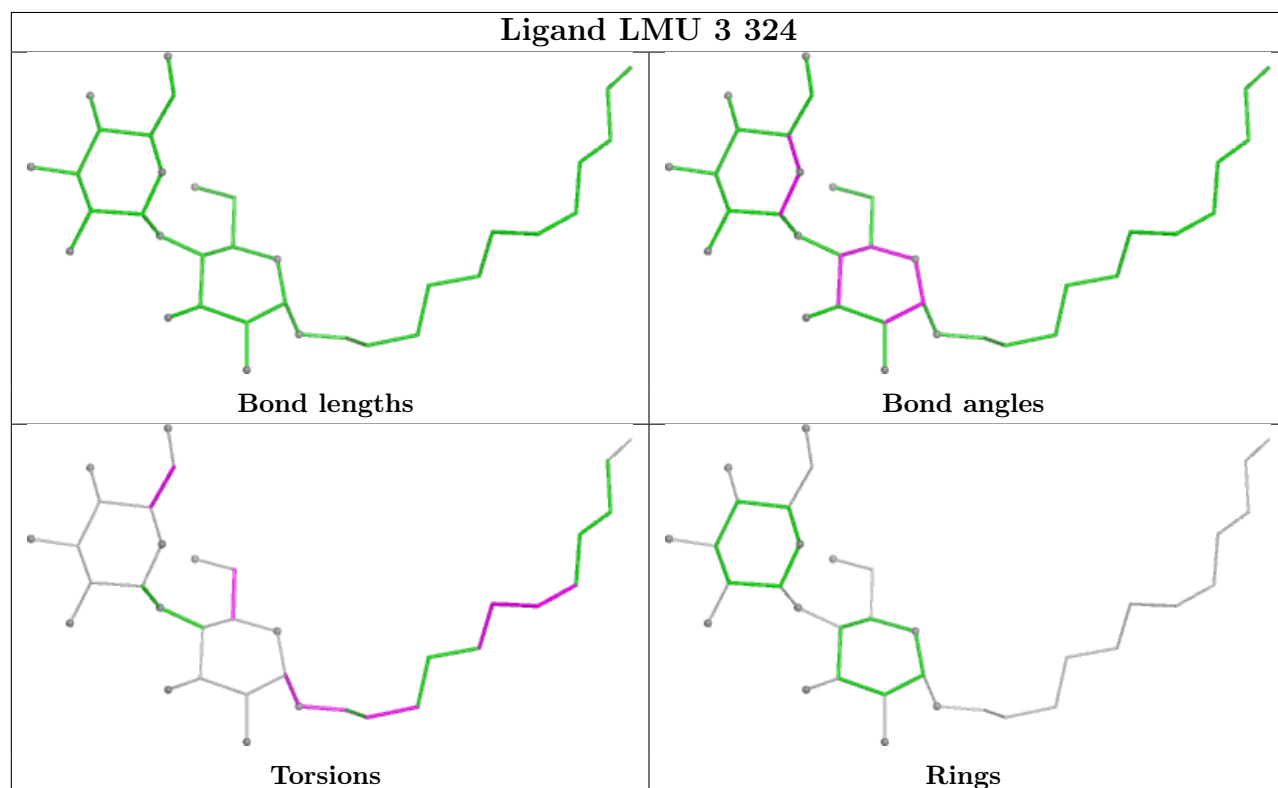
Ligand LUT 4 616**Ligand CLA J 102**

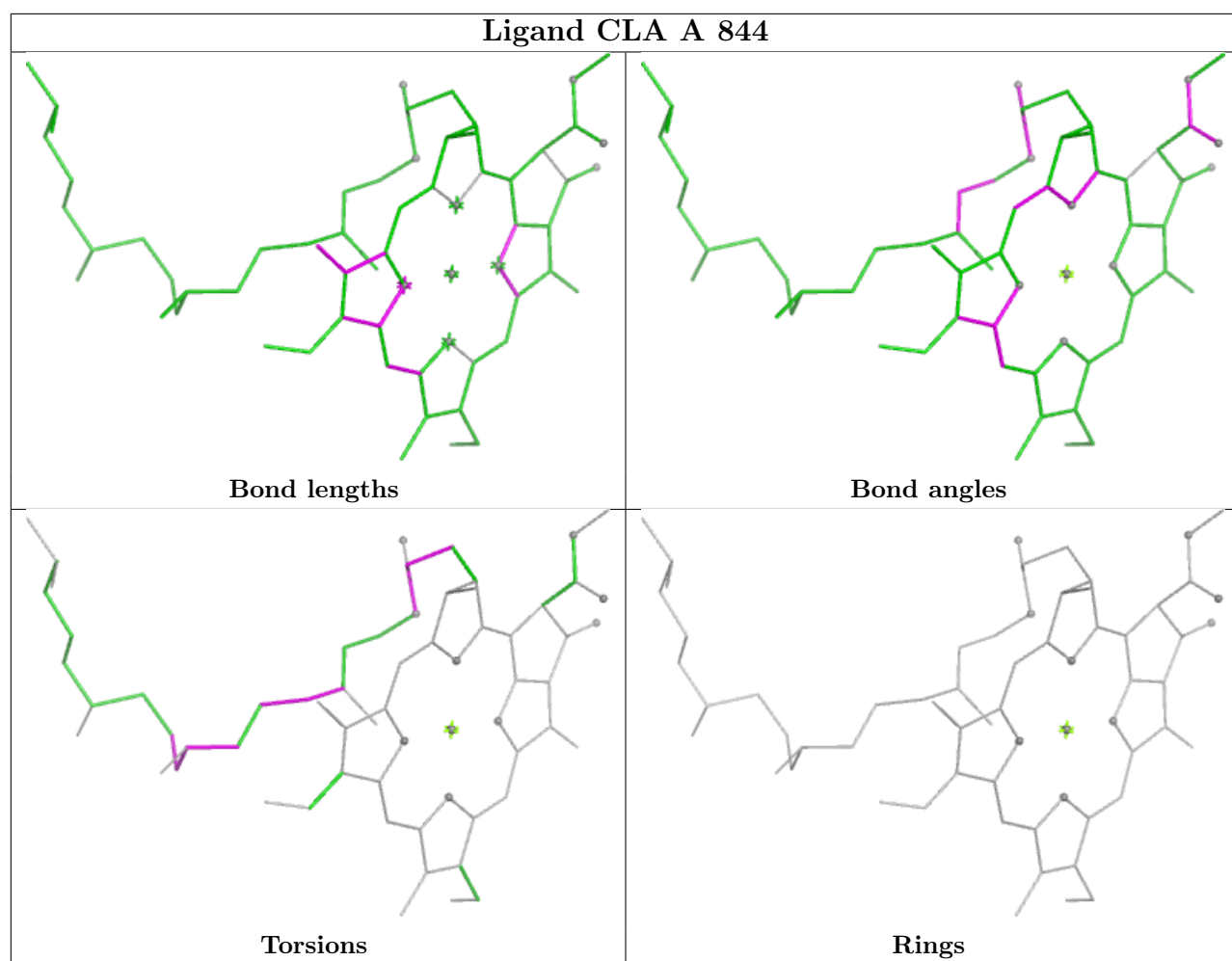


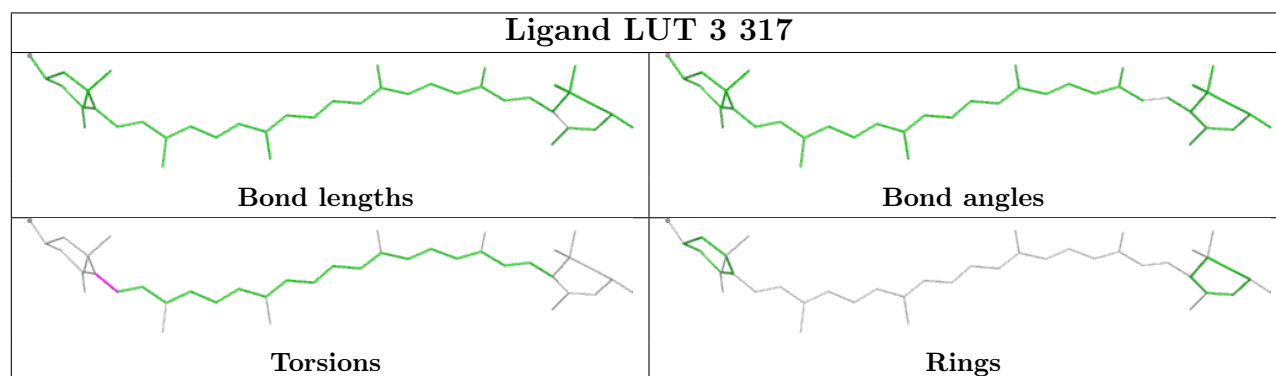
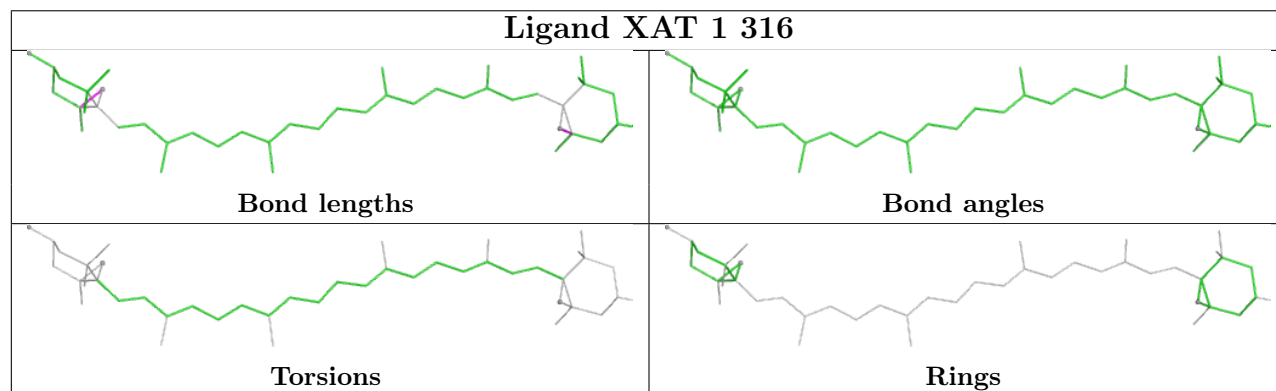
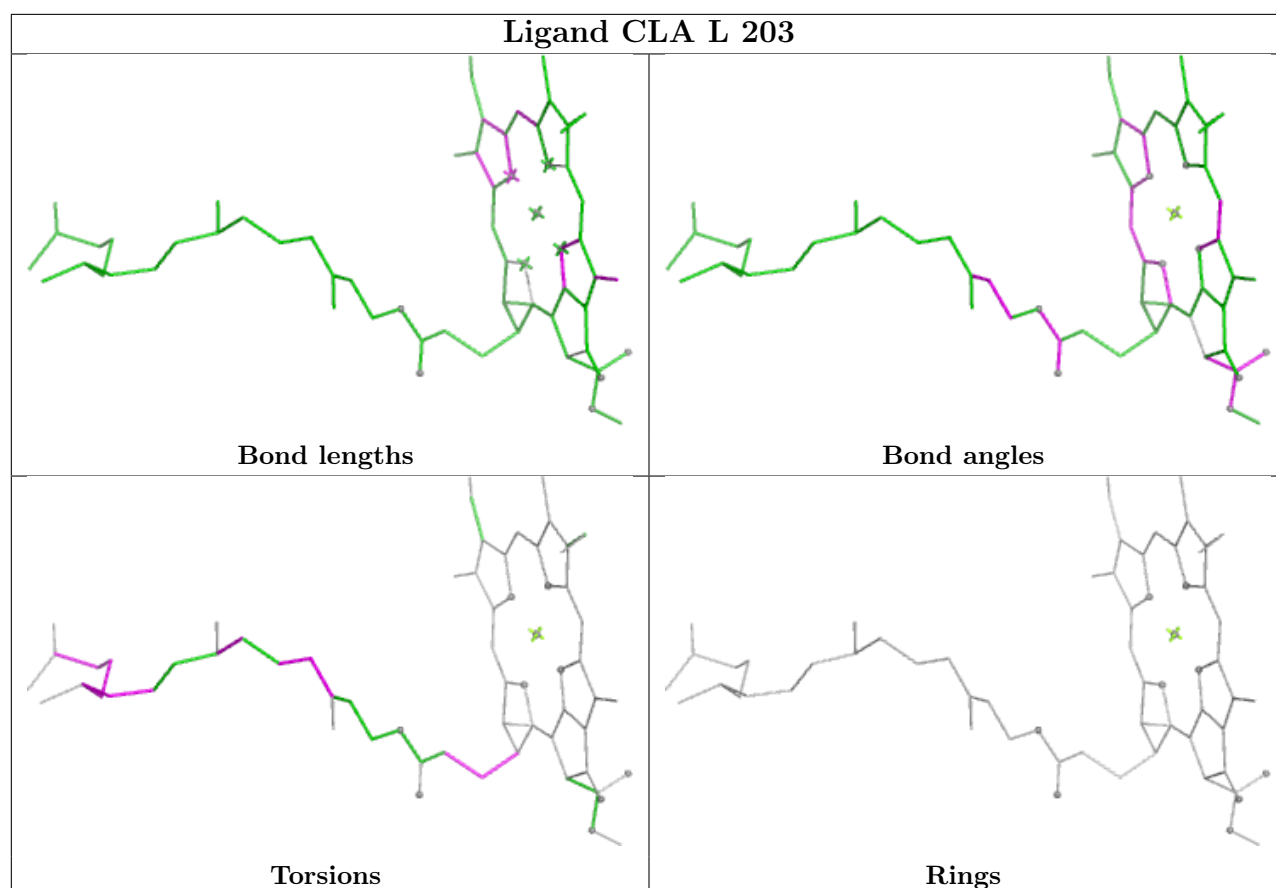
Ligand CLA B 835

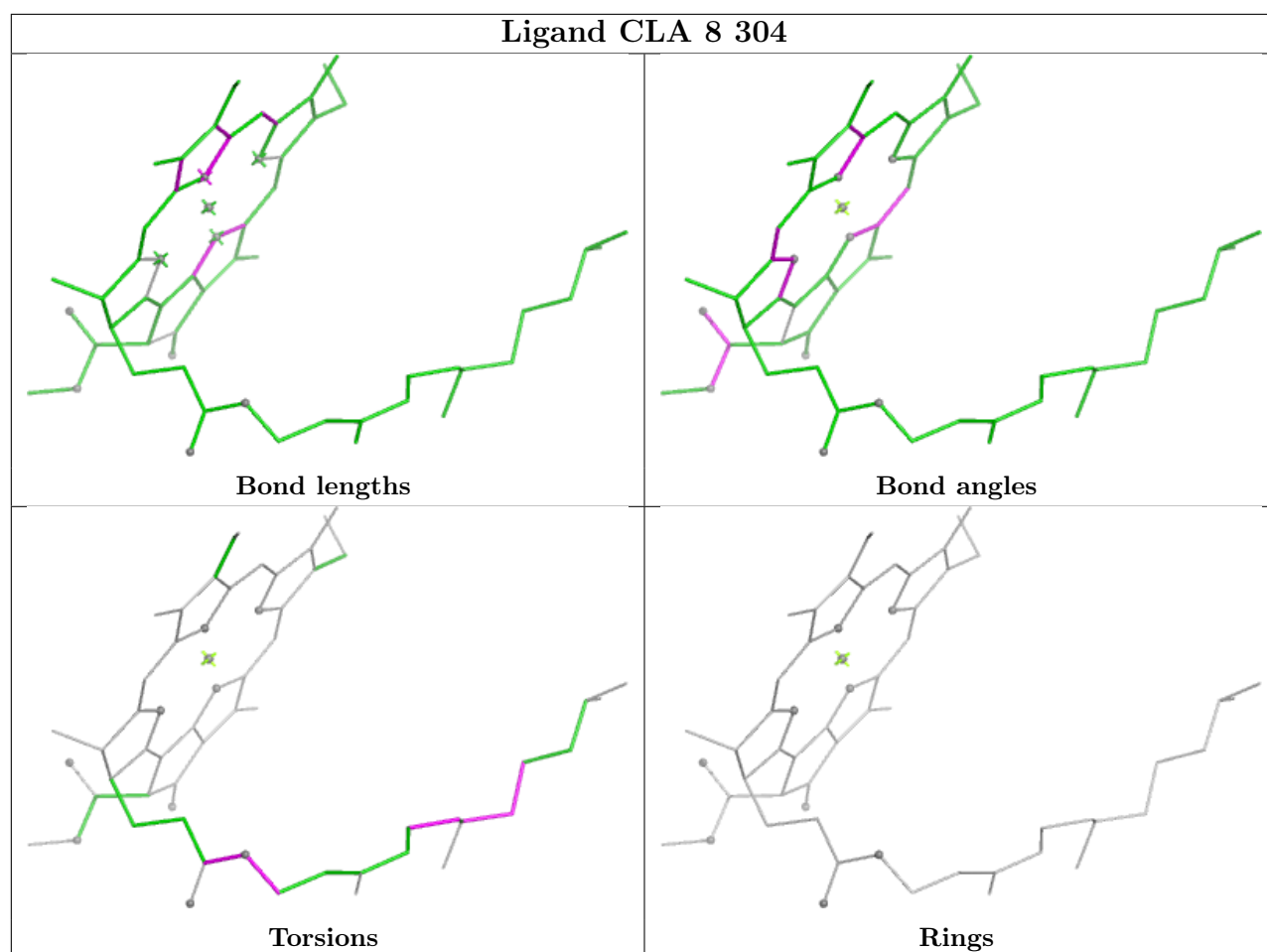


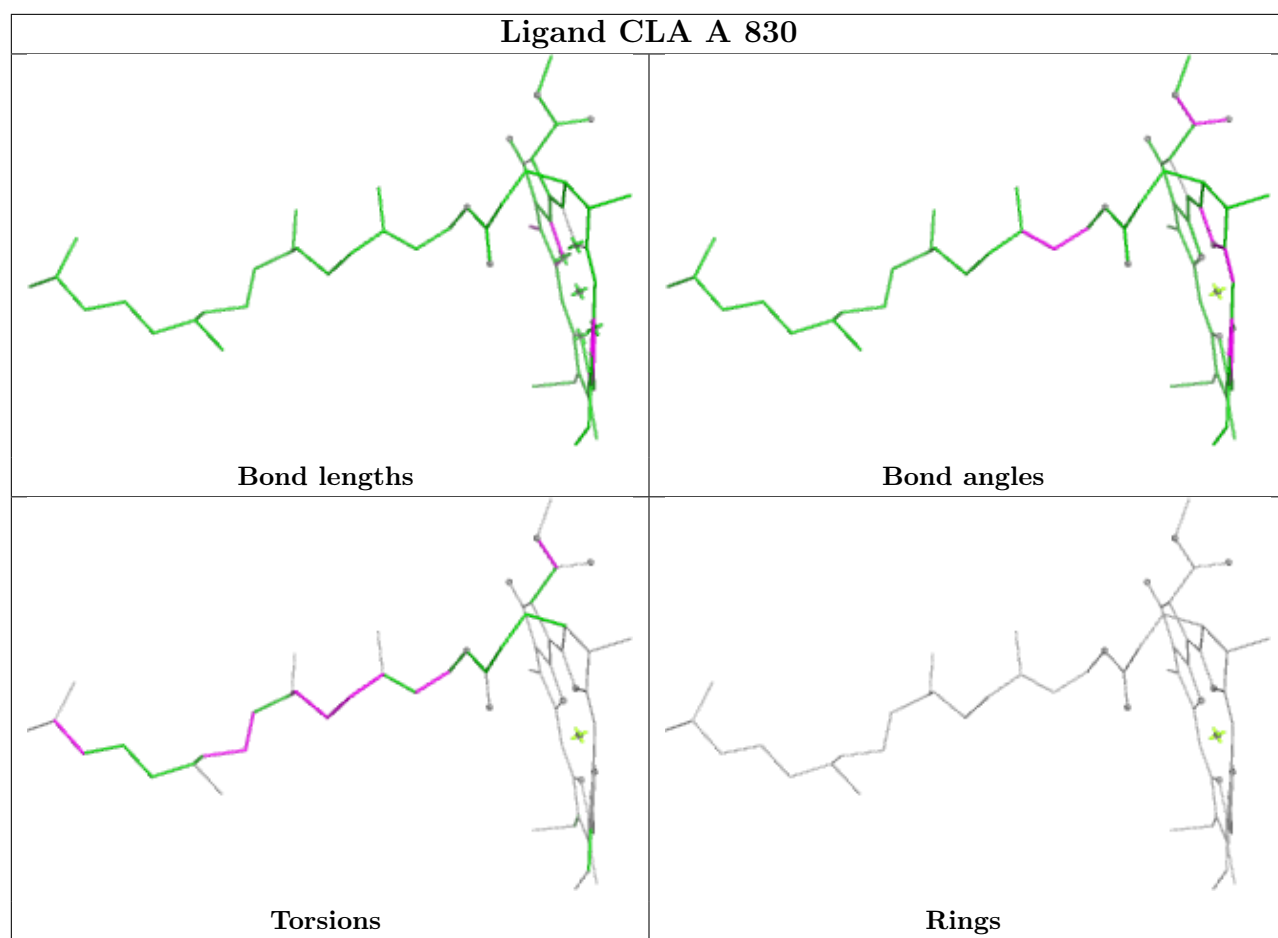
Ligand LMU 3 324

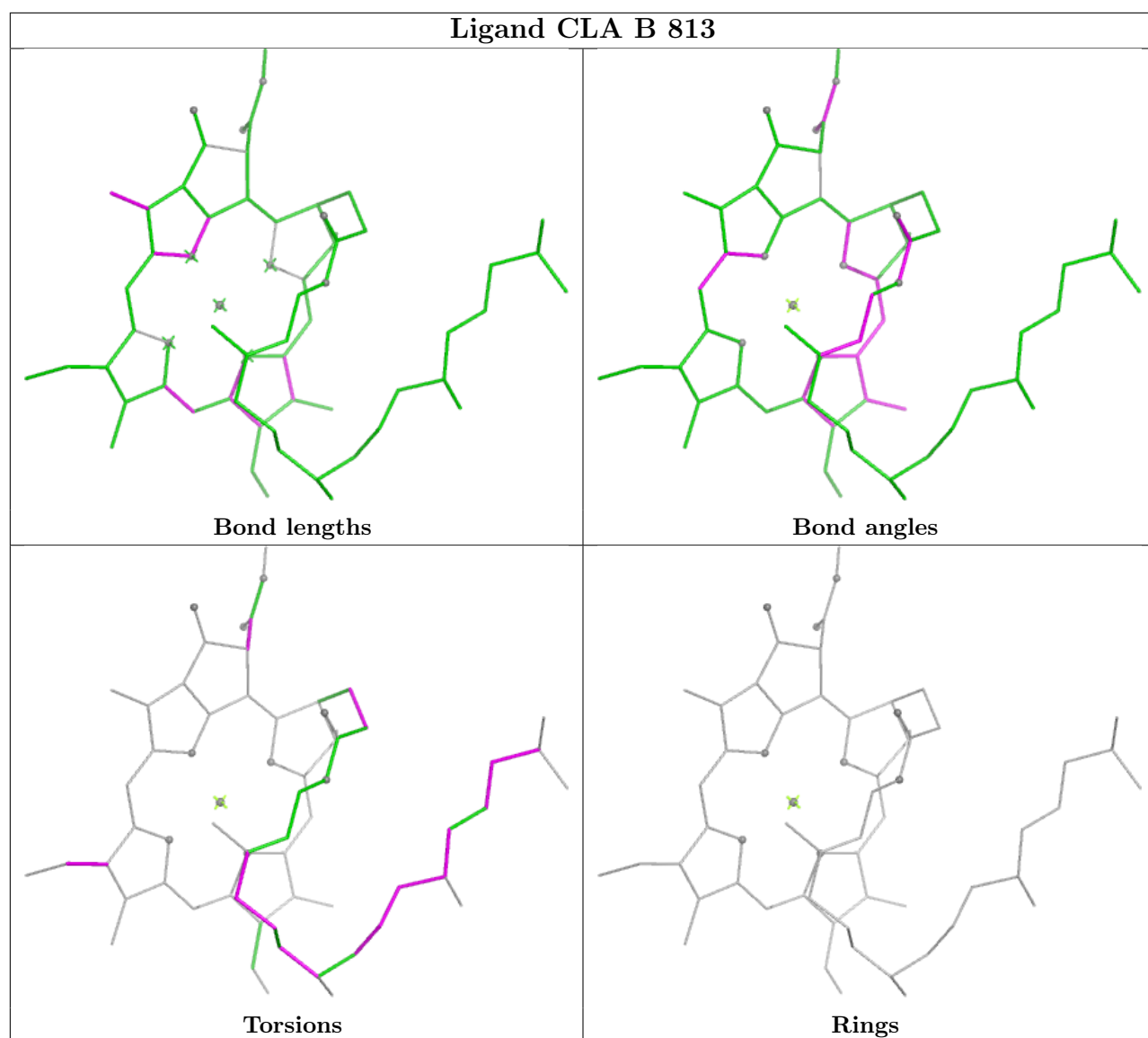




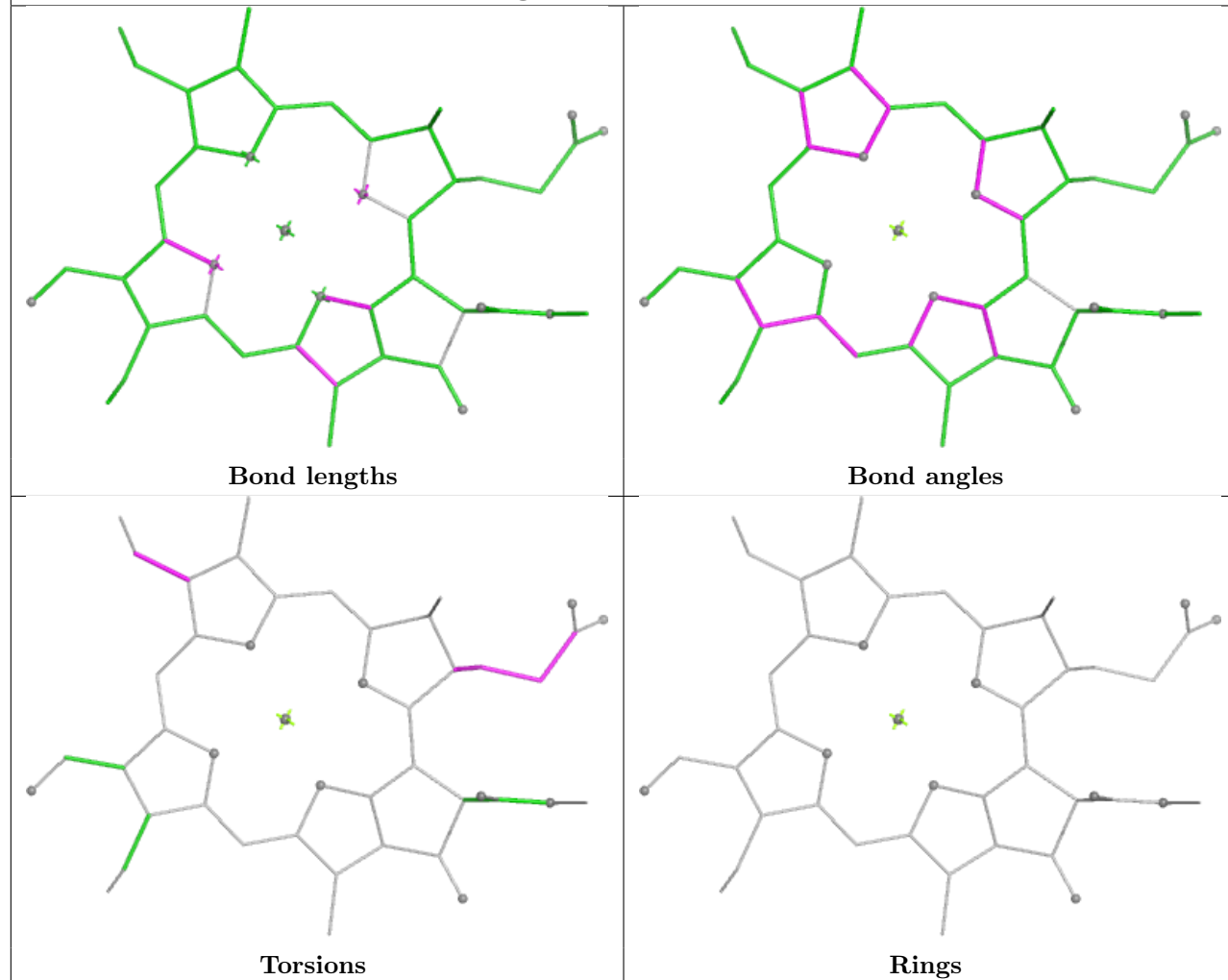


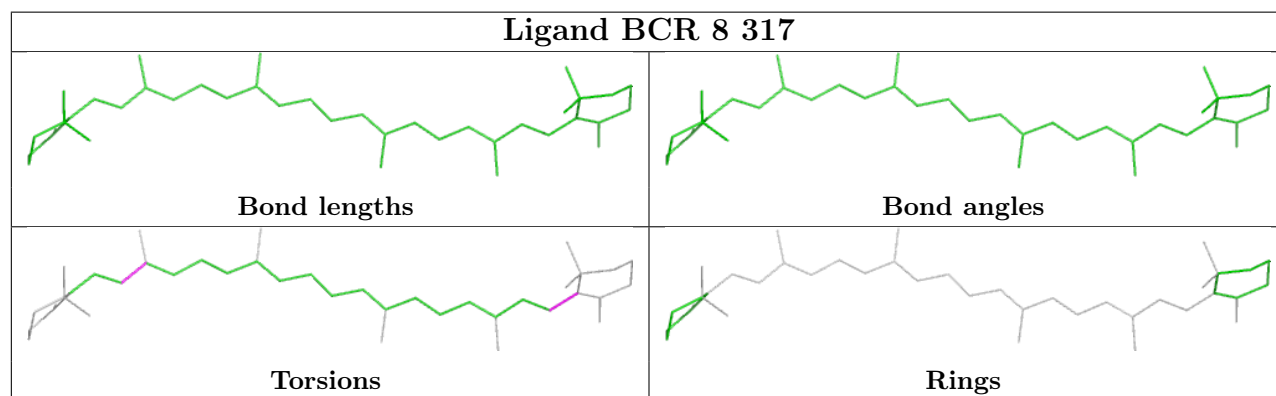
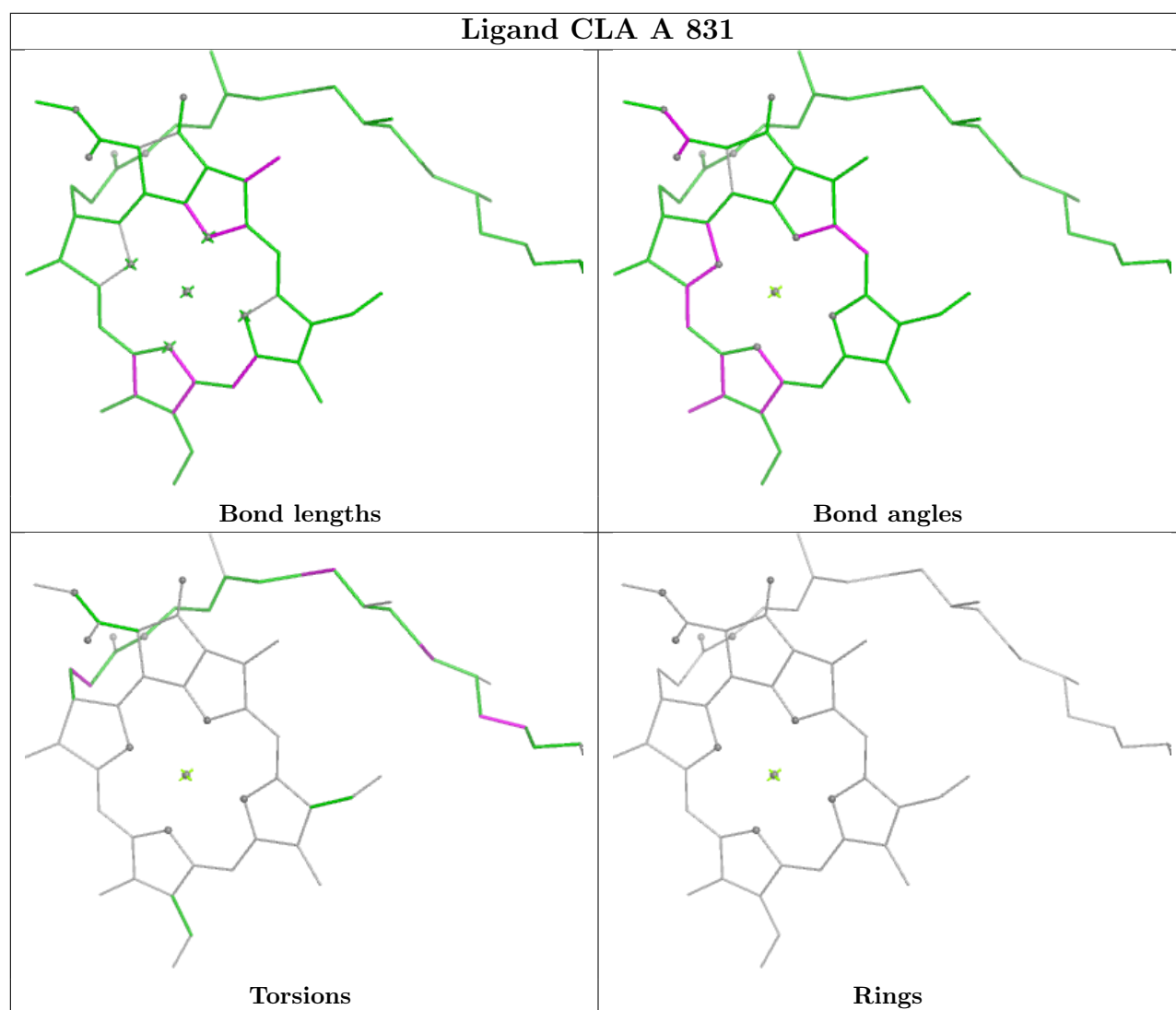




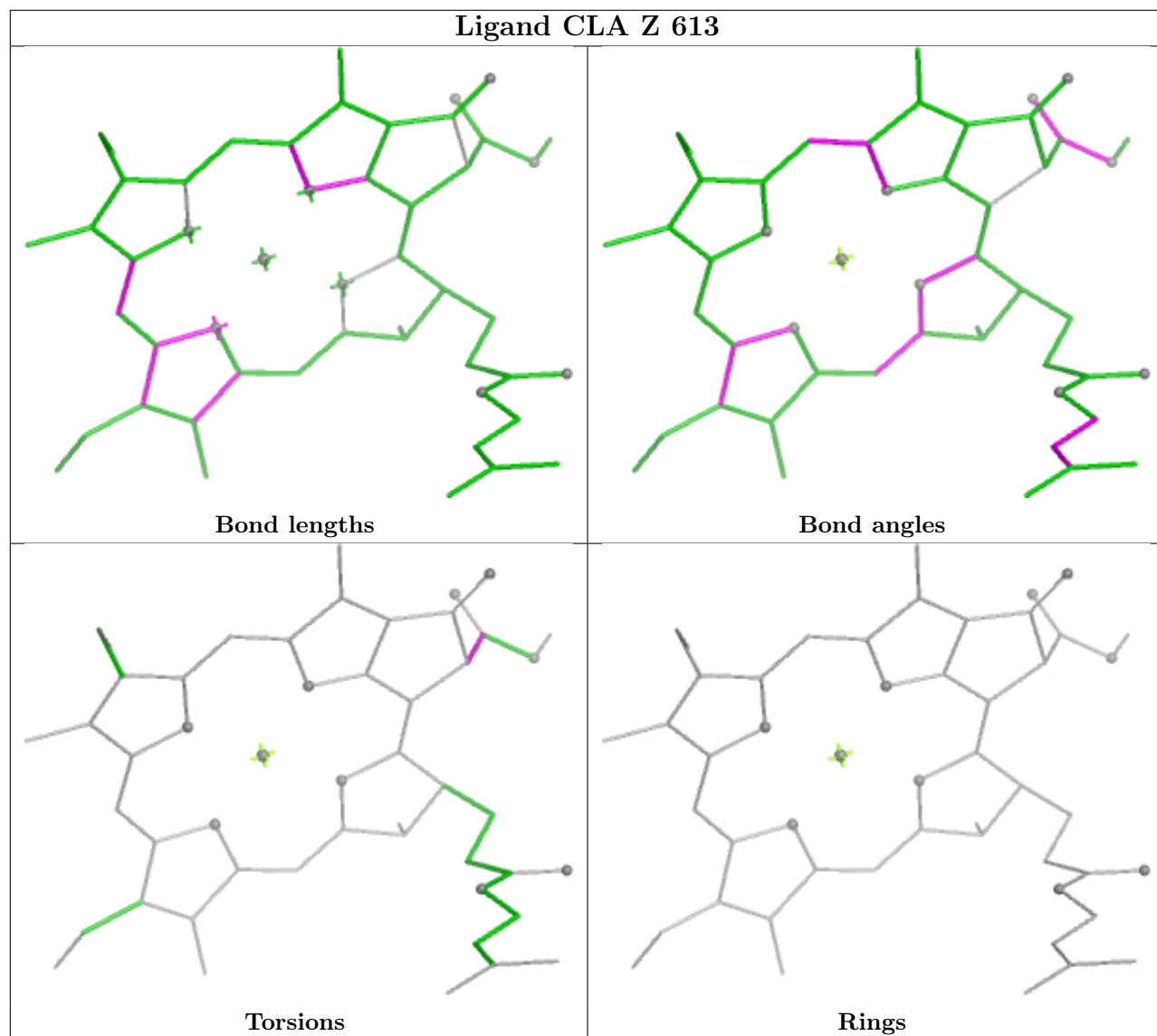


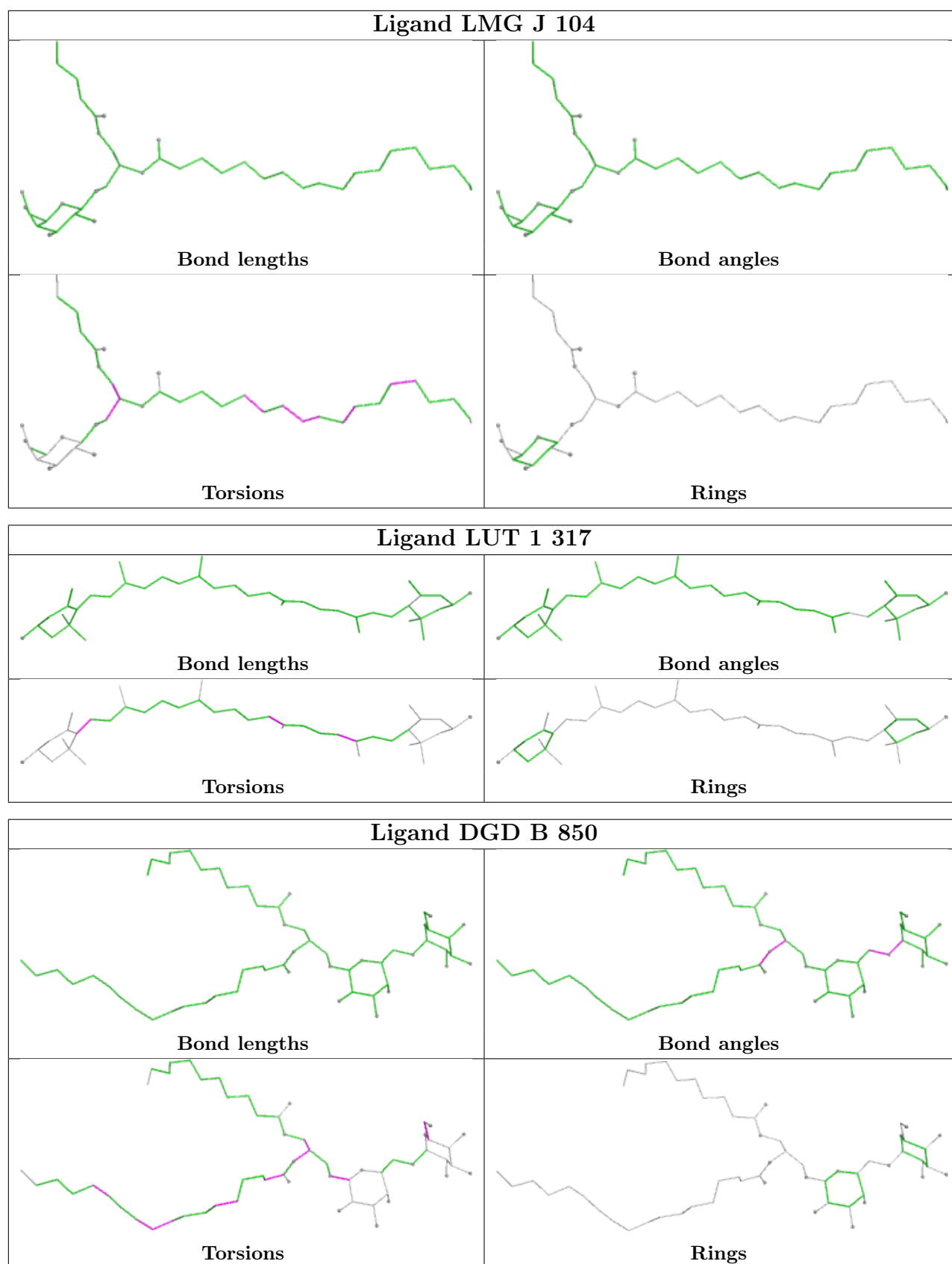
Ligand CHL 5 306

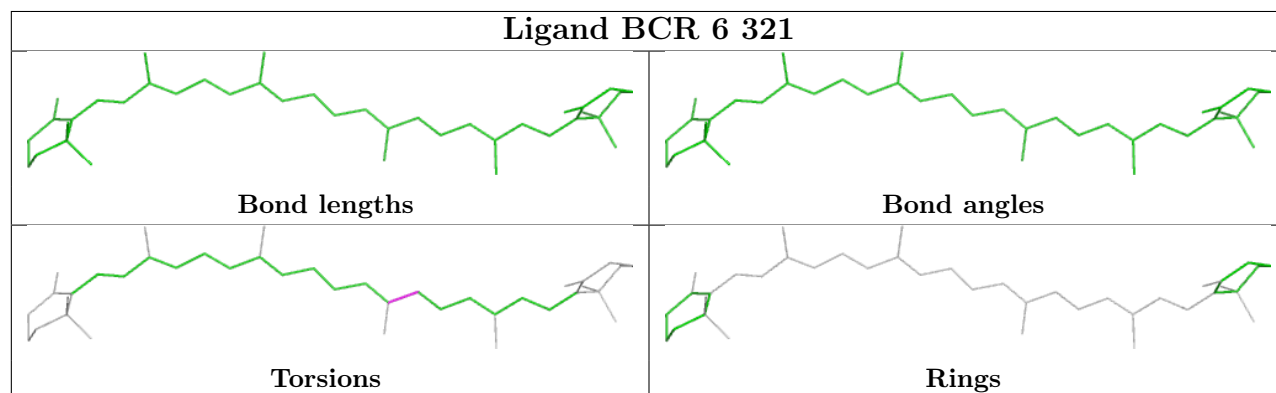
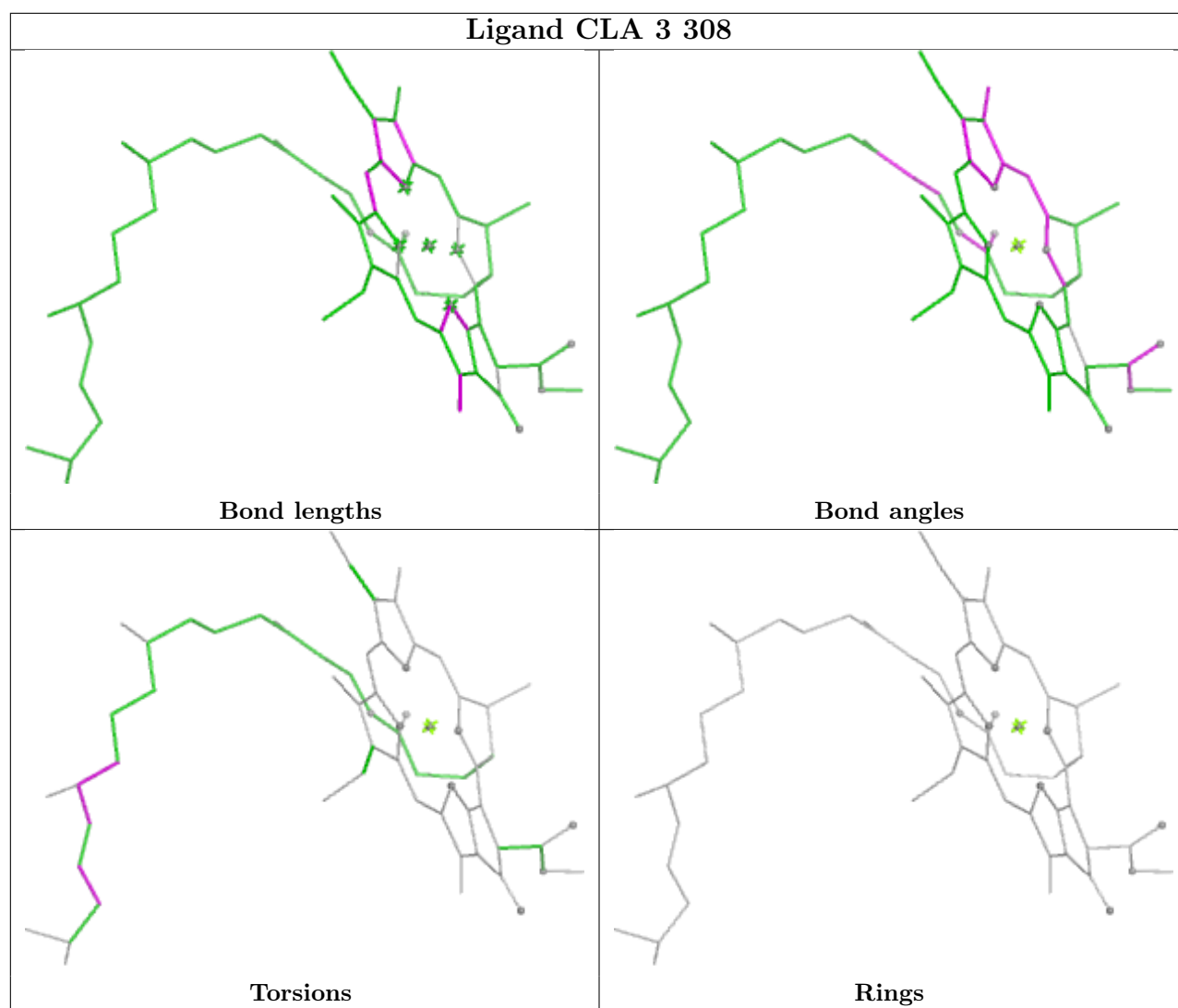




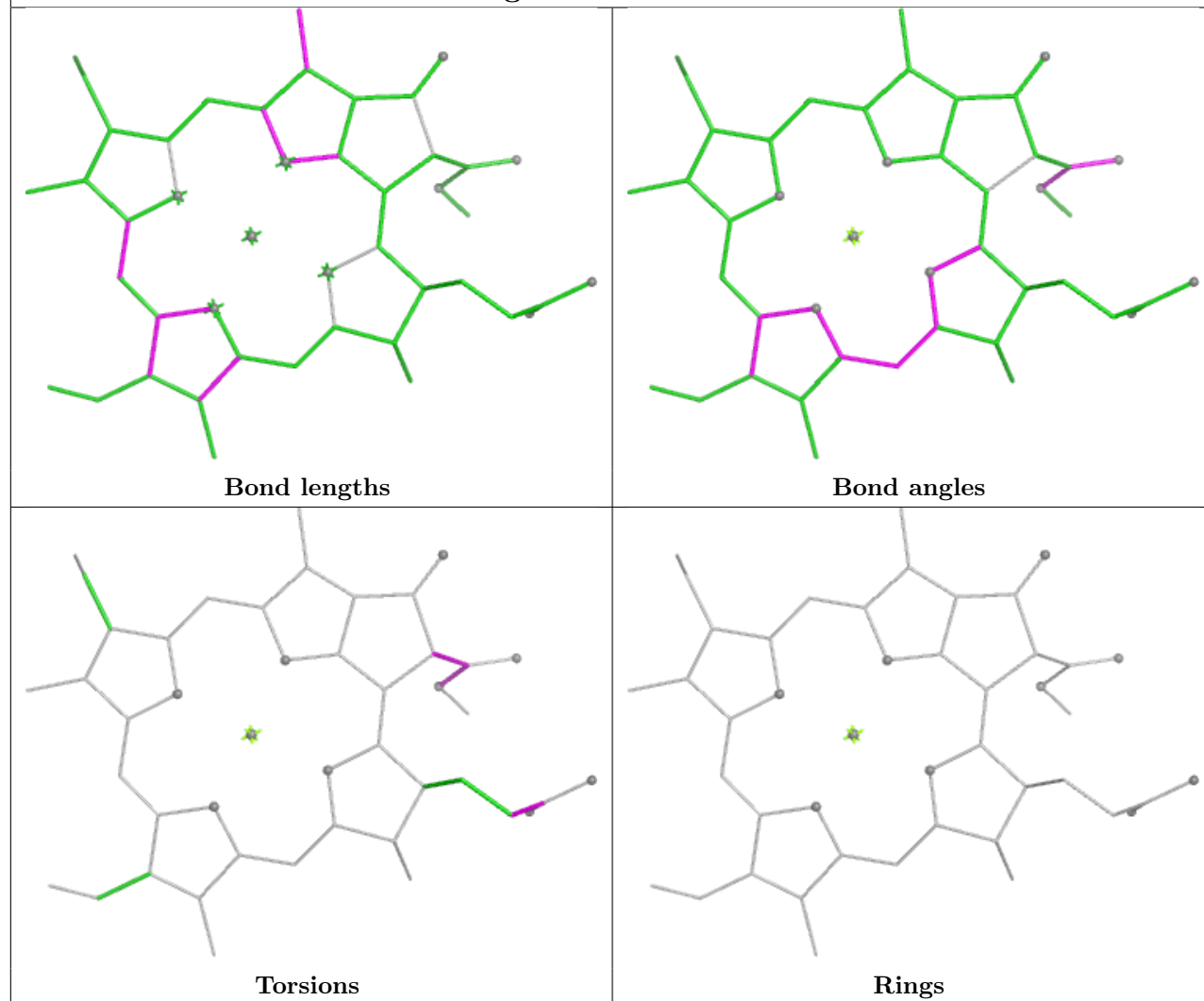
Ligand CLA Z 613



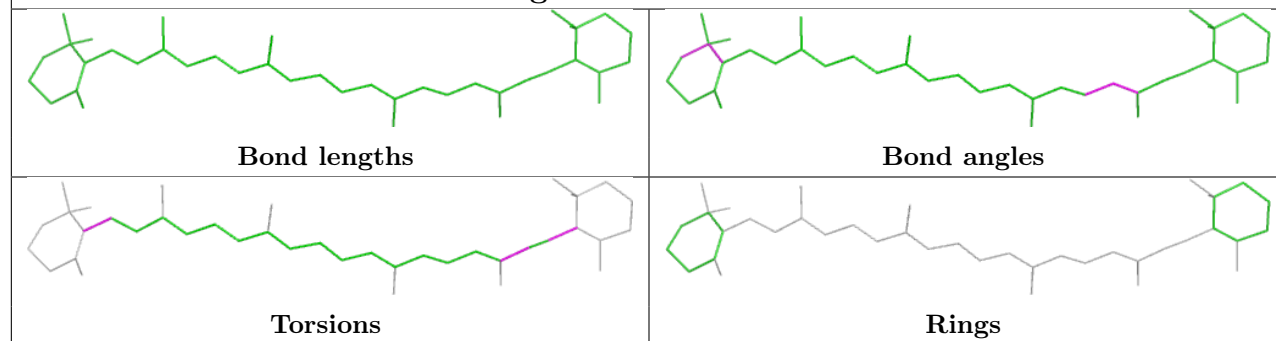


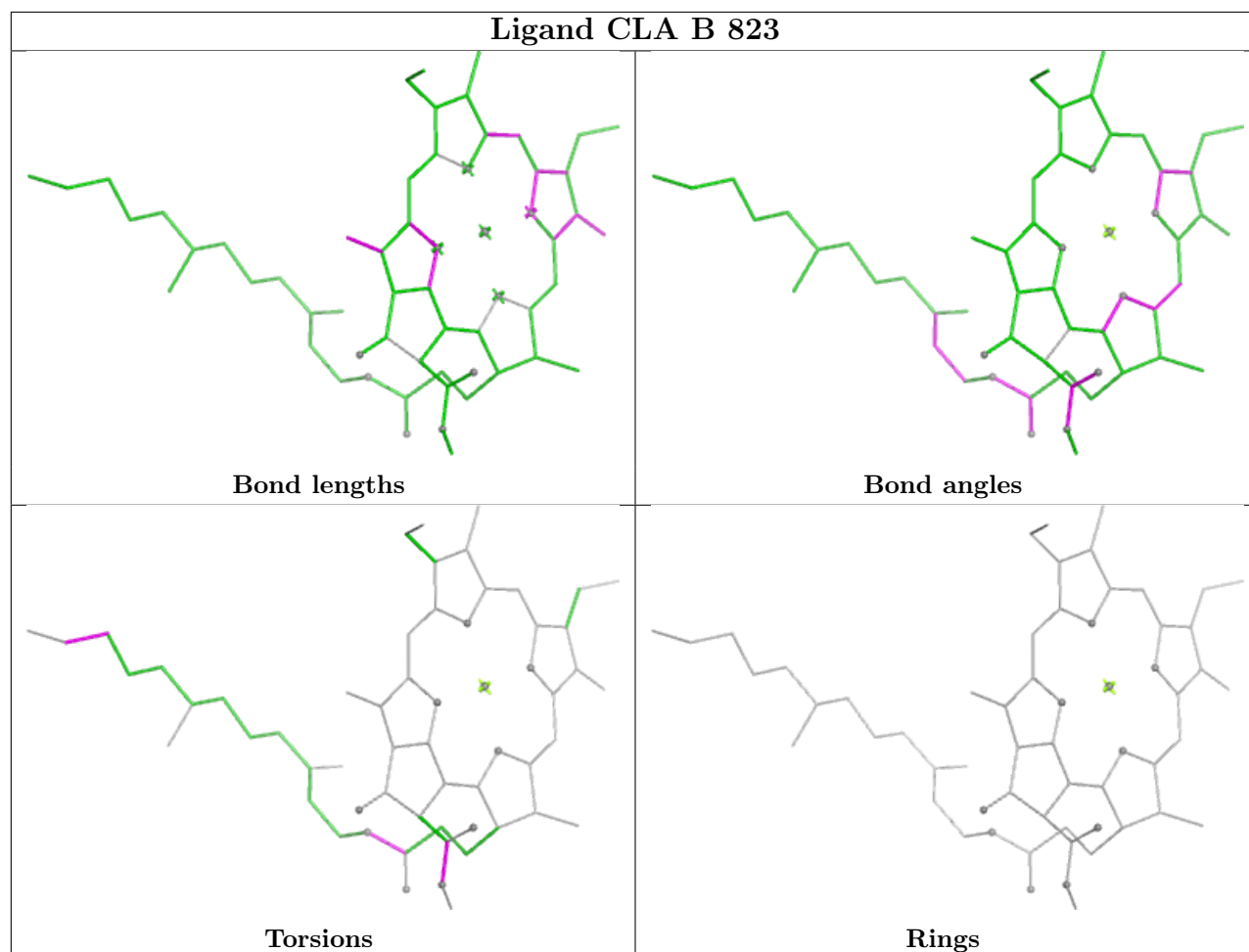
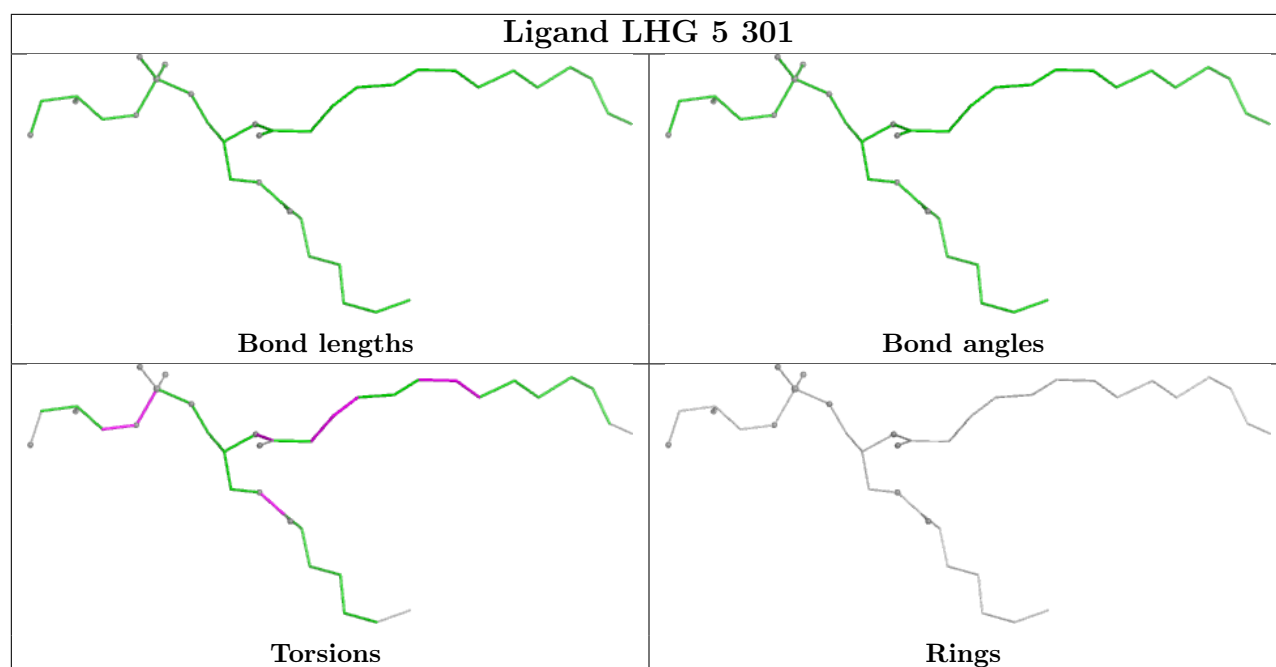


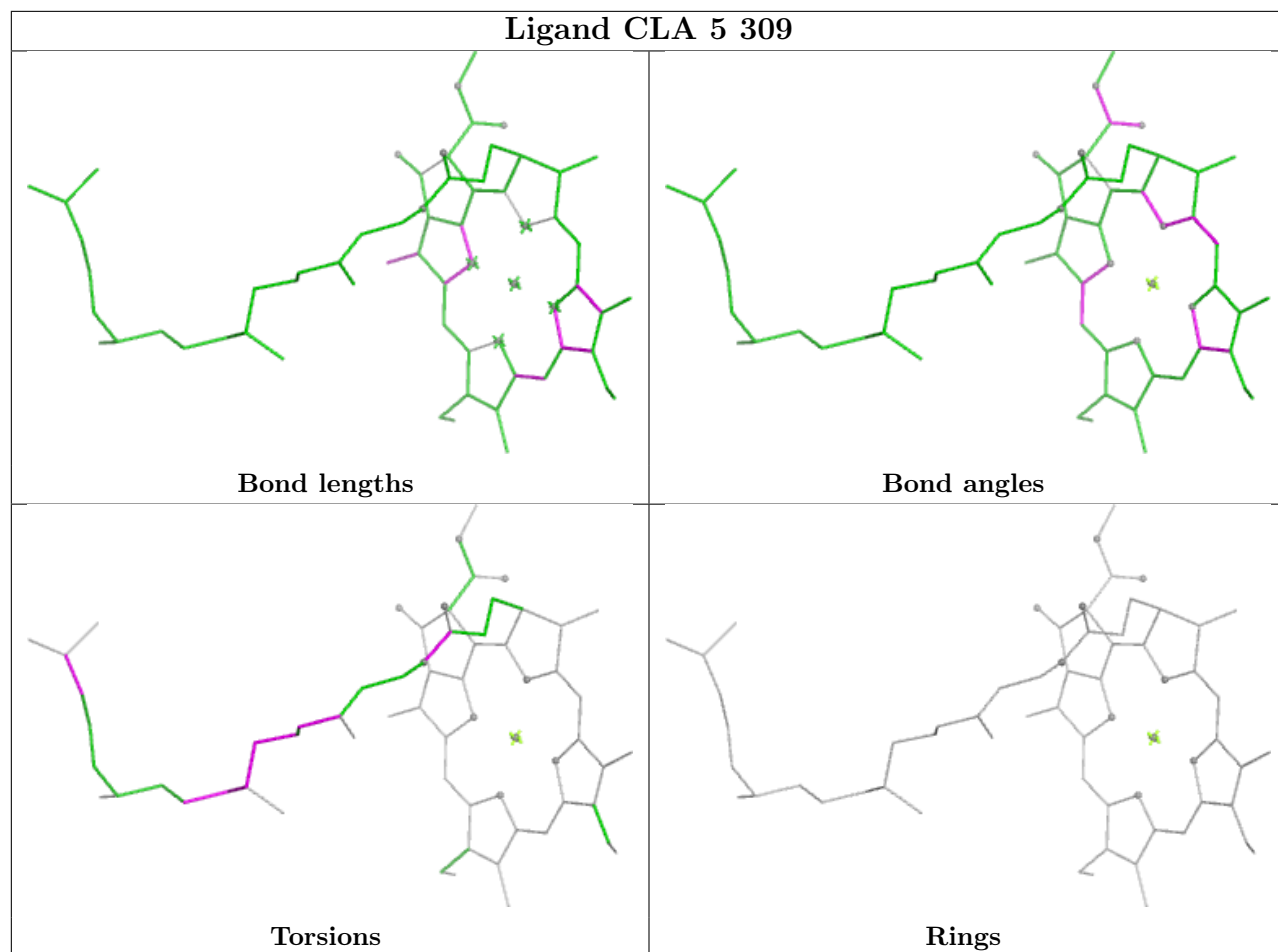
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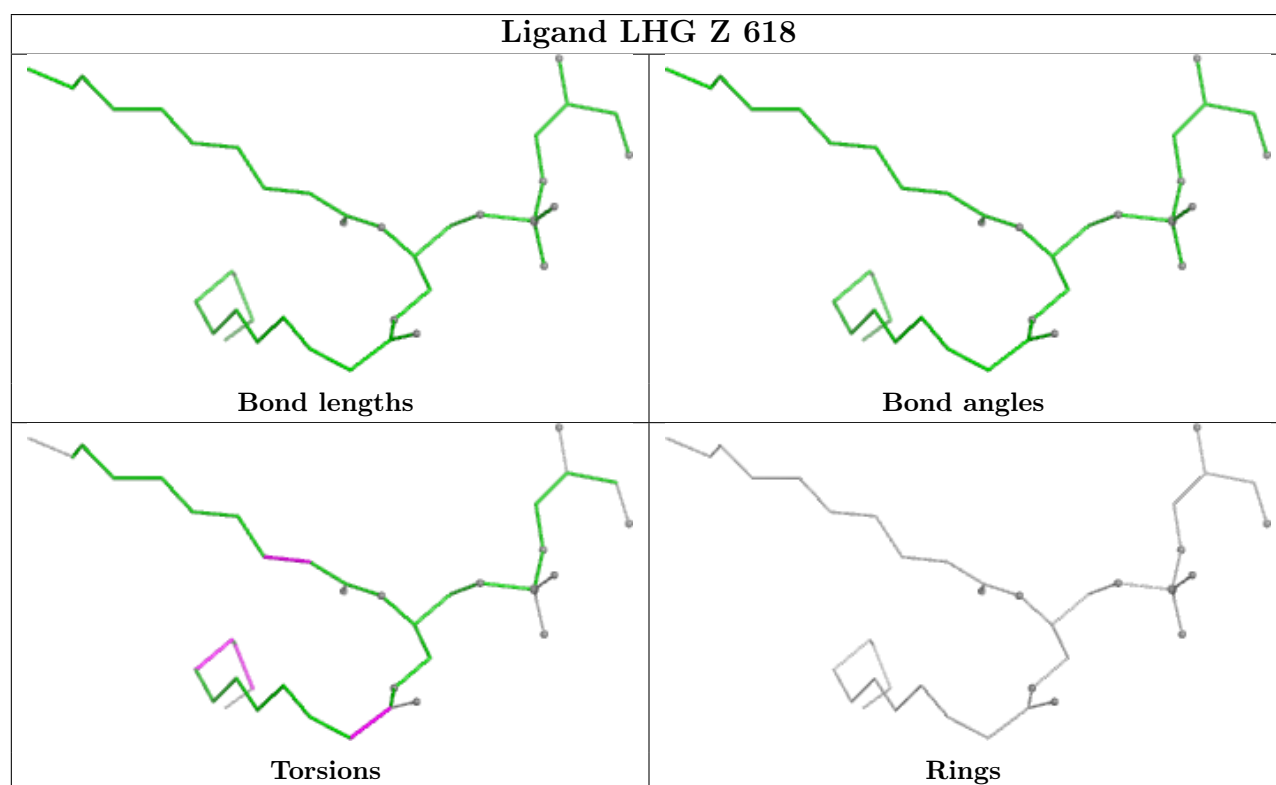
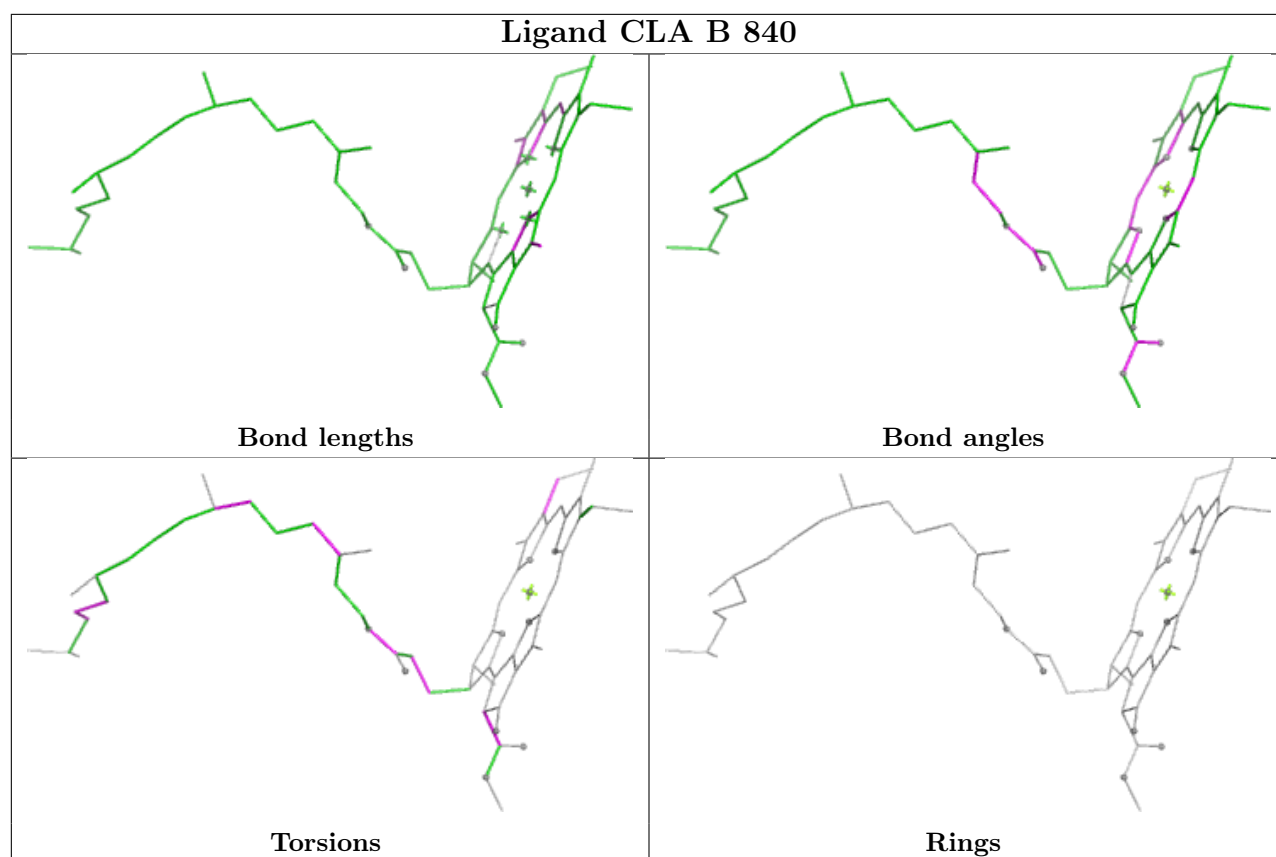


Ligand BCR A 858

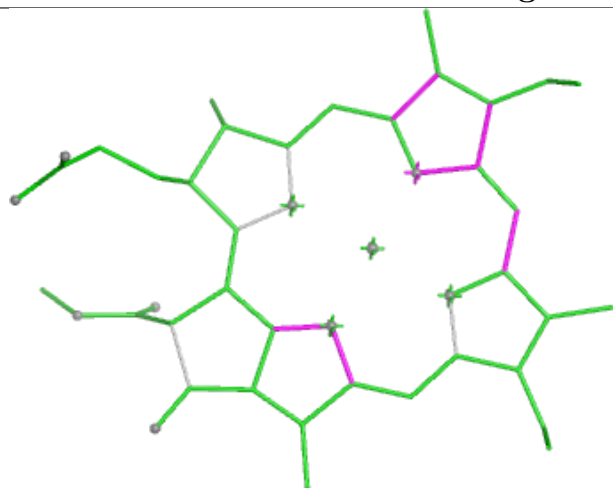




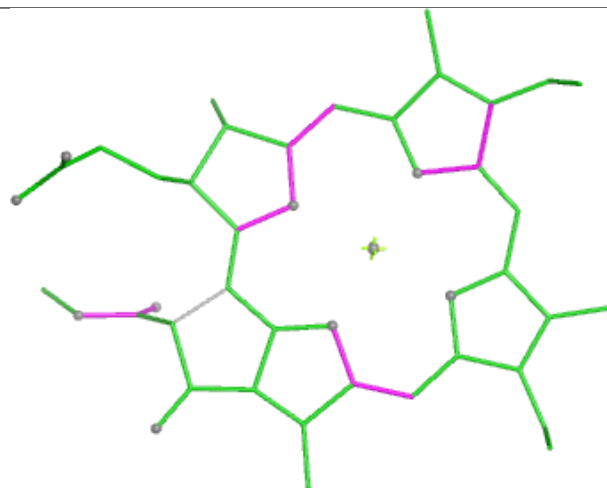




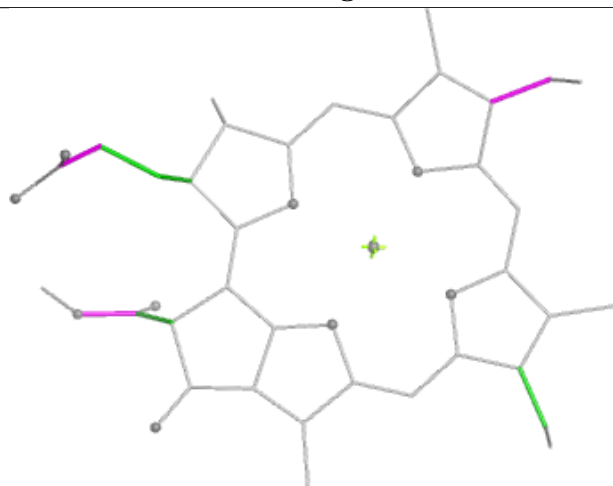
Ligand CLA 3 312



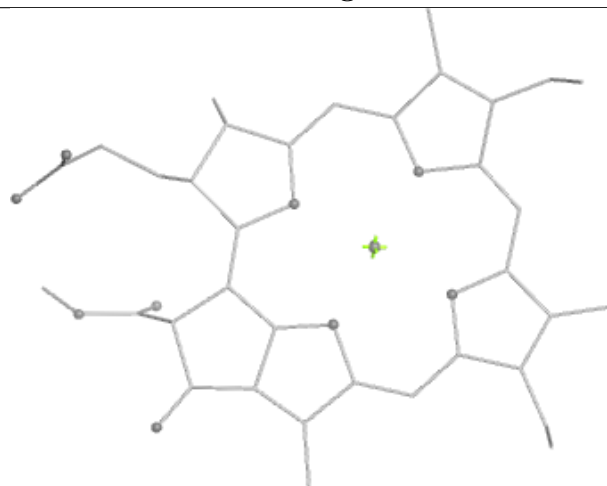
Bond lengths



Bond angles

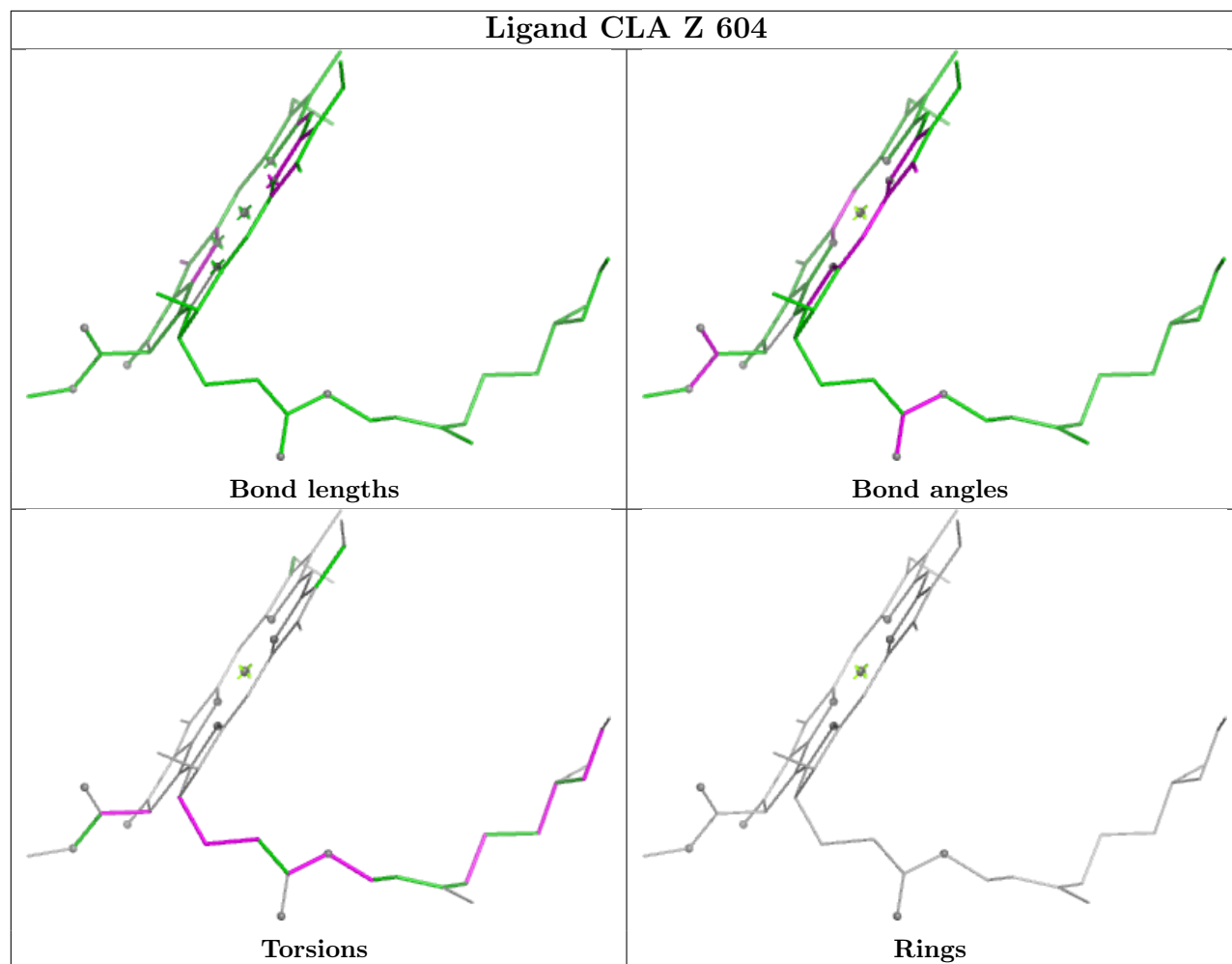


Torsions

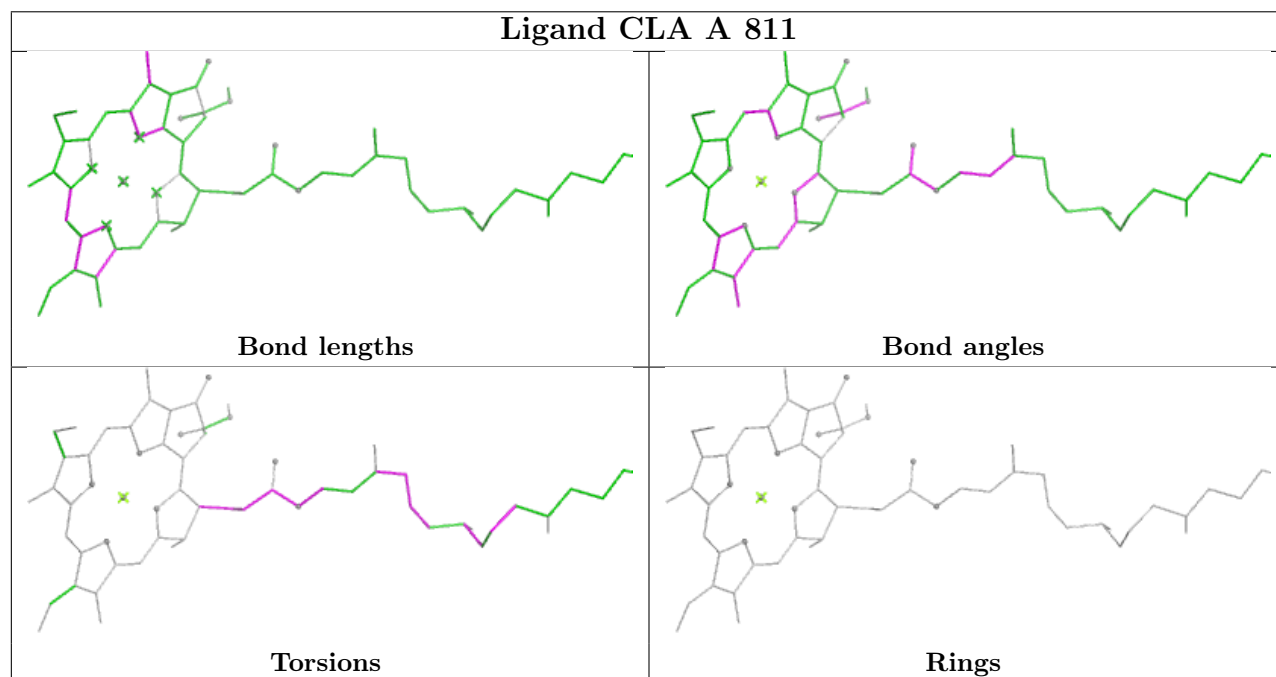


Rings

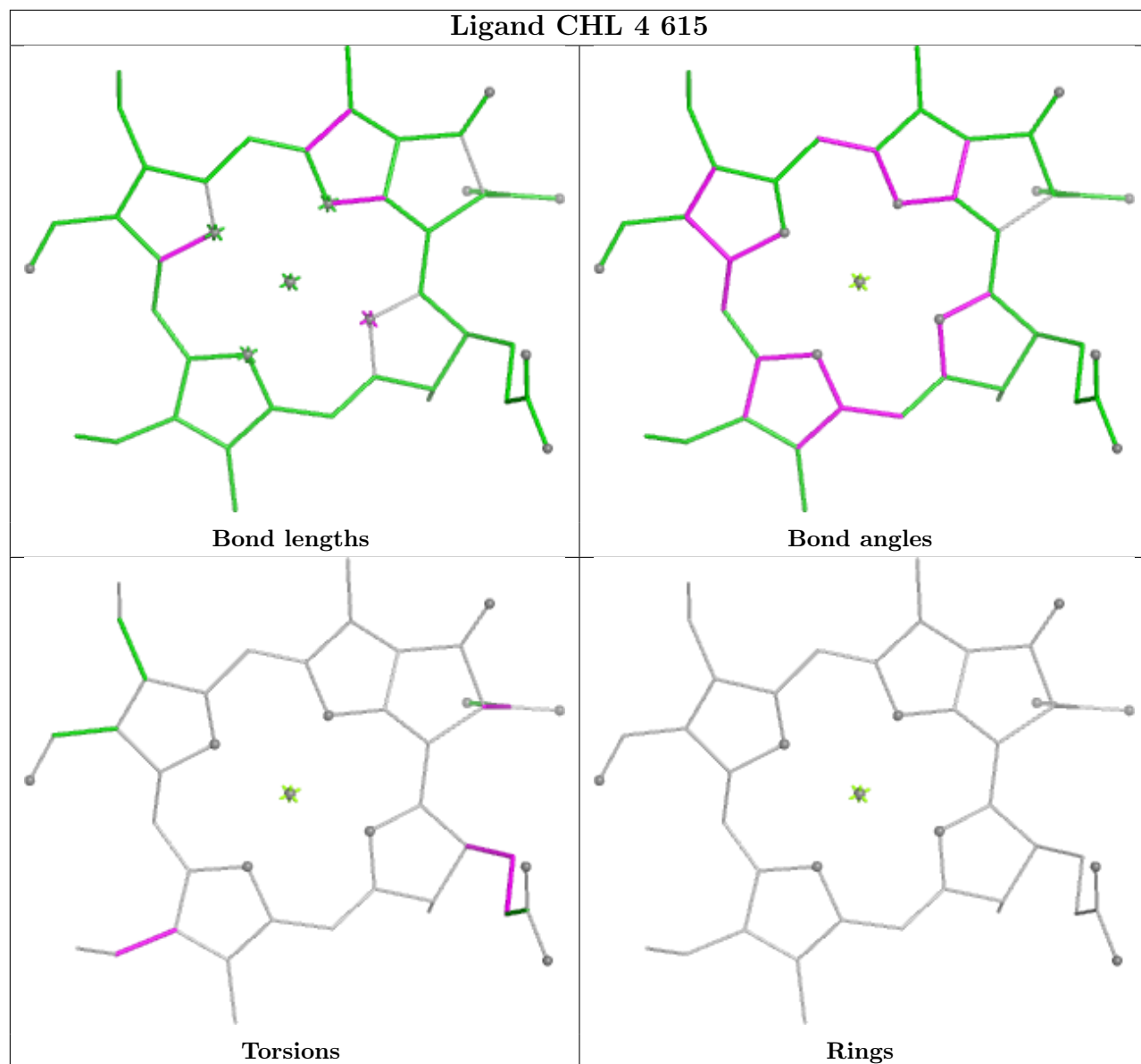
Ligand CLA Z 604



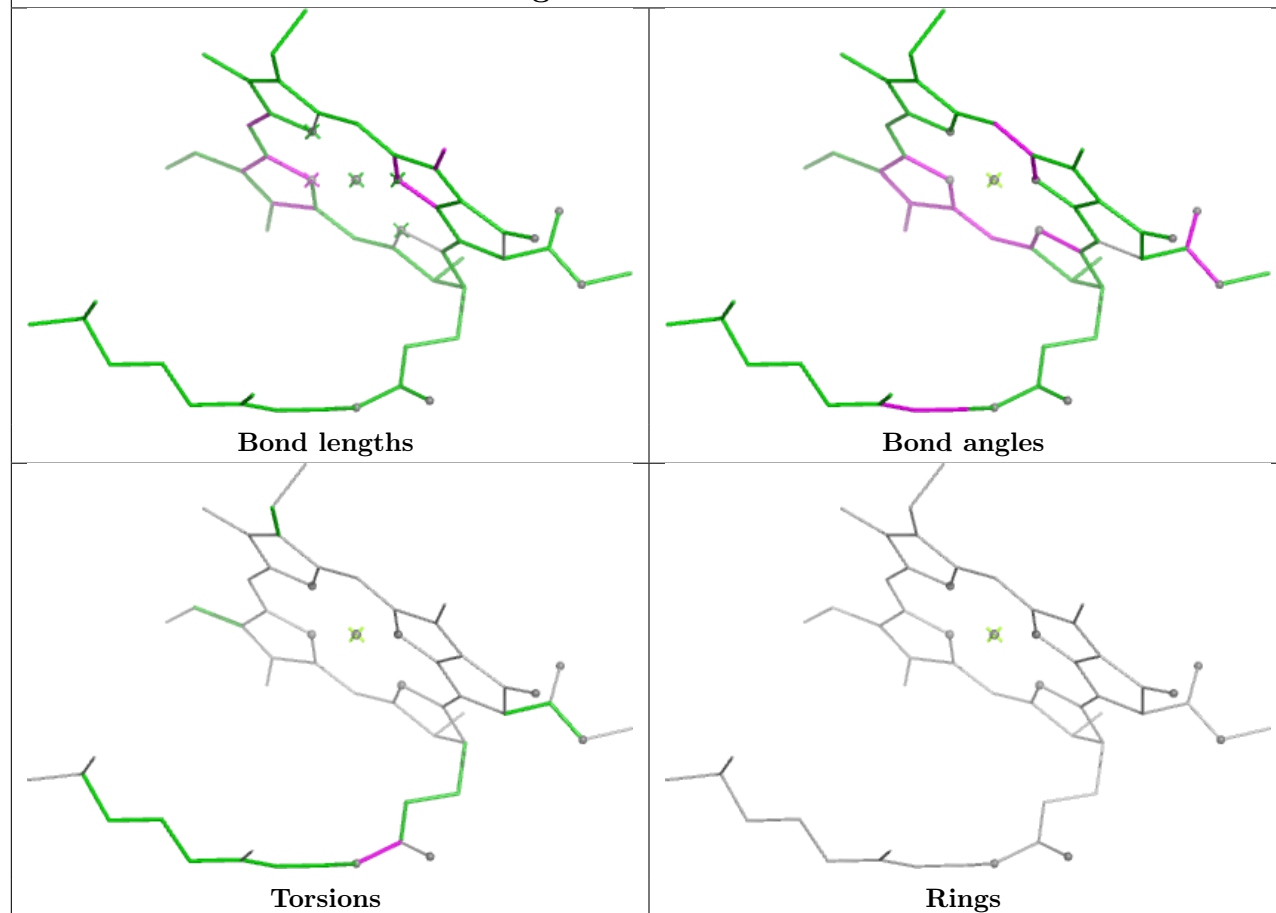
Ligand CLA A 811



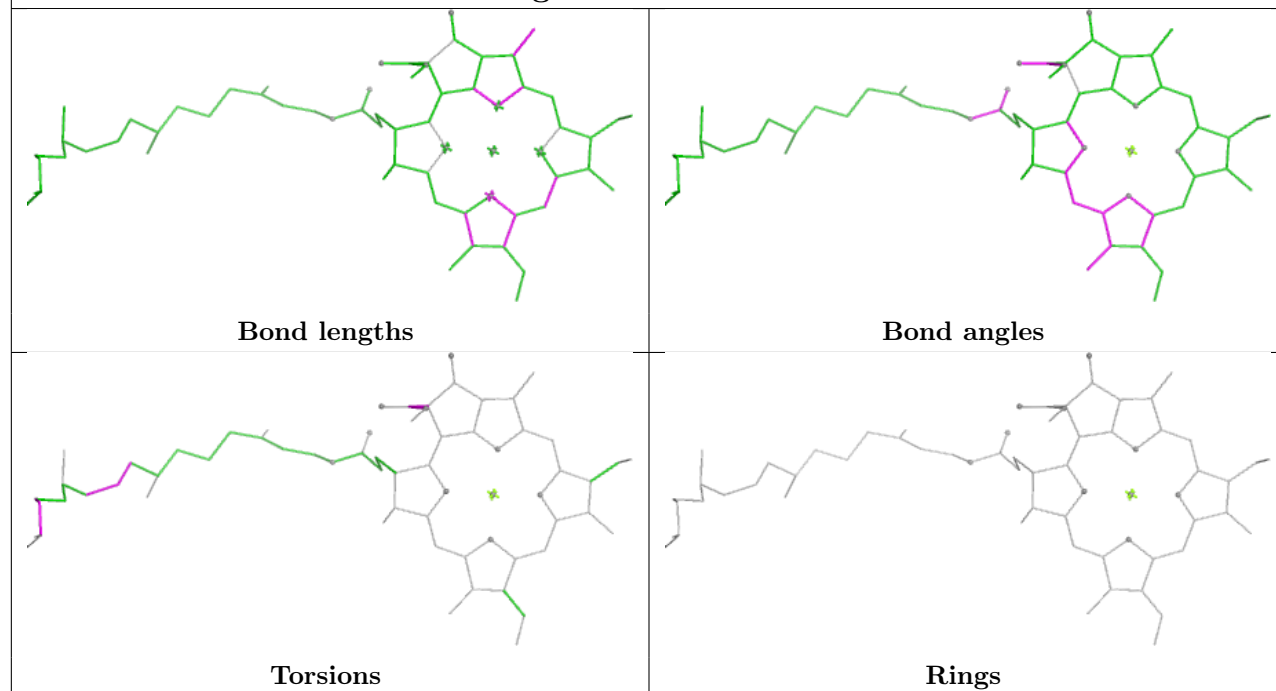
Ligand CHL 4 615

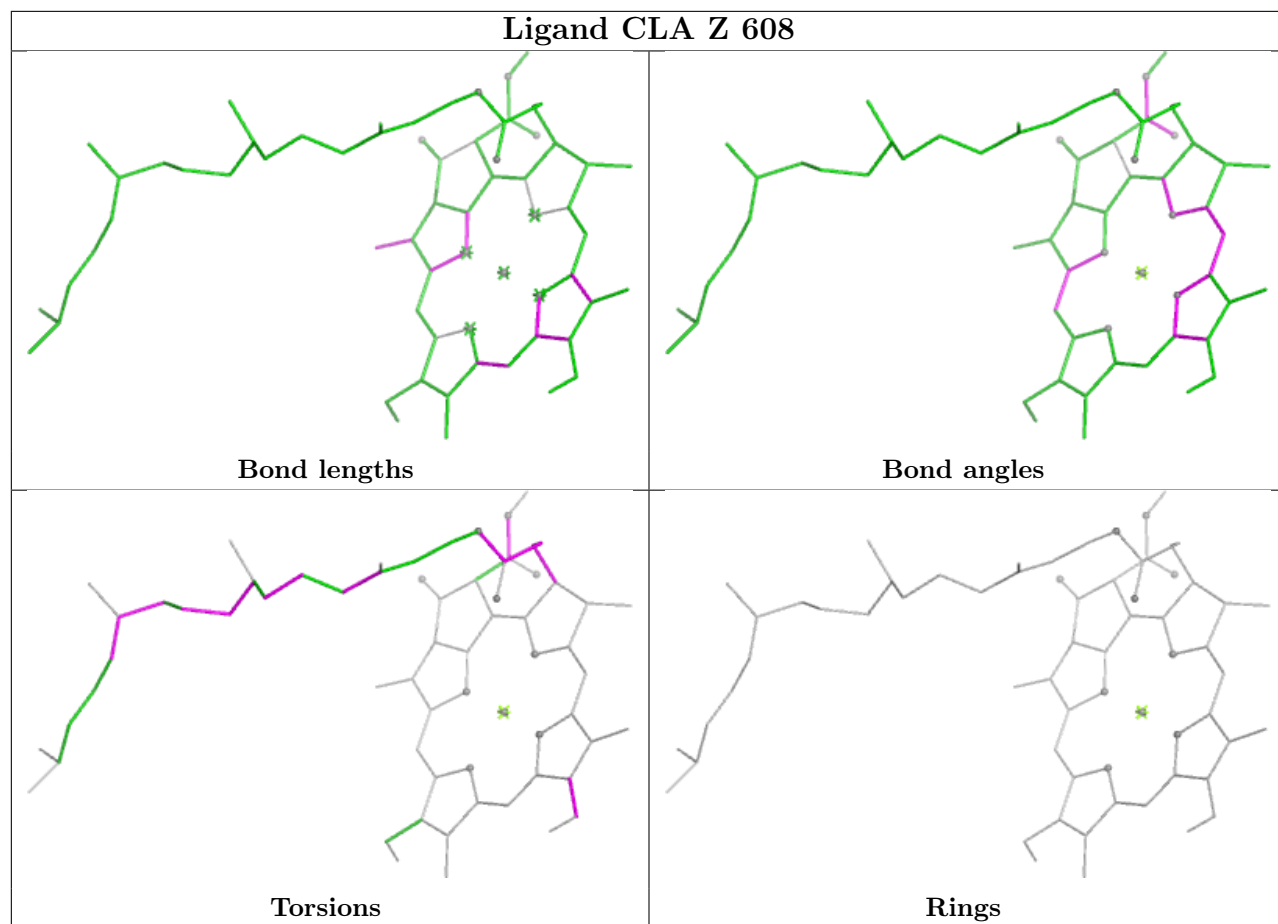


Ligand CLA B 832

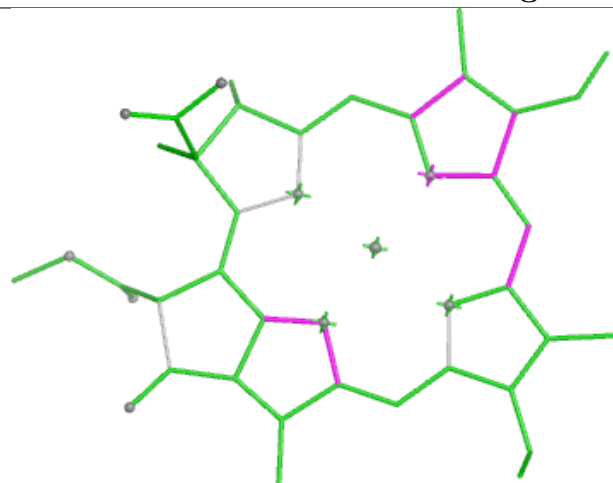


Ligand CLA B 842

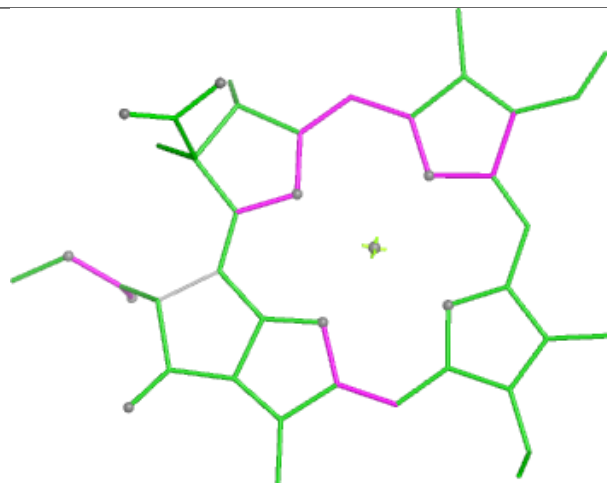




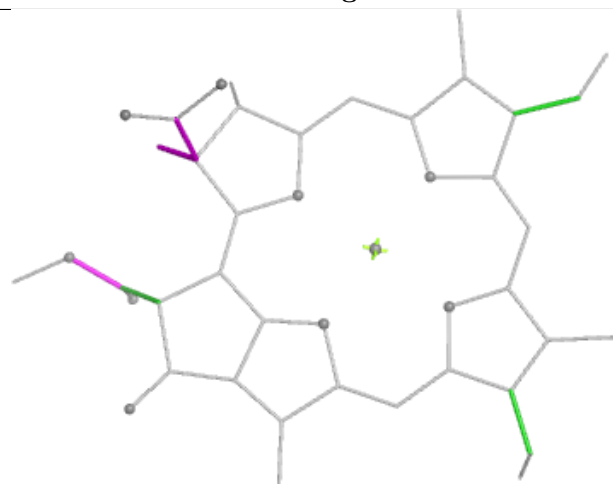
Ligand CLA 5 314



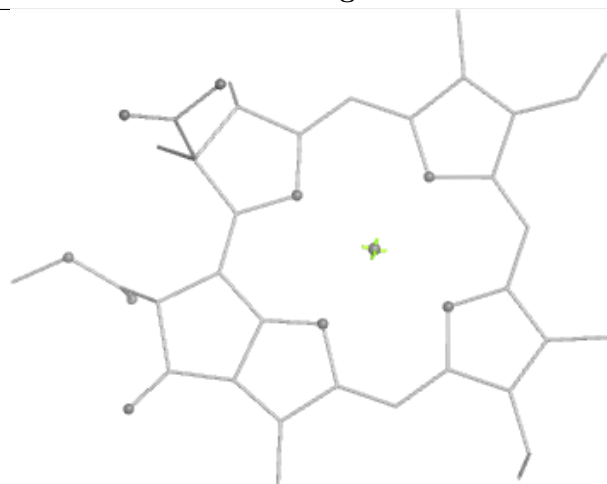
Bond lengths



Bond angles

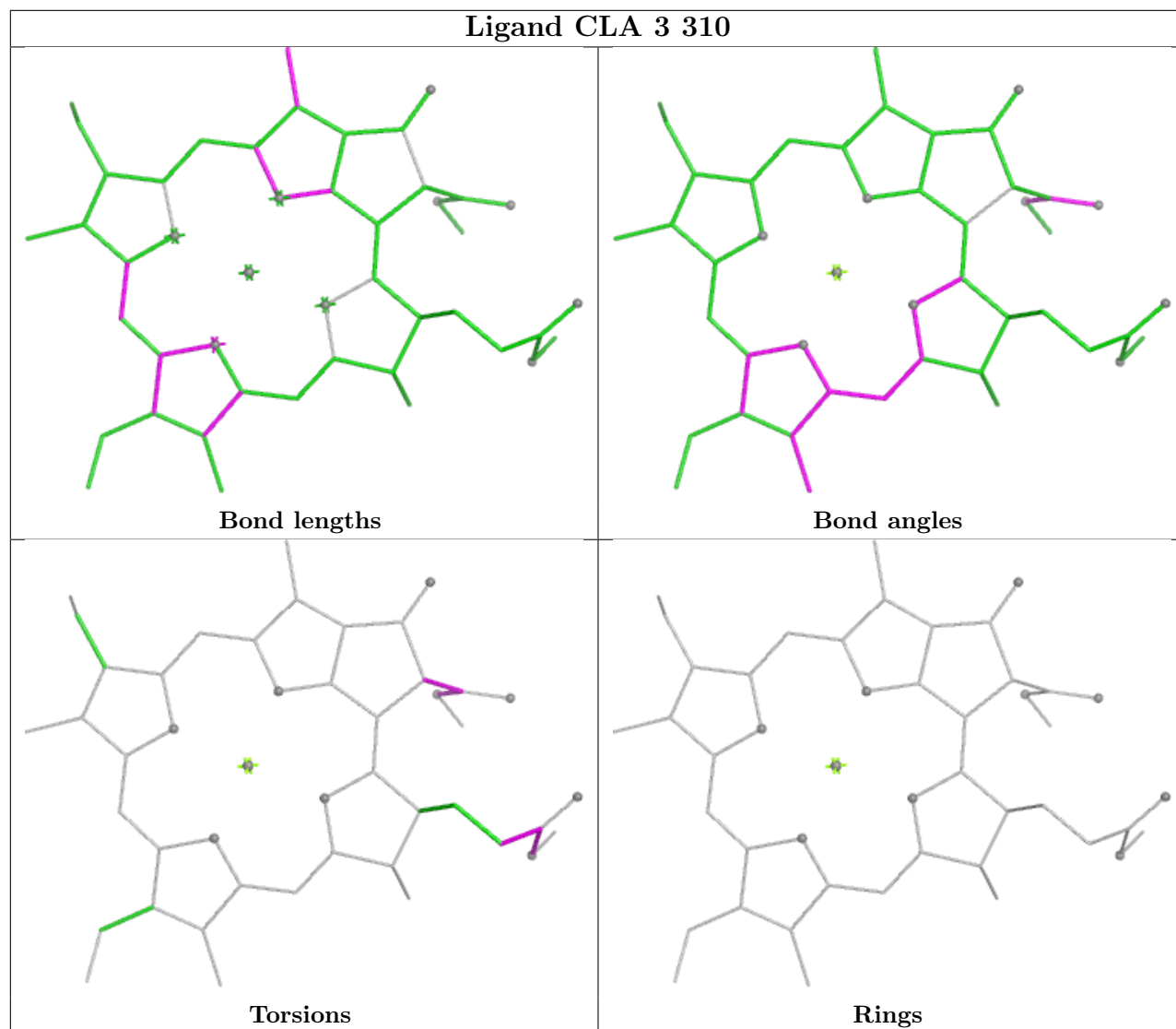


Torsions

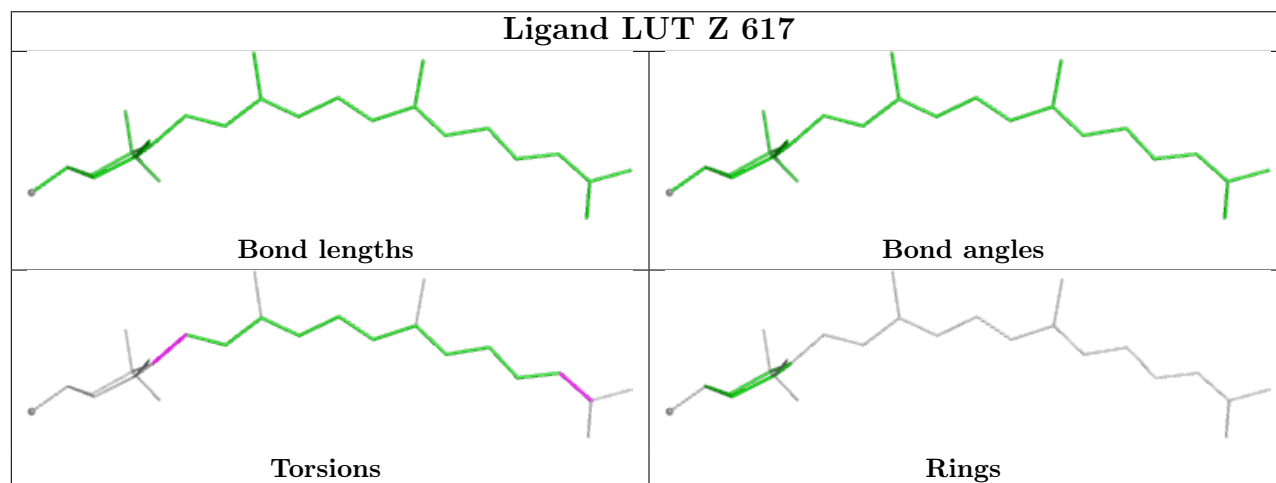


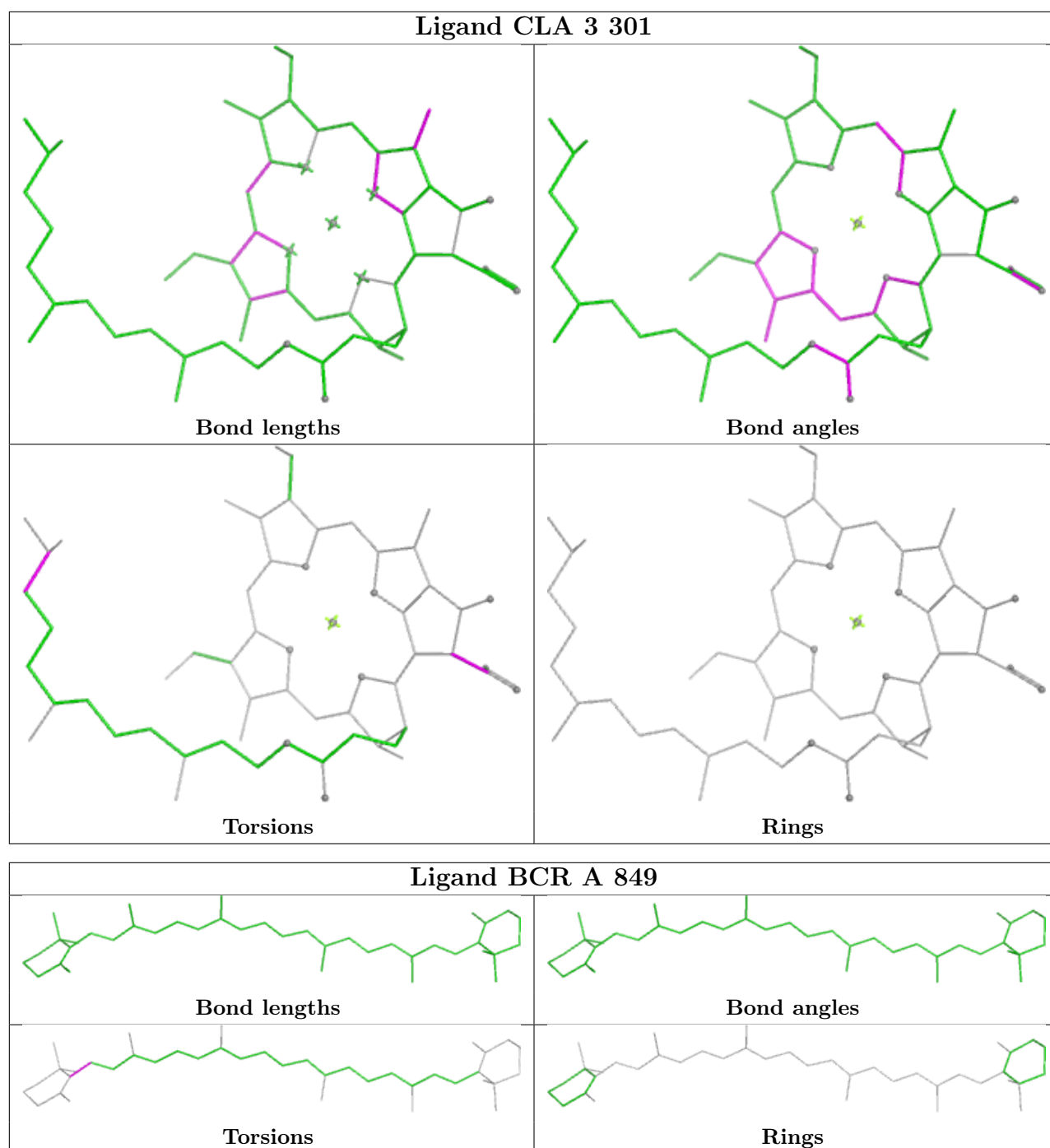
Rings

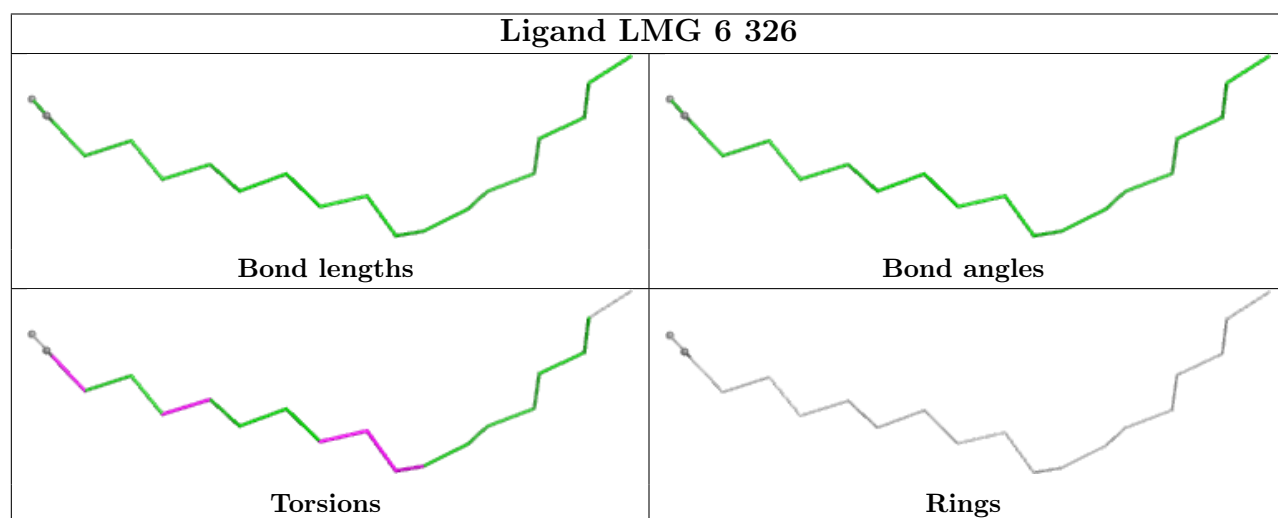
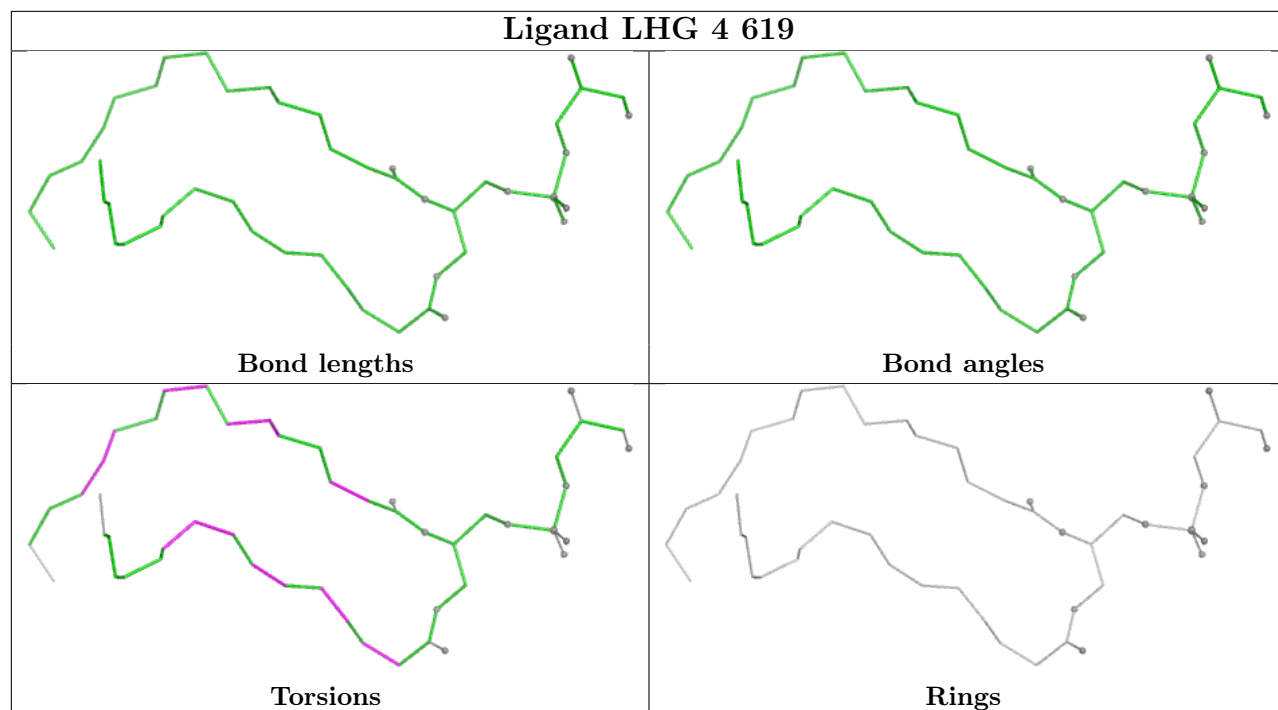
Ligand CLA 3 310

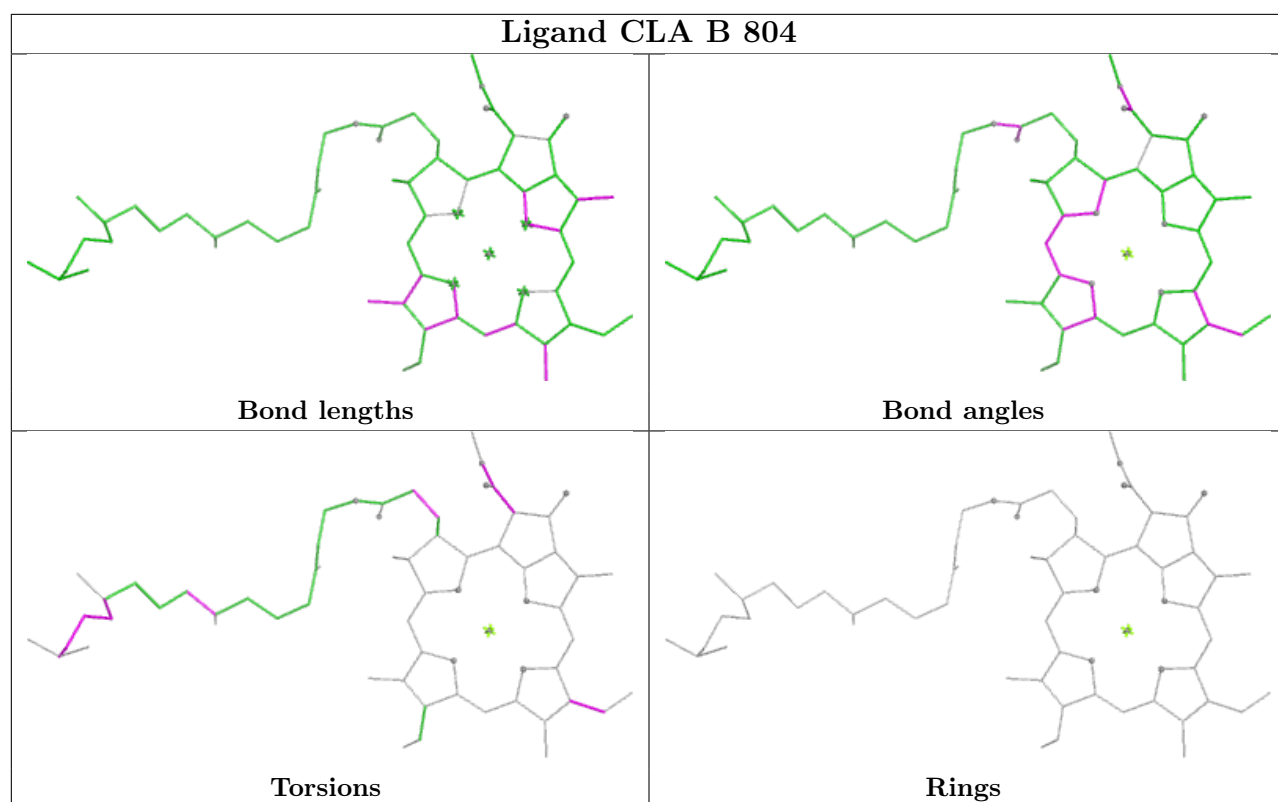


Ligand LUT Z 617

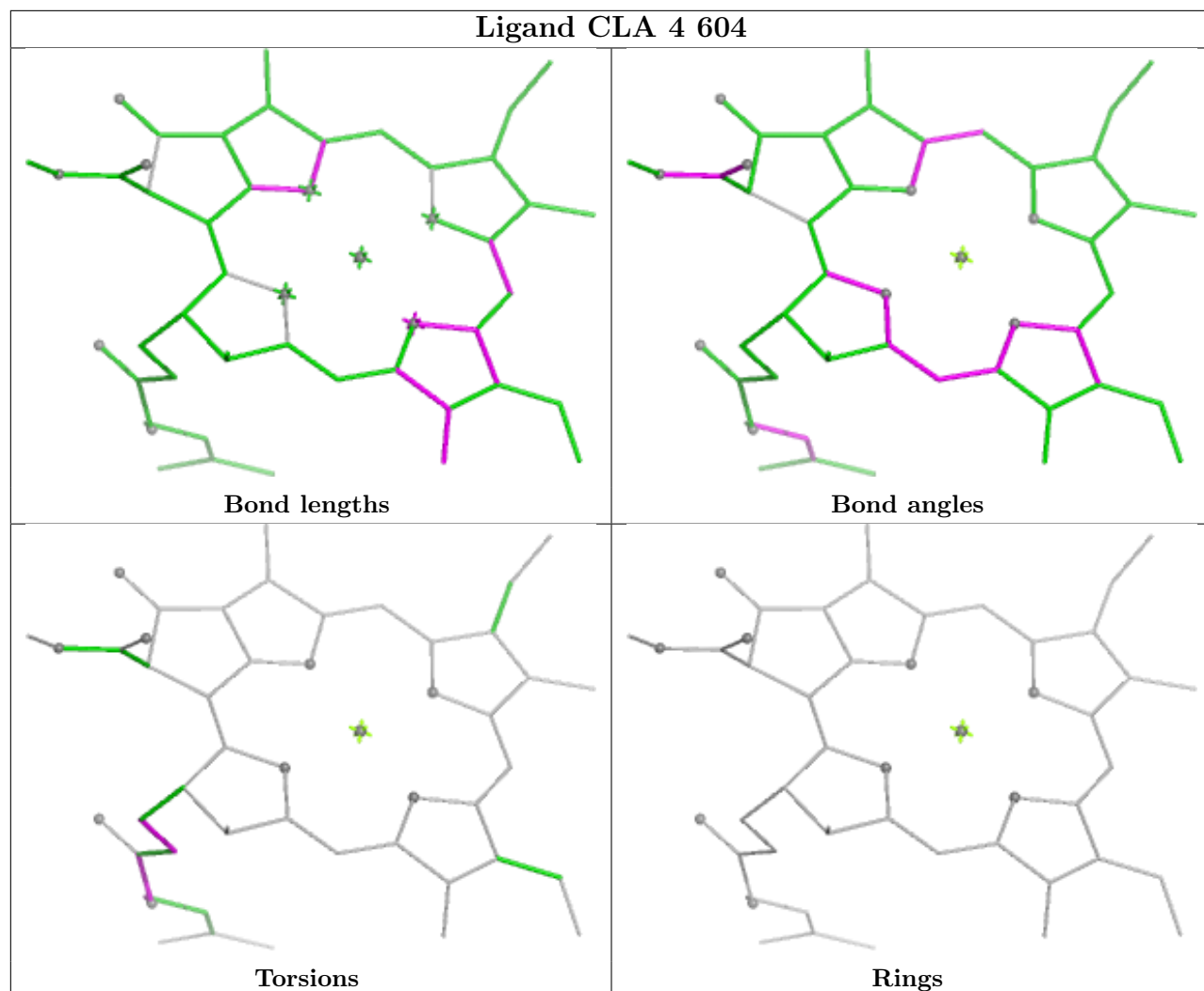


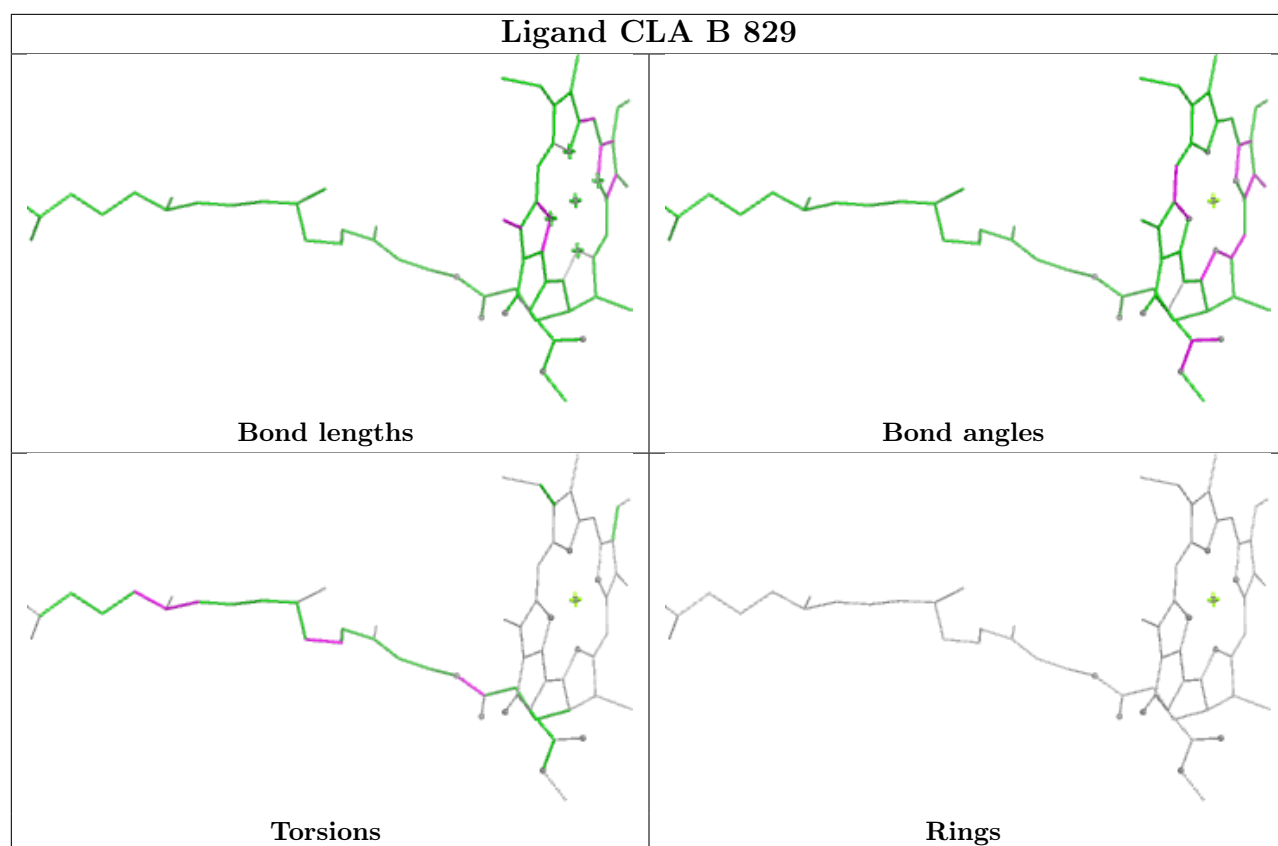


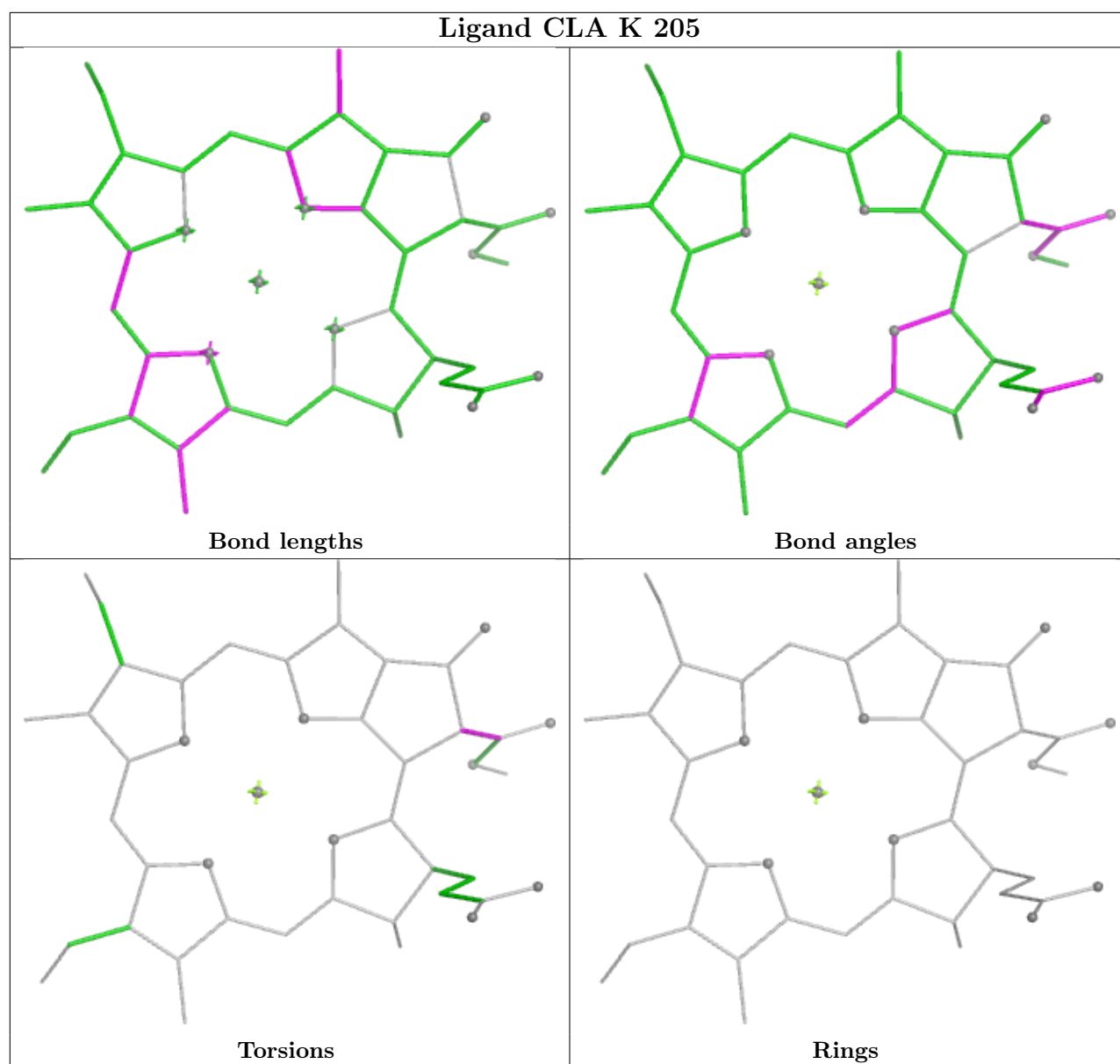


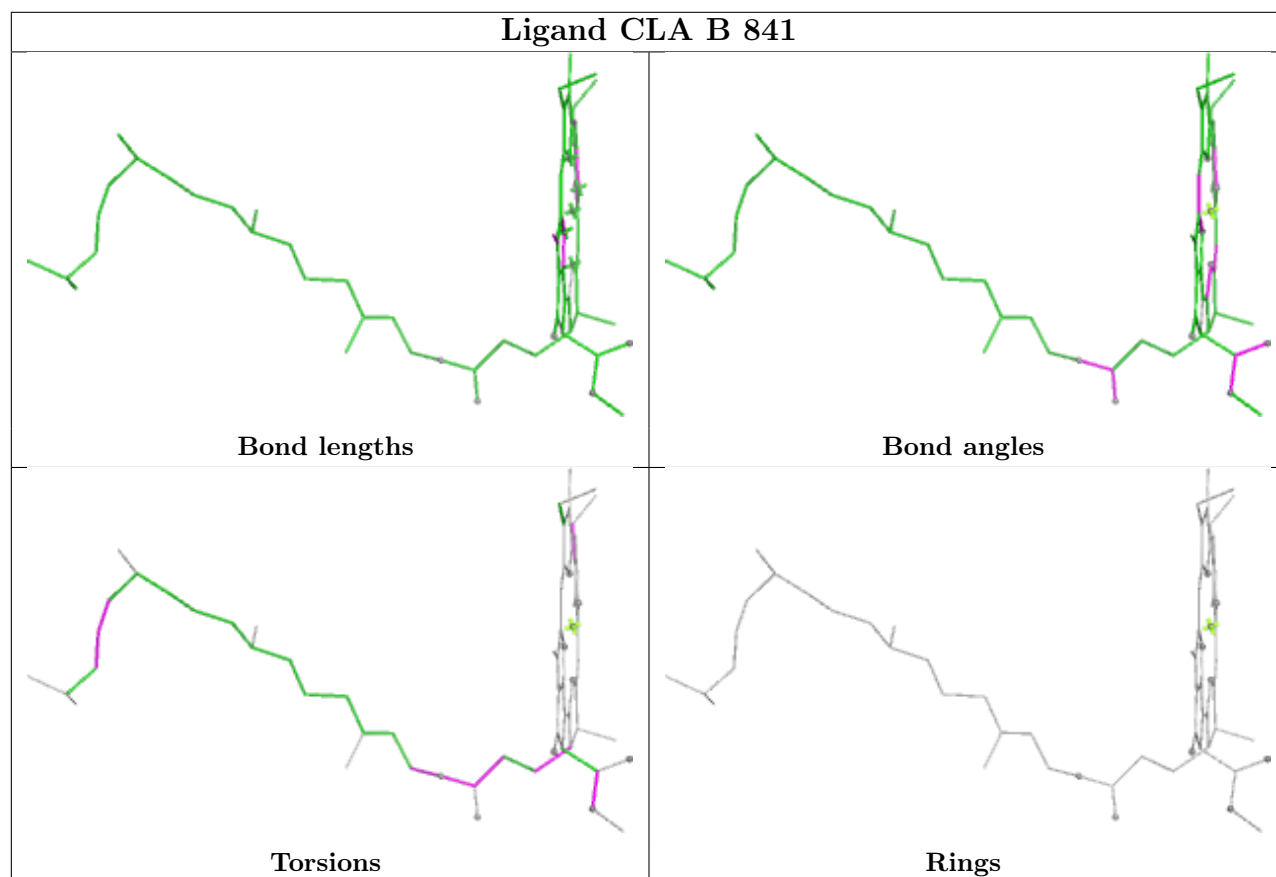
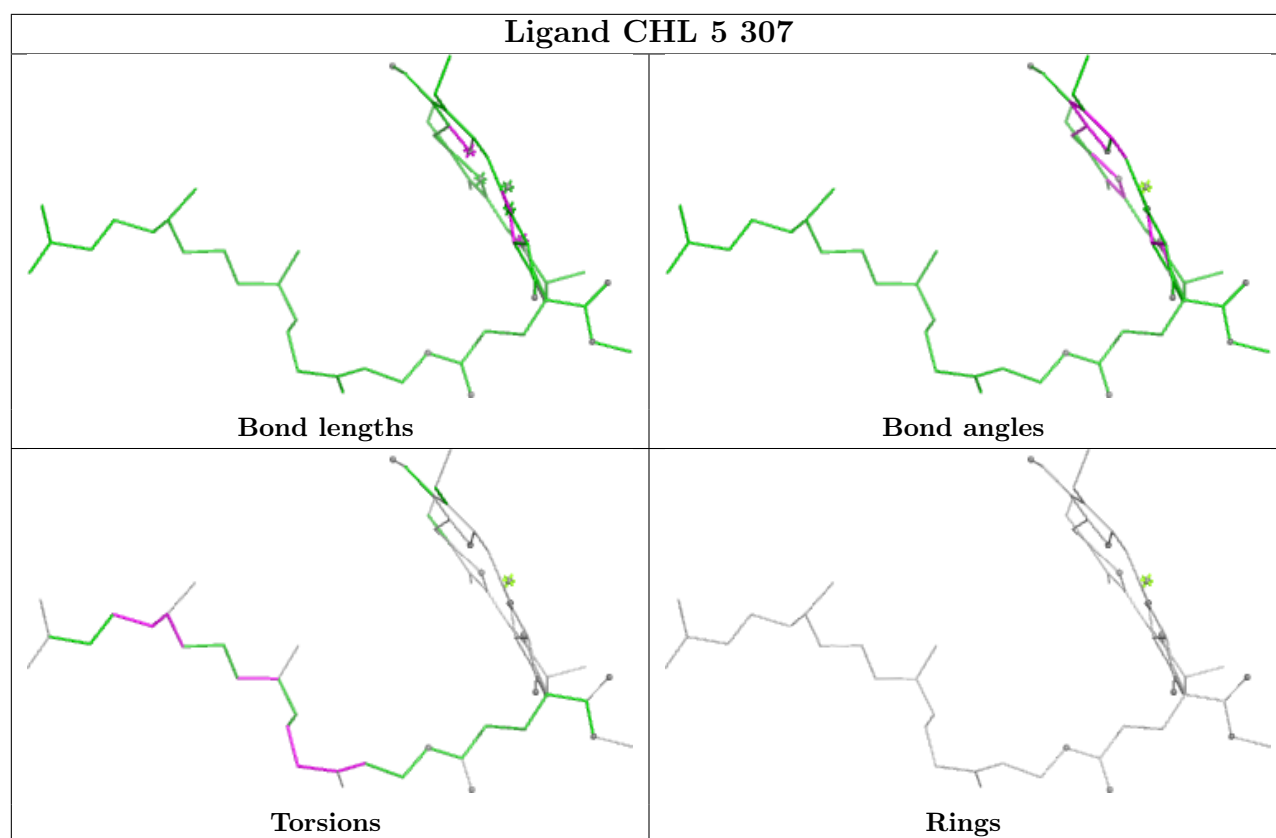


Ligand CLA 4 604

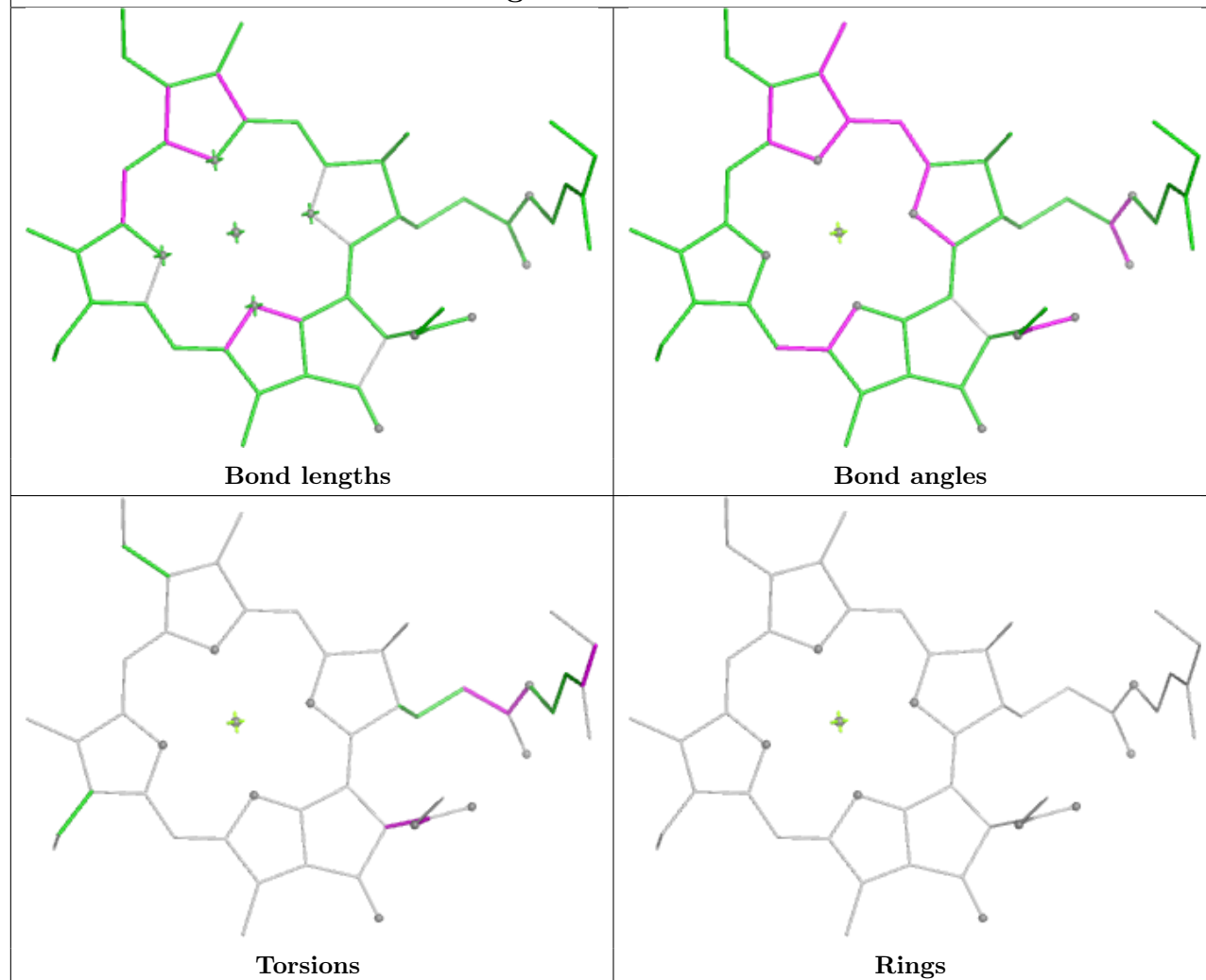




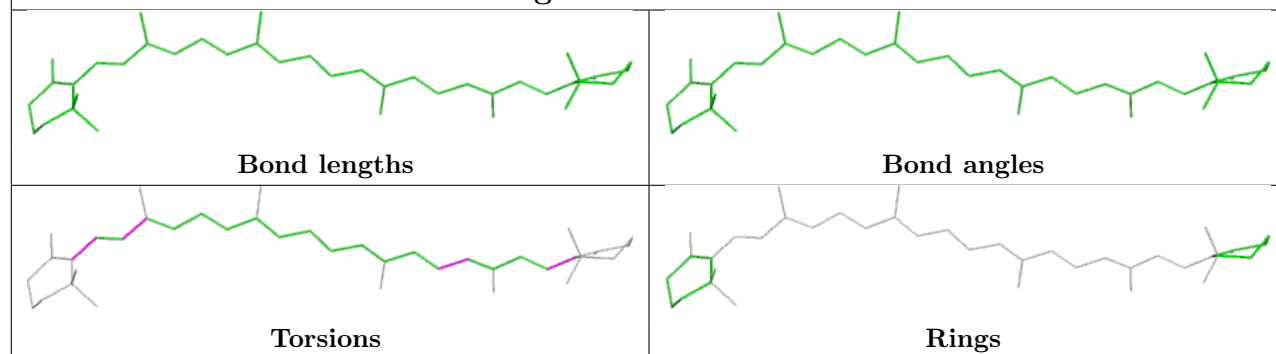


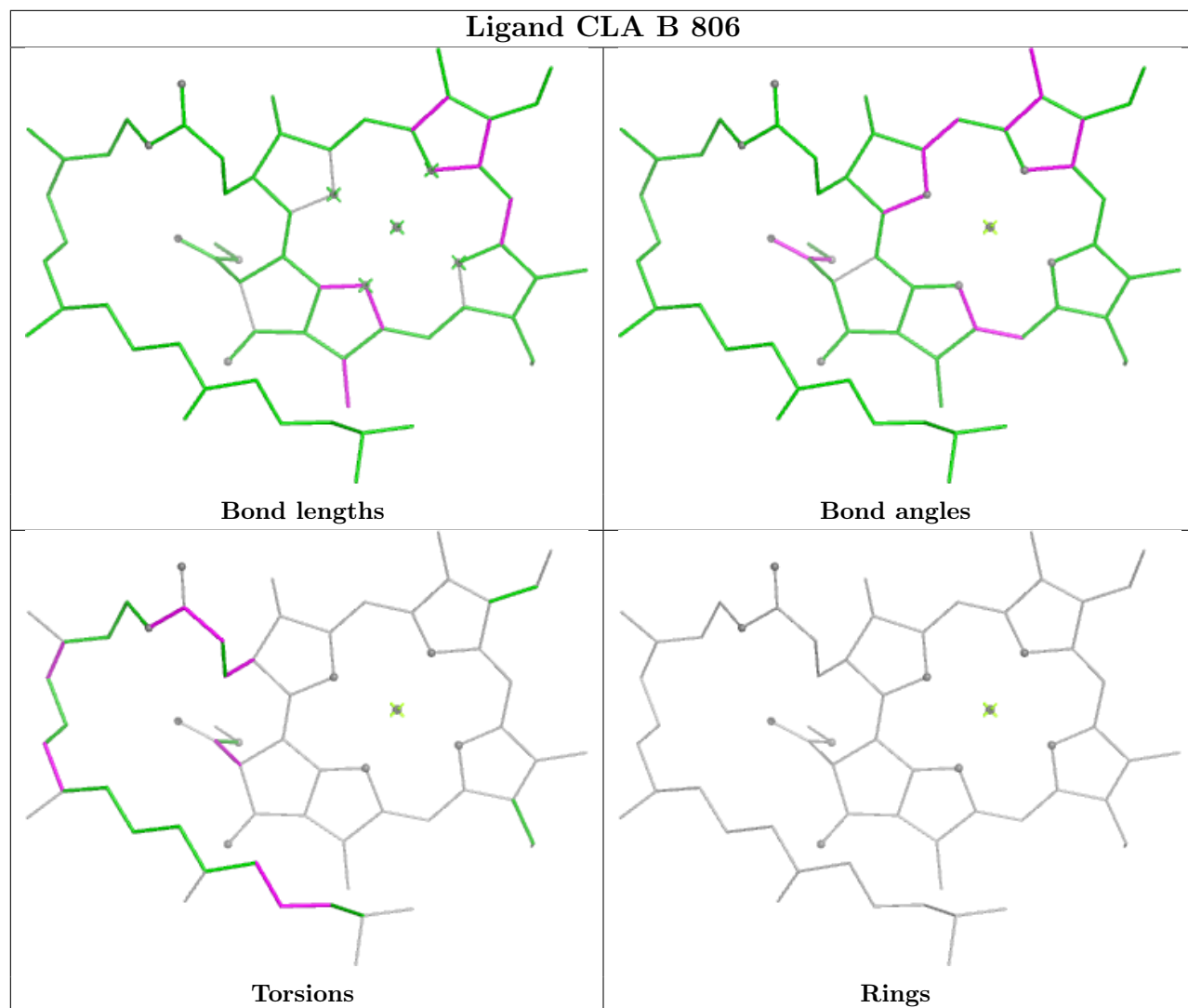


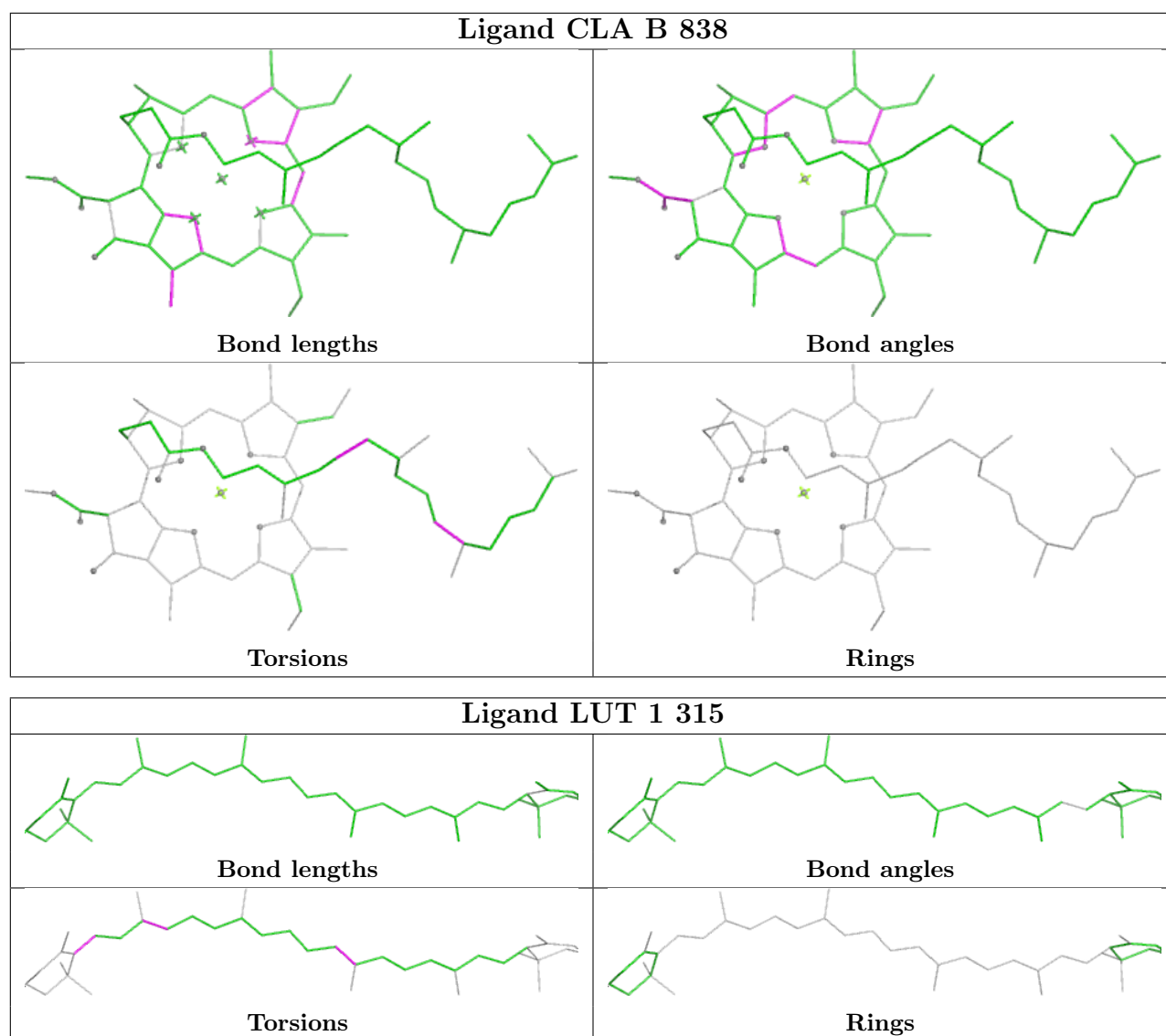
Ligand CLA 6 304



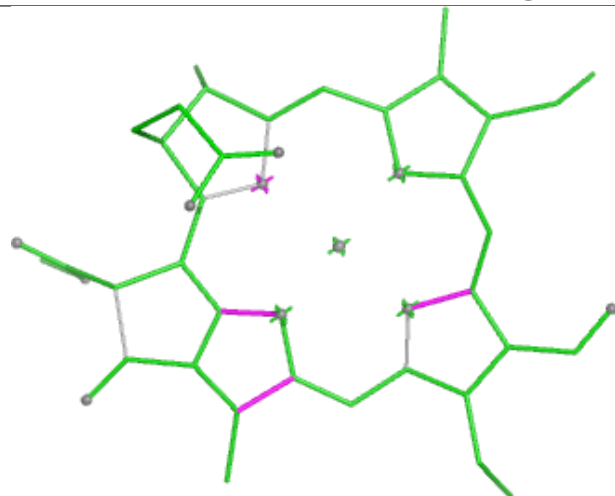
Ligand BCR 3 315



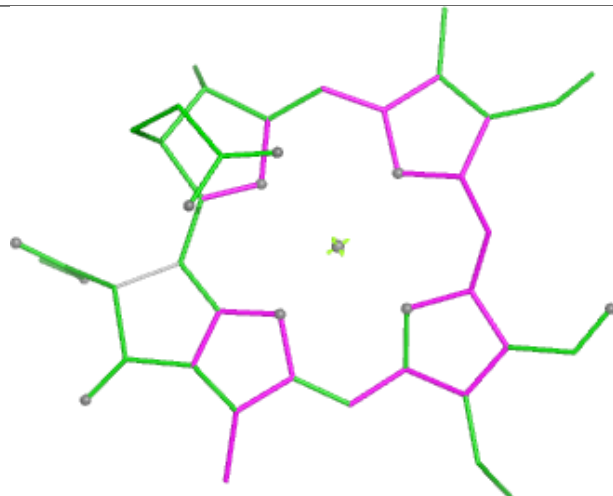




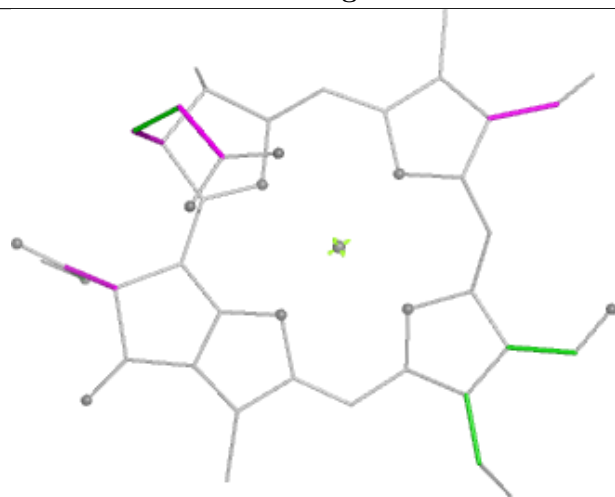
Ligand CHL 1 306



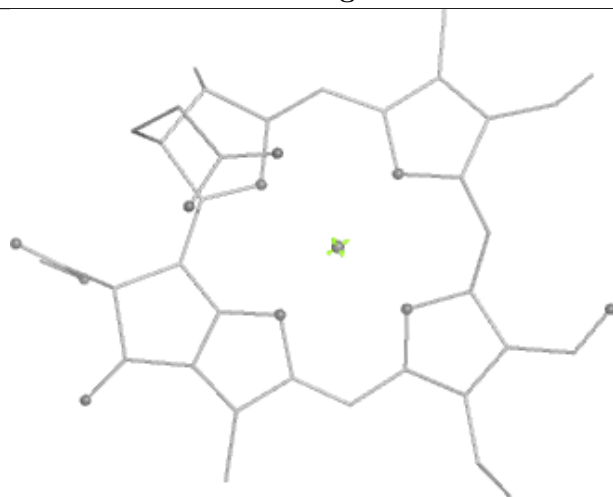
Bond lengths



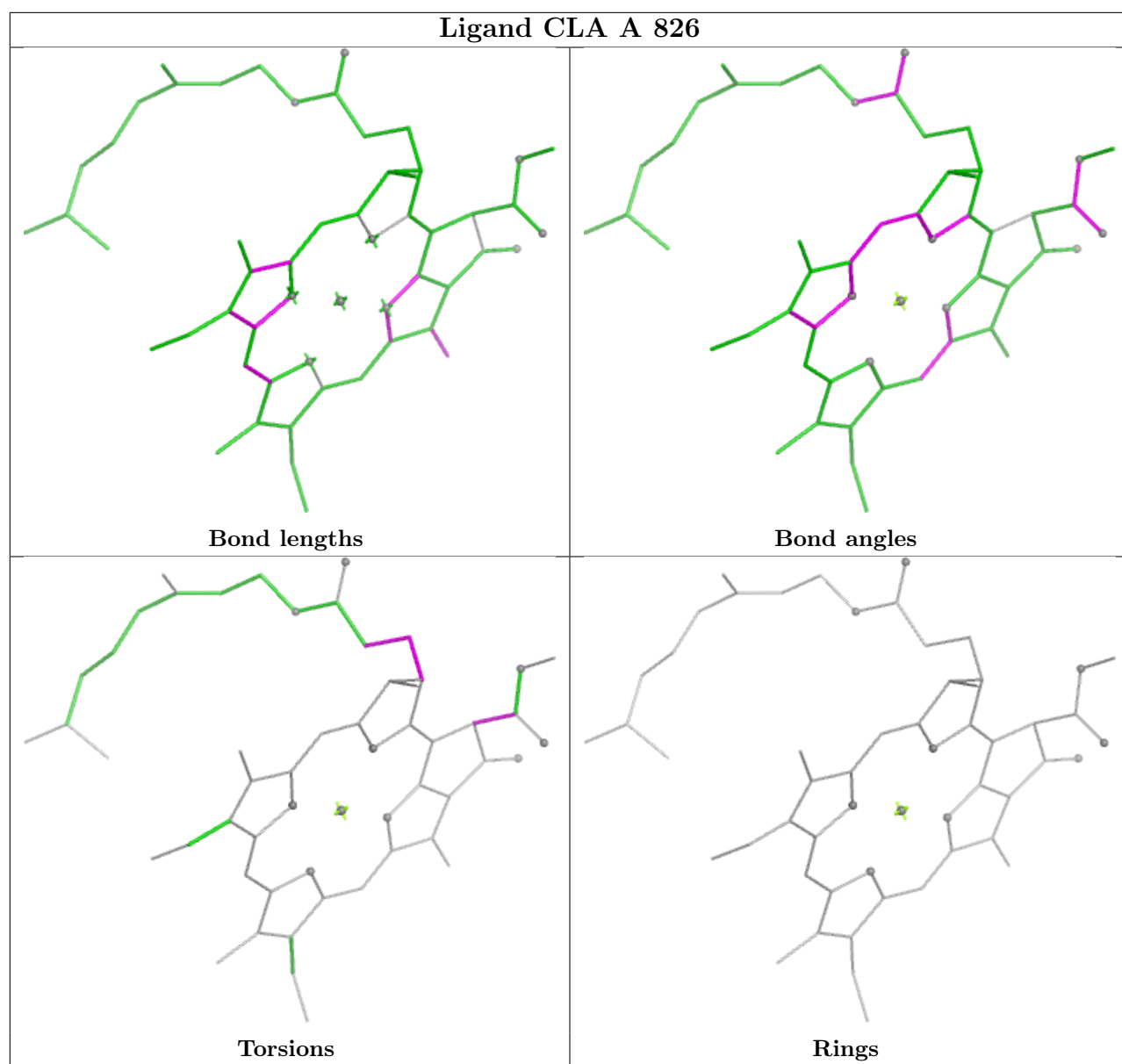
Bond angles

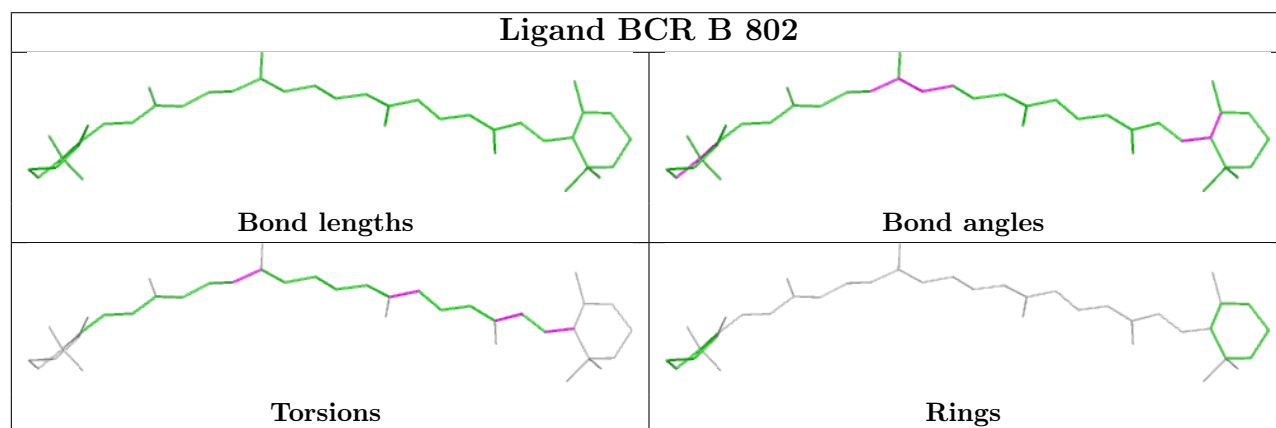
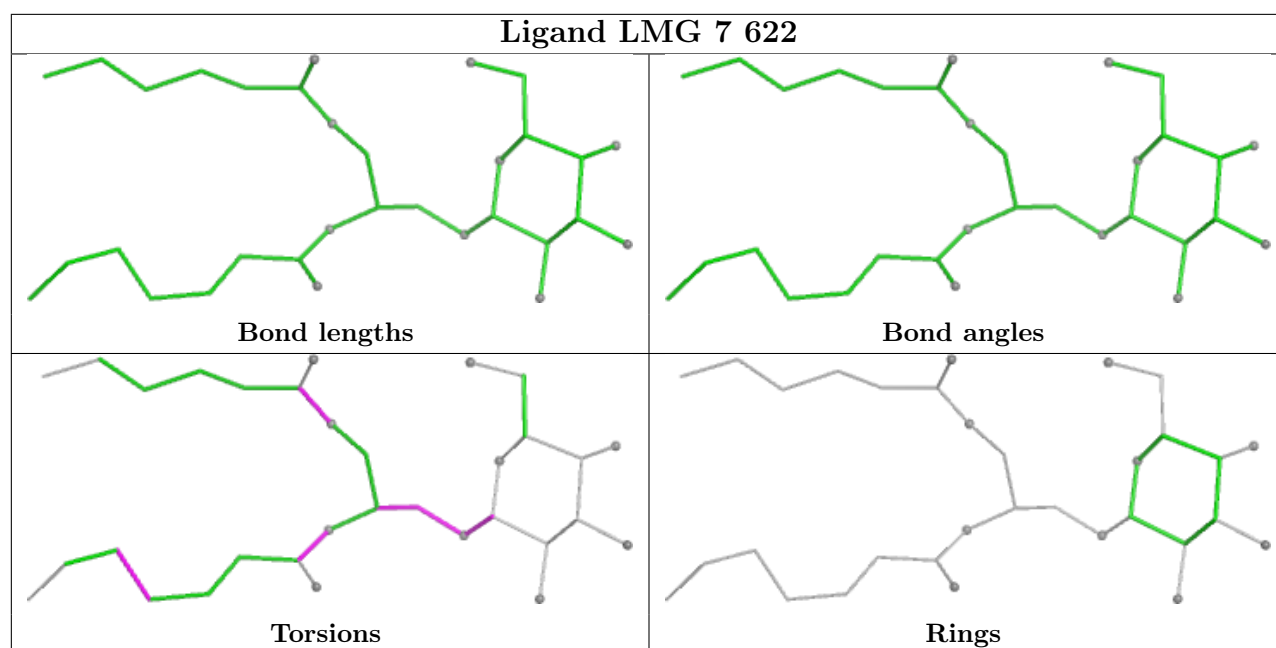


Torsions

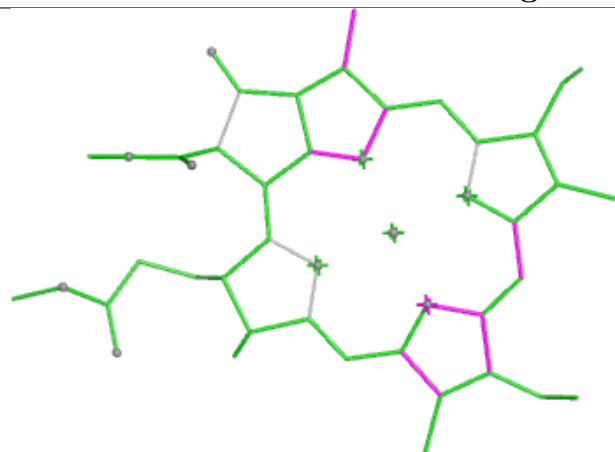


Rings

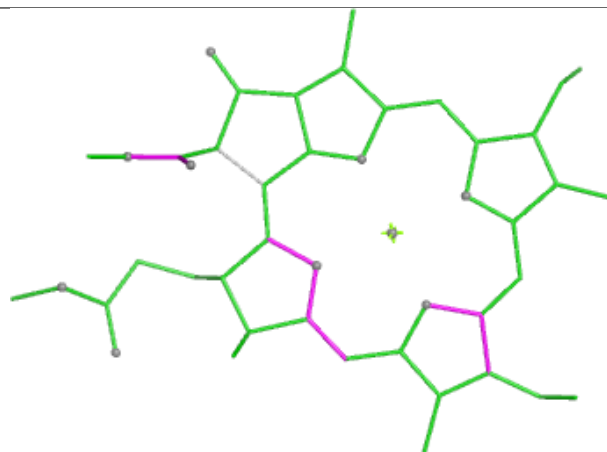




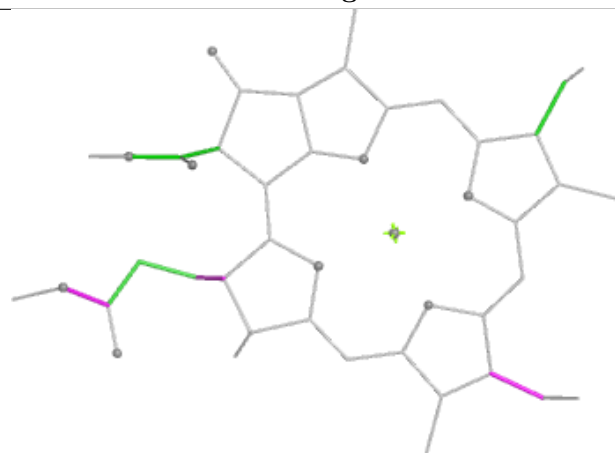
Ligand CLA 7 614



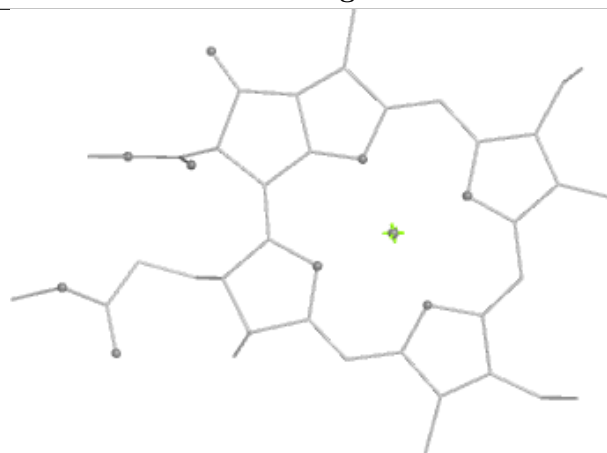
Bond lengths



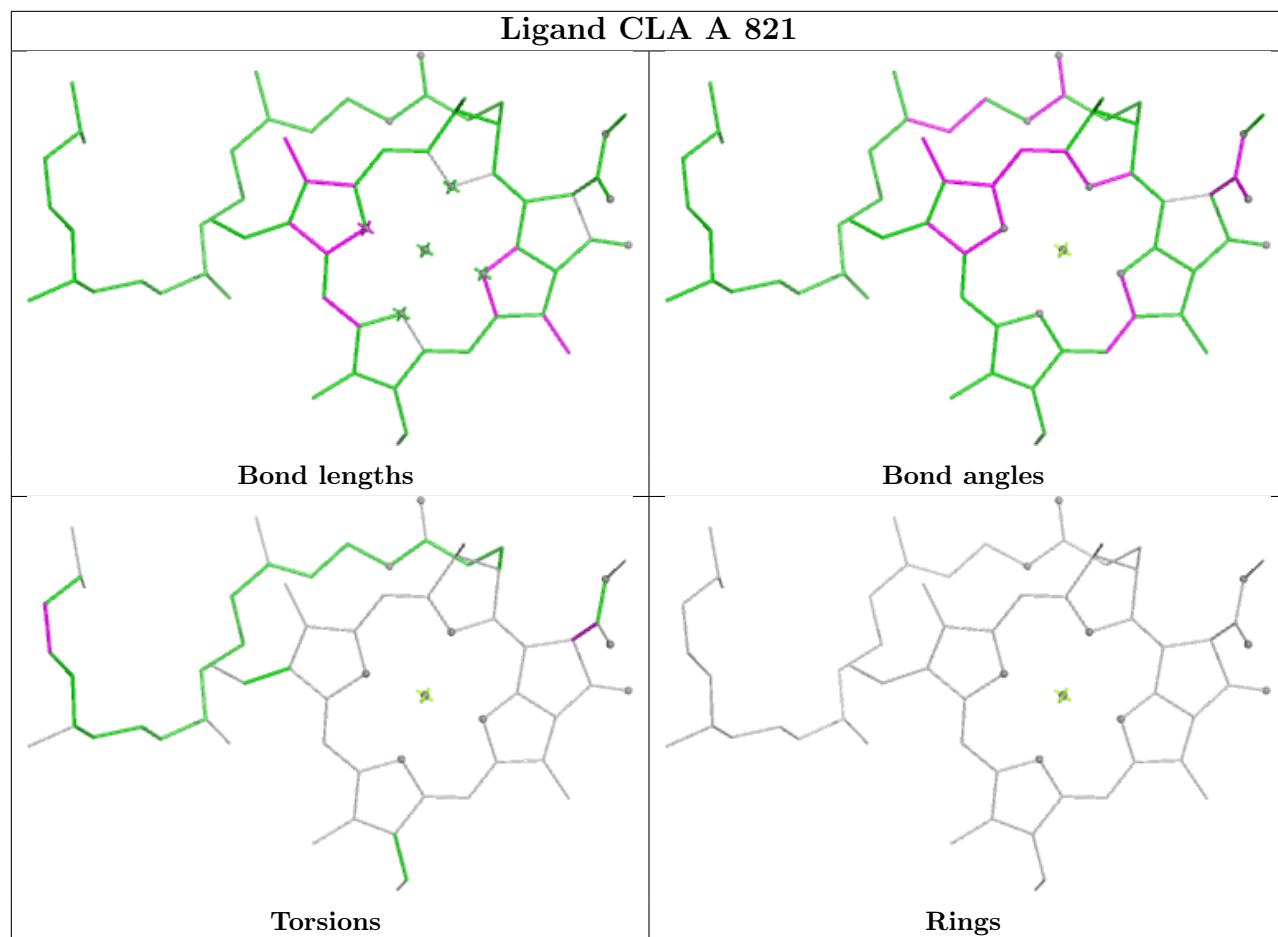
Bond angles

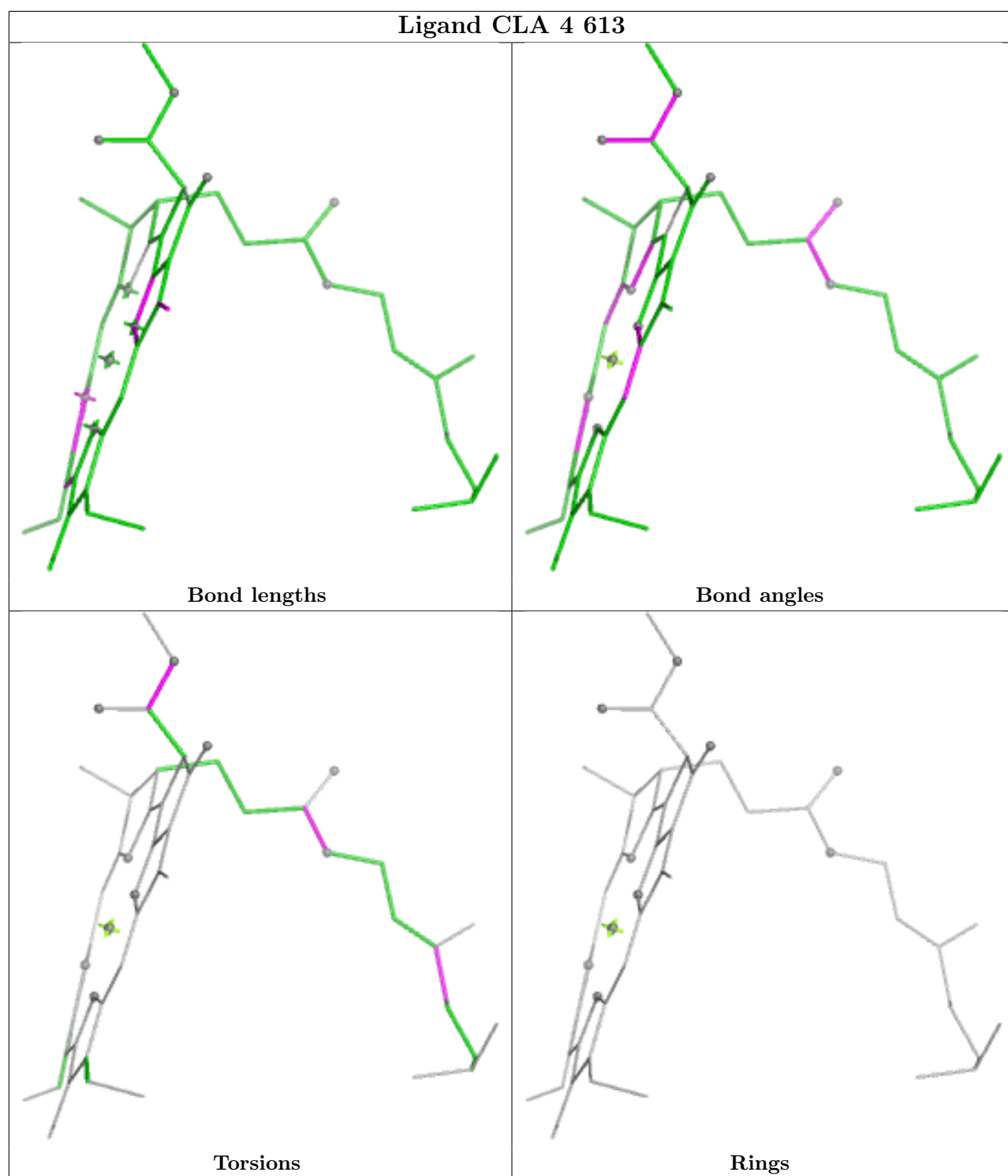


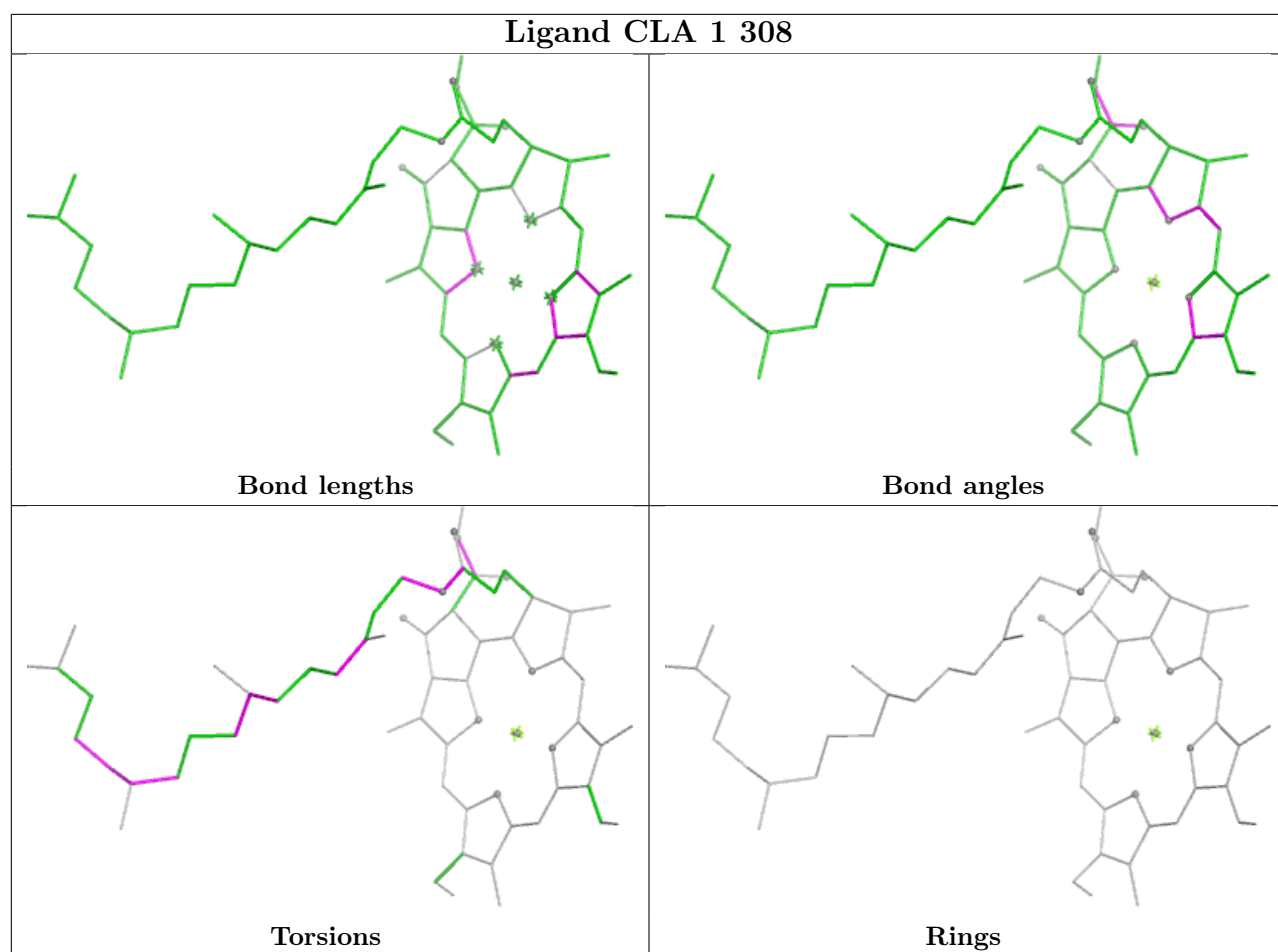
Torsions

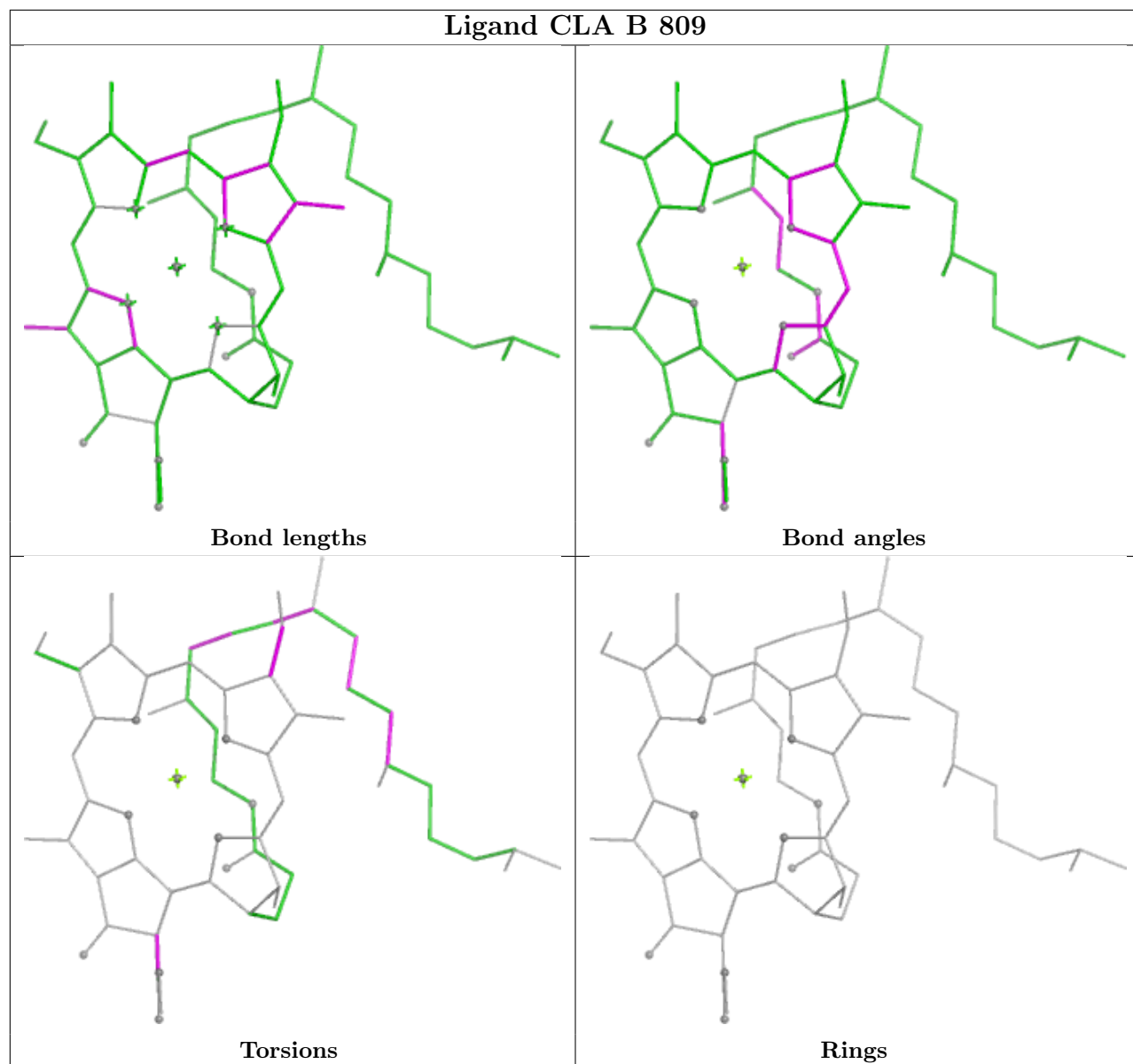


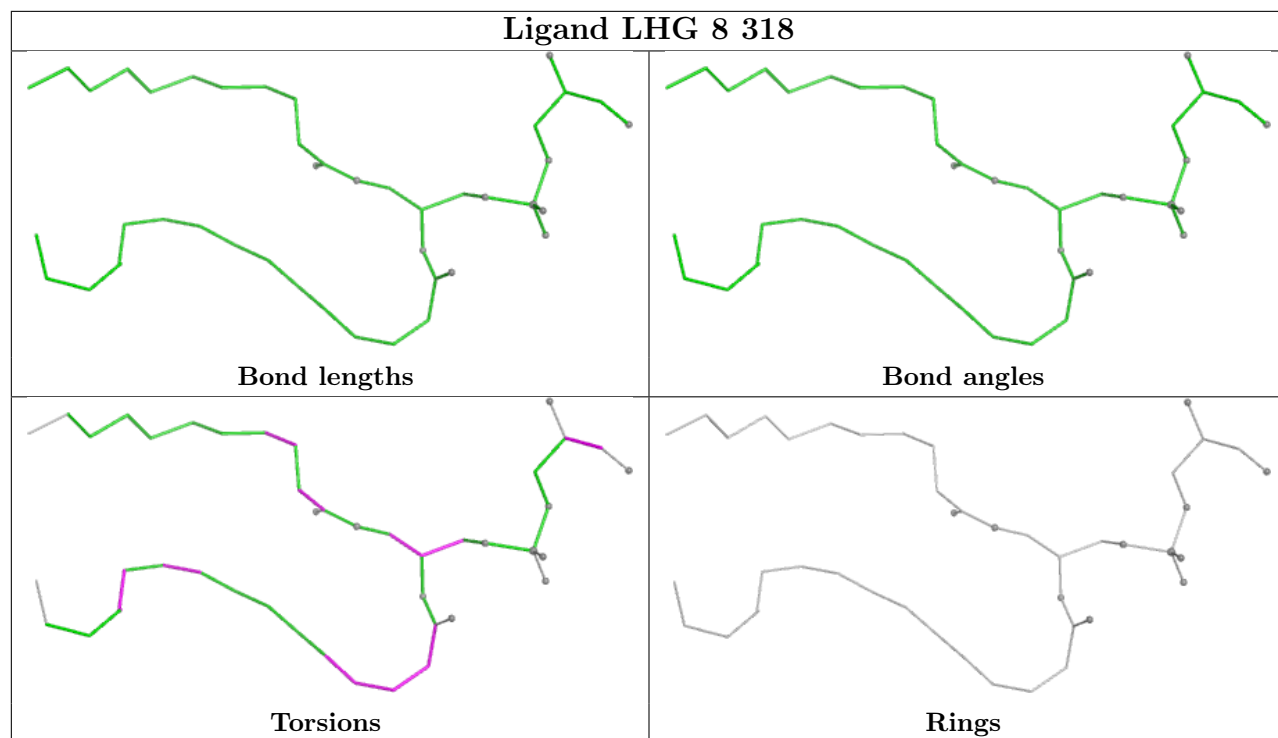
Rings



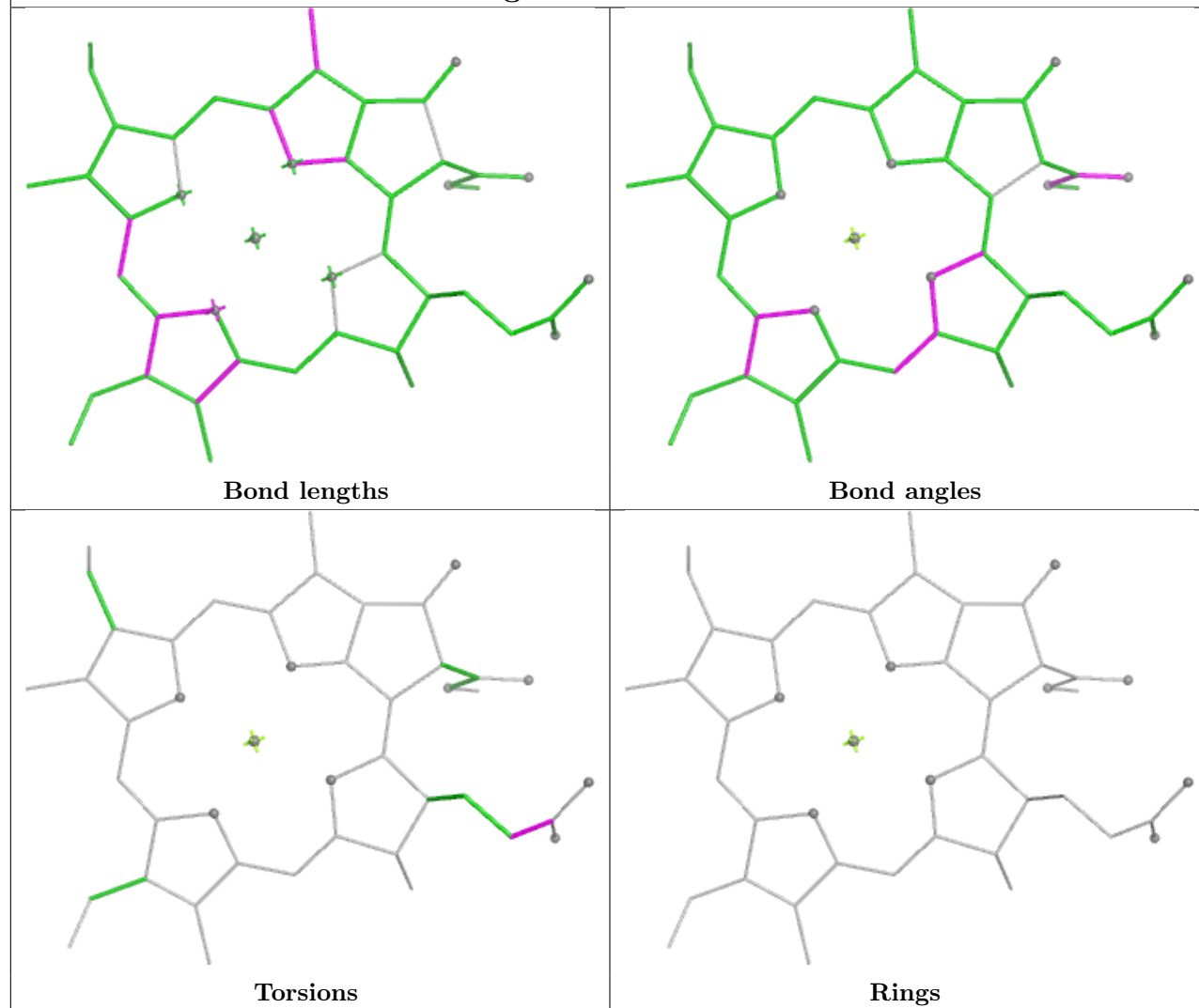




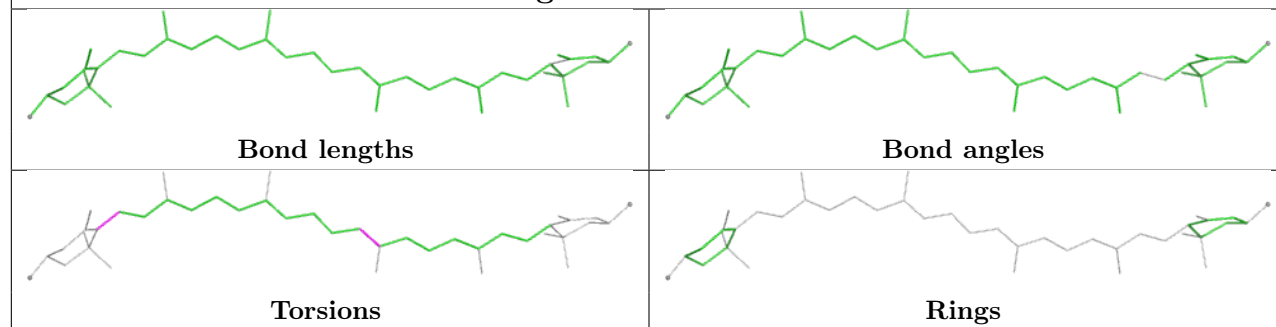




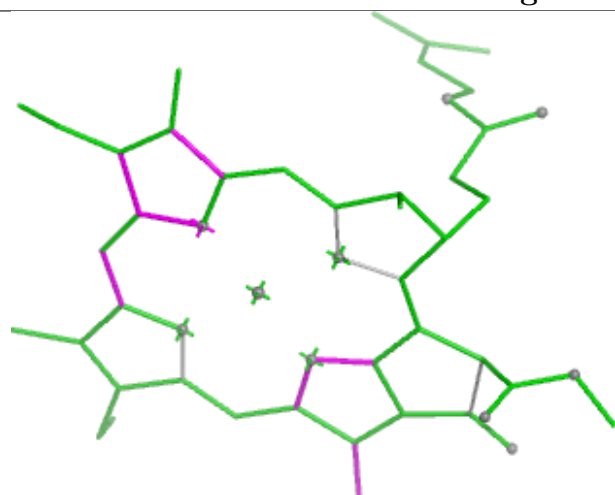
Ligand CLA 6 312



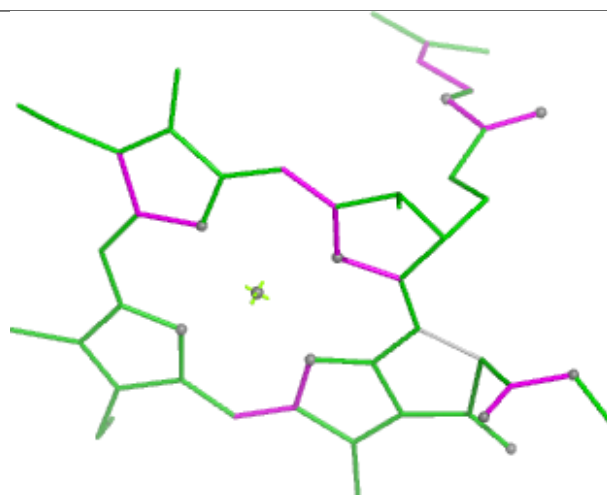
Ligand LUT 3 316



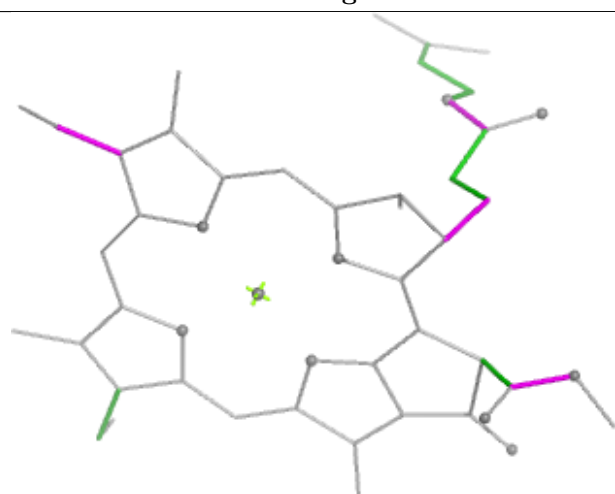
Ligand CLA 6 314



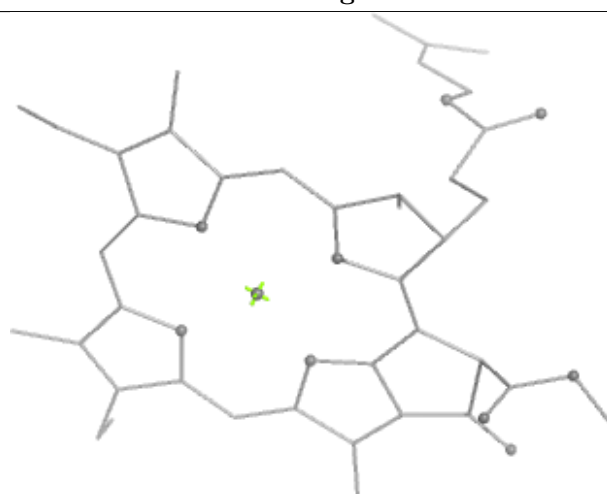
Bond lengths



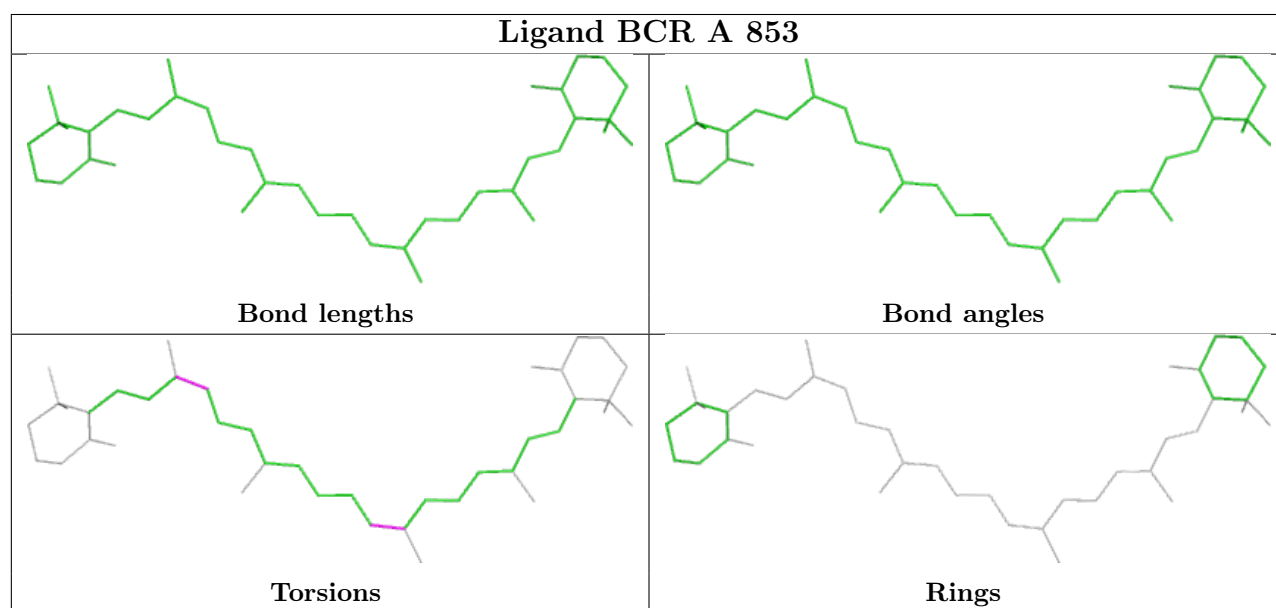
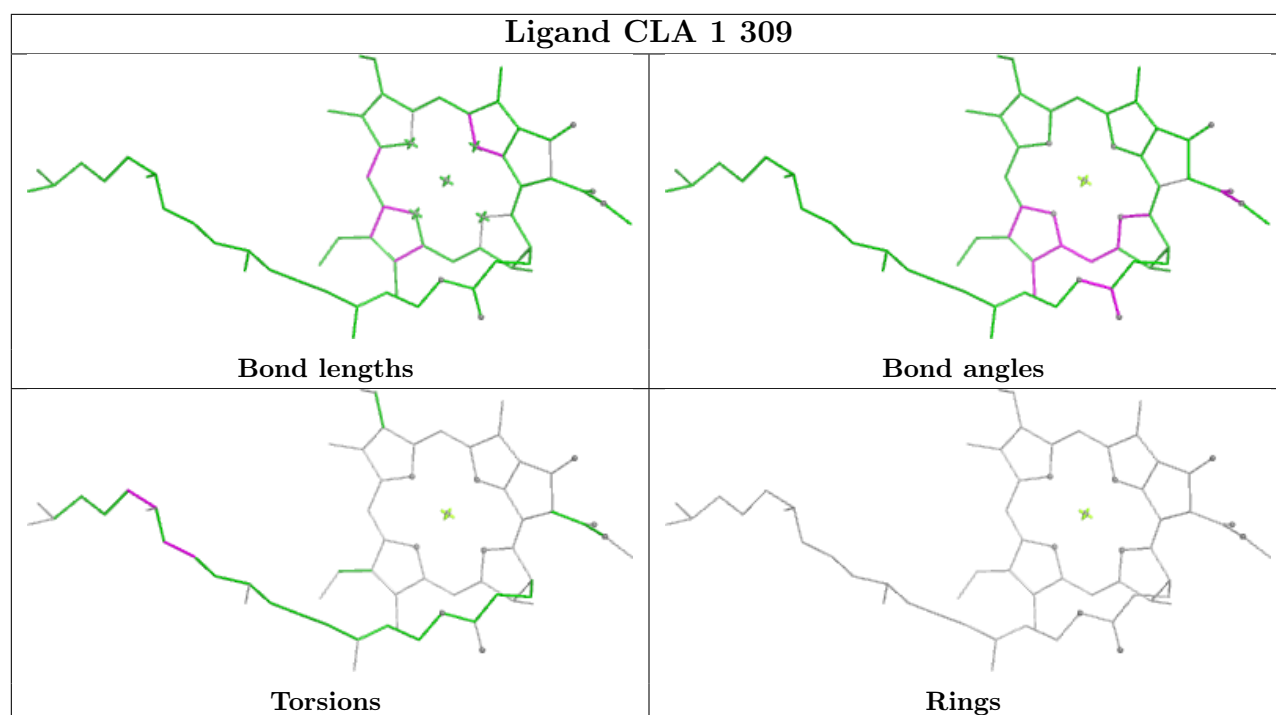
Bond angles



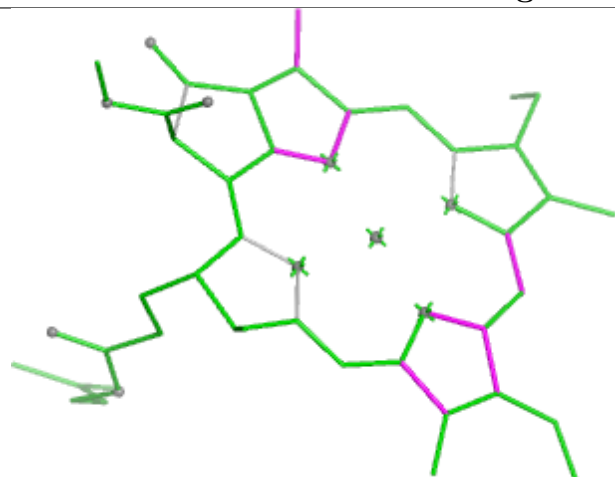
Torsions



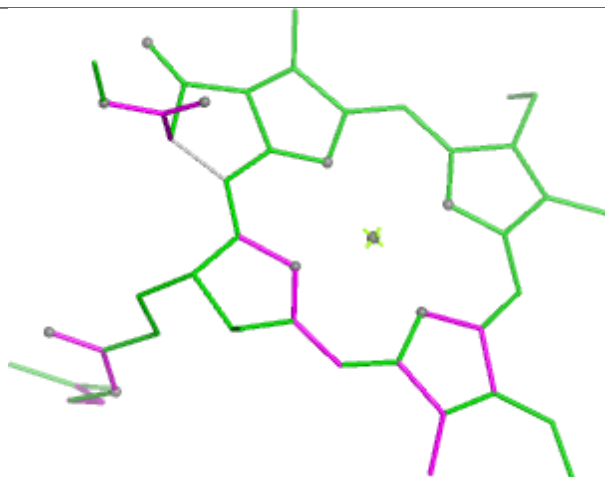
Rings



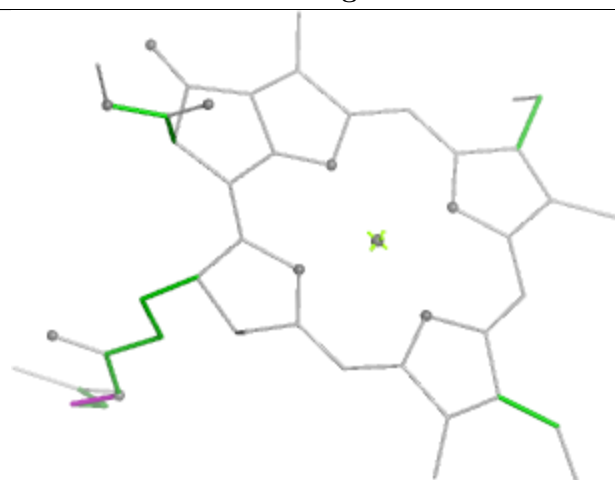
Ligand CLA B 839



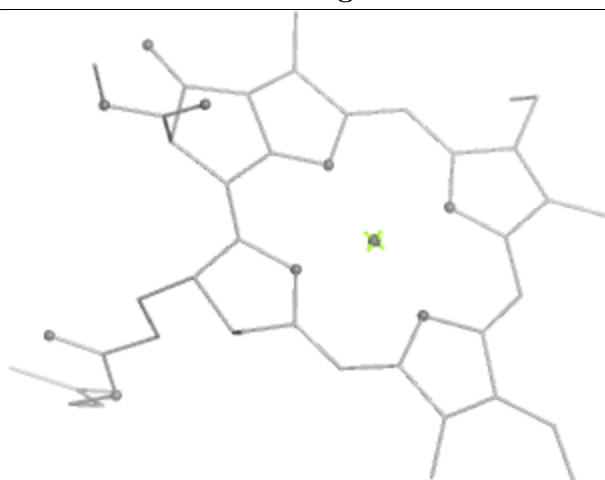
Bond lengths



Bond angles

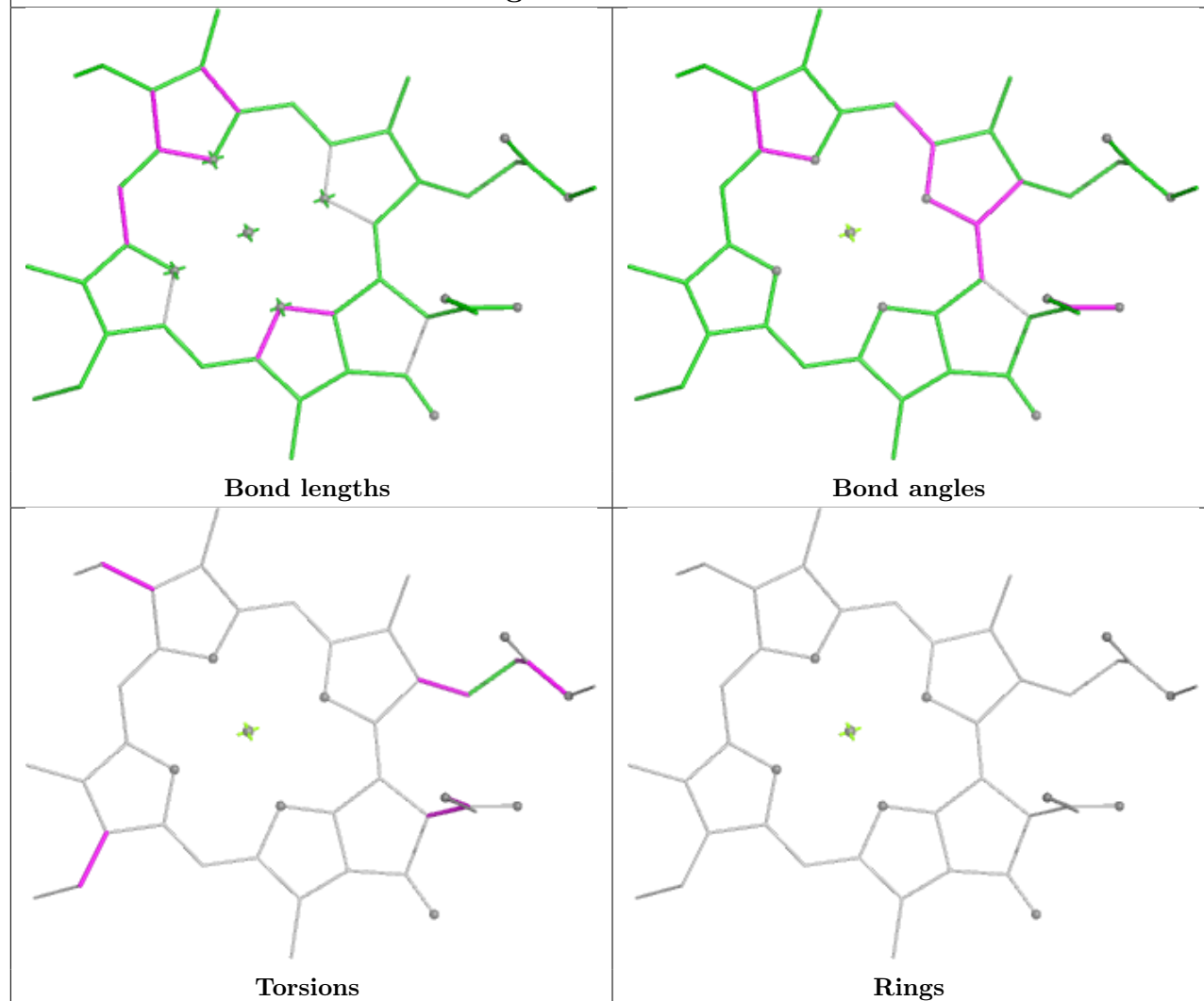


Torsions

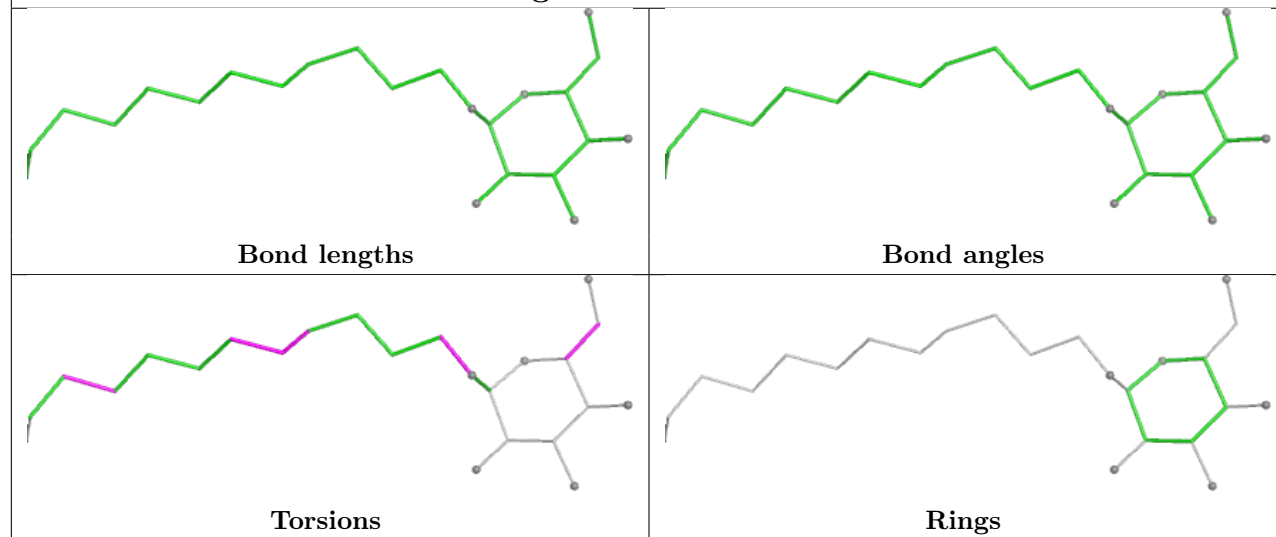


Rings

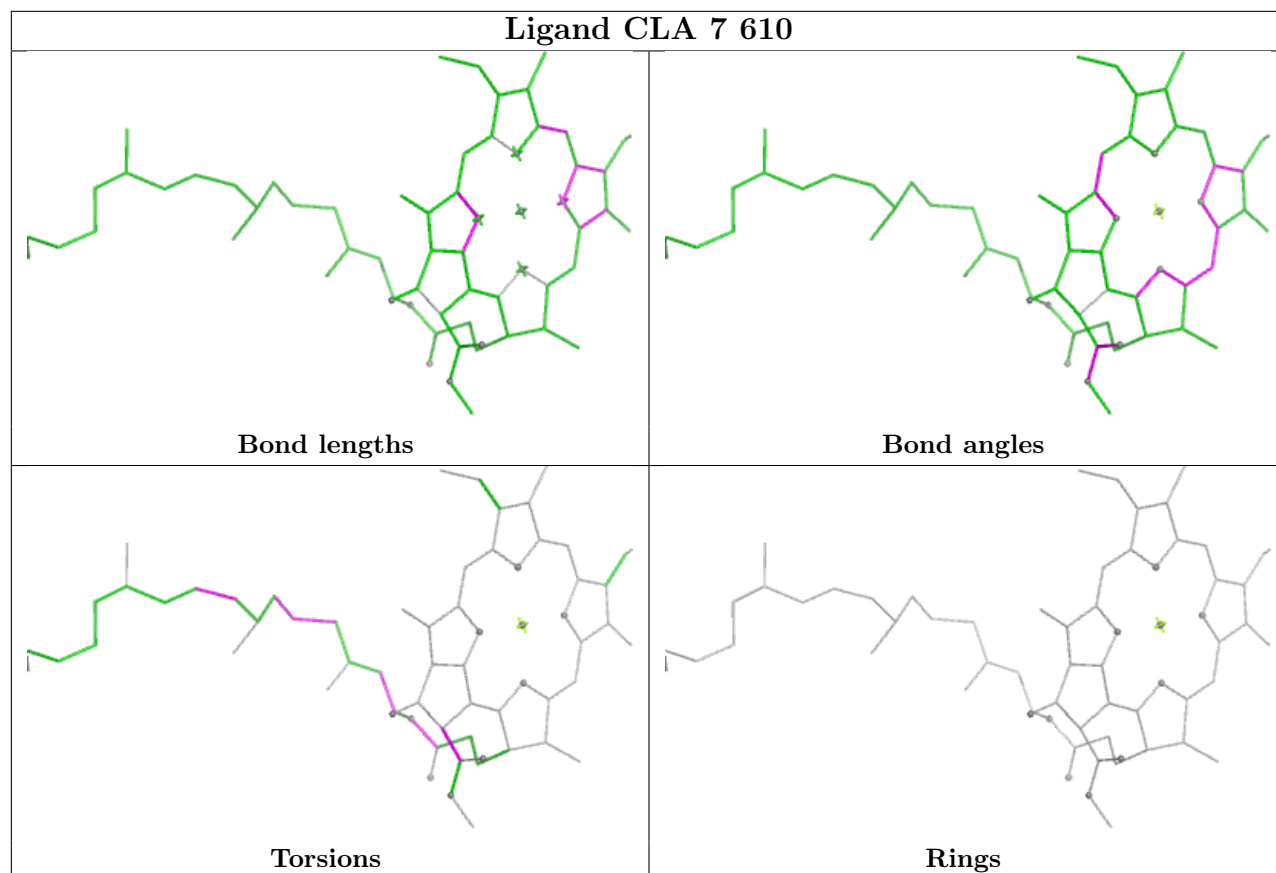
Ligand CLA 5 319



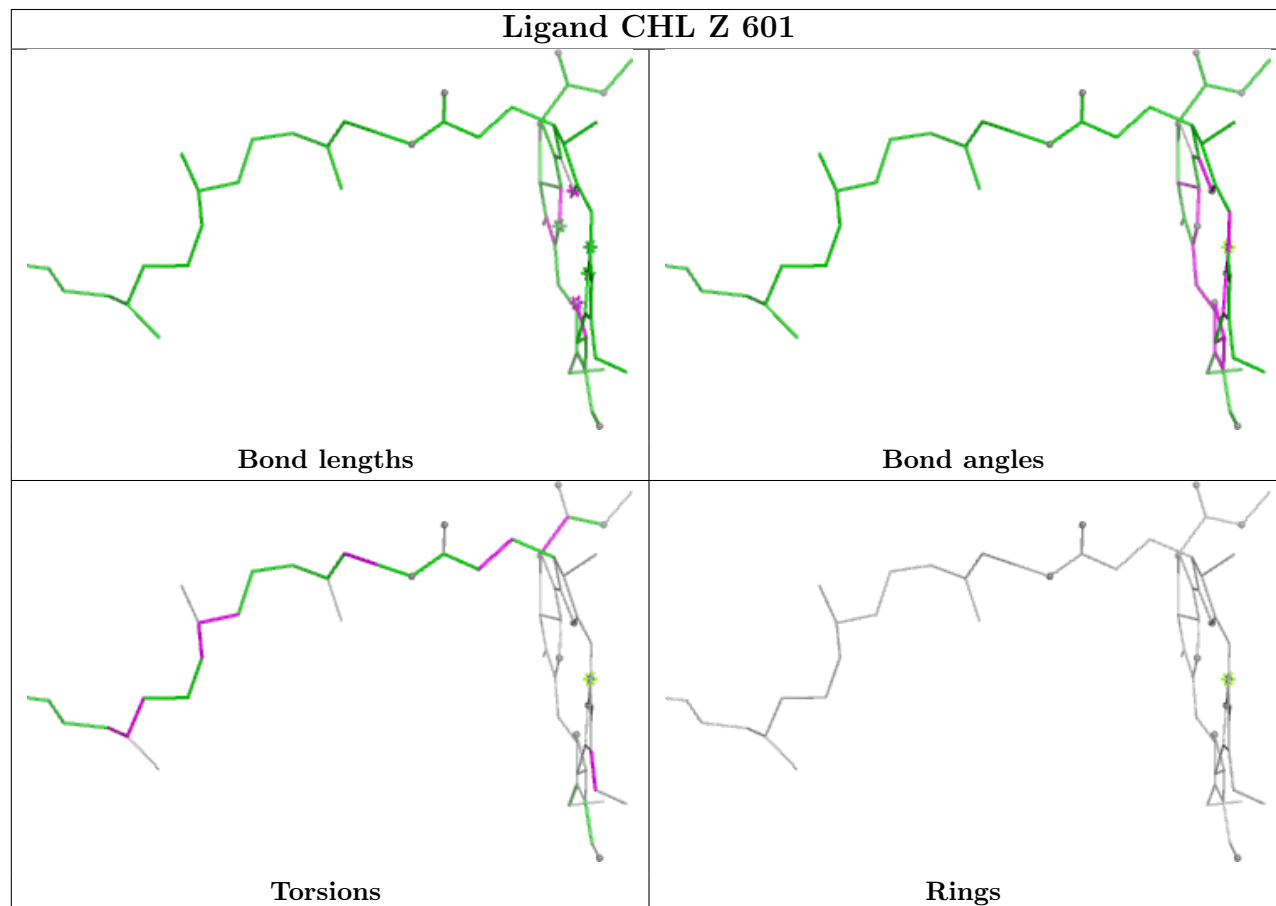
Ligand LMU 6 324

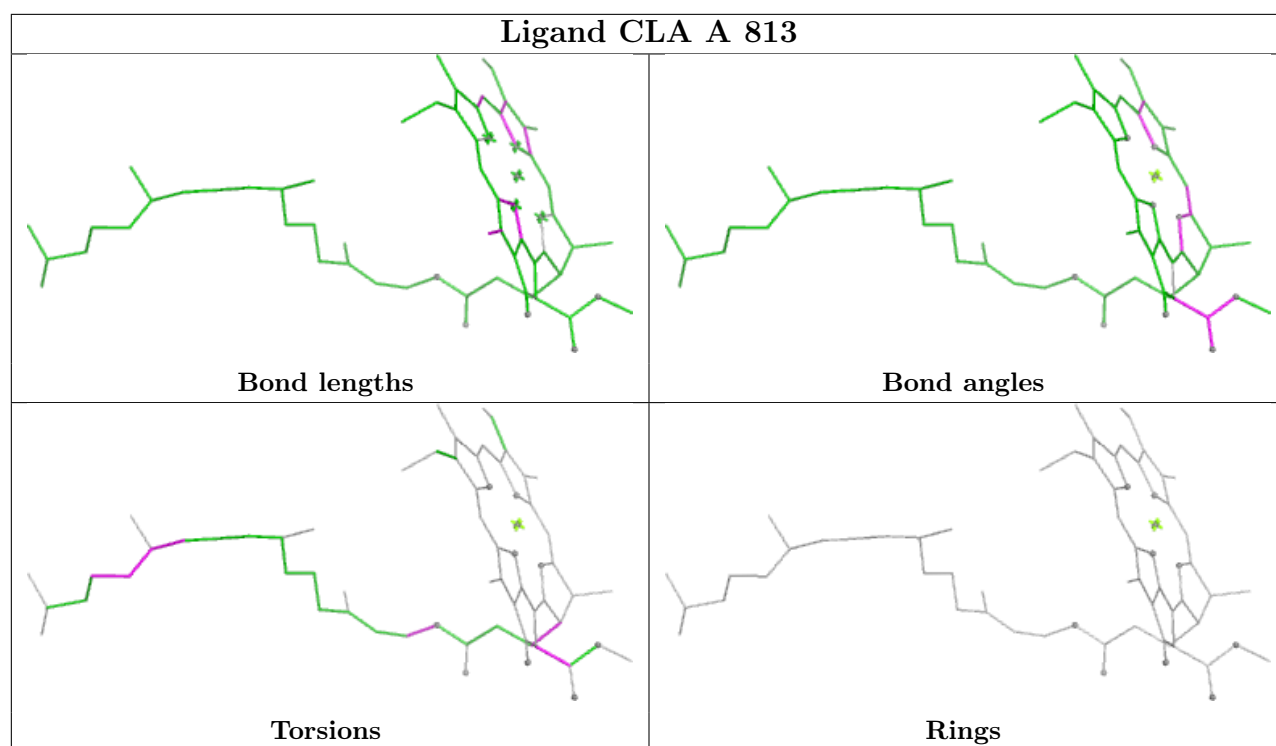


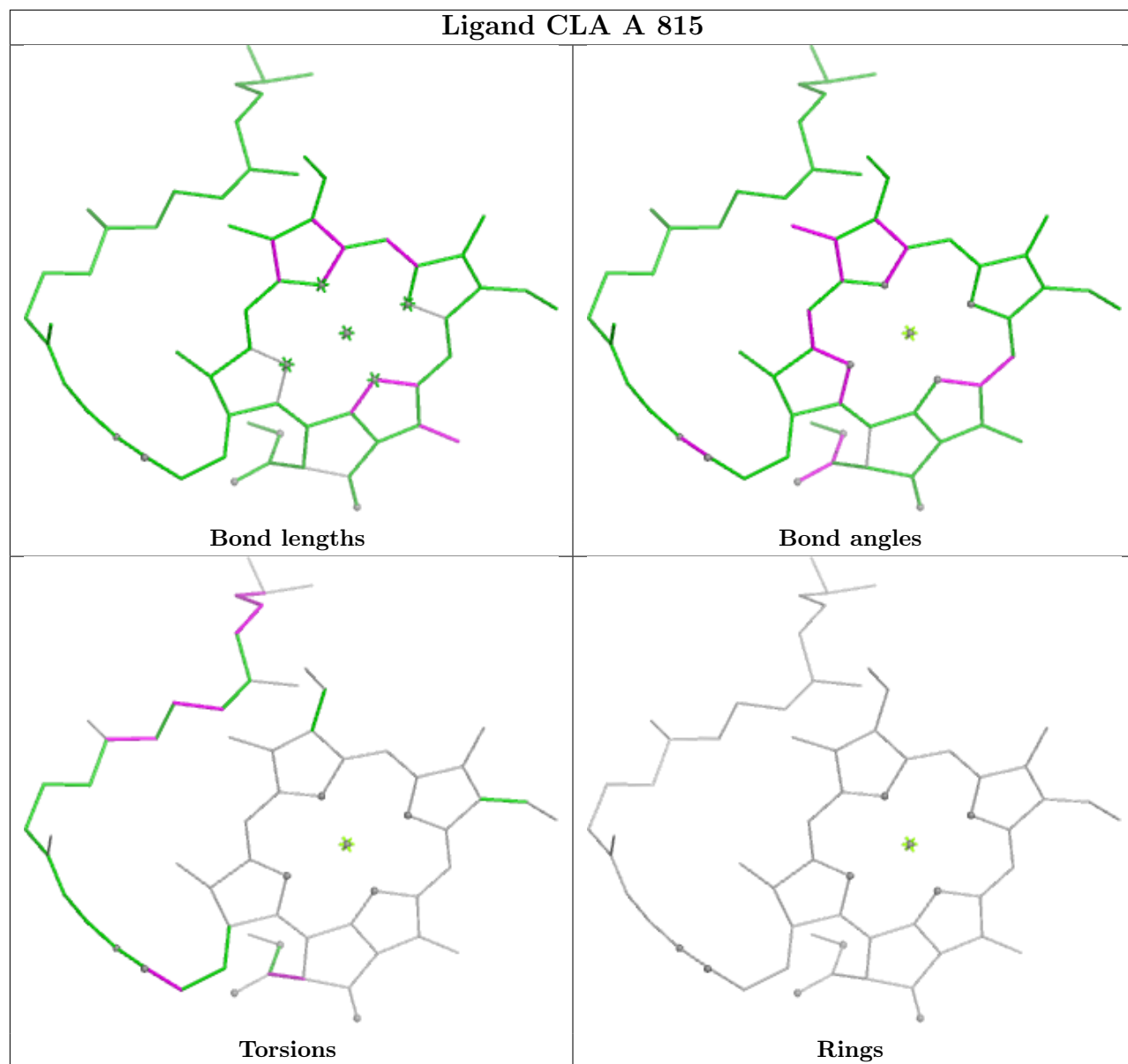
Ligand CLA 7 610

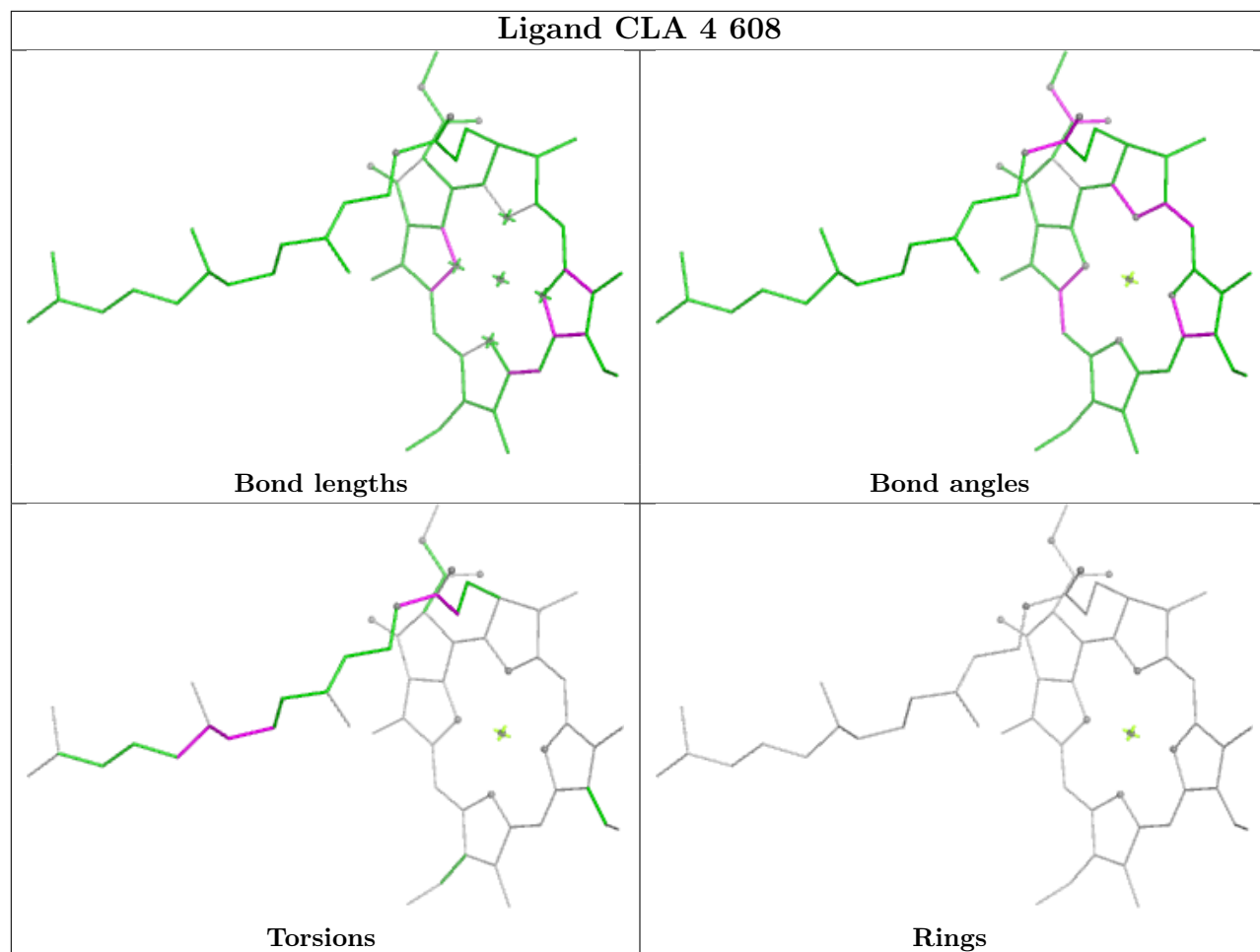


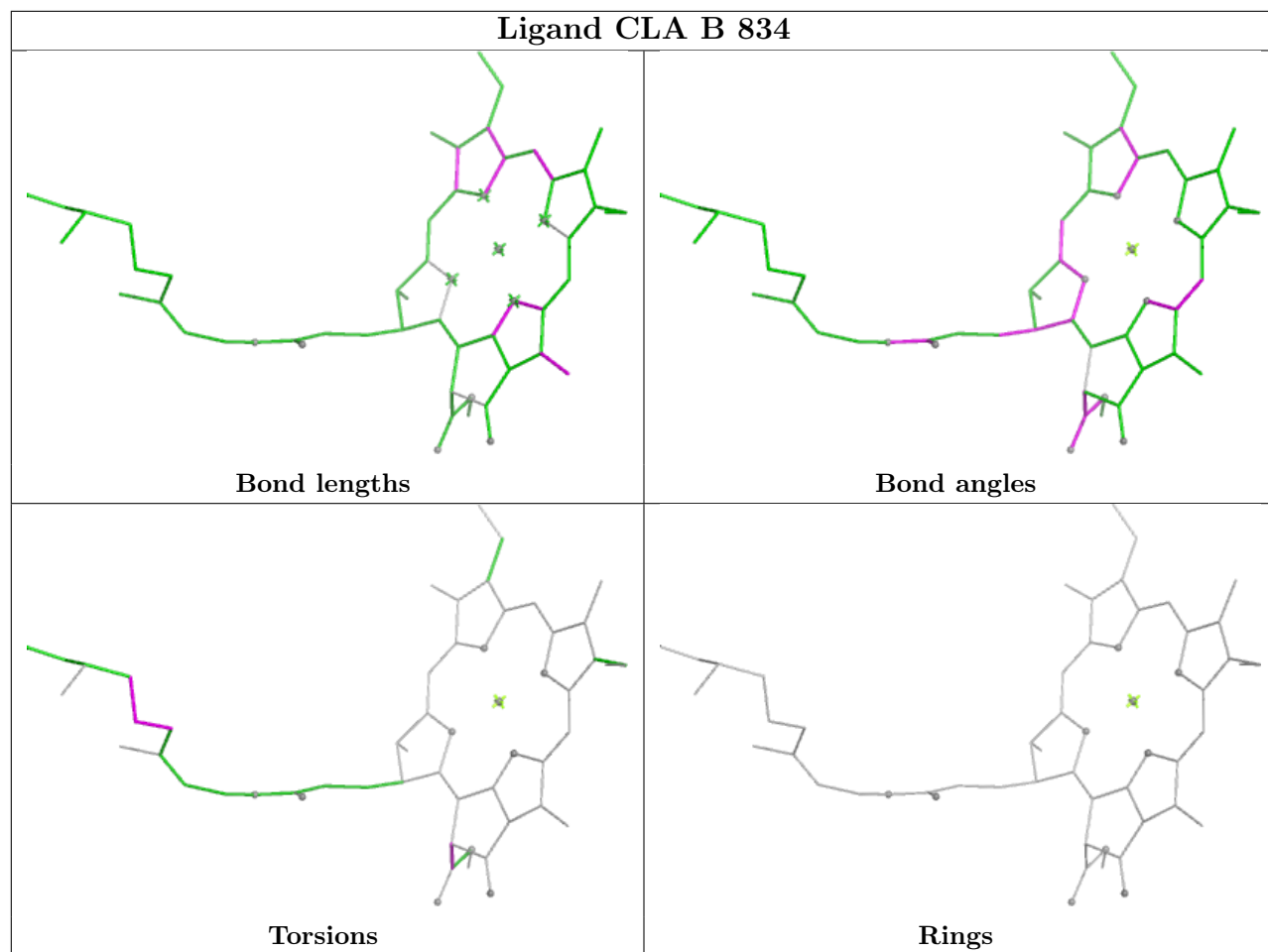
Ligand CHL Z 601

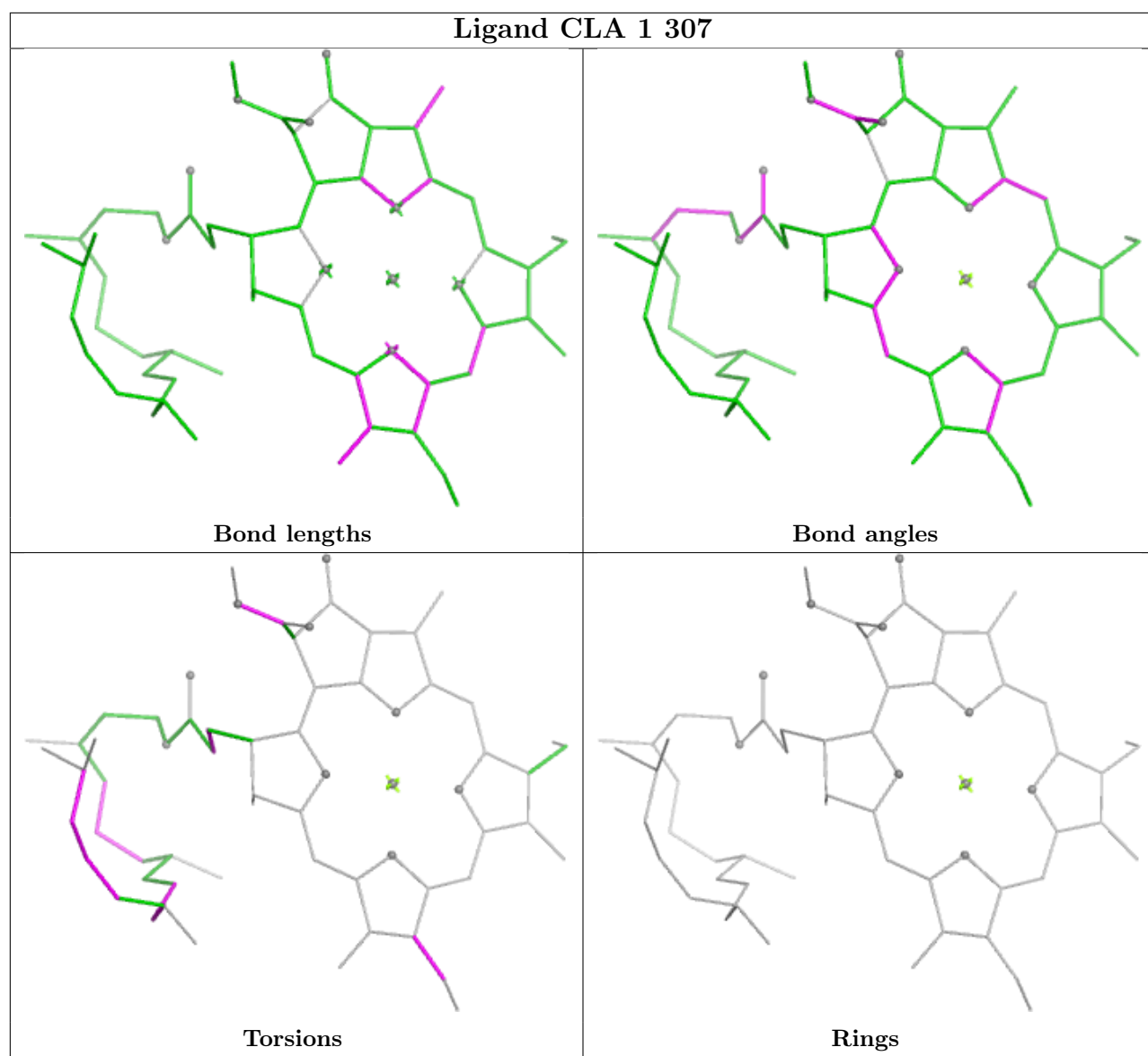


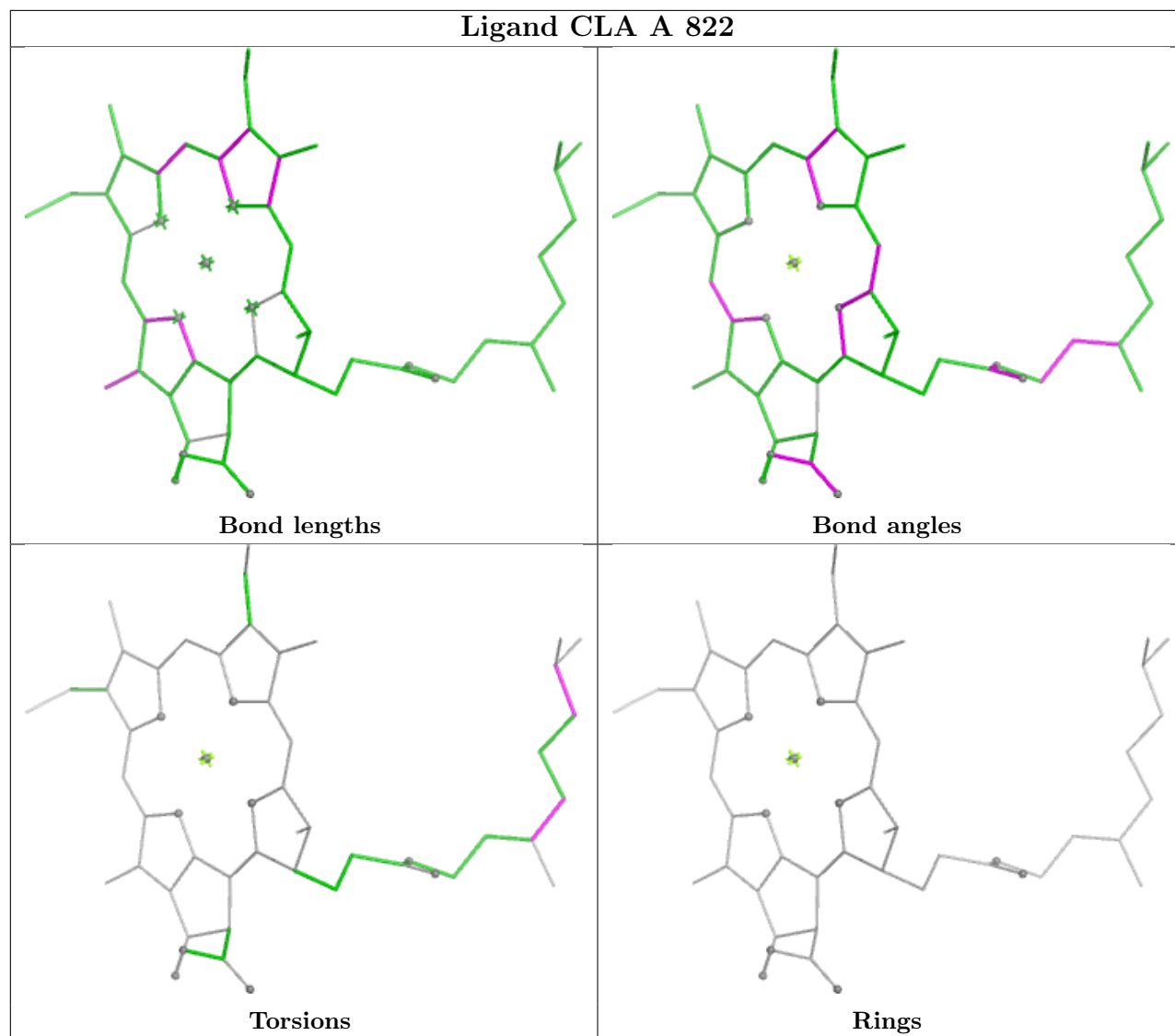


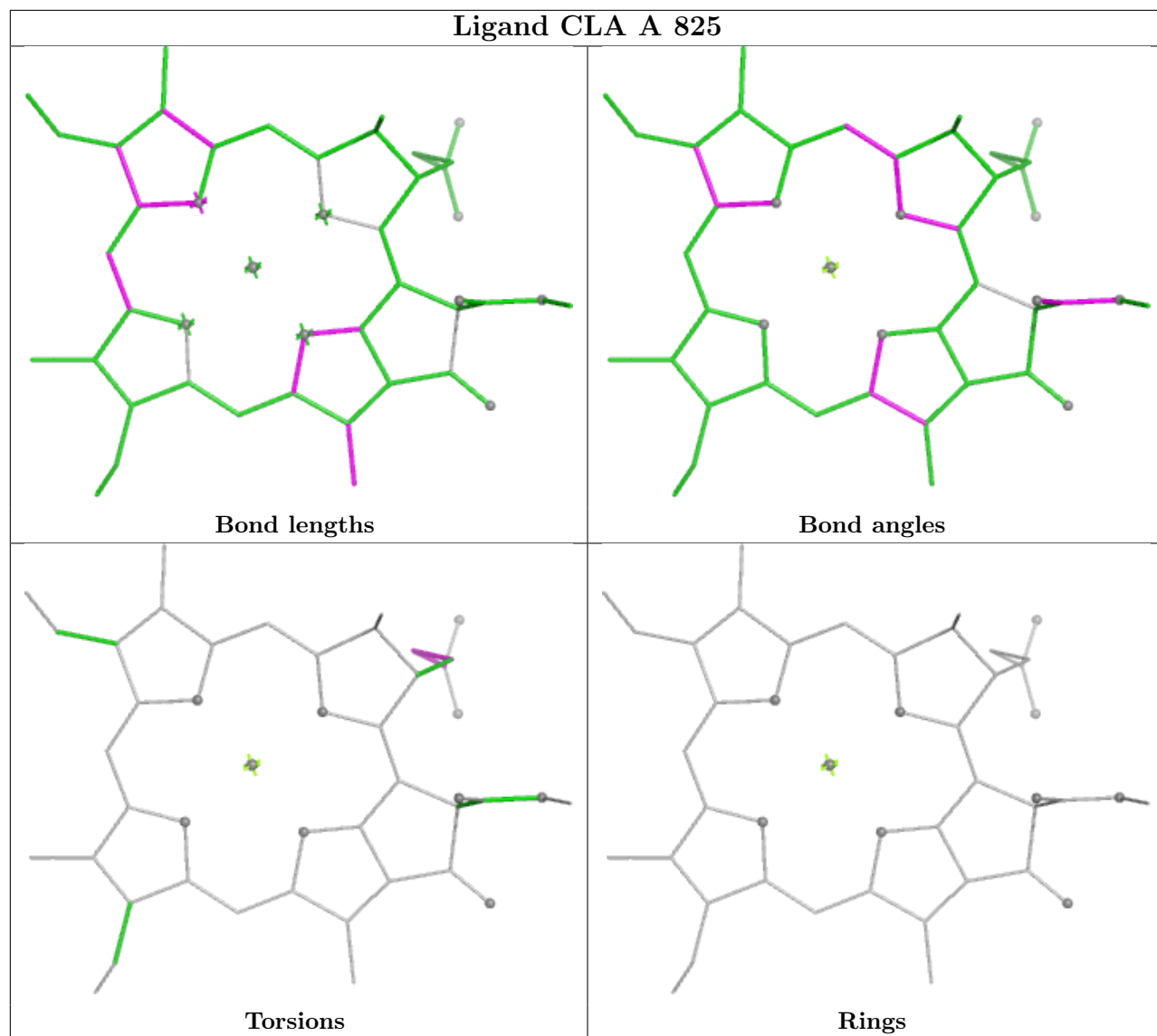


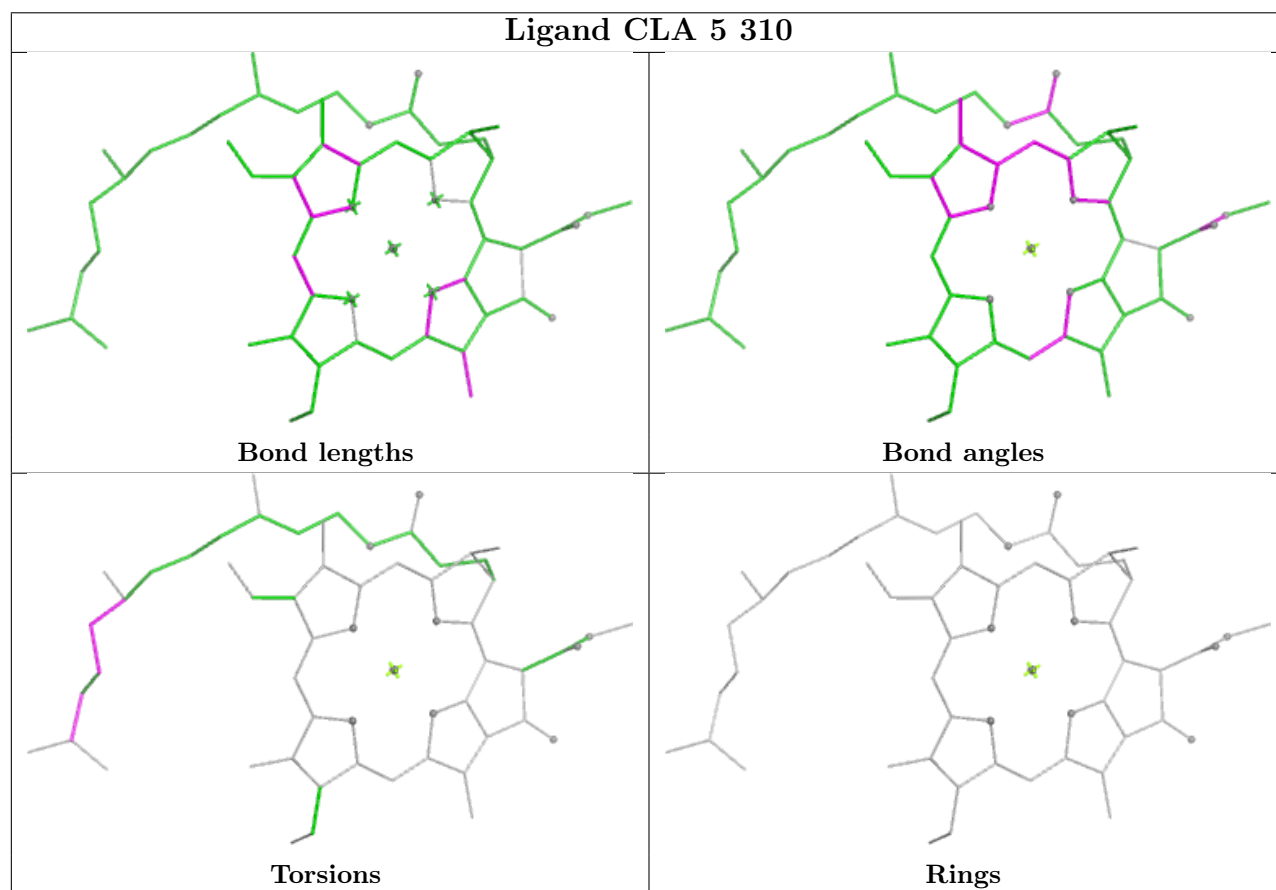
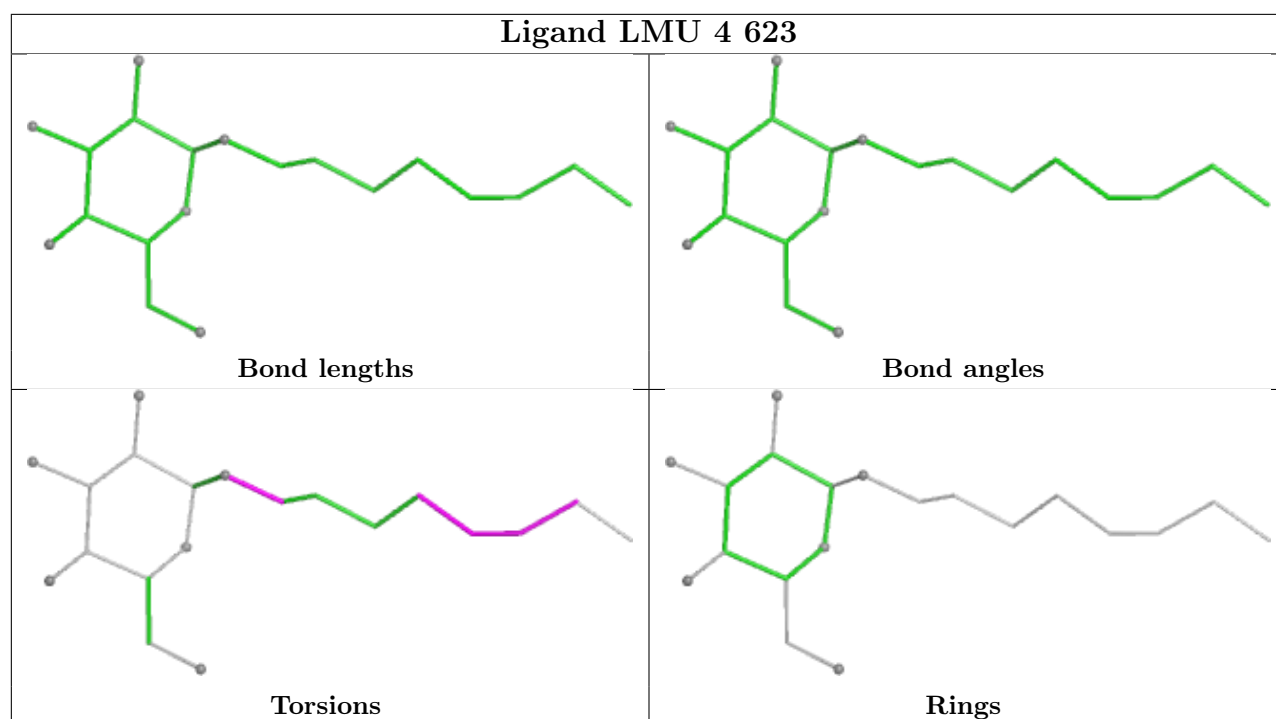


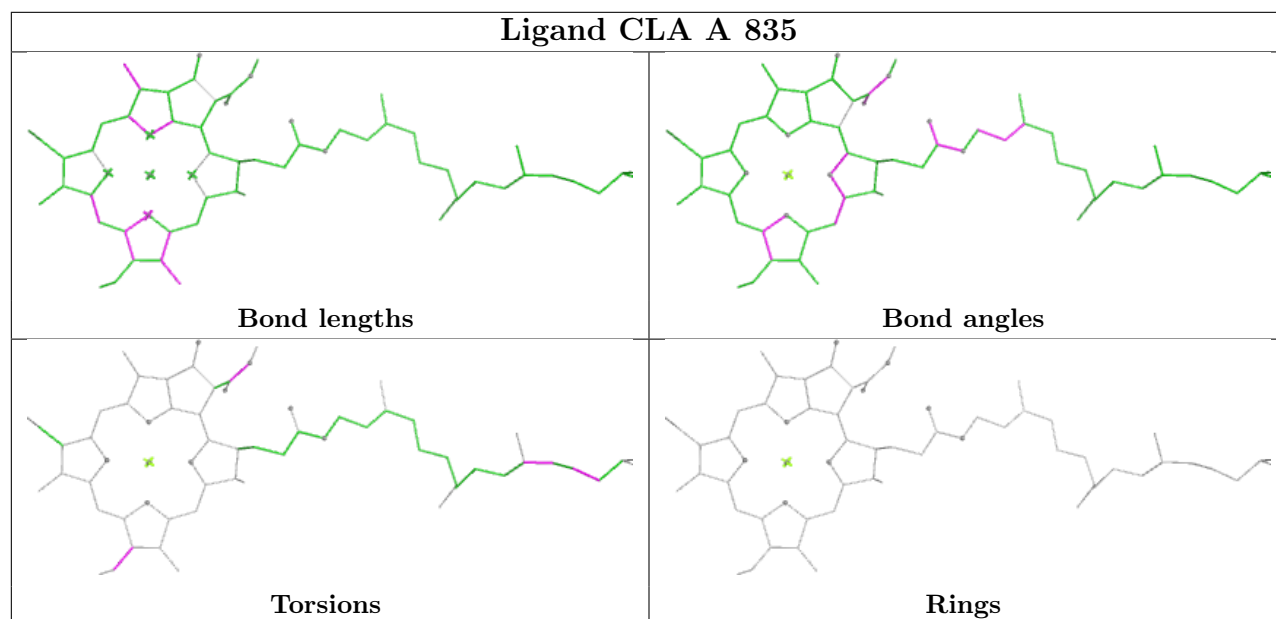
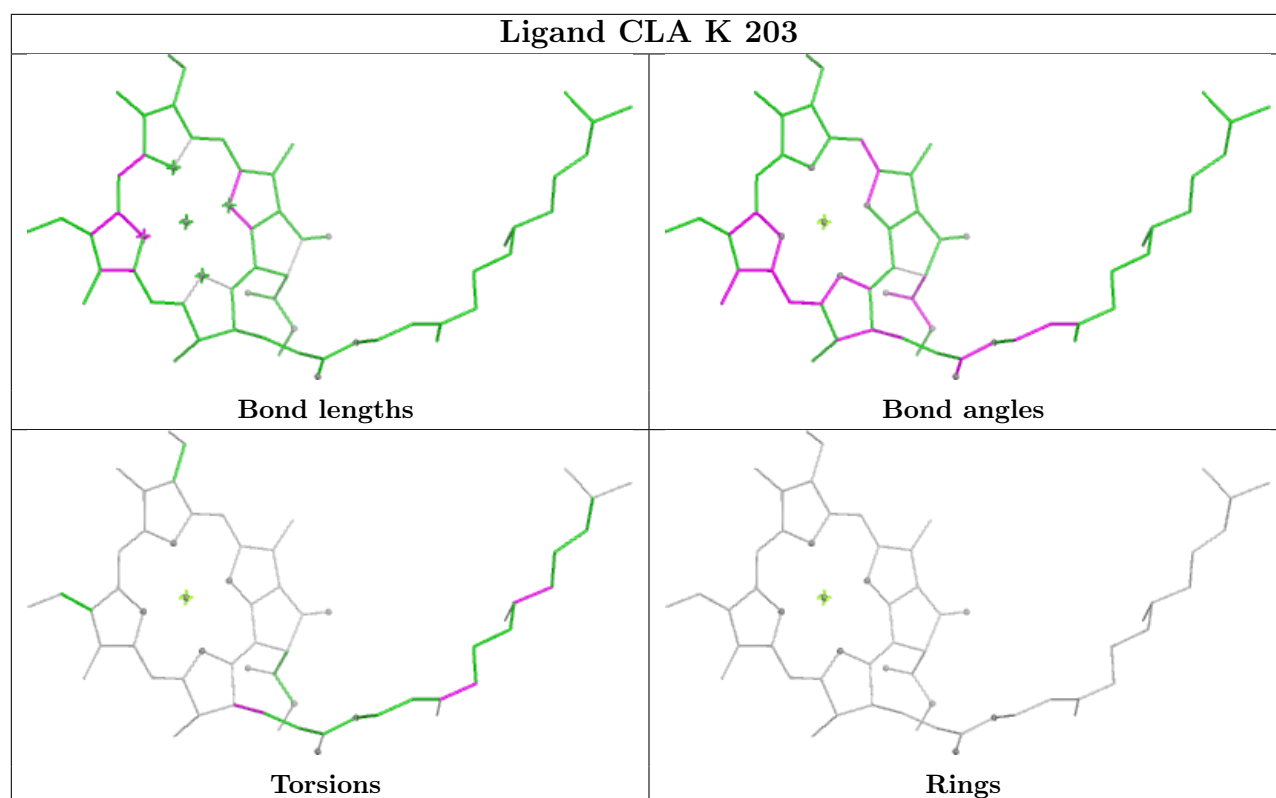


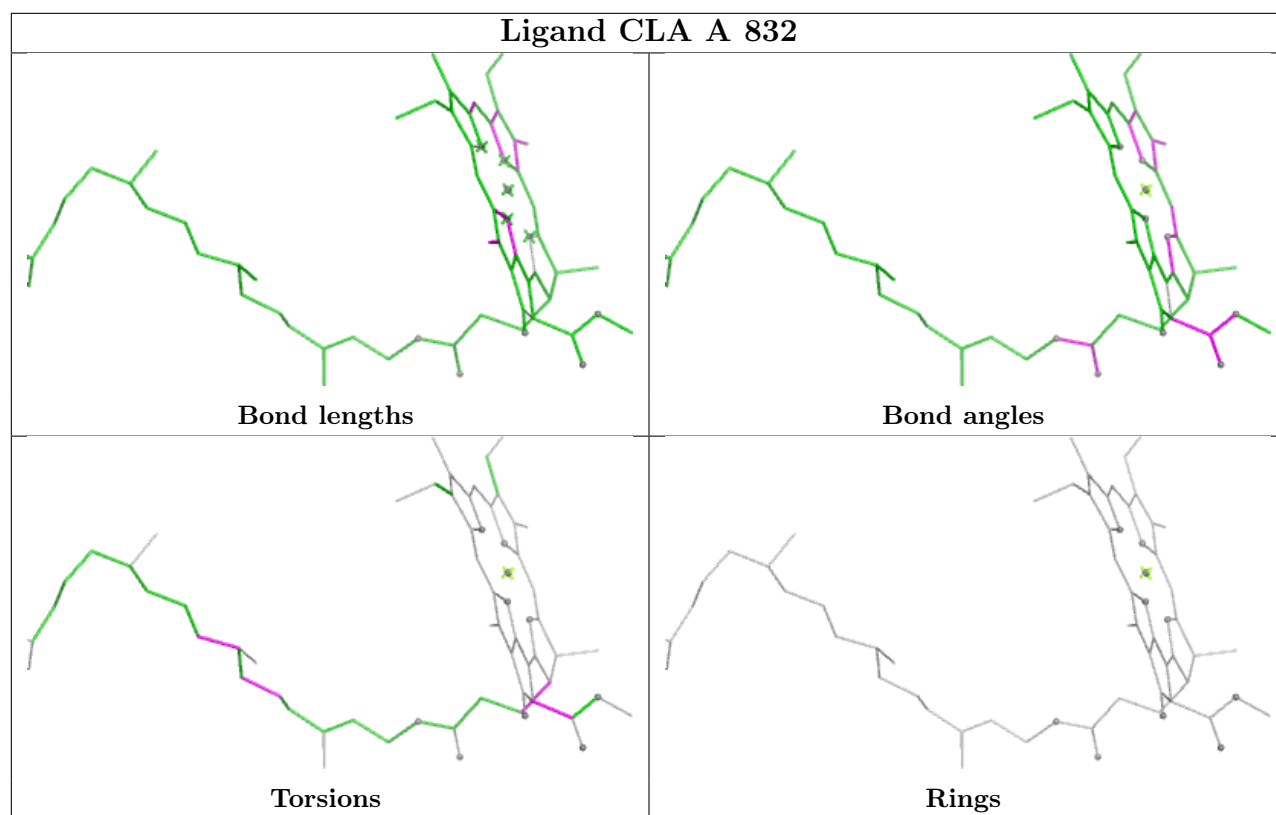
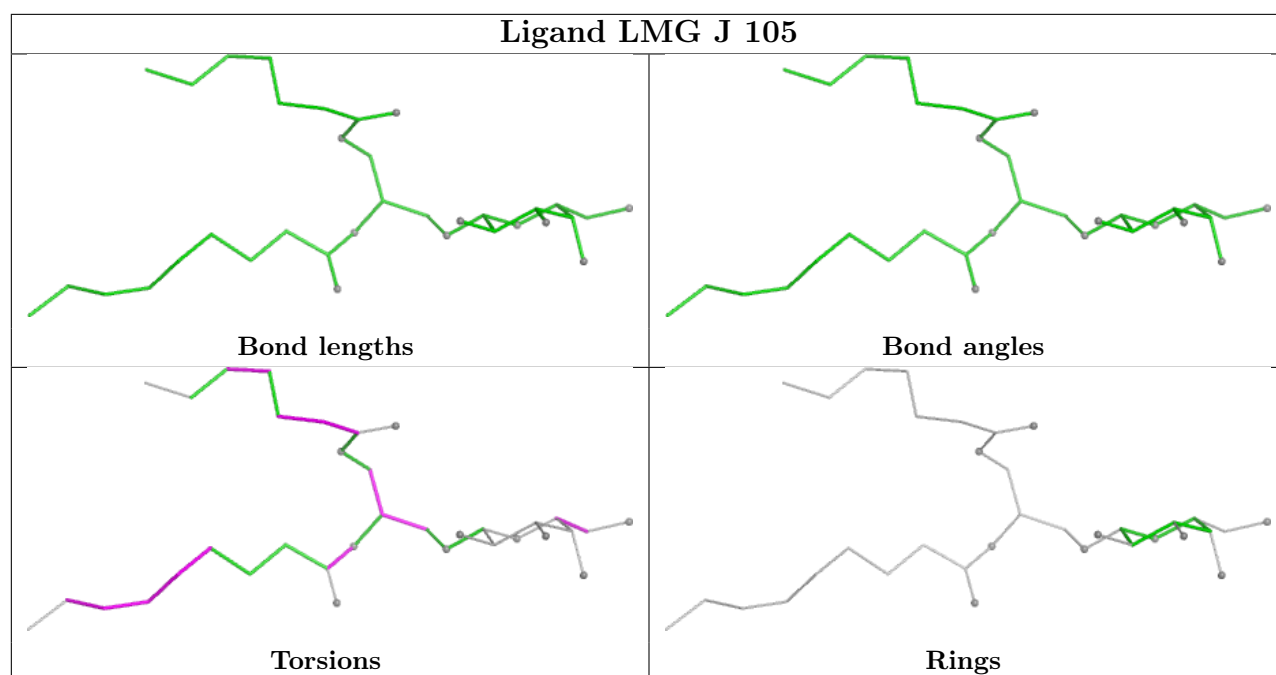


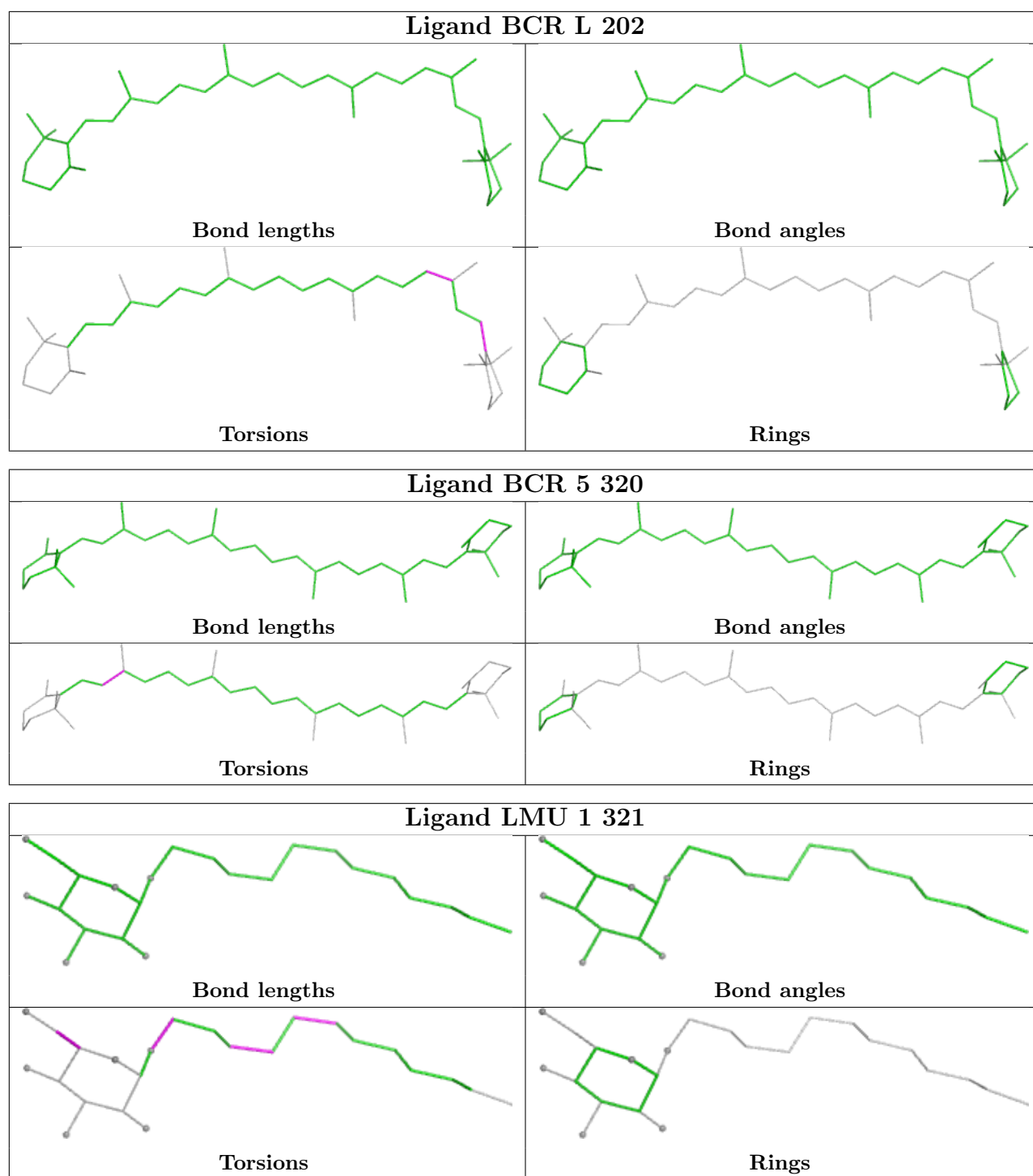




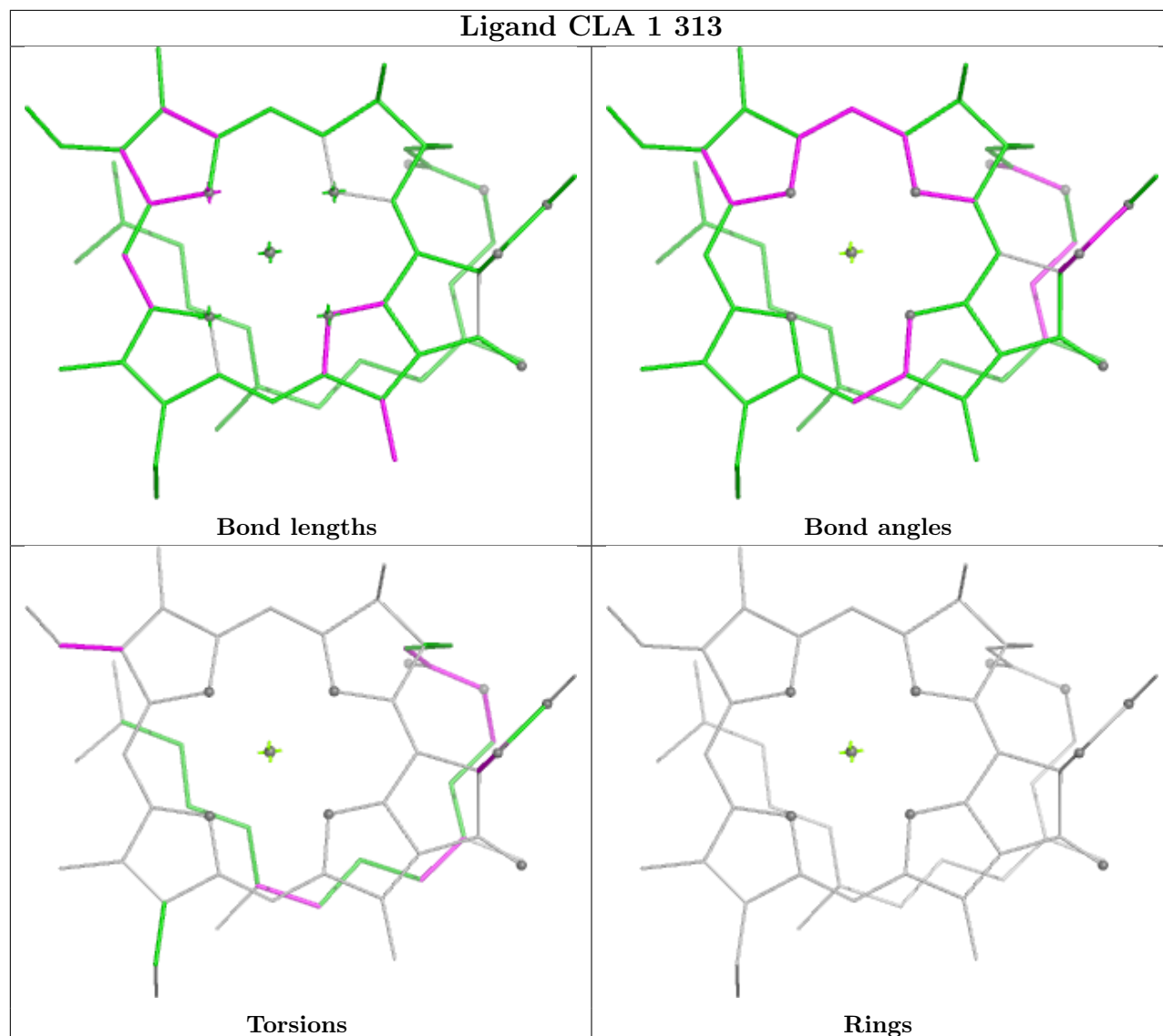


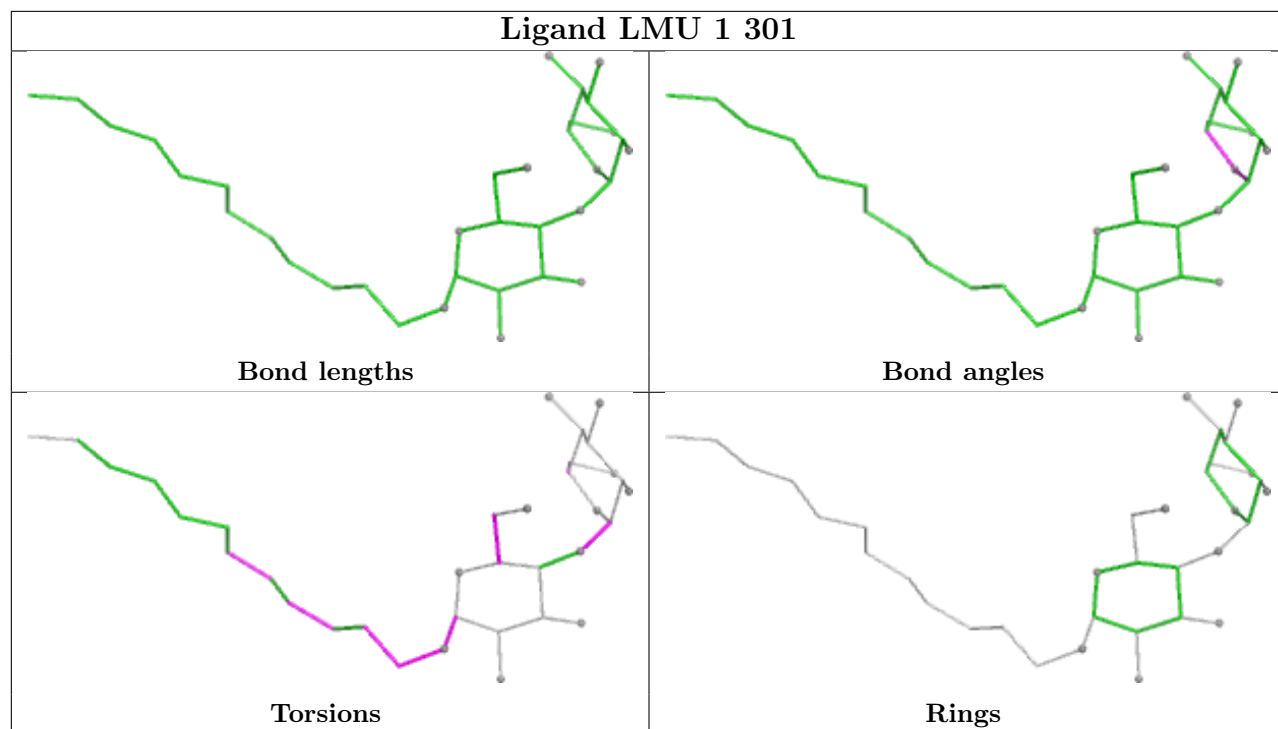




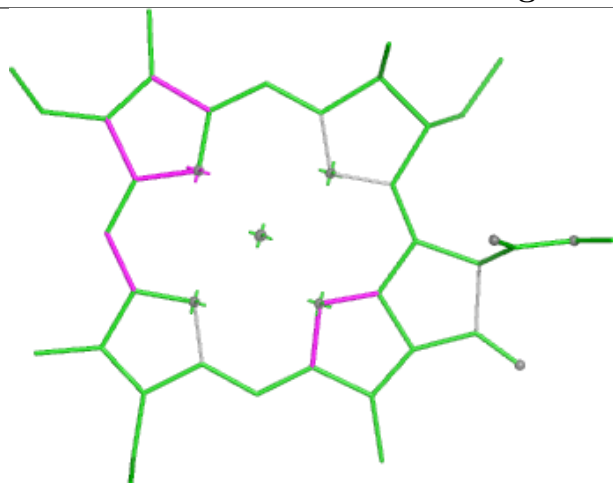


Ligand CLA 1 313

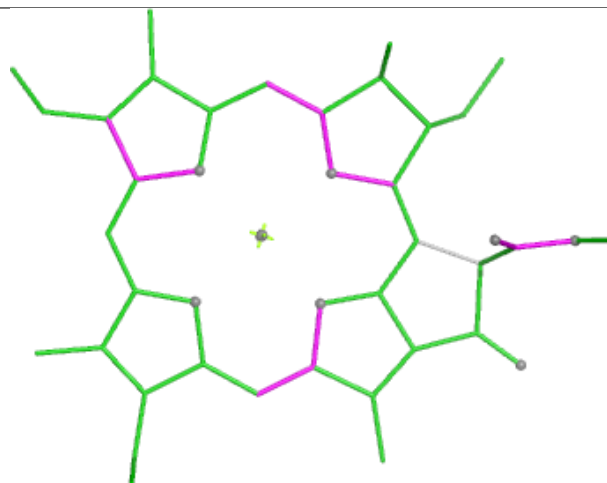




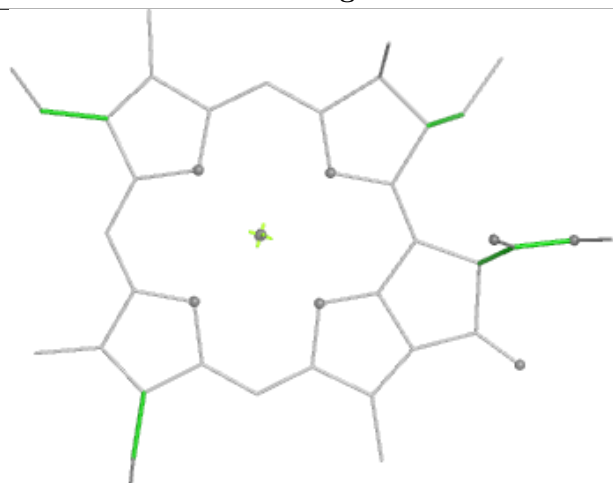
Ligand CLA 3 304



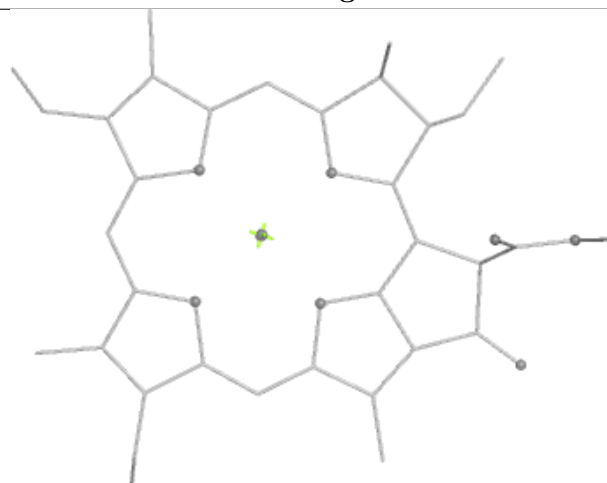
Bond lengths



Bond angles



Torsions



Rings

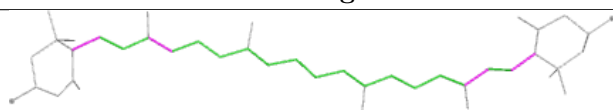
Ligand LUT 8 301



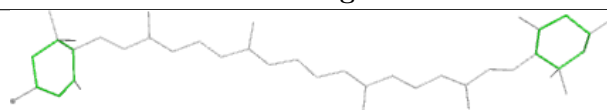
Bond lengths



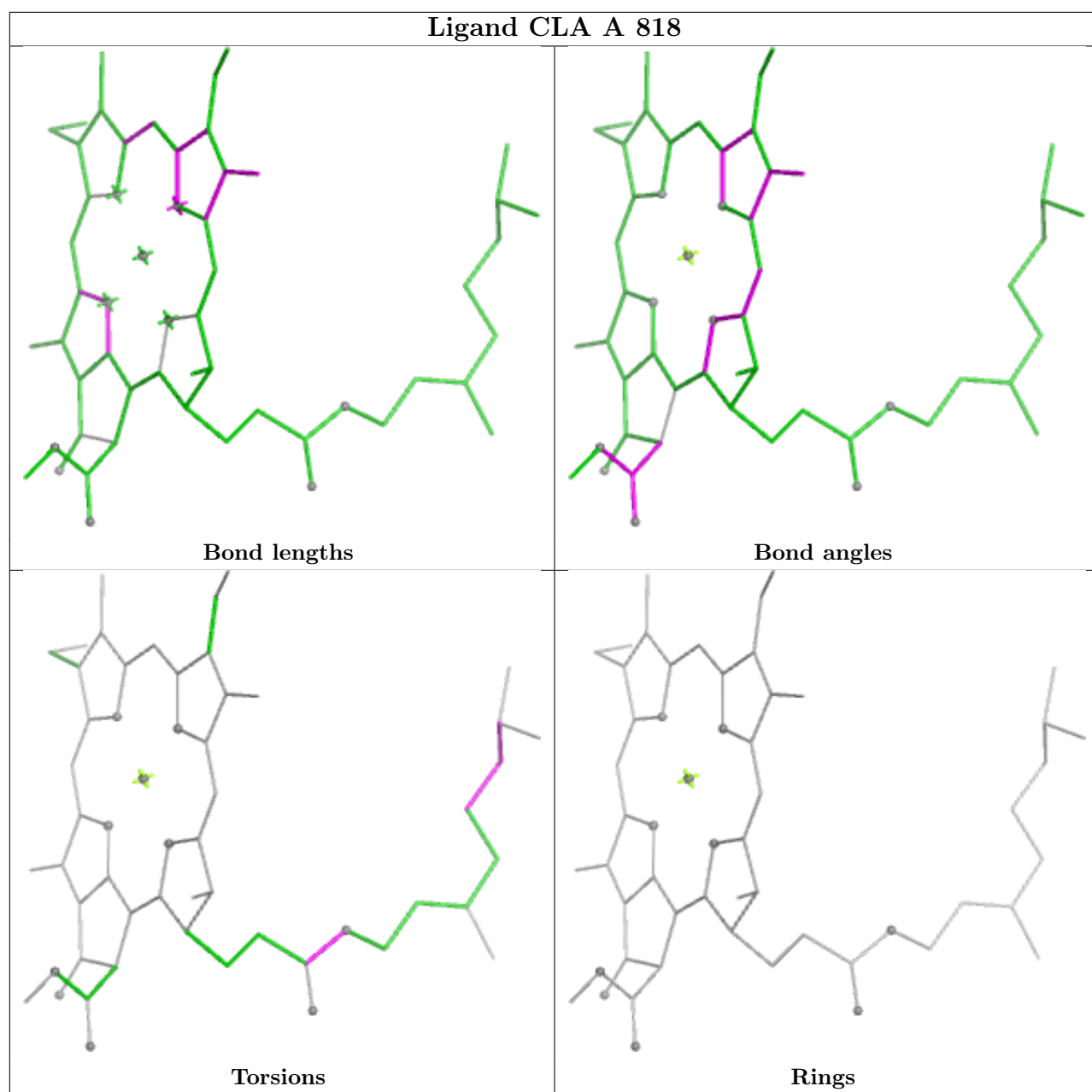
Bond angles

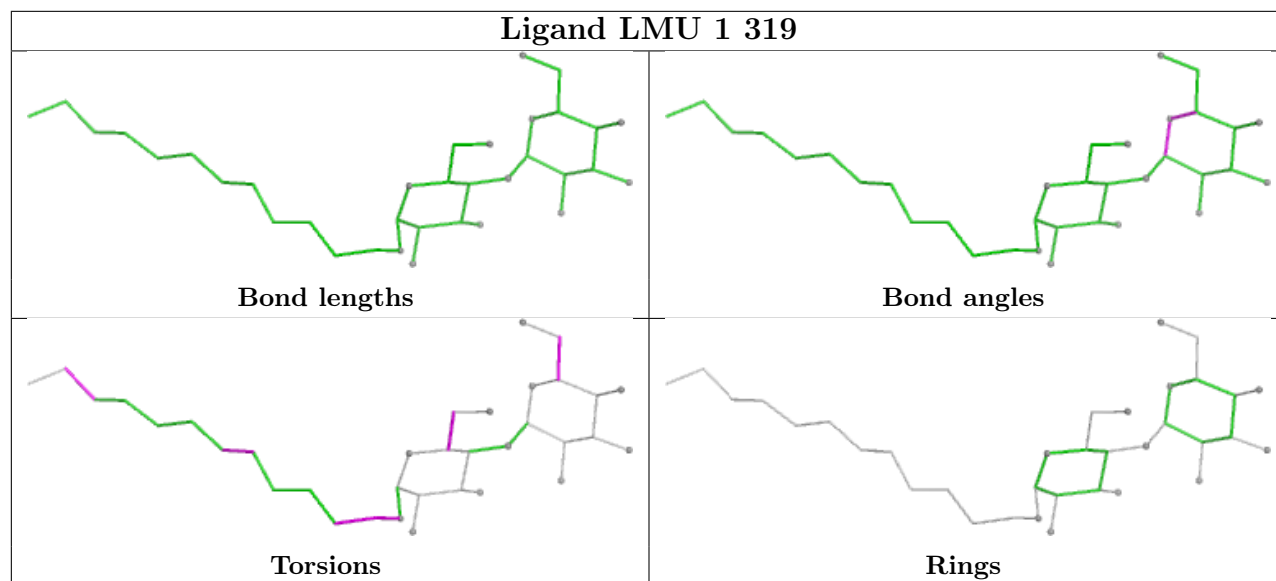
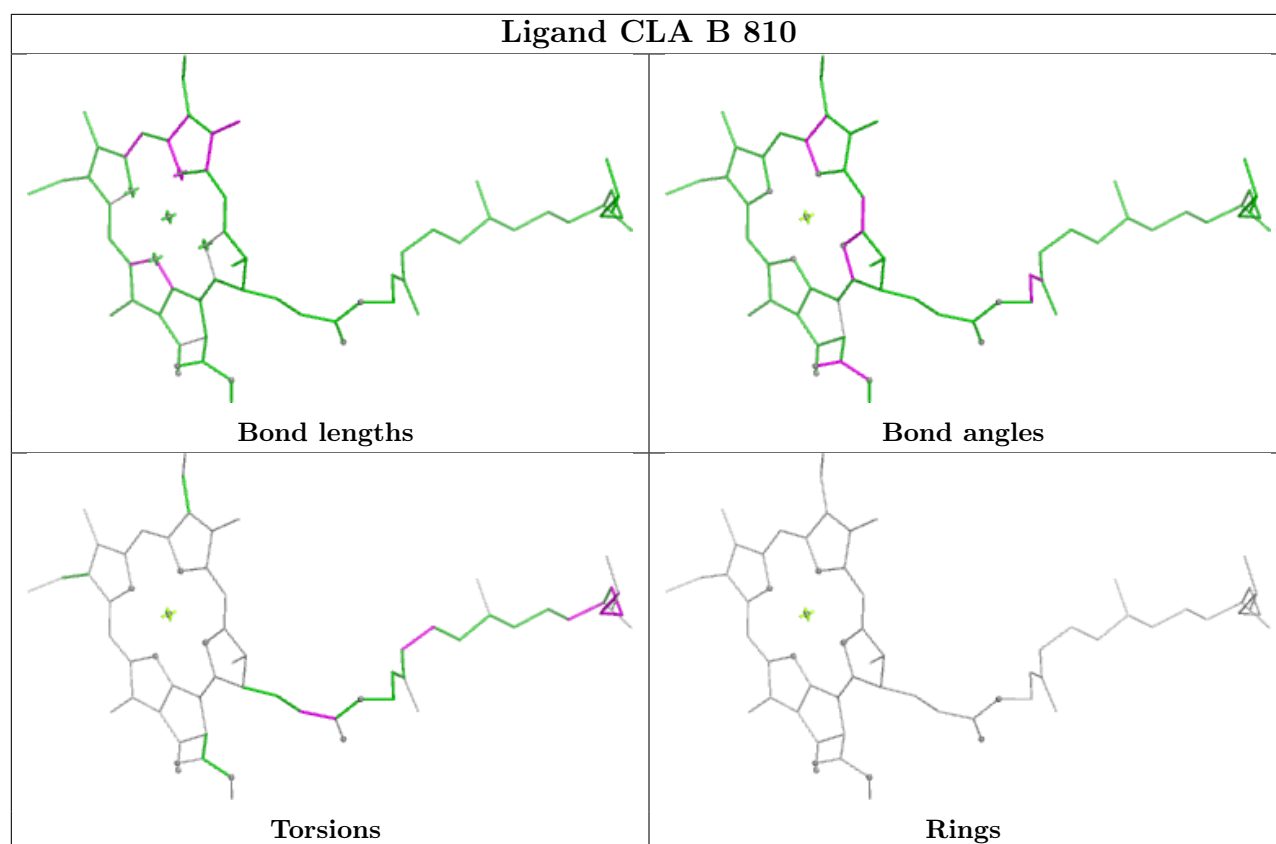


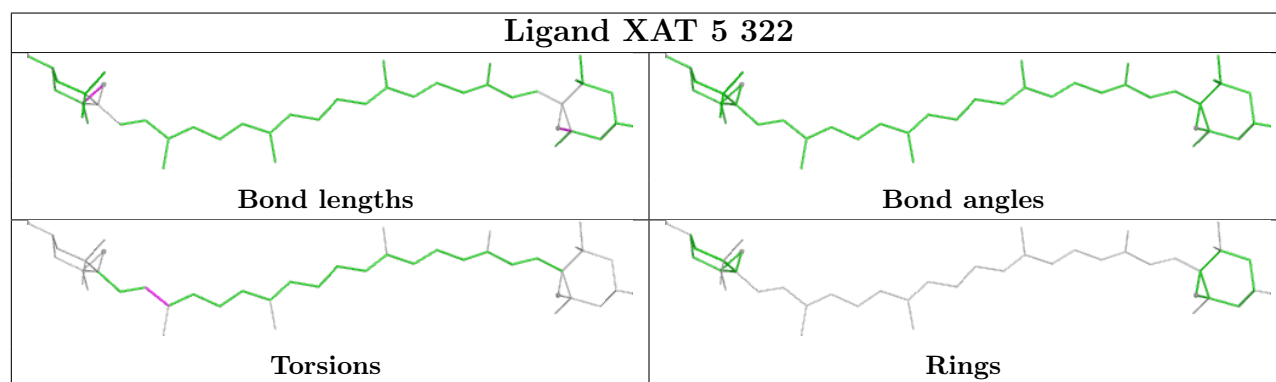
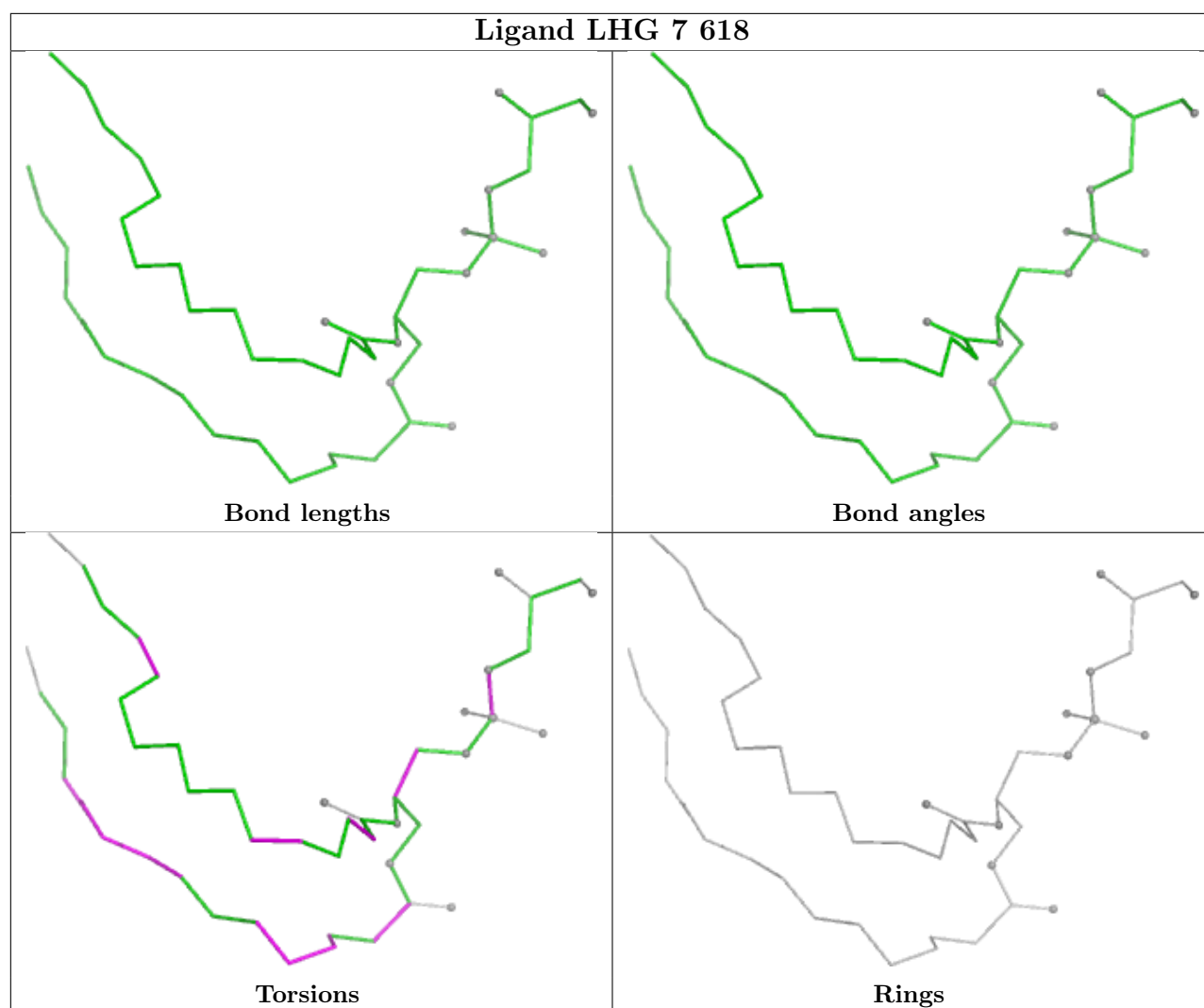
Torsions



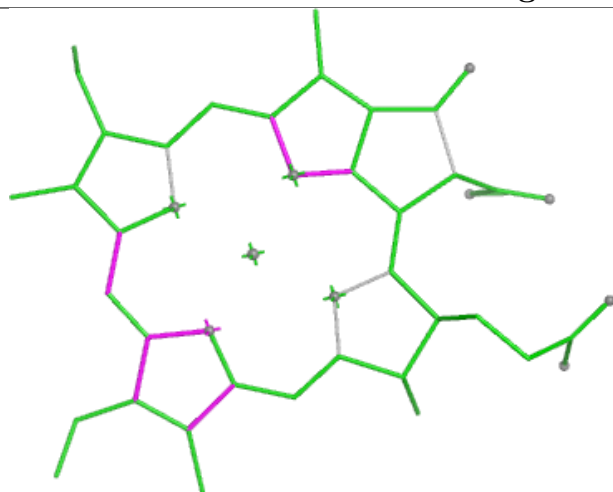
Rings



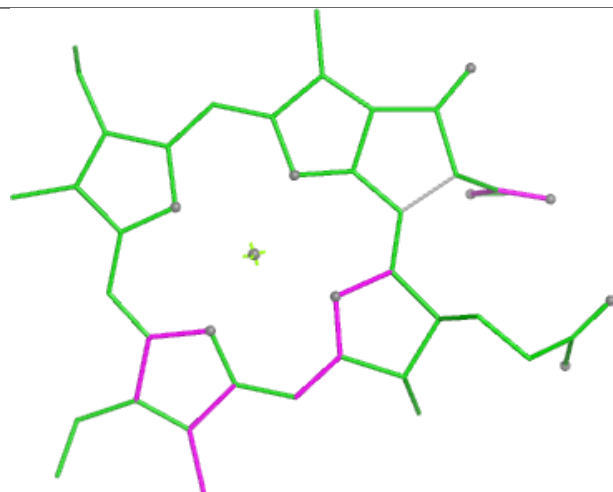




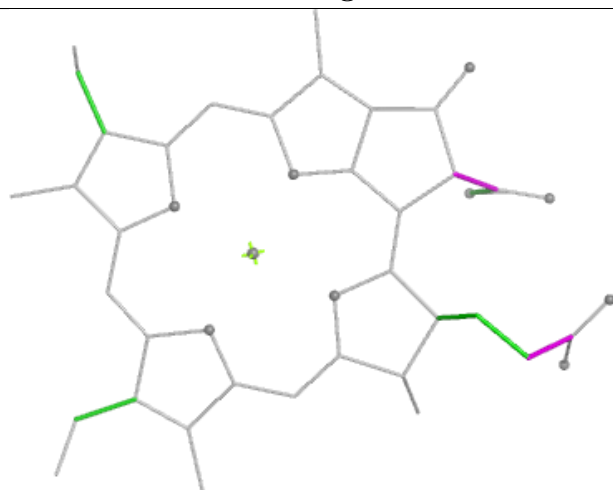
Ligand CLA 4 611



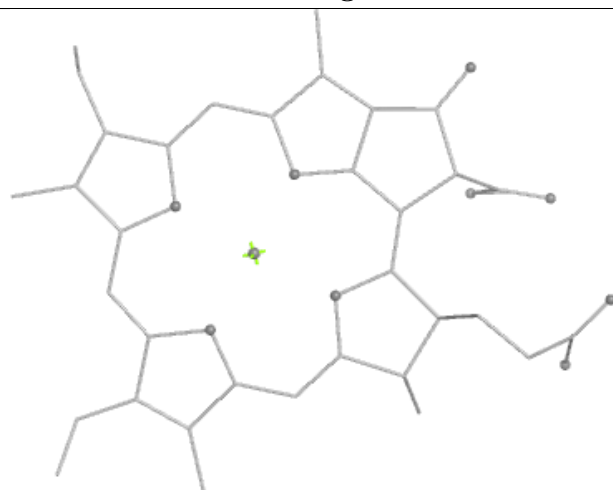
Bond lengths



Bond angles

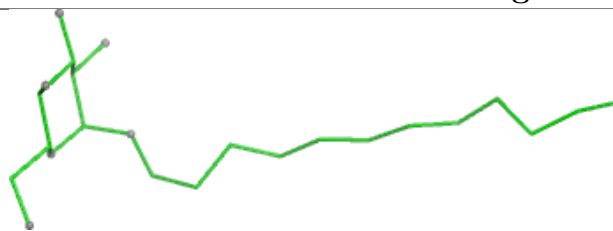


Torsions

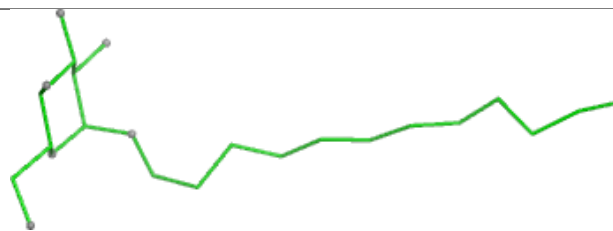


Rings

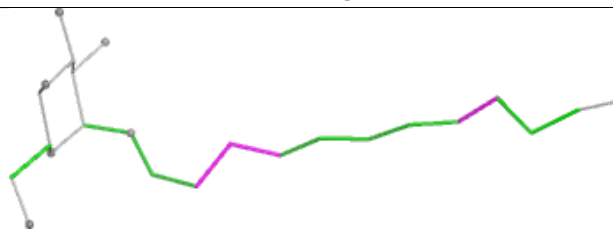
Ligand LMU Z 621



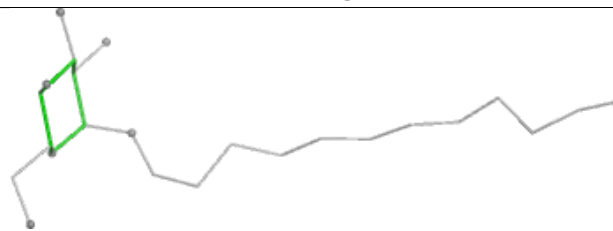
Bond lengths



Bond angles

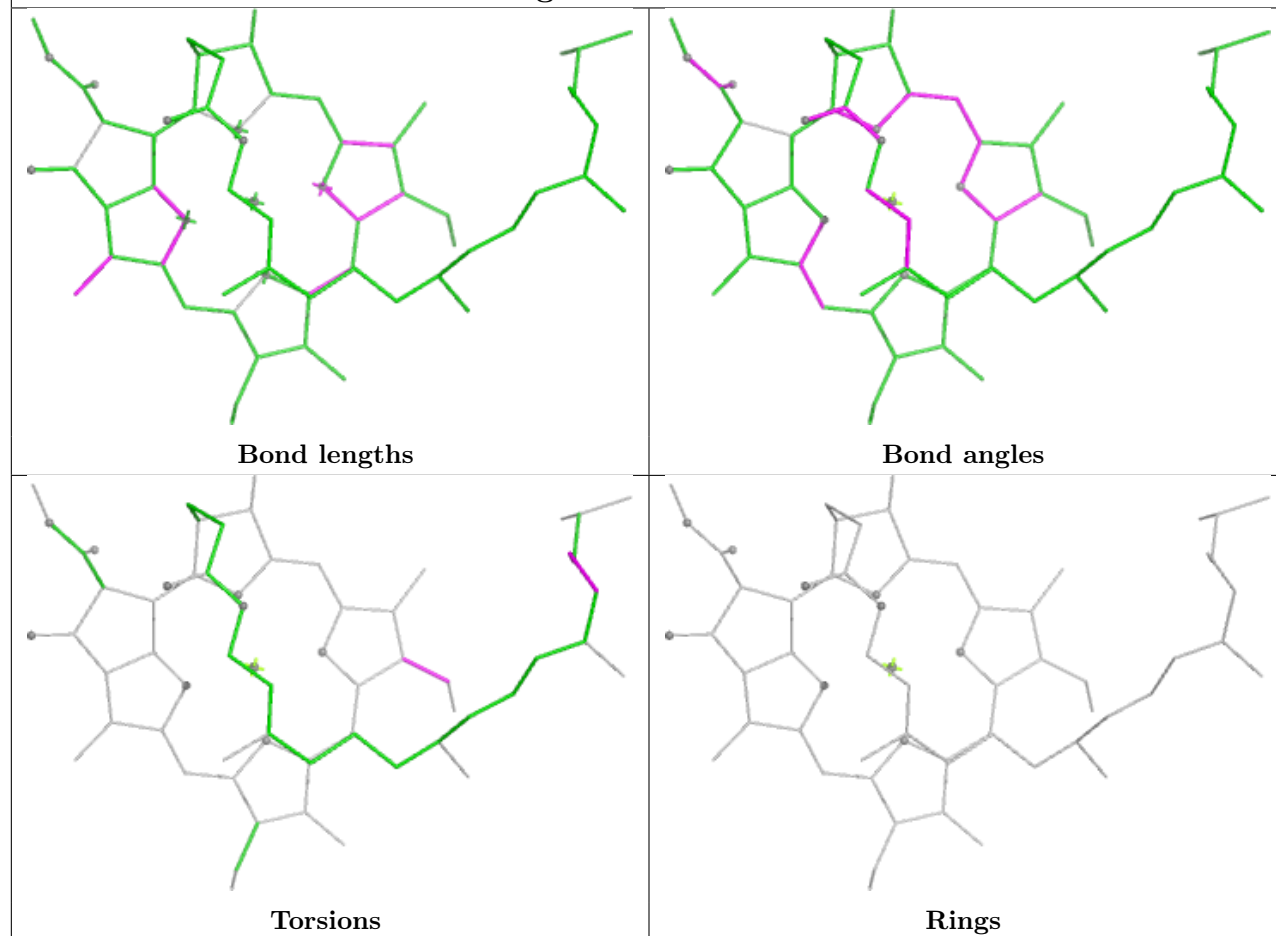


Torsions

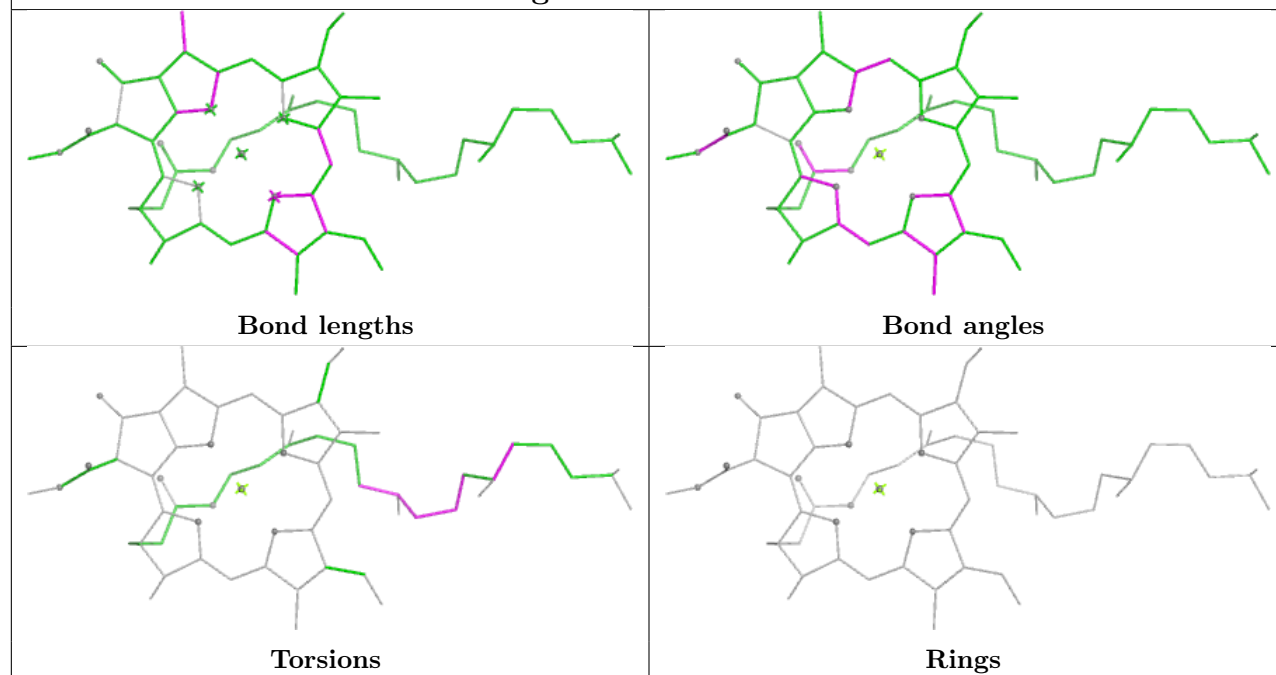


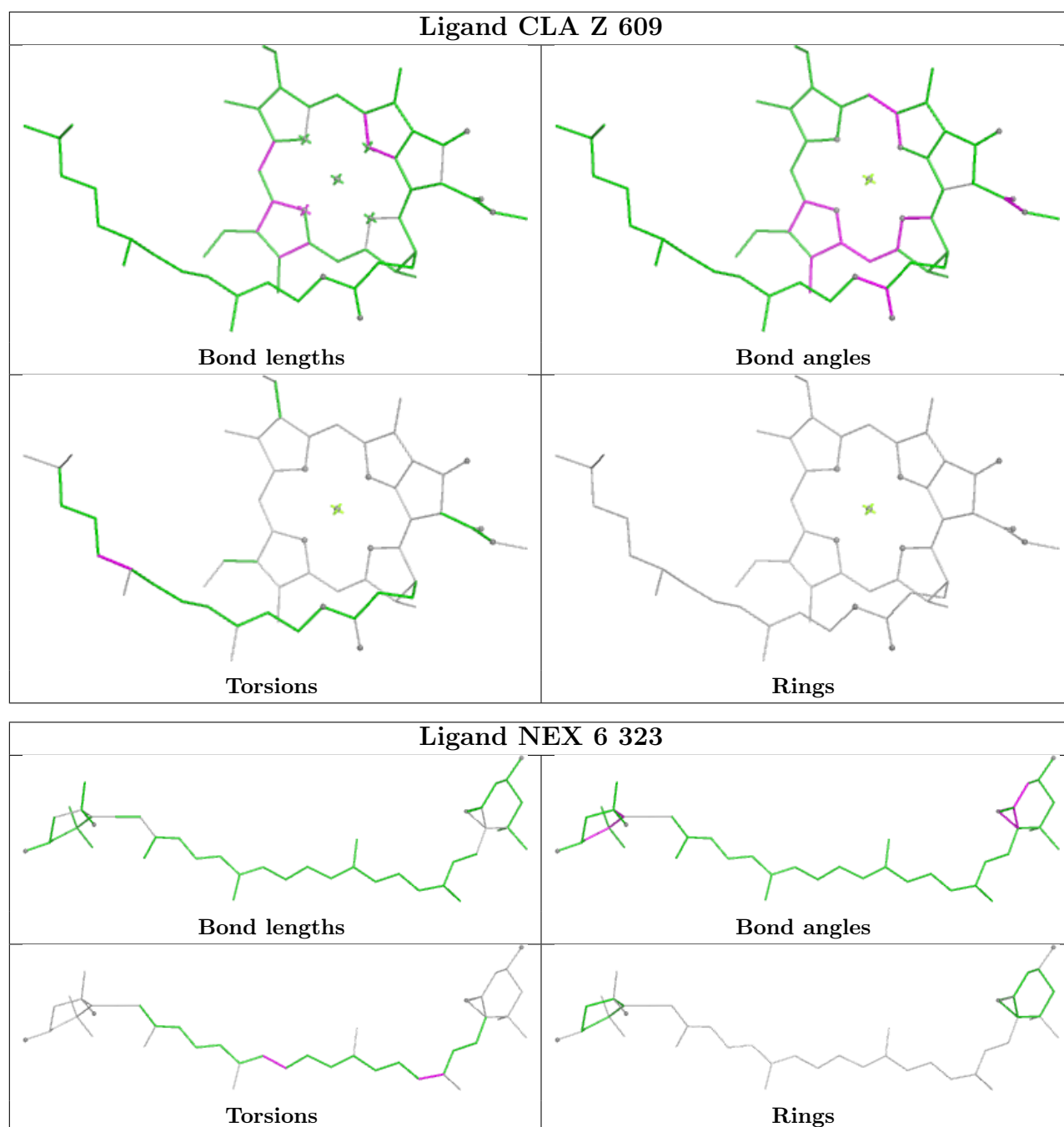
Rings

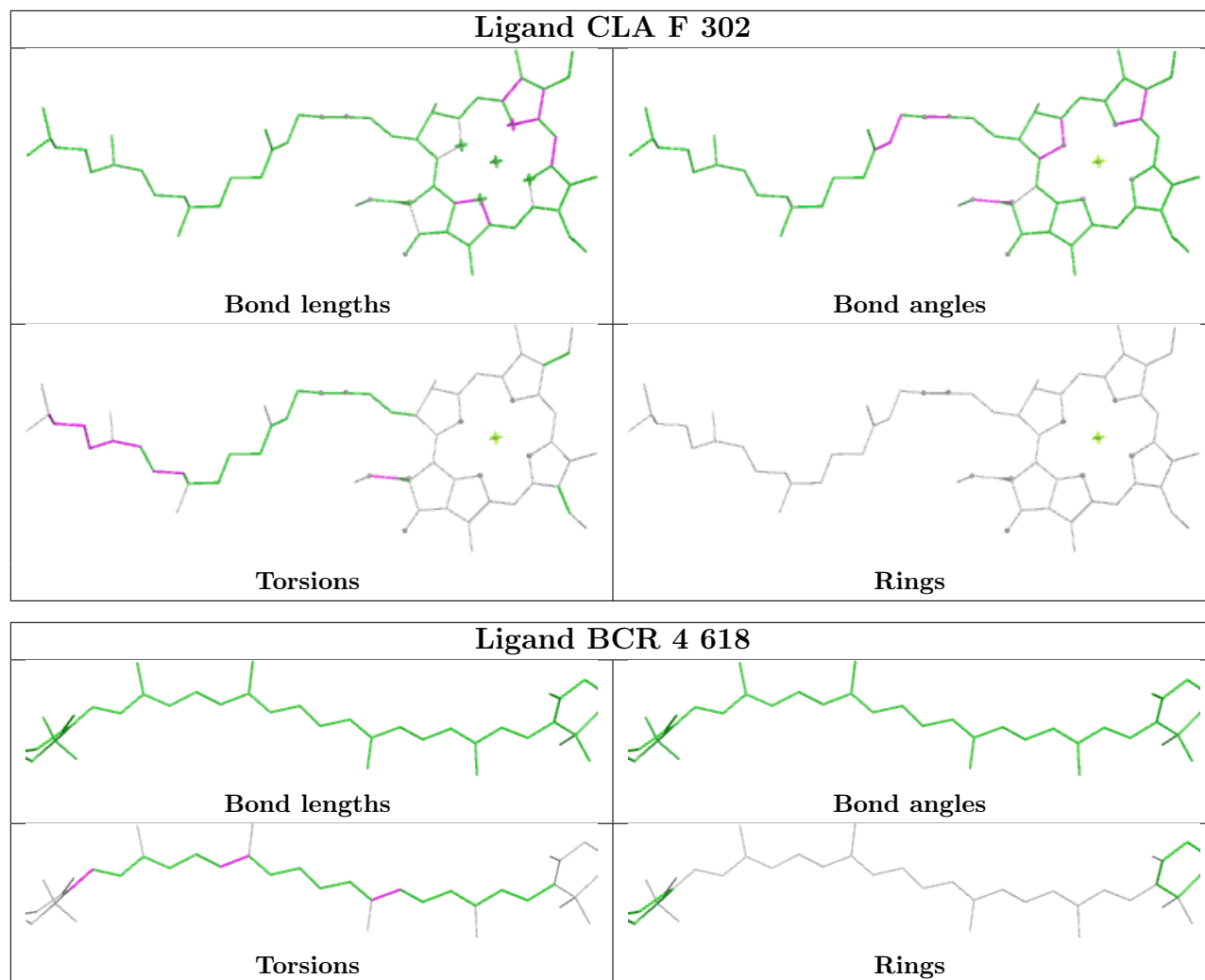
Ligand CLA 6 313



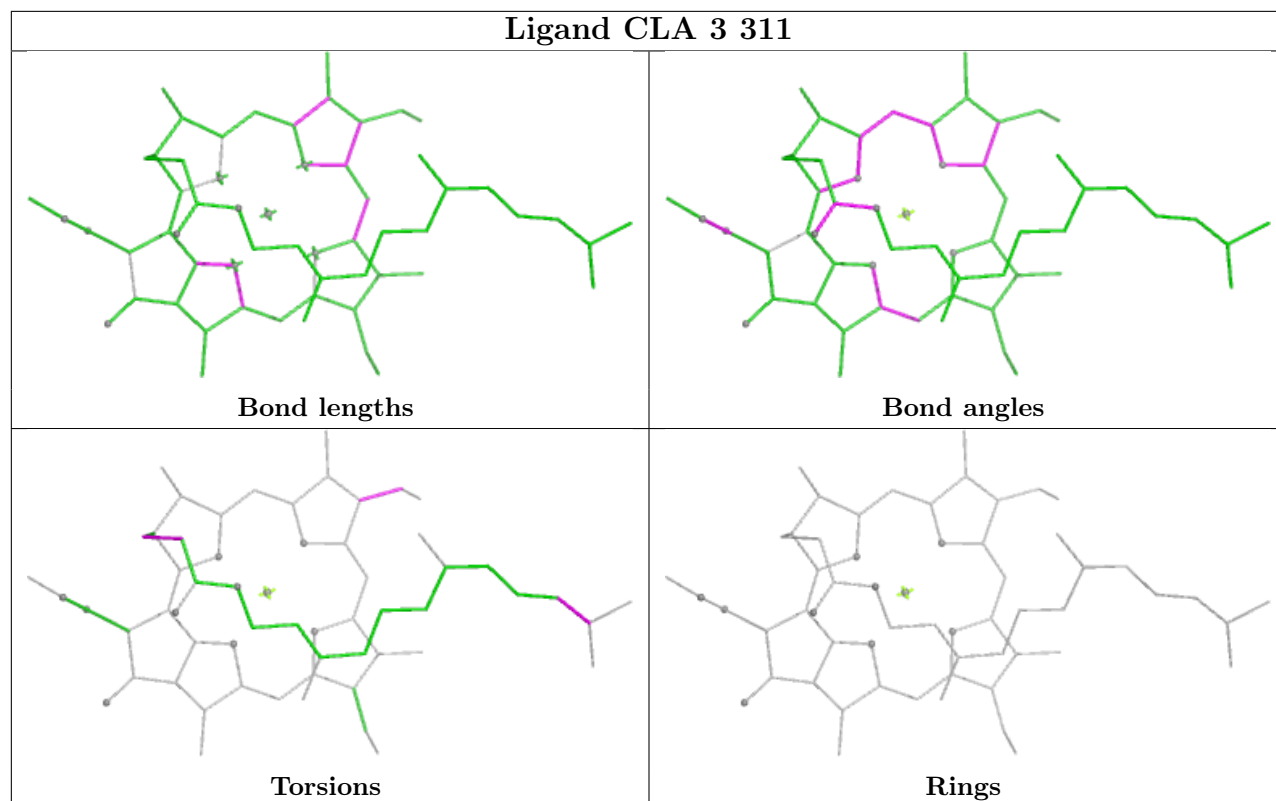
Ligand CLA A 840



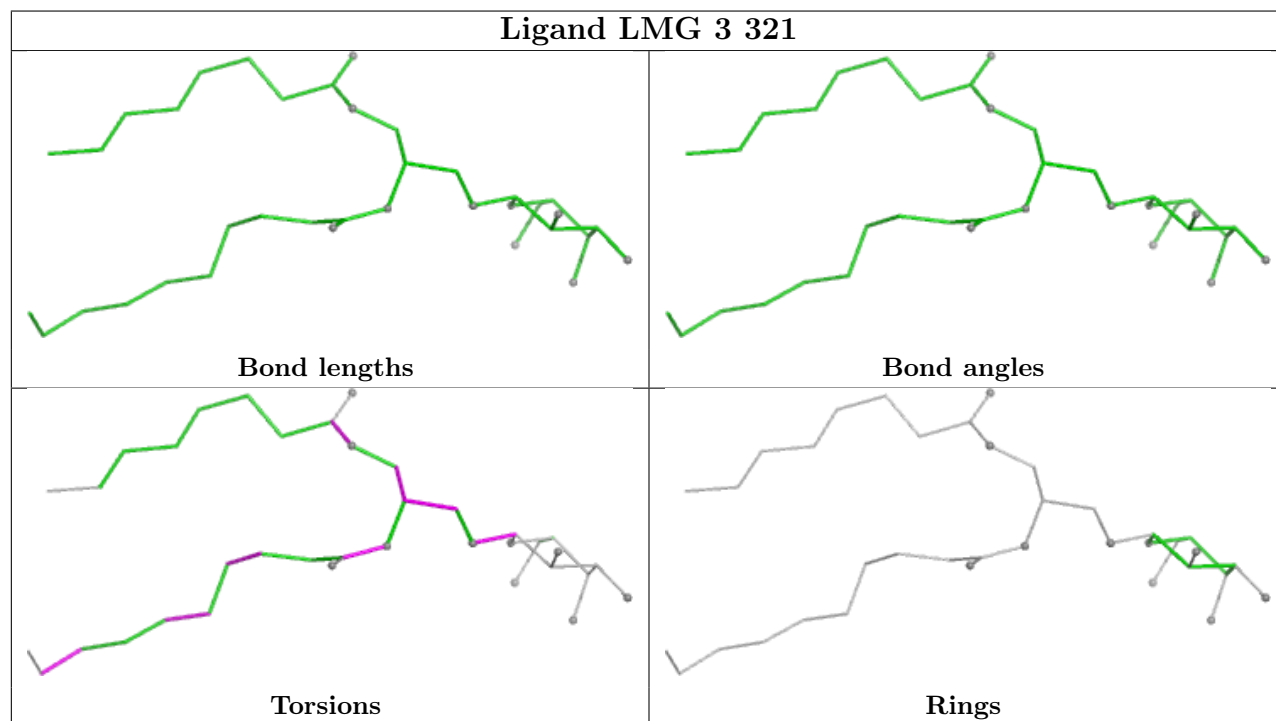


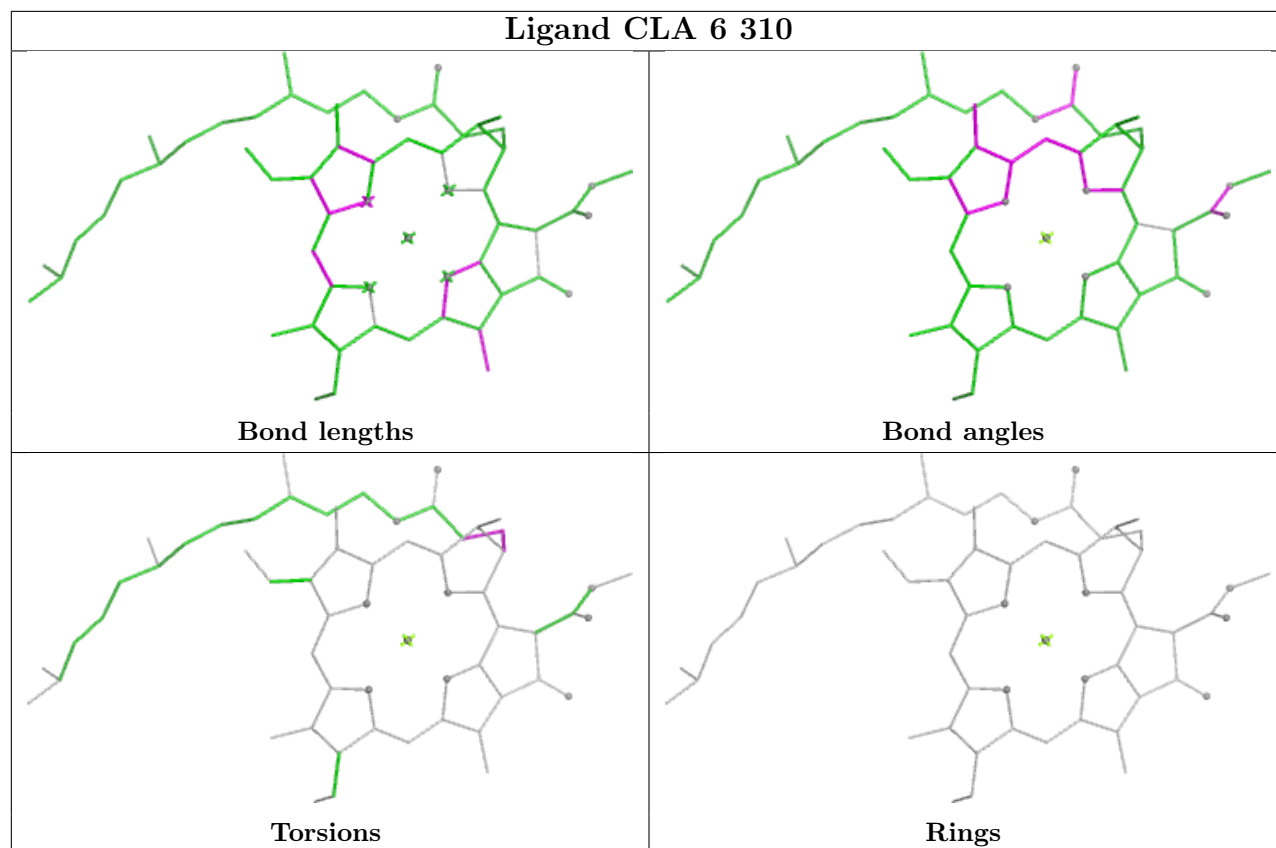
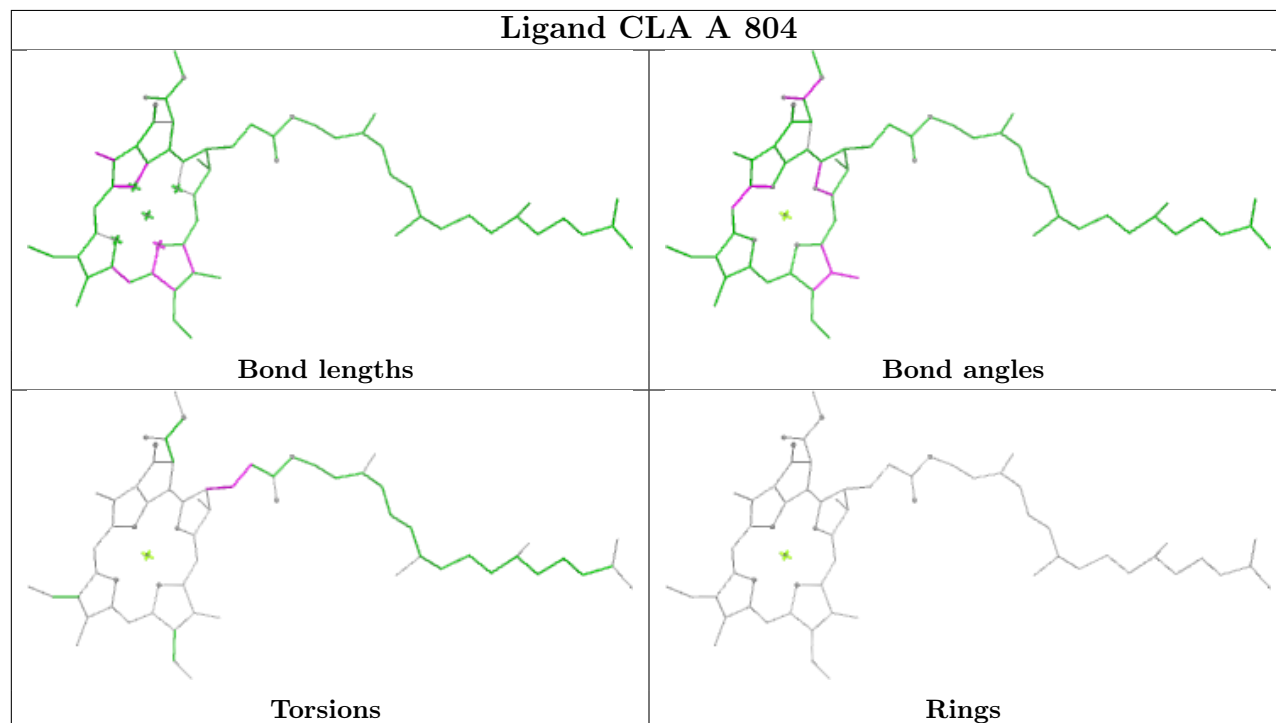


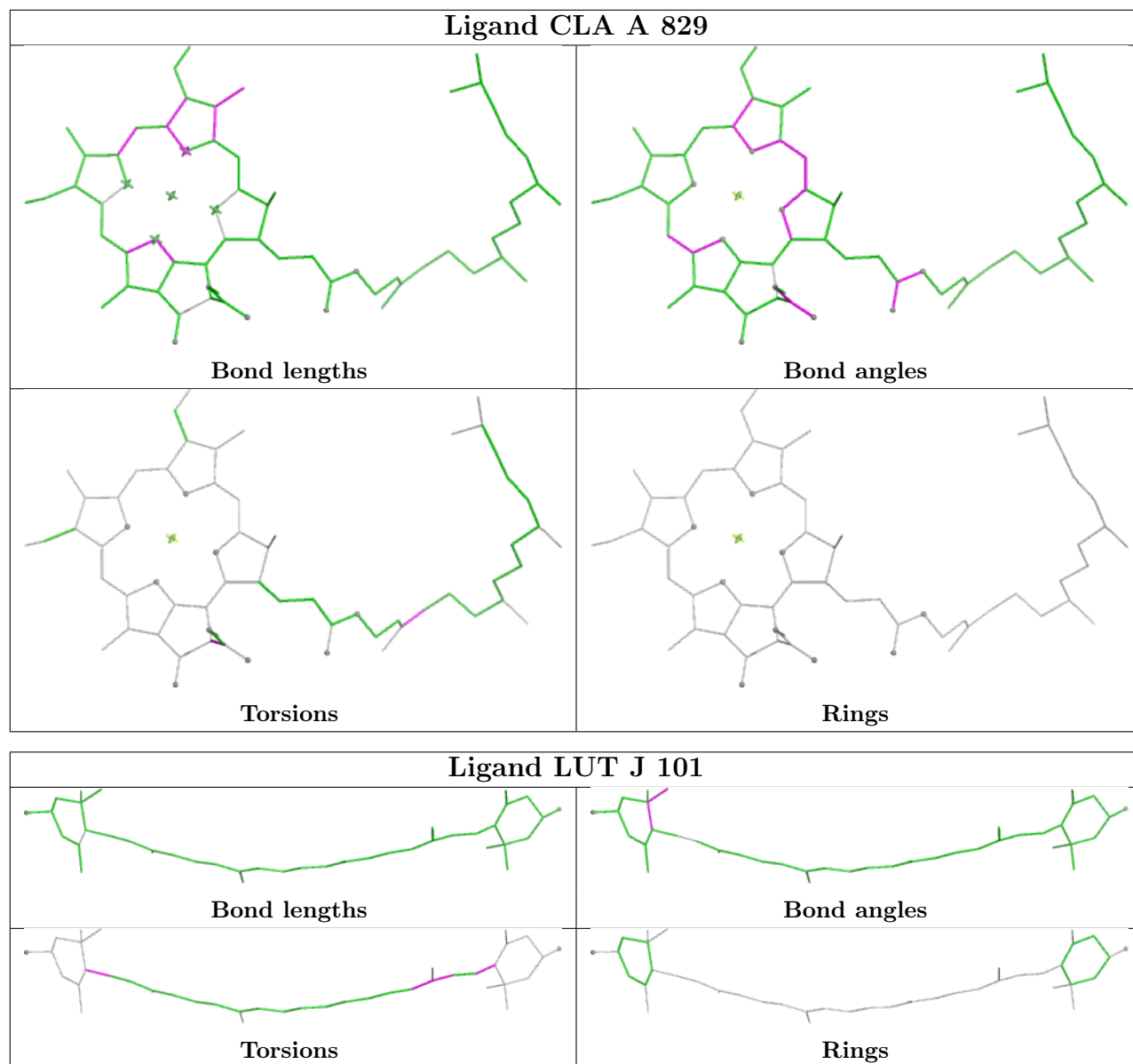
Ligand CLA 3 311

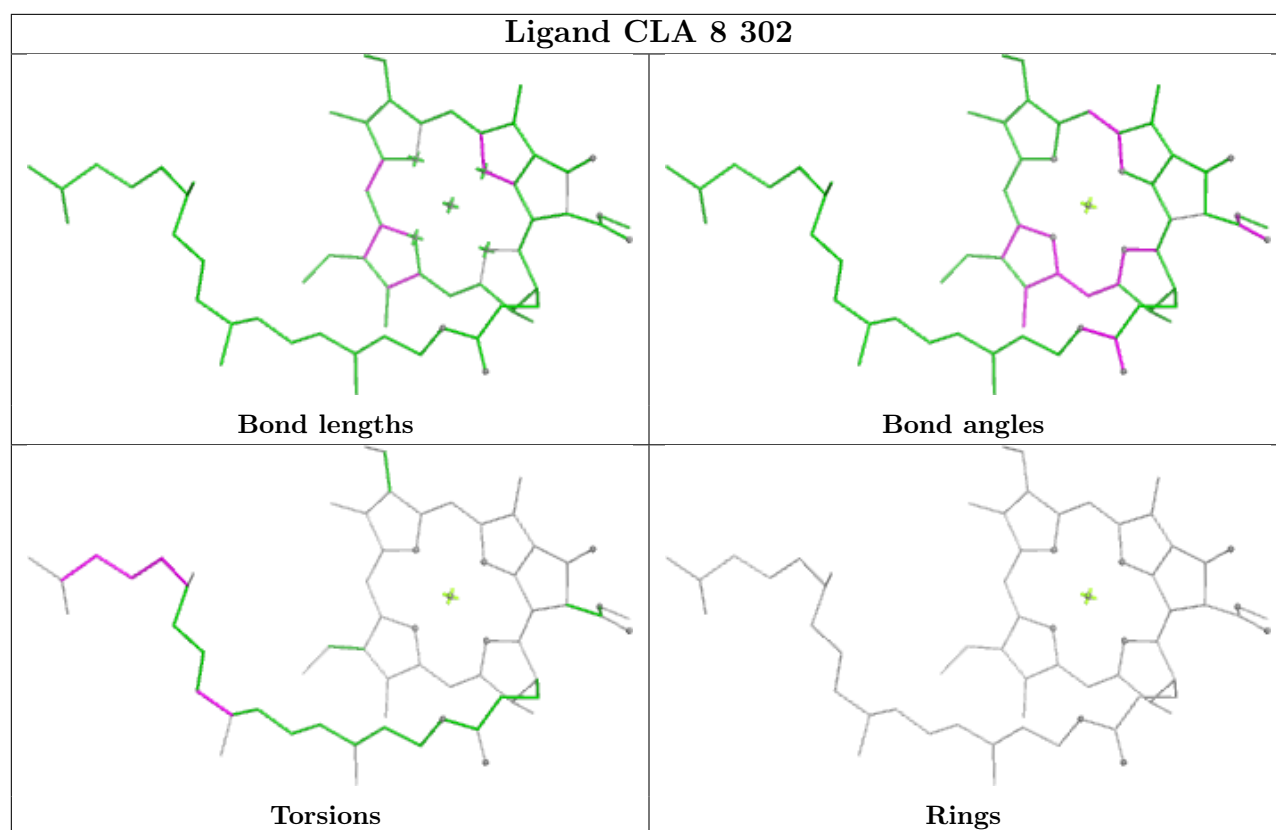


Ligand LMG 3 321

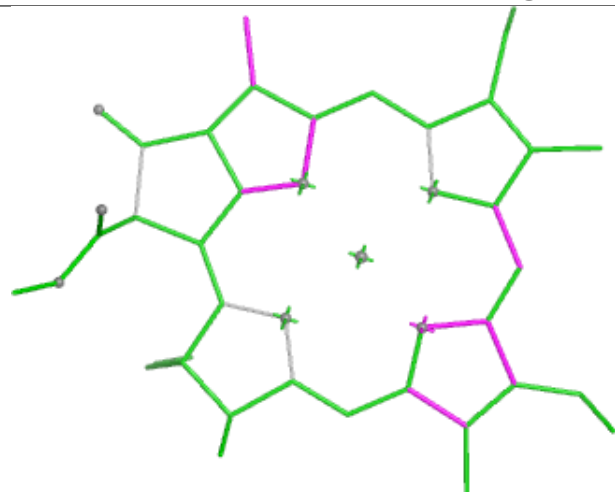


Ligand CLA 6 310**Ligand CLA A 804**

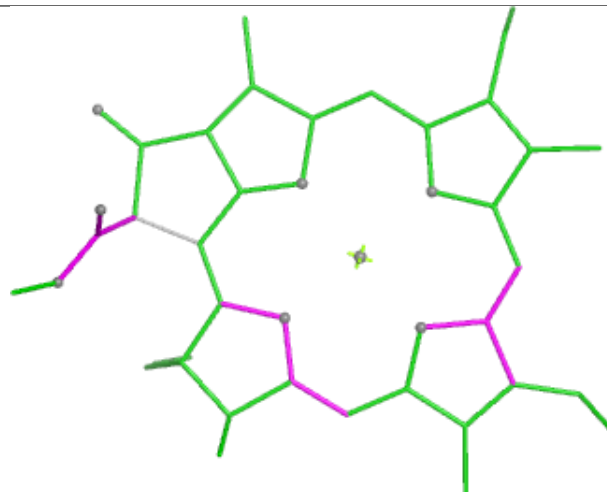




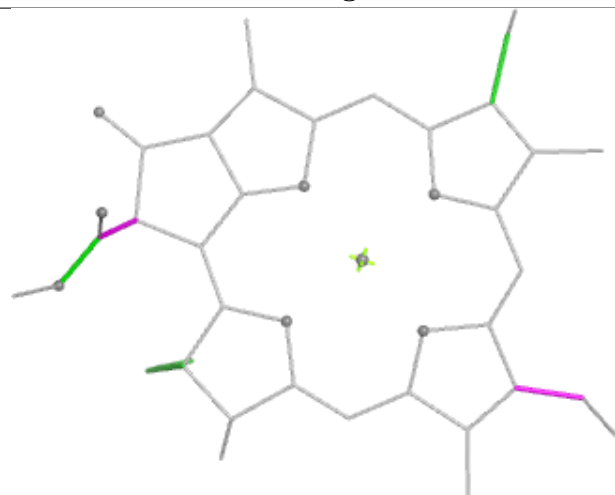
Ligand CLA 7 613



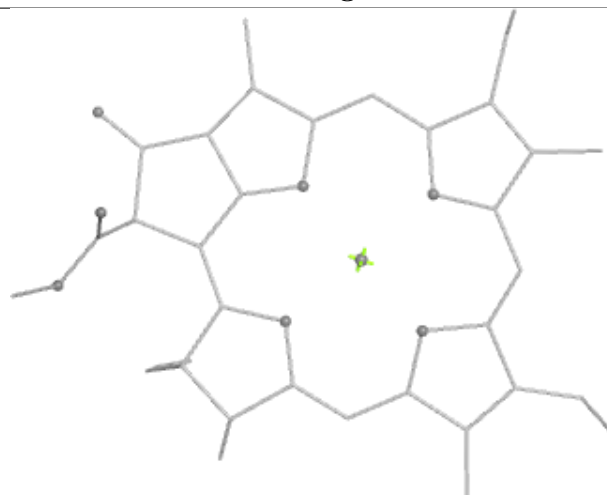
Bond lengths



Bond angles

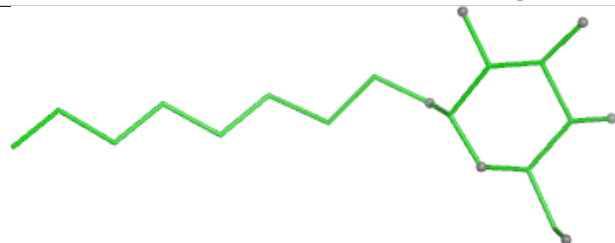


Torsions

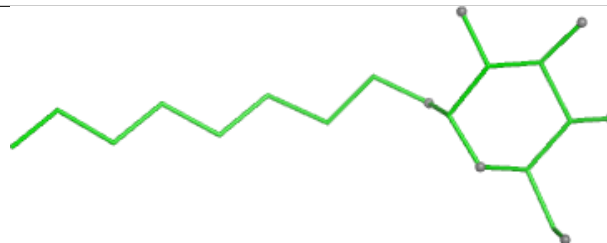


Rings

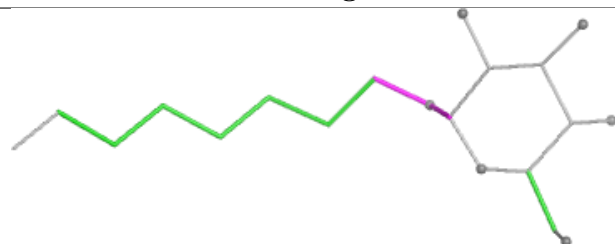
Ligand LMU A 856



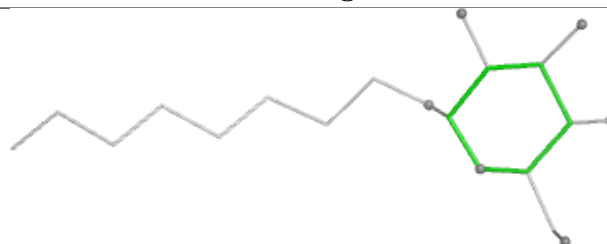
Bond lengths



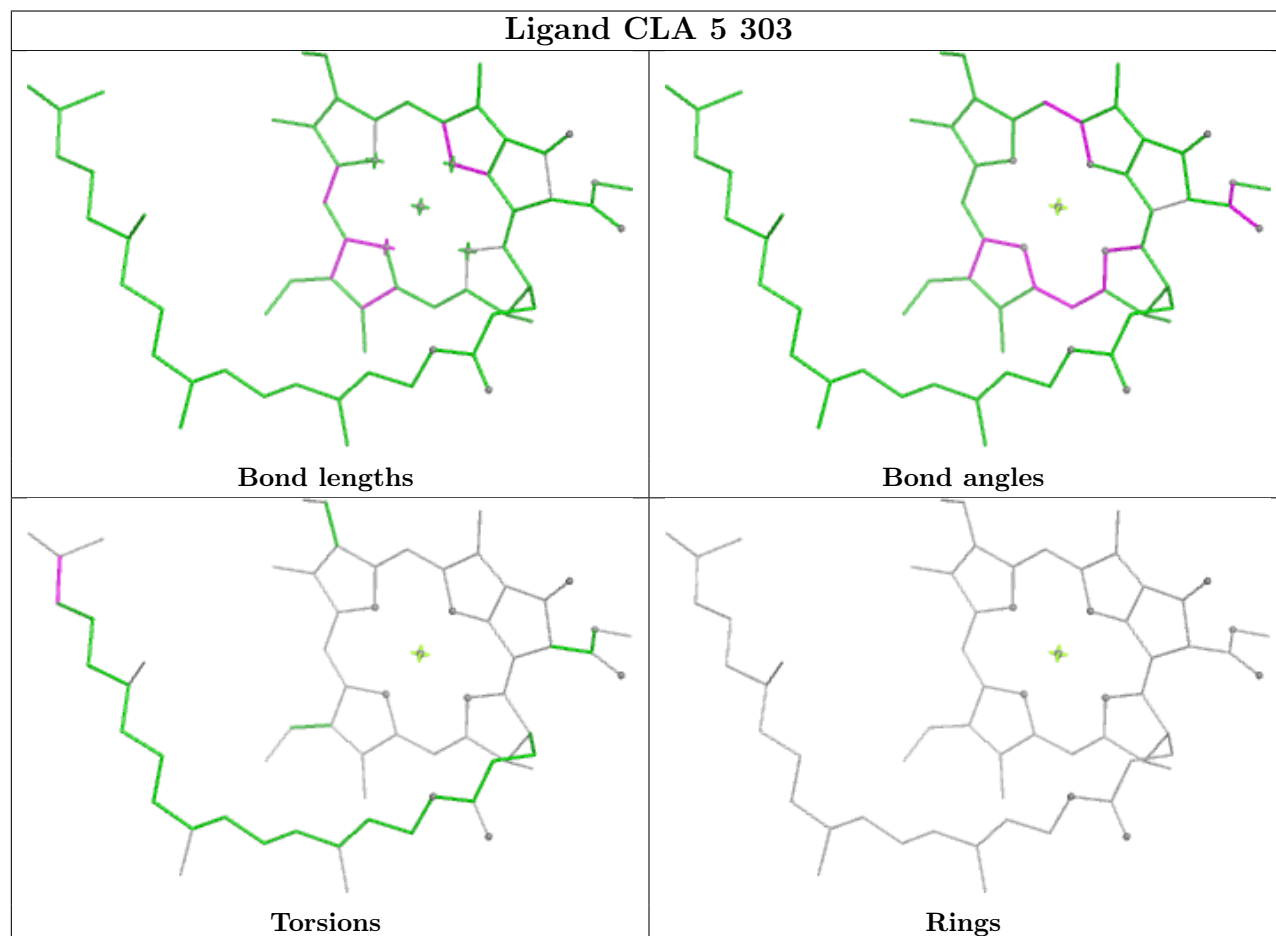
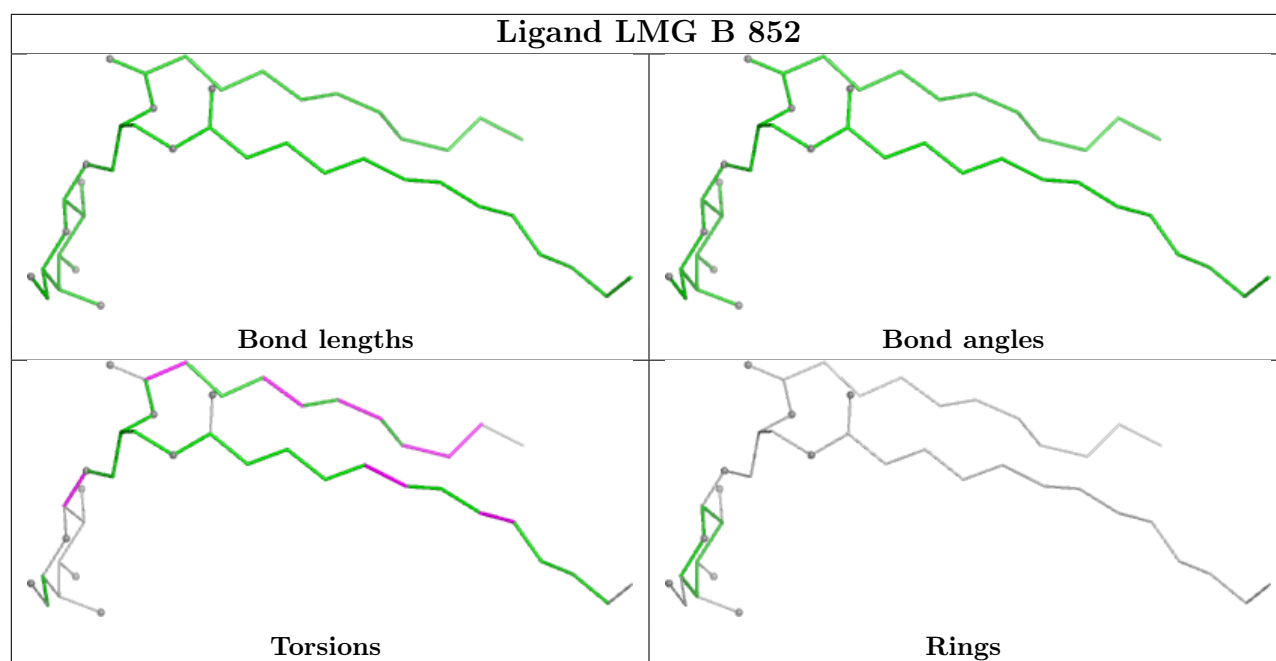
Bond angles

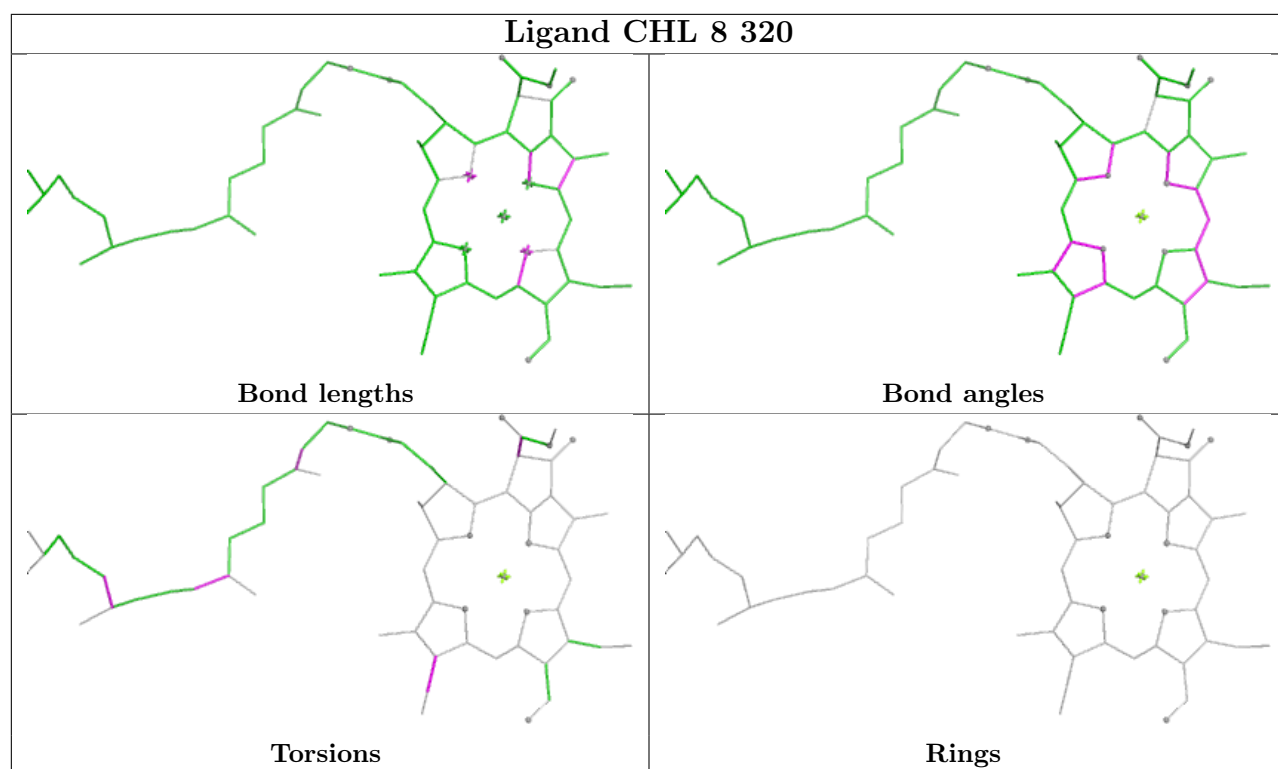


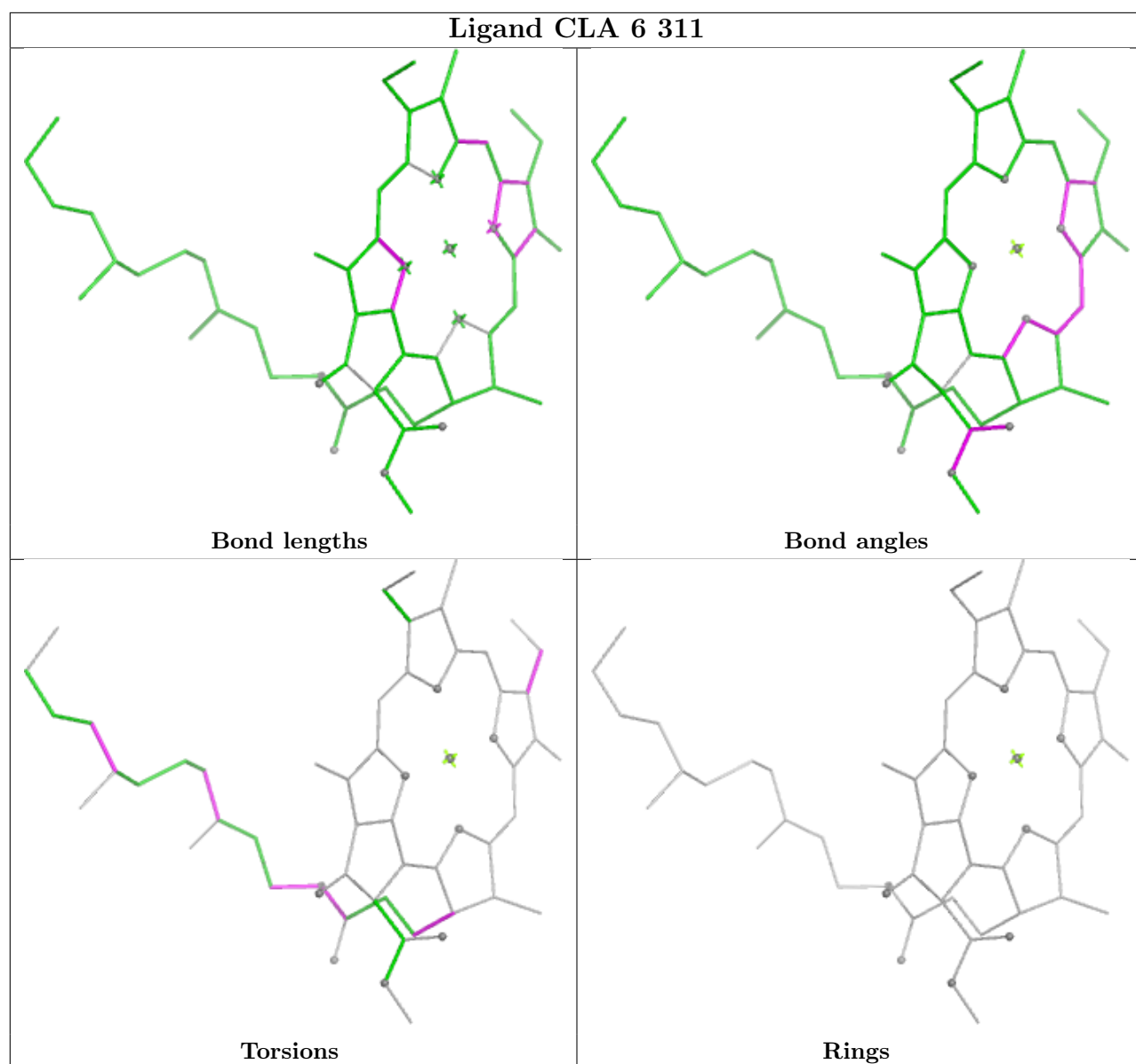
Torsions

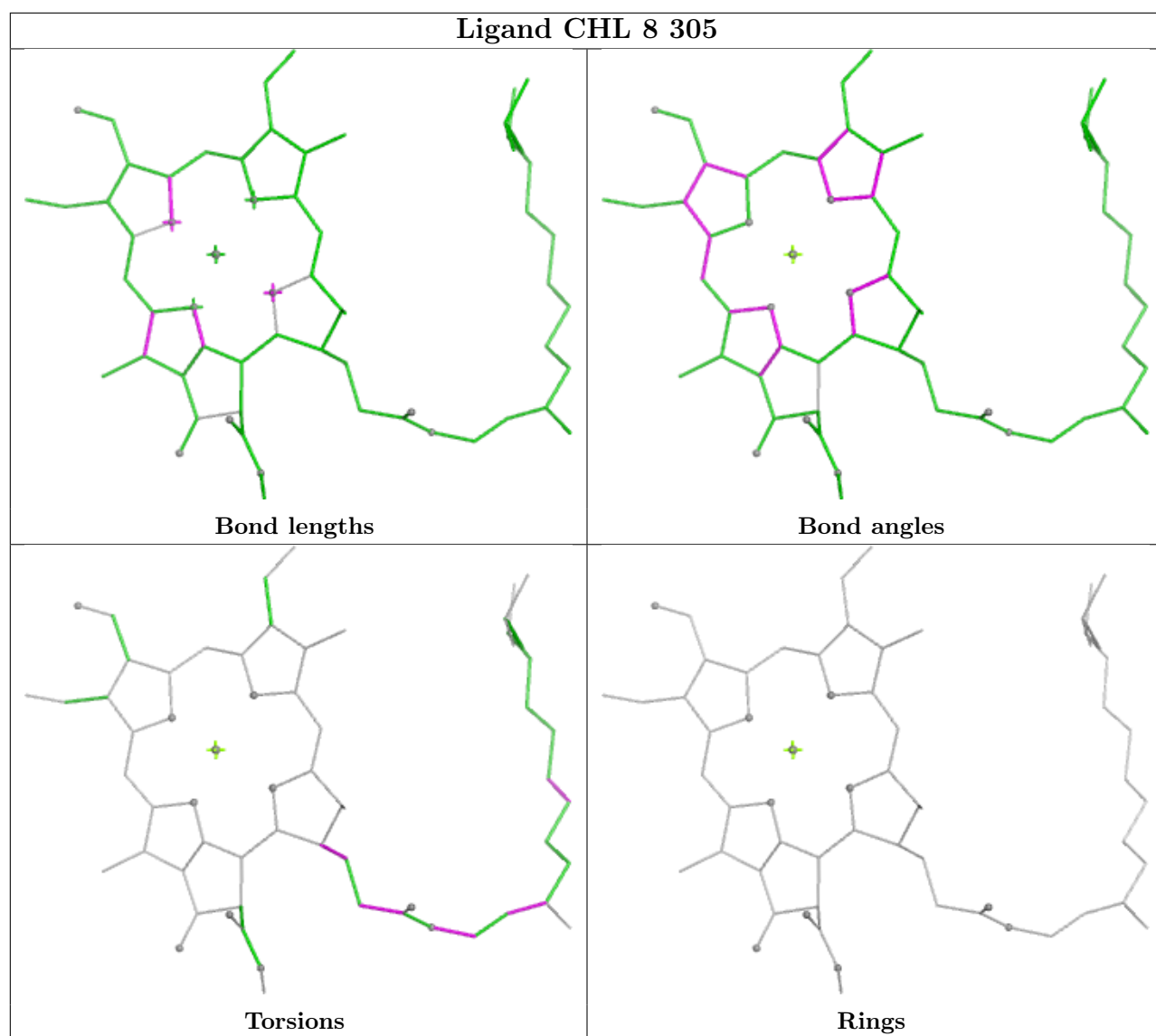


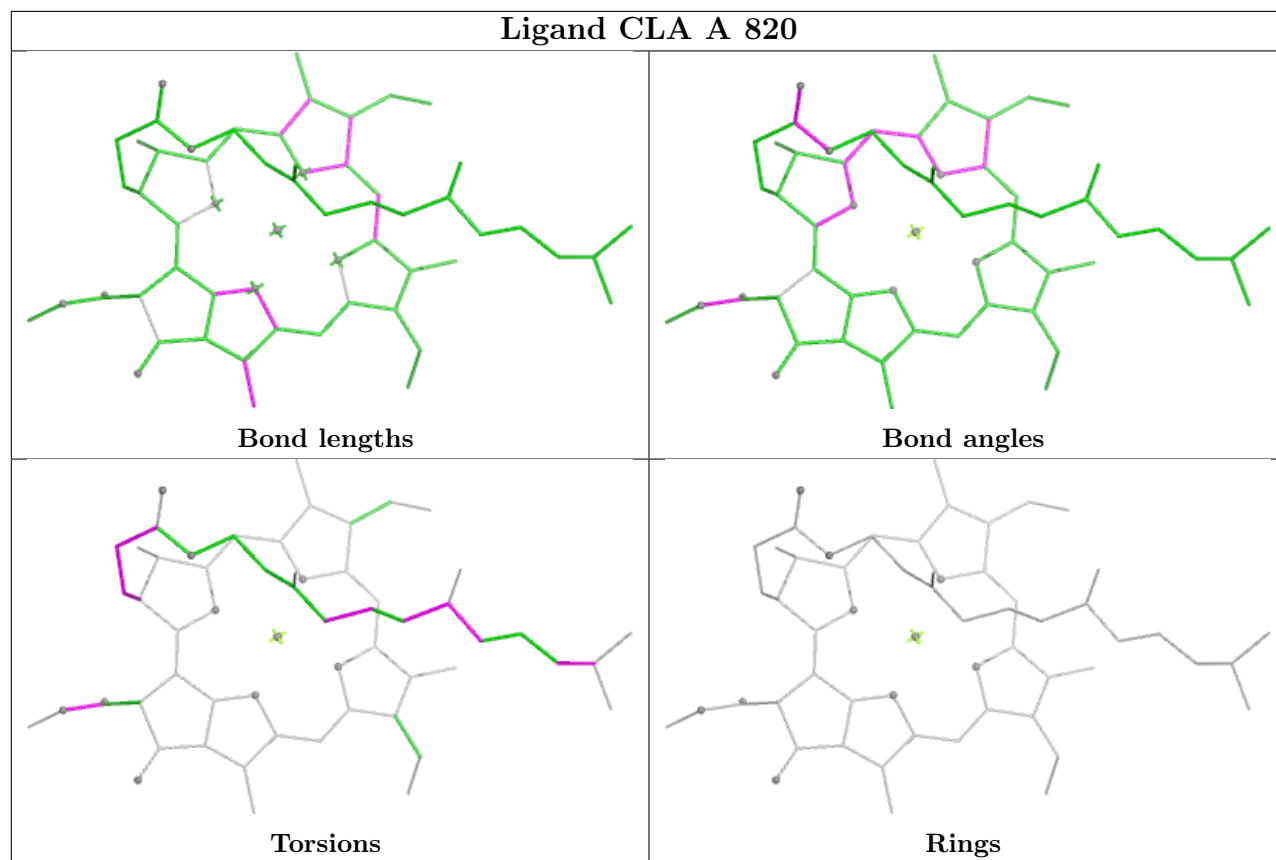
Rings



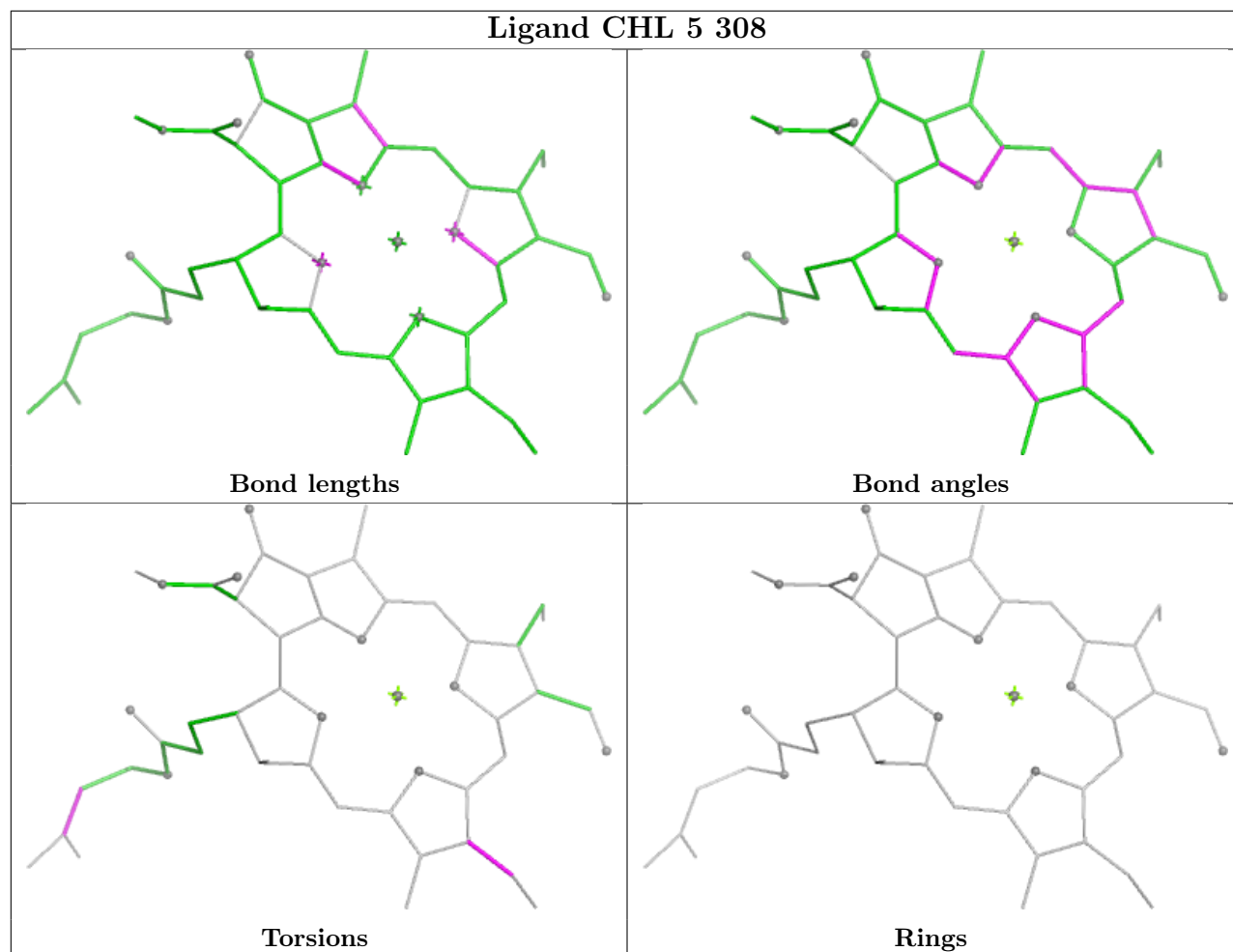




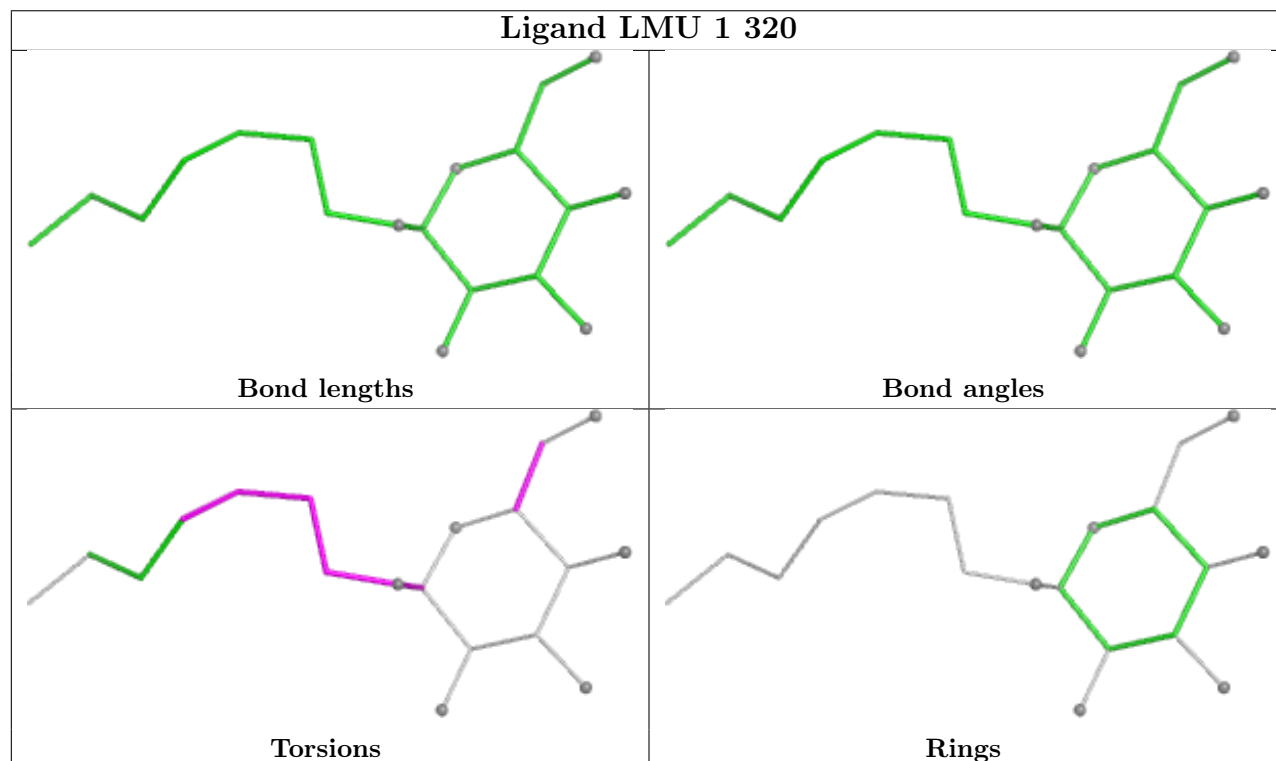


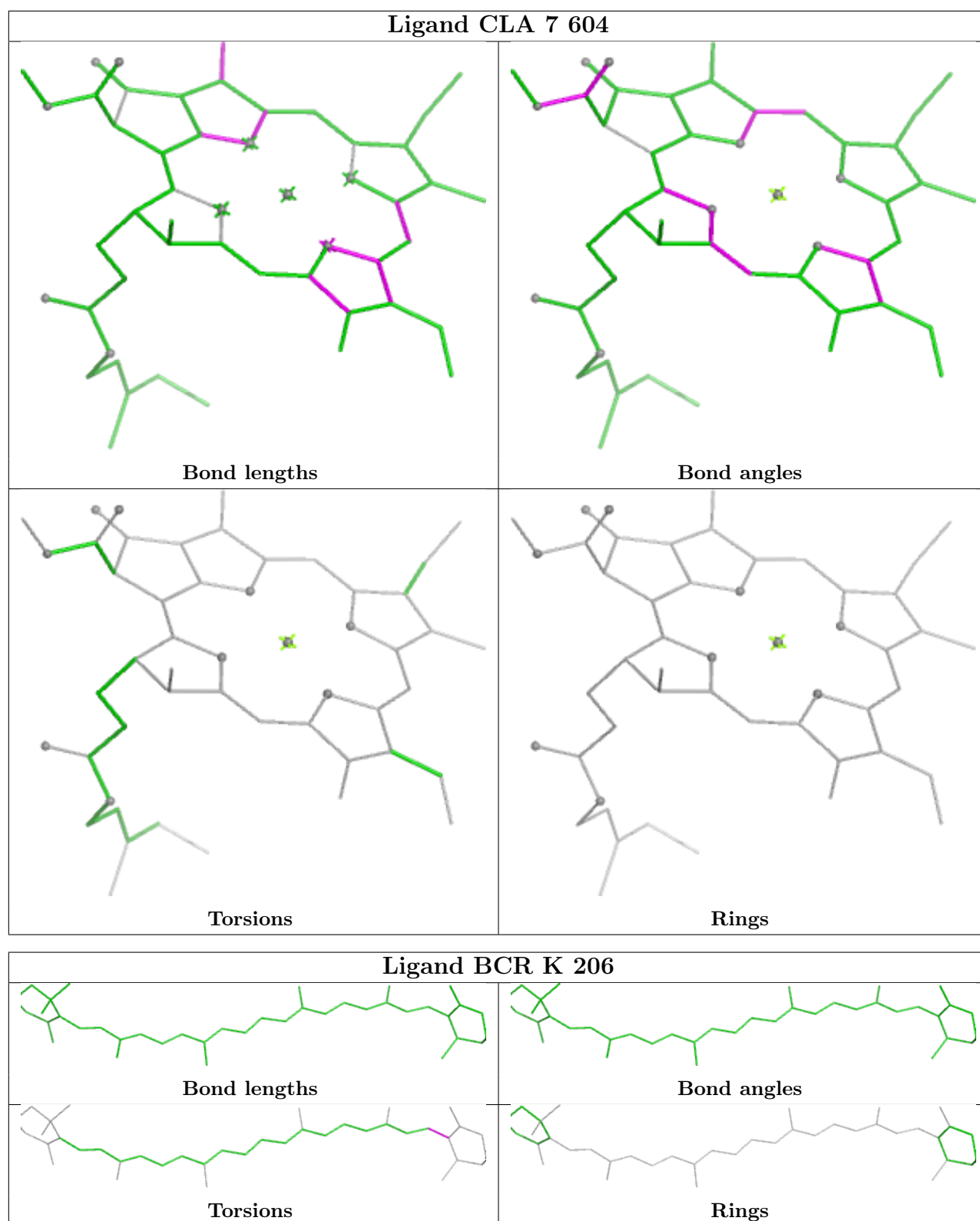


Ligand CHL 5 308



Ligand LMU 1 320





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	142:SER	C	157:ALA	N	10.13

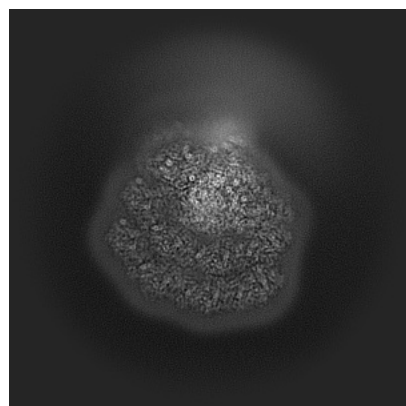
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54803. These allow visual inspection of the internal detail of the map and identification of artifacts.

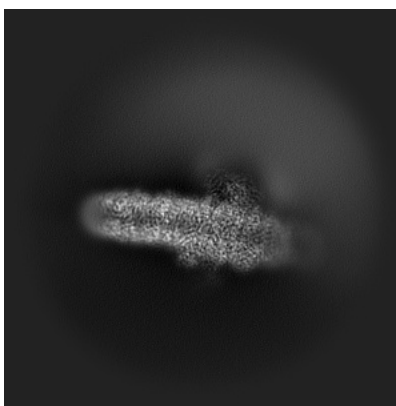
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

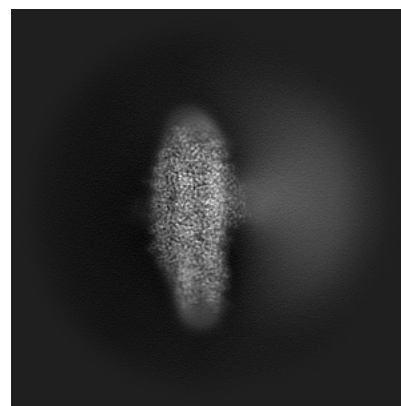
6.1.1 Primary map



X

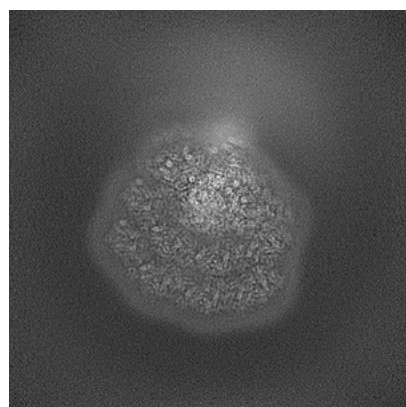


Y

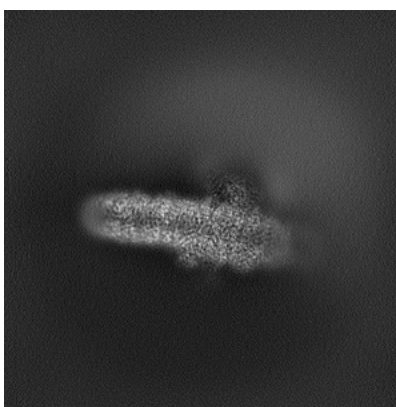


Z

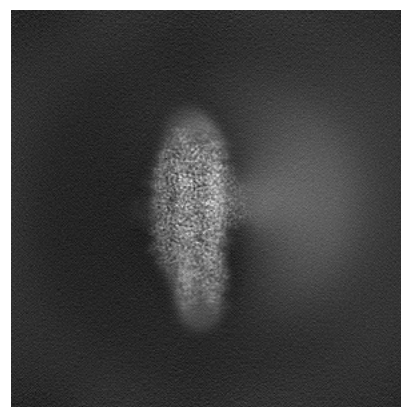
6.1.2 Raw map



X



Y

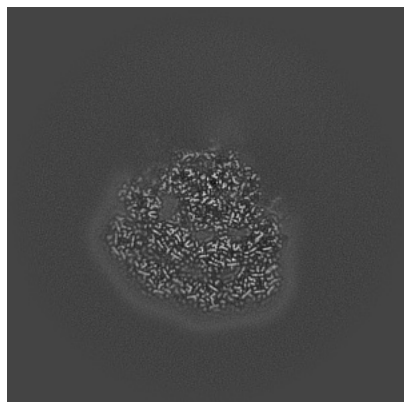


Z

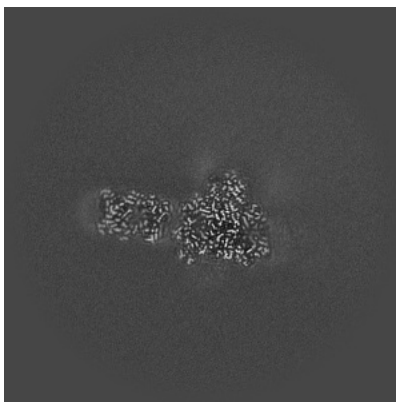
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

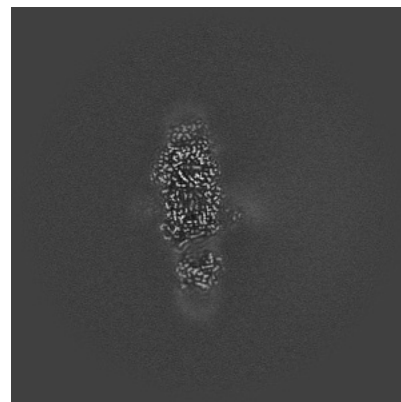
6.2.1 Primary map



X Index: 256

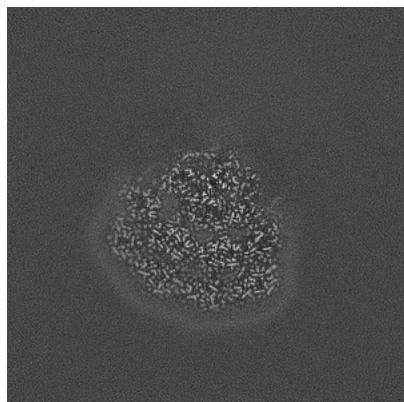


Y Index: 256

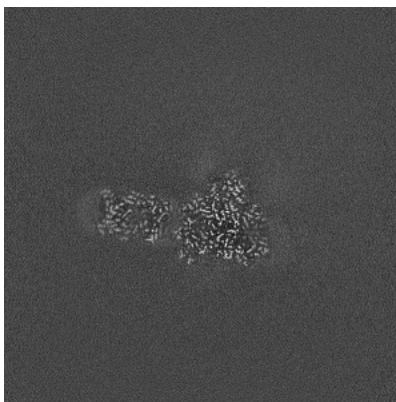


Z Index: 256

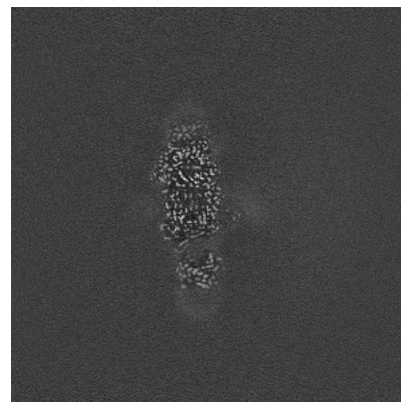
6.2.2 Raw map



X Index: 256



Y Index: 256

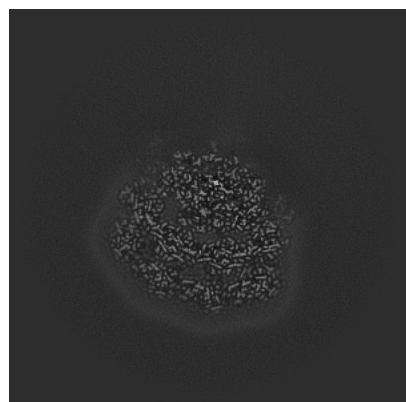


Z Index: 256

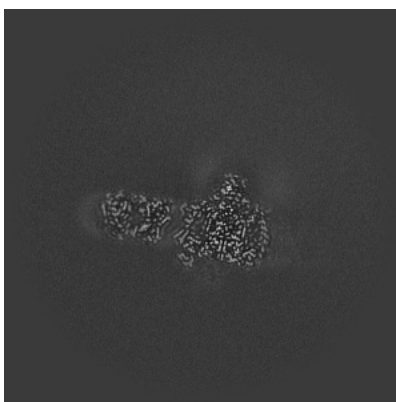
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

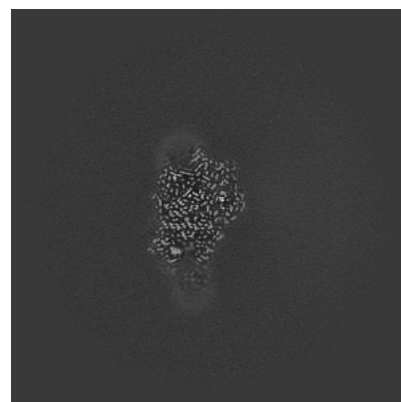
6.3.1 Primary map



X Index: 253

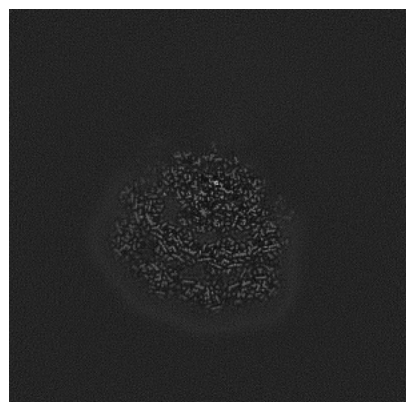


Y Index: 261

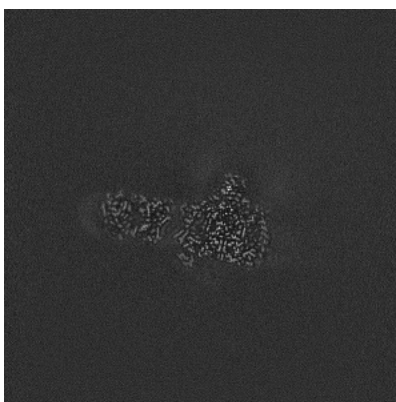


Z Index: 296

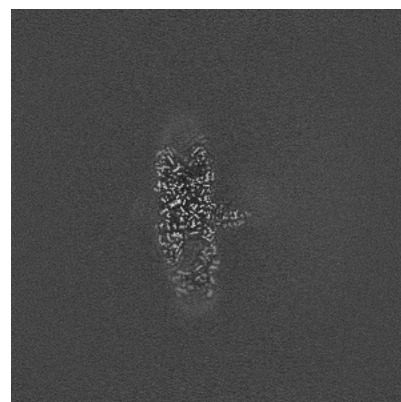
6.3.2 Raw map



X Index: 253



Y Index: 261

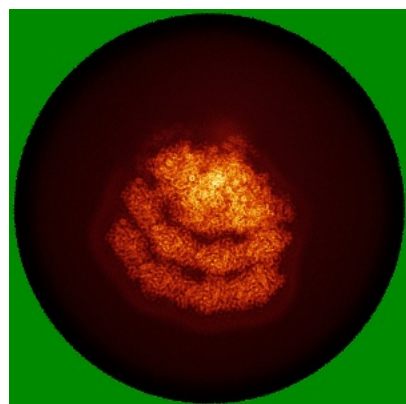


Z Index: 276

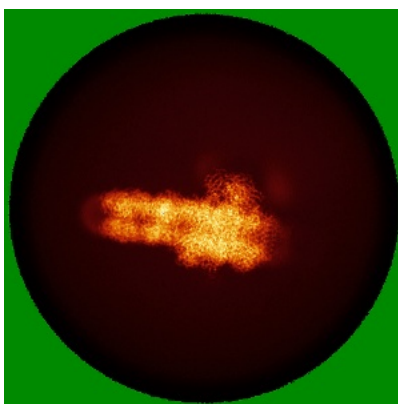
The images above show the largest variance slices of the map in three orthogonal directions.

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

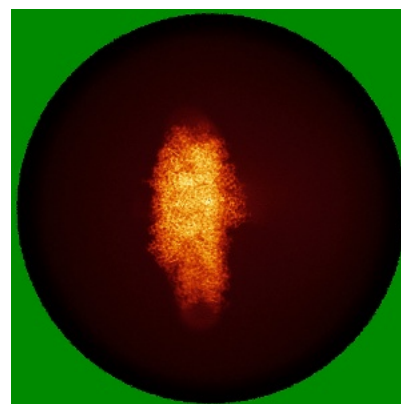
6.4.1 Primary map



X

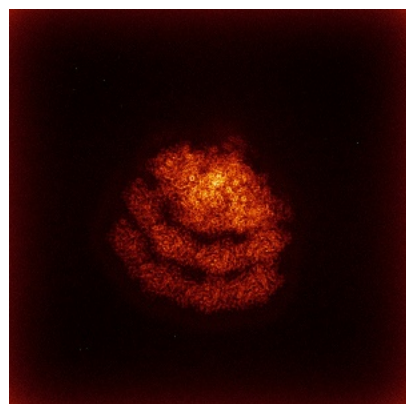


Y

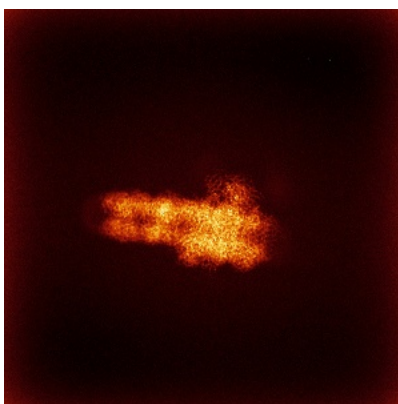


Z

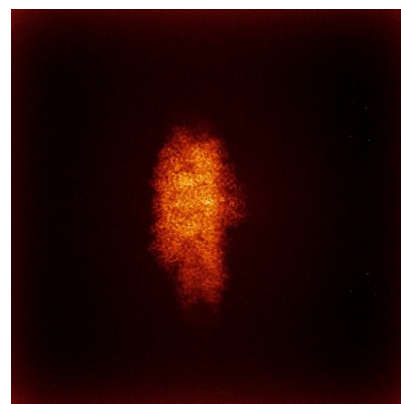
6.4.2 Raw map



X



Y

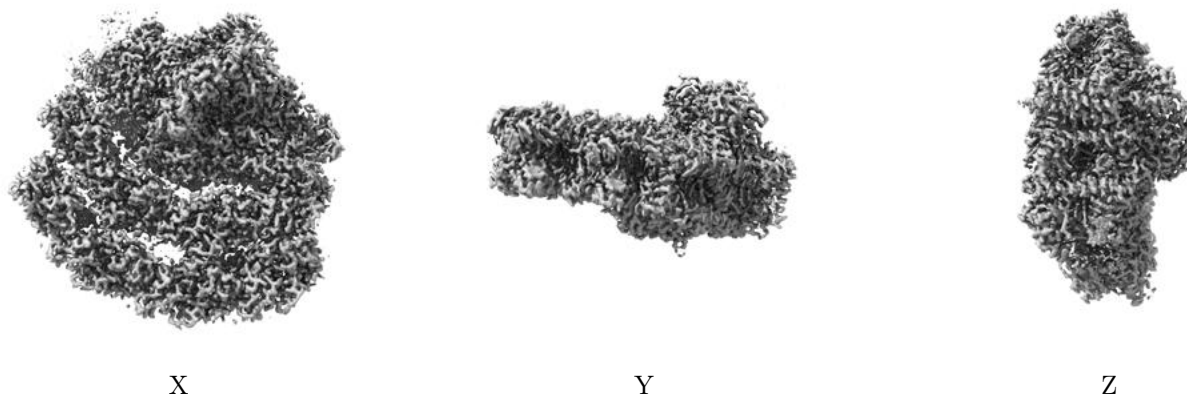


Z

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

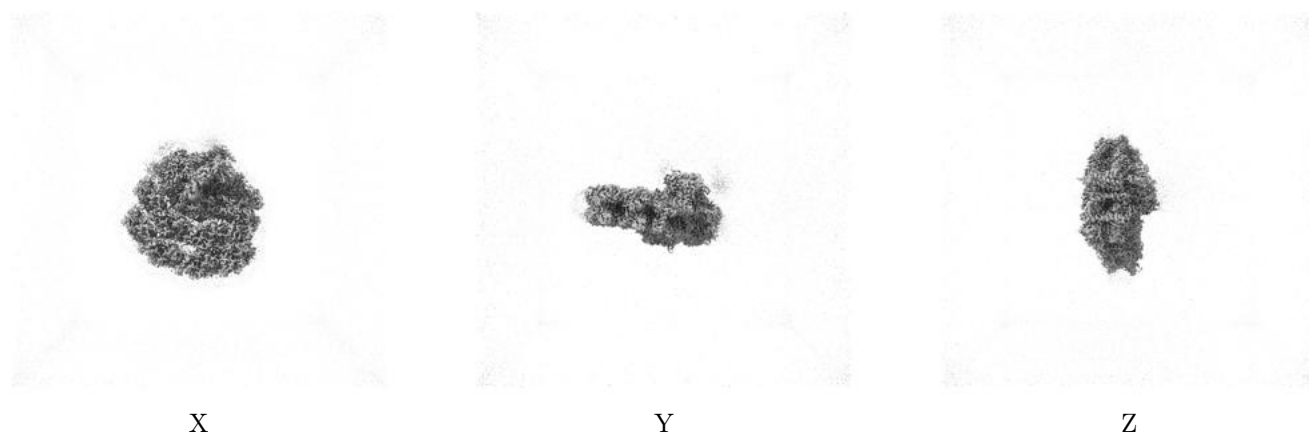
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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

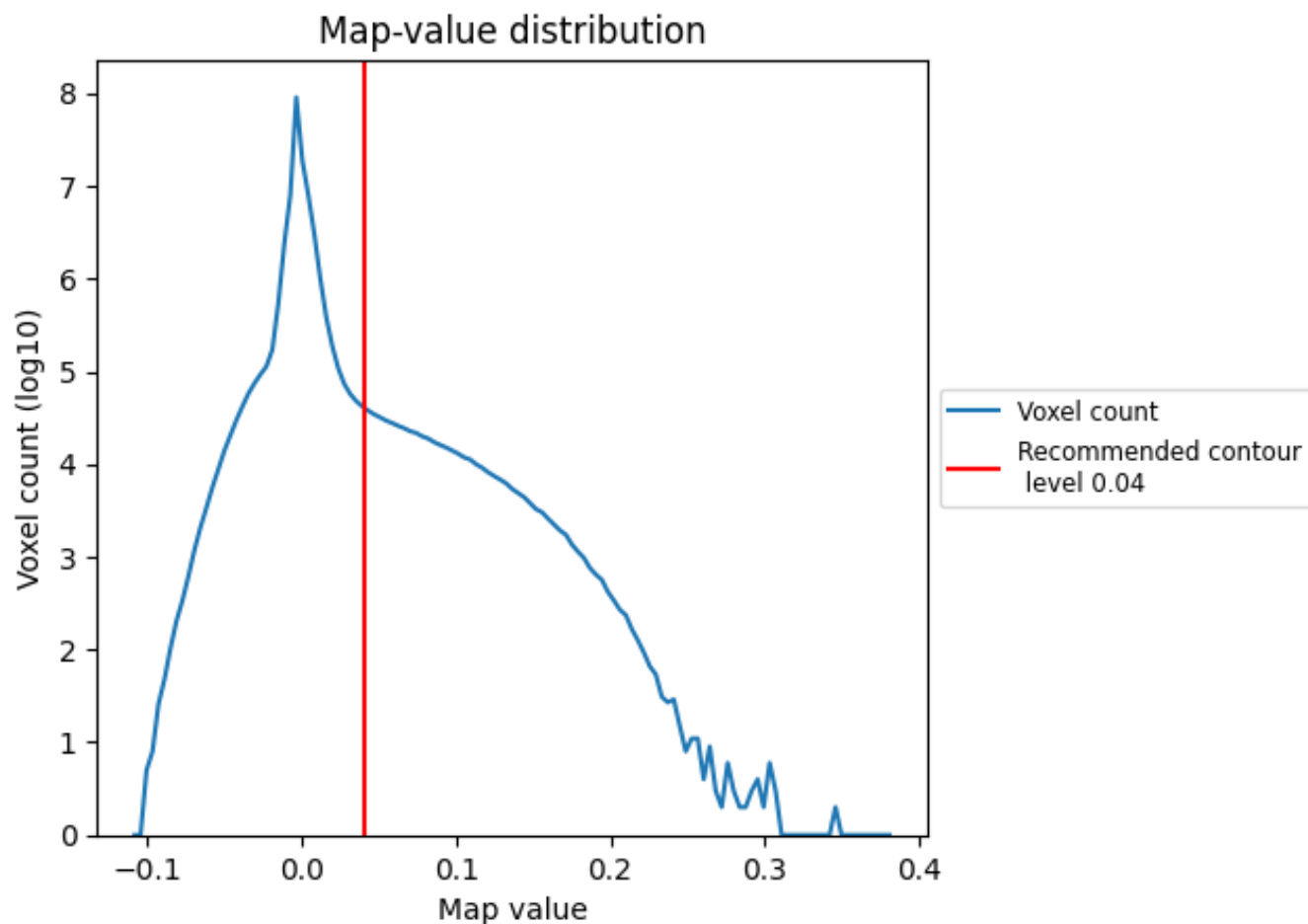
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

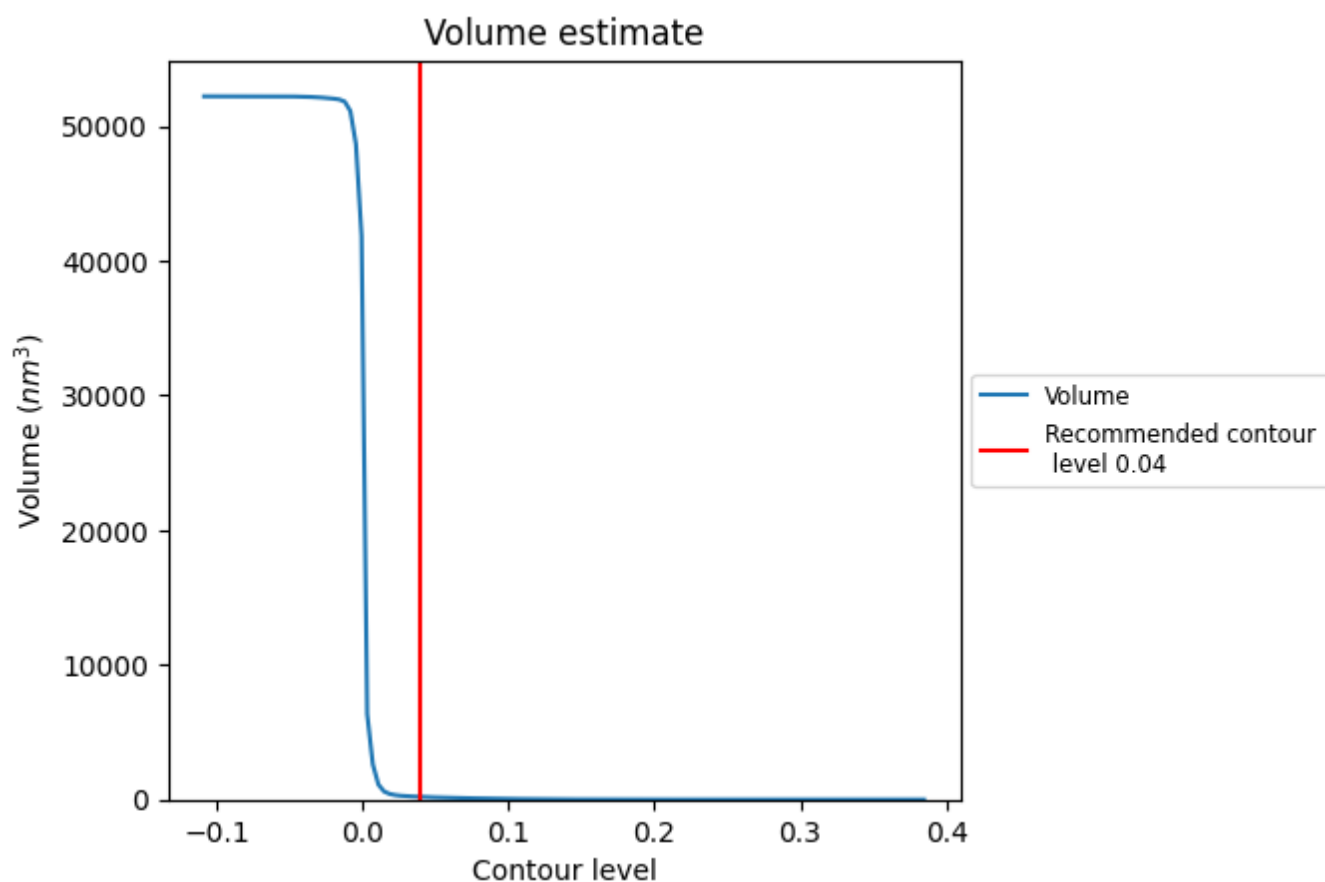
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

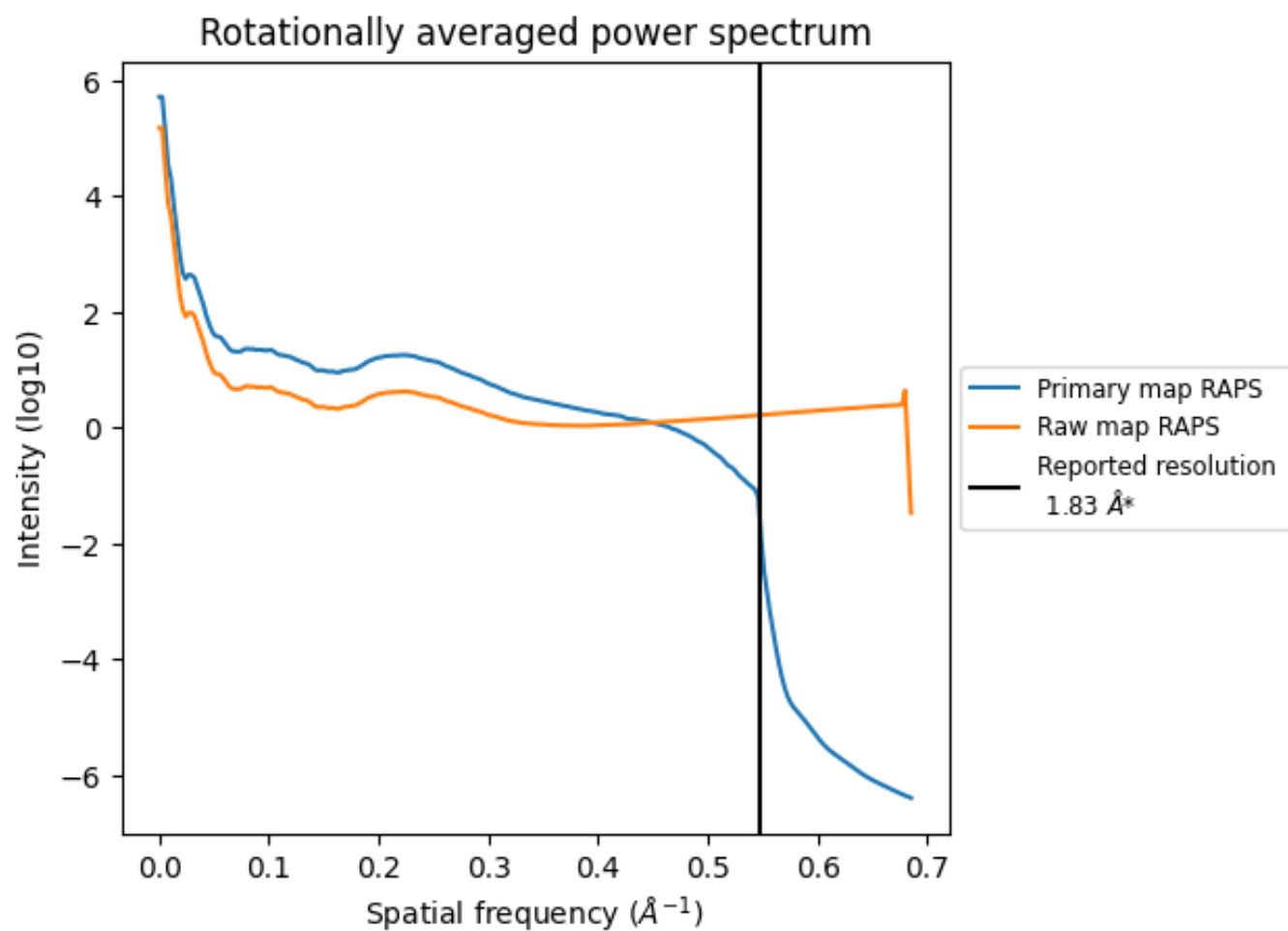
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 200 nm^3 ; this corresponds to an approximate mass of 181 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

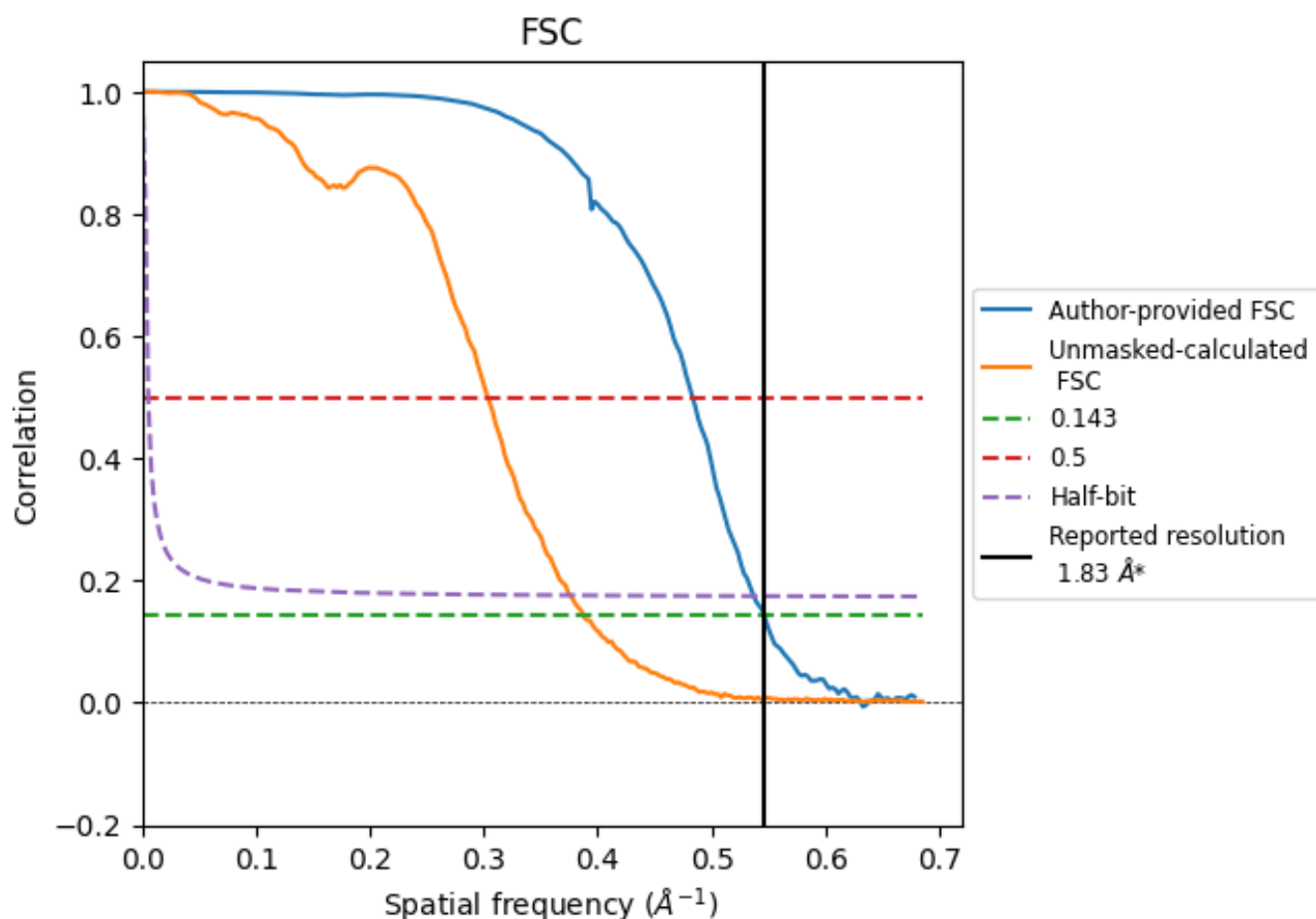


*Reported resolution corresponds to spatial frequency of 0.546 $\text{\AA}^{-1}$

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 0.546 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

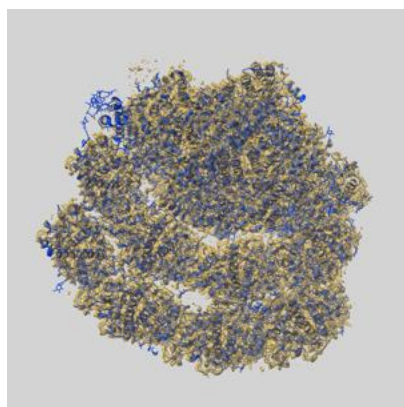
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.83	-	-
Author-provided FSC curve	1.83	2.07	1.86
Unmasked-calculated*	2.58	3.30	2.66

*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 2.58 differs from the reported value 1.83 by more than 10 %

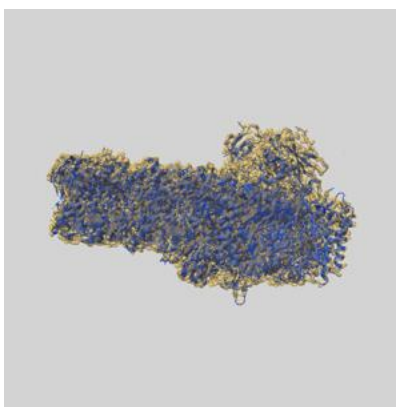
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54803 and PDB model 9SE6. Per-residue inclusion information can be found in [section 3](#) on [page 30](#).

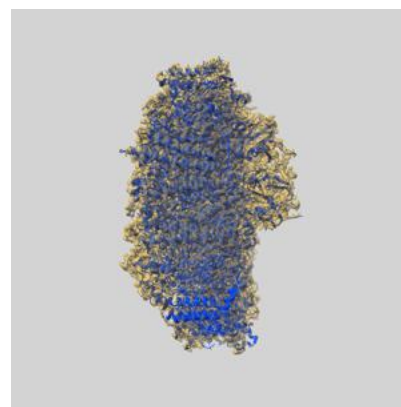
9.1 Map-model overlay [i](#)



X



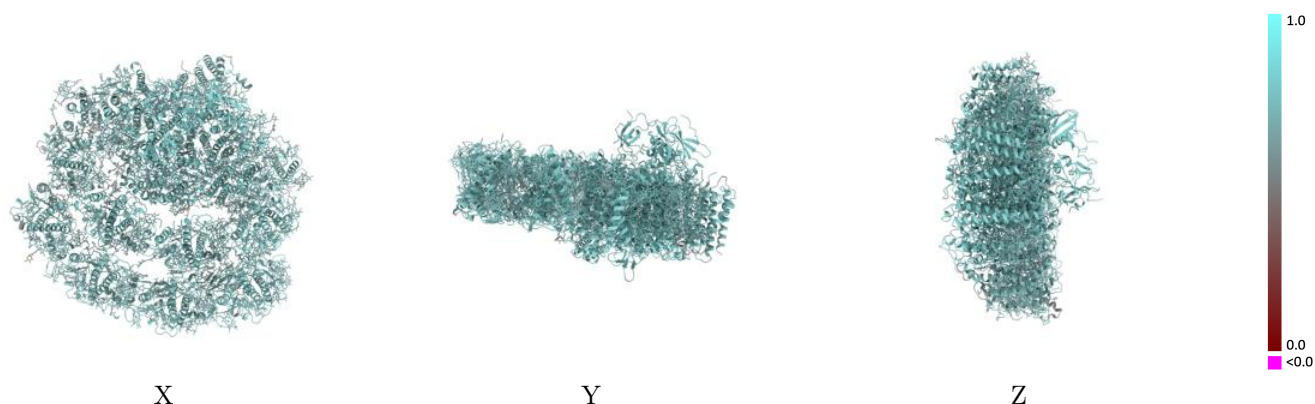
Y



Z

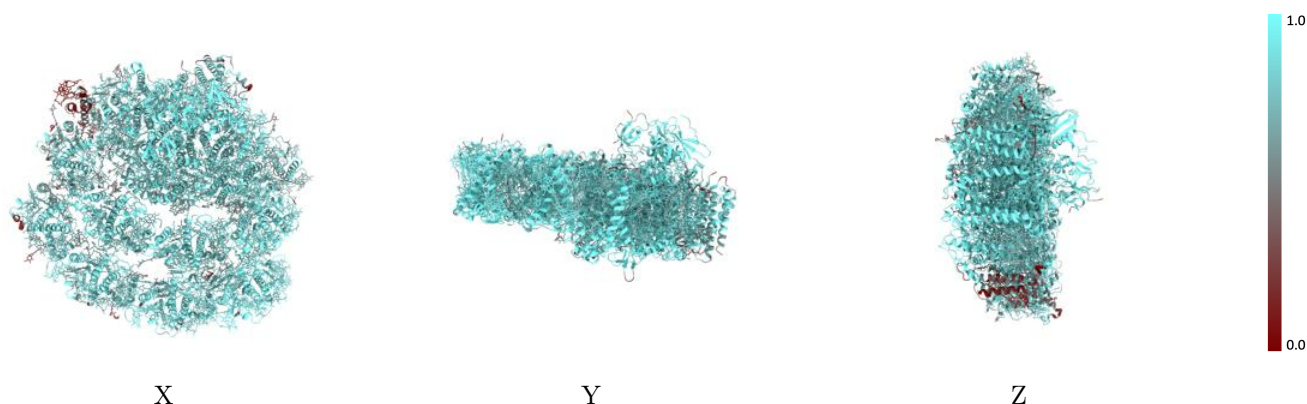
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



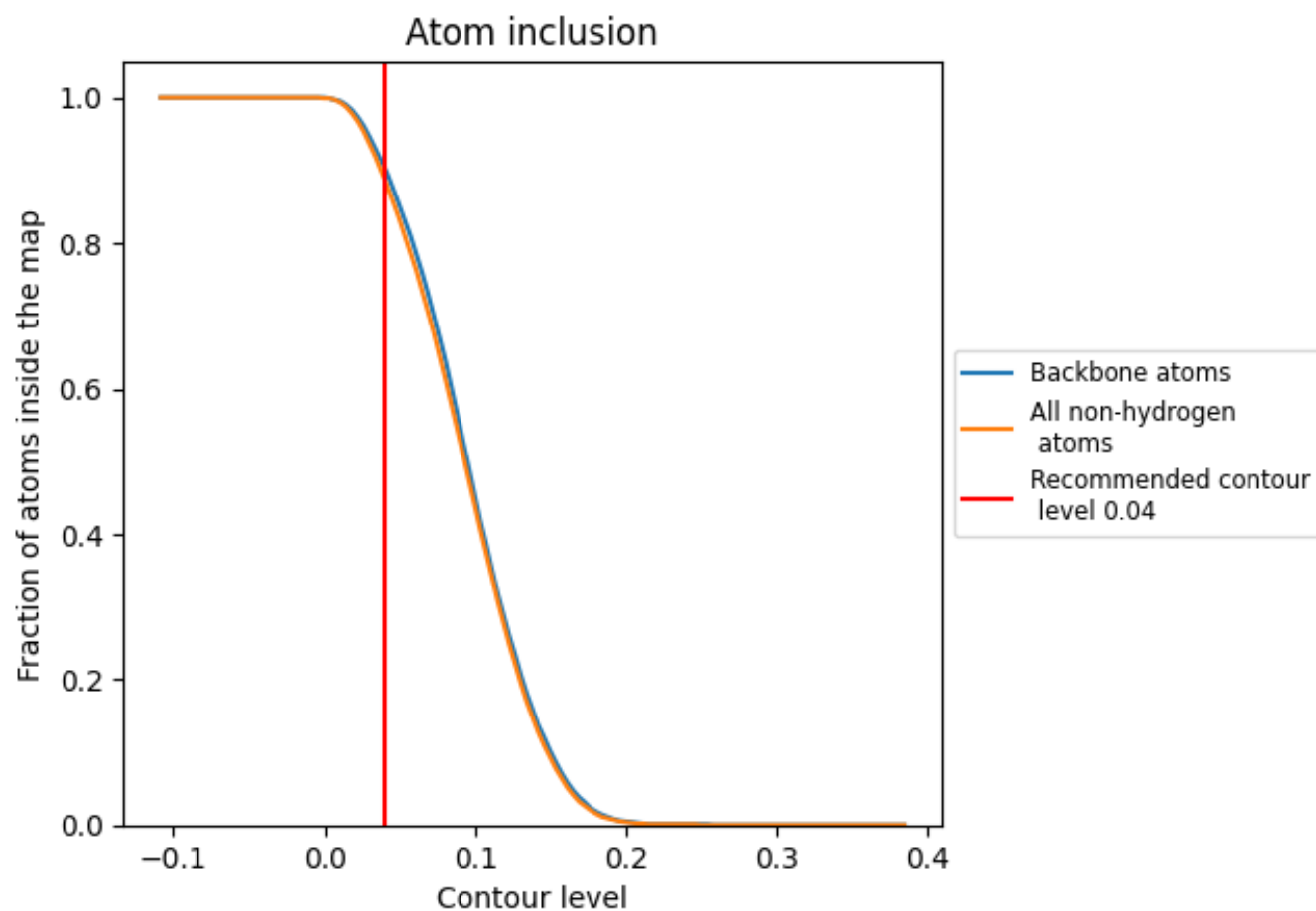
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 90% of all backbone atoms, 89% 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	 0.8890	 0.7200
1	 0.8090	 0.6830
3	 0.9120	 0.7230
4	 0.8430	 0.6810
5	 0.9080	 0.7020
6	 0.8810	 0.6960
7	 0.9240	 0.7300
8	 0.9120	 0.7250
A	 0.9490	 0.7540
B	 0.9300	 0.7430
C	 0.9820	 0.7630
D	 0.9240	 0.7400
E	 0.8900	 0.7250
F	 0.8920	 0.7270
G	 0.1770	 0.6260
I	 0.8650	 0.7140
J	 0.9100	 0.7350
K	 0.7540	 0.6890
L	 0.7230	 0.6770
Z	 0.7830	 0.6680

