



Full wwPDB EM Validation Report ⓘ

Jul 2, 2023 – 12:31 AM JST

PDB ID : 7WZN
EMDB ID : EMD-32907
Title : PSI-LHCI from Chlamydomonas reinhardtii with bound ferredoxin
Authors : Kurisu, G.; Gerle, C.; Mitsuoka, K.; Kawamoto, A.; Tanaka, H.
Deposited on : 2022-02-18
Resolution : 4.90 Å (reported)
Based on initial model : 6JO5

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:

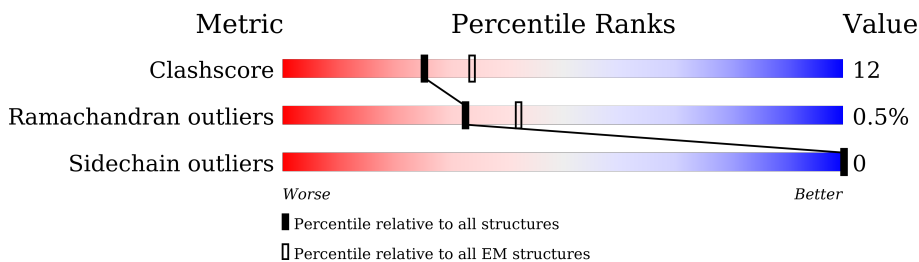
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

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 4.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	
2	B	735	
3	C	81	
4	D	196	
5	E	97	
6	F	227	
7	J	41	
8	1	224	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	3	298	
10	7	241	
11	8	243	
12	Z	228	
13	4	264	
14	5	257	
15	6	257	
16	G	126	

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
17	CL0	A	801	X	-	-	-
18	CLA	1	602	X	-	-	-
18	CLA	1	603	X	-	-	-
18	CLA	1	604	X	-	-	-
18	CLA	1	605	X	-	-	-
18	CLA	1	607	X	-	-	-
18	CLA	1	608	X	-	-	-
18	CLA	1	609	X	-	-	-
18	CLA	1	610	X	-	-	-
18	CLA	1	611	X	-	-	-
18	CLA	1	612	X	-	-	-
18	CLA	1	613	X	-	-	-
18	CLA	1	614	X	-	-	-
18	CLA	3	301	X	-	-	-
18	CLA	3	302	X	-	-	-
18	CLA	3	303	X	-	-	-
18	CLA	3	304	X	-	-	-
18	CLA	3	305	X	-	-	-
18	CLA	3	307	X	-	-	-
18	CLA	3	308	X	-	-	-
18	CLA	3	309	X	-	-	-
18	CLA	3	310	X	-	-	-
18	CLA	3	311	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	3	312	X	-	-	-
18	CLA	3	313	X	-	-	-
18	CLA	3	314	X	-	-	-
18	CLA	4	601	X	-	-	-
18	CLA	4	602	X	-	-	-
18	CLA	4	603	X	-	-	-
18	CLA	4	606	X	-	-	-
18	CLA	4	607	X	-	-	-
18	CLA	4	608	X	-	-	-
18	CLA	4	609	X	-	-	-
18	CLA	4	610	X	-	-	-
18	CLA	4	611	X	-	-	-
18	CLA	4	612	X	-	-	-
18	CLA	5	601	X	-	-	-
18	CLA	5	602	X	-	-	-
18	CLA	5	603	X	-	-	-
18	CLA	5	604	X	-	-	-
18	CLA	5	605	X	-	-	-
18	CLA	5	608	X	-	-	-
18	CLA	5	609	X	-	-	-
18	CLA	5	610	X	-	-	-
18	CLA	5	611	X	-	-	-
18	CLA	5	612	X	-	-	-
18	CLA	5	613	X	-	-	-
18	CLA	5	614	X	-	-	-
18	CLA	5	615	X	-	-	-
18	CLA	5	617	X	-	-	-
18	CLA	6	301	X	-	-	-
18	CLA	6	302	X	-	-	-
18	CLA	6	303	X	-	-	-
18	CLA	6	304	X	-	-	-
18	CLA	6	308	X	-	-	-
18	CLA	6	309	X	-	-	-
18	CLA	6	310	X	-	-	-
18	CLA	6	311	X	-	-	-
18	CLA	6	312	X	-	-	-
18	CLA	6	313	X	-	-	-
18	CLA	6	314	X	-	-	-
18	CLA	6	315	X	-	-	-
18	CLA	6	317	X	-	-	-
18	CLA	7	601	X	-	-	-
18	CLA	7	602	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	7	603	X	-	-	-
18	CLA	7	604	X	-	-	-
18	CLA	7	605	X	-	-	-
18	CLA	7	607	X	-	-	-
18	CLA	7	608	X	-	-	-
18	CLA	7	609	X	-	-	-
18	CLA	7	610	X	-	-	-
18	CLA	7	611	X	-	-	-
18	CLA	7	612	X	-	-	-
18	CLA	7	613	X	-	-	-
18	CLA	7	614	X	-	-	-
18	CLA	8	601	X	-	-	-
18	CLA	8	602	X	-	-	-
18	CLA	8	603	X	-	-	-
18	CLA	8	604	X	-	-	-
18	CLA	8	605	X	-	-	-
18	CLA	8	607	X	-	-	-
18	CLA	8	608	X	-	-	-
18	CLA	8	609	X	-	-	-
18	CLA	8	610	X	-	-	-
18	CLA	8	611	X	-	-	-
18	CLA	8	612	X	-	-	-
18	CLA	8	613	X	-	-	-
18	CLA	8	614	X	-	-	-
18	CLA	8	615	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-
18	CLA	A	821	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	841	X	-	-	-
18	CLA	A	843	X	-	-	-
18	CLA	A	844	X	-	-	-
18	CLA	A	845	X	-	-	-
18	CLA	B	801	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-
18	CLA	B	811	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	838	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	841	X	-	-	-
18	CLA	B	842	X	-	-	-
18	CLA	B	843	X	-	-	-
18	CLA	F	301	X	-	-	-
18	CLA	F	302	X	-	-	-
18	CLA	J	101	X	-	-	-
18	CLA	Z	602	X	-	-	-
18	CLA	Z	603	X	-	-	-
18	CLA	Z	604	X	-	-	-
18	CLA	Z	606	X	-	-	-
18	CLA	Z	607	X	-	-	-
18	CLA	Z	608	X	-	-	-
18	CLA	Z	609	X	-	-	-
18	CLA	Z	610	X	-	-	-
18	CLA	Z	611	X	-	-	-
18	CLA	Z	612	X	-	-	-
18	CLA	Z	613	X	-	-	-
20	SF4	C	101	-	-	X	-
21	CHL	1	601	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHL	1	606	X	-	-	-
21	CHL	3	306	X	-	-	-
21	CHL	4	604	X	-	-	-
21	CHL	4	605	X	-	-	-
21	CHL	5	606	X	-	-	-
21	CHL	5	607	X	-	-	-
21	CHL	5	616	X	-	-	-
21	CHL	6	305	X	-	-	-
21	CHL	6	306	X	-	-	-
21	CHL	6	307	X	-	-	-
21	CHL	6	316	X	-	-	-
21	CHL	7	606	X	-	-	-
21	CHL	8	606	X	-	-	-
21	CHL	Z	601	X	-	-	-
21	CHL	Z	605	X	-	-	-

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 27190 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	738	3628	2151	739	738	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	732	3601	2136	733	732	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	80	395	235	80	80	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	144	706	418	144	144	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	61	300	178	61	61	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	F	165	810	480	165	165	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	J	39	194	116	39	39	0	0

- Molecule 8 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	1	194	942	554	194	194	0	0

- Molecule 9 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	3	202	985	581	202	202	0	0

- Molecule 10 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	7	212	1033	609	212	212	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	8	217	1059	625	217	217	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	Z	192	934	550	192	192	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	4	203	992	586	203	203	0	0

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

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
14	5	223	1091	645	223	223	0	0

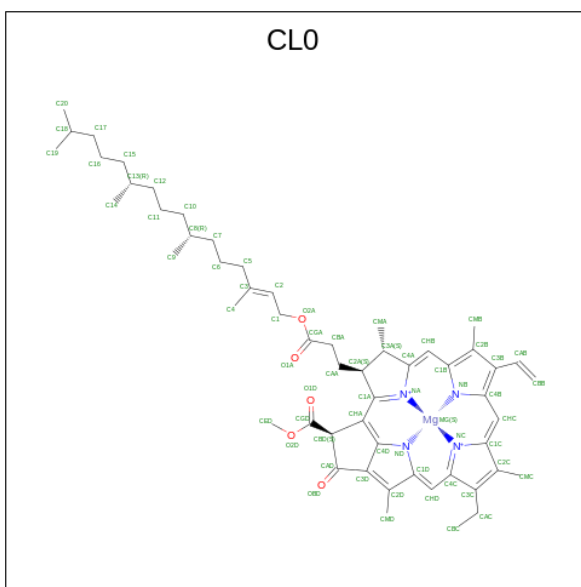
- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
15	6	229	1122	664	229	229	0	0

- Molecule 16 is a protein called Ferredoxin, chloroplastic.

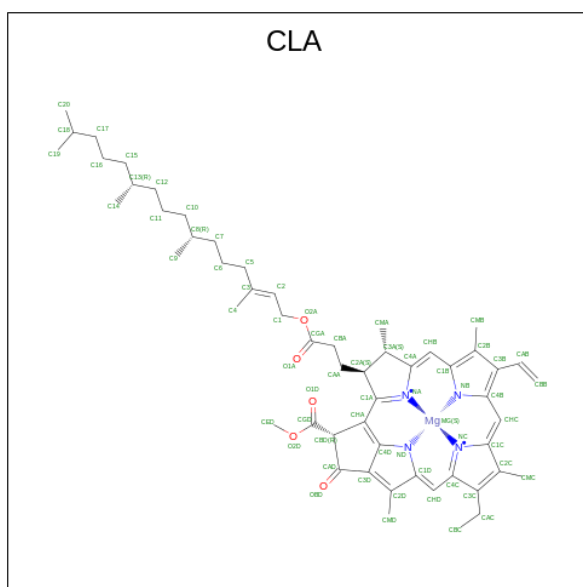
Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
16	G	95	493	293	100	100	5	0

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



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
17	A	1	42	34	1	4	3	0

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



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	43	35	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	42	34	1	4	3	0
18	A	1	47	37	1	4	5	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	51	41	1	4	5	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	A	1	52	42	1	4	5	0
18	A	1	42	34	1	4	3	0
18	A	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	46	36	1	4	5	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	45	35	1	4	5	0
18	B	1	50	42	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	41	33	1	4	3	0
18	B	1	42	34	1	4	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	45	35	1	4	5	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	39	31	1	4	3	0
18	B	1	42	34	1	4	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	43	35	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	B	1	42	34	1	4	3	0
18	F	1	45	35	1	4	5	0
18	F	1	65	55	1	4	5	0
18	J	1	42	34	1	4	3	0
18	1	1	42	34	1	4	3	0
18	1	1	42	34	1	4	3	0
18	1	1	42	34	1	4	3	0
18	1	1	42	34	1	4	3	0
18	1	1	42	34	1	4	3	0
18	1	1	42	34	1	4	3	0
18	1	1	42	34	1	4	3	0
18	1	1	42	34	1	4	3	0
18	1	1	42	34	1	4	3	0
18	1	1	42	34	1	4	3	0
18	1	1	46	36	1	4	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	1	1	42	34	1	4	3	0
18	1	1	46	36	1	4	5	0
18	3	1	42	34	1	4	3	0
18	3	1	42	34	1	4	3	0
18	3	1	42	34	1	4	3	0
18	3	1	42	34	1	4	3	0
18	3	1	42	34	1	4	3	0
18	3	1	42	34	1	4	3	0
18	3	1	42	34	1	4	3	0
18	3	1	41	33	1	4	3	0
18	3	1	46	36	1	4	5	0
18	3	1	45	35	1	4	5	0
18	3	1	45	35	1	4	5	0
18	3	1	46	36	1	4	5	0
18	3	1	42	34	1	4	3	0
18	7	1	42	34	1	4	3	0
18	7	1	42	34	1	4	3	0
18	7	1	46	36	1	4	5	0
18	7	1	43	35	1	4	3	0
18	7	1	42	34	1	4	3	0
18	7	1	42	34	1	4	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
18	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	8	1	Total 42	C 34	Mg 1	N 4	O 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	Z	1	42	34	1	4	3	0
18	Z	1	42	34	1	4	3	0
18	Z	1	43	35	1	4	3	0
18	Z	1	42	34	1	4	3	0
18	Z	1	42	34	1	4	3	0
18	Z	1	42	34	1	4	3	0
18	Z	1	42	34	1	4	3	0
18	Z	1	42	34	1	4	3	0
18	Z	1	45	35	1	4	5	0
18	Z	1	42	34	1	4	3	0
18	Z	1	42	34	1	4	3	0
18	4	1	42	34	1	4	3	0
18	4	1	42	34	1	4	3	0
18	4	1	46	36	1	4	5	0
18	4	1	42	34	1	4	3	0
18	4	1	42	34	1	4	3	0
18	4	1	42	34	1	4	3	0
18	4	1	42	34	1	4	3	0
18	4	1	42	34	1	4	3	0
18	4	1	42	34	1	4	3	0
18	4	1	41	33	1	4	3	0

Continued on next page...

Continued from previous page...

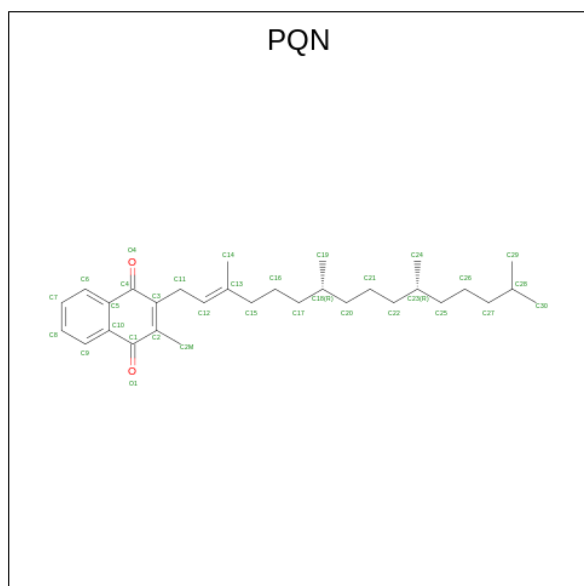
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	5	1	42	34	1	4	3	0
18	5	1	42	34	1	4	3	0
18	5	1	46	36	1	4	5	0
18	5	1	42	34	1	4	3	0
18	5	1	42	34	1	4	3	0
18	5	1	42	34	1	4	3	0
18	5	1	42	34	1	4	3	0
18	5	1	55	45	1	4	5	0
18	5	1	42	34	1	4	3	0
18	5	1	42	34	1	4	3	0
18	5	1	42	34	1	4	3	0
18	5	1	42	34	1	4	3	0
18	5	1	42	34	1	4	3	0
18	5	1	46	36	1	4	5	0
18	5	1	46	36	1	4	5	0
18	6	1	42	34	1	4	3	0
18	6	1	42	34	1	4	3	0
18	6	1	46	36	1	4	5	0
18	6	1	42	34	1	4	3	0
18	6	1	42	34	1	4	3	0
18	6	1	45	35	1	4	5	0
18	6	1	42	34	1	4	3	0

Continued on next page...

Continued from previous page...

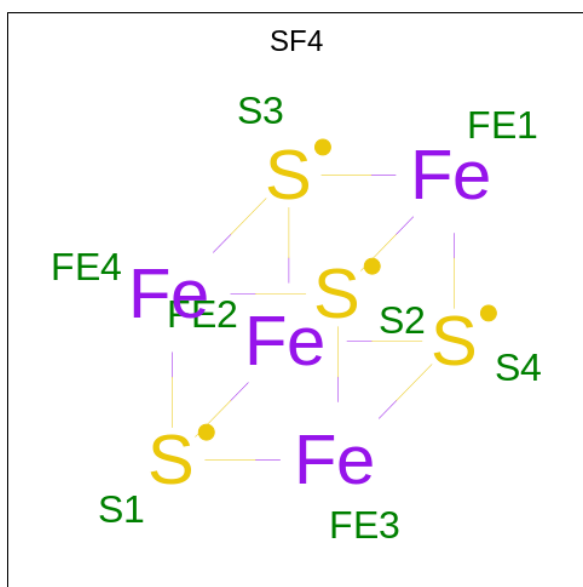
Mol	Chain	Residues	Atoms					AltConf
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 19 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



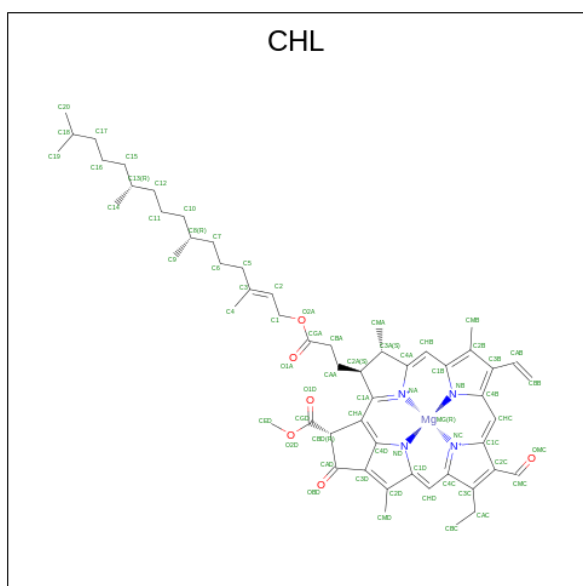
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			33	31	2	
19	B	1	Total	C	O	0
			33	31	2	

- Molecule 20 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



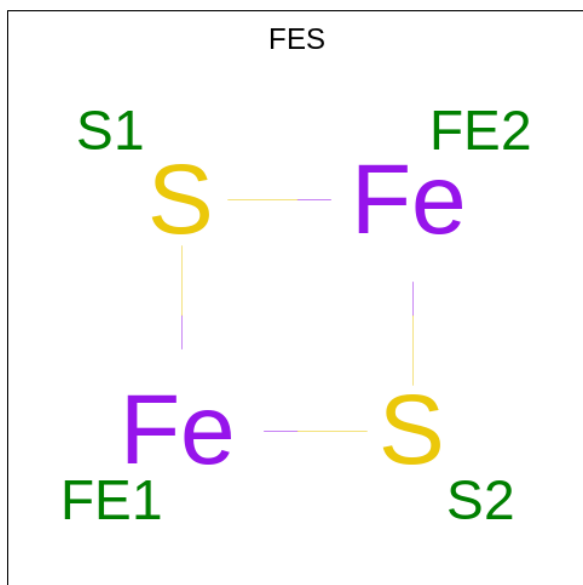
Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total	Fe	S	0
			8	4	4	
20	C	1	Total	Fe	S	0
			8	4	4	
20	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 21 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	7	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	Z	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	Z	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
21	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).

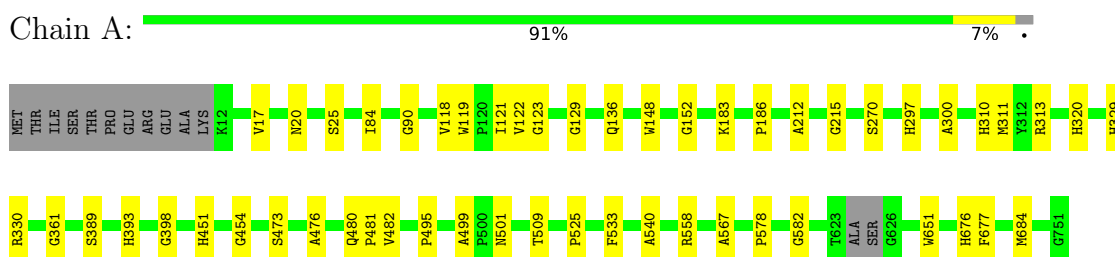


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
22	G	1	4	2	2	0

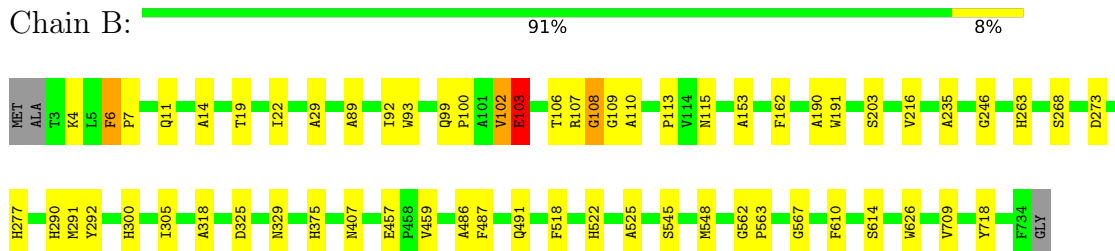
3 Residue-property plots

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

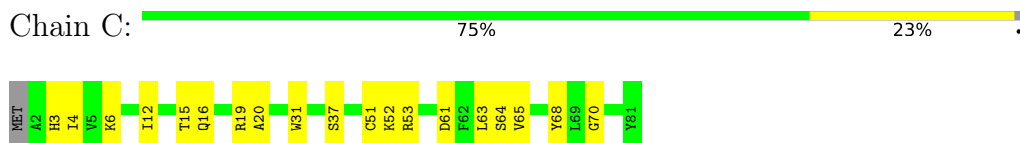
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



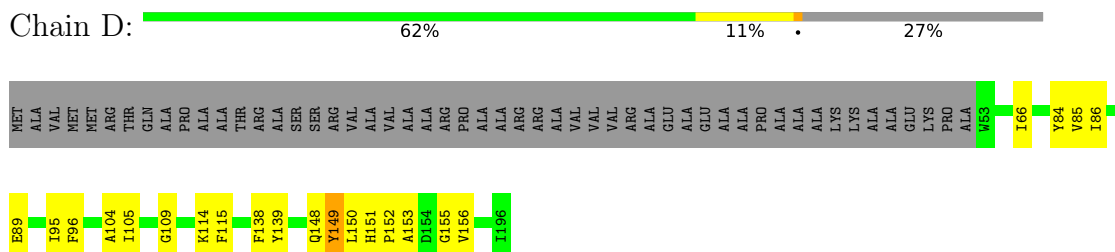
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



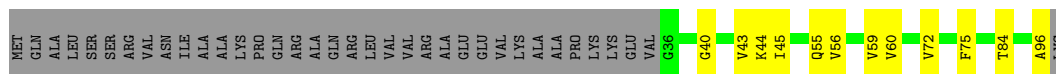
- Molecule 3: Photosystem I iron-sulfur center



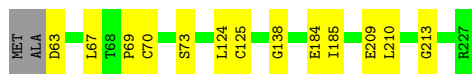
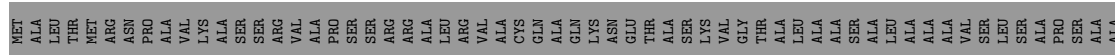
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



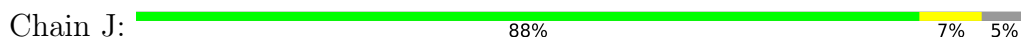
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



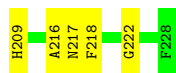
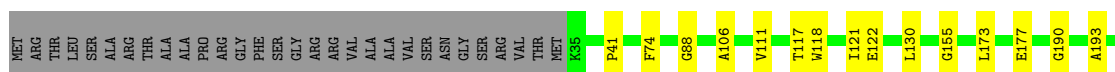
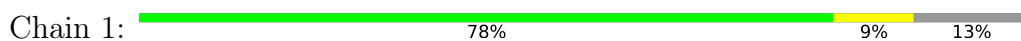
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic



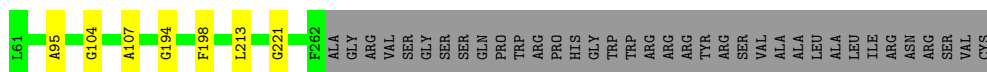
• Molecule 7: Photosystem I reaction center subunit IX



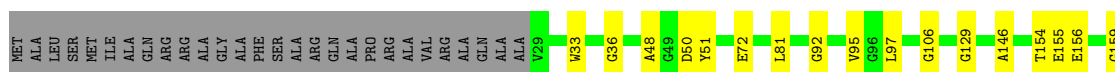
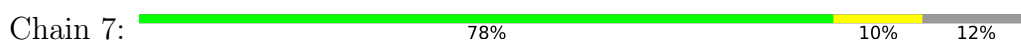
• Molecule 8: Chlorophyll a-b binding protein, chloroplastic



• Molecule 9: Chlorophyll a-b binding protein, chloroplastic



• Molecule 10: Chlorophyll a-b binding protein, chloroplastic





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

Chain 8:
84% 6% 11%

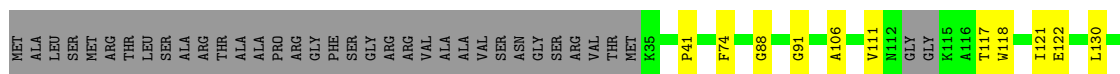
The quality bar for Chain 8 shows 84% green (good), 6% yellow (medium), and 11% grey (poor) segments.



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

Chain Z:
75% 9% 16%

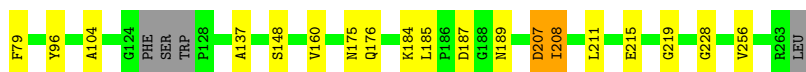
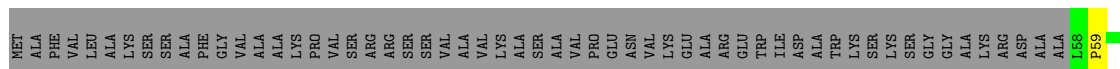
The quality bar for Chain Z shows 75% green (good), 9% yellow (medium), and 16% grey (poor) segments.



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

Chain 4:
69% 7% 23%

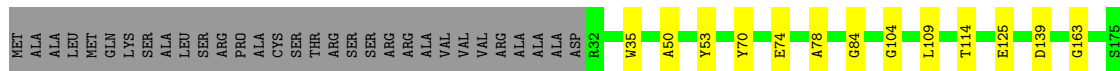
The quality bar for Chain 4 shows 69% green (good), 7% yellow (medium), and 23% grey (poor) segments.



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

Chain 5:
77% 10% 13%

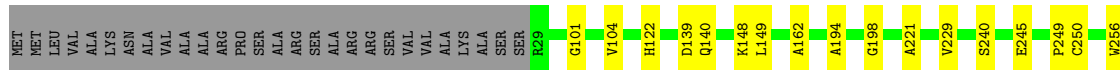
The quality bar for Chain 5 shows 77% green (good), 10% yellow (medium), and 13% grey (poor) segments.



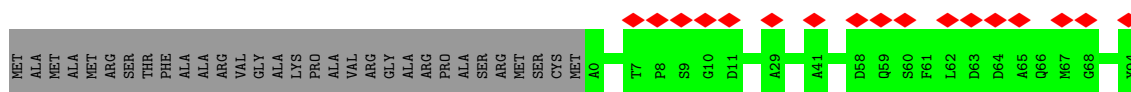
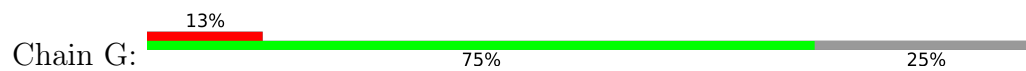
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 6:
82% 7% 11%

The quality bar for Chain 6 shows 82% green (good), 7% yellow (medium), and 11% grey (poor) segments.



● Molecule 16: Ferredoxin, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48941	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	91	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	3.579	Depositor
Minimum map value	-0.699	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	431.2, 431.2, 431.2	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, PQN, CHL, SF4, CLA, CLO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/3628	0.48	0/5034
2	B	0.34	0/3602	0.59	3/5001 (0.1%)
3	C	0.35	0/394	0.55	0/547
4	D	0.37	0/705	0.52	0/977
5	E	0.30	0/299	0.48	0/414
6	F	0.31	0/809	0.44	0/1122
7	J	0.31	0/193	0.46	0/268
8	1	0.32	0/941	0.47	0/1299
9	3	0.33	0/984	0.46	0/1361
10	7	0.34	0/1032	0.48	1/1427 (0.1%)
11	8	0.33	0/1058	0.46	0/1464
12	Z	0.33	0/932	0.47	0/1286
13	4	0.32	0/990	0.52	0/1369
14	5	0.32	0/1089	0.47	0/1507
15	6	0.34	0/1121	0.47	0/1554
16	G	0.40	0/492	0.65	0/683
All	All	0.34	0/18269	0.51	4/25313 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
13	4	0	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	103	GLU	N-CA-CB	14.49	136.68	110.60
2	B	102	VAL	N-CA-C	-10.71	82.08	111.00
2	B	102	VAL	CB-CA-C	-8.29	95.65	111.40
10	7	36	GLY	C-N-CA	-5.14	108.84	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	4	207	ASP	Peptide
13	4	208	ILE	Peptide
4	D	149	TYR	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	0	1728	56	0
2	B	3601	0	1713	75	0
3	C	395	0	178	14	0
4	D	706	0	316	11	0
5	E	300	0	135	6	0
6	F	810	0	404	10	0
7	J	194	0	87	4	0
8	1	942	0	489	19	0
9	3	985	0	480	7	0
10	7	1033	0	498	18	0
11	8	1059	0	527	15	0
12	Z	934	0	482	20	0
13	4	992	0	471	17	0
14	5	1091	0	504	19	0
15	6	1122	0	524	16	0
16	G	493	0	239	0	0
17	A	42	0	31	9	0
18	1	512	0	376	24	0
18	3	559	0	409	20	0
18	4	423	0	310	10	0
18	5	613	0	458	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	6	566	0	415	24	0
18	7	565	0	419	24	0
18	8	599	0	440	22	0
18	A	1831	0	1361	79	0
18	B	1782	0	1314	79	0
18	F	110	0	105	12	0
18	J	42	0	31	2	0
18	Z	466	0	345	25	0
19	A	33	0	46	6	0
19	B	33	0	46	5	0
20	B	8	0	0	1	0
20	C	16	0	0	3	0
21	1	96	0	70	5	0
21	3	43	0	29	0	0
21	4	89	0	59	5	0
21	5	129	0	87	4	0
21	6	172	0	116	3	0
21	7	43	0	29	1	0
21	8	43	0	29	3	0
21	Z	86	0	58	3	0
22	G	4	0	0	0	0
All	All	27190	0	15358	490	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 12.

All (490) 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)
2:B:102:VAL:CA	2:B:106:THR:CB	1.79	1.59
2:B:103:GLU:N	2:B:106:THR:CB	1.71	1.51
2:B:102:VAL:C	2:B:106:THR:CB	1.97	1.32
2:B:103:GLU:CA	2:B:107:ARG:H	1.46	1.25
2:B:103:GLU:C	2:B:107:ARG:H	1.44	1.12
2:B:103:GLU:CA	2:B:107:ARG:N	2.13	1.10
2:B:102:VAL:HA	2:B:106:THR:CB	1.65	1.06
1:A:651:TRP:CE2	2:B:626:TRP:CZ2	2.44	1.06
1:A:651:TRP:CH2	2:B:626:TRP:CE2	2.45	0.98
14:5:226:ASN:CB	18:5:613:CLA:HED2	1.94	0.98
1:A:651:TRP:CZ2	2:B:626:TRP:CE2	2.53	0.96
2:B:103:GLU:C	2:B:107:ARG:N	2.15	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:GLU:N	2:B:107:ARG:H	1.65	0.94
12:Z:111:VAL:CB	21:Z:605:CHL:OBD	2.15	0.93
8:1:111:VAL:CB	21:1:606:CHL:OBD	2.15	0.93
1:A:212:ALA:HA	18:A:815:CLA:HBB2	1.53	0.91
2:B:102:VAL:CB	2:B:106:THR:CB	2.48	0.91
10:7:72:GLU:HA	18:7:602:CLA:HBB1	1.56	0.88
4:D:139:TYR:HA	4:D:150:LEU:N	1.65	0.88
1:A:509:THR:HA	1:A:525:PRO:HA	1.55	0.87
11:8:131:GLY:HA2	18:8:608:CLA:HAB	1.55	0.86
2:B:103:GLU:N	2:B:107:ARG:N	2.24	0.85
12:Z:177:GLU:HA	18:Z:608:CLA:HBB1	1.60	0.84
2:B:518:PHE:HA	18:B:839:CLA:HED1	1.57	0.84
8:1:177:GLU:HA	18:1:609:CLA:HBB1	1.60	0.83
15:6:249:PRO:CB	18:6:301:CLA:HBB	2.09	0.82
18:A:835:CLA:HBB1	18:A:837:CLA:HED2	1.61	0.82
17:A:801:CL0:H15	18:A:844:CLA:HED1	1.62	0.81
15:6:249:PRO:CB	18:6:301:CLA:HMA1	2.11	0.81
12:Z:88:GLY:HA2	18:Z:603:CLA:HAB	1.65	0.79
2:B:93:TRP:H	18:B:811:CLA:HED2	1.47	0.79
8:1:88:GLY:HA2	18:1:604:CLA:HAB	1.65	0.78
15:6:101:GLY:HA2	21:6:305:CHL:HAC2	1.65	0.78
18:B:809:CLA:HBB	18:B:810:CLA:HMB3	1.64	0.78
14:5:74:GLU:HA	18:5:602:CLA:HBB1	1.65	0.78
18:F:302:CLA:C1B	18:F:302:CLA:H2	2.14	0.78
18:A:802:CLA:HAA1	18:A:844:CLA:HBB2	1.65	0.77
18:A:808:CLA:HMC3	18:A:809:CLA:HMD2	1.66	0.77
2:B:103:GLU:N	2:B:106:THR:CA	2.48	0.77
1:A:495:PRO:HA	1:A:499:ALA:HB3	1.67	0.76
14:5:241:ASP:HA	14:5:246:THR:HA	1.69	0.74
9:3:95:ALA:HB1	9:3:221:GLY:HA3	1.69	0.74
18:3:302:CLA:HHC	18:3:302:CLA:HBB1	1.70	0.74
10:7:129:GLY:HA2	18:7:608:CLA:HAB	1.69	0.74
1:A:533:PHE:HA	18:A:838:CLA:HED1	1.70	0.73
4:D:148:GLN:O	4:D:150:LEU:CB	2.38	0.72
18:6:312:CLA:HHC	18:6:312:CLA:HBB1	1.71	0.72
15:6:162:ALA:HB2	18:6:309:CLA:HBD	1.70	0.71
1:A:651:TRP:CZ2	2:B:626:TRP:CZ2	2.75	0.71
18:A:803:CLA:HHC	18:A:803:CLA:HBB1	1.72	0.71
1:A:684:MET:HA	18:A:802:CLA:HBC2	1.73	0.70
2:B:89:ALA:N	2:B:115:ASN:O	2.21	0.70
11:8:188:TRP:O	18:8:609:CLA:HMB3	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:6:249:PRO:CB	18:6:301:CLA:CHB	2.69	0.69
4:D:148:GLN:O	4:D:150:LEU:N	2.26	0.69
5:E:40:GLY:N	5:E:59:VAL:O	2.23	0.69
2:B:6:PHE:CB	2:B:14:ALA:HA	2.23	0.69
18:B:821:CLA:HAA2	18:B:826:CLA:HAB	1.73	0.69
2:B:709:VAL:HA	18:B:842:CLA:HED2	1.74	0.69
18:5:611:CLA:HHC	18:5:611:CLA:HBB1	1.74	0.69
8:1:217:ASN:HA	18:1:612:CLA:HAA1	1.74	0.68
4:D:139:TYR:HA	4:D:150:LEU:H	1.57	0.68
18:1:611:CLA:HHC	18:1:611:CLA:HBB1	1.76	0.68
3:C:4:ILE:O	3:C:68:TYR:N	2.27	0.68
2:B:203:SER:HA	2:B:246:GLY:HA2	1.76	0.68
18:A:843:CLA:HHC	18:A:843:CLA:HBB1	1.75	0.68
12:Z:217:ASN:HA	18:Z:611:CLA:HAA1	1.74	0.68
18:Z:610:CLA:HHC	18:Z:610:CLA:HBB1	1.76	0.68
18:A:823:CLA:HHB	18:A:843:CLA:HAC2	1.76	0.67
2:B:103:GLU:HA	2:B:107:ARG:N	2.08	0.67
14:5:242:VAL:N	14:5:245:LEU:O	2.28	0.67
1:A:473:SER:H	1:A:476:ALA:HB3	1.59	0.66
12:Z:130:LEU:HA	18:Z:604:CLA:HED2	1.77	0.66
2:B:92:ILE:N	2:B:113:PRO:O	2.27	0.66
18:A:826:CLA:HAA1	18:A:839:CLA:HED1	1.76	0.66
2:B:563:PRO:HA	2:B:567:GLY:HA2	1.77	0.66
18:8:609:CLA:HMB1	18:8:609:CLA:HBB1	1.78	0.66
1:A:578:PRO:HA	1:A:582:GLY:HA2	1.78	0.66
1:A:300:ALA:HA	18:A:817:CLA:HMC3	1.76	0.65
12:Z:216:ALA:HB1	18:Z:611:CLA:HED1	1.78	0.65
8:1:130:LEU:HA	18:1:605:CLA:HED2	1.77	0.65
18:A:843:CLA:H2	18:A:843:CLA:C4D	2.26	0.65
1:A:389:SER:HA	18:A:828:CLA:HMB3	1.78	0.65
10:7:81:LEU:CB	18:7:604:CLA:HBB2	2.27	0.65
18:F:301:CLA:HHC	18:F:301:CLA:HBB1	1.79	0.65
4:D:84:TYR:N	4:D:115:PHE:O	2.29	0.65
10:7:159:GLY:HA2	10:7:165:PRO:HA	1.78	0.65
18:8:615:CLA:HBC2	18:Z:607:CLA:HMD2	1.78	0.65
14:5:125:GLU:HA	18:5:605:CLA:HMA3	1.78	0.65
13:4:215:GLU:HA	18:4:607:CLA:HBB1	1.79	0.64
11:8:88:LEU:O	11:8:92:LEU:N	2.28	0.64
18:5:612:CLA:HHC	18:5:612:CLA:HBB1	1.79	0.64
1:A:329:HIS:HA	18:A:843:CLA:HBC2	1.79	0.64
18:B:829:CLA:O1D	18:B:830:CLA:HBB	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:216:ALA:HB1	18:1:612:CLA:HED1	1.78	0.64
18:1:603:CLA:HBC2	18:1:608:CLA:HMD2	1.78	0.64
18:A:816:CLA:HHC	18:A:816:CLA:HBB1	1.80	0.63
18:8:611:CLA:HHC	18:8:611:CLA:HBB1	1.80	0.63
21:1:601:CHL:H43	18:8:608:CLA:HMB1	1.81	0.63
11:8:69:TYR:O	18:8:602:CLA:HMB3	1.99	0.63
18:6:314:CLA:HBB2	18:6:317:CLA:HMD3	1.81	0.63
2:B:562:GLY:HA2	20:B:803:SF4:S1	2.39	0.63
10:7:81:LEU:CB	18:7:604:CLA:CBB	2.77	0.63
18:B:805:CLA:HMB1	18:B:805:CLA:HBB1	1.79	0.63
18:B:814:CLA:HHC	18:B:814:CLA:HBB1	1.81	0.62
18:A:806:CLA:H3A	18:A:830:CLA:HAB	1.81	0.62
18:B:842:CLA:HBD	19:B:844:PQN:H28	1.80	0.62
14:5:226:ASN:CB	18:5:613:CLA:CED	2.73	0.62
6:F:70:CYS:CB	6:F:125:CYS:CB	2.78	0.62
18:A:807:CLA:HMB3	18:A:808:CLA:H3A	1.82	0.62
10:7:146:ALA:HB1	10:7:155:GLU:H	1.64	0.62
18:B:806:CLA:HHC	18:B:808:CLA:OBD	2.00	0.61
18:A:812:CLA:HAC2	18:A:813:CLA:HAB	1.81	0.61
3:C:4:ILE:N	3:C:68:TYR:O	2.31	0.61
2:B:263:HIS:N	2:B:268:SER:O	2.23	0.61
18:1:612:CLA:HHB	18:1:613:CLA:HBC3	1.82	0.61
15:6:240:SER:HA	15:6:245:GLU:HA	1.82	0.61
1:A:20:ASN:N	1:A:183:LYS:O	2.31	0.61
18:Z:611:CLA:HHB	18:Z:612:CLA:HBC3	1.82	0.61
1:A:451:HIS:HA	18:A:834:CLA:HBB2	1.82	0.61
18:B:842:CLA:ND	19:B:844:PQN:H23	2.15	0.61
1:A:651:TRP:CG	2:B:626:TRP:HH2	2.12	0.60
21:5:607:CHL:OMC	21:5:616:CHL:HMC	2.01	0.60
18:6:312:CLA:HMA1	18:6:313:CLA:HAC2	1.83	0.60
15:6:122:HIS:HA	18:6:308:CLA:HAB	1.84	0.60
19:A:842:PQN:H23	18:A:845:CLA:C1B	2.32	0.59
18:B:814:CLA:HHD	18:B:815:CLA:HAB	1.84	0.59
3:C:53:ARG:N	20:C:101:SF4:S4	2.75	0.59
18:5:610:CLA:HBD	18:5:611:CLA:OBD	2.02	0.59
18:A:845:CLA:ND	18:B:802:CLA:HMC3	2.16	0.59
13:4:176:GLN:HA	13:4:184:LYS:HA	1.83	0.59
7:J:25:LEU:HA	18:J:101:CLA:HAB	1.85	0.59
1:A:121:ILE:O	1:A:123:GLY:N	2.35	0.59
2:B:487:PHE:O	2:B:491:GLN:CB	2.51	0.59
10:7:92:GLY:HA3	18:6:301:CLA:HED3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:804:CLA:HHC	18:B:804:CLA:HBB1	1.85	0.59
10:7:48:ALA:HB1	10:7:188:GLN:HA	1.85	0.59
14:5:50:ALA:HB1	14:5:184:THR:HA	1.85	0.59
4:D:95:ILE:HA	4:D:105:ILE:HA	1.84	0.58
18:A:835:CLA:HMD2	18:A:836:CLA:CBB	2.33	0.58
18:7:604:CLA:HBA1	18:7:605:CLA:C4C	2.33	0.58
4:D:85:VAL:HA	4:D:114:LYS:HA	1.86	0.58
5:E:60:VAL:N	5:E:72:VAL:O	2.35	0.57
1:A:558:ARG:O	1:A:567:ALA:N	2.37	0.57
19:A:842:PQN:H211	18:A:845:CLA:C3B	2.34	0.57
4:D:96:PHE:N	4:D:104:ALA:O	2.27	0.57
21:1:601:CHL:H2	11:8:131:GLY:HA3	1.87	0.57
18:Z:612:CLA:HHC	18:Z:612:CLA:HBB1	1.86	0.57
15:6:140:GLN:HA	15:6:148:LYS:HA	1.87	0.57
18:3:307:CLA:HBB1	18:3:313:CLA:CHC	2.34	0.57
2:B:4:LYS:C	2:B:6:PHE:H	2.08	0.56
18:1:613:CLA:HHC	18:1:613:CLA:HBB1	1.86	0.56
1:A:17:VAL:HA	1:A:186:PRO:HA	1.85	0.56
18:A:844:CLA:HBB1	18:A:844:CLA:HMB1	1.87	0.56
3:C:63:LEU:C	3:C:65:VAL:H	2.07	0.56
9:3:194:GLY:O	9:3:198:PHE:CB	2.54	0.56
18:A:825:CLA:HAA2	18:A:825:CLA:HBD	1.87	0.56
18:B:807:CLA:HMA3	18:B:831:CLA:HBB2	1.87	0.56
6:F:69:PRO:HA	6:F:124:LEU:HA	1.87	0.56
13:4:137:ALA:HB1	21:4:604:CHL:HAC2	1.87	0.56
18:5:614:CLA:HHC	18:5:614:CLA:HBB1	1.86	0.56
11:8:43:PRO:O	11:8:47:ALA:HB3	2.06	0.56
18:B:832:CLA:HMB2	18:B:833:CLA:C3D	2.35	0.56
18:A:845:CLA:HMD1	18:B:802:CLA:HBB1	1.87	0.56
18:Z:604:CLA:HMC3	21:Z:605:CHL:C1C	2.36	0.56
5:E:75:PHE:N	5:E:84:THR:O	2.38	0.56
18:7:612:CLA:HHC	18:7:612:CLA:HBB1	1.88	0.56
18:3:314:CLA:HHC	18:3:314:CLA:HBB1	1.88	0.56
12:Z:74:PHE:O	18:Z:602:CLA:HMB3	2.06	0.56
18:B:823:CLA:HMB3	18:B:824:CLA:C4D	2.35	0.56
8:1:74:PHE:O	18:1:602:CLA:HMB3	2.06	0.55
11:8:43:PRO:O	11:8:47:ALA:CB	2.54	0.55
3:C:31:TRP:N	3:C:37:SER:O	2.39	0.55
8:1:118:TRP:N	8:1:121:ILE:O	2.32	0.55
18:A:814:CLA:HAC1	18:A:815:CLA:HMB3	1.89	0.55
18:5:605:CLA:HBB1	18:5:605:CLA:HHC	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:605:CLA:HMC3	21:1:606:CHL:C1C	2.36	0.55
1:A:311:MET:HA	18:A:822:CLA:HAC2	1.88	0.55
9:3:107:ALA:HB2	18:3:303:CLA:HAC2	1.88	0.55
1:A:651:TRP:HH2	2:B:626:TRP:O	1.89	0.54
18:3:304:CLA:C2C	18:3:305:CLA:HED2	2.37	0.54
13:4:137:ALA:HB1	21:4:604:CHL:HMC	1.89	0.54
18:3:307:CLA:CBB	18:3:313:CLA:HBB1	2.37	0.54
2:B:545:SER:N	2:B:548:MET:O	2.39	0.54
12:Z:117:THR:HA	12:Z:122:GLU:HA	1.89	0.54
18:A:838:CLA:HHC	18:A:838:CLA:HBB1	1.90	0.54
8:1:117:THR:HA	8:1:122:GLU:HA	1.89	0.54
17:A:801:CL0:H14	18:B:804:CLA:NA	2.23	0.54
5:E:44:LYS:HA	5:E:56:VAL:HA	1.90	0.54
15:6:249:PRO:CB	18:6:301:CLA:CMA	2.86	0.54
13:4:228:GLY:HA2	18:4:610:CLA:HMC3	1.89	0.54
2:B:191:TRP:N	18:B:816:CLA:HAB	2.24	0.53
1:A:651:TRP:CA	2:B:626:TRP:HH2	2.21	0.53
17:A:801:CL0:H14	18:B:804:CLA:C1A	2.38	0.53
18:Z:612:CLA:HED1	13:4:148:SER:HA	1.91	0.53
1:A:297:HIS:HA	18:A:818:CLA:C4B	2.39	0.53
18:3:311:CLA:C4A	18:3:312:CLA:HMD3	2.38	0.53
18:7:604:CLA:HHD	18:6:301:CLA:HMD3	1.90	0.53
18:8:612:CLA:C4A	18:8:613:CLA:HMD3	2.38	0.53
18:A:841:CLA:HMC3	18:B:841:CLA:C1D	2.38	0.53
18:A:845:CLA:C1D	18:B:802:CLA:HMC3	2.39	0.53
4:D:89:GLU:HA	4:D:109:GLY:O	2.09	0.53
19:A:842:PQN:H252	18:A:845:CLA:C4A	2.39	0.52
18:B:801:CLA:HBB1	18:B:801:CLA:HMB1	1.90	0.52
18:F:302:CLA:H2	18:F:302:CLA:NB	2.24	0.52
18:3:313:CLA:HED2	18:7:601:CLA:CHB	2.39	0.52
12:Z:173:LEU:O	18:Z:608:CLA:HMB3	2.10	0.52
3:C:63:LEU:C	3:C:65:VAL:N	2.61	0.52
11:8:239:SER:HA	18:8:614:CLA:O1D	2.09	0.52
12:Z:118:TRP:N	12:Z:121:ILE:O	2.32	0.52
18:B:842:CLA:CHA	19:B:844:PQN:H261	2.39	0.52
8:1:173:LEU:O	18:1:609:CLA:HMB3	2.10	0.52
8:1:209:HIS:HA	8:1:216:ALA:HB3	1.92	0.52
13:4:160:VAL:HA	21:4:605:CHL:NB	2.24	0.52
18:4:602:CLA:HBB1	18:4:603:CLA:HAA1	1.90	0.52
1:A:473:SER:N	1:A:476:ALA:HB3	2.25	0.52
1:A:651:TRP:HA	2:B:626:TRP:HH2	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:845:CLA:HED3	6:F:184:GLU:HA	1.92	0.52
2:B:273:ASP:O	18:B:819:CLA:HMB3	2.09	0.52
2:B:162:PHE:HA	18:B:813:CLA:HED2	1.92	0.52
13:4:187:ASP:O	13:4:189:ASN:N	2.40	0.52
18:B:834:CLA:HAB	18:B:835:CLA:HBB1	1.93	0.51
14:5:70:TYR:O	18:5:602:CLA:HMB3	2.10	0.51
14:5:139:ASP:CB	21:5:607:CHL:HAC2	2.40	0.51
18:A:802:CLA:HHC	18:A:802:CLA:HBB1	1.92	0.51
18:6:315:CLA:HHC	18:6:315:CLA:HBB1	1.91	0.51
3:C:12:ILE:N	20:C:102:SF4:S2	2.81	0.51
12:Z:209:HIS:HA	12:Z:216:ALA:HB3	1.92	0.51
18:A:827:CLA:NA	18:A:835:CLA:HMB2	2.26	0.51
1:A:300:ALA:HB1	18:A:817:CLA:HBC2	1.92	0.51
2:B:277:HIS:HA	18:B:819:CLA:C3B	2.41	0.51
13:4:175:ASN:O	13:4:185:LEU:N	2.28	0.50
18:B:826:CLA:HAA2	18:B:826:CLA:HBD	1.93	0.50
18:B:834:CLA:C3B	18:B:835:CLA:HBB1	2.41	0.50
18:1:605:CLA:HAA2	18:1:605:CLA:HBD	1.93	0.50
18:Z:604:CLA:HAA2	18:Z:604:CLA:HBD	1.93	0.50
18:A:824:CLA:HHB	18:A:843:CLA:CBB	2.42	0.50
8:1:218:PHE:O	8:1:222:GLY:N	2.43	0.50
12:Z:218:PHE:O	12:Z:222:GLY:N	2.43	0.50
19:A:842:PQN:H252	18:A:845:CLA:NA	2.27	0.50
15:6:139:ASP:O	15:6:149:LEU:N	2.34	0.50
2:B:235:ALA:HB2	18:B:818:CLA:HMA2	1.93	0.50
3:C:52:LYS:N	20:C:101:SF4:S2	2.78	0.50
18:F:302:CLA:H93	18:F:302:CLA:HBC3	1.93	0.50
18:4:603:CLA:HMD2	18:4:606:CLA:C1D	2.41	0.50
2:B:103:GLU:CA	2:B:107:ARG:CA	2.84	0.50
2:B:318:ALA:HB3	2:B:407:ASN:HA	1.92	0.50
13:4:256:VAL:HA	18:4:610:CLA:CAD	2.42	0.50
11:8:131:GLY:CA	18:8:608:CLA:HAB	2.36	0.50
18:B:824:CLA:HMB3	18:B:843:CLA:CHD	2.42	0.50
18:F:302:CLA:H52	18:F:302:CLA:C4B	2.42	0.50
12:Z:155:GLY:N	18:Z:608:CLA:OBD	2.41	0.49
1:A:84:ILE:HA	18:A:806:CLA:HAC2	1.94	0.49
17:A:801:CL0:H13	18:A:844:CLA:OBD	2.12	0.49
18:7:604:CLA:HMD2	18:6:301:CLA:HMD3	1.95	0.49
11:8:210:LYS:O	11:8:214:GLY:HA2	2.12	0.49
18:B:825:CLA:HMA1	18:B:843:CLA:CGD	2.43	0.49
18:3:311:CLA:CHB	18:3:312:CLA:HMD3	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:96:TYR:O	18:4:602:CLA:HMB3	2.12	0.49
8:1:155:GLY:N	18:1:609:CLA:OBD	2.41	0.49
18:B:814:CLA:HAC2	18:B:815:CLA:HAB	1.95	0.49
18:8:605:CLA:HMC3	21:8:606:CHL:NC	2.28	0.49
4:D:66:ILE:N	4:D:105:ILE:O	2.38	0.49
18:3:313:CLA:O2A	18:3:313:CLA:HBD	2.13	0.49
18:B:821:CLA:HMD3	18:B:823:CLA:HMC3	1.94	0.49
3:C:63:LEU:O	3:C:65:VAL:N	2.46	0.49
1:A:651:TRP:O	2:B:626:TRP:CH2	2.65	0.49
2:B:103:GLU:N	2:B:106:THR:C	2.67	0.49
18:B:832:CLA:HMB2	18:B:833:CLA:C2D	2.42	0.49
1:A:651:TRP:CH2	2:B:626:TRP:CG	2.74	0.48
18:A:841:CLA:HMC3	18:B:841:CLA:ND	2.28	0.48
18:3:304:CLA:HBB1	18:3:305:CLA:OBD	2.13	0.48
19:A:842:PQN:H211	18:A:845:CLA:C2B	2.43	0.48
2:B:103:GLU:O	2:B:108:GLY:N	2.42	0.48
10:7:50:ASP:HA	18:7:602:CLA:CGD	2.43	0.48
14:5:78:ALA:HB1	14:5:190:GLY:HA3	1.95	0.48
1:A:313:ARG:H	1:A:320:HIS:H	1.62	0.48
18:B:834:CLA:CAB	18:B:835:CLA:HBB1	2.44	0.48
3:C:3:HIS:HA	3:C:70:GLY:N	2.28	0.48
2:B:290:HIS:HA	18:B:822:CLA:HED1	1.96	0.48
14:5:253:TRP:CB	18:5:614:CLA:HMA3	2.43	0.48
21:6:305:CHL:HBC2	21:6:306:CHL:CHD	2.44	0.48
18:A:803:CLA:HED2	7:J:12:PRO:HA	1.96	0.47
14:5:35:TRP:N	14:5:53:TYR:O	2.45	0.47
18:A:833:CLA:HHC	18:A:833:CLA:HBB1	1.96	0.47
1:A:454:GLY:HA2	18:A:834:CLA:HMC3	1.94	0.47
18:A:804:CLA:HMB3	18:A:805:CLA:HBB1	1.95	0.47
3:C:51:CYS:O	3:C:53:ARG:N	2.48	0.47
6:F:63:ASP:N	6:F:67:LEU:O	2.47	0.47
2:B:4:LYS:C	2:B:6:PHE:N	2.68	0.47
6:F:185:ILE:O	7:J:11:ALA:HB2	2.15	0.47
18:7:612:CLA:HBA2	18:7:613:CLA:C2D	2.45	0.47
12:Z:41:PRO:O	21:Z:601:CHL:HED1	2.15	0.47
18:B:814:CLA:CHD	18:B:815:CLA:HAB	2.44	0.47
18:A:822:CLA:HMB3	18:A:823:CLA:C3D	2.45	0.47
2:B:216:VAL:O	18:B:817:CLA:HED3	2.15	0.47
18:B:802:CLA:C1A	18:B:802:CLA:CGA	2.92	0.47
18:B:825:CLA:HBB1	18:B:832:CLA:HBC2	1.96	0.47
18:B:842:CLA:CHD	19:B:844:PQN:H211	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ILE:HA	18:B:824:CLA:HED2	1.96	0.47
18:7:604:CLA:HMD2	18:6:301:CLA:CHD	2.45	0.47
5:E:43:VAL:HA	5:E:96:ALA:H	1.80	0.46
18:8:612:CLA:CHB	18:8:613:CLA:HMD3	2.45	0.46
1:A:215:GLY:HA3	18:A:815:CLA:CAB	2.46	0.46
10:7:33:TRP:HA	18:7:601:CLA:C1C	2.45	0.46
1:A:148:TRP:O	1:A:152:GLY:N	2.48	0.46
8:1:41:PRO:O	21:1:601:CHL:HED1	2.15	0.46
18:Z:603:CLA:HBB1	18:Z:603:CLA:HMB1	1.96	0.46
18:5:610:CLA:H2	18:5:611:CLA:CMD	2.46	0.46
15:6:256:TRP:HA	18:6:317:CLA:O1D	2.16	0.46
18:6:312:CLA:CHB	18:6:313:CLA:HMD3	2.45	0.46
18:A:807:CLA:H3A	18:A:808:CLA:HMB3	1.96	0.46
18:A:812:CLA:C2D	18:A:813:CLA:HMC3	2.45	0.46
15:6:249:PRO:CB	18:6:301:CLA:C3A	2.93	0.46
18:B:810:CLA:HMC3	18:B:811:CLA:C3D	2.45	0.46
18:8:603:CLA:HMD2	18:8:608:CLA:C4C	2.46	0.46
18:1:604:CLA:HBB1	18:1:604:CLA:HMB1	1.96	0.46
1:A:361:GLY:HA2	1:A:398:GLY:HA2	1.98	0.46
18:5:612:CLA:CHB	18:5:613:CLA:HMD3	2.45	0.46
1:A:118:VAL:HA	18:A:809:CLA:HED2	1.98	0.46
10:7:186:TYR:O	18:7:609:CLA:HMB3	2.16	0.46
18:7:612:CLA:C4A	18:7:613:CLA:HMD3	2.46	0.46
18:4:610:CLA:CHB	18:4:611:CLA:HMD3	2.45	0.46
1:A:677:PHE:HA	18:A:844:CLA:HAA2	1.98	0.45
15:6:250:CYS:O	18:6:301:CLA:CBA	2.64	0.45
18:6:301:CLA:HAA1	18:6:301:CLA:HBD	1.98	0.45
1:A:651:TRP:CG	2:B:626:TRP:CH2	2.61	0.45
2:B:19:THR:O	2:B:22:ILE:N	2.49	0.45
10:7:225:ASP:O	10:7:229:VAL:N	2.49	0.45
2:B:292:TYR:HA	2:B:300:HIS:H	1.82	0.45
9:3:104:GLY:HA2	18:3:303:CLA:C3C	2.45	0.45
18:3:303:CLA:CHA	18:3:314:CLA:HMB3	2.47	0.45
12:Z:190:GLY:HA2	18:Z:611:CLA:C2C	2.47	0.45
14:5:199:ALA:HB2	18:5:612:CLA:HMC3	1.99	0.45
2:B:29:ALA:O	18:B:806:CLA:HED1	2.16	0.45
1:A:651:TRP:HH2	2:B:626:TRP:CG	2.32	0.45
6:F:69:PRO:O	6:F:73:SER:N	2.48	0.45
6:F:138:GLY:HA3	18:F:302:CLA:C3D	2.47	0.45
18:7:604:CLA:CMD	18:6:301:CLA:HMD3	2.47	0.45
14:5:163:GLY:HA2	21:5:607:CHL:HMD1	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:812:CLA:HED2	18:A:813:CLA:HBC1	1.98	0.45
2:B:610:PHE:O	2:B:614:SER:CB	2.65	0.45
1:A:676:HIS:HA	17:A:801:CL0:CMA	2.47	0.45
18:A:814:CLA:HHC	18:A:814:CLA:HBB1	1.99	0.45
8:1:190:GLY:HA2	18:1:612:CLA:C2C	2.47	0.45
18:7:605:CLA:HMC3	21:7:606:CHL:C4C	2.47	0.45
11:8:83:GLY:HA2	18:8:604:CLA:HAB	1.98	0.45
1:A:330:ARG:O	18:A:843:CLA:HBC3	2.17	0.45
17:A:801:CL0:H7	18:B:804:CLA:HAB	1.99	0.45
18:B:826:CLA:HAA2	18:B:826:CLA:CBD	2.47	0.45
18:B:811:CLA:HHB	18:B:812:CLA:HBB1	1.97	0.44
21:6:307:CHL:HAA1	21:6:307:CHL:HBD	1.98	0.44
18:F:302:CLA:H111	18:F:302:CLA:H72	1.69	0.44
18:A:827:CLA:C2B	18:A:835:CLA:H3A	2.47	0.44
11:8:30:TRP:HA	18:8:601:CLA:C1C	2.47	0.44
18:B:808:CLA:HHB	18:B:831:CLA:HAB	1.99	0.44
18:B:829:CLA:C3D	18:B:830:CLA:HMB3	2.47	0.44
18:F:302:CLA:H52	18:F:302:CLA:C3B	2.47	0.44
18:F:302:CLA:C1C	18:F:302:CLA:H71	2.47	0.44
18:F:302:CLA:CAD	18:F:302:CLA:H152	2.47	0.44
18:8:612:CLA:HBA2	18:8:613:CLA:C2D	2.47	0.44
18:A:817:CLA:C1A	18:A:817:CLA:CGA	2.95	0.44
18:B:836:CLA:CHA	18:B:837:CLA:HMB3	2.47	0.44
1:A:270:SER:HA	18:A:817:CLA:HAA2	1.98	0.44
19:A:842:PQN:H23	18:A:845:CLA:CHB	2.48	0.44
18:B:806:CLA:NA	18:B:806:CLA:HBA2	2.32	0.44
18:A:827:CLA:HBB1	18:A:827:CLA:HMB1	1.99	0.44
5:E:45:ILE:N	5:E:55:GLN:O	2.42	0.44
10:7:234:ASN:C	10:7:236:VAL:H	2.22	0.44
18:Z:611:CLA:CHB	18:Z:612:CLA:HMD3	2.48	0.44
14:5:182:LEU:O	18:5:609:CLA:HMB3	2.18	0.44
15:6:104:VAL:HA	18:6:304:CLA:HED1	1.99	0.44
2:B:190:ALA:HA	18:B:817:CLA:HBB2	2.00	0.44
1:A:129:GLY:O	1:A:136:GLN:HA	2.18	0.43
10:7:106:GLY:HA2	18:7:605:CLA:HAC2	2.00	0.43
18:7:614:CLA:HED3	18:7:614:CLA:HMA2	1.99	0.43
18:Z:604:CLA:HAA2	18:Z:604:CLA:CBD	2.47	0.43
18:5:608:CLA:HMB2	18:5:615:CLA:C2C	2.48	0.43
1:A:651:TRP:HA	2:B:626:TRP:CH2	2.52	0.43
1:A:651:TRP:O	2:B:626:TRP:HH2	2.01	0.43
2:B:89:ALA:HB3	2:B:115:ASN:CB	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:825:CLA:HBB	18:B:843:CLA:O1D	2.19	0.43
18:8:605:CLA:HBC2	21:8:606:CHL:CHD	2.48	0.43
18:A:823:CLA:HMB3	18:A:843:CLA:C3C	2.48	0.43
18:1:605:CLA:HAA2	18:1:605:CLA:CB	2.47	0.43
2:B:325:ASP:O	2:B:329:ASN:N	2.51	0.43
18:F:302:CLA:H2	18:F:302:CLA:C2B	2.49	0.43
10:7:154:THR:C	10:7:156:GLU:H	2.21	0.43
2:B:93:TRP:H	18:B:811:CLA:CED	2.25	0.43
2:B:291:MET:HA	18:B:823:CLA:HAC2	2.00	0.43
18:1:612:CLA:CHB	18:1:613:CLA:HMD3	2.48	0.43
18:8:603:CLA:HMD2	18:8:608:CLA:CHD	2.48	0.43
1:A:393:HIS:HA	18:A:828:CLA:CHC	2.49	0.43
2:B:92:ILE:CB	2:B:113:PRO:CB	2.96	0.43
6:F:210:LEU:O	6:F:213:GLY:N	2.49	0.43
14:5:84:GLY:HA2	18:5:604:CLA:HBB1	2.00	0.43
15:6:194:ALA:O	15:6:198:GLY:N	2.40	0.43
17:A:801:CL0:H11	18:B:804:CLA:HAA2	2.01	0.43
13:4:137:ALA:HB1	21:4:604:CHL:CMC	2.49	0.43
3:C:16:GLN:O	3:C:20:ALA:N	2.52	0.43
14:5:109:LEU:CB	14:5:114:THR:HA	2.49	0.43
18:5:610:CLA:H52	18:5:611:CLA:C2D	2.49	0.43
18:A:836:CLA:HHC	18:A:836:CLA:HBB1	1.99	0.43
2:B:153:ALA:HB2	18:B:813:CLA:HBC2	1.99	0.43
11:8:30:TRP:CB	18:8:601:CLA:HBB1	2.49	0.43
2:B:191:TRP:HA	18:B:816:CLA:HAB	2.01	0.42
18:3:302:CLA:HBC1	18:3:307:CLA:HAC1	2.01	0.42
18:4:610:CLA:C1B	18:4:611:CLA:HMD3	2.49	0.42
17:A:801:CL0:H14	18:B:804:CLA:HAA2	2.01	0.42
13:4:256:VAL:H	18:4:611:CLA:HED2	1.85	0.42
2:B:11:GLN:HA	2:B:14:ALA:HB3	2.01	0.42
2:B:457:GLU:O	2:B:459:VAL:N	2.48	0.42
10:7:95:VAL:O	10:7:97:LEU:N	2.52	0.42
2:B:522:HIS:HA	18:B:839:CLA:HMA1	2.01	0.42
1:A:310:HIS:HA	18:A:820:CLA:HED1	1.99	0.42
18:6:309:CLA:CBB	18:6:311:CLA:H3A	2.50	0.42
1:A:480:GLN:O	1:A:482:VAL:N	2.51	0.42
18:B:827:CLA:HMB2	18:B:840:CLA:CBA	2.49	0.42
18:F:302:CLA:H61	18:F:302:CLA:H41	1.89	0.42
9:3:107:ALA:CB	18:3:303:CLA:HAC2	2.49	0.42
18:8:612:CLA:CGA	18:8:612:CLA:C1A	2.98	0.42
18:8:615:CLA:HMD2	18:Z:607:CLA:ND	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:106:ALA:HA	18:Z:603:CLA:HED3	2.02	0.42
14:5:239:SER:HA	14:5:247:ILE:O	2.19	0.42
18:6:301:CLA:HAA1	18:6:301:CLA:CB	2.49	0.42
2:B:486:ALA:HB2	18:B:837:CLA:C3D	2.50	0.42
15:6:221:ALA:HB1	15:6:229:VAL:O	2.20	0.42
1:A:676:HIS:HA	17:A:801:CL0:H6	2.01	0.42
4:D:86:ILE:HA	4:D:138:PHE:CB	2.49	0.42
12:Z:173:LEU:CB	18:Z:608:CLA:HBB	2.50	0.42
2:B:99:GLN:O	2:B:100:PRO:C	2.56	0.42
13:4:104:ALA:HB1	13:4:219:GLY:HA3	2.02	0.42
14:5:104:GLY:O	21:5:606:CHL:HMD3	2.19	0.42
1:A:481:PRO:HA	18:A:838:CLA:HMD1	2.02	0.41
8:1:118:TRP:HA	18:1:604:CLA:OBD	2.20	0.41
18:5:610:CLA:H93	18:5:611:CLA:C1C	2.50	0.41
1:A:119:TRP:N	18:A:809:CLA:O1D	2.54	0.41
2:B:718:TYR:O	18:B:804:CLA:HED2	2.20	0.41
18:B:808:CLA:HMC3	18:B:830:CLA:CBB	2.50	0.41
18:1:603:CLA:HMD2	18:1:608:CLA:ND	2.35	0.41
18:A:835:CLA:CAD	18:A:836:CLA:HMB3	2.50	0.41
3:C:6:LYS:O	3:C:65:VAL:HA	2.19	0.41
18:3:314:CLA:HBD	18:3:314:CLA:HAA1	2.02	0.41
12:Z:118:TRP:HA	18:Z:603:CLA:OBD	2.20	0.41
18:A:806:CLA:H3A	18:A:830:CLA:CAB	2.48	0.41
2:B:191:TRP:CA	18:B:816:CLA:HAB	2.51	0.41
13:4:211:LEU:O	18:4:607:CLA:HMB3	2.20	0.41
9:3:194:GLY:N	18:3:308:CLA:OBD	2.33	0.41
18:7:605:CLA:HHC	18:7:605:CLA:HBB1	2.02	0.41
13:4:59:PRO:O	13:4:79:PHE:HA	2.21	0.41
1:A:311:MET:CA	18:A:822:CLA:HAC2	2.51	0.41
8:1:173:LEU:CB	18:1:609:CLA:HBB	2.50	0.41
18:1:614:CLA:HBA1	18:1:614:CLA:H3A	1.92	0.41
18:3:302:CLA:OBD	18:3:307:CLA:HAA2	2.21	0.41
13:4:137:ALA:C	21:4:604:CHL:HAC2	2.41	0.41
18:6:312:CLA:C4A	18:6:313:CLA:HMD3	2.50	0.41
9:3:213:LEU:O	18:3:308:CLA:HMB3	2.20	0.41
10:7:230:ASN:HA	18:7:612:CLA:HAA1	2.02	0.41
1:A:540:ALA:HB1	18:A:838:CLA:HMB3	2.03	0.41
18:A:845:CLA:CMD	18:B:802:CLA:HBB1	2.50	0.41
2:B:190:ALA:C	18:B:816:CLA:HAB	2.41	0.41
18:B:809:CLA:HMB3	18:B:810:CLA:HBB	2.03	0.41
18:B:824:CLA:HMB3	18:B:843:CLA:C1D	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:THR:O	3:C:19:ARG:N	2.36	0.41
10:7:51:TYR:N	18:7:602:CLA:OBD	2.38	0.41
18:7:608:CLA:H3A	18:7:608:CLA:HBA2	1.87	0.41
12:Z:88:GLY:HA2	18:Z:603:CLA:CAB	2.44	0.41
18:5:601:CLA:HAA2	18:5:601:CLA:HBD	2.02	0.41
18:B:814:CLA:HMD3	18:B:815:CLA:CHC	2.51	0.41
6:F:70:CYS:HA	6:F:73:SER:CB	2.51	0.41
18:3:307:CLA:HBB1	18:3:313:CLA:HHC	2.02	0.41
18:B:814:CLA:HBD	18:B:814:CLA:HAA1	2.02	0.40
11:8:106:ASP:HA	21:8:606:CHL:CED	2.51	0.40
18:B:842:CLA:C1D	19:B:844:PQN:H23	2.51	0.40
8:1:106:ALA:HA	18:1:604:CLA:HED3	2.02	0.40
18:7:603:CLA:HMD2	18:7:608:CLA:C1D	2.52	0.40
18:A:818:CLA:O1D	18:A:819:CLA:HHB	2.22	0.40
2:B:375:HIS:HA	18:B:829:CLA:C4B	2.52	0.40
2:B:525:ALA:HB2	18:B:840:CLA:HED2	2.03	0.40
11:8:126:GLN:CB	18:8:605:CLA:HMA3	2.51	0.40
12:Z:91:GLY:HA3	18:Z:603:CLA:C1C	2.51	0.40
1:A:501:ASN:CB	18:A:836:CLA:HED2	2.51	0.40
18:A:814:CLA:CHA	18:A:816:CLA:HMB3	2.52	0.40
7:J:25:LEU:CA	18:J:101:CLA:HAB	2.49	0.40
8:1:193:ALA:CB	18:1:612:CLA:HAC2	2.52	0.40
1:A:25:SER:N	18:A:811:CLA:HMB3	2.37	0.40
1:A:90:GLY:HA3	18:A:807:CLA:CBB	2.51	0.40
18:A:805:CLA:HBB1	18:A:805:CLA:HMB1	2.04	0.40
18:B:822:CLA:CGA	18:B:822:CLA:C4A	2.98	0.40
6:F:209:GLU:O	6:F:213:GLY:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	734/751 (98%)	670 (91%)	63 (9%)	1 (0%)	51	85
2	B	730/735 (99%)	656 (90%)	68 (9%)	6 (1%)	19	60
3	C	78/81 (96%)	64 (82%)	12 (15%)	2 (3%)	5	34
4	D	142/196 (72%)	120 (84%)	16 (11%)	6 (4%)	3	24
5	E	59/97 (61%)	55 (93%)	4 (7%)	0	100	100
6	F	163/227 (72%)	154 (94%)	9 (6%)	0	100	100
7	J	37/41 (90%)	32 (86%)	5 (14%)	0	100	100
8	1	192/224 (86%)	175 (91%)	17 (9%)	0	100	100
9	3	200/298 (67%)	182 (91%)	18 (9%)	0	100	100
10	7	210/241 (87%)	193 (92%)	17 (8%)	0	100	100
11	8	215/243 (88%)	192 (89%)	23 (11%)	0	100	100
12	Z	188/228 (82%)	172 (92%)	16 (8%)	0	100	100
13	4	199/264 (75%)	175 (88%)	22 (11%)	2 (1%)	15	54
14	5	219/257 (85%)	194 (89%)	25 (11%)	0	100	100
15	6	227/257 (88%)	205 (90%)	22 (10%)	0	100	100
16	G	98/126 (78%)	93 (95%)	5 (5%)	0	100	100
All	All	3691/4266 (86%)	3332 (90%)	342 (9%)	17 (0%)	32	68

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	6	PHE
2	B	7	PRO
2	B	103	GLU
3	C	64	SER
4	D	149	TYR
4	D	151	HIS
1	A	122	VAL
2	B	108	GLY
2	B	110	ALA
4	D	152	PRO
4	D	155	GLY
4	D	156	VAL
13	4	207	ASP
3	C	61	ASP
4	D	153	ALA
13	4	208	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	109	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1/610 (0%)	1 (100%)	0	100	100
2	B	1/597 (0%)	1 (100%)	0	100	100
All	All	2/1207 (0%)	2 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

211 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	3	304	-	42,50,73	2.66	10 (23%)	48,85,113	1.58	9 (18%)
18	CLA	Z	604	-	43,51,73	2.80	9 (20%)	49,86,113	1.55	8 (16%)
21	CHL	6	306	-	43,51,74	2.48	10 (23%)	45,86,114	1.95	8 (17%)
18	CLA	A	845	-	42,50,73	2.85	9 (21%)	48,85,113	1.46	9 (18%)
18	CLA	B	823	-	42,50,73	2.97	9 (21%)	48,85,113	1.58	7 (14%)
18	CLA	B	815	-	42,50,73	2.85	9 (21%)	48,85,113	1.94	12 (25%)
18	CLA	Z	602	-	42,50,73	2.85	8 (19%)	48,85,113	1.51	8 (16%)
21	CHL	8	606	-	43,51,74	2.51	9 (20%)	45,86,114	2.17	10 (22%)
18	CLA	A	809	-	42,50,73	2.76	11 (26%)	48,85,113	1.45	7 (14%)
18	CLA	A	836	1	42,50,73	2.88	10 (23%)	48,85,113	1.55	7 (14%)
18	CLA	A	807	-	42,50,73	2.79	10 (23%)	48,85,113	1.59	9 (18%)
18	CLA	A	841	-	42,50,73	2.72	11 (26%)	48,85,113	1.49	9 (18%)
18	CLA	F	301	-	45,53,73	2.66	8 (17%)	52,89,113	1.52	7 (13%)
18	CLA	1	612	-	46,54,73	2.59	9 (19%)	53,90,113	1.41	8 (15%)
18	CLA	B	827	-	42,50,73	2.69	9 (21%)	48,85,113	1.86	11 (22%)
18	CLA	A	810	-	42,50,73	2.82	10 (23%)	48,85,113	1.48	7 (14%)
18	CLA	8	608	-	42,50,73	2.81	9 (21%)	48,85,113	1.65	10 (20%)
18	CLA	Z	613	-	42,50,73	2.85	9 (21%)	48,85,113	1.55	7 (14%)
18	CLA	6	309	-	45,53,73	2.77	9 (20%)	52,89,113	1.47	8 (15%)
18	CLA	6	312	-	45,53,73	2.72	11 (24%)	52,89,113	1.37	8 (15%)
18	CLA	A	812	-	42,50,73	2.78	11 (26%)	48,85,113	1.57	9 (18%)
18	CLA	A	826	-	42,50,73	2.85	10 (23%)	48,85,113	1.72	7 (14%)
18	CLA	A	818	-	42,50,73	2.72	10 (23%)	48,85,113	1.51	8 (16%)
18	CLA	A	806	-	42,50,73	2.76	10 (23%)	48,85,113	1.59	8 (16%)
18	CLA	8	612	-	46,54,73	2.73	11 (23%)	53,90,113	1.46	9 (16%)
18	CLA	4	601	13	42,50,73	2.89	8 (19%)	48,85,113	1.86	9 (18%)
18	CLA	6	311	-	45,53,73	2.70	10 (22%)	52,89,113	1.48	9 (17%)
18	CLA	A	815	-	42,50,73	2.78	9 (21%)	48,85,113	1.48	7 (14%)
18	CLA	B	838	-	43,51,73	2.63	9 (20%)	49,86,113	1.46	8 (16%)
18	CLA	4	608	-	42,50,73	2.78	7 (16%)	48,85,113	1.95	11 (22%)
18	CLA	A	821	-	42,50,73	2.76	10 (23%)	48,85,113	1.45	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	7	613	-	43,51,73	2.71	9 (20%)	49,86,113	1.63	8 (16%)
21	CHL	1	601	8	53,61,74	2.22	10 (18%)	57,98,114	1.51	6 (10%)
18	CLA	Z	612	-	42,50,73	2.84	9 (21%)	48,85,113	1.61	9 (18%)
18	CLA	B	831	-	42,50,73	2.82	10 (23%)	48,85,113	1.56	9 (18%)
18	CLA	A	803	-	42,50,73	2.95	12 (28%)	48,85,113	1.77	9 (18%)
18	CLA	A	814	-	42,50,73	2.79	9 (21%)	48,85,113	1.57	7 (14%)
18	CLA	B	817	-	42,50,73	2.80	8 (19%)	48,85,113	1.63	9 (18%)
18	CLA	A	817	-	47,55,73	2.62	11 (23%)	54,91,113	1.47	8 (14%)
18	CLA	B	828	-	42,50,73	2.69	10 (23%)	48,85,113	1.49	7 (14%)
18	CLA	4	612	-	41,49,73	2.81	8 (19%)	47,84,113	1.32	6 (12%)
18	CLA	3	313	-	46,54,73	2.59	8 (17%)	53,90,113	1.47	9 (16%)
18	CLA	A	816	-	42,50,73	2.78	10 (23%)	48,85,113	1.47	7 (14%)
18	CLA	3	302	-	42,50,73	2.84	10 (23%)	48,85,113	1.53	7 (14%)
18	CLA	B	809	-	42,50,73	2.80	9 (21%)	48,85,113	1.58	9 (18%)
18	CLA	B	836	-	42,50,73	2.75	9 (21%)	48,85,113	1.64	9 (18%)
18	CLA	3	310	-	46,54,73	2.64	10 (21%)	53,90,113	1.45	7 (13%)
19	PQN	A	842	-	34,34,34	0.24	0	42,45,45	0.35	0
18	CLA	7	611	-	42,50,73	2.81	10 (23%)	48,85,113	1.50	8 (16%)
18	CLA	B	835	-	42,50,73	2.85	8 (19%)	48,85,113	1.79	9 (18%)
18	CLA	B	826	-	42,50,73	2.79	10 (23%)	48,85,113	1.48	8 (16%)
18	CLA	B	812	-	42,50,73	2.75	10 (23%)	48,85,113	1.97	12 (25%)
18	CLA	7	614	10	42,50,73	2.72	9 (21%)	48,85,113	2.22	10 (20%)
18	CLA	8	611	-	42,50,73	2.80	10 (23%)	48,85,113	1.78	8 (16%)
18	CLA	A	823	-	51,59,73	2.45	9 (17%)	59,96,113	1.70	12 (20%)
21	CHL	5	616	-	43,51,74	2.54	11 (25%)	45,86,114	1.73	7 (15%)
21	CHL	4	604	-	43,51,74	2.60	11 (25%)	45,86,114	2.09	14 (31%)
18	CLA	6	308	-	42,50,73	2.75	8 (19%)	48,85,113	1.56	8 (16%)
18	CLA	5	617	-	46,54,73	2.44	9 (19%)	53,90,113	1.63	9 (16%)
18	CLA	A	813	-	42,50,73	2.79	10 (23%)	48,85,113	1.49	8 (16%)
18	CLA	3	314	-	42,50,73	2.68	10 (23%)	48,85,113	1.45	8 (16%)
18	CLA	A	808	-	42,50,73	2.98	10 (23%)	48,85,113	1.69	9 (18%)
18	CLA	8	602	-	42,50,73	2.78	8 (19%)	48,85,113	1.44	8 (16%)
18	CLA	6	314	15	46,54,73	2.68	9 (19%)	53,90,113	1.49	10 (18%)
21	CHL	6	307	-	43,51,74	2.48	10 (23%)	45,86,114	1.71	8 (17%)
18	CLA	A	831	-	42,50,73	2.77	8 (19%)	48,85,113	1.67	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CHL	1	606	-	43,51,74	2.57	11 (25%)	45,86,114	1.89	9 (20%)
21	CHL	4	605	-	46,54,74	2.32	11 (23%)	49,90,114	2.38	11 (22%)
18	CLA	B	829	-	42,50,73	2.57	9 (21%)	48,85,113	1.53	8 (16%)
18	CLA	7	605	-	42,50,73	2.80	10 (23%)	48,85,113	1.63	9 (18%)
18	CLA	5	601	14	42,50,73	2.76	8 (19%)	48,85,113	1.42	7 (14%)
18	CLA	B	816	-	42,50,73	2.82	9 (21%)	48,85,113	1.55	7 (14%)
18	CLA	7	608	-	50,58,73	2.52	10 (20%)	58,95,113	1.49	10 (17%)
18	CLA	A	819	-	42,50,73	2.74	8 (19%)	48,85,113	1.69	7 (14%)
18	CLA	A	802	-	42,50,73	2.65	10 (23%)	48,85,113	1.87	10 (20%)
18	CLA	8	605	-	42,50,73	2.84	9 (21%)	48,85,113	1.48	8 (16%)
18	CLA	5	608	-	42,50,73	2.84	9 (21%)	48,85,113	1.41	6 (12%)
18	CLA	A	843	-	52,60,73	2.60	8 (15%)	60,97,113	1.32	9 (15%)
21	CHL	Z	605	-	43,51,74	2.56	11 (25%)	45,86,114	1.88	9 (20%)
18	CLA	A	837	-	42,50,73	2.77	10 (23%)	48,85,113	1.53	9 (18%)
20	SF4	C	102	3	0,12,12	-	-	-	-	-
18	CLA	A	832	-	42,50,73	2.67	9 (21%)	48,85,113	1.55	8 (16%)
18	CLA	5	609	-	42,50,73	2.71	9 (21%)	48,85,113	1.51	10 (20%)
18	CLA	A	835	-	42,50,73	2.89	9 (21%)	48,85,113	1.55	10 (20%)
18	CLA	B	818	-	42,50,73	2.78	9 (21%)	48,85,113	1.58	8 (16%)
18	CLA	B	801	-	42,50,73	2.65	9 (21%)	48,85,113	1.58	10 (20%)
18	CLA	B	840	-	42,50,73	2.64	9 (21%)	48,85,113	1.55	9 (18%)
18	CLA	3	303	-	42,50,73	2.70	10 (23%)	48,85,113	1.52	8 (16%)
18	CLA	8	604	-	42,50,73	2.80	8 (19%)	48,85,113	1.46	8 (16%)
18	CLA	8	614	-	42,50,73	2.79	8 (19%)	48,85,113	1.73	9 (18%)
18	CLA	8	601	11	42,50,73	2.77	9 (21%)	48,85,113	1.46	8 (16%)
18	CLA	1	610	-	42,50,73	2.62	8 (19%)	48,85,113	1.69	9 (18%)
18	CLA	3	312	-	45,53,73	2.74	8 (17%)	52,89,113	1.50	8 (15%)
18	CLA	1	611	-	42,50,73	2.85	10 (23%)	48,85,113	1.56	9 (18%)
18	CLA	A	820	-	42,50,73	2.63	10 (23%)	48,85,113	1.58	9 (18%)
18	CLA	3	309	-	41,49,73	2.78	9 (21%)	47,84,113	2.02	11 (23%)
18	CLA	5	612	-	42,50,73	2.69	10 (23%)	48,85,113	1.50	8 (16%)
18	CLA	Z	606	-	42,50,73	2.75	9 (21%)	48,85,113	1.50	7 (14%)
18	CLA	A	834	-	42,50,73	2.83	10 (23%)	48,85,113	2.02	12 (25%)
18	CLA	7	609	-	45,53,73	2.71	9 (20%)	52,89,113	1.44	8 (15%)
18	CLA	B	811	-	42,50,73	2.60	10 (23%)	48,85,113	1.56	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	837	-	42,50,73	2.70	9 (21%)	48,85,113	1.45	8 (16%)
18	CLA	A	833	-	42,50,73	2.91	10 (23%)	48,85,113	1.47	7 (14%)
19	PQN	B	844	-	34,34,34	0.24	0	42,45,45	0.37	0
18	CLA	B	802	-	46,54,73	2.59	10 (21%)	53,90,113	1.44	7 (13%)
18	CLA	8	615	-	42,50,73	2.81	11 (26%)	48,85,113	1.49	7 (14%)
18	CLA	A	824	-	42,50,73	2.65	12 (28%)	48,85,113	1.73	9 (18%)
18	CLA	3	305	9	42,50,73	2.72	9 (21%)	48,85,113	2.17	13 (27%)
18	CLA	Z	610	-	42,50,73	2.85	10 (23%)	48,85,113	1.55	9 (18%)
18	CLA	Z	611	-	45,53,73	2.62	9 (20%)	52,89,113	1.43	8 (15%)
18	CLA	B	832	-	42,50,73	2.81	8 (19%)	48,85,113	1.52	7 (14%)
18	CLA	4	609	-	42,50,73	2.87	7 (16%)	48,85,113	1.51	7 (14%)
18	CLA	B	822	-	45,53,73	2.56	9 (20%)	52,89,113	1.60	8 (15%)
18	CLA	5	611	-	42,50,73	2.73	10 (23%)	48,85,113	1.65	10 (20%)
18	CLA	8	610	-	46,54,73	2.33	7 (15%)	53,90,113	1.64	10 (18%)
18	CLA	1	607	-	42,50,73	2.75	8 (19%)	48,85,113	1.50	8 (16%)
18	CLA	A	829	-	42,50,73	2.63	10 (23%)	48,85,113	1.56	8 (16%)
18	CLA	1	614	-	46,54,73	2.73	9 (19%)	53,90,113	1.45	7 (13%)
18	CLA	Z	609	-	42,50,73	2.63	8 (19%)	48,85,113	1.70	9 (18%)
18	CLA	4	610	-	42,50,73	2.77	10 (23%)	48,85,113	1.53	8 (16%)
18	CLA	5	604	-	42,50,73	2.80	8 (19%)	48,85,113	1.57	9 (18%)
18	CLA	7	607	-	42,50,73	2.78	11 (26%)	48,85,113	1.52	9 (18%)
22	FES	G	101	-	0,4,4	-	-	-	-	-
18	CLA	B	805	-	42,50,73	2.70	9 (21%)	48,85,113	1.73	9 (18%)
18	CLA	3	308	-	42,50,73	2.75	10 (23%)	48,85,113	1.47	9 (18%)
18	CLA	1	605	-	42,50,73	2.83	9 (21%)	48,85,113	1.58	8 (16%)
18	CLA	6	313	-	42,50,73	2.75	9 (21%)	48,85,113	1.67	10 (20%)
21	CHL	3	306	-	43,51,74	2.49	12 (27%)	45,86,114	1.88	7 (15%)
18	CLA	3	301	-	42,50,73	2.71	9 (21%)	48,85,113	1.62	9 (18%)
18	CLA	B	808	-	42,50,73	2.67	11 (26%)	48,85,113	1.60	8 (16%)
18	CLA	5	602	-	42,50,73	2.79	10 (23%)	48,85,113	1.60	8 (16%)
18	CLA	4	602	-	42,50,73	2.89	10 (23%)	48,85,113	1.59	10 (20%)
20	SF4	B	803	-	0,12,12	-	-	-	-	-
18	CLA	B	824	-	42,50,73	2.81	8 (19%)	48,85,113	1.55	7 (14%)
18	CLA	8	607	-	42,50,73	2.80	10 (23%)	48,85,113	1.57	9 (18%)
18	CLA	8	609	-	42,50,73	2.82	9 (21%)	48,85,113	1.57	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	834	-	38,46,73	4.73	12 (31%)	37,77,113	1.75	8 (21%)
21	CHL	5	606	-	43,51,74	2.54	8 (18%)	45,86,114	2.67	11 (24%)
18	CLA	B	825	-	42,50,73	2.87	9 (21%)	48,85,113	1.47	7 (14%)
18	CLA	A	804	-	42,50,73	2.75	10 (23%)	48,85,113	1.58	8 (16%)
18	CLA	6	315	-	42,50,73	2.66	8 (19%)	48,85,113	1.73	9 (18%)
18	CLA	7	603	-	46,54,73	2.64	9 (19%)	53,90,113	1.46	6 (11%)
18	CLA	B	821	-	42,50,73	2.71	8 (19%)	48,85,113	1.45	8 (16%)
21	CHL	6	305	-	43,51,74	2.48	10 (23%)	45,86,114	1.84	9 (20%)
18	CLA	5	613	-	42,50,73	2.79	9 (21%)	48,85,113	1.63	8 (16%)
18	CLA	A	828	-	42,50,73	2.65	11 (26%)	48,85,113	1.46	8 (16%)
18	CLA	3	311	-	45,53,73	2.70	11 (24%)	52,89,113	1.39	9 (17%)
18	CLA	6	304	-	42,50,73	2.86	9 (21%)	48,85,113	1.50	10 (20%)
18	CLA	4	606	-	42,50,73	2.82	8 (19%)	48,85,113	1.49	7 (14%)
18	CLA	1	602	-	42,50,73	2.84	9 (21%)	48,85,113	1.51	8 (16%)
18	CLA	A	844	-	42,50,73	2.56	8 (19%)	48,85,113	1.47	8 (16%)
18	CLA	A	827	-	42,50,73	2.57	7 (16%)	48,85,113	1.87	12 (25%)
18	CLA	B	814	-	42,50,73	2.90	8 (19%)	48,85,113	1.45	6 (12%)
18	CLA	1	604	-	42,50,73	2.82	9 (21%)	48,85,113	1.45	9 (18%)
18	CLA	5	605	-	42,50,73	2.84	9 (21%)	48,85,113	1.53	8 (16%)
21	CHL	6	316	-	43,51,74	2.55	9 (20%)	45,86,114	1.74	6 (13%)
18	CLA	Z	603	-	42,50,73	2.82	8 (19%)	48,85,113	1.45	9 (18%)
18	CLA	1	613	-	42,50,73	2.83	9 (21%)	48,85,113	1.61	9 (18%)
18	CLA	6	302	-	42,50,73	2.68	9 (21%)	48,85,113	1.63	9 (18%)
18	CLA	A	822	-	42,50,73	2.84	10 (23%)	48,85,113	1.65	10 (20%)
18	CLA	B	819	-	42,50,73	2.80	10 (23%)	48,85,113	1.86	10 (20%)
18	CLA	A	805	-	42,50,73	2.76	10 (23%)	48,85,113	1.64	8 (16%)
18	CLA	8	603	-	45,53,73	2.69	8 (17%)	52,89,113	1.51	8 (15%)
18	CLA	A	838	-	42,50,73	2.58	9 (21%)	48,85,113	1.66	9 (18%)
18	CLA	A	811	-	43,51,73	2.68	9 (20%)	49,86,113	1.51	7 (14%)
18	CLA	B	843	-	42,50,73	2.69	10 (23%)	48,85,113	1.60	8 (16%)
18	CLA	7	610	-	41,49,73	2.91	9 (21%)	47,84,113	2.15	11 (23%)
20	SF4	C	101	3	0,12,12	-	-	-	-	-
18	CLA	B	839	-	42,50,73	2.62	8 (19%)	48,85,113	1.51	7 (14%)
18	CLA	5	610	-	55,63,73	2.14	8 (14%)	64,101,113	1.36	7 (10%)
18	CLA	B	804	-	42,50,73	2.76	10 (23%)	48,85,113	1.86	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	4	611	-	42,50,73	2.70	8 (19%)	48,85,113	1.48	8 (16%)
18	CLA	B	830	-	45,53,73	2.60	8 (17%)	52,89,113	1.37	8 (15%)
18	CLA	A	825	-	42,50,73	2.77	9 (21%)	48,85,113	1.81	11 (22%)
18	CLA	6	301	-	42,50,73	2.96	9 (21%)	48,85,113	1.43	9 (18%)
18	CLA	B	813	-	41,49,73	2.71	9 (21%)	51,84,113	1.53	9 (17%)
18	CLA	7	612	-	45,53,73	2.76	11 (24%)	52,89,113	1.44	8 (15%)
18	CLA	4	603	-	46,54,73	2.69	11 (23%)	53,90,113	1.45	7 (13%)
18	CLA	Z	608	-	42,50,73	2.85	9 (21%)	48,85,113	1.46	7 (14%)
21	CHL	7	606	-	43,51,74	2.54	9 (20%)	45,86,114	1.93	6 (13%)
18	CLA	1	608	-	42,50,73	2.70	8 (19%)	48,85,113	1.95	12 (25%)
18	CLA	B	820	-	42,50,73	2.58	7 (16%)	48,85,113	1.87	11 (22%)
18	CLA	B	842	-	42,50,73	2.71	11 (26%)	48,85,113	1.71	8 (16%)
18	CLA	6	303	-	46,54,73	2.65	9 (19%)	53,90,113	1.39	6 (11%)
18	CLA	B	841	-	42,50,73	2.73	9 (21%)	48,85,113	1.72	10 (20%)
18	CLA	3	307	-	42,50,73	2.74	9 (21%)	48,85,113	1.81	8 (16%)
18	CLA	6	310	-	42,50,73	2.27	7 (16%)	48,85,113	2.17	7 (14%)
18	CLA	1	603	-	42,50,73	2.83	10 (23%)	48,85,113	1.48	7 (14%)
18	CLA	A	840	-	42,50,73	2.81	11 (26%)	48,85,113	1.71	7 (14%)
18	CLA	B	833	-	42,50,73	2.75	9 (21%)	48,85,113	1.44	8 (16%)
18	CLA	F	302	-	65,73,73	2.16	9 (13%)	76,113,113	1.25	9 (11%)
18	CLA	4	607	-	42,50,73	2.86	9 (21%)	48,85,113	1.58	9 (18%)
18	CLA	5	614	14	42,50,73	2.65	8 (19%)	48,85,113	1.49	10 (20%)
18	CLA	A	830	-	42,50,73	2.77	10 (23%)	48,85,113	1.46	7 (14%)
21	CHL	Z	601	12	43,51,74	2.45	10 (23%)	45,86,114	1.69	7 (15%)
21	CHL	5	607	-	43,51,74	2.45	10 (23%)	45,86,114	1.87	10 (22%)
18	CLA	1	609	-	42,50,73	2.86	9 (21%)	48,85,113	1.46	7 (14%)
18	CLA	J	101	-	42,50,73	2.82	8 (19%)	48,85,113	1.55	9 (18%)
18	CLA	8	613	-	42,50,73	2.72	10 (23%)	48,85,113	1.55	7 (14%)
18	CLA	Z	607	-	42,50,73	2.70	8 (19%)	48,85,113	1.95	12 (25%)
18	CLA	B	807	-	49,57,73	2.59	10 (20%)	55,92,113	1.57	11 (20%)
18	CLA	5	615	-	46,54,73	2.55	7 (15%)	53,90,113	2.04	11 (20%)
18	CLA	5	603	-	46,54,73	2.68	10 (21%)	53,90,113	1.39	8 (15%)
18	CLA	B	810	-	42,50,73	2.60	9 (21%)	48,85,113	1.50	7 (14%)
18	CLA	7	604	-	43,51,73	2.98	9 (20%)	49,86,113	1.64	11 (22%)
17	CL0	A	801	-	42,50,73	2.66	10 (23%)	48,85,113	1.59	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	7	601	10	42,50,73	2.76	9 (21%)	48,85,113	1.56	8 (16%)
18	CLA	B	806	-	45,53,73	2.76	10 (22%)	52,89,113	1.86	8 (15%)
18	CLA	7	602	-	42,50,73	2.77	11 (26%)	48,85,113	1.58	9 (18%)
18	CLA	A	839	-	42,50,73	2.73	11 (26%)	48,85,113	1.57	9 (18%)
18	CLA	6	317	-	45,53,73	2.72	10 (22%)	52,89,113	1.41	8 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3	304	-	1/1/10/20	1/10/88/115	-
18	CLA	Z	604	-	1/1/10/20	4/11/89/115	-
21	CHL	6	306	-	3/3/15/26	0/12/110/137	-
18	CLA	A	845	-	1/1/10/20	2/10/88/115	-
18	CLA	B	823	-	1/1/10/20	2/10/88/115	-
18	CLA	B	815	-	1/1/10/20	5/10/88/115	-
18	CLA	Z	602	-	1/1/10/20	2/10/88/115	-
21	CHL	8	606	-	3/3/15/26	1/12/110/137	-
18	CLA	A	809	-	1/1/10/20	0/10/88/115	-
18	CLA	A	836	1	1/1/10/20	3/10/88/115	-
18	CLA	A	807	-	1/1/10/20	2/10/88/115	-
18	CLA	A	841	-	1/1/10/20	1/10/88/115	-
18	CLA	F	301	-	1/1/11/20	2/13/91/115	-
18	CLA	1	612	-	1/1/11/20	3/15/93/115	-
18	CLA	B	827	-	1/1/10/20	1/10/88/115	-
18	CLA	A	810	-	1/1/10/20	0/10/88/115	-
18	CLA	8	608	-	1/1/10/20	0/10/88/115	-
18	CLA	Z	613	-	1/1/10/20	2/10/88/115	-
18	CLA	6	309	-	1/1/11/20	3/13/91/115	-
18	CLA	6	312	-	1/1/11/20	5/13/91/115	-
18	CLA	A	812	-	1/1/10/20	1/10/88/115	-
18	CLA	A	826	-	1/1/10/20	1/10/88/115	-
18	CLA	A	818	-	1/1/10/20	2/10/88/115	-
18	CLA	A	806	-	1/1/10/20	4/10/88/115	-
18	CLA	8	612	-	1/1/11/20	4/15/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	4	601	13	1/1/10/20	2/10/88/115	-
18	CLA	6	311	-	1/1/11/20	6/13/91/115	-
18	CLA	A	815	-	1/1/10/20	0/10/88/115	-
18	CLA	B	838	-	1/1/10/20	2/11/89/115	-
18	CLA	4	608	-	1/1/10/20	2/10/88/115	-
18	CLA	A	821	-	1/1/10/20	2/10/88/115	-
18	CLA	7	613	-	1/1/10/20	3/11/89/115	-
21	CHL	1	601	8	3/3/17/26	4/24/122/137	-
18	CLA	Z	612	-	1/1/10/20	3/10/88/115	-
18	CLA	B	831	-	1/1/10/20	2/10/88/115	-
18	CLA	A	803	-	1/1/10/20	6/10/88/115	-
18	CLA	A	814	-	1/1/10/20	2/10/88/115	-
18	CLA	B	817	-	1/1/10/20	3/10/88/115	-
18	CLA	A	817	-	1/1/11/20	4/16/94/115	-
18	CLA	B	828	-	1/1/10/20	4/10/88/115	-
18	CLA	4	612	-	1/1/10/20	0/8/86/115	-
18	CLA	3	313	-	1/1/11/20	3/15/93/115	-
18	CLA	A	816	-	1/1/10/20	1/10/88/115	-
18	CLA	3	302	-	1/1/10/20	1/10/88/115	-
18	CLA	B	809	-	1/1/10/20	2/10/88/115	-
18	CLA	B	836	-	1/1/10/20	1/10/88/115	-
18	CLA	3	310	-	1/1/11/20	5/15/93/115	-
19	PQN	A	842	-	-	7/23/43/43	0/2/2/2
18	CLA	7	611	-	1/1/10/20	0/10/88/115	-
18	CLA	B	835	-	1/1/10/20	1/10/88/115	-
18	CLA	B	826	-	1/1/10/20	1/10/88/115	-
18	CLA	B	812	-	1/1/10/20	4/10/88/115	-
18	CLA	7	614	10	1/1/10/20	3/10/88/115	-
18	CLA	8	611	-	1/1/10/20	2/10/88/115	-
18	CLA	A	823	-	1/1/12/20	4/21/99/115	-
21	CHL	5	616	-	3/3/15/26	2/12/110/137	-
21	CHL	4	604	-	3/3/15/26	1/12/110/137	-
18	CLA	6	308	-	1/1/10/20	0/10/88/115	-
18	CLA	5	617	-	1/1/11/20	8/15/93/115	-
18	CLA	A	813	-	1/1/10/20	7/10/88/115	-
18	CLA	3	314	-	1/1/10/20	0/10/88/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	808	-	1/1/10/20	2/10/88/115	-
18	CLA	8	602	-	1/1/10/20	2/10/88/115	-
18	CLA	6	314	15	1/1/11/20	2/15/93/115	-
21	CHL	6	307	-	3/3/15/26	2/12/110/137	-
18	CLA	A	831	-	1/1/10/20	3/10/88/115	-
21	CHL	1	606	-	3/3/15/26	3/12/110/137	-
21	CHL	4	605	-	3/3/16/26	4/15/113/137	-
18	CLA	B	829	-	1/1/10/20	4/10/88/115	-
18	CLA	7	605	-	1/1/10/20	1/10/88/115	-
18	CLA	5	601	14	1/1/10/20	2/10/88/115	-
18	CLA	B	816	-	1/1/10/20	2/10/88/115	-
18	CLA	7	608	-	1/1/12/20	3/19/97/115	-
18	CLA	A	819	-	1/1/10/20	2/10/88/115	-
18	CLA	A	802	-	1/1/10/20	4/10/88/115	-
18	CLA	8	605	-	1/1/10/20	2/10/88/115	-
18	CLA	5	608	-	1/1/10/20	2/10/88/115	-
18	CLA	A	843	-	1/1/12/20	7/22/100/115	-
21	CHL	Z	605	-	3/3/15/26	3/12/110/137	-
18	CLA	A	837	-	1/1/10/20	1/10/88/115	-
20	SF4	C	102	3	-	-	0/6/5/5
18	CLA	A	832	-	1/1/10/20	0/10/88/115	-
18	CLA	5	609	-	1/1/10/20	1/10/88/115	-
18	CLA	A	835	-	1/1/10/20	1/10/88/115	-
18	CLA	B	818	-	1/1/10/20	1/10/88/115	-
18	CLA	B	801	-	1/1/10/20	2/10/88/115	-
18	CLA	B	840	-	1/1/10/20	2/10/88/115	-
18	CLA	3	303	-	1/1/10/20	0/10/88/115	-
18	CLA	8	604	-	1/1/10/20	0/10/88/115	-
18	CLA	8	614	-	1/1/10/20	0/10/88/115	-
18	CLA	8	601	11	1/1/10/20	5/10/88/115	-
18	CLA	1	610	-	1/1/10/20	1/10/88/115	-
18	CLA	3	312	-	1/1/11/20	2/13/91/115	-
18	CLA	1	611	-	1/1/10/20	2/10/88/115	-
18	CLA	A	820	-	1/1/10/20	3/10/88/115	-
18	CLA	3	309	-	1/1/10/20	2/8/86/115	-
18	CLA	5	612	-	1/1/10/20	2/10/88/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	Z	606	-	1/1/10/20	0/10/88/115	-
18	CLA	A	834	-	1/1/10/20	3/10/88/115	-
18	CLA	7	609	-	1/1/11/20	0/13/91/115	-
18	CLA	B	811	-	1/1/10/20	2/10/88/115	-
18	CLA	B	837	-	1/1/10/20	0/10/88/115	-
18	CLA	A	833	-	1/1/10/20	2/10/88/115	-
19	PQN	B	844	-	-	5/23/43/43	0/2/2/2
18	CLA	B	802	-	1/1/11/20	1/15/93/115	-
18	CLA	8	615	-	1/1/10/20	2/10/88/115	-
18	CLA	A	824	-	1/1/10/20	4/10/88/115	-
18	CLA	3	305	9	1/1/10/20	1/10/88/115	-
18	CLA	Z	610	-	1/1/10/20	2/10/88/115	-
18	CLA	Z	611	-	1/1/11/20	4/13/91/115	-
18	CLA	B	832	-	1/1/10/20	2/10/88/115	-
18	CLA	4	609	-	1/1/10/20	3/10/88/115	-
18	CLA	B	822	-	1/1/11/20	4/13/91/115	-
18	CLA	5	611	-	1/1/10/20	3/10/88/115	-
18	CLA	8	610	-	1/1/11/20	1/15/93/115	-
18	CLA	1	607	-	1/1/10/20	0/10/88/115	-
18	CLA	A	829	-	1/1/10/20	0/10/88/115	-
18	CLA	1	614	-	1/1/11/20	3/15/93/115	-
18	CLA	Z	609	-	1/1/10/20	1/10/88/115	-
18	CLA	4	610	-	1/1/10/20	2/10/88/115	-
18	CLA	5	604	-	1/1/10/20	1/10/88/115	-
18	CLA	7	607	-	1/1/10/20	2/10/88/115	-
22	FES	G	101	-	-	-	0/1/1/1
18	CLA	B	805	-	1/1/10/20	2/10/88/115	-
18	CLA	3	308	-	1/1/10/20	1/10/88/115	-
18	CLA	1	605	-	1/1/10/20	3/10/88/115	-
18	CLA	6	313	-	1/1/10/20	3/10/88/115	-
21	CHL	3	306	-	3/3/15/26	1/12/110/137	-
18	CLA	3	301	-	1/1/10/20	2/10/88/115	-
18	CLA	B	808	-	1/1/10/20	0/10/88/115	-
18	CLA	5	602	-	1/1/10/20	4/10/88/115	-
18	CLA	4	602	-	1/1/10/20	1/10/88/115	-
20	SF4	B	803	-	-	-	0/6/5/5
18	CLA	B	824	-	1/1/10/20	2/10/88/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	8	607	-	1/1/10/20	1/10/88/115	-
18	CLA	8	609	-	1/1/10/20	2/10/88/115	-
18	CLA	B	834	-	1/1/10/20	2/10/85/115	-
21	CHL	5	606	-	3/3/15/26	3/12/110/137	-
18	CLA	B	825	-	1/1/10/20	3/10/88/115	-
18	CLA	A	804	-	1/1/10/20	3/10/88/115	-
18	CLA	6	315	-	1/1/10/20	2/10/88/115	-
18	CLA	7	603	-	1/1/11/20	2/15/93/115	-
18	CLA	B	821	-	1/1/10/20	1/10/88/115	-
21	CHL	6	305	-	3/3/15/26	0/12/110/137	-
18	CLA	5	613	-	1/1/10/20	1/10/88/115	-
18	CLA	A	828	-	1/1/10/20	0/10/88/115	-
18	CLA	3	311	-	1/1/11/20	2/13/91/115	-
18	CLA	6	304	-	1/1/10/20	2/10/88/115	-
18	CLA	4	606	-	1/1/10/20	3/10/88/115	-
18	CLA	1	602	-	1/1/10/20	2/10/88/115	-
18	CLA	A	844	-	1/1/10/20	6/10/88/115	-
18	CLA	A	827	-	1/1/10/20	1/10/88/115	-
18	CLA	B	814	-	1/1/10/20	0/10/88/115	-
18	CLA	1	604	-	1/1/10/20	1/10/88/115	-
18	CLA	5	605	-	1/1/10/20	0/10/88/115	-
21	CHL	6	316	-	3/3/15/26	2/12/110/137	-
18	CLA	Z	603	-	1/1/10/20	1/10/88/115	-
18	CLA	1	613	-	1/1/10/20	3/10/88/115	-
18	CLA	6	302	-	1/1/10/20	3/10/88/115	-
18	CLA	A	822	-	1/1/10/20	5/10/88/115	-
18	CLA	B	819	-	1/1/10/20	2/10/88/115	-
18	CLA	A	805	-	1/1/10/20	2/10/88/115	-
18	CLA	8	603	-	1/1/11/20	0/13/91/115	-
18	CLA	A	838	-	1/1/10/20	2/10/88/115	-
18	CLA	A	811	-	1/1/10/20	1/11/89/115	-
18	CLA	B	843	-	1/1/10/20	3/10/88/115	-
18	CLA	7	610	-	1/1/10/20	2/8/86/115	-
20	SF4	C	101	3	-	-	0/6/5/5
18	CLA	B	839	-	1/1/10/20	3/10/88/115	-
18	CLA	5	610	-	1/1/13/20	4/25/103/115	-
18	CLA	B	804	-	1/1/10/20	1/10/88/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	4	611	-	1/1/10/20	2/10/88/115	-
18	CLA	B	830	-	1/1/11/20	4/13/91/115	-
18	CLA	A	825	-	1/1/10/20	2/10/88/115	-
18	CLA	6	301	-	1/1/10/20	4/10/88/115	-
18	CLA	B	813	-	1/1/10/20	1/10/86/115	-
18	CLA	7	612	-	1/1/11/20	4/13/91/115	-
18	CLA	4	603	-	1/1/11/20	4/15/93/115	-
18	CLA	Z	608	-	1/1/10/20	2/10/88/115	-
21	CHL	7	606	-	3/3/15/26	1/12/110/137	-
18	CLA	1	608	-	1/1/10/20	2/10/88/115	-
18	CLA	B	820	-	1/1/10/20	2/10/88/115	-
18	CLA	B	842	-	1/1/10/20	1/10/88/115	-
18	CLA	6	303	-	1/1/11/20	4/15/93/115	-
18	CLA	B	841	-	1/1/10/20	1/10/88/115	-
18	CLA	3	307	-	1/1/10/20	1/10/88/115	-
18	CLA	6	310	-	1/1/10/20	2/10/88/115	-
18	CLA	1	603	-	1/1/10/20	2/10/88/115	-
18	CLA	A	840	-	1/1/10/20	2/10/88/115	-
18	CLA	B	833	-	1/1/10/20	3/10/88/115	-
18	CLA	F	302	-	1/1/15/20	5/37/115/115	-
18	CLA	4	607	-	1/1/10/20	1/10/88/115	-
18	CLA	5	614	14	1/1/10/20	1/10/88/115	-
18	CLA	A	830	-	1/1/10/20	1/10/88/115	-
21	CHL	Z	601	12	3/3/15/26	1/12/110/137	-
21	CHL	5	607	-	3/3/15/26	2/12/110/137	-
18	CLA	1	609	-	1/1/10/20	2/10/88/115	-
18	CLA	J	101	-	1/1/10/20	4/10/88/115	-
18	CLA	8	613	-	1/1/10/20	1/10/88/115	-
18	CLA	Z	607	-	1/1/10/20	2/10/88/115	-
18	CLA	B	807	-	1/1/11/20	4/15/93/115	-
18	CLA	5	615	-	1/1/11/20	3/15/93/115	-
18	CLA	5	603	-	1/1/11/20	4/15/93/115	-
18	CLA	B	810	-	1/1/10/20	2/10/88/115	-
18	CLA	7	604	-	1/1/10/20	2/11/89/115	-
17	CL0	A	801	-	3/3/15/25	2/10/108/135	-
18	CLA	7	601	10	1/1/10/20	5/10/88/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	806	-	1/1/11/20	4/13/91/115	-
18	CLA	7	602	-	1/1/10/20	2/10/88/115	-
18	CLA	A	839	-	1/1/10/20	2/10/88/115	-
18	CLA	6	317	-	1/1/11/20	2/13/91/115	-

All (1910) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	834	CLA	C4C-NC	22.91	1.47	1.30
18	7	604	CLA	C4B-NB	15.66	1.49	1.35
18	B	823	CLA	C4B-NB	15.01	1.48	1.35
18	6	301	CLA	C4B-NB	14.68	1.48	1.35
18	A	833	CLA	C4B-NB	14.61	1.48	1.35
18	B	814	CLA	C4B-NB	14.34	1.48	1.35
18	A	808	CLA	C4B-NB	14.27	1.47	1.35
18	A	843	CLA	C4B-NB	14.24	1.47	1.35
18	3	302	CLA	C4B-NB	14.13	1.47	1.35
18	5	605	CLA	C4B-NB	14.04	1.47	1.35
18	B	825	CLA	C4B-NB	14.00	1.47	1.35
18	Z	604	CLA	C4B-NB	14.00	1.47	1.35
18	8	605	CLA	C4B-NB	13.99	1.47	1.35
18	1	605	CLA	C4B-NB	13.96	1.47	1.35
18	4	602	CLA	C4B-NB	13.94	1.47	1.35
18	Z	612	CLA	C4B-NB	13.88	1.47	1.35
18	Z	602	CLA	C4B-NB	13.87	1.47	1.35
18	1	603	CLA	C4B-NB	13.85	1.47	1.35
18	A	836	CLA	C4B-NB	13.84	1.47	1.35
18	1	613	CLA	C4B-NB	13.82	1.47	1.35
18	1	602	CLA	C4B-NB	13.75	1.47	1.35
18	8	615	CLA	C4B-NB	13.73	1.47	1.35
18	5	603	CLA	C4B-NB	13.71	1.47	1.35
18	8	612	CLA	C4B-NB	13.71	1.47	1.35
18	B	824	CLA	C4B-NB	13.69	1.47	1.35
18	7	612	CLA	C4B-NB	13.69	1.47	1.35
18	Z	610	CLA	C4B-NB	13.66	1.47	1.35
18	6	317	CLA	C4B-NB	13.65	1.47	1.35
18	1	611	CLA	C4B-NB	13.64	1.47	1.35
18	Z	613	CLA	C4B-NB	13.63	1.47	1.35
18	1	609	CLA	C4B-NB	13.62	1.47	1.35
18	1	614	CLA	C4B-NB	13.62	1.47	1.35
18	Z	608	CLA	C4B-NB	13.60	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	J	101	CLA	C4B-NB	13.59	1.47	1.35
18	6	304	CLA	C4B-NB	13.58	1.47	1.35
18	6	309	CLA	C4B-NB	13.56	1.47	1.35
18	4	609	CLA	C4B-NB	13.55	1.47	1.35
18	6	303	CLA	C4B-NB	13.50	1.47	1.35
18	5	608	CLA	C4B-NB	13.47	1.47	1.35
18	A	804	CLA	C4B-NB	13.45	1.47	1.35
18	8	602	CLA	C4B-NB	13.43	1.47	1.35
18	6	312	CLA	C4B-NB	13.43	1.47	1.35
18	1	604	CLA	C4B-NB	13.41	1.47	1.35
18	A	834	CLA	C4B-NB	13.41	1.47	1.35
18	4	606	CLA	C4B-NB	13.40	1.47	1.35
18	B	816	CLA	C4B-NB	13.40	1.47	1.35
18	Z	603	CLA	C4B-NB	13.40	1.47	1.35
18	3	312	CLA	C4B-NB	13.37	1.47	1.35
18	7	609	CLA	C4B-NB	13.37	1.47	1.35
18	A	817	CLA	C4B-NB	13.36	1.47	1.35
18	A	803	CLA	C4B-NB	13.36	1.47	1.35
18	B	834	CLA	C4B-NB	13.36	1.47	1.35
18	B	809	CLA	C4B-NB	13.35	1.47	1.35
18	8	604	CLA	C4B-NB	13.34	1.47	1.35
18	A	831	CLA	C4B-NB	13.31	1.47	1.35
18	A	814	CLA	C4B-NB	13.30	1.47	1.35
18	A	845	CLA	C4B-NB	13.29	1.47	1.35
18	A	816	CLA	C4B-NB	13.29	1.47	1.35
18	B	826	CLA	C4B-NB	13.26	1.47	1.35
18	8	601	CLA	C4B-NB	13.26	1.47	1.35
18	A	826	CLA	C4B-NB	13.25	1.47	1.35
18	4	601	CLA	C4B-NB	13.24	1.47	1.35
18	B	819	CLA	C4B-NB	13.23	1.47	1.35
18	A	812	CLA	C4B-NB	13.22	1.47	1.35
18	4	610	CLA	C4B-NB	13.20	1.47	1.35
18	A	815	CLA	C4B-NB	13.18	1.47	1.35
18	A	835	CLA	C4B-NB	13.18	1.47	1.35
18	6	311	CLA	C4B-NB	13.18	1.47	1.35
18	B	804	CLA	C4B-NB	13.18	1.47	1.35
18	Z	606	CLA	C4B-NB	13.18	1.47	1.35
18	A	813	CLA	C4B-NB	13.17	1.47	1.35
18	1	607	CLA	C4B-NB	13.17	1.47	1.35
18	B	837	CLA	C4B-NB	13.16	1.46	1.35
18	4	603	CLA	C4B-NB	13.14	1.46	1.35
18	A	805	CLA	C4B-NB	13.13	1.46	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	832	CLA	C4B-NB	13.13	1.46	1.35
18	3	311	CLA	C4B-NB	13.13	1.46	1.35
18	A	810	CLA	C4B-NB	13.12	1.46	1.35
18	B	817	CLA	C4B-NB	13.12	1.46	1.35
18	B	835	CLA	C4B-NB	13.11	1.46	1.35
18	B	831	CLA	C4B-NB	13.10	1.46	1.35
18	5	601	CLA	C4B-NB	13.10	1.46	1.35
18	7	605	CLA	C4B-NB	13.09	1.46	1.35
18	8	603	CLA	C4B-NB	13.09	1.46	1.35
18	B	833	CLA	C4B-NB	13.09	1.46	1.35
18	5	604	CLA	C4B-NB	13.08	1.46	1.35
18	7	611	CLA	C4B-NB	13.06	1.46	1.35
18	4	607	CLA	C4B-NB	13.05	1.46	1.35
18	A	809	CLA	C4B-NB	13.05	1.46	1.35
18	B	830	CLA	C4B-NB	13.03	1.46	1.35
18	6	314	CLA	C4B-NB	13.03	1.46	1.35
18	A	830	CLA	C4B-NB	13.02	1.46	1.35
18	A	818	CLA	C4B-NB	12.98	1.46	1.35
18	B	818	CLA	C4B-NB	12.98	1.46	1.35
18	7	602	CLA	C4B-NB	12.97	1.46	1.35
18	7	603	CLA	C4B-NB	12.97	1.46	1.35
18	7	607	CLA	C4B-NB	12.97	1.46	1.35
18	5	602	CLA	C4B-NB	12.95	1.46	1.35
18	B	828	CLA	C4B-NB	12.94	1.46	1.35
18	5	611	CLA	C4B-NB	12.94	1.46	1.35
18	B	815	CLA	C4B-NB	12.94	1.46	1.35
18	A	822	CLA	C4B-NB	12.94	1.46	1.35
18	F	301	CLA	C4B-NB	12.93	1.46	1.35
18	B	821	CLA	C4B-NB	12.92	1.46	1.35
18	6	308	CLA	C4B-NB	12.90	1.46	1.35
18	A	840	CLA	C4B-NB	12.89	1.46	1.35
18	B	836	CLA	C4B-NB	12.87	1.46	1.35
18	8	607	CLA	C4B-NB	12.86	1.46	1.35
18	8	609	CLA	C4B-NB	12.84	1.46	1.35
18	A	837	CLA	C4B-NB	12.82	1.46	1.35
18	A	825	CLA	C4B-NB	12.82	1.46	1.35
18	3	308	CLA	C4B-NB	12.82	1.46	1.35
18	8	611	CLA	C4B-NB	12.81	1.46	1.35
18	3	310	CLA	C4B-NB	12.79	1.46	1.35
18	6	313	CLA	C4B-NB	12.78	1.46	1.35
18	A	819	CLA	C4B-NB	12.77	1.46	1.35
18	A	839	CLA	C4B-NB	12.77	1.46	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	7	601	CLA	C4B-NB	12.72	1.46	1.35
18	B	806	CLA	C4B-NB	12.72	1.46	1.35
18	A	807	CLA	C4B-NB	12.71	1.46	1.35
18	4	612	CLA	C4B-NB	12.71	1.46	1.35
18	A	806	CLA	C4B-NB	12.69	1.46	1.35
18	3	314	CLA	C4B-NB	12.67	1.46	1.35
18	Z	611	CLA	C4B-NB	12.66	1.46	1.35
18	3	313	CLA	C4B-NB	12.65	1.46	1.35
18	B	802	CLA	C4B-NB	12.64	1.46	1.35
18	8	608	CLA	C4B-NB	12.63	1.46	1.35
18	F	302	CLA	C4B-NB	12.61	1.46	1.35
18	8	613	CLA	C4B-NB	12.60	1.46	1.35
18	A	821	CLA	C4B-NB	12.60	1.46	1.35
18	8	614	CLA	C4B-NB	12.60	1.46	1.35
18	B	807	CLA	C4B-NB	12.59	1.46	1.35
18	1	612	CLA	C4B-NB	12.58	1.46	1.35
18	4	611	CLA	C4B-NB	12.58	1.46	1.35
18	A	828	CLA	C4B-NB	12.57	1.46	1.35
18	7	608	CLA	C4B-NB	12.49	1.46	1.35
18	B	843	CLA	C4B-NB	12.48	1.46	1.35
18	7	613	CLA	C4B-NB	12.43	1.46	1.35
18	5	609	CLA	C4B-NB	12.42	1.46	1.35
18	5	613	CLA	C4B-NB	12.42	1.46	1.35
18	A	832	CLA	C4B-NB	12.41	1.46	1.35
18	Z	607	CLA	C4B-NB	12.36	1.46	1.35
18	A	841	CLA	C4B-NB	12.35	1.46	1.35
18	1	608	CLA	C4B-NB	12.35	1.46	1.35
18	B	840	CLA	C4B-NB	12.31	1.46	1.35
18	A	844	CLA	C4B-NB	12.26	1.46	1.35
18	3	304	CLA	C4B-NB	12.25	1.46	1.35
18	5	614	CLA	C4B-NB	12.25	1.46	1.35
18	5	612	CLA	C4B-NB	12.24	1.46	1.35
18	3	301	CLA	C4B-NB	12.23	1.46	1.35
18	6	302	CLA	C4B-NB	12.22	1.46	1.35
18	B	842	CLA	C4B-NB	12.15	1.46	1.35
18	3	307	CLA	C4B-NB	12.15	1.46	1.35
18	B	822	CLA	C4B-NB	12.13	1.46	1.35
18	4	608	CLA	C4B-NB	12.09	1.46	1.35
18	3	303	CLA	C4B-NB	12.09	1.46	1.35
18	A	823	CLA	C4B-NB	12.08	1.46	1.35
21	6	316	CHL	C4B-NB	12.06	1.46	1.35
18	A	820	CLA	C4B-NB	12.00	1.45	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	7	614	CLA	C4B-NB	12.00	1.45	1.35
18	B	808	CLA	C4B-NB	11.99	1.45	1.35
18	A	811	CLA	C4B-NB	11.99	1.45	1.35
18	B	813	CLA	C4B-NB	11.98	1.45	1.35
18	B	811	CLA	C4B-NB	11.98	1.45	1.35
18	B	801	CLA	C4B-NB	11.97	1.45	1.35
18	3	309	CLA	C4B-NB	11.97	1.45	1.35
18	B	838	CLA	C4B-NB	11.96	1.45	1.35
21	5	616	CHL	C4B-NB	11.95	1.45	1.35
18	B	839	CLA	C4B-NB	11.93	1.45	1.35
18	6	315	CLA	C4B-NB	11.90	1.45	1.35
18	A	829	CLA	C4B-NB	11.84	1.45	1.35
21	6	305	CHL	C4B-NB	11.78	1.45	1.35
17	A	801	CL0	C4B-NB	11.77	1.45	1.35
18	B	812	CLA	C4B-NB	11.76	1.45	1.35
21	1	606	CHL	C4B-NB	11.70	1.45	1.35
18	B	827	CLA	C4B-NB	11.70	1.45	1.35
18	B	829	CLA	C4B-NB	11.69	1.45	1.35
18	Z	609	CLA	C4B-NB	11.67	1.45	1.35
18	B	810	CLA	C4B-NB	11.64	1.45	1.35
18	B	841	CLA	C4B-NB	11.64	1.45	1.35
21	Z	605	CHL	C4B-NB	11.64	1.45	1.35
18	1	610	CLA	C4B-NB	11.62	1.45	1.35
18	A	838	CLA	C4B-NB	11.59	1.45	1.35
18	7	610	CLA	C4B-NB	11.58	1.45	1.35
18	B	805	CLA	C4B-NB	11.57	1.45	1.35
21	4	604	CHL	C4B-NB	11.54	1.45	1.35
18	3	305	CLA	C4B-NB	11.51	1.45	1.35
18	5	617	CLA	C4B-NB	11.48	1.45	1.35
18	A	824	CLA	C4B-NB	11.45	1.45	1.35
18	B	820	CLA	C4B-NB	11.44	1.45	1.35
21	6	307	CHL	C4B-NB	11.38	1.45	1.35
18	A	802	CLA	C4B-NB	11.34	1.45	1.35
21	4	605	CHL	C4B-NB	11.15	1.45	1.35
21	3	306	CHL	C4B-NB	11.12	1.45	1.35
21	6	306	CHL	C4B-NB	11.08	1.45	1.35
21	5	607	CHL	C4B-NB	11.05	1.45	1.35
18	5	615	CLA	C4B-NB	11.04	1.45	1.35
18	A	827	CLA	C4B-NB	10.92	1.44	1.35
21	1	601	CHL	C4B-NB	10.92	1.44	1.35
21	Z	601	CHL	C4B-NB	10.85	1.44	1.35
21	7	606	CHL	C4B-NB	10.69	1.44	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	610	CLA	C4B-NB	10.65	1.44	1.35
21	8	606	CHL	C4B-NB	10.50	1.44	1.35
21	5	606	CHL	C4B-NB	10.17	1.44	1.35
18	8	610	CLA	C4B-NB	9.95	1.44	1.35
18	7	610	CLA	C3A-C2A	-8.06	1.47	1.54
18	6	310	CLA	C4B-NB	7.36	1.41	1.35
18	8	610	CLA	MG-ND	-7.27	1.91	2.05
18	6	310	CLA	MG-ND	-7.27	1.91	2.05
18	7	604	CLA	MG-ND	-7.20	1.91	2.05
21	8	606	CHL	MG-ND	-7.14	1.91	2.05
18	4	606	CLA	C1B-NB	7.14	1.41	1.35
21	5	606	CHL	MG-ND	-7.05	1.91	2.05
21	7	606	CHL	MG-ND	-7.04	1.91	2.05
18	A	835	CLA	C1B-NB	7.01	1.41	1.35
21	4	604	CHL	MG-ND	-6.91	1.92	2.05
21	1	606	CHL	MG-ND	-6.88	1.92	2.05
21	Z	605	CHL	MG-ND	-6.87	1.92	2.05
18	6	301	CLA	C1B-NB	6.83	1.41	1.35
21	1	601	CHL	MG-ND	-6.80	1.92	2.05
21	Z	601	CHL	MG-ND	-6.78	1.92	2.05
18	B	805	CLA	MG-ND	-6.76	1.92	2.05
18	6	309	CLA	C1B-NB	6.74	1.41	1.35
18	B	823	CLA	C1B-NB	6.73	1.41	1.35
21	3	306	CHL	MG-ND	-6.71	1.92	2.05
18	B	815	CLA	MG-ND	-6.69	1.92	2.05
21	5	607	CHL	MG-ND	-6.69	1.92	2.05
18	3	312	CLA	C1B-NB	6.64	1.41	1.35
18	A	824	CLA	MG-ND	-6.62	1.92	2.05
18	5	604	CLA	C1B-NB	6.62	1.41	1.35
21	6	316	CHL	MG-ND	-6.61	1.92	2.05
18	A	822	CLA	MG-ND	-6.59	1.92	2.05
18	B	809	CLA	C1B-NB	6.54	1.41	1.35
18	4	607	CLA	C1B-NB	6.53	1.41	1.35
18	5	615	CLA	MG-ND	-6.53	1.92	2.05
18	4	608	CLA	C1B-NB	6.53	1.41	1.35
18	A	840	CLA	MG-ND	-6.53	1.92	2.05
18	8	614	CLA	C1B-NB	6.53	1.41	1.35
17	A	801	CL0	MG-ND	-6.53	1.92	2.05
18	8	608	CLA	MG-ND	-6.52	1.92	2.05
18	4	601	CLA	C1B-NB	6.48	1.41	1.35
18	A	811	CLA	MG-ND	-6.47	1.93	2.05
21	5	616	CHL	MG-ND	-6.46	1.93	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	306	CHL	MG-ND	-6.46	1.93	2.05
18	Z	613	CLA	C1B-NB	6.45	1.41	1.35
18	3	310	CLA	C1B-NB	6.45	1.41	1.35
18	4	612	CLA	MG-ND	-6.45	1.93	2.05
21	6	307	CHL	MG-ND	-6.45	1.93	2.05
18	B	811	CLA	MG-ND	-6.45	1.93	2.05
18	B	838	CLA	MG-ND	-6.44	1.93	2.05
18	1	614	CLA	C1B-NB	6.43	1.40	1.35
21	6	305	CHL	MG-ND	-6.42	1.93	2.05
18	4	608	CLA	MG-ND	-6.41	1.93	2.05
18	1	605	CLA	C1B-NB	6.40	1.40	1.35
18	B	806	CLA	MG-ND	-6.39	1.93	2.05
18	A	841	CLA	MG-ND	-6.37	1.93	2.05
18	A	822	CLA	C1B-NB	6.37	1.40	1.35
18	Z	604	CLA	C1B-NB	6.36	1.40	1.35
18	6	304	CLA	C1B-NB	6.36	1.40	1.35
18	J	101	CLA	C1B-NB	6.34	1.40	1.35
18	B	802	CLA	MG-ND	-6.33	1.93	2.05
18	A	802	CLA	MG-ND	-6.33	1.93	2.05
18	Z	609	CLA	MG-ND	-6.33	1.93	2.05
18	B	813	CLA	C1B-NB	6.33	1.40	1.35
18	7	609	CLA	C1B-NB	6.32	1.40	1.35
18	1	610	CLA	MG-ND	-6.31	1.93	2.05
18	B	840	CLA	MG-ND	-6.30	1.93	2.05
18	B	829	CLA	MG-ND	-6.30	1.93	2.05
18	A	821	CLA	C1B-NB	6.30	1.40	1.35
18	A	843	CLA	C1B-NB	6.29	1.40	1.35
18	6	315	CLA	MG-ND	-6.29	1.93	2.05
18	4	603	CLA	MG-ND	-6.29	1.93	2.05
18	8	604	CLA	C1B-NB	6.29	1.40	1.35
18	7	614	CLA	C1B-NB	6.28	1.40	1.35
18	B	841	CLA	MG-ND	-6.28	1.93	2.05
18	B	801	CLA	MG-ND	-6.27	1.93	2.05
18	8	607	CLA	MG-ND	-6.27	1.93	2.05
18	A	813	CLA	MG-ND	-6.26	1.93	2.05
18	5	608	CLA	C1B-NB	6.26	1.40	1.35
18	1	608	CLA	MG-ND	-6.26	1.93	2.05
18	8	612	CLA	C1B-NB	6.25	1.40	1.35
18	Z	607	CLA	MG-ND	-6.25	1.93	2.05
18	A	834	CLA	MG-ND	-6.25	1.93	2.05
18	5	613	CLA	C1B-NB	6.25	1.40	1.35
18	4	602	CLA	C1B-NB	6.25	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	832	CLA	C1B-NB	6.25	1.40	1.35
18	A	803	CLA	MG-ND	-6.24	1.93	2.05
18	A	827	CLA	MG-ND	-6.24	1.93	2.05
18	3	309	CLA	C1B-NB	6.24	1.40	1.35
18	1	609	CLA	C1B-NB	6.24	1.40	1.35
18	7	605	CLA	MG-ND	-6.24	1.93	2.05
18	Z	608	CLA	C1B-NB	6.23	1.40	1.35
18	B	808	CLA	MG-ND	-6.22	1.93	2.05
18	A	828	CLA	MG-ND	-6.22	1.93	2.05
18	B	835	CLA	MG-ND	-6.21	1.93	2.05
18	A	844	CLA	MG-ND	-6.21	1.93	2.05
18	B	839	CLA	MG-ND	-6.21	1.93	2.05
18	6	314	CLA	MG-ND	-6.21	1.93	2.05
18	B	825	CLA	C1B-NB	6.21	1.40	1.35
18	4	609	CLA	C1B-NB	6.21	1.40	1.35
18	3	303	CLA	MG-ND	-6.20	1.93	2.05
18	5	615	CLA	MG-NA	-6.20	1.91	2.06
18	A	837	CLA	MG-ND	-6.20	1.93	2.05
18	5	612	CLA	MG-ND	-6.20	1.93	2.05
18	8	608	CLA	C1B-NB	6.19	1.40	1.35
18	B	804	CLA	MG-ND	-6.19	1.93	2.05
18	B	831	CLA	MG-ND	-6.19	1.93	2.05
18	3	305	CLA	MG-ND	-6.19	1.93	2.05
18	B	815	CLA	C1B-NB	6.18	1.40	1.35
18	6	317	CLA	C1B-NB	6.17	1.40	1.35
18	B	820	CLA	MG-ND	-6.16	1.93	2.05
18	A	820	CLA	MG-ND	-6.16	1.93	2.05
18	A	807	CLA	MG-ND	-6.16	1.93	2.05
18	Z	602	CLA	C1B-NB	6.15	1.40	1.35
18	1	602	CLA	C1B-NB	6.15	1.40	1.35
18	A	845	CLA	MG-ND	-6.13	1.93	2.05
18	B	806	CLA	MG-NA	-6.12	1.91	2.06
18	7	601	CLA	MG-ND	-6.12	1.93	2.05
18	B	835	CLA	C1B-NB	6.11	1.40	1.35
18	6	314	CLA	C1B-NB	6.11	1.40	1.35
18	8	614	CLA	MG-ND	-6.11	1.93	2.05
18	8	609	CLA	MG-NA	-6.10	1.91	2.06
18	8	609	CLA	C1B-NB	6.10	1.40	1.35
18	4	601	CLA	MG-ND	-6.10	1.93	2.05
18	3	303	CLA	C1B-NB	6.09	1.40	1.35
18	3	311	CLA	MG-ND	-6.08	1.93	2.05
18	B	812	CLA	MG-NA	-6.07	1.91	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	816	CLA	C1B-NB	6.06	1.40	1.35
18	A	835	CLA	MG-ND	-6.05	1.93	2.05
18	A	830	CLA	MG-ND	-6.05	1.93	2.05
18	B	821	CLA	C1B-NB	6.04	1.40	1.35
18	6	310	CLA	MG-NA	-6.03	1.91	2.06
18	Z	603	CLA	C1B-NB	6.03	1.40	1.35
18	5	610	CLA	MG-ND	-6.02	1.93	2.05
18	A	808	CLA	C1B-NB	6.02	1.40	1.35
18	4	603	CLA	C1B-NB	6.02	1.40	1.35
18	4	610	CLA	C1B-NB	6.01	1.40	1.35
18	3	307	CLA	MG-ND	-6.01	1.93	2.05
18	B	817	CLA	MG-ND	-6.01	1.93	2.05
18	F	301	CLA	MG-ND	-6.00	1.93	2.05
18	7	610	CLA	MG-ND	-6.00	1.93	2.05
18	B	827	CLA	MG-ND	-5.99	1.93	2.05
18	B	807	CLA	MG-ND	-5.99	1.93	2.05
18	6	308	CLA	C1B-NB	5.99	1.40	1.35
18	8	605	CLA	C1B-NB	5.98	1.40	1.35
18	8	603	CLA	C1B-NB	5.98	1.40	1.35
18	8	601	CLA	MG-ND	-5.98	1.93	2.05
18	A	836	CLA	C1B-NB	5.98	1.40	1.35
18	7	612	CLA	C1B-NB	5.98	1.40	1.35
18	B	817	CLA	C1B-NB	5.98	1.40	1.35
18	5	613	CLA	MG-ND	-5.97	1.93	2.05
18	3	305	CLA	MG-NA	-5.97	1.92	2.06
18	8	615	CLA	C1B-NB	5.97	1.40	1.35
18	7	614	CLA	MG-ND	-5.97	1.94	2.05
18	B	841	CLA	MG-NA	-5.97	1.92	2.06
18	6	302	CLA	MG-ND	-5.97	1.94	2.05
18	A	821	CLA	MG-ND	-5.96	1.94	2.05
18	5	602	CLA	MG-ND	-5.96	1.94	2.05
18	3	308	CLA	C1B-NB	5.96	1.40	1.35
18	B	833	CLA	MG-ND	-5.95	1.94	2.05
18	B	812	CLA	MG-ND	-5.95	1.94	2.05
21	5	606	CHL	MG-NA	-5.95	1.92	2.06
18	6	303	CLA	C1B-NB	5.94	1.40	1.35
18	A	839	CLA	MG-ND	-5.94	1.94	2.05
18	1	604	CLA	C1B-NB	5.94	1.40	1.35
18	1	603	CLA	C1B-NB	5.93	1.40	1.35
18	7	613	CLA	MG-ND	-5.93	1.94	2.05
18	A	810	CLA	MG-ND	-5.93	1.94	2.05
18	A	818	CLA	MG-ND	-5.93	1.94	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	845	CLA	C1B-NB	5.93	1.40	1.35
18	B	836	CLA	MG-ND	-5.92	1.94	2.05
18	B	816	CLA	MG-ND	-5.92	1.94	2.05
18	5	605	CLA	C1B-NB	5.92	1.40	1.35
18	A	809	CLA	MG-ND	-5.91	1.94	2.05
18	A	826	CLA	C1B-NB	5.91	1.40	1.35
18	B	806	CLA	C1B-NB	5.91	1.40	1.35
18	F	302	CLA	C1B-NB	5.90	1.40	1.35
18	7	607	CLA	MG-ND	-5.90	1.94	2.05
18	A	808	CLA	MG-ND	-5.90	1.94	2.05
18	1	611	CLA	C1B-NB	5.89	1.40	1.35
18	B	812	CLA	C1B-NB	5.89	1.40	1.35
18	B	826	CLA	C1B-NB	5.89	1.40	1.35
18	A	823	CLA	MG-ND	-5.89	1.94	2.05
18	1	605	CLA	MG-ND	-5.88	1.94	2.05
18	7	612	CLA	MG-ND	-5.88	1.94	2.05
18	3	305	CLA	C1B-NB	5.88	1.40	1.35
18	B	827	CLA	C1B-NB	5.87	1.40	1.35
18	B	818	CLA	MG-ND	-5.87	1.94	2.05
18	A	805	CLA	MG-ND	-5.87	1.94	2.05
18	A	819	CLA	MG-ND	-5.87	1.94	2.05
18	5	603	CLA	MG-ND	-5.86	1.94	2.05
18	Z	607	CLA	C1B-NB	5.86	1.40	1.35
18	3	307	CLA	C1B-NB	5.86	1.40	1.35
18	8	603	CLA	MG-ND	-5.86	1.94	2.05
18	1	609	CLA	MG-ND	-5.85	1.94	2.05
18	A	823	CLA	C1B-NB	5.85	1.40	1.35
18	1	608	CLA	C1B-NB	5.85	1.40	1.35
18	5	614	CLA	MG-ND	-5.85	1.94	2.05
18	B	842	CLA	MG-ND	-5.85	1.94	2.05
18	7	602	CLA	C1B-NB	5.85	1.40	1.35
18	A	817	CLA	MG-ND	-5.85	1.94	2.05
18	A	827	CLA	MG-NA	-5.84	1.92	2.06
18	4	608	CLA	MG-NA	-5.84	1.92	2.06
18	3	304	CLA	MG-ND	-5.84	1.94	2.05
18	Z	604	CLA	MG-ND	-5.83	1.94	2.05
18	A	832	CLA	MG-ND	-5.83	1.94	2.05
18	B	805	CLA	MG-NA	-5.83	1.92	2.06
18	A	829	CLA	MG-ND	-5.83	1.94	2.05
18	A	803	CLA	C1B-NB	5.83	1.40	1.35
18	3	301	CLA	C1B-NB	5.83	1.40	1.35
18	8	605	CLA	MG-ND	-5.83	1.94	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	804	CLA	MG-ND	-5.82	1.94	2.05
18	4	611	CLA	MG-ND	-5.82	1.94	2.05
18	8	602	CLA	C1B-NB	5.82	1.40	1.35
18	B	834	CLA	MG-ND	-5.82	1.94	2.05
18	7	608	CLA	C1B-NB	5.82	1.40	1.35
18	7	611	CLA	C1B-NB	5.81	1.40	1.35
18	A	826	CLA	MG-ND	-5.80	1.94	2.05
18	8	611	CLA	MG-ND	-5.80	1.94	2.05
18	Z	608	CLA	MG-ND	-5.80	1.94	2.05
18	B	810	CLA	MG-ND	-5.80	1.94	2.05
18	6	313	CLA	MG-ND	-5.80	1.94	2.05
18	5	617	CLA	MG-ND	-5.80	1.94	2.05
18	4	607	CLA	MG-ND	-5.79	1.94	2.05
18	Z	610	CLA	C1B-NB	5.79	1.40	1.35
18	A	843	CLA	MG-ND	-5.79	1.94	2.05
18	6	302	CLA	C1B-NB	5.78	1.40	1.35
18	6	311	CLA	C1B-NB	5.78	1.40	1.35
18	A	806	CLA	MG-ND	-5.78	1.94	2.05
18	5	611	CLA	C1B-NB	5.78	1.40	1.35
18	1	612	CLA	MG-ND	-5.78	1.94	2.05
18	B	843	CLA	C1B-NB	5.78	1.40	1.35
18	5	608	CLA	MG-ND	-5.77	1.94	2.05
18	4	601	CLA	MG-NA	-5.77	1.92	2.06
18	A	814	CLA	MG-ND	-5.77	1.94	2.05
18	Z	611	CLA	MG-ND	-5.77	1.94	2.05
18	7	603	CLA	MG-ND	-5.75	1.94	2.05
18	3	313	CLA	MG-ND	-5.75	1.94	2.05
18	1	613	CLA	C1B-NB	5.75	1.40	1.35
18	3	309	CLA	MG-ND	-5.75	1.94	2.05
18	7	613	CLA	C1B-NB	5.74	1.40	1.35
18	3	311	CLA	C1B-NB	5.74	1.40	1.35
18	5	601	CLA	MG-ND	-5.73	1.94	2.05
18	5	609	CLA	MG-ND	-5.73	1.94	2.05
18	Z	612	CLA	C1B-NB	5.72	1.40	1.35
18	3	314	CLA	MG-ND	-5.72	1.94	2.05
18	B	830	CLA	MG-ND	-5.71	1.94	2.05
18	8	612	CLA	MG-ND	-5.71	1.94	2.05
18	8	613	CLA	MG-ND	-5.71	1.94	2.05
18	B	831	CLA	C1B-NB	5.69	1.40	1.35
18	B	822	CLA	C1B-NB	5.69	1.40	1.35
18	Z	609	CLA	C1B-NB	5.69	1.40	1.35
18	A	833	CLA	C1B-NB	5.68	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	825	CLA	MG-ND	-5.68	1.94	2.05
18	3	302	CLA	C1B-NB	5.68	1.40	1.35
18	A	831	CLA	MG-ND	-5.68	1.94	2.05
18	B	842	CLA	C1B-NB	5.67	1.40	1.35
18	1	610	CLA	C1B-NB	5.67	1.40	1.35
18	4	610	CLA	MG-ND	-5.67	1.94	2.05
18	B	837	CLA	MG-ND	-5.67	1.94	2.05
18	3	307	CLA	MG-NA	-5.67	1.92	2.06
18	B	813	CLA	MG-ND	-5.67	1.94	2.05
18	B	819	CLA	C1B-NB	5.67	1.40	1.35
18	F	302	CLA	MG-ND	-5.67	1.94	2.05
18	8	604	CLA	MG-ND	-5.66	1.94	2.05
18	3	304	CLA	C1B-NB	5.66	1.40	1.35
18	A	802	CLA	C1B-NB	5.66	1.40	1.35
18	5	614	CLA	C1B-NB	5.65	1.40	1.35
18	B	832	CLA	MG-ND	-5.65	1.94	2.05
18	6	312	CLA	MG-ND	-5.65	1.94	2.05
18	B	820	CLA	MG-NA	-5.65	1.92	2.06
18	6	315	CLA	C1B-NB	5.65	1.40	1.35
18	5	605	CLA	MG-ND	-5.64	1.94	2.05
18	B	815	CLA	MG-NA	-5.63	1.92	2.06
18	4	612	CLA	MG-NA	-5.63	1.92	2.06
18	5	602	CLA	C1B-NB	5.63	1.40	1.35
18	7	610	CLA	MG-NA	-5.62	1.92	2.06
18	B	826	CLA	MG-ND	-5.62	1.94	2.05
18	Z	603	CLA	MG-ND	-5.62	1.94	2.05
18	Z	606	CLA	C1B-NB	5.61	1.40	1.35
18	3	313	CLA	C1B-NB	5.61	1.40	1.35
18	6	312	CLA	C1B-NB	5.61	1.40	1.35
18	Z	606	CLA	MG-ND	-5.61	1.94	2.05
18	7	602	CLA	MG-ND	-5.61	1.94	2.05
18	A	831	CLA	C1B-NB	5.61	1.40	1.35
18	7	605	CLA	C1B-NB	5.61	1.40	1.35
18	1	604	CLA	MG-ND	-5.61	1.94	2.05
18	1	607	CLA	MG-ND	-5.60	1.94	2.05
18	B	819	CLA	MG-NA	-5.59	1.93	2.06
18	A	803	CLA	MG-NA	-5.59	1.93	2.06
18	6	301	CLA	MG-ND	-5.59	1.94	2.05
18	A	824	CLA	MG-NA	-5.59	1.93	2.06
18	7	607	CLA	C1B-NB	5.58	1.40	1.35
18	A	837	CLA	C1B-NB	5.58	1.40	1.35
18	A	816	CLA	MG-ND	-5.58	1.94	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Z	613	CLA	MG-ND	-5.58	1.94	2.05
18	B	843	CLA	MG-ND	-5.57	1.94	2.05
18	A	814	CLA	C1B-NB	5.56	1.40	1.35
18	3	308	CLA	MG-ND	-5.56	1.94	2.05
18	1	614	CLA	MG-ND	-5.56	1.94	2.05
18	7	611	CLA	MG-ND	-5.56	1.94	2.05
18	4	609	CLA	MG-ND	-5.54	1.94	2.05
18	8	611	CLA	C1B-NB	5.54	1.40	1.35
18	A	815	CLA	MG-ND	-5.53	1.94	2.05
18	6	308	CLA	MG-ND	-5.53	1.94	2.05
18	4	612	CLA	C1B-NB	5.53	1.40	1.35
18	7	608	CLA	MG-ND	-5.53	1.94	2.05
18	A	825	CLA	MG-NA	-5.52	1.93	2.06
18	B	839	CLA	C1B-NB	5.52	1.40	1.35
18	5	609	CLA	C1B-NB	5.52	1.40	1.35
18	3	301	CLA	MG-ND	-5.51	1.94	2.05
18	B	827	CLA	MG-NA	-5.50	1.93	2.06
18	A	829	CLA	C1B-NB	5.50	1.40	1.35
18	A	825	CLA	MG-ND	-5.50	1.94	2.05
18	A	838	CLA	C1B-NB	5.49	1.40	1.35
18	1	607	CLA	C1B-NB	5.49	1.40	1.35
18	6	313	CLA	C1B-NB	5.49	1.40	1.35
18	A	808	CLA	MG-NA	-5.49	1.93	2.06
18	8	611	CLA	MG-NA	-5.49	1.93	2.06
18	A	810	CLA	C1B-NB	5.49	1.40	1.35
18	1	612	CLA	C1B-NB	5.49	1.40	1.35
18	4	602	CLA	MG-ND	-5.49	1.94	2.05
18	A	811	CLA	C1B-NB	5.49	1.40	1.35
18	B	818	CLA	C1B-NB	5.49	1.40	1.35
18	5	615	CLA	C1B-NB	5.48	1.40	1.35
18	A	806	CLA	C1B-NB	5.48	1.40	1.35
18	5	603	CLA	C1B-NB	5.47	1.40	1.35
18	6	304	CLA	MG-ND	-5.47	1.94	2.05
18	B	822	CLA	MG-ND	-5.47	1.94	2.05
18	A	807	CLA	C1B-NB	5.46	1.40	1.35
18	5	604	CLA	MG-ND	-5.46	1.95	2.05
18	A	840	CLA	C1B-NB	5.46	1.40	1.35
18	Z	611	CLA	C1B-NB	5.46	1.40	1.35
18	4	611	CLA	C1B-NB	5.46	1.40	1.35
18	7	603	CLA	C1B-NB	5.45	1.40	1.35
21	8	606	CHL	MG-NC	-5.45	1.93	2.06
18	A	809	CLA	C1B-NB	5.45	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	810	CLA	MG-NA	-5.45	1.93	2.06
18	B	833	CLA	C1B-NB	5.45	1.40	1.35
18	B	836	CLA	C1B-NB	5.44	1.40	1.35
18	8	615	CLA	MG-ND	-5.44	1.95	2.05
18	B	814	CLA	C1B-NB	5.44	1.40	1.35
18	A	812	CLA	MG-ND	-5.43	1.95	2.05
18	B	824	CLA	MG-ND	-5.43	1.95	2.05
18	A	812	CLA	C1B-NB	5.43	1.40	1.35
18	B	834	CLA	C1B-NB	5.43	1.40	1.35
18	8	613	CLA	C1B-NB	5.43	1.40	1.35
18	1	603	CLA	MG-ND	-5.43	1.95	2.05
18	7	608	CLA	MG-NA	-5.43	1.93	2.06
18	6	309	CLA	MG-ND	-5.43	1.95	2.05
18	B	821	CLA	MG-ND	-5.42	1.95	2.05
18	Z	610	CLA	MG-ND	-5.42	1.95	2.05
18	1	611	CLA	MG-ND	-5.41	1.95	2.05
18	8	610	CLA	MG-NA	-5.41	1.93	2.06
18	3	301	CLA	MG-NA	-5.41	1.93	2.06
18	4	607	CLA	MG-NA	-5.40	1.93	2.06
18	F	301	CLA	C1B-NB	5.39	1.40	1.35
21	7	606	CHL	MG-NC	-5.39	1.93	2.06
18	B	824	CLA	C1B-NB	5.38	1.40	1.35
18	A	827	CLA	MG-NC	-5.38	1.93	2.06
18	A	819	CLA	C1B-NB	5.37	1.40	1.35
18	B	828	CLA	MG-ND	-5.37	1.95	2.05
18	A	838	CLA	MG-ND	-5.37	1.95	2.05
18	5	613	CLA	MG-NA	-5.36	1.93	2.06
18	B	801	CLA	C1B-NB	5.34	1.40	1.35
18	A	815	CLA	C1B-NB	5.34	1.40	1.35
18	B	807	CLA	C1B-NB	5.33	1.40	1.35
21	5	606	CHL	MG-NC	-5.33	1.93	2.06
18	3	312	CLA	MG-ND	-5.33	1.95	2.05
21	7	606	CHL	MG-NA	-5.33	1.93	2.06
18	A	833	CLA	MG-ND	-5.33	1.95	2.05
18	A	802	CLA	MG-NA	-5.32	1.93	2.06
18	A	811	CLA	MG-NA	-5.32	1.93	2.06
18	5	612	CLA	C1B-NB	5.32	1.40	1.35
21	8	606	CHL	MG-NA	-5.31	1.93	2.06
18	6	311	CLA	MG-ND	-5.31	1.95	2.05
18	B	808	CLA	C1B-NB	5.31	1.39	1.35
18	A	825	CLA	MG-NC	-5.31	1.93	2.06
18	B	841	CLA	C1B-NB	5.31	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	809	CLA	MG-ND	-5.30	1.95	2.05
18	7	614	CLA	MG-NA	-5.30	1.93	2.06
18	3	310	CLA	MG-ND	-5.29	1.95	2.05
18	7	609	CLA	MG-ND	-5.29	1.95	2.05
18	5	617	CLA	MG-NA	-5.28	1.93	2.06
18	A	836	CLA	MG-ND	-5.28	1.95	2.05
18	A	804	CLA	C1B-NB	5.28	1.39	1.35
18	B	814	CLA	MG-ND	-5.28	1.95	2.05
18	4	612	CLA	MG-NC	-5.27	1.93	2.06
18	6	303	CLA	MG-ND	-5.26	1.95	2.05
18	B	835	CLA	MG-NA	-5.26	1.93	2.06
18	6	317	CLA	MG-ND	-5.26	1.95	2.05
18	7	613	CLA	MG-NA	-5.26	1.93	2.06
18	A	813	CLA	MG-NA	-5.25	1.93	2.06
18	8	609	CLA	MG-ND	-5.25	1.95	2.05
18	B	804	CLA	MG-NA	-5.25	1.93	2.06
18	3	302	CLA	MG-ND	-5.24	1.95	2.05
18	A	834	CLA	MG-NA	-5.24	1.93	2.06
18	Z	607	CLA	MG-NA	-5.23	1.93	2.06
18	1	608	CLA	MG-NA	-5.22	1.93	2.06
18	1	602	CLA	MG-ND	-5.21	1.95	2.05
18	Z	602	CLA	MG-ND	-5.21	1.95	2.05
18	3	309	CLA	MG-NA	-5.20	1.93	2.06
18	7	610	CLA	C1B-NB	5.20	1.39	1.35
18	1	613	CLA	MG-ND	-5.20	1.95	2.05
18	Z	612	CLA	MG-ND	-5.20	1.95	2.05
18	6	313	CLA	MG-NA	-5.19	1.93	2.06
18	A	803	CLA	MG-NC	-5.19	1.93	2.06
18	8	601	CLA	C1B-NB	5.18	1.39	1.35
18	8	614	CLA	MG-NA	-5.18	1.94	2.06
21	4	604	CHL	MG-NA	-5.18	1.94	2.06
18	B	819	CLA	MG-ND	-5.18	1.95	2.05
18	7	601	CLA	C1B-NB	5.17	1.39	1.35
18	8	602	CLA	MG-ND	-5.16	1.95	2.05
18	A	839	CLA	C1B-NB	5.16	1.39	1.35
18	B	805	CLA	MG-NC	-5.15	1.94	2.06
18	4	611	CLA	MG-NA	-5.14	1.94	2.06
18	5	615	CLA	MG-NC	-5.14	1.94	2.06
18	A	813	CLA	C1B-NB	5.14	1.39	1.35
18	A	838	CLA	MG-NA	-5.13	1.94	2.06
18	B	818	CLA	MG-NA	-5.13	1.94	2.06
18	A	807	CLA	MG-NC	-5.12	1.94	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	602	CLA	MG-NA	-5.12	1.94	2.06
18	B	824	CLA	MG-NA	-5.12	1.94	2.06
18	7	611	CLA	MG-NA	-5.11	1.94	2.06
18	5	611	CLA	MG-ND	-5.10	1.95	2.05
18	B	810	CLA	MG-NA	-5.10	1.94	2.06
18	B	805	CLA	C1B-NB	5.10	1.39	1.35
18	A	819	CLA	MG-NA	-5.10	1.94	2.06
21	4	604	CHL	MG-NC	-5.08	1.94	2.06
18	B	838	CLA	MG-NA	-5.08	1.94	2.06
18	A	807	CLA	MG-NA	-5.07	1.94	2.06
18	A	823	CLA	MG-NA	-5.07	1.94	2.06
18	B	841	CLA	MG-NC	-5.07	1.94	2.06
18	B	817	CLA	MG-NA	-5.06	1.94	2.06
18	4	609	CLA	MG-NA	-5.05	1.94	2.06
18	A	827	CLA	C1B-NB	5.05	1.39	1.35
18	4	602	CLA	MG-NA	-5.05	1.94	2.06
21	4	605	CHL	MG-NC	-5.04	1.94	2.06
18	7	601	CLA	MG-NA	-5.04	1.94	2.06
18	B	807	CLA	MG-NA	-5.04	1.94	2.06
18	A	840	CLA	MG-NA	-5.03	1.94	2.06
18	A	830	CLA	C1B-NB	5.03	1.39	1.35
18	A	816	CLA	C1B-NB	5.03	1.39	1.35
18	5	601	CLA	MG-NA	-5.03	1.94	2.06
18	B	822	CLA	MG-NA	-5.03	1.94	2.06
18	6	315	CLA	MG-NA	-5.02	1.94	2.06
18	7	603	CLA	MG-NA	-5.01	1.94	2.06
18	A	830	CLA	MG-NA	-5.01	1.94	2.06
18	6	309	CLA	MG-NA	-5.01	1.94	2.06
18	A	808	CLA	MG-NC	-5.01	1.94	2.06
18	B	802	CLA	MG-NA	-5.01	1.94	2.06
18	3	309	CLA	C3A-C2A	-5.00	1.49	1.54
18	F	301	CLA	MG-NA	-5.00	1.94	2.06
18	A	836	CLA	MG-NA	-4.99	1.94	2.06
18	5	613	CLA	MG-NC	-4.99	1.94	2.06
18	B	832	CLA	MG-NA	-4.99	1.94	2.06
18	B	837	CLA	C1B-NB	4.99	1.39	1.35
18	6	308	CLA	MG-NA	-4.99	1.94	2.06
18	A	826	CLA	MG-NA	-4.98	1.94	2.06
18	B	842	CLA	MG-NA	-4.98	1.94	2.06
18	5	610	CLA	MG-NA	-4.97	1.94	2.06
18	8	613	CLA	MG-NA	-4.97	1.94	2.06
18	4	601	CLA	MG-NC	-4.97	1.94	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	805	CLA	MG-NA	-4.97	1.94	2.06
18	J	101	CLA	MG-ND	-4.96	1.96	2.05
18	A	817	CLA	C1B-NB	4.96	1.39	1.35
18	A	835	CLA	MG-NA	-4.95	1.94	2.06
18	B	829	CLA	MG-NA	-4.95	1.94	2.06
18	8	603	CLA	MG-NA	-4.95	1.94	2.06
18	8	607	CLA	MG-NA	-4.95	1.94	2.06
18	4	606	CLA	MG-ND	-4.94	1.96	2.05
18	1	609	CLA	MG-NA	-4.93	1.94	2.06
18	3	305	CLA	MG-NC	-4.93	1.94	2.06
18	A	841	CLA	C1B-NB	4.92	1.39	1.35
18	A	836	CLA	MG-NC	-4.92	1.94	2.06
18	A	815	CLA	MG-NA	-4.92	1.94	2.06
18	B	830	CLA	C1B-NB	4.91	1.39	1.35
18	6	310	CLA	MG-NC	-4.91	1.94	2.06
18	A	806	CLA	MG-NA	-4.91	1.94	2.06
18	Z	608	CLA	MG-NA	-4.91	1.94	2.06
18	6	312	CLA	MG-NA	-4.90	1.94	2.06
18	4	606	CLA	MG-NA	-4.90	1.94	2.06
18	B	830	CLA	MG-NA	-4.89	1.94	2.06
18	Z	611	CLA	MG-NA	-4.89	1.94	2.06
18	5	610	CLA	C1B-NB	4.89	1.39	1.35
18	A	821	CLA	MG-NA	-4.88	1.94	2.06
18	5	611	CLA	MG-NA	-4.88	1.94	2.06
18	1	612	CLA	MG-NA	-4.87	1.94	2.06
18	1	607	CLA	MG-NA	-4.87	1.94	2.06
18	B	835	CLA	MG-NC	-4.87	1.94	2.06
18	3	310	CLA	MG-NA	-4.86	1.94	2.06
18	3	308	CLA	MG-NA	-4.86	1.94	2.06
18	4	609	CLA	MG-NC	-4.86	1.94	2.06
18	7	602	CLA	MG-NA	-4.86	1.94	2.06
18	8	609	CLA	MG-NC	-4.86	1.94	2.06
18	B	827	CLA	MG-NC	-4.85	1.94	2.06
18	B	813	CLA	MG-NA	-4.84	1.94	2.06
18	Z	606	CLA	MG-NA	-4.84	1.94	2.06
18	8	607	CLA	C1B-NB	4.84	1.39	1.35
18	B	810	CLA	C1B-NB	4.84	1.39	1.35
18	B	821	CLA	MG-NA	-4.84	1.94	2.06
18	A	841	CLA	MG-NA	-4.83	1.94	2.06
18	A	832	CLA	C1B-NB	4.83	1.39	1.35
18	A	805	CLA	C1B-NB	4.83	1.39	1.35
18	5	601	CLA	C1B-NB	4.82	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	601	CHL	MG-NA	-4.82	1.94	2.06
18	5	609	CLA	MG-NA	-4.81	1.94	2.06
18	B	838	CLA	MG-NC	-4.81	1.94	2.06
18	Z	602	CLA	MG-NA	-4.80	1.94	2.06
18	4	607	CLA	MG-NC	-4.80	1.94	2.06
18	1	611	CLA	MG-NA	-4.80	1.94	2.06
18	B	839	CLA	MG-NA	-4.80	1.94	2.06
18	8	602	CLA	MG-NA	-4.80	1.94	2.06
18	8	604	CLA	MG-NA	-4.80	1.94	2.06
18	B	826	CLA	MG-NA	-4.80	1.94	2.06
21	Z	601	CHL	MG-NA	-4.80	1.94	2.06
18	A	802	CLA	MG-NC	-4.80	1.94	2.06
18	B	806	CLA	MG-NC	-4.80	1.94	2.06
18	7	609	CLA	MG-NA	-4.79	1.94	2.06
18	B	801	CLA	MG-NA	-4.78	1.94	2.06
18	A	816	CLA	MG-NA	-4.78	1.94	2.06
18	B	834	CLA	MG-NA	-4.78	1.94	2.06
18	1	602	CLA	MG-NA	-4.78	1.94	2.06
18	7	607	CLA	MG-NA	-4.77	1.94	2.06
18	A	824	CLA	MG-NC	-4.77	1.94	2.06
21	5	607	CHL	MG-NA	-4.77	1.94	2.06
18	A	832	CLA	MG-NA	-4.77	1.94	2.06
18	1	604	CLA	MG-NA	-4.77	1.94	2.06
18	1	610	CLA	MG-NA	-4.77	1.94	2.06
18	A	845	CLA	MG-NA	-4.77	1.94	2.06
18	6	311	CLA	MG-NA	-4.76	1.95	2.06
18	A	814	CLA	MG-NA	-4.76	1.95	2.06
18	7	611	CLA	MG-NC	-4.76	1.95	2.06
18	B	820	CLA	C1B-NB	4.76	1.39	1.35
18	Z	610	CLA	MG-NA	-4.76	1.95	2.06
18	Z	603	CLA	MG-NA	-4.76	1.95	2.06
18	8	607	CLA	MG-NC	-4.76	1.95	2.06
18	Z	603	CLA	MG-NC	-4.76	1.95	2.06
18	8	608	CLA	MG-NA	-4.75	1.95	2.06
18	B	833	CLA	MG-NA	-4.75	1.95	2.06
18	B	831	CLA	MG-NA	-4.75	1.95	2.06
18	4	608	CLA	MG-NC	-4.75	1.95	2.06
18	1	604	CLA	MG-NC	-4.74	1.95	2.06
21	1	606	CHL	MG-NC	-4.74	1.95	2.06
18	3	301	CLA	MG-NC	-4.74	1.95	2.06
18	B	809	CLA	MG-NA	-4.74	1.95	2.06
18	B	804	CLA	MG-NC	-4.74	1.95	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	818	CLA	MG-NA	-4.74	1.95	2.06
18	Z	609	CLA	MG-NA	-4.73	1.95	2.06
18	8	611	CLA	MG-NC	-4.73	1.95	2.06
21	Z	605	CHL	MG-NC	-4.73	1.95	2.06
18	B	812	CLA	MG-NC	-4.73	1.95	2.06
18	A	816	CLA	MG-NC	-4.73	1.95	2.06
18	1	613	CLA	MG-NA	-4.73	1.95	2.06
18	3	314	CLA	C1B-NB	4.73	1.39	1.35
18	3	312	CLA	MG-NA	-4.73	1.95	2.06
18	6	302	CLA	MG-NA	-4.73	1.95	2.06
18	B	828	CLA	MG-NA	-4.73	1.95	2.06
18	Z	612	CLA	MG-NA	-4.73	1.95	2.06
21	6	307	CHL	MG-NA	-4.72	1.95	2.06
18	A	837	CLA	MG-NA	-4.72	1.95	2.06
18	8	601	CLA	MG-NA	-4.71	1.95	2.06
18	A	820	CLA	C1B-NB	4.71	1.39	1.35
18	A	831	CLA	MG-NA	-4.70	1.95	2.06
18	3	307	CLA	MG-NC	-4.70	1.95	2.06
18	B	814	CLA	MG-NC	-4.70	1.95	2.06
18	3	303	CLA	MG-NA	-4.70	1.95	2.06
21	6	307	CHL	MG-NC	-4.69	1.95	2.06
18	8	610	CLA	MG-NC	-4.68	1.95	2.06
18	A	823	CLA	MG-NC	-4.68	1.95	2.06
18	A	809	CLA	MG-NA	-4.68	1.95	2.06
18	6	304	CLA	MG-NA	-4.67	1.95	2.06
18	7	605	CLA	MG-NA	-4.67	1.95	2.06
18	8	614	CLA	MG-NC	-4.66	1.95	2.06
17	A	801	CL0	MG-NA	-4.66	1.95	2.06
18	J	101	CLA	MG-NA	-4.66	1.95	2.06
18	B	840	CLA	MG-NA	-4.65	1.95	2.06
18	B	814	CLA	MG-NA	-4.65	1.95	2.06
18	A	812	CLA	MG-NA	-4.64	1.95	2.06
18	7	612	CLA	MG-NA	-4.64	1.95	2.06
18	7	614	CLA	MG-NC	-4.64	1.95	2.06
18	7	608	CLA	MG-NC	-4.63	1.95	2.06
18	A	818	CLA	MG-NC	-4.63	1.95	2.06
21	6	306	CHL	MG-NA	-4.62	1.95	2.06
18	5	604	CLA	MG-NA	-4.62	1.95	2.06
18	5	612	CLA	MG-NA	-4.62	1.95	2.06
18	B	819	CLA	MG-NC	-4.61	1.95	2.06
18	B	836	CLA	MG-NA	-4.60	1.95	2.06
18	5	608	CLA	MG-NA	-4.60	1.95	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	823	CLA	MG-NA	-4.60	1.95	2.06
18	B	838	CLA	C1B-NB	4.59	1.39	1.35
18	A	818	CLA	C1B-NB	4.59	1.39	1.35
18	1	614	CLA	MG-NA	-4.59	1.95	2.06
18	B	815	CLA	MG-NC	-4.59	1.95	2.06
18	A	845	CLA	MG-NC	-4.58	1.95	2.06
18	A	820	CLA	MG-NA	-4.58	1.95	2.06
18	B	816	CLA	MG-NA	-4.58	1.95	2.06
18	3	313	CLA	MG-NA	-4.58	1.95	2.06
18	Z	613	CLA	MG-NA	-4.58	1.95	2.06
18	7	607	CLA	MG-NC	-4.58	1.95	2.06
21	6	306	CHL	MG-NC	-4.58	1.95	2.06
18	A	825	CLA	C1B-NB	4.58	1.39	1.35
18	7	613	CLA	MG-NC	-4.58	1.95	2.06
18	Z	613	CLA	MG-NC	-4.58	1.95	2.06
18	3	314	CLA	MG-NA	-4.58	1.95	2.06
18	B	840	CLA	C1B-NB	4.57	1.39	1.35
18	A	840	CLA	MG-NC	-4.57	1.95	2.06
18	A	829	CLA	MG-NA	-4.57	1.95	2.06
18	A	835	CLA	MG-NC	-4.57	1.95	2.06
18	A	810	CLA	MG-NC	-4.57	1.95	2.06
18	6	314	CLA	MG-NA	-4.57	1.95	2.06
18	A	839	CLA	MG-NA	-4.55	1.95	2.06
18	5	614	CLA	MG-NA	-4.55	1.95	2.06
18	A	812	CLA	MG-NC	-4.55	1.95	2.06
18	1	614	CLA	MG-NC	-4.55	1.95	2.06
18	A	826	CLA	MG-NC	-4.55	1.95	2.06
18	B	802	CLA	C1B-NB	4.53	1.39	1.35
18	A	819	CLA	MG-NC	-4.53	1.95	2.06
18	A	830	CLA	MG-NC	-4.52	1.95	2.06
18	5	601	CLA	MG-NC	-4.51	1.95	2.06
18	A	843	CLA	MG-NA	-4.51	1.95	2.06
18	3	302	CLA	MG-NA	-4.51	1.95	2.06
18	8	603	CLA	MG-NC	-4.51	1.95	2.06
18	3	312	CLA	MG-NC	-4.51	1.95	2.06
18	A	828	CLA	MG-NA	-4.50	1.95	2.06
18	A	817	CLA	MG-NA	-4.50	1.95	2.06
18	A	806	CLA	MG-NC	-4.50	1.95	2.06
18	B	831	CLA	MG-NC	-4.50	1.95	2.06
18	B	807	CLA	MG-NC	-4.49	1.95	2.06
18	B	842	CLA	MG-NC	-4.49	1.95	2.06
21	5	607	CHL	MG-NC	-4.48	1.95	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	311	CLA	MG-NA	-4.48	1.95	2.06
18	7	610	CLA	MG-NC	-4.48	1.95	2.06
18	B	829	CLA	MG-NC	-4.48	1.95	2.06
18	B	818	CLA	MG-NC	-4.48	1.95	2.06
18	B	811	CLA	C1B-NB	4.48	1.39	1.35
18	3	310	CLA	MG-NC	-4.47	1.95	2.06
18	6	313	CLA	MG-NC	-4.47	1.95	2.06
18	7	601	CLA	MG-NC	-4.47	1.95	2.06
21	1	601	CHL	MG-NC	-4.47	1.95	2.06
18	A	844	CLA	C1B-NB	4.47	1.39	1.35
18	6	315	CLA	MG-NC	-4.46	1.95	2.06
18	B	820	CLA	MG-NC	-4.46	1.95	2.06
18	F	302	CLA	MG-NA	-4.46	1.95	2.06
18	A	822	CLA	MG-NA	-4.46	1.95	2.06
18	A	815	CLA	MG-NC	-4.45	1.95	2.06
21	Z	601	CHL	MG-NC	-4.45	1.95	2.06
18	A	838	CLA	MG-NC	-4.45	1.95	2.06
21	Z	605	CHL	MG-NA	-4.45	1.95	2.06
18	6	303	CLA	MG-NA	-4.44	1.95	2.06
18	A	834	CLA	MG-NC	-4.43	1.95	2.06
21	1	606	CHL	MG-NA	-4.43	1.95	2.06
18	3	308	CLA	MG-NC	-4.43	1.95	2.06
18	A	805	CLA	MG-NC	-4.43	1.95	2.06
18	J	101	CLA	MG-NC	-4.43	1.95	2.06
18	4	603	CLA	MG-NA	-4.42	1.95	2.06
17	A	801	CL0	C1B-NB	4.42	1.39	1.35
18	6	311	CLA	MG-NC	-4.41	1.95	2.06
18	5	617	CLA	C1B-NB	4.41	1.39	1.35
18	5	602	CLA	MG-NC	-4.41	1.95	2.06
18	A	824	CLA	C1B-NB	4.41	1.39	1.35
18	A	820	CLA	MG-NC	-4.40	1.95	2.06
18	B	828	CLA	C1B-NB	4.40	1.39	1.35
21	6	316	CHL	MG-NC	-4.40	1.95	2.06
18	A	833	CLA	MG-NA	-4.40	1.95	2.06
18	B	825	CLA	MG-NA	-4.39	1.95	2.06
18	7	602	CLA	MG-NC	-4.38	1.95	2.06
18	F	301	CLA	MG-NC	-4.38	1.95	2.06
18	3	304	CLA	MG-NA	-4.37	1.95	2.06
21	5	616	CHL	MG-NA	-4.37	1.95	2.06
18	B	837	CLA	MG-NA	-4.37	1.95	2.06
21	5	616	CHL	MG-NC	-4.36	1.95	2.06
18	B	833	CLA	MG-NC	-4.36	1.95	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	834	CLA	C1B-NB	4.36	1.39	1.35
18	A	822	CLA	MG-NC	-4.36	1.95	2.06
18	6	317	CLA	MG-NA	-4.36	1.95	2.06
18	5	617	CLA	MG-NC	-4.35	1.95	2.06
18	A	814	CLA	MG-NC	-4.35	1.95	2.06
18	A	844	CLA	MG-NA	-4.35	1.95	2.06
18	B	801	CLA	MG-NC	-4.35	1.95	2.06
18	7	609	CLA	MG-NC	-4.35	1.95	2.06
18	B	826	CLA	MG-NC	-4.35	1.95	2.06
18	7	603	CLA	MG-NC	-4.34	1.96	2.06
18	3	314	CLA	MG-NC	-4.34	1.96	2.06
18	8	612	CLA	MG-NA	-4.34	1.96	2.06
18	A	837	CLA	MG-NC	-4.33	1.96	2.06
18	B	843	CLA	MG-NA	-4.33	1.96	2.06
18	5	603	CLA	MG-NA	-4.32	1.96	2.06
18	B	816	CLA	MG-NC	-4.32	1.96	2.06
18	B	810	CLA	MG-NC	-4.32	1.96	2.06
18	5	611	CLA	MG-NC	-4.32	1.96	2.06
18	1	608	CLA	MG-NC	-4.31	1.96	2.06
21	3	306	CHL	MG-NA	-4.31	1.96	2.06
18	4	610	CLA	MG-NA	-4.30	1.96	2.06
18	6	304	CLA	MG-NC	-4.30	1.96	2.06
18	Z	607	CLA	MG-NC	-4.30	1.96	2.06
18	1	602	CLA	MG-NC	-4.30	1.96	2.06
17	A	801	CL0	MG-NC	-4.30	1.96	2.06
18	B	808	CLA	MG-NA	-4.29	1.96	2.06
18	1	603	CLA	MG-NA	-4.29	1.96	2.06
18	3	309	CLA	MG-NC	-4.29	1.96	2.06
18	A	817	CLA	MG-NC	-4.28	1.96	2.06
18	B	822	CLA	MG-NC	-4.28	1.96	2.06
18	Z	602	CLA	MG-NC	-4.28	1.96	2.06
18	8	608	CLA	MG-NC	-4.28	1.96	2.06
18	A	811	CLA	MG-NC	-4.27	1.96	2.06
18	B	824	CLA	MG-NC	-4.27	1.96	2.06
18	B	802	CLA	MG-NC	-4.27	1.96	2.06
18	8	615	CLA	MG-NA	-4.27	1.96	2.06
18	A	841	CLA	MG-NC	-4.27	1.96	2.06
18	4	602	CLA	MG-NC	-4.26	1.96	2.06
21	3	306	CHL	MG-NC	-4.26	1.96	2.06
18	1	613	CLA	MG-NC	-4.25	1.96	2.06
18	6	301	CLA	MG-NA	-4.25	1.96	2.06
18	A	809	CLA	MG-NC	-4.25	1.96	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Z	612	CLA	MG-NC	-4.24	1.96	2.06
18	B	813	CLA	MG-NC	-4.24	1.96	2.06
18	B	817	CLA	MG-NC	-4.23	1.96	2.06
18	6	302	CLA	MG-NC	-4.23	1.96	2.06
18	A	832	CLA	MG-NC	-4.23	1.96	2.06
21	6	305	CHL	MG-NC	-4.23	1.96	2.06
18	A	804	CLA	MG-NA	-4.23	1.96	2.06
18	3	313	CLA	MG-NC	-4.22	1.96	2.06
18	B	843	CLA	MG-NC	-4.22	1.96	2.06
18	4	603	CLA	MG-NC	-4.22	1.96	2.06
18	B	811	CLA	MG-NA	-4.21	1.96	2.06
18	8	613	CLA	MG-NC	-4.21	1.96	2.06
18	3	303	CLA	MG-NC	-4.21	1.96	2.06
21	6	316	CHL	MG-NA	-4.21	1.96	2.06
18	6	308	CLA	MG-NC	-4.21	1.96	2.06
18	A	831	CLA	MG-NC	-4.20	1.96	2.06
18	5	609	CLA	MG-NC	-4.20	1.96	2.06
18	B	809	CLA	MG-NC	-4.20	1.96	2.06
18	8	605	CLA	MG-NA	-4.20	1.96	2.06
18	5	612	CLA	MG-NC	-4.20	1.96	2.06
18	4	611	CLA	MG-NC	-4.20	1.96	2.06
18	Z	610	CLA	MG-NC	-4.19	1.96	2.06
21	4	605	CHL	C3B-C2B	-4.19	1.34	1.40
18	6	312	CLA	MG-NC	-4.19	1.96	2.06
18	A	829	CLA	MG-NC	-4.18	1.96	2.06
18	Z	609	CLA	MG-NC	-4.18	1.96	2.06
18	B	832	CLA	MG-NC	-4.18	1.96	2.06
18	B	839	CLA	MG-NC	-4.17	1.96	2.06
18	8	602	CLA	MG-NC	-4.16	1.96	2.06
18	1	611	CLA	MG-NC	-4.16	1.96	2.06
18	B	836	CLA	MG-NC	-4.16	1.96	2.06
18	5	608	CLA	MG-NC	-4.16	1.96	2.06
18	8	604	CLA	MG-NC	-4.15	1.96	2.06
18	1	610	CLA	MG-NC	-4.15	1.96	2.06
18	7	605	CLA	MG-NC	-4.15	1.96	2.06
18	A	821	CLA	MG-NC	-4.14	1.96	2.06
18	3	311	CLA	MG-NC	-4.13	1.96	2.06
18	B	808	CLA	MG-NC	-4.12	1.96	2.06
18	B	823	CLA	MG-ND	-4.12	1.97	2.05
18	5	605	CLA	MG-NA	-4.12	1.96	2.06
18	Z	608	CLA	MG-NC	-4.11	1.96	2.06
18	6	309	CLA	MG-NC	-4.11	1.96	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	609	CLA	MG-NC	-4.10	1.96	2.06
18	6	303	CLA	MG-NC	-4.10	1.96	2.06
18	3	304	CLA	MG-NC	-4.10	1.96	2.06
18	B	828	CLA	MG-NC	-4.09	1.96	2.06
18	8	612	CLA	MG-NC	-4.09	1.96	2.06
18	B	825	CLA	MG-NC	-4.08	1.96	2.06
18	5	604	CLA	MG-NC	-4.08	1.96	2.06
18	A	839	CLA	MG-NC	-4.07	1.96	2.06
18	8	601	CLA	MG-NC	-4.06	1.96	2.06
18	A	813	CLA	MG-NC	-4.05	1.96	2.06
18	7	612	CLA	MG-NC	-4.05	1.96	2.06
18	3	302	CLA	MG-NC	-4.05	1.96	2.06
18	B	840	CLA	MG-NC	-4.03	1.96	2.06
18	A	843	CLA	MG-NC	-4.02	1.96	2.06
18	A	828	CLA	MG-NC	-4.01	1.96	2.06
21	6	305	CHL	MG-NA	-3.99	1.96	2.06
18	1	607	CLA	MG-NC	-3.99	1.96	2.06
18	B	830	CLA	MG-NC	-3.99	1.96	2.06
18	F	302	CLA	MG-NC	-3.99	1.96	2.06
18	6	317	CLA	MG-NC	-3.98	1.96	2.06
18	Z	606	CLA	MG-NC	-3.97	1.96	2.06
18	A	833	CLA	MG-NC	-3.96	1.96	2.06
18	5	610	CLA	MG-NC	-3.96	1.96	2.06
18	B	821	CLA	MG-NC	-3.96	1.96	2.06
18	B	834	CLA	MG-NC	-3.94	1.96	2.06
18	1	605	CLA	MG-NA	-3.92	1.97	2.06
18	Z	604	CLA	MG-NA	-3.91	1.97	2.06
18	1	612	CLA	MG-NC	-3.91	1.97	2.06
18	6	314	CLA	MG-NC	-3.91	1.97	2.06
18	4	606	CLA	MG-NC	-3.91	1.97	2.06
18	Z	611	CLA	MG-NC	-3.91	1.97	2.06
18	8	615	CLA	MG-NC	-3.90	1.97	2.06
18	7	604	CLA	MG-NA	-3.90	1.97	2.06
18	5	614	CLA	MG-NC	-3.89	1.97	2.06
18	1	603	CLA	MG-NC	-3.88	1.97	2.06
21	4	605	CHL	MG-ND	-3.86	1.98	2.05
18	8	605	CLA	MG-NC	-3.82	1.97	2.06
18	A	844	CLA	MG-NC	-3.82	1.97	2.06
18	B	804	CLA	C1B-NB	3.81	1.38	1.35
18	6	310	CLA	C1B-NB	3.77	1.38	1.35
18	A	828	CLA	C1B-NB	3.77	1.38	1.35
18	B	837	CLA	MG-NC	-3.75	1.97	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	603	CLA	MG-NC	-3.75	1.97	2.06
18	5	601	CLA	C1D-ND	3.72	1.42	1.37
18	6	301	CLA	C1D-ND	3.72	1.42	1.37
18	7	604	CLA	C1D-ND	3.71	1.42	1.37
18	A	804	CLA	MG-NC	-3.71	1.97	2.06
18	6	304	CLA	C1D-ND	3.70	1.42	1.37
18	Z	612	CLA	C1D-ND	3.70	1.42	1.37
18	J	101	CLA	C1D-ND	3.69	1.42	1.37
18	8	608	CLA	C1D-ND	3.69	1.42	1.37
18	1	613	CLA	C1D-ND	3.67	1.42	1.37
18	4	610	CLA	MG-NC	-3.67	1.97	2.06
18	1	611	CLA	C1D-ND	3.65	1.42	1.37
18	6	301	CLA	MG-NC	-3.65	1.97	2.06
18	B	843	CLA	C1D-ND	3.64	1.42	1.37
18	B	811	CLA	MG-NC	-3.64	1.97	2.06
18	B	829	CLA	C1B-NB	3.63	1.38	1.35
18	Z	610	CLA	C1D-ND	3.63	1.42	1.37
18	B	823	CLA	MG-NC	-3.63	1.97	2.06
18	B	807	CLA	C2-C3	3.60	1.52	1.28
18	8	610	CLA	C1B-NB	3.59	1.38	1.35
18	A	825	CLA	C3A-C2A	-3.58	1.44	1.54
18	3	312	CLA	C1D-ND	3.58	1.42	1.37
21	5	606	CHL	C1B-NB	3.57	1.38	1.35
18	5	605	CLA	MG-NC	-3.55	1.97	2.06
21	3	306	CHL	C3B-C2B	-3.53	1.35	1.40
18	Z	604	CLA	MG-NC	-3.53	1.97	2.06
18	1	605	CLA	MG-NC	-3.52	1.97	2.06
18	1	604	CLA	C1D-ND	3.51	1.42	1.37
18	5	604	CLA	C1D-ND	3.50	1.42	1.37
18	4	606	CLA	C1D-ND	3.48	1.42	1.37
18	Z	603	CLA	C1D-ND	3.45	1.42	1.37
18	8	609	CLA	C1D-ND	3.45	1.42	1.37
18	B	814	CLA	C1D-ND	3.43	1.42	1.37
18	A	833	CLA	C1D-ND	3.38	1.41	1.37
18	6	312	CLA	C1D-ND	3.33	1.41	1.37
21	1	601	CHL	C3B-C2B	-3.33	1.35	1.40
18	5	614	CLA	C1D-ND	3.33	1.41	1.37
21	6	307	CHL	C3B-C2B	-3.32	1.35	1.40
18	6	317	CLA	C1D-ND	3.31	1.41	1.37
21	Z	601	CHL	C3B-C2B	-3.31	1.35	1.40
18	1	603	CLA	C1D-ND	3.30	1.41	1.37
18	8	615	CLA	C1D-ND	3.29	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	808	CLA	C1D-ND	3.27	1.41	1.37
18	B	828	CLA	C1D-ND	3.27	1.41	1.37
18	5	605	CLA	C1D-ND	3.25	1.41	1.37
18	5	609	CLA	C1D-ND	3.25	1.41	1.37
18	B	823	CLA	C1D-ND	3.24	1.41	1.37
18	A	822	CLA	C1D-ND	3.24	1.41	1.37
21	Z	605	CHL	C3B-C2B	-3.24	1.35	1.40
18	A	832	CLA	C1D-ND	3.24	1.41	1.37
18	A	829	CLA	C1D-ND	3.23	1.41	1.37
18	3	313	CLA	C1D-ND	3.23	1.41	1.37
18	A	839	CLA	C1D-ND	3.22	1.41	1.37
18	A	816	CLA	C1D-ND	3.21	1.41	1.37
18	B	810	CLA	C1D-ND	3.21	1.41	1.37
21	1	606	CHL	C3B-C2B	-3.21	1.35	1.40
18	5	603	CLA	C1D-ND	3.20	1.41	1.37
18	6	311	CLA	C1D-ND	3.19	1.41	1.37
18	B	826	CLA	C1D-ND	3.19	1.41	1.37
18	3	314	CLA	C1D-ND	3.19	1.41	1.37
18	7	613	CLA	C1D-ND	3.19	1.41	1.37
21	5	606	CHL	C3B-C2B	-3.19	1.35	1.40
21	4	605	CHL	C1B-NB	3.19	1.38	1.35
21	4	605	CHL	MG-NA	-3.18	1.98	2.06
18	6	309	CLA	C1D-ND	3.18	1.41	1.37
18	B	825	CLA	C1D-ND	3.18	1.41	1.37
18	A	834	CLA	C3A-C2A	-3.18	1.45	1.54
17	A	801	CL0	C3B-C2B	-3.17	1.36	1.40
21	4	605	CHL	C1D-ND	3.17	1.41	1.37
18	1	614	CLA	C1D-ND	3.16	1.41	1.37
18	4	609	CLA	C1D-ND	3.16	1.41	1.37
18	B	831	CLA	C1D-ND	3.16	1.41	1.37
21	4	604	CHL	C1B-NB	3.16	1.38	1.35
21	7	606	CHL	C3B-C2B	-3.16	1.36	1.40
18	7	604	CLA	MG-NC	-3.15	1.98	2.06
18	8	612	CLA	C1D-ND	3.14	1.41	1.37
18	7	609	CLA	C1D-ND	3.13	1.41	1.37
18	4	610	CLA	C1D-ND	3.13	1.41	1.37
21	6	306	CHL	C3B-C2B	-3.12	1.36	1.40
18	Z	613	CLA	C1D-ND	3.12	1.41	1.37
18	3	310	CLA	C1D-ND	3.12	1.41	1.37
18	8	605	CLA	C1D-ND	3.12	1.41	1.37
18	Z	602	CLA	C1D-ND	3.12	1.41	1.37
18	1	609	CLA	C1D-ND	3.11	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	311	CLA	C1D-ND	3.11	1.41	1.37
18	B	812	CLA	C1D-ND	3.10	1.41	1.37
18	Z	608	CLA	C1D-ND	3.10	1.41	1.37
18	8	602	CLA	C1D-ND	3.10	1.41	1.37
18	Z	606	CLA	C1D-ND	3.09	1.41	1.37
18	6	313	CLA	C1D-ND	3.09	1.41	1.37
18	A	803	CLA	C3A-C2A	-3.09	1.45	1.54
21	5	607	CHL	C3B-C2B	-3.07	1.36	1.40
18	1	602	CLA	C1D-ND	3.07	1.41	1.37
18	8	613	CLA	C1D-ND	3.07	1.41	1.37
17	A	801	CL0	C1D-ND	3.07	1.41	1.37
18	1	607	CLA	C1D-ND	3.06	1.41	1.37
21	1	606	CHL	C3D-C4D	-3.06	1.37	1.44
21	Z	605	CHL	C3D-C4D	-3.06	1.37	1.44
18	8	607	CLA	C3B-C2B	-3.03	1.36	1.40
18	1	612	CLA	C1D-ND	3.03	1.41	1.37
18	3	308	CLA	C1D-ND	3.03	1.41	1.37
21	4	604	CHL	C3A-C2A	-3.03	1.46	1.54
21	5	616	CHL	C3B-C2B	-3.03	1.36	1.40
18	4	607	CLA	C1D-ND	3.03	1.41	1.37
18	A	812	CLA	C1D-ND	3.02	1.41	1.37
18	A	845	CLA	C1D-ND	3.02	1.41	1.37
18	7	614	CLA	C1D-ND	3.02	1.41	1.37
18	A	823	CLA	C1D-ND	3.00	1.41	1.37
18	7	611	CLA	C1D-ND	3.00	1.41	1.37
18	B	836	CLA	C1D-ND	3.00	1.41	1.37
18	8	607	CLA	C3A-C2A	-3.00	1.46	1.54
18	B	837	CLA	C1D-ND	3.00	1.41	1.37
18	B	832	CLA	C1D-ND	2.99	1.41	1.37
18	B	823	CLA	C1C-C2C	2.98	1.50	1.44
18	5	608	CLA	C1D-ND	2.97	1.41	1.37
18	8	607	CLA	C1D-ND	2.96	1.41	1.37
18	6	303	CLA	C1D-ND	2.95	1.41	1.37
18	1	605	CLA	C1D-ND	2.94	1.41	1.37
18	A	828	CLA	C3B-C2B	-2.94	1.36	1.40
18	B	821	CLA	C1D-ND	2.94	1.41	1.37
18	Z	611	CLA	C1D-ND	2.94	1.41	1.37
18	7	608	CLA	C1D-ND	2.93	1.41	1.37
18	B	824	CLA	C1D-ND	2.93	1.41	1.37
18	A	806	CLA	C1D-ND	2.93	1.41	1.37
18	A	820	CLA	C1D-ND	2.92	1.41	1.37
18	Z	604	CLA	C1D-ND	2.91	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	834	CLA	C1D-ND	2.91	1.41	1.37
18	B	822	CLA	C1D-ND	2.91	1.41	1.37
18	3	302	CLA	C1D-ND	2.91	1.41	1.37
18	B	816	CLA	C1D-ND	2.91	1.41	1.37
18	6	314	CLA	C1D-ND	2.91	1.41	1.37
21	5	616	CHL	C1D-ND	2.91	1.41	1.37
18	8	611	CLA	C3A-C2A	-2.89	1.46	1.54
18	6	308	CLA	C1D-ND	2.89	1.41	1.37
18	B	817	CLA	C1D-ND	2.89	1.41	1.37
18	B	838	CLA	C1D-ND	2.88	1.41	1.37
18	B	813	CLA	C1D-ND	2.88	1.41	1.37
18	8	604	CLA	C1D-ND	2.87	1.41	1.37
18	A	807	CLA	C1D-ND	2.87	1.41	1.37
18	B	811	CLA	C3A-C2A	-2.86	1.46	1.54
18	A	830	CLA	C1D-ND	2.86	1.41	1.37
18	A	835	CLA	C1D-ND	2.86	1.41	1.37
18	A	843	CLA	C1D-ND	2.86	1.41	1.37
18	A	815	CLA	C3B-C2B	-2.85	1.36	1.40
18	7	607	CLA	C1D-ND	2.84	1.41	1.37
18	A	841	CLA	C1D-ND	2.83	1.41	1.37
18	7	603	CLA	C1D-ND	2.83	1.41	1.37
18	A	804	CLA	C1D-ND	2.82	1.41	1.37
18	A	837	CLA	C3A-C2A	-2.82	1.46	1.54
18	7	601	CLA	C3B-C2B	-2.82	1.36	1.40
18	A	821	CLA	C1D-ND	2.81	1.41	1.37
21	6	306	CHL	C1D-ND	2.81	1.41	1.37
18	B	840	CLA	C1D-ND	2.80	1.41	1.37
21	3	306	CHL	C3A-C2A	-2.80	1.46	1.54
18	4	603	CLA	C1D-C2D	-2.80	1.39	1.45
18	5	612	CLA	C1D-ND	2.79	1.41	1.37
21	8	606	CHL	C3B-C2B	-2.79	1.36	1.40
18	A	836	CLA	C1D-ND	2.78	1.41	1.37
18	A	839	CLA	C3A-C2A	-2.78	1.46	1.54
21	6	316	CHL	C3B-C2B	-2.78	1.36	1.40
18	F	302	CLA	C1D-ND	2.78	1.41	1.37
18	4	607	CLA	C1C-C2C	2.78	1.49	1.44
18	A	833	CLA	C3B-C2B	-2.77	1.36	1.40
17	A	801	CL0	C3A-C2A	-2.77	1.46	1.54
18	A	806	CLA	C3A-C2A	-2.76	1.46	1.54
18	A	825	CLA	C3B-C2B	-2.76	1.36	1.40
18	A	811	CLA	C1D-ND	2.75	1.41	1.37
18	B	830	CLA	C1D-ND	2.75	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	828	CLA	C3B-C2B	-2.73	1.36	1.40
18	3	304	CLA	C1D-ND	2.73	1.41	1.37
21	6	306	CHL	C1B-NB	2.73	1.37	1.35
18	3	303	CLA	C1D-ND	2.73	1.41	1.37
18	A	809	CLA	C1D-ND	2.72	1.41	1.37
18	3	309	CLA	C1D-ND	2.72	1.41	1.37
21	6	316	CHL	C1D-ND	2.72	1.41	1.37
18	B	833	CLA	C1D-ND	2.72	1.41	1.37
18	B	811	CLA	C1D-ND	2.71	1.41	1.37
18	A	826	CLA	C3A-C2A	-2.71	1.46	1.54
18	5	608	CLA	C1D-C2D	-2.71	1.40	1.45
18	8	601	CLA	C3B-C2B	-2.70	1.36	1.40
18	A	845	CLA	C1D-C2D	-2.70	1.40	1.45
21	4	604	CHL	C3B-C2B	-2.69	1.36	1.40
18	B	825	CLA	C3A-C2A	-2.69	1.46	1.54
18	A	810	CLA	C1D-ND	2.69	1.41	1.37
18	B	819	CLA	C1D-ND	2.69	1.41	1.37
18	6	302	CLA	C1D-ND	2.69	1.41	1.37
18	4	611	CLA	C1D-ND	2.68	1.41	1.37
18	6	304	CLA	C1D-C2D	-2.68	1.40	1.45
18	A	828	CLA	C1D-ND	2.68	1.41	1.37
18	5	603	CLA	C1D-C2D	-2.68	1.40	1.45
18	B	829	CLA	C1D-C2D	-2.68	1.40	1.45
18	A	826	CLA	C1D-ND	2.68	1.41	1.37
21	8	606	CHL	C1B-NB	2.68	1.37	1.35
18	4	602	CLA	C1D-ND	2.67	1.41	1.37
18	5	605	CLA	C3A-C2A	-2.67	1.47	1.54
18	8	608	CLA	C1D-C2D	-2.66	1.40	1.45
18	8	603	CLA	C1D-ND	2.66	1.41	1.37
21	6	305	CHL	C3B-C2B	-2.66	1.36	1.40
18	5	611	CLA	C1D-ND	2.66	1.41	1.37
18	B	812	CLA	C3A-C2A	-2.66	1.47	1.54
18	A	838	CLA	C1D-ND	2.66	1.41	1.37
18	A	835	CLA	C1D-C2D	-2.65	1.40	1.45
18	8	615	CLA	C1D-C2D	-2.65	1.40	1.45
18	B	808	CLA	C1D-C2D	-2.65	1.40	1.45
18	B	807	CLA	C3A-C2A	-2.65	1.47	1.54
18	A	821	CLA	C1D-C2D	-2.64	1.40	1.45
18	1	603	CLA	C1D-C2D	-2.64	1.40	1.45
18	5	601	CLA	C1D-C2D	-2.64	1.40	1.45
18	7	612	CLA	C1D-ND	2.64	1.41	1.37
18	7	602	CLA	C1D-ND	2.63	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	841	CLA	C1D-ND	2.63	1.41	1.37
18	8	607	CLA	C1D-C2D	-2.62	1.40	1.45
18	A	839	CLA	C1D-C2D	-2.62	1.40	1.45
18	B	807	CLA	C1D-ND	2.62	1.41	1.37
18	B	833	CLA	C1D-C2D	-2.62	1.40	1.45
18	A	813	CLA	C1D-ND	2.62	1.41	1.37
18	B	842	CLA	C1D-ND	2.62	1.41	1.37
18	8	602	CLA	C3B-C2B	-2.62	1.36	1.40
18	5	602	CLA	C1D-C2D	-2.62	1.40	1.45
18	A	809	CLA	C1D-C2D	-2.61	1.40	1.45
18	A	815	CLA	C1D-ND	2.61	1.41	1.37
18	A	841	CLA	C1D-C2D	-2.61	1.40	1.45
18	3	311	CLA	C1D-C2D	-2.61	1.40	1.45
18	6	317	CLA	C1D-C2D	-2.61	1.40	1.45
18	B	804	CLA	C3B-C2B	-2.61	1.36	1.40
18	6	303	CLA	C1D-C2D	-2.60	1.40	1.45
18	5	612	CLA	C1D-C2D	-2.60	1.40	1.45
18	7	601	CLA	C1D-ND	2.60	1.41	1.37
18	7	611	CLA	C3B-C2B	-2.59	1.36	1.40
18	3	314	CLA	C1D-C2D	-2.59	1.40	1.45
18	5	609	CLA	C3B-C2B	-2.59	1.36	1.40
18	4	611	CLA	C1D-C2D	-2.59	1.40	1.45
18	5	610	CLA	C1D-ND	2.59	1.41	1.37
18	1	614	CLA	C1D-C2D	-2.59	1.40	1.45
18	5	613	CLA	C1D-C2D	-2.58	1.40	1.45
18	8	614	CLA	C1D-ND	2.58	1.41	1.37
18	6	301	CLA	C1D-C2D	-2.58	1.40	1.45
18	7	603	CLA	C1D-C2D	-2.58	1.40	1.45
18	A	818	CLA	C1D-C2D	-2.57	1.40	1.45
18	8	602	CLA	C1D-C2D	-2.57	1.40	1.45
18	Z	613	CLA	C1D-C2D	-2.57	1.40	1.45
18	B	838	CLA	C1D-C2D	-2.57	1.40	1.45
18	8	612	CLA	C1D-C2D	-2.57	1.40	1.45
18	A	817	CLA	C1D-ND	2.57	1.40	1.37
18	A	834	CLA	C1D-ND	2.57	1.40	1.37
18	7	607	CLA	C1D-C2D	-2.56	1.40	1.45
18	6	315	CLA	C1D-ND	2.56	1.40	1.37
18	A	828	CLA	C1D-C2D	-2.56	1.40	1.45
18	7	604	CLA	C3D-C4D	-2.56	1.38	1.44
18	8	601	CLA	C1D-ND	2.56	1.40	1.37
18	A	830	CLA	C3B-C2B	-2.56	1.36	1.40
18	6	311	CLA	C3B-C2B	-2.56	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	302	CLA	C1D-C2D	-2.55	1.40	1.45
18	B	814	CLA	C3B-C2B	-2.55	1.36	1.40
18	4	608	CLA	C1D-C2D	-2.55	1.40	1.45
18	5	611	CLA	C3B-C2B	-2.54	1.36	1.40
18	B	802	CLA	C1D-C2D	-2.54	1.40	1.45
18	8	601	CLA	C1D-C2D	-2.54	1.40	1.45
18	A	811	CLA	C1D-C2D	-2.54	1.40	1.45
18	A	815	CLA	C1D-C2D	-2.54	1.40	1.45
18	Z	607	CLA	C1D-C2D	-2.54	1.40	1.45
18	A	833	CLA	C1D-C2D	-2.53	1.40	1.45
21	6	305	CHL	C1D-ND	2.53	1.40	1.37
18	7	602	CLA	C1D-C2D	-2.53	1.40	1.45
18	B	809	CLA	C1D-C2D	-2.53	1.40	1.45
18	6	302	CLA	C1D-C2D	-2.53	1.40	1.45
18	A	818	CLA	C1D-ND	2.53	1.40	1.37
18	A	830	CLA	C1D-C2D	-2.53	1.40	1.45
18	A	836	CLA	C1D-C2D	-2.53	1.40	1.45
21	Z	601	CHL	C1D-ND	2.53	1.40	1.37
18	7	608	CLA	C1D-C2D	-2.53	1.40	1.45
18	3	302	CLA	C1D-C2D	-2.53	1.40	1.45
18	A	808	CLA	C1D-ND	2.53	1.40	1.37
18	B	809	CLA	C1D-ND	2.53	1.40	1.37
18	3	308	CLA	C1D-C2D	-2.53	1.40	1.45
18	6	312	CLA	C1D-C2D	-2.53	1.40	1.45
18	B	818	CLA	C1D-ND	2.52	1.40	1.37
18	B	825	CLA	C1D-C2D	-2.52	1.40	1.45
18	8	603	CLA	C1D-C2D	-2.52	1.40	1.45
18	A	806	CLA	C3B-C2B	-2.52	1.36	1.40
18	A	814	CLA	C3B-C2B	-2.52	1.36	1.40
21	8	606	CHL	C1D-C2D	-2.52	1.40	1.45
18	A	804	CLA	C1D-C2D	-2.52	1.40	1.45
18	A	817	CLA	C1D-C2D	-2.51	1.40	1.45
18	A	837	CLA	C1D-C2D	-2.51	1.40	1.45
18	B	840	CLA	C1D-C2D	-2.51	1.40	1.45
21	1	606	CHL	C1D-ND	2.51	1.40	1.37
18	A	808	CLA	C1D-C2D	-2.51	1.40	1.45
18	3	307	CLA	C1D-C2D	-2.51	1.40	1.45
18	8	614	CLA	C1D-C2D	-2.51	1.40	1.45
18	4	603	CLA	C1D-ND	2.51	1.40	1.37
18	A	834	CLA	C3D-C4D	-2.51	1.38	1.44
18	1	608	CLA	C1D-C2D	-2.51	1.40	1.45
18	B	801	CLA	C1D-ND	2.51	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	601	CHL	C1D-C2D	-2.51	1.40	1.45
21	4	605	CHL	C1D-C2D	-2.50	1.40	1.45
18	6	314	CLA	C3A-C2A	-2.50	1.47	1.54
18	B	811	CLA	C1D-C2D	-2.50	1.40	1.45
18	B	826	CLA	C1D-C2D	-2.50	1.40	1.45
21	6	307	CHL	C1D-C2D	-2.50	1.40	1.45
18	B	836	CLA	C3A-C2A	-2.50	1.47	1.54
18	B	806	CLA	C1D-C2D	-2.50	1.40	1.45
18	3	301	CLA	C1D-ND	2.50	1.40	1.37
18	4	602	CLA	C1D-C2D	-2.50	1.40	1.45
18	A	816	CLA	C1D-C2D	-2.50	1.40	1.45
18	A	819	CLA	C1D-ND	2.50	1.40	1.37
18	1	612	CLA	C1D-C2D	-2.50	1.40	1.45
18	4	612	CLA	C1D-C2D	-2.49	1.40	1.45
18	A	810	CLA	C1D-C2D	-2.49	1.40	1.45
18	B	823	CLA	C1D-C2D	-2.49	1.40	1.45
18	Z	603	CLA	C1D-C2D	-2.49	1.40	1.45
18	Z	604	CLA	C1D-C2D	-2.49	1.40	1.45
18	A	806	CLA	C1D-C2D	-2.49	1.40	1.45
18	5	609	CLA	C1D-C2D	-2.49	1.40	1.45
18	Z	602	CLA	C1D-C2D	-2.49	1.40	1.45
18	1	612	CLA	C3B-C2B	-2.49	1.36	1.40
18	B	805	CLA	C1D-C2D	-2.49	1.40	1.45
18	B	836	CLA	C1D-C2D	-2.49	1.40	1.45
18	1	602	CLA	C1D-C2D	-2.49	1.40	1.45
18	7	604	CLA	C3B-C2B	2.48	1.43	1.40
18	5	604	CLA	C1D-C2D	-2.48	1.40	1.45
18	B	831	CLA	C1D-C2D	-2.48	1.40	1.45
18	3	304	CLA	C1D-C2D	-2.48	1.40	1.45
21	Z	605	CHL	C1D-ND	2.48	1.40	1.37
18	B	818	CLA	C1D-C2D	-2.48	1.40	1.45
18	8	610	CLA	C3D-C4D	-2.48	1.38	1.44
18	B	842	CLA	C1D-C2D	-2.48	1.40	1.45
18	A	839	CLA	C3B-C2B	-2.48	1.36	1.40
18	A	805	CLA	C3A-C2A	-2.48	1.47	1.54
18	A	817	CLA	C3B-C2B	-2.48	1.36	1.40
18	B	816	CLA	C3B-C2B	-2.48	1.36	1.40
18	1	611	CLA	C1D-C2D	-2.47	1.40	1.45
18	Z	608	CLA	C1D-C2D	-2.47	1.40	1.45
18	B	841	CLA	C1D-C2D	-2.47	1.40	1.45
18	7	605	CLA	C3A-C2A	-2.47	1.47	1.54
18	B	815	CLA	C3A-C2A	-2.47	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	843	CLA	C1D-C2D	-2.47	1.40	1.45
18	7	611	CLA	C1D-C2D	-2.47	1.40	1.45
21	1	601	CHL	C1D-ND	2.47	1.40	1.37
18	1	605	CLA	C1D-C2D	-2.47	1.40	1.45
18	A	805	CLA	C1D-C2D	-2.47	1.40	1.45
18	A	844	CLA	C1D-C2D	-2.47	1.40	1.45
18	8	609	CLA	C1D-C2D	-2.47	1.40	1.45
18	6	309	CLA	C1D-C2D	-2.47	1.40	1.45
18	F	301	CLA	C1D-ND	2.47	1.40	1.37
18	4	601	CLA	C1D-C2D	-2.46	1.40	1.45
18	8	613	CLA	C1D-C2D	-2.46	1.40	1.45
21	6	316	CHL	C1B-NB	2.46	1.37	1.35
18	7	609	CLA	C1D-C2D	-2.46	1.40	1.45
18	A	829	CLA	C1D-C2D	-2.46	1.40	1.45
18	B	837	CLA	C1D-C2D	-2.46	1.40	1.45
18	8	611	CLA	C1D-ND	2.46	1.40	1.37
21	5	607	CHL	C1D-C2D	-2.46	1.40	1.45
18	B	804	CLA	C3A-C2A	-2.46	1.47	1.54
18	A	831	CLA	C1D-ND	2.46	1.40	1.37
18	B	830	CLA	C1D-C2D	-2.46	1.40	1.45
18	Z	609	CLA	C1D-C2D	-2.46	1.40	1.45
18	A	817	CLA	C3D-C4D	-2.46	1.38	1.44
18	7	612	CLA	C1D-C2D	-2.46	1.40	1.45
21	6	316	CHL	C1D-C2D	-2.45	1.40	1.45
18	Z	612	CLA	C1D-C2D	-2.45	1.40	1.45
21	7	606	CHL	C1B-NB	2.45	1.37	1.35
18	1	609	CLA	C1D-C2D	-2.45	1.40	1.45
18	B	814	CLA	C1D-C2D	-2.45	1.40	1.45
18	4	607	CLA	C1D-C2D	-2.45	1.40	1.45
18	1	604	CLA	C1D-C2D	-2.45	1.40	1.45
18	Z	610	CLA	C3A-C2A	-2.45	1.47	1.54
18	F	301	CLA	C1D-C2D	-2.45	1.40	1.45
18	6	308	CLA	C1D-C2D	-2.45	1.40	1.45
18	6	311	CLA	C3A-C2A	-2.45	1.47	1.54
18	7	605	CLA	C1D-ND	2.45	1.40	1.37
18	B	813	CLA	CAB-C3B	-2.44	1.46	1.51
18	A	814	CLA	C1D-C2D	-2.44	1.40	1.45
18	A	841	CLA	C3A-C2A	-2.44	1.47	1.54
18	Z	611	CLA	C3B-C2B	-2.44	1.37	1.40
18	A	807	CLA	C1D-C2D	-2.44	1.40	1.45
18	Z	611	CLA	C1D-C2D	-2.44	1.40	1.45
18	B	832	CLA	C1D-C2D	-2.44	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	313	CLA	C1D-C2D	-2.44	1.40	1.45
18	B	808	CLA	C3B-C2B	-2.44	1.37	1.40
18	3	305	CLA	C1D-C2D	-2.43	1.40	1.45
18	A	826	CLA	C3B-C2B	-2.43	1.37	1.40
18	B	834	CLA	C1D-C2D	-2.43	1.40	1.45
18	B	812	CLA	C1D-C2D	-2.43	1.40	1.45
18	B	839	CLA	C1D-C2D	-2.43	1.40	1.45
18	6	314	CLA	C1D-C2D	-2.43	1.40	1.45
18	A	841	CLA	C3B-C2B	-2.43	1.37	1.40
18	8	605	CLA	C1D-C2D	-2.43	1.40	1.45
18	A	802	CLA	C1D-C2D	-2.43	1.40	1.45
18	7	613	CLA	C1D-C2D	-2.43	1.40	1.45
18	Z	610	CLA	C1D-C2D	-2.43	1.40	1.45
18	7	604	CLA	C1D-C2D	-2.42	1.40	1.45
18	B	821	CLA	C1D-C2D	-2.42	1.40	1.45
18	B	813	CLA	C1D-C2D	-2.42	1.40	1.45
18	A	831	CLA	C3D-C4D	-2.42	1.38	1.44
18	1	610	CLA	C1D-C2D	-2.42	1.40	1.45
18	A	823	CLA	C1D-C2D	-2.42	1.40	1.45
18	5	612	CLA	C3B-C2B	-2.42	1.37	1.40
18	A	812	CLA	C1D-C2D	-2.42	1.40	1.45
18	8	604	CLA	C1D-C2D	-2.42	1.40	1.45
21	5	606	CHL	C3D-C4D	-2.42	1.38	1.44
21	1	601	CHL	C1D-C2D	-2.42	1.40	1.45
18	1	611	CLA	C3A-C2A	-2.42	1.47	1.54
18	A	826	CLA	C1D-C2D	-2.42	1.40	1.45
18	5	614	CLA	C3B-C2B	-2.42	1.37	1.40
18	A	840	CLA	C3D-C4D	-2.42	1.38	1.44
18	3	307	CLA	C3D-C4D	-2.42	1.38	1.44
18	B	804	CLA	C1D-C2D	-2.41	1.40	1.45
18	B	824	CLA	C1D-C2D	-2.41	1.40	1.45
18	6	315	CLA	C1D-C2D	-2.41	1.40	1.45
18	B	843	CLA	C1D-C2D	-2.41	1.40	1.45
18	4	610	CLA	C3A-C2A	-2.41	1.47	1.54
18	6	310	CLA	C1D-C2D	-2.41	1.40	1.45
18	7	614	CLA	C3A-C2A	-2.41	1.47	1.54
18	3	303	CLA	C1D-C2D	-2.41	1.40	1.45
18	B	835	CLA	C1D-ND	2.40	1.40	1.37
18	6	313	CLA	C3D-C4D	-2.40	1.38	1.44
18	A	844	CLA	C1D-ND	2.40	1.40	1.37
18	A	824	CLA	C3B-C2B	-2.40	1.37	1.40
18	A	832	CLA	C1D-C2D	-2.40	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	840	CLA	C1D-C2D	-2.40	1.40	1.45
18	A	820	CLA	C3B-C2B	-2.40	1.37	1.40
18	1	613	CLA	C1D-C2D	-2.40	1.40	1.45
18	5	614	CLA	C1D-C2D	-2.40	1.40	1.45
18	B	819	CLA	C3A-C2A	-2.40	1.47	1.54
18	5	615	CLA	C1D-C2D	-2.40	1.40	1.45
18	A	824	CLA	C1D-C2D	-2.39	1.40	1.45
18	3	301	CLA	C1D-C2D	-2.39	1.40	1.45
18	7	605	CLA	C1D-C2D	-2.39	1.40	1.45
18	B	806	CLA	C3A-C2A	-2.39	1.47	1.54
18	4	610	CLA	C1D-C2D	-2.39	1.40	1.45
18	6	304	CLA	C3A-C2A	-2.39	1.47	1.54
18	B	801	CLA	C3A-C2A	-2.39	1.47	1.54
18	A	837	CLA	C1D-ND	2.39	1.40	1.37
18	A	813	CLA	C1D-C2D	-2.39	1.40	1.45
18	A	820	CLA	C1D-C2D	-2.39	1.40	1.45
18	8	611	CLA	C1D-C2D	-2.38	1.40	1.45
21	3	306	CHL	C1D-C2D	-2.38	1.40	1.45
18	A	803	CLA	C3D-C4D	-2.38	1.38	1.44
18	7	601	CLA	C1D-C2D	-2.38	1.40	1.45
18	B	835	CLA	C1D-C2D	-2.38	1.40	1.45
18	3	304	CLA	C3B-C2B	-2.38	1.37	1.40
21	5	607	CHL	C1D-ND	2.38	1.40	1.37
18	A	822	CLA	C1D-C2D	-2.38	1.40	1.45
18	B	805	CLA	C3D-C4D	-2.38	1.38	1.44
18	B	822	CLA	C1D-C2D	-2.38	1.40	1.45
18	4	601	CLA	C1D-ND	2.37	1.40	1.37
21	5	606	CHL	C1D-C2D	-2.37	1.40	1.45
21	7	606	CHL	C1D-C2D	-2.37	1.40	1.45
18	5	611	CLA	C1D-C2D	-2.37	1.40	1.45
18	3	305	CLA	C3A-C2A	-2.37	1.47	1.54
18	3	303	CLA	C3B-C2B	-2.37	1.37	1.40
18	Z	606	CLA	C1D-C2D	-2.37	1.40	1.45
18	B	815	CLA	C3D-C4D	-2.36	1.38	1.44
18	5	605	CLA	C1D-C2D	-2.36	1.40	1.45
18	4	609	CLA	C1D-C2D	-2.36	1.40	1.45
21	7	606	CHL	C3D-C4D	-2.36	1.38	1.44
18	5	617	CLA	C1D-C2D	-2.36	1.40	1.45
18	3	303	CLA	C3D-C4D	-2.36	1.38	1.44
18	5	602	CLA	C1D-ND	2.36	1.40	1.37
18	A	816	CLA	C3B-C2B	-2.36	1.37	1.40
18	B	808	CLA	C3A-C2A	-2.36	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	812	CLA	C3B-C2B	-2.36	1.37	1.40
18	J	101	CLA	C1D-C2D	-2.35	1.40	1.45
21	1	606	CHL	C1D-C2D	-2.35	1.40	1.45
18	5	613	CLA	C1D-ND	2.35	1.40	1.37
18	5	608	CLA	CHD-C4C	-2.35	1.33	1.39
18	A	832	CLA	C3A-C2A	-2.35	1.47	1.54
18	B	820	CLA	C3D-C4D	-2.35	1.38	1.44
18	B	831	CLA	C3A-C2A	-2.35	1.47	1.54
18	3	312	CLA	C1D-C2D	-2.35	1.40	1.45
18	B	835	CLA	C3D-C4D	-2.35	1.38	1.44
18	B	828	CLA	C1D-C2D	-2.35	1.40	1.45
18	B	836	CLA	C3D-C4D	-2.35	1.38	1.44
18	B	807	CLA	C1D-C2D	-2.35	1.40	1.45
18	A	831	CLA	C1D-C2D	-2.35	1.40	1.45
21	6	307	CHL	C1D-ND	2.34	1.40	1.37
18	B	808	CLA	C3D-C4D	-2.34	1.38	1.44
18	B	805	CLA	C3A-C2A	-2.34	1.47	1.54
18	6	311	CLA	C1D-C2D	-2.34	1.40	1.45
18	A	811	CLA	C3D-C4D	-2.34	1.38	1.44
18	5	617	CLA	C3D-C4D	-2.34	1.38	1.44
18	Z	607	CLA	C1D-ND	2.34	1.40	1.37
18	A	812	CLA	C3B-C2B	-2.34	1.37	1.40
18	1	607	CLA	C1D-C2D	-2.34	1.40	1.45
18	A	819	CLA	C1D-C2D	-2.34	1.40	1.45
18	8	612	CLA	C3A-C2A	-2.34	1.47	1.54
18	5	613	CLA	C3B-C2B	-2.33	1.37	1.40
18	8	610	CLA	C1D-C2D	-2.33	1.40	1.45
18	B	810	CLA	C3B-C2B	-2.33	1.37	1.40
21	6	306	CHL	C1D-C2D	-2.33	1.40	1.45
21	5	616	CHL	C1D-C2D	-2.33	1.40	1.45
18	7	607	CLA	C3A-C2A	-2.33	1.48	1.54
18	B	818	CLA	C3B-C2B	-2.33	1.37	1.40
17	A	801	CL0	C3D-C4D	-2.33	1.38	1.44
18	B	827	CLA	C1D-ND	2.33	1.40	1.37
18	1	608	CLA	C3D-C4D	-2.33	1.38	1.44
18	7	612	CLA	C3B-C2B	-2.32	1.37	1.40
18	5	610	CLA	C1D-C2D	-2.32	1.40	1.45
18	Z	609	CLA	C3D-C4D	-2.32	1.38	1.44
18	A	814	CLA	C1D-ND	2.32	1.40	1.37
18	Z	607	CLA	C3D-C4D	-2.32	1.38	1.44
18	B	834	CLA	C3D-C4D	-2.32	1.38	1.44
18	4	606	CLA	C1D-C2D	-2.32	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	605	CHL	C1D-C2D	-2.32	1.40	1.45
18	B	810	CLA	C1D-C2D	-2.32	1.40	1.45
18	B	827	CLA	C1D-C2D	-2.32	1.40	1.45
18	B	816	CLA	C1D-C2D	-2.31	1.40	1.45
21	6	316	CHL	C3D-C4D	-2.31	1.39	1.44
17	A	801	CL0	C1D-C2D	-2.31	1.40	1.45
21	1	601	CHL	C3D-C4D	-2.31	1.39	1.44
18	4	603	CLA	C3B-C2B	-2.31	1.37	1.40
18	7	613	CLA	C3B-C2B	-2.31	1.37	1.40
18	B	801	CLA	C1D-C2D	-2.31	1.40	1.45
18	B	817	CLA	C1D-C2D	-2.31	1.40	1.45
18	A	819	CLA	C3D-C4D	-2.30	1.39	1.44
18	B	820	CLA	C1D-C2D	-2.30	1.40	1.45
18	3	305	CLA	C3D-C4D	-2.30	1.39	1.44
18	A	802	CLA	C3A-C2A	-2.30	1.48	1.54
18	B	802	CLA	C3D-C4D	-2.30	1.39	1.44
18	8	603	CLA	C3D-C4D	-2.30	1.39	1.44
18	A	805	CLA	C3D-C4D	-2.30	1.39	1.44
21	4	605	CHL	C1B-CHB	-2.30	1.34	1.41
18	A	826	CLA	C3D-C4D	-2.30	1.39	1.44
18	B	829	CLA	C1D-ND	2.30	1.40	1.37
18	7	602	CLA	C3B-C2B	-2.30	1.37	1.40
18	7	605	CLA	C3D-C4D	-2.29	1.39	1.44
21	6	305	CHL	C3D-C4D	-2.29	1.39	1.44
18	7	605	CLA	C3B-C2B	-2.29	1.37	1.40
18	3	310	CLA	C1D-C2D	-2.29	1.40	1.45
18	A	814	CLA	C3D-C4D	-2.29	1.39	1.44
21	3	306	CHL	C1D-ND	2.29	1.40	1.37
18	3	308	CLA	C3B-C2B	-2.29	1.37	1.40
18	B	806	CLA	C3D-C4D	-2.28	1.39	1.44
18	6	310	CLA	C3D-C4D	-2.28	1.39	1.44
18	1	608	CLA	C1D-ND	2.28	1.40	1.37
18	B	841	CLA	C3D-C4D	-2.28	1.39	1.44
21	Z	601	CHL	C3D-C4D	-2.28	1.39	1.44
18	4	603	CLA	C3A-C2A	-2.28	1.48	1.54
18	A	827	CLA	C1D-C2D	-2.28	1.40	1.45
18	A	803	CLA	C1A-CHA	-2.28	1.33	1.43
18	A	802	CLA	C3D-C4D	-2.28	1.39	1.44
18	4	610	CLA	C1C-C2C	2.27	1.49	1.44
21	8	606	CHL	C3D-C4D	-2.27	1.39	1.44
18	A	824	CLA	C3A-C2A	-2.27	1.48	1.54
18	3	303	CLA	C3A-C2A	-2.27	1.48	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	843	CLA	C3D-C4D	-2.27	1.39	1.44
18	B	842	CLA	C3D-C4D	-2.27	1.39	1.44
18	6	313	CLA	C1D-C2D	-2.27	1.40	1.45
18	8	613	CLA	C3B-C2B	-2.27	1.37	1.40
18	A	829	CLA	C3B-C2B	-2.26	1.37	1.40
18	3	314	CLA	C3B-C2B	-2.26	1.37	1.40
18	A	804	CLA	C3A-C2A	-2.26	1.48	1.54
18	A	805	CLA	C1D-ND	2.26	1.40	1.37
18	B	806	CLA	C1C-C2C	2.26	1.48	1.44
18	B	815	CLA	C1D-C2D	-2.26	1.40	1.45
18	7	610	CLA	C1D-C2D	-2.26	1.40	1.45
21	6	305	CHL	C1D-C2D	-2.26	1.40	1.45
18	3	305	CLA	C1D-ND	2.26	1.40	1.37
18	7	604	CLA	C1B-NB	2.26	1.37	1.35
18	A	803	CLA	C1D-ND	2.26	1.40	1.37
18	B	801	CLA	C3D-C4D	-2.26	1.39	1.44
18	7	610	CLA	C1D-ND	2.26	1.40	1.37
18	1	610	CLA	C3D-C4D	-2.25	1.39	1.44
18	5	602	CLA	C3D-C4D	-2.25	1.39	1.44
18	B	837	CLA	C3B-C2B	-2.25	1.37	1.40
18	6	309	CLA	C1C-C2C	2.25	1.48	1.44
18	6	312	CLA	C3A-C2A	-2.25	1.48	1.54
18	5	608	CLA	C3D-C4D	-2.25	1.39	1.44
18	4	603	CLA	CHD-C4C	-2.25	1.34	1.39
18	A	835	CLA	C3D-C4D	-2.25	1.39	1.44
18	B	819	CLA	C3B-C2B	-2.25	1.37	1.40
18	A	813	CLA	C3D-C4D	-2.25	1.39	1.44
18	A	803	CLA	C1D-C2D	-2.25	1.40	1.45
18	3	309	CLA	C1D-C2D	-2.25	1.40	1.45
21	4	605	CHL	C4B-CHC	-2.24	1.34	1.41
18	A	822	CLA	C3D-C4D	-2.24	1.39	1.44
18	3	302	CLA	C3B-C2B	-2.24	1.37	1.40
18	A	825	CLA	C1D-C2D	-2.24	1.40	1.45
18	A	818	CLA	C3D-C4D	-2.24	1.39	1.44
18	3	311	CLA	C3B-C2B	-2.24	1.37	1.40
18	1	603	CLA	C3B-C2B	-2.24	1.37	1.40
18	B	827	CLA	C3D-C4D	-2.24	1.39	1.44
18	8	611	CLA	C3D-C4D	-2.24	1.39	1.44
18	5	613	CLA	C3D-C4D	-2.23	1.39	1.44
18	5	603	CLA	C3B-C2B	-2.23	1.37	1.40
18	B	819	CLA	C1D-C2D	-2.23	1.40	1.45
21	1	601	CHL	C4B-CHC	-2.23	1.34	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	307	CHL	C1B-CHB	-2.23	1.34	1.41
18	A	810	CLA	C3D-C4D	-2.23	1.39	1.44
18	7	601	CLA	C3D-C4D	-2.23	1.39	1.44
21	Z	601	CHL	C4B-CHC	-2.22	1.34	1.41
21	8	606	CHL	C4B-CHC	-2.22	1.34	1.41
18	B	842	CLA	C3B-C2B	-2.22	1.37	1.40
21	4	604	CHL	C3D-C4D	-2.22	1.39	1.44
18	A	818	CLA	C3B-C2B	-2.22	1.37	1.40
18	4	608	CLA	C3D-C4D	-2.22	1.39	1.44
18	A	803	CLA	C3B-C2B	-2.22	1.37	1.40
18	A	805	CLA	C1C-C2C	2.22	1.48	1.44
18	B	841	CLA	C3B-C2B	-2.21	1.37	1.40
18	5	604	CLA	C3D-C4D	-2.21	1.39	1.44
18	8	608	CLA	CHD-C4C	-2.21	1.34	1.39
18	B	832	CLA	C3D-C4D	-2.21	1.39	1.44
18	A	844	CLA	C3D-C4D	-2.21	1.39	1.44
18	4	612	CLA	C1D-ND	2.21	1.40	1.37
18	5	615	CLA	C3D-C4D	-2.21	1.39	1.44
18	F	301	CLA	C3D-C4D	-2.21	1.39	1.44
18	4	603	CLA	C3D-C4D	-2.21	1.39	1.44
18	A	803	CLA	C4D-CHA	-2.21	1.30	1.38
18	A	837	CLA	C3D-C4D	-2.21	1.39	1.44
21	6	305	CHL	C1B-NB	2.21	1.37	1.35
18	A	815	CLA	C3D-C4D	-2.21	1.39	1.44
18	7	607	CLA	CHD-C4C	-2.21	1.34	1.39
18	B	813	CLA	C3D-C4D	-2.21	1.39	1.44
18	8	601	CLA	C3D-C4D	-2.21	1.39	1.44
18	A	809	CLA	C3B-C2B	-2.20	1.37	1.40
18	3	301	CLA	C3D-C4D	-2.20	1.39	1.44
18	B	815	CLA	C1D-ND	2.20	1.40	1.37
18	B	834	CLA	C2C-C1C	-2.20	1.46	1.51
18	B	809	CLA	C3D-C4D	-2.20	1.39	1.44
18	A	845	CLA	CHD-C4C	-2.20	1.34	1.39
18	4	601	CLA	C3D-C4D	-2.20	1.39	1.44
18	A	824	CLA	C3D-C4D	-2.20	1.39	1.44
18	3	311	CLA	C3A-C2A	-2.20	1.48	1.54
21	5	616	CHL	C1B-NB	2.20	1.37	1.35
18	A	834	CLA	C1D-C2D	-2.20	1.41	1.45
21	5	616	CHL	C3D-C4D	-2.20	1.39	1.44
18	A	829	CLA	C3D-C4D	-2.20	1.39	1.44
18	A	821	CLA	C3D-C4D	-2.20	1.39	1.44
18	6	308	CLA	C3D-C4D	-2.20	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	315	CLA	C3D-C4D	-2.20	1.39	1.44
18	B	818	CLA	C3D-C4D	-2.19	1.39	1.44
18	A	841	CLA	CHD-C4C	-2.19	1.34	1.39
18	Z	604	CLA	C3A-C2A	-2.19	1.48	1.54
18	7	613	CLA	C3D-C4D	-2.19	1.39	1.44
18	A	813	CLA	C3A-C2A	-2.19	1.48	1.54
18	8	615	CLA	C3B-C2B	-2.19	1.37	1.40
18	B	840	CLA	C3D-C4D	-2.19	1.39	1.44
18	7	614	CLA	C3D-C4D	-2.19	1.39	1.44
18	A	808	CLA	C3D-C4D	-2.19	1.39	1.44
18	B	811	CLA	C3D-C4D	-2.18	1.39	1.44
21	5	607	CHL	C1B-CHB	-2.18	1.34	1.41
18	1	605	CLA	C3A-C2A	-2.18	1.48	1.54
18	8	604	CLA	C3D-C4D	-2.18	1.39	1.44
18	B	807	CLA	C3D-C4D	-2.18	1.39	1.44
18	B	830	CLA	C3D-C4D	-2.18	1.39	1.44
18	B	804	CLA	C1D-ND	2.18	1.40	1.37
18	B	829	CLA	CHD-C4C	-2.18	1.34	1.39
18	A	824	CLA	C1C-NC	-2.18	1.34	1.37
18	3	304	CLA	C3A-C2A	-2.18	1.48	1.54
18	B	827	CLA	C3B-C2B	-2.18	1.37	1.40
21	6	306	CHL	C3D-C4D	-2.18	1.39	1.44
18	B	839	CLA	C3D-C4D	-2.18	1.39	1.44
18	7	612	CLA	C3D-C4D	-2.18	1.39	1.44
18	B	811	CLA	C3B-C2B	-2.18	1.37	1.40
18	B	816	CLA	C3D-C4D	-2.18	1.39	1.44
18	B	838	CLA	C3D-C4D	-2.18	1.39	1.44
18	8	614	CLA	C3D-C4D	-2.18	1.39	1.44
18	B	839	CLA	C1D-ND	2.18	1.40	1.37
18	B	829	CLA	C3D-C4D	-2.17	1.39	1.44
18	7	603	CLA	C3D-C4D	-2.17	1.39	1.44
18	7	608	CLA	C3B-C2B	-2.17	1.37	1.40
18	1	614	CLA	CHD-C4C	-2.17	1.34	1.39
18	A	811	CLA	C3B-C2B	-2.17	1.37	1.40
18	B	802	CLA	C1D-ND	2.17	1.40	1.37
21	Z	605	CHL	C1B-NB	2.17	1.37	1.35
18	6	302	CLA	C3D-C4D	-2.17	1.39	1.44
18	B	831	CLA	C3D-C4D	-2.17	1.39	1.44
18	8	607	CLA	CHD-C4C	-2.17	1.34	1.39
18	5	612	CLA	C3D-C4D	-2.17	1.39	1.44
18	5	617	CLA	C3A-C2A	-2.17	1.48	1.54
18	8	613	CLA	C3D-C4D	-2.16	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	306	CHL	C3D-C4D	-2.16	1.39	1.44
18	4	612	CLA	C3D-C4D	-2.16	1.39	1.44
18	B	817	CLA	C3D-C4D	-2.16	1.39	1.44
18	B	824	CLA	C3D-C4D	-2.16	1.39	1.44
18	B	840	CLA	C3A-C2A	-2.16	1.48	1.54
18	5	601	CLA	CHD-C4C	-2.16	1.34	1.39
18	7	611	CLA	C3D-C4D	-2.16	1.39	1.44
18	A	804	CLA	C3D-C4D	-2.16	1.39	1.44
18	7	607	CLA	C3B-C2B	-2.15	1.37	1.40
18	8	615	CLA	C3A-C2A	-2.15	1.48	1.54
18	A	812	CLA	C3D-C4D	-2.15	1.39	1.44
18	A	820	CLA	C3A-C2A	-2.15	1.48	1.54
18	4	602	CLA	C3D-C4D	-2.15	1.39	1.44
18	B	834	CLA	C3B-C2B	-2.15	1.37	1.40
18	3	304	CLA	C3D-C4D	-2.15	1.39	1.44
18	7	610	CLA	C3D-C4D	-2.15	1.39	1.44
18	A	838	CLA	C1D-C2D	-2.15	1.41	1.45
18	B	806	CLA	C1D-ND	2.15	1.40	1.37
18	1	610	CLA	C1D-ND	2.15	1.40	1.37
18	Z	612	CLA	C3B-C2B	-2.15	1.37	1.40
18	3	314	CLA	C3D-C4D	-2.15	1.39	1.44
18	Z	613	CLA	CHD-C4C	-2.15	1.34	1.39
18	1	603	CLA	C3A-C2A	-2.14	1.48	1.54
18	A	823	CLA	C3D-C4D	-2.14	1.39	1.44
18	B	826	CLA	C3B-C2B	-2.14	1.37	1.40
18	A	828	CLA	C3A-C2A	-2.14	1.48	1.54
21	6	307	CHL	C4B-CHC	-2.14	1.35	1.41
18	A	832	CLA	C3D-C4D	-2.14	1.39	1.44
18	A	845	CLA	C3D-C4D	-2.14	1.39	1.44
18	B	808	CLA	CHD-C4C	-2.14	1.34	1.39
18	3	310	CLA	C3B-C2B	-2.14	1.37	1.40
18	8	612	CLA	C3D-C4D	-2.14	1.39	1.44
21	1	606	CHL	C1B-NB	2.14	1.37	1.35
18	A	808	CLA	C3A-C2A	-2.14	1.48	1.54
18	A	809	CLA	C3D-C4D	-2.14	1.39	1.44
21	Z	601	CHL	C1B-CHB	-2.13	1.35	1.41
18	A	807	CLA	C3D-C4D	-2.13	1.39	1.44
18	5	610	CLA	C3D-C4D	-2.13	1.39	1.44
18	Z	609	CLA	C1D-ND	2.13	1.40	1.37
18	A	817	CLA	C3A-C2A	-2.13	1.48	1.54
18	4	611	CLA	C3D-C4D	-2.13	1.39	1.44
18	3	310	CLA	C3A-C2A	-2.13	1.48	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	607	CHL	C4B-CHC	-2.13	1.35	1.41
18	B	842	CLA	C3A-C2A	-2.13	1.48	1.54
18	8	609	CLA	CHD-C4C	-2.13	1.34	1.39
21	6	307	CHL	C3D-C4D	-2.13	1.39	1.44
18	3	312	CLA	C3D-C4D	-2.13	1.39	1.44
18	A	806	CLA	C3D-C4D	-2.13	1.39	1.44
18	3	311	CLA	CHD-C4C	-2.13	1.34	1.39
18	3	311	CLA	C3D-C4D	-2.13	1.39	1.44
18	A	809	CLA	CHD-C4C	-2.13	1.34	1.39
18	A	813	CLA	C3B-C2B	-2.13	1.37	1.40
18	A	810	CLA	C3A-C2A	-2.13	1.48	1.54
18	7	614	CLA	C1D-C2D	-2.12	1.41	1.45
18	6	304	CLA	CHD-C4C	-2.12	1.34	1.39
18	A	821	CLA	C3A-C2A	-2.12	1.48	1.54
18	4	607	CLA	C3D-C4D	-2.12	1.39	1.44
18	A	839	CLA	C3D-C4D	-2.12	1.39	1.44
18	A	840	CLA	C3B-C2B	-2.12	1.37	1.40
18	8	605	CLA	C3A-C2A	-2.12	1.48	1.54
18	5	605	CLA	C3D-C4D	-2.12	1.39	1.44
18	A	830	CLA	C3D-C4D	-2.12	1.39	1.44
18	1	607	CLA	C3D-C4D	-2.12	1.39	1.44
18	A	821	CLA	CHD-C4C	-2.12	1.34	1.39
18	A	820	CLA	C3D-C4D	-2.12	1.39	1.44
18	3	307	CLA	C1D-ND	2.12	1.40	1.37
18	4	602	CLA	CHD-C4C	-2.12	1.34	1.39
18	A	836	CLA	C3D-C4D	-2.11	1.39	1.44
18	A	836	CLA	CHD-C4C	-2.11	1.34	1.39
18	Z	610	CLA	C3B-C2B	-2.11	1.37	1.40
18	1	611	CLA	C3D-C4D	-2.11	1.39	1.44
18	1	611	CLA	C3B-C2B	-2.11	1.37	1.40
21	3	306	CHL	C1B-NB	2.11	1.37	1.35
18	A	840	CLA	C4D-CHA	-2.11	1.31	1.38
21	1	601	CHL	C1B-CHB	-2.11	1.35	1.41
21	3	306	CHL	C1B-CHB	-2.11	1.35	1.41
18	B	823	CLA	C3D-C4D	-2.11	1.39	1.44
18	B	838	CLA	CHD-C4C	-2.11	1.34	1.39
18	7	603	CLA	CHD-C4C	-2.11	1.34	1.39
18	1	609	CLA	C1C-C2C	2.11	1.48	1.44
18	A	807	CLA	C3A-C2A	-2.11	1.48	1.54
18	3	309	CLA	C3D-C4D	-2.10	1.39	1.44
21	4	605	CHL	C3D-C4D	-2.10	1.39	1.44
18	6	301	CLA	C1C-C2C	2.10	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	834	CLA	C3A-C2A	-2.10	1.48	1.54
18	8	605	CLA	C3D-C4D	-2.10	1.39	1.44
18	6	314	CLA	C3D-C4D	-2.10	1.39	1.44
18	4	606	CLA	C3D-C4D	-2.10	1.39	1.44
18	A	827	CLA	C3D-C4D	-2.10	1.39	1.44
18	A	840	CLA	C1D-ND	2.10	1.40	1.37
18	F	302	CLA	C3D-C4D	-2.10	1.39	1.44
18	5	611	CLA	C3A-C2A	-2.10	1.48	1.54
18	5	611	CLA	C3D-C4D	-2.10	1.39	1.44
18	7	602	CLA	CHD-C4C	-2.10	1.34	1.39
18	5	617	CLA	C1D-ND	2.10	1.40	1.37
18	B	843	CLA	C3B-C2B	-2.10	1.37	1.40
18	6	317	CLA	C3A-C2A	-2.10	1.48	1.54
18	B	833	CLA	C3D-C4D	-2.10	1.39	1.44
18	7	602	CLA	C3D-C4D	-2.10	1.39	1.44
18	B	802	CLA	C3A-C2A	-2.10	1.48	1.54
18	Z	610	CLA	C3D-C4D	-2.10	1.39	1.44
18	Z	608	CLA	C1C-C2C	2.10	1.48	1.44
18	A	822	CLA	C3A-C2A	-2.10	1.48	1.54
18	B	826	CLA	C3A-C2A	-2.10	1.48	1.54
18	4	602	CLA	C1C-C2C	2.10	1.48	1.44
18	A	841	CLA	C3D-C4D	-2.09	1.39	1.44
18	A	834	CLA	C1A-CHA	-2.09	1.34	1.43
18	5	602	CLA	CHD-C4C	-2.09	1.34	1.39
18	1	603	CLA	CHD-C4C	-2.09	1.34	1.39
18	B	828	CLA	C3A-C2A	-2.09	1.48	1.54
18	B	804	CLA	C3D-C4D	-2.09	1.39	1.44
18	A	823	CLA	CHD-C4C	-2.09	1.34	1.39
18	A	829	CLA	C3A-C2A	-2.09	1.48	1.54
18	A	802	CLA	C1D-ND	2.09	1.40	1.37
18	7	612	CLA	C3A-C2A	-2.09	1.48	1.54
18	A	828	CLA	C3D-C4D	-2.09	1.39	1.44
18	Z	606	CLA	C3D-C4D	-2.09	1.39	1.44
18	F	302	CLA	CHD-C4C	-2.09	1.34	1.39
18	6	301	CLA	CHD-C4C	-2.08	1.34	1.39
18	B	837	CLA	C3D-C4D	-2.08	1.39	1.44
18	4	610	CLA	C3D-C4D	-2.08	1.39	1.44
18	A	809	CLA	C3A-C2A	-2.08	1.48	1.54
18	3	313	CLA	C3D-C4D	-2.08	1.39	1.44
18	5	603	CLA	CHD-C4C	-2.08	1.34	1.39
18	8	613	CLA	C3A-C2A	-2.08	1.48	1.54
18	3	314	CLA	CHD-C4C	-2.08	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	604	CHL	C1D-ND	2.08	1.40	1.37
18	6	303	CLA	C3D-C4D	-2.08	1.39	1.44
18	B	825	CLA	C3D-C4D	-2.08	1.39	1.44
18	A	828	CLA	CHD-C4C	-2.08	1.34	1.39
18	A	838	CLA	C3D-C4D	-2.08	1.39	1.44
18	1	614	CLA	C3D-C4D	-2.08	1.39	1.44
18	B	812	CLA	C3D-C4D	-2.08	1.39	1.44
18	7	611	CLA	C3A-C2A	-2.08	1.48	1.54
21	5	616	CHL	C4B-CHC	-2.08	1.35	1.41
18	B	843	CLA	C3D-C4D	-2.08	1.39	1.44
18	A	812	CLA	CHD-C4C	-2.07	1.34	1.39
18	B	805	CLA	CHD-C4C	-2.07	1.34	1.39
18	A	837	CLA	CHD-C4C	-2.07	1.34	1.39
18	1	605	CLA	C3D-C4D	-2.07	1.39	1.44
18	Z	602	CLA	C3D-C4D	-2.07	1.39	1.44
18	6	317	CLA	CHD-C4C	-2.07	1.34	1.39
18	5	609	CLA	C3D-C4D	-2.07	1.39	1.44
18	J	101	CLA	C3D-C4D	-2.07	1.39	1.44
18	A	838	CLA	C3B-C2B	-2.07	1.37	1.40
18	1	609	CLA	C3D-C4D	-2.07	1.39	1.44
18	B	826	CLA	C3D-C4D	-2.07	1.39	1.44
18	1	604	CLA	C3A-C2A	-2.07	1.48	1.54
18	6	312	CLA	C3D-C4D	-2.07	1.39	1.44
18	1	602	CLA	C3D-C4D	-2.07	1.39	1.44
18	8	608	CLA	C3D-C4D	-2.06	1.39	1.44
18	A	835	CLA	CHD-C4C	-2.06	1.34	1.39
21	1	606	CHL	C1B-CHB	-2.06	1.35	1.41
18	B	822	CLA	C3B-C2B	-2.06	1.37	1.40
18	A	818	CLA	CHD-C4C	-2.06	1.34	1.39
18	Z	608	CLA	C3D-C4D	-2.06	1.39	1.44
18	B	822	CLA	C3D-C4D	-2.06	1.39	1.44
18	1	613	CLA	C3B-C2B	-2.06	1.37	1.40
18	Z	612	CLA	C3D-C4D	-2.06	1.39	1.44
18	A	808	CLA	CHD-C4C	-2.06	1.34	1.39
18	Z	604	CLA	C3D-C4D	-2.06	1.39	1.44
18	3	301	CLA	C3B-C2B	-2.06	1.37	1.40
18	Z	603	CLA	C3A-C2A	-2.06	1.48	1.54
18	3	310	CLA	C3D-C4D	-2.05	1.39	1.44
18	7	609	CLA	C3D-C4D	-2.05	1.39	1.44
18	6	302	CLA	CHD-C4C	-2.05	1.34	1.39
18	3	307	CLA	C3A-C2A	-2.05	1.48	1.54
18	A	833	CLA	CHD-C4C	-2.05	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	802	CLA	CHD-C4C	-2.05	1.34	1.39
18	7	608	CLA	C3D-C4D	-2.05	1.39	1.44
18	A	836	CLA	C3B-C2B	-2.05	1.37	1.40
18	1	612	CLA	C3D-C4D	-2.05	1.39	1.44
18	Z	611	CLA	C3D-C4D	-2.05	1.39	1.44
18	8	609	CLA	C3D-C4D	-2.05	1.39	1.44
18	6	309	CLA	C3D-C4D	-2.05	1.39	1.44
18	A	812	CLA	C3A-C2A	-2.05	1.48	1.54
18	8	615	CLA	CHD-C4C	-2.05	1.34	1.39
18	7	609	CLA	CHD-C4C	-2.05	1.34	1.39
21	5	607	CHL	C3D-C4D	-2.05	1.39	1.44
18	6	312	CLA	C3B-C2B	-2.05	1.37	1.40
18	6	313	CLA	C3A-C2A	-2.05	1.48	1.54
18	A	830	CLA	CHD-C4C	-2.05	1.34	1.39
21	4	604	CHL	C4B-CHC	-2.05	1.35	1.41
18	5	612	CLA	CHD-C4C	-2.05	1.34	1.39
21	4	604	CHL	C1D-C2D	-2.05	1.41	1.45
18	3	302	CLA	C3A-C2A	-2.04	1.48	1.54
18	Z	613	CLA	C3D-C4D	-2.04	1.39	1.44
18	A	833	CLA	C3D-C4D	-2.04	1.39	1.44
18	5	603	CLA	C3D-C4D	-2.04	1.39	1.44
18	B	810	CLA	C3A-C2A	-2.04	1.48	1.54
21	6	305	CHL	C4B-CHC	-2.04	1.35	1.41
18	B	809	CLA	CHD-C4C	-2.04	1.34	1.39
18	A	839	CLA	CHD-C4C	-2.04	1.34	1.39
18	A	824	CLA	CHD-C4C	-2.04	1.34	1.39
18	A	802	CLA	CHD-C4C	-2.03	1.34	1.39
18	A	810	CLA	C3B-C2B	-2.03	1.37	1.40
21	6	306	CHL	C1B-CHB	-2.03	1.35	1.41
18	A	807	CLA	C3B-C2B	-2.03	1.37	1.40
18	6	317	CLA	C3D-C4D	-2.03	1.39	1.44
18	B	833	CLA	CHD-C4C	-2.03	1.34	1.39
18	3	308	CLA	CHD-C4C	-2.03	1.34	1.39
18	1	613	CLA	C3D-C4D	-2.03	1.39	1.44
21	1	606	CHL	C4B-CHC	-2.03	1.35	1.41
21	Z	605	CHL	C1B-CHB	-2.03	1.35	1.41
18	Z	606	CLA	C3B-C2B	-2.03	1.37	1.40
18	A	822	CLA	C1C-NC	-2.03	1.34	1.37
18	B	828	CLA	C3D-C4D	-2.03	1.39	1.44
18	3	308	CLA	C3D-C4D	-2.03	1.39	1.44
18	6	303	CLA	CHD-C4C	-2.03	1.34	1.39
18	B	821	CLA	C3D-C4D	-2.03	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	302	CLA	C3D-C4D	-2.03	1.39	1.44
18	8	612	CLA	C3B-C2B	-2.03	1.37	1.40
18	8	612	CLA	CHD-C4C	-2.03	1.34	1.39
18	B	843	CLA	C3A-C2A	-2.03	1.48	1.54
21	7	606	CHL	C1D-ND	2.03	1.40	1.37
18	A	824	CLA	C1D-ND	2.02	1.40	1.37
18	7	607	CLA	C3D-C4D	-2.02	1.39	1.44
21	Z	605	CHL	C4B-CHC	-2.02	1.35	1.41
21	3	306	CHL	C4B-CHC	-2.02	1.35	1.41
18	B	831	CLA	CHD-C4C	-2.02	1.34	1.39
18	1	602	CLA	CHD-C4C	-2.02	1.34	1.39
18	A	840	CLA	C3A-C2A	-2.02	1.48	1.54
18	A	816	CLA	CHD-C4C	-2.02	1.34	1.39
18	B	842	CLA	CHD-C4C	-2.02	1.34	1.39
18	A	816	CLA	C3D-C4D	-2.02	1.39	1.44
18	7	612	CLA	CHD-C4C	-2.02	1.34	1.39
18	6	312	CLA	CHD-C4C	-2.01	1.34	1.39
18	A	804	CLA	C3B-C2B	-2.01	1.37	1.40
18	1	604	CLA	C3D-C4D	-2.01	1.39	1.44
18	A	825	CLA	C3D-C4D	-2.01	1.39	1.44
18	7	602	CLA	C3A-C2A	-2.01	1.48	1.54
21	5	616	CHL	C1B-CHB	-2.01	1.35	1.41
18	6	311	CLA	C3D-C4D	-2.01	1.39	1.44
18	A	817	CLA	CHD-C4C	-2.01	1.34	1.39
18	8	615	CLA	C3D-C4D	-2.01	1.39	1.44
18	8	611	CLA	C3B-C2B	-2.00	1.37	1.40
18	5	602	CLA	C3B-C2B	-2.00	1.37	1.40
18	B	819	CLA	C3D-C4D	-2.00	1.39	1.44
18	7	608	CLA	CHD-C4C	-2.00	1.34	1.39

All (1748) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	606	CHL	C4A-NA-C1A	-12.99	100.87	106.71
21	4	605	CHL	C4A-NA-C1A	-12.67	101.01	106.71
18	7	614	CLA	C4A-NA-C1A	-10.95	101.78	106.71
18	7	610	CLA	C4A-NA-C1A	-10.06	102.18	106.71
18	A	834	CLA	C4A-NA-C1A	-9.90	102.26	106.71
18	3	305	CLA	C4A-NA-C1A	-9.76	102.32	106.71
18	5	615	CLA	C4A-NA-C1A	-9.45	102.46	106.71
21	8	606	CHL	C4A-NA-C1A	-9.37	102.49	106.71
18	6	310	CLA	C4A-NA-C1A	-9.26	102.54	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	306	CHL	C4A-NA-C1A	-8.93	102.69	106.71
18	3	309	CLA	C4A-NA-C1A	-8.91	102.70	106.71
18	B	815	CLA	C4A-NA-C1A	-8.87	102.72	106.71
21	7	606	CHL	C4A-NA-C1A	-8.81	102.75	106.71
18	4	608	CLA	C4A-NA-C1A	-8.72	102.79	106.71
18	B	804	CLA	C4A-NA-C1A	-8.47	102.90	106.71
21	3	306	CHL	C4A-NA-C1A	-8.41	102.93	106.71
18	B	806	CLA	C4A-NA-C1A	-8.20	103.02	106.71
18	A	802	CLA	C4A-NA-C1A	-8.19	103.03	106.71
18	Z	607	CLA	C4A-NA-C1A	-8.17	103.03	106.71
21	4	604	CHL	C4A-NA-C1A	-8.13	103.05	106.71
18	1	608	CLA	C4A-NA-C1A	-8.11	103.06	106.71
21	1	606	CHL	C4A-NA-C1A	-8.04	103.09	106.71
21	Z	605	CHL	C4A-NA-C1A	-7.99	103.11	106.71
18	4	601	CLA	C4A-NA-C1A	-7.87	103.17	106.71
18	8	611	CLA	C4A-NA-C1A	-7.81	103.20	106.71
18	8	614	CLA	C4A-NA-C1A	-7.58	103.30	106.71
18	B	835	CLA	C4A-NA-C1A	-7.48	103.34	106.71
18	3	307	CLA	C4A-NA-C1A	-7.45	103.36	106.71
18	B	827	CLA	C4A-NA-C1A	-7.39	103.38	106.71
21	6	316	CHL	C4A-NA-C1A	-7.32	103.42	106.71
18	B	812	CLA	C4A-NA-C1A	-7.30	103.42	106.71
18	A	824	CLA	C4A-NA-C1A	-7.27	103.44	106.71
18	A	805	CLA	C4A-NA-C1A	-7.23	103.45	106.71
18	A	840	CLA	C4A-NA-C1A	-7.20	103.47	106.71
18	6	315	CLA	C4A-NA-C1A	-7.17	103.48	106.71
18	Z	609	CLA	C4A-NA-C1A	-7.11	103.51	106.71
18	1	610	CLA	C4A-NA-C1A	-7.07	103.53	106.71
18	B	820	CLA	C4A-NA-C1A	-7.02	103.55	106.71
21	5	616	CHL	C4A-NA-C1A	-6.98	103.57	106.71
18	5	617	CLA	C4A-NA-C1A	-6.94	103.58	106.71
18	B	836	CLA	C4A-NA-C1A	-6.93	103.59	106.71
18	A	822	CLA	C4A-NA-C1A	-6.92	103.60	106.71
21	6	305	CHL	C4A-NA-C1A	-6.87	103.62	106.71
18	A	823	CLA	C4A-NA-C1A	-6.82	103.64	106.71
18	B	819	CLA	C4A-NA-C1A	-6.81	103.64	106.71
18	B	841	CLA	C4A-NA-C1A	-6.81	103.64	106.71
18	A	804	CLA	C4A-NA-C1A	-6.73	103.68	106.71
18	A	803	CLA	C4A-NA-C1A	-6.70	103.69	106.71
21	5	607	CHL	C4A-NA-C1A	-6.67	103.71	106.71
18	8	610	CLA	C4A-NA-C1A	-6.57	103.75	106.71
18	B	808	CLA	C4A-NA-C1A	-6.56	103.76	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	822	CLA	C4A-NA-C1A	-6.54	103.77	106.71
18	7	613	CLA	C4A-NA-C1A	-6.51	103.78	106.71
18	7	605	CLA	C4A-NA-C1A	-6.49	103.79	106.71
18	B	805	CLA	C4A-NA-C1A	-6.48	103.79	106.71
18	A	806	CLA	C4A-NA-C1A	-6.45	103.81	106.71
21	Z	601	CHL	C4A-NA-C1A	-6.40	103.83	106.71
18	B	831	CLA	C4A-NA-C1A	-6.39	103.83	106.71
18	F	301	CLA	C4A-NA-C1A	-6.37	103.84	106.71
18	A	831	CLA	C4A-NA-C1A	-6.37	103.84	106.71
21	1	601	CHL	C4A-NA-C1A	-6.34	103.86	106.71
18	B	807	CLA	C4A-NA-C1A	-6.31	103.87	106.71
18	5	613	CLA	C4A-NA-C1A	-6.28	103.88	106.71
18	B	811	CLA	C4A-NA-C1A	-6.28	103.88	106.71
18	B	842	CLA	C4A-NA-C1A	-6.22	103.91	106.71
21	6	307	CHL	C4A-NA-C1A	-6.18	103.93	106.71
18	A	838	CLA	C4A-NA-C1A	-6.17	103.93	106.71
18	3	304	CLA	C4A-NA-C1A	-6.16	103.94	106.71
18	A	826	CLA	C4A-NA-C1A	-6.15	103.94	106.71
18	6	314	CLA	C4A-NA-C1A	-6.14	103.95	106.71
18	5	610	CLA	C4A-NA-C1A	-6.13	103.95	106.71
18	6	308	CLA	C4A-NA-C1A	-6.13	103.95	106.71
18	B	832	CLA	C4A-NA-C1A	-6.09	103.97	106.71
18	B	840	CLA	C4A-NA-C1A	-6.06	103.98	106.71
18	B	843	CLA	C4A-NA-C1A	-6.05	103.99	106.71
18	4	610	CLA	C4A-NA-C1A	-6.04	103.99	106.71
18	A	808	CLA	C4A-NA-C1A	-6.04	103.99	106.71
18	4	603	CLA	C4A-NA-C1A	-6.03	103.99	106.71
18	6	302	CLA	C4A-NA-C1A	-6.02	104.00	106.71
18	8	603	CLA	C4A-NA-C1A	-5.98	104.02	106.71
18	B	802	CLA	C4A-NA-C1A	-5.98	104.02	106.71
18	A	827	CLA	C4A-NA-C1A	-5.96	104.03	106.71
18	4	602	CLA	C4A-NA-C1A	-5.95	104.03	106.71
18	1	605	CLA	C4A-NA-C1A	-5.95	104.03	106.71
18	A	825	CLA	C4A-NA-C1A	-5.91	104.05	106.71
18	Z	604	CLA	C4A-NA-C1A	-5.91	104.05	106.71
18	6	313	CLA	C4A-NA-C1A	-5.90	104.05	106.71
18	4	607	CLA	C4A-NA-C1A	-5.89	104.06	106.71
18	B	817	CLA	C4A-NA-C1A	-5.89	104.06	106.71
18	5	602	CLA	C4A-NA-C1A	-5.89	104.06	106.71
18	6	309	CLA	C4A-NA-C1A	-5.81	104.10	106.71
18	5	605	CLA	C4A-NA-C1A	-5.80	104.10	106.71
18	B	818	CLA	C4A-NA-C1A	-5.77	104.11	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	303	CLA	C4A-NA-C1A	-5.76	104.12	106.71
18	A	811	CLA	C4A-NA-C1A	-5.76	104.12	106.71
18	A	819	CLA	C4A-NA-C1A	-5.75	104.12	106.71
18	5	612	CLA	C4A-NA-C1A	-5.73	104.13	106.71
18	A	832	CLA	C4A-NA-C1A	-5.73	104.13	106.71
18	A	829	CLA	C4A-NA-C1A	-5.73	104.13	106.71
18	B	819	CLA	CAA-C2A-C1A	-5.68	99.58	112.14
18	B	839	CLA	C4A-NA-C1A	-5.65	104.17	106.71
18	8	615	CLA	C4A-NA-C1A	-5.57	104.20	106.71
18	8	605	CLA	C4A-NA-C1A	-5.55	104.21	106.71
18	3	302	CLA	C4A-NA-C1A	-5.54	104.22	106.71
18	1	603	CLA	C4A-NA-C1A	-5.52	104.22	106.71
18	8	612	CLA	C4A-NA-C1A	-5.50	104.23	106.71
18	6	310	CLA	C1B-CHB-C4A	-5.48	119.27	130.12
18	1	611	CLA	C4A-NA-C1A	-5.48	104.24	106.71
18	B	824	CLA	C4A-NA-C1A	-5.44	104.26	106.71
18	Z	610	CLA	C4A-NA-C1A	-5.44	104.26	106.71
18	6	311	CLA	C4A-NA-C1A	-5.43	104.26	106.71
18	1	609	CLA	C4A-NA-C1A	-5.42	104.27	106.71
18	A	807	CLA	C4A-NA-C1A	-5.41	104.27	106.71
18	B	801	CLA	C4A-NA-C1A	-5.39	104.28	106.71
18	6	310	CLA	C3A-C2A-C1A	-5.38	93.28	101.34
18	5	611	CLA	C4A-NA-C1A	-5.38	104.29	106.71
18	A	835	CLA	C4A-NA-C1A	-5.38	104.29	106.71
18	Z	613	CLA	C4A-NA-C1A	-5.38	104.29	106.71
18	3	301	CLA	C4A-NA-C1A	-5.37	104.29	106.71
18	Z	608	CLA	C4A-NA-C1A	-5.37	104.29	106.71
18	8	608	CLA	C4A-NA-C1A	-5.37	104.29	106.71
18	3	312	CLA	C4A-NA-C1A	-5.35	104.30	106.71
18	A	825	CLA	CHD-C1D-ND	-5.35	119.54	124.45
18	3	313	CLA	C4A-NA-C1A	-5.33	104.31	106.71
18	7	603	CLA	C4A-NA-C1A	-5.32	104.31	106.71
18	B	813	CLA	C4A-NA-C1A	-5.30	104.32	106.71
18	1	613	CLA	C4A-NA-C1A	-5.30	104.32	106.71
18	1	614	CLA	C4A-NA-C1A	-5.29	104.33	106.71
18	A	839	CLA	C4A-NA-C1A	-5.29	104.33	106.71
18	A	812	CLA	C4A-NA-C1A	-5.29	104.33	106.71
18	Z	612	CLA	C4A-NA-C1A	-5.28	104.33	106.71
18	7	608	CLA	C4A-NA-C1A	-5.27	104.34	106.71
18	A	820	CLA	C4A-NA-C1A	-5.27	104.34	106.71
18	7	612	CLA	C4A-NA-C1A	-5.26	104.34	106.71
18	B	812	CLA	CAA-C2A-C1A	-5.26	100.50	112.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	836	CLA	C4A-NA-C1A	-5.25	104.34	106.71
18	A	837	CLA	C4A-NA-C1A	-5.24	104.35	106.71
18	3	310	CLA	C4A-NA-C1A	-5.23	104.35	106.71
18	B	837	CLA	C4A-NA-C1A	-5.23	104.35	106.71
18	8	604	CLA	C4A-NA-C1A	-5.23	104.35	106.71
18	B	809	CLA	C4A-NA-C1A	-5.23	104.36	106.71
18	7	602	CLA	C4A-NA-C1A	-5.18	104.38	106.71
18	A	814	CLA	C4A-NA-C1A	-5.15	104.39	106.71
18	B	834	CLA	C4A-NA-C1A	-5.14	104.39	106.71
18	8	613	CLA	C4A-NA-C1A	-5.14	104.40	106.71
18	5	604	CLA	C4A-NA-C1A	-5.13	104.40	106.71
18	5	609	CLA	C4A-NA-C1A	-5.11	104.41	106.71
18	4	606	CLA	C4A-NA-C1A	-5.10	104.41	106.71
18	5	603	CLA	C4A-NA-C1A	-5.10	104.41	106.71
18	B	816	CLA	C4A-NA-C1A	-5.10	104.41	106.71
18	B	825	CLA	C4A-NA-C1A	-5.10	104.41	106.71
18	Z	611	CLA	C4A-NA-C1A	-5.10	104.42	106.71
17	A	801	CL0	C4A-NA-C1A	-5.09	104.42	106.71
18	A	826	CLA	CAA-C2A-C1A	-5.08	100.89	112.14
18	A	810	CLA	C4A-NA-C1A	-5.08	104.42	106.71
18	B	823	CLA	C4A-NA-C1A	-5.06	104.43	106.71
18	B	828	CLA	C4A-NA-C1A	-5.05	104.43	106.71
18	A	830	CLA	C4A-NA-C1A	-5.04	104.44	106.71
18	7	604	CLA	C4A-NA-C1A	-5.02	104.45	106.71
18	Z	606	CLA	C4A-NA-C1A	-5.02	104.45	106.71
18	1	612	CLA	C4A-NA-C1A	-5.01	104.45	106.71
18	1	607	CLA	C4A-NA-C1A	-5.00	104.46	106.71
18	6	301	CLA	C4A-NA-C1A	-5.00	104.46	106.71
18	5	615	CLA	C3A-C2A-C1A	-4.98	93.88	101.34
18	A	821	CLA	C4A-NA-C1A	-4.98	104.47	106.71
18	A	809	CLA	C4A-NA-C1A	-4.97	104.47	106.71
18	7	601	CLA	C4A-NA-C1A	-4.97	104.47	106.71
18	4	611	CLA	C4A-NA-C1A	-4.97	104.47	106.71
18	3	311	CLA	C4A-NA-C1A	-4.95	104.48	106.71
18	4	608	CLA	C3A-C2A-C1A	-4.94	93.94	101.34
18	7	607	CLA	C4A-NA-C1A	-4.94	104.49	106.71
18	B	838	CLA	C4A-NA-C1A	-4.91	104.50	106.71
18	F	302	CLA	C4A-NA-C1A	-4.90	104.50	106.71
21	5	606	CHL	C1B-CHB-C4A	-4.87	120.48	130.12
18	B	833	CLA	C4A-NA-C1A	-4.86	104.52	106.71
18	6	317	CLA	C4A-NA-C1A	-4.85	104.53	106.71
18	J	101	CLA	C4A-NA-C1A	-4.81	104.54	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	8	609	CLA	CHD-C1D-ND	-4.81	120.04	124.45
18	8	601	CLA	C4A-NA-C1A	-4.81	104.55	106.71
21	4	604	CHL	CAA-C2A-C1A	4.81	122.78	112.14
18	B	826	CLA	C4A-NA-C1A	-4.80	104.55	106.71
18	7	614	CLA	C3A-C2A-C1A	-4.80	94.15	101.34
18	A	816	CLA	C4A-NA-C1A	-4.80	104.55	106.71
18	A	843	CLA	C4A-NA-C1A	-4.78	104.56	106.71
18	A	817	CLA	C4A-NA-C1A	-4.75	104.57	106.71
18	A	841	CLA	C4A-NA-C1A	-4.74	104.58	106.71
18	B	829	CLA	C4A-NA-C1A	-4.71	104.59	106.71
18	A	827	CLA	CAA-C2A-C1A	-4.71	101.71	112.14
18	7	609	CLA	C4A-NA-C1A	-4.70	104.59	106.71
18	B	806	CLA	C3A-C2A-C1A	-4.69	94.31	101.34
18	A	813	CLA	C4A-NA-C1A	-4.66	104.61	106.71
18	A	827	CLA	CHD-C1D-ND	-4.64	120.19	124.45
18	1	604	CLA	C4A-NA-C1A	-4.64	104.62	106.71
18	A	833	CLA	C4A-NA-C1A	-4.62	104.63	106.71
18	Z	603	CLA	C4A-NA-C1A	-4.62	104.63	106.71
18	A	808	CLA	CAA-C2A-C1A	-4.61	101.93	112.14
18	B	821	CLA	C4A-NA-C1A	-4.60	104.64	106.71
18	A	845	CLA	C4A-NA-C1A	-4.60	104.64	106.71
18	8	607	CLA	C4A-NA-C1A	-4.59	104.64	106.71
18	5	614	CLA	C4A-NA-C1A	-4.57	104.65	106.71
18	A	828	CLA	C4A-NA-C1A	-4.57	104.65	106.71
18	3	314	CLA	C4A-NA-C1A	-4.55	104.66	106.71
18	6	303	CLA	C4A-NA-C1A	-4.53	104.67	106.71
18	B	823	CLA	CHD-C1D-ND	-4.52	120.30	124.45
18	6	313	CLA	CHD-C1D-ND	-4.51	120.31	124.45
18	A	815	CLA	C4A-NA-C1A	-4.50	104.68	106.71
21	5	606	CHL	C3A-C2A-C1A	-4.48	94.62	101.34
18	B	823	CLA	C1D-ND-C4D	-4.48	103.15	106.33
18	A	838	CLA	CHD-C1D-ND	-4.46	120.35	124.45
18	A	803	CLA	CAA-C2A-C1A	-4.46	102.28	112.14
18	A	818	CLA	C4A-NA-C1A	-4.46	104.70	106.71
18	Z	602	CLA	C4A-NA-C1A	-4.44	104.71	106.71
18	4	609	CLA	C4A-NA-C1A	-4.44	104.71	106.71
18	B	814	CLA	C4A-NA-C1A	-4.42	104.72	106.71
18	A	844	CLA	C4A-NA-C1A	-4.41	104.72	106.71
18	B	820	CLA	CHD-C1D-ND	-4.40	120.41	124.45
18	A	819	CLA	CHD-C1D-ND	-4.40	120.41	124.45
18	B	810	CLA	C4A-NA-C1A	-4.39	104.73	106.71
18	A	803	CLA	CHD-C1D-ND	-4.38	120.43	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	7	614	CLA	CHD-C1D-ND	-4.37	120.44	124.45
18	8	609	CLA	C4A-NA-C1A	-4.37	104.74	106.71
18	1	602	CLA	C4A-NA-C1A	-4.37	104.74	106.71
18	4	612	CLA	CHD-C1D-ND	-4.34	120.46	124.45
18	8	611	CLA	CHD-C1D-ND	-4.30	120.50	124.45
18	5	611	CLA	CHD-C1D-ND	-4.30	120.50	124.45
18	5	608	CLA	C4A-NA-C1A	-4.30	104.77	106.71
18	4	601	CLA	CHD-C1D-ND	-4.30	120.50	124.45
18	3	301	CLA	CHD-C1D-ND	-4.29	120.51	124.45
18	4	607	CLA	CHD-C1D-ND	-4.27	120.53	124.45
18	8	610	CLA	C1B-CHB-C4A	-4.26	121.68	130.12
18	5	615	CLA	CHD-C1D-ND	-4.24	120.56	124.45
18	7	611	CLA	C4A-NA-C1A	-4.22	104.81	106.71
18	4	609	CLA	CHD-C1D-ND	-4.22	120.58	124.45
18	B	827	CLA	CHD-C1D-ND	-4.22	120.58	124.45
18	B	807	CLA	CHD-C1D-ND	-4.21	120.58	124.45
21	7	606	CHL	C1B-CHB-C4A	-4.21	121.78	130.12
18	3	308	CLA	C4A-NA-C1A	-4.21	104.81	106.71
18	6	311	CLA	CHD-C1D-ND	-4.20	120.59	124.45
18	A	819	CLA	CAA-C2A-C1A	-4.20	102.84	112.14
18	5	617	CLA	CHD-C1D-ND	-4.19	120.60	124.45
18	5	601	CLA	C4A-NA-C1A	-4.19	104.82	106.71
18	B	828	CLA	CHD-C1D-ND	-4.18	120.61	124.45
18	B	819	CLA	CHD-C1D-ND	-4.17	120.62	124.45
18	A	807	CLA	CHD-C1D-ND	-4.16	120.63	124.45
18	3	310	CLA	CHD-C1D-ND	-4.16	120.63	124.45
18	1	608	CLA	CAA-C2A-C1A	-4.15	102.94	112.14
18	7	610	CLA	CHD-C1D-ND	-4.15	120.64	124.45
18	3	305	CLA	C3A-C2A-C1A	-4.15	95.12	101.34
18	Z	607	CLA	CAA-C2A-C1A	-4.15	102.96	112.14
18	B	815	CLA	C3A-C2A-C1A	-4.15	95.13	101.34
18	B	804	CLA	CHD-C1D-ND	-4.14	120.64	124.45
18	8	608	CLA	CHD-C1D-ND	-4.14	120.65	124.45
18	7	610	CLA	C3A-C2A-C1A	-4.14	94.63	101.64
18	3	307	CLA	CAA-C2A-C1A	-4.13	103.00	112.14
18	3	305	CLA	CAA-C2A-C1A	-4.13	103.00	112.14
18	A	820	CLA	CHD-C1D-ND	-4.12	120.67	124.45
18	4	606	CLA	CHD-C1D-ND	-4.12	120.67	124.45
21	8	606	CHL	C1B-CHB-C4A	-4.12	121.96	130.12
18	B	805	CLA	CHD-C1D-ND	-4.11	120.67	124.45
18	B	822	CLA	CHD-C1D-ND	-4.11	120.68	124.45
18	B	841	CLA	CHD-C1D-ND	-4.11	120.68	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	101	CLA	CHD-C1D-ND	-4.10	120.69	124.45
18	5	613	CLA	CHD-C1D-ND	-4.09	120.69	124.45
18	7	602	CLA	CHD-C1D-ND	-4.08	120.70	124.45
18	6	312	CLA	C4A-NA-C1A	-4.08	104.87	106.71
18	8	603	CLA	CHD-C1D-ND	-4.08	120.70	124.45
18	A	808	CLA	CHD-C1D-ND	-4.06	120.72	124.45
18	B	806	CLA	CHD-C1D-ND	-4.06	120.72	124.45
18	A	836	CLA	CHD-C1D-ND	-4.06	120.73	124.45
18	3	312	CLA	CHD-C1D-ND	-4.05	120.73	124.45
18	7	611	CLA	CHD-C1D-ND	-4.03	120.75	124.45
18	3	309	CLA	CHD-C1D-ND	-4.03	120.75	124.45
18	7	609	CLA	CHD-C1D-ND	-4.03	120.75	124.45
18	B	813	CLA	CHD-C1D-ND	-4.03	120.75	124.45
21	4	604	CHL	C1B-CHB-C4A	-4.02	122.16	130.12
18	B	835	CLA	CHD-C1D-ND	-4.02	120.76	124.45
18	A	826	CLA	CHD-C1D-ND	-4.01	120.77	124.45
18	A	802	CLA	CHD-C1D-ND	-4.01	120.77	124.45
18	A	814	CLA	CHD-C1D-ND	-4.01	120.77	124.45
18	B	829	CLA	CAA-C2A-C1A	-4.01	103.27	112.14
18	6	302	CLA	CHD-C1D-ND	-4.00	120.78	124.45
21	5	607	CHL	CAA-C2A-C1A	4.00	120.98	112.14
18	A	825	CLA	CAA-C2A-C1A	-3.99	103.30	112.14
18	A	823	CLA	CHD-C1D-ND	-3.99	120.79	124.45
18	B	816	CLA	CHD-C1D-ND	-3.99	120.79	124.45
18	A	815	CLA	CHD-C1D-ND	-3.99	120.79	124.45
18	A	812	CLA	CHD-C1D-ND	-3.99	120.79	124.45
18	B	842	CLA	CHD-C1D-ND	-3.98	120.80	124.45
18	3	307	CLA	CHD-C1D-ND	-3.98	120.80	124.45
18	6	304	CLA	C4A-NA-C1A	-3.97	104.92	106.71
18	7	613	CLA	CHD-C1D-ND	-3.96	120.82	124.45
18	F	301	CLA	CHD-C1D-ND	-3.95	120.82	124.45
18	8	610	CLA	CHD-C1D-ND	-3.95	120.82	124.45
18	A	830	CLA	CHD-C1D-ND	-3.95	120.82	124.45
18	B	830	CLA	C4A-NA-C1A	-3.94	104.93	106.71
17	A	801	CL0	CHD-C1D-ND	-3.94	120.83	124.45
18	5	604	CLA	CHD-C1D-ND	-3.94	120.83	124.45
18	A	817	CLA	CHD-C1D-ND	-3.94	120.84	124.45
18	1	602	CLA	CHD-C1D-ND	-3.93	120.84	124.45
18	Z	602	CLA	CHD-C1D-ND	-3.93	120.85	124.45
18	A	824	CLA	CHD-C1D-ND	-3.92	120.85	124.45
18	1	602	CLA	C1D-ND-C4D	-3.91	103.56	106.33
18	A	810	CLA	CHD-C1D-ND	-3.91	120.86	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	310	CLA	C3B-C4B-NB	-3.91	104.15	109.21
18	B	842	CLA	CAA-C2A-C1A	-3.90	103.50	112.14
21	Z	605	CHL	C1B-CHB-C4A	-3.90	122.39	130.12
21	1	606	CHL	C1B-CHB-C4A	-3.90	122.40	130.12
18	B	801	CLA	CHD-C1D-ND	-3.89	120.88	124.45
18	B	809	CLA	CHD-C1D-ND	-3.89	120.88	124.45
18	B	843	CLA	CHD-C1D-ND	-3.89	120.88	124.45
18	Z	602	CLA	C1D-ND-C4D	-3.89	103.57	106.33
18	A	805	CLA	CHD-C1D-ND	-3.88	120.89	124.45
18	6	308	CLA	CHD-C1D-ND	-3.88	120.89	124.45
18	4	602	CLA	CHD-C1D-ND	-3.88	120.89	124.45
18	B	818	CLA	CHD-C1D-ND	-3.87	120.89	124.45
18	B	824	CLA	CHD-C1D-ND	-3.87	120.90	124.45
18	1	605	CLA	C2C-C1C-NC	3.86	113.59	109.97
18	5	602	CLA	CHD-C1D-ND	-3.86	120.91	124.45
18	A	831	CLA	CHD-C1D-ND	-3.85	120.91	124.45
18	4	610	CLA	CHD-C1D-ND	-3.85	120.92	124.45
18	A	816	CLA	CHD-C1D-ND	-3.84	120.92	124.45
18	B	832	CLA	CHD-C1D-ND	-3.84	120.93	124.45
18	Z	604	CLA	C2C-C1C-NC	3.83	113.56	109.97
18	B	820	CLA	C3A-C2A-C1A	-3.83	95.60	101.34
18	8	602	CLA	CHD-C1D-ND	-3.83	120.93	124.45
18	5	615	CLA	C1B-CHB-C4A	-3.83	122.53	130.12
18	B	814	CLA	CHD-C1D-ND	-3.83	120.94	124.45
18	3	302	CLA	CHD-C1D-ND	-3.81	120.95	124.45
18	8	604	CLA	CHD-C1D-ND	-3.81	120.95	124.45
18	6	309	CLA	CHD-C1D-ND	-3.81	120.95	124.45
18	3	305	CLA	CHD-C1D-ND	-3.80	120.96	124.45
18	3	309	CLA	C3A-C2A-C1A	-3.80	95.21	101.64
18	8	609	CLA	C1D-ND-C4D	-3.79	103.64	106.33
18	7	608	CLA	CHD-C1D-ND	-3.79	120.97	124.45
18	A	840	CLA	CHD-C1D-ND	-3.79	120.97	124.45
18	B	834	CLA	C4B-CHC-C1C	-3.79	122.61	130.12
18	8	608	CLA	C1D-ND-C4D	-3.78	103.65	106.33
18	6	315	CLA	CHD-C1D-ND	-3.78	120.98	124.45
18	5	614	CLA	CHD-C1D-ND	-3.78	120.98	124.45
18	A	818	CLA	CHD-C1D-ND	-3.77	120.99	124.45
18	Z	612	CLA	CHD-C1D-ND	-3.76	121.00	124.45
21	6	306	CHL	C1B-CHB-C4A	-3.76	122.66	130.12
18	A	829	CLA	CHD-C1D-ND	-3.76	121.00	124.45
18	8	613	CLA	CHD-C1D-ND	-3.76	121.00	124.45
21	5	606	CHL	CHA-C1A-NA	-3.76	117.79	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	313	CLA	CHD-C1D-ND	-3.76	121.00	124.45
21	5	606	CHL	C2A-C3A-C4A	-3.75	95.81	101.87
18	5	609	CLA	CHD-C1D-ND	-3.75	121.01	124.45
18	B	815	CLA	CHD-C1D-ND	-3.74	121.02	124.45
18	5	611	CLA	C1D-ND-C4D	-3.74	103.68	106.33
18	4	601	CLA	C3A-C2A-C1A	-3.74	95.74	101.34
18	7	602	CLA	C1D-ND-C4D	-3.73	103.69	106.33
18	A	836	CLA	C1D-ND-C4D	-3.72	103.69	106.33
18	A	832	CLA	CHD-C1D-ND	-3.72	121.03	124.45
18	B	817	CLA	CHD-C1D-ND	-3.72	121.03	124.45
18	1	613	CLA	CHD-C1D-ND	-3.72	121.04	124.45
18	B	809	CLA	C1D-ND-C4D	-3.71	103.70	106.33
18	3	301	CLA	C1D-ND-C4D	-3.71	103.70	106.33
18	B	810	CLA	CHD-C1D-ND	-3.70	121.05	124.45
18	1	614	CLA	CHD-C1D-ND	-3.70	121.05	124.45
18	Z	613	CLA	CHD-C1D-ND	-3.70	121.05	124.45
18	B	801	CLA	CAA-C2A-C1A	-3.70	103.94	112.14
18	B	821	CLA	CHD-C1D-ND	-3.70	121.05	124.45
18	B	834	CLA	CMC-C2C-C1C	3.70	126.06	113.11
18	B	839	CLA	CHD-C1D-ND	-3.70	121.05	124.45
21	5	606	CHL	CHD-C1D-ND	-3.70	121.05	124.45
18	7	601	CLA	CHD-C1D-ND	-3.70	121.06	124.45
18	6	303	CLA	CHD-C1D-ND	-3.69	121.06	124.45
18	6	310	CLA	CHD-C1D-ND	-3.69	121.06	124.45
18	3	308	CLA	CHD-C1D-ND	-3.68	121.07	124.45
18	A	817	CLA	C1D-ND-C4D	-3.68	103.72	106.33
18	F	302	CLA	CHD-C1D-ND	-3.67	121.08	124.45
18	6	302	CLA	C1D-ND-C4D	-3.67	103.73	106.33
21	Z	605	CHL	CMB-C2B-C1B	-3.67	122.83	128.46
18	B	829	CLA	CHD-C1D-ND	-3.66	121.09	124.45
21	8	606	CHL	CHA-C1A-NA	-3.66	118.01	126.40
18	5	602	CLA	C1D-ND-C4D	-3.66	103.74	106.33
18	Z	606	CLA	CHD-C1D-ND	-3.66	121.09	124.45
18	4	602	CLA	C1D-ND-C4D	-3.65	103.74	106.33
18	A	835	CLA	CHD-C1D-ND	-3.65	121.10	124.45
21	1	606	CHL	CMB-C2B-C1B	-3.65	122.86	128.46
18	A	834	CLA	CHD-C1D-ND	-3.65	121.10	124.45
18	B	802	CLA	CHD-C1D-ND	-3.65	121.10	124.45
21	5	606	CHL	C2A-C1A-CHA	3.65	130.23	123.86
18	5	610	CLA	CHD-C1D-ND	-3.65	121.10	124.45
18	A	837	CLA	CHD-C1D-ND	-3.64	121.11	124.45
18	1	607	CLA	CHD-C1D-ND	-3.64	121.11	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	8	614	CLA	CHD-C1D-ND	-3.63	121.11	124.45
18	1	608	CLA	CHD-C1D-ND	-3.63	121.11	124.45
18	5	615	CLA	C2A-C3A-C4A	-3.63	96.01	101.87
18	7	603	CLA	CHD-C1D-ND	-3.63	121.12	124.45
18	B	831	CLA	CHD-C1D-ND	-3.62	121.12	124.45
18	4	611	CLA	CHD-C1D-ND	-3.62	121.13	124.45
18	1	611	CLA	CHD-C1D-ND	-3.62	121.13	124.45
18	Z	603	CLA	CHD-C1D-ND	-3.62	121.13	124.45
18	4	609	CLA	C1D-ND-C4D	-3.61	103.77	106.33
18	Z	607	CLA	CHD-C1D-ND	-3.61	121.14	124.45
18	B	838	CLA	CHD-C1D-ND	-3.61	121.14	124.45
18	Z	608	CLA	CHD-C1D-ND	-3.60	121.14	124.45
18	B	812	CLA	CHD-C1D-ND	-3.60	121.14	124.45
18	1	609	CLA	CHD-C1D-ND	-3.60	121.15	124.45
18	1	612	CLA	CHD-C1D-ND	-3.59	121.15	124.45
18	7	605	CLA	CHD-C1D-ND	-3.59	121.16	124.45
18	1	604	CLA	CHD-C1D-ND	-3.59	121.16	124.45
18	B	808	CLA	C2C-C1C-NC	3.59	113.33	109.97
18	8	612	CLA	CHD-C1D-ND	-3.58	121.16	124.45
18	Z	610	CLA	CHD-C1D-ND	-3.58	121.16	124.45
18	B	836	CLA	CHD-C1D-ND	-3.58	121.16	124.45
18	3	303	CLA	CHD-C1D-ND	-3.58	121.17	124.45
18	A	806	CLA	CHD-C1D-ND	-3.58	121.17	124.45
18	B	825	CLA	CHD-C1D-ND	-3.58	121.17	124.45
18	5	610	CLA	C1B-CHB-C4A	-3.57	123.04	130.12
18	B	830	CLA	CHD-C1D-ND	-3.57	121.17	124.45
18	Z	609	CLA	CHD-C1D-ND	-3.56	121.18	124.45
18	8	601	CLA	CHD-C1D-ND	-3.56	121.18	124.45
18	B	805	CLA	CAA-C2A-C1A	-3.56	104.26	112.14
18	A	845	CLA	CHD-C1D-ND	-3.56	121.19	124.45
18	5	603	CLA	C2C-C1C-NC	3.56	113.30	109.97
18	B	842	CLA	C1D-ND-C4D	-3.55	103.81	106.33
18	A	812	CLA	C1D-ND-C4D	-3.55	103.81	106.33
18	8	602	CLA	C4A-NA-C1A	-3.55	105.11	106.71
18	6	311	CLA	C1D-ND-C4D	-3.55	103.81	106.33
18	A	811	CLA	CHD-C1D-ND	-3.55	121.19	124.45
21	8	606	CHL	CAA-C2A-C1A	3.55	119.99	112.14
18	B	826	CLA	CHD-C1D-ND	-3.53	121.21	124.45
18	A	808	CLA	C1D-ND-C4D	-3.53	103.83	106.33
21	Z	601	CHL	C1B-CHB-C4A	-3.53	123.12	130.12
21	1	601	CHL	C1B-CHB-C4A	-3.53	123.13	130.12
18	1	610	CLA	CHD-C1D-ND	-3.53	121.21	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	8	611	CLA	C1D-ND-C4D	-3.52	103.83	106.33
18	B	806	CLA	C1B-CHB-C4A	-3.52	123.14	130.12
21	4	605	CHL	CHD-C1D-ND	-3.52	121.22	124.45
21	8	606	CHL	CHD-C1D-ND	-3.52	121.22	124.45
18	7	607	CLA	CHD-C1D-ND	-3.51	121.23	124.45
18	8	607	CLA	CHD-C1D-ND	-3.51	121.23	124.45
18	6	304	CLA	CHD-C1D-ND	-3.50	121.23	124.45
18	A	814	CLA	C1D-ND-C4D	-3.50	103.85	106.33
18	B	818	CLA	C1D-ND-C4D	-3.50	103.85	106.33
18	7	603	CLA	C1D-ND-C4D	-3.50	103.85	106.33
18	B	812	CLA	C1B-CHB-C4A	-3.50	123.19	130.12
18	Z	611	CLA	CHD-C1D-ND	-3.50	121.24	124.45
18	6	317	CLA	CHD-C1D-ND	-3.50	121.24	124.45
18	A	819	CLA	C1D-ND-C4D	-3.50	103.85	106.33
18	A	813	CLA	CHD-C1D-ND	-3.50	121.24	124.45
21	5	607	CHL	C1B-CHB-C4A	-3.49	123.20	130.12
18	3	314	CLA	CHD-C1D-ND	-3.49	121.25	124.45
18	6	314	CLA	CHD-C1D-ND	-3.49	121.25	124.45
21	7	606	CHL	CHD-C1D-ND	-3.49	121.25	124.45
21	4	604	CHL	CHD-C1D-ND	-3.48	121.25	124.45
18	5	608	CLA	CHD-C1D-ND	-3.48	121.25	124.45
18	7	611	CLA	C1D-ND-C4D	-3.48	103.86	106.33
18	7	612	CLA	CHD-C1D-ND	-3.48	121.26	124.45
18	6	315	CLA	CAA-C2A-C1A	-3.48	104.44	112.14
21	3	306	CHL	C1B-CHB-C4A	-3.47	123.25	130.12
18	7	610	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
18	B	820	CLA	CAA-C2A-C1A	-3.46	104.48	112.14
18	3	304	CLA	CHD-C1D-ND	-3.46	121.28	124.45
18	A	814	CLA	C2C-C1C-NC	3.46	113.21	109.97
18	A	833	CLA	CHD-C1D-ND	-3.45	121.28	124.45
18	A	827	CLA	C1B-CHB-C4A	-3.45	123.29	130.12
18	A	815	CLA	C1D-ND-C4D	-3.45	103.89	106.33
18	6	303	CLA	C1D-ND-C4D	-3.44	103.89	106.33
18	B	837	CLA	CHD-C1D-ND	-3.43	121.30	124.45
18	7	604	CLA	CHA-C1A-NA	-3.43	118.54	126.40
18	A	803	CLA	C1D-ND-C4D	-3.42	103.90	106.33
18	5	614	CLA	CAA-C2A-C1A	-3.42	104.57	112.14
18	B	817	CLA	CAA-C2A-C1A	-3.42	104.57	112.14
18	5	613	CLA	C1D-ND-C4D	-3.41	103.91	106.33
18	7	609	CLA	C1D-ND-C4D	-3.41	103.92	106.33
18	7	604	CLA	CHD-C1D-ND	-3.40	121.33	124.45
21	6	306	CHL	CHD-C1D-ND	-3.40	121.33	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	5	605	CLA	C2C-C1C-NC	3.40	113.16	109.97
18	B	822	CLA	C1D-ND-C4D	-3.40	103.92	106.33
18	1	608	CLA	C3A-C2A-C1A	-3.40	96.24	101.34
21	6	305	CHL	CMB-C2B-C1B	-3.40	123.24	128.46
21	6	305	CHL	C1B-CHB-C4A	-3.40	123.39	130.12
18	Z	607	CLA	C3A-C2A-C1A	-3.40	96.25	101.34
18	A	826	CLA	C1D-ND-C4D	-3.39	103.92	106.33
18	8	602	CLA	C1D-ND-C4D	-3.39	103.92	106.33
18	A	844	CLA	C2C-C1C-NC	3.39	113.14	109.97
18	A	821	CLA	CHD-C1D-ND	-3.39	121.34	124.45
18	4	608	CLA	CHD-C1D-ND	-3.39	121.34	124.45
21	6	305	CHL	CHD-C1D-ND	-3.38	121.34	124.45
18	B	817	CLA	C2C-C1C-NC	3.38	113.14	109.97
18	A	843	CLA	CHD-C1D-ND	-3.38	121.35	124.45
17	A	801	CL0	CHC-C1C-NC	3.38	129.33	124.20
18	J	101	CLA	C1D-ND-C4D	-3.38	103.94	106.33
18	A	841	CLA	CHD-C1D-ND	-3.37	121.36	124.45
18	B	840	CLA	CHD-C1D-ND	-3.37	121.36	124.45
18	3	310	CLA	C1D-ND-C4D	-3.37	103.94	106.33
18	B	833	CLA	CHD-C1D-ND	-3.37	121.36	124.45
18	3	304	CLA	C2C-C1C-NC	3.37	113.12	109.97
21	6	305	CHL	CAA-C2A-C1A	3.36	119.57	112.14
18	5	612	CLA	CHD-C1D-ND	-3.36	121.37	124.45
18	A	844	CLA	CHD-C1D-ND	-3.35	121.37	124.45
18	B	805	CLA	C1B-CHB-C4A	-3.35	123.47	130.12
18	7	603	CLA	C2C-C1C-NC	3.35	113.11	109.97
18	B	814	CLA	C1D-ND-C4D	-3.35	103.95	106.33
18	B	819	CLA	C1D-ND-C4D	-3.35	103.95	106.33
18	A	828	CLA	CHD-C1D-ND	-3.35	121.38	124.45
18	6	312	CLA	CHD-C1D-ND	-3.34	121.38	124.45
21	5	616	CHL	C1B-CHB-C4A	-3.34	123.50	130.12
18	8	612	CLA	C1D-ND-C4D	-3.33	103.97	106.33
18	A	835	CLA	C1D-ND-C4D	-3.33	103.97	106.33
18	3	302	CLA	C1D-ND-C4D	-3.33	103.97	106.33
21	4	604	CHL	CMB-C2B-C1B	-3.33	123.35	128.46
18	A	802	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
21	4	605	CHL	C4D-CHA-C1A	-3.32	117.21	121.25
18	5	604	CLA	C1D-ND-C4D	-3.32	103.98	106.33
18	6	313	CLA	C1D-ND-C4D	-3.31	103.98	106.33
18	B	832	CLA	C1D-ND-C4D	-3.31	103.98	106.33
18	1	611	CLA	C1D-ND-C4D	-3.31	103.99	106.33
18	7	608	CLA	C1D-ND-C4D	-3.31	103.99	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	309	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
18	A	839	CLA	CHD-C1D-ND	-3.31	121.42	124.45
18	F	302	CLA	C1D-ND-C4D	-3.30	103.99	106.33
18	B	828	CLA	C1D-ND-C4D	-3.30	103.99	106.33
18	B	824	CLA	C1D-ND-C4D	-3.30	103.99	106.33
18	4	601	CLA	C1D-ND-C4D	-3.30	103.99	106.33
18	3	308	CLA	C1D-ND-C4D	-3.29	104.00	106.33
18	A	823	CLA	C1D-ND-C4D	-3.28	104.00	106.33
18	A	839	CLA	C2C-C1C-NC	3.28	113.05	109.97
18	5	608	CLA	C1D-ND-C4D	-3.28	104.00	106.33
18	A	804	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	Z	606	CLA	C2C-C1C-NC	3.27	113.04	109.97
18	A	831	CLA	C1D-ND-C4D	-3.27	104.01	106.33
18	3	312	CLA	C1D-ND-C4D	-3.27	104.01	106.33
21	6	316	CHL	C1B-CHB-C4A	-3.27	123.64	130.12
18	B	816	CLA	C2C-C1C-NC	3.27	113.03	109.97
18	Z	610	CLA	C1D-ND-C4D	-3.27	104.01	106.33
21	1	606	CHL	CHD-C1D-ND	-3.26	121.46	124.45
18	4	608	CLA	C1B-CHB-C4A	-3.26	123.66	130.12
18	7	612	CLA	C1D-ND-C4D	-3.26	104.02	106.33
18	B	827	CLA	C3A-C2A-C1A	-3.25	96.47	101.34
18	3	311	CLA	C2C-C1C-NC	3.25	113.02	109.97
18	B	820	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
18	A	809	CLA	CHD-C1D-ND	-3.25	121.47	124.45
18	B	834	CLA	CHD-C1D-ND	-3.25	121.13	124.40
18	3	311	CLA	CHD-C1D-ND	-3.24	121.47	124.45
18	A	823	CLA	O2A-C1-C2	3.24	117.15	108.64
18	A	818	CLA	C1D-ND-C4D	-3.24	104.03	106.33
18	1	607	CLA	C2C-C1C-NC	3.24	113.01	109.97
18	B	843	CLA	C2C-C1C-NC	3.24	113.00	109.97
18	5	611	CLA	CAA-C2A-C1A	-3.23	104.99	112.14
18	Z	612	CLA	C1D-ND-C4D	-3.22	104.04	106.33
18	5	617	CLA	C1B-CHB-C4A	-3.22	123.73	130.12
21	5	607	CHL	CMB-C2B-C1B	-3.22	123.51	128.46
18	7	601	CLA	C2C-C1C-NC	3.22	112.99	109.97
18	8	613	CLA	C1D-ND-C4D	-3.22	104.05	106.33
18	3	305	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
21	Z	605	CHL	CHD-C1D-ND	-3.22	121.50	124.45
18	6	315	CLA	C1B-CHB-C4A	-3.21	123.76	130.12
18	1	613	CLA	C1D-ND-C4D	-3.21	104.05	106.33
18	A	833	CLA	C2C-C1C-NC	3.21	112.98	109.97
18	7	614	CLA	C1B-CHB-C4A	-3.21	123.76	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	302	CLA	C2C-C1C-NC	3.21	112.98	109.97
18	5	605	CLA	CHD-C1D-ND	-3.21	121.51	124.45
18	B	834	CLA	C1D-ND-C4D	-3.20	104.06	106.33
18	A	822	CLA	CHD-C1D-ND	-3.20	121.52	124.45
18	8	615	CLA	CHD-C1D-ND	-3.19	121.52	124.45
17	A	801	CL0	CHC-C1C-C2C	-3.19	117.89	126.72
18	Z	604	CLA	CHC-C1C-C2C	-3.19	117.89	126.72
18	6	309	CLA	C1D-ND-C4D	-3.19	104.07	106.33
18	B	804	CLA	C3A-C2A-C1A	-3.19	96.56	101.34
18	B	807	CLA	CAA-C2A-C1A	-3.19	105.08	112.14
18	7	607	CLA	CAA-C2A-C1A	-3.19	105.08	112.14
21	5	607	CHL	CHA-C1A-NA	-3.18	119.11	126.40
18	1	605	CLA	CHC-C1C-C2C	-3.18	117.92	126.72
21	6	316	CHL	CHD-C1D-ND	-3.18	121.53	124.45
18	A	815	CLA	C2C-C1C-NC	3.18	112.95	109.97
21	4	605	CHL	C3A-C2A-C1A	3.18	106.10	101.34
18	8	605	CLA	CHD-C1D-ND	-3.18	121.53	124.45
18	Z	613	CLA	C1D-ND-C4D	-3.18	104.08	106.33
18	8	603	CLA	C1D-ND-C4D	-3.18	104.08	106.33
18	1	603	CLA	CHD-C1D-ND	-3.17	121.54	124.45
18	3	314	CLA	C1D-ND-C4D	-3.17	104.08	106.33
18	A	833	CLA	C1D-ND-C4D	-3.17	104.08	106.33
21	Z	601	CHL	CHD-C1D-ND	-3.17	121.55	124.45
18	1	614	CLA	C1D-ND-C4D	-3.16	104.09	106.33
18	B	842	CLA	C2C-C1C-NC	3.16	112.93	109.97
18	8	612	CLA	C2C-C1C-NC	3.15	112.92	109.97
18	7	608	CLA	C1-C2-C3	-3.15	121.66	126.75
21	3	306	CHL	CHD-C1D-ND	-3.14	121.56	124.45
18	B	835	CLA	CHC-C1C-NC	3.14	128.97	124.20
21	6	307	CHL	CHD-C1D-ND	-3.14	121.57	124.45
18	7	605	CLA	C2C-C1C-NC	3.14	112.92	109.97
18	B	816	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
21	8	606	CHL	CMB-C2B-C1B	-3.13	123.65	128.46
18	B	827	CLA	CAA-C2A-C1A	-3.13	105.20	112.14
18	A	825	CLA	C1D-ND-C4D	-3.13	104.11	106.33
18	6	303	CLA	C2C-C1C-NC	3.13	112.91	109.97
18	6	308	CLA	C1D-ND-C4D	-3.13	104.11	106.33
21	5	607	CHL	C2A-C1A-CHA	3.13	129.33	123.86
18	8	615	CLA	C2C-C1C-NC	3.13	112.91	109.97
21	1	606	CHL	C1D-ND-C4D	-3.13	104.11	106.33
18	B	830	CLA	C2C-C1C-NC	3.13	112.90	109.97
18	1	603	CLA	C2C-C1C-NC	3.13	112.90	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	608	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
18	A	824	CLA	C2C-C1C-NC	3.13	112.90	109.97
18	4	606	CLA	C1D-ND-C4D	-3.13	104.11	106.33
18	B	827	CLA	C1D-ND-C4D	-3.12	104.12	106.33
21	6	306	CHL	CHA-C1A-NA	-3.12	119.25	126.40
18	A	816	CLA	C1D-ND-C4D	-3.12	104.12	106.33
18	4	610	CLA	C1D-ND-C4D	-3.12	104.12	106.33
18	B	835	CLA	C1D-ND-C4D	-3.12	104.12	106.33
18	B	841	CLA	C1D-ND-C4D	-3.12	104.12	106.33
18	A	825	CLA	CHC-C1C-NC	3.12	128.94	124.20
18	Z	611	CLA	C2C-C1C-NC	3.11	112.89	109.97
18	A	834	CLA	CAA-C2A-C1A	-3.11	105.25	112.14
18	B	816	CLA	CHC-C1C-NC	3.11	128.93	124.20
18	B	843	CLA	C1D-ND-C4D	-3.11	104.12	106.33
18	Z	607	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
18	A	813	CLA	C2C-C1C-NC	3.11	112.89	109.97
21	1	601	CHL	CHD-C1D-ND	-3.11	121.60	124.45
18	1	613	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
18	A	814	CLA	CHC-C1C-C2C	-3.11	118.13	126.72
18	5	601	CLA	C2C-C1C-NC	3.10	112.88	109.97
21	6	307	CHL	C1B-CHB-C4A	-3.10	123.98	130.12
18	B	829	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
18	B	810	CLA	CHC-C1C-C2C	-3.09	118.16	126.72
18	Z	612	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
18	J	101	CLA	CAA-C2A-C1A	-3.09	105.30	112.14
18	7	601	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
18	B	808	CLA	CHD-C1D-ND	-3.09	121.62	124.45
18	1	613	CLA	C2C-C1C-NC	3.09	112.86	109.97
21	Z	605	CHL	C1D-ND-C4D	-3.09	104.14	106.33
18	1	613	CLA	CHC-C1C-NC	3.09	128.88	124.20
18	4	611	CLA	C2C-C1C-NC	3.08	112.86	109.97
18	Z	612	CLA	CHC-C1C-NC	3.08	128.88	124.20
18	1	612	CLA	C2C-C1C-NC	3.08	112.85	109.97
18	B	811	CLA	CHD-C1D-ND	-3.07	121.63	124.45
18	B	835	CLA	CAA-C2A-C1A	-3.07	105.34	112.14
21	3	306	CHL	C2C-C3C-C4C	3.07	108.68	106.49
18	B	816	CLA	C1D-ND-C4D	-3.07	104.16	106.33
18	5	601	CLA	CHD-C1D-ND	-3.07	121.63	124.45
21	5	606	CHL	CMB-C2B-C1B	-3.07	123.75	128.46
18	A	805	CLA	C1D-ND-C4D	-3.06	104.16	106.33
18	5	617	CLA	C1D-ND-C4D	-3.06	104.16	106.33
18	Z	612	CLA	C2C-C1C-NC	3.06	112.83	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	603	CLA	C2C-C1C-NC	3.05	112.83	109.97
18	A	843	CLA	C2C-C1C-NC	3.05	112.83	109.97
18	1	610	CLA	C2C-C1C-NC	3.05	112.83	109.97
18	A	807	CLA	C1D-ND-C4D	-3.05	104.17	106.33
21	3	306	CHL	CHA-C1A-NA	-3.05	119.41	126.40
18	3	305	CLA	C2A-C3A-C4A	-3.05	96.94	101.87
18	7	601	CLA	CHC-C1C-NC	3.05	128.83	124.20
18	B	813	CLA	C1D-ND-C4D	-3.05	104.17	106.33
18	B	808	CLA	CHC-C1C-C2C	-3.04	118.30	126.72
18	5	609	CLA	C1D-ND-C4D	-3.04	104.17	106.33
18	B	838	CLA	C1D-ND-C4D	-3.04	104.17	106.33
18	A	840	CLA	C1D-ND-C4D	-3.04	104.17	106.33
18	5	603	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
18	4	611	CLA	C1D-ND-C4D	-3.04	104.18	106.33
18	B	812	CLA	C2A-C1A-CHA	3.04	129.17	123.86
18	A	813	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
18	F	302	CLA	C2C-C1C-NC	3.03	112.81	109.97
18	A	838	CLA	C1D-ND-C4D	-3.03	104.18	106.33
18	Z	609	CLA	C2C-C1C-NC	3.03	112.81	109.97
18	7	601	CLA	C1D-ND-C4D	-3.02	104.19	106.33
18	6	317	CLA	C2C-C1C-NC	3.02	112.80	109.97
21	5	616	CHL	CHD-C1D-ND	-3.02	121.68	124.45
18	1	607	CLA	C1D-ND-C4D	-3.02	104.19	106.33
18	B	840	CLA	C2C-C1C-NC	3.02	112.80	109.97
18	A	820	CLA	C1D-ND-C4D	-3.02	104.19	106.33
18	A	827	CLA	C3A-C2A-C1A	-3.02	96.82	101.34
21	4	605	CHL	CMA-C3A-C4A	3.01	119.88	111.77
18	B	810	CLA	C1D-ND-C4D	-3.01	104.20	106.33
18	Z	606	CLA	C1D-ND-C4D	-3.01	104.20	106.33
21	4	605	CHL	C1D-ND-C4D	-3.01	104.20	106.33
18	A	804	CLA	C2C-C1C-NC	3.01	112.79	109.97
18	B	836	CLA	C1D-ND-C4D	-3.00	104.20	106.33
18	8	604	CLA	C1D-ND-C4D	-3.00	104.20	106.33
18	A	833	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
21	6	306	CHL	CMB-C2B-C1B	-3.00	123.85	128.46
18	A	841	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
18	3	309	CLA	C2A-C3A-C4A	-2.99	97.96	101.78
17	A	801	CL0	C2C-C1C-NC	2.99	112.77	109.97
18	A	828	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
18	8	605	CLA	C2C-C1C-NC	2.99	112.77	109.97
18	Z	604	CLA	CHD-C1D-ND	-2.98	121.71	124.45
18	5	603	CLA	CHD-C1D-ND	-2.98	121.71	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	841	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
18	A	813	CLA	CHC-C1C-NC	2.98	128.73	124.20
18	A	806	CLA	C1D-ND-C4D	-2.98	104.22	106.33
18	B	810	CLA	C2C-C1C-NC	2.98	112.76	109.97
21	6	316	CHL	CMB-C2B-C1B	-2.98	123.88	128.46
18	B	827	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
18	A	816	CLA	CHC-C1C-NC	2.97	128.71	124.20
18	A	839	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
18	A	802	CLA	C2C-C1C-NC	2.96	112.75	109.97
18	A	829	CLA	C1D-ND-C4D	-2.96	104.23	106.33
18	B	815	CLA	CAA-C2A-C1A	-2.96	105.59	112.14
18	3	314	CLA	CHC-C1C-NC	2.96	128.69	124.20
18	8	601	CLA	C2C-C1C-NC	2.96	112.74	109.97
18	B	807	CLA	C1D-ND-C4D	-2.96	104.23	106.33
18	1	605	CLA	CHD-C1D-ND	-2.95	121.74	124.45
18	A	816	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
18	F	301	CLA	C1D-ND-C4D	-2.95	104.24	106.33
18	A	827	CLA	C2A-C3A-C4A	-2.95	97.11	101.87
18	8	611	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
21	Z	601	CHL	CHA-C1A-NA	-2.95	119.65	126.40
18	7	613	CLA	C1D-ND-C4D	-2.94	104.24	106.33
18	Z	603	CLA	C1D-ND-C4D	-2.94	104.25	106.33
18	6	303	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
18	A	831	CLA	CAA-C2A-C1A	-2.94	105.64	112.14
18	B	817	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
21	1	601	CHL	CHA-C1A-NA	-2.94	119.67	126.40
18	A	832	CLA	C1D-ND-C4D	-2.94	104.25	106.33
18	4	603	CLA	C1D-ND-C4D	-2.93	104.25	106.33
18	5	611	CLA	C2C-C1C-NC	2.93	112.72	109.97
18	A	810	CLA	C1D-ND-C4D	-2.93	104.25	106.33
18	3	307	CLA	C1D-ND-C4D	-2.93	104.25	106.33
18	A	825	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
18	6	302	CLA	C2C-C1C-NC	2.93	112.72	109.97
18	Z	609	CLA	CAA-C2A-C1A	-2.93	105.66	112.14
18	B	809	CLA	C2C-C1C-NC	2.93	112.72	109.97
18	8	613	CLA	C2C-C1C-NC	2.93	112.71	109.97
18	A	836	CLA	CHC-C1C-NC	2.93	128.64	124.20
18	A	820	CLA	CHC-C1C-C2C	-2.93	118.63	126.72
21	6	307	CHL	CHA-C1A-NA	-2.93	119.70	126.40
21	6	316	CHL	CHA-C1A-NA	-2.92	119.70	126.40
18	A	803	CLA	CHC-C1C-NC	2.92	128.64	124.20
18	A	815	CLA	CHC-C1C-C2C	-2.92	118.64	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	8	607	CLA	CHC-C1C-NC	2.92	128.63	124.20
18	6	317	CLA	C1D-ND-C4D	-2.92	104.26	106.33
21	7	606	CHL	CMB-C2B-C1B	-2.92	123.98	128.46
18	7	610	CLA	CAA-C2A-C1A	-2.92	104.61	111.81
18	A	844	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
18	7	613	CLA	C2C-C1C-NC	2.92	112.70	109.97
18	5	605	CLA	CHC-C1C-C2C	-2.92	118.66	126.72
18	5	601	CLA	CHC-C1C-C2C	-2.91	118.66	126.72
18	A	823	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
18	8	602	CLA	C2C-C1C-NC	2.91	112.70	109.97
21	6	307	CHL	CMB-C2B-C1B	-2.91	124.00	128.46
18	6	312	CLA	C1D-ND-C4D	-2.91	104.27	106.33
18	A	828	CLA	CHC-C1C-NC	2.90	128.61	124.20
18	B	810	CLA	CHC-C1C-NC	2.90	128.61	124.20
18	B	826	CLA	C1D-ND-C4D	-2.90	104.27	106.33
18	A	830	CLA	CHC-C1C-NC	2.90	128.60	124.20
18	A	838	CLA	C2C-C1C-NC	2.90	112.69	109.97
18	B	820	CLA	C2C-C1C-NC	2.90	112.69	109.97
18	1	610	CLA	CAA-C2A-C1A	-2.90	105.73	112.14
18	A	833	CLA	CHC-C1C-NC	2.89	128.59	124.20
21	5	616	CHL	CMB-C2B-C1B	-2.89	124.02	128.46
21	7	606	CHL	CHA-C1A-NA	-2.89	119.78	126.40
18	J	101	CLA	CHC-C1C-NC	2.89	128.59	124.20
18	8	607	CLA	CAA-C2A-C3A	-2.89	107.03	114.26
18	7	604	CLA	C2C-C1C-NC	2.89	112.68	109.97
18	1	604	CLA	C1D-ND-C4D	-2.89	104.28	106.33
18	7	611	CLA	CHC-C1C-NC	2.89	128.58	124.20
18	A	837	CLA	C2C-C1C-NC	2.88	112.67	109.97
18	B	830	CLA	C1D-ND-C4D	-2.88	104.29	106.33
18	6	312	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
18	A	828	CLA	C2C-C1C-NC	2.88	112.67	109.97
18	B	826	CLA	C2C-C1C-NC	2.88	112.67	109.97
21	6	305	CHL	CHA-C1A-NA	-2.88	119.80	126.40
17	A	801	CL0	C1D-ND-C4D	-2.88	104.29	106.33
18	Z	611	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
18	1	613	CLA	CGD-CBD-CAD	-2.88	101.41	110.73
18	8	601	CLA	C1D-ND-C4D	-2.87	104.29	106.33
18	3	314	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
18	6	314	CLA	C2C-C1C-NC	2.87	112.66	109.97
18	6	310	CLA	C2A-C3A-C4A	-2.87	97.23	101.87
18	1	612	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
18	6	317	CLA	CHC-C1C-C2C	-2.87	118.78	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	303	CLA	C2C-C1C-NC	2.87	112.66	109.97
18	A	814	CLA	CHC-C1C-NC	2.87	128.55	124.20
18	8	601	CLA	CHC-C1C-C2C	-2.87	118.80	126.72
18	B	811	CLA	C1B-CHB-C4A	-2.86	124.44	130.12
18	B	809	CLA	CHC-C1C-C2C	-2.86	118.80	126.72
18	A	812	CLA	CHC-C1C-C2C	-2.86	118.80	126.72
18	Z	612	CLA	CGD-CBD-CAD	-2.86	101.46	110.73
18	B	811	CLA	C2C-C1C-NC	2.86	112.65	109.97
18	B	830	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
18	3	304	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
18	B	817	CLA	C1D-ND-C4D	-2.86	104.30	106.33
18	A	820	CLA	CHC-C1C-NC	2.86	128.54	124.20
18	5	617	CLA	CGD-CBD-CAD	-2.85	101.49	110.73
18	A	835	CLA	CAA-C2A-C1A	-2.85	105.82	112.14
18	7	613	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
18	3	313	CLA	C1D-ND-C4D	-2.85	104.31	106.33
18	7	603	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
18	3	312	CLA	CAA-C2A-C1A	-2.85	102.64	111.97
18	3	310	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
18	7	604	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
18	7	614	CLA	CHA-C1A-NA	-2.85	119.88	126.40
21	5	607	CHL	C2C-C3C-C4C	2.85	108.52	106.49
18	A	830	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
18	A	841	CLA	CHC-C1C-NC	2.85	128.52	124.20
18	3	302	CLA	CHC-C1C-C2C	-2.84	118.85	126.72
18	8	615	CLA	C1D-ND-C4D	-2.84	104.31	106.33
18	4	607	CLA	C1D-ND-C4D	-2.84	104.31	106.33
18	B	831	CLA	C1D-ND-C4D	-2.84	104.32	106.33
18	A	824	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
21	1	601	CHL	CMB-C2B-C1B	-2.84	124.10	128.46
21	6	306	CHL	CAA-C2A-C1A	2.84	118.43	112.14
18	B	840	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
18	A	802	CLA	C1D-ND-C4D	-2.84	104.32	106.33
18	A	809	CLA	CHC-C1C-C2C	-2.83	118.88	126.72
18	F	302	CLA	C1-C2-C3	-2.83	121.14	126.04
18	A	832	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
21	Z	601	CHL	CMB-C2B-C1B	-2.83	124.11	128.46
18	A	812	CLA	CHC-C1C-NC	2.83	128.50	124.20
18	6	313	CLA	CHC-C1C-NC	2.83	128.50	124.20
18	6	303	CLA	CHC-C1C-NC	2.83	128.50	124.20
18	6	304	CLA	CAA-C2A-C3A	-2.83	107.19	114.26
18	B	843	CLA	CHC-C1C-C2C	-2.83	118.90	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	307	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
18	A	827	CLA	CHC-C1C-NC	2.83	128.49	124.20
18	7	614	CLA	C1D-ND-C4D	-2.83	104.33	106.33
21	6	305	CHL	C2C-C3C-C4C	2.82	108.50	106.49
21	Z	601	CHL	CHC-C1C-NC	2.82	128.49	124.20
18	1	607	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
18	6	304	CLA	C1D-ND-C4D	-2.82	104.33	106.33
18	5	601	CLA	CHA-C1A-NA	-2.82	119.94	126.40
18	8	603	CLA	C2C-C1C-NC	2.82	112.61	109.97
18	3	303	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
18	Z	613	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
18	A	838	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
18	B	833	CLA	C1D-ND-C4D	-2.82	104.33	106.33
18	1	603	CLA	C1D-ND-C4D	-2.82	104.33	106.33
21	6	307	CHL	C2C-C3C-C4C	2.82	108.50	106.49
18	7	611	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
18	4	603	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
18	6	304	CLA	CHC-C1C-NC	2.81	128.47	124.20
18	Z	606	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
18	B	822	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
18	A	840	CLA	C2C-C1C-NC	2.81	112.61	109.97
18	8	602	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
18	B	839	CLA	C2C-C1C-NC	2.81	112.60	109.97
18	A	824	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
18	1	603	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
18	8	601	CLA	CHC-C1C-NC	2.81	128.46	124.20
18	4	611	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
18	Z	613	CLA	CHC-C1C-NC	2.81	128.46	124.20
18	8	612	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
18	1	614	CLA	CHC-C1C-C2C	-2.80	118.96	126.72
18	1	614	CLA	CHC-C1C-NC	2.80	128.45	124.20
18	1	610	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
18	7	613	CLA	CHC-C1C-NC	2.80	128.45	124.20
18	8	615	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
18	1	611	CLA	C2C-C1C-NC	2.80	112.59	109.97
18	B	825	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
18	A	811	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
18	A	809	CLA	C1D-ND-C4D	-2.80	104.35	106.33
18	8	607	CLA	CAA-C2A-C1A	-2.79	105.95	112.14
18	B	839	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
18	B	826	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
18	3	313	CLA	C2C-C1C-NC	2.79	112.59	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	307	CLA	C3A-C2A-C1A	-2.79	97.16	101.34
18	A	822	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
18	8	607	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
18	Z	604	CLA	CHC-C1C-NC	2.79	128.43	124.20
18	A	803	CLA	CHC-C1C-C2C	-2.78	119.02	126.72
18	B	835	CLA	CHC-C1C-C2C	-2.78	119.02	126.72
18	A	830	CLA	C1D-ND-C4D	-2.78	104.36	106.33
18	Z	610	CLA	C2C-C1C-NC	2.78	112.58	109.97
18	8	613	CLA	CHC-C1C-C2C	-2.78	119.02	126.72
18	B	809	CLA	CHC-C1C-NC	2.78	128.42	124.20
18	5	611	CLA	CHC-C1C-C2C	-2.78	119.03	126.72
18	3	310	CLA	CHC-C1C-NC	2.78	128.42	124.20
18	7	610	CLA	C2A-C3A-C4A	-2.78	98.24	101.78
18	B	825	CLA	C2C-C1C-NC	2.78	112.58	109.97
18	Z	609	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
18	4	603	CLA	CHD-C1D-ND	-2.78	121.90	124.45
18	6	314	CLA	CAA-C2A-C1A	-2.77	102.88	111.97
18	8	614	CLA	C2C-C1C-NC	2.77	112.57	109.97
18	A	802	CLA	C3A-C2A-C1A	-2.77	97.18	101.34
18	Z	610	CLA	CAA-C2A-C1A	-2.77	106.01	112.14
18	B	825	CLA	CHC-C1C-NC	2.77	128.40	124.20
18	B	823	CLA	CAA-C2A-C1A	-2.77	106.02	112.14
18	B	802	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
18	5	614	CLA	C2C-C1C-NC	2.76	112.56	109.97
18	A	806	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
18	1	611	CLA	CAA-C2A-C1A	-2.76	106.02	112.14
18	B	828	CLA	C2C-C1C-NC	2.76	112.56	109.97
18	3	304	CLA	C1D-ND-C4D	-2.76	104.37	106.33
18	A	829	CLA	CHC-C1C-NC	2.76	128.39	124.20
18	3	303	CLA	CHC-C1C-NC	2.76	128.39	124.20
18	B	842	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
18	A	807	CLA	CHC-C1C-C2C	-2.76	119.10	126.72
18	7	604	CLA	CHC-C1C-NC	2.75	128.38	124.20
18	6	301	CLA	CHD-C1D-ND	-2.75	121.92	124.45
18	B	833	CLA	C2C-C1C-NC	2.75	112.55	109.97
21	1	601	CHL	CHC-C1C-NC	2.75	128.38	124.20
18	7	607	CLA	C1D-ND-C4D	-2.75	104.38	106.33
18	Z	609	CLA	C1D-ND-C4D	-2.75	104.38	106.33
18	A	817	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
18	3	308	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
18	3	301	CLA	CAA-C2A-C1A	-2.75	106.05	112.14
21	8	606	CHL	CHC-C1C-NC	2.75	128.37	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	836	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
18	B	838	CLA	C2C-C1C-NC	2.75	112.55	109.97
18	1	605	CLA	CHC-C1C-NC	2.75	128.37	124.20
18	5	612	CLA	CHC-C1C-C2C	-2.75	119.13	126.72
18	A	832	CLA	CHC-C1C-NC	2.74	128.37	124.20
18	A	808	CLA	CHC-C1C-NC	2.74	128.36	124.20
18	A	815	CLA	CHC-C1C-NC	2.74	128.36	124.20
18	A	817	CLA	CHC-C1C-NC	2.74	128.36	124.20
18	A	845	CLA	CHC-C1C-NC	2.74	128.36	124.20
21	4	605	CHL	CHC-C1C-NC	2.74	128.36	124.20
18	8	608	CLA	CHA-C1A-NA	-2.74	120.12	126.40
18	1	602	CLA	CHC-C1C-NC	2.74	128.36	124.20
18	5	613	CLA	C2C-C1C-NC	2.74	112.54	109.97
18	5	613	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
18	A	843	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
18	A	829	CLA	CHC-C1C-C2C	-2.74	119.16	126.72
18	6	304	CLA	CHC-C1C-C2C	-2.73	119.16	126.72
18	7	602	CLA	C2C-C1C-NC	2.73	112.53	109.97
18	B	822	CLA	CHC-C1C-NC	2.73	128.35	124.20
18	5	612	CLA	C1D-ND-C4D	-2.73	104.39	106.33
18	B	822	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
18	B	833	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
18	8	603	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
18	Z	613	CLA	C2C-C1C-NC	2.73	112.53	109.97
18	A	809	CLA	CHC-C1C-NC	2.73	128.34	124.20
18	3	305	CLA	C1D-ND-C4D	-2.73	104.40	106.33
18	Z	610	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
18	A	804	CLA	CHC-C1C-C2C	-2.72	119.18	126.72
18	Z	602	CLA	CHC-C1C-NC	2.72	128.34	124.20
18	6	312	CLA	CHC-C1C-NC	2.72	128.34	124.20
18	6	301	CLA	CHA-C1A-NA	-2.72	120.16	126.40
18	5	603	CLA	CHC-C1C-NC	2.72	128.33	124.20
18	A	845	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
18	3	311	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
18	8	608	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
18	1	609	CLA	C1D-ND-C4D	-2.72	104.40	106.33
18	8	605	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
18	B	815	CLA	CHA-C1A-NA	-2.72	120.17	126.40
18	7	605	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
18	A	827	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
18	4	612	CLA	CAA-C2A-C1A	-2.72	105.09	111.81
18	1	611	CLA	CHC-C1C-C2C	-2.72	119.20	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Z	608	CLA	C1D-ND-C4D	-2.72	104.41	106.33
18	4	601	CLA	CHA-C1A-NA	-2.72	120.18	126.40
18	8	602	CLA	CHC-C1C-NC	2.71	128.32	124.20
18	3	313	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
18	3	308	CLA	CHC-C1C-NC	2.71	128.32	124.20
18	B	821	CLA	C1D-ND-C4D	-2.71	104.41	106.33
18	A	821	CLA	C2C-C1C-NC	2.71	112.51	109.97
18	A	818	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
18	B	826	CLA	CHC-C1C-NC	2.71	128.31	124.20
18	F	301	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
18	6	313	CLA	CHC-C1C-C2C	-2.71	119.24	126.72
18	A	822	CLA	CHC-C1C-NC	2.71	128.31	124.20
18	5	603	CLA	C1D-ND-C4D	-2.71	104.41	106.33
18	B	838	CLA	CHC-C1C-C2C	-2.70	119.24	126.72
18	3	301	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
18	7	612	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
21	5	616	CHL	CHA-C1A-NA	-2.70	120.21	126.40
18	F	302	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
18	B	804	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
18	6	317	CLA	CHC-C1C-NC	2.70	128.30	124.20
18	B	838	CLA	CHA-C1A-NA	-2.70	120.22	126.40
18	A	823	CLA	CHC-C1C-NC	2.70	128.30	124.20
18	1	614	CLA	C2C-C1C-NC	2.70	112.50	109.97
18	A	807	CLA	CHC-C1C-NC	2.70	128.29	124.20
18	3	310	CLA	C2C-C1C-NC	2.70	112.50	109.97
18	B	839	CLA	CHC-C1C-C2C	-2.70	119.27	126.72
18	J	101	CLA	CHC-C1C-C2C	-2.69	119.27	126.72
18	B	814	CLA	CHC-C1C-NC	2.69	128.29	124.20
18	A	810	CLA	CHC-C1C-NC	2.69	128.29	124.20
18	A	840	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
18	4	607	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
18	A	806	CLA	C2C-C1C-NC	2.69	112.49	109.97
21	8	606	CHL	C3A-C2A-C1A	-2.69	97.31	101.34
18	1	612	CLA	C1D-ND-C4D	-2.69	104.42	106.33
18	A	819	CLA	CHC-C1C-NC	2.69	128.28	124.20
18	A	825	CLA	CAA-C2A-C3A	-2.69	107.55	114.26
18	A	838	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
18	5	604	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
18	8	614	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
18	A	809	CLA	C2C-C1C-NC	2.69	112.49	109.97
18	B	808	CLA	CHC-C1C-NC	2.69	128.28	124.20
18	A	813	CLA	CAA-C2A-C1A	-2.68	106.20	112.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	601	CLA	CHC-C1C-NC	2.68	128.27	124.20
18	7	605	CLA	CAA-C2A-C1A	-2.68	106.22	112.14
18	8	608	CLA	C2C-C1C-NC	2.68	112.48	109.97
18	B	817	CLA	CHC-C1C-NC	2.68	128.26	124.20
18	A	821	CLA	C1D-ND-C4D	-2.68	104.43	106.33
18	B	828	CLA	CHC-C1C-C2C	-2.67	119.32	126.72
18	1	609	CLA	CAA-C2A-C1A	-2.67	106.22	112.14
18	A	818	CLA	CAA-C2A-C1A	-2.67	106.22	112.14
18	A	823	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
21	4	605	CHL	C1B-CHB-C4A	-2.67	124.82	130.12
18	A	837	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
18	A	804	CLA	C1D-ND-C4D	-2.67	104.44	106.33
18	8	610	CLA	CHA-C1A-NA	-2.67	120.29	126.40
18	6	311	CLA	CHC-C1C-C2C	-2.67	119.34	126.72
18	A	822	CLA	C2C-C1C-NC	2.67	112.47	109.97
18	A	832	CLA	C2C-C1C-NC	2.66	112.47	109.97
18	6	301	CLA	C1D-ND-C4D	-2.66	104.44	106.33
18	A	811	CLA	CGD-CBD-CAD	-2.66	102.11	110.73
18	7	613	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
18	B	819	CLA	CHC-C1C-NC	2.66	128.24	124.20
18	6	314	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
18	A	839	CLA	CHC-C1C-NC	2.66	128.23	124.20
18	B	810	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
18	5	611	CLA	CHC-C1C-NC	2.65	128.23	124.20
18	5	615	CLA	C1D-ND-C4D	-2.65	104.45	106.33
21	6	307	CHL	CAA-C2A-C1A	2.65	118.02	112.14
21	6	307	CHL	CHC-C1C-NC	2.65	128.23	124.20
18	A	835	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
18	A	818	CLA	CHC-C1C-NC	2.65	128.23	124.20
18	5	609	CLA	C2C-C1C-NC	2.65	112.46	109.97
18	8	613	CLA	CHC-C1C-NC	2.65	128.23	124.20
18	B	824	CLA	CHC-C1C-NC	2.65	128.23	124.20
18	Z	608	CLA	CAA-C2A-C1A	-2.65	106.28	112.14
18	B	830	CLA	CHC-C1C-NC	2.65	128.22	124.20
18	5	613	CLA	CHC-C1C-NC	2.65	128.22	124.20
18	Z	603	CLA	CAA-C2A-C1A	-2.65	106.28	112.14
18	8	603	CLA	CHC-C1C-NC	2.65	128.22	124.20
18	A	841	CLA	C1D-ND-C4D	-2.65	104.46	106.33
18	B	820	CLA	C1D-ND-C4D	-2.64	104.46	106.33
18	1	605	CLA	CHA-C1A-NA	-2.64	120.34	126.40
21	5	607	CHL	CHD-C1D-ND	-2.64	122.03	124.45
18	1	604	CLA	CAA-C2A-C1A	-2.64	106.29	112.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	801	CLA	C2C-C1C-NC	2.64	112.45	109.97
18	B	838	CLA	CHC-C1C-NC	2.64	128.21	124.20
21	5	616	CHL	CHC-C1C-NC	2.64	128.21	124.20
18	Z	602	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
18	1	602	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
18	B	820	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
18	B	818	CLA	C2C-C1C-NC	2.64	112.44	109.97
18	B	836	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
18	4	603	CLA	CHC-C1C-NC	2.64	128.20	124.20
18	B	824	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
18	B	818	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
18	1	610	CLA	C1D-ND-C4D	-2.63	104.46	106.33
18	8	614	CLA	C1D-ND-C4D	-2.63	104.46	106.33
18	8	611	CLA	CHC-C1C-NC	2.63	128.20	124.20
18	A	823	CLA	C1-C2-C3	-2.63	121.50	126.04
18	Z	604	CLA	CHA-C1A-NA	-2.63	120.38	126.40
18	7	612	CLA	CHC-C1C-NC	2.63	128.19	124.20
18	B	840	CLA	CHC-C1C-NC	2.63	128.19	124.20
18	7	608	CLA	CHC-C1C-NC	2.63	128.19	124.20
18	B	821	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
18	5	601	CLA	CHC-C1C-NC	2.62	128.19	124.20
18	A	802	CLA	CHC-C1C-C2C	-2.62	119.46	126.72
18	A	844	CLA	CHC-C1C-NC	2.62	128.18	124.20
18	4	611	CLA	CHC-C1C-NC	2.62	128.18	124.20
18	B	833	CLA	CHC-C1C-NC	2.62	128.18	124.20
18	B	825	CLA	C1D-ND-C4D	-2.62	104.47	106.33
18	B	819	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
18	1	612	CLA	CHC-C1C-NC	2.62	128.17	124.20
18	8	614	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
18	A	806	CLA	CHC-C1C-NC	2.61	128.17	124.20
18	A	821	CLA	CHC-C1C-C2C	-2.61	119.49	126.72
18	7	604	CLA	C3B-C4B-NB	-2.61	105.83	109.21
18	A	831	CLA	C2C-C1C-NC	2.61	112.42	109.97
18	Z	611	CLA	CHC-C1C-NC	2.61	128.16	124.20
18	6	312	CLA	C2C-C1C-NC	2.61	112.42	109.97
18	3	302	CLA	CHC-C1C-NC	2.61	128.16	124.20
18	A	834	CLA	C1D-ND-C4D	-2.61	104.48	106.33
18	5	602	CLA	C2C-C1C-NC	2.61	112.41	109.97
18	6	311	CLA	C2C-C1C-NC	2.60	112.41	109.97
18	A	811	CLA	C1D-ND-C4D	-2.60	104.49	106.33
18	5	604	CLA	C2C-C1C-NC	2.60	112.41	109.97
18	Z	611	CLA	C1D-ND-C4D	-2.60	104.49	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	309	CLA	CAA-C2A-C1A	-2.60	105.39	111.81
18	3	312	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
18	6	309	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
18	8	614	CLA	CHC-C1C-NC	2.59	128.14	124.20
18	B	829	CLA	C1D-ND-C4D	-2.59	104.49	106.33
18	F	301	CLA	C2C-C1C-NC	2.59	112.40	109.97
21	1	606	CHL	CHA-C1A-NA	-2.59	120.46	126.40
18	B	812	CLA	C3A-C2A-C1A	-2.59	97.46	101.34
18	A	831	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
18	F	301	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
18	A	825	CLA	C2C-C1C-NC	2.59	112.40	109.97
18	Z	610	CLA	CHC-C1C-NC	2.59	128.13	124.20
18	B	805	CLA	CHC-C1C-NC	2.59	128.13	124.20
18	7	602	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
18	7	608	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
18	B	821	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
18	7	605	CLA	C1D-ND-C4D	-2.58	104.50	106.33
18	B	813	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
18	1	608	CLA	CHA-C1A-NA	-2.58	120.48	126.40
21	Z	605	CHL	CHA-C1A-NA	-2.58	120.48	126.40
18	7	607	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
18	8	607	CLA	CHA-C1A-NA	-2.58	120.49	126.40
18	Z	607	CLA	CHA-C1A-NA	-2.58	120.49	126.40
18	A	845	CLA	C1D-ND-C4D	-2.58	104.50	106.33
18	6	311	CLA	CHC-C1C-NC	2.58	128.12	124.20
18	5	612	CLA	C2C-C1C-NC	2.58	112.39	109.97
18	8	609	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
18	A	822	CLA	C1D-ND-C4D	-2.57	104.51	106.33
18	1	603	CLA	CHC-C1C-NC	2.57	128.11	124.20
18	B	814	CLA	CHC-C1C-C2C	-2.57	119.60	126.72
18	7	607	CLA	C2C-C1C-NC	2.57	112.38	109.97
18	8	608	CLA	CAA-C2A-C1A	-2.57	106.45	112.14
18	5	602	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
18	8	608	CLA	CHC-C1C-NC	2.57	128.10	124.20
18	B	841	CLA	CHC-C1C-C2C	-2.57	119.61	126.72
18	B	828	CLA	CHC-C1C-NC	2.57	128.10	124.20
18	3	312	CLA	CHC-C1C-NC	2.57	128.10	124.20
18	A	808	CLA	CHC-C1C-C2C	-2.57	119.62	126.72
18	1	611	CLA	CHC-C1C-NC	2.57	128.10	124.20
18	3	308	CLA	C2C-C1C-NC	2.57	112.38	109.97
18	4	609	CLA	CHC-C1C-C2C	-2.56	119.63	126.72
18	A	823	CLA	C2C-C1C-NC	2.56	112.37	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	834	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
18	A	825	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
18	8	615	CLA	CHC-C1C-NC	2.56	128.09	124.20
18	A	820	CLA	C2C-C1C-NC	2.56	112.37	109.97
18	A	826	CLA	CHC-C1C-NC	2.56	128.08	124.20
18	8	612	CLA	CHC-C1C-NC	2.56	128.08	124.20
18	1	610	CLA	CHC-C1C-C2C	-2.56	119.65	126.72
18	B	804	CLA	CHA-C1A-NA	-2.56	120.54	126.40
18	B	801	CLA	CHC-C1C-C2C	-2.56	119.65	126.72
18	B	827	CLA	CHC-C1C-C2C	-2.56	119.65	126.72
18	A	819	CLA	CHC-C1C-C2C	-2.55	119.66	126.72
18	A	829	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
18	6	304	CLA	CHA-C1A-NA	-2.55	120.55	126.40
18	5	602	CLA	CHC-C1C-C2C	-2.55	119.66	126.72
18	4	609	CLA	CHC-C1C-NC	2.55	128.08	124.20
18	7	604	CLA	CGD-CBD-CAD	-2.55	102.47	110.73
18	6	310	CLA	CHA-C1A-NA	-2.55	120.56	126.40
18	6	314	CLA	C1D-ND-C4D	-2.55	104.52	106.33
18	A	835	CLA	C2C-C1C-NC	2.55	112.36	109.97
18	Z	609	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
18	5	612	CLA	CHC-C1C-NC	2.55	128.07	124.20
18	7	604	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
18	5	601	CLA	C1D-ND-C4D	-2.54	104.53	106.33
18	1	607	CLA	CHC-C1C-NC	2.54	128.06	124.20
18	A	824	CLA	C1D-ND-C4D	-2.54	104.53	106.33
18	B	837	CLA	C1D-ND-C4D	-2.54	104.53	106.33
18	A	839	CLA	CHA-C1A-NA	-2.54	120.58	126.40
18	B	822	CLA	C2C-C1C-NC	2.54	112.35	109.97
18	B	837	CLA	CHC-C1C-C2C	-2.54	119.70	126.72
18	5	604	CLA	CHC-C1C-NC	2.54	128.05	124.20
18	6	315	CLA	CHC-C1C-C2C	-2.54	119.70	126.72
18	A	841	CLA	CAA-C2A-C1A	-2.54	106.53	112.14
18	3	313	CLA	CHC-C1C-NC	2.54	128.05	124.20
18	7	603	CLA	CHC-C1C-NC	2.54	128.05	124.20
17	A	801	CL0	CHA-C1A-NA	-2.53	120.59	126.40
18	B	819	CLA	CHC-C1C-C2C	-2.53	119.71	126.72
18	B	841	CLA	CHC-C1C-NC	2.53	128.05	124.20
18	B	815	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
18	B	804	CLA	CHC-C1C-NC	2.53	128.04	124.20
18	B	843	CLA	CHC-C1C-NC	2.53	128.04	124.20
18	8	611	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
18	A	835	CLA	CHC-C1C-C2C	-2.53	119.73	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	8	609	CLA	CHC-C1C-C2C	-2.52	119.74	126.72
18	3	311	CLA	CHA-C1A-NA	-2.52	120.62	126.40
18	B	827	CLA	CHC-C1C-NC	2.52	128.03	124.20
18	B	811	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
18	B	809	CLA	CAA-C2A-C1A	-2.52	106.56	112.14
18	6	302	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
18	B	806	CLA	C1D-ND-C4D	-2.52	104.55	106.33
18	Z	613	CLA	CHA-C1A-NA	-2.52	120.64	126.40
18	B	821	CLA	C2C-C1C-NC	2.51	112.33	109.97
18	A	844	CLA	CHA-C1A-NA	-2.51	120.64	126.40
18	8	610	CLA	C3A-C2A-C1A	-2.51	97.57	101.34
18	6	315	CLA	C2C-C1C-NC	2.51	112.33	109.97
18	1	614	CLA	CHA-C1A-NA	-2.51	120.64	126.40
18	6	308	CLA	CHC-C1C-C2C	-2.51	119.77	126.72
18	4	612	CLA	CHC-C1C-NC	2.51	128.01	124.20
18	B	820	CLA	CHA-C1A-NA	-2.51	120.65	126.40
18	6	301	CLA	C2C-C1C-NC	2.51	112.32	109.97
18	5	614	CLA	C1D-ND-C4D	-2.51	104.55	106.33
18	A	831	CLA	CHC-C1C-NC	2.51	128.01	124.20
18	3	304	CLA	CHC-C1C-NC	2.51	128.01	124.20
18	A	834	CLA	CHC-C1C-C2C	-2.51	119.78	126.72
18	A	804	CLA	CHC-C1C-NC	2.51	128.01	124.20
18	B	818	CLA	CHC-C1C-NC	2.51	128.01	124.20
18	B	837	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
18	A	817	CLA	CGD-CBD-CAD	-2.51	102.62	110.73
18	3	313	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
18	Z	606	CLA	CHC-C1C-NC	2.50	128.00	124.20
18	8	605	CLA	C1D-ND-C4D	-2.50	104.56	106.33
18	5	605	CLA	CHC-C1C-NC	2.50	128.00	124.20
18	A	823	CLA	C3A-C2A-C1A	-2.50	97.59	101.34
18	A	824	CLA	CHC-C1C-NC	2.50	127.99	124.20
18	A	828	CLA	CHA-C1A-NA	-2.50	120.68	126.40
18	A	838	CLA	CHC-C1C-NC	2.50	127.99	124.20
18	8	609	CLA	CAA-C2A-C1A	-2.49	106.62	112.14
18	A	807	CLA	CAA-C2A-C1A	-2.49	106.62	112.14
18	A	803	CLA	C2C-C1C-NC	2.49	112.31	109.97
18	A	818	CLA	C2C-C1C-NC	2.49	112.31	109.97
21	8	606	CHL	C2A-C1A-CHA	2.49	128.21	123.86
18	B	807	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
18	1	608	CLA	CHC-C1C-NC	2.49	127.98	124.20
18	A	821	CLA	CHC-C1C-NC	2.49	127.98	124.20
21	3	306	CHL	CMB-C2B-C1B	-2.49	124.64	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	839	CLA	C1D-ND-C4D	-2.48	104.57	106.33
18	B	836	CLA	CHC-C1C-C2C	-2.48	119.85	126.72
18	4	601	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
18	Z	606	CLA	CAA-C2A-C1A	-2.48	106.65	112.14
18	B	840	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
18	8	609	CLA	CHC-C1C-NC	2.48	127.97	124.20
21	1	606	CHL	CHC-C1C-NC	2.48	127.97	124.20
18	5	614	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
18	B	842	CLA	CHC-C1C-NC	2.48	127.96	124.20
18	B	833	CLA	CHA-C1A-NA	-2.48	120.72	126.40
21	4	604	CHL	CMA-C3A-C2A	-2.48	103.83	113.83
18	4	606	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
18	A	810	CLA	CHC-C1C-C2C	-2.47	119.88	126.72
18	5	603	CLA	CHA-C1A-NA	-2.47	120.73	126.40
18	3	301	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
18	3	307	CLA	CHC-C1C-NC	2.47	127.95	124.20
18	3	303	CLA	C1D-ND-C4D	-2.47	104.58	106.33
18	5	609	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
18	1	604	CLA	CHC-C1C-NC	2.47	127.95	124.20
18	B	821	CLA	CAA-C2A-C1A	-2.47	106.67	112.14
18	B	839	CLA	CHC-C1C-NC	2.47	127.95	124.20
18	A	819	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
18	B	812	CLA	CHC-C1C-C2C	-2.47	119.90	126.72
18	B	813	CLA	CAB-C3B-C4B	-2.47	124.67	128.46
18	A	840	CLA	CHC-C1C-NC	2.47	127.95	124.20
18	B	837	CLA	C2C-C1C-NC	2.47	112.28	109.97
18	B	821	CLA	CHC-C1C-NC	2.47	127.94	124.20
18	7	614	CLA	CHC-C1C-C2C	-2.47	119.90	126.72
18	1	607	CLA	CAA-C2A-C1A	-2.47	106.68	112.14
18	1	604	CLA	CHA-C1A-NA	-2.46	120.76	126.40
18	1	612	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
18	Z	607	CLA	CHC-C1C-NC	2.46	127.94	124.20
21	Z	605	CHL	CHC-C1C-NC	2.46	127.94	124.20
18	B	813	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
18	B	837	CLA	CHC-C1C-NC	2.46	127.94	124.20
18	3	305	CLA	CHC-C1C-NC	2.46	127.94	124.20
18	6	301	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
18	4	601	CLA	CHC-C1C-C2C	-2.45	119.93	126.72
18	Z	603	CLA	CHA-C1A-NA	-2.45	120.78	126.40
18	7	609	CLA	CHC-C1C-C2C	-2.45	119.93	126.72
18	A	831	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
18	4	608	CLA	CHA-C1A-NA	-2.45	120.78	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	F	302	CLA	CHC-C1C-NC	2.45	127.92	124.20
18	Z	603	CLA	CHC-C1C-NC	2.45	127.92	124.20
18	A	843	CLA	C1-C2-C3	-2.45	121.80	126.04
18	5	608	CLA	CHC-C1C-NC	2.45	127.92	124.20
21	Z	601	CHL	CAA-C2A-C1A	2.45	117.56	112.14
18	A	816	CLA	C2C-C1C-NC	2.45	112.26	109.97
18	1	603	CLA	CHA-C1A-NA	-2.45	120.80	126.40
21	4	604	CHL	CHA-C1A-NA	-2.45	120.80	126.40
18	A	843	CLA	C1D-ND-C4D	-2.45	104.60	106.33
18	B	814	CLA	CHA-C1A-NA	-2.44	120.80	126.40
18	8	615	CLA	CHA-C1A-NA	-2.44	120.81	126.40
18	Z	611	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
18	B	813	CLA	CHC-C1C-NC	2.44	127.91	124.20
18	B	841	CLA	C3A-C2A-C1A	-2.44	97.69	101.34
18	F	301	CLA	CHC-C1C-NC	2.44	127.90	124.20
18	A	807	CLA	C2C-C1C-NC	2.44	112.25	109.97
21	4	605	CHL	CMB-C2B-C1B	-2.44	124.72	128.46
18	8	604	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
18	B	827	CLA	C2C-C1C-NC	2.44	112.25	109.97
18	B	812	CLA	C2A-C3A-C4A	-2.44	97.93	101.87
18	B	801	CLA	CHC-C1C-NC	2.44	127.90	124.20
18	A	837	CLA	C1D-ND-C4D	-2.44	104.61	106.33
18	A	820	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
18	7	602	CLA	CHC-C1C-NC	2.43	127.89	124.20
21	Z	605	CHL	C3D-C4D-ND	2.43	114.17	110.24
21	4	604	CHL	CHC-C1C-NC	2.43	127.89	124.20
18	A	832	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
18	A	835	CLA	CHC-C1C-NC	2.43	127.89	124.20
18	B	823	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
18	A	830	CLA	C2C-C1C-NC	2.43	112.25	109.97
18	B	820	CLA	CHC-C1C-NC	2.43	127.89	124.20
18	1	608	CLA	CHC-C1C-C2C	-2.43	120.01	126.72
18	B	836	CLA	C2C-C1C-NC	2.43	112.24	109.97
18	B	831	CLA	CHC-C1C-C2C	-2.42	120.02	126.72
18	7	614	CLA	C2C-C1C-NC	2.42	112.24	109.97
18	5	602	CLA	CHC-C1C-NC	2.42	127.88	124.20
18	3	305	CLA	CHC-C1C-C2C	-2.42	120.02	126.72
18	5	615	CLA	CAA-C2A-C1A	-2.42	104.04	111.97
21	7	606	CHL	CHC-C1C-NC	2.42	127.87	124.20
18	Z	607	CLA	C2A-C3A-C4A	-2.42	97.96	101.87
18	A	837	CLA	CHC-C1C-NC	2.42	127.87	124.20
18	A	811	CLA	CHC-C1C-C2C	-2.42	120.04	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	308	CLA	CHC-C1C-NC	2.42	127.87	124.20
18	5	617	CLA	CHC-C1C-C2C	-2.42	120.04	126.72
18	B	824	CLA	CHC-C1C-C2C	-2.42	120.04	126.72
18	5	605	CLA	CHA-C1A-NA	-2.42	120.87	126.40
18	7	610	CLA	CHC-C1C-C2C	-2.42	120.04	126.72
21	1	606	CHL	C3D-C4D-ND	2.41	114.14	110.24
18	A	826	CLA	CHC-C1C-C2C	-2.41	120.04	126.72
18	A	823	CLA	CHA-C1A-NA	-2.41	120.87	126.40
18	4	609	CLA	C2C-C1C-NC	2.41	112.23	109.97
18	Z	607	CLA	CHC-C1C-C2C	-2.41	120.05	126.72
18	B	808	CLA	C1D-ND-C4D	-2.41	104.62	106.33
18	7	604	CLA	C1D-ND-C4D	-2.41	104.62	106.33
18	A	836	CLA	C2C-C1C-NC	2.41	112.23	109.97
18	B	805	CLA	CHC-C1C-C2C	-2.41	120.06	126.72
18	B	829	CLA	CHC-C1C-NC	2.41	127.86	124.20
18	1	608	CLA	C2A-C3A-C4A	-2.41	97.98	101.87
18	A	804	CLA	CHA-C1A-NA	-2.41	120.89	126.40
18	A	817	CLA	CHA-C1A-NA	-2.41	120.89	126.40
18	8	614	CLA	CHA-C1A-NA	-2.41	120.89	126.40
18	B	815	CLA	CHC-C1C-NC	2.41	127.85	124.20
18	6	313	CLA	C2C-C1C-NC	2.40	112.22	109.97
18	A	821	CLA	C1B-CHB-C4A	-2.40	125.35	130.12
18	3	309	CLA	C1D-ND-C4D	-2.40	104.63	106.33
18	3	305	CLA	CGD-CBD-CAD	-2.40	102.95	110.73
18	6	302	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
18	3	314	CLA	C2C-C1C-NC	2.40	112.22	109.97
18	A	805	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
18	A	821	CLA	CHA-C1A-NA	-2.40	120.90	126.40
18	A	834	CLA	CHA-C1A-NA	-2.40	120.90	126.40
21	6	316	CHL	CHC-C1C-NC	2.40	127.84	124.20
18	A	827	CLA	C2A-C1A-CHA	2.40	128.06	123.86
18	5	604	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
18	6	313	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
18	A	834	CLA	CHC-C1C-NC	2.40	127.84	124.20
21	5	607	CHL	CHC-C1C-NC	2.40	127.84	124.20
18	A	833	CLA	CHA-C1A-NA	-2.40	120.91	126.40
18	8	612	CLA	CHA-C1A-NA	-2.39	120.91	126.40
18	5	608	CLA	CHC-C1C-C2C	-2.39	120.10	126.72
18	B	843	CLA	CHA-C1A-NA	-2.39	120.92	126.40
18	3	309	CLA	CHC-C1C-NC	2.39	127.83	124.20
18	5	617	CLA	CHC-C1C-NC	2.39	127.83	124.20
18	3	307	CLA	CHC-C1C-C2C	-2.39	120.12	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	802	CLA	CAA-C2A-C1A	-2.38	106.86	112.14
18	A	843	CLA	CHC-C1C-NC	2.38	127.82	124.20
18	B	827	CLA	CGD-CBD-CAD	-2.38	103.02	110.73
18	8	604	CLA	CHC-C1C-NC	2.38	127.81	124.20
18	B	808	CLA	CHA-C1A-NA	-2.38	120.95	126.40
18	B	836	CLA	CHC-C1C-NC	2.38	127.81	124.20
18	3	305	CLA	C2A-C1A-CHA	2.37	128.01	123.86
18	3	309	CLA	CHC-C1C-C2C	-2.37	120.16	126.72
18	A	805	CLA	CAA-C2A-C1A	-2.37	106.89	112.14
18	A	822	CLA	CHA-C1A-NA	-2.37	120.96	126.40
18	B	842	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
18	A	806	CLA	CAA-C2A-C1A	-2.37	106.89	112.14
18	7	605	CLA	CHC-C1C-NC	2.37	127.80	124.20
18	6	308	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
18	A	834	CLA	C2C-C1C-NC	2.37	112.19	109.97
18	B	812	CLA	CHC-C1C-NC	2.36	127.79	124.20
18	8	604	CLA	C2C-C1C-NC	2.36	112.19	109.97
18	7	610	CLA	C1D-ND-C4D	-2.36	104.66	106.33
18	B	815	CLA	CHC-C1C-C2C	-2.36	120.19	126.72
18	A	802	CLA	CHC-C1C-NC	2.36	127.79	124.20
18	A	828	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
21	4	605	CHL	C2A-C1A-CHA	-2.36	119.73	123.86
18	A	811	CLA	CHC-C1C-NC	2.36	127.78	124.20
18	B	829	CLA	CHC-C1C-C2C	-2.36	120.20	126.72
18	B	827	CLA	CHA-C1A-NA	-2.36	121.00	126.40
18	5	614	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
18	7	611	CLA	C2C-C1C-NC	2.35	112.18	109.97
18	3	301	CLA	CHC-C1C-NC	2.35	127.78	124.20
18	B	813	CLA	C2C-C1C-NC	2.35	112.18	109.97
18	8	608	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
18	B	826	CLA	CHA-C1A-NA	-2.35	121.01	126.40
18	7	607	CLA	CHC-C1C-NC	2.35	127.77	124.20
18	5	604	CLA	CAA-C2A-C1A	-2.35	106.94	112.14
18	3	303	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
18	B	840	CLA	C1D-ND-C4D	-2.35	104.67	106.33
18	B	831	CLA	CHC-C1C-NC	2.35	127.77	124.20
18	A	839	CLA	CAA-C2A-C3A	-2.35	108.39	114.26
18	8	610	CLA	CHC-C1C-C2C	-2.35	120.23	126.72
18	8	605	CLA	CHC-C1C-NC	2.35	127.76	124.20
18	6	315	CLA	CHC-C1C-NC	2.35	127.76	124.20
21	6	305	CHL	CHC-C1C-NC	2.34	127.76	124.20
18	3	309	CLA	CHA-C1A-NA	-2.34	121.03	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	311	CLA	C1D-ND-C4D	-2.34	104.67	106.33
18	F	302	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
18	5	613	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
18	8	610	CLA	CHC-C1C-NC	2.34	127.75	124.20
18	6	314	CLA	CHC-C1C-NC	2.33	127.74	124.20
18	B	835	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
18	7	602	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
18	7	610	CLA	CHA-C1A-NA	-2.33	121.06	126.40
18	A	807	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
18	8	613	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
18	B	835	CLA	C3A-C2A-C1A	-2.33	97.86	101.34
18	B	807	CLA	C5-C3-C2	-2.32	111.04	126.84
18	4	607	CLA	CHA-C1A-NA	-2.32	121.08	126.40
18	6	314	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	Z	602	CLA	C2C-C1C-NC	2.32	112.15	109.97
18	7	614	CLA	CHC-C1C-NC	2.32	127.72	124.20
21	6	306	CHL	CHC-C1C-NC	2.32	127.72	124.20
18	7	608	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	B	840	CLA	CHA-C1A-NA	-2.32	121.09	126.40
18	7	609	CLA	CHC-C1C-NC	2.32	127.72	124.20
18	6	309	CLA	CHC-C1C-C2C	-2.32	120.31	126.72
18	A	812	CLA	C2C-C1C-NC	2.32	112.14	109.97
18	B	802	CLA	C1D-ND-C4D	-2.31	104.69	106.33
18	B	841	CLA	C2C-C1C-NC	2.31	112.14	109.97
18	6	301	CLA	CHC-C1C-NC	2.31	127.71	124.20
18	3	312	CLA	C2C-C1C-NC	2.31	112.14	109.97
18	5	617	CLA	C2C-C1C-NC	2.31	112.14	109.97
18	A	820	CLA	CHA-C1A-NA	-2.31	121.11	126.40
18	A	824	CLA	CHA-C1A-NA	-2.31	121.11	126.40
18	B	804	CLA	CHC-C1C-C2C	-2.31	120.34	126.72
18	3	314	CLA	CHA-C1A-NA	-2.31	121.11	126.40
21	1	606	CHL	CMB-C2B-C3B	2.31	128.99	124.68
18	8	610	CLA	C3B-C4B-NB	-2.30	106.23	109.21
21	4	604	CHL	CMA-C3A-C4A	-2.30	105.58	111.77
18	B	807	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
18	5	612	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	8	605	CLA	CHA-C1A-NA	-2.30	121.13	126.40
18	1	602	CLA	C2C-C1C-NC	2.30	112.12	109.97
18	A	810	CLA	CAA-C2A-C1A	-2.30	107.06	112.14
18	4	611	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
18	A	809	CLA	CHA-C1A-NA	-2.30	121.14	126.40
21	Z	605	CHL	CMB-C2B-C3B	2.29	128.97	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	305	CLA	CHA-C1A-NA	-2.29	121.15	126.40
18	3	301	CLA	C2C-C1C-NC	2.29	112.12	109.97
18	3	308	CLA	CAA-C2A-C1A	-2.29	107.07	112.14
18	3	311	CLA	CHC-C1C-NC	2.29	127.68	124.20
18	B	802	CLA	CHC-C1C-C2C	-2.29	120.39	126.72
18	B	811	CLA	C1D-ND-C4D	-2.29	104.71	106.33
18	5	615	CLA	CHA-C1A-NA	-2.29	121.16	126.40
18	7	610	CLA	CHC-C1C-NC	2.29	127.67	124.20
18	3	303	CLA	CHA-C1A-NA	-2.29	121.16	126.40
18	5	609	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
18	5	613	CLA	CHA-C1A-NA	-2.29	121.16	126.40
21	4	604	CHL	CHD-C1D-C2D	2.29	130.28	125.48
18	B	811	CLA	CHA-C1A-NA	-2.29	121.16	126.40
18	4	606	CLA	CHC-C1C-NC	2.29	127.67	124.20
18	A	813	CLA	C1D-ND-C4D	-2.28	104.71	106.33
18	5	615	CLA	C2A-C1A-CHA	2.28	127.85	123.86
18	A	827	CLA	C2C-C1C-NC	2.28	112.11	109.97
18	4	607	CLA	C1D-CHD-C4C	-2.28	121.14	126.06
18	Z	604	CLA	C1D-ND-C4D	-2.28	104.72	106.33
18	4	608	CLA	C2A-C3A-C4A	-2.28	98.19	101.87
18	6	308	CLA	C2C-C1C-NC	2.27	112.10	109.97
18	A	803	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
18	B	807	CLA	CHC-C1C-NC	2.27	127.65	124.20
18	5	610	CLA	C2C-C1C-NC	2.27	112.10	109.97
18	B	801	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
18	B	828	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
18	A	841	CLA	C2C-C1C-NC	2.27	112.10	109.97
21	3	306	CHL	CHC-C1C-NC	2.27	127.65	124.20
18	8	614	CLA	C3A-C2A-C1A	-2.27	97.94	101.34
18	A	810	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
18	A	817	CLA	C2C-C1C-NC	2.26	112.09	109.97
18	7	612	CLA	C2C-C1C-NC	2.26	112.09	109.97
18	B	825	CLA	CHA-C1A-NA	-2.26	121.22	126.40
18	B	832	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
18	5	610	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
18	Z	607	CLA	C2A-C1A-CHA	2.26	127.81	123.86
18	1	605	CLA	C1D-ND-C4D	-2.26	104.73	106.33
18	B	807	CLA	CGD-CBD-CAD	-2.26	103.43	110.73
18	A	818	CLA	CHA-C1A-NA	-2.26	121.23	126.40
18	4	610	CLA	CHC-C1C-C2C	-2.26	120.48	126.72
18	B	818	CLA	CAA-C2A-C1A	-2.25	107.15	112.14
18	A	806	CLA	C1B-CHB-C4A	-2.25	125.66	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	832	CLA	CHA-C1A-NA	-2.25	121.24	126.40
18	B	802	CLA	CHA-C1A-NA	-2.25	121.24	126.40
18	A	834	CLA	CGD-CBD-CAD	-2.25	103.45	110.73
18	4	610	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
18	B	838	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
18	4	602	CLA	CAA-C2A-C1A	-2.24	107.17	112.14
18	8	609	CLA	C2C-C1C-NC	2.24	112.07	109.97
18	7	614	CLA	C2A-C3A-C4A	-2.24	98.25	101.87
18	B	806	CLA	CGD-CBD-CAD	-2.24	103.48	110.73
18	A	845	CLA	C2C-C1C-NC	2.24	112.07	109.97
18	7	601	CLA	CGD-CBD-CAD	-2.24	103.48	110.73
21	4	604	CHL	CHD-C4C-C3C	2.24	128.13	124.84
18	A	802	CLA	CHA-C1A-NA	-2.24	121.28	126.40
18	A	829	CLA	C2C-C1C-NC	2.24	112.07	109.97
18	8	604	CLA	CHA-C1A-NA	-2.24	121.28	126.40
18	4	612	CLA	CHA-C1A-NA	-2.24	121.28	126.40
18	A	844	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
18	1	608	CLA	C2A-C1A-CHA	2.24	127.77	123.86
18	7	609	CLA	CGD-CBD-CAD	-2.24	103.49	110.73
18	8	603	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
18	A	844	CLA	CAA-C2A-C1A	-2.23	107.19	112.14
18	5	602	CLA	CAA-C2A-C1A	-2.23	107.20	112.14
18	4	608	CLA	CHC-C1C-C2C	-2.23	120.55	126.72
18	5	614	CLA	CHA-C1A-NA	-2.23	121.29	126.40
18	B	818	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
18	6	312	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
18	A	830	CLA	CHA-C1A-NA	-2.23	121.29	126.40
18	5	609	CLA	CAA-C2A-C1A	-2.23	107.21	112.14
18	Z	608	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
18	B	819	CLA	C3A-C2A-C1A	-2.22	98.01	101.34
18	6	313	CLA	CAA-C2A-C1A	-2.22	107.23	112.14
18	A	829	CLA	CHA-C1A-NA	-2.22	121.31	126.40
18	3	313	CLA	CHA-C1A-NA	-2.22	121.31	126.40
18	5	611	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
18	3	304	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
18	5	615	CLA	CHC-C1C-C2C	-2.22	120.59	126.72
18	7	610	CLA	C2C-C1C-NC	2.22	112.05	109.97
18	B	823	CLA	C3D-C4D-ND	2.22	113.83	110.24
18	5	609	CLA	CHC-C1C-NC	2.22	127.57	124.20
21	4	604	CHL	C2D-C1D-ND	-2.22	108.47	110.10
18	1	604	CLA	CHC-C1C-C2C	-2.22	120.59	126.72
18	5	605	CLA	C1D-ND-C4D	-2.22	104.76	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	301	CLA	C2A-C1A-CHA	2.21	127.73	123.86
18	5	614	CLA	CHC-C1C-NC	2.21	127.56	124.20
18	A	835	CLA	CHA-C1A-NA	-2.21	121.33	126.40
18	4	607	CLA	C3A-C2A-C1A	-2.21	98.03	101.34
18	4	606	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
21	6	305	CHL	CMB-C2B-C3B	2.21	128.81	124.68
18	7	608	CLA	CHA-C1A-NA	-2.21	121.34	126.40
18	B	806	CLA	CHA-C1A-NA	-2.21	121.34	126.40
18	B	835	CLA	CHA-C1A-NA	-2.21	121.34	126.40
18	6	315	CLA	C1D-ND-C4D	-2.21	104.77	106.33
18	4	610	CLA	CHA-C1A-NA	-2.20	121.35	126.40
18	B	805	CLA	C3A-C2A-C1A	-2.20	98.04	101.34
18	8	607	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
18	B	816	CLA	CHA-C1A-NA	-2.20	121.36	126.40
18	7	609	CLA	C2C-C1C-NC	2.20	112.03	109.97
18	7	613	CLA	CHA-C1A-NA	-2.20	121.36	126.40
18	8	604	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
18	4	602	CLA	CHC-C1C-C2C	-2.20	120.65	126.72
18	B	831	CLA	CAA-C2A-C1A	-2.20	107.28	112.14
18	A	845	CLA	CHA-C1A-NA	-2.20	121.37	126.40
18	A	841	CLA	CHA-C1A-NA	-2.20	121.37	126.40
18	Z	603	CLA	CMB-C2B-C1B	-2.19	125.09	128.46
18	5	604	CLA	CHA-C1A-NA	-2.19	121.37	126.40
18	Z	603	CLA	CHC-C1C-C2C	-2.19	120.65	126.72
18	B	808	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
18	A	839	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
18	1	604	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
17	A	801	CL0	C1B-CHB-C4A	-2.19	125.78	130.12
18	B	802	CLA	CHC-C1C-NC	2.19	127.53	124.20
18	5	611	CLA	CGD-CBD-CAD	-2.19	103.65	110.73
18	B	826	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
18	5	610	CLA	CHA-C1A-NA	-2.18	121.40	126.40
18	B	801	CLA	C1D-ND-C4D	-2.18	104.78	106.33
18	1	609	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
18	A	805	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
18	1	608	CLA	C1D-ND-C4D	-2.18	104.78	106.33
18	Z	607	CLA	C1D-ND-C4D	-2.18	104.78	106.33
18	A	803	CLA	C3D-C4D-ND	2.18	113.76	110.24
18	6	317	CLA	CHA-C1A-NA	-2.18	121.41	126.40
18	B	805	CLA	C1D-ND-C4D	-2.18	104.79	106.33
18	B	834	CLA	CHA-C1A-NA	-2.18	121.41	126.40
18	1	609	CLA	C1B-CHB-C4A	-2.18	125.80	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	309	CLA	C2C-C1C-NC	2.18	112.01	109.97
18	B	832	CLA	CHC-C1C-NC	2.18	127.51	124.20
18	B	831	CLA	CHA-C1A-NA	-2.18	121.41	126.40
18	4	603	CLA	CHA-C1A-NA	-2.18	121.42	126.40
18	Z	608	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
18	4	611	CLA	CAA-C2A-C1A	-2.17	107.33	112.14
18	A	827	CLA	CHA-C1A-NA	-2.17	121.42	126.40
18	5	612	CLA	CHA-C1A-NA	-2.17	121.43	126.40
18	A	822	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
18	A	834	CLA	C3A-C2A-C1A	-2.17	98.09	101.34
18	B	841	CLA	CBA-CAA-C2A	2.17	118.30	113.47
18	4	606	CLA	CHA-C1A-NA	-2.17	121.43	126.40
18	6	302	CLA	CAA-C2A-C1A	-2.17	107.34	112.14
18	A	805	CLA	CHC-C1C-NC	2.17	127.49	124.20
18	6	309	CLA	CHC-C1C-NC	2.17	127.49	124.20
18	J	101	CLA	C2C-C1C-NC	2.17	112.00	109.97
18	7	612	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
18	B	813	CLA	CHA-C1A-NA	-2.17	121.44	126.40
18	Z	609	CLA	CHC-C1C-NC	2.17	127.49	124.20
18	7	602	CLA	CAA-C2A-C1A	-2.17	107.35	112.14
18	B	832	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
18	B	832	CLA	C2C-C1C-NC	2.16	112.00	109.97
18	4	608	CLA	CAA-C2A-C1A	-2.16	107.35	112.14
18	B	841	CLA	CHA-C1A-NA	-2.16	121.44	126.40
18	3	312	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
18	1	610	CLA	CHC-C1C-NC	2.16	127.48	124.20
18	8	607	CLA	C2C-C1C-NC	2.16	112.00	109.97
18	B	801	CLA	CGD-CBD-CAD	-2.16	103.74	110.73
18	6	302	CLA	CHC-C1C-NC	2.16	127.48	124.20
18	6	304	CLA	C2C-C1C-NC	2.16	112.00	109.97
18	4	609	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
18	Z	607	CLA	C2C-C1C-NC	2.16	111.99	109.97
18	A	816	CLA	CHA-C1A-NA	-2.16	121.46	126.40
18	5	609	CLA	CHA-C1A-NA	-2.15	121.46	126.40
18	4	608	CLA	C2C-C1C-NC	2.15	111.99	109.97
18	A	831	CLA	C3D-C4D-ND	2.15	113.72	110.24
18	1	608	CLA	C2C-C1C-NC	2.15	111.99	109.97
18	8	611	CLA	C2C-C1C-NC	2.15	111.99	109.97
18	4	602	CLA	C2C-C1C-NC	2.15	111.99	109.97
18	B	839	CLA	CHA-C1A-NA	-2.15	121.47	126.40
18	1	613	CLA	CHA-C1A-NA	-2.15	121.47	126.40
18	B	801	CLA	CMB-C2B-C1B	-2.15	125.16	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	101	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
18	4	608	CLA	C1D-ND-C4D	-2.15	104.81	106.33
18	6	313	CLA	CHD-C1D-C2D	2.15	129.99	125.48
18	4	610	CLA	C2C-C1C-NC	2.15	111.99	109.97
18	7	612	CLA	CHA-C1A-NA	-2.15	121.48	126.40
18	5	615	CLA	CHC-C1C-NC	2.15	127.46	124.20
18	B	831	CLA	C2C-C1C-NC	2.15	111.98	109.97
18	A	845	CLA	CAA-C2A-C1A	-2.15	107.39	112.14
18	B	823	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
18	8	601	CLA	CHA-C1A-NA	-2.14	121.49	126.40
18	Z	612	CLA	CHA-C1A-NA	-2.14	121.49	126.40
18	B	811	CLA	CHC-C1C-NC	2.14	127.45	124.20
18	7	608	CLA	C2C-C1C-NC	2.14	111.97	109.97
18	3	313	CLA	CAA-C2A-C1A	-2.14	104.97	111.97
18	7	609	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
21	5	606	CHL	CHC-C1C-NC	2.14	127.44	124.20
18	B	837	CLA	CHA-C1A-NA	-2.14	121.51	126.40
18	B	807	CLA	C2C-C1C-NC	2.13	111.97	109.97
18	3	301	CLA	C3D-C4D-ND	2.13	113.69	110.24
18	7	604	CLA	C1D-CHD-C4C	-2.13	121.46	126.06
18	6	309	CLA	C2C-C1C-NC	2.13	111.97	109.97
18	7	607	CLA	CHA-C1A-NA	-2.13	121.52	126.40
18	A	808	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
18	1	610	CLA	CHA-C1A-NA	-2.13	121.52	126.40
18	Z	609	CLA	CHA-C1A-NA	-2.13	121.52	126.40
18	3	314	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
18	4	602	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
18	A	824	CLA	C3A-C2A-C1A	-2.12	98.16	101.34
18	A	828	CLA	C1D-ND-C4D	-2.12	104.83	106.33
18	6	302	CLA	CHA-C1A-NA	-2.12	121.54	126.40
18	B	805	CLA	CHA-C1A-NA	-2.12	121.54	126.40
18	5	610	CLA	CHC-C1C-NC	2.12	127.42	124.20
18	A	834	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
18	A	840	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
18	6	315	CLA	CHA-C1A-NA	-2.12	121.55	126.40
18	5	605	CLA	CMB-C2B-C1B	-2.11	125.21	128.46
18	3	305	CLA	C2C-C1C-NC	2.11	111.95	109.97
18	6	314	CLA	CMB-C2B-C1B	-2.11	125.22	128.46
21	5	606	CHL	CMB-C2B-C3B	2.11	128.63	124.68
18	8	610	CLA	CHD-C1D-C2D	2.11	129.91	125.48
18	B	817	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
18	Z	610	CLA	C1B-CHB-C4A	-2.11	125.94	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	823	CLA	CGD-CBD-CAD	-2.11	103.91	110.73
18	1	604	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
18	6	312	CLA	CHA-C1A-NA	-2.10	121.58	126.40
18	1	611	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
18	3	304	CLA	CAA-C2A-C1A	-2.10	107.49	112.14
18	1	605	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
21	5	607	CHL	CMB-C2B-C3B	2.10	128.61	124.68
18	6	314	CLA	CHA-C1A-NA	-2.10	121.59	126.40
18	6	301	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
18	A	827	CLA	CHD-C1D-C2D	2.10	129.88	125.48
18	4	607	CLA	CHC-C1C-NC	2.10	127.39	124.20
18	Z	603	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
18	4	607	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
18	B	836	CLA	CHA-C1A-NA	-2.10	121.60	126.40
18	A	804	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
18	Z	612	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
18	8	608	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
18	A	841	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
18	8	612	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
18	8	611	CLA	C3D-C4D-ND	2.09	113.62	110.24
18	B	834	CLA	C2C-C1C-CHC	-2.09	118.78	124.50
18	B	815	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
18	A	825	CLA	CHD-C1D-C2D	2.09	129.86	125.48
18	B	830	CLA	CGD-CBD-CAD	-2.09	103.97	110.73
18	B	807	CLA	CMB-C2B-C1B	-2.09	125.26	128.46
18	1	611	CLA	CMB-C2B-C1B	-2.09	125.26	128.46
18	6	304	CLA	CMB-C2B-C1B	-2.09	125.26	128.46
18	B	804	CLA	C2A-C3A-C4A	-2.09	98.50	101.87
18	3	310	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
18	F	302	CLA	CHA-C1A-NA	-2.08	121.62	126.40
18	B	819	CLA	C2C-C1C-NC	2.08	111.92	109.97
18	8	610	CLA	C2C-C1C-NC	2.08	111.92	109.97
18	5	611	CLA	C3D-C4D-ND	2.08	113.61	110.24
18	4	602	CLA	CMB-C2B-C1B	-2.08	125.26	128.46
18	8	602	CLA	CAA-C2A-C1A	-2.08	107.53	112.14
18	7	605	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
18	B	836	CLA	CAA-C2A-C1A	-2.08	107.54	112.14
18	B	815	CLA	C2C-C1C-NC	2.08	111.92	109.97
18	J	101	CLA	CHA-C1A-NA	-2.08	121.64	126.40
18	B	843	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
18	5	608	CLA	CHA-C1A-NA	-2.08	121.64	126.40
21	5	616	CHL	C2C-C3C-C4C	2.08	107.97	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	835	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
18	A	837	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
18	A	807	CLA	CHA-C1A-NA	-2.07	121.65	126.40
18	A	808	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
21	4	605	CHL	C2A-C3A-C4A	-2.07	98.52	101.87
18	1	613	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
18	7	607	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
18	A	812	CLA	CHA-C1A-NA	-2.07	121.65	126.40
18	A	843	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
18	B	831	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
18	8	612	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
18	A	826	CLA	C3D-C4D-ND	2.07	113.58	110.24
18	4	608	CLA	CHC-C1C-NC	2.07	127.34	124.20
18	A	822	CLA	CAC-C3C-C4C	2.07	127.49	124.81
18	B	804	CLA	C2A-C1A-CHA	2.07	127.47	123.86
18	A	836	CLA	CAA-C2A-C1A	-2.06	107.57	112.14
18	8	602	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
18	3	304	CLA	CHA-C1A-NA	-2.06	121.67	126.40
18	Z	604	CLA	CMB-C2B-C1B	-2.06	125.29	128.46
21	4	604	CHL	C3C-C4C-NC	-2.06	108.26	110.57
18	8	601	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
18	A	843	CLA	CHA-C1A-NA	-2.06	121.69	126.40
18	7	611	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
18	B	840	CLA	CAA-C2A-C1A	-2.06	107.59	112.14
21	4	604	CHL	CMB-C2B-C3B	2.06	128.53	124.68
18	4	612	CLA	C1D-ND-C4D	-2.06	104.87	106.33
18	8	605	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
18	A	837	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
18	Z	610	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
18	B	812	CLA	CHB-C4A-NA	2.05	127.35	124.51
18	3	302	CLA	CAA-C2A-C1A	-2.05	107.60	112.14
18	B	812	CLA	C1D-ND-C4D	-2.05	104.88	106.33
18	Z	602	CLA	CHA-C1A-NA	-2.05	121.70	126.40
18	A	805	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
18	A	812	CLA	CGD-CBD-CAD	-2.05	104.09	110.73
18	B	815	CLA	C1D-ND-C4D	-2.05	104.88	106.33
21	6	306	CHL	CMB-C2B-C3B	2.05	128.51	124.68
18	6	304	CLA	C1B-CHB-C4A	-2.04	126.07	130.12
18	A	845	CLA	C1D-CHD-C4C	-2.04	121.65	126.06
18	B	822	CLA	CHA-C1A-NA	-2.04	121.72	126.40
18	7	608	CLA	CAA-C2A-C1A	-2.04	105.28	111.97
18	1	602	CLA	CHA-C1A-NA	-2.04	121.72	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	609	CLA	CHC-C1C-NC	2.04	127.30	124.20
18	3	311	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
18	B	819	CLA	C3D-C4D-ND	2.04	113.54	110.24
18	3	311	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
18	7	605	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
18	A	815	CLA	CHA-C1A-NA	-2.04	121.73	126.40
18	6	308	CLA	CHA-C1A-NA	-2.04	121.74	126.40
18	Z	608	CLA	CHC-C1C-NC	2.03	127.29	124.20
18	A	825	CLA	CHA-C1A-NA	-2.03	121.74	126.40
18	B	804	CLA	C1D-ND-C4D	-2.03	104.89	106.33
18	3	308	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
18	B	809	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
18	B	815	CLA	CHD-C1D-C2D	2.03	129.74	125.48
18	A	838	CLA	CAA-C2A-C1A	-2.03	107.64	112.14
18	6	317	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
18	B	833	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
18	7	601	CLA	CAA-C2A-C1A	-2.03	107.65	112.14
18	B	829	CLA	CHA-C1A-NA	-2.03	121.76	126.40
18	1	602	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
18	3	308	CLA	CHA-C1A-NA	-2.03	121.76	126.40
18	A	838	CLA	CHD-C1D-C2D	2.03	129.73	125.48
18	4	602	CLA	C3D-C4D-ND	2.03	113.51	110.24
18	5	617	CLA	C3D-C4D-ND	2.02	113.51	110.24
18	4	601	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
18	1	607	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
18	B	830	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
18	A	820	CLA	CAA-C2A-C1A	-2.02	107.67	112.14
18	4	602	CLA	CHC-C1C-NC	2.02	127.27	124.20
18	6	309	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
18	5	609	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
18	1	612	CLA	CHA-C1A-NA	-2.02	121.78	126.40
18	5	614	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
18	A	808	CLA	C3D-C4D-ND	2.02	113.50	110.24
18	6	311	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
18	7	611	CLA	CAA-C2A-C1A	-2.02	107.68	112.14
18	A	813	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
21	5	606	CHL	CHD-C1D-C2D	2.01	129.70	125.48
18	Z	611	CLA	CHA-C1A-NA	-2.01	121.79	126.40
18	6	311	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
18	A	814	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
18	6	313	CLA	CHA-C1A-NA	-2.01	121.80	126.40
18	B	817	CLA	CMB-C2B-C1B	-2.01	125.38	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	834	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
18	4	610	CLA	CHC-C1C-NC	2.01	127.25	124.20
18	A	812	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
18	A	837	CLA	CHA-C1A-NA	-2.01	121.80	126.40
18	7	602	CLA	CHA-C1A-NA	-2.01	121.80	126.40
18	8	603	CLA	CHA-C1A-NA	-2.01	121.80	126.40
18	B	820	CLA	CHD-C1D-C2D	2.01	129.69	125.48
18	Z	602	CLA	C3D-C4D-ND	2.00	113.48	110.24
21	8	606	CHL	CMB-C2B-C3B	2.00	128.43	124.68
18	A	822	CLA	CMB-C2B-C1B	-2.00	125.38	128.46
18	6	311	CLA	C3D-C4D-ND	2.00	113.48	110.24
18	B	812	CLA	C2C-C1C-NC	2.00	111.85	109.97
18	B	806	CLA	CMB-C2B-C1B	-2.00	125.39	128.46
18	4	612	CLA	CHC-C1C-C2C	-2.00	121.19	126.72
18	5	603	CLA	CMB-C2B-C1B	-2.00	125.39	128.46
18	B	809	CLA	CMB-C2B-C1B	-2.00	125.39	128.46
18	B	824	CLA	CAA-C2A-C1A	-2.00	107.71	112.14

All (239) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	801	CL0	ND
17	A	801	CL0	NC
17	A	801	CL0	NA
18	A	802	CLA	ND
18	A	803	CLA	ND
18	A	804	CLA	ND
18	A	805	CLA	ND
18	A	806	CLA	ND
18	A	807	CLA	ND
18	A	808	CLA	ND
18	A	809	CLA	ND
18	A	810	CLA	ND
18	A	811	CLA	ND
18	A	812	CLA	ND
18	A	813	CLA	ND
18	A	814	CLA	ND
18	A	815	CLA	ND
18	A	816	CLA	ND
18	A	817	CLA	ND
18	A	818	CLA	ND
18	A	819	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
18	A	820	CLA	ND
18	A	821	CLA	ND
18	A	822	CLA	ND
18	A	823	CLA	ND
18	A	824	CLA	ND
18	A	825	CLA	ND
18	A	826	CLA	ND
18	A	827	CLA	ND
18	A	828	CLA	ND
18	A	829	CLA	ND
18	A	830	CLA	ND
18	A	831	CLA	ND
18	A	832	CLA	ND
18	A	833	CLA	ND
18	A	834	CLA	ND
18	A	835	CLA	ND
18	A	836	CLA	ND
18	A	837	CLA	ND
18	A	838	CLA	ND
18	A	839	CLA	ND
18	A	840	CLA	ND
18	A	841	CLA	ND
18	A	843	CLA	ND
18	A	844	CLA	ND
18	A	845	CLA	ND
18	B	801	CLA	ND
18	B	802	CLA	ND
18	B	804	CLA	ND
18	B	805	CLA	ND
18	B	806	CLA	ND
18	B	807	CLA	ND
18	B	808	CLA	ND
18	B	809	CLA	ND
18	B	810	CLA	ND
18	B	811	CLA	ND
18	B	812	CLA	ND
18	B	813	CLA	ND
18	B	814	CLA	ND
18	B	815	CLA	ND
18	B	816	CLA	ND
18	B	817	CLA	ND
18	B	818	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
18	B	819	CLA	ND
18	B	820	CLA	ND
18	B	821	CLA	ND
18	B	822	CLA	ND
18	B	823	CLA	ND
18	B	824	CLA	ND
18	B	825	CLA	ND
18	B	826	CLA	ND
18	B	827	CLA	ND
18	B	828	CLA	ND
18	B	829	CLA	ND
18	B	830	CLA	ND
18	B	831	CLA	ND
18	B	832	CLA	ND
18	B	833	CLA	ND
18	B	834	CLA	ND
18	B	835	CLA	ND
18	B	836	CLA	ND
18	B	837	CLA	ND
18	B	838	CLA	ND
18	B	839	CLA	ND
18	B	840	CLA	ND
18	B	841	CLA	ND
18	B	842	CLA	ND
18	B	843	CLA	ND
18	F	301	CLA	ND
18	F	302	CLA	ND
18	J	101	CLA	ND
18	1	602	CLA	ND
18	1	603	CLA	ND
18	1	604	CLA	ND
18	1	605	CLA	ND
18	1	607	CLA	ND
18	1	608	CLA	ND
18	1	609	CLA	ND
18	1	610	CLA	ND
18	1	611	CLA	ND
18	1	612	CLA	ND
18	1	613	CLA	ND
18	1	614	CLA	ND
18	3	301	CLA	ND
18	3	302	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
18	3	303	CLA	ND
18	3	304	CLA	ND
18	3	305	CLA	ND
18	3	307	CLA	ND
18	3	308	CLA	ND
18	3	309	CLA	ND
18	3	310	CLA	ND
18	3	311	CLA	ND
18	3	312	CLA	ND
18	3	313	CLA	ND
18	3	314	CLA	ND
18	7	601	CLA	ND
18	7	602	CLA	ND
18	7	603	CLA	ND
18	7	604	CLA	ND
18	7	605	CLA	ND
18	7	607	CLA	ND
18	7	608	CLA	ND
18	7	609	CLA	ND
18	7	610	CLA	ND
18	7	611	CLA	ND
18	7	612	CLA	ND
18	7	613	CLA	ND
18	7	614	CLA	ND
18	8	601	CLA	ND
18	8	602	CLA	ND
18	8	603	CLA	ND
18	8	604	CLA	ND
18	8	605	CLA	ND
18	8	607	CLA	ND
18	8	608	CLA	ND
18	8	609	CLA	ND
18	8	610	CLA	ND
18	8	611	CLA	ND
18	8	612	CLA	ND
18	8	613	CLA	ND
18	8	614	CLA	ND
18	8	615	CLA	ND
18	Z	602	CLA	ND
18	Z	603	CLA	ND
18	Z	604	CLA	ND
18	Z	606	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
18	Z	607	CLA	ND
18	Z	608	CLA	ND
18	Z	609	CLA	ND
18	Z	610	CLA	ND
18	Z	611	CLA	ND
18	Z	612	CLA	ND
18	Z	613	CLA	ND
18	4	601	CLA	ND
18	4	602	CLA	ND
18	4	603	CLA	ND
18	4	606	CLA	ND
18	4	607	CLA	ND
18	4	608	CLA	ND
18	4	609	CLA	ND
18	4	610	CLA	ND
18	4	611	CLA	ND
18	4	612	CLA	ND
18	5	601	CLA	ND
18	5	602	CLA	ND
18	5	603	CLA	ND
18	5	604	CLA	ND
18	5	605	CLA	ND
18	5	608	CLA	ND
18	5	609	CLA	ND
18	5	610	CLA	ND
18	5	611	CLA	ND
18	5	612	CLA	ND
18	5	613	CLA	ND
18	5	614	CLA	ND
18	5	615	CLA	ND
18	5	617	CLA	ND
18	6	301	CLA	ND
18	6	302	CLA	ND
18	6	303	CLA	ND
18	6	304	CLA	ND
18	6	308	CLA	ND
18	6	309	CLA	ND
18	6	310	CLA	ND
18	6	311	CLA	ND
18	6	312	CLA	ND
18	6	313	CLA	ND
18	6	314	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
18	6	315	CLA	ND
18	6	317	CLA	ND
21	1	601	CHL	ND
21	1	601	CHL	NC
21	1	601	CHL	NA
21	1	606	CHL	ND
21	1	606	CHL	NC
21	1	606	CHL	NA
21	3	306	CHL	ND
21	3	306	CHL	NC
21	3	306	CHL	NA
21	7	606	CHL	ND
21	7	606	CHL	NC
21	7	606	CHL	NA
21	8	606	CHL	ND
21	8	606	CHL	NC
21	8	606	CHL	NA
21	Z	601	CHL	ND
21	Z	601	CHL	NC
21	Z	601	CHL	NA
21	Z	605	CHL	ND
21	Z	605	CHL	NC
21	Z	605	CHL	NA
21	4	604	CHL	ND
21	4	604	CHL	NC
21	4	604	CHL	NA
21	4	605	CHL	ND
21	4	605	CHL	NC
21	4	605	CHL	NA
21	5	606	CHL	ND
21	5	606	CHL	NC
21	5	606	CHL	NA
21	5	607	CHL	ND
21	5	607	CHL	NC
21	5	607	CHL	NA
21	5	616	CHL	ND
21	5	616	CHL	NC
21	5	616	CHL	NA
21	6	305	CHL	ND
21	6	305	CHL	NC
21	6	305	CHL	NA
21	6	306	CHL	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
21	6	306	CHL	NC
21	6	306	CHL	NA
21	6	307	CHL	ND
21	6	307	CHL	NC
21	6	307	CHL	NA
21	6	316	CHL	ND
21	6	316	CHL	NC
21	6	316	CHL	NA

All (458) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	802	CLA	C1A-C2A-CAA-CBA
18	A	802	CLA	C3A-C2A-CAA-CBA
18	A	802	CLA	CHA-CBD-CGD-O1D
18	A	802	CLA	CHA-CBD-CGD-O2D
18	A	803	CLA	C1A-C2A-CAA-CBA
18	A	803	CLA	C3A-C2A-CAA-CBA
18	A	803	CLA	CHA-CBD-CGD-O1D
18	A	803	CLA	CAD-CBD-CGD-O1D
18	A	803	CLA	CAD-CBD-CGD-O2D
18	A	804	CLA	CHA-CBD-CGD-O1D
18	A	804	CLA	CHA-CBD-CGD-O2D
18	A	806	CLA	C1A-C2A-CAA-CBA
18	A	813	CLA	C1A-C2A-CAA-CBA
18	A	813	CLA	C3A-C2A-CAA-CBA
18	A	818	CLA	C1A-C2A-CAA-CBA
18	A	818	CLA	C3A-C2A-CAA-CBA
18	A	819	CLA	C1A-C2A-CAA-CBA
18	A	819	CLA	C3A-C2A-CAA-CBA
18	A	821	CLA	CHA-CBD-CGD-O1D
18	A	821	CLA	CHA-CBD-CGD-O2D
18	A	822	CLA	C3A-C2A-CAA-CBA
18	A	823	CLA	C1A-C2A-CAA-CBA
18	A	823	CLA	C3A-C2A-CAA-CBA
18	A	824	CLA	C1A-C2A-CAA-CBA
18	A	824	CLA	C3A-C2A-CAA-CBA
18	A	831	CLA	C1A-C2A-CAA-CBA
18	A	833	CLA	C1A-C2A-CAA-CBA
18	A	833	CLA	C3A-C2A-CAA-CBA
18	A	834	CLA	CHA-CBD-CGD-O1D
18	A	834	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	840	CLA	C1A-C2A-CAA-CBA
18	A	843	CLA	CHA-CBD-CGD-O1D
18	A	843	CLA	CHA-CBD-CGD-O2D
18	A	843	CLA	CAD-CBD-CGD-O1D
18	A	843	CLA	CAD-CBD-CGD-O2D
18	A	844	CLA	C1A-C2A-CAA-CBA
18	A	844	CLA	C3A-C2A-CAA-CBA
18	A	844	CLA	CHA-CBD-CGD-O1D
18	A	844	CLA	CHA-CBD-CGD-O2D
18	A	844	CLA	CAD-CBD-CGD-O1D
18	A	844	CLA	CAD-CBD-CGD-O2D
18	A	845	CLA	CHA-CBD-CGD-O1D
18	B	801	CLA	C1A-C2A-CAA-CBA
18	B	801	CLA	C3A-C2A-CAA-CBA
18	B	804	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C1A-C2A-CAA-CBA
18	B	806	CLA	C1A-C2A-CAA-CBA
18	B	809	CLA	C1A-C2A-CAA-CBA
18	B	811	CLA	C1A-C2A-CAA-CBA
18	B	812	CLA	C1A-C2A-CAA-CBA
18	B	812	CLA	C3A-C2A-CAA-CBA
18	B	815	CLA	C1A-C2A-CAA-CBA
18	B	815	CLA	CAD-CBD-CGD-O1D
18	B	816	CLA	C3A-C2A-CAA-CBA
18	B	817	CLA	C1A-C2A-CAA-CBA
18	B	819	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C3A-C2A-CAA-CBA
18	B	825	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	828	CLA	CHA-CBD-CGD-O1D
18	B	828	CLA	CHA-CBD-CGD-O2D
18	B	828	CLA	CAD-CBD-CGD-O1D
18	B	829	CLA	C1A-C2A-CAA-CBA
18	B	829	CLA	C3A-C2A-CAA-CBA
18	B	829	CLA	CHA-CBD-CGD-O1D
18	B	829	CLA	CHA-CBD-CGD-O2D
18	B	830	CLA	C1A-C2A-CAA-CBA
18	B	830	CLA	C3A-C2A-CAA-CBA
18	B	833	CLA	CHA-CBD-CGD-O1D
18	B	833	CLA	CHA-CBD-CGD-O2D
18	B	840	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	843	CLA	C3A-C2A-CAA-CBA
18	F	302	CLA	CHA-CBD-CGD-O1D
18	F	302	CLA	CHA-CBD-CGD-O2D
18	J	101	CLA	CAD-CBD-CGD-O1D
18	J	101	CLA	CAD-CBD-CGD-O2D
18	1	602	CLA	C1A-C2A-CAA-CBA
18	1	608	CLA	C1A-C2A-CAA-CBA
18	1	609	CLA	C1A-C2A-CAA-CBA
18	1	610	CLA	C1A-C2A-CAA-CBA
18	1	611	CLA	C1A-C2A-CAA-CBA
18	1	612	CLA	CHA-CBD-CGD-O1D
18	1	612	CLA	CHA-CBD-CGD-O2D
18	1	613	CLA	CHA-CBD-CGD-O1D
18	1	613	CLA	CHA-CBD-CGD-O2D
18	1	614	CLA	CHA-CBD-CGD-O1D
18	1	614	CLA	CHA-CBD-CGD-O2D
18	3	305	CLA	C3A-C2A-CAA-CBA
18	3	308	CLA	C1A-C2A-CAA-CBA
18	3	309	CLA	CHA-CBD-CGD-O1D
18	3	309	CLA	CHA-CBD-CGD-O2D
18	3	313	CLA	C1A-C2A-CAA-CBA
18	7	602	CLA	C1A-C2A-CAA-CBA
18	7	603	CLA	CHA-CBD-CGD-O1D
18	7	603	CLA	CHA-CBD-CGD-O2D
18	7	610	CLA	CHA-CBD-CGD-O1D
18	7	610	CLA	CHA-CBD-CGD-O2D
18	7	614	CLA	CHA-CBD-CGD-O1D
18	7	614	CLA	CHA-CBD-CGD-O2D
18	8	601	CLA	C3A-C2A-CAA-CBA
18	8	602	CLA	C1A-C2A-CAA-CBA
18	8	609	CLA	C1A-C2A-CAA-CBA
18	8	610	CLA	C1A-C2A-CAA-CBA
18	8	611	CLA	C1A-C2A-CAA-CBA
18	8	611	CLA	C3A-C2A-CAA-CBA
18	8	612	CLA	CHA-CBD-CGD-O2D
18	Z	602	CLA	C1A-C2A-CAA-CBA
18	Z	607	CLA	C1A-C2A-CAA-CBA
18	Z	608	CLA	C1A-C2A-CAA-CBA
18	Z	609	CLA	C1A-C2A-CAA-CBA
18	Z	610	CLA	C1A-C2A-CAA-CBA
18	Z	611	CLA	CHA-CBD-CGD-O1D
18	Z	611	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	Z	612	CLA	CHA-CBD-CGD-O1D
18	Z	612	CLA	CHA-CBD-CGD-O2D
18	Z	613	CLA	CHA-CBD-CGD-O1D
18	Z	613	CLA	CHA-CBD-CGD-O2D
18	4	602	CLA	C1A-C2A-CAA-CBA
18	4	606	CLA	C1A-C2A-CAA-CBA
18	4	607	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C3A-C2A-CAA-CBA
18	4	609	CLA	C1A-C2A-CAA-CBA
18	4	609	CLA	C3A-C2A-CAA-CBA
18	4	610	CLA	CHA-CBD-CGD-O1D
18	4	610	CLA	CHA-CBD-CGD-O2D
18	5	601	CLA	C1A-C2A-CAA-CBA
18	5	601	CLA	C3A-C2A-CAA-CBA
18	5	608	CLA	C3A-C2A-CAA-CBA
18	5	609	CLA	C1A-C2A-CAA-CBA
18	5	610	CLA	CHA-CBD-CGD-O1D
18	5	610	CLA	CHA-CBD-CGD-O2D
18	5	611	CLA	C1A-C2A-CAA-CBA
18	5	611	CLA	C3A-C2A-CAA-CBA
18	5	612	CLA	CHA-CBD-CGD-O1D
18	5	612	CLA	CHA-CBD-CGD-O2D
18	5	615	CLA	CHA-CBD-CGD-O1D
18	5	615	CLA	CHA-CBD-CGD-O2D
18	6	302	CLA	CHA-CBD-CGD-O2D
18	6	304	CLA	CHA-CBD-CGD-O1D
18	6	304	CLA	CHA-CBD-CGD-O2D
18	6	310	CLA	C1A-C2A-CAA-CBA
18	6	310	CLA	C3A-C2A-CAA-CBA
18	6	313	CLA	CAD-CBD-CGD-O1D
18	6	315	CLA	C1A-C2A-CAA-CBA
18	6	315	CLA	C3A-C2A-CAA-CBA
21	1	601	CHL	O2A-C1-C2-C3
21	1	601	CHL	C2-C3-C5-C6
21	1	601	CHL	C4-C3-C5-C6
21	1	606	CHL	C1A-C2A-CAA-CBA
21	1	606	CHL	CHA-CBD-CGD-O1D
21	1	606	CHL	CHA-CBD-CGD-O2D
21	3	306	CHL	C1A-C2A-CAA-CBA
21	7	606	CHL	C1A-C2A-CAA-CBA
21	8	606	CHL	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	Z	605	CHL	C1A-C2A-CAA-CBA
21	Z	605	CHL	CHA-CBD-CGD-O1D
21	Z	605	CHL	CHA-CBD-CGD-O2D
21	5	606	CHL	CHA-CBD-CGD-O1D
21	5	607	CHL	C1A-C2A-CAA-CBA
21	5	607	CHL	C3A-C2A-CAA-CBA
21	5	616	CHL	CHA-CBD-CGD-O1D
21	6	307	CHL	C1A-C2A-CAA-CBA
21	6	307	CHL	C3A-C2A-CAA-CBA
21	6	316	CHL	C1A-C2A-CAA-CBA
18	3	310	CLA	C2A-CAA-CBA-CGA
18	5	617	CLA	C2A-CAA-CBA-CGA
18	4	603	CLA	C2C-C3C-CAC-CBC
18	3	313	CLA	C2A-CAA-CBA-CGA
21	4	605	CHL	C2A-CAA-CBA-CGA
19	A	842	PQN	C24-C23-C25-C26
19	B	844	PQN	C24-C23-C25-C26
18	A	823	CLA	C2-C1-O2A-CGA
18	6	311	CLA	C2A-CAA-CBA-CGA
19	B	844	PQN	C20-C21-C22-C23
18	7	604	CLA	C2A-CAA-CBA-CGA
18	B	806	CLA	C3A-C2A-CAA-CBA
18	6	311	CLA	C3A-C2A-CAA-CBA
19	A	842	PQN	C22-C23-C25-C26
18	B	822	CLA	C1A-C2A-CAA-CBA
18	F	302	CLA	C1A-C2A-CAA-CBA
18	5	603	CLA	C2C-C3C-CAC-CBC
18	A	806	CLA	C3A-C2A-CAA-CBA
18	B	805	CLA	C3A-C2A-CAA-CBA
18	B	811	CLA	C3A-C2A-CAA-CBA
18	1	611	CLA	C3A-C2A-CAA-CBA
18	Z	610	CLA	C3A-C2A-CAA-CBA
21	6	316	CHL	C3A-C2A-CAA-CBA
18	A	843	CLA	C2A-CAA-CBA-CGA
18	B	807	CLA	C2-C3-C5-C6
19	A	842	PQN	C19-C18-C20-C21
18	6	303	CLA	C2C-C3C-CAC-CBC
18	3	313	CLA	C3A-C2A-CAA-CBA
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	807	CLA	C1A-C2A-CAA-CBA
18	A	820	CLA	C1A-C2A-CAA-CBA
18	A	826	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	A	834	CLA	C1A-C2A-CAA-CBA
18	A	838	CLA	C1A-C2A-CAA-CBA
18	B	816	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C1A-C2A-CAA-CBA
18	B	821	CLA	C1A-C2A-CAA-CBA
18	B	824	CLA	C1A-C2A-CAA-CBA
18	B	834	CLA	C1A-C2A-CAA-CBA
18	1	613	CLA	C1A-C2A-CAA-CBA
18	3	301	CLA	C1A-C2A-CAA-CBA
18	7	607	CLA	C1A-C2A-CAA-CBA
18	7	614	CLA	C1A-C2A-CAA-CBA
18	8	613	CLA	C1A-C2A-CAA-CBA
18	Z	612	CLA	C1A-C2A-CAA-CBA
18	4	611	CLA	C1A-C2A-CAA-CBA
18	5	602	CLA	C1A-C2A-CAA-CBA
18	5	608	CLA	C1A-C2A-CAA-CBA
18	5	613	CLA	C1A-C2A-CAA-CBA
18	5	614	CLA	C1A-C2A-CAA-CBA
18	6	302	CLA	C1A-C2A-CAA-CBA
18	6	313	CLA	C1A-C2A-CAA-CBA
21	5	606	CHL	C1A-C2A-CAA-CBA
21	4	604	CHL	C4C-C3C-CAC-CBC
18	4	603	CLA	C4C-C3C-CAC-CBC
19	A	842	PQN	C17-C18-C20-C21
18	B	807	CLA	C5-C6-C7-C8
18	A	811	CLA	CAD-CBD-CGD-O2D
18	A	816	CLA	CAD-CBD-CGD-O2D
18	A	827	CLA	CAD-CBD-CGD-O2D
18	A	835	CLA	CAD-CBD-CGD-O2D
18	A	840	CLA	CAD-CBD-CGD-O2D
18	A	841	CLA	CAD-CBD-CGD-O2D
18	B	813	CLA	CAD-CBD-CGD-O2D
18	B	831	CLA	CAD-CBD-CGD-O2D
18	B	842	CLA	CAD-CBD-CGD-O2D
18	3	304	CLA	CAD-CBD-CGD-O2D
18	3	307	CLA	CAD-CBD-CGD-O2D
18	7	607	CLA	CAD-CBD-CGD-O2D
18	8	602	CLA	CAD-CBD-CGD-O2D
18	8	607	CLA	CAD-CBD-CGD-O2D
18	8	609	CLA	CAD-CBD-CGD-O2D
18	4	611	CLA	CAD-CBD-CGD-O2D
18	5	611	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	5	617	CLA	CAD-CBD-CGD-O2D
18	6	311	CLA	CAD-CBD-CGD-O2D
19	A	842	PQN	C18-C20-C21-C22
18	4	601	CLA	C2C-C3C-CAC-CBC
18	A	803	CLA	CHA-CBD-CGD-O2D
18	A	806	CLA	CHA-CBD-CGD-O1D
18	A	806	CLA	CHA-CBD-CGD-O2D
18	A	808	CLA	CHA-CBD-CGD-O1D
18	A	808	CLA	CHA-CBD-CGD-O2D
18	A	813	CLA	CHA-CBD-CGD-O1D
18	A	817	CLA	CHA-CBD-CGD-O1D
18	A	817	CLA	CHA-CBD-CGD-O2D
18	B	807	CLA	CHA-CBD-CGD-O1D
18	B	810	CLA	CHA-CBD-CGD-O1D
18	B	810	CLA	CHA-CBD-CGD-O2D
18	B	815	CLA	CHA-CBD-CGD-O1D
18	B	815	CLA	CHA-CBD-CGD-O2D
18	B	823	CLA	CHA-CBD-CGD-O1D
18	B	823	CLA	CHA-CBD-CGD-O2D
18	B	825	CLA	CHA-CBD-CGD-O1D
18	B	825	CLA	CHA-CBD-CGD-O2D
18	B	832	CLA	CHA-CBD-CGD-O1D
18	B	832	CLA	CHA-CBD-CGD-O2D
18	B	839	CLA	CHA-CBD-CGD-O1D
18	B	839	CLA	CHA-CBD-CGD-O2D
18	J	101	CLA	CHA-CBD-CGD-O1D
18	7	613	CLA	CHA-CBD-CGD-O1D
18	7	613	CLA	CHA-CBD-CGD-O2D
18	8	601	CLA	CHA-CBD-CGD-O1D
18	6	301	CLA	CHA-CBD-CGD-O1D
18	6	301	CLA	CHA-CBD-CGD-O2D
18	6	302	CLA	CHA-CBD-CGD-O1D
21	5	606	CHL	CHA-CBD-CGD-O2D
21	5	616	CHL	CHA-CBD-CGD-O2D
18	B	831	CLA	C2C-C3C-CAC-CBC
18	B	802	CLA	C1A-C2A-CAA-CBA
18	7	608	CLA	C1A-C2A-CAA-CBA
18	7	613	CLA	C1A-C2A-CAA-CBA
18	6	309	CLA	C1A-C2A-CAA-CBA
18	6	311	CLA	C1A-C2A-CAA-CBA
18	Z	604	CLA	C2C-C3C-CAC-CBC
19	A	842	PQN	C3-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	B	844	PQN	C3-C11-C12-C13
18	A	822	CLA	C2C-C3C-CAC-CBC
18	1	605	CLA	C2C-C3C-CAC-CBC
18	A	805	CLA	CAD-CBD-CGD-O1D
18	A	813	CLA	CAD-CBD-CGD-O1D
18	A	825	CLA	CAD-CBD-CGD-O1D
18	A	838	CLA	CAD-CBD-CGD-O1D
18	B	839	CLA	CAD-CBD-CGD-O1D
18	8	601	CLA	CAD-CBD-CGD-O1D
18	6	301	CLA	CAD-CBD-CGD-O1D
18	Z	604	CLA	C2A-CAA-CBA-CGA
18	B	815	CLA	C3A-C2A-CAA-CBA
18	7	601	CLA	C3A-C2A-CAA-CBA
18	5	617	CLA	C3A-C2A-CAA-CBA
18	6	301	CLA	C3A-C2A-CAA-CBA
18	8	612	CLA	C2C-C3C-CAC-CBC
18	7	608	CLA	CAA-CBA-CGA-O2A
18	6	312	CLA	C2C-C3C-CAC-CBC
18	B	838	CLA	C2C-C3C-CAC-CBC
18	Z	604	CLA	C4C-C3C-CAC-CBC
18	1	604	CLA	C2C-C3C-CAC-CBC
18	1	605	CLA	C4C-C3C-CAC-CBC
18	Z	603	CLA	C2C-C3C-CAC-CBC
19	B	844	PQN	C14-C13-C15-C16
18	7	601	CLA	C2C-C3C-CAC-CBC
18	6	317	CLA	C2A-CAA-CBA-CGA
18	A	824	CLA	C2C-C3C-CAC-CBC
18	7	601	CLA	C4C-C3C-CAC-CBC
21	4	605	CHL	CAA-CBA-CGA-O1A
21	4	605	CHL	CAA-CBA-CGA-O2A
18	3	302	CLA	C2C-C3C-CAC-CBC
18	A	824	CLA	C4C-C3C-CAC-CBC
18	3	311	CLA	CAA-CBA-CGA-O2A
18	5	617	CLA	C1A-C2A-CAA-CBA
18	F	302	CLA	C6-C7-C8-C10
18	5	615	CLA	C2A-CAA-CBA-CGA
18	3	311	CLA	CAA-CBA-CGA-O1A
18	6	312	CLA	CAA-CBA-CGA-O2A
18	F	301	CLA	CAA-CBA-CGA-O1A
18	A	807	CLA	C2C-C3C-CAC-CBC
18	5	617	CLA	C2C-C3C-CAC-CBC
18	6	311	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	B	822	CLA	C2C-C3C-CAC-CBC
18	6	311	CLA	CAA-CBA-CGA-O2A
18	A	836	CLA	C2C-C3C-CAC-CBC
18	6	312	CLA	CAA-CBA-CGA-O1A
18	A	822	CLA	C1A-C2A-CAA-CBA
18	B	843	CLA	C1A-C2A-CAA-CBA
18	8	601	CLA	C1A-C2A-CAA-CBA
18	7	612	CLA	CAA-CBA-CGA-O2A
18	6	309	CLA	CAA-CBA-CGA-O2A
18	B	830	CLA	CAA-CBA-CGA-O2A
18	5	610	CLA	C2A-CAA-CBA-CGA
19	B	844	PQN	C12-C13-C15-C16
18	Z	611	CLA	CAA-CBA-CGA-O2A
18	B	830	CLA	CAA-CBA-CGA-O1A
18	7	608	CLA	C3A-C2A-CAA-CBA
18	3	312	CLA	CAA-CBA-CGA-O2A
18	7	612	CLA	CAA-CBA-CGA-O1A
18	A	812	CLA	CAD-CBD-CGD-O2D
18	A	817	CLA	CAD-CBD-CGD-O2D
18	A	823	CLA	CAD-CBD-CGD-O2D
18	A	837	CLA	CAD-CBD-CGD-O2D
18	B	824	CLA	CAD-CBD-CGD-O2D
18	B	826	CLA	CAD-CBD-CGD-O2D
18	B	828	CLA	CAD-CBD-CGD-O2D
18	B	834	CLA	CAD-CBD-CGD-O2D
18	B	835	CLA	CAD-CBD-CGD-O2D
18	B	836	CLA	CAD-CBD-CGD-O2D
18	B	838	CLA	CAD-CBD-CGD-O2D
18	B	840	CLA	CAD-CBD-CGD-O2D
18	B	841	CLA	CAD-CBD-CGD-O2D
18	1	605	CLA	CAD-CBD-CGD-O2D
18	1	609	CLA	CAD-CBD-CGD-O2D
18	3	301	CLA	CAD-CBD-CGD-O2D
18	3	310	CLA	CAD-CBD-CGD-O2D
18	7	602	CLA	CAD-CBD-CGD-O2D
18	Z	604	CLA	CAD-CBD-CGD-O2D
18	Z	608	CLA	CAD-CBD-CGD-O2D
18	4	601	CLA	CAD-CBD-CGD-O2D
18	4	609	CLA	CAD-CBD-CGD-O2D
18	6	313	CLA	CAD-CBD-CGD-O2D
18	6	317	CLA	CAD-CBD-CGD-O2D
18	5	602	CLA	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	4	603	CLA	CAA-CBA-CGA-O2A
18	6	309	CLA	CAA-CBA-CGA-O1A
18	5	603	CLA	CAA-CBA-CGA-O2A
18	F	301	CLA	CAA-CBA-CGA-O2A
17	A	801	CL0	CHA-CBD-CGD-O1D
17	A	801	CL0	CHA-CBD-CGD-O2D
18	A	805	CLA	CHA-CBD-CGD-O1D
18	A	813	CLA	CHA-CBD-CGD-O2D
18	A	814	CLA	CHA-CBD-CGD-O1D
18	A	814	CLA	CHA-CBD-CGD-O2D
18	A	820	CLA	CHA-CBD-CGD-O1D
18	A	820	CLA	CHA-CBD-CGD-O2D
18	A	822	CLA	CHA-CBD-CGD-O1D
18	A	822	CLA	CHA-CBD-CGD-O2D
18	A	825	CLA	CHA-CBD-CGD-O1D
18	A	830	CLA	CHA-CBD-CGD-O2D
18	A	831	CLA	CHA-CBD-CGD-O1D
18	A	831	CLA	CHA-CBD-CGD-O2D
18	A	836	CLA	CHA-CBD-CGD-O1D
18	A	836	CLA	CHA-CBD-CGD-O2D
18	A	839	CLA	CHA-CBD-CGD-O1D
18	A	839	CLA	CHA-CBD-CGD-O2D
18	A	845	CLA	CHA-CBD-CGD-O2D
18	B	806	CLA	CHA-CBD-CGD-O1D
18	B	806	CLA	CHA-CBD-CGD-O2D
18	B	812	CLA	CHA-CBD-CGD-O1D
18	B	812	CLA	CHA-CBD-CGD-O2D
18	B	817	CLA	CHA-CBD-CGD-O1D
18	B	817	CLA	CHA-CBD-CGD-O2D
18	B	822	CLA	CHA-CBD-CGD-O1D
18	B	822	CLA	CHA-CBD-CGD-O2D
18	B	843	CLA	CHA-CBD-CGD-O2D
18	J	101	CLA	CHA-CBD-CGD-O2D
18	1	602	CLA	CHA-CBD-CGD-O2D
18	1	603	CLA	CHA-CBD-CGD-O1D
18	1	603	CLA	CHA-CBD-CGD-O2D
18	7	601	CLA	CHA-CBD-CGD-O1D
18	7	601	CLA	CHA-CBD-CGD-O2D
18	7	612	CLA	CHA-CBD-CGD-O1D
18	7	612	CLA	CHA-CBD-CGD-O2D
18	8	601	CLA	CHA-CBD-CGD-O2D
18	8	605	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	8	605	CLA	CHA-CBD-CGD-O2D
18	8	612	CLA	CHA-CBD-CGD-O1D
18	8	615	CLA	CHA-CBD-CGD-O1D
18	8	615	CLA	CHA-CBD-CGD-O2D
18	Z	602	CLA	CHA-CBD-CGD-O2D
18	4	606	CLA	CHA-CBD-CGD-O1D
18	4	606	CLA	CHA-CBD-CGD-O2D
18	5	602	CLA	CHA-CBD-CGD-O1D
18	5	602	CLA	CHA-CBD-CGD-O2D
18	5	603	CLA	CHA-CBD-CGD-O2D
18	5	604	CLA	CHA-CBD-CGD-O2D
18	6	303	CLA	CHA-CBD-CGD-O2D
18	6	312	CLA	CHA-CBD-CGD-O1D
18	6	312	CLA	CHA-CBD-CGD-O2D
18	6	314	CLA	CHA-CBD-CGD-O1D
18	6	314	CLA	CHA-CBD-CGD-O2D
21	4	605	CHL	CHA-CBD-CGD-O2D
18	3	312	CLA	CAA-CBA-CGA-O1A
18	Z	611	CLA	CAA-CBA-CGA-O1A
18	5	617	CLA	CAA-CBA-CGA-O2A
18	6	303	CLA	CAA-CBA-CGA-O2A
18	A	843	CLA	CAA-CBA-CGA-O2A
18	3	310	CLA	CAA-CBA-CGA-O2A
18	A	813	CLA	C4C-C3C-CAC-CBC
18	A	813	CLA	C2C-C3C-CAC-CBC
18	1	614	CLA	C1A-C2A-CAA-CBA
18	3	310	CLA	C1A-C2A-CAA-CBA
18	4	603	CLA	CAA-CBA-CGA-O1A
18	5	603	CLA	CAA-CBA-CGA-O1A
18	6	303	CLA	CAA-CBA-CGA-O1A
18	A	843	CLA	CAA-CBA-CGA-O1A
18	5	617	CLA	CAA-CBA-CGA-O1A
18	B	807	CLA	C6-C7-C8-C9
18	B	809	CLA	CAD-CBD-CGD-O1D
18	7	604	CLA	CAD-CBD-CGD-O1D
18	7	605	CLA	CAD-CBD-CGD-O1D
18	5	617	CLA	CAD-CBD-CGD-O1D
21	1	601	CHL	CAD-CBD-CGD-O1D
21	Z	601	CHL	CAD-CBD-CGD-O1D
18	8	612	CLA	CAA-CBA-CGA-O2A
18	F	302	CLA	C6-C7-C8-C9
18	B	833	CLA	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	1	612	CLA	CAA-CBA-CGA-O2A
19	A	842	PQN	C23-C25-C26-C27
18	B	819	CLA	C3A-C2A-CAA-CBA
18	1	608	CLA	C3A-C2A-CAA-CBA
18	Z	607	CLA	C3A-C2A-CAA-CBA
18	3	310	CLA	CAA-CBA-CGA-O1A
18	A	817	CLA	CAA-CBA-CGA-O2A
18	5	610	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

177 monomers are involved in 352 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3	304	CLA	2	0
18	Z	604	CLA	4	0
21	6	306	CHL	1	0
18	A	845	CLA	11	0
18	B	823	CLA	3	0
18	B	815	CLA	4	0
18	Z	602	CLA	1	0
21	8	606	CHL	3	0
18	A	809	CLA	3	0
18	A	836	CLA	4	0
18	A	807	CLA	3	0
18	A	841	CLA	2	0
18	F	301	CLA	1	0
18	1	612	CLA	6	0
18	B	827	CLA	1	0
18	8	608	CLA	5	0
18	6	309	CLA	2	0
18	6	312	CLA	4	0
18	A	812	CLA	3	0
18	A	826	CLA	1	0
18	A	818	CLA	2	0
18	A	806	CLA	3	0
18	8	612	CLA	4	0
18	6	311	CLA	1	0
18	A	815	CLA	3	0
18	7	613	CLA	2	0
21	1	601	CHL	3	0
18	Z	612	CLA	4	0
18	B	831	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	803	CLA	2	0
18	A	814	CLA	3	0
18	B	817	CLA	2	0
18	A	817	CLA	4	0
18	3	313	CLA	5	0
18	A	816	CLA	2	0
18	3	302	CLA	3	0
18	B	809	CLA	2	0
18	B	836	CLA	1	0
19	A	842	PQN	6	0
18	B	835	CLA	3	0
18	B	826	CLA	3	0
18	B	812	CLA	1	0
18	7	614	CLA	1	0
18	8	611	CLA	1	0
18	A	823	CLA	3	0
21	5	616	CHL	1	0
21	4	604	CHL	4	0
18	6	308	CLA	1	0
18	A	813	CLA	3	0
18	3	314	CLA	3	0
18	A	808	CLA	3	0
18	8	602	CLA	1	0
18	6	314	CLA	1	0
21	6	307	CHL	1	0
21	1	606	CHL	2	0
21	4	605	CHL	1	0
18	B	829	CLA	3	0
18	7	605	CLA	4	0
18	5	601	CLA	1	0
18	B	816	CLA	4	0
18	7	608	CLA	3	0
18	A	819	CLA	1	0
18	A	802	CLA	3	0
18	8	605	CLA	3	0
18	5	608	CLA	1	0
18	A	843	CLA	7	0
21	Z	605	CHL	2	0
18	A	837	CLA	1	0
20	C	102	SF4	1	0
18	5	609	CLA	1	0
18	A	835	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	818	CLA	1	0
18	B	801	CLA	1	0
18	B	840	CLA	2	0
18	3	303	CLA	4	0
18	8	604	CLA	1	0
18	8	614	CLA	1	0
18	8	601	CLA	2	0
18	3	312	CLA	2	0
18	1	611	CLA	1	0
18	A	820	CLA	1	0
18	5	612	CLA	3	0
18	A	834	CLA	2	0
18	7	609	CLA	1	0
18	B	811	CLA	4	0
18	B	837	CLA	2	0
18	A	833	CLA	1	0
19	B	844	PQN	5	0
18	B	802	CLA	5	0
18	8	615	CLA	2	0
18	A	824	CLA	1	0
18	3	305	CLA	2	0
18	Z	610	CLA	1	0
18	Z	611	CLA	5	0
18	B	832	CLA	3	0
18	B	822	CLA	2	0
18	5	611	CLA	5	0
18	1	614	CLA	1	0
18	4	610	CLA	4	0
18	5	604	CLA	1	0
18	B	805	CLA	1	0
18	3	308	CLA	2	0
18	1	605	CLA	4	0
18	6	313	CLA	3	0
18	B	808	CLA	3	0
18	5	602	CLA	2	0
18	4	602	CLA	2	0
20	B	803	SF4	1	0
18	B	824	CLA	4	0
18	8	609	CLA	2	0
18	B	834	CLA	3	0
21	5	606	CHL	1	0
18	B	825	CLA	3	0

Continued on next page...

Continued from previous page...

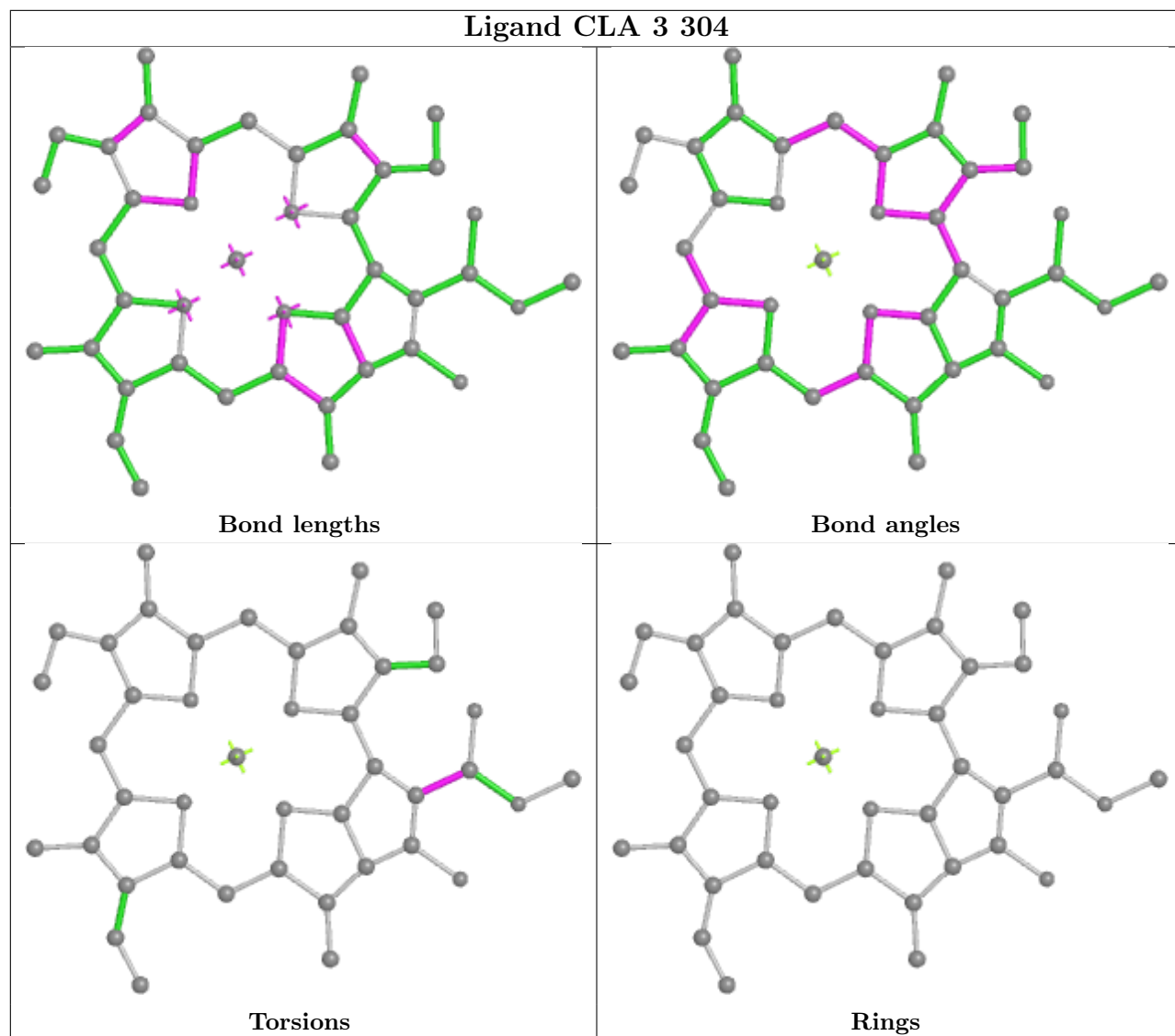
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	804	CLA	1	0
18	6	315	CLA	1	0
18	7	603	CLA	1	0
18	B	821	CLA	2	0
21	6	305	CHL	2	0
18	5	613	CLA	3	0
18	A	828	CLA	2	0
18	3	311	CLA	2	0
18	6	304	CLA	1	0
18	4	606	CLA	1	0
18	1	602	CLA	1	0
18	A	844	CLA	5	0
18	A	827	CLA	3	0
18	B	814	CLA	6	0
18	1	604	CLA	4	0
18	5	605	CLA	2	0
18	Z	603	CLA	6	0
18	1	613	CLA	3	0
18	A	822	CLA	3	0
18	B	819	CLA	2	0
18	A	805	CLA	2	0
18	8	603	CLA	2	0
18	A	838	CLA	4	0
18	A	811	CLA	1	0
18	B	843	CLA	4	0
20	C	101	SF4	2	0
18	B	839	CLA	2	0
18	5	610	CLA	4	0
18	B	804	CLA	7	0
18	4	611	CLA	3	0
18	B	830	CLA	3	0
18	A	825	CLA	1	0
18	6	301	CLA	13	0
18	B	813	CLA	2	0
18	7	612	CLA	4	0
18	4	603	CLA	2	0
18	Z	608	CLA	4	0
21	7	606	CHL	1	0
18	1	608	CLA	2	0
18	B	842	CLA	6	0
18	B	841	CLA	2	0
18	3	307	CLA	5	0

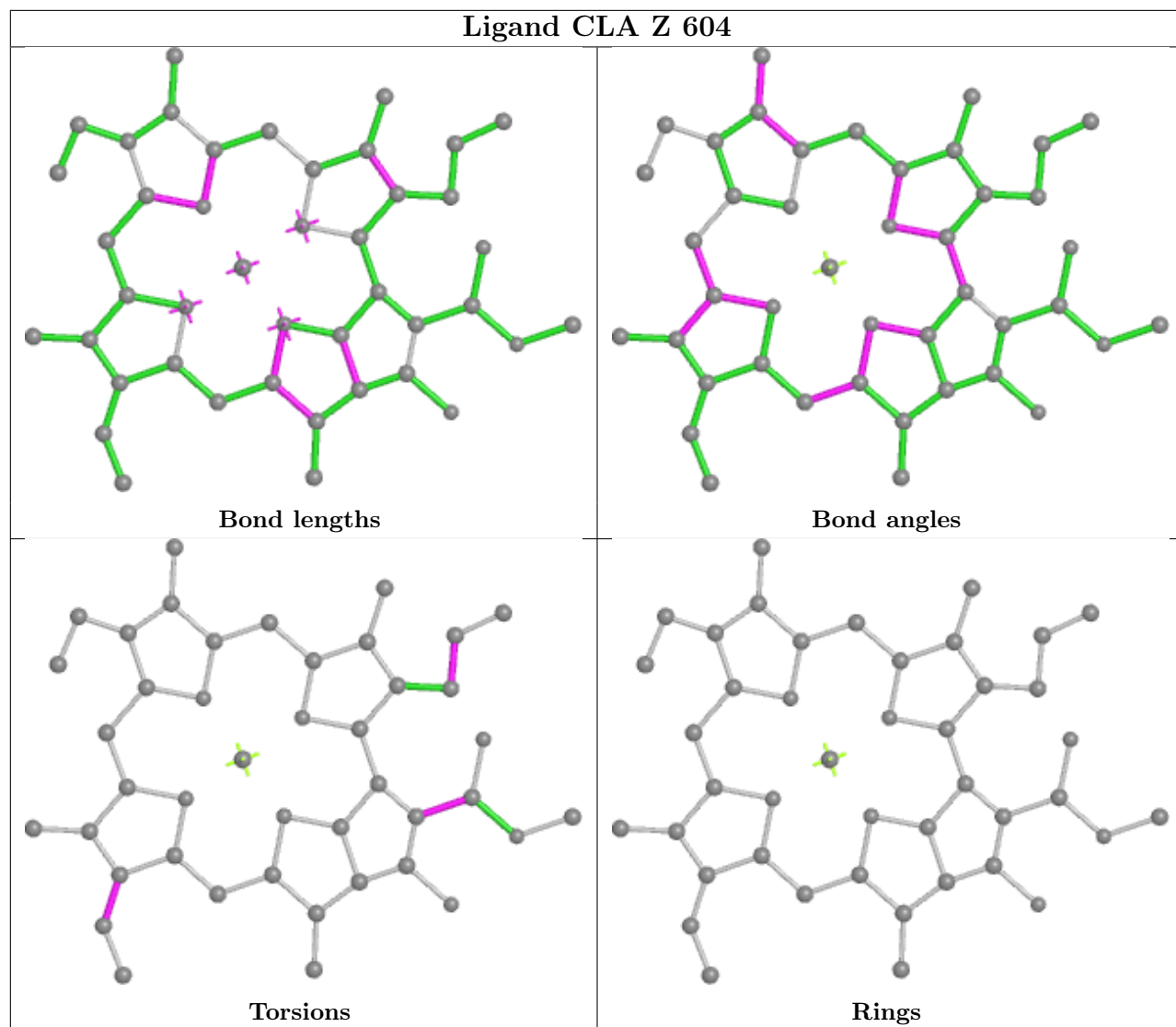
Continued on next page...

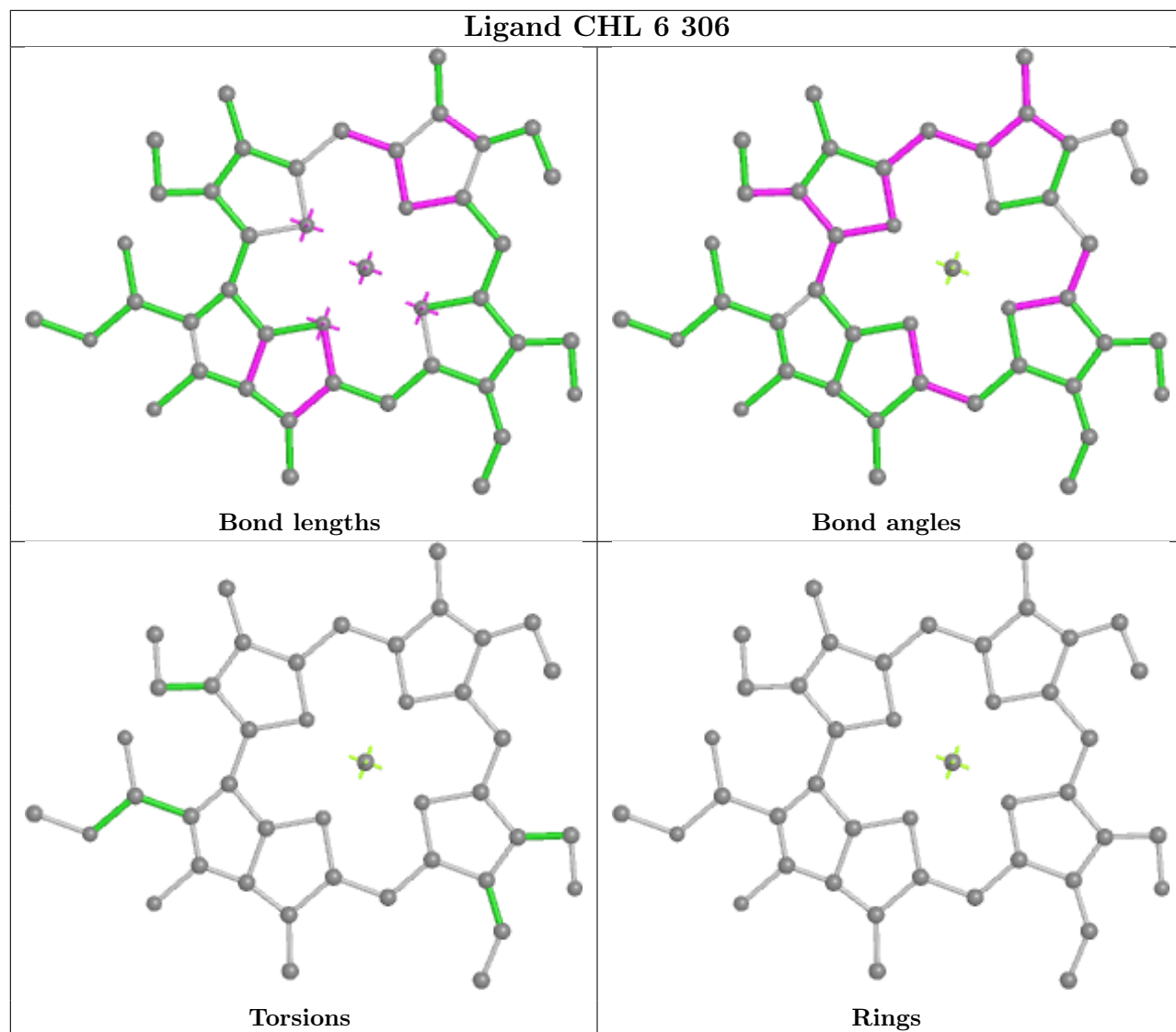
Continued from previous page...

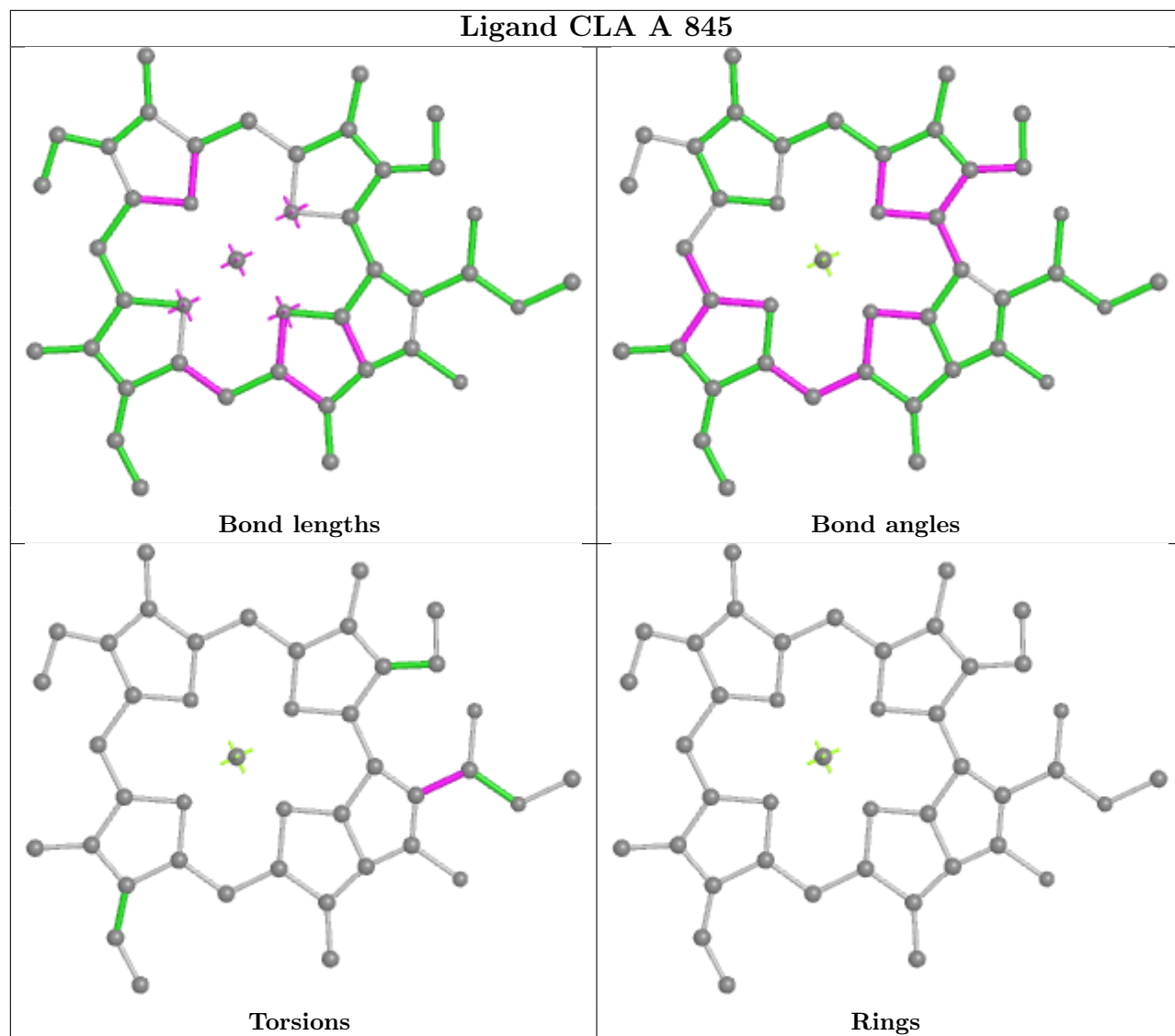
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	1	603	CLA	2	0
18	B	833	CLA	2	0
18	F	302	CLA	11	0
18	4	607	CLA	2	0
18	5	614	CLA	2	0
18	A	830	CLA	2	0
21	Z	601	CHL	1	0
21	5	607	CHL	3	0
18	1	609	CLA	4	0
18	J	101	CLA	2	0
18	8	613	CLA	3	0
18	Z	607	CLA	2	0
18	B	807	CLA	1	0
18	5	615	CLA	1	0
18	B	810	CLA	3	0
18	7	604	CLA	7	0
17	A	801	CL0	9	0
18	7	601	CLA	2	0
18	B	806	CLA	3	0
18	7	602	CLA	3	0
18	A	839	CLA	1	0
18	6	317	CLA	2	0

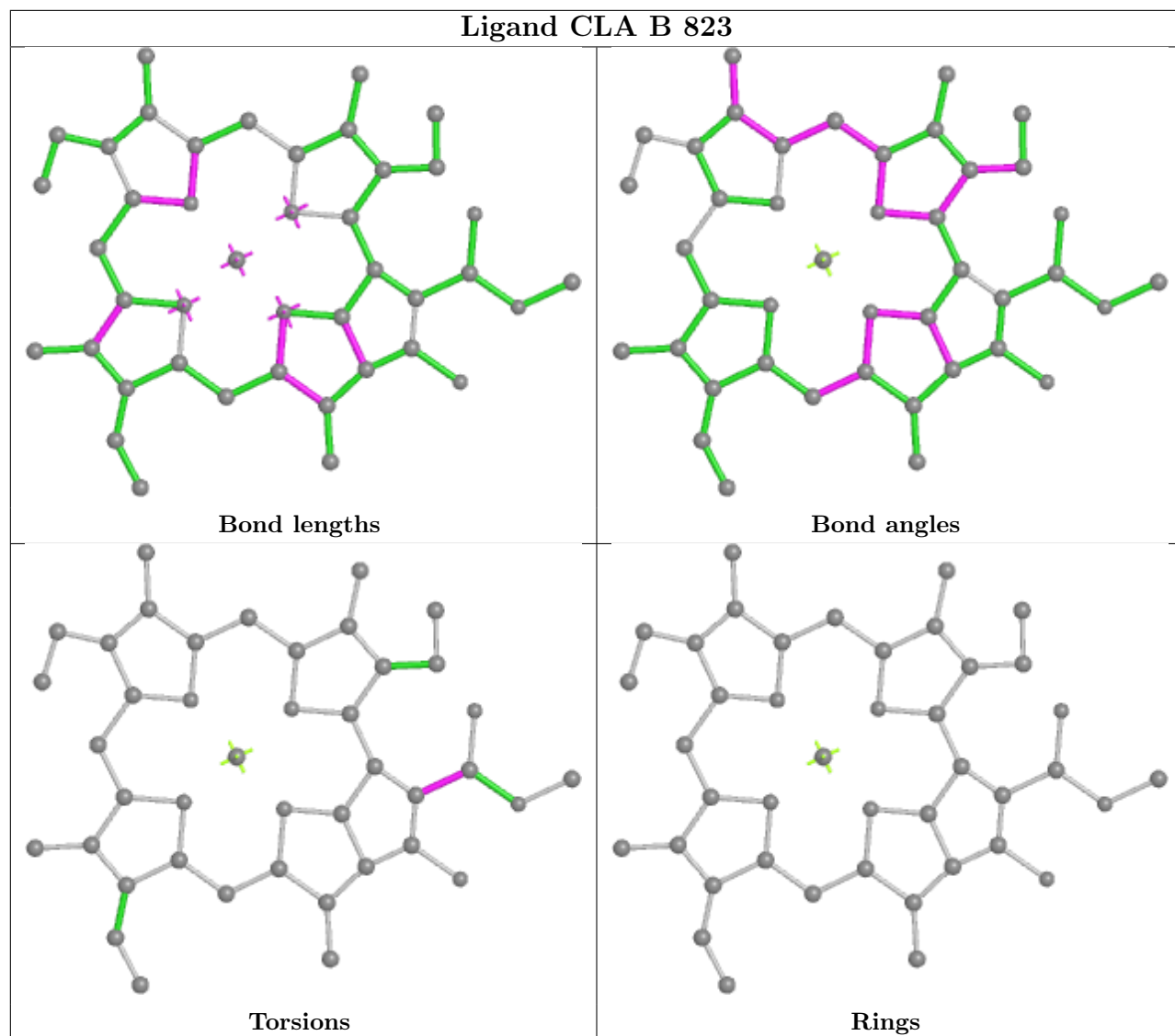
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

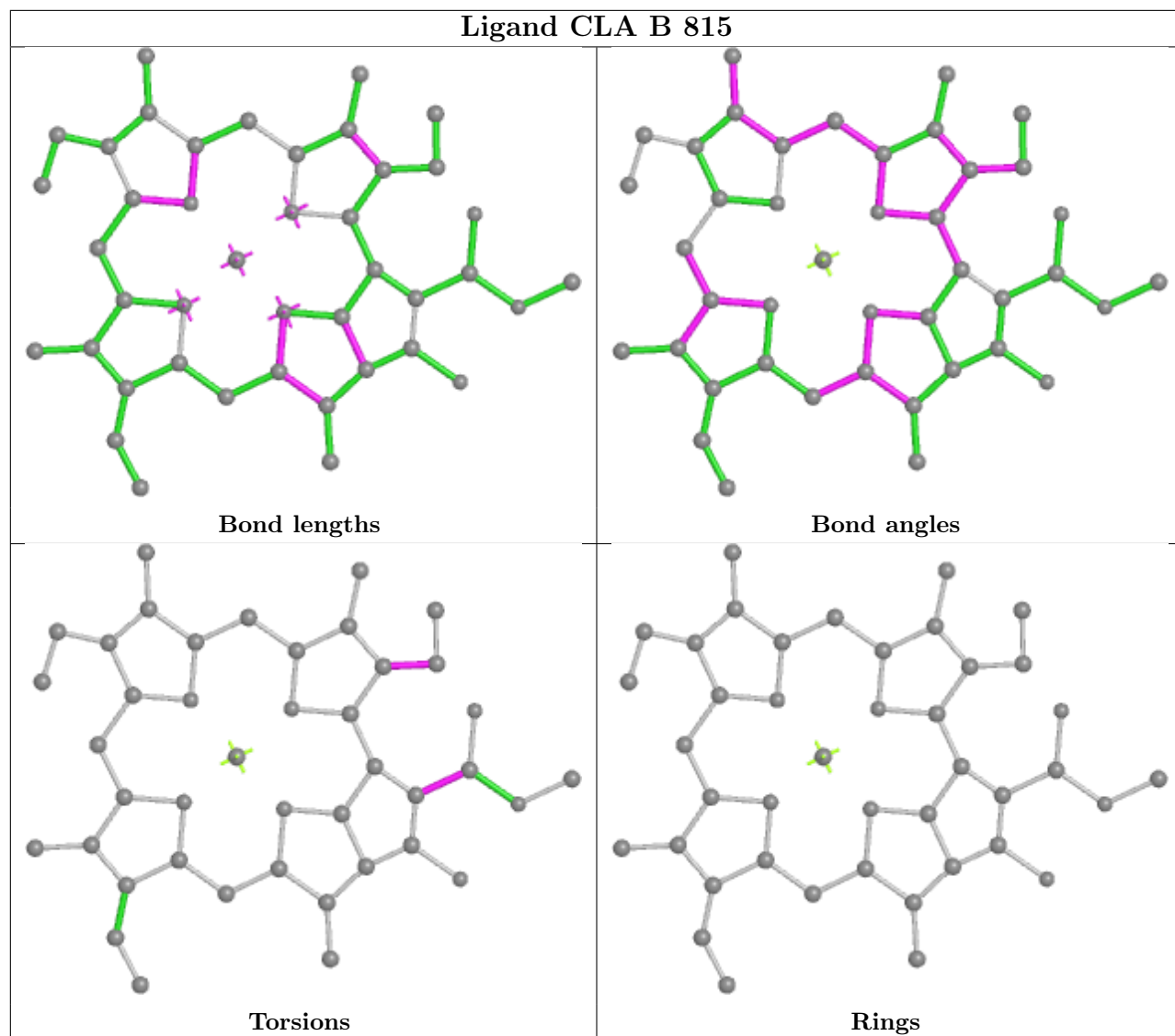


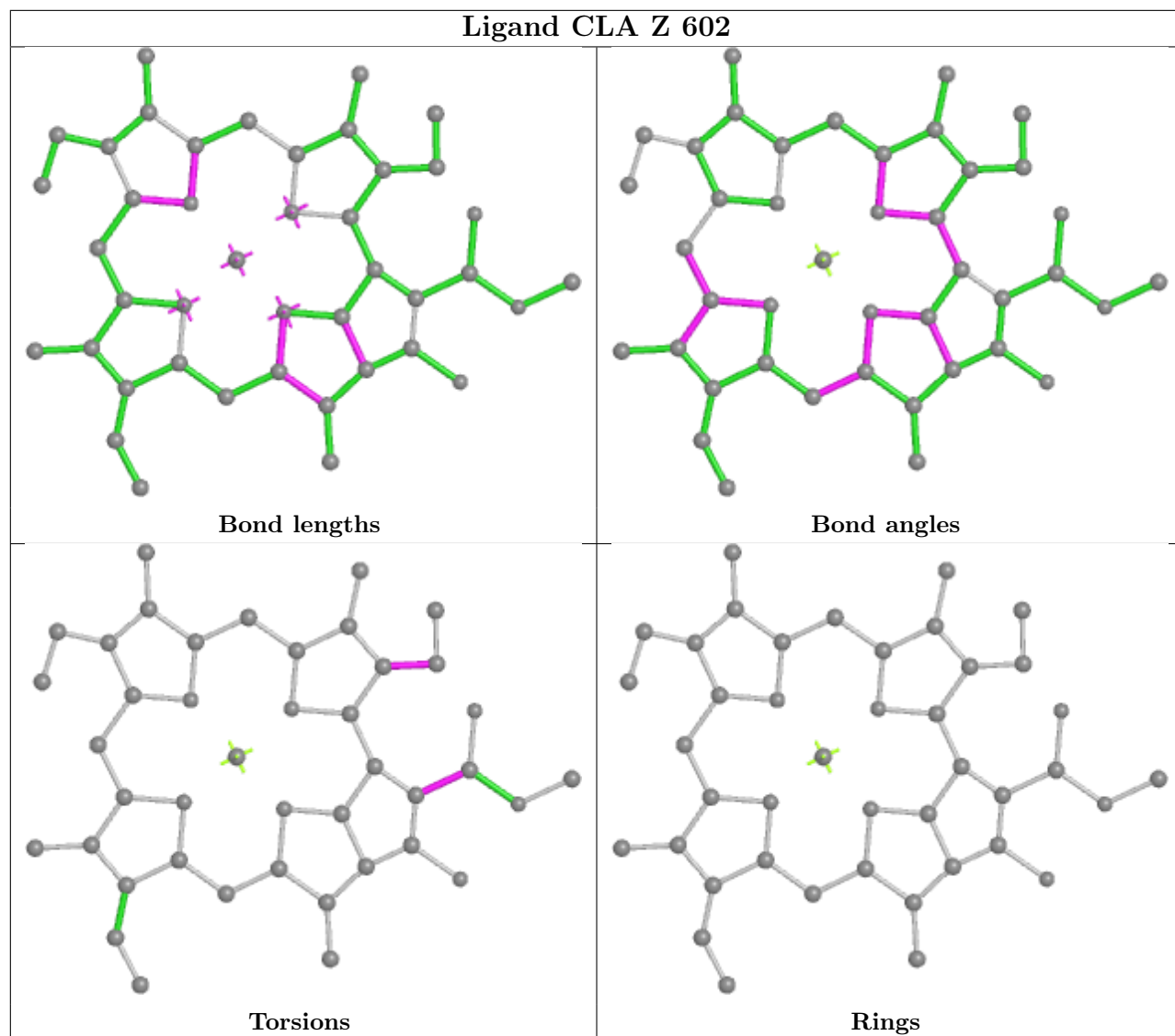


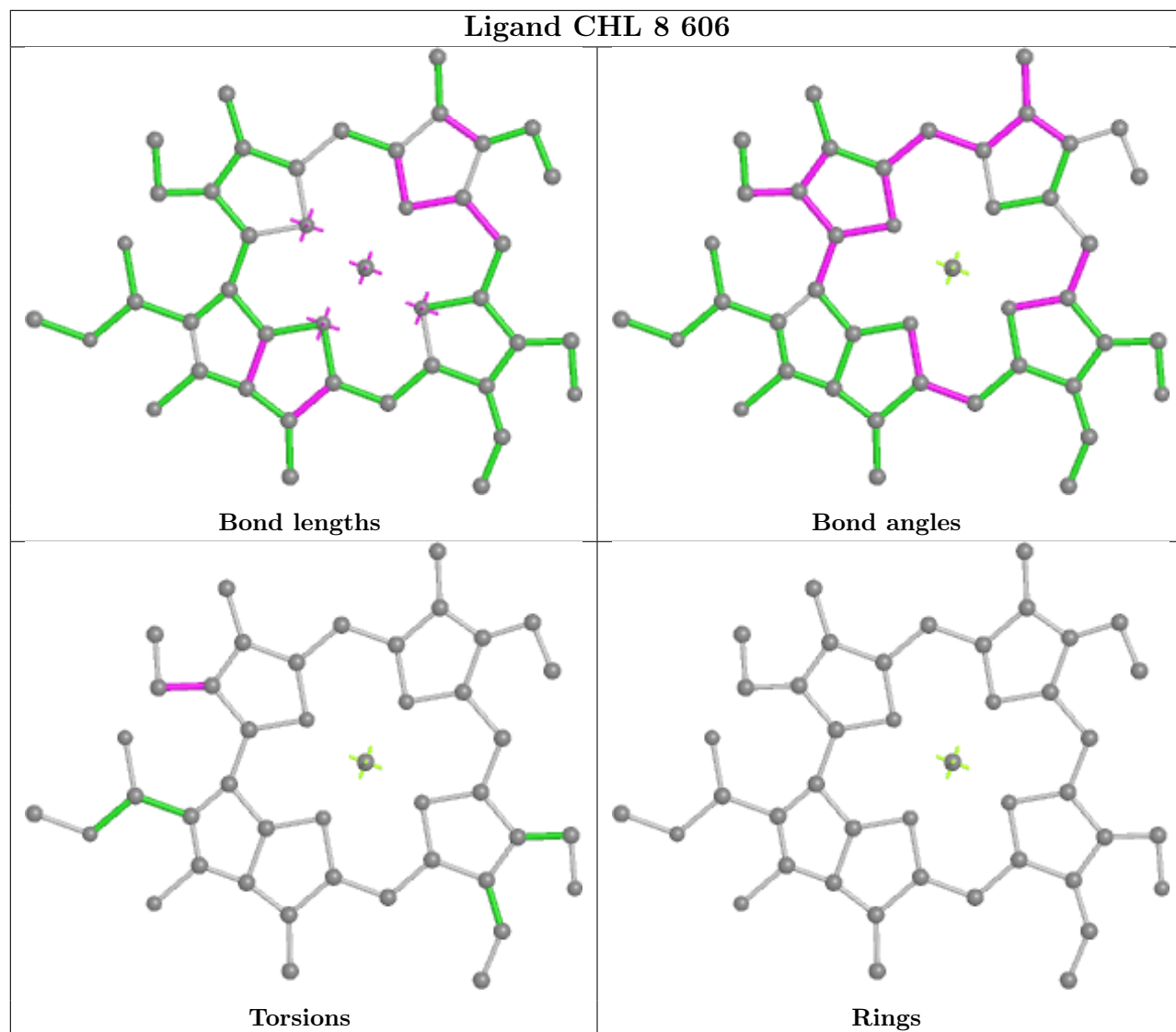


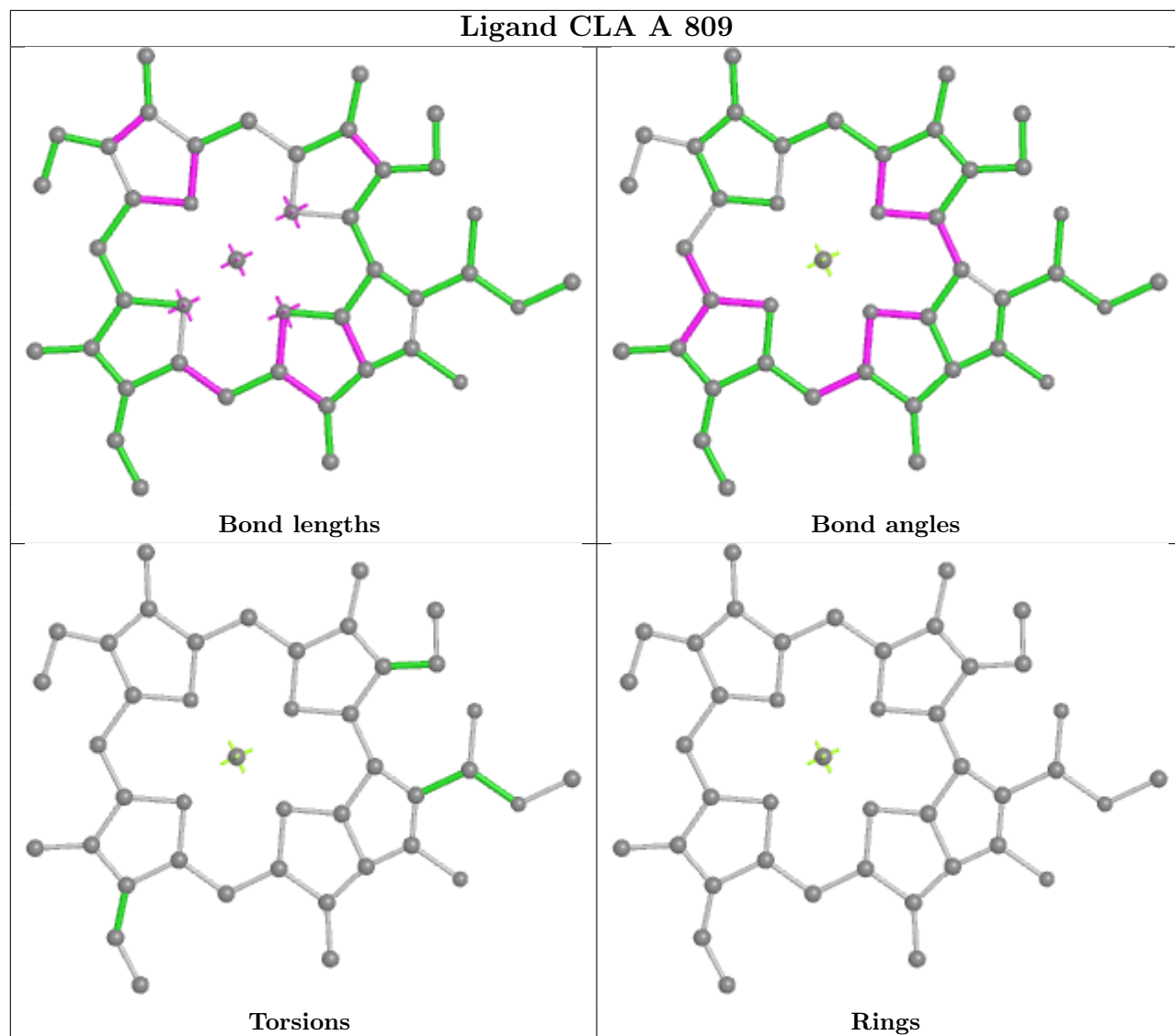


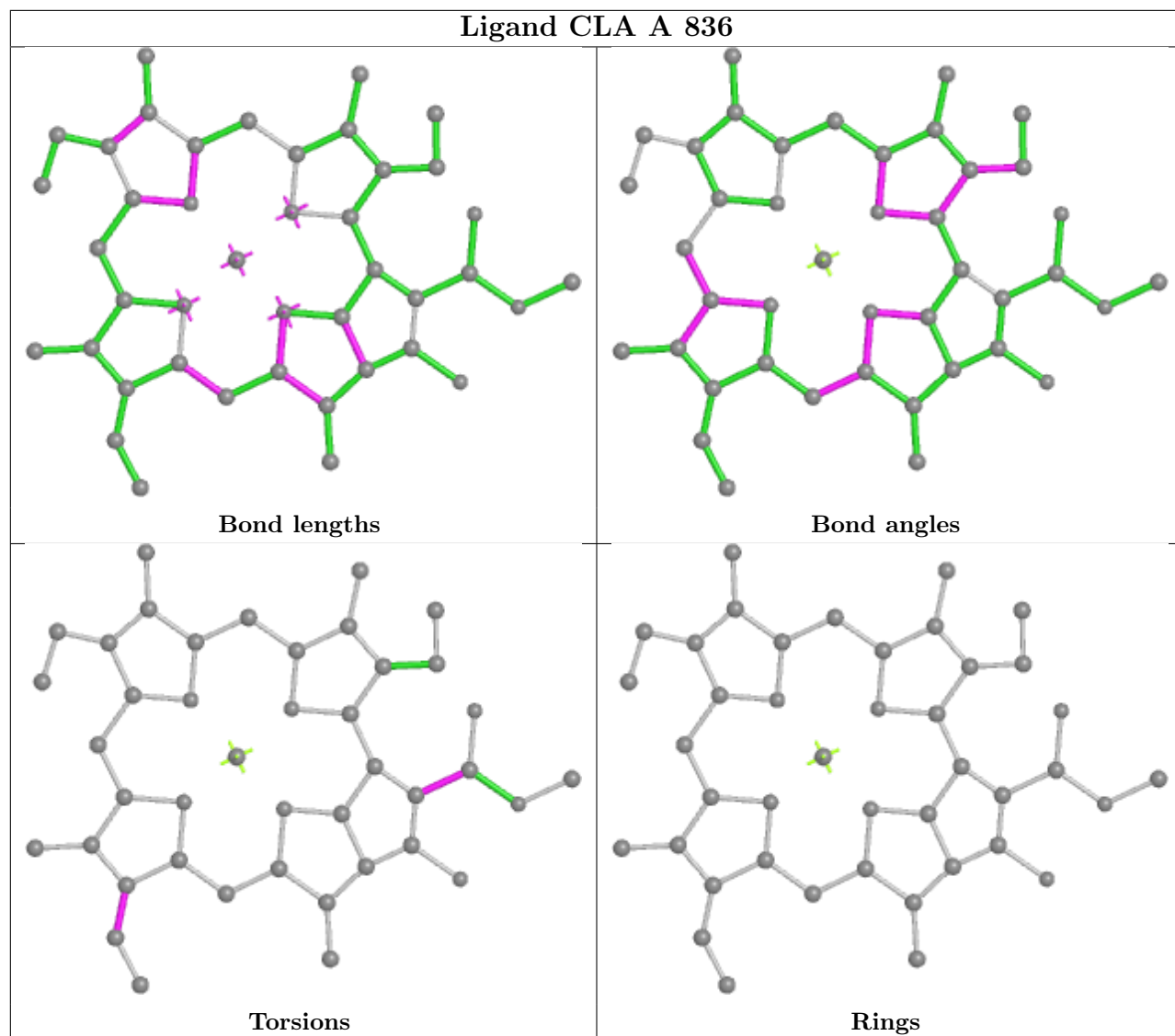


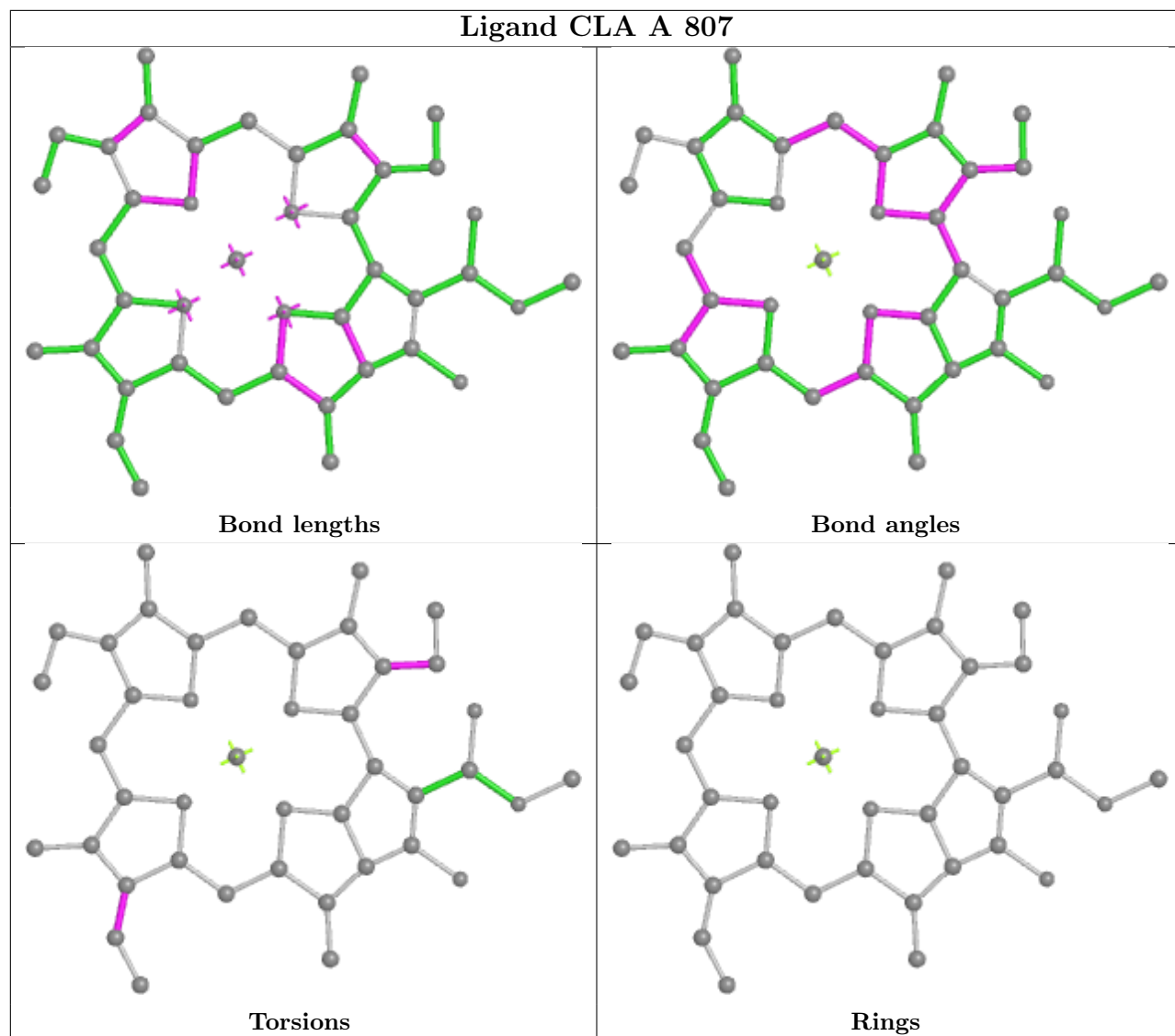


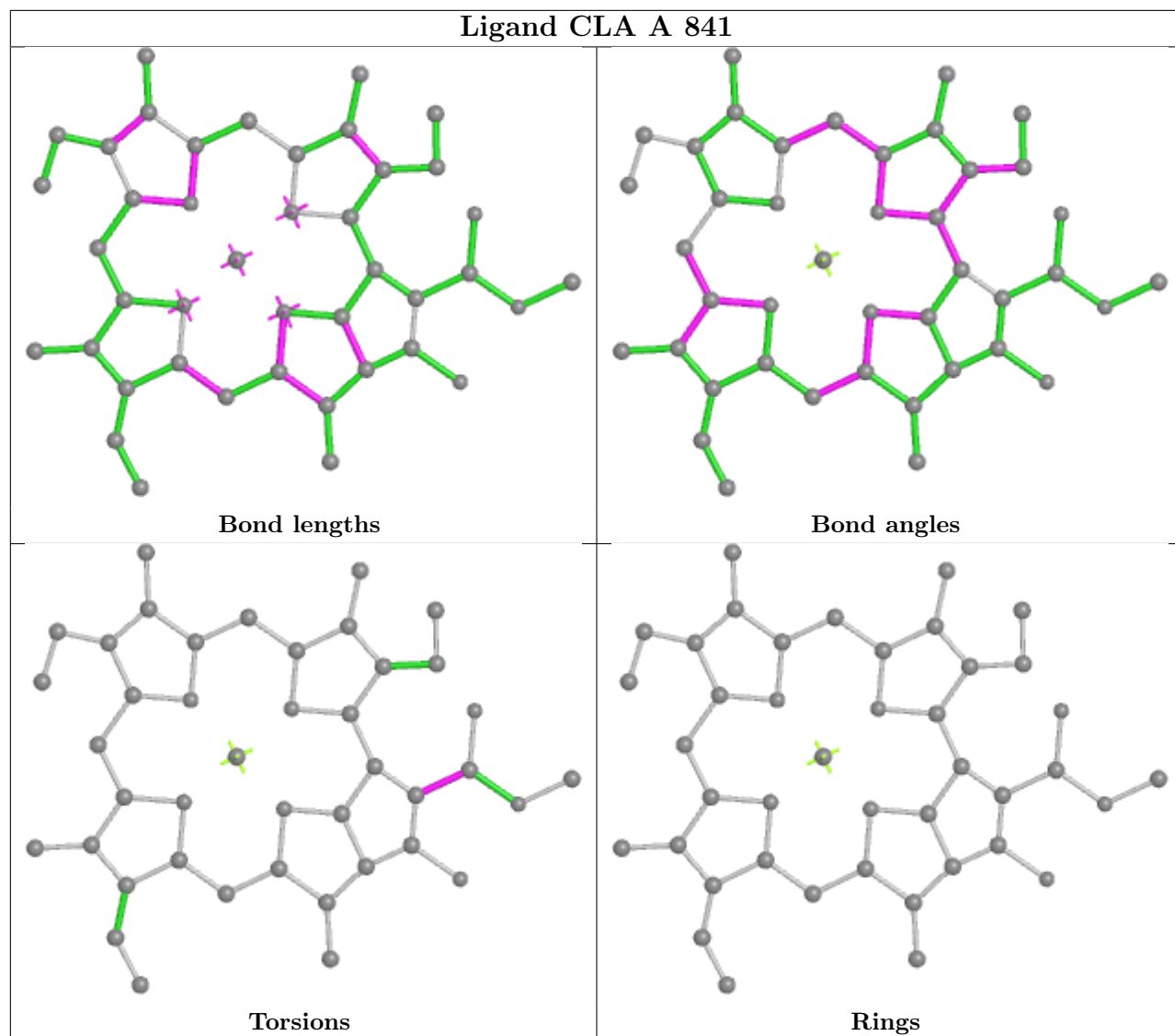


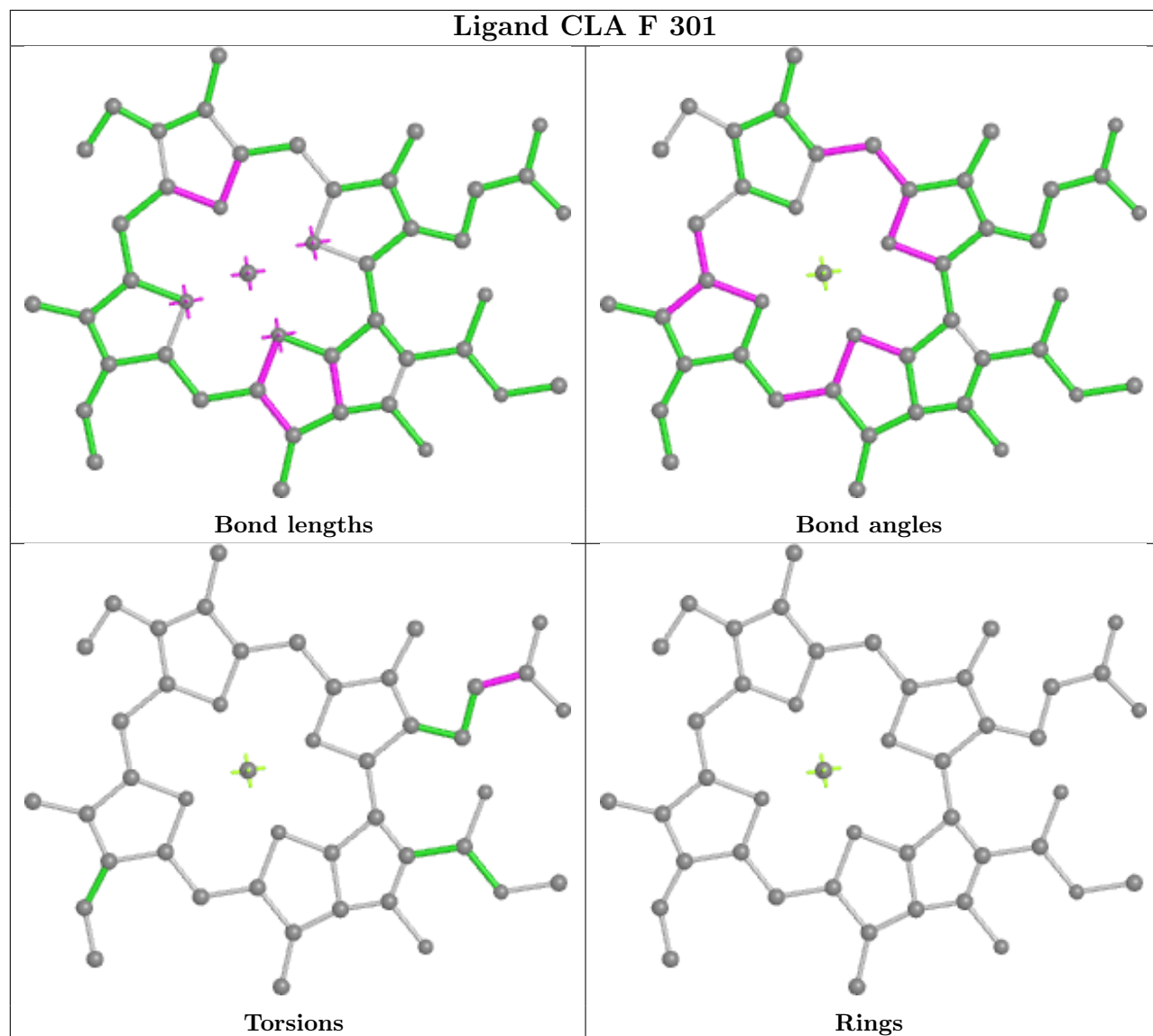


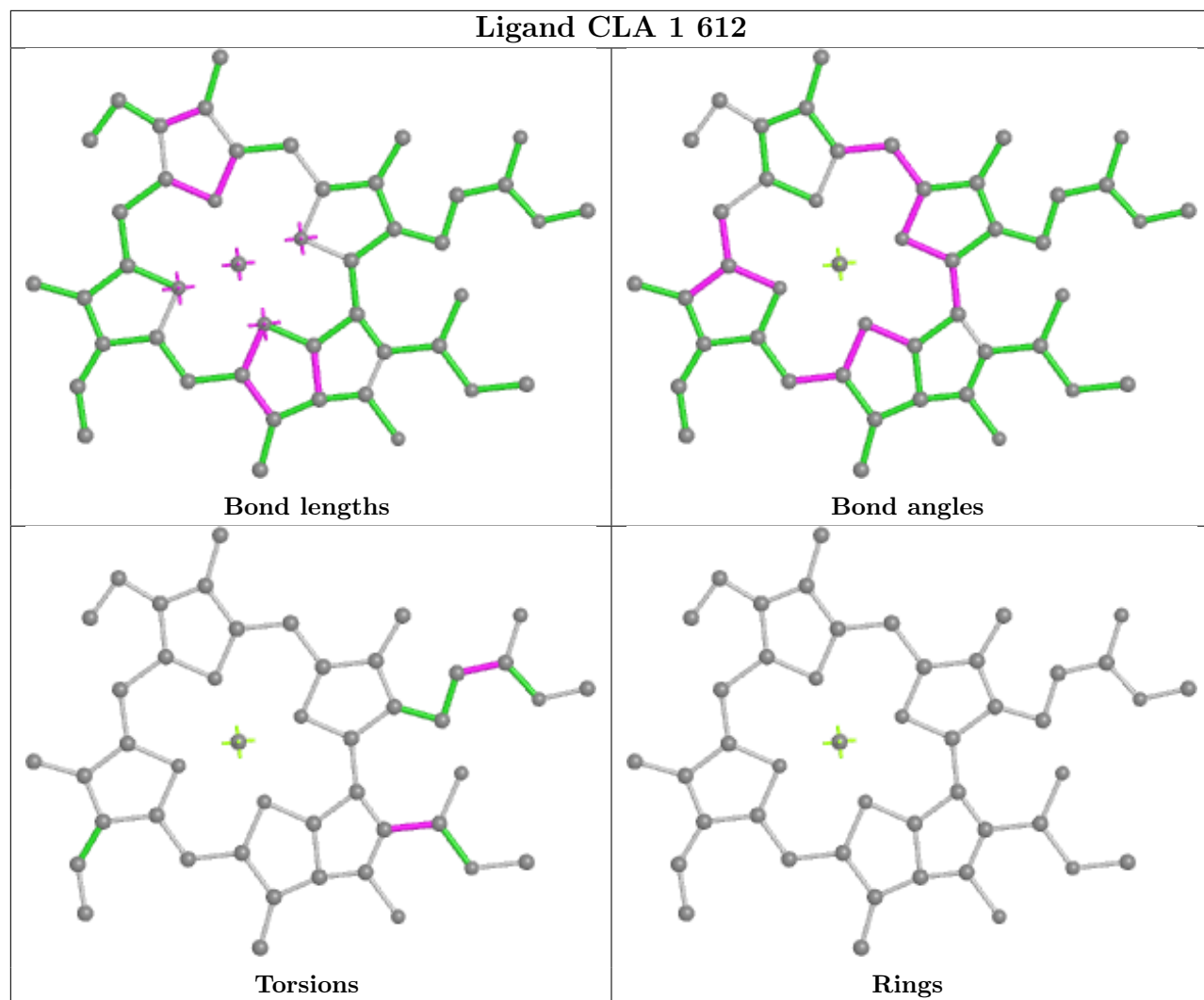


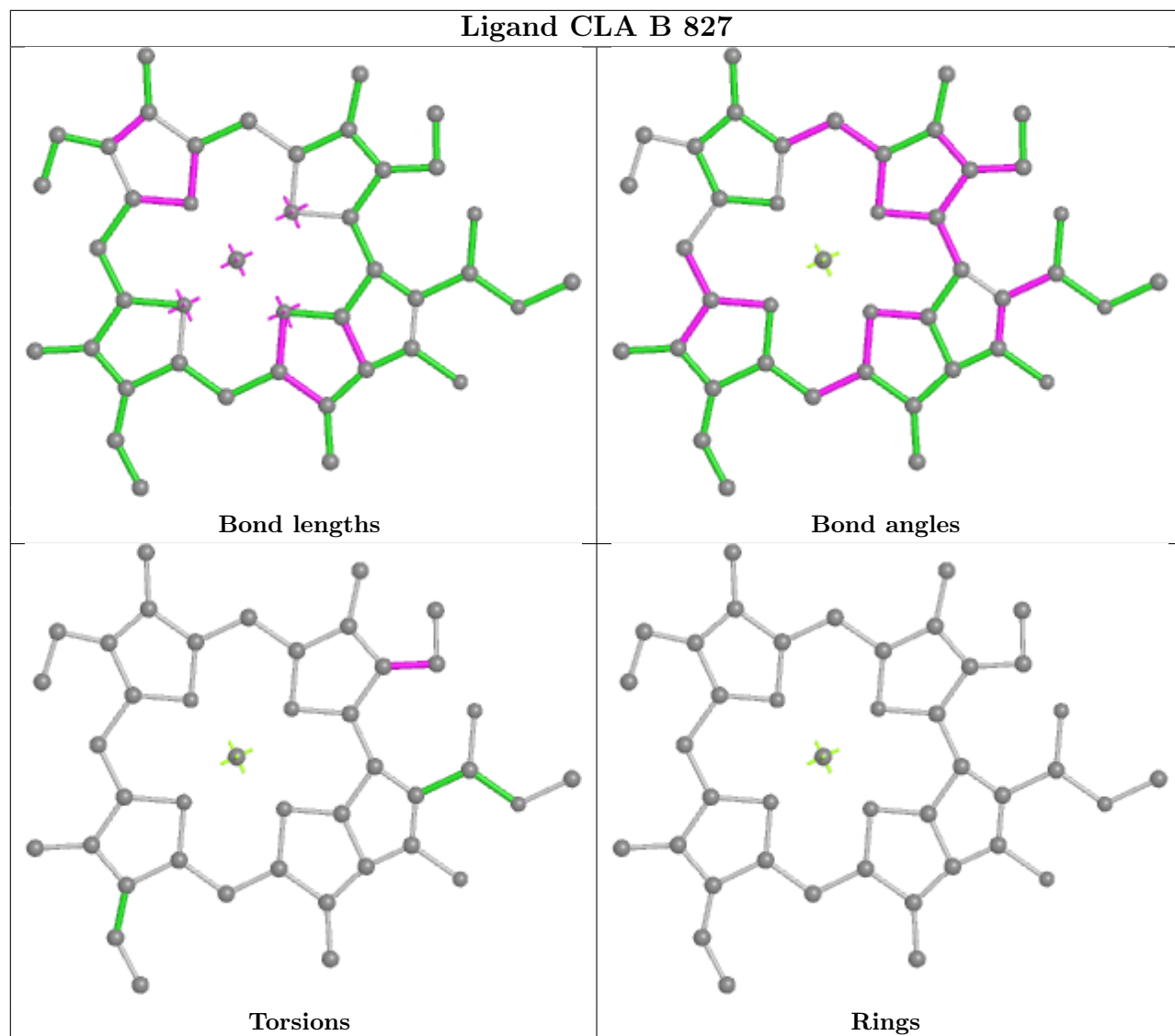


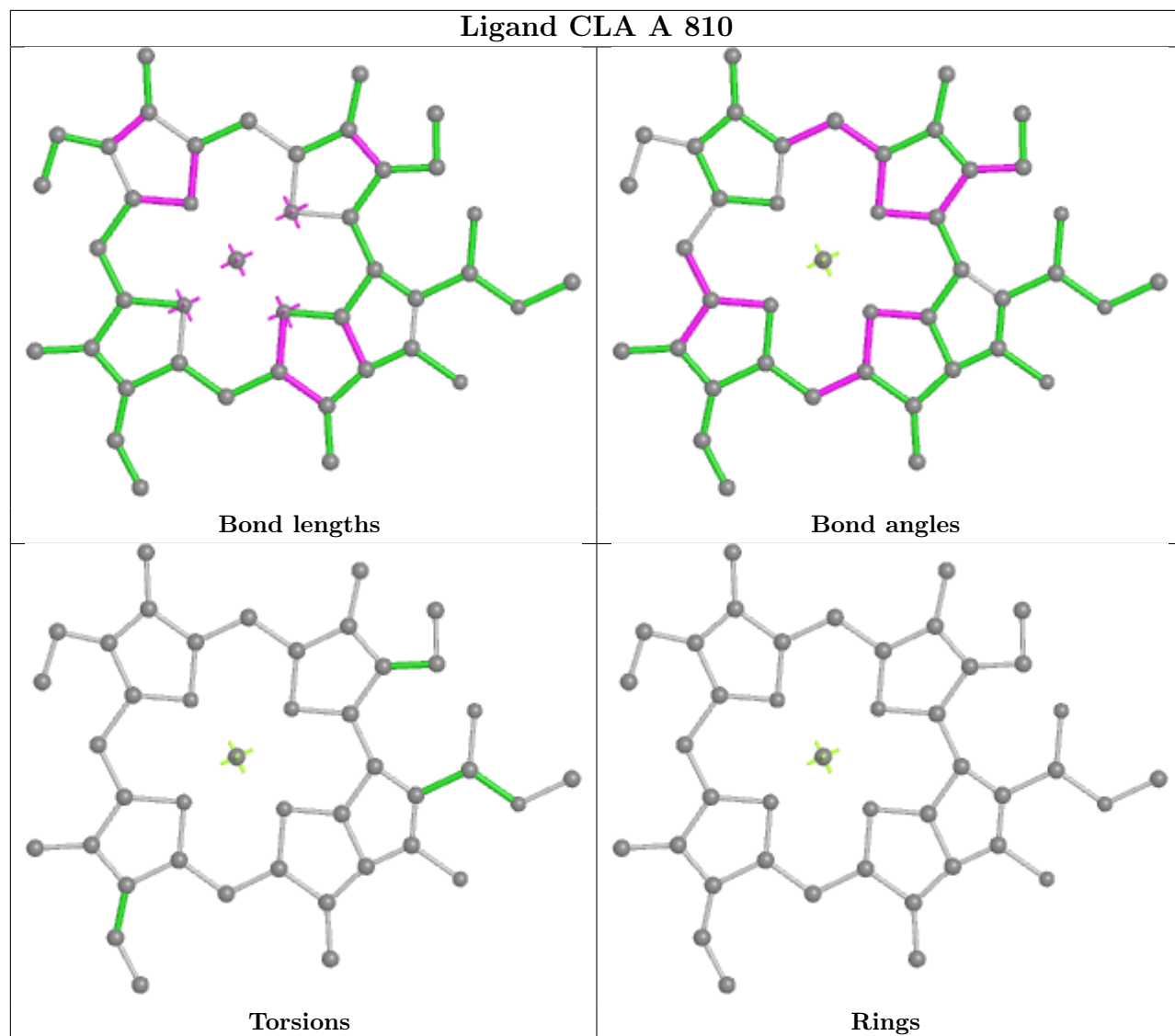


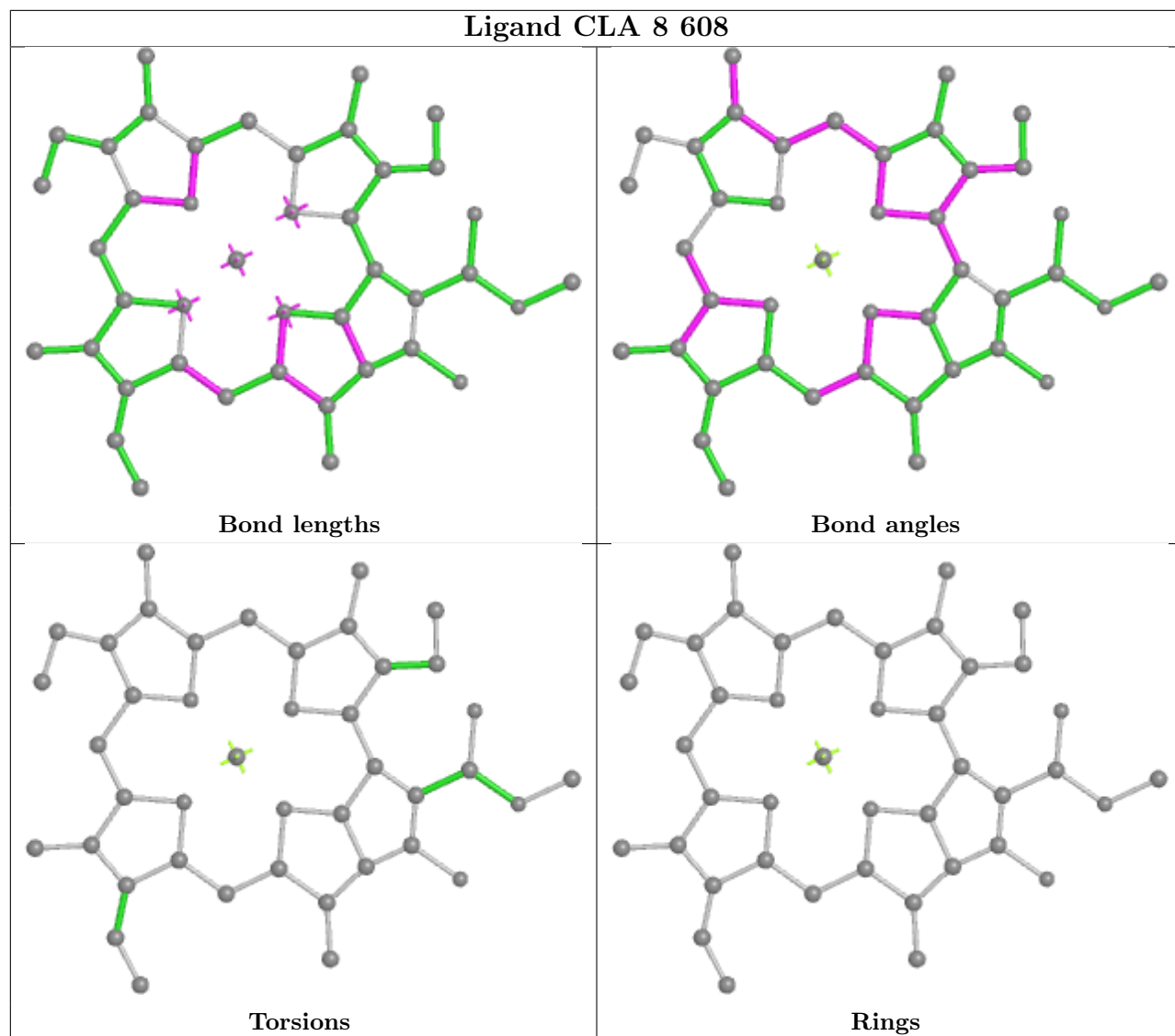


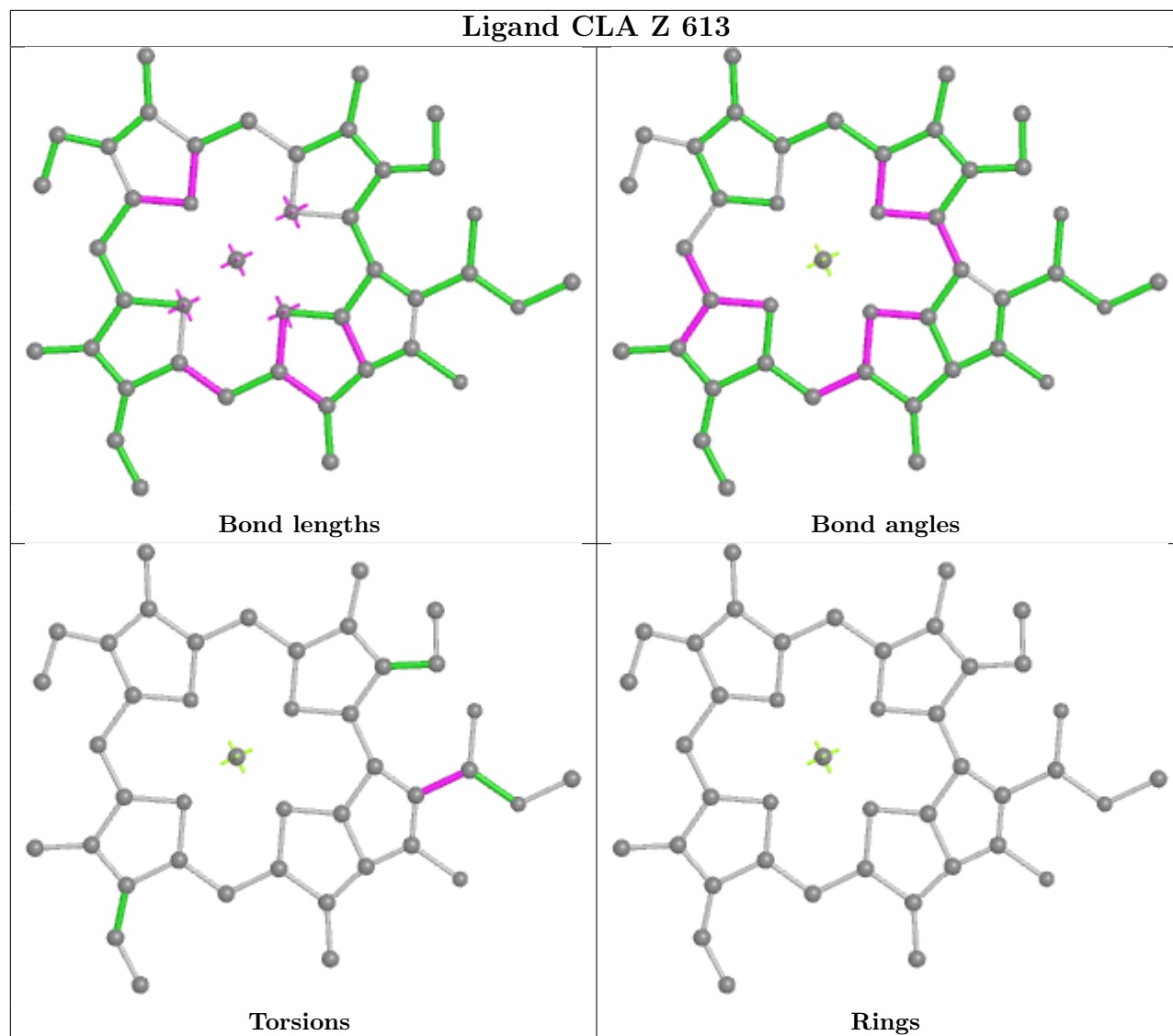


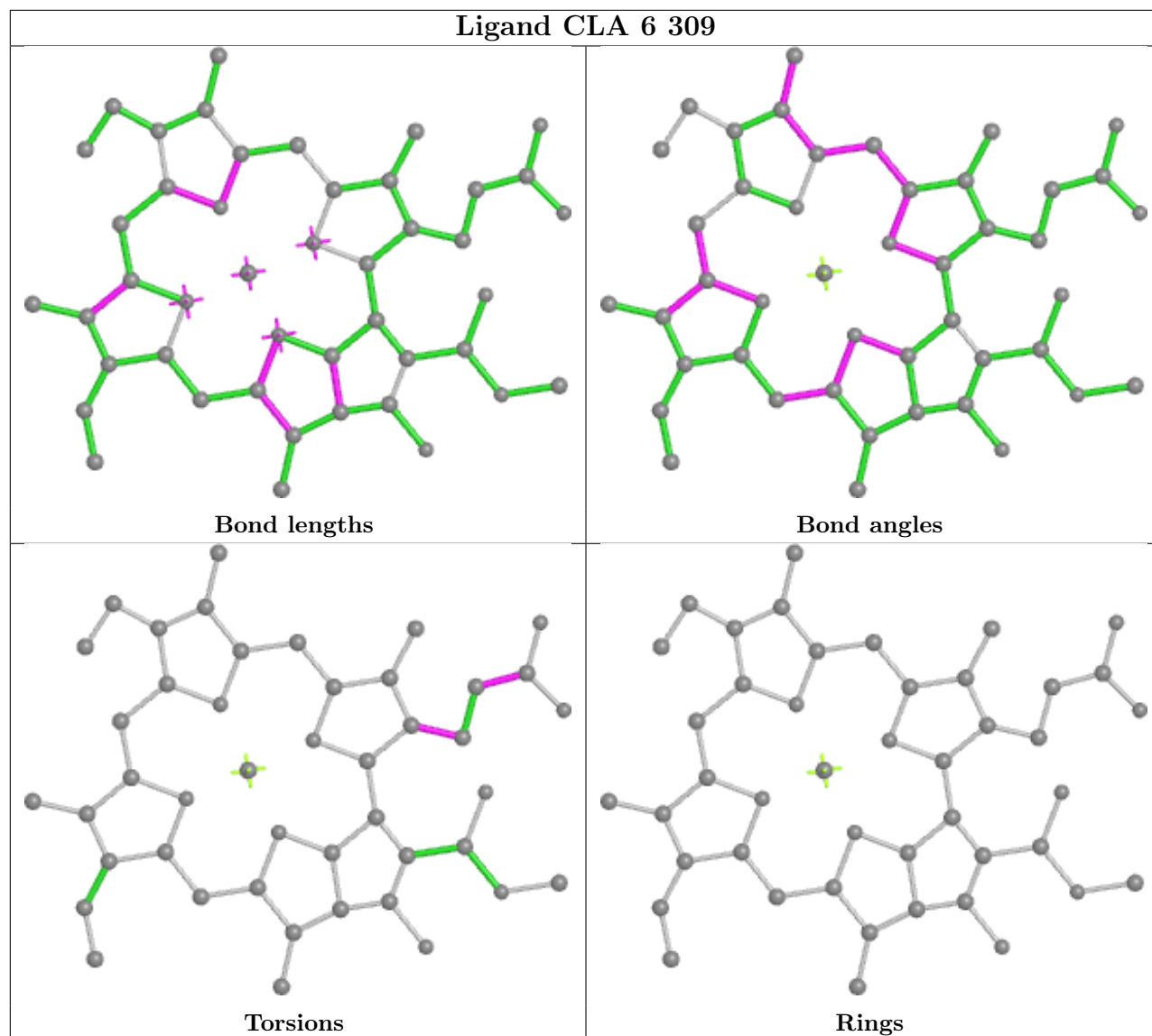


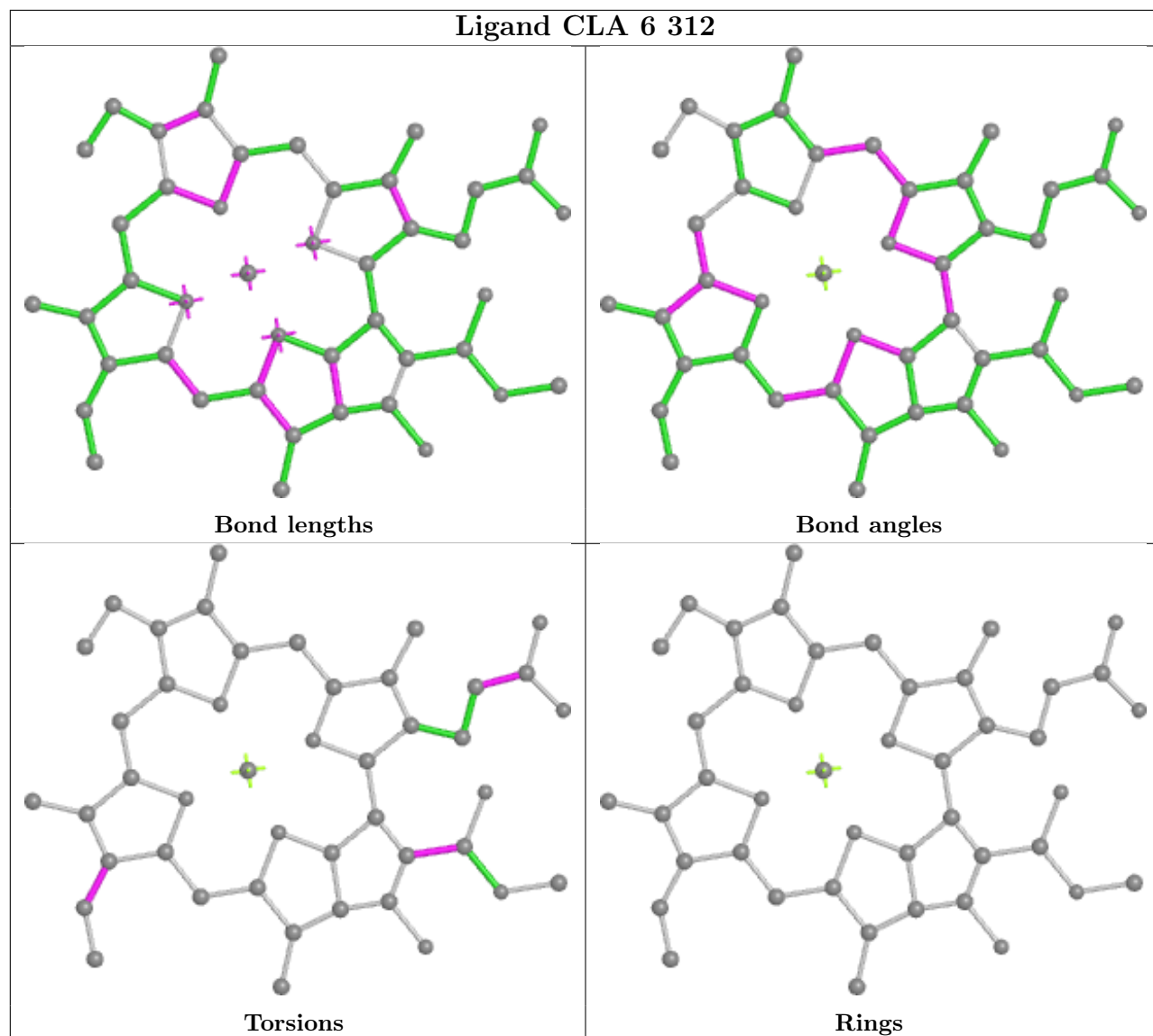


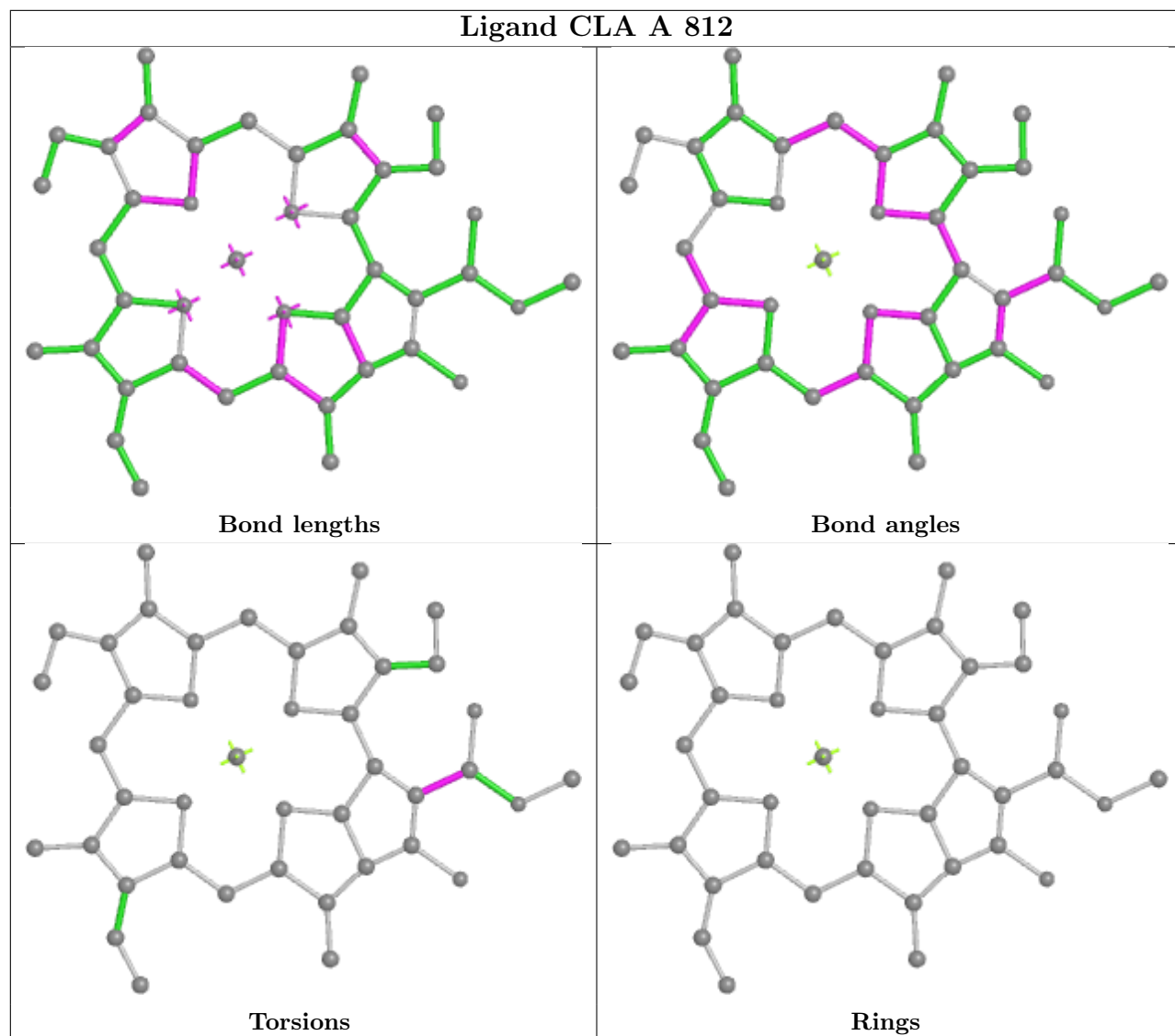


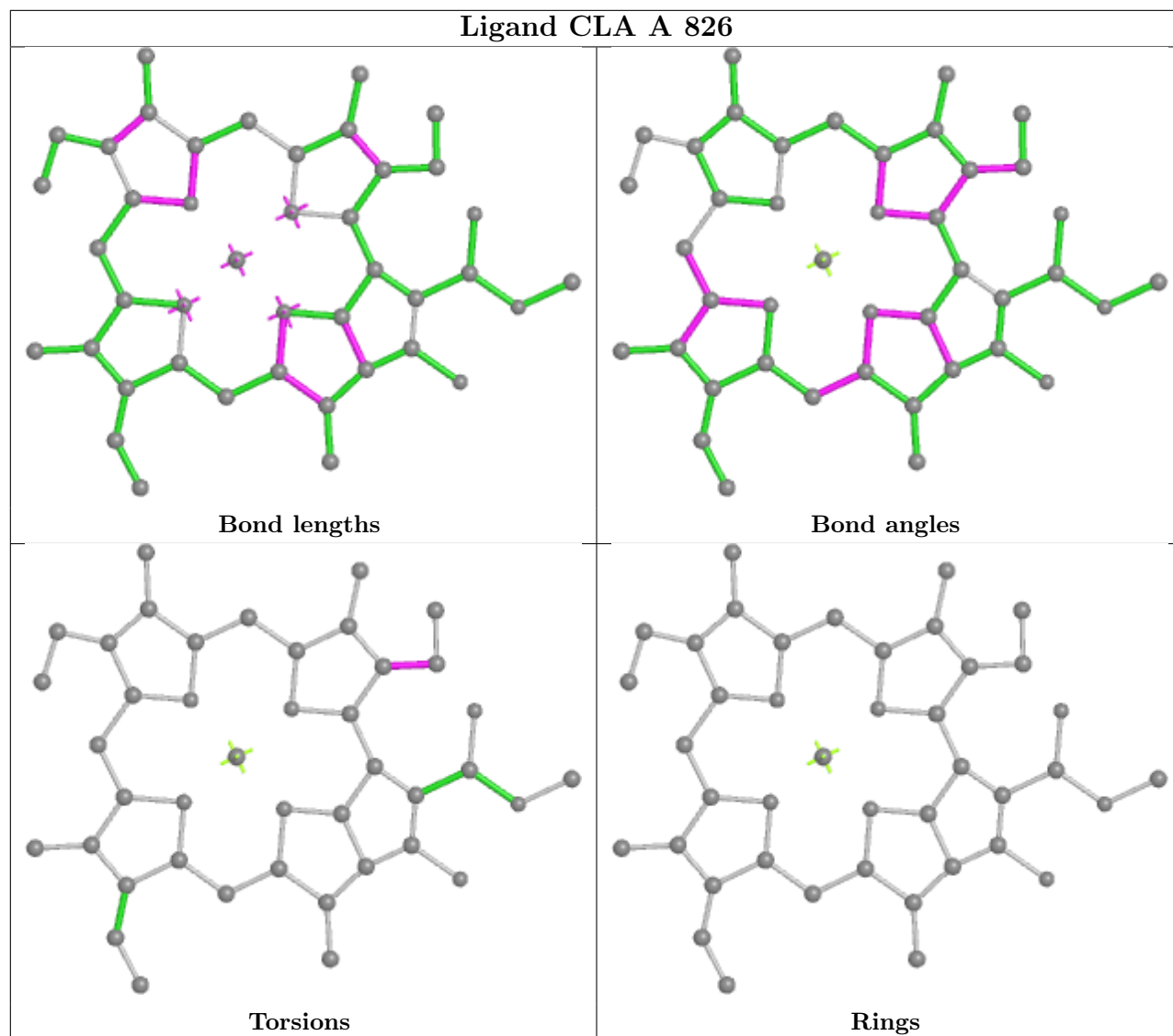


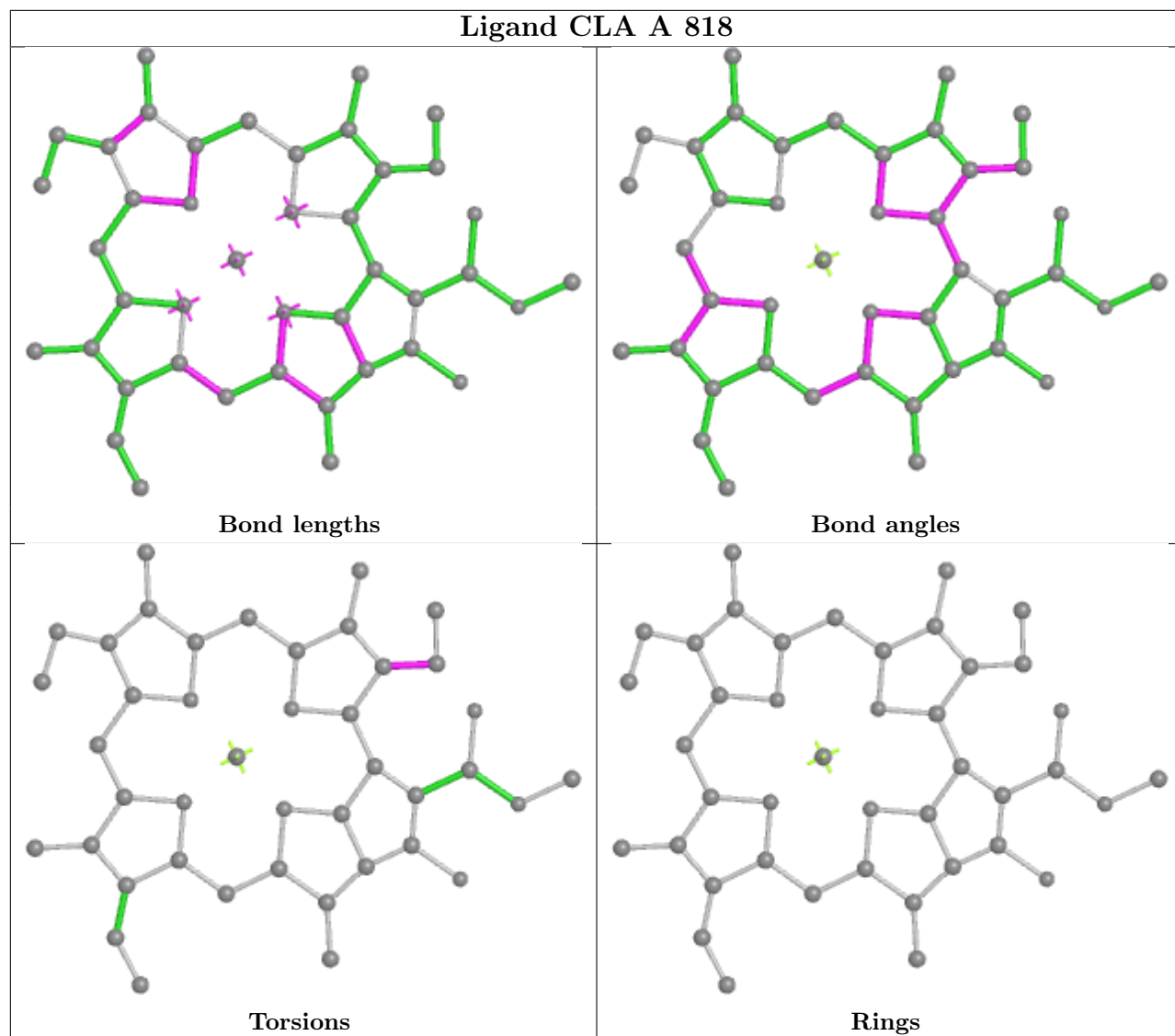


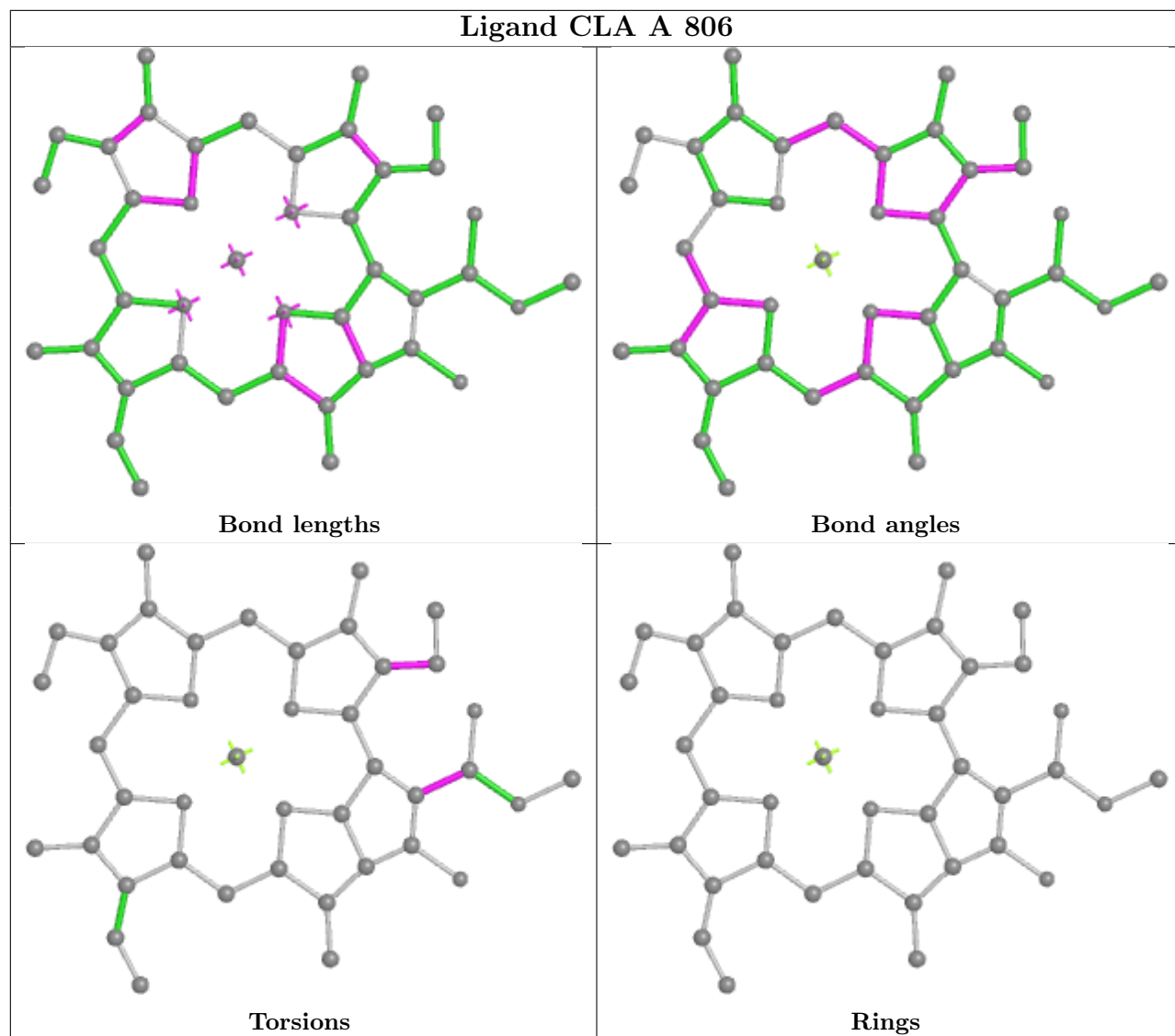


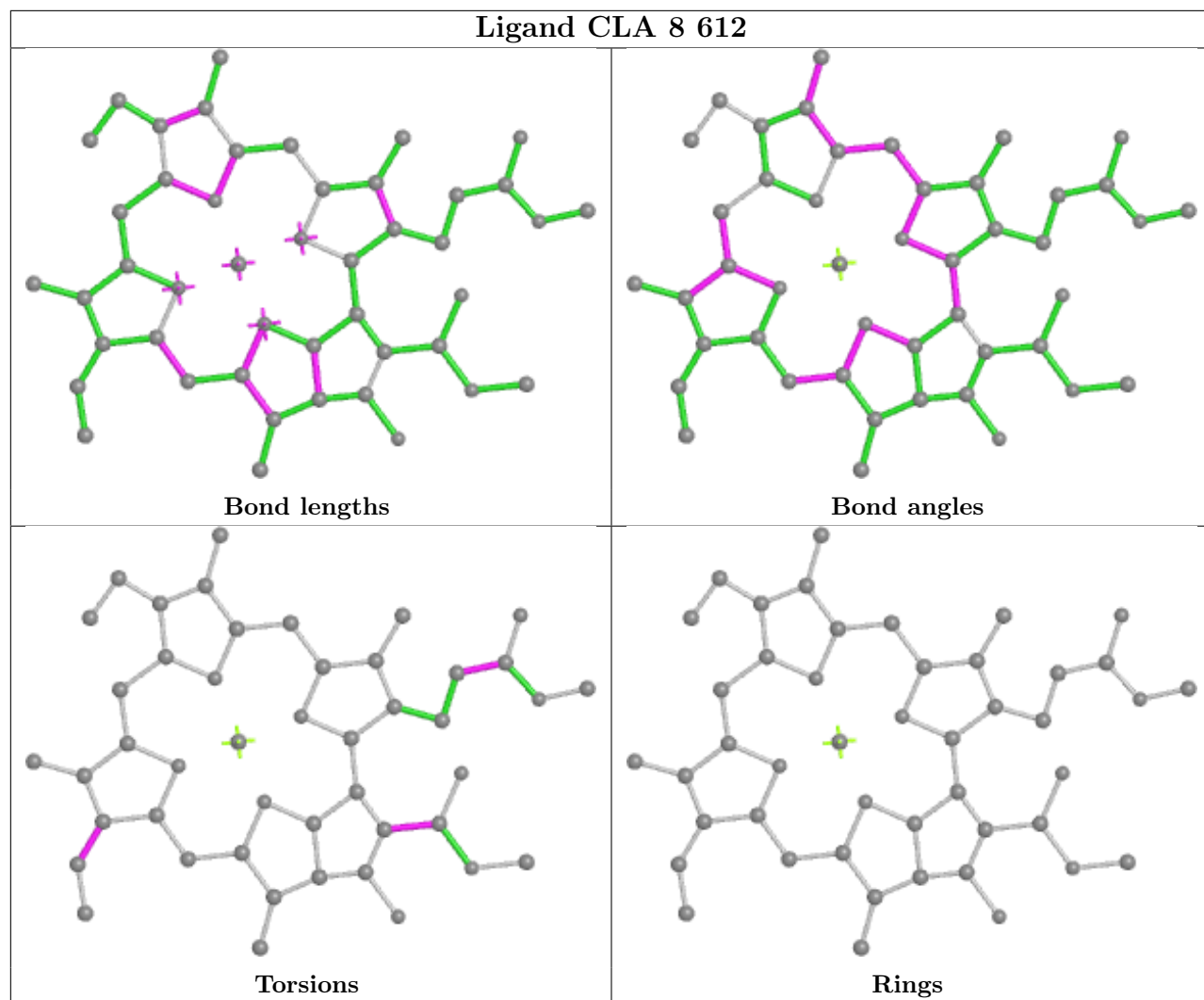


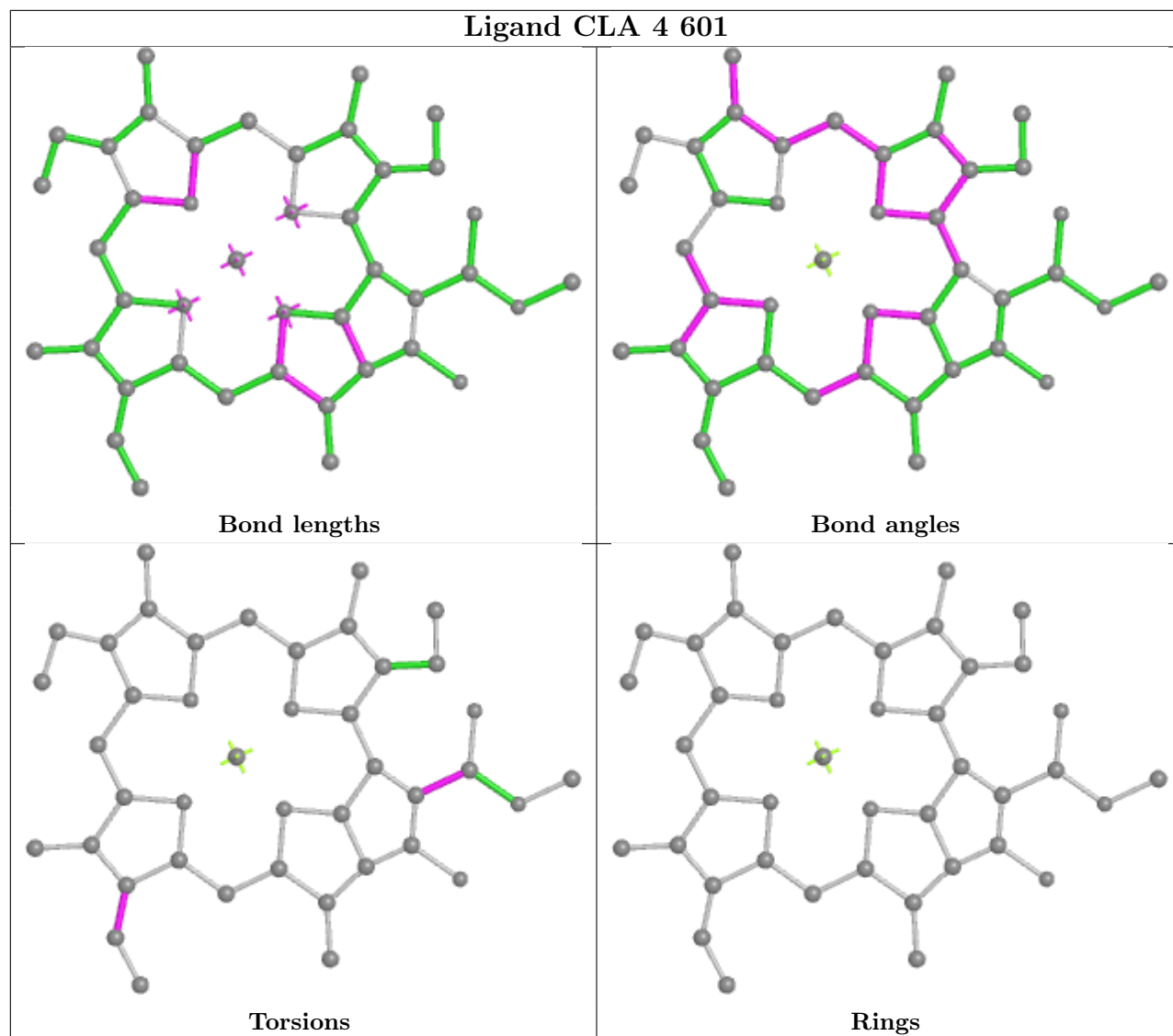


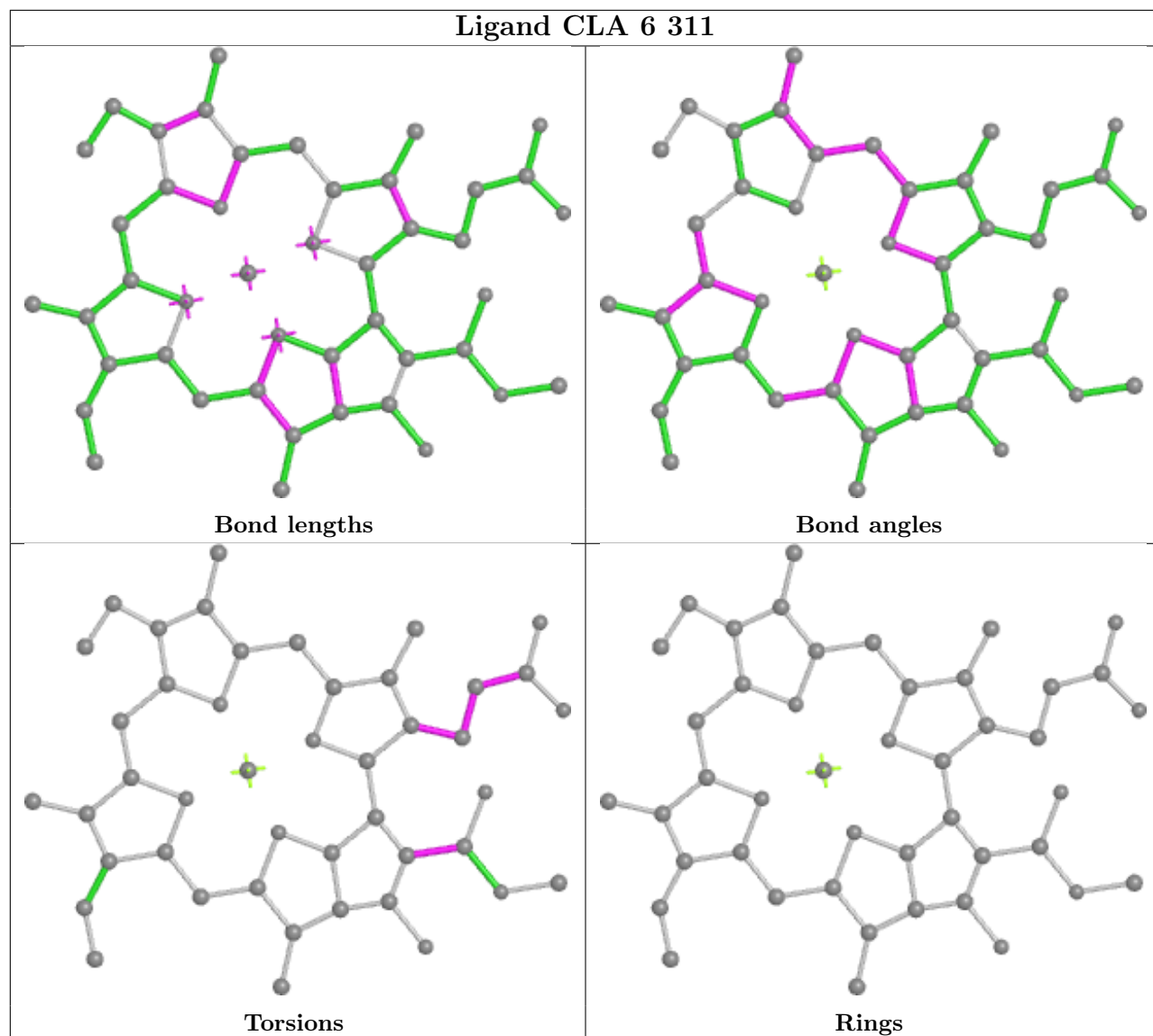


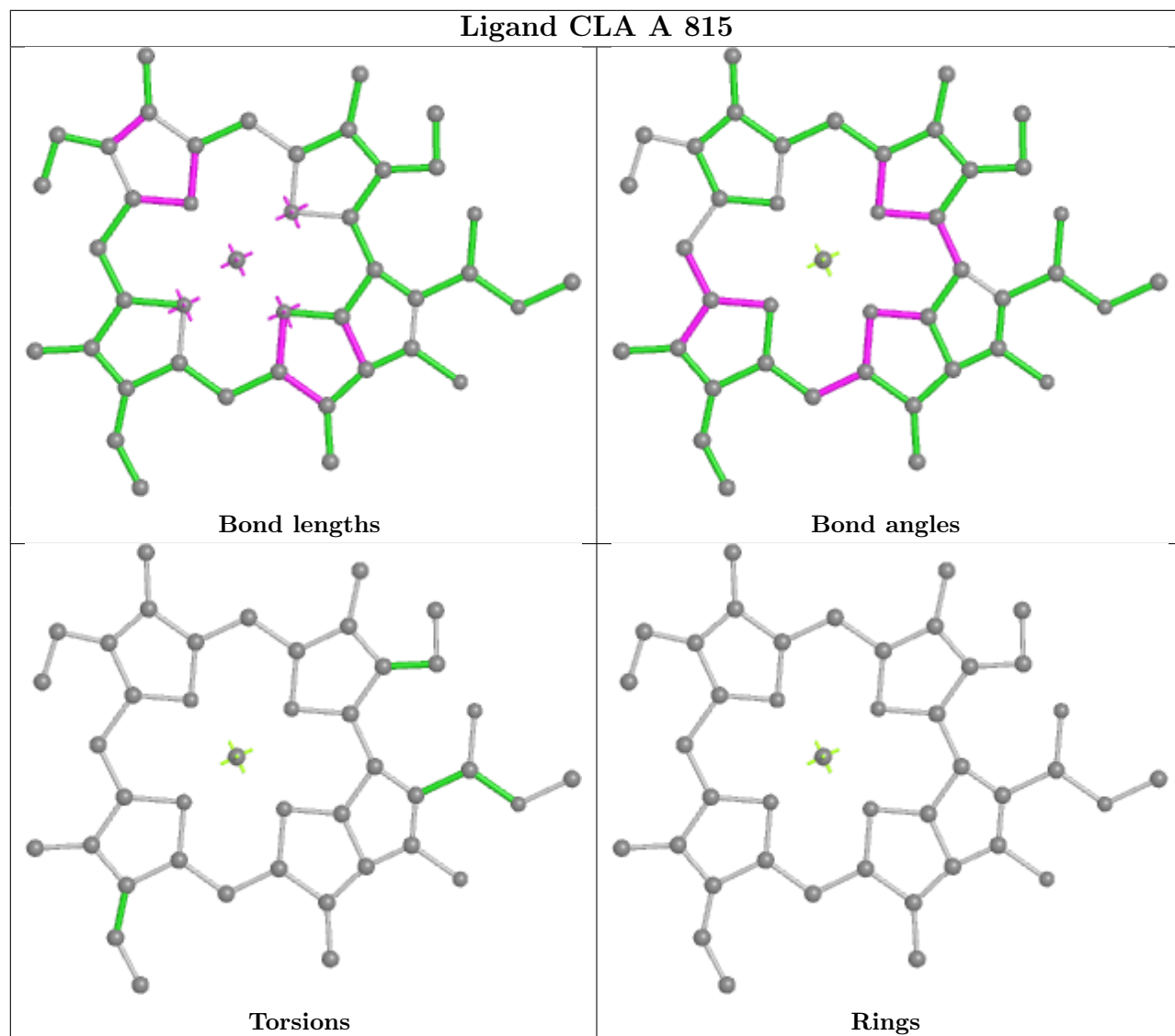


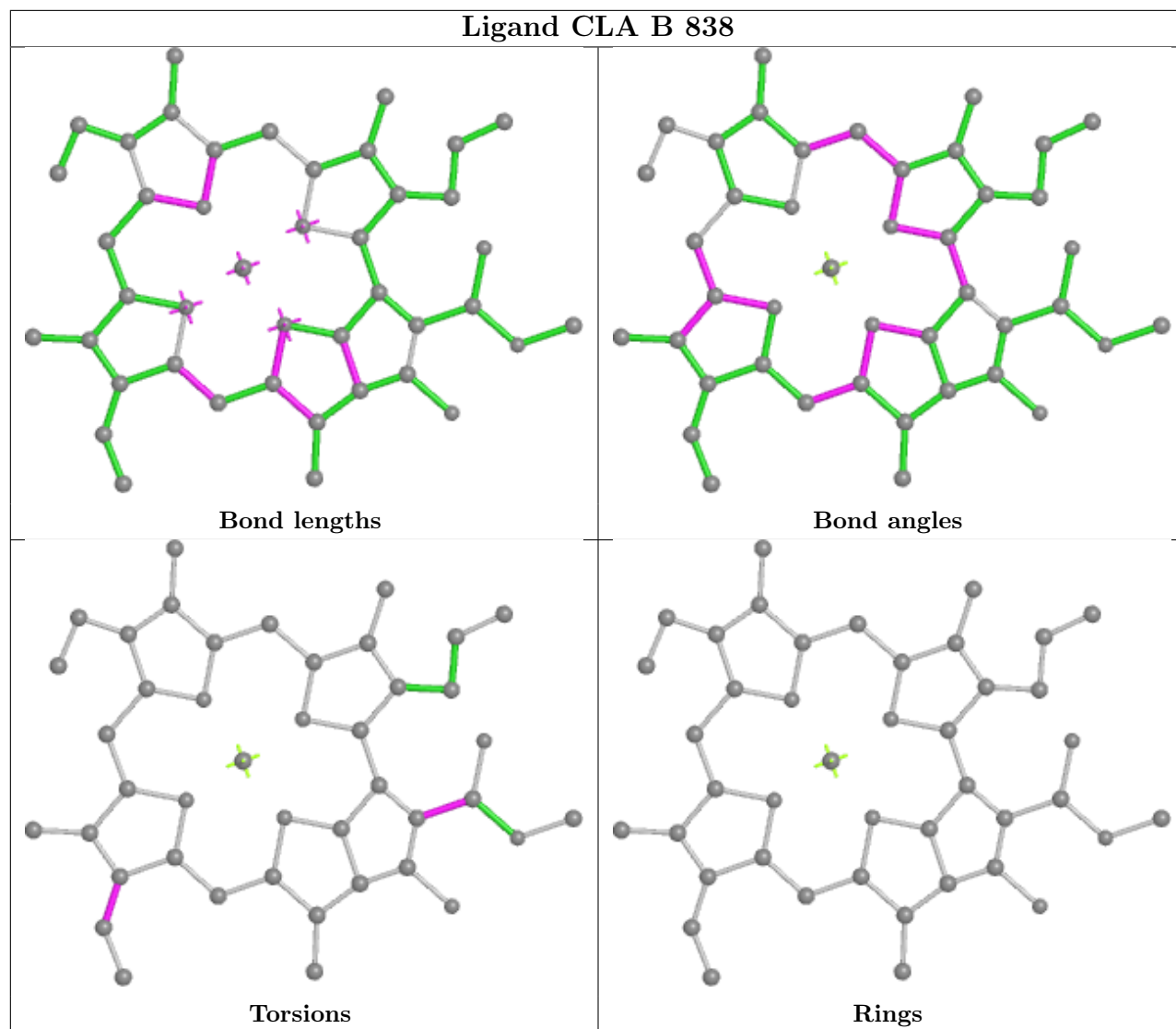


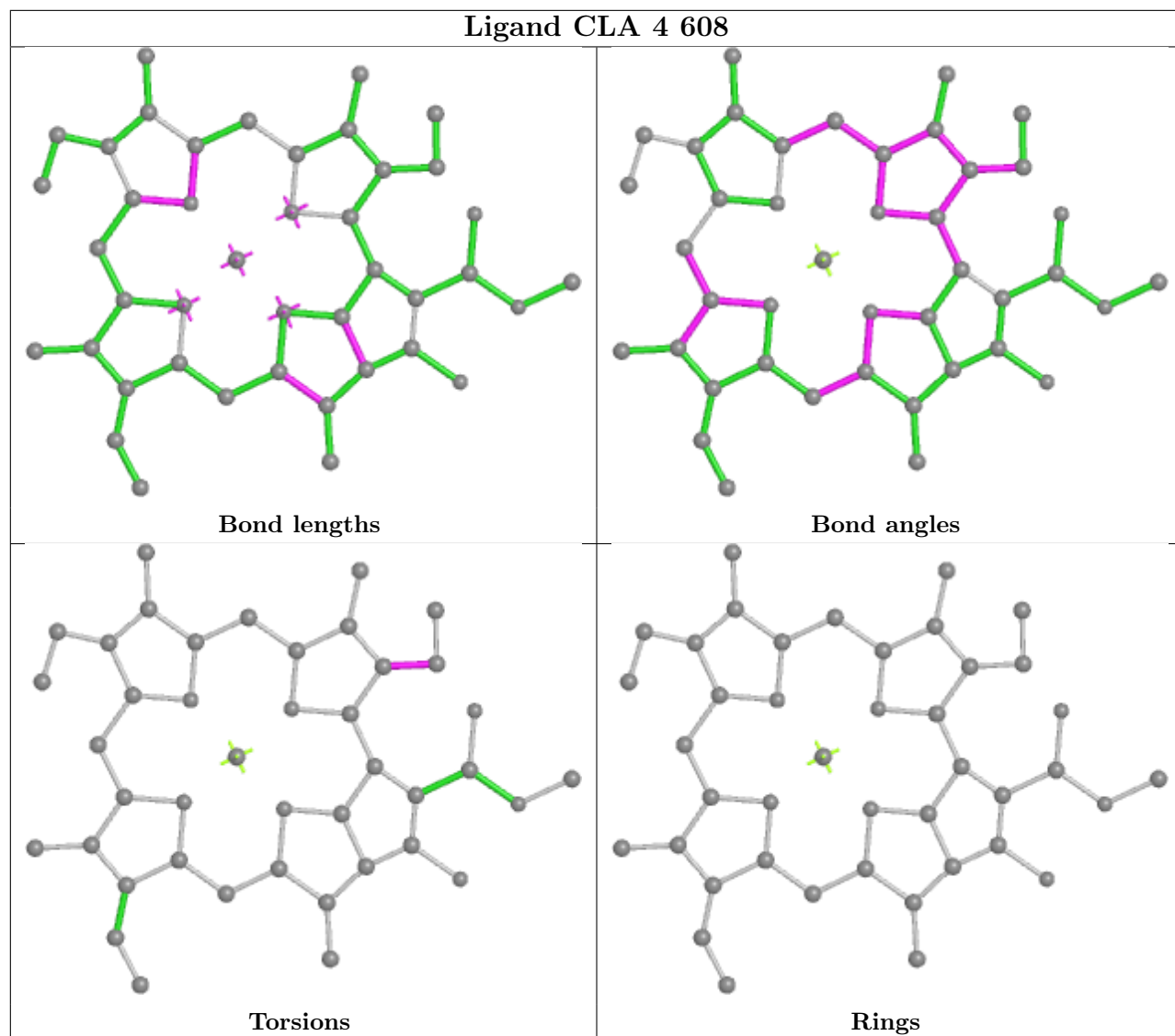


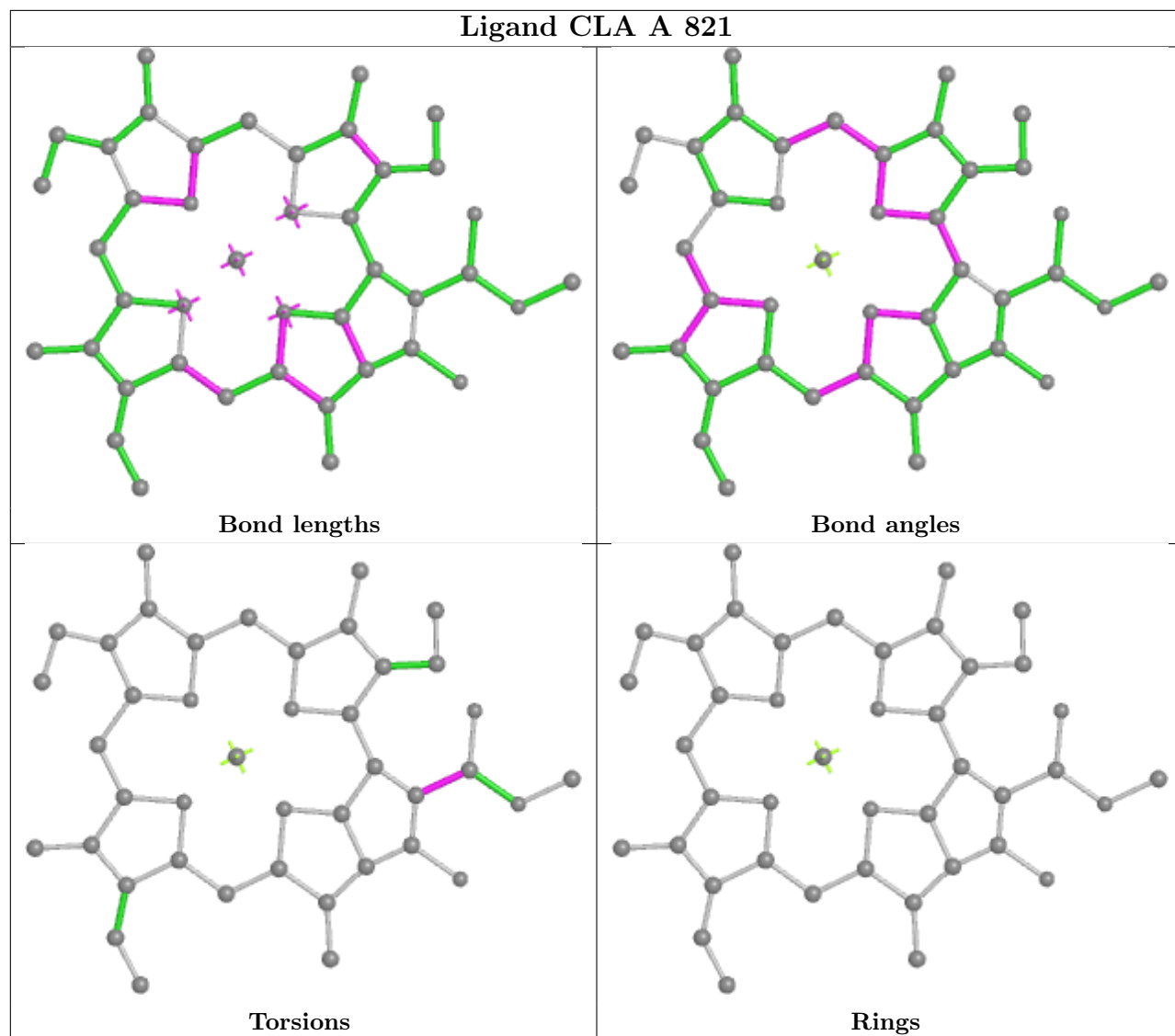


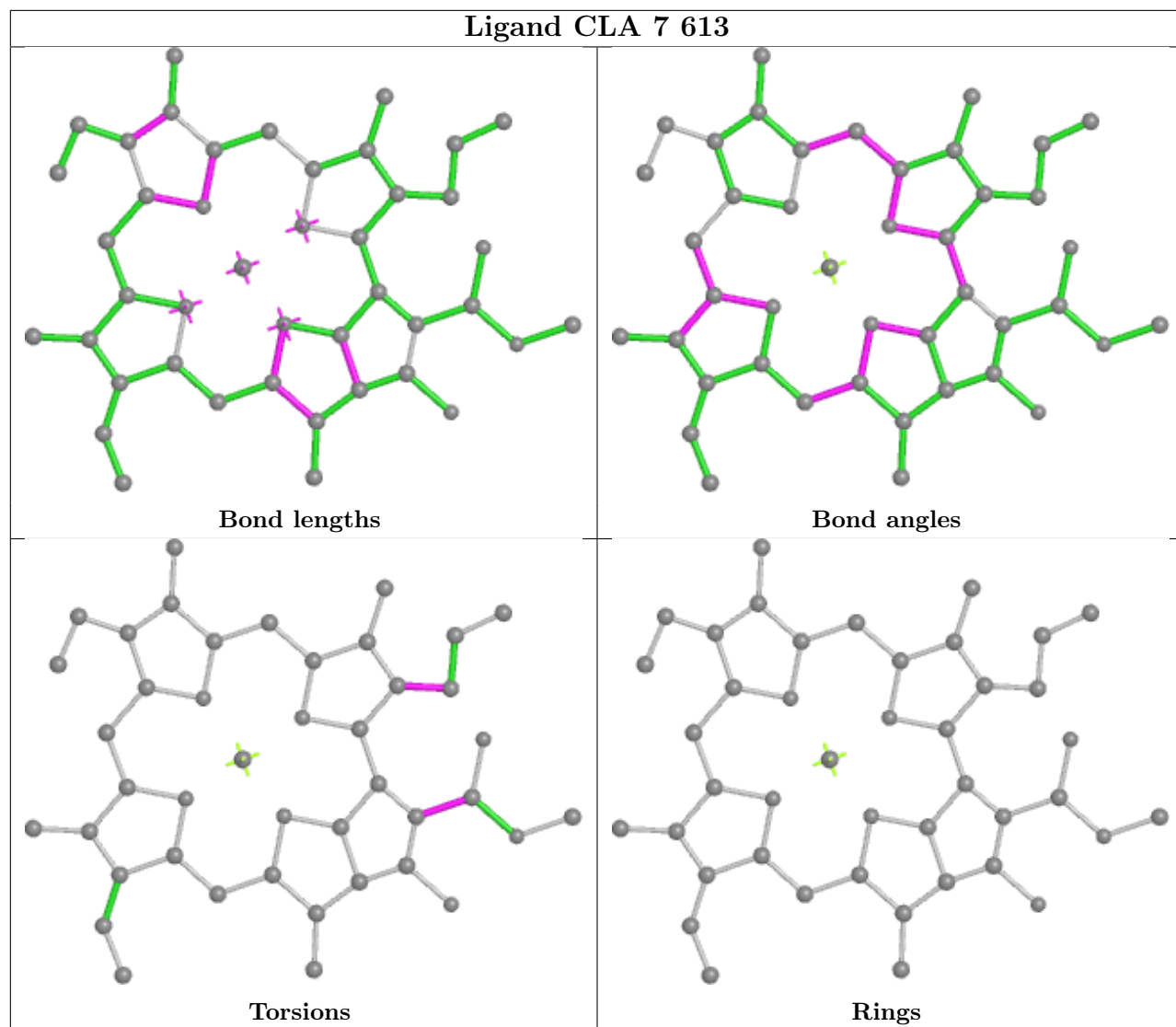


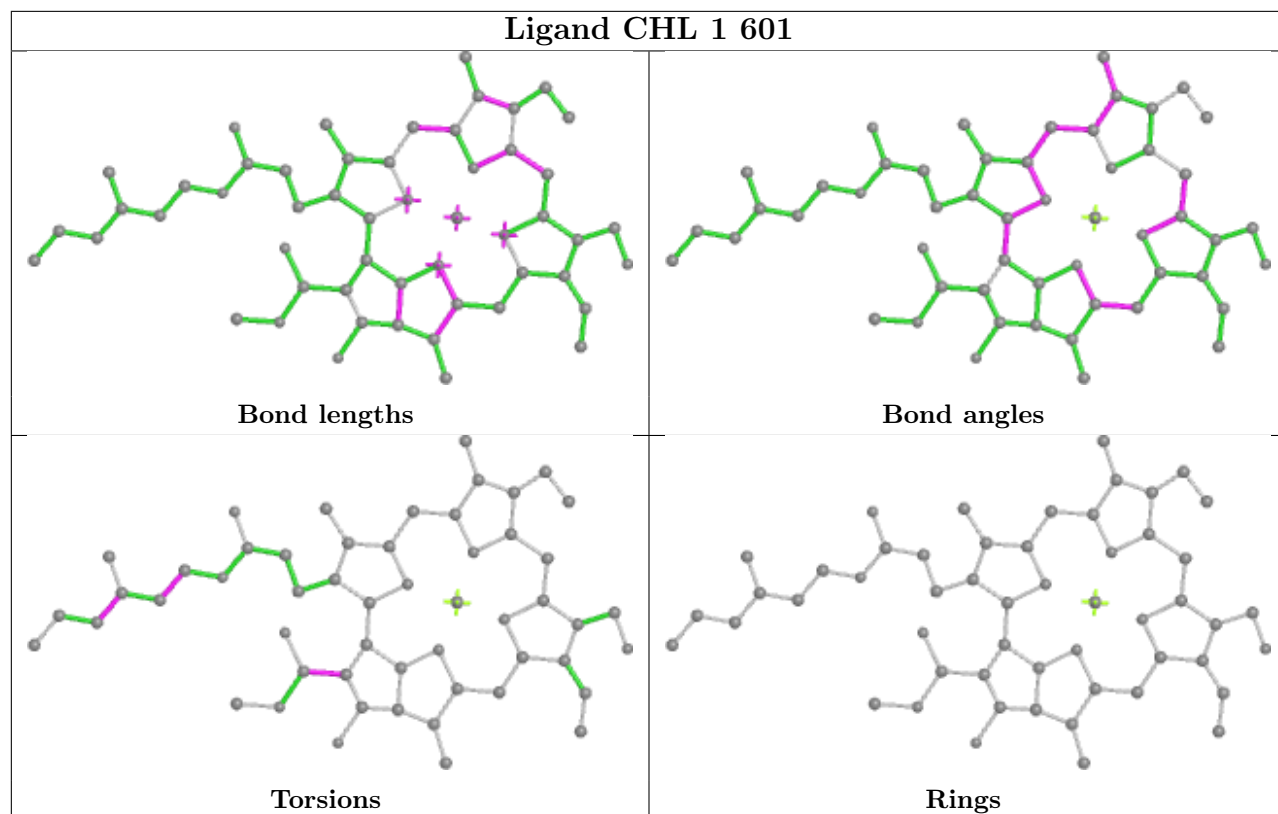


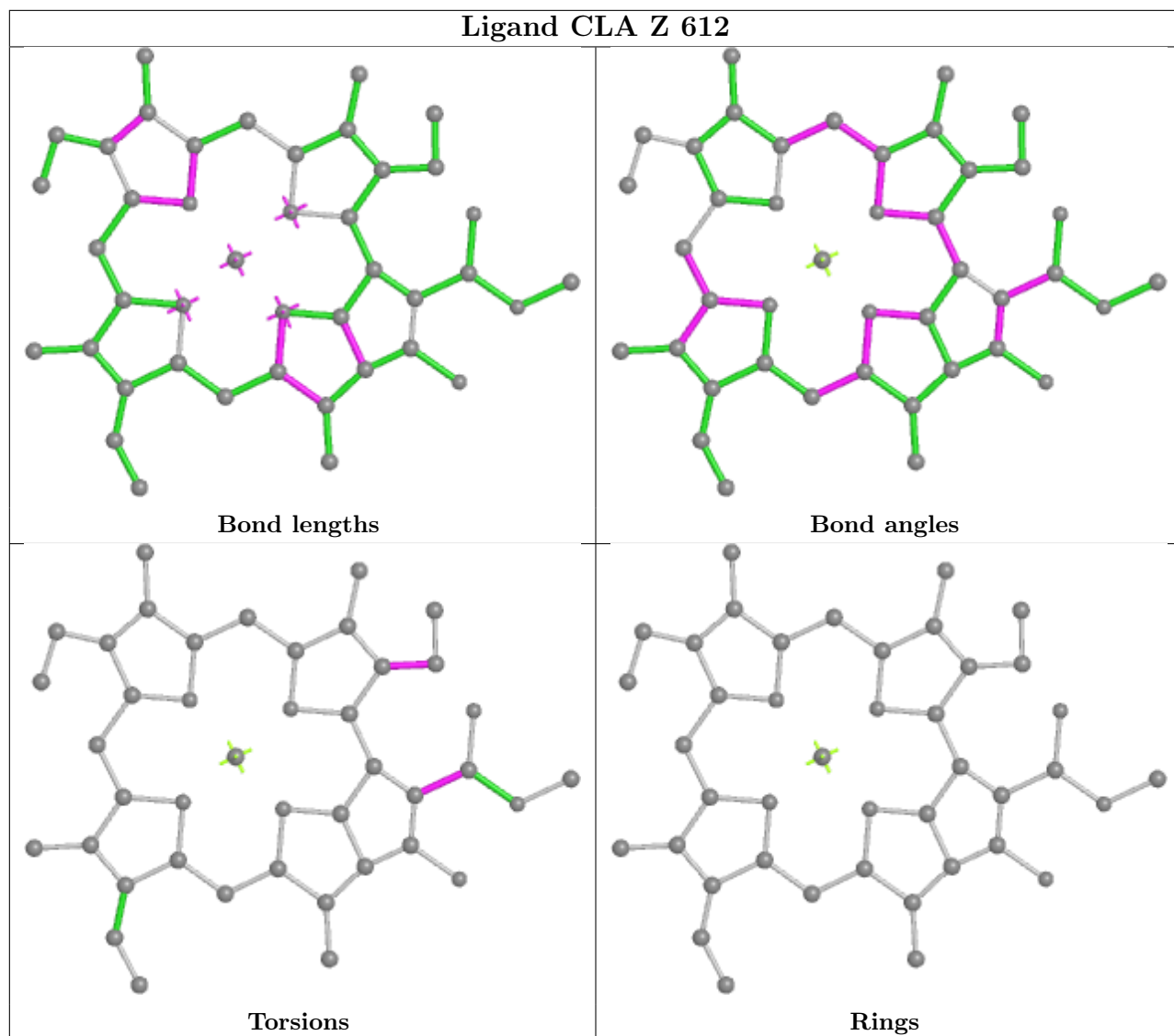


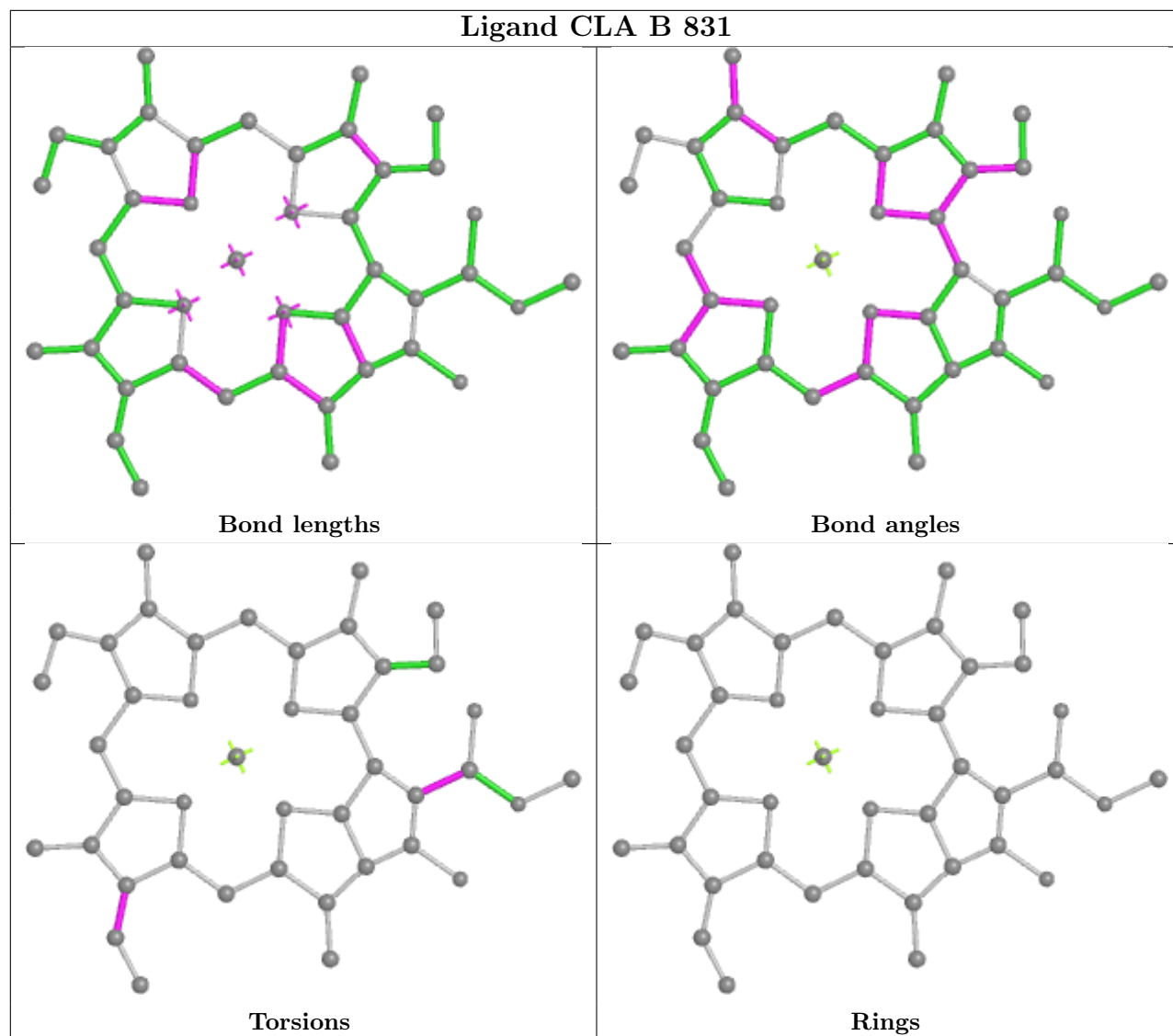


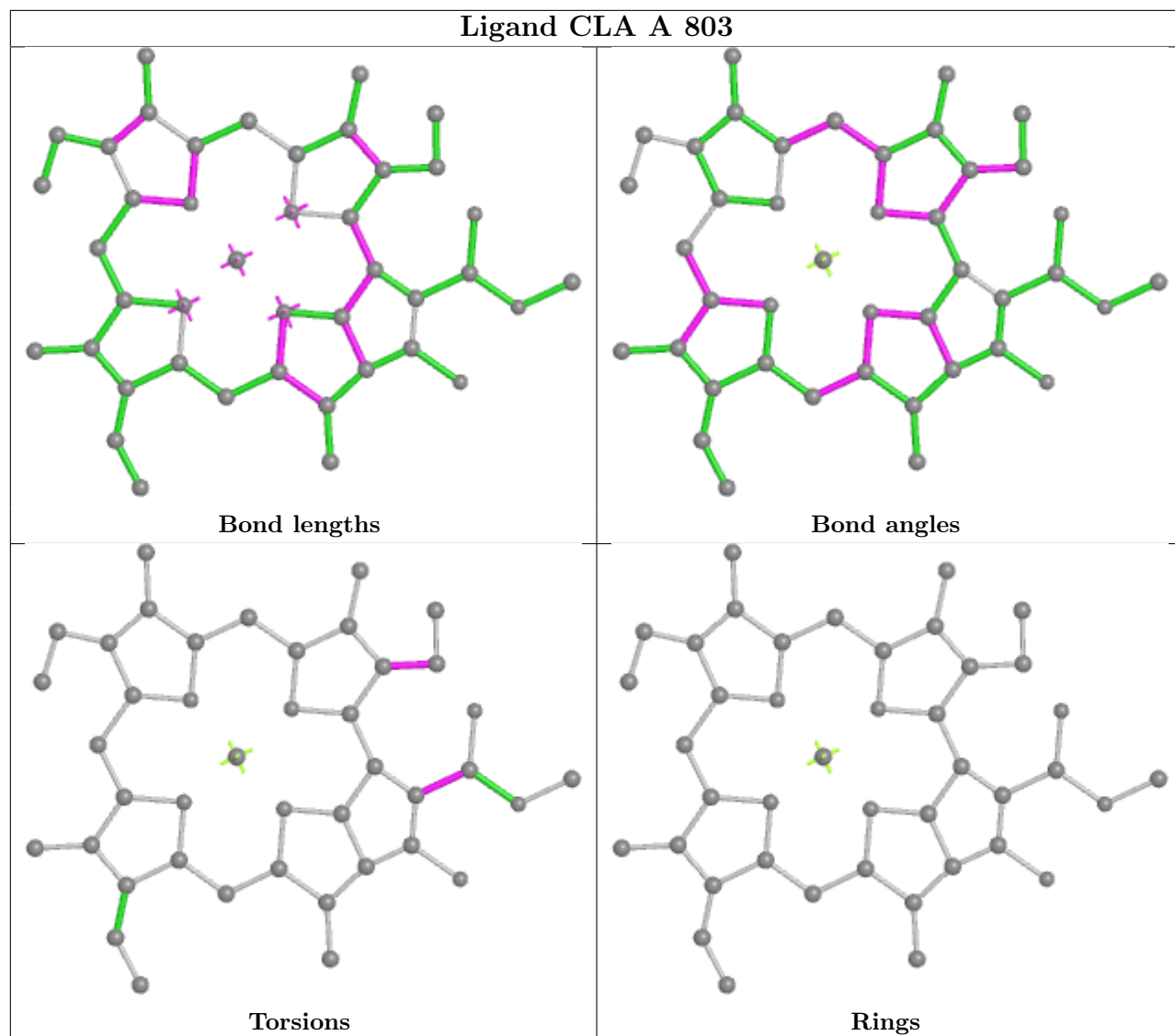


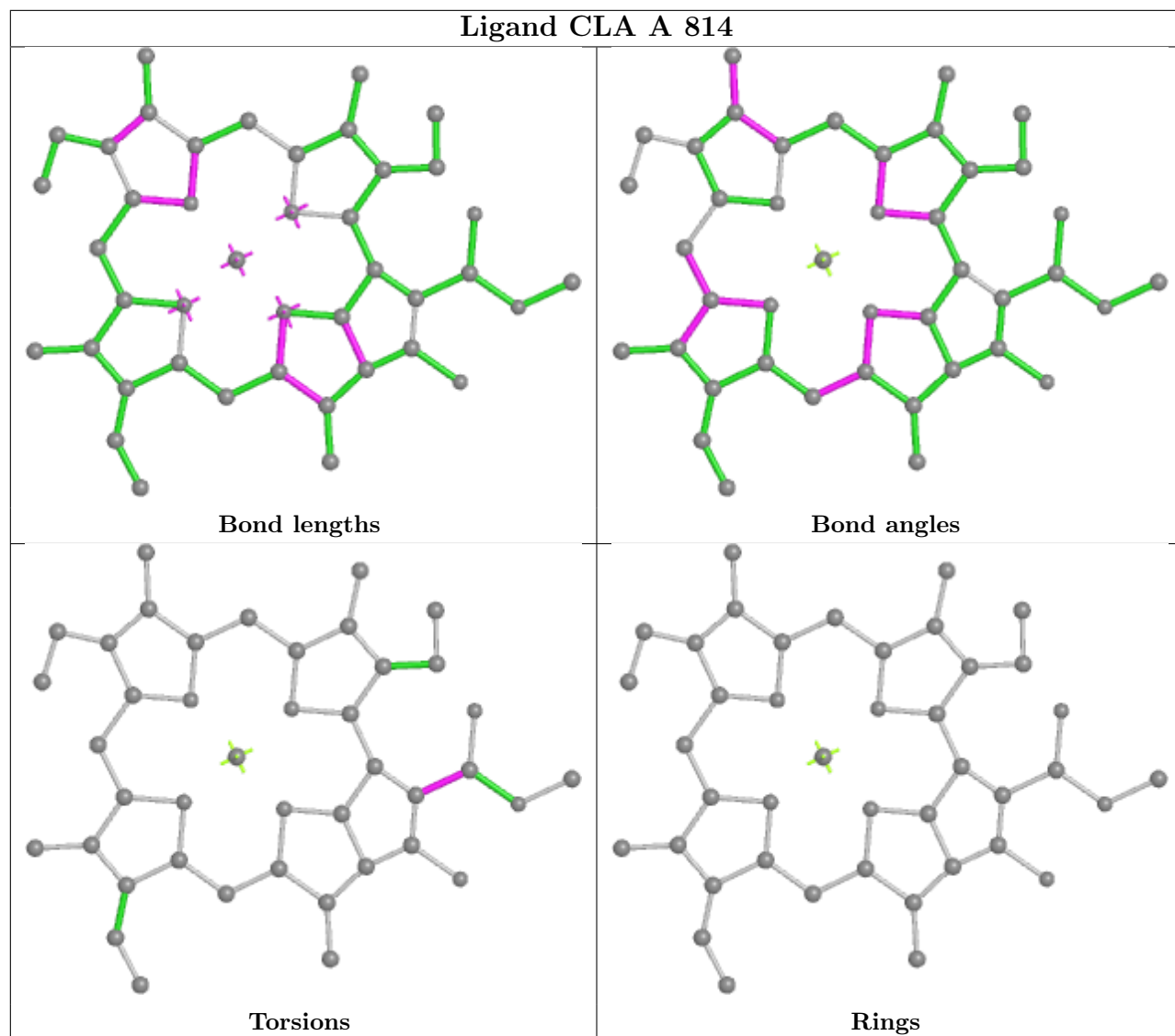


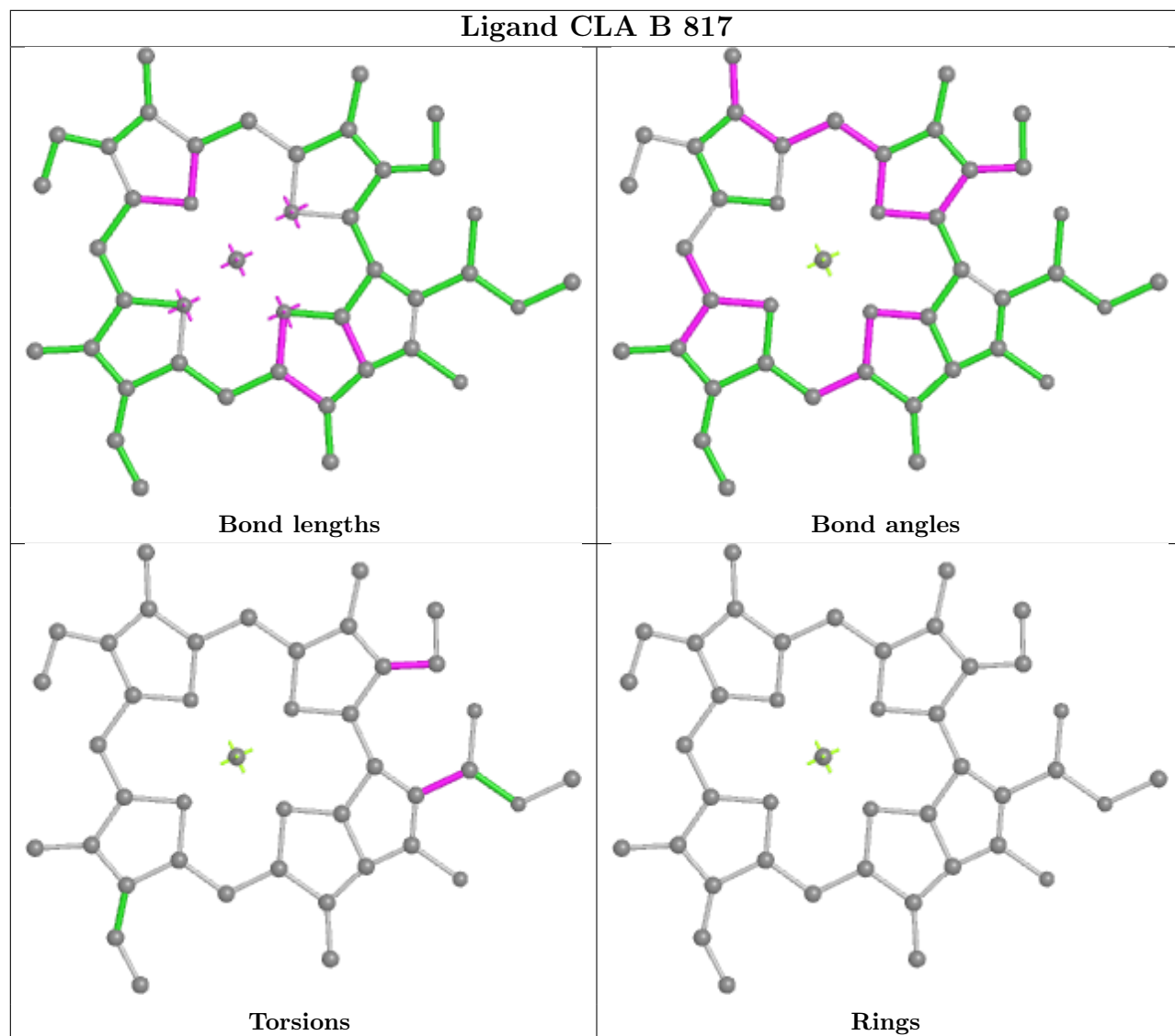


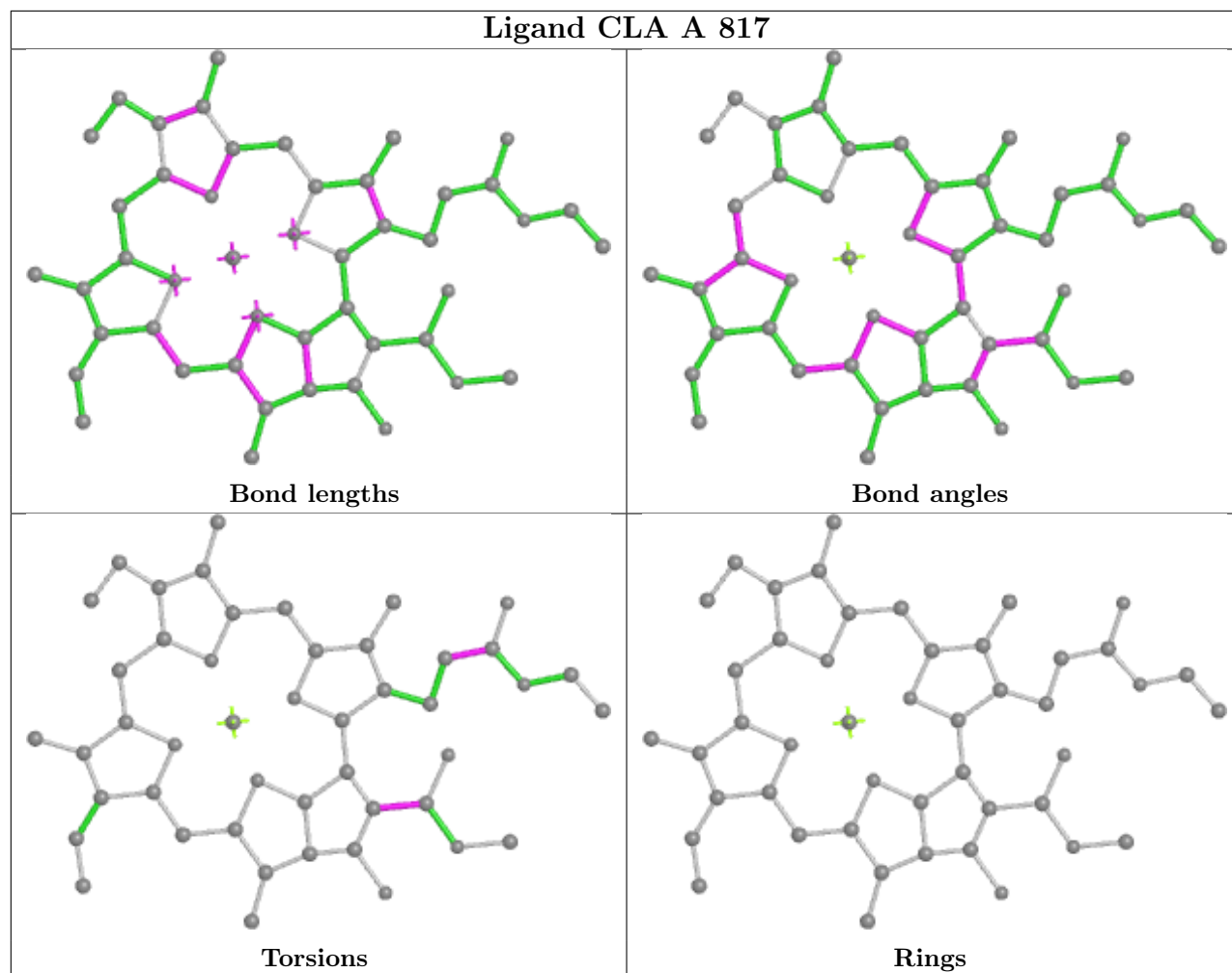


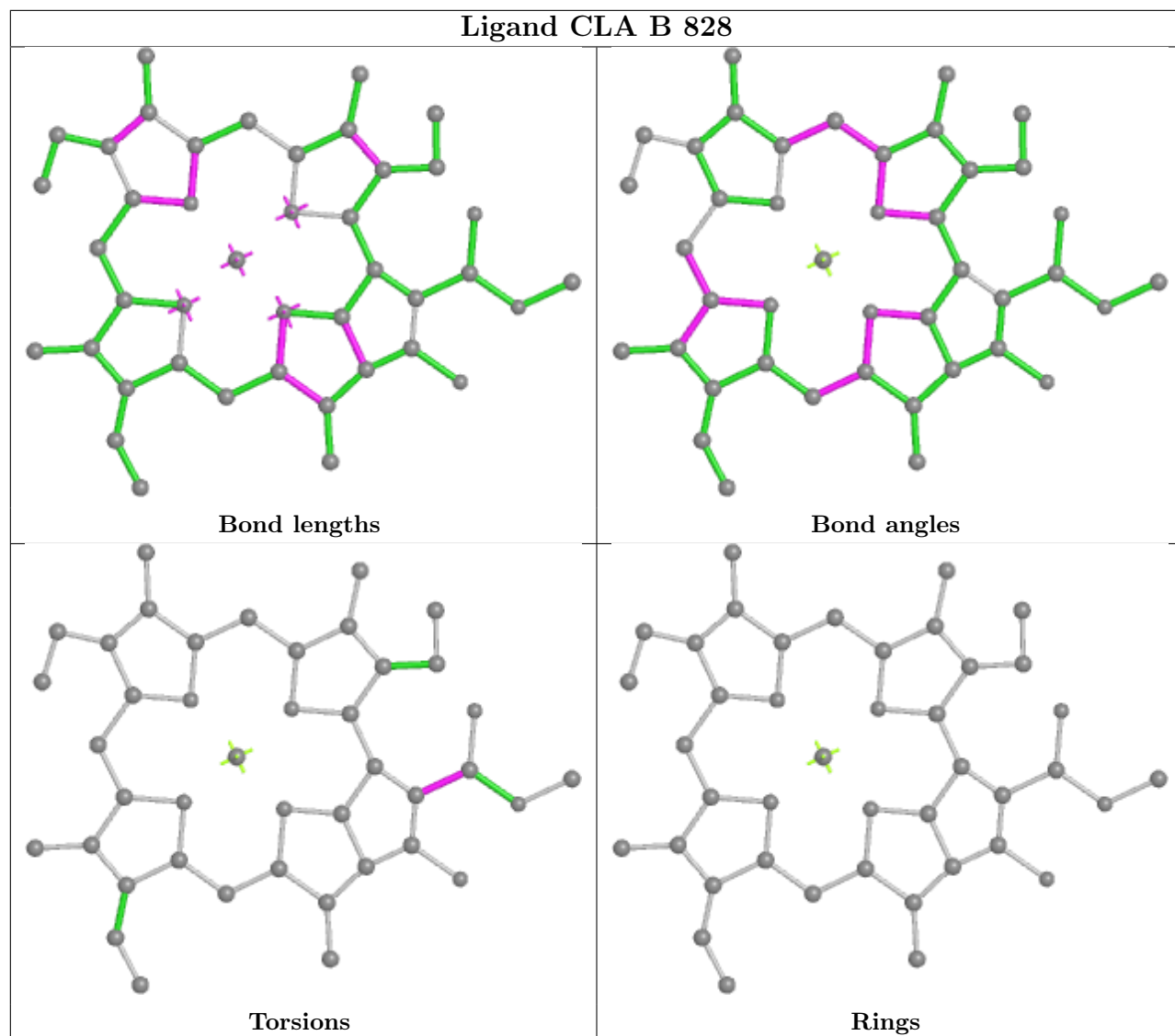


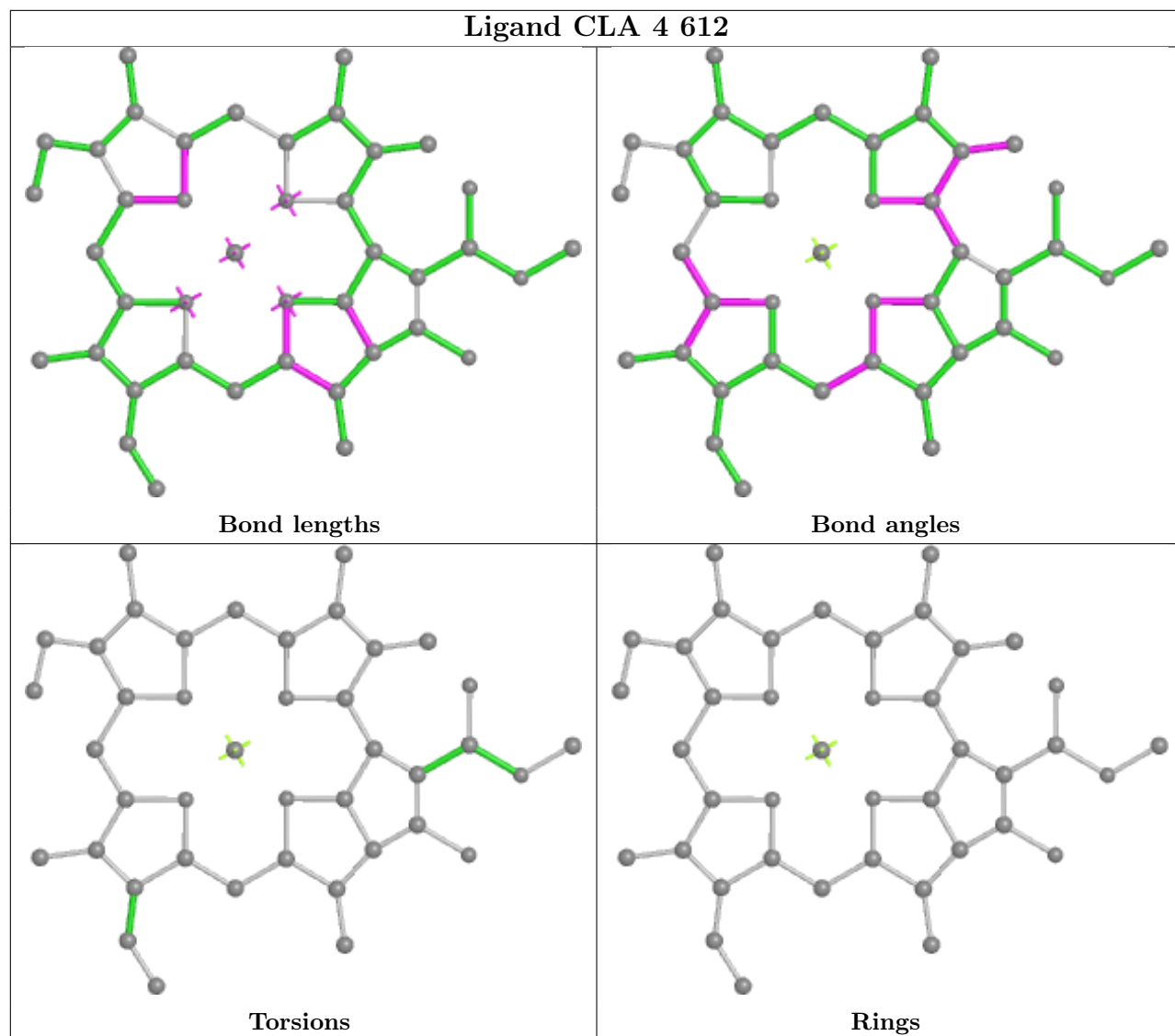


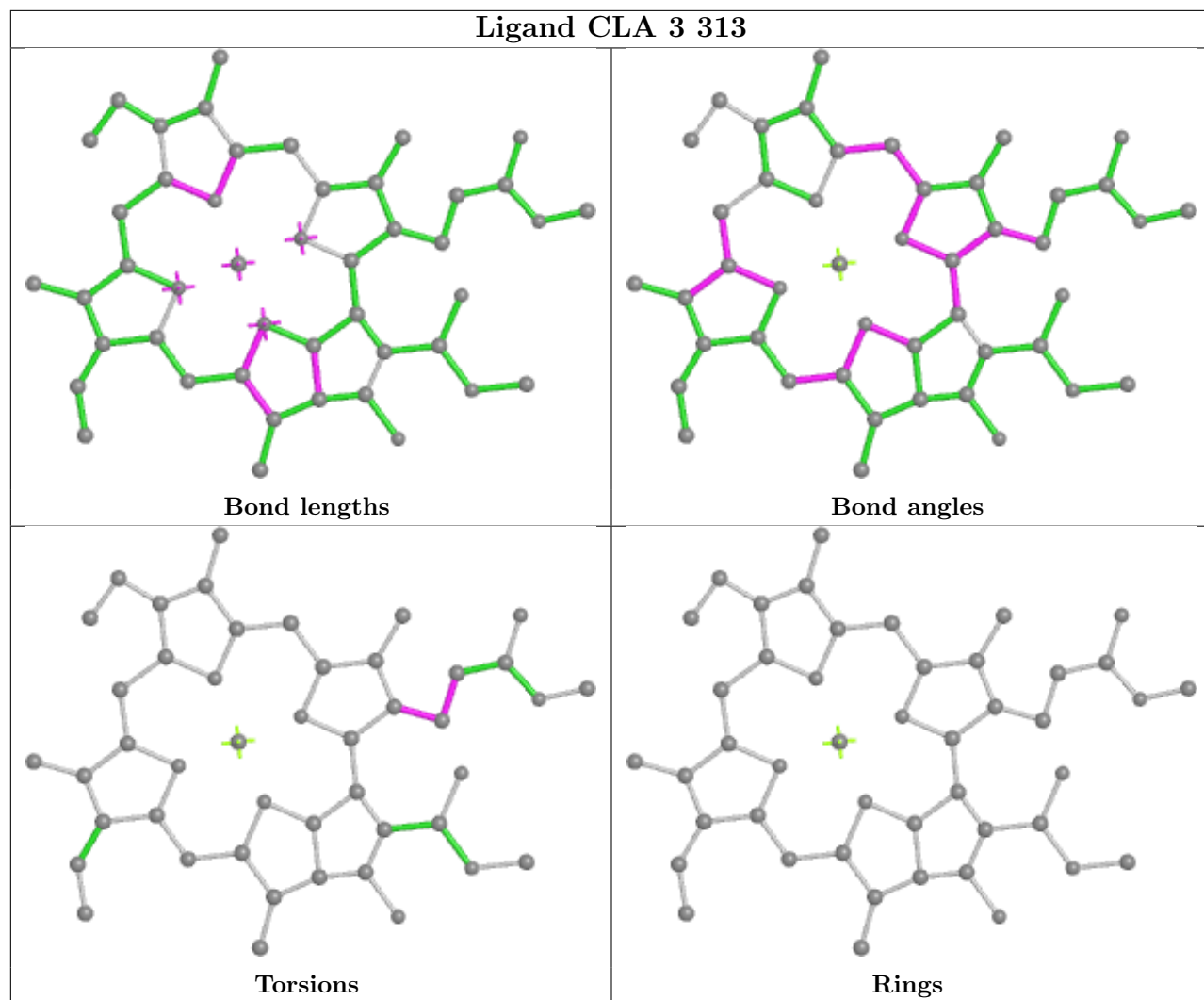


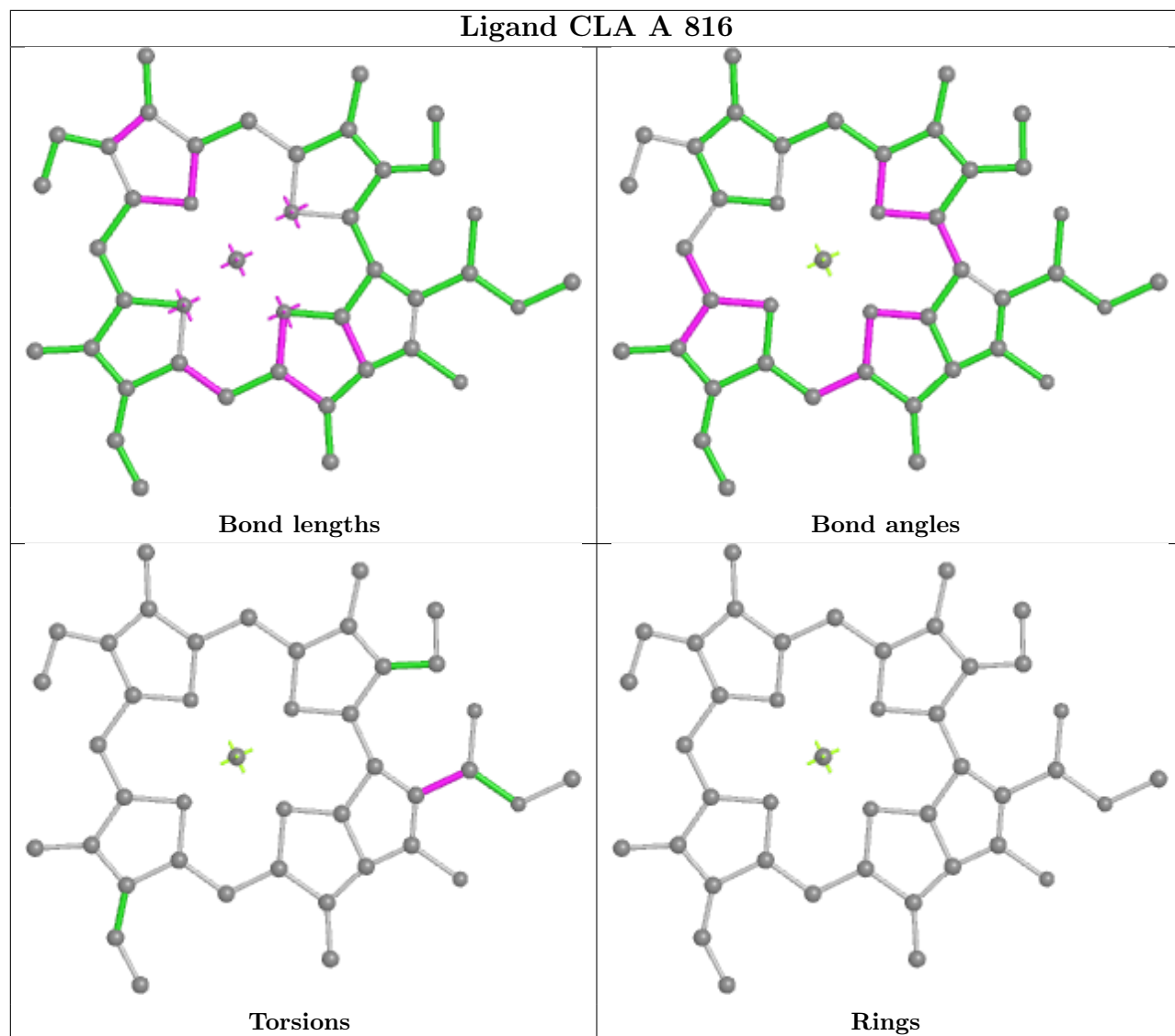


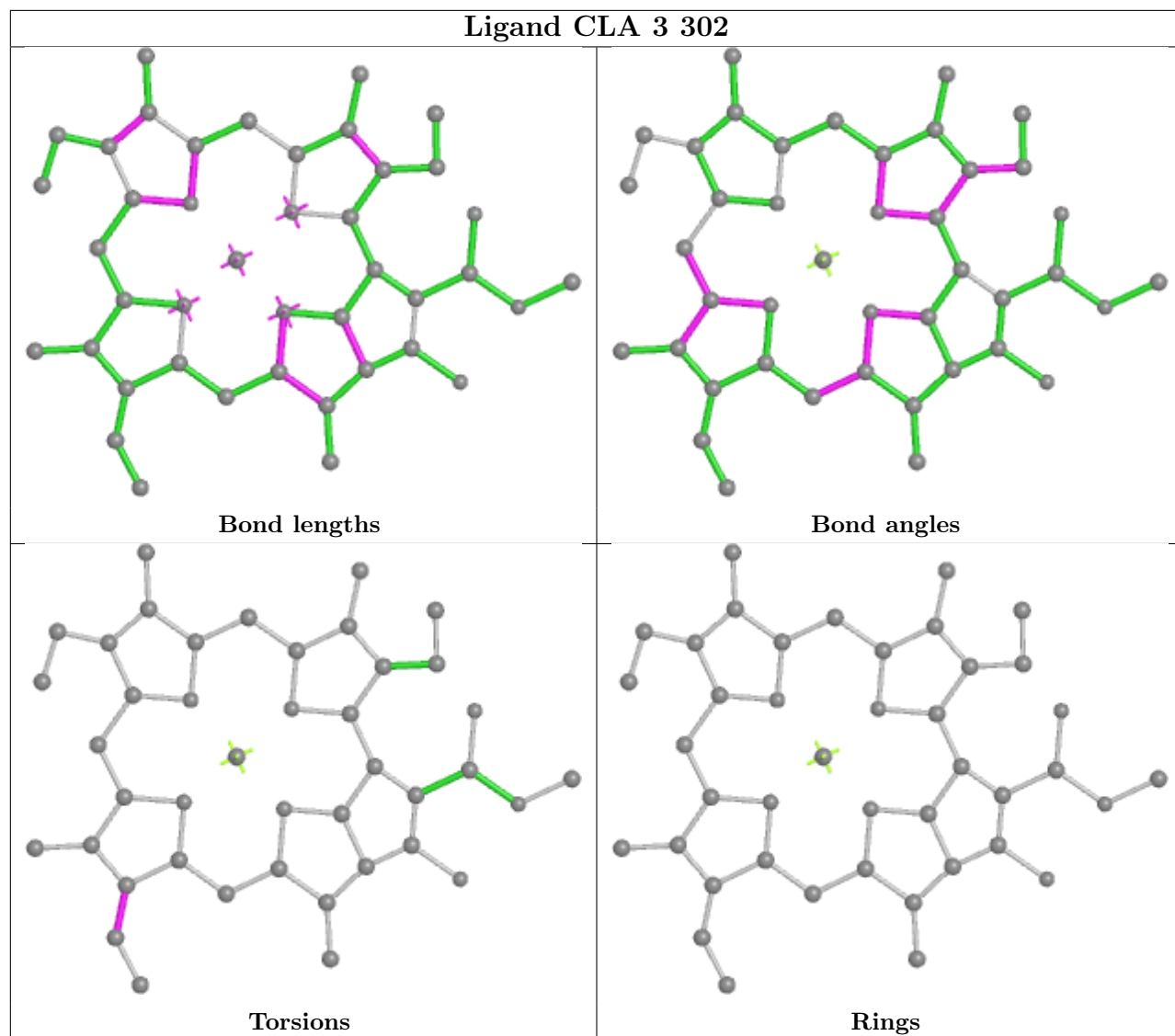


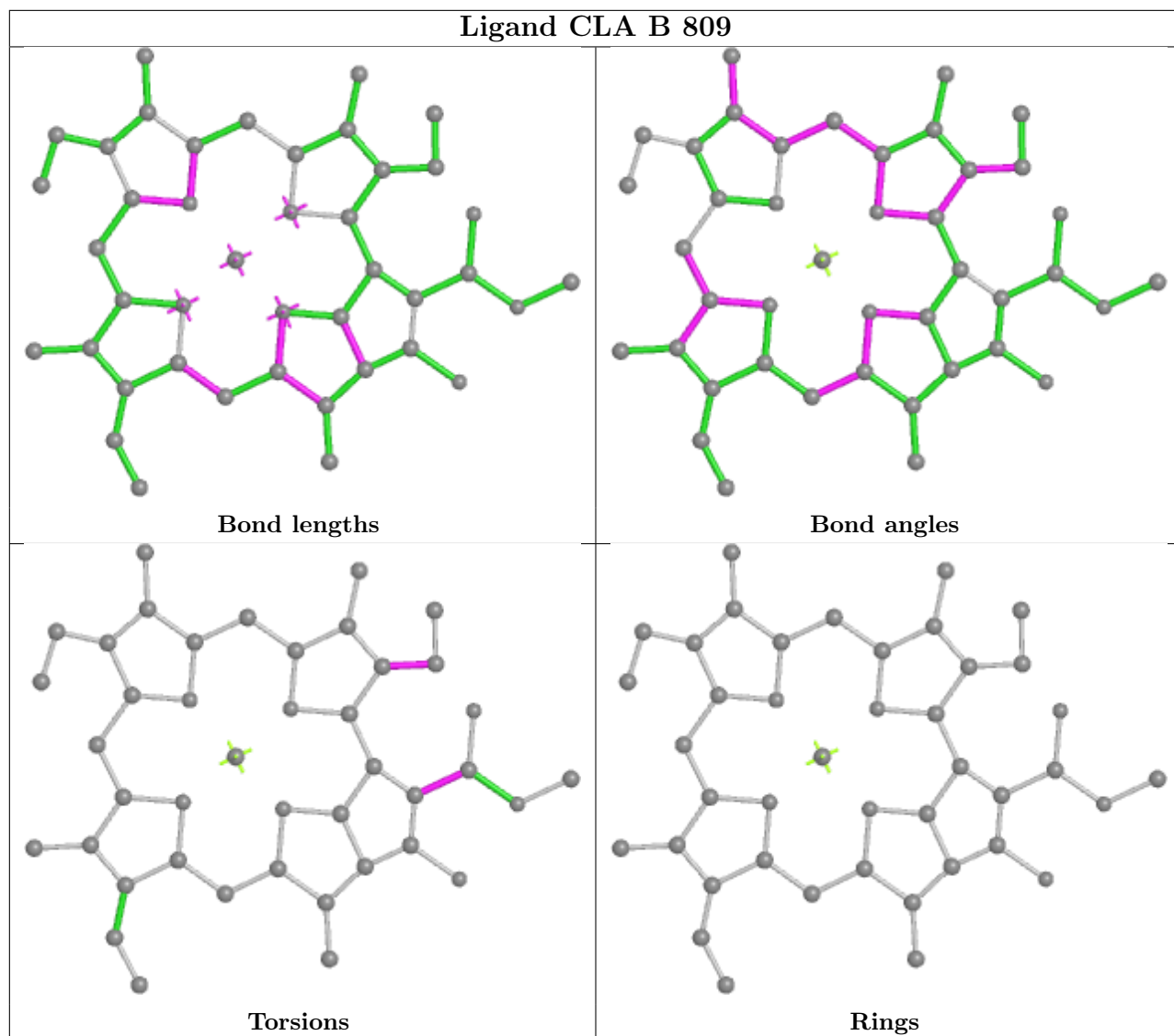


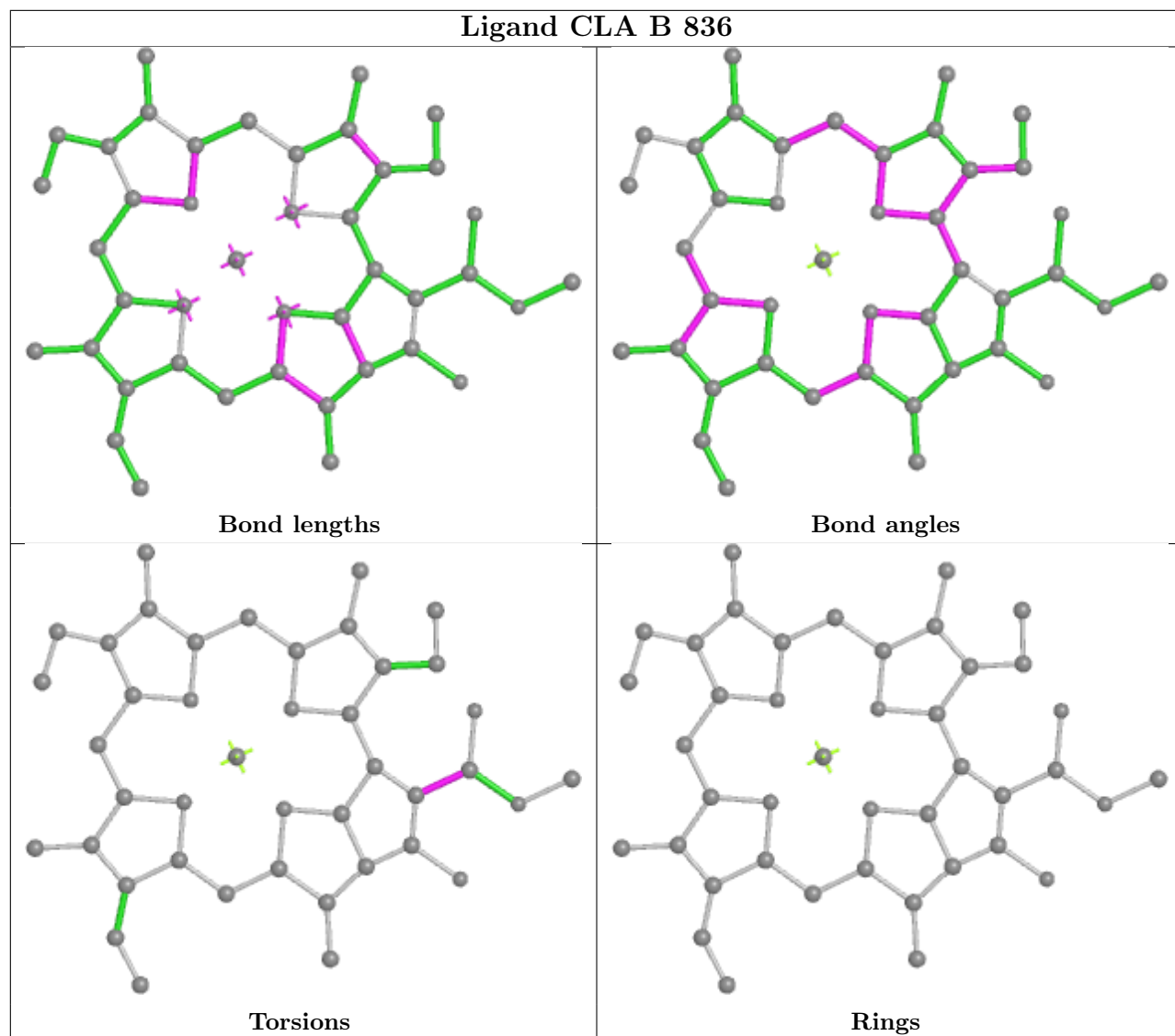


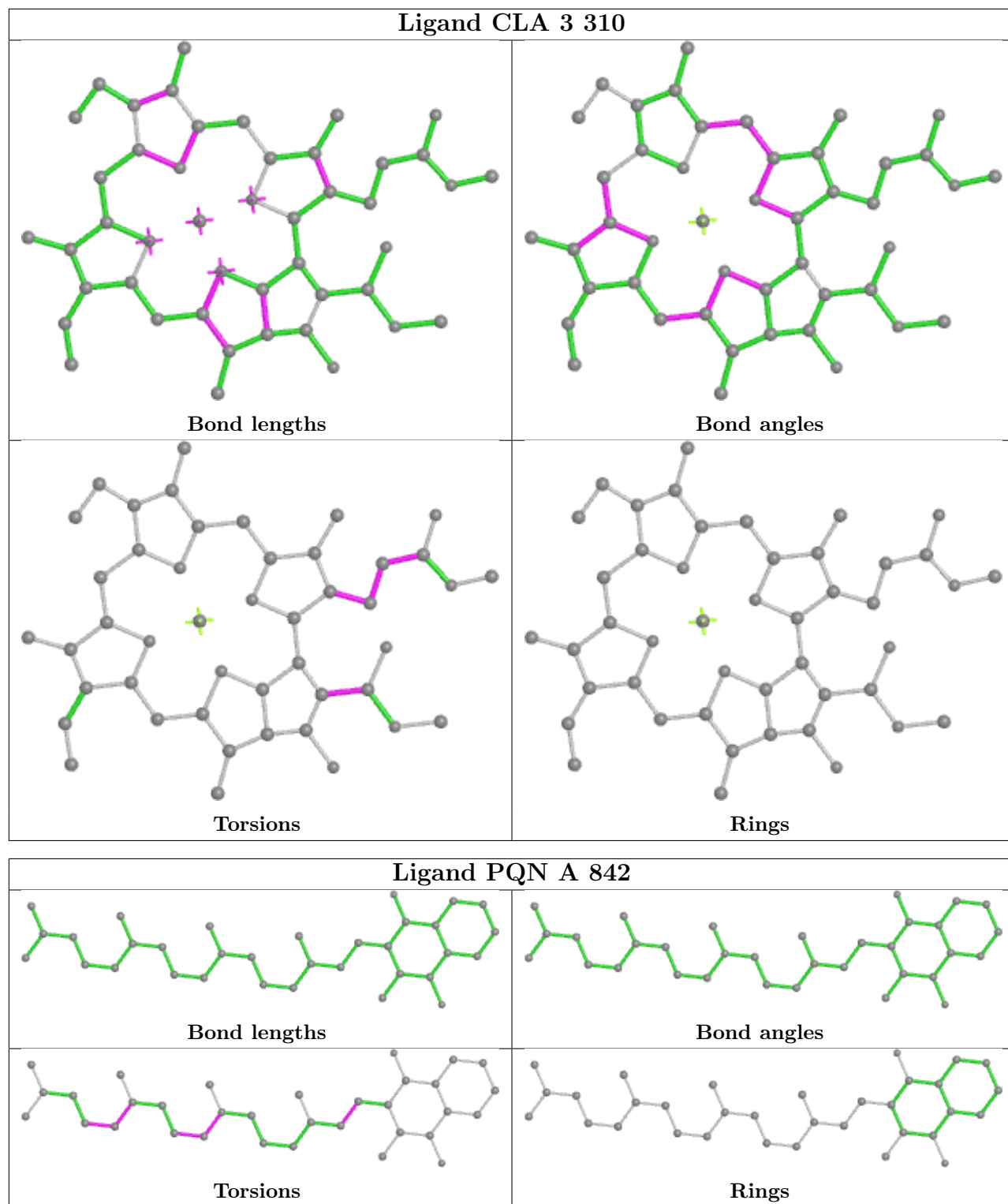


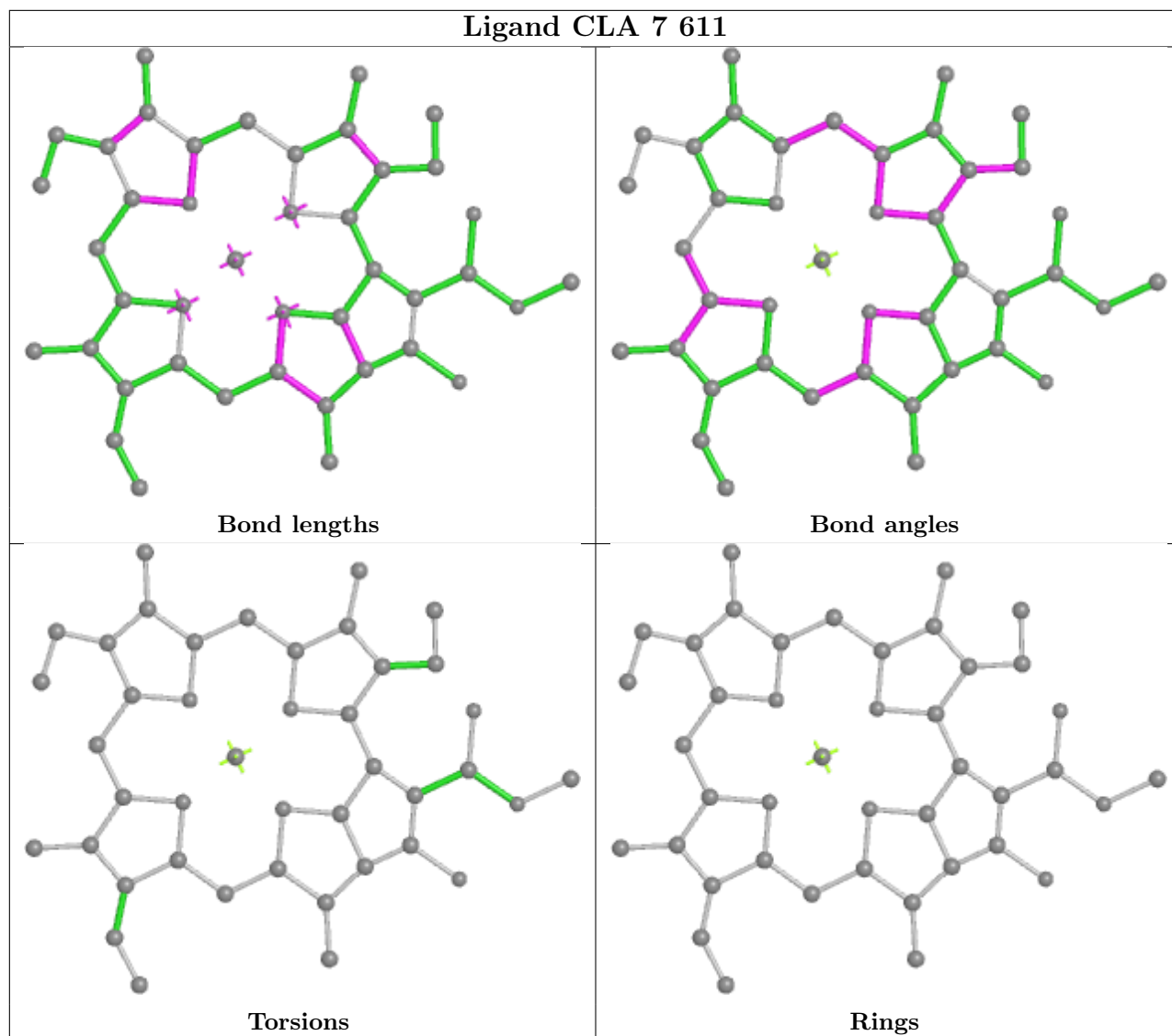


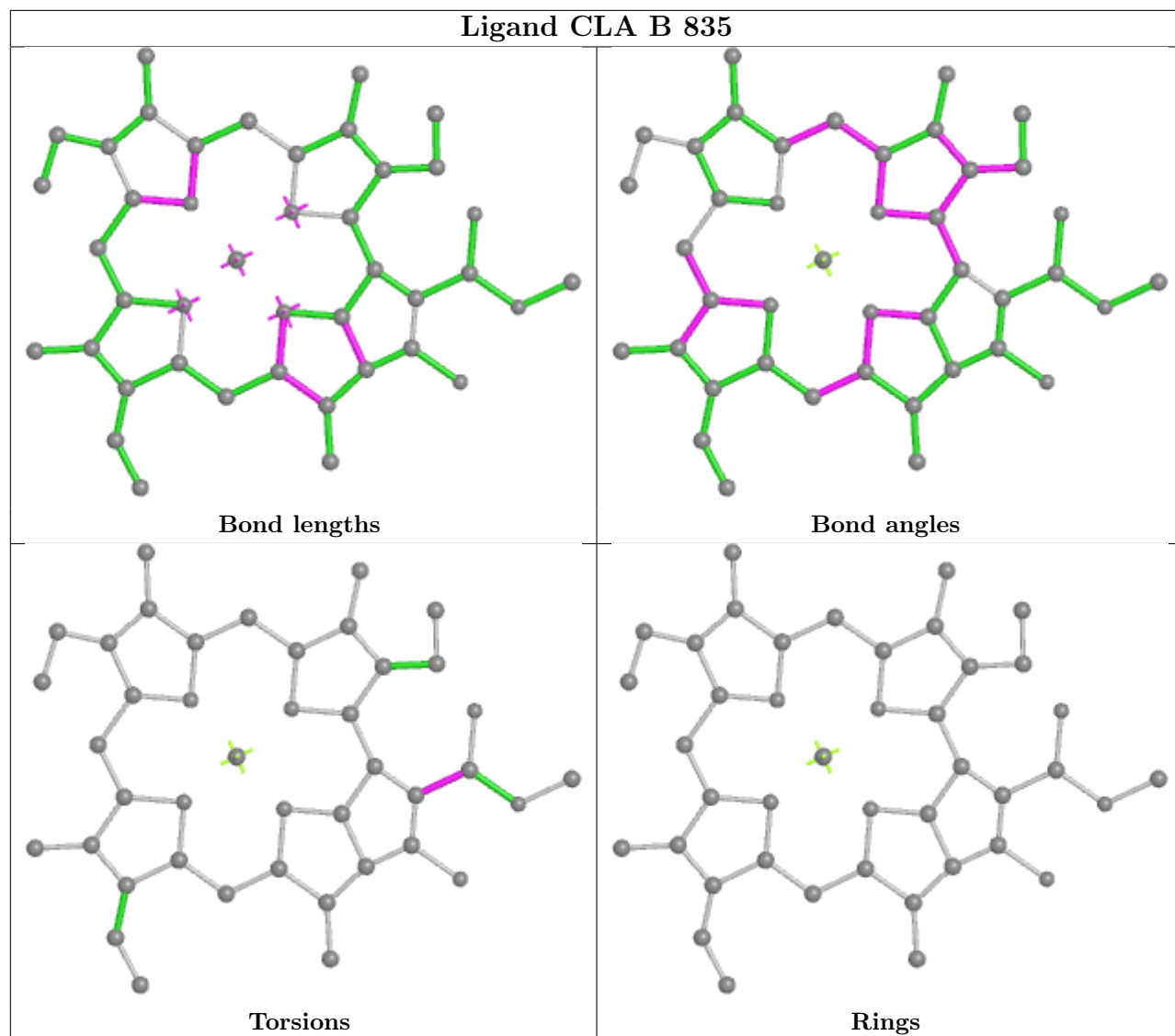


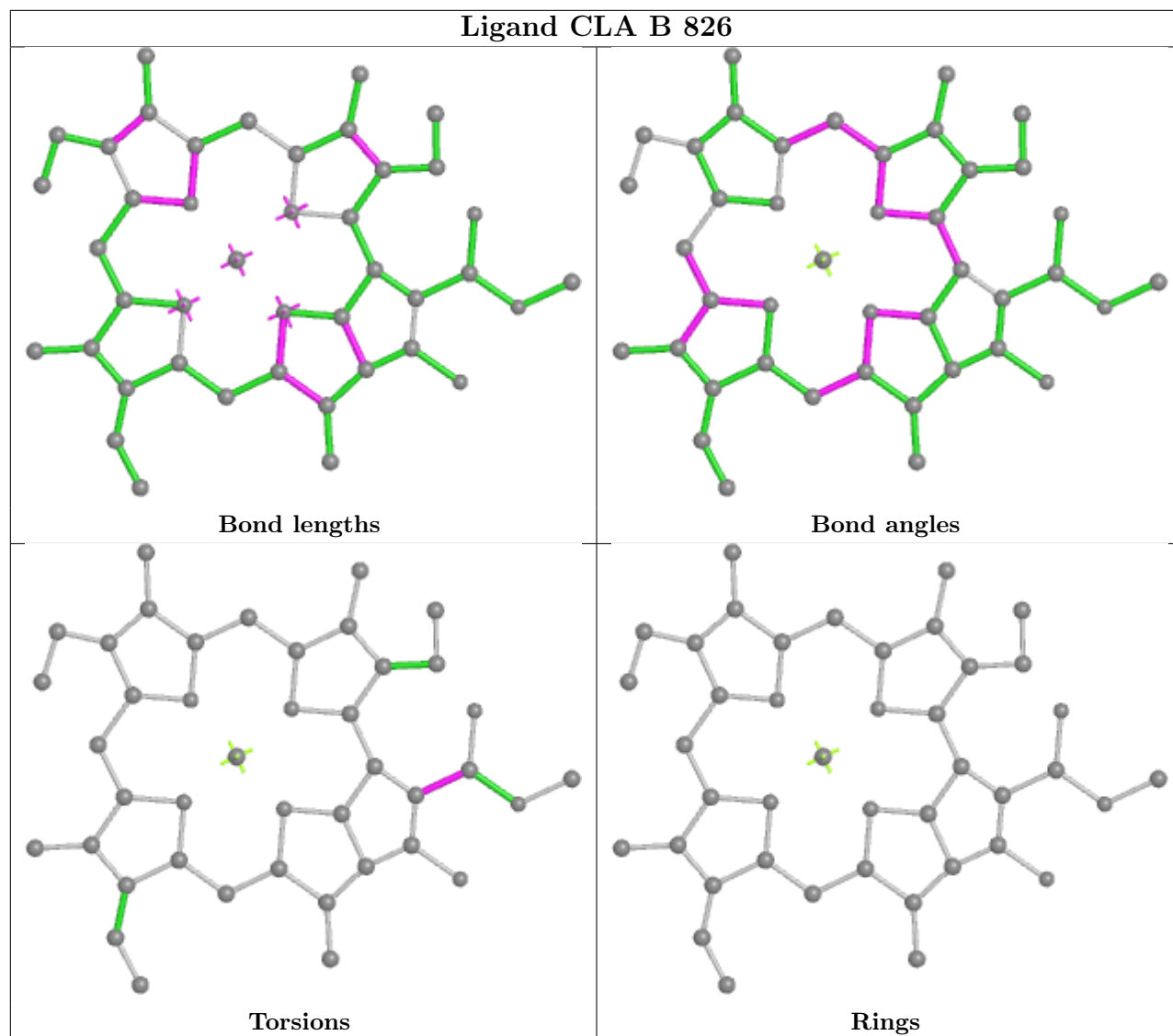


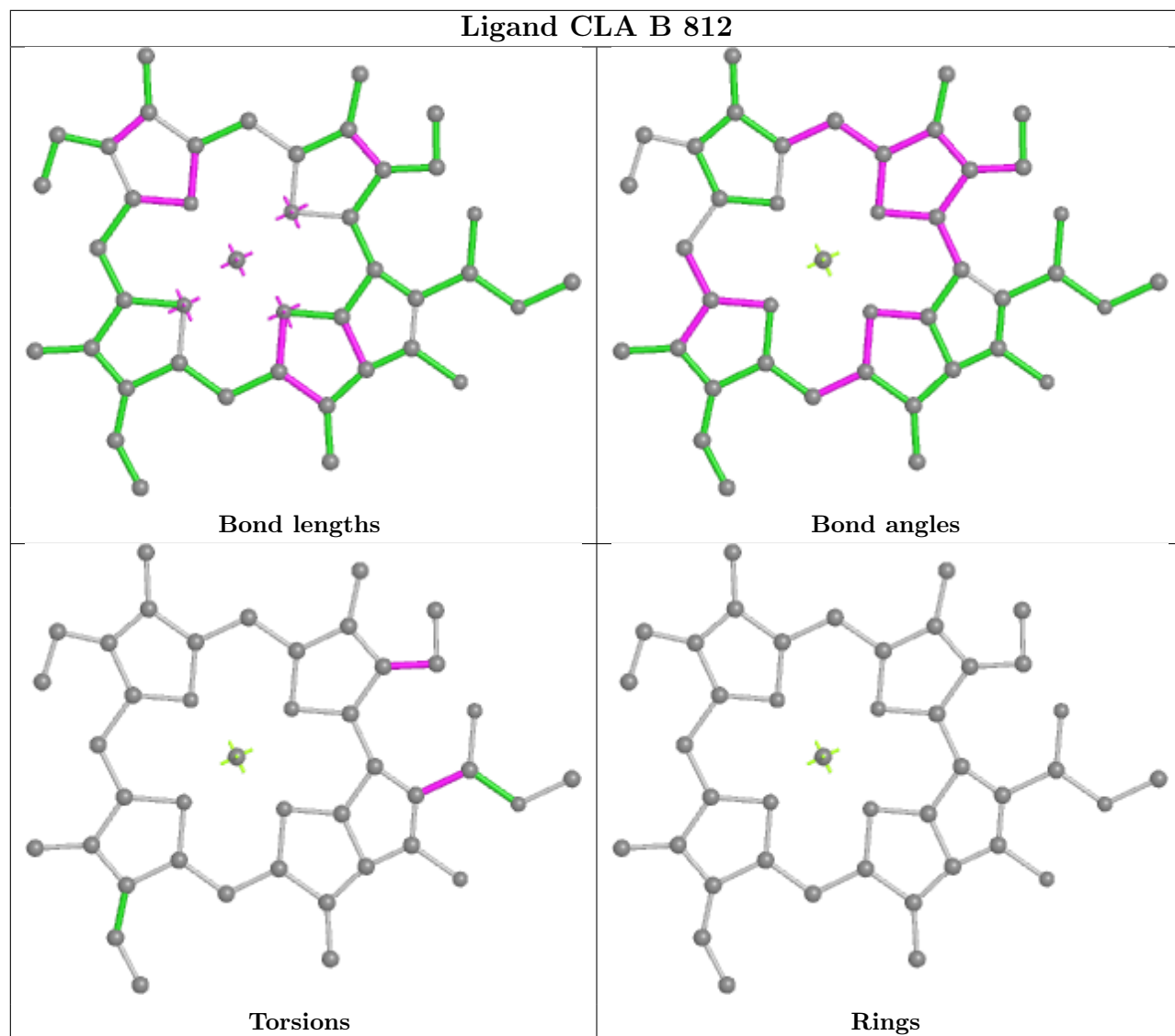


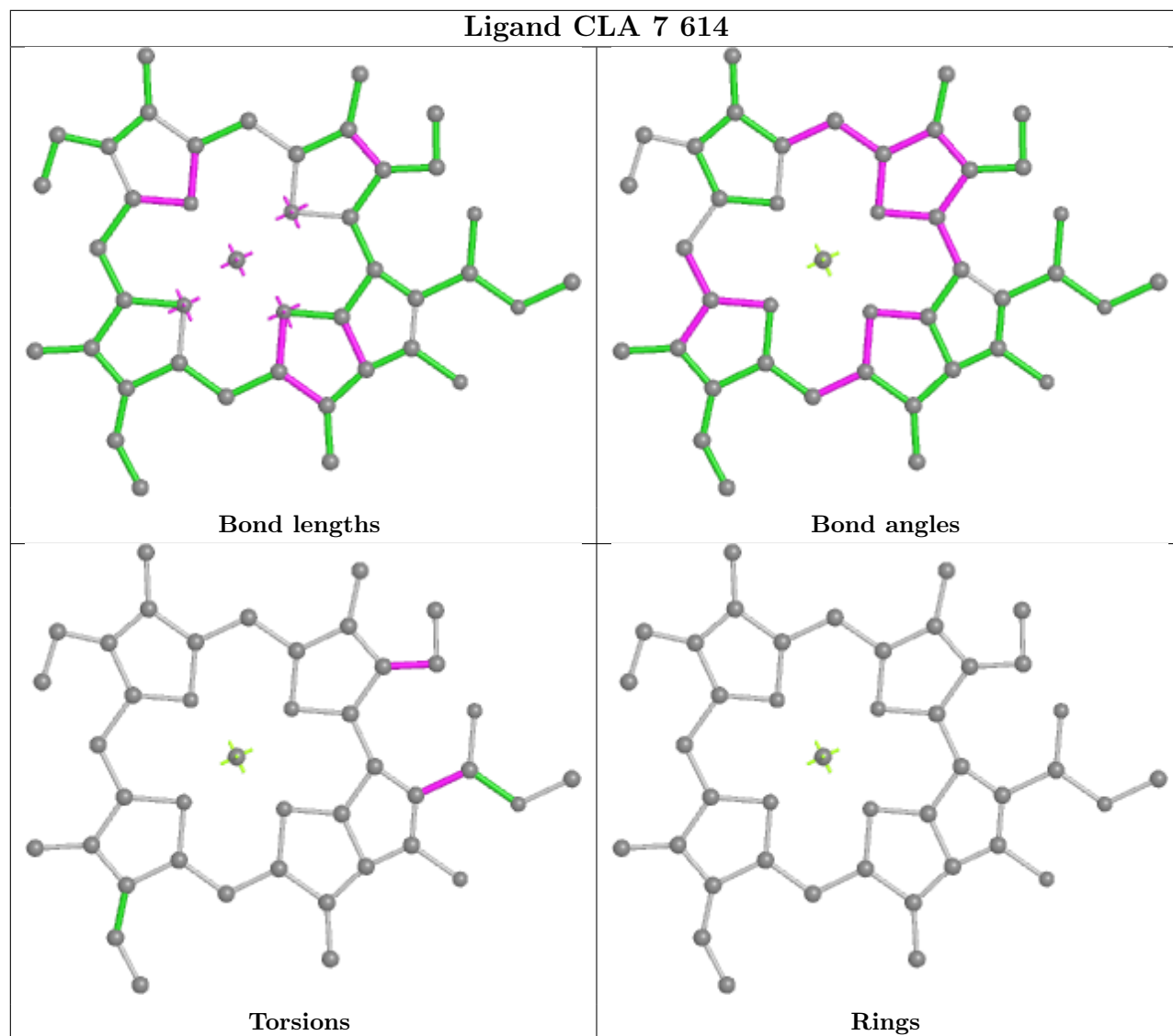


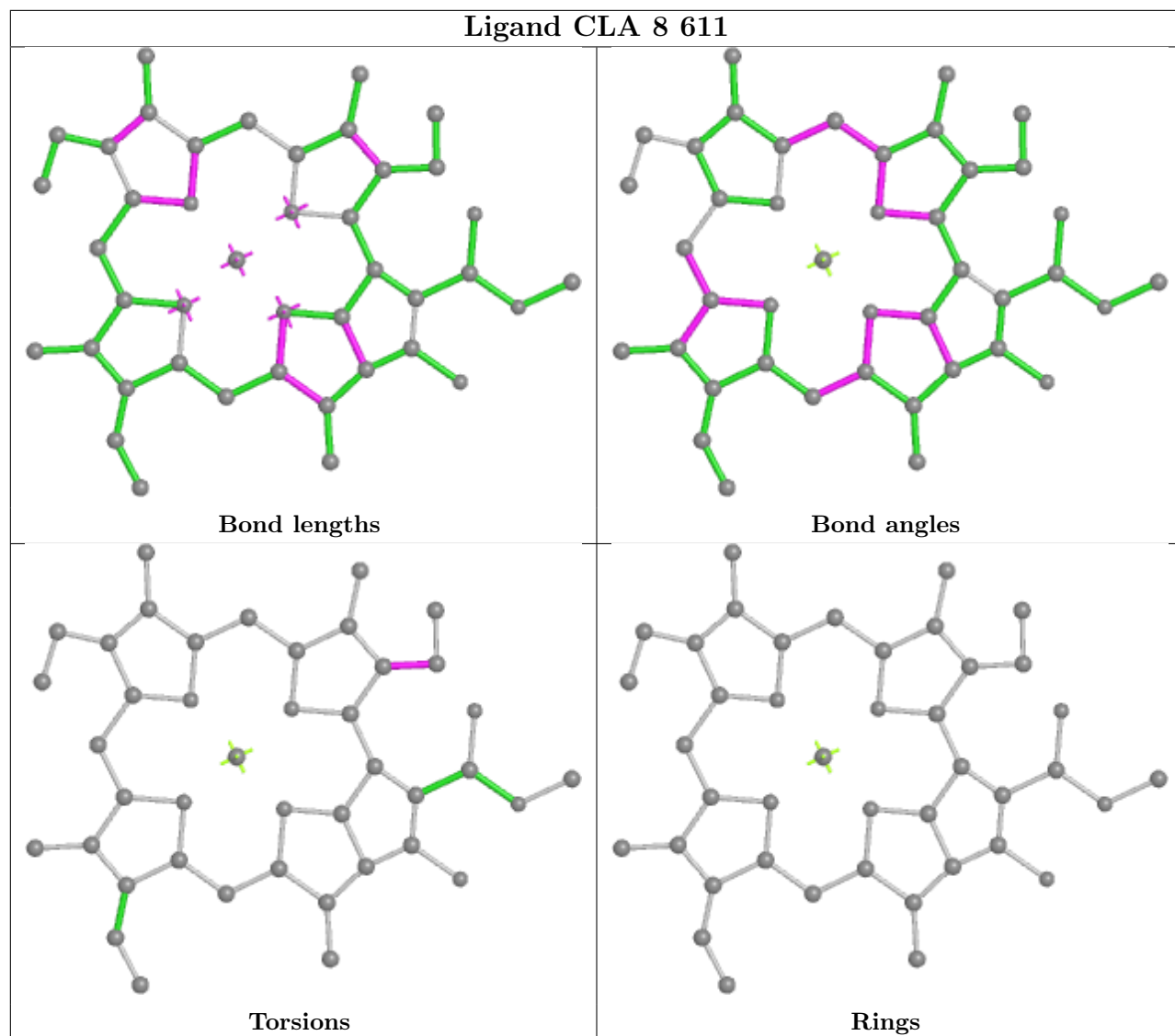


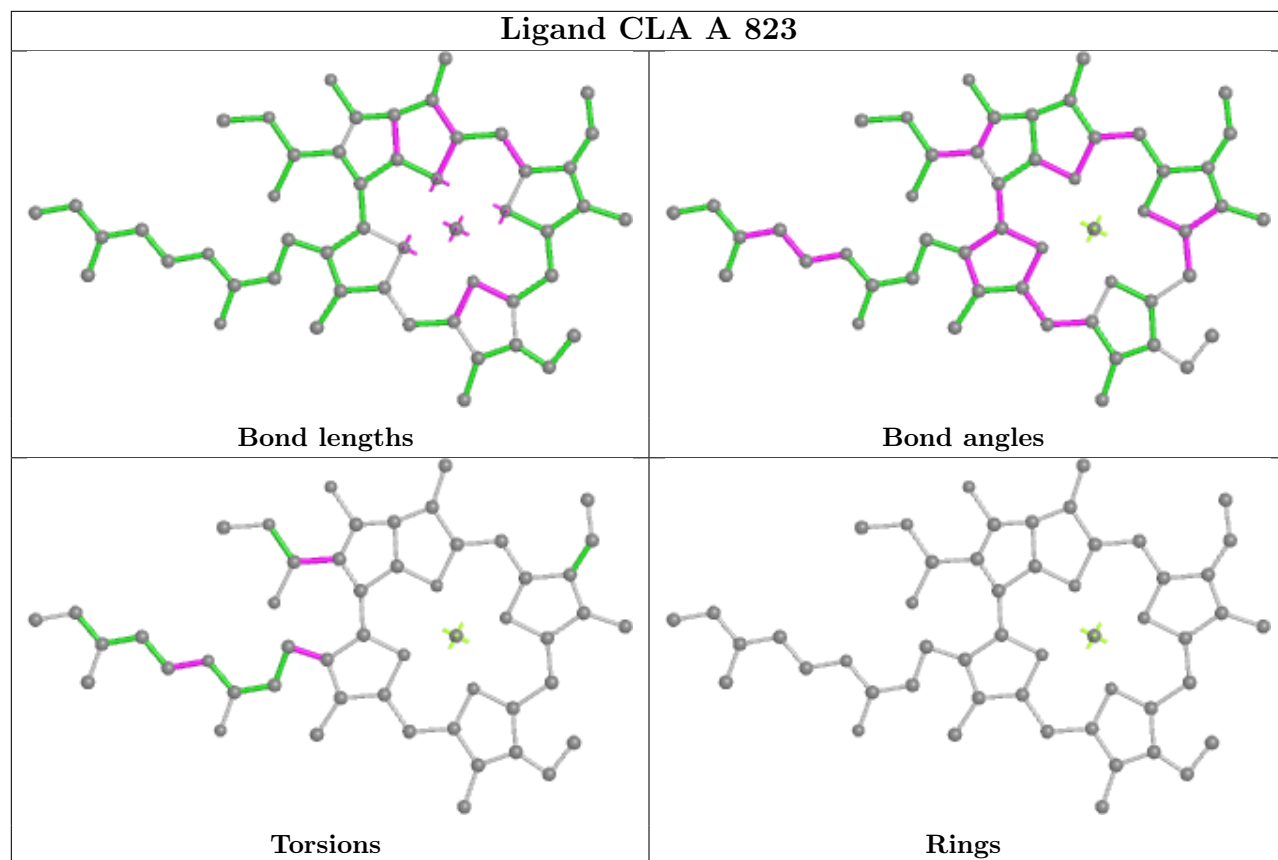


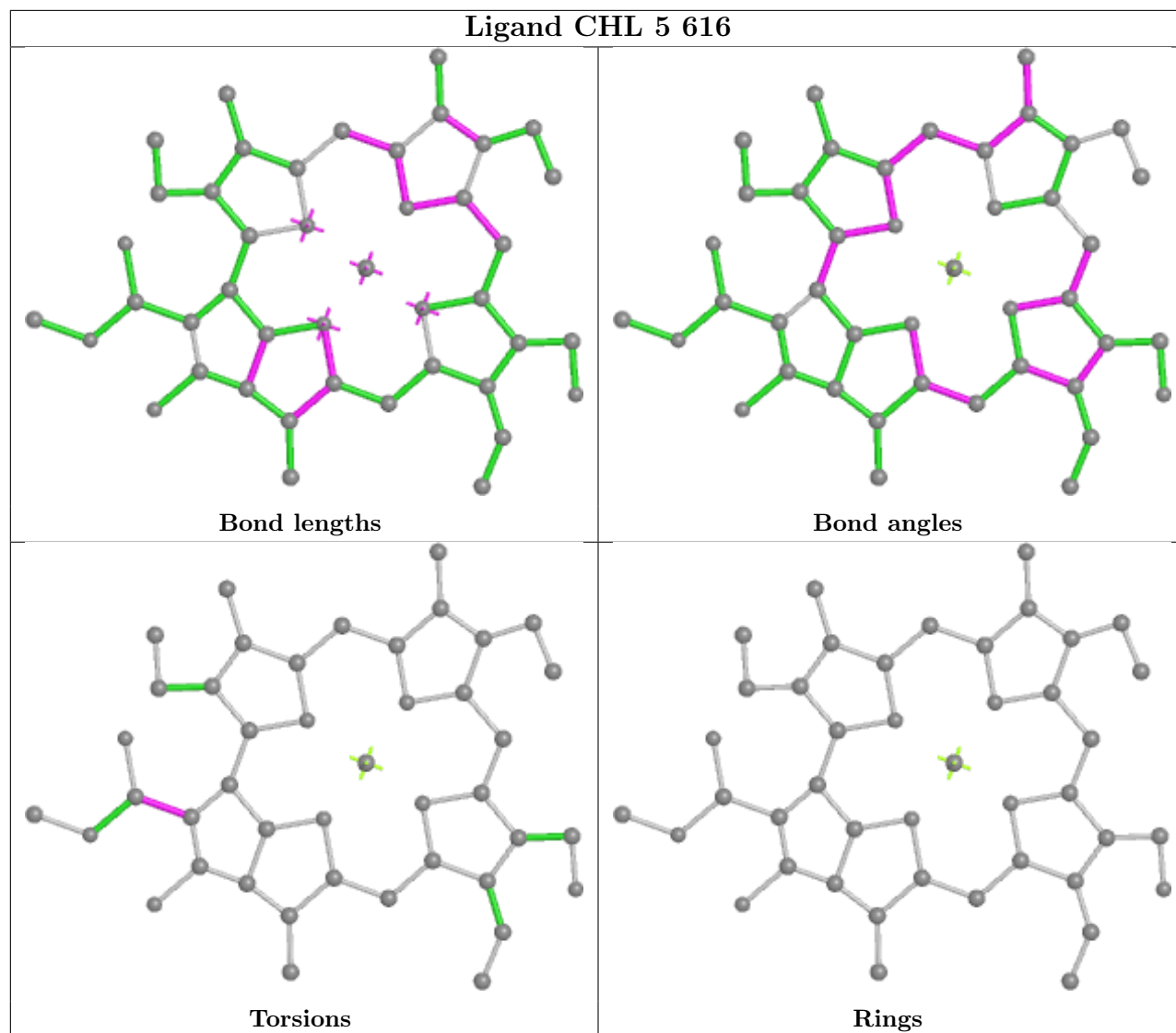


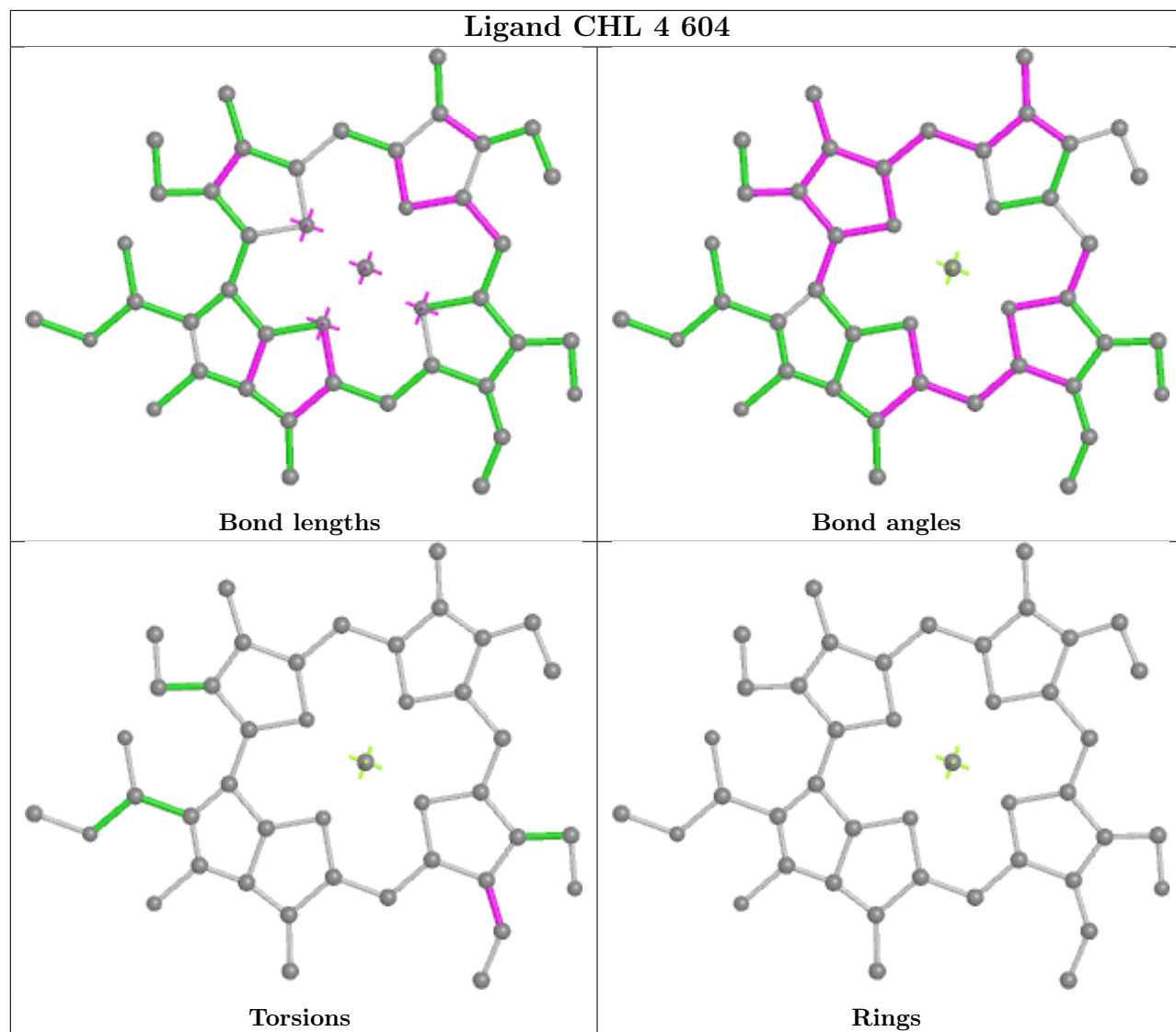


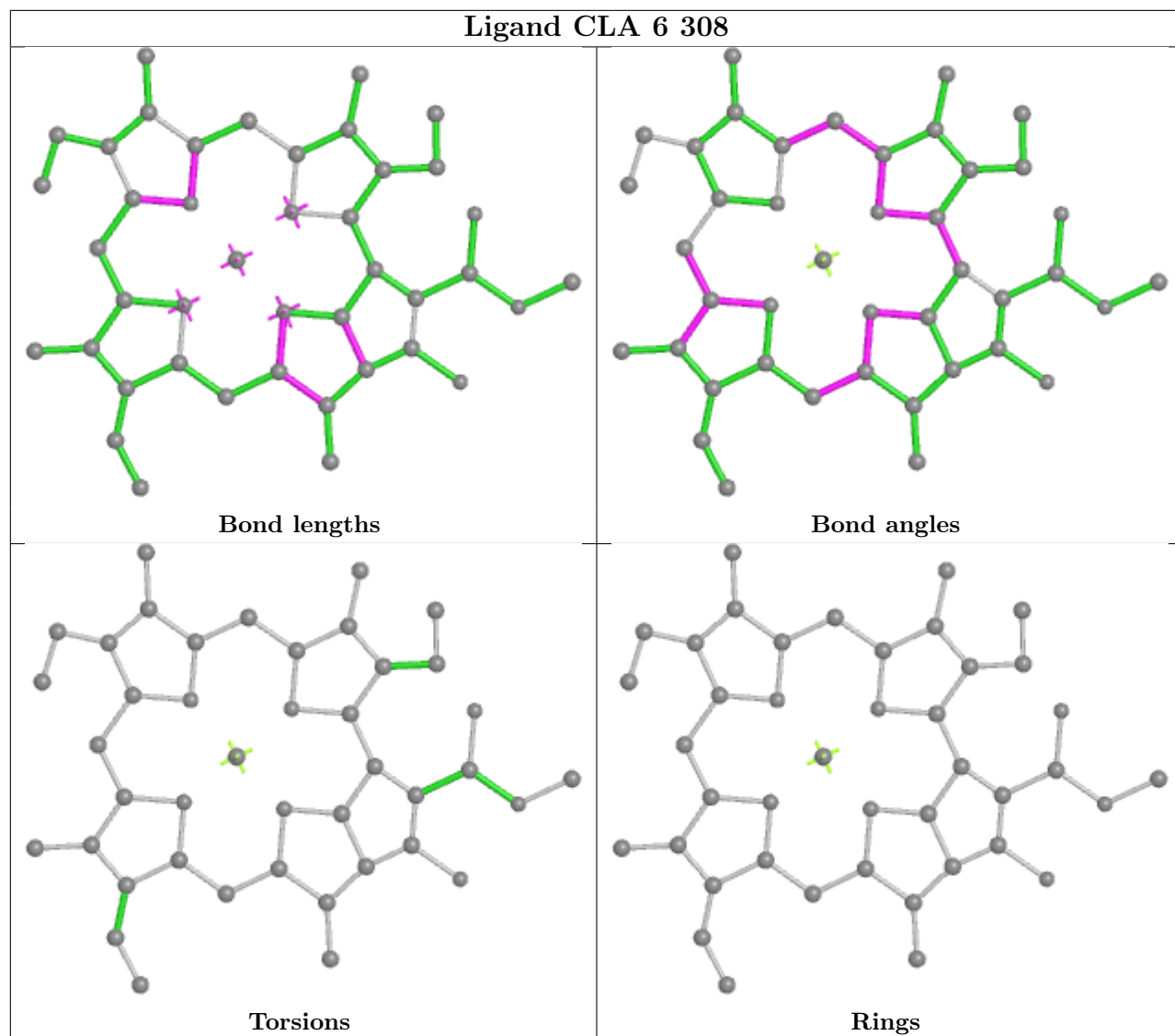


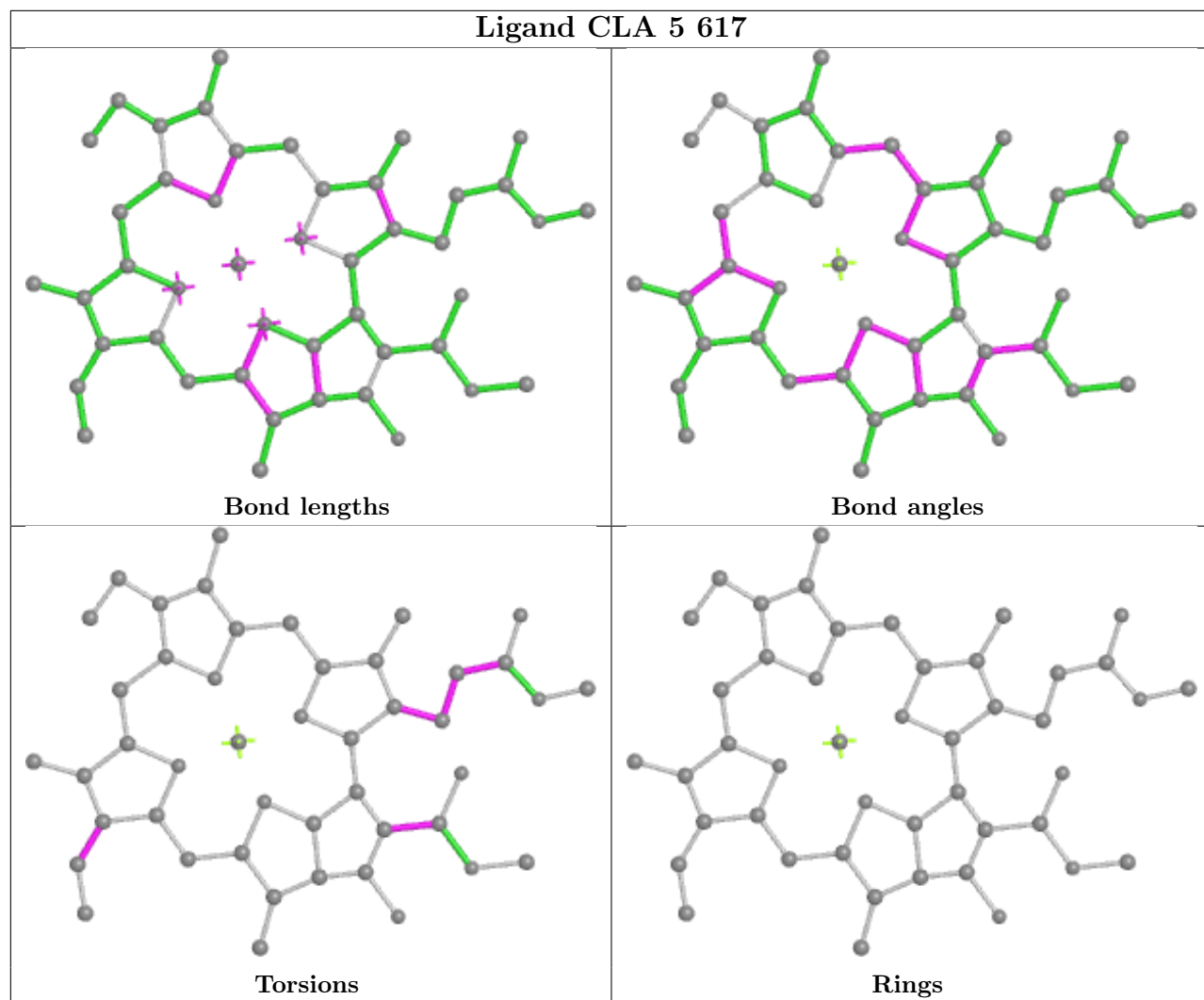


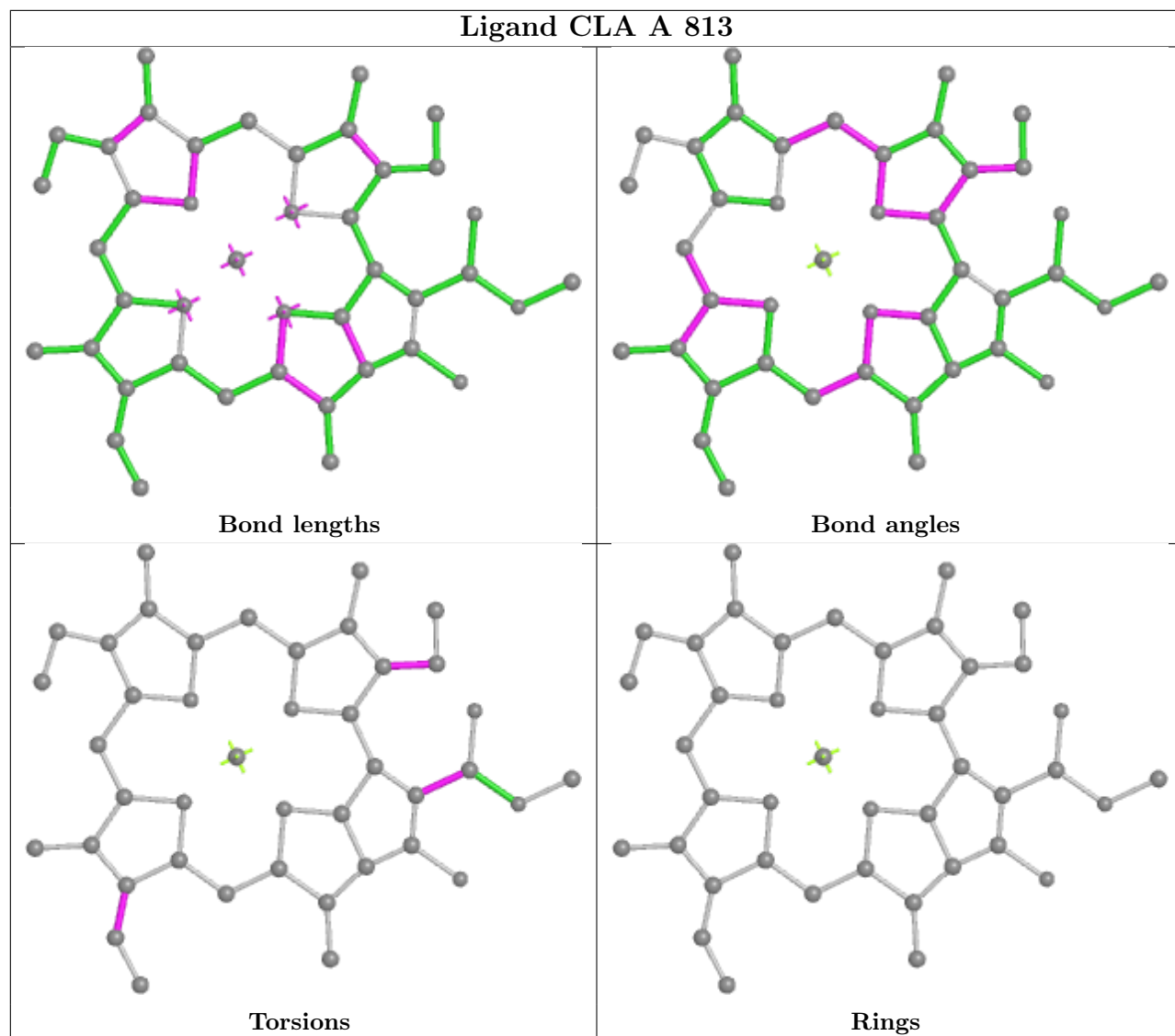


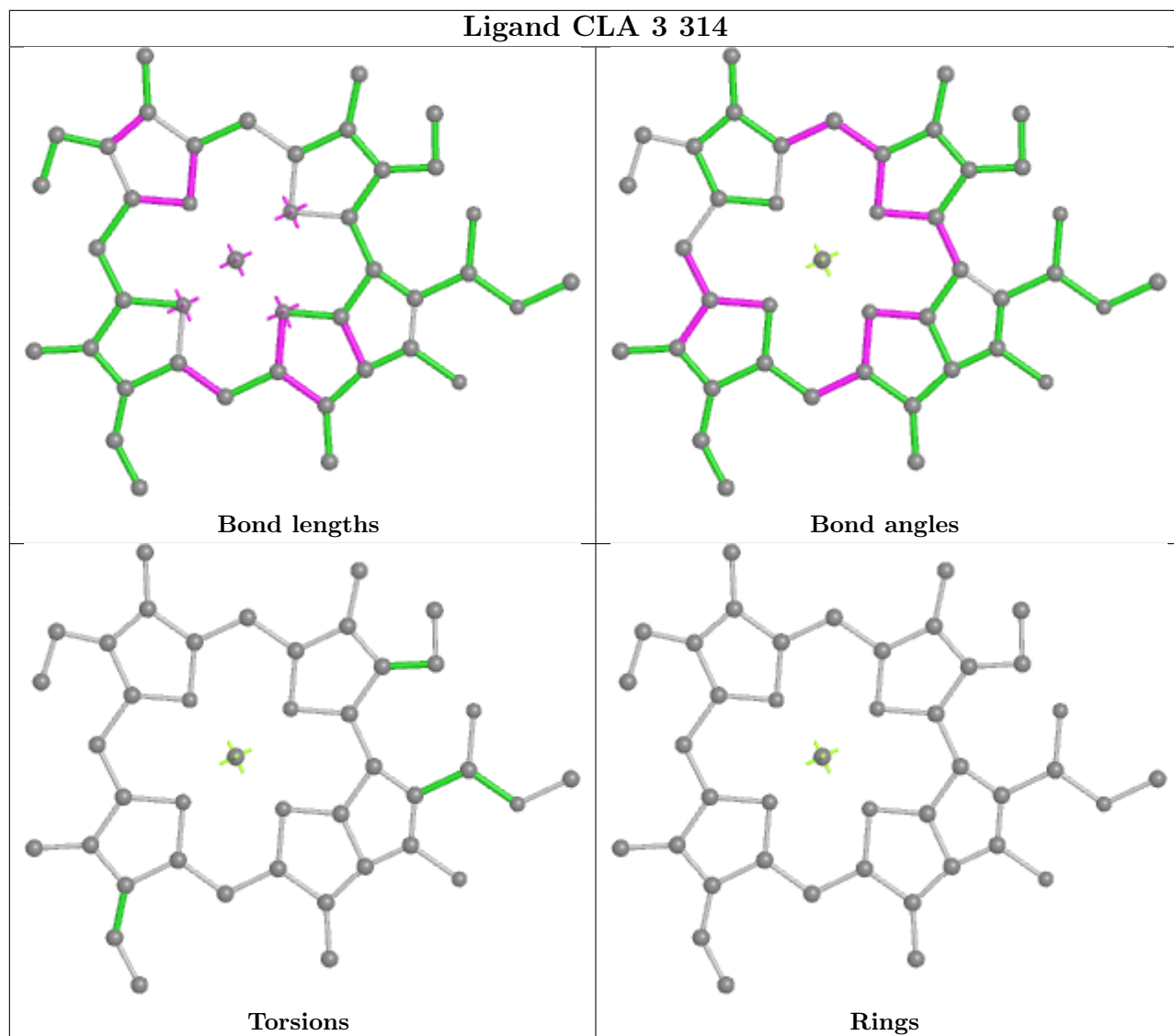


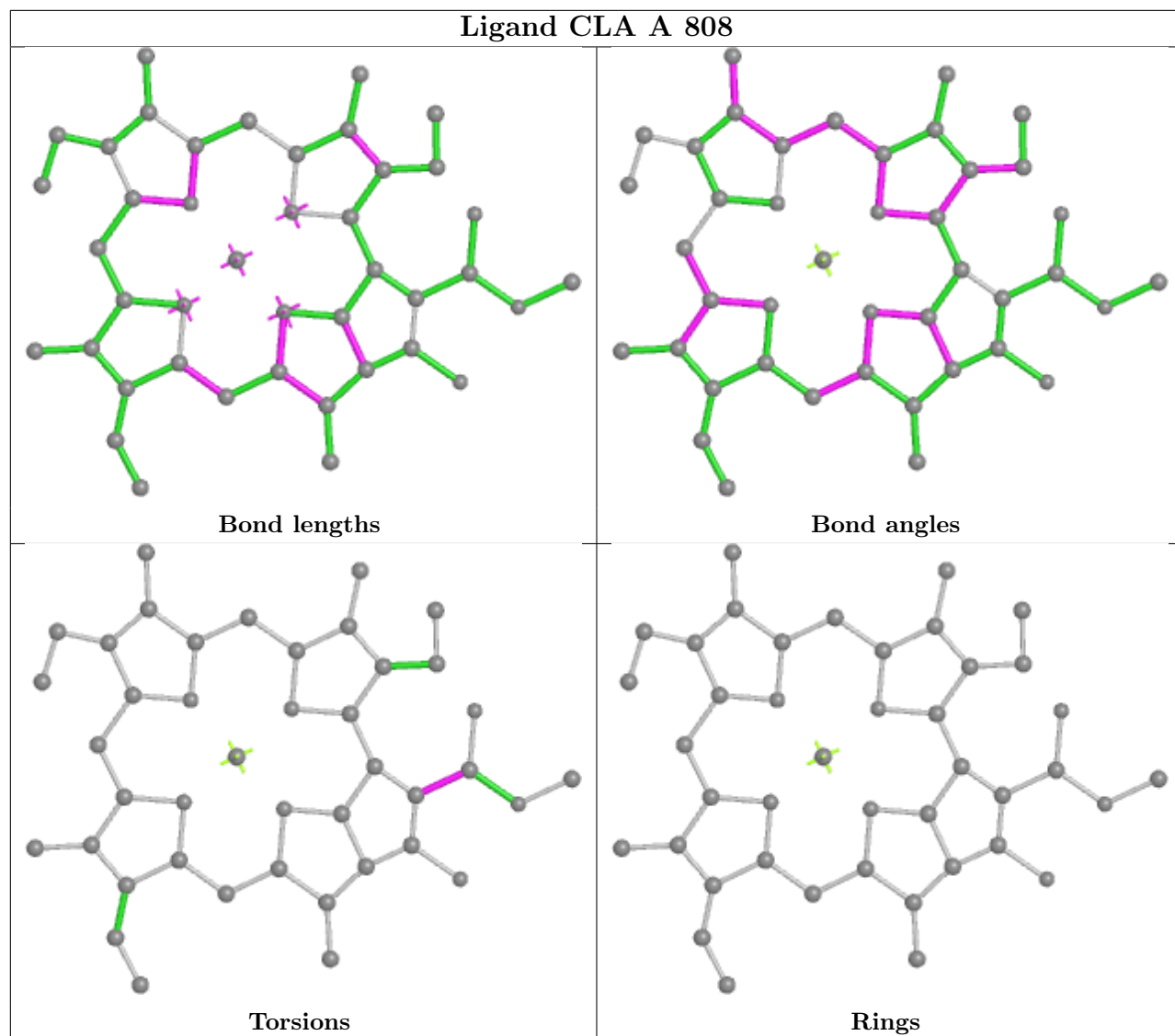


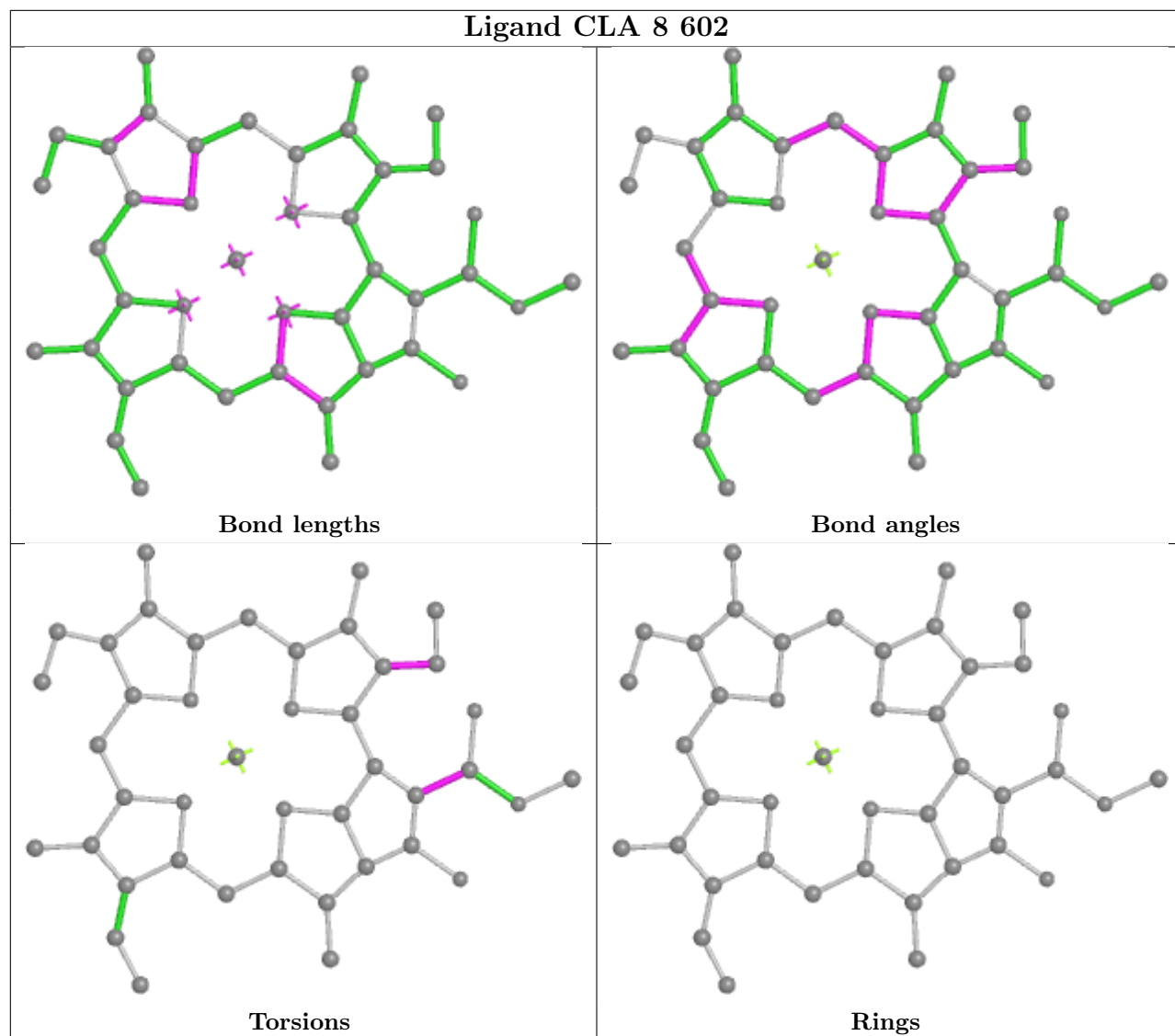


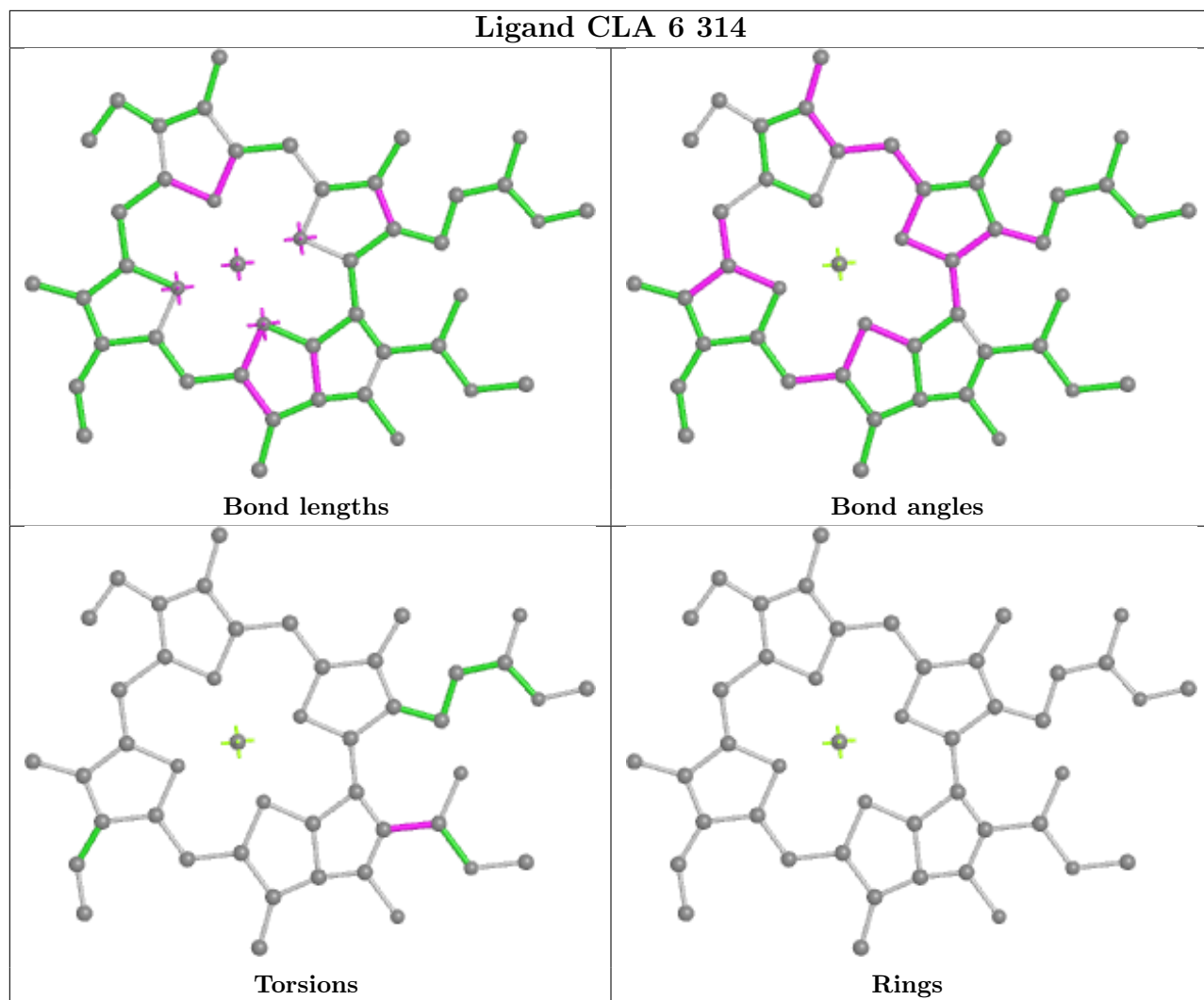


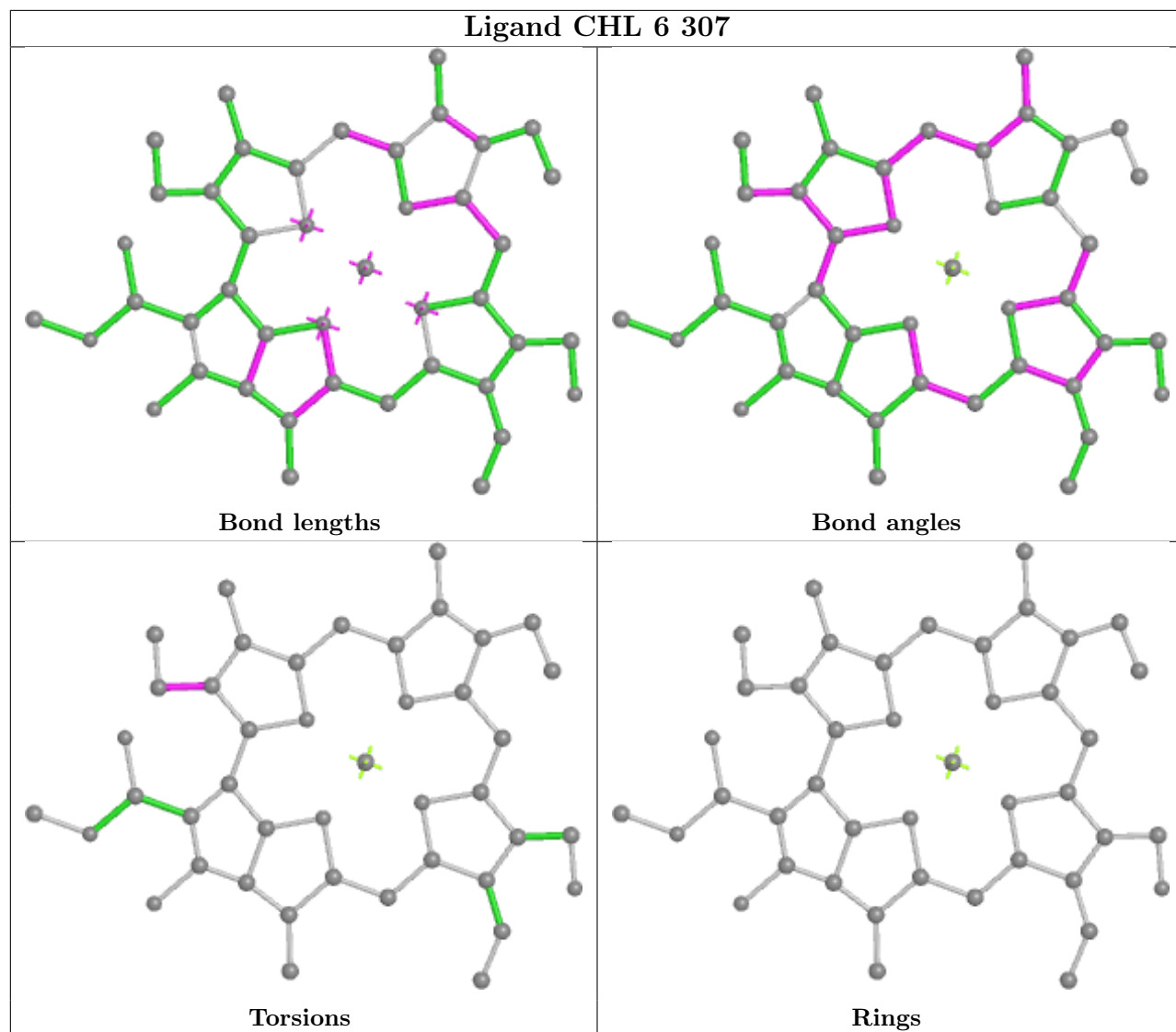


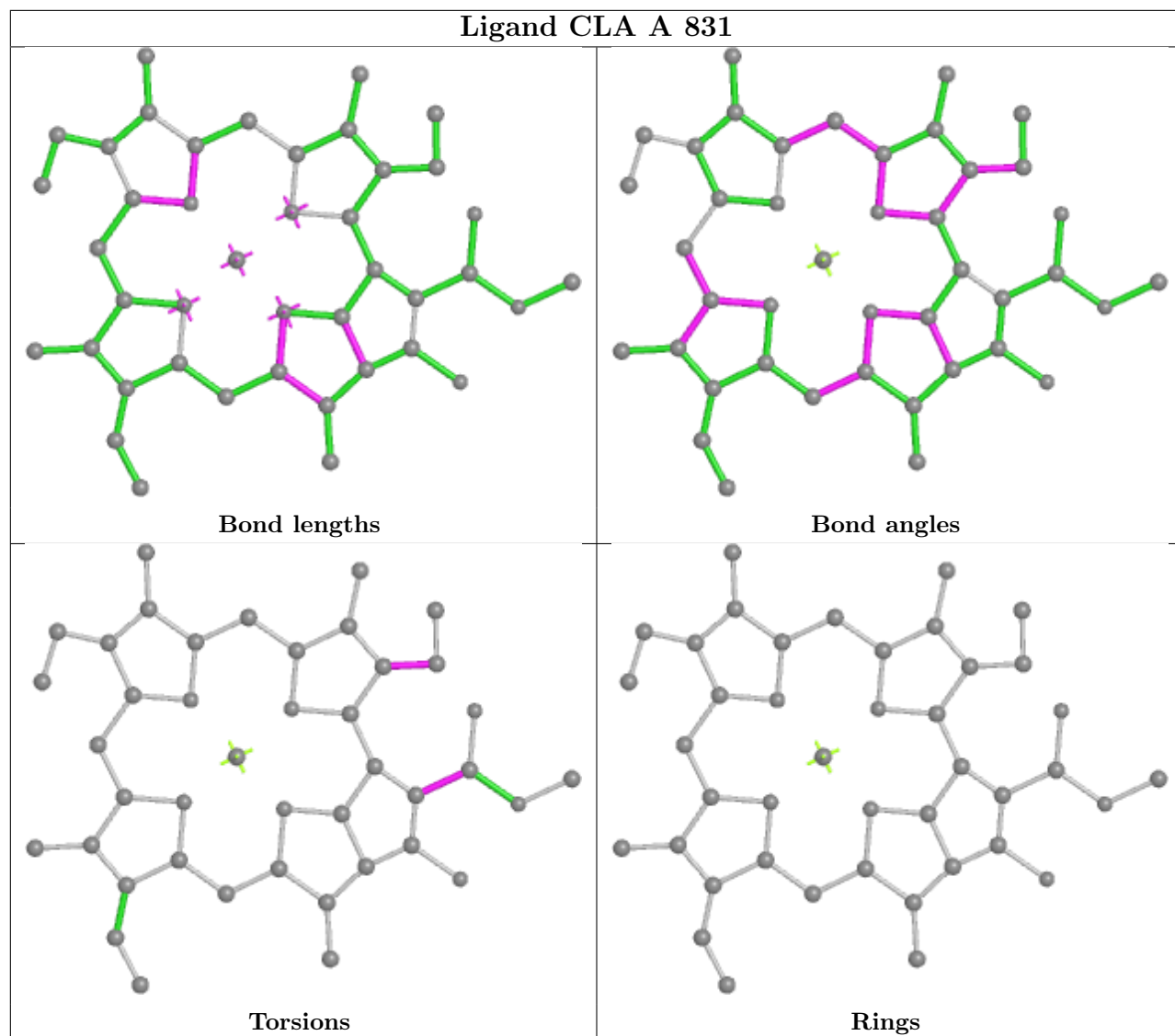


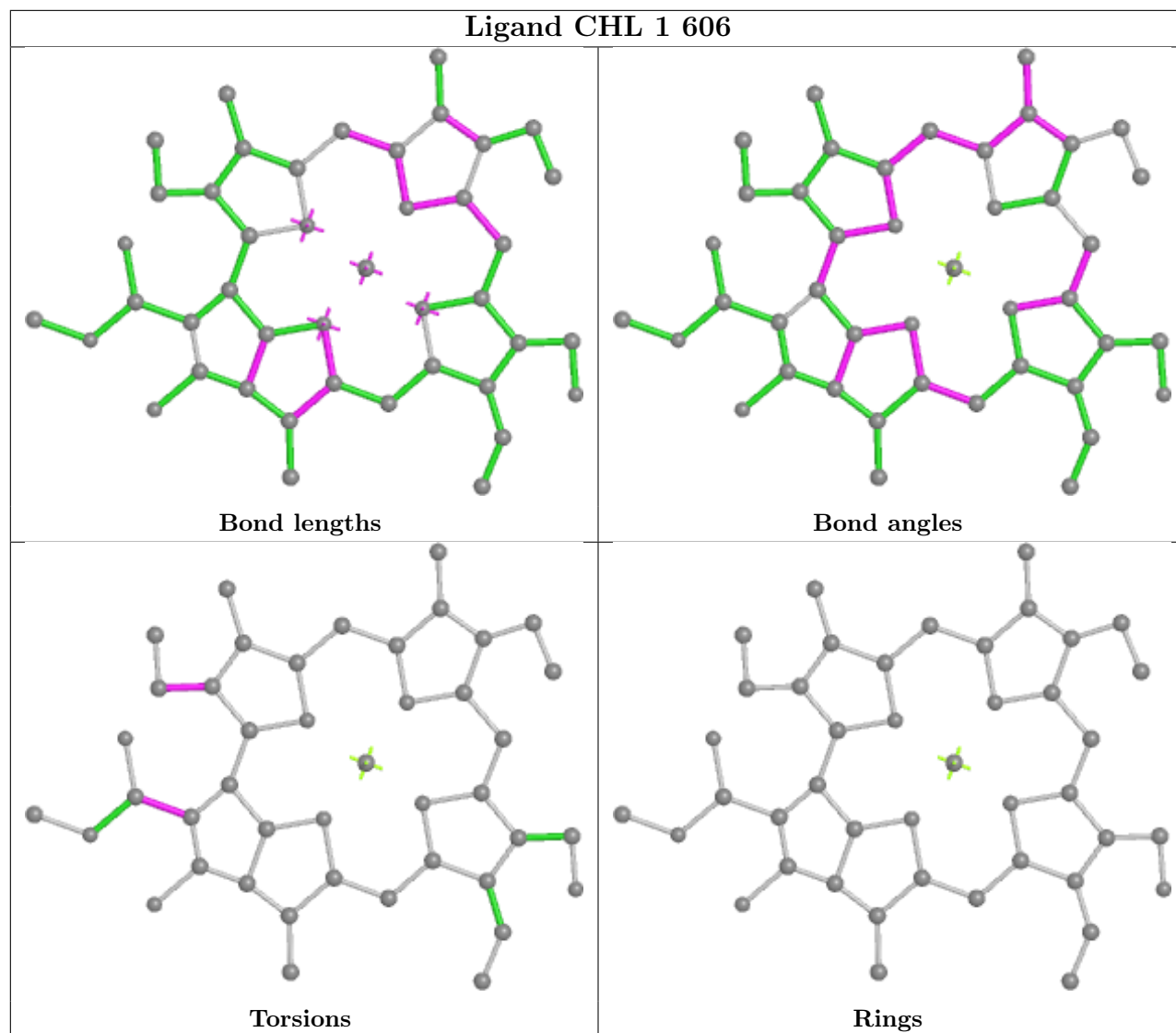


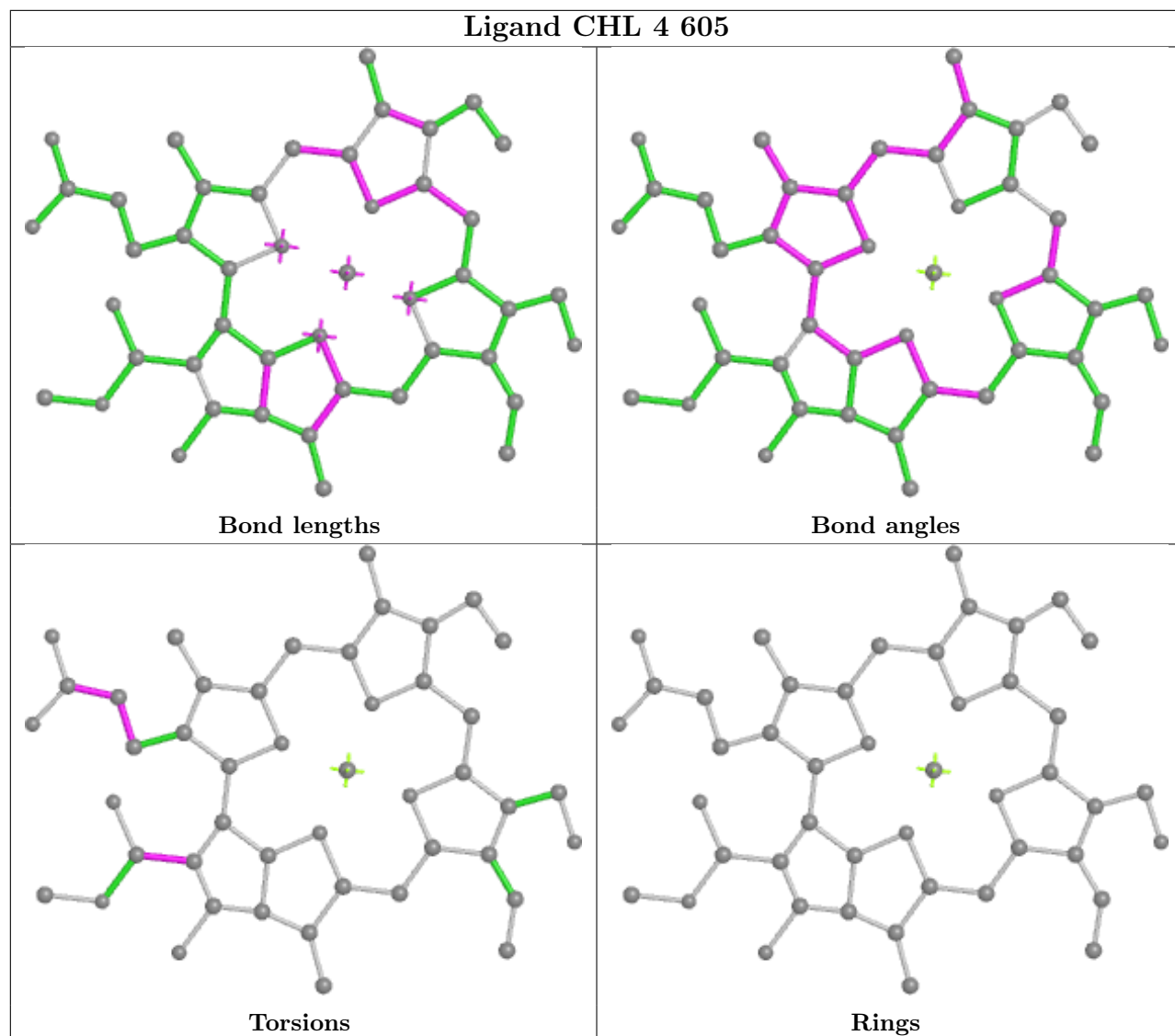


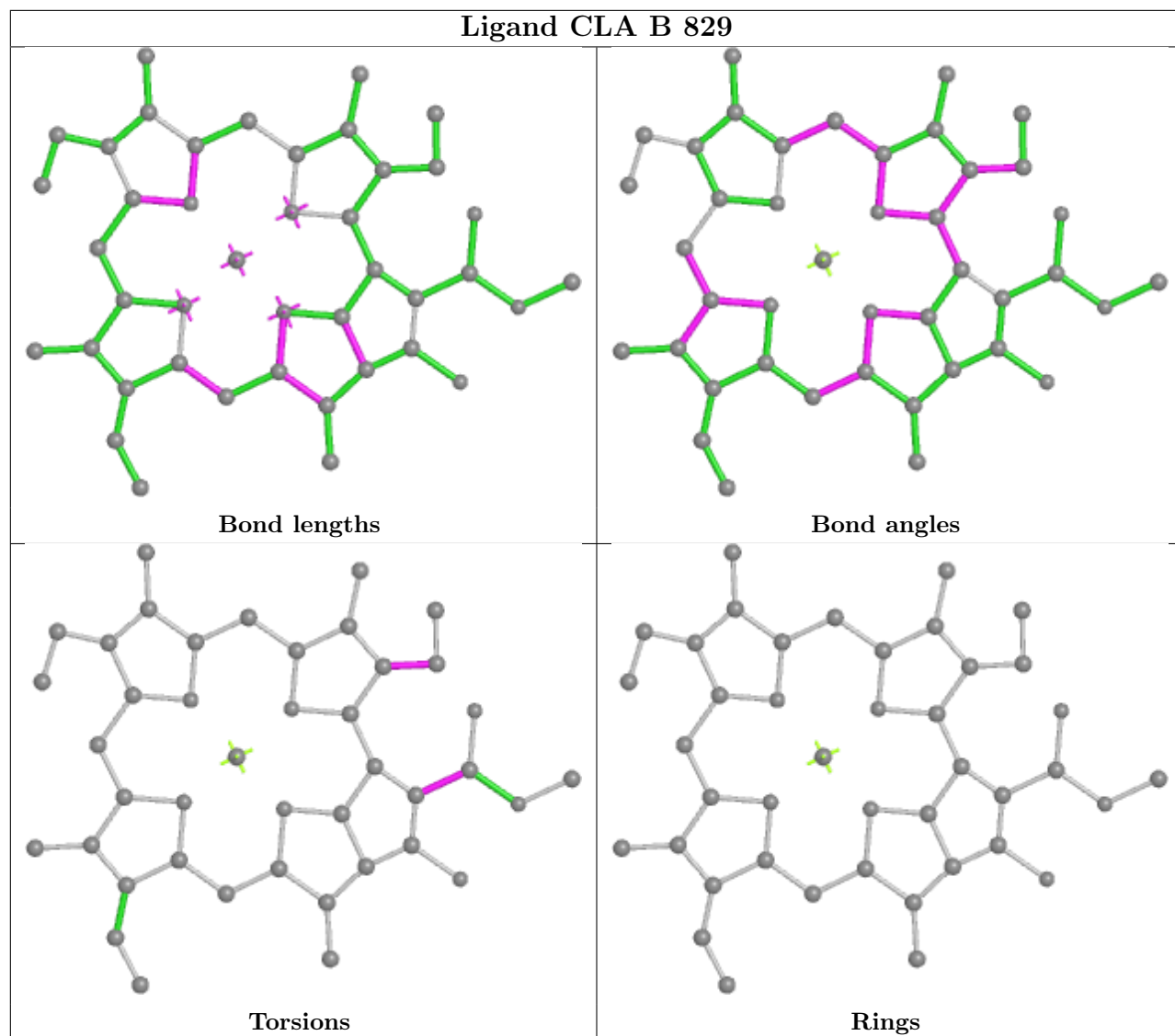


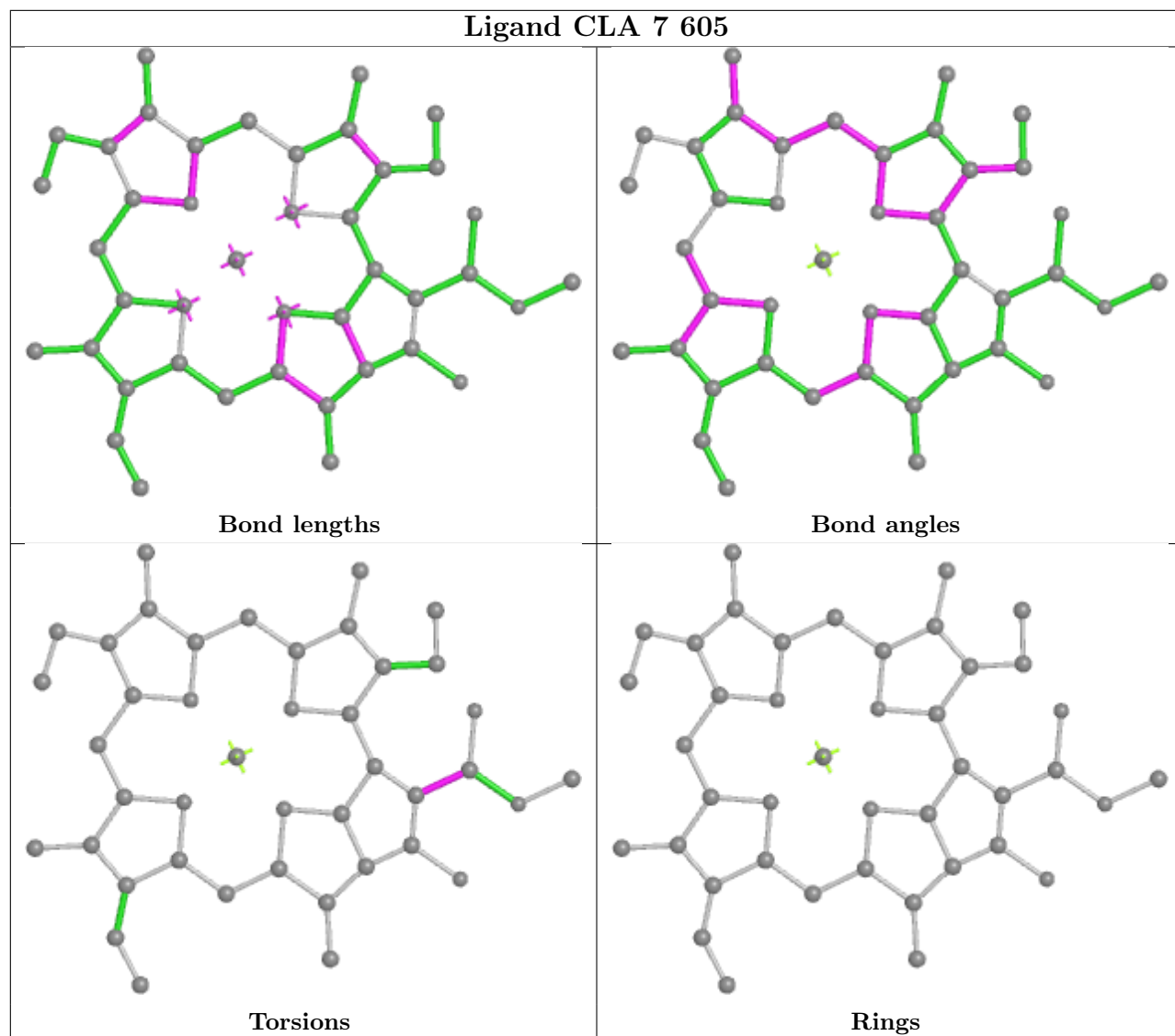


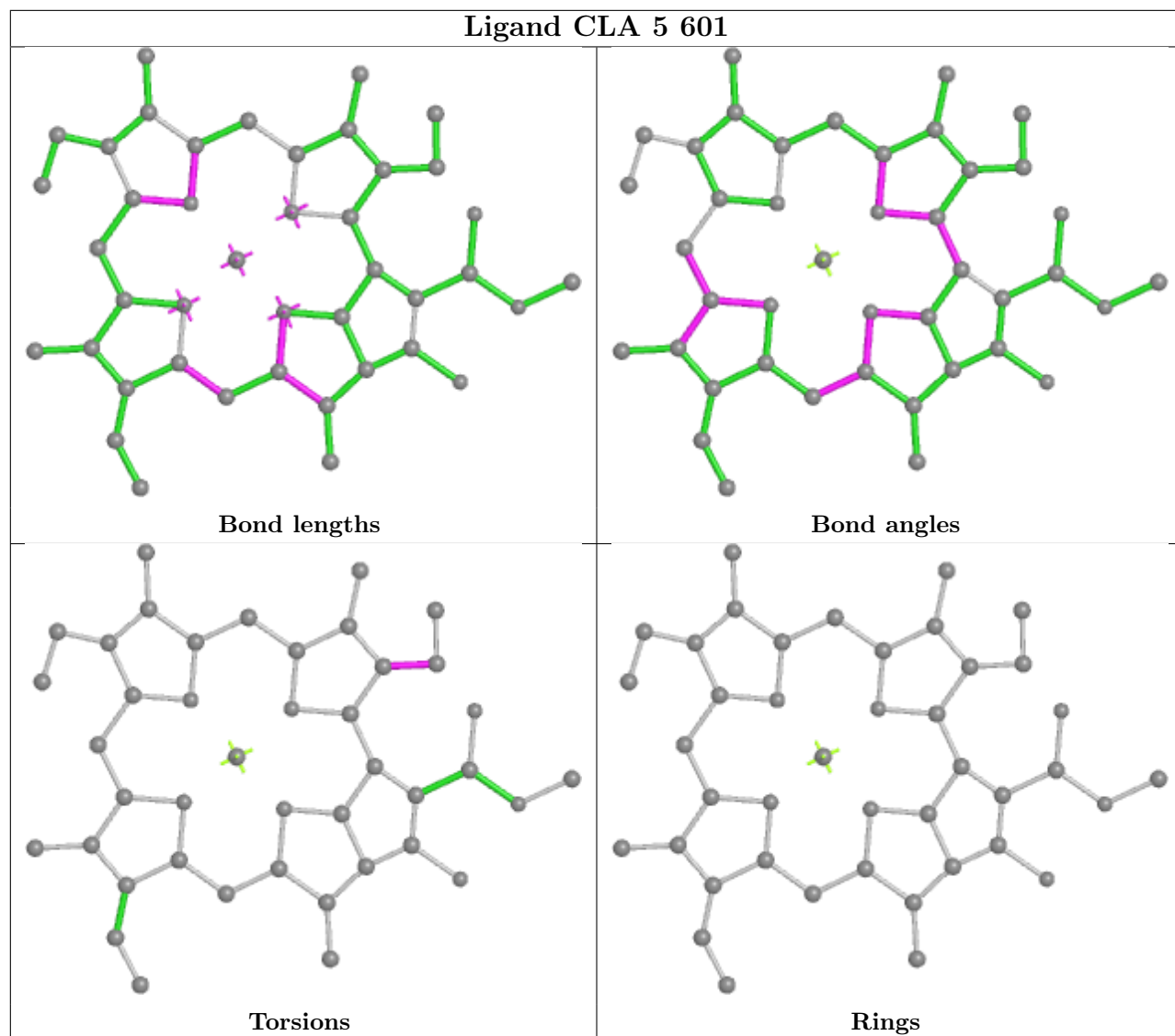


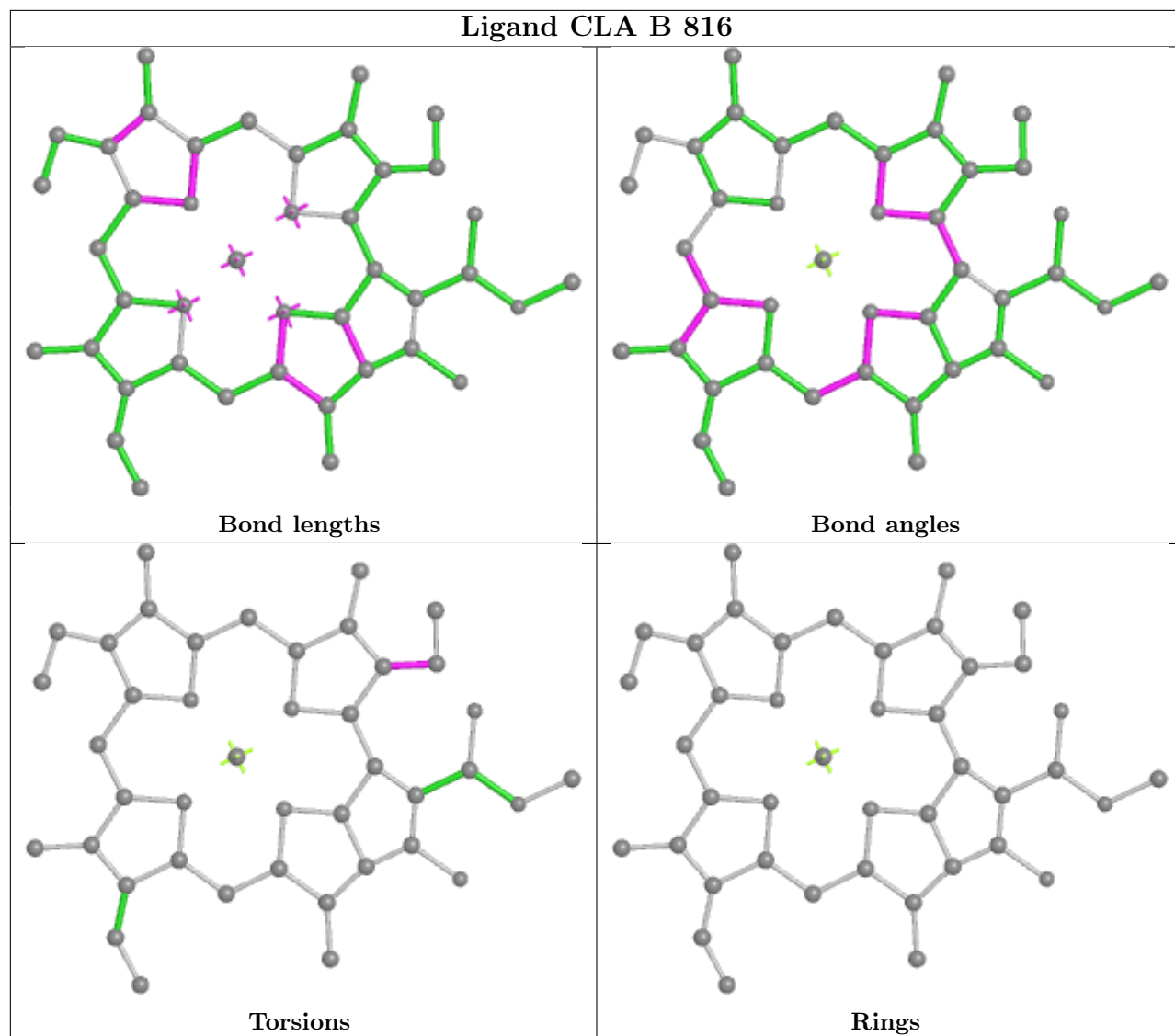


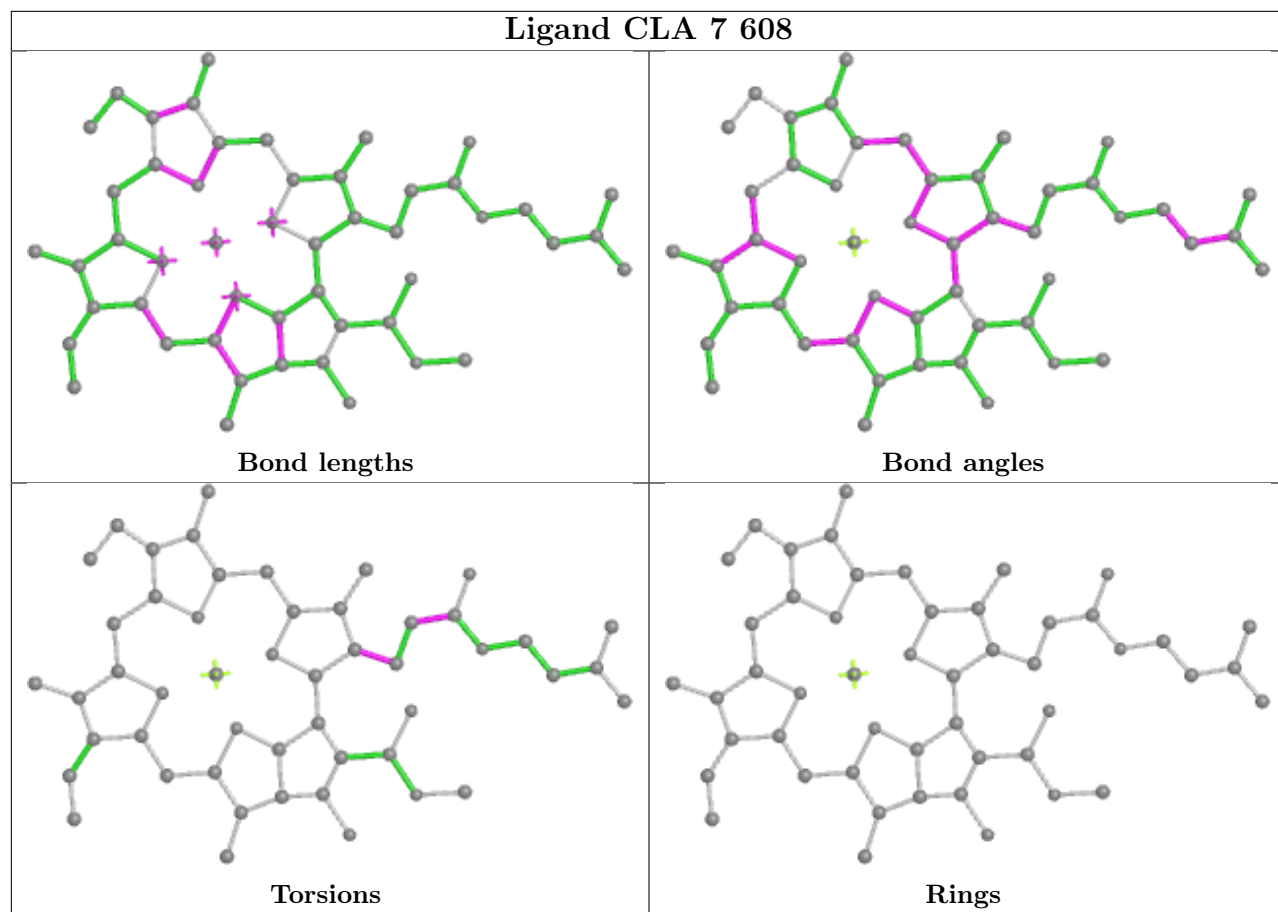


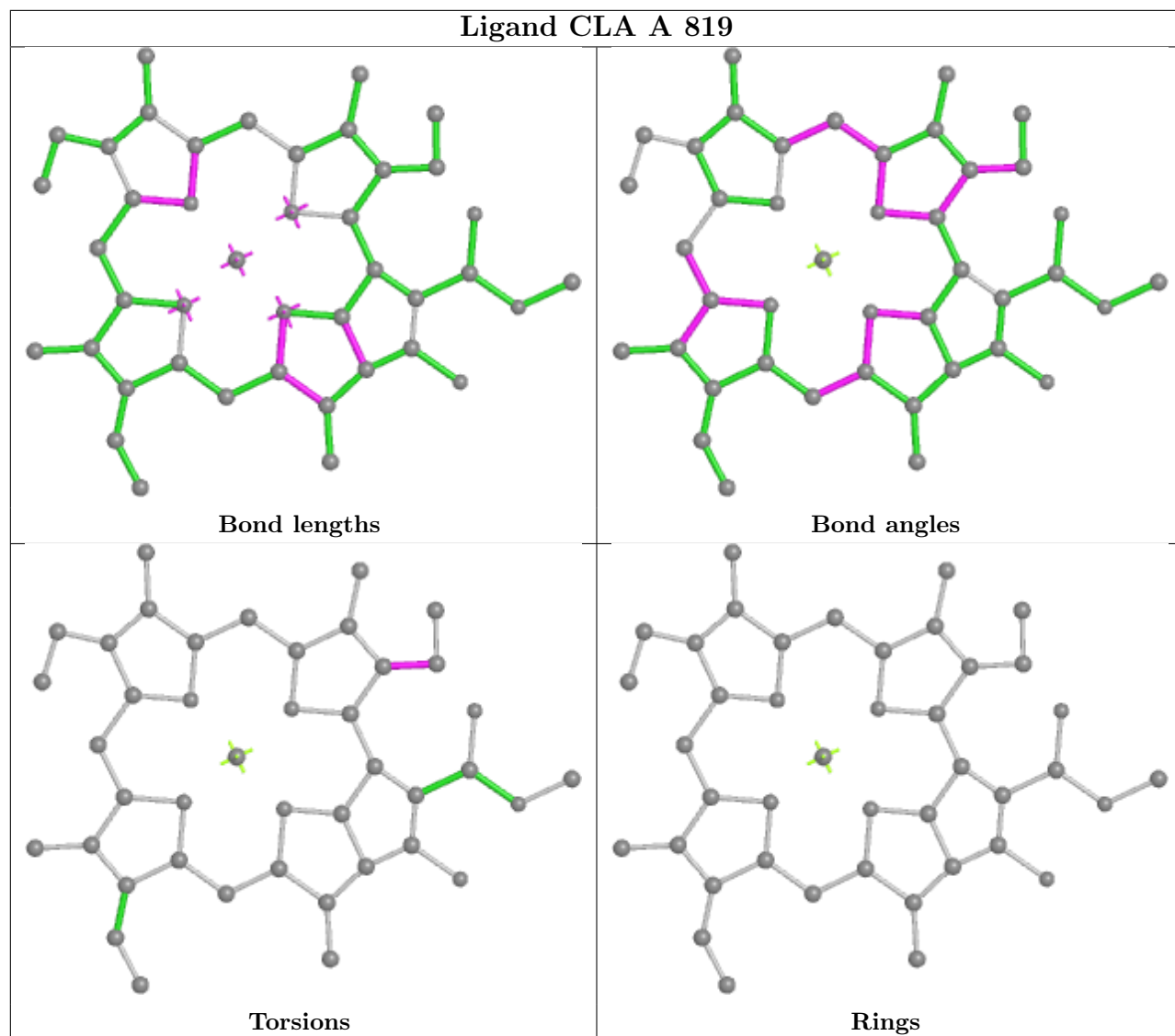


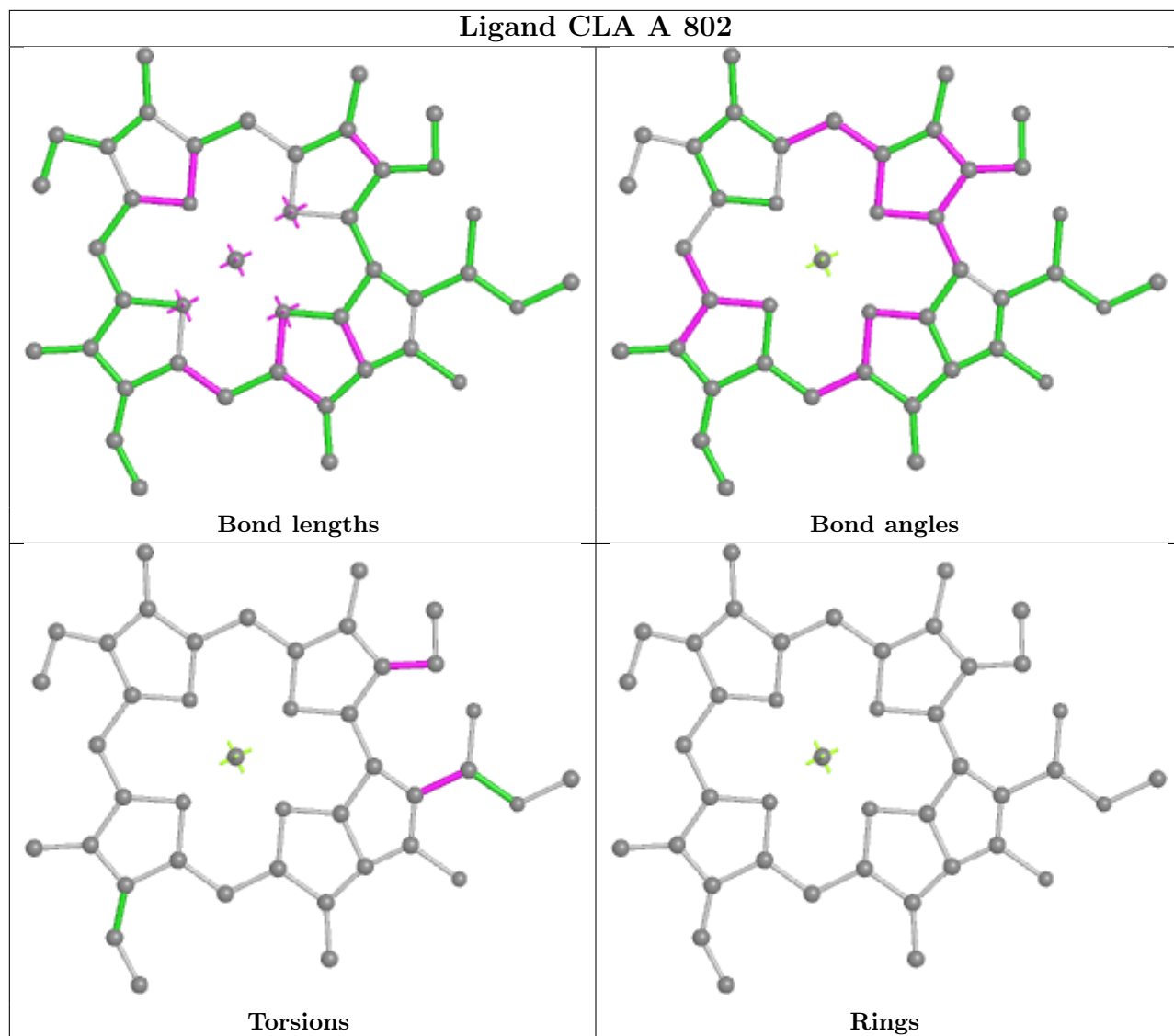


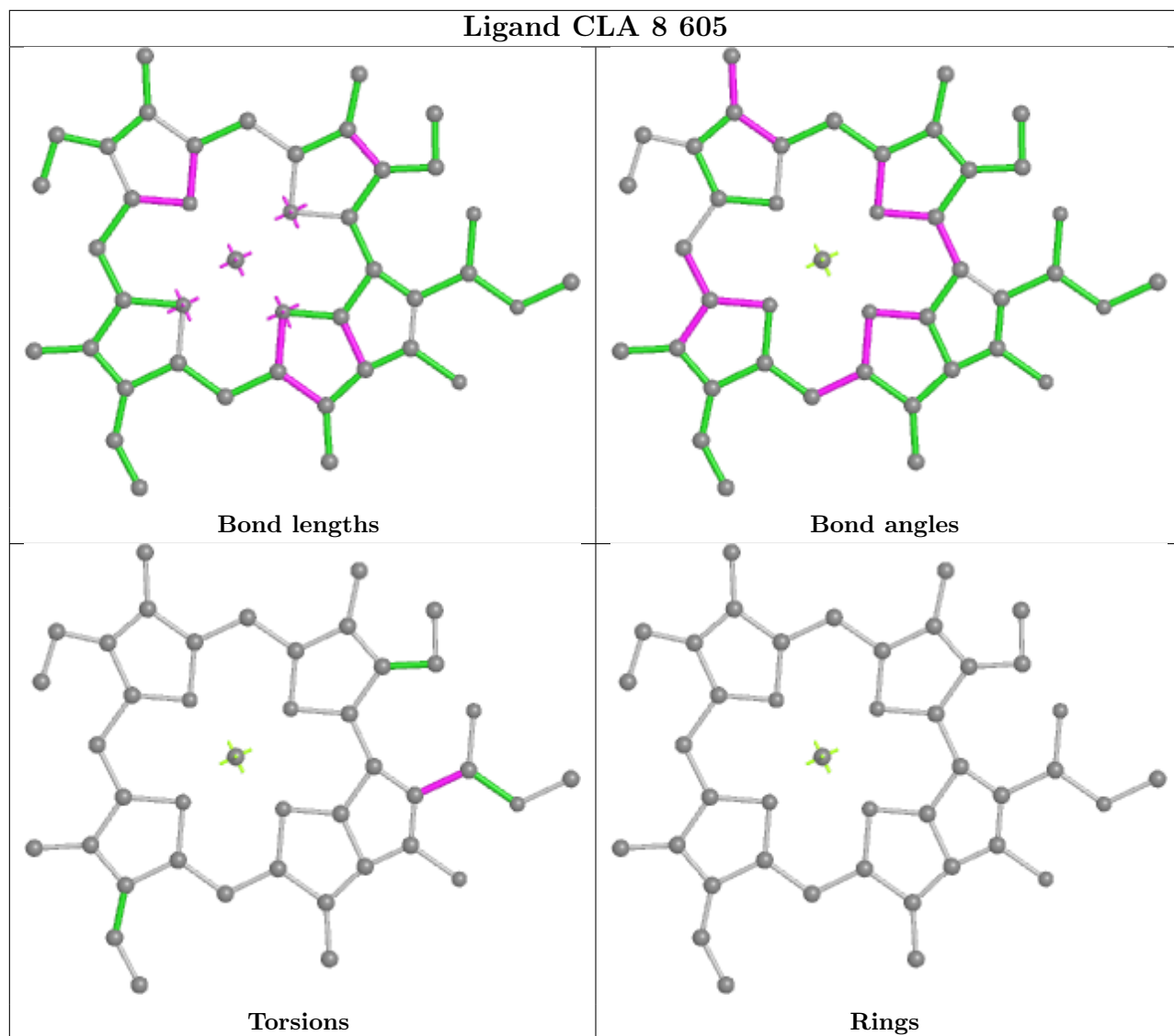


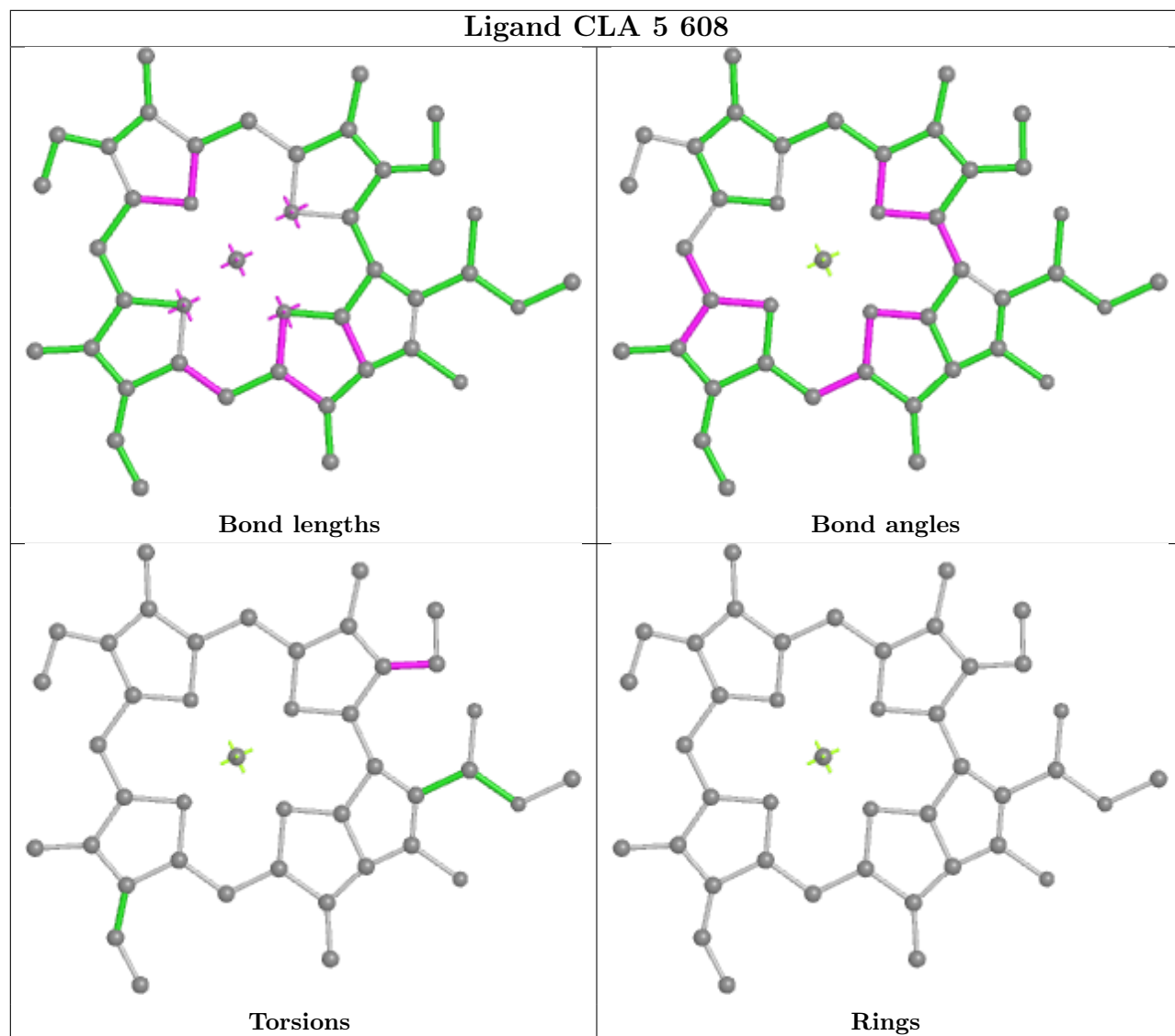


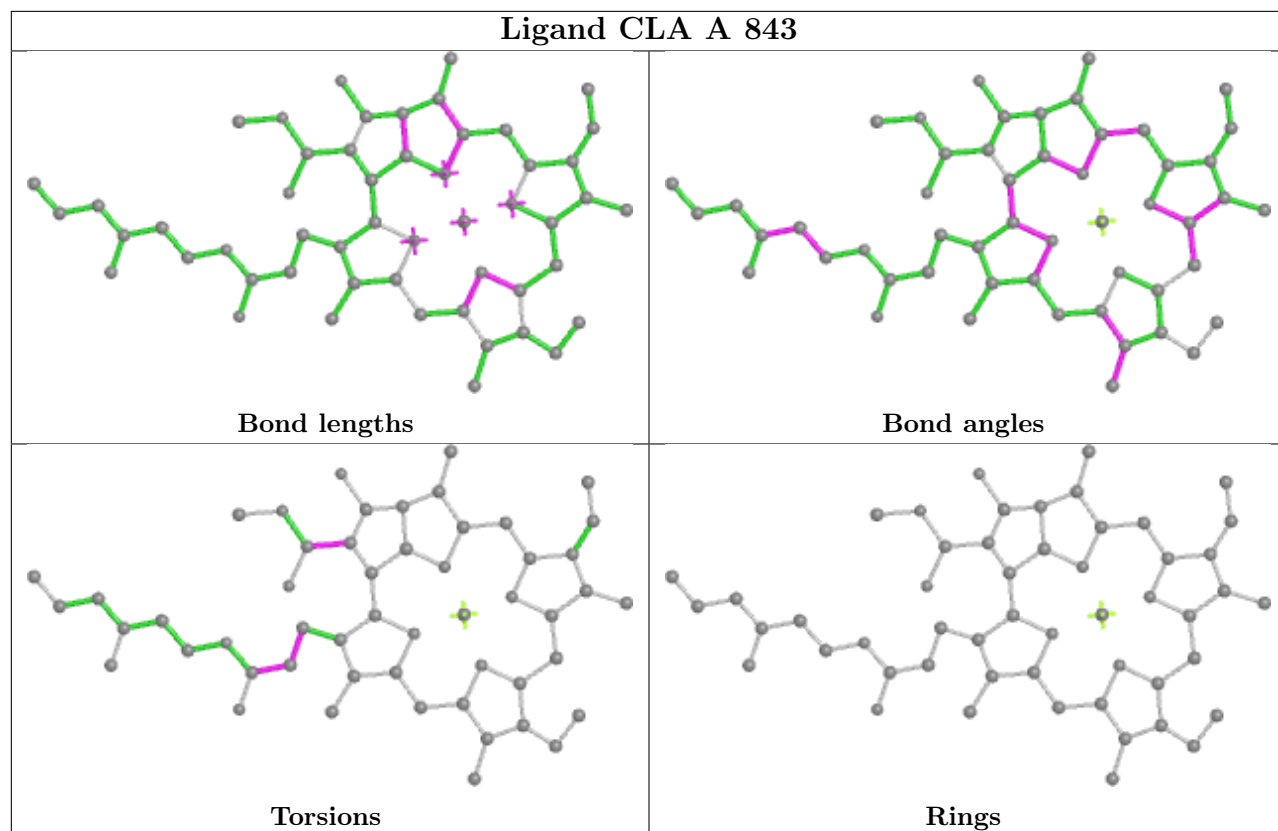


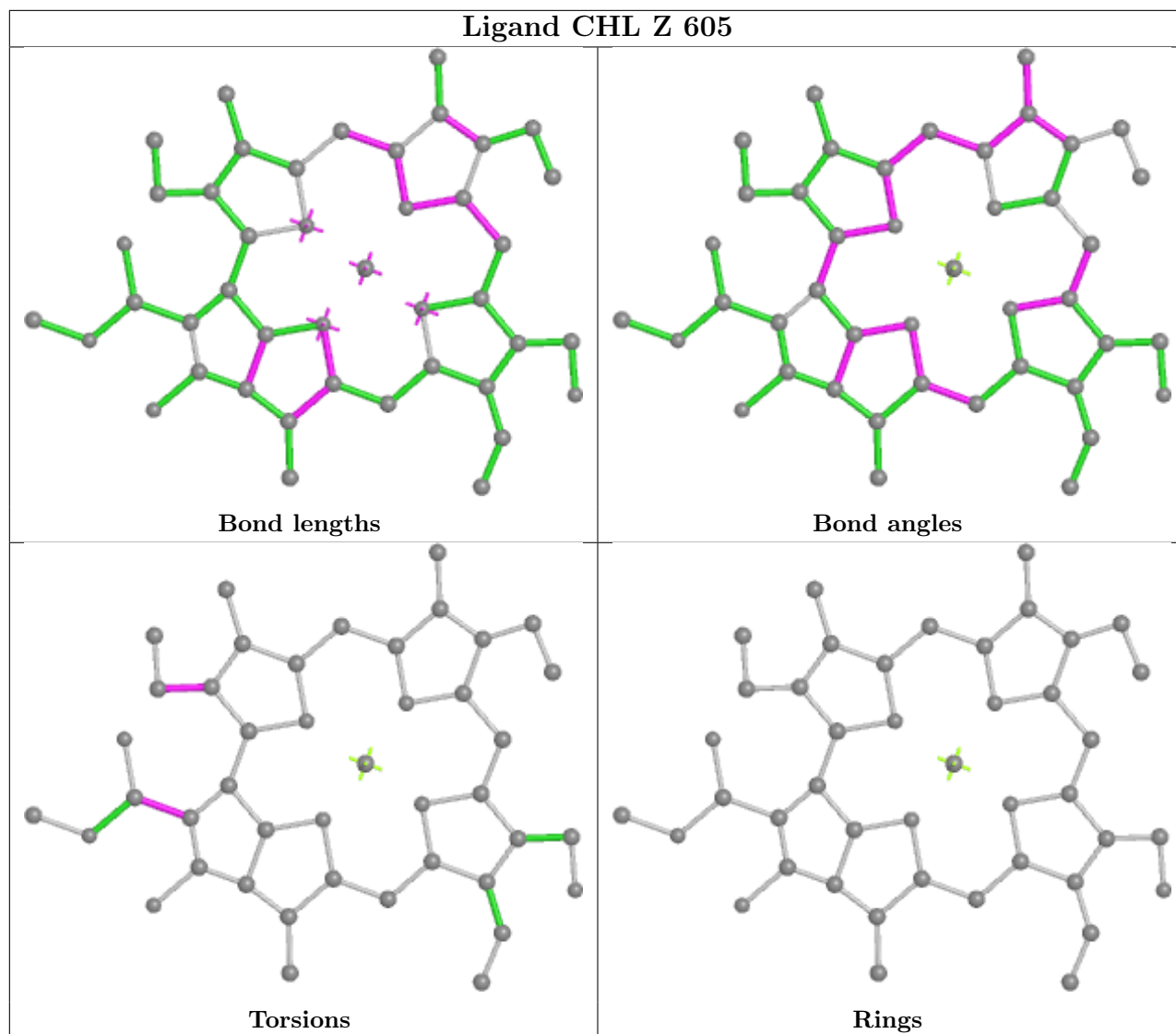


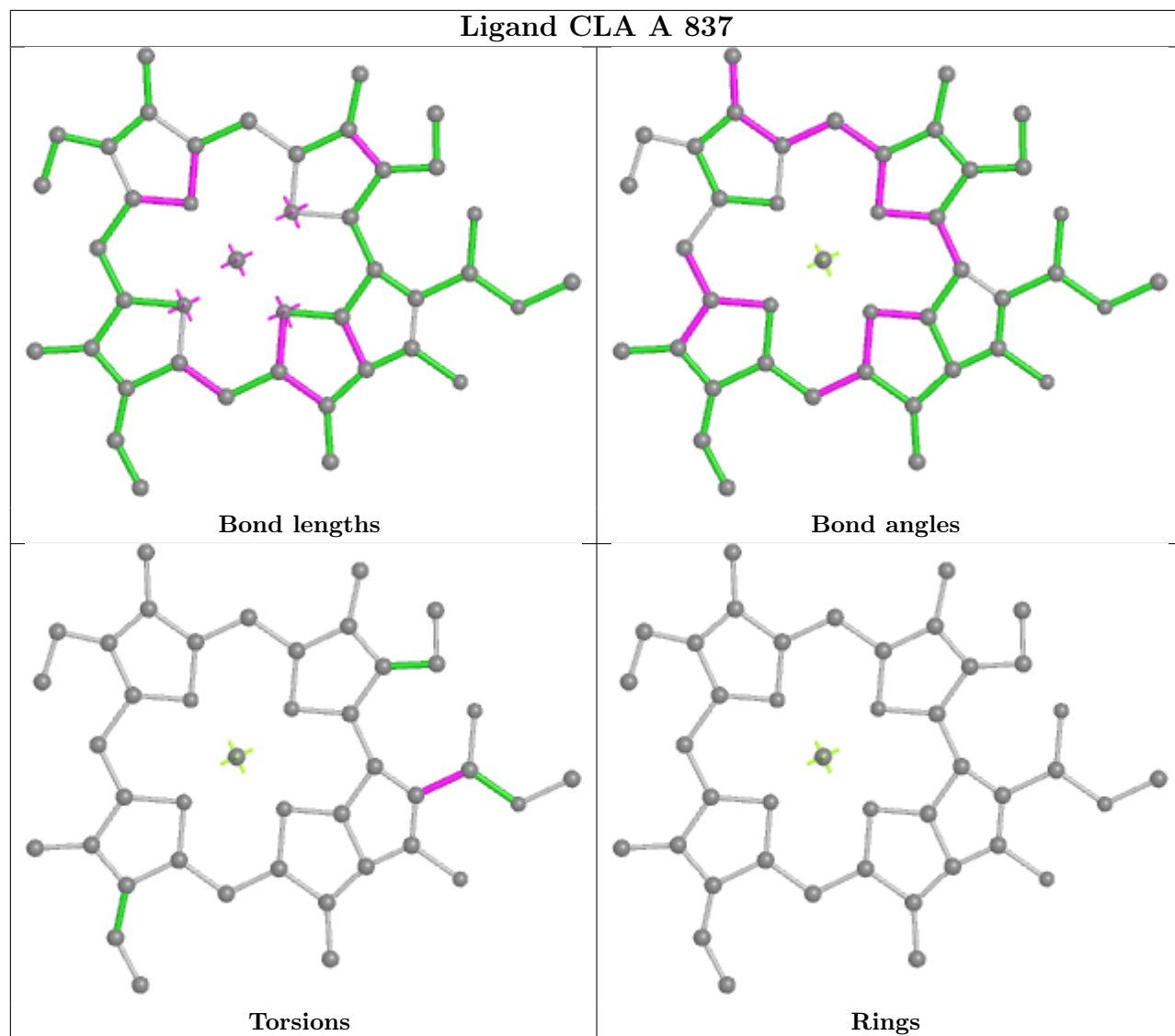


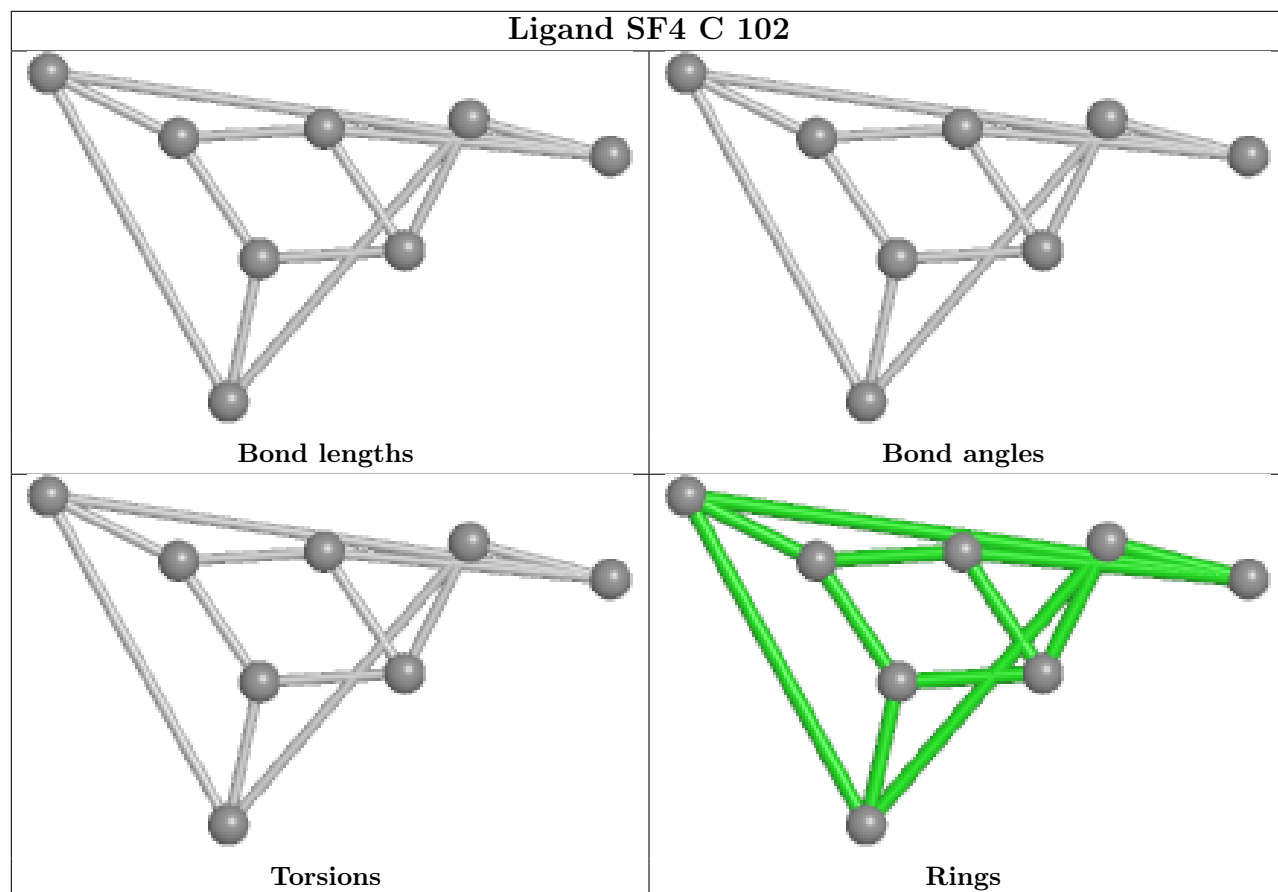


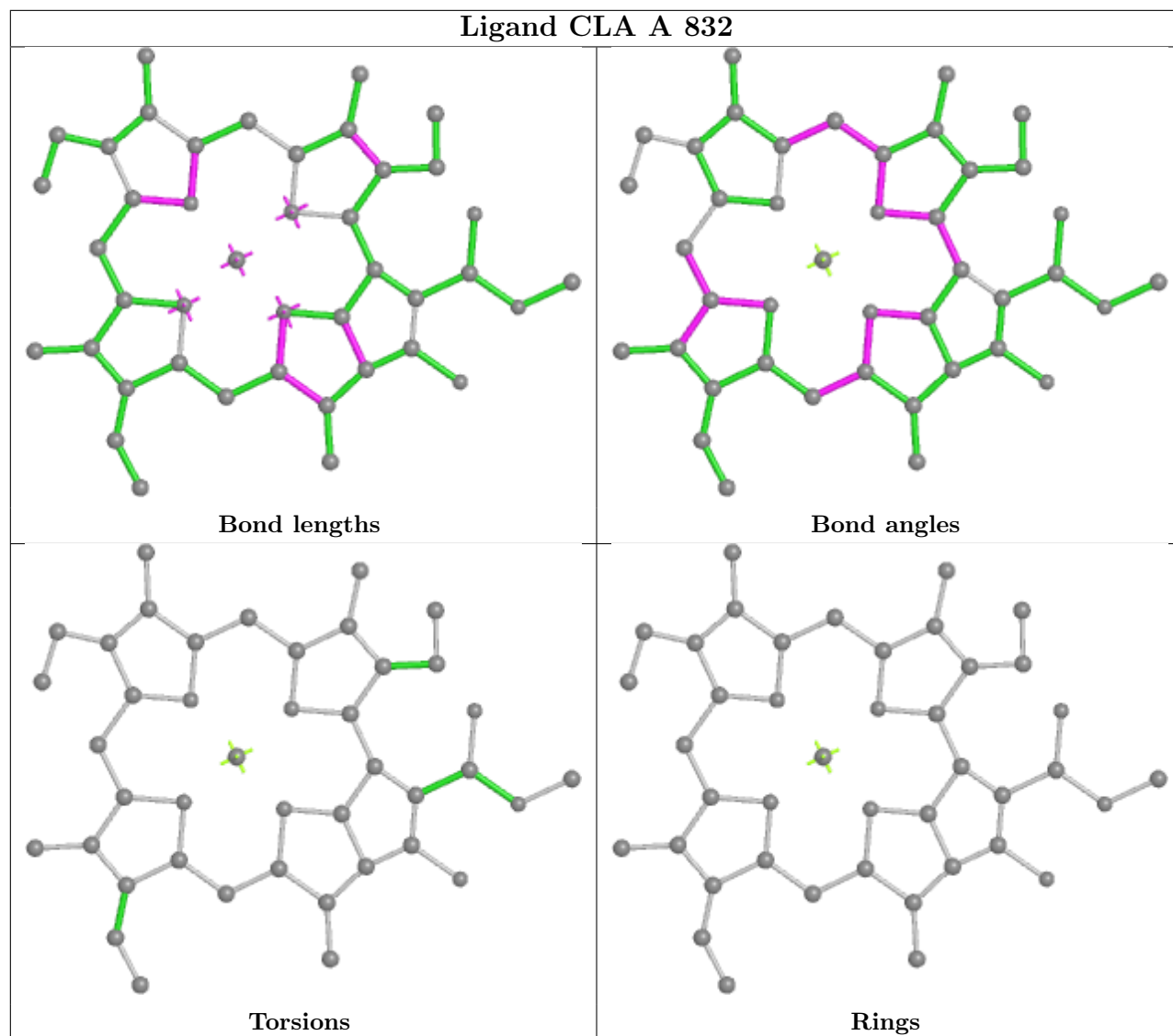


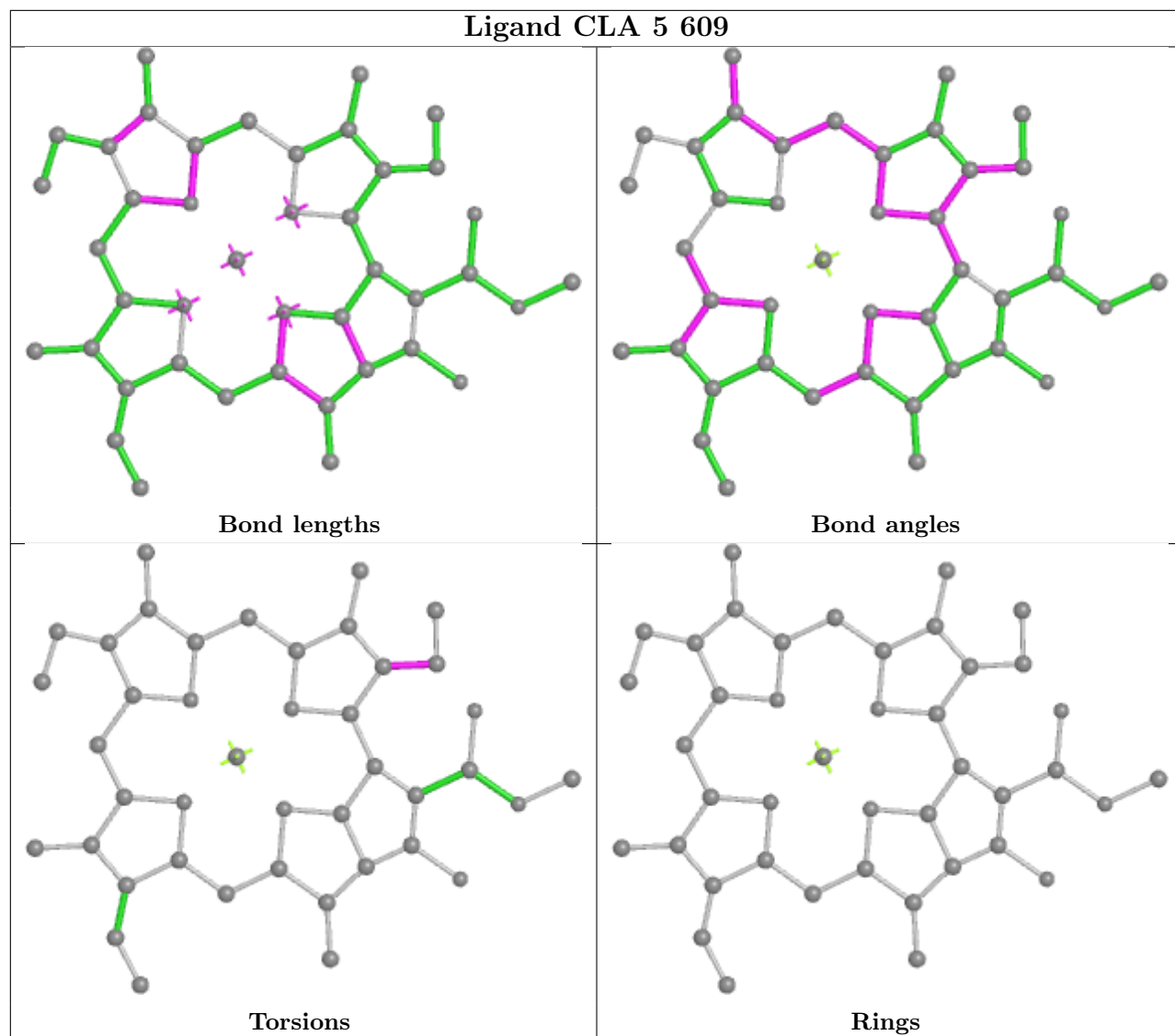


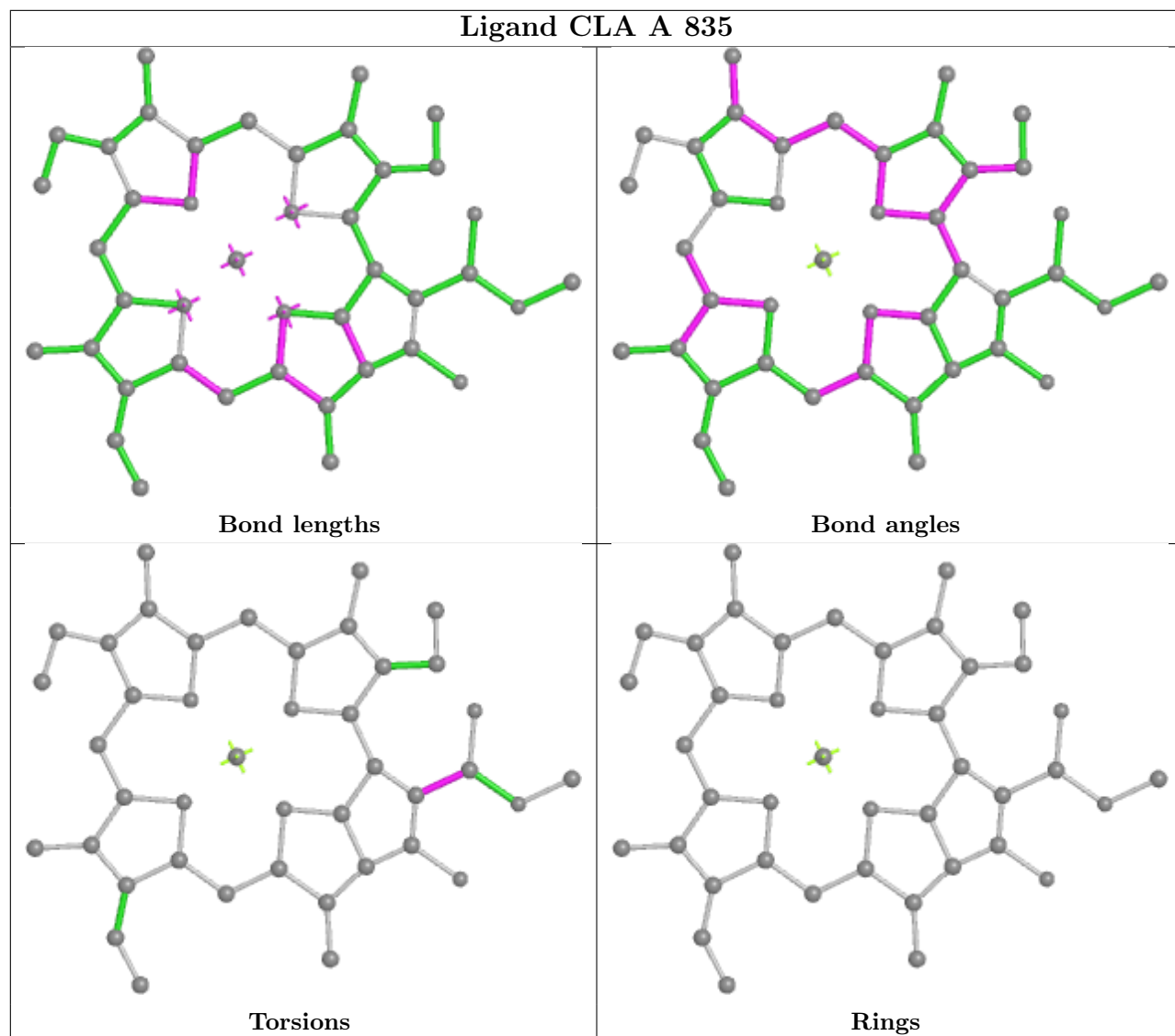


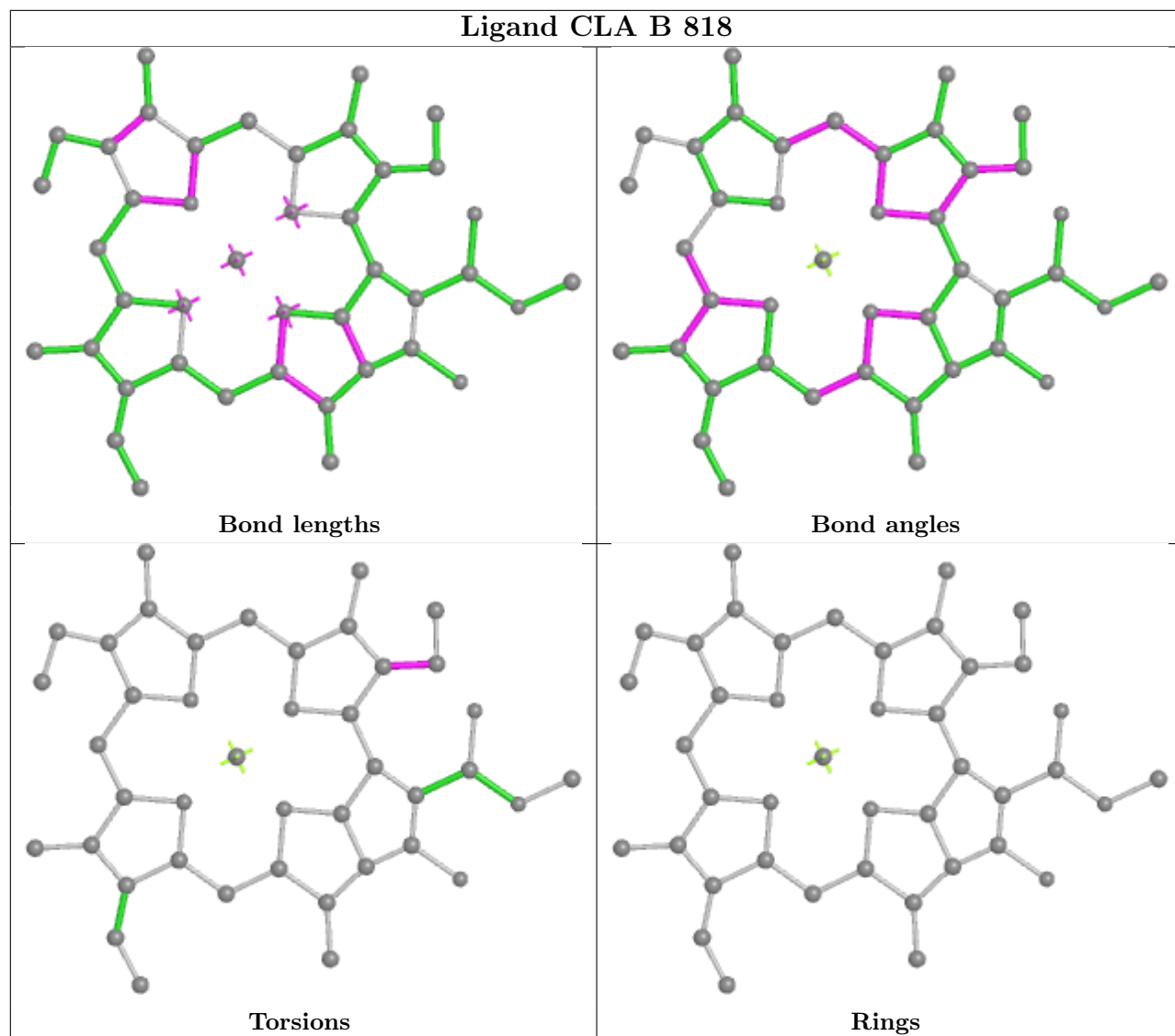


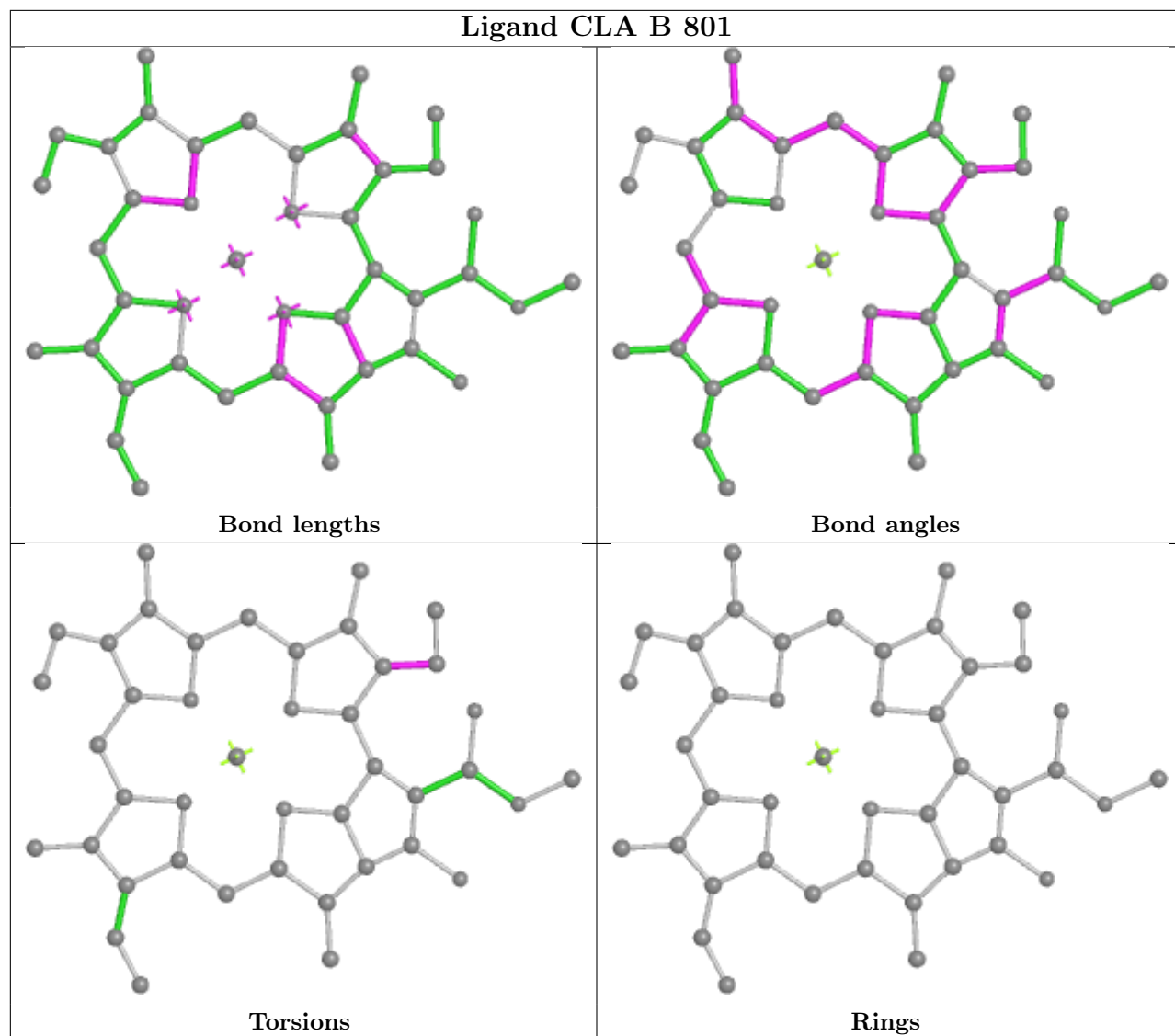


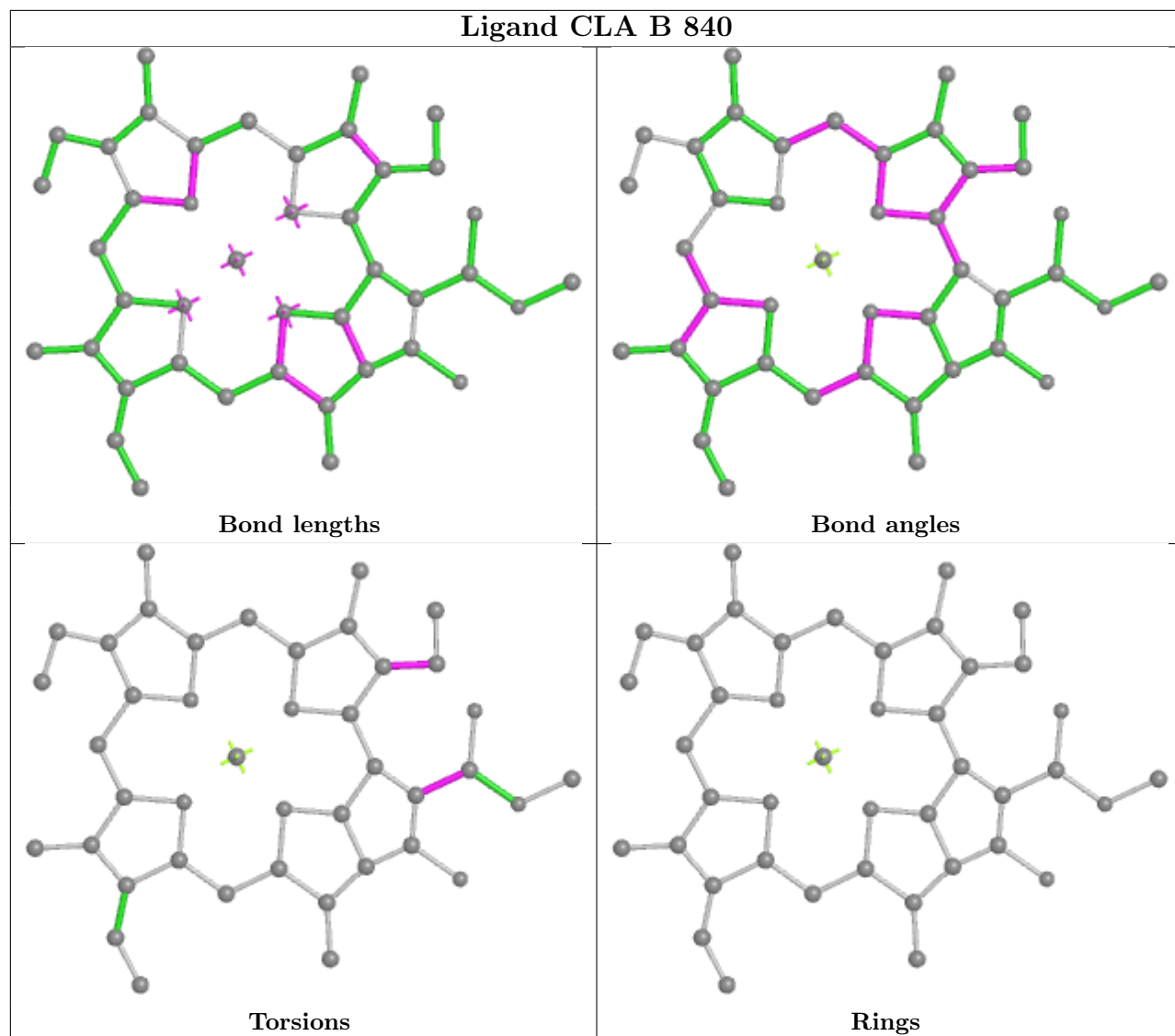


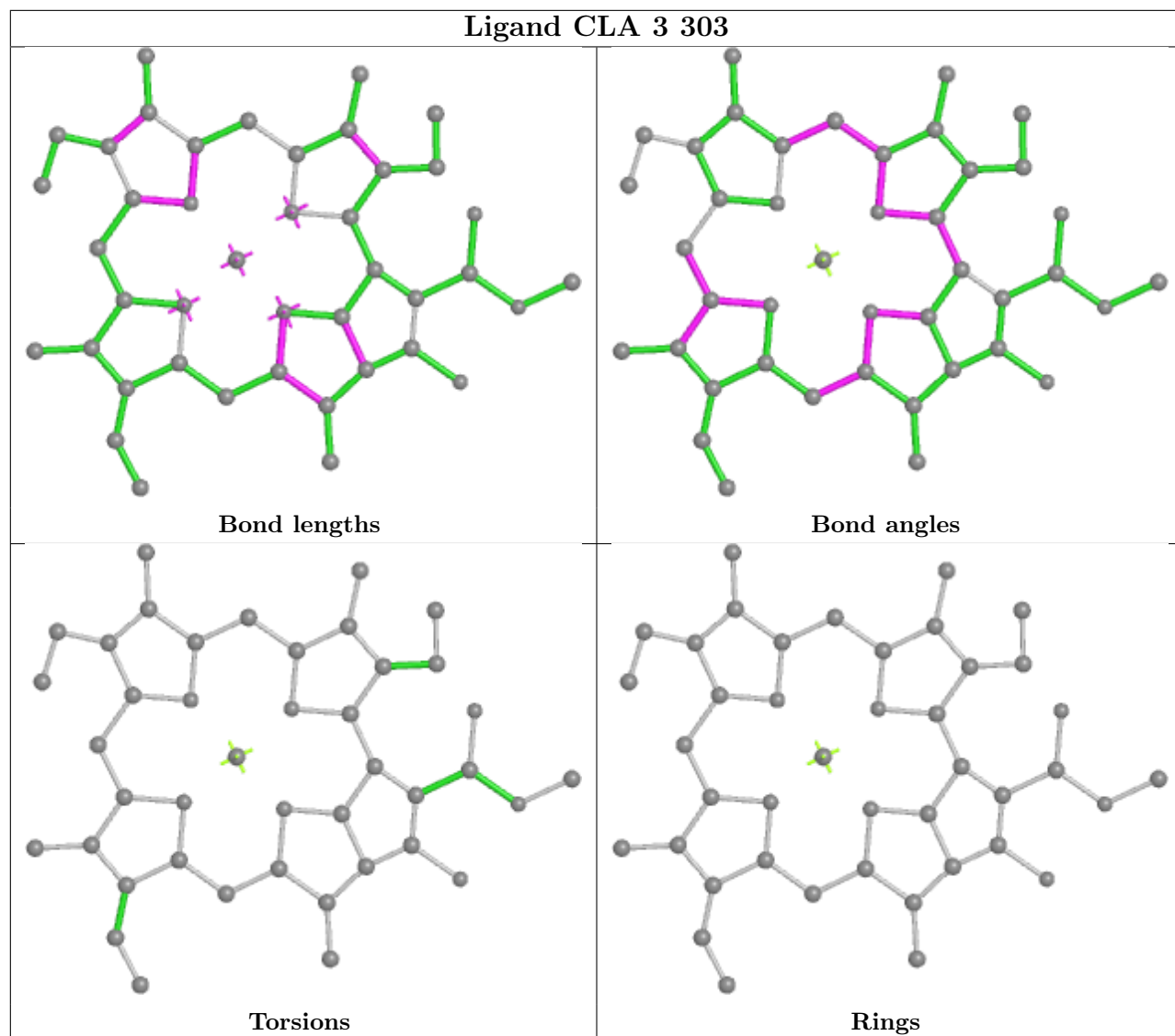


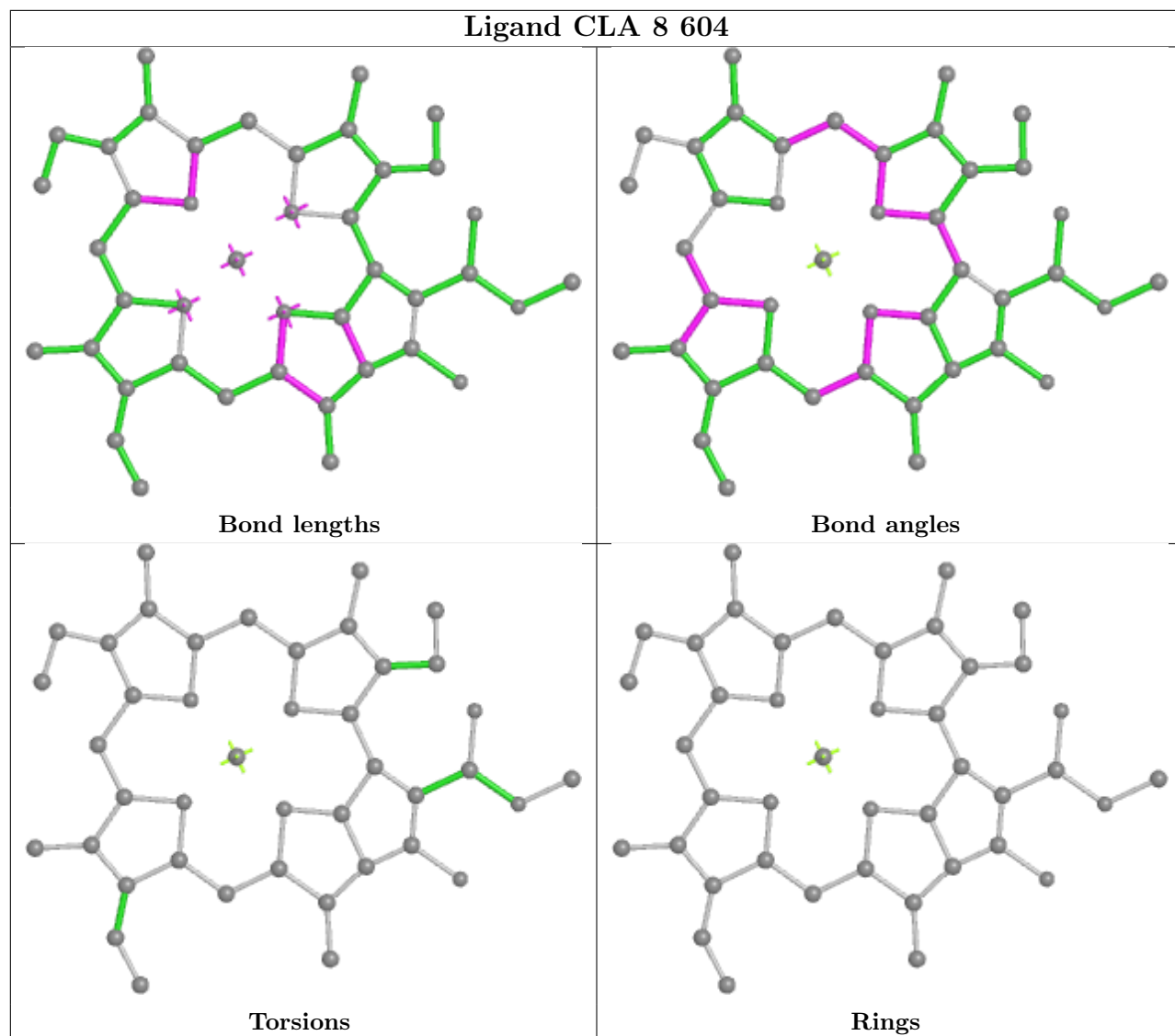


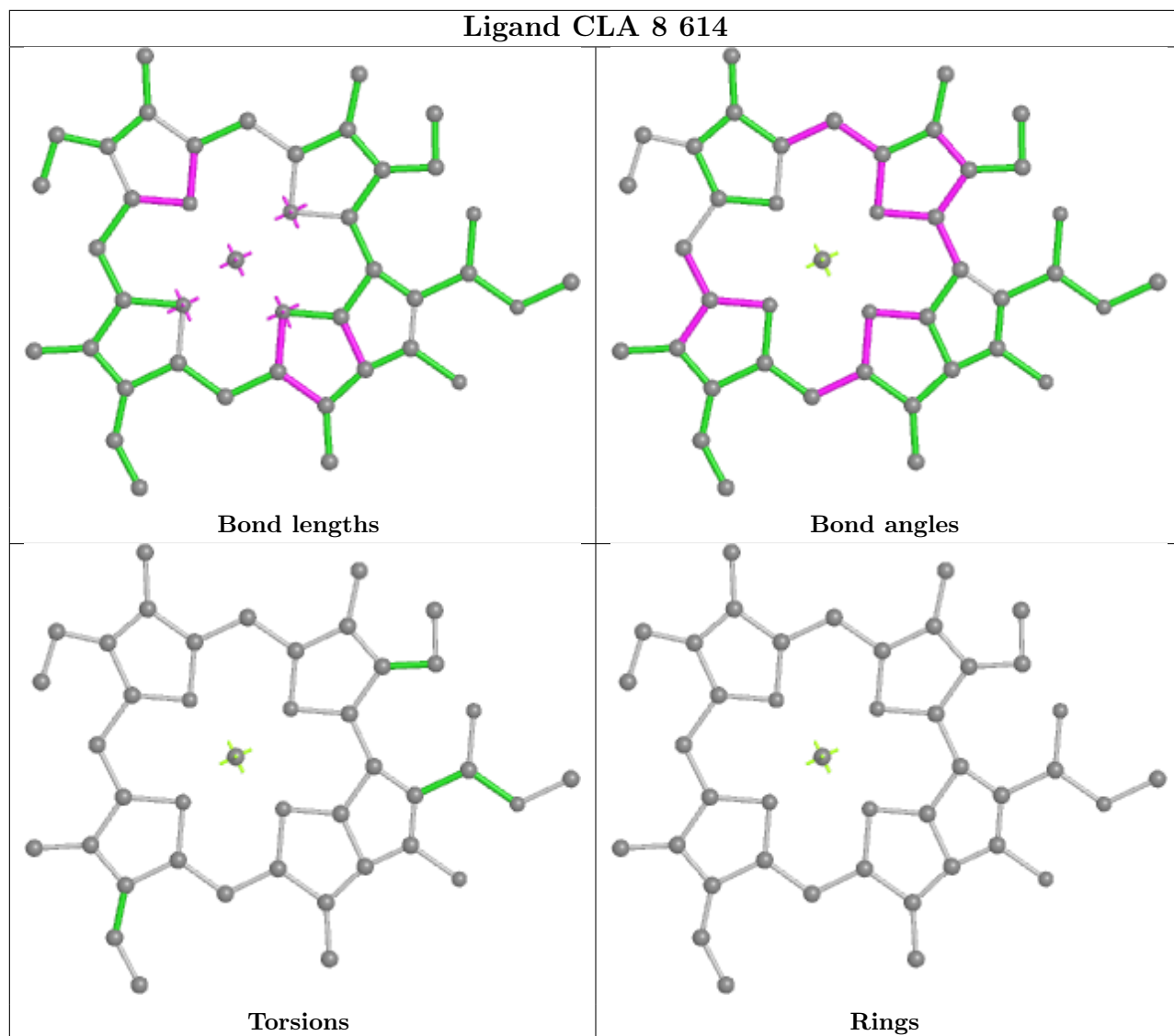


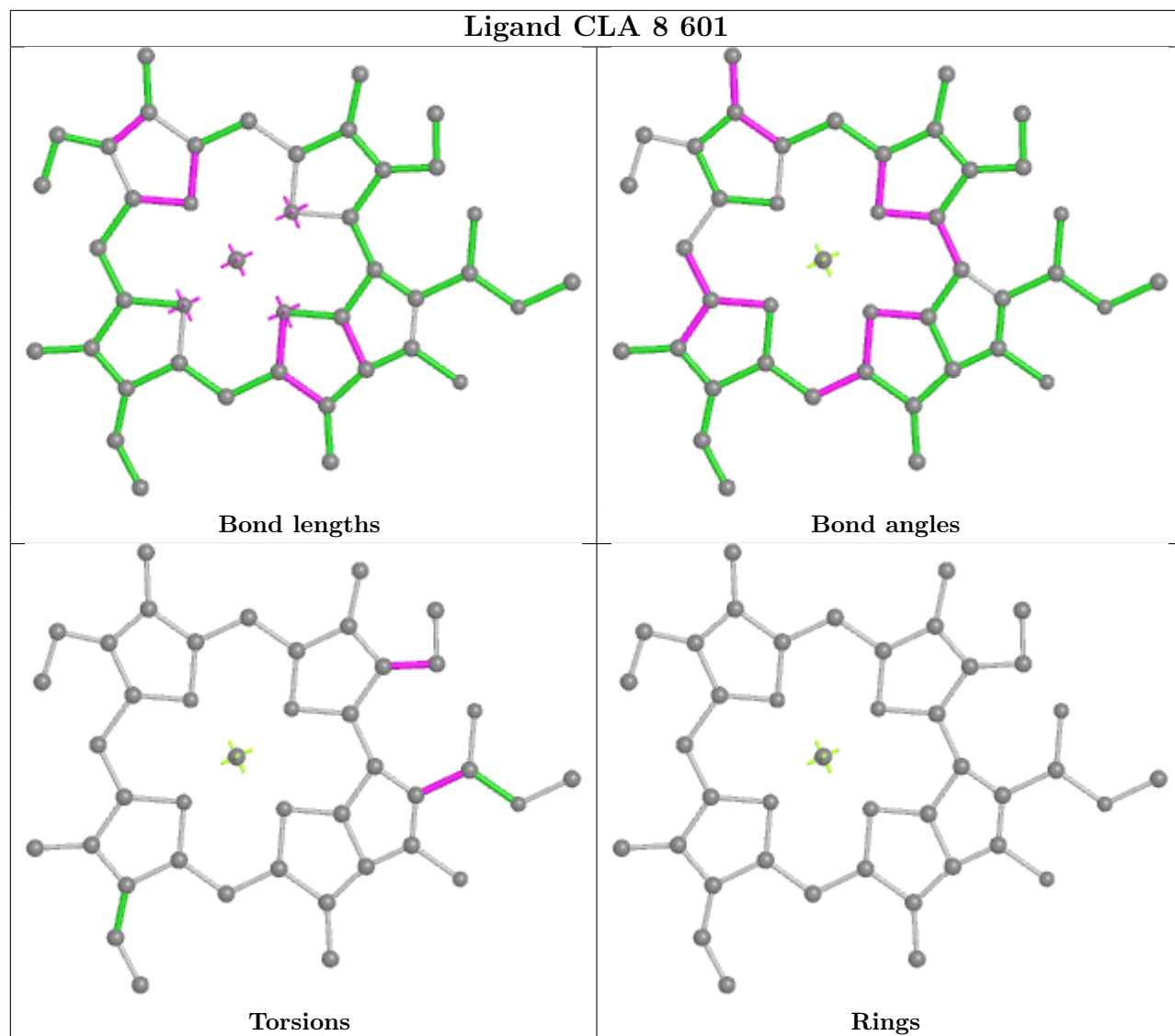


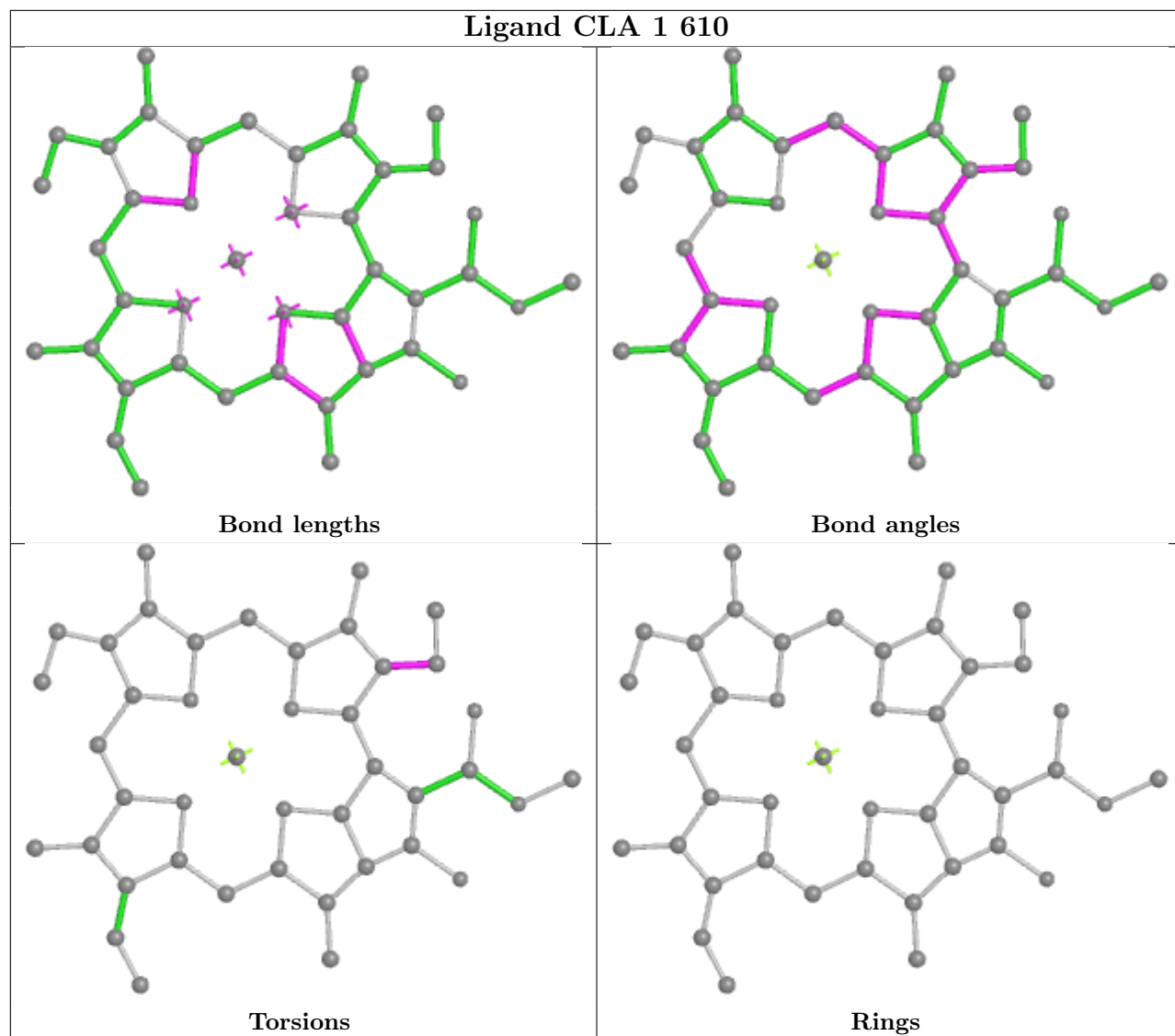


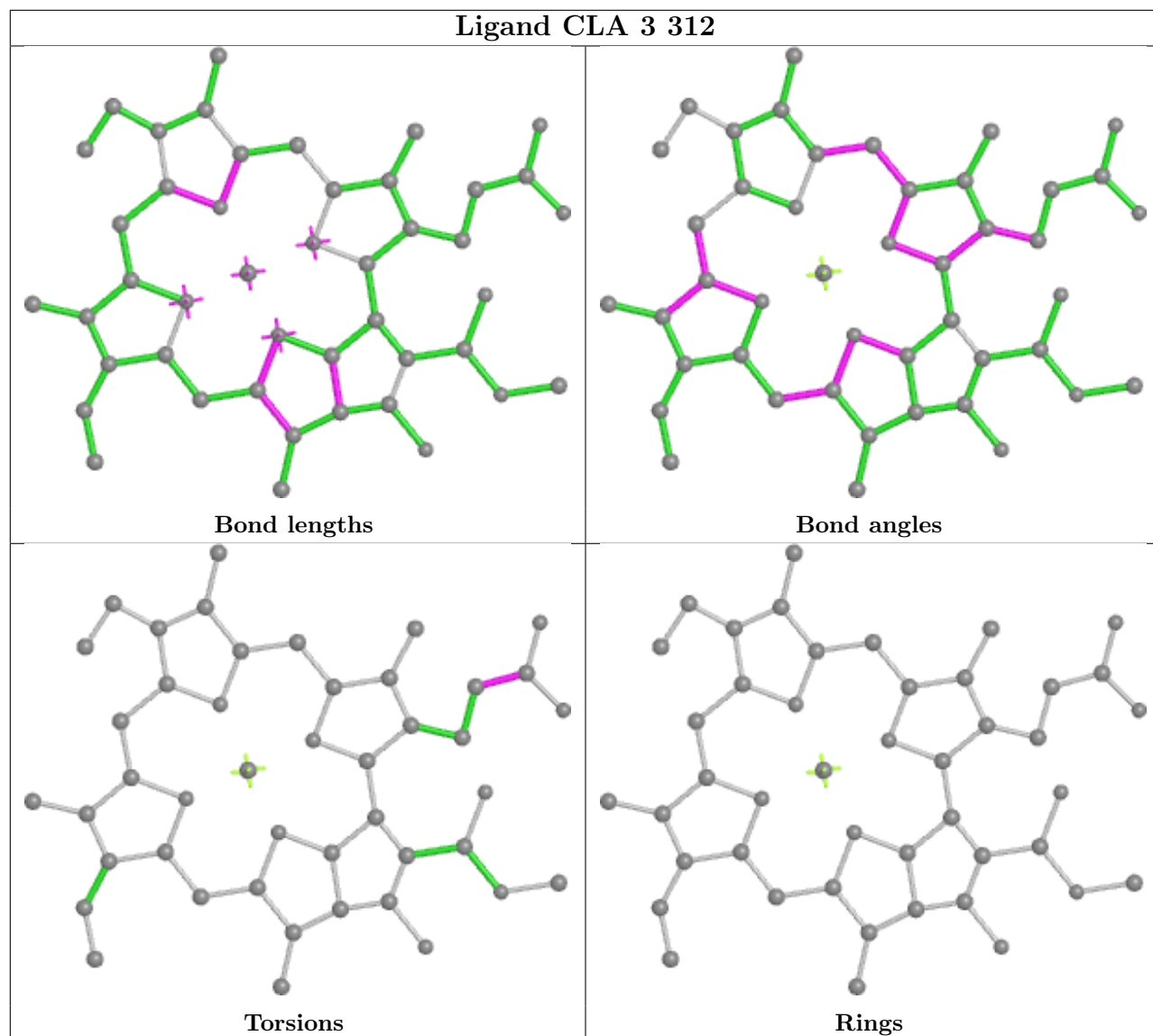


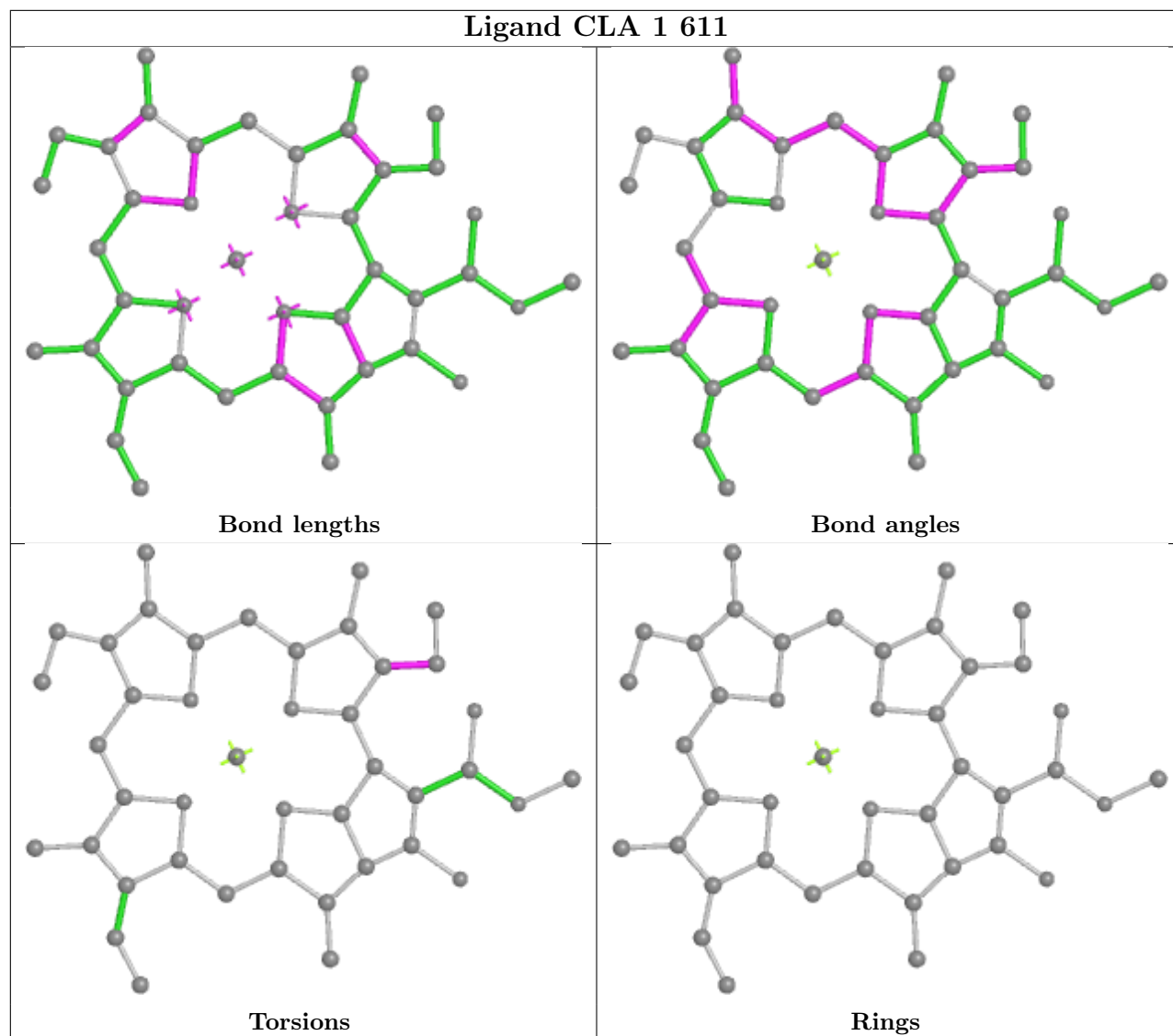


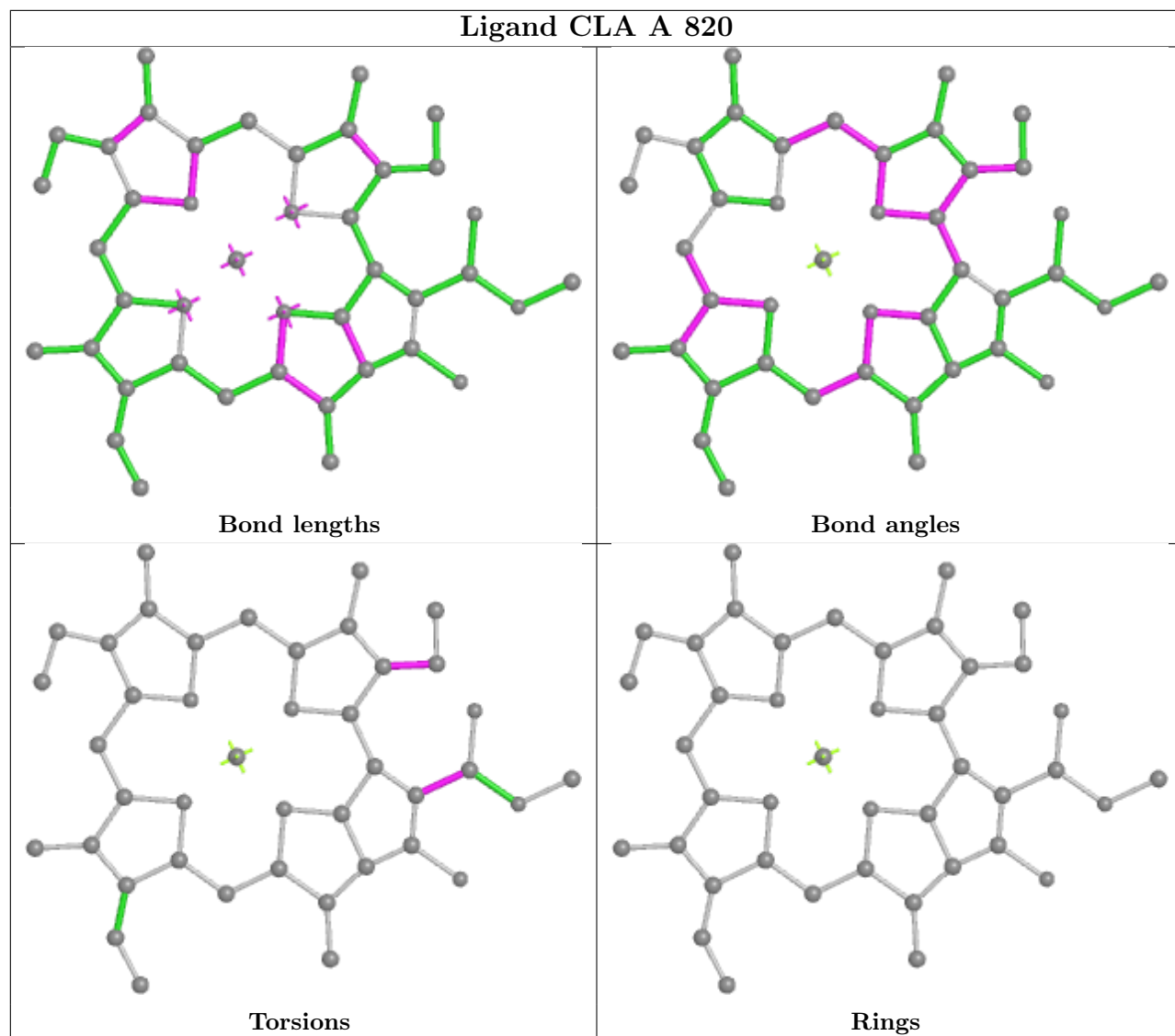


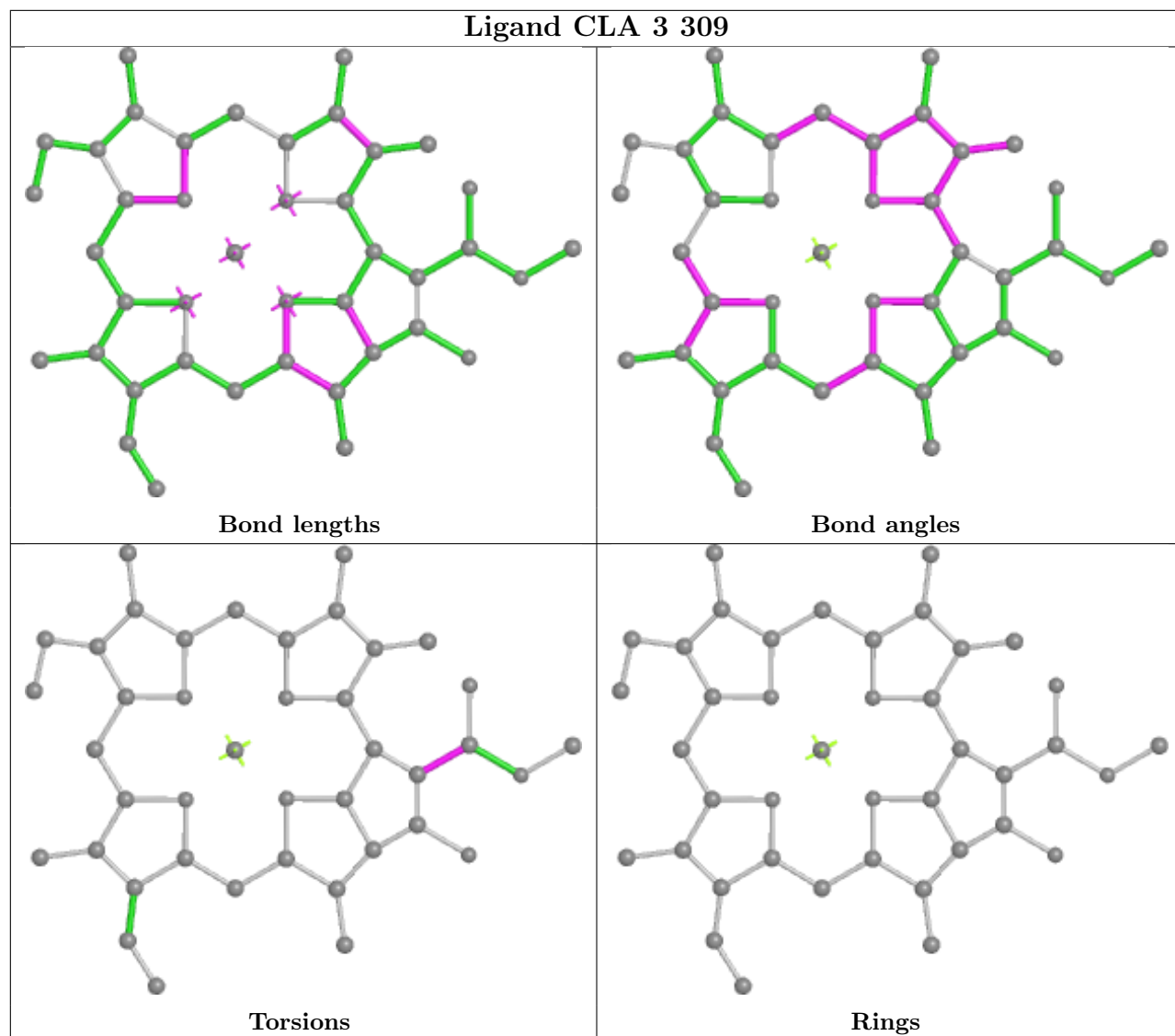




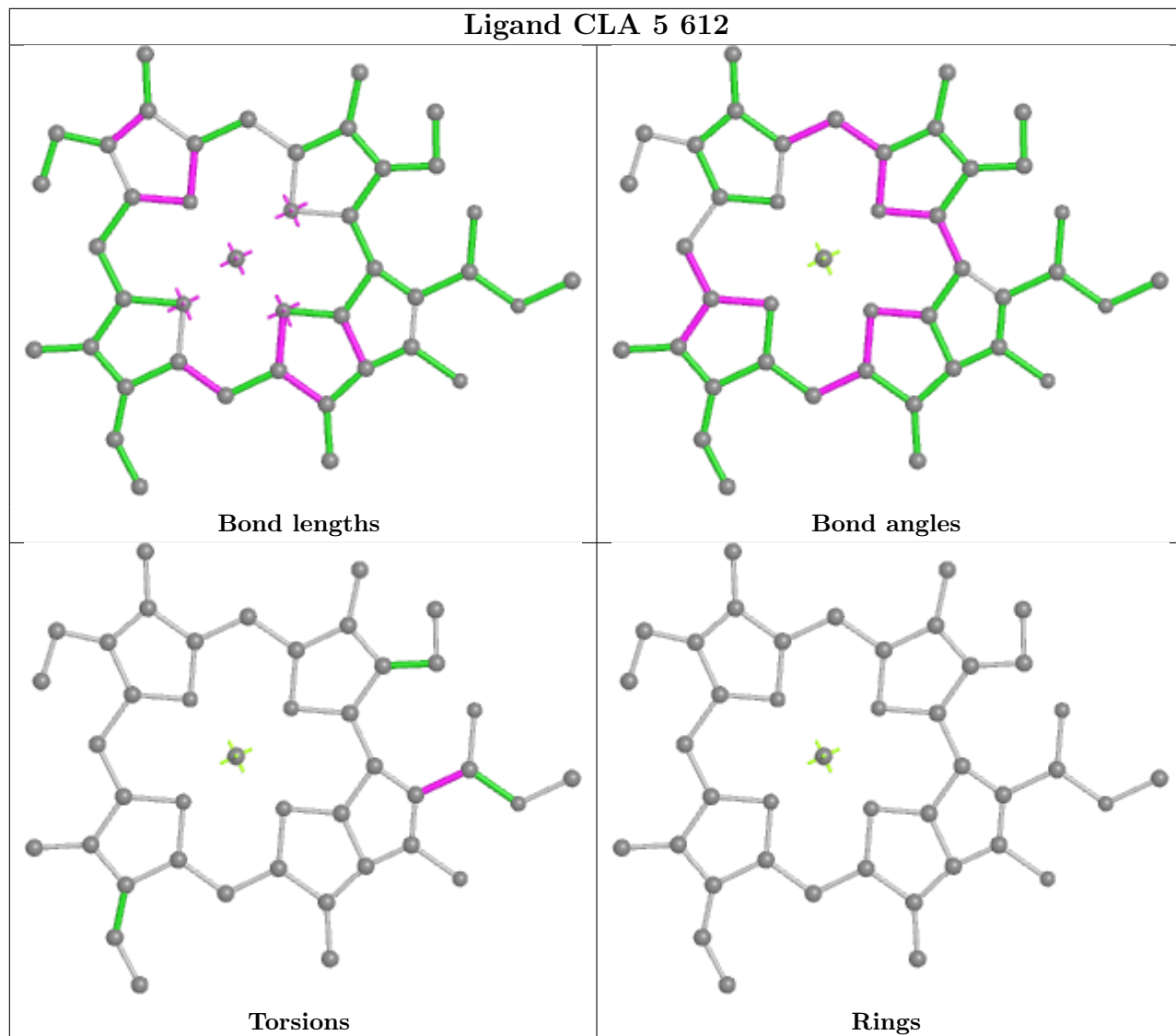


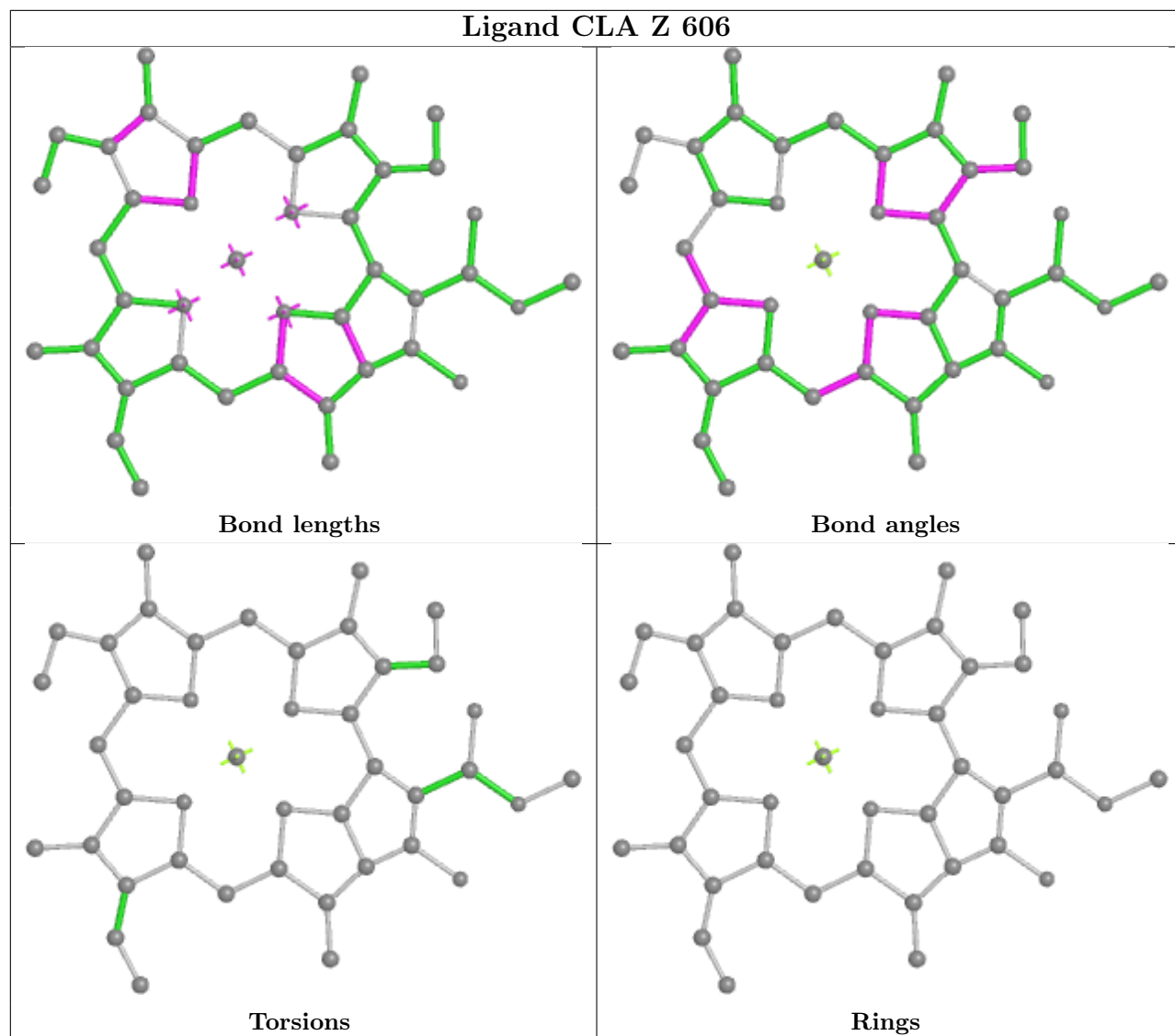


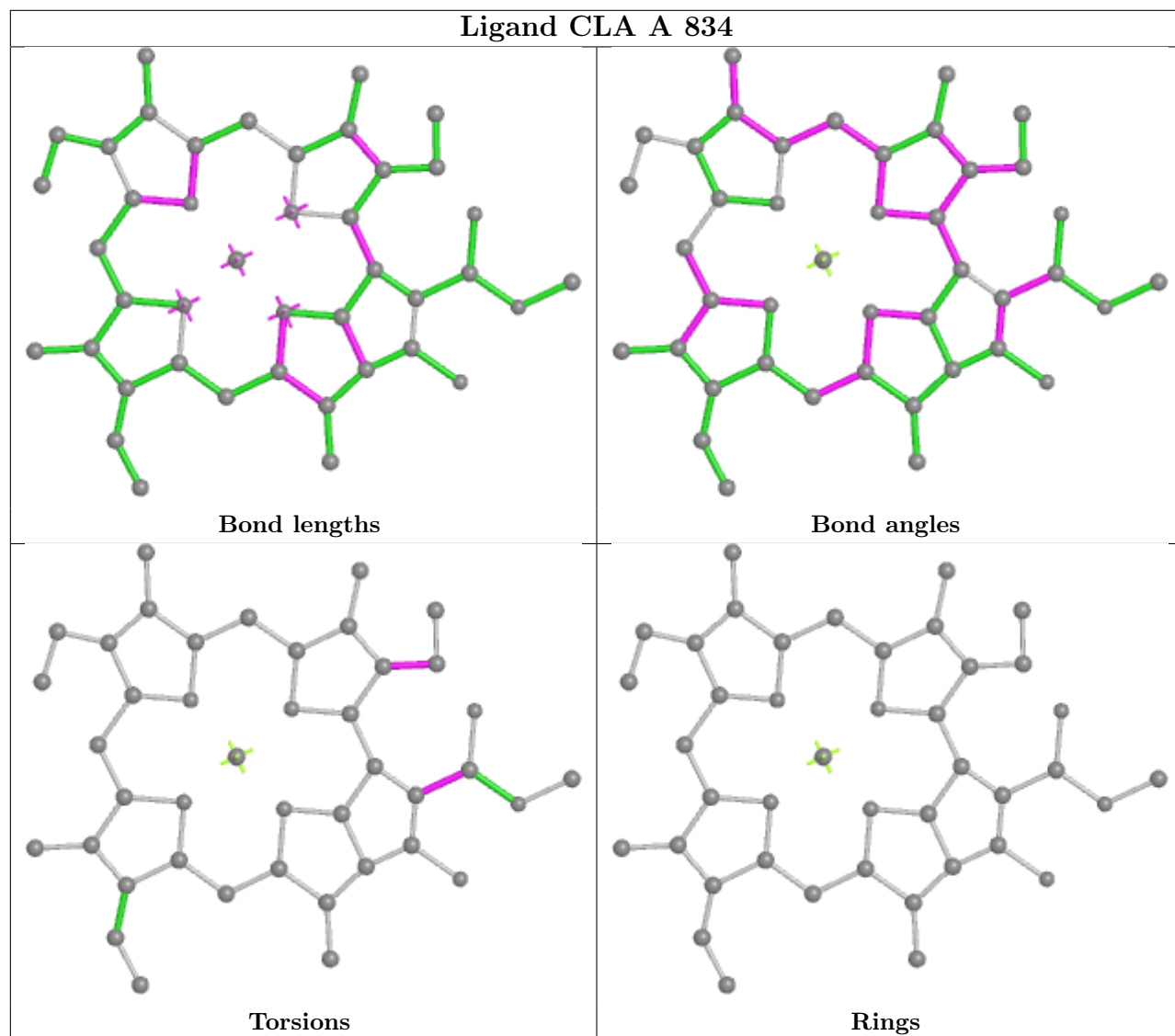


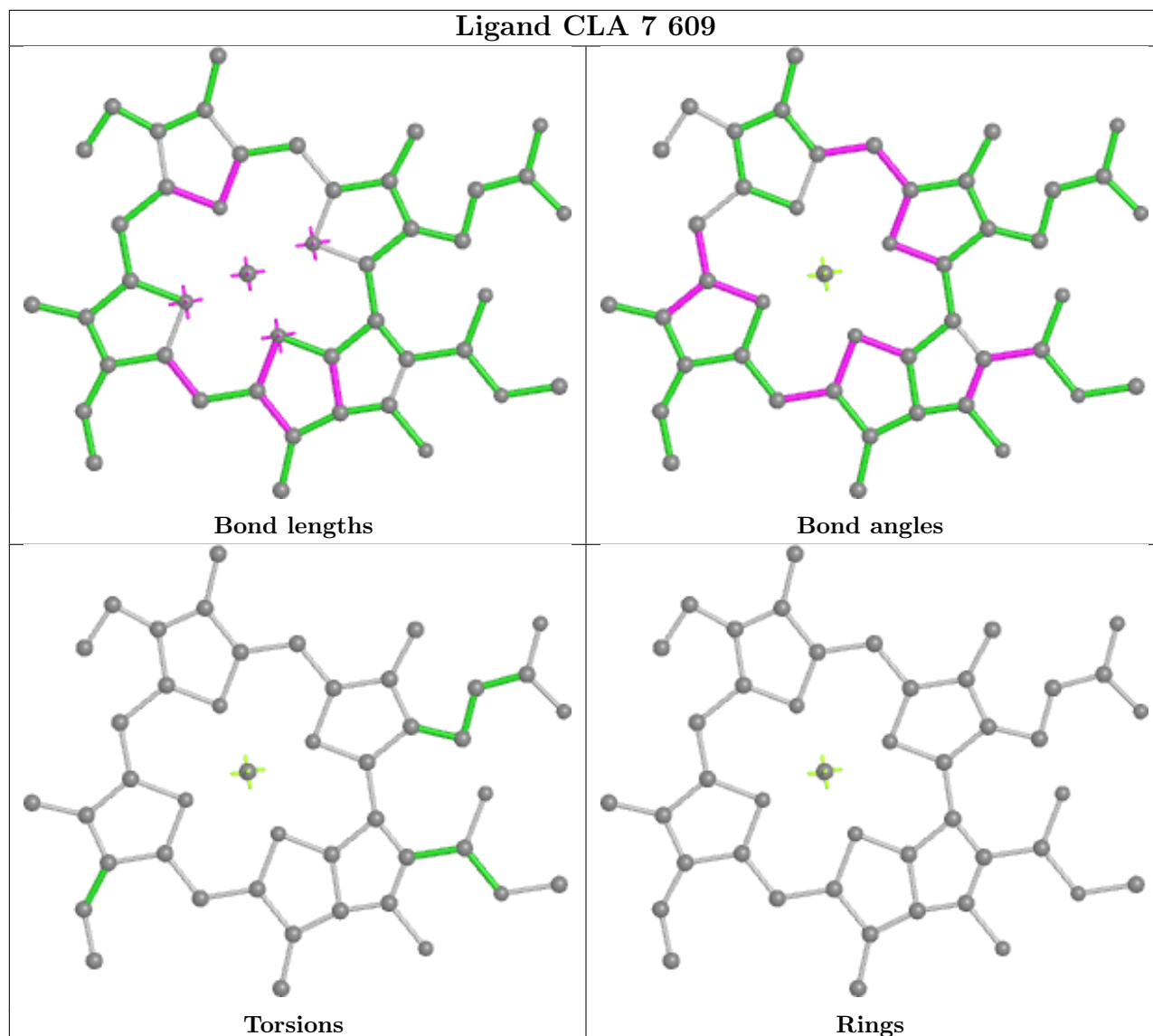


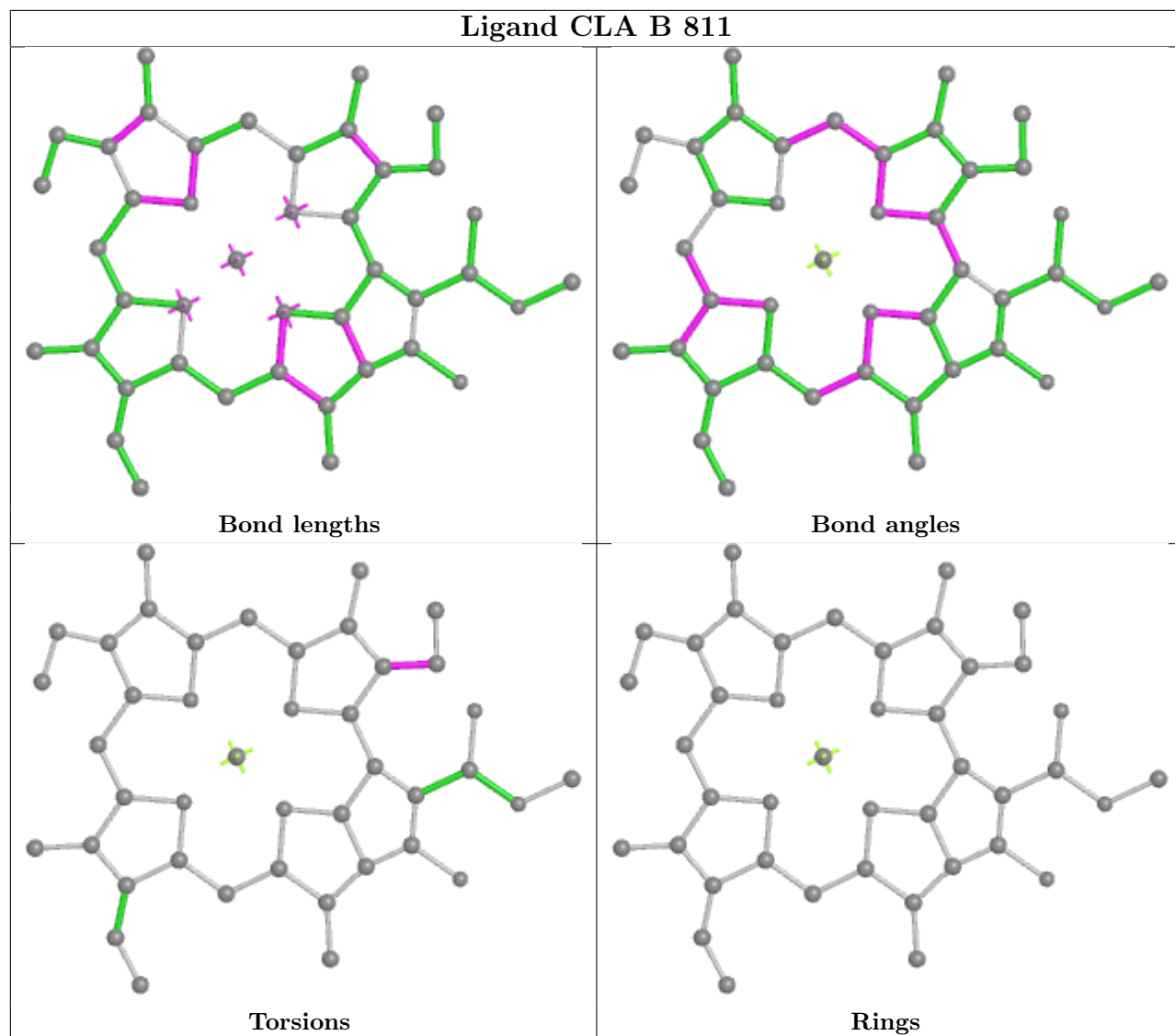
Ligand CLA 5 612

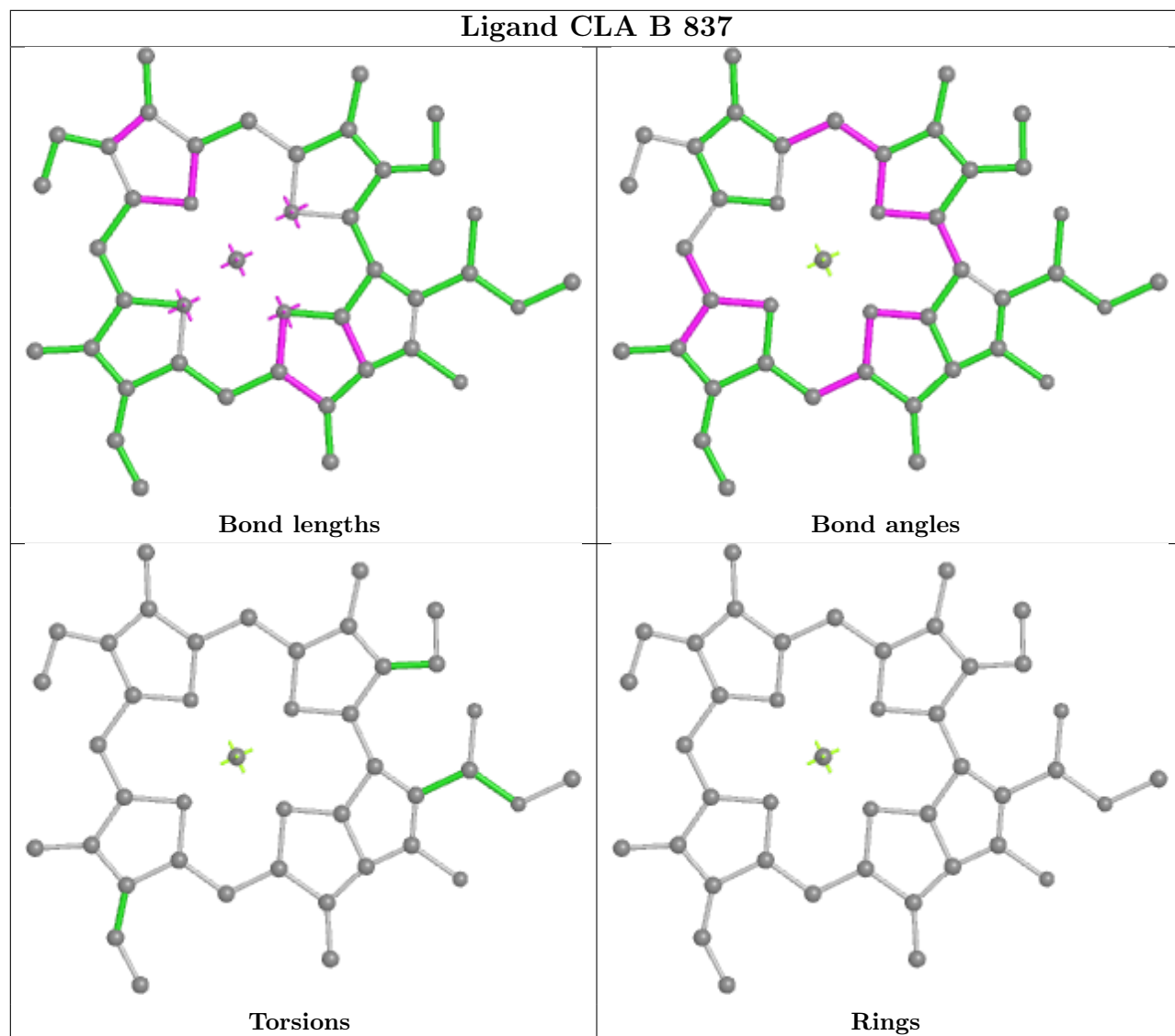


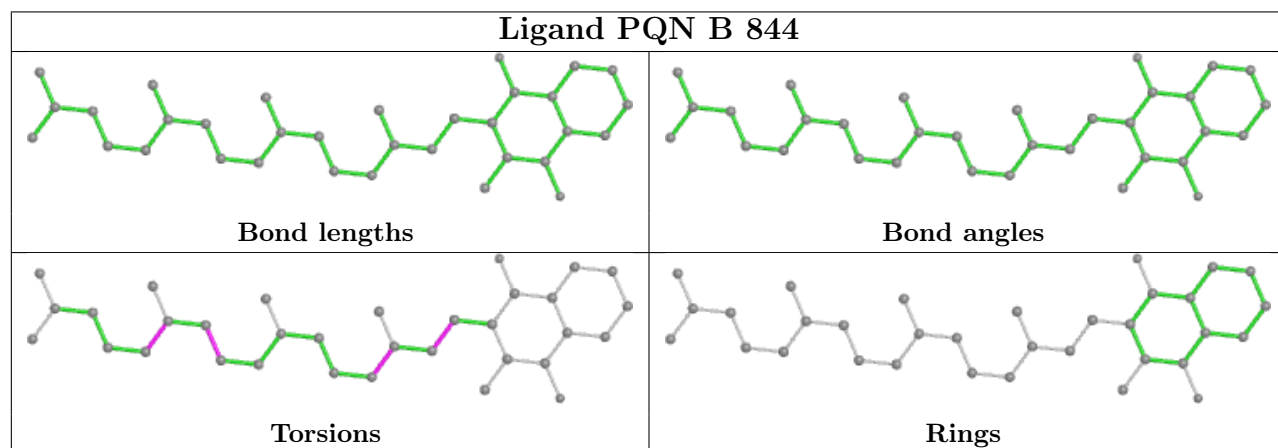
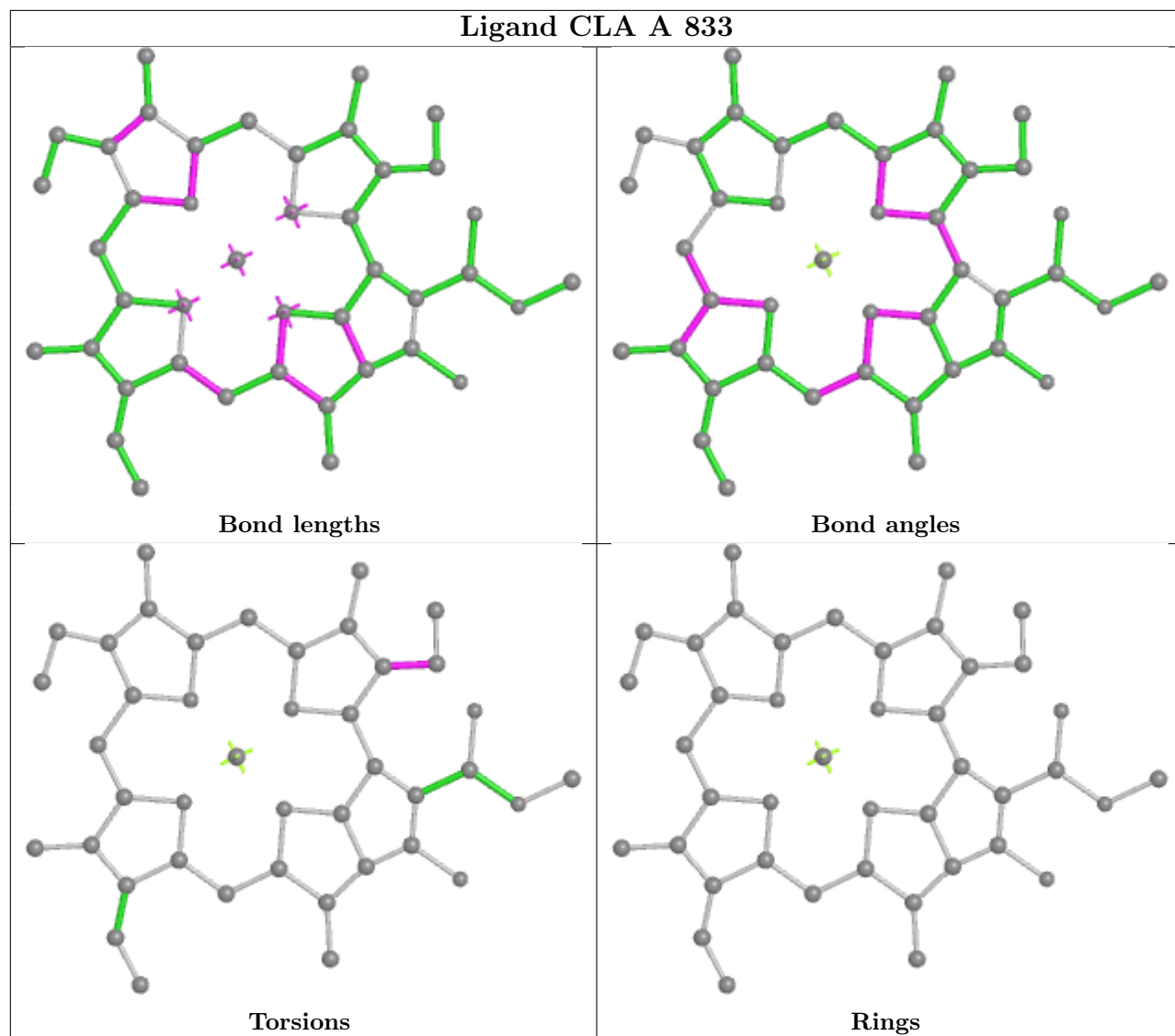


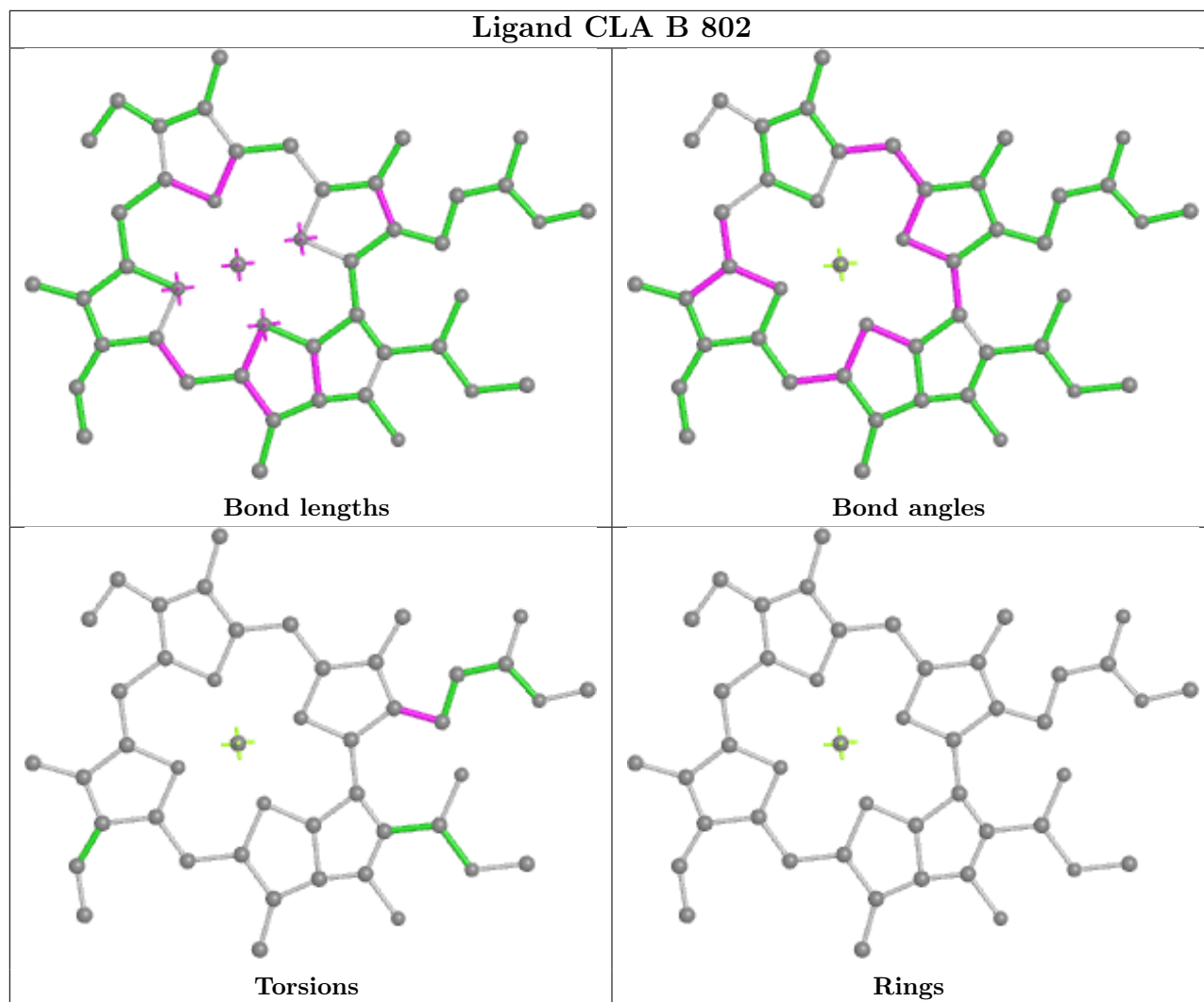




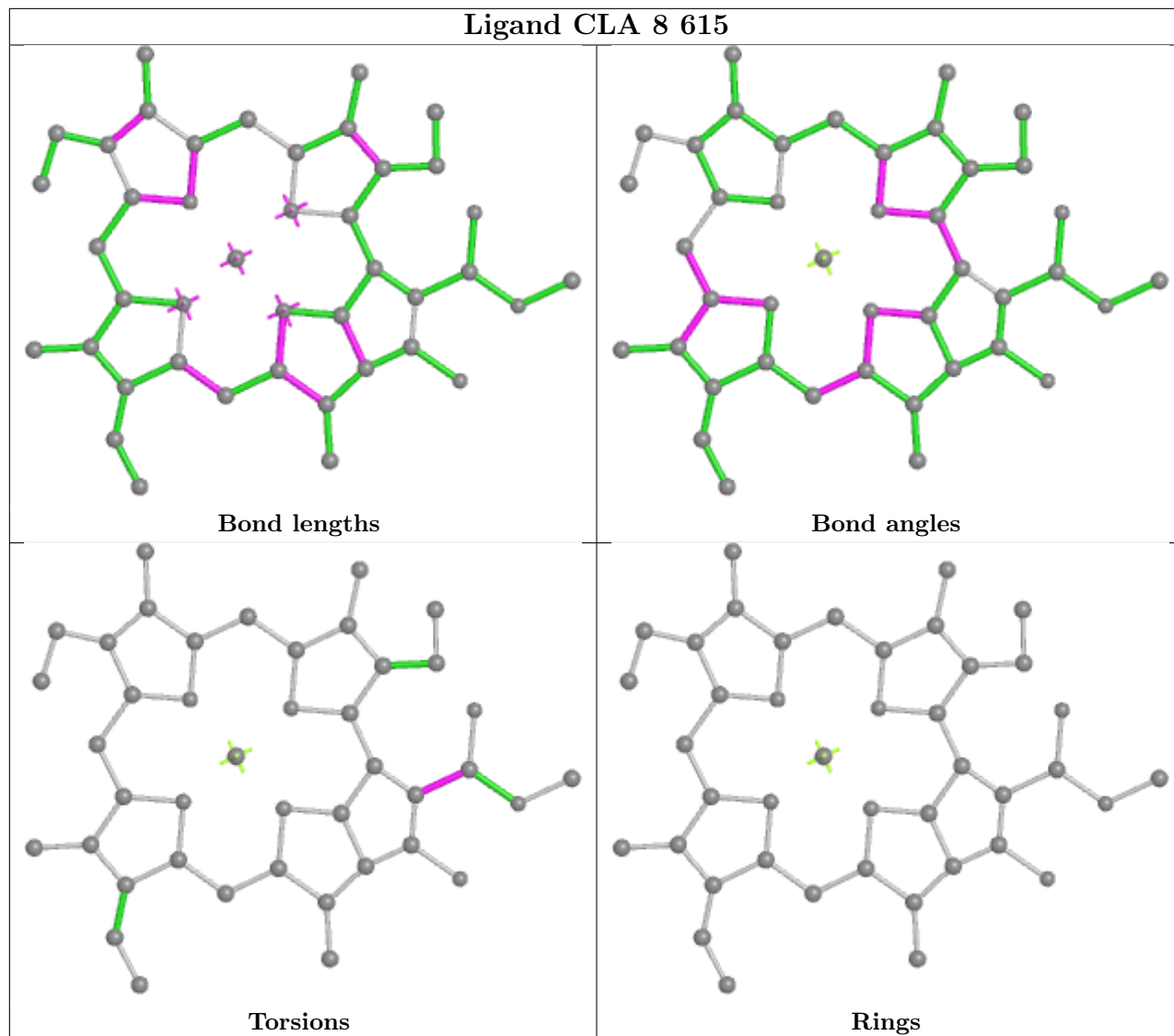


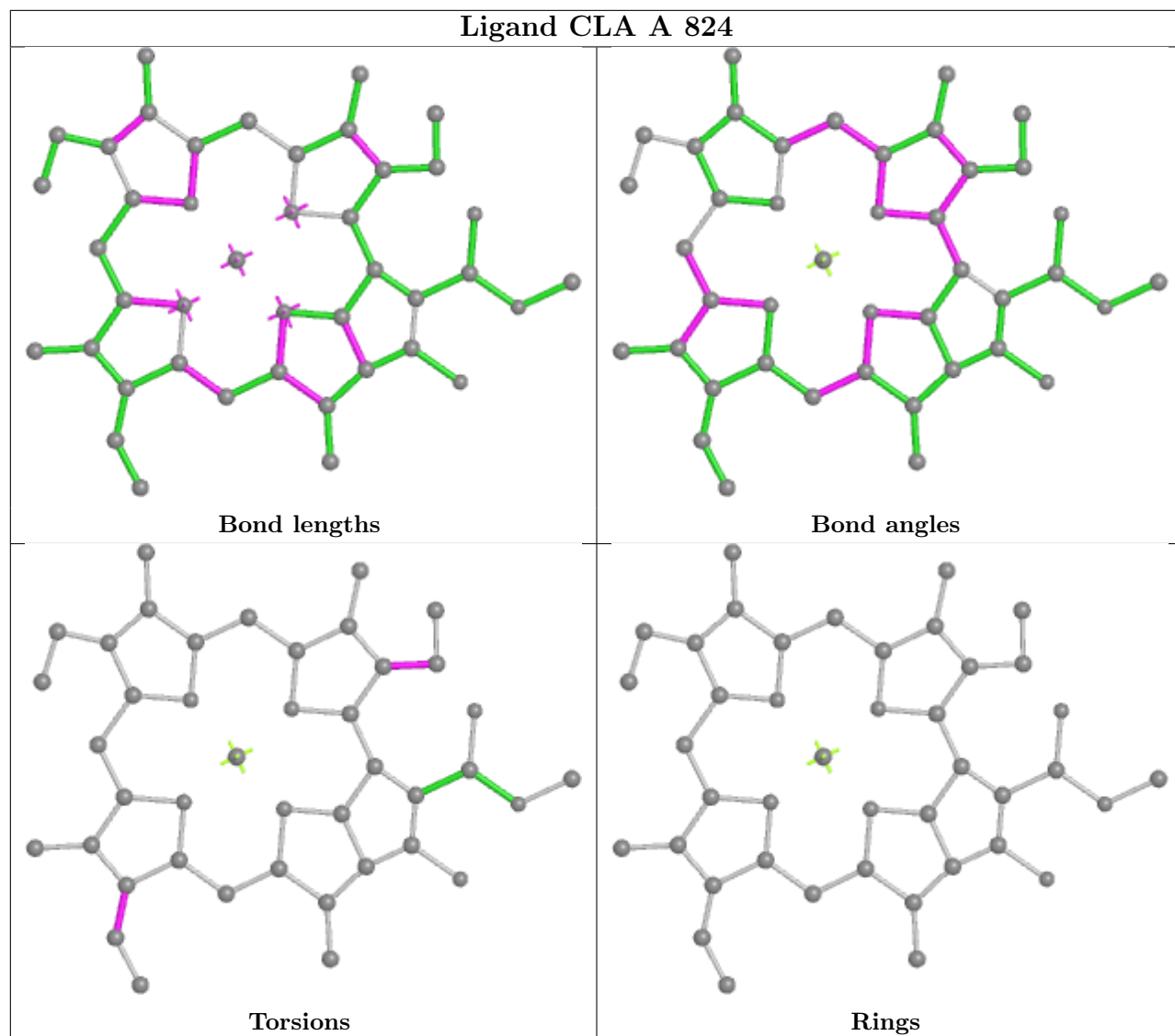


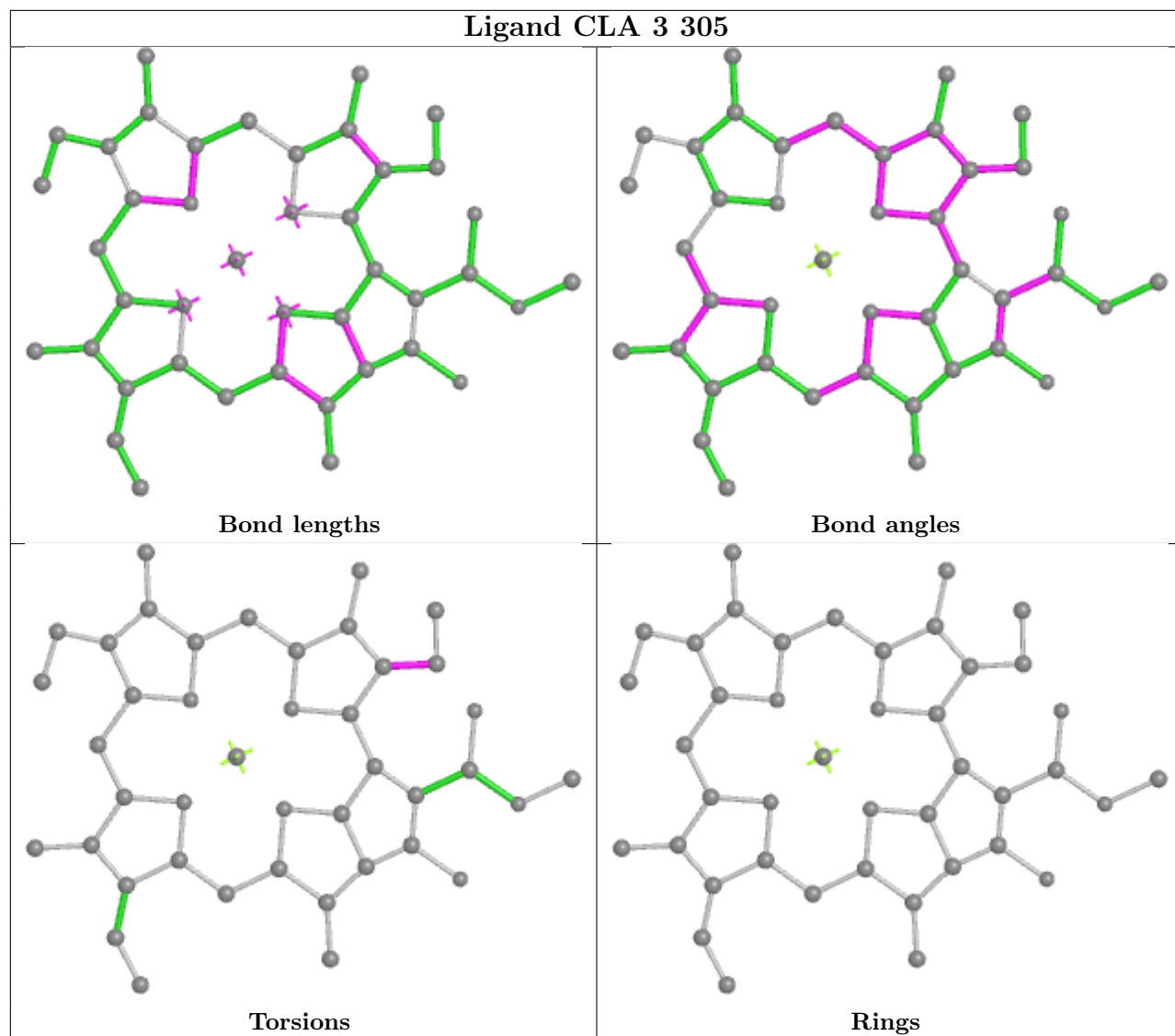


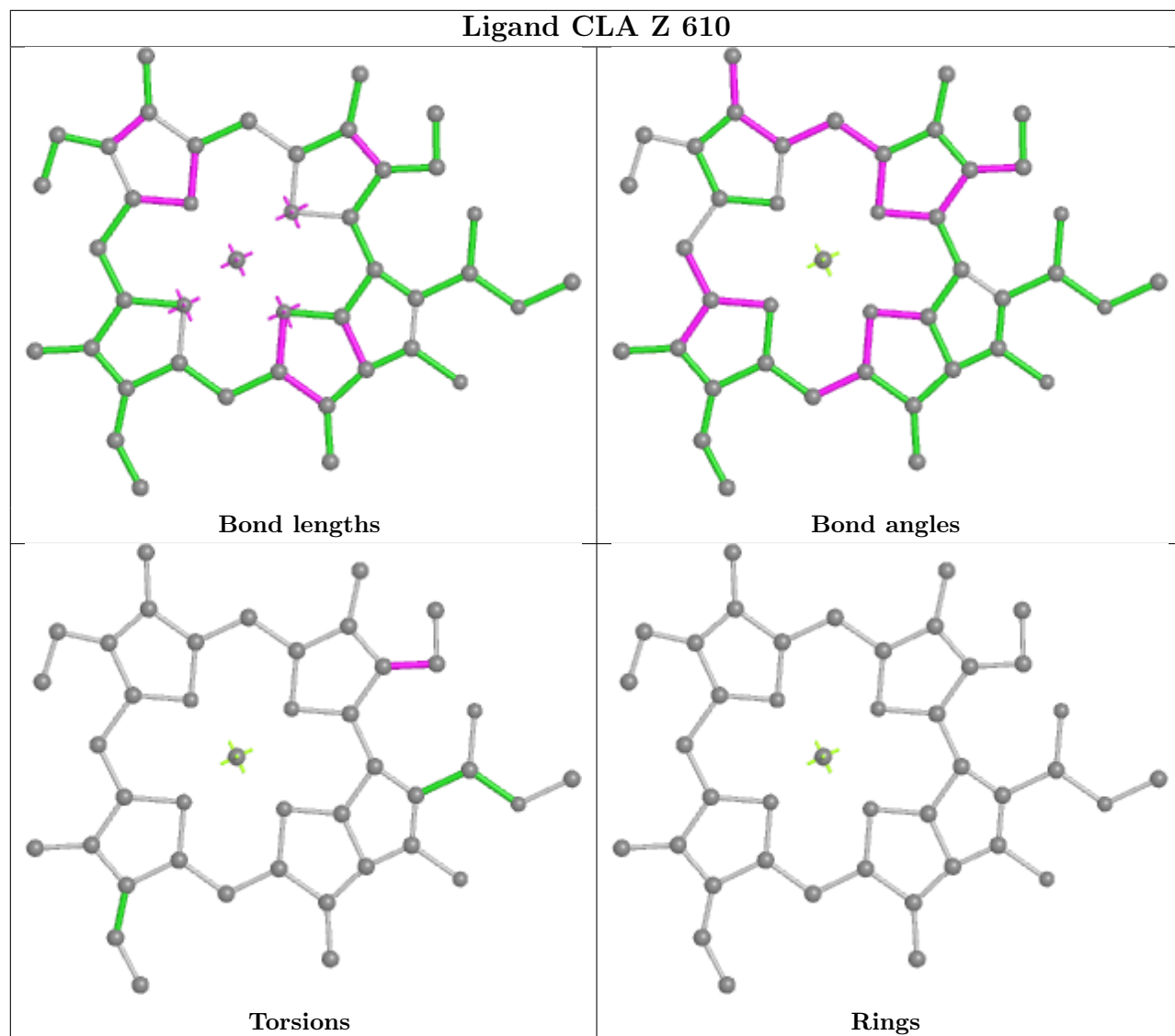


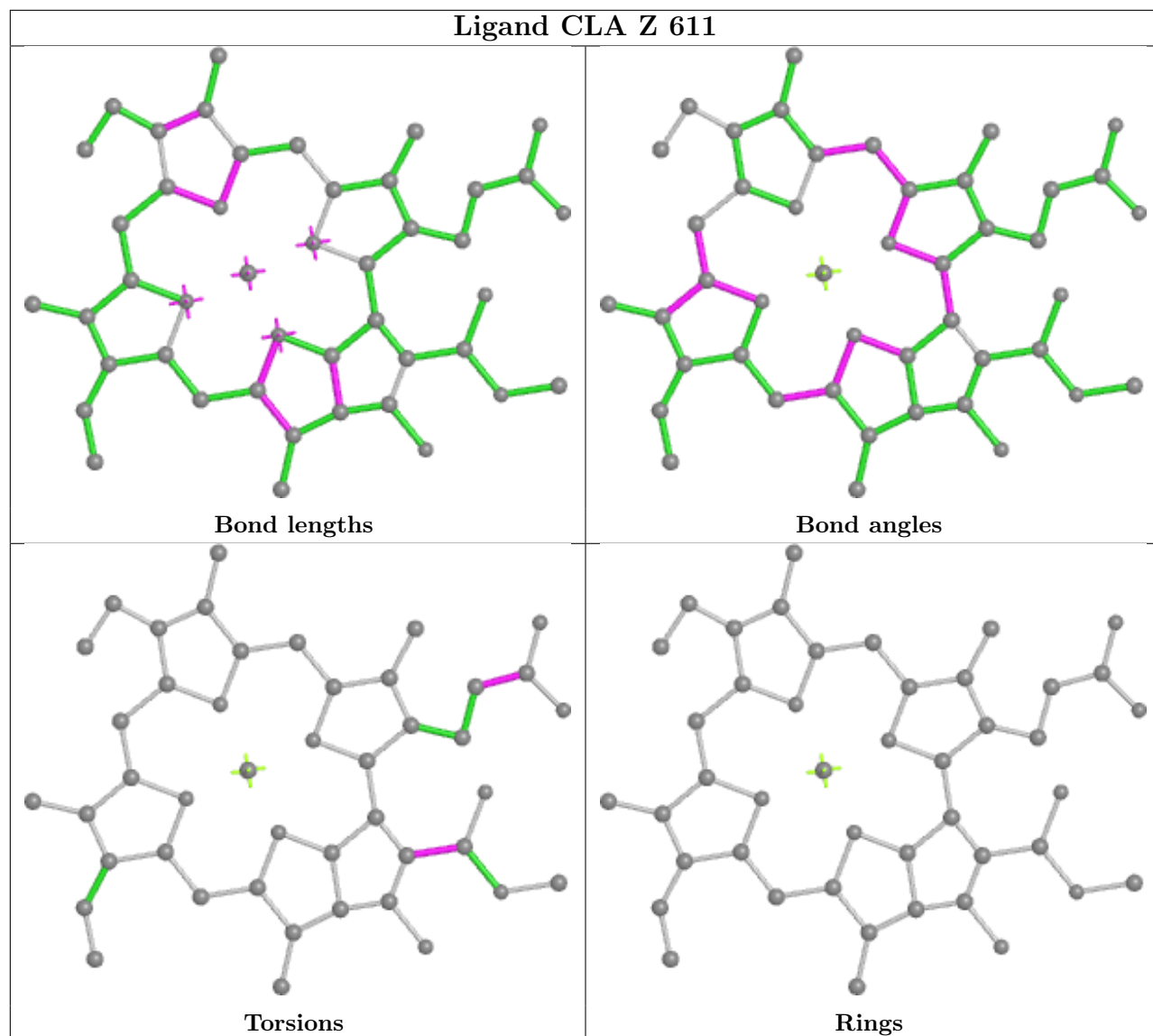
Ligand CLA 8 615

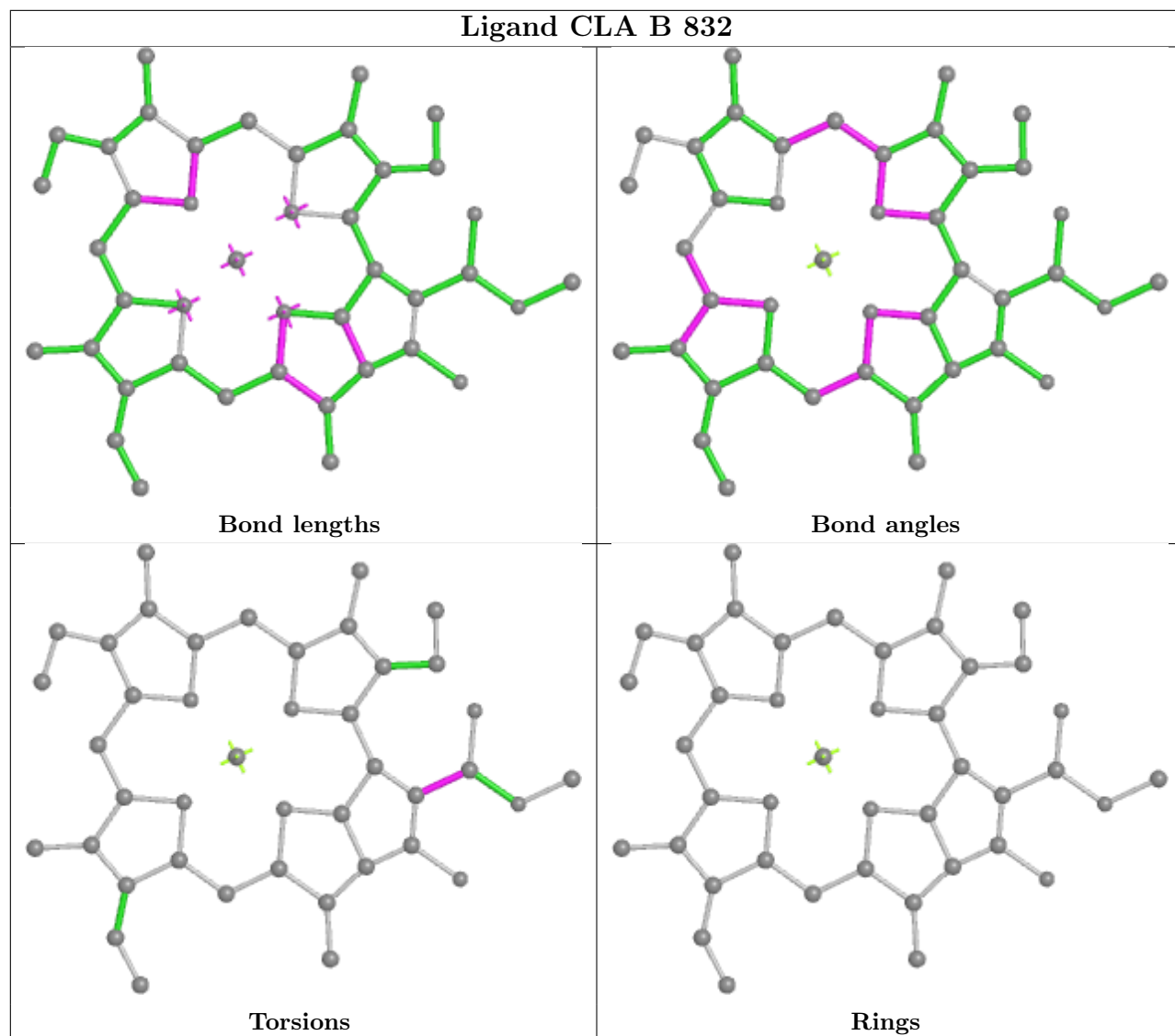


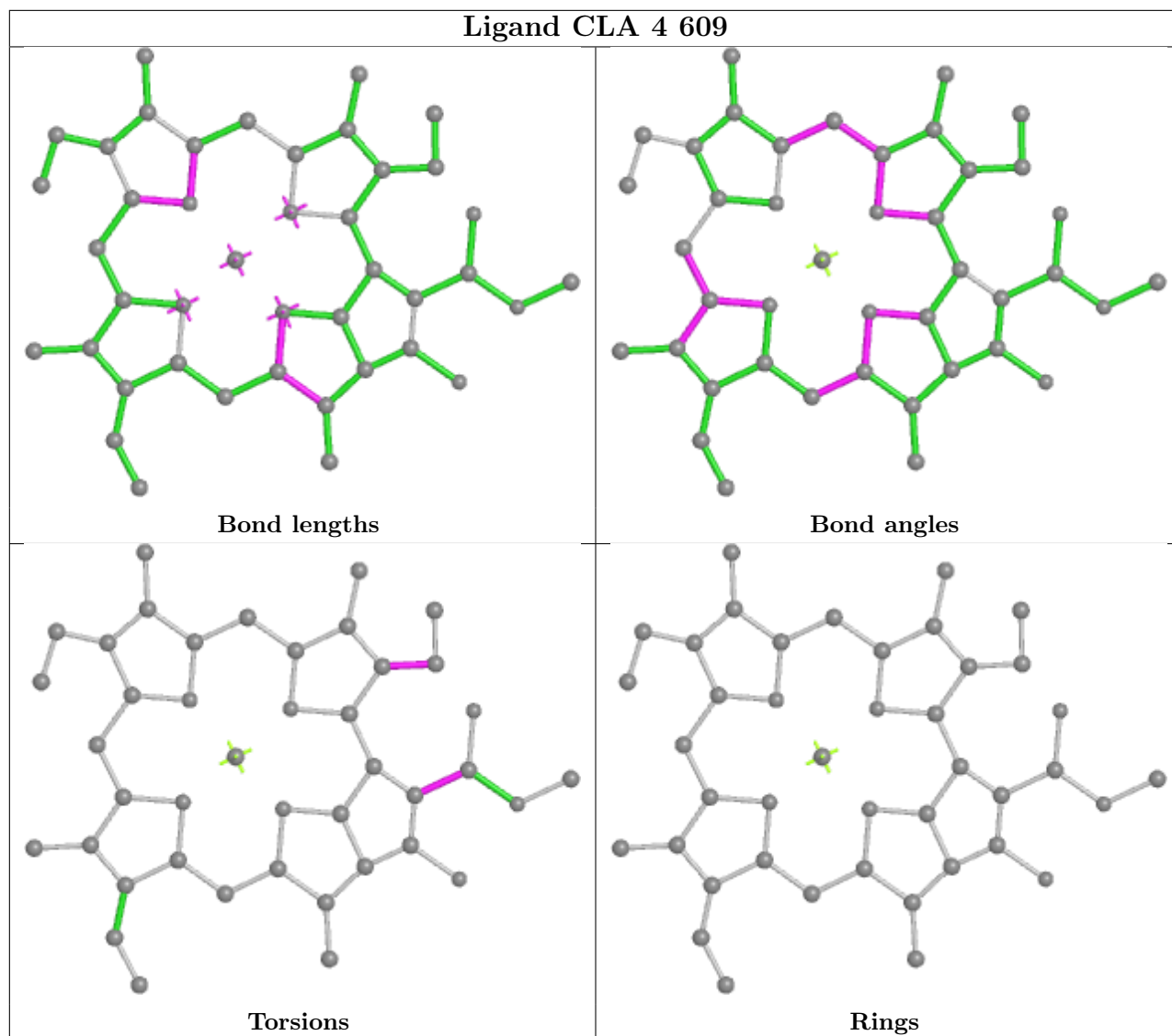


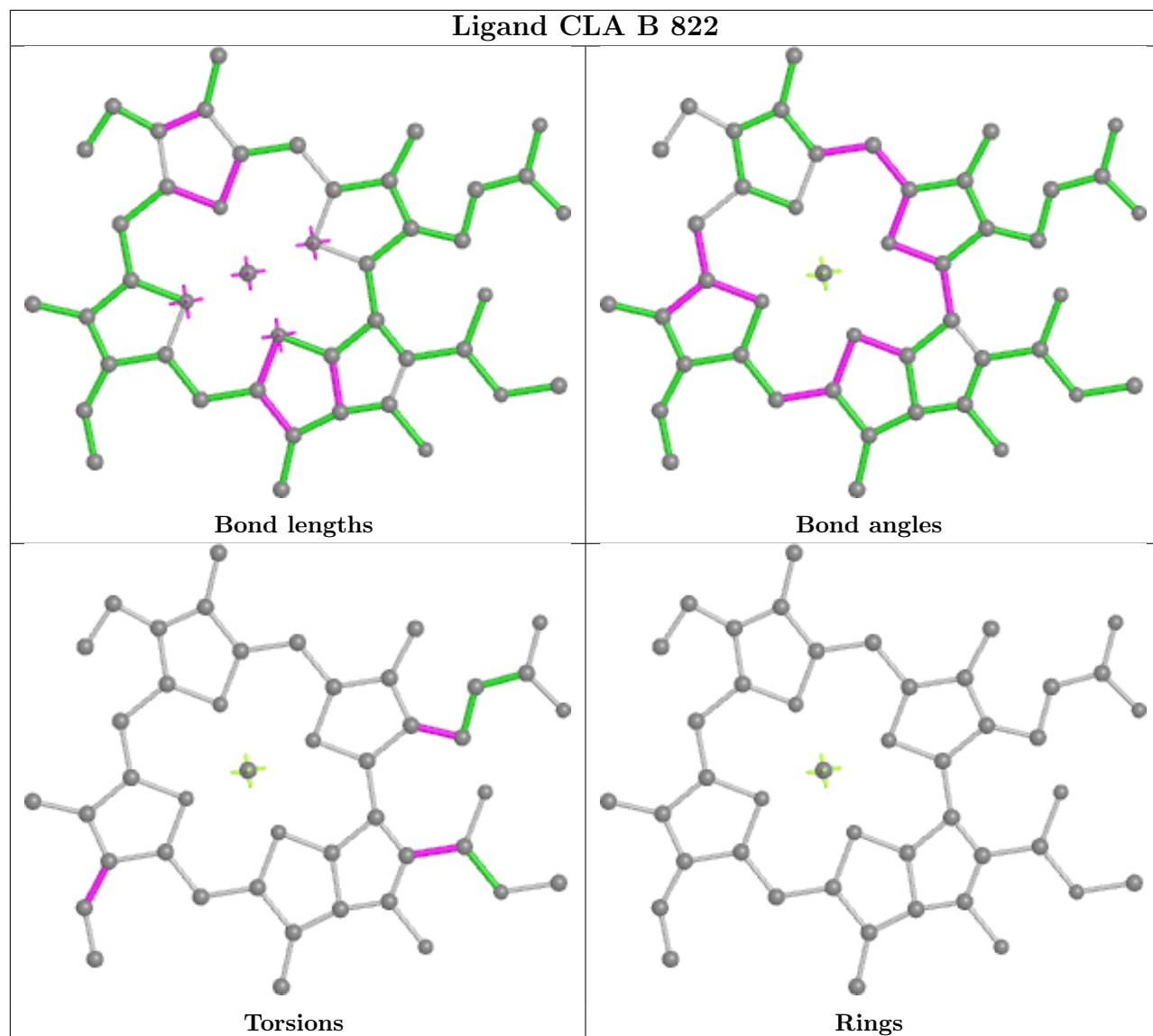


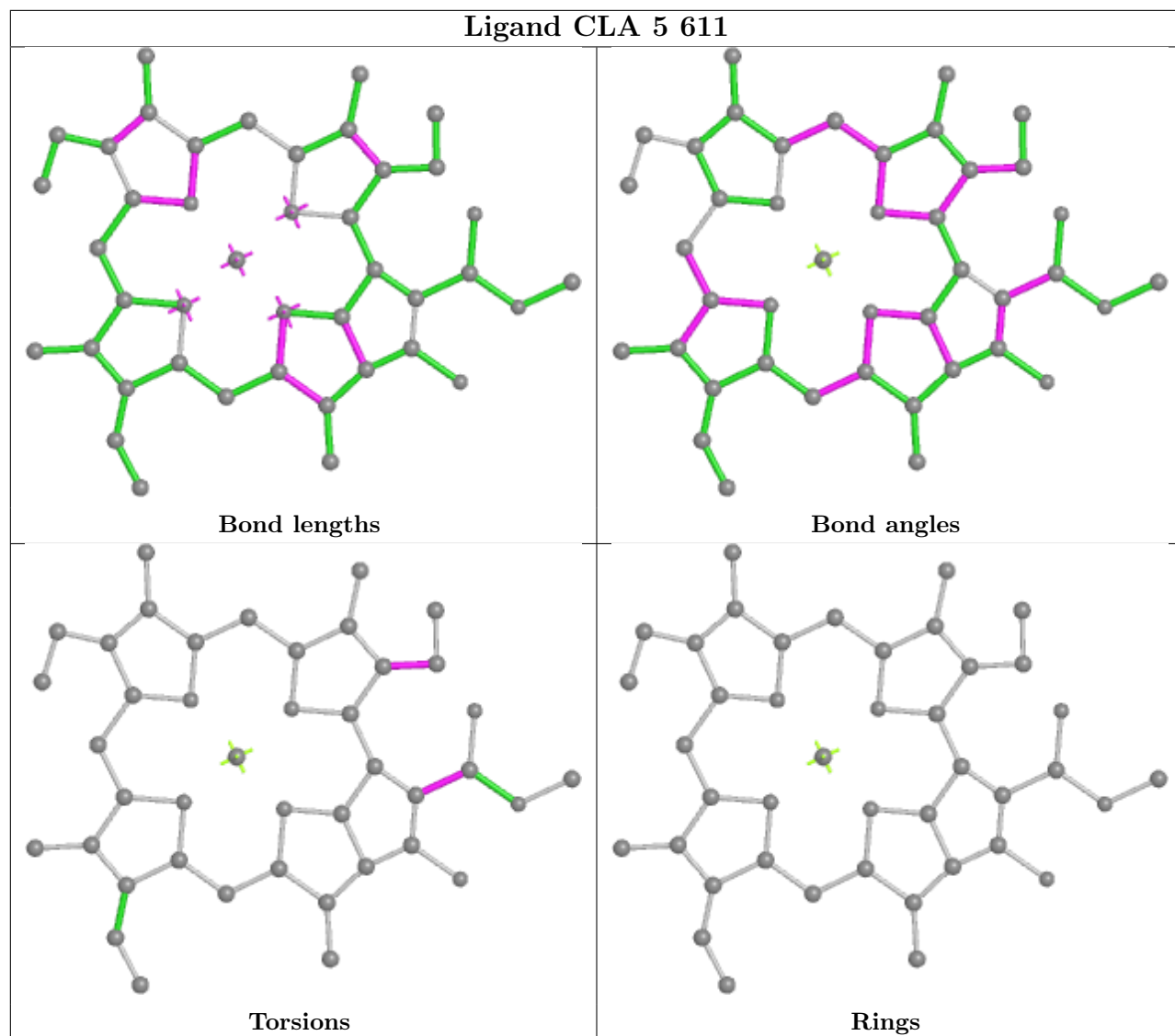


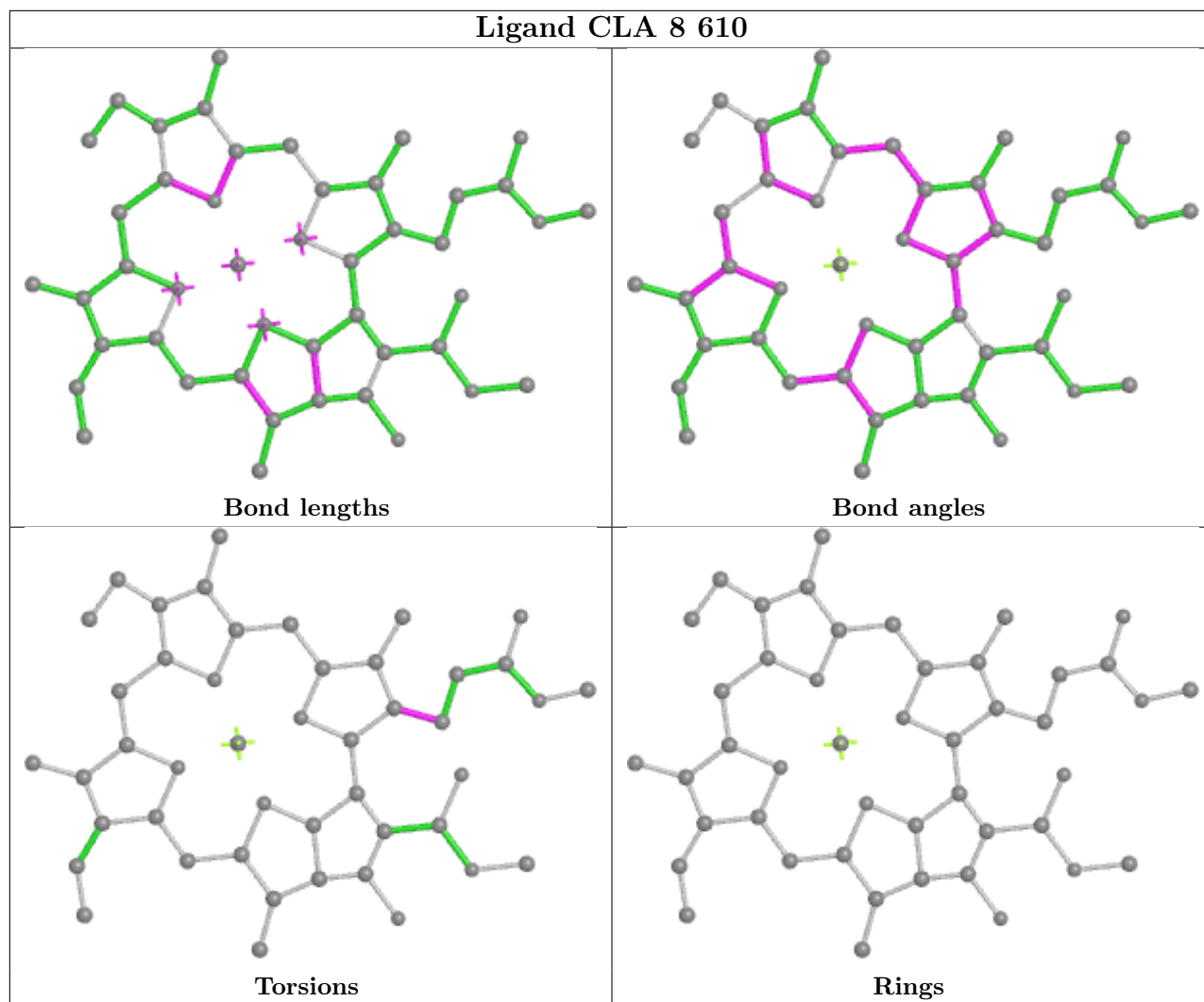


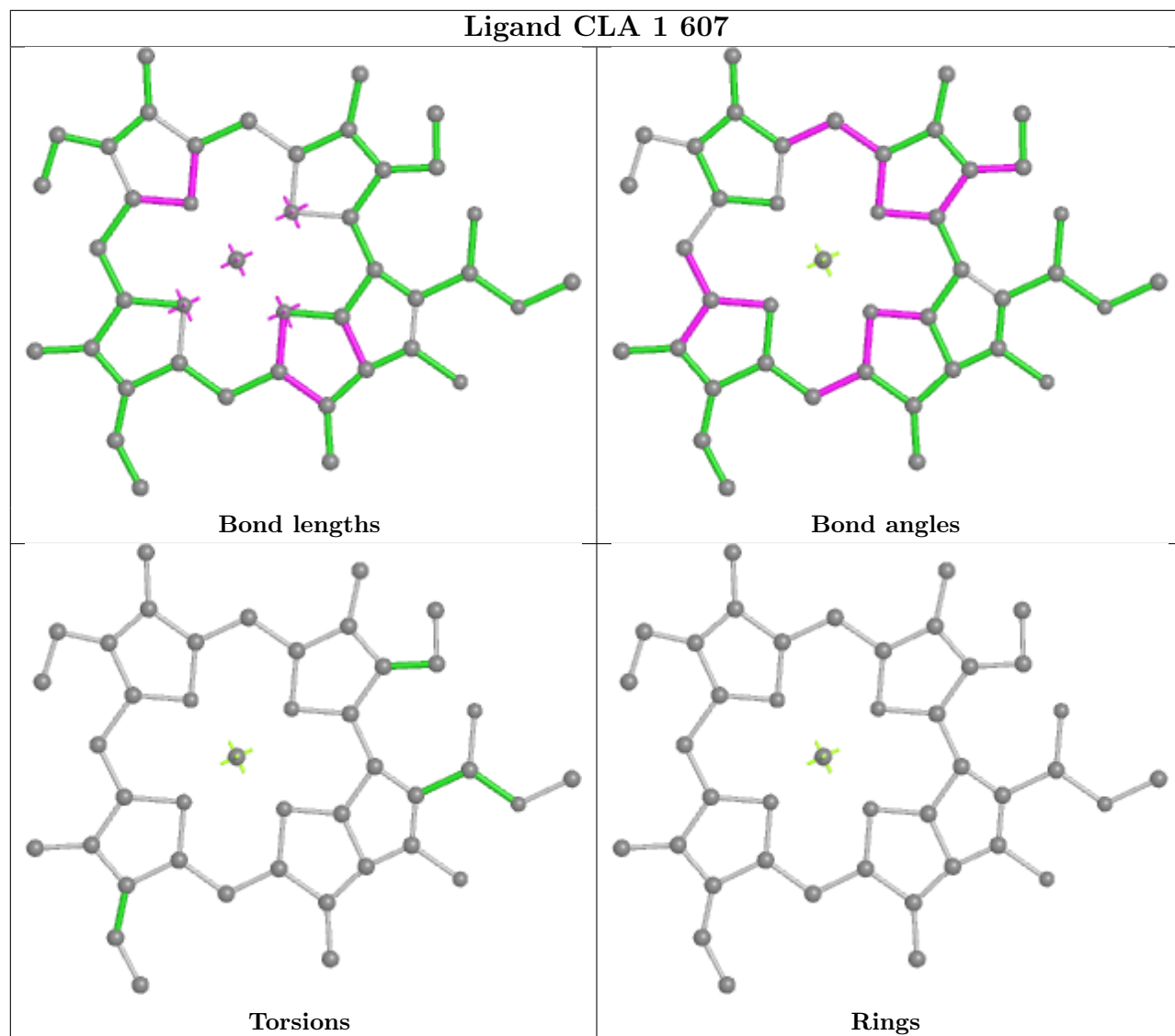


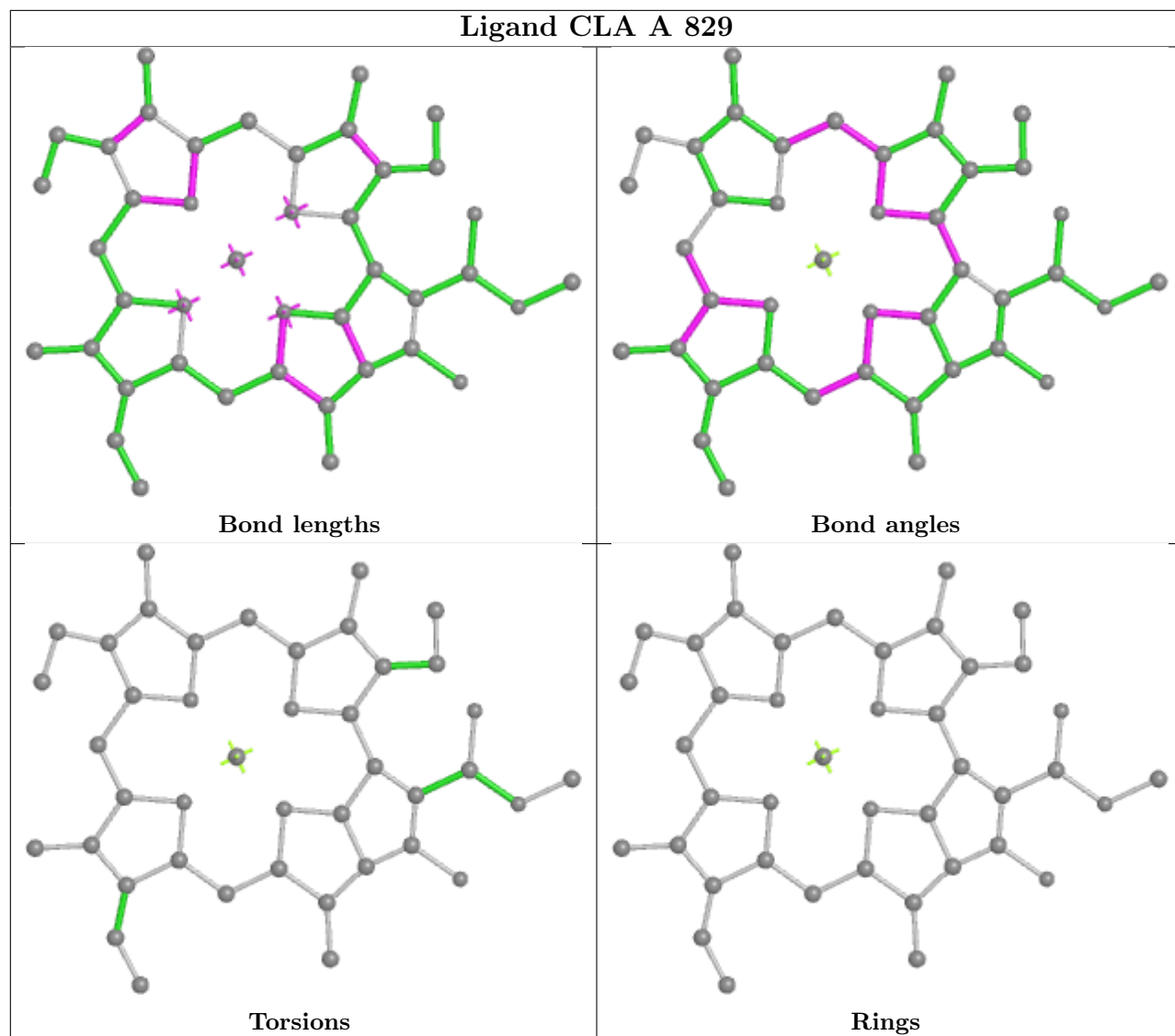


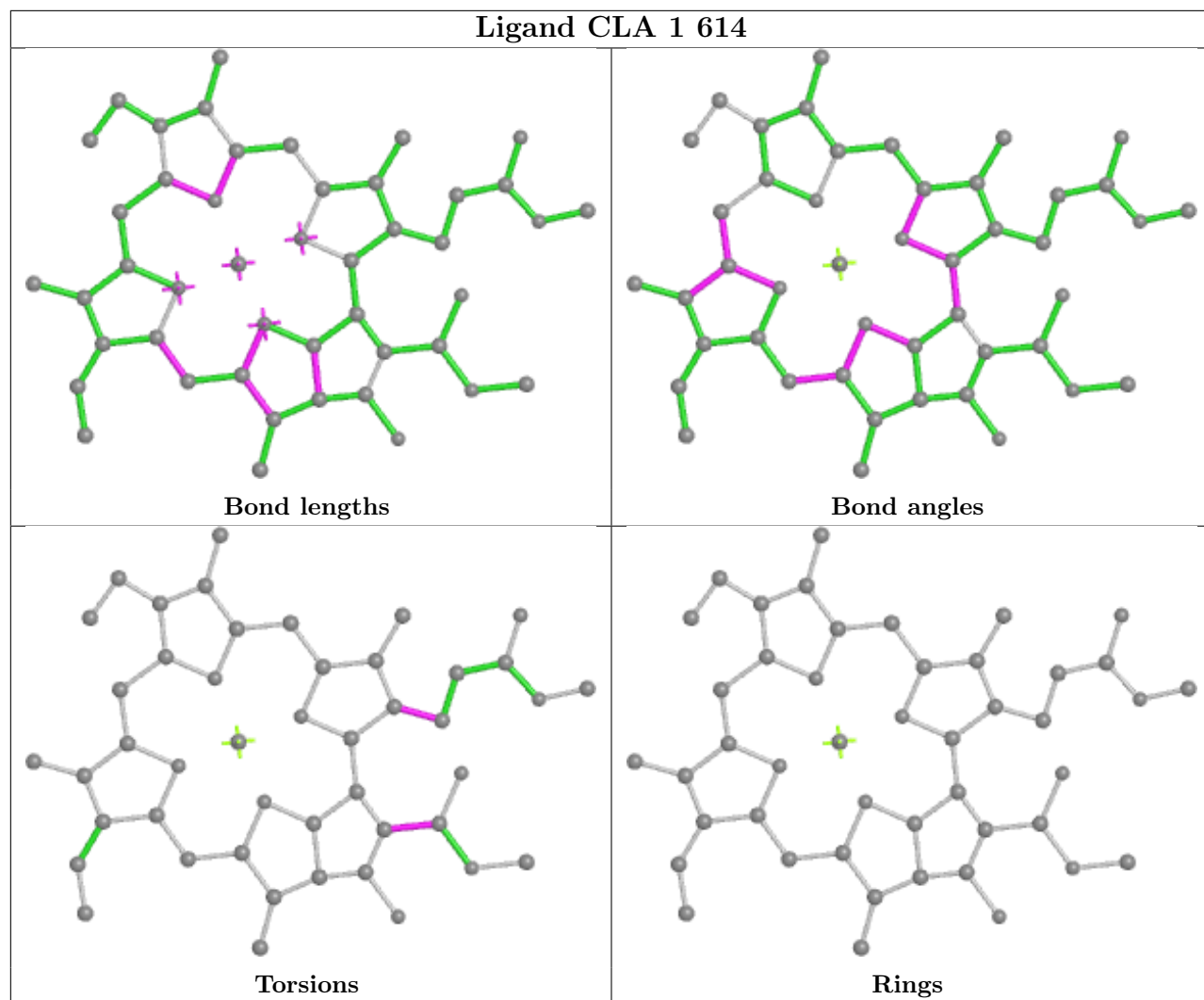


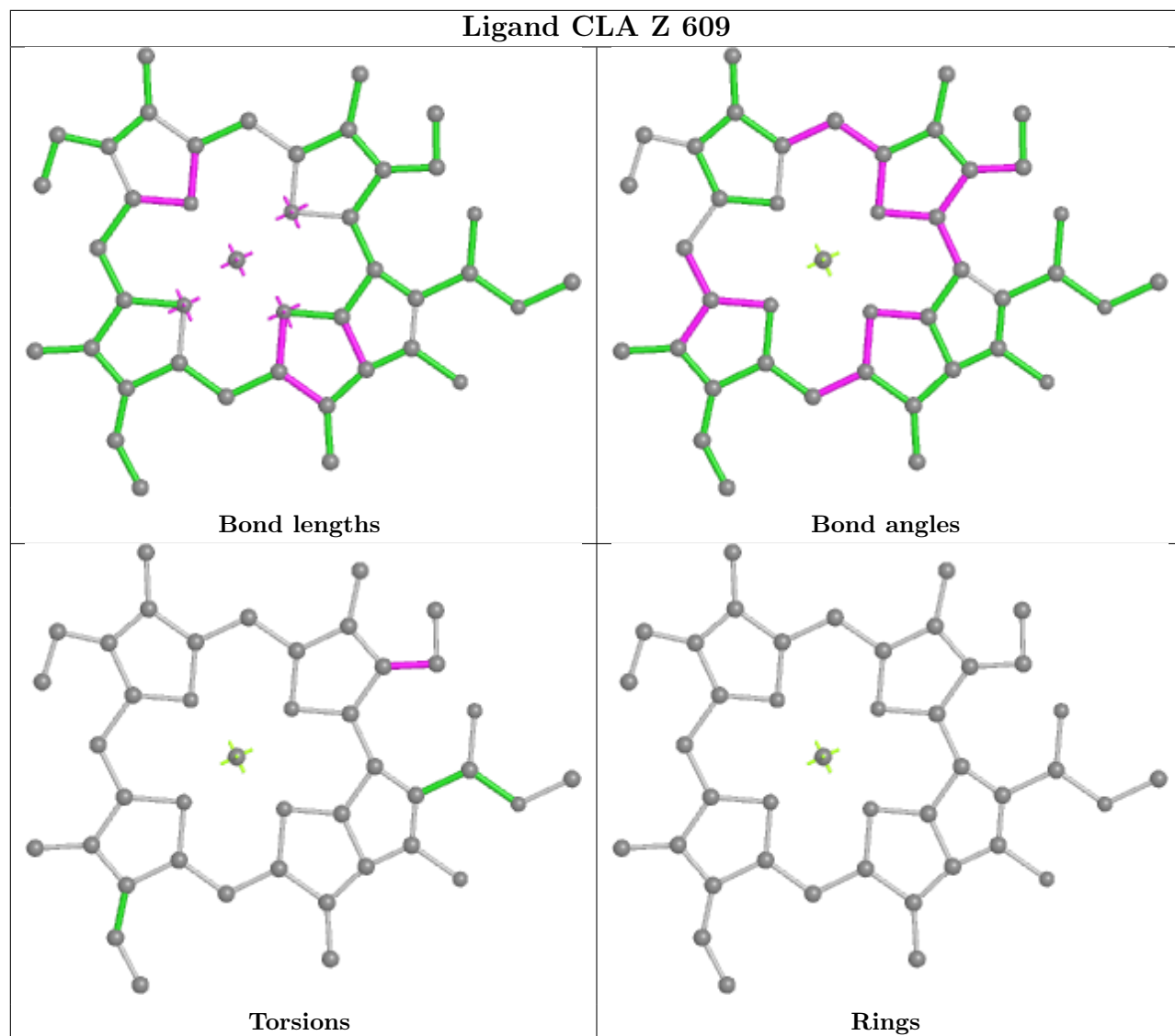


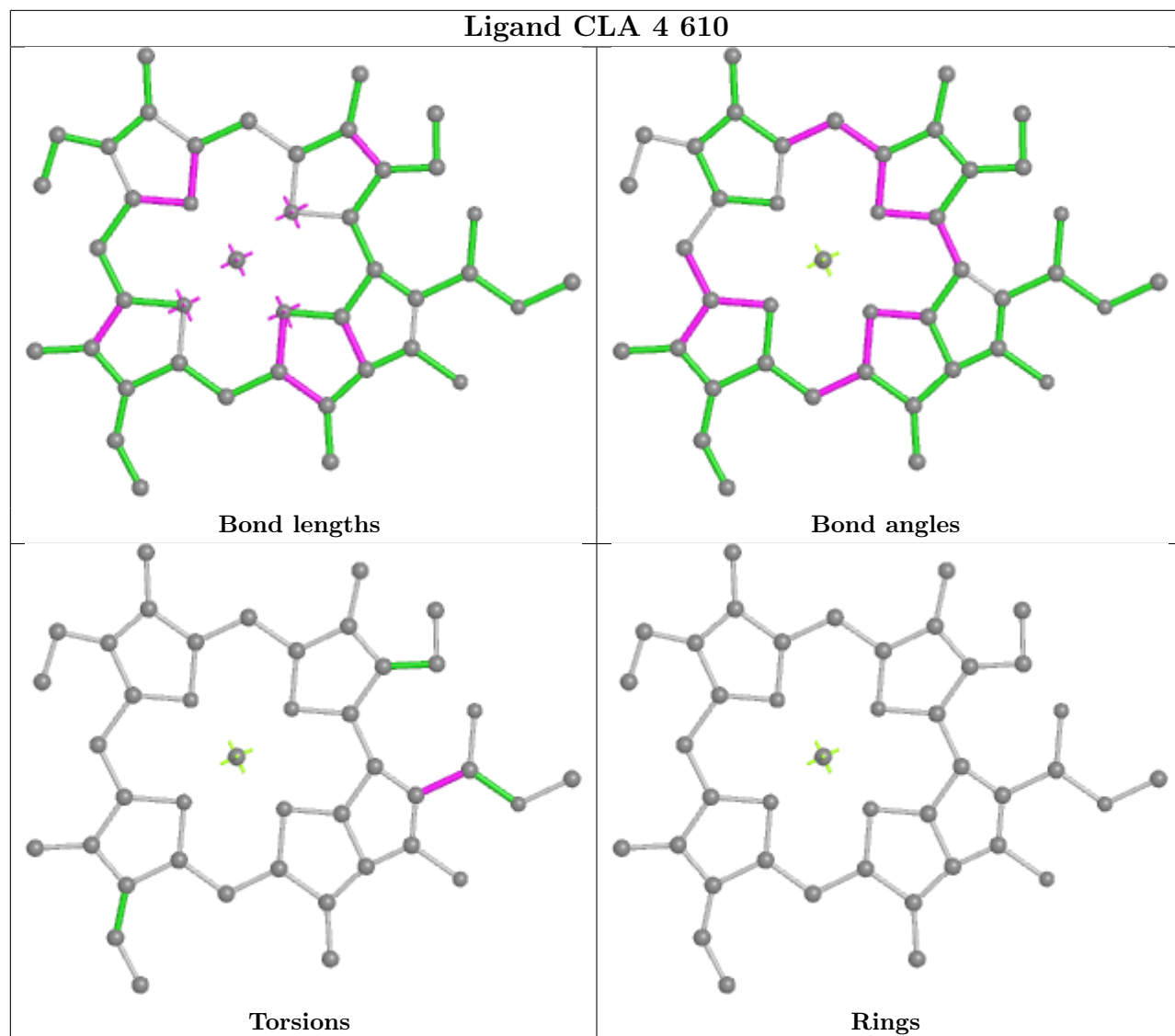


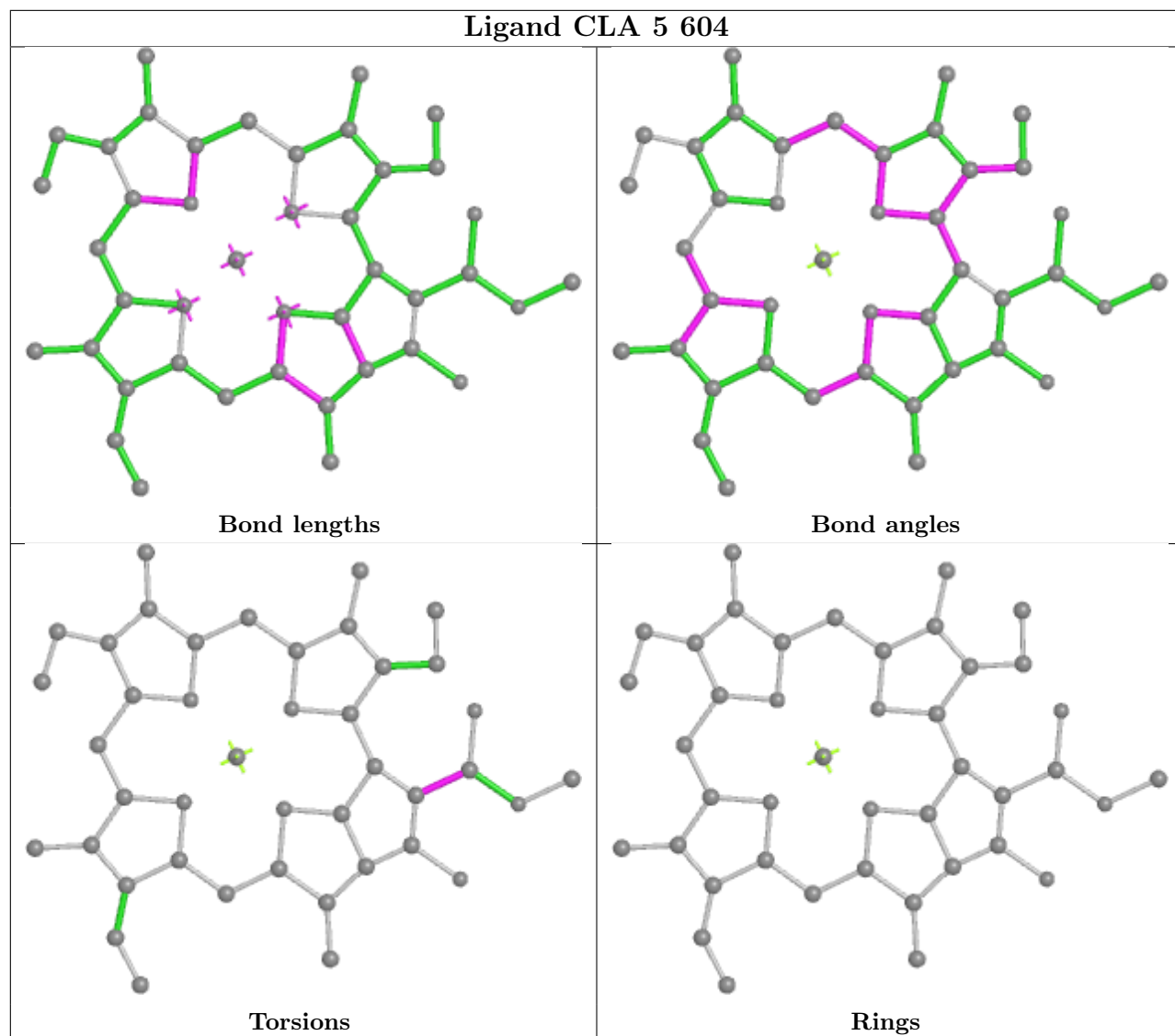


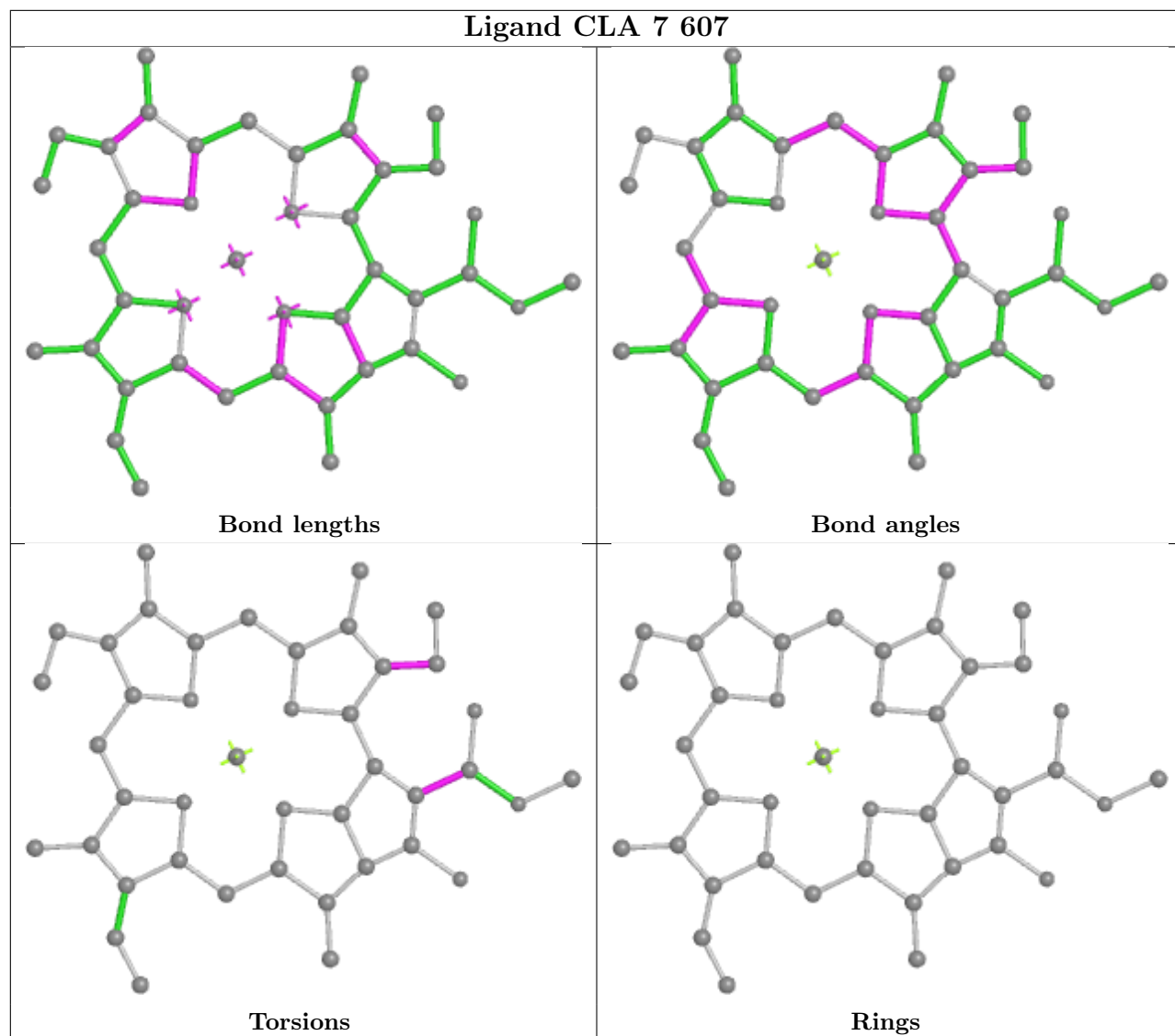


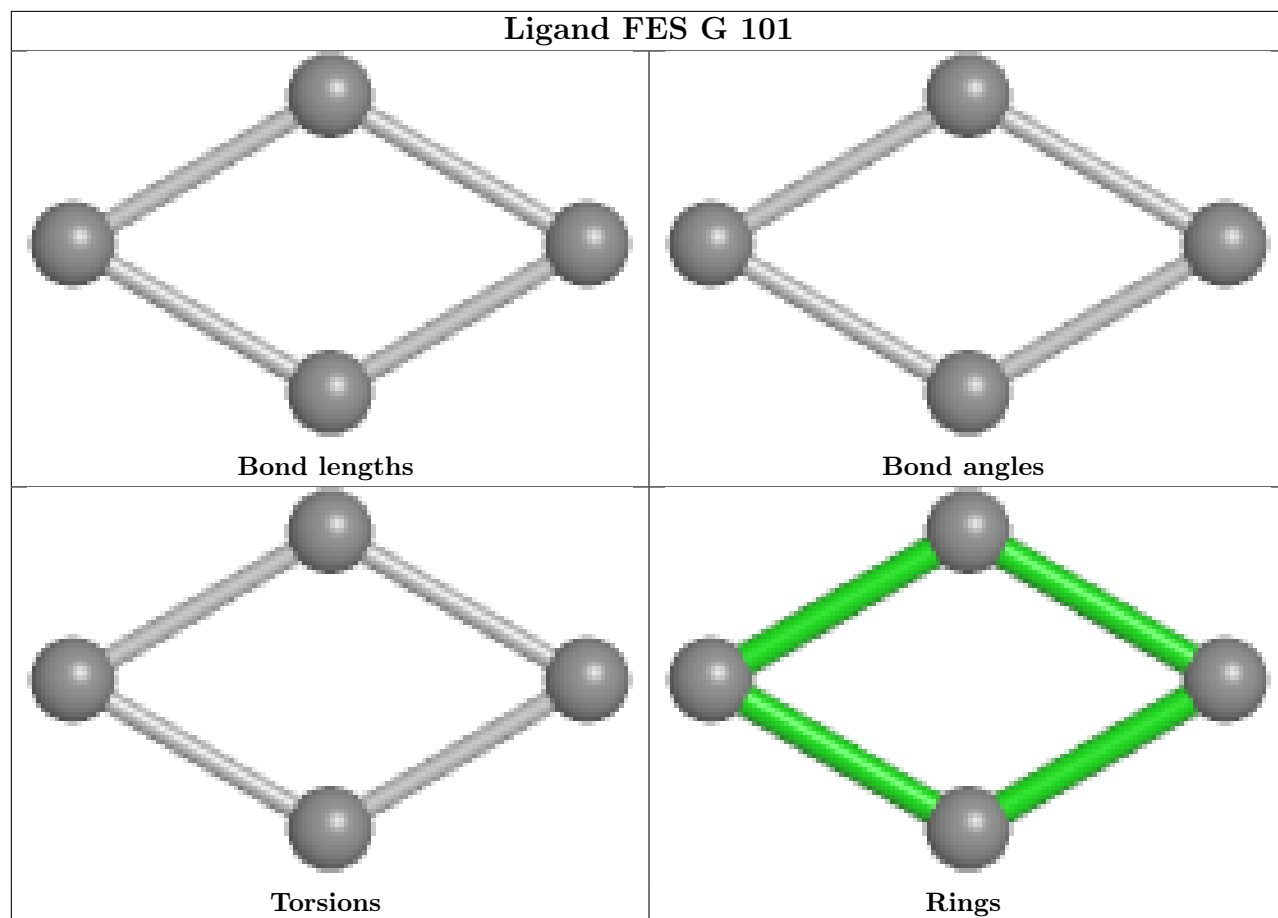


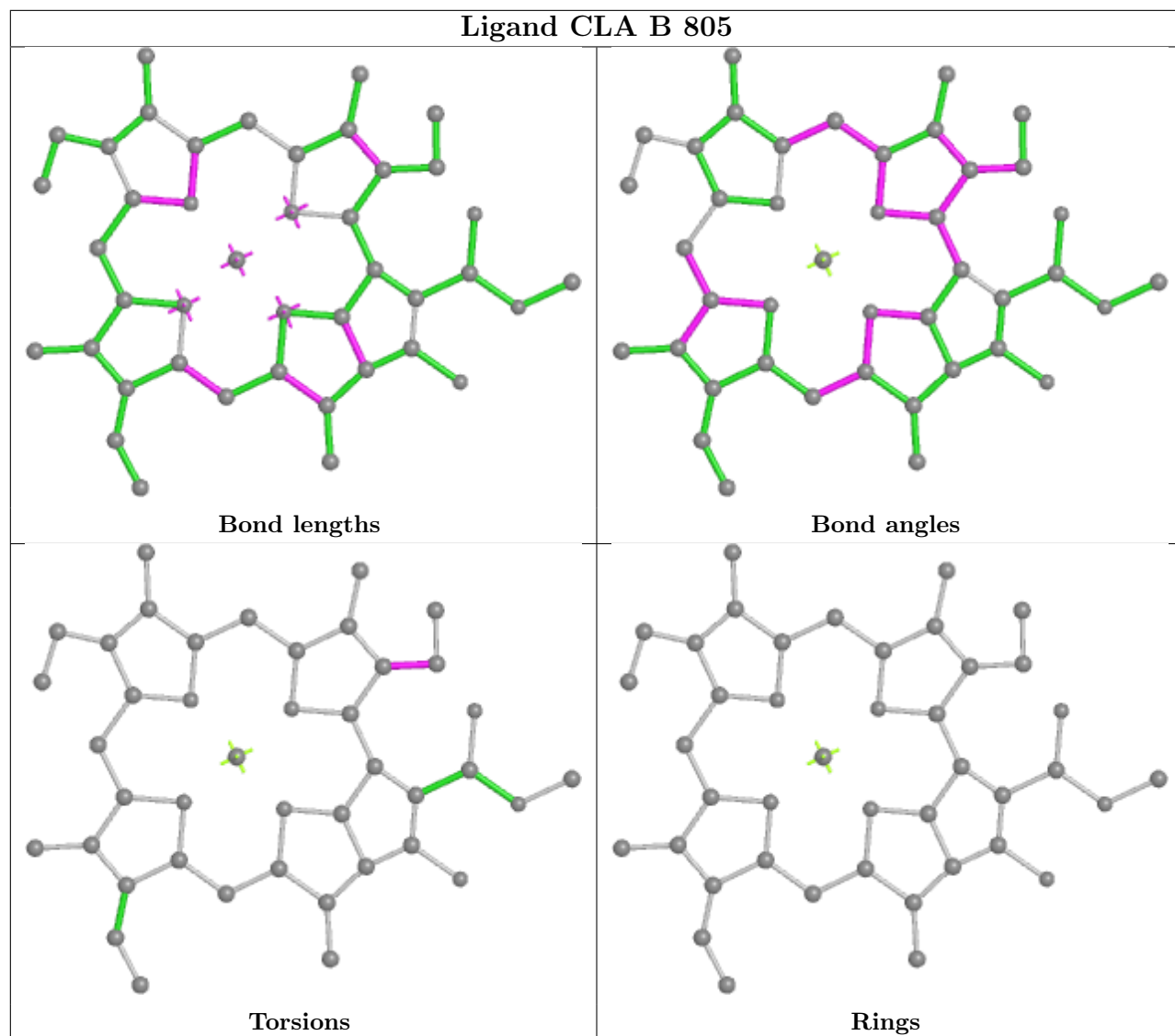


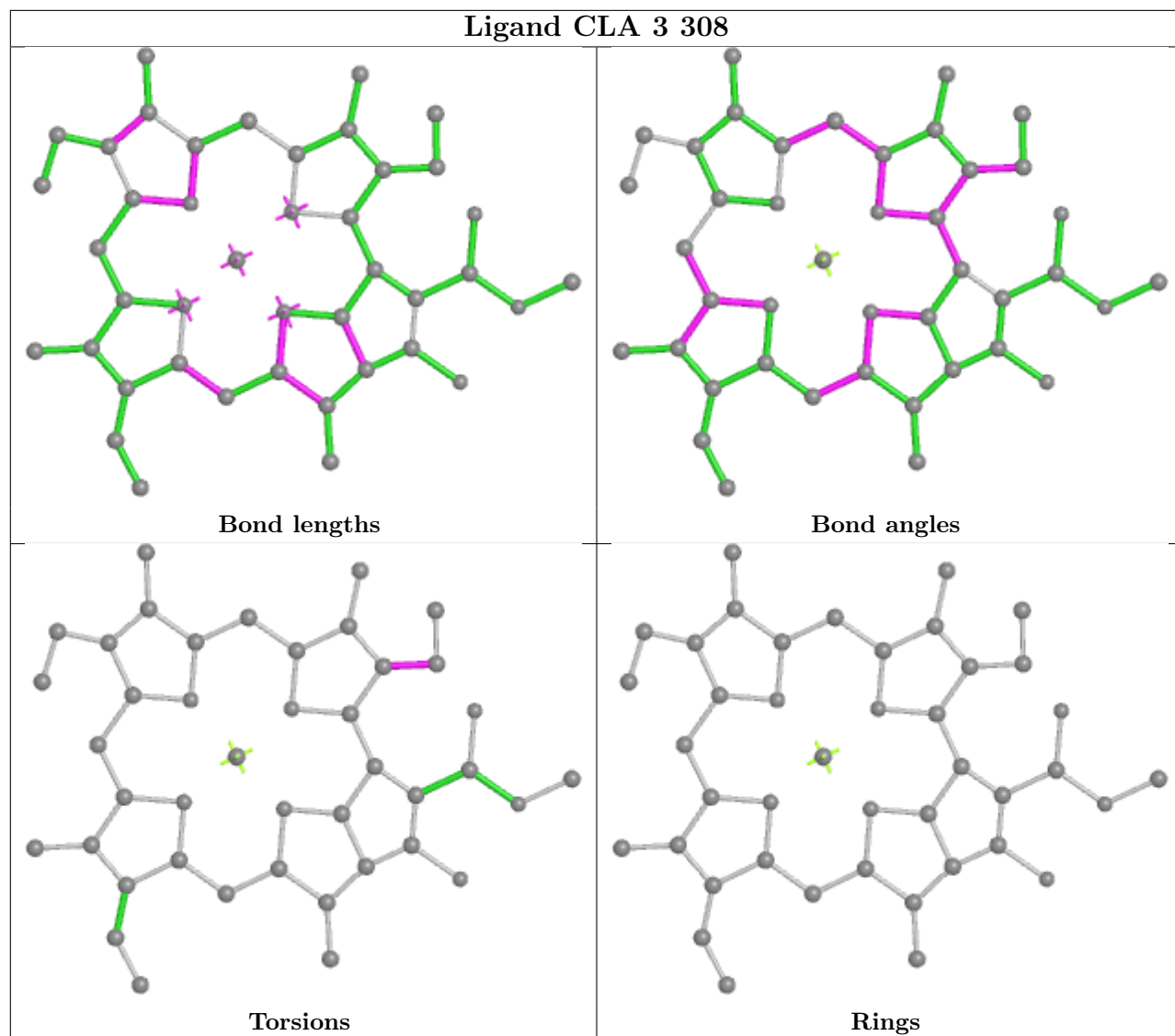


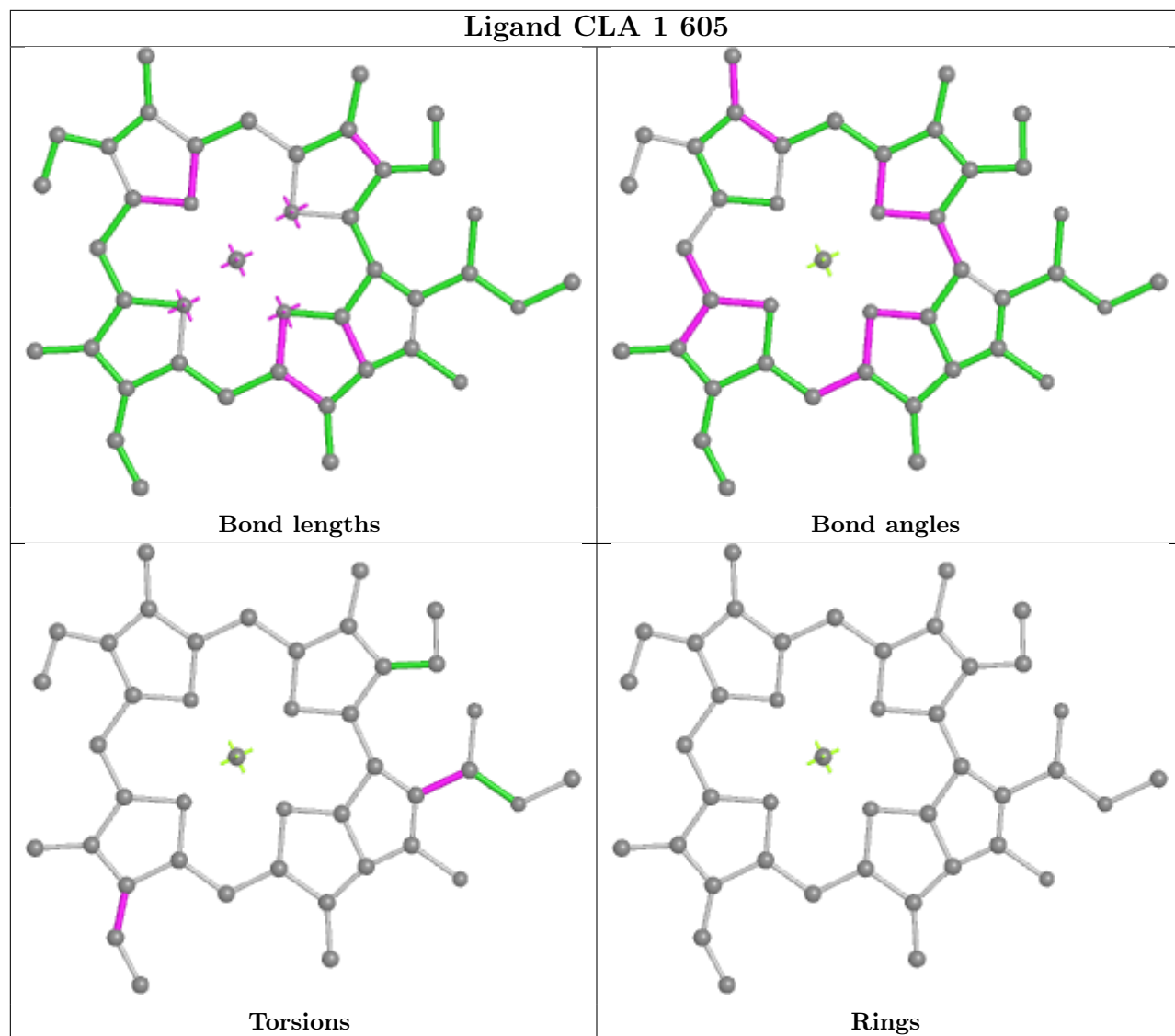




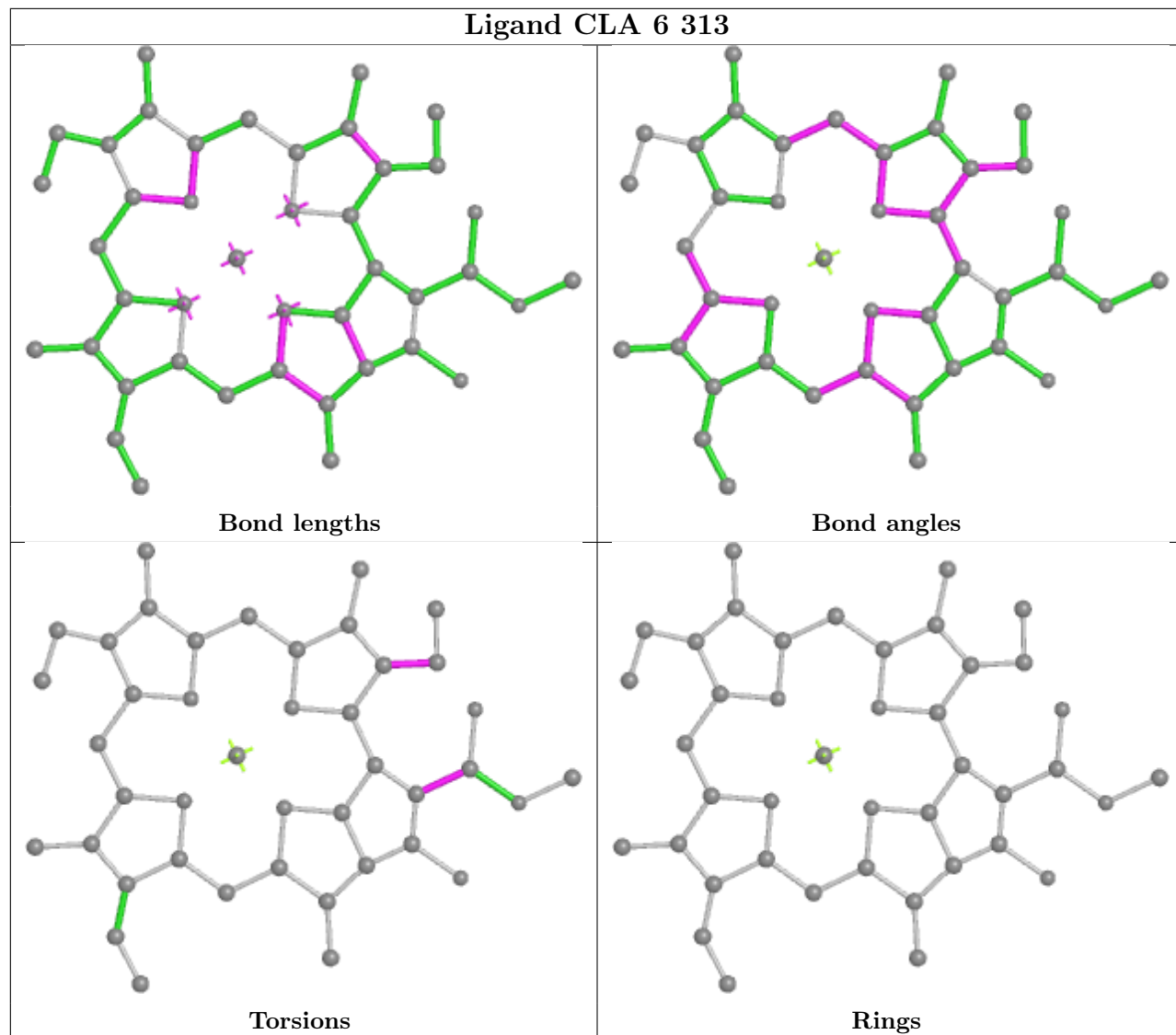


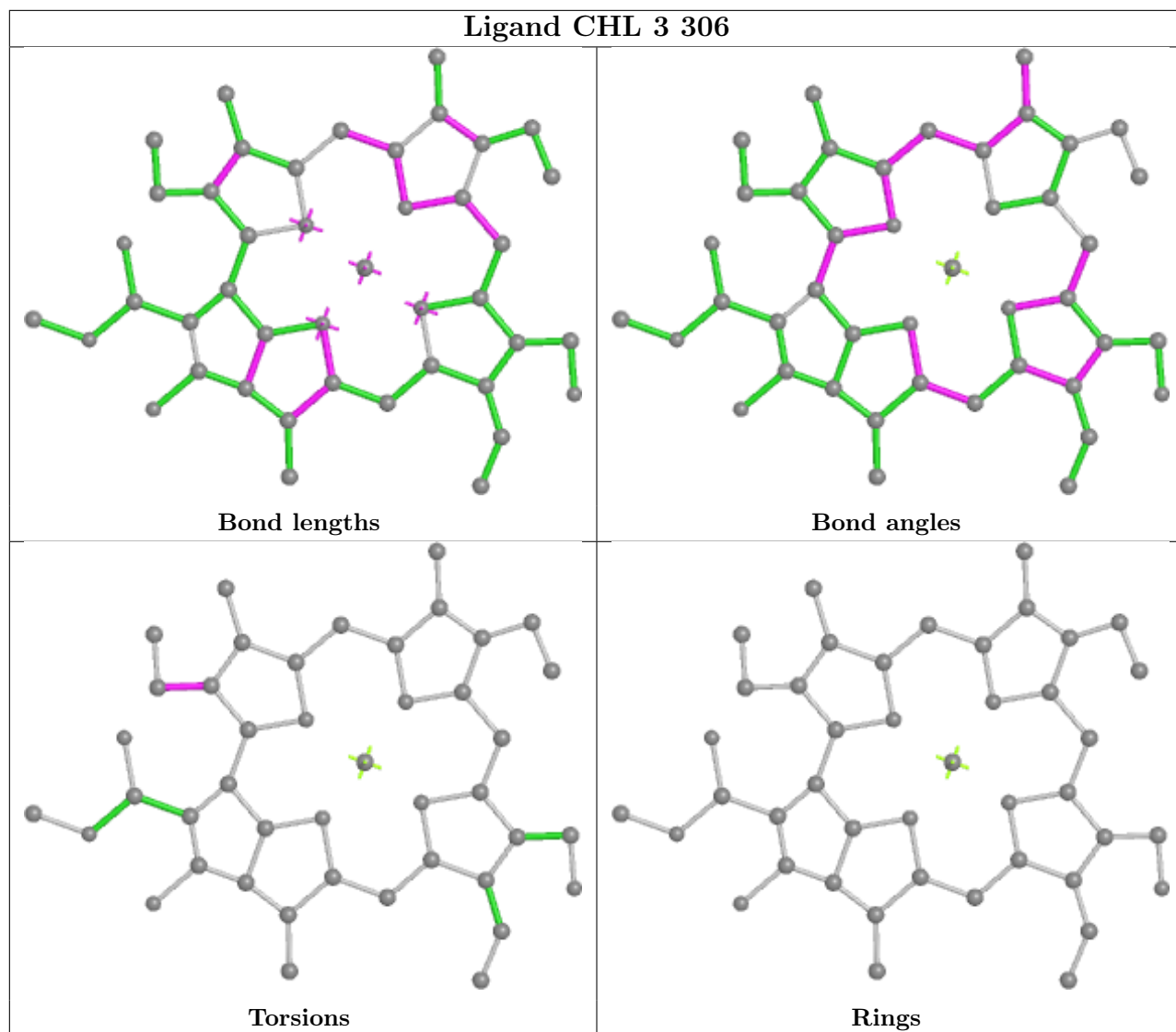


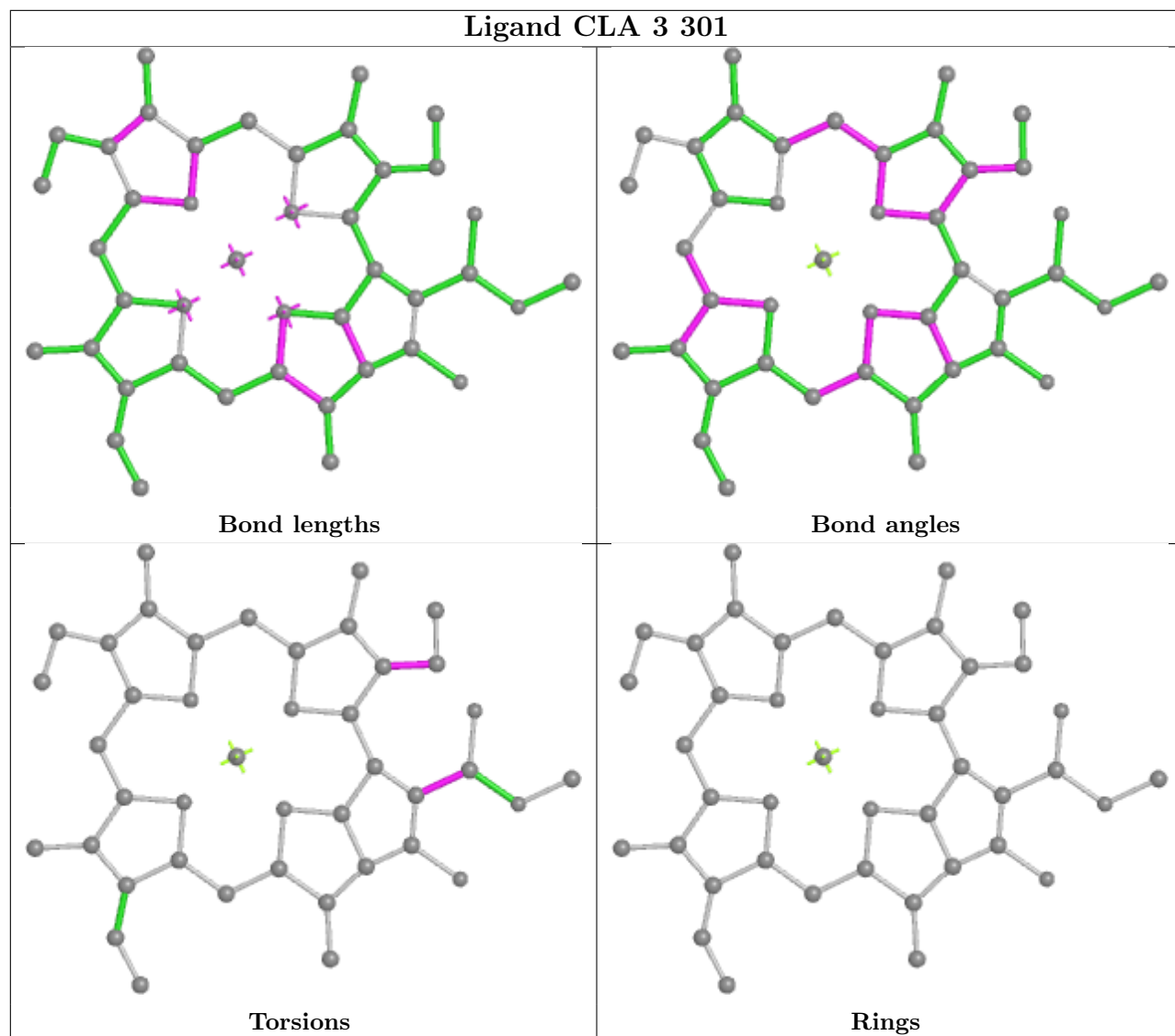


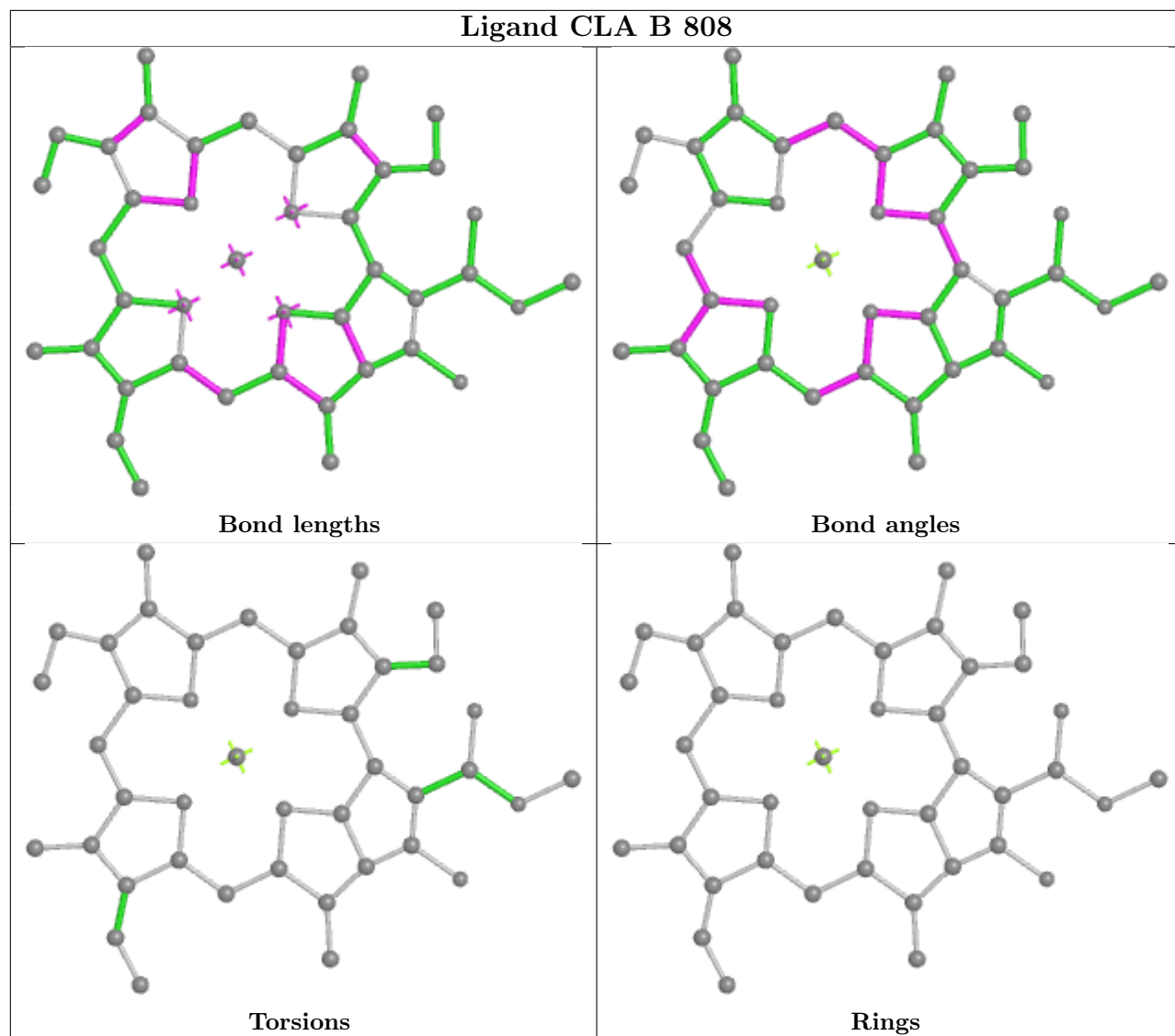


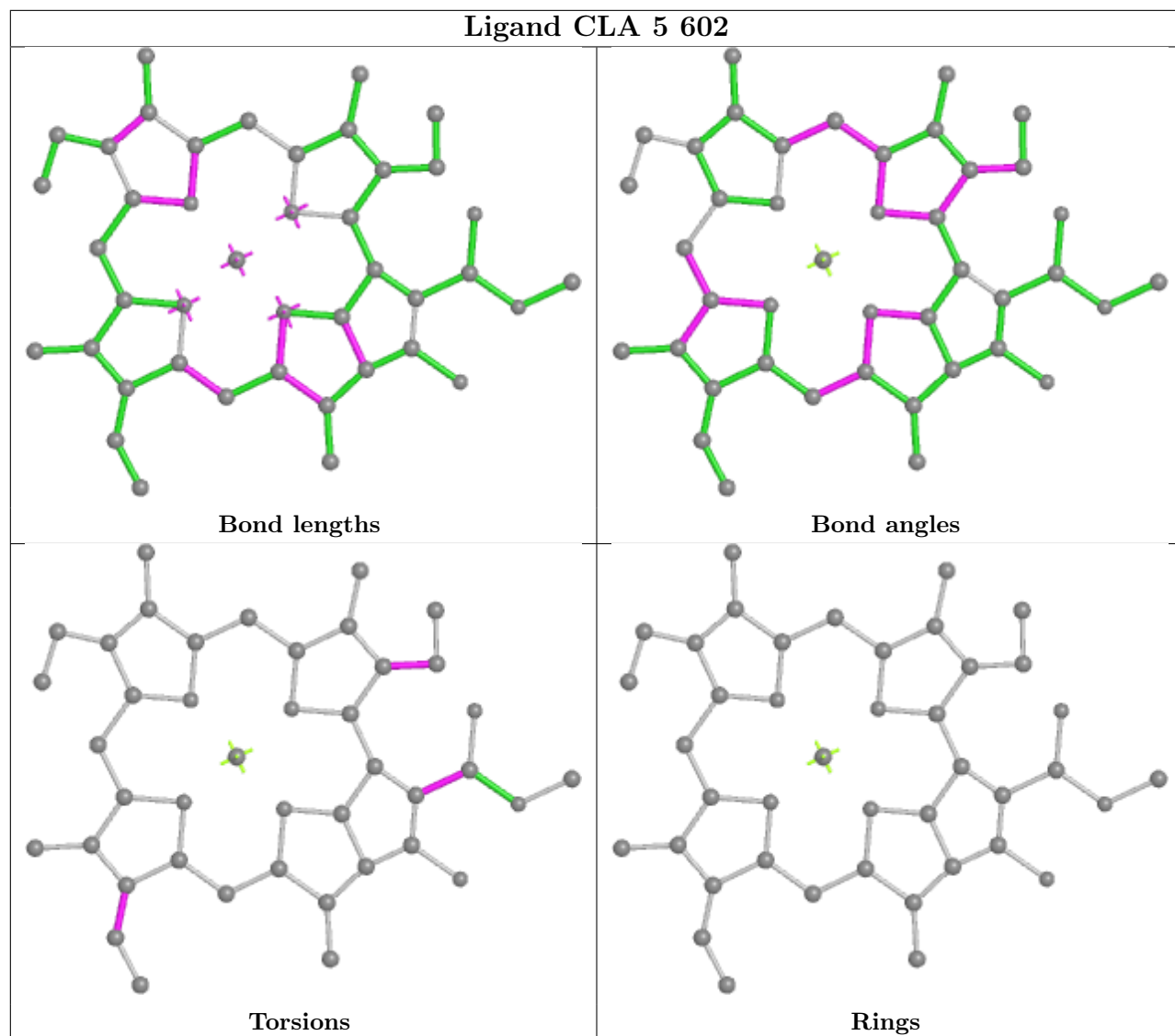
Ligand CLA 6 313

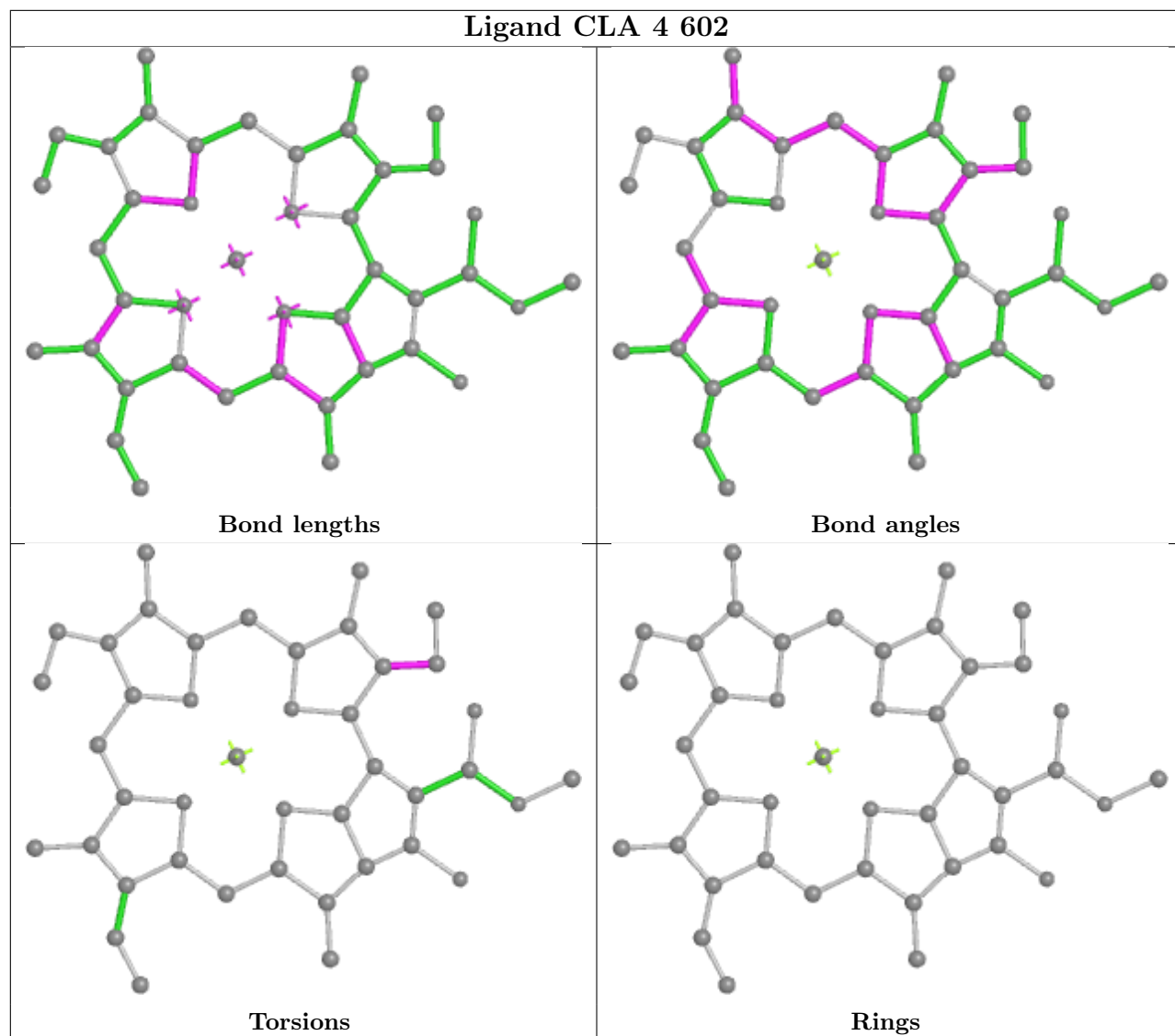


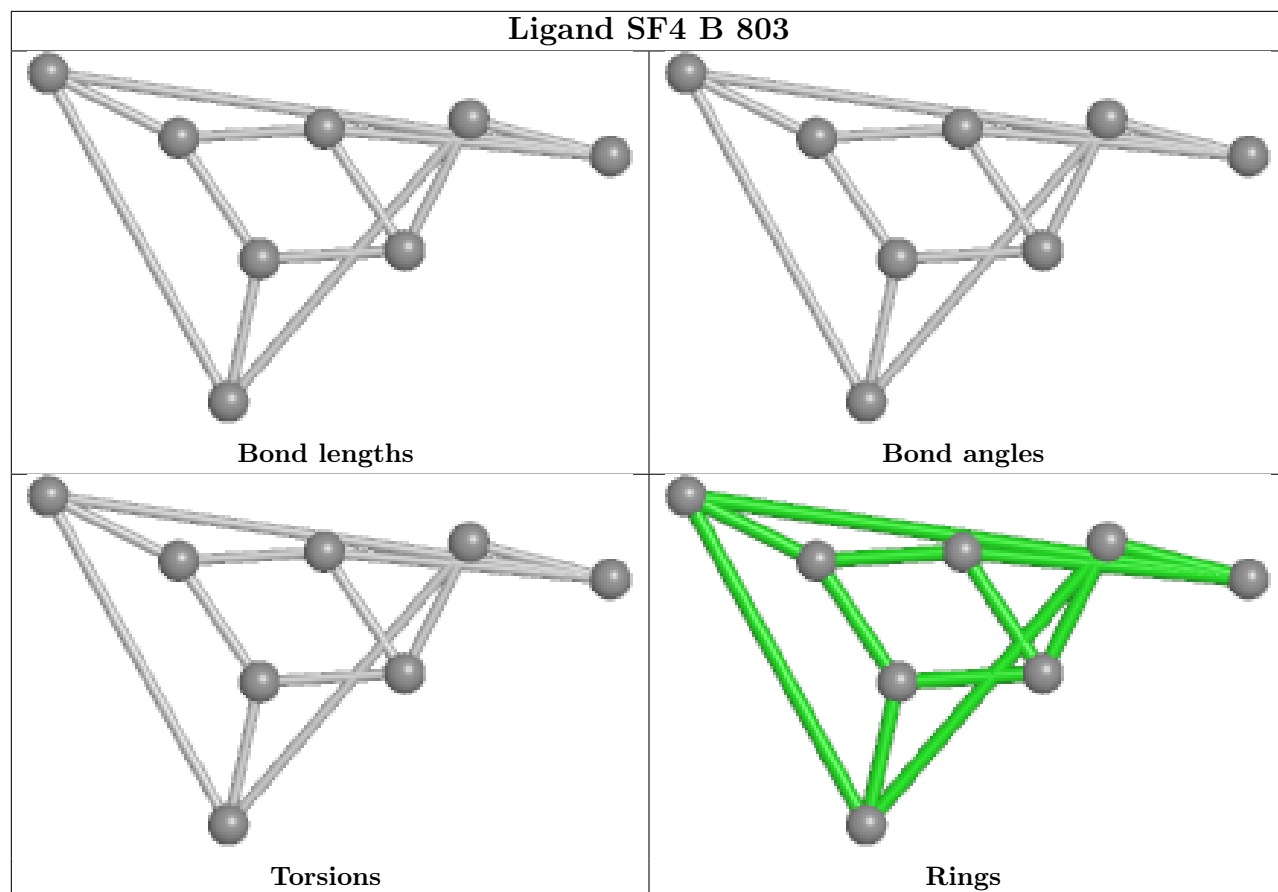


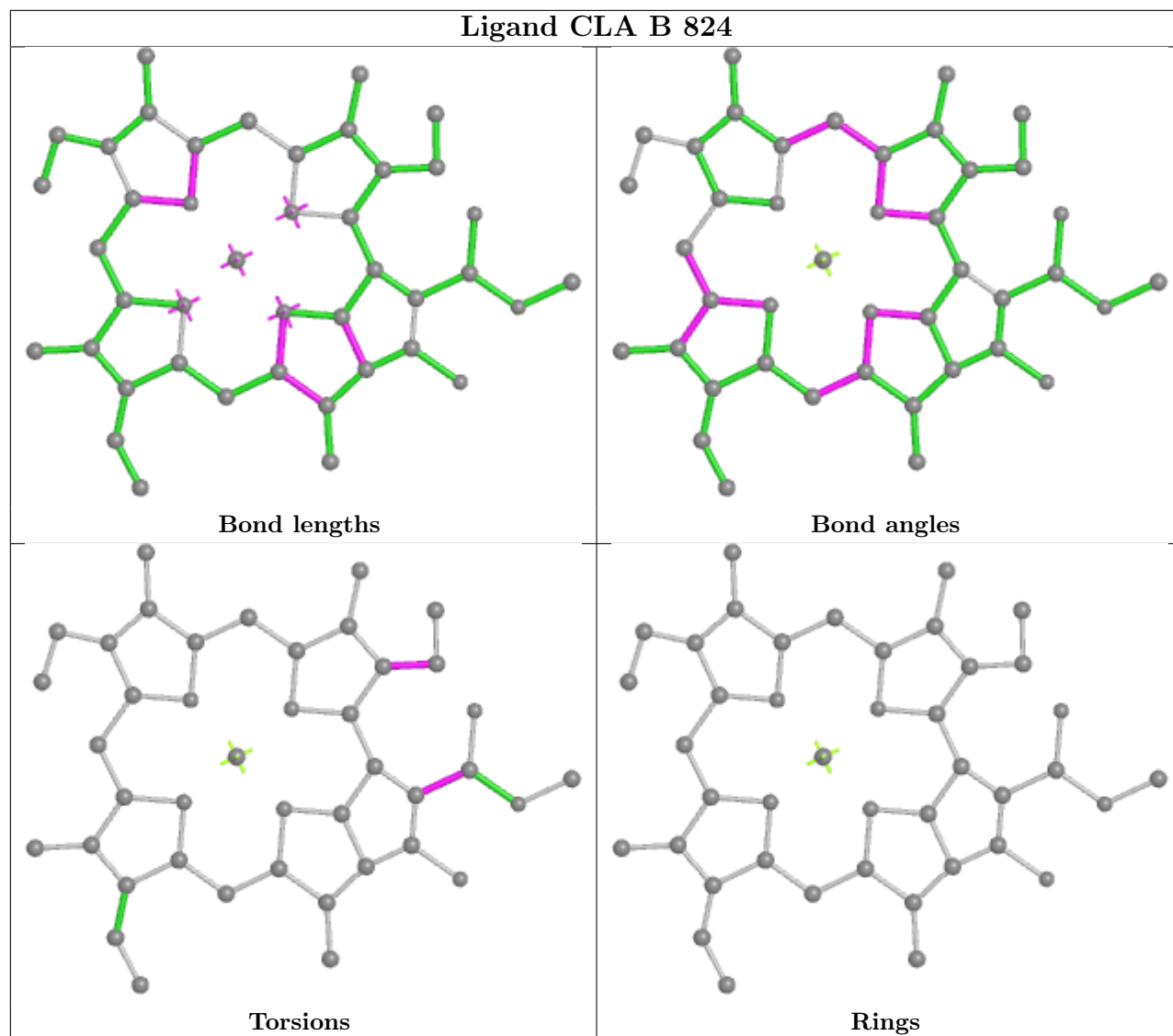


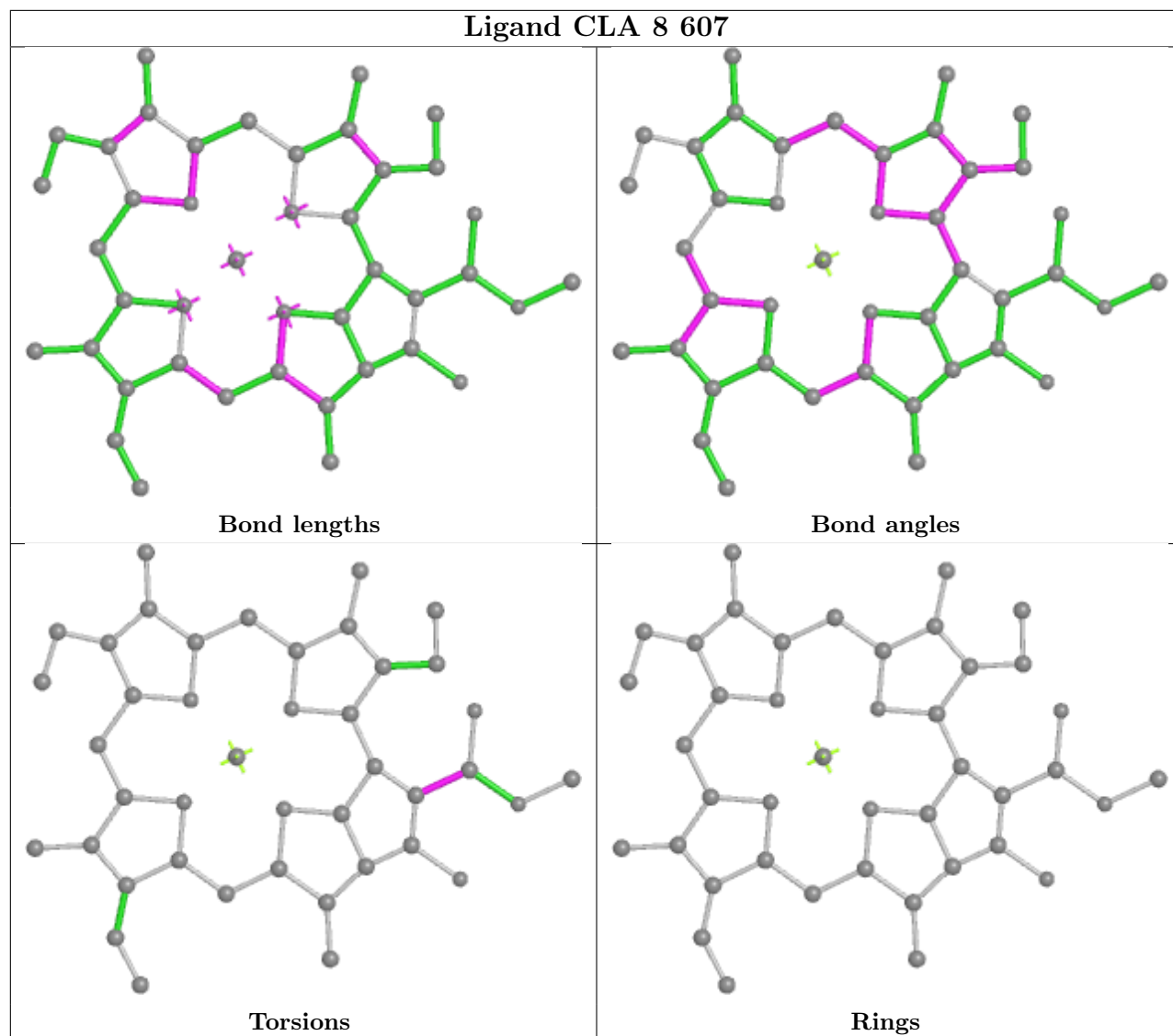


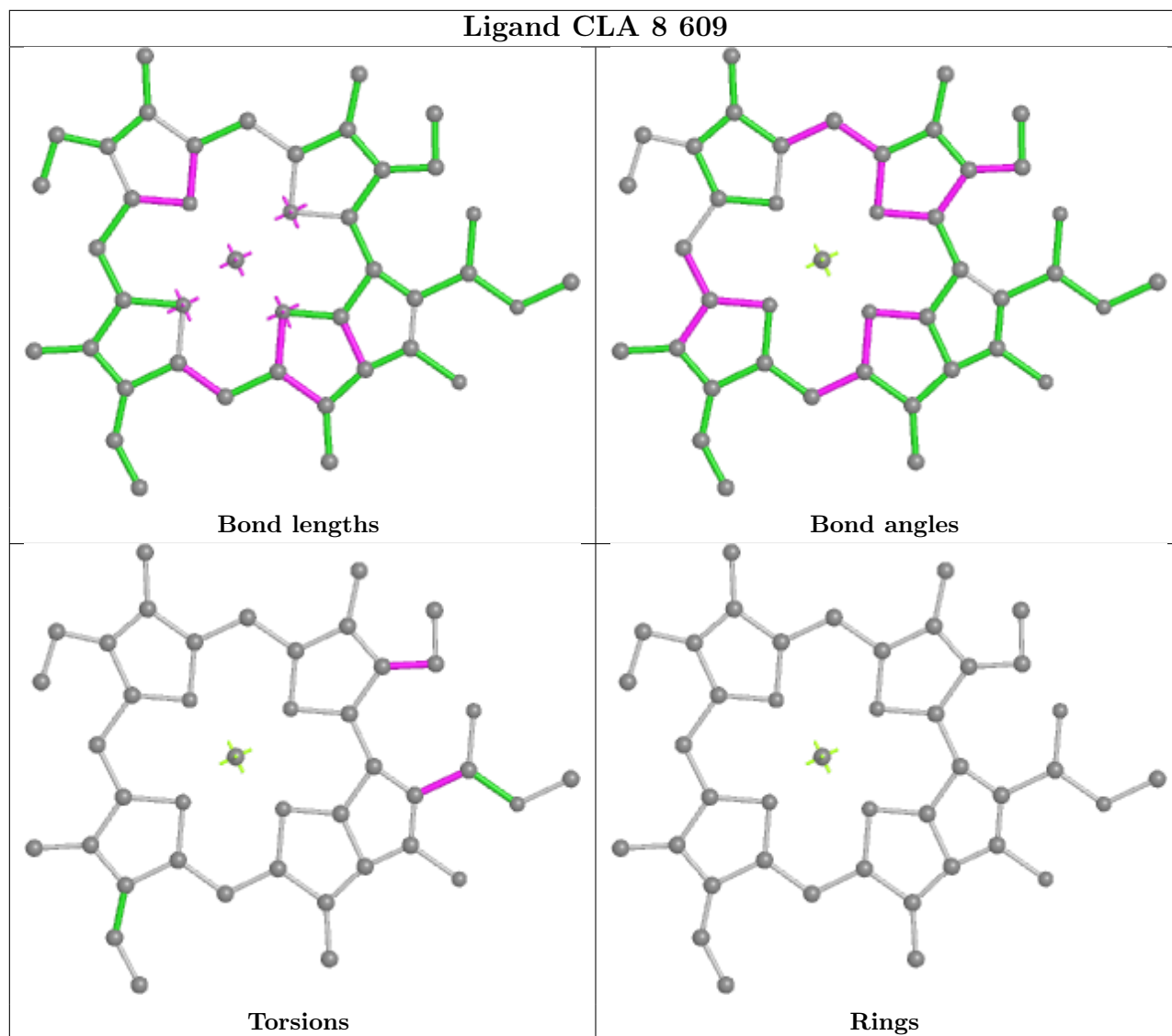


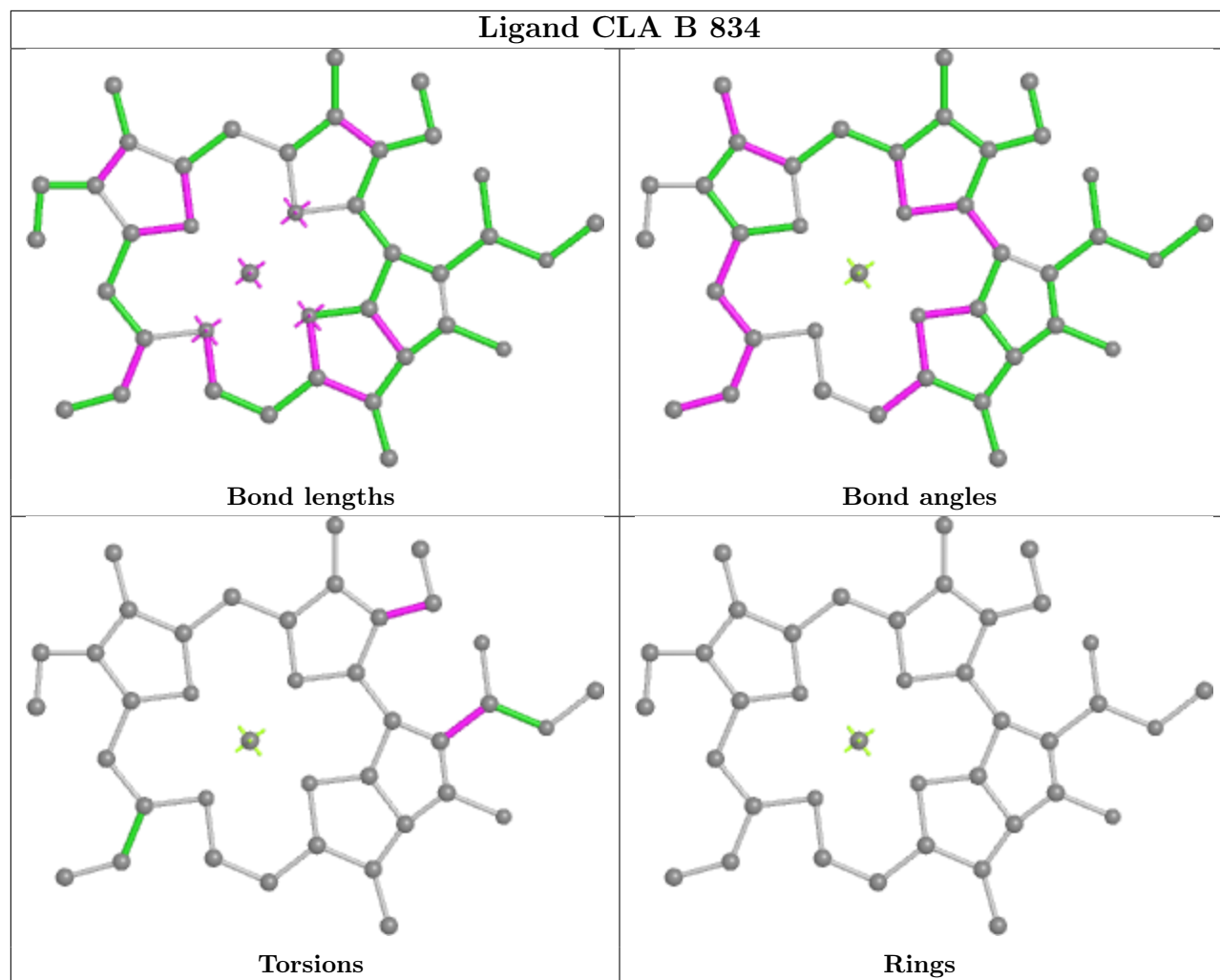


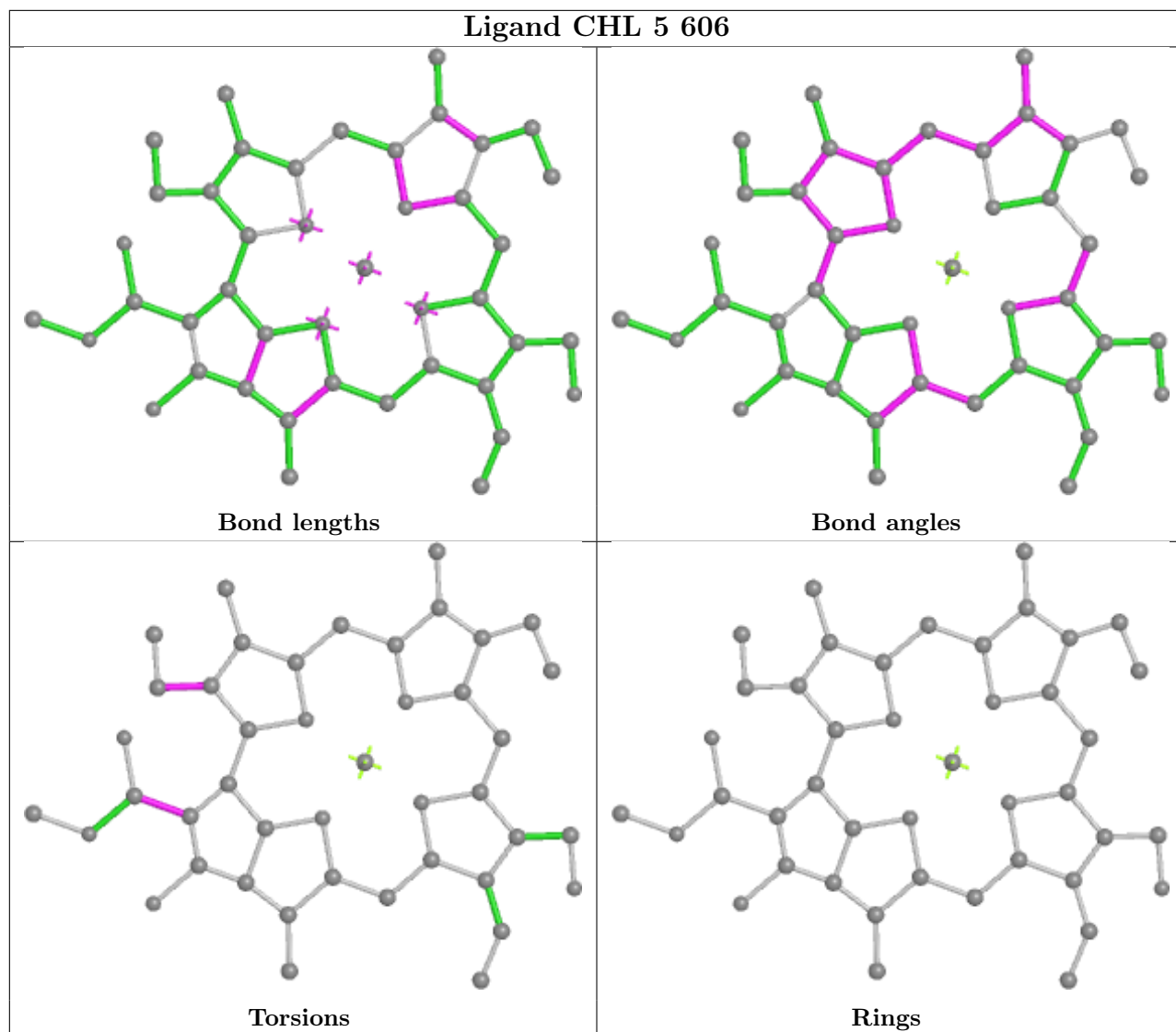


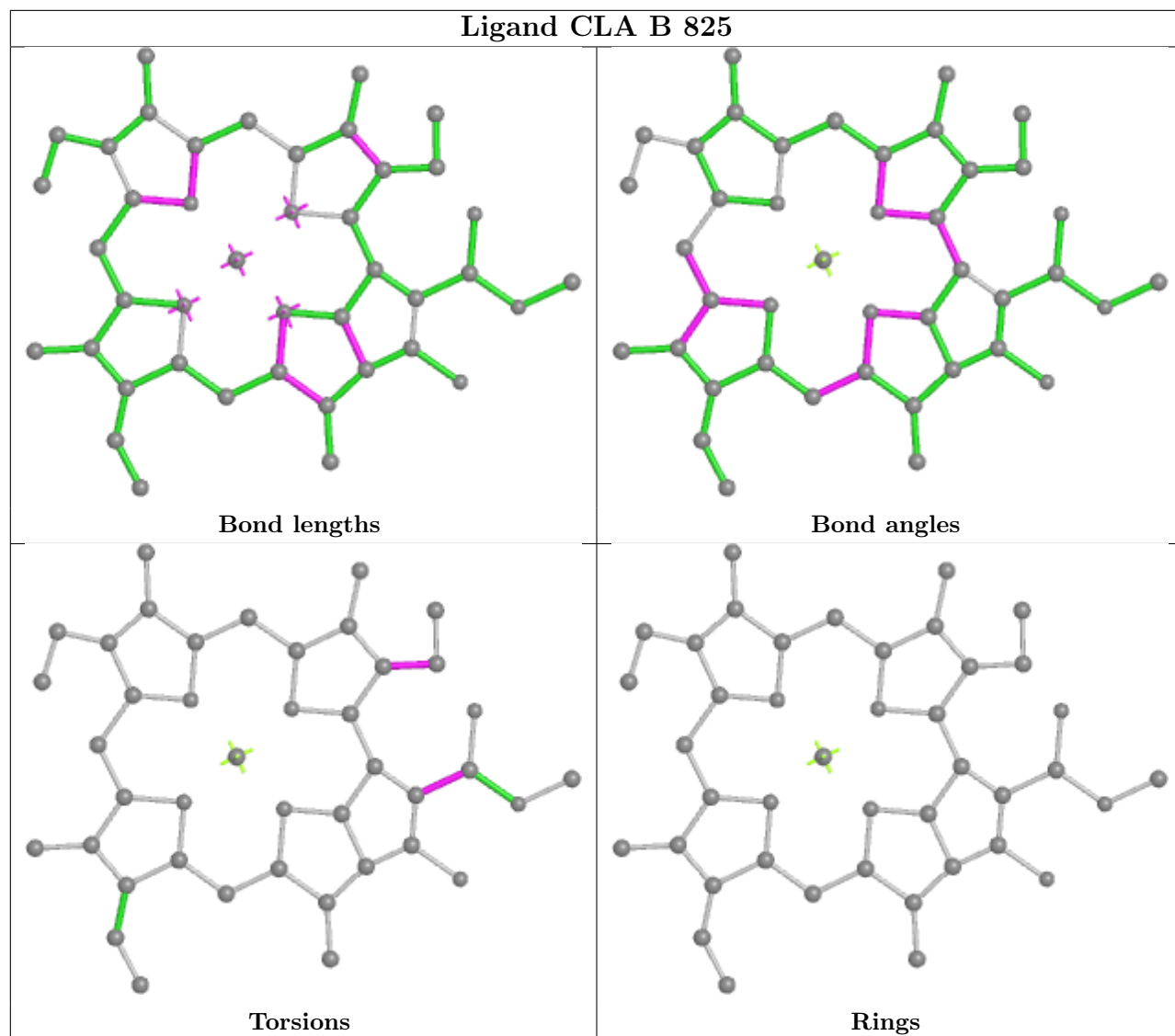


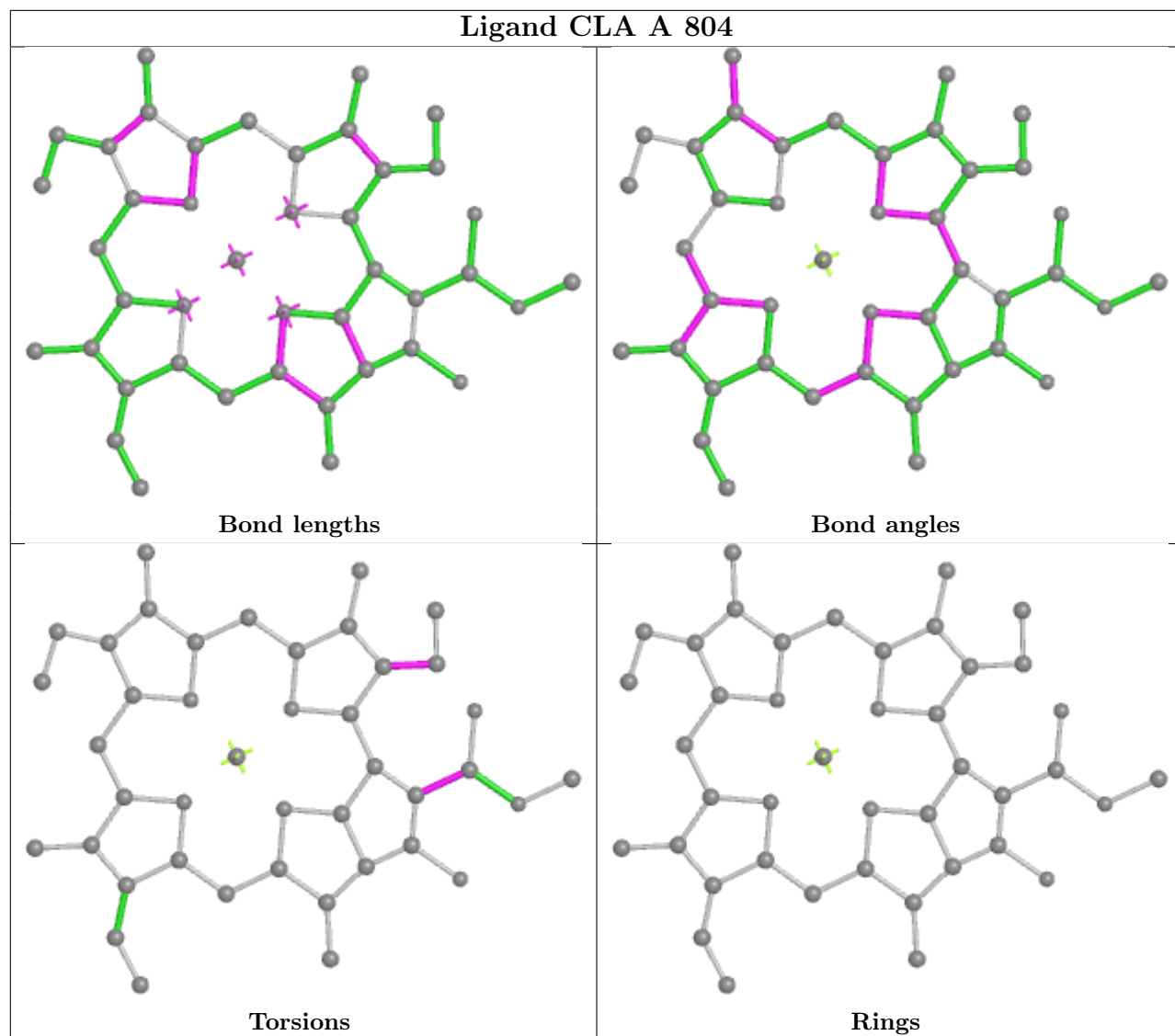


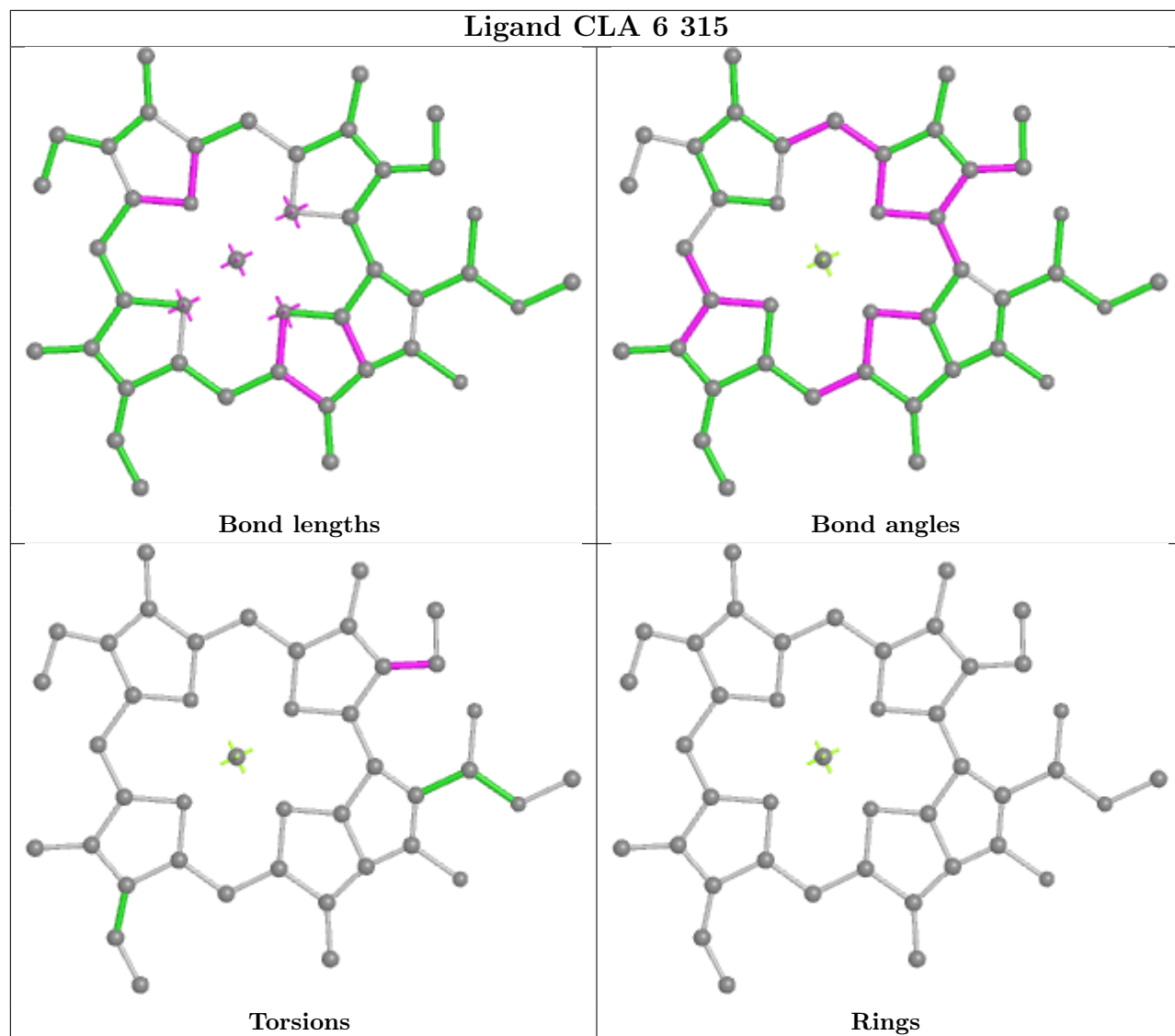




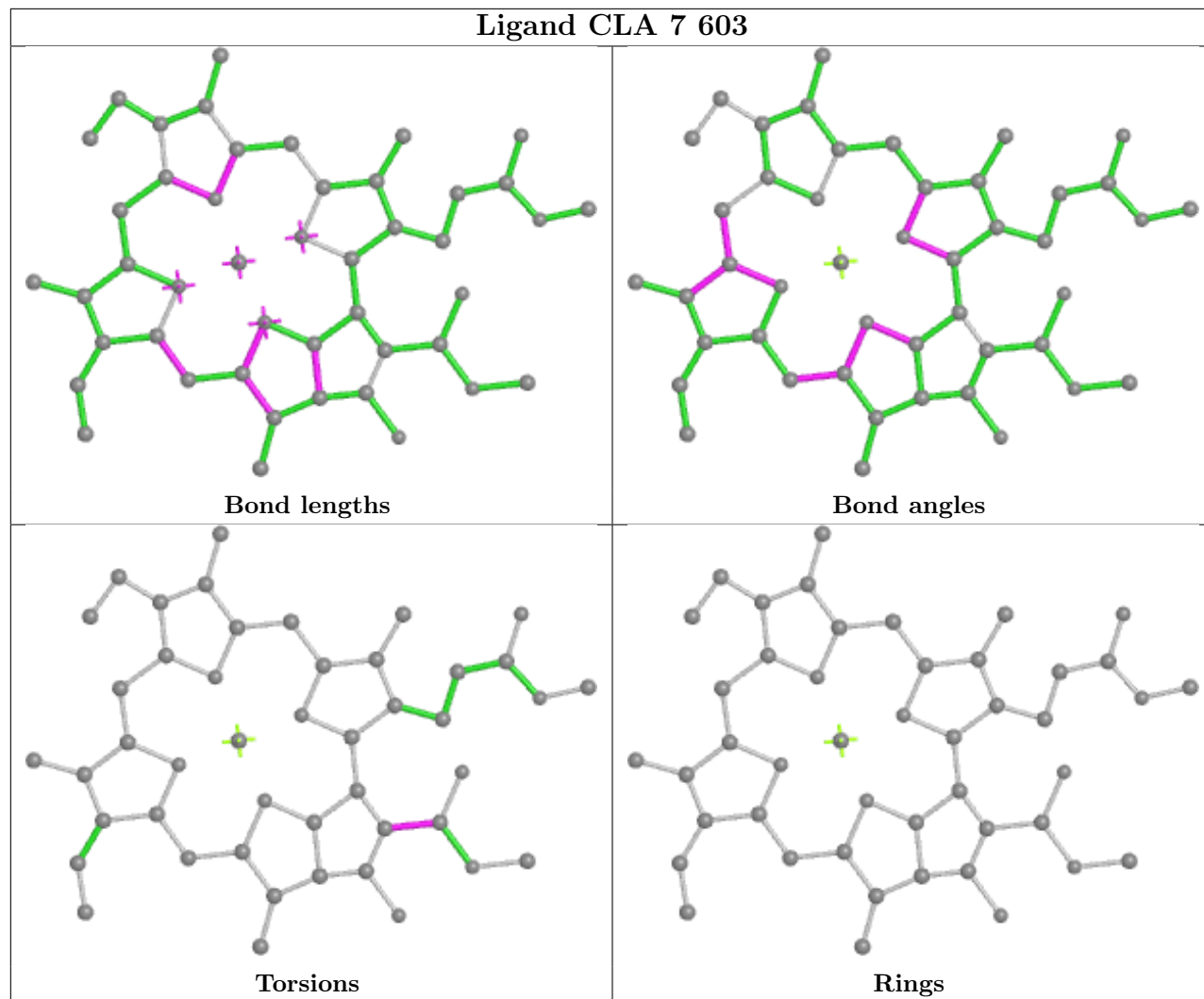


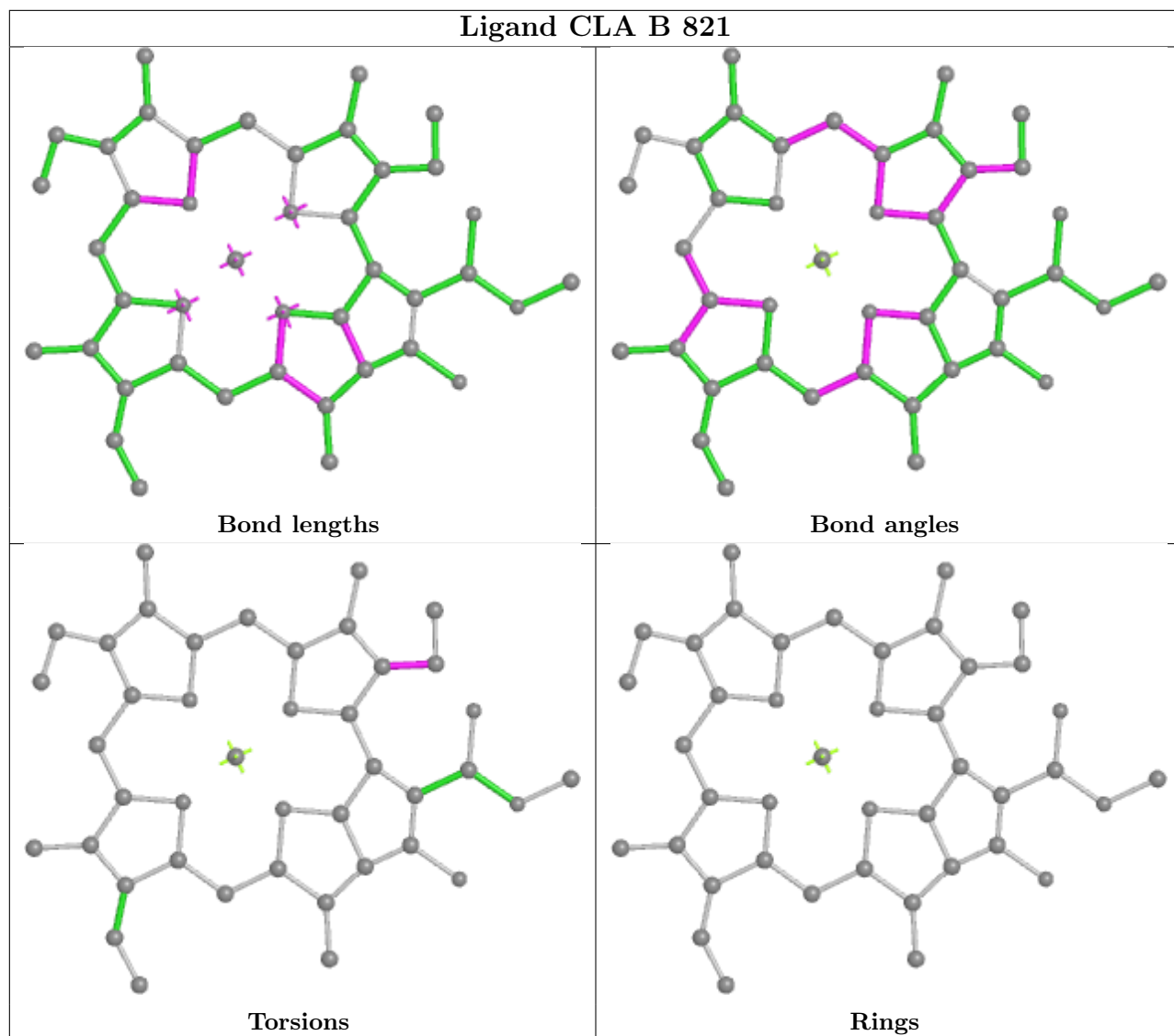


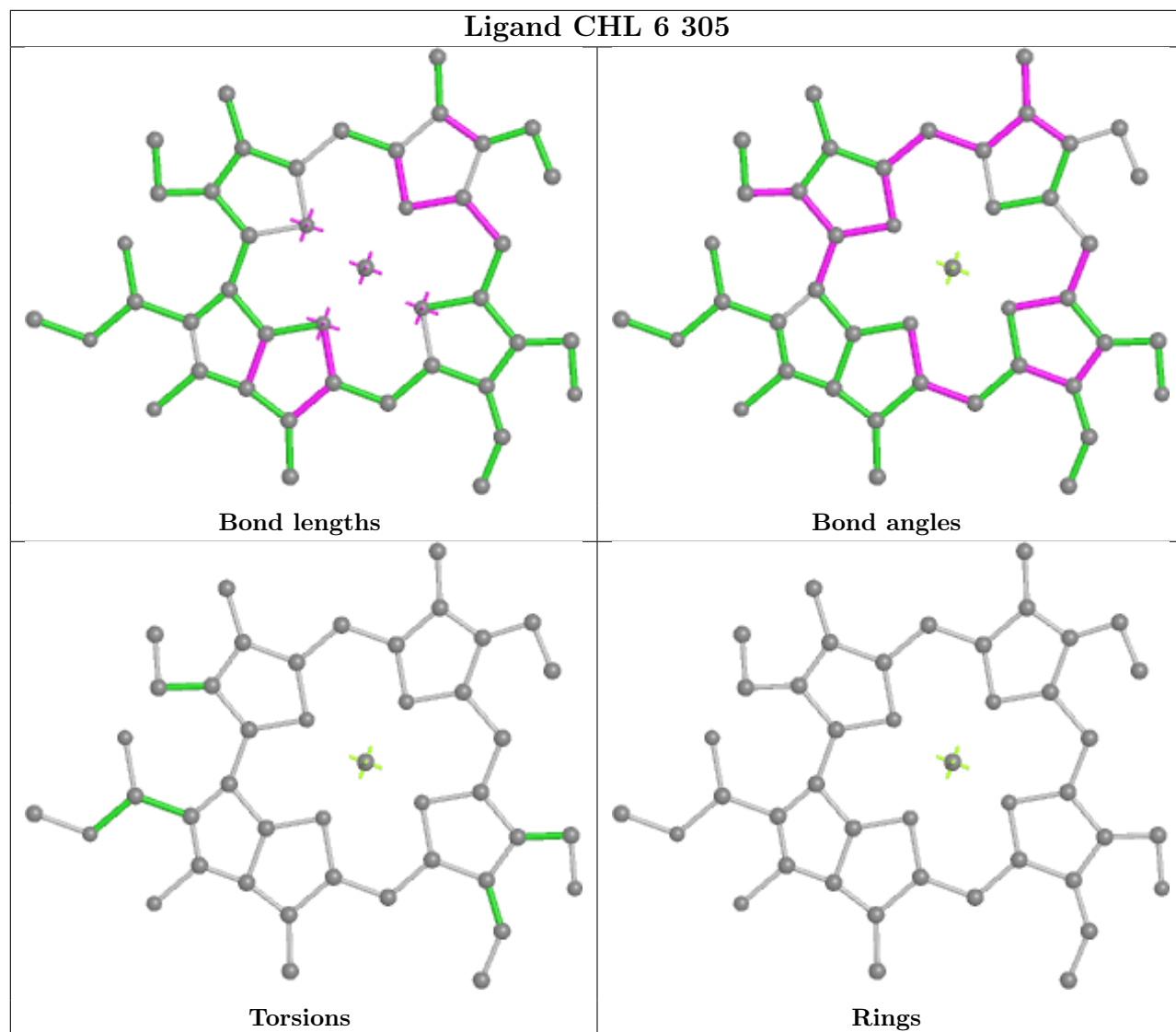


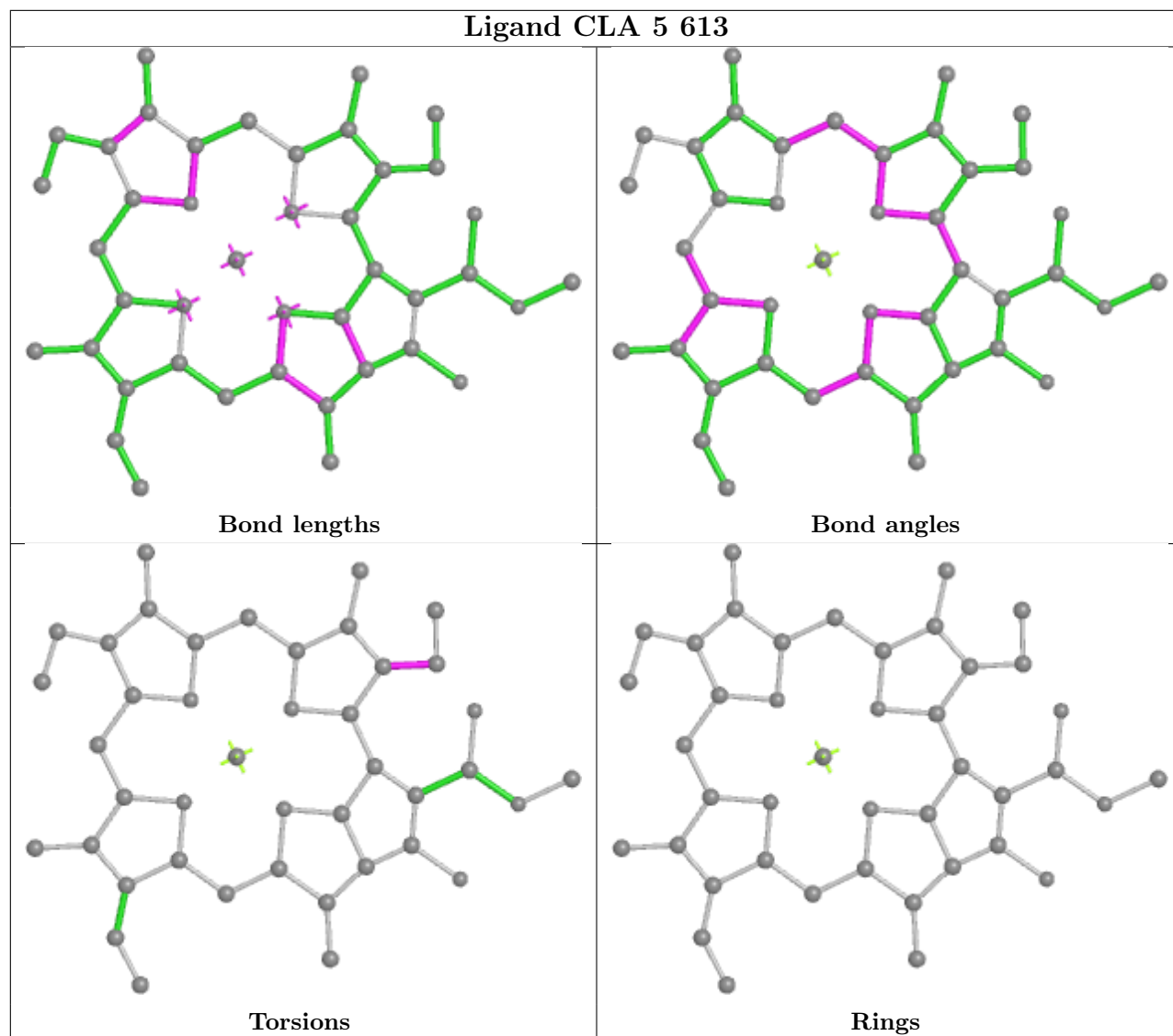


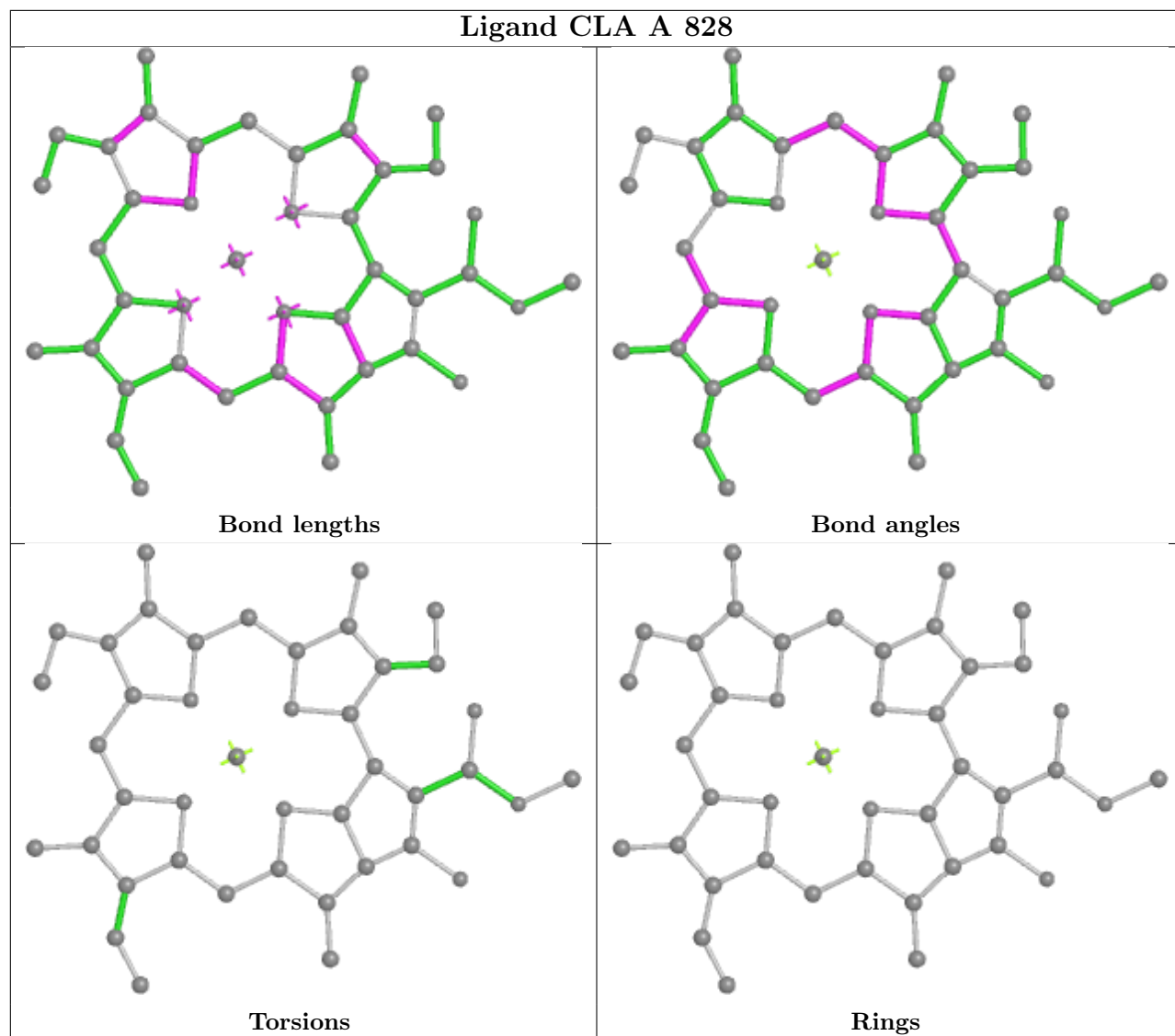
Ligand CLA 7 603

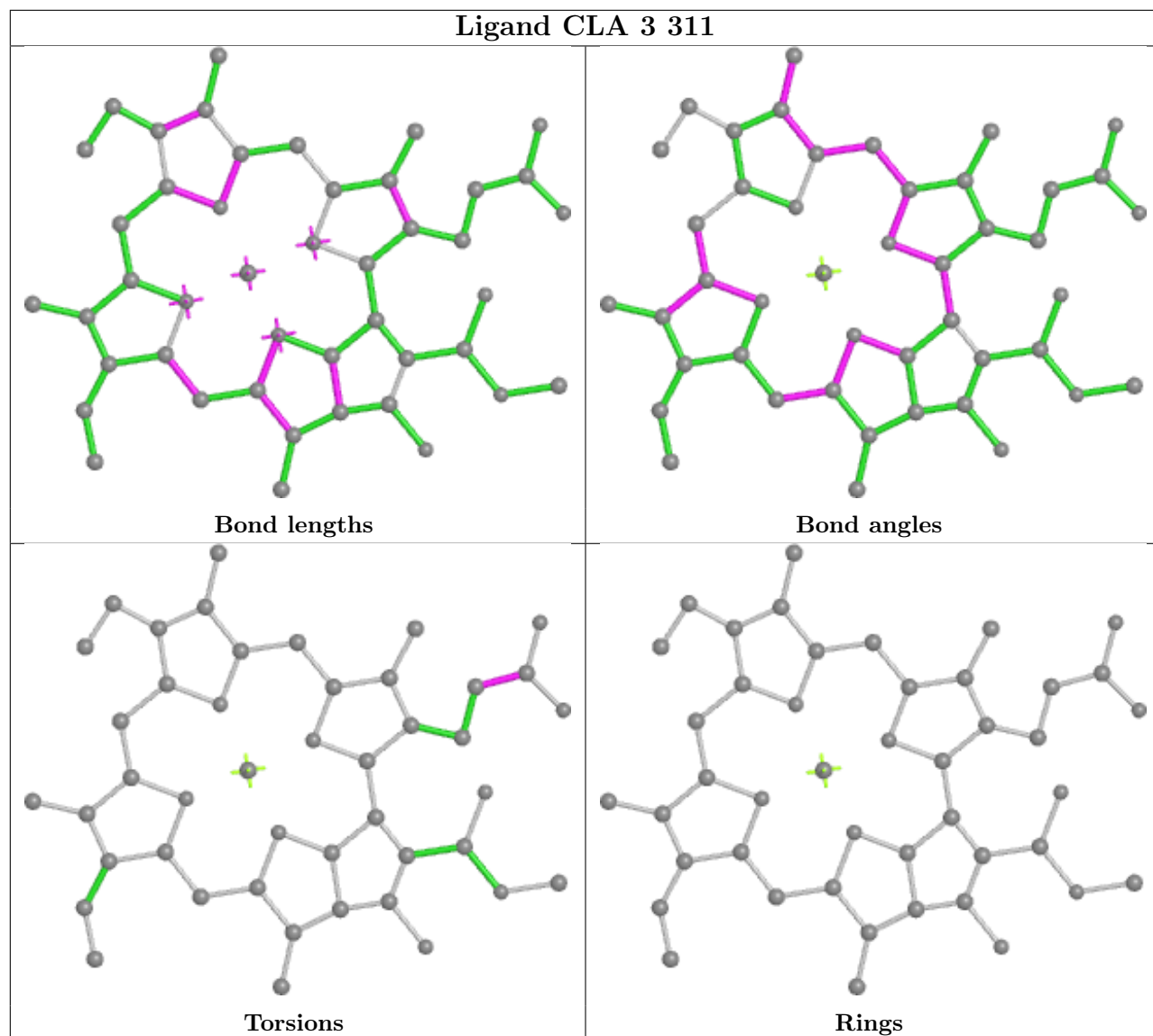


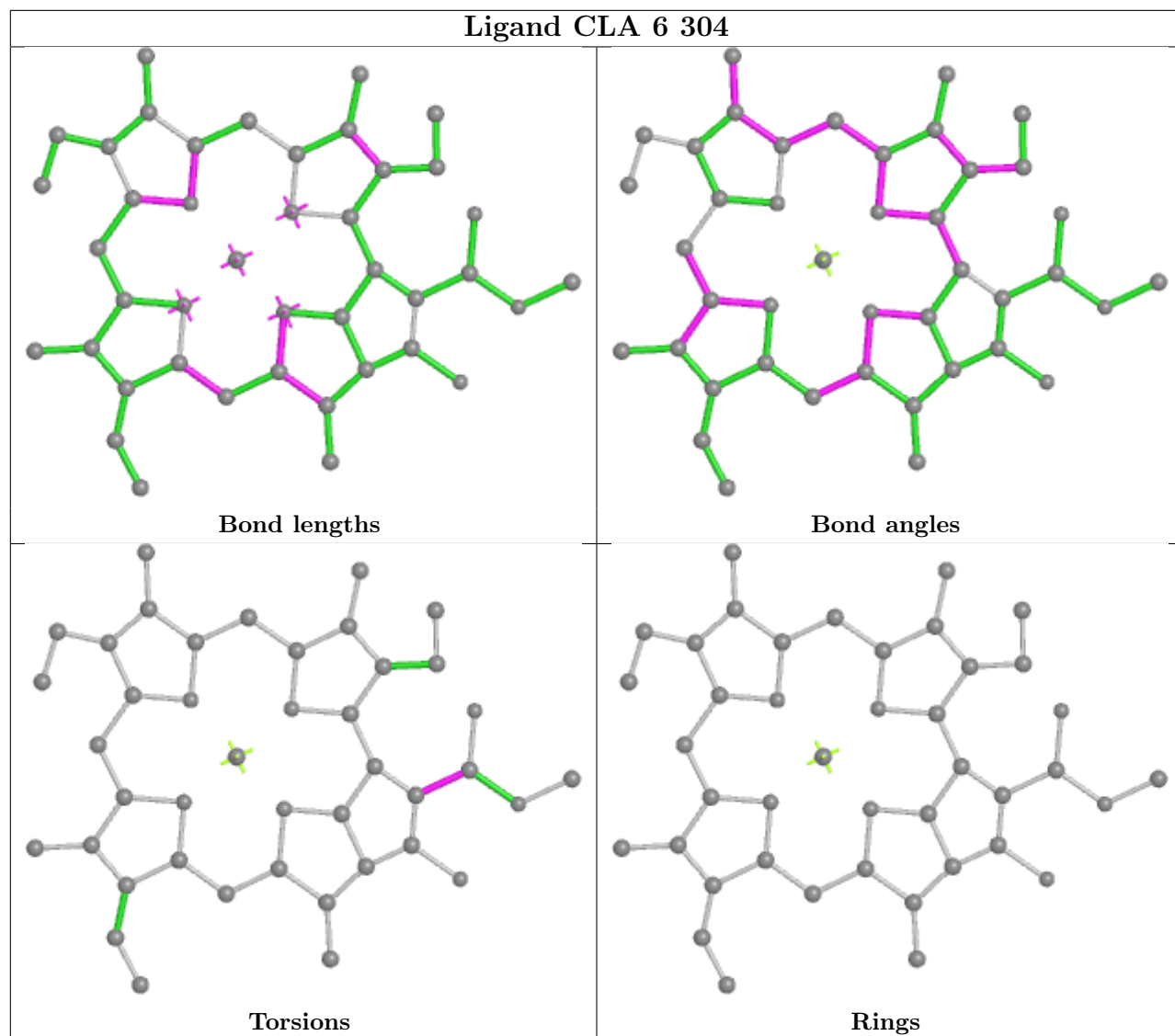


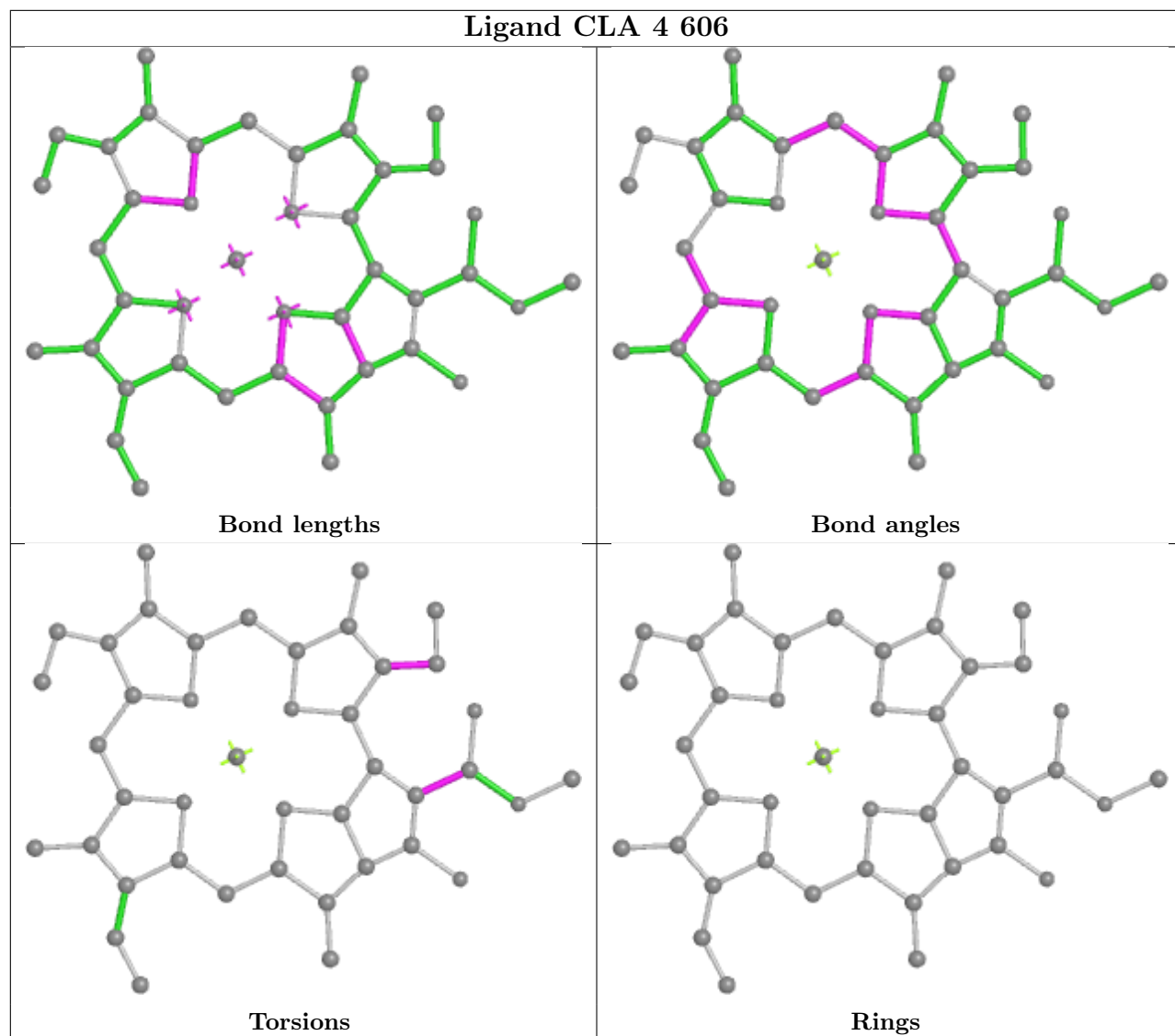


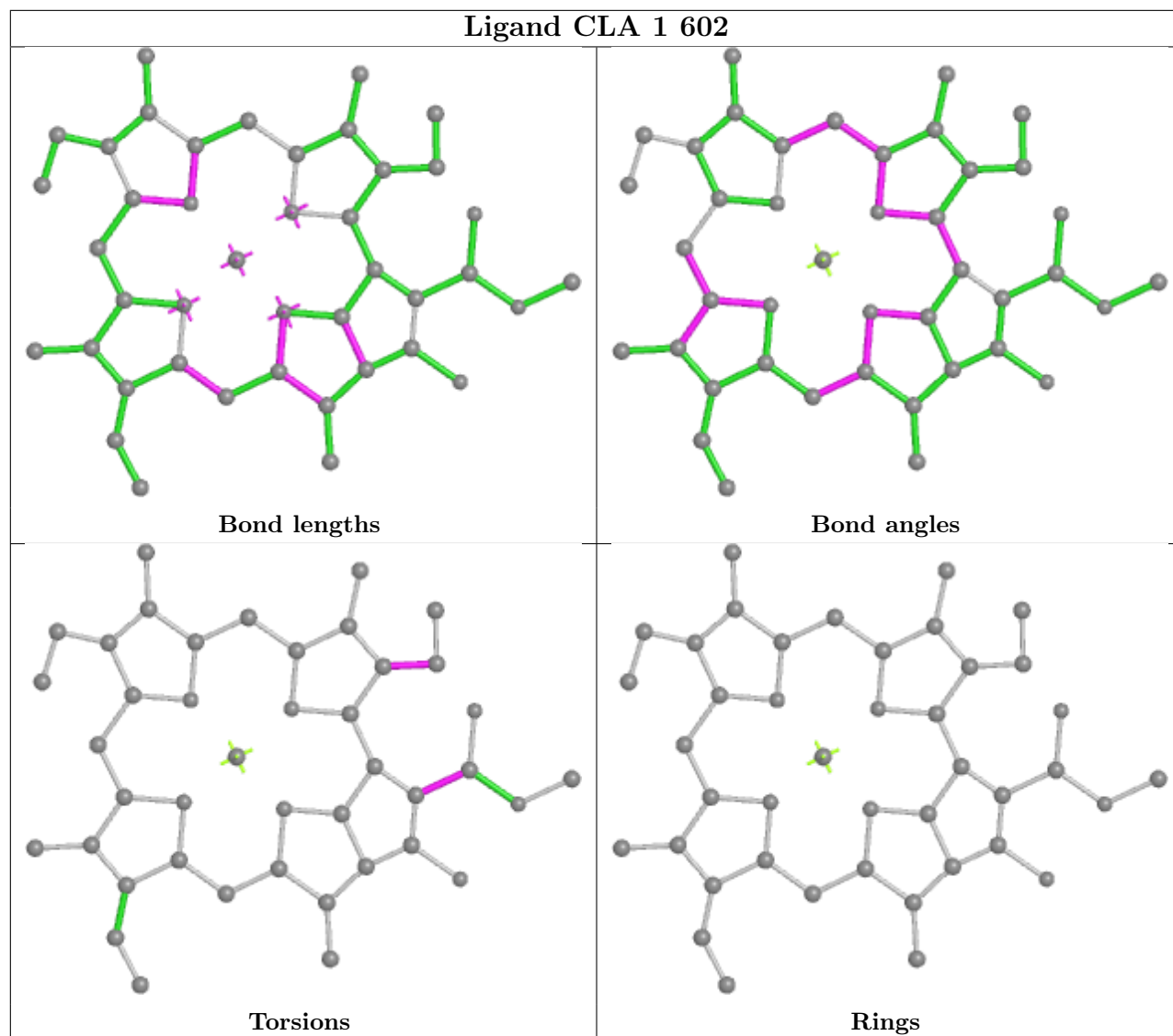


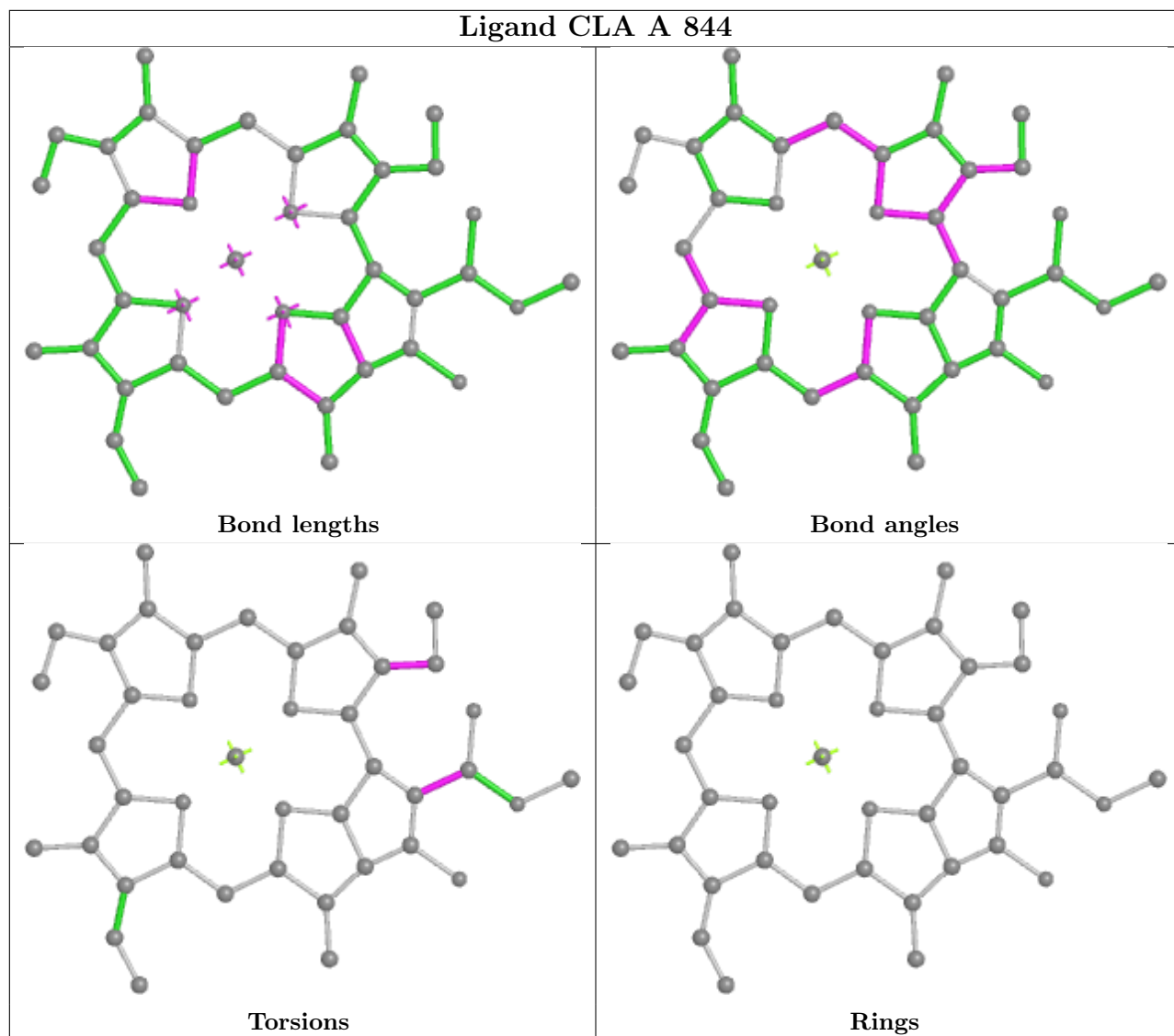


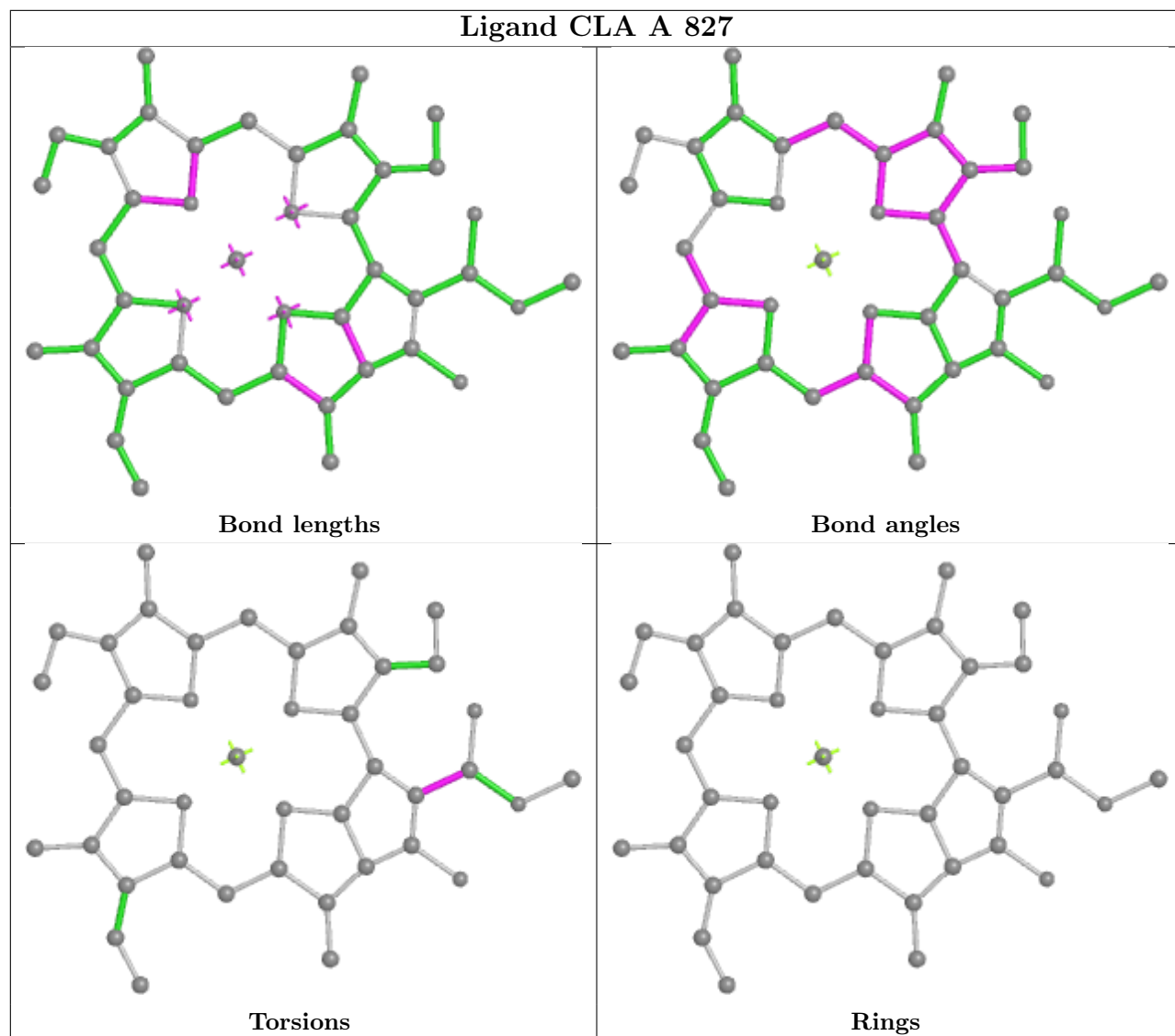


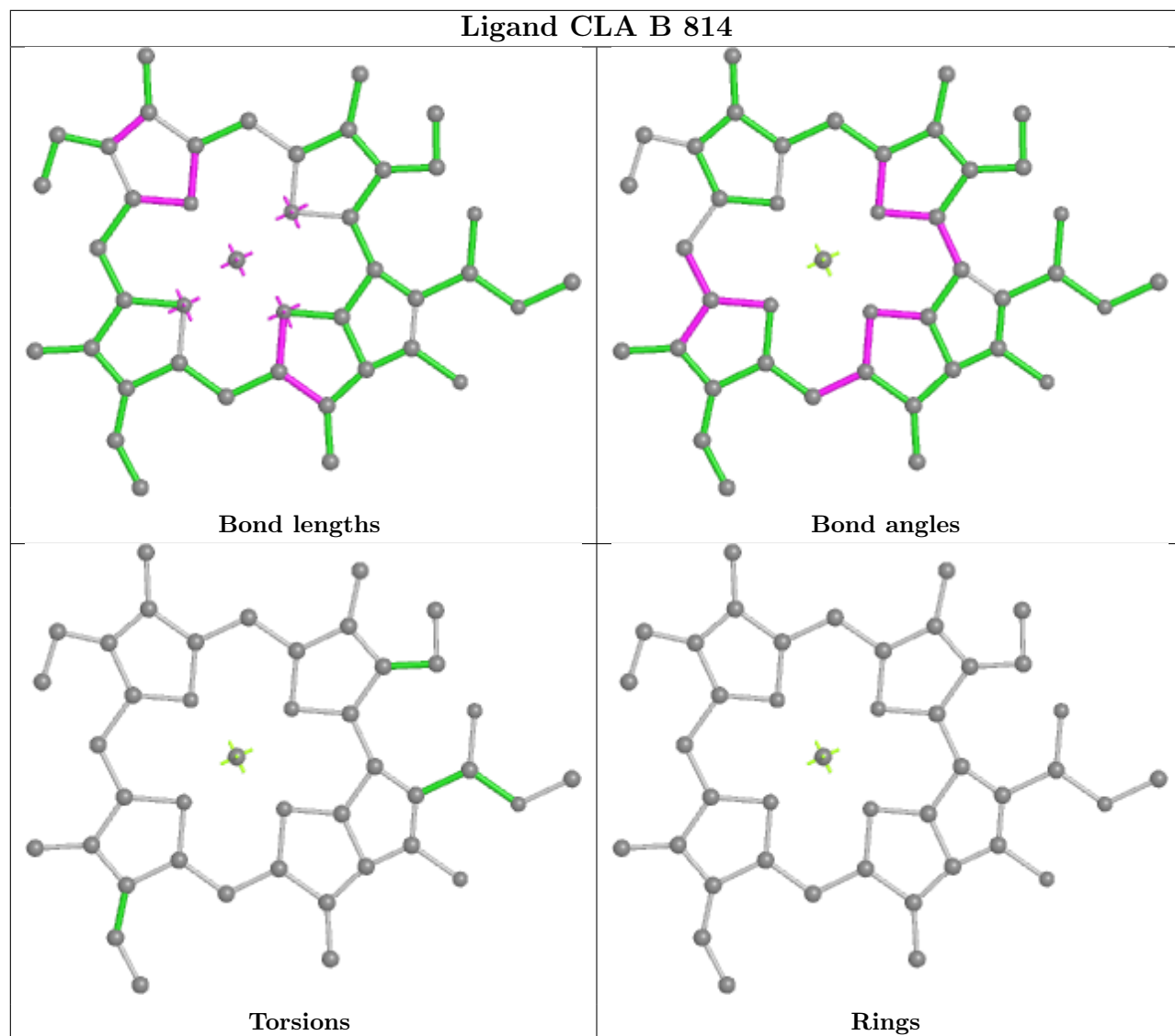


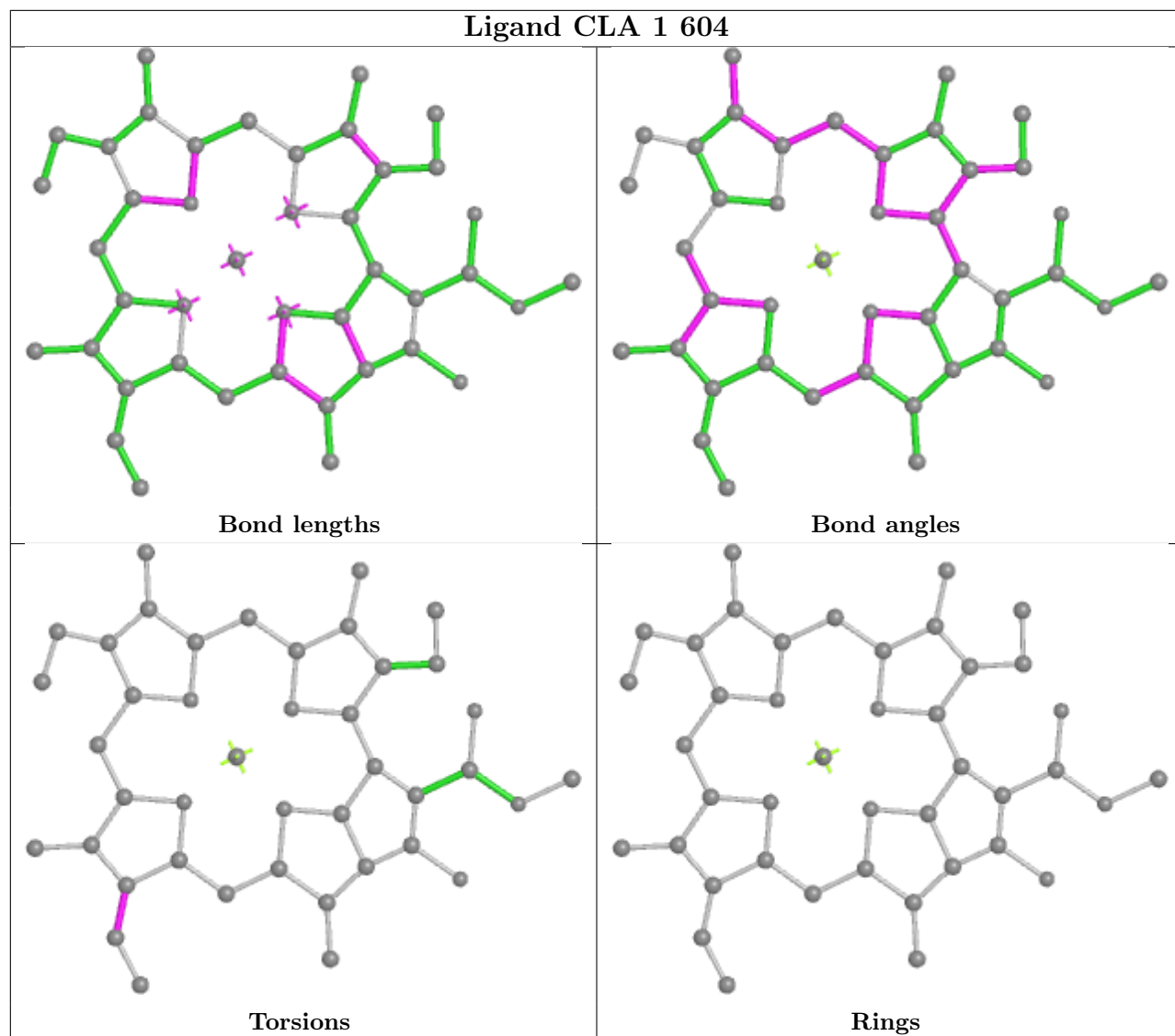


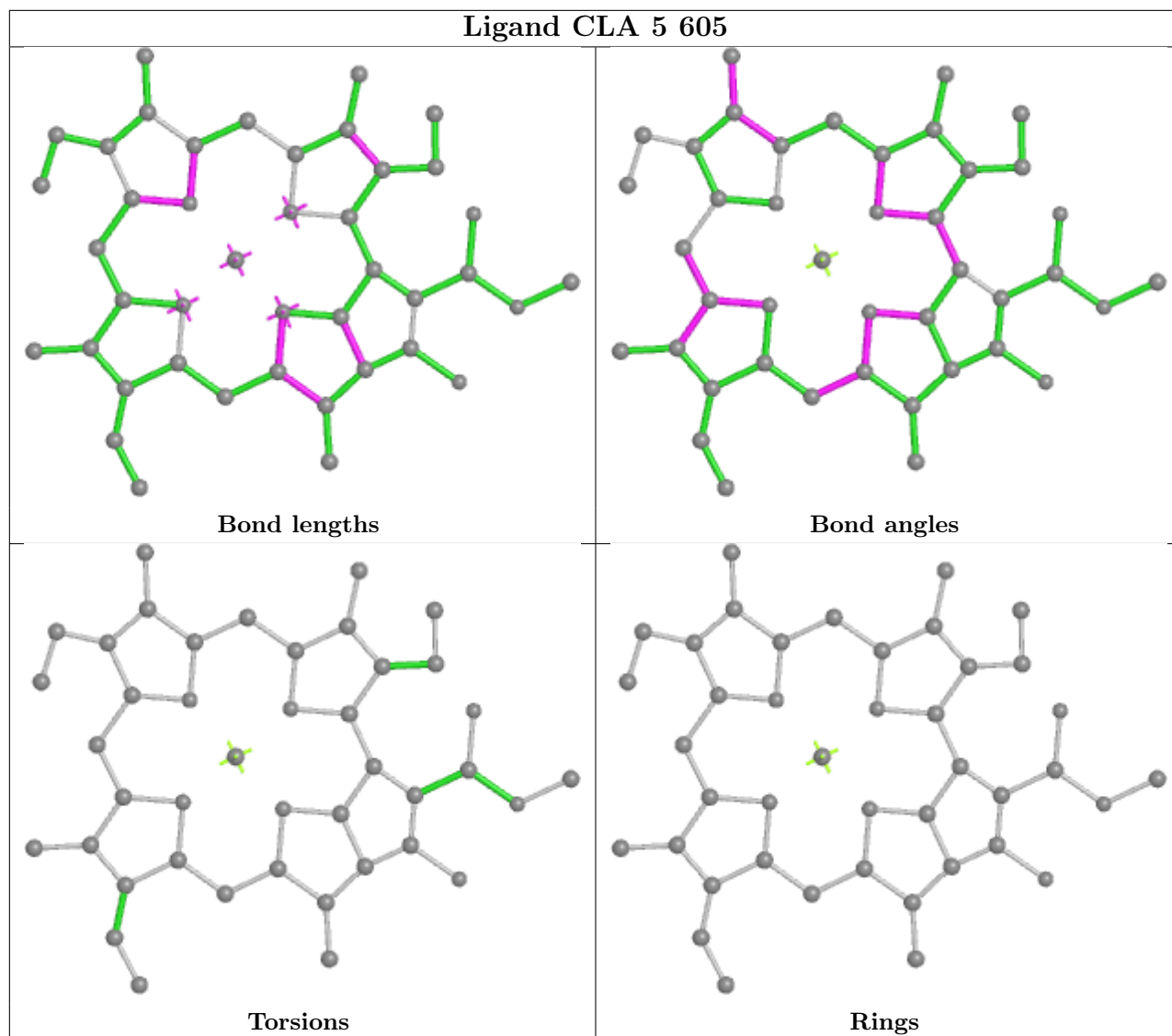


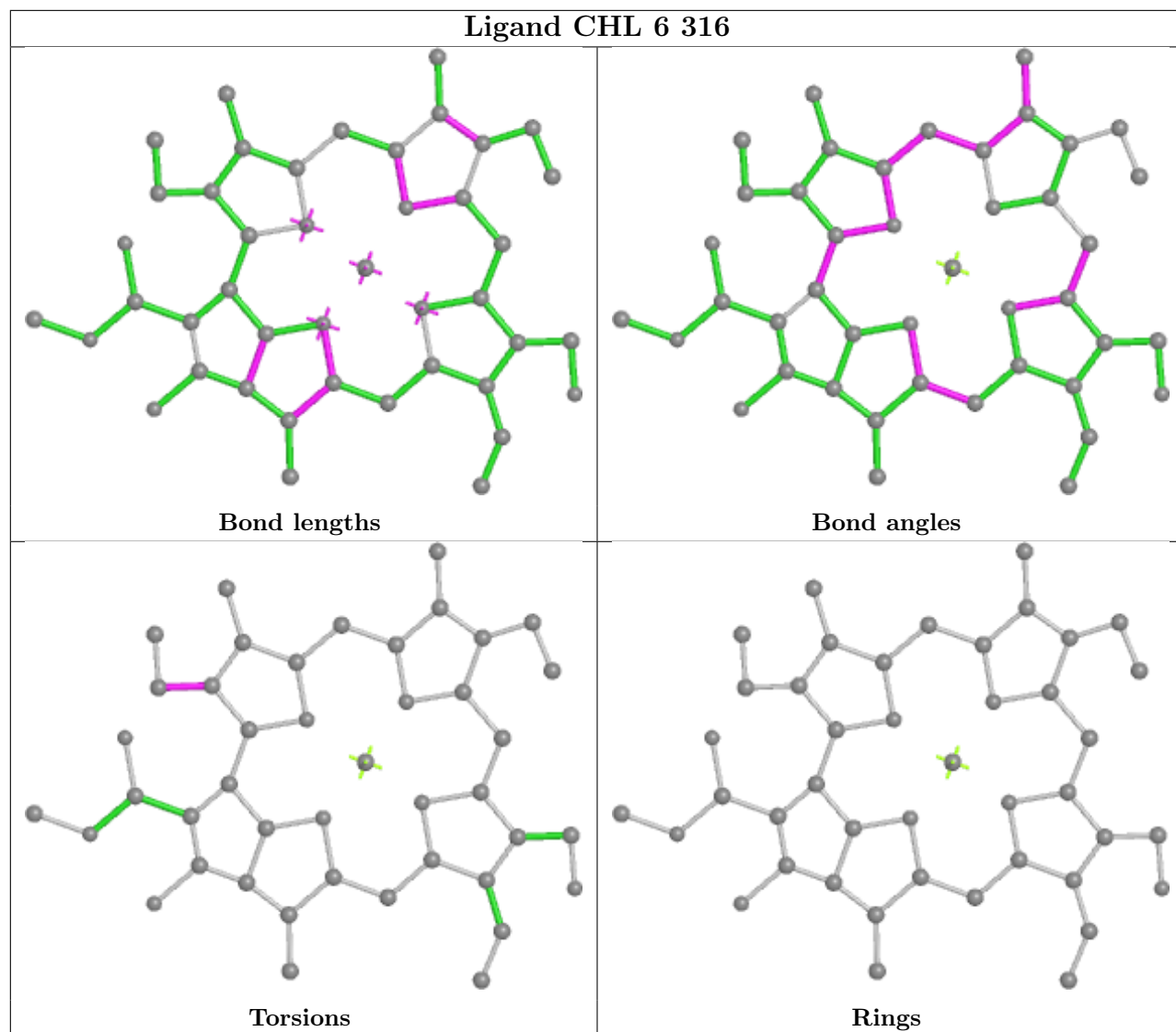


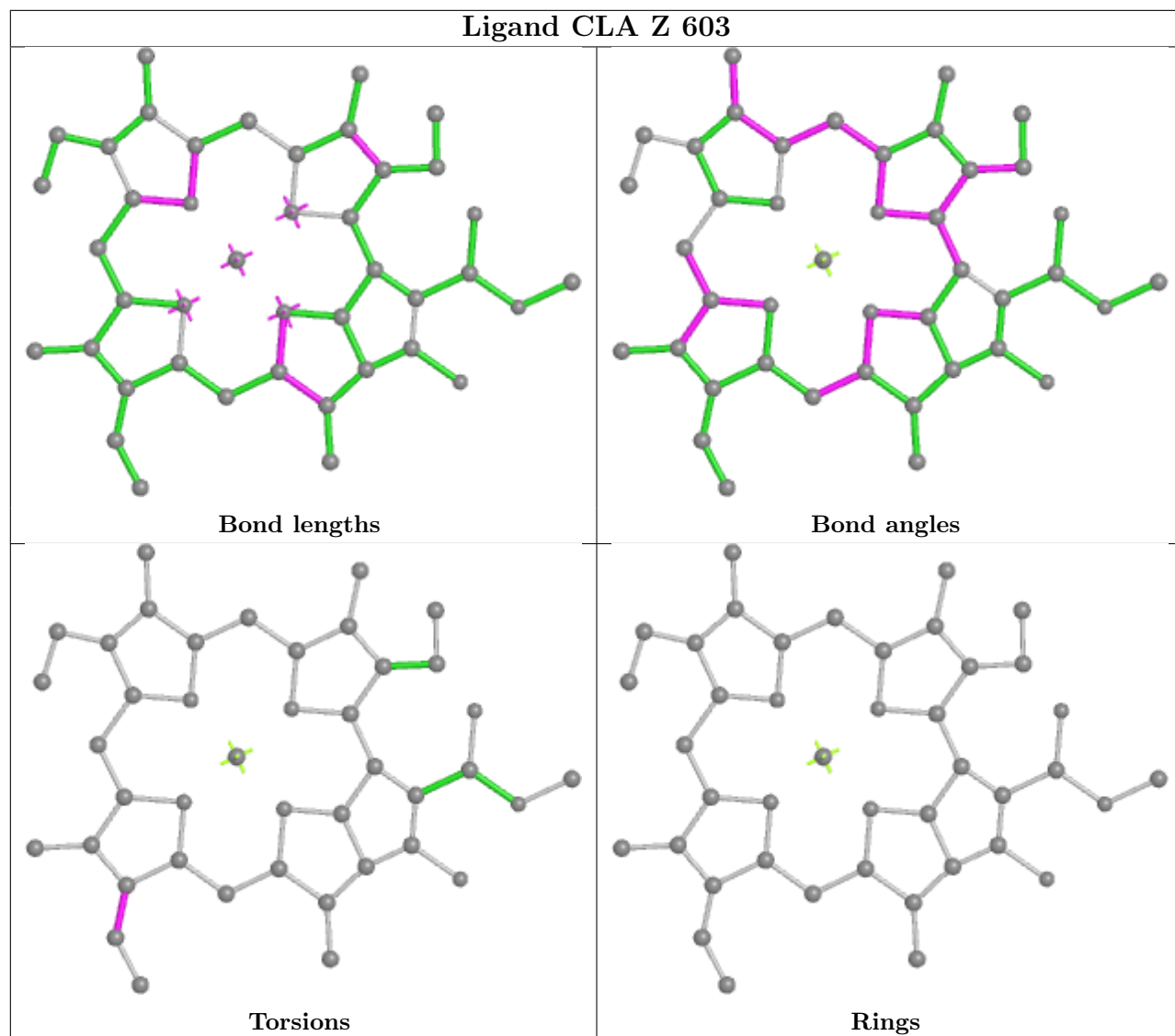


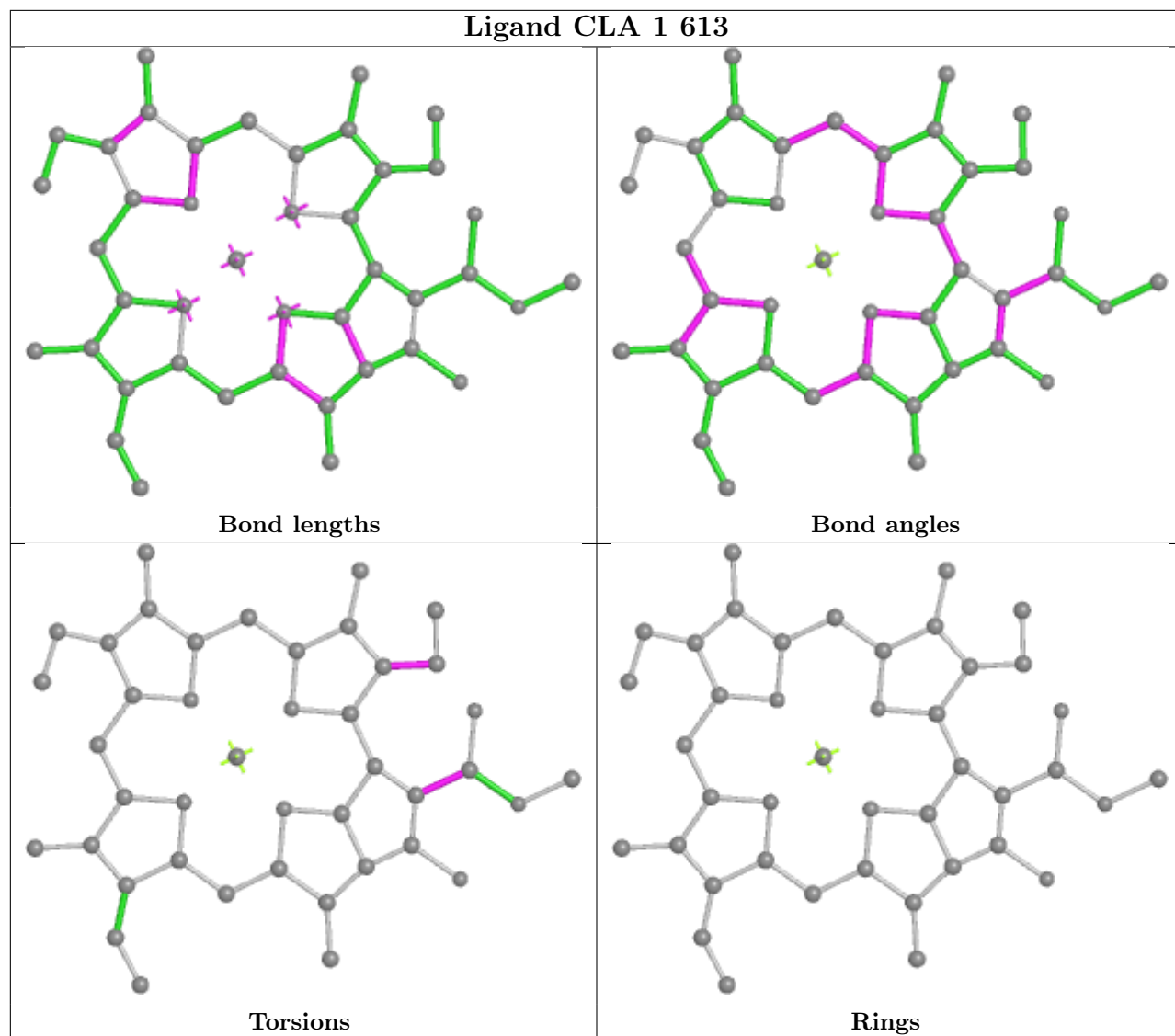


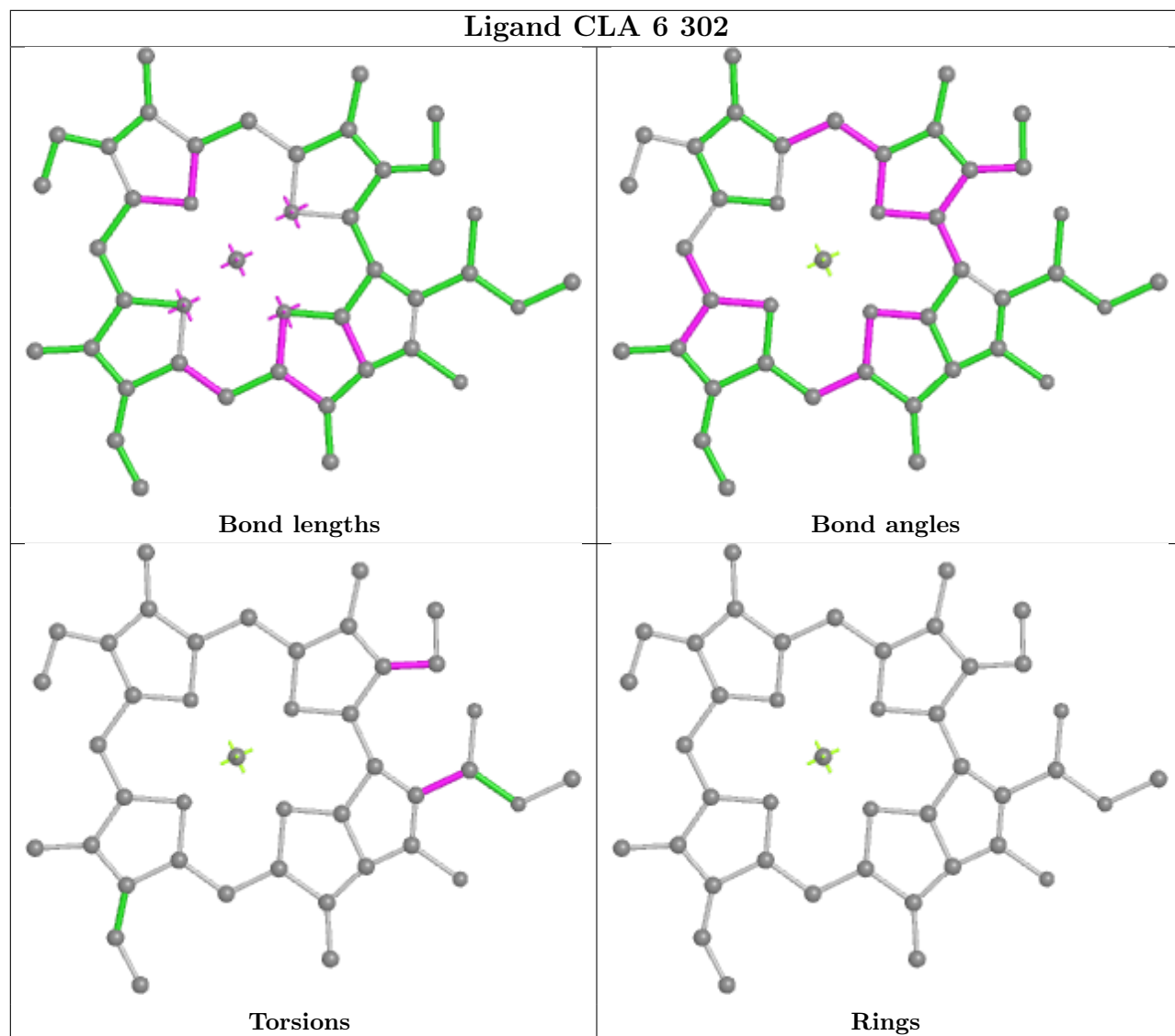


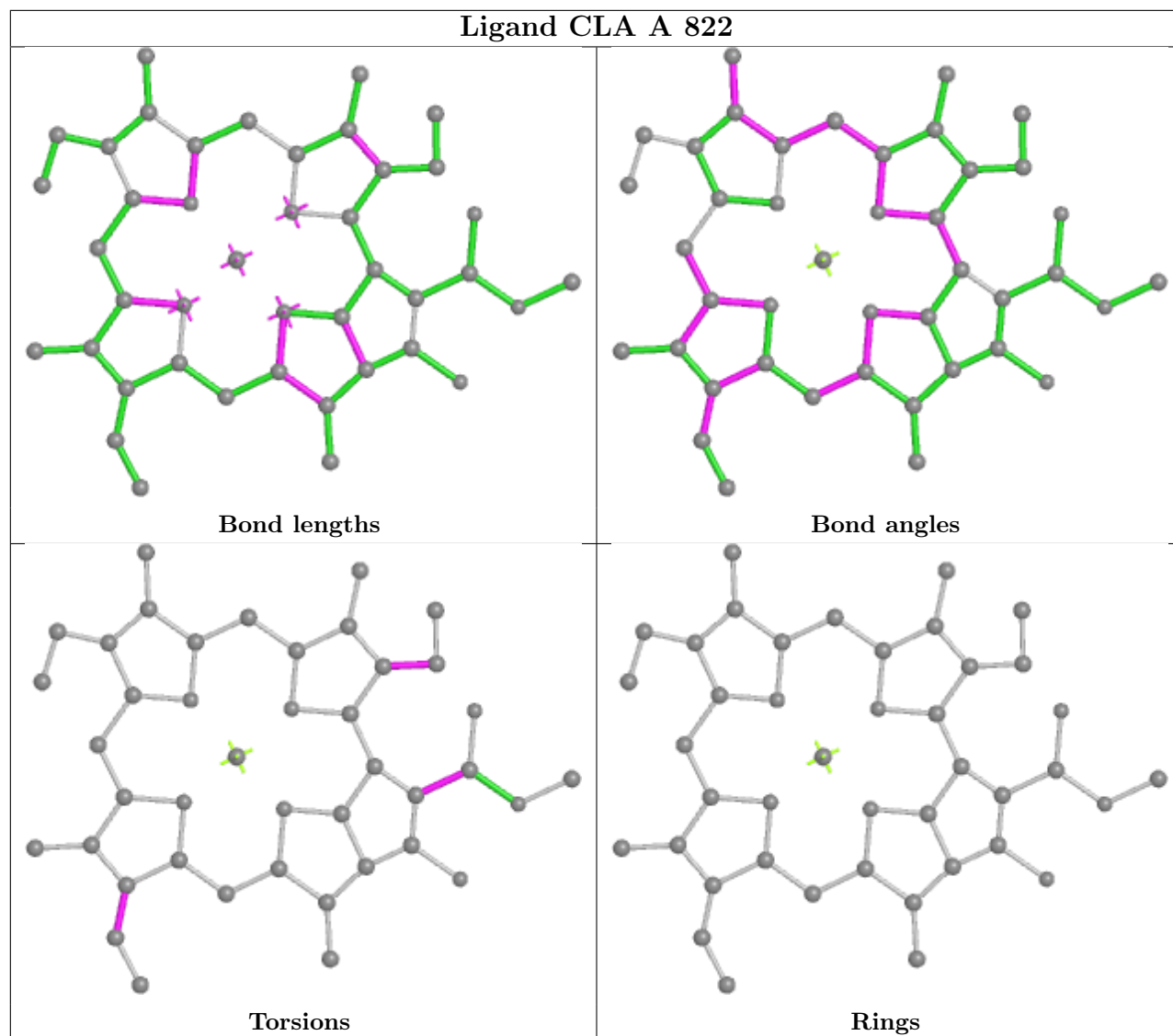


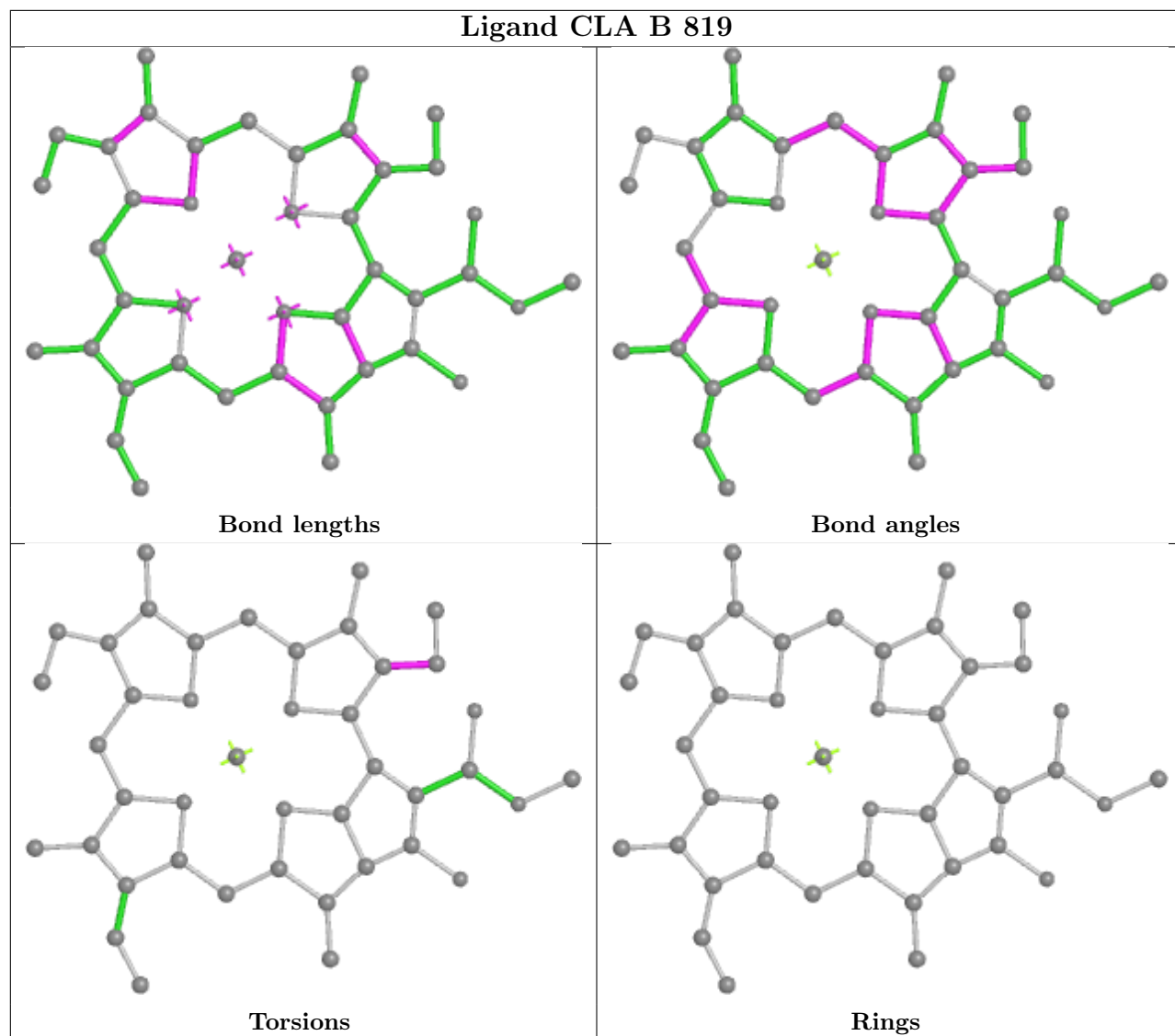


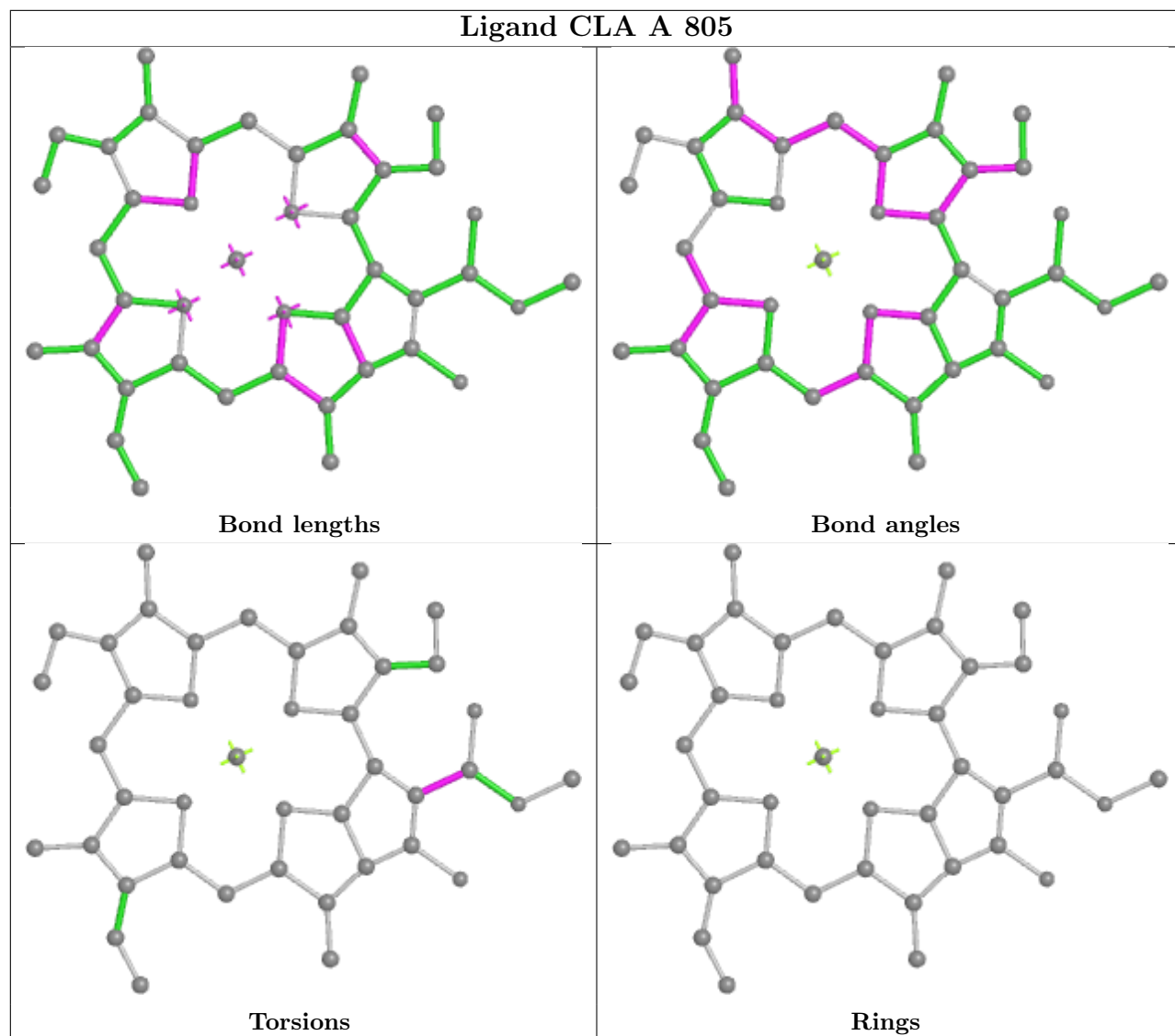


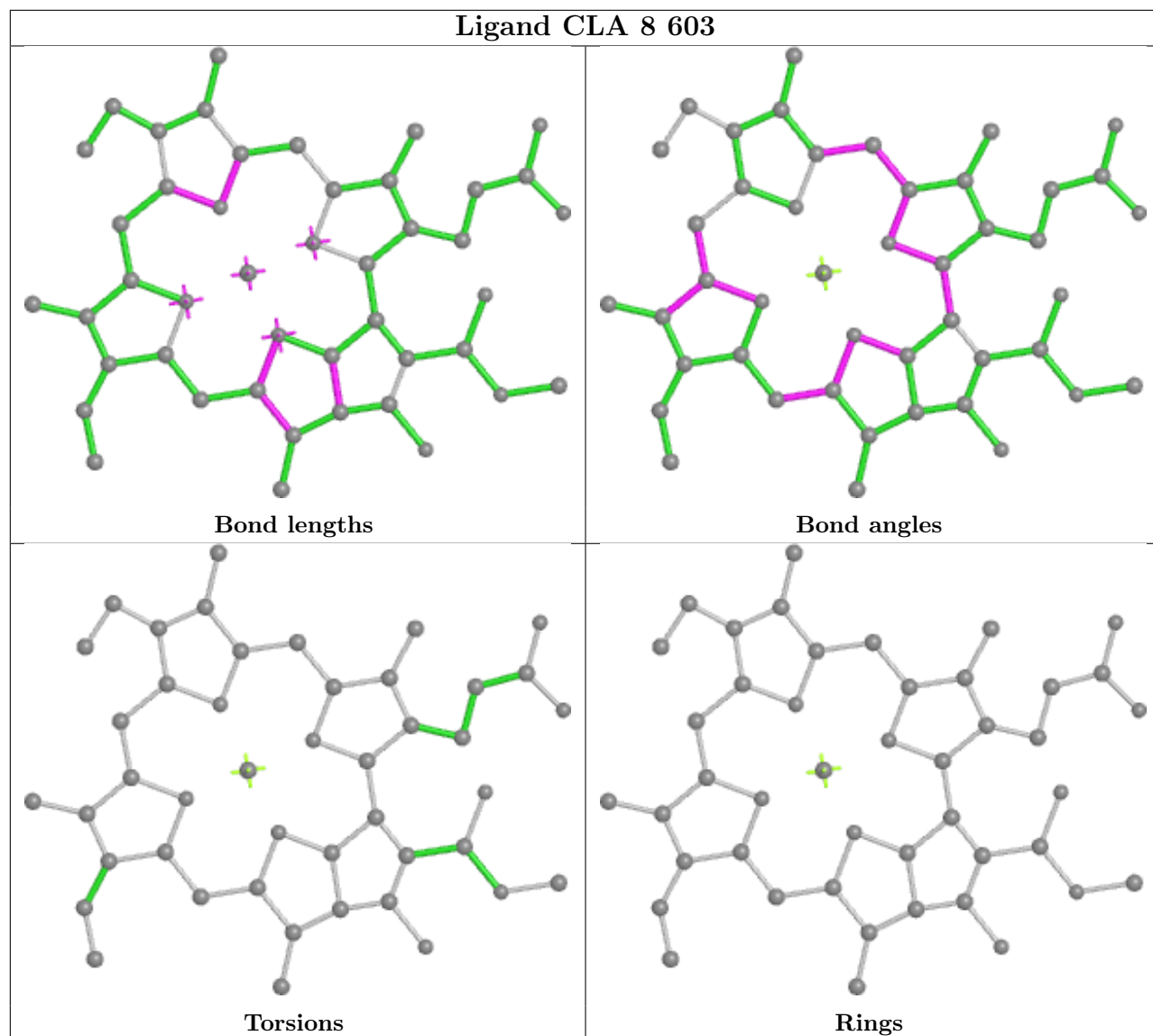


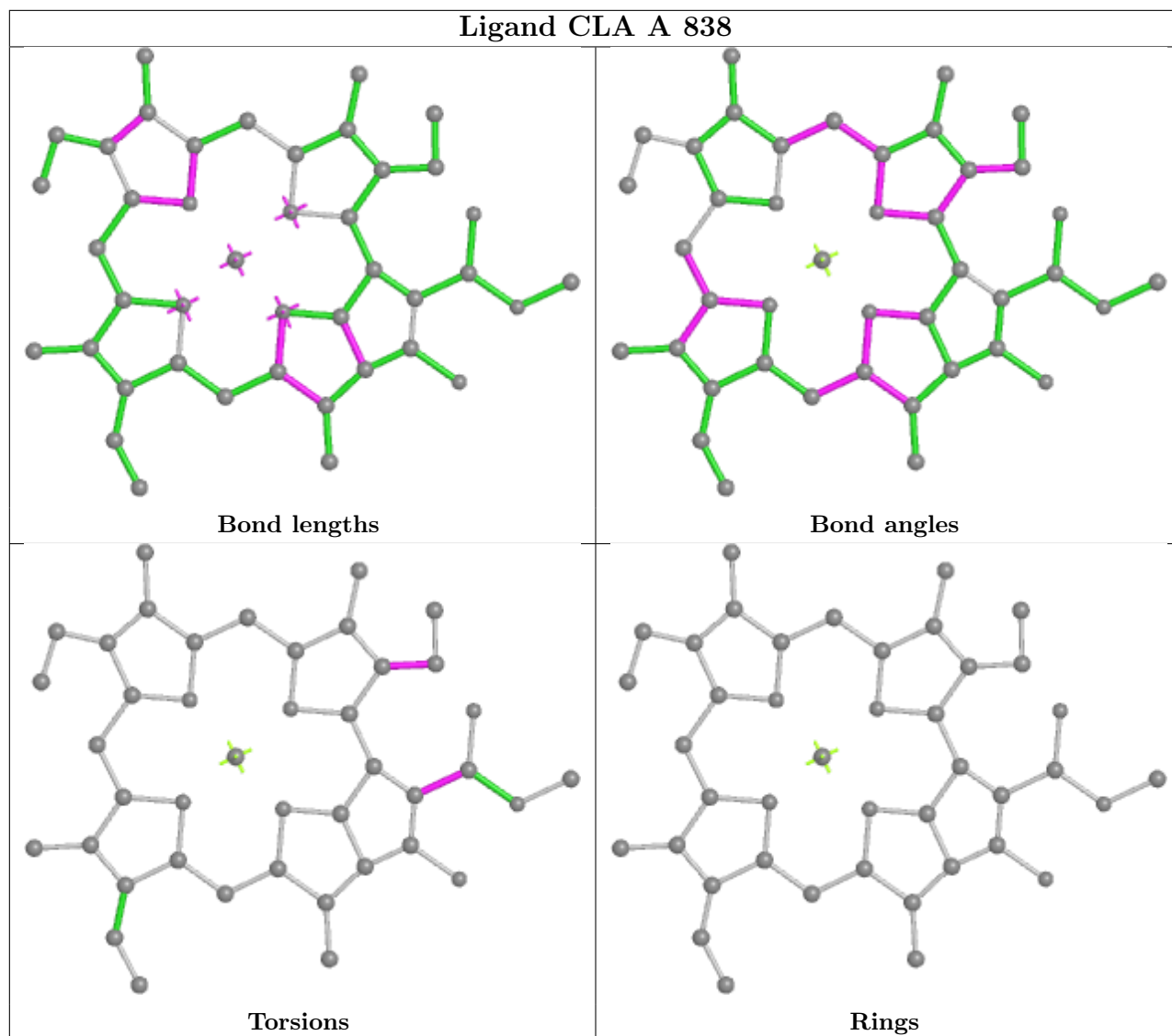


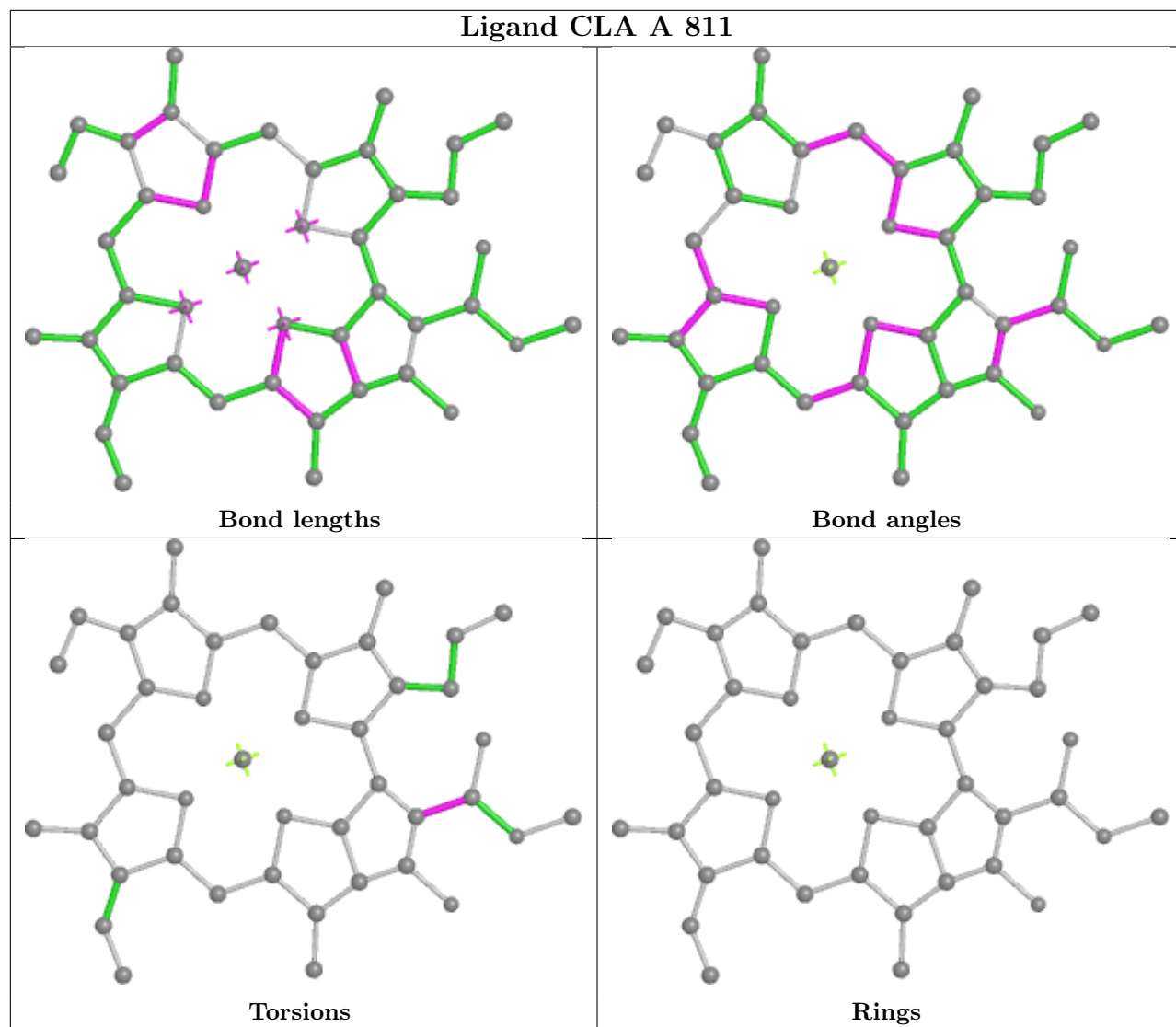


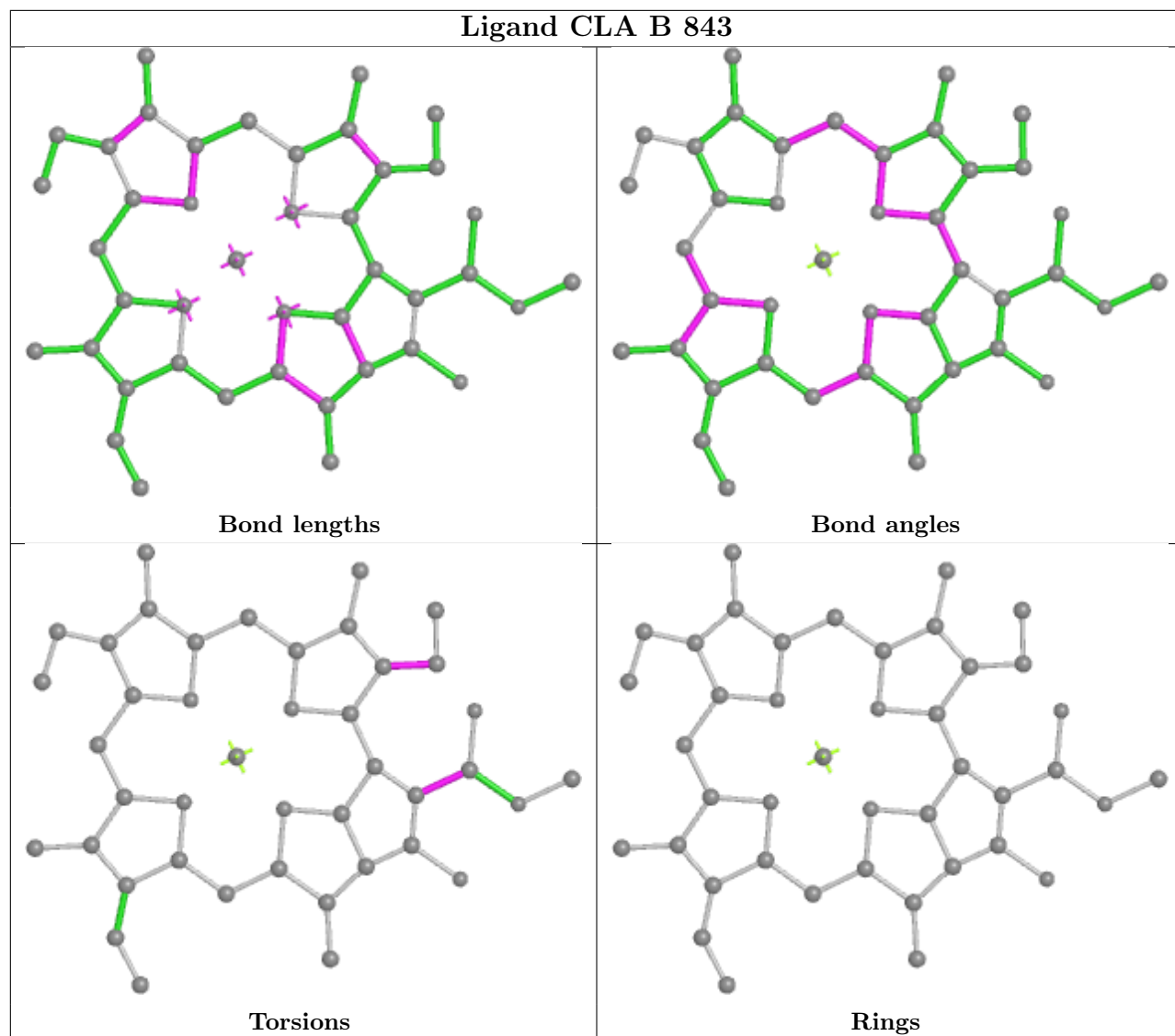


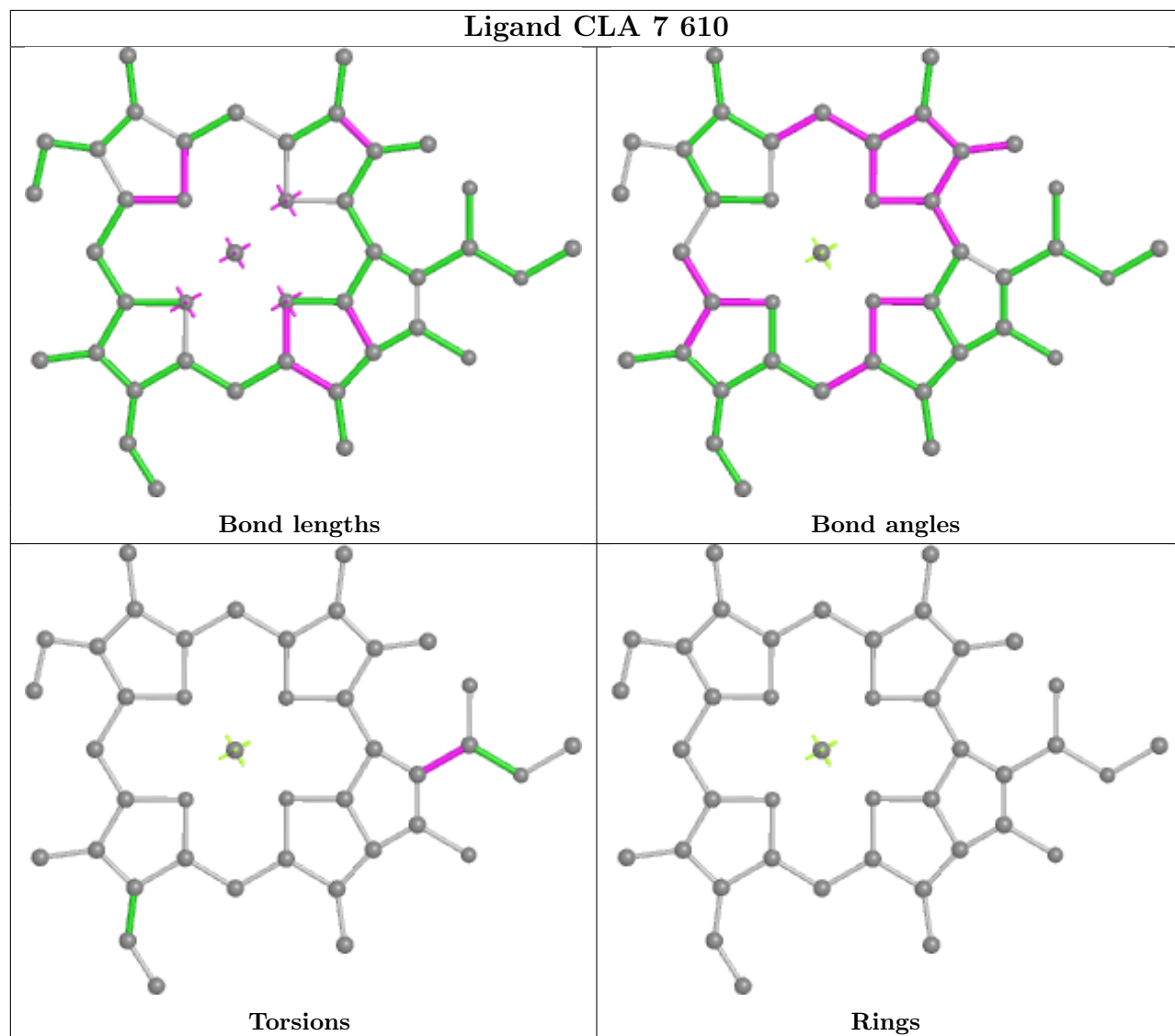


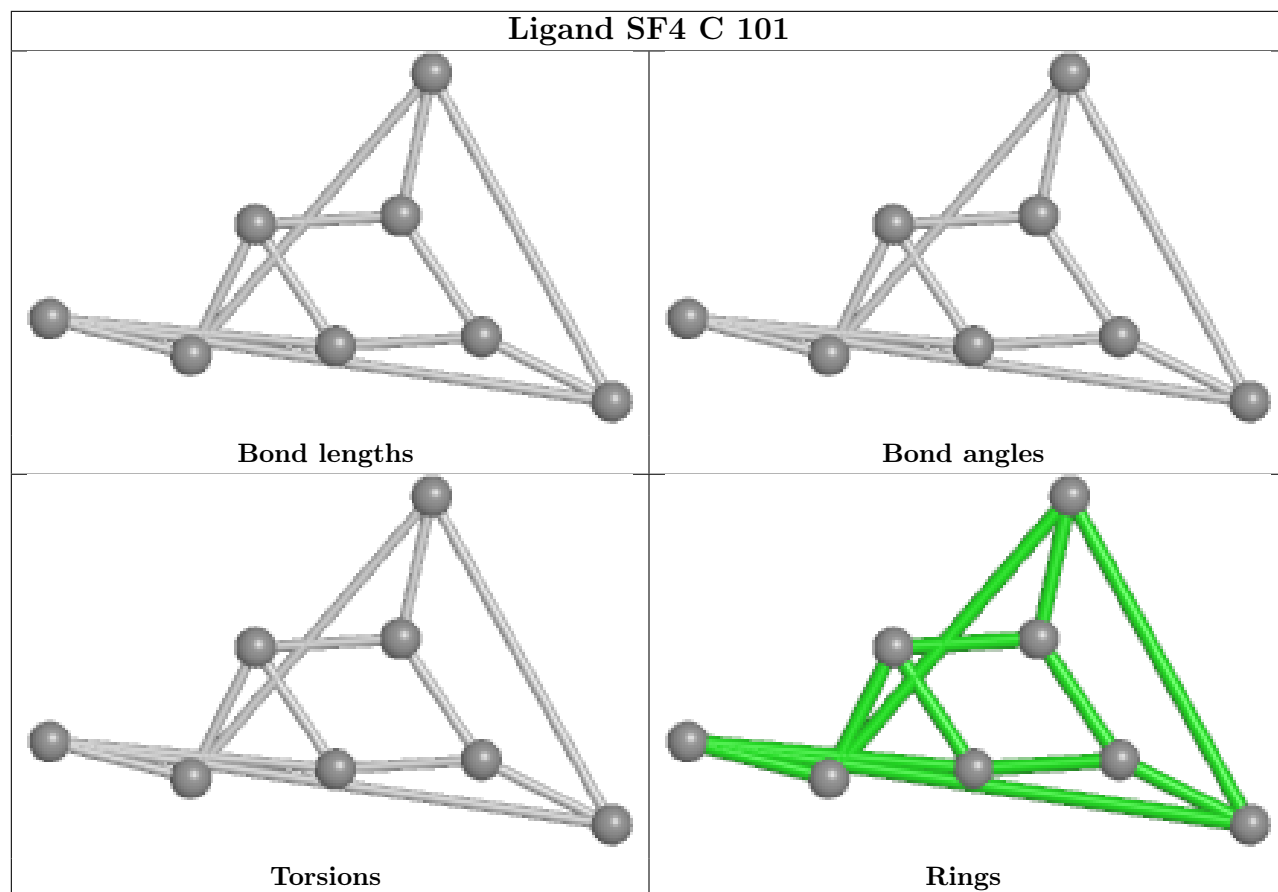


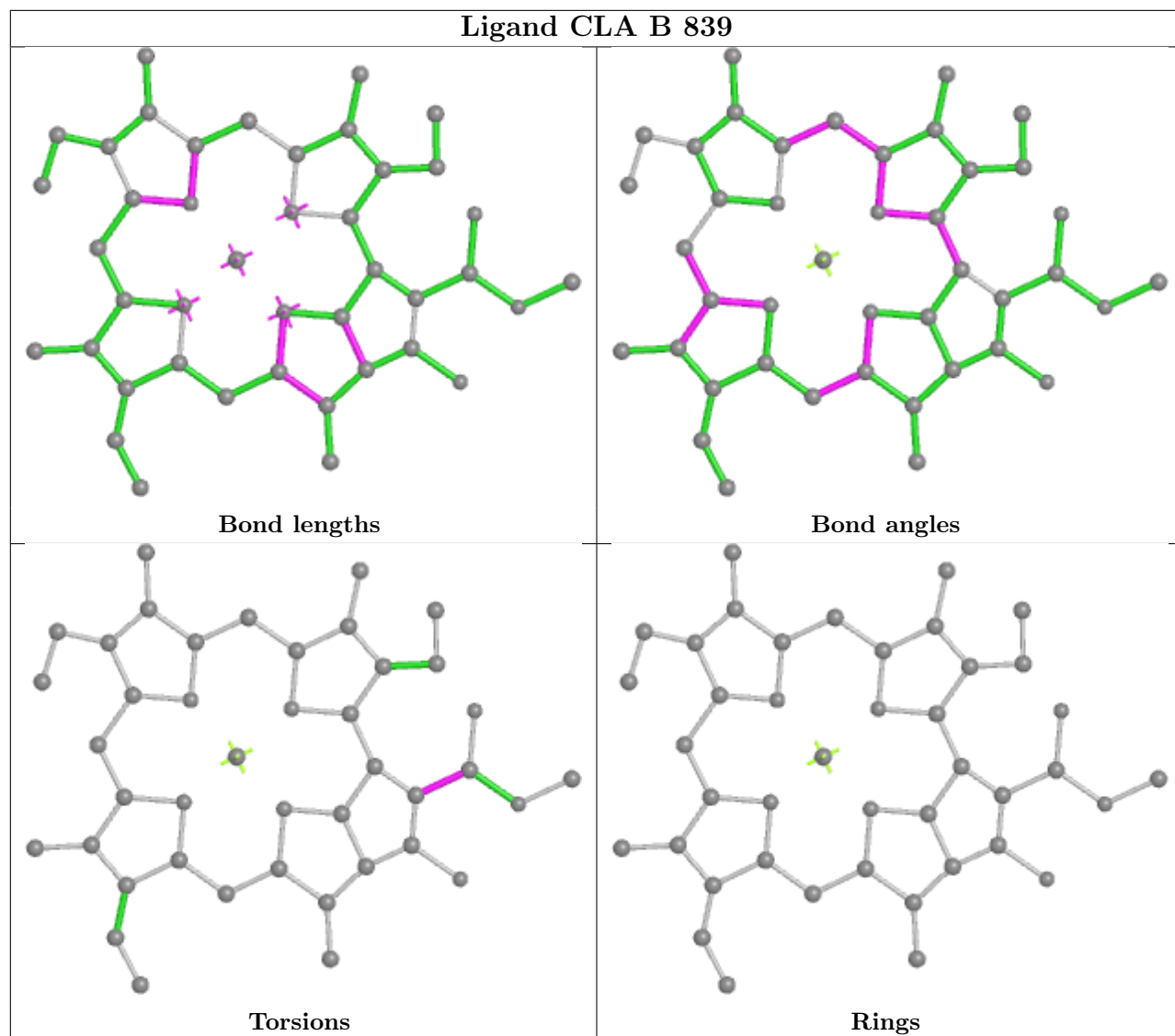


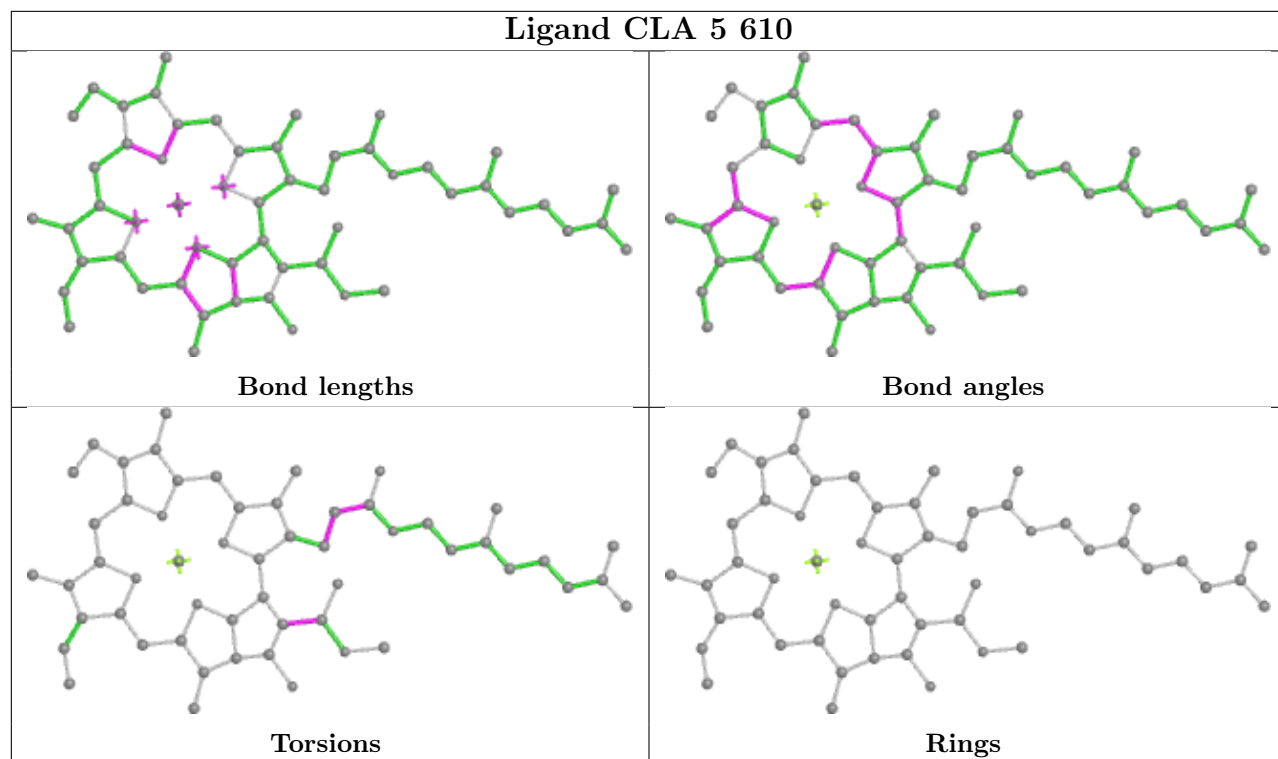


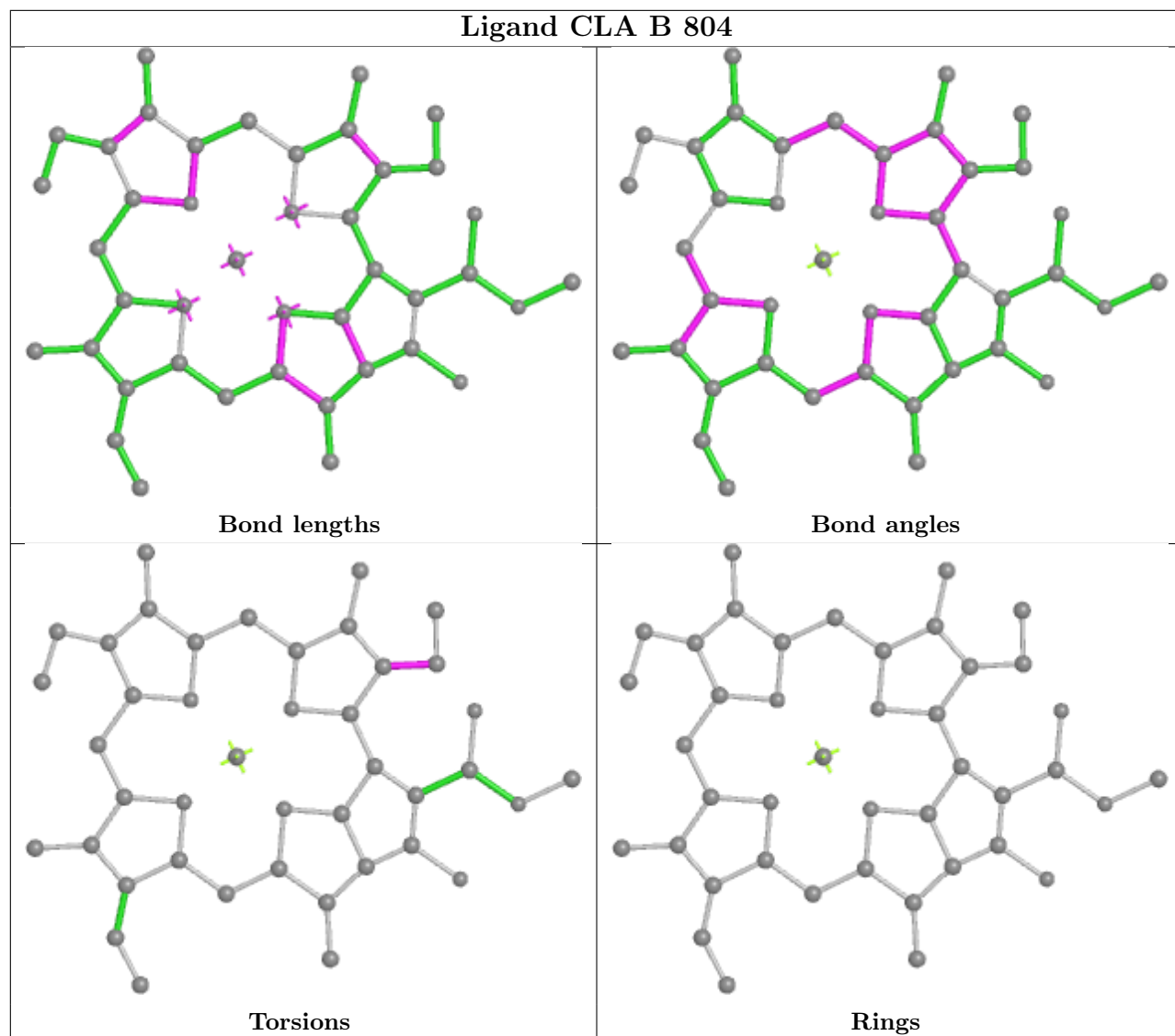


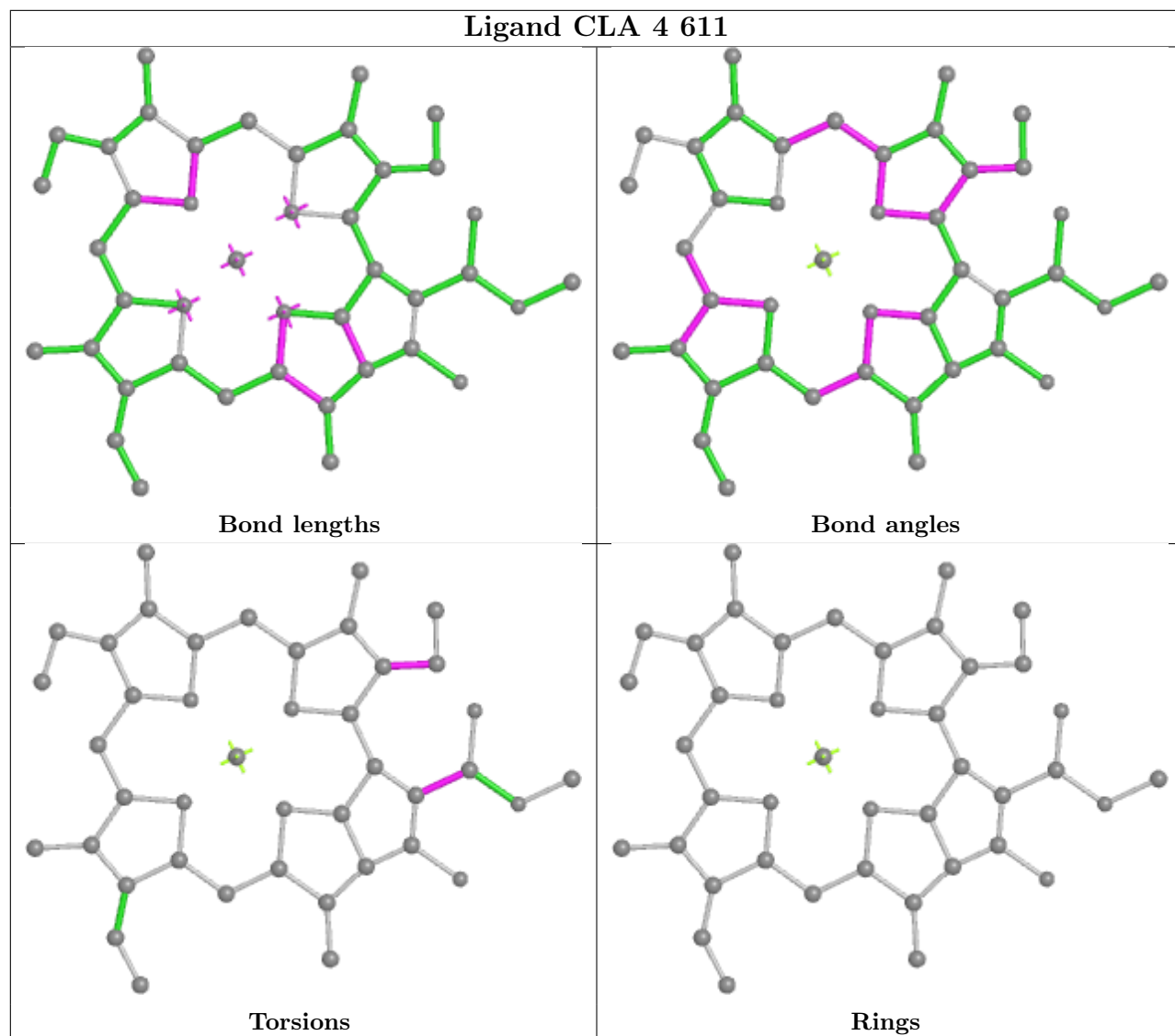


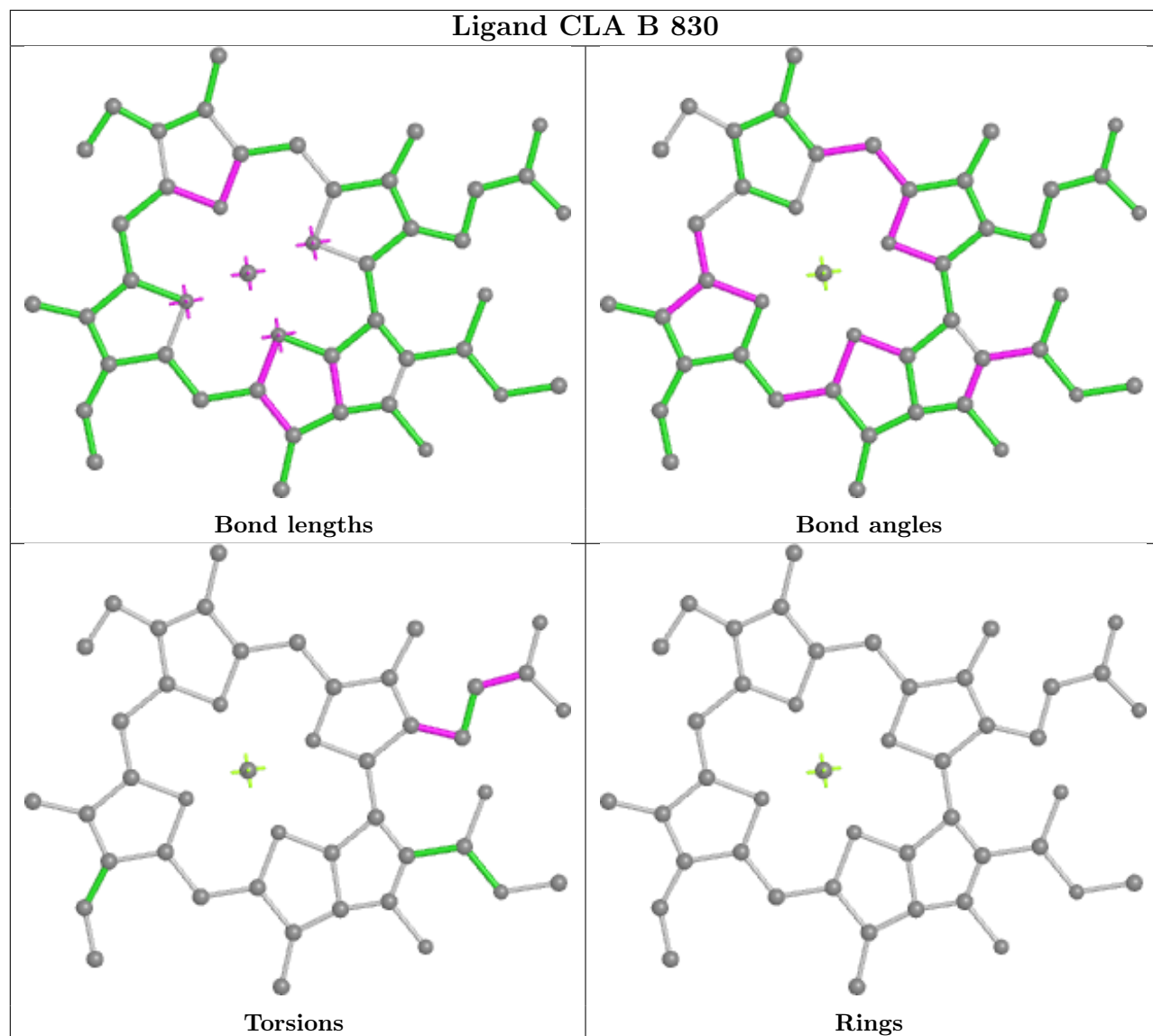


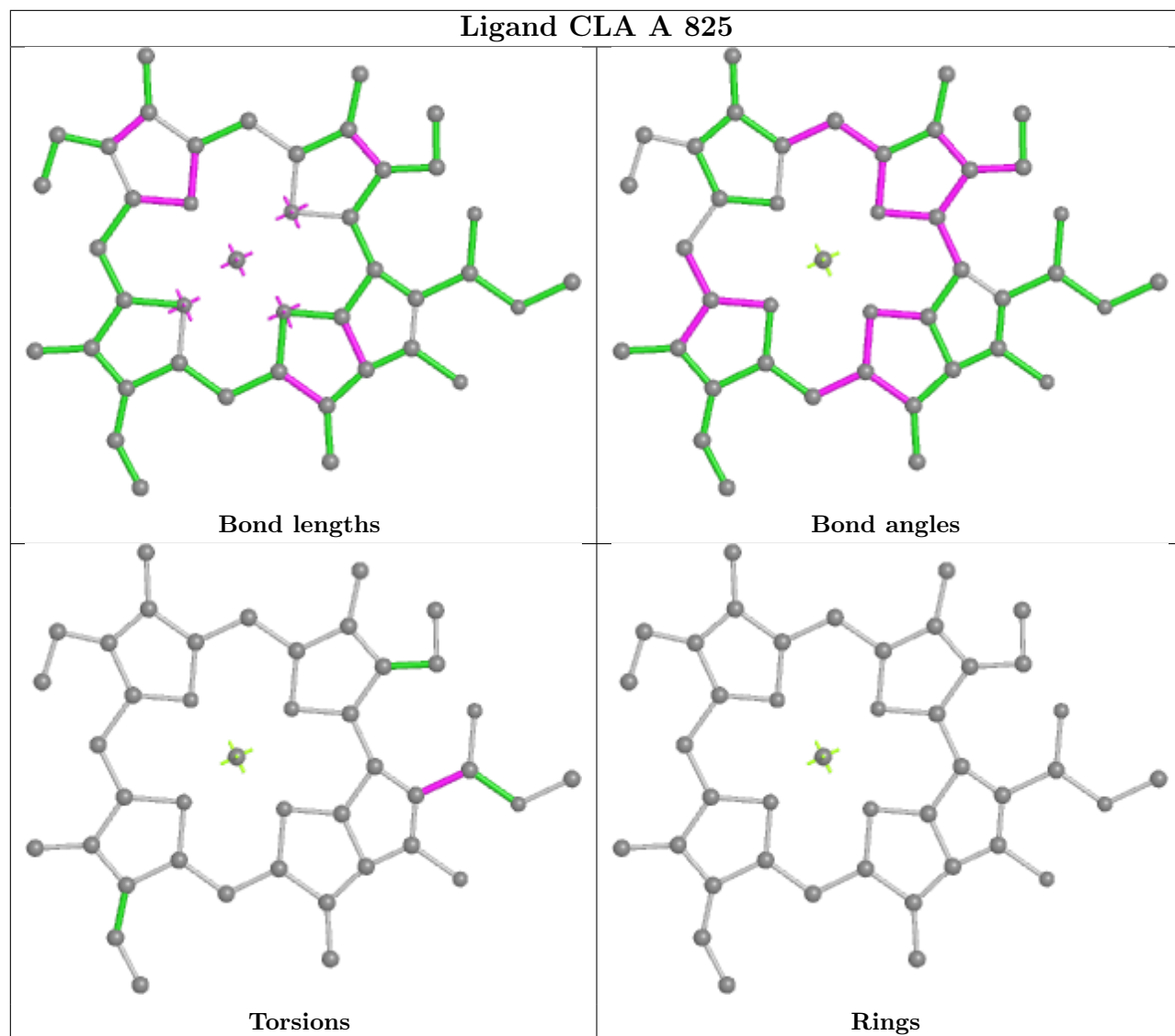


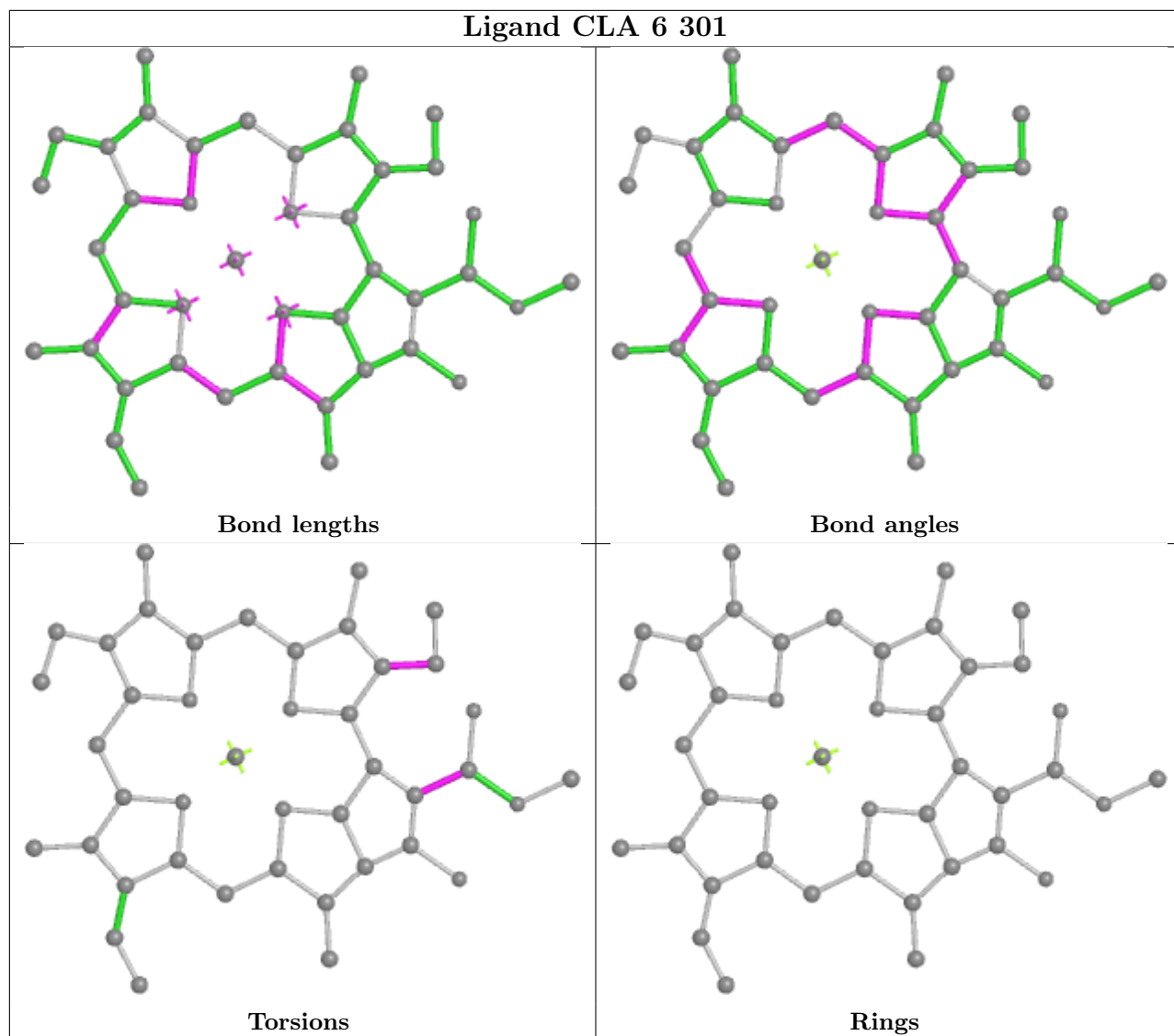


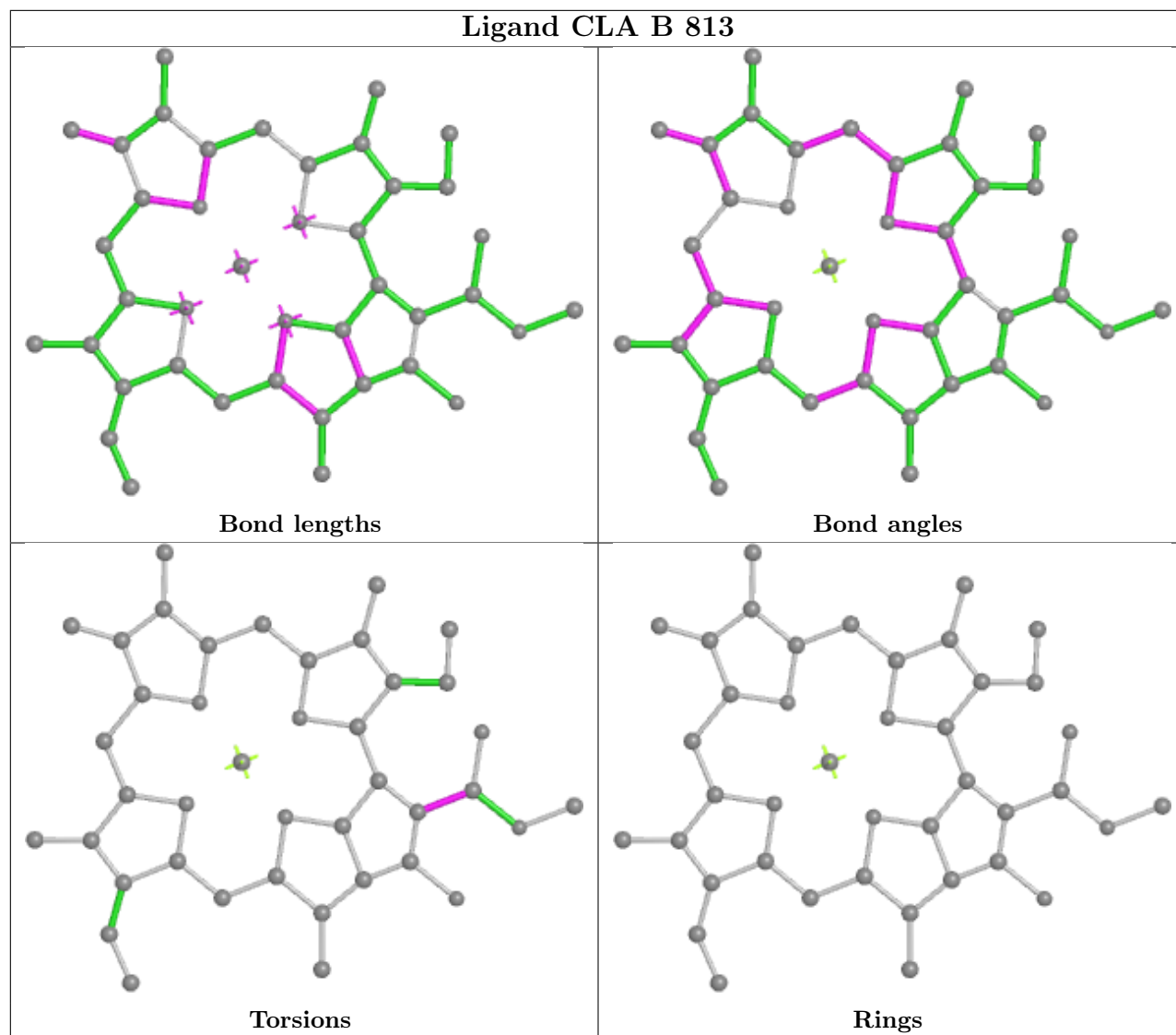


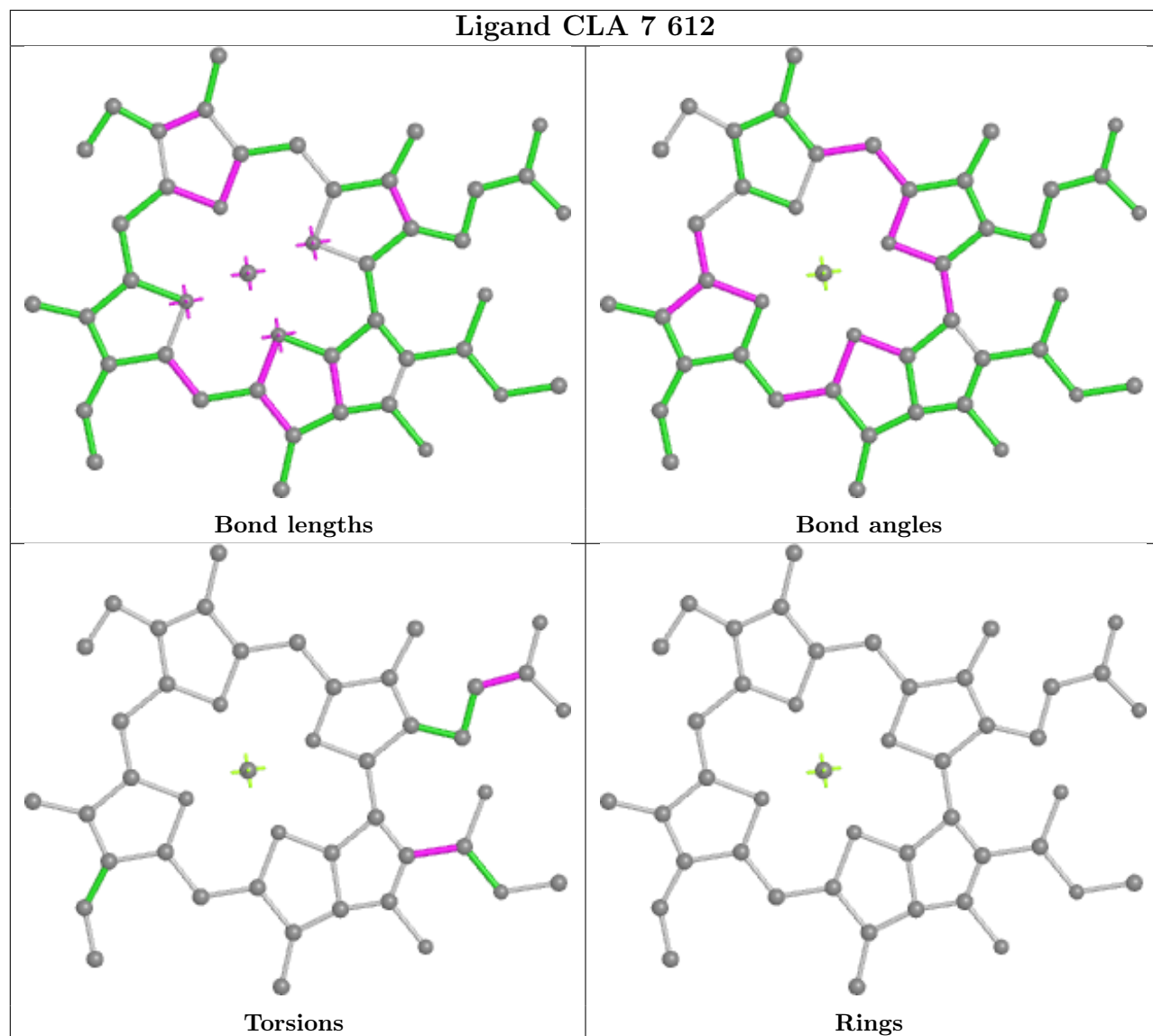


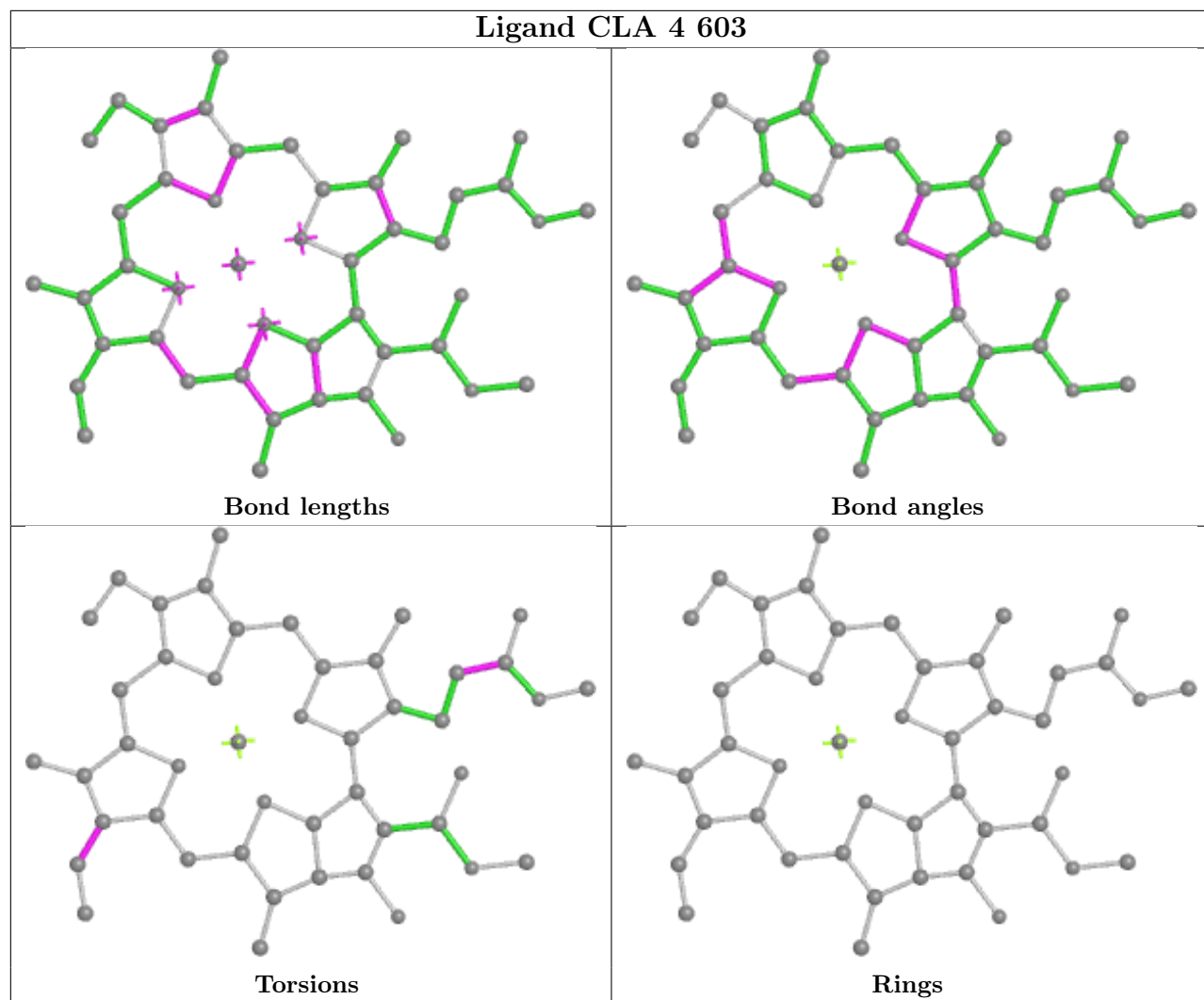


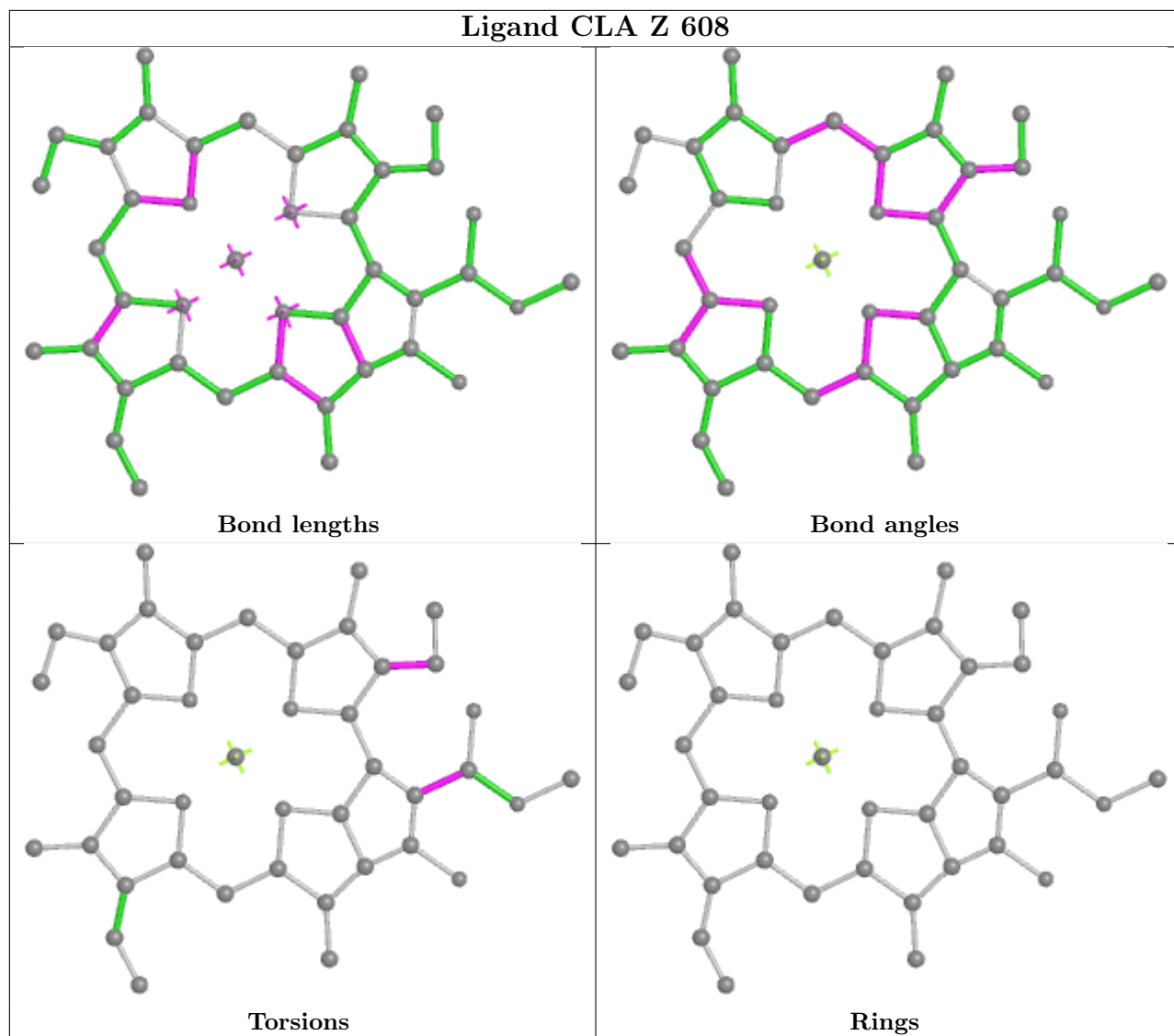


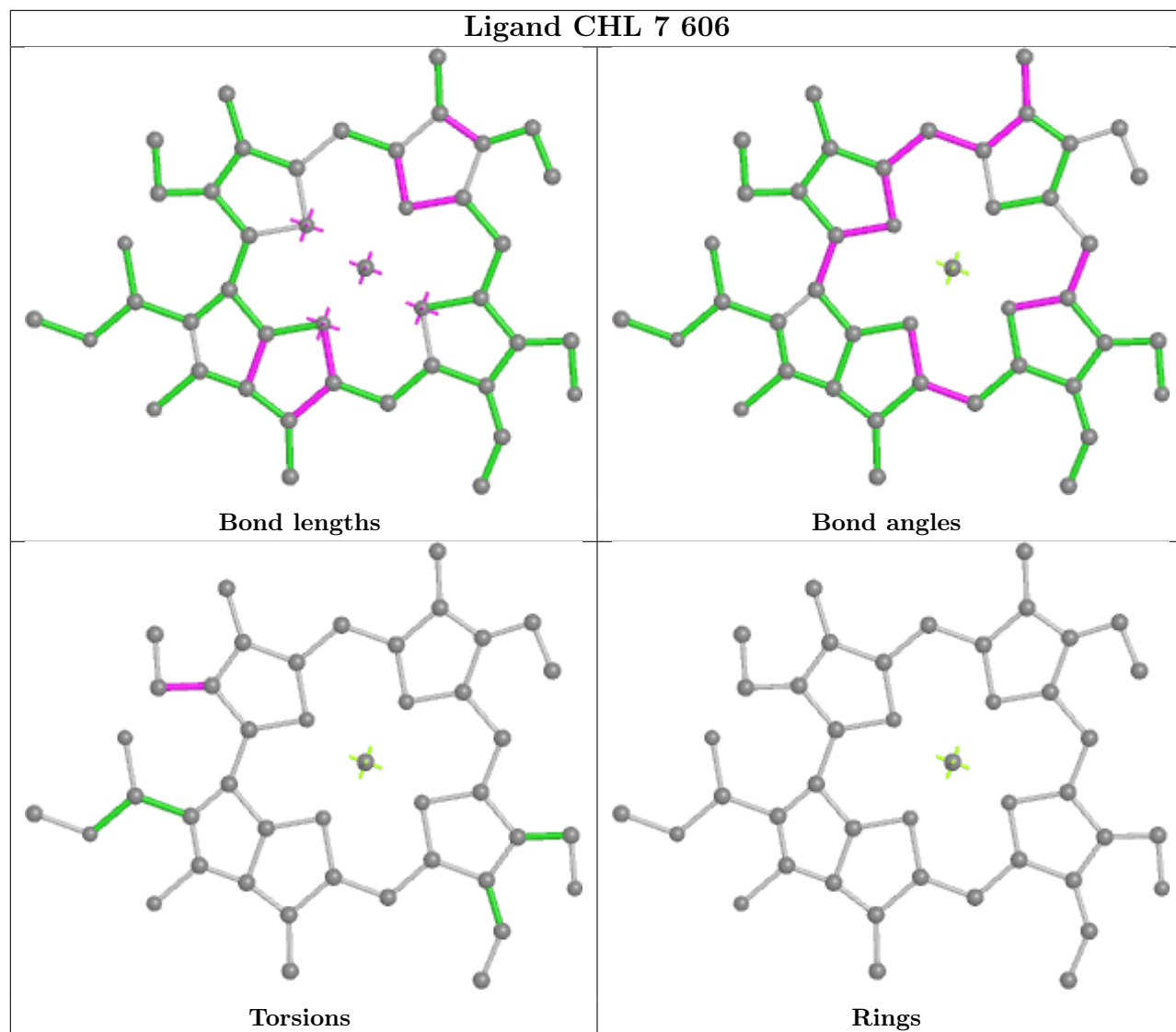


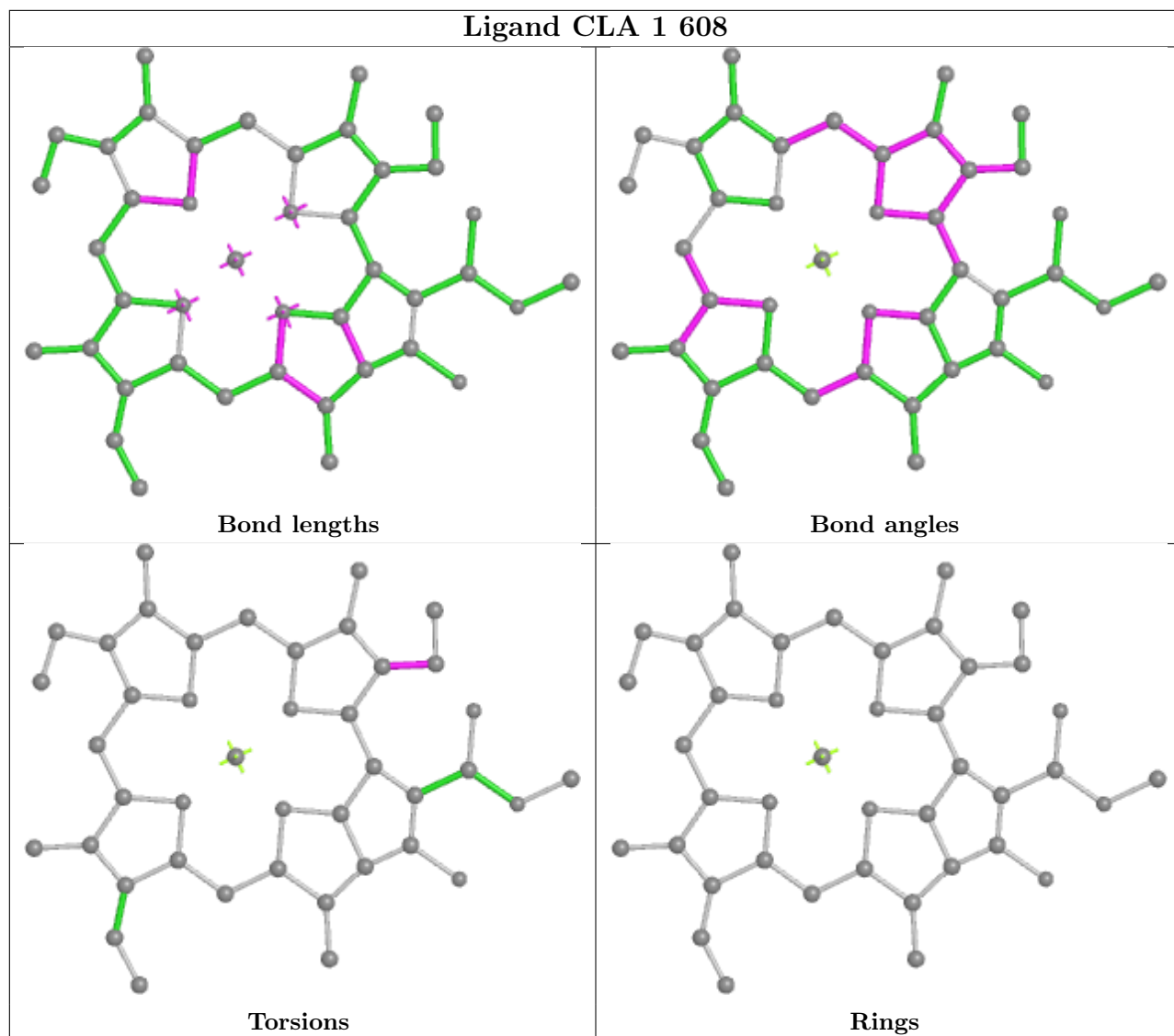


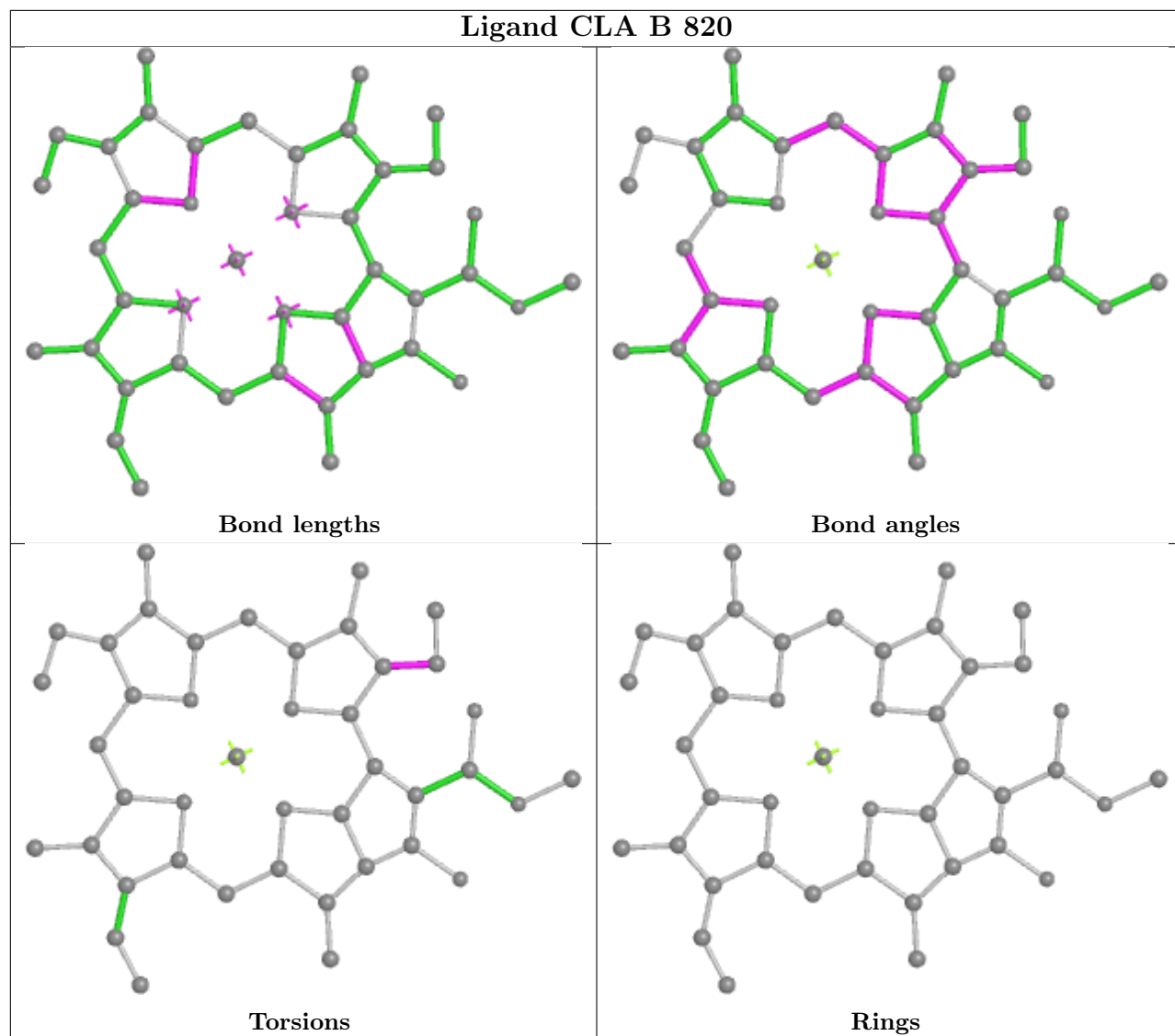


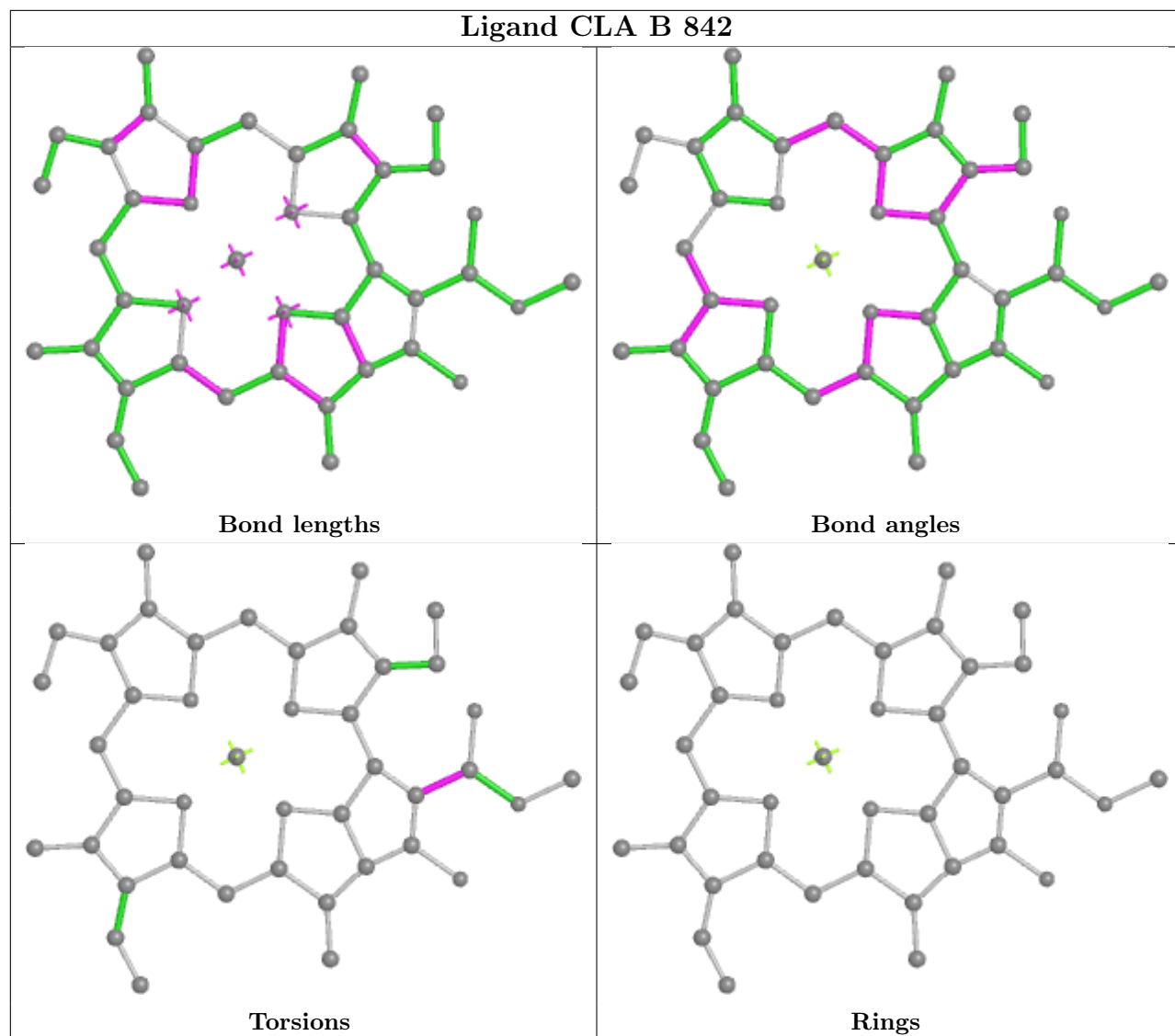


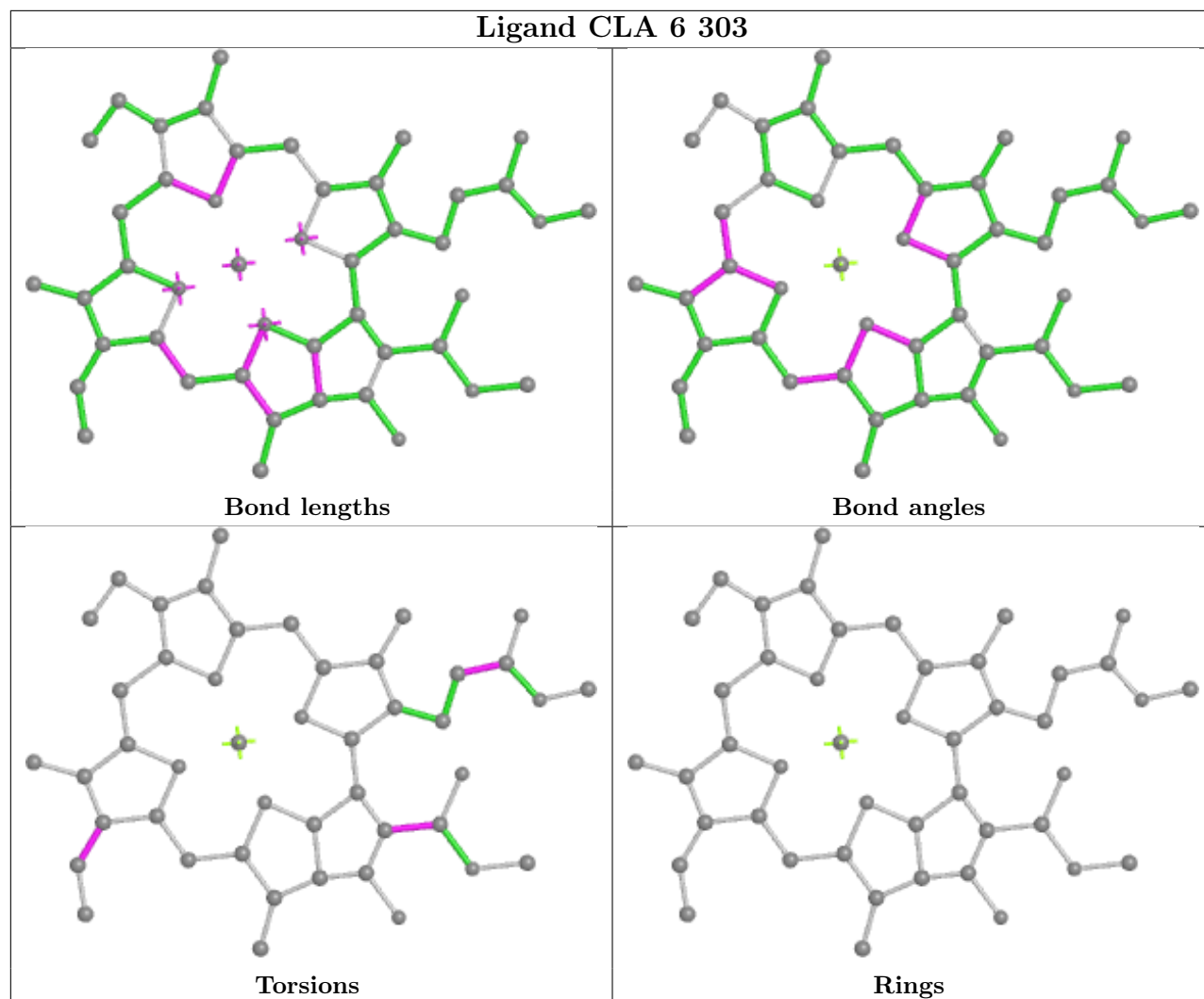


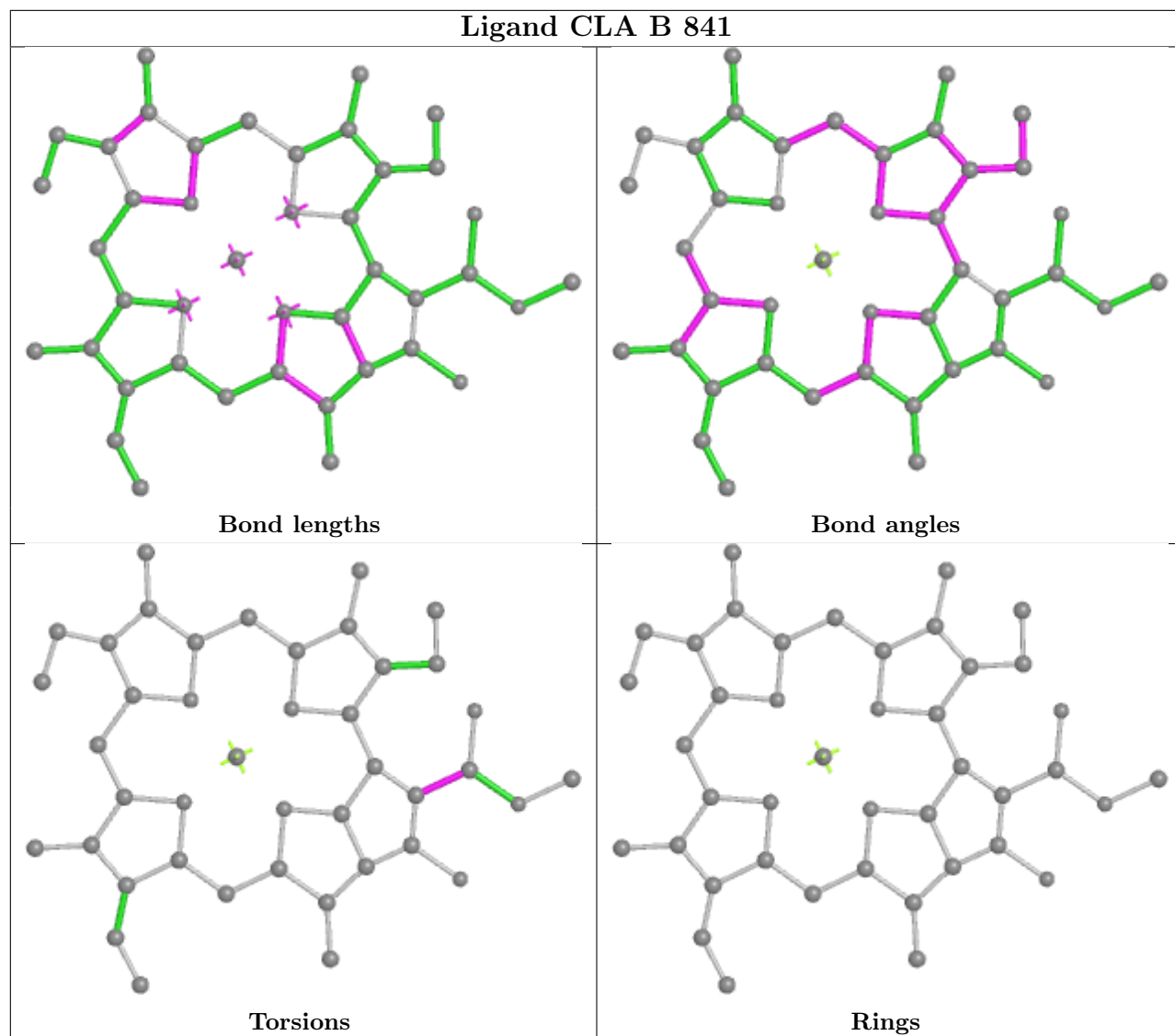




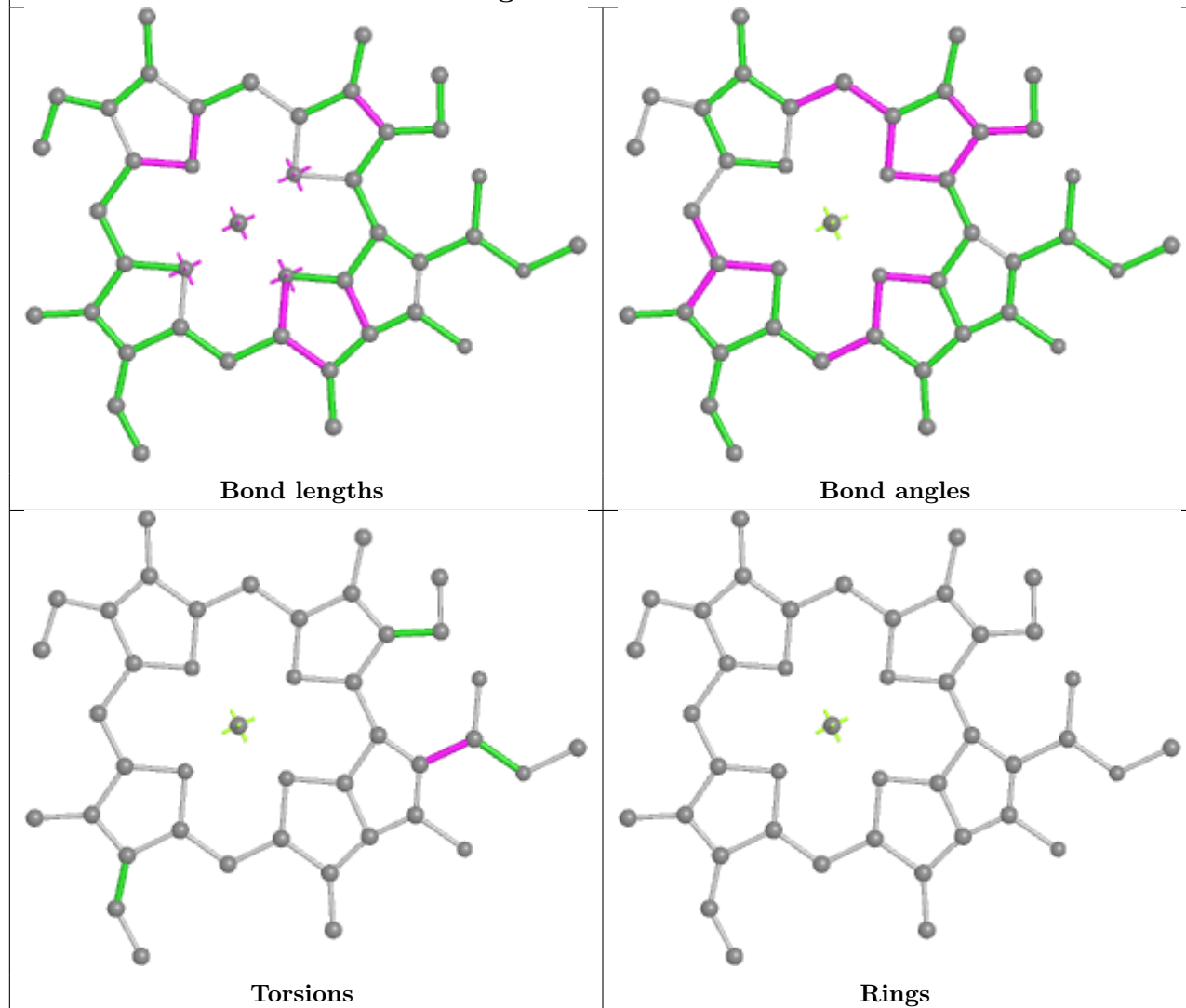




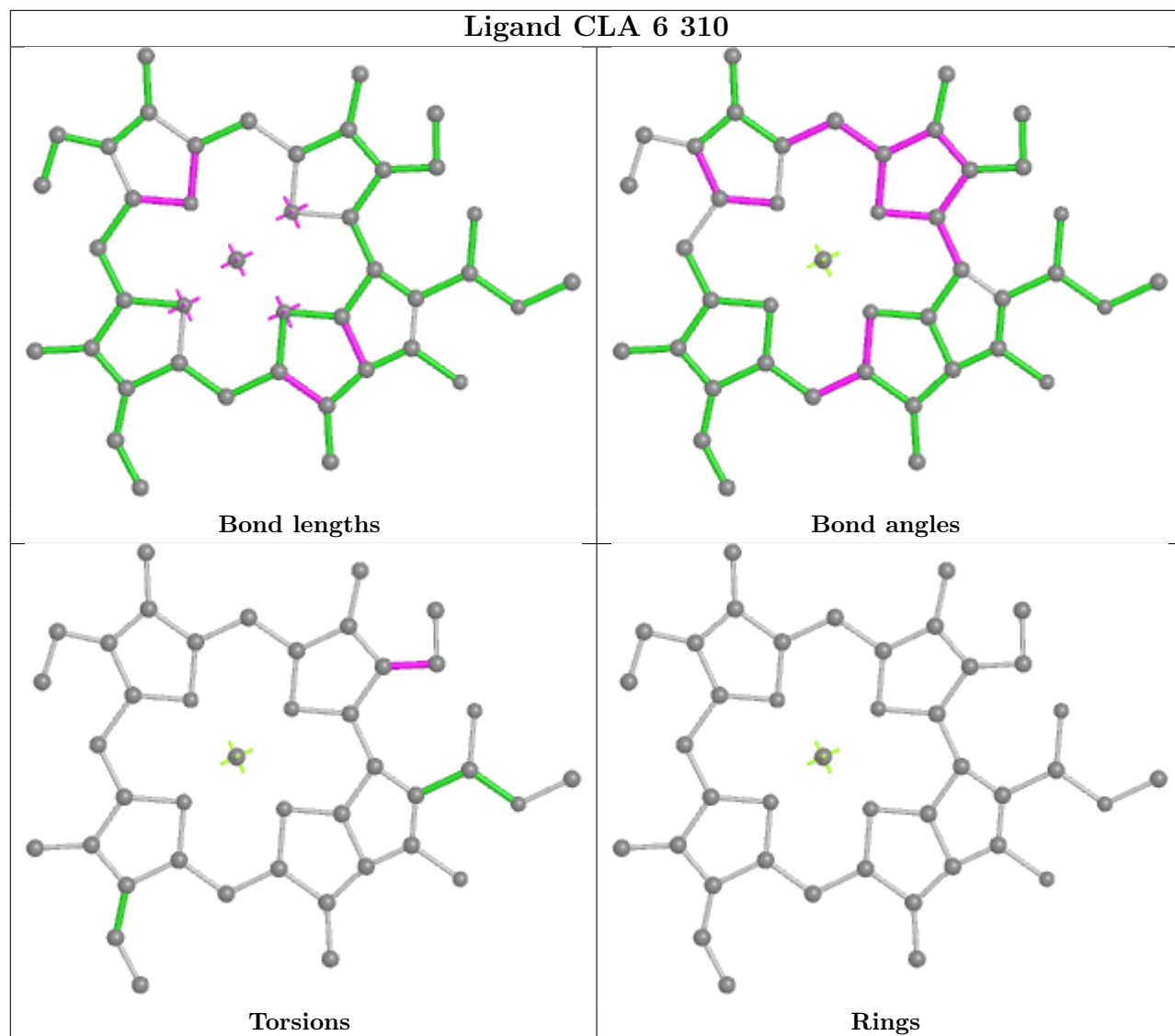


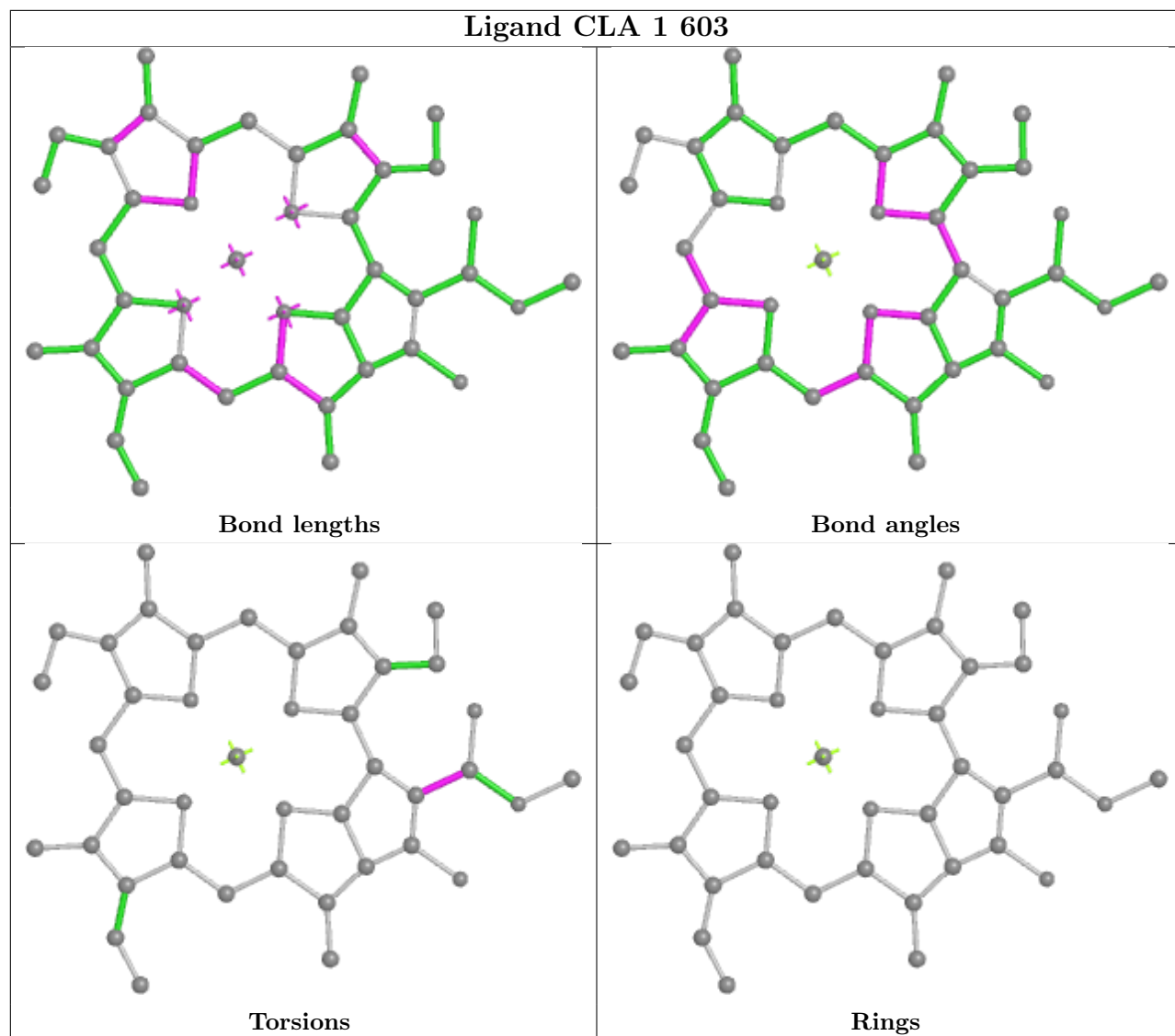


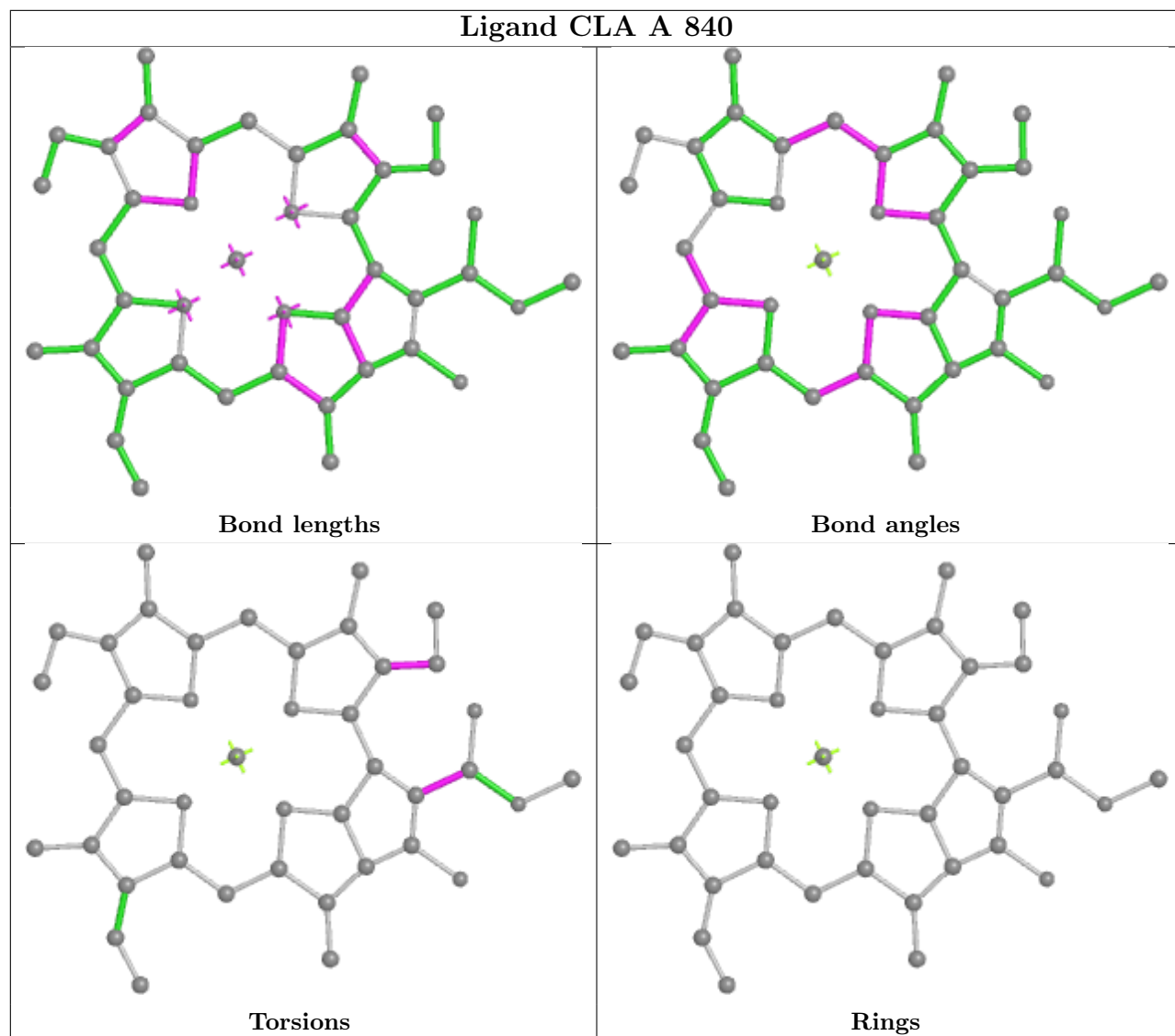
Ligand CLA 3 307

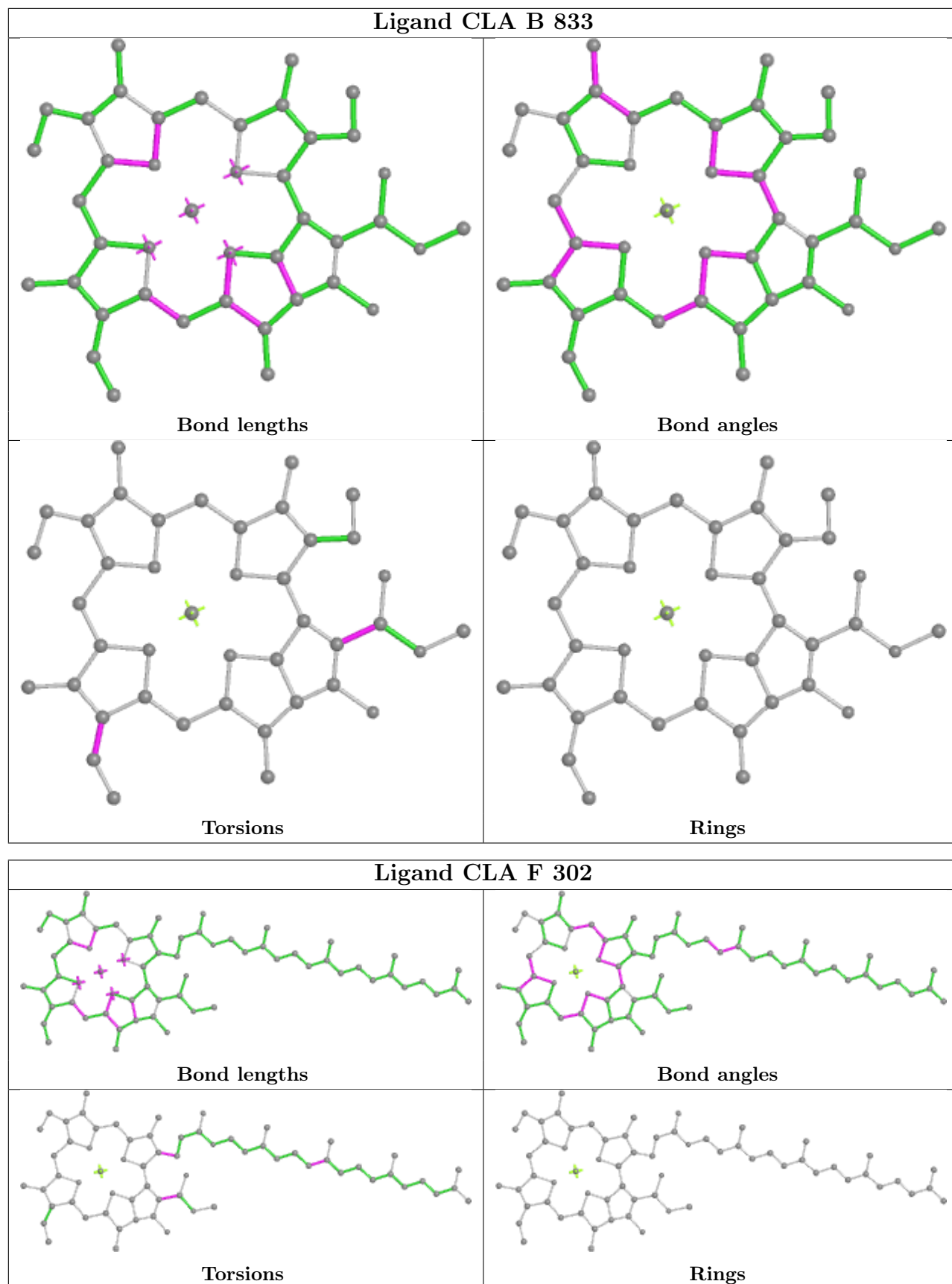


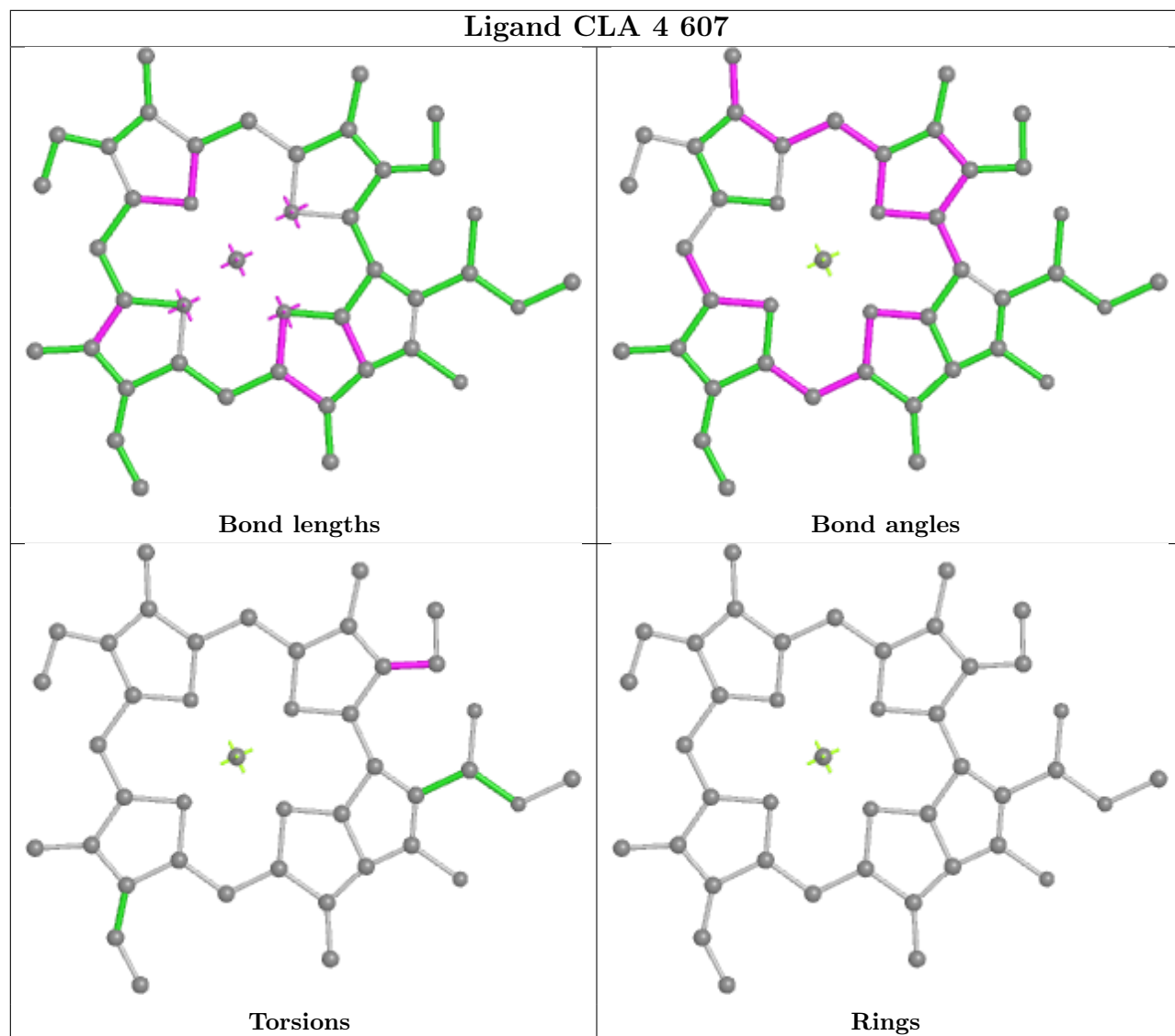
Ligand CLA 6 310



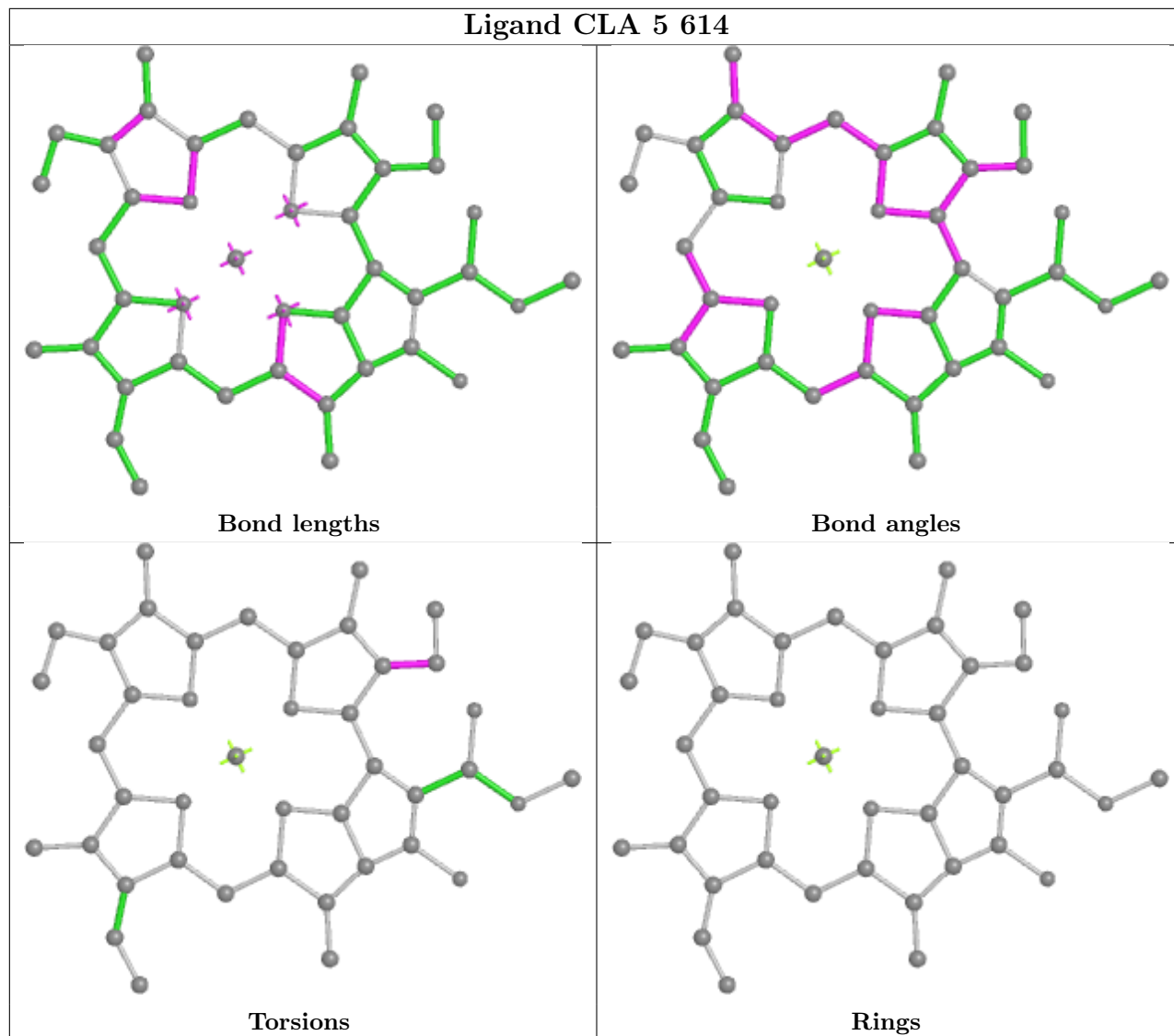


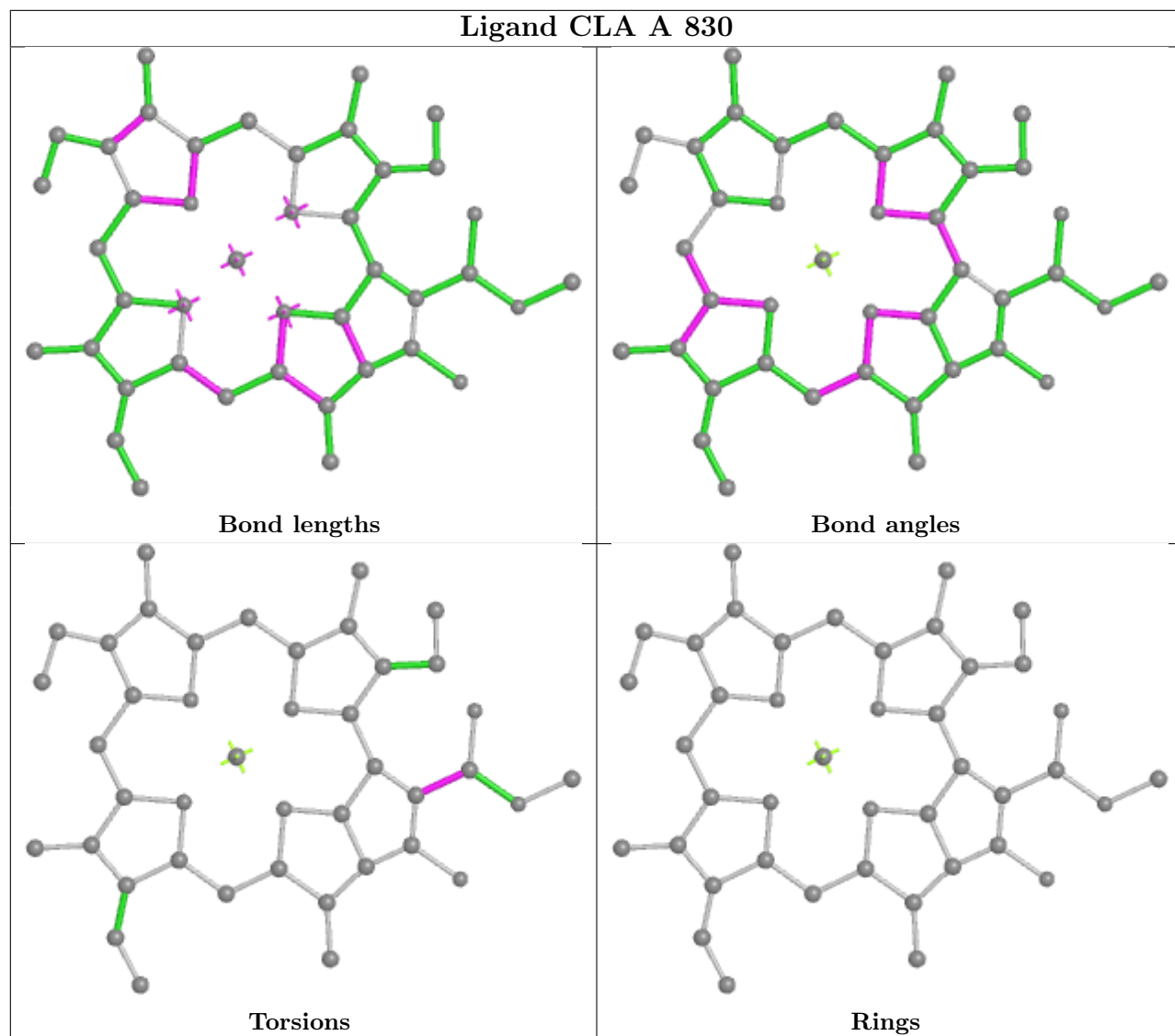


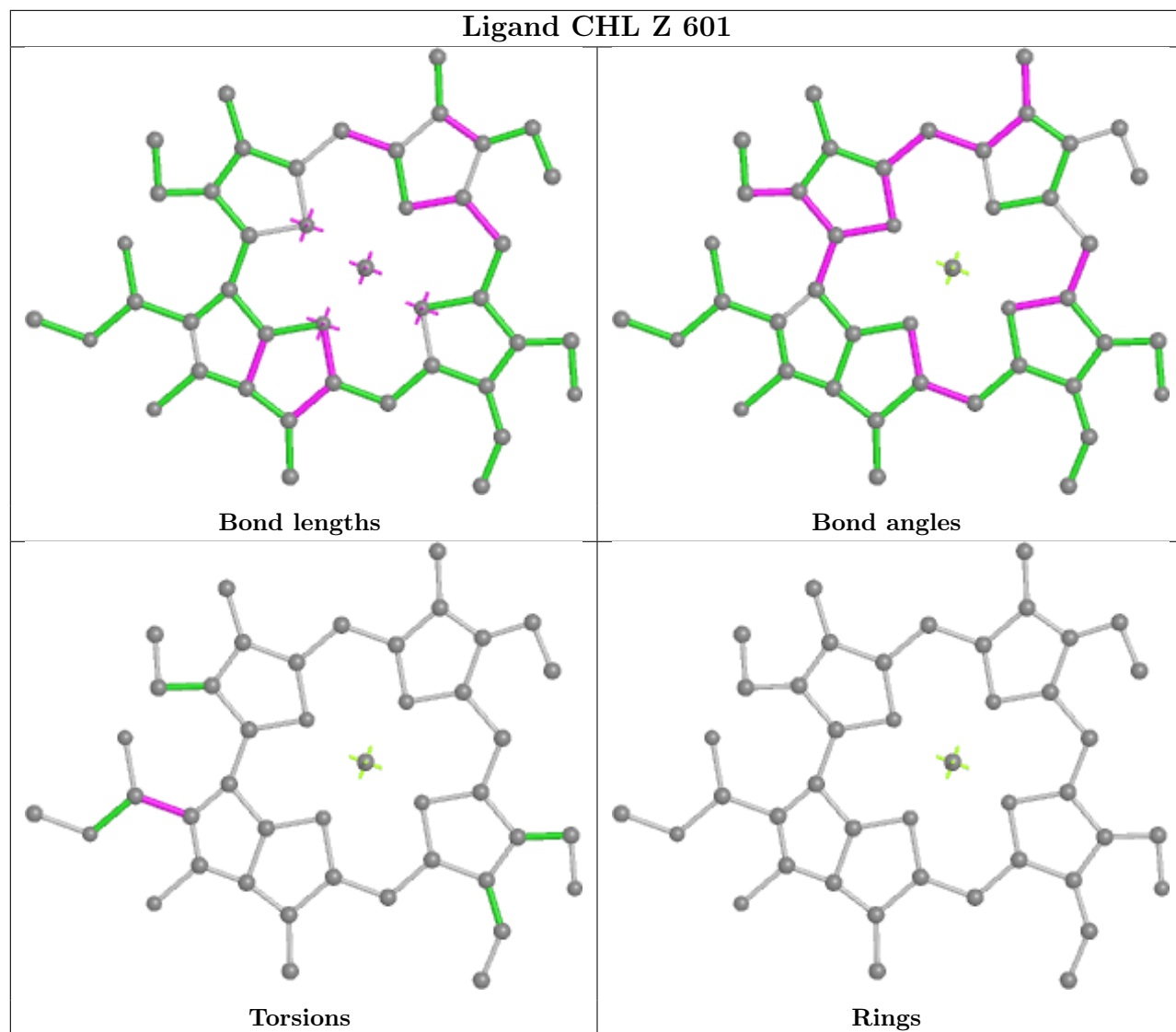


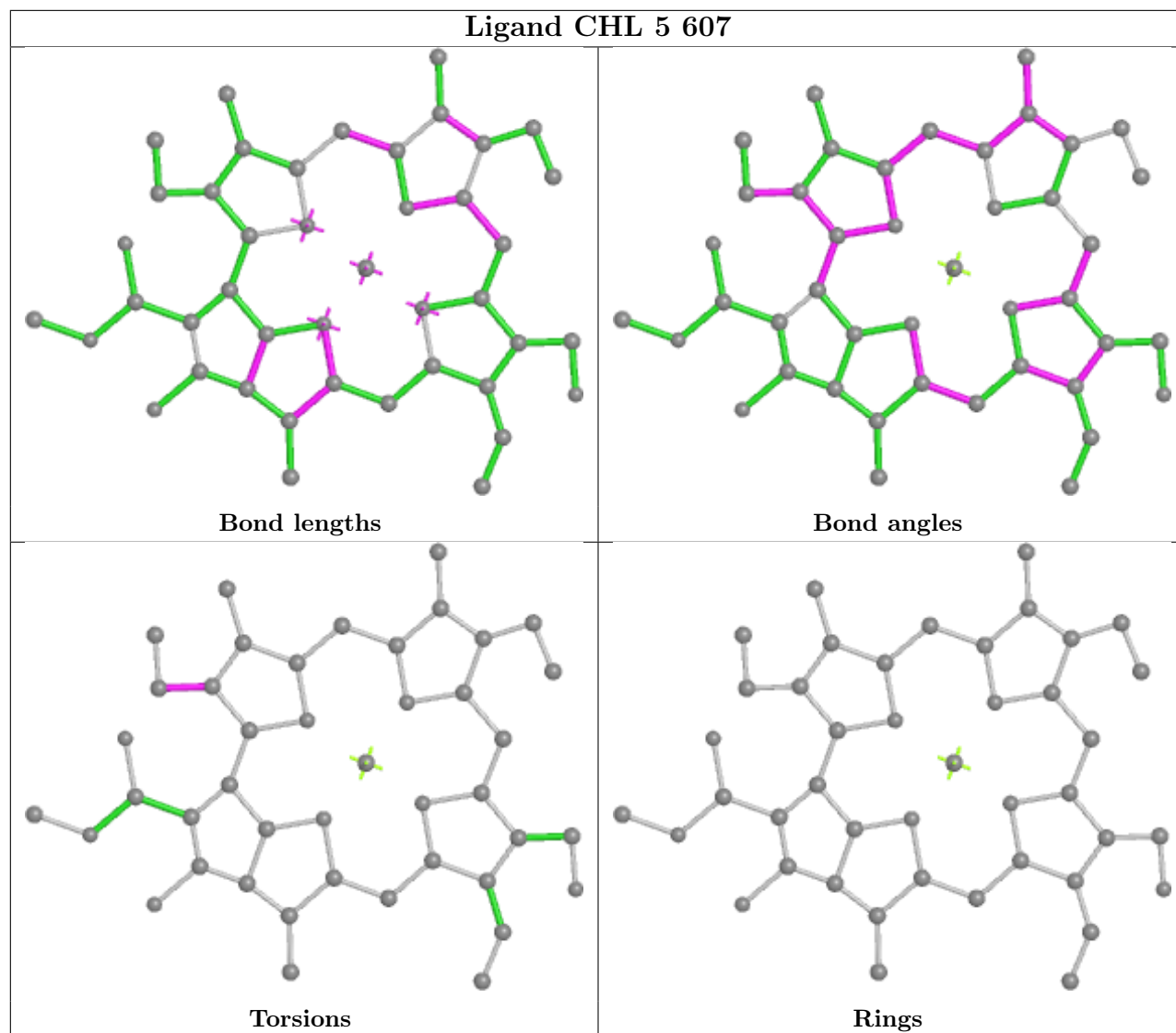


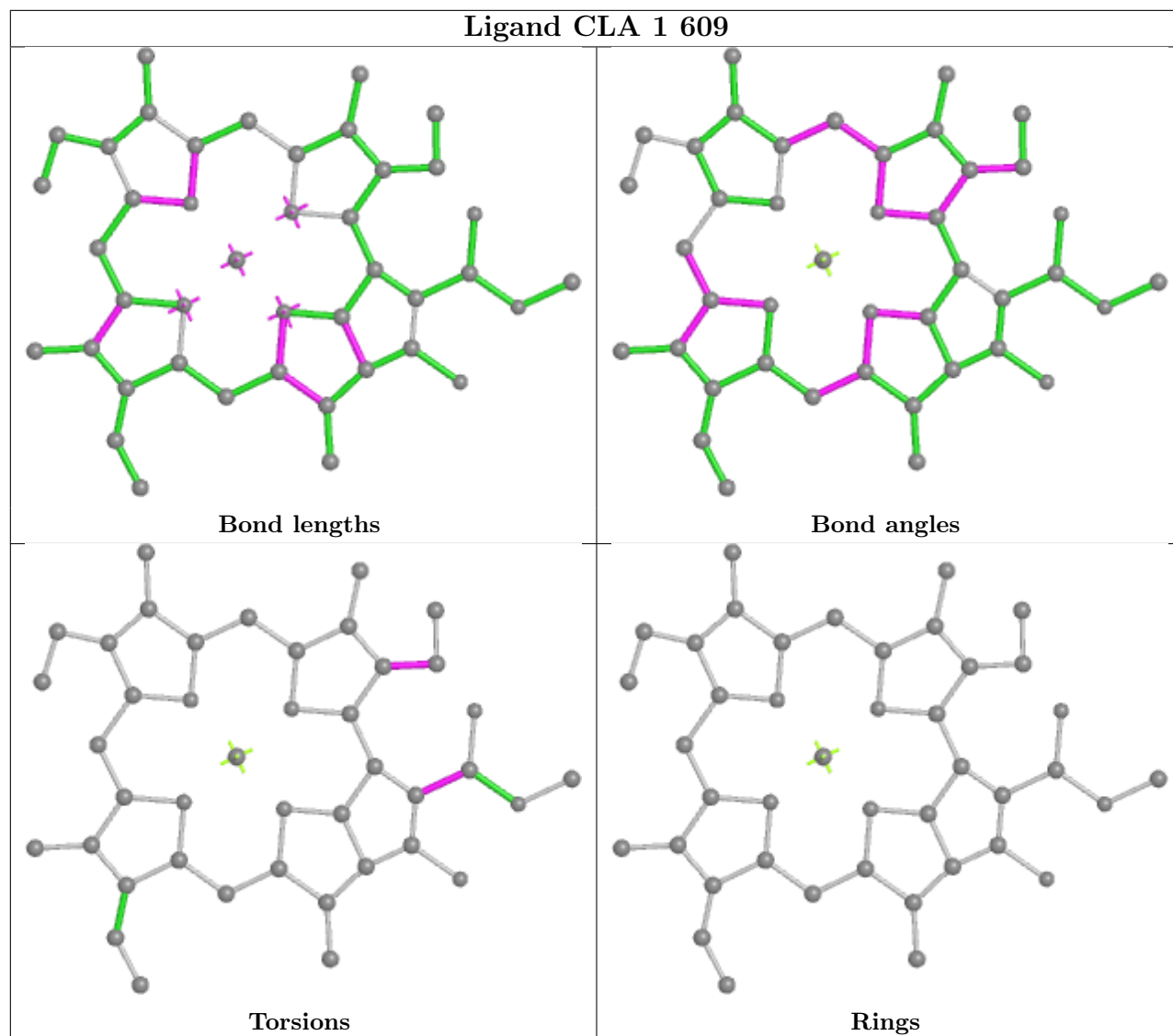
Ligand CLA 5 614

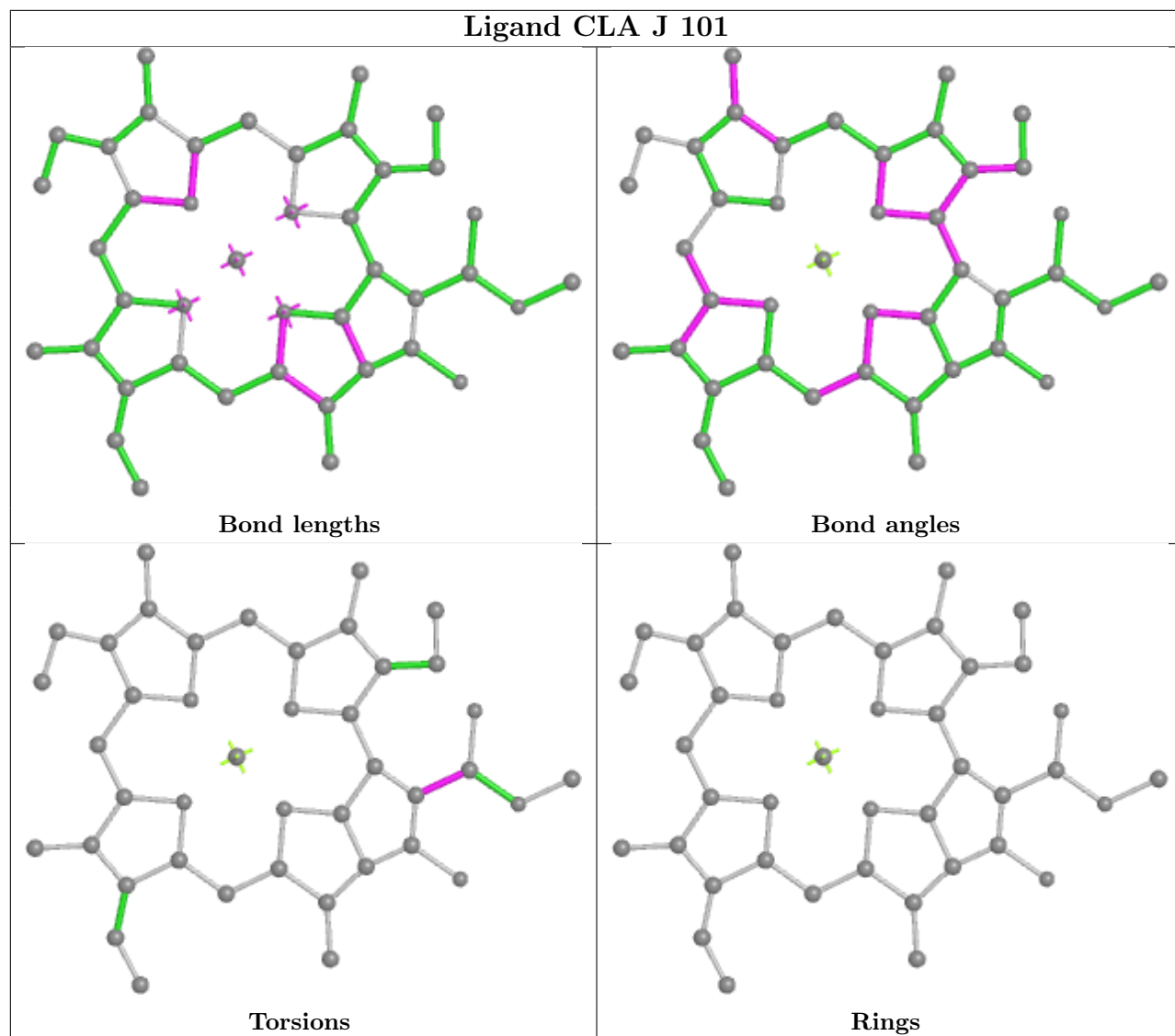




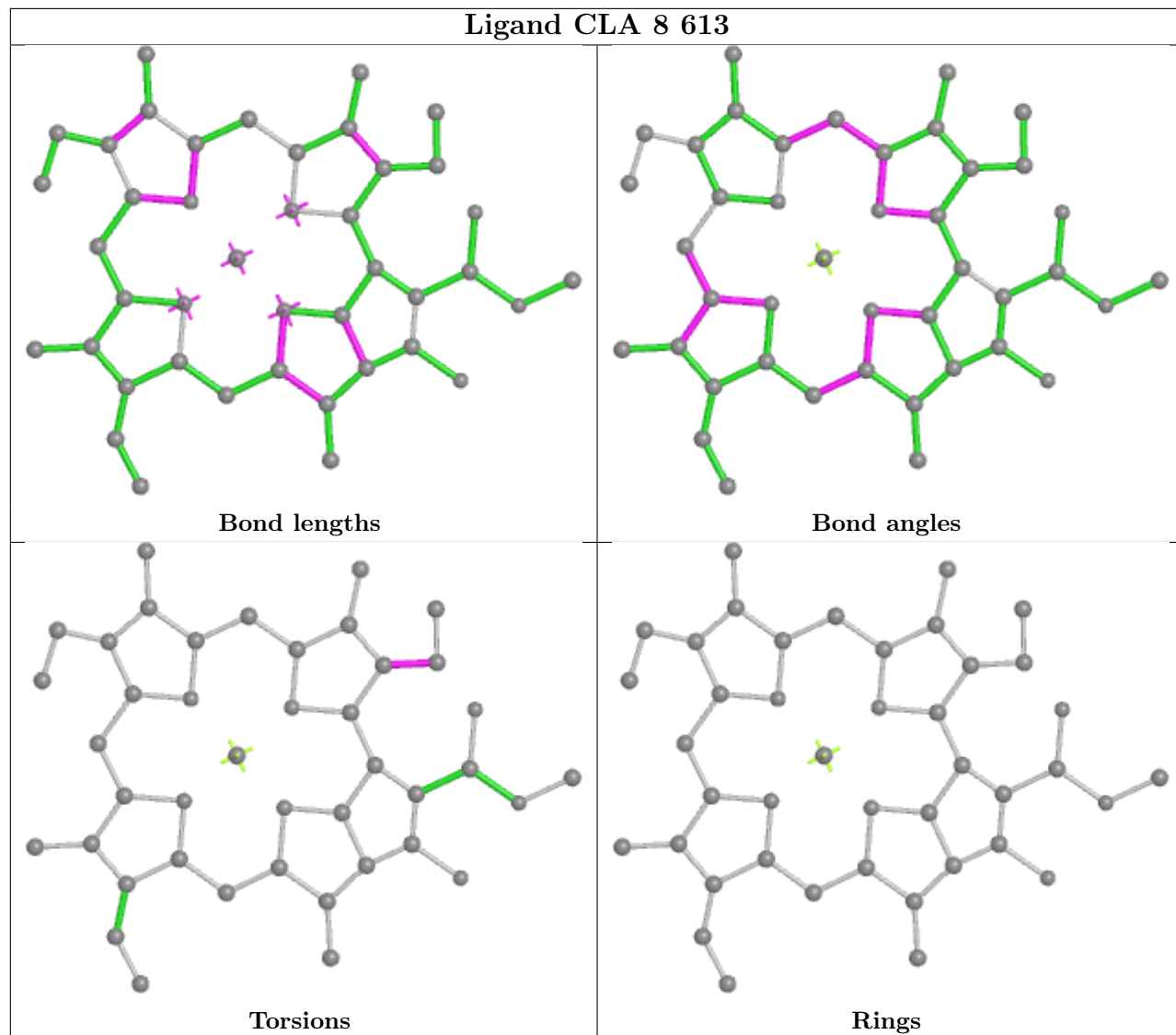


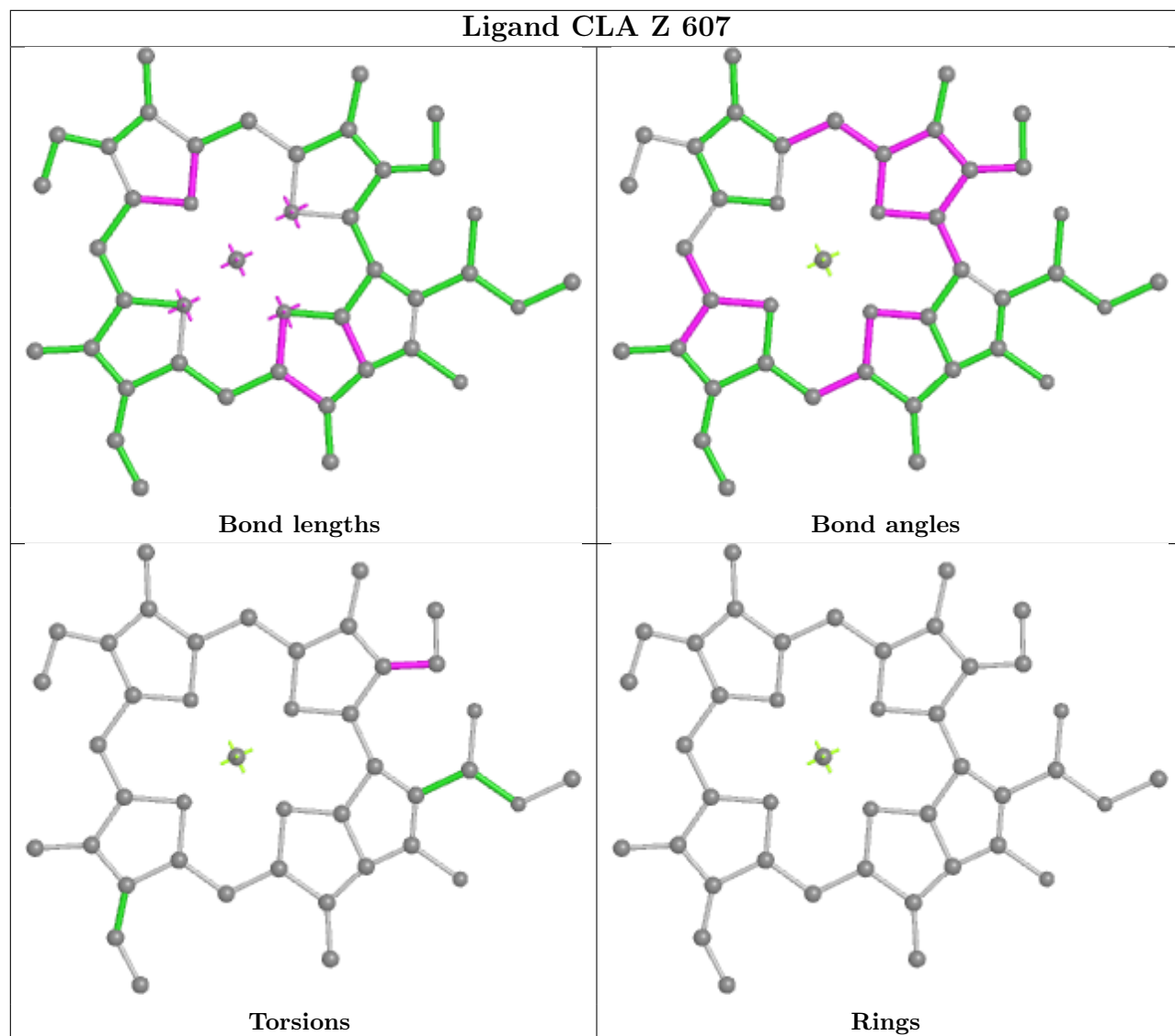


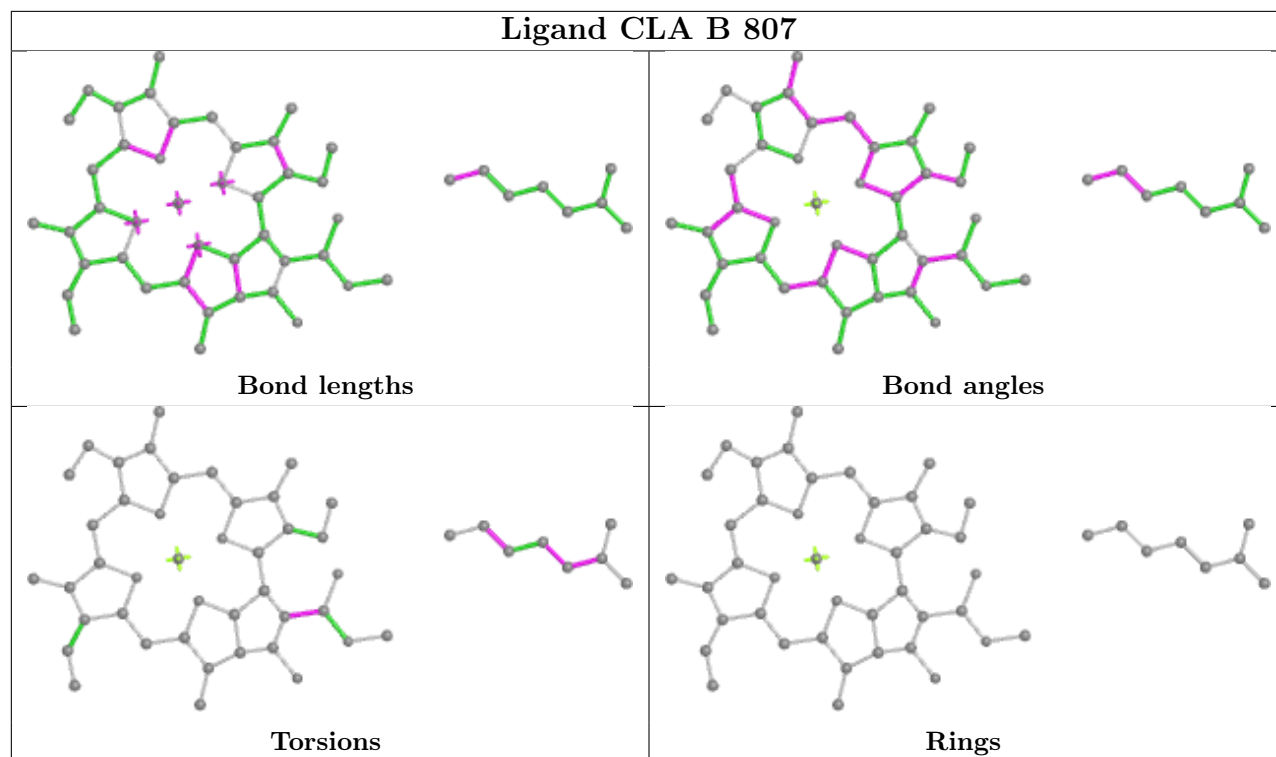


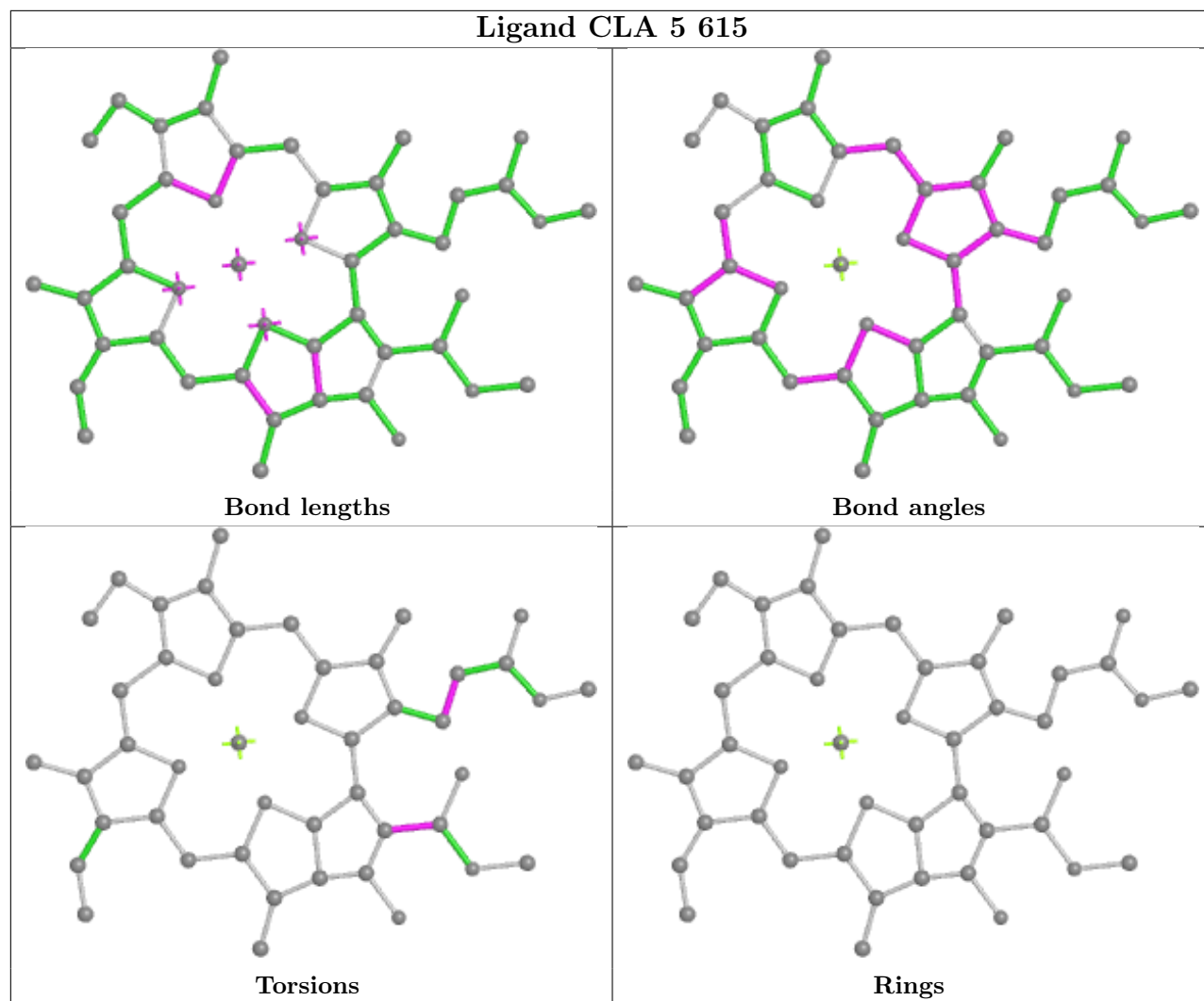


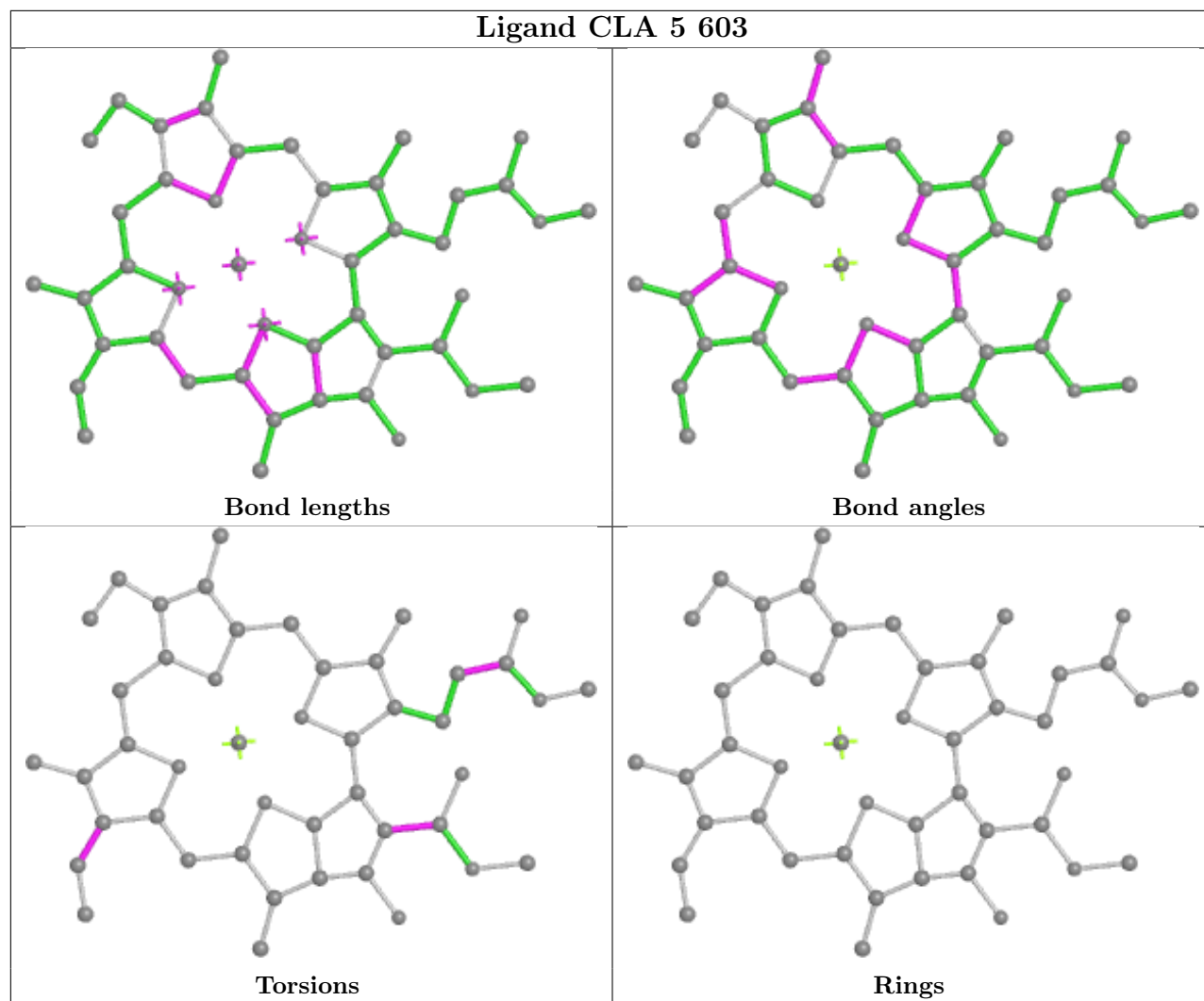
Ligand CLA 8 613

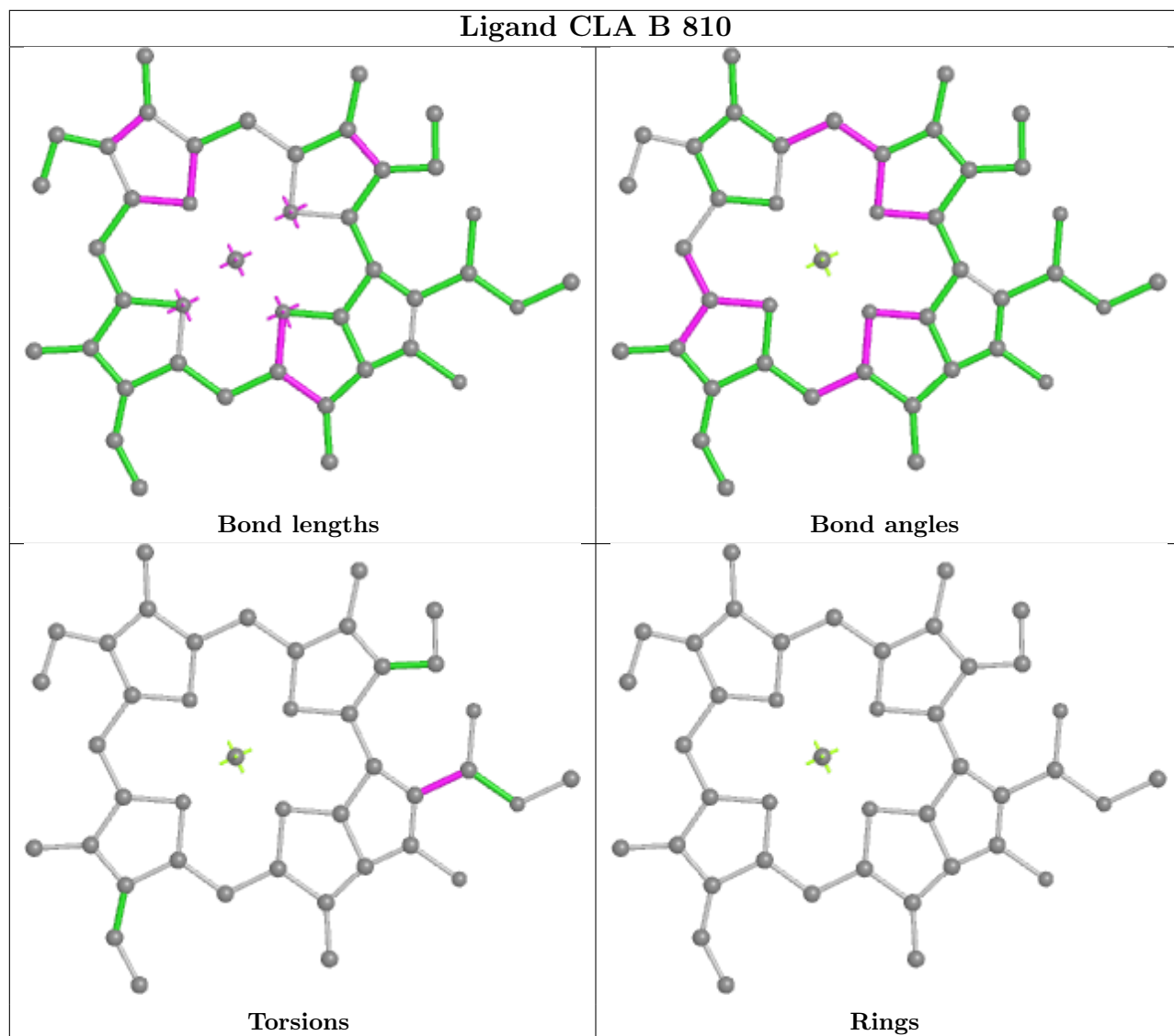


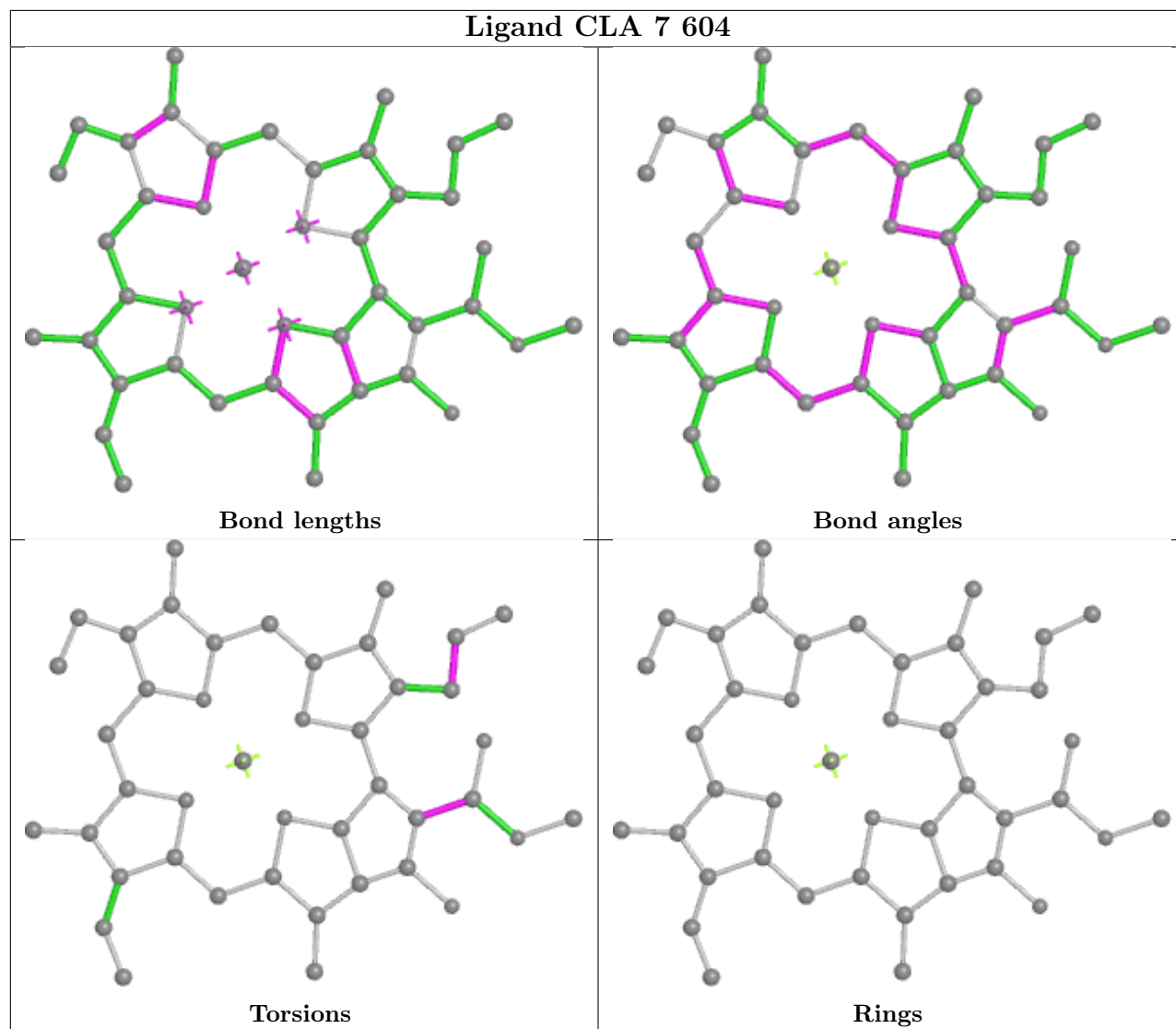


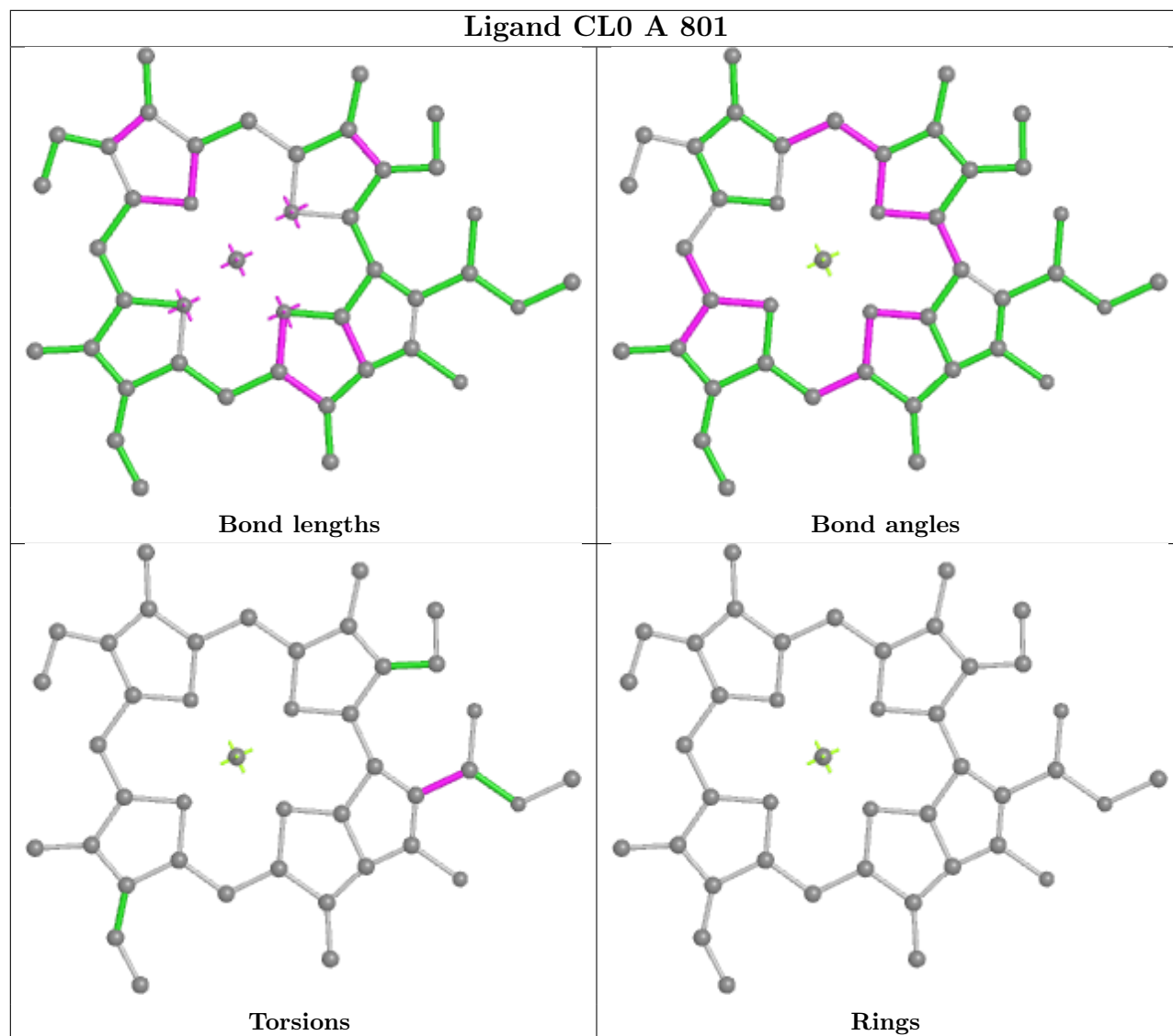




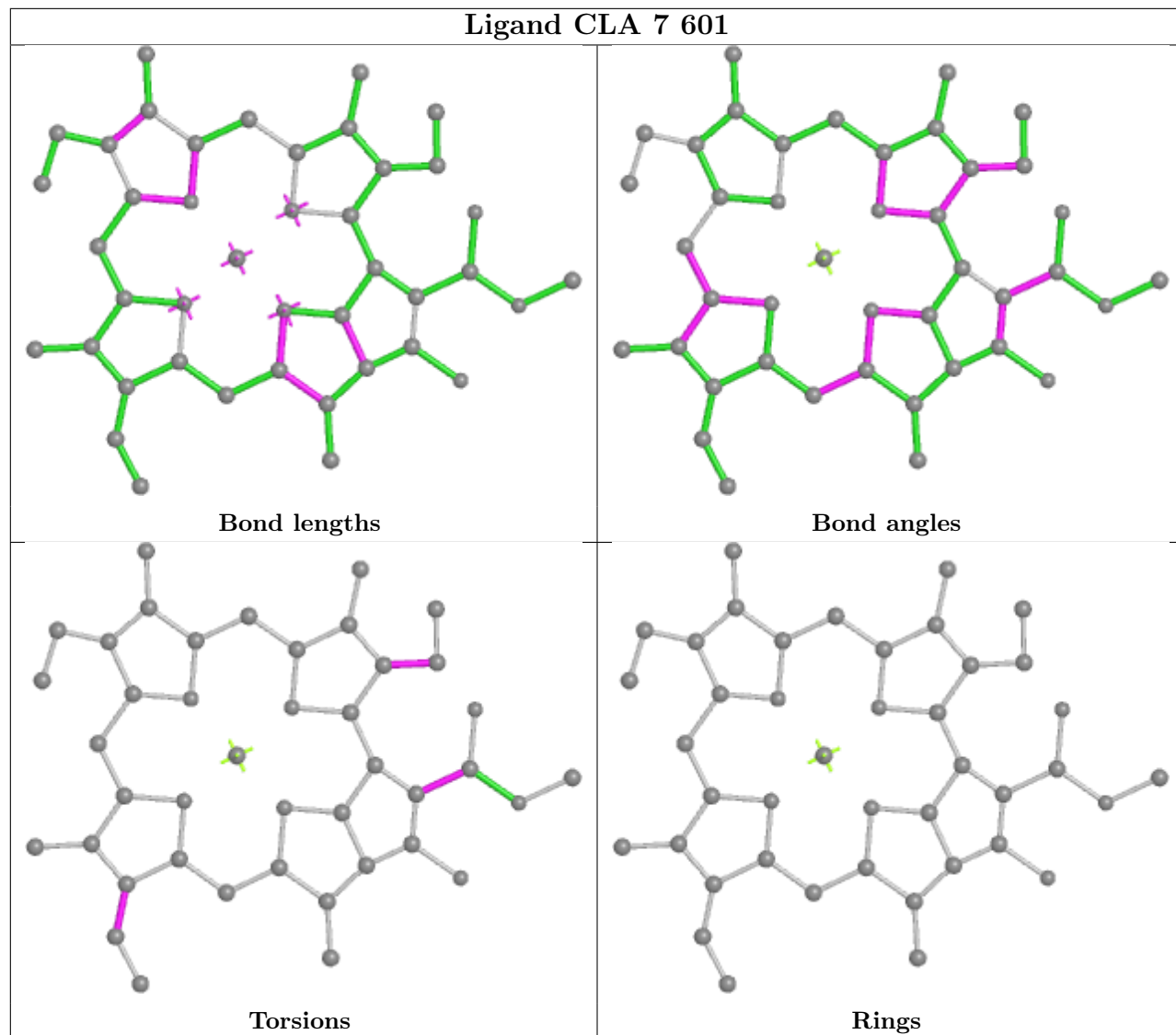


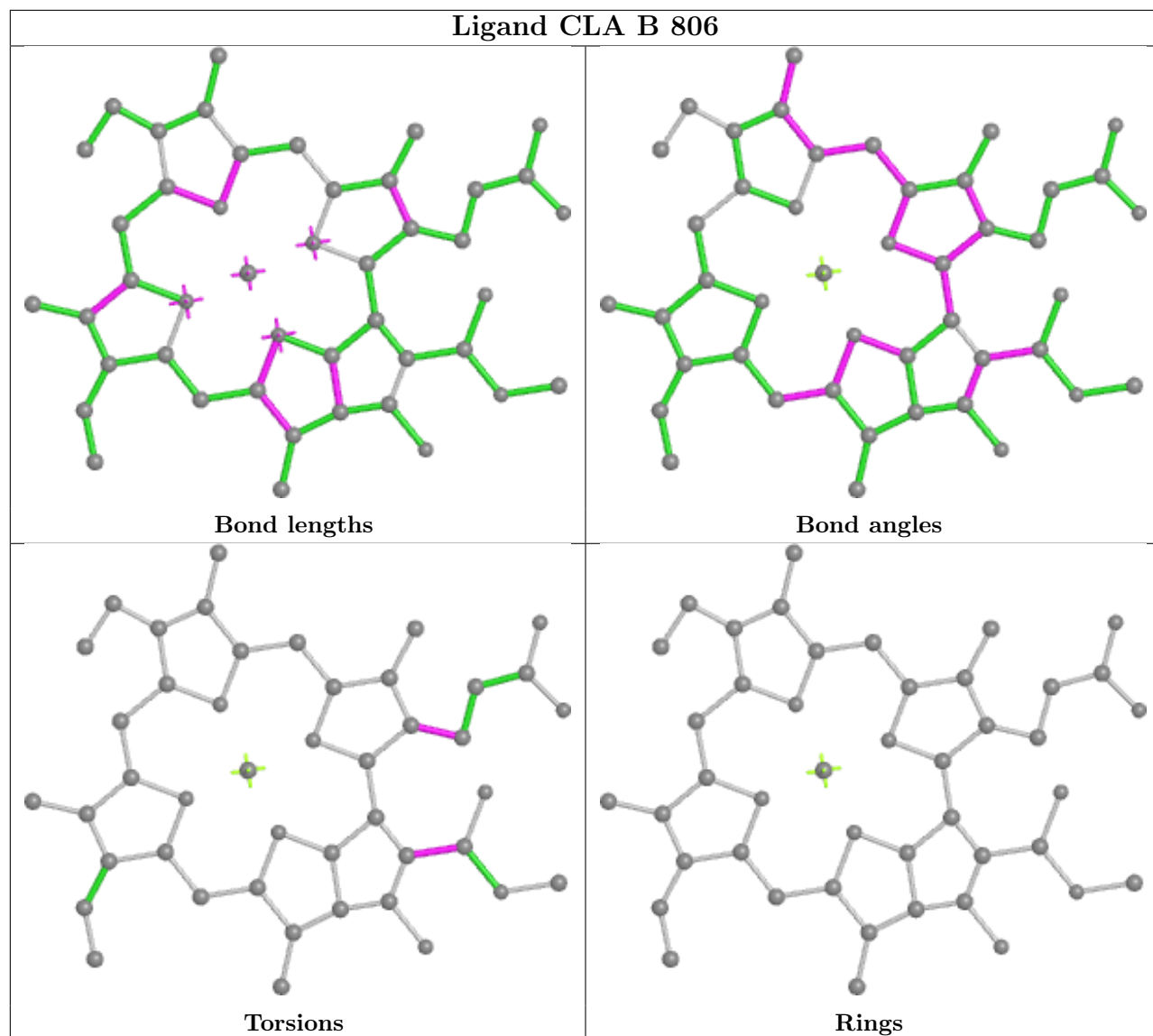




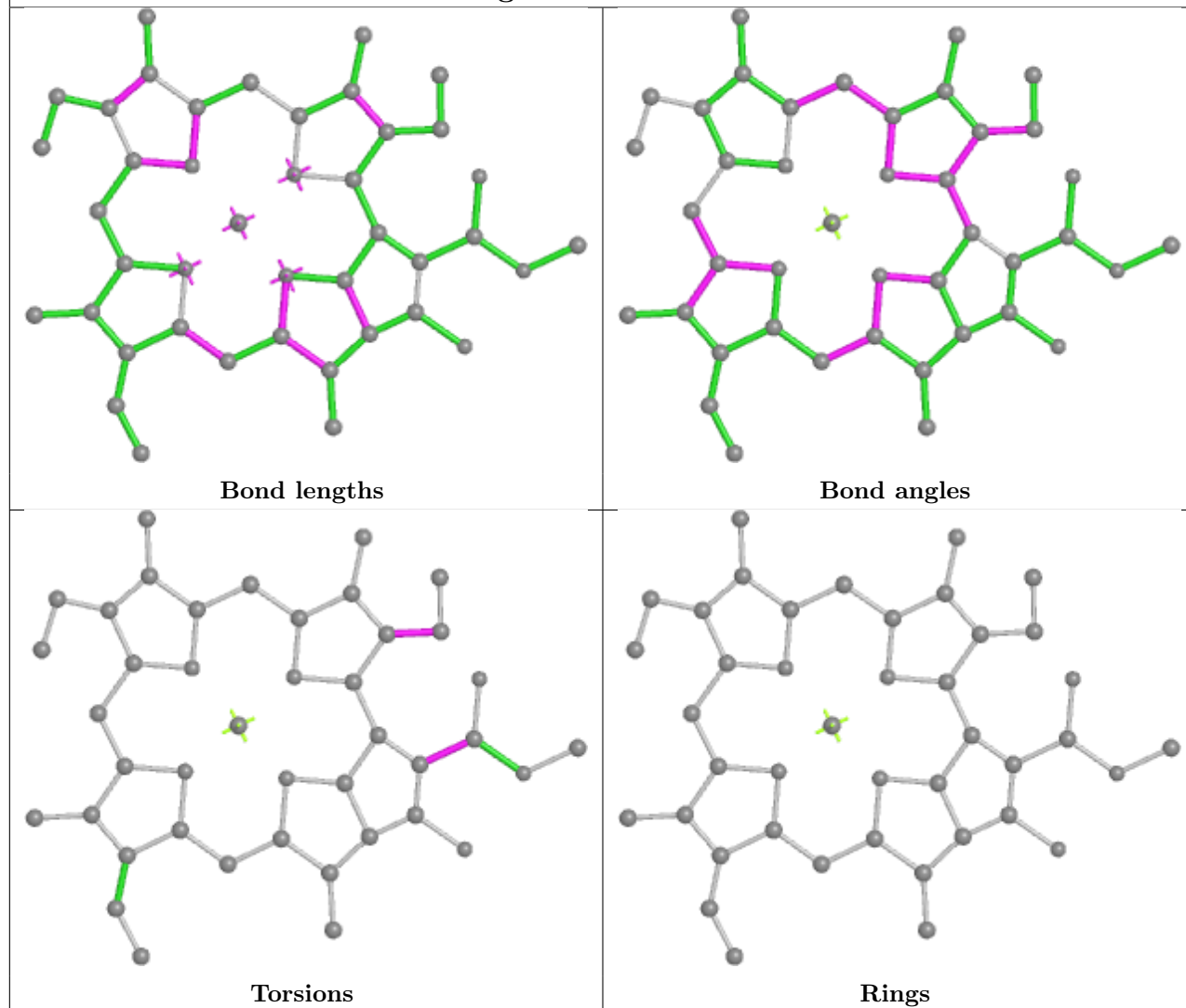


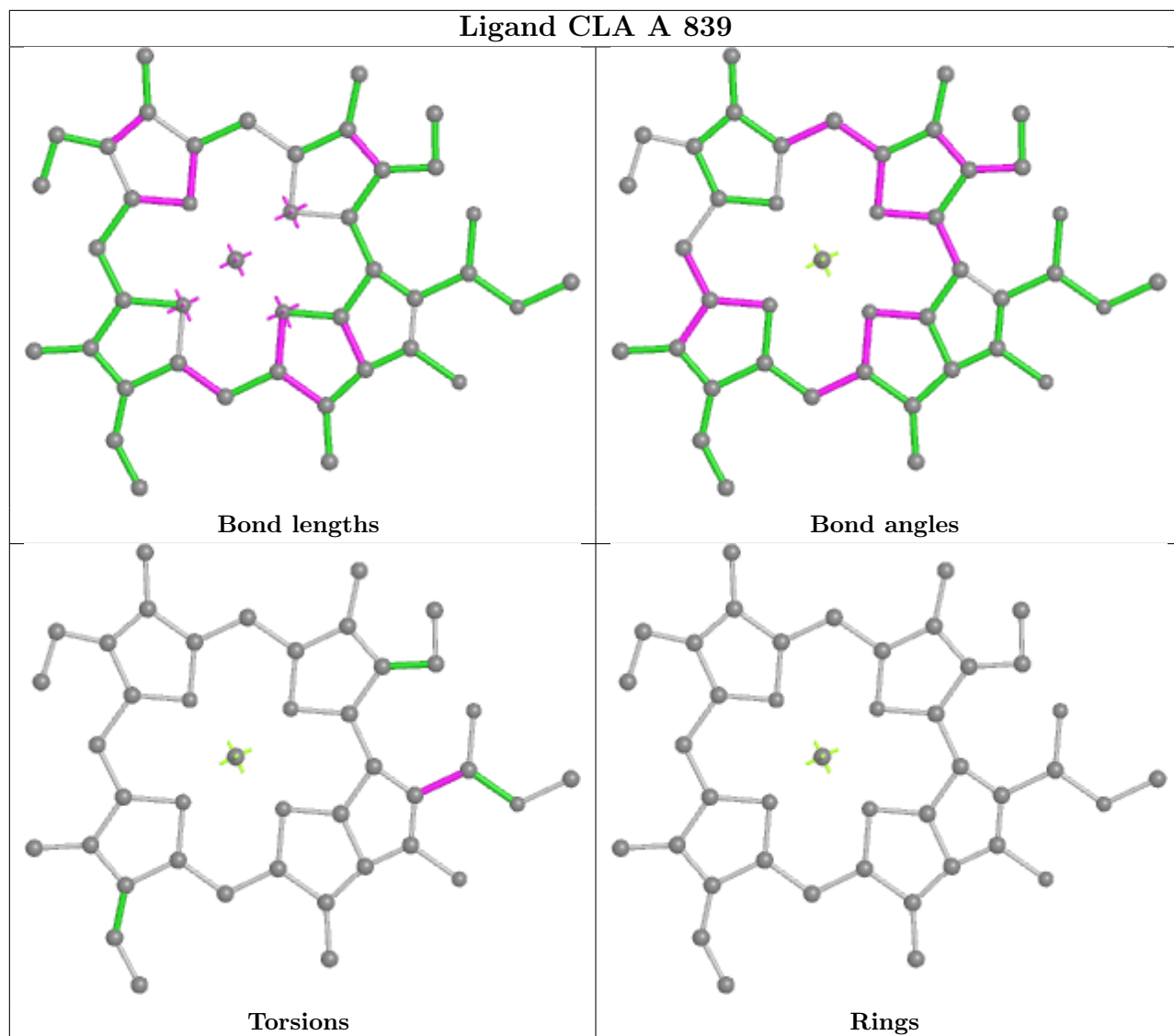
Ligand CLA 7 601

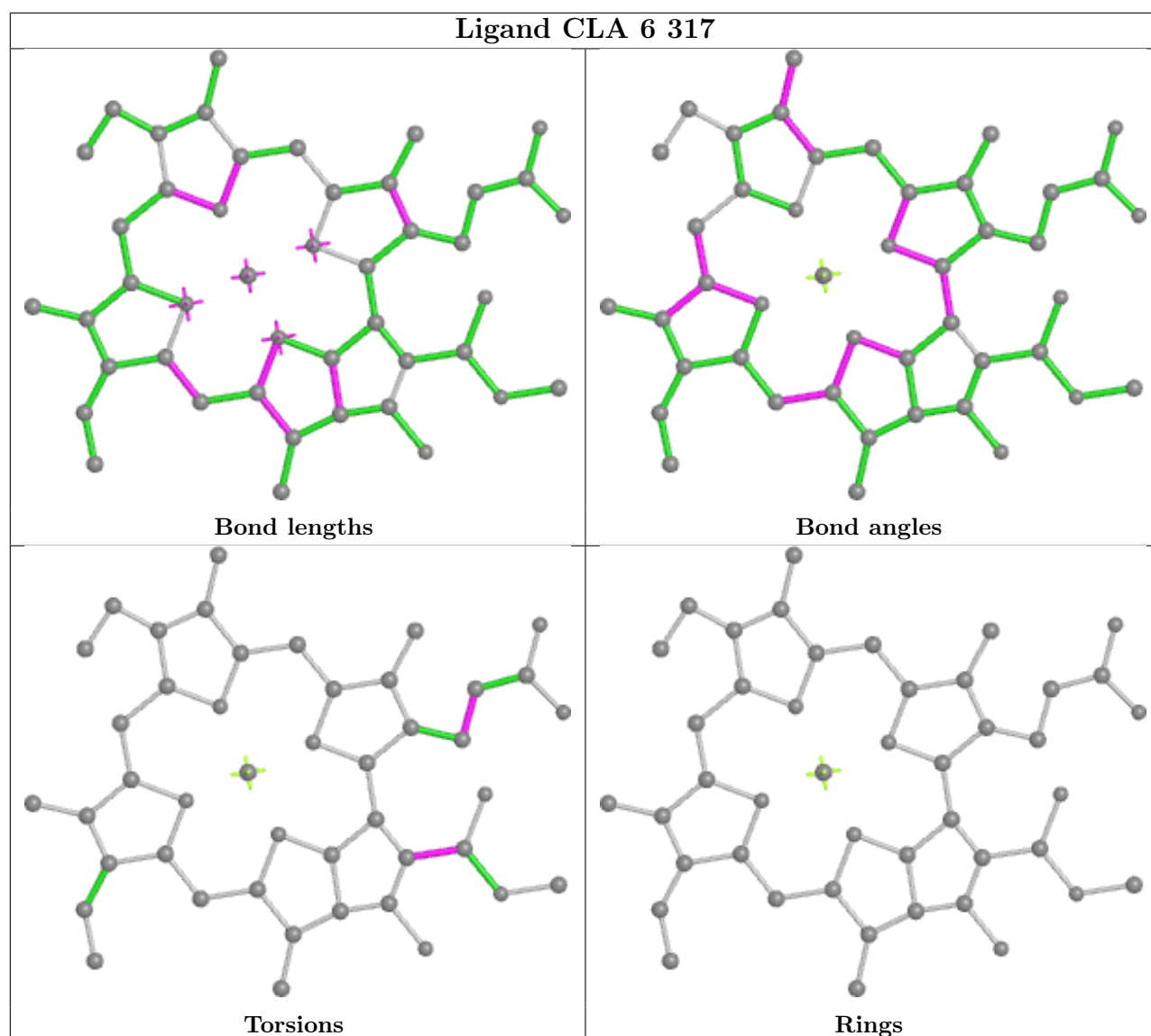




Ligand CLA 7 602







5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

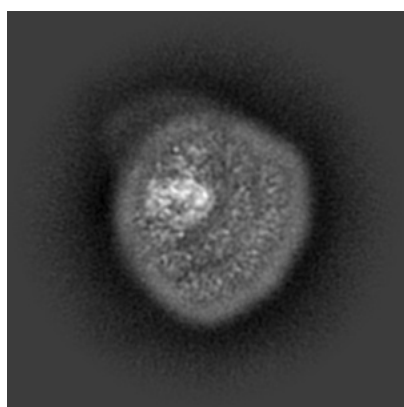
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32907. These allow visual inspection of the internal detail of the map and identification of artifacts.

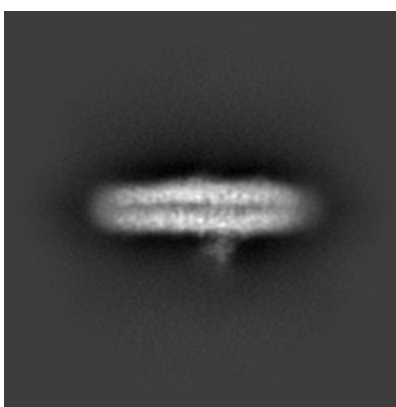
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

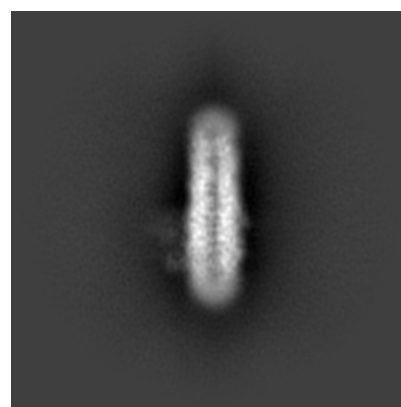
6.1.1 Primary map



X



Y

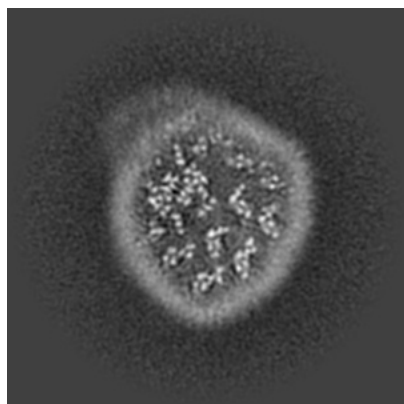


Z

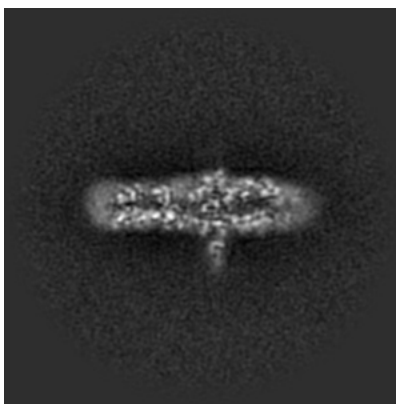
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

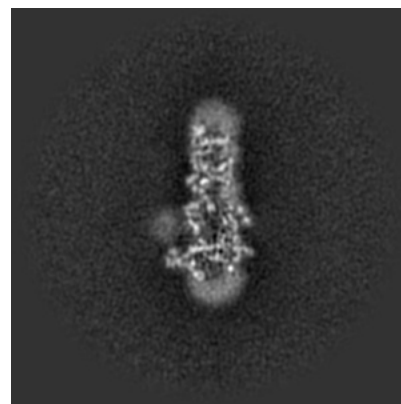
6.2.1 Primary map



X Index: 196



Y Index: 196

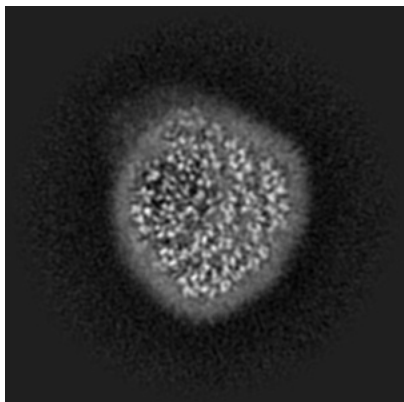


Z Index: 196

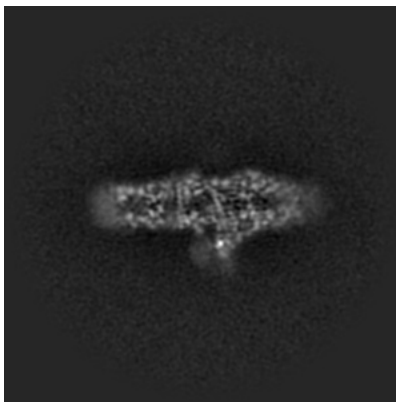
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

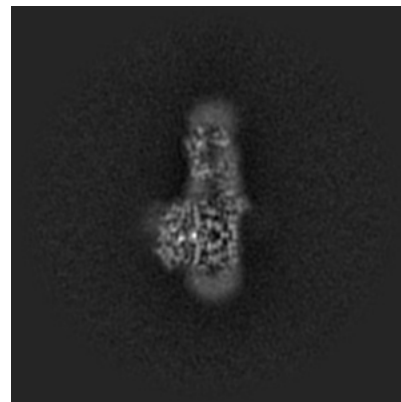
6.3.1 Primary map



X Index: 186



Y Index: 172

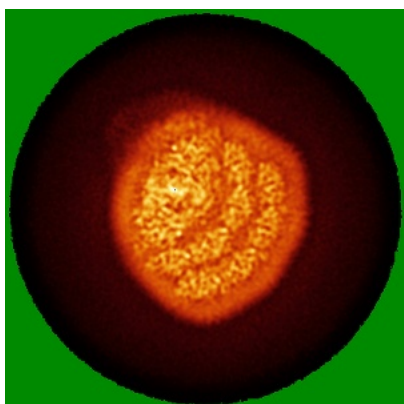


Z Index: 214

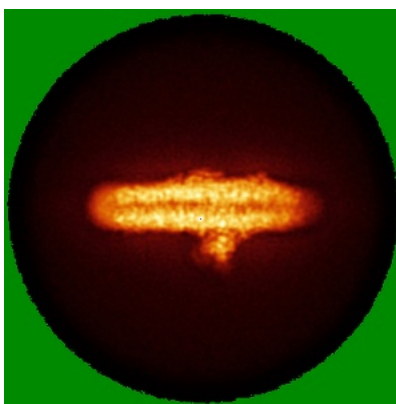
The images above show the largest variance slices of the map in three orthogonal directions.

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

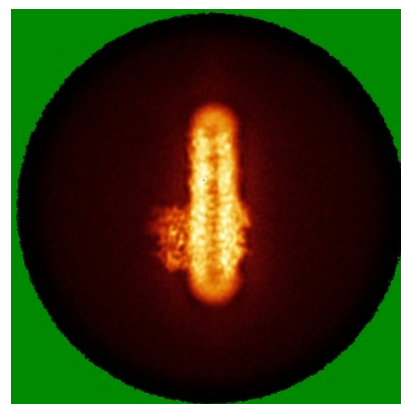
6.4.1 Primary map



X



Y

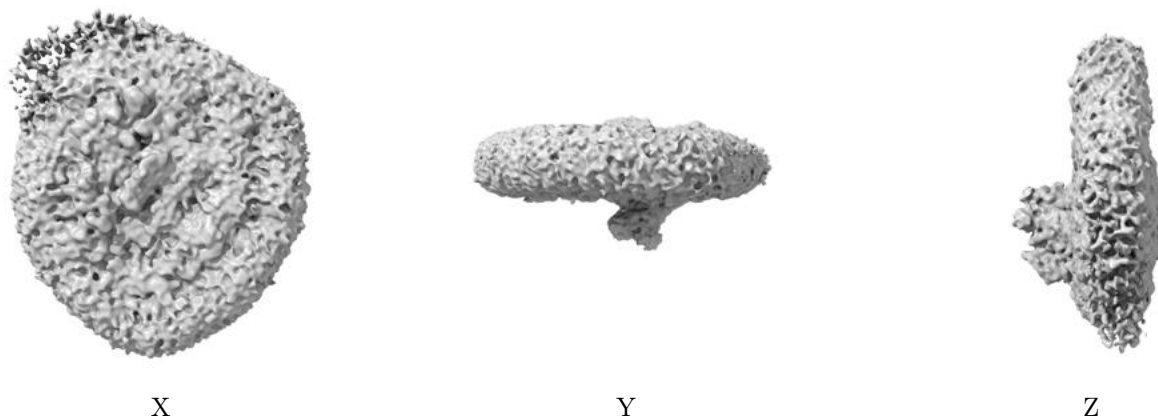


Z

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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

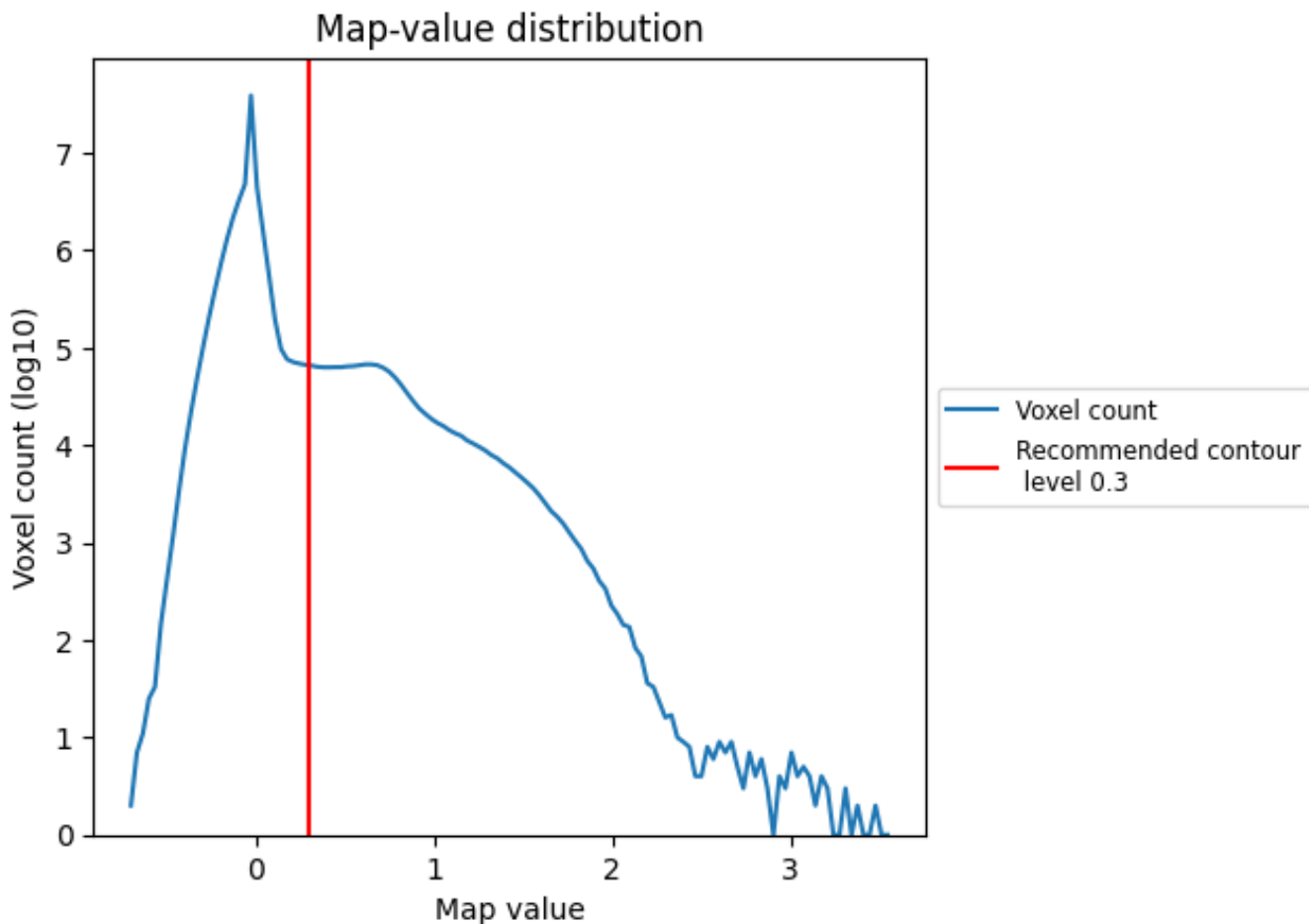
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

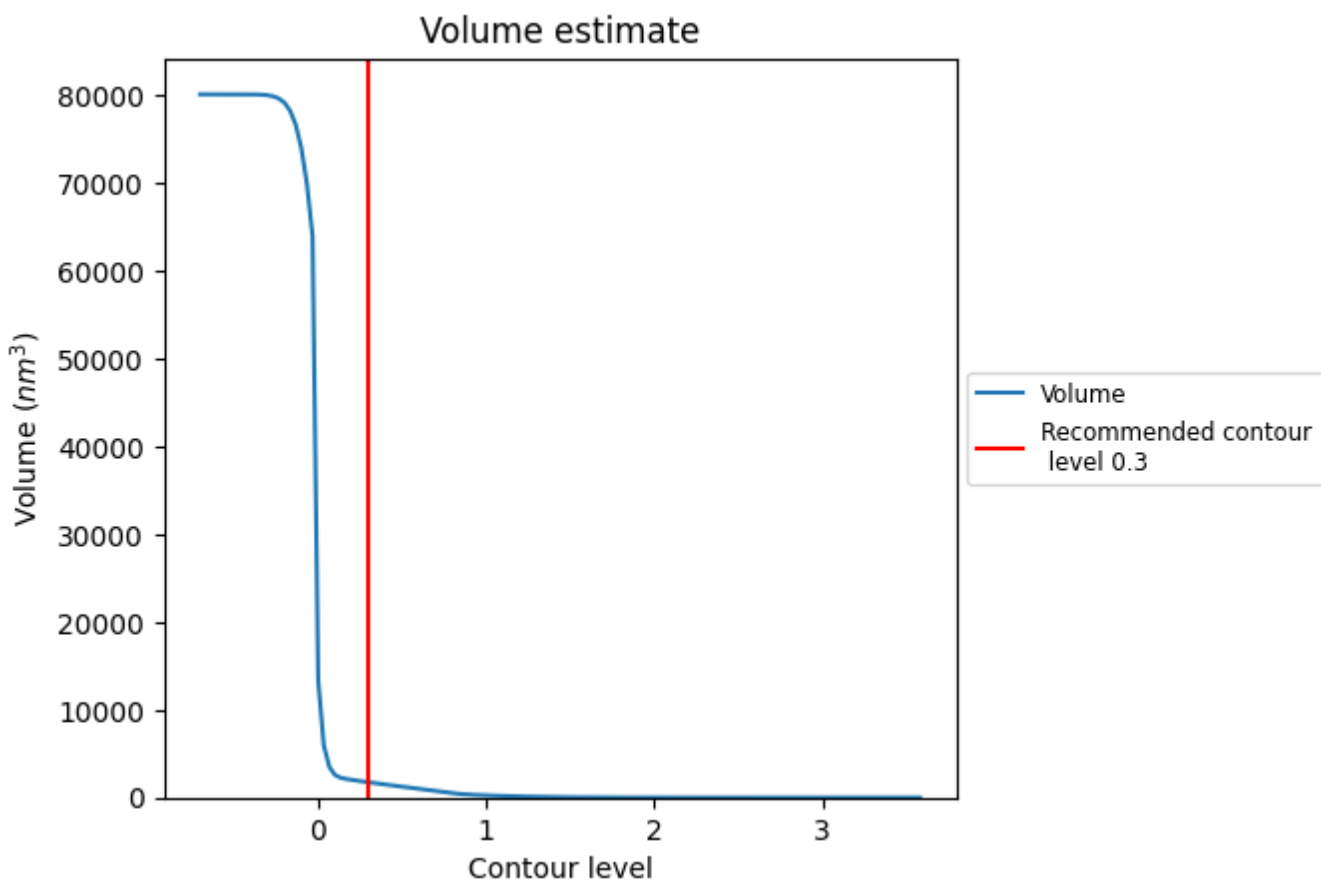
This section contains the results of statistical analysis of the map.

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.

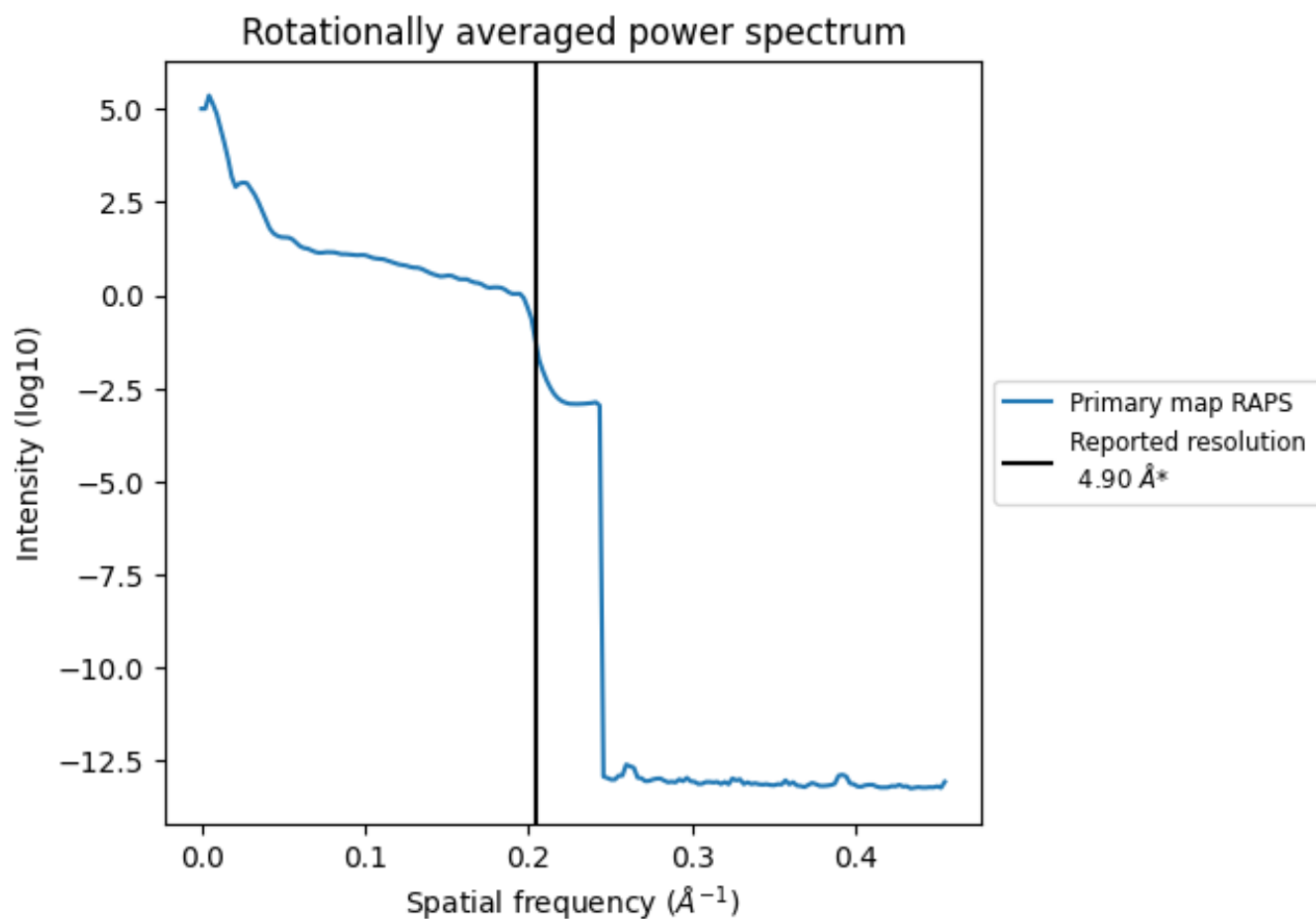
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1747 nm^3 ; this corresponds to an approximate mass of 1578 kDa.

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

7.3 Rotationally averaged power spectrum [\(i\)](#)

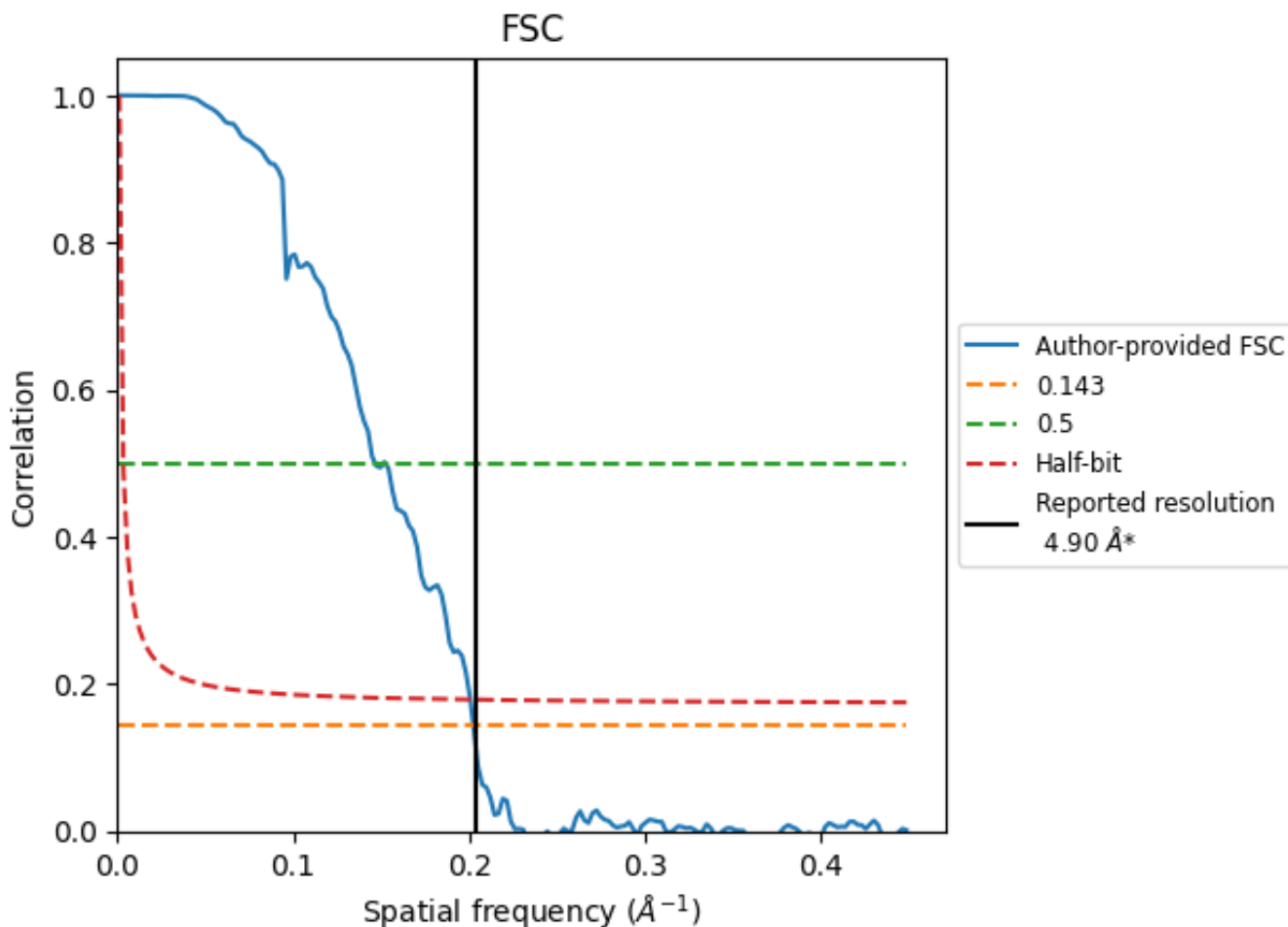


*Reported resolution corresponds to spatial frequency of 0.204 \AA^{-1}

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 0.204 Å⁻¹

8.2 Resolution estimates [i](#)

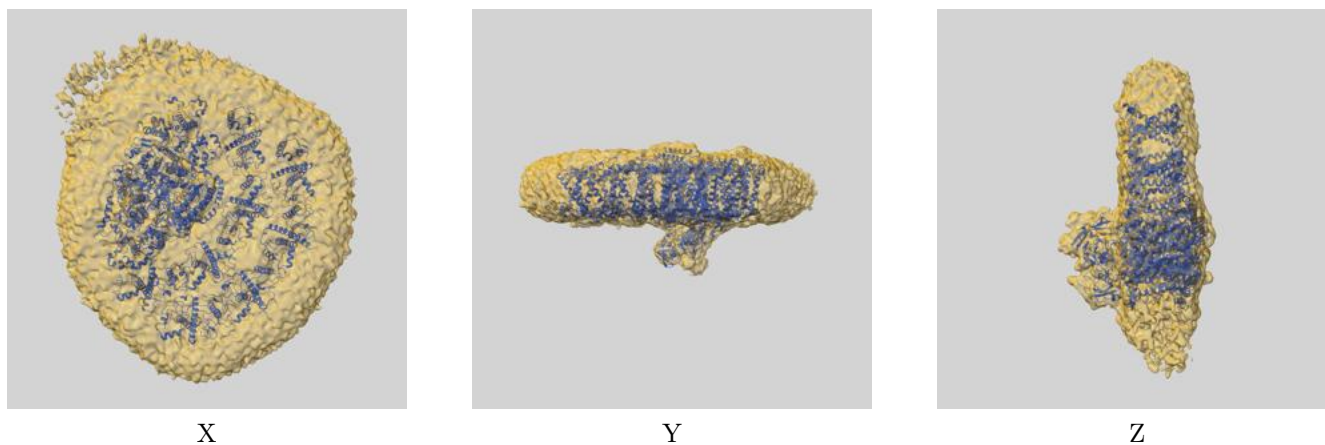
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	4.94	6.82	4.98
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32907 and PDB model 7WZN. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



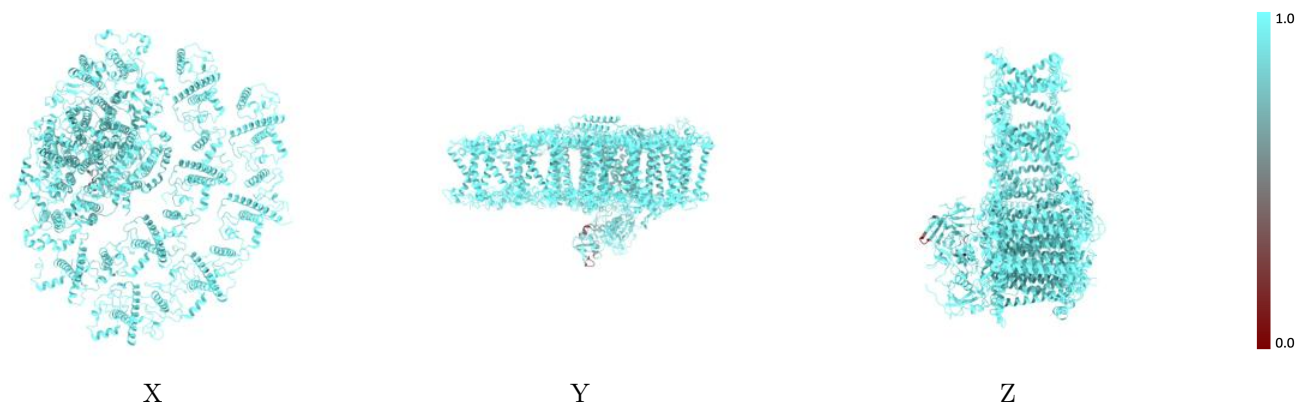
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



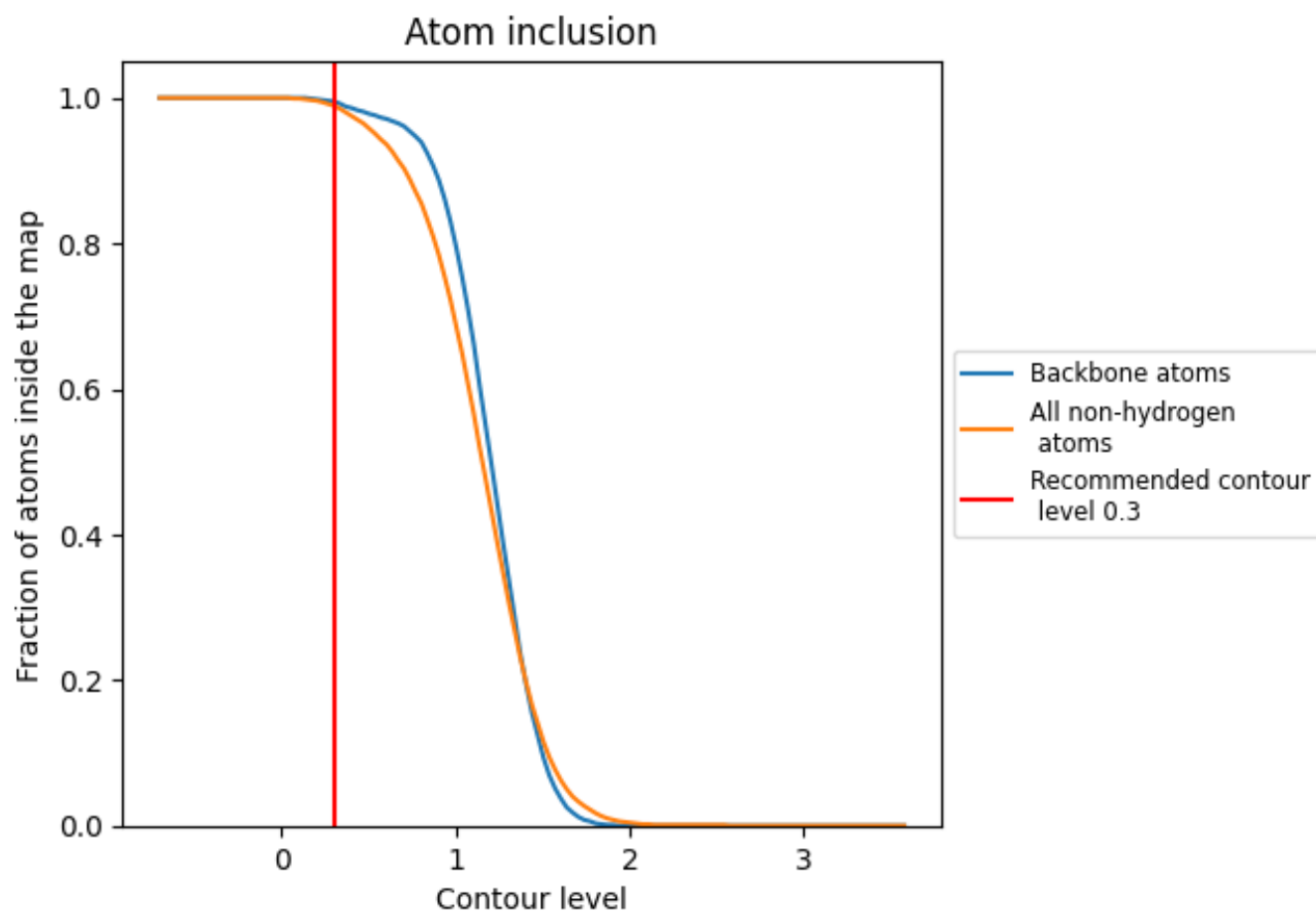
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9890	 0.2950
1	 0.9930	 0.2740
3	 0.9970	 0.3020
4	 0.9920	 0.2710
5	 0.9970	 0.2920
6	 0.9960	 0.2900
7	 0.9930	 0.3080
8	 0.9960	 0.2980
A	 0.9920	 0.3100
B	 0.9890	 0.2970
C	 1.0000	 0.3050
D	 1.0000	 0.3520
E	 1.0000	 0.3480
F	 0.9960	 0.2970
G	 0.7650	 0.1610
J	 1.0000	 0.2920
Z	 0.9990	 0.2560

