



# Full wwPDB EM Validation Report ⓘ

Nov 9, 2022 – 04:51 AM JST

PDB ID : 6IJJ  
EMDB ID : EMD-9678  
Title : Photosystem I of Chlamydomonas reinhardtii  
Authors : Pan, X.; Ma, J.; Su, X.; Liu, Z.; Zhang, X.; Li, M.  
Deposited on : 2018-10-10  
Resolution : 2.89 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

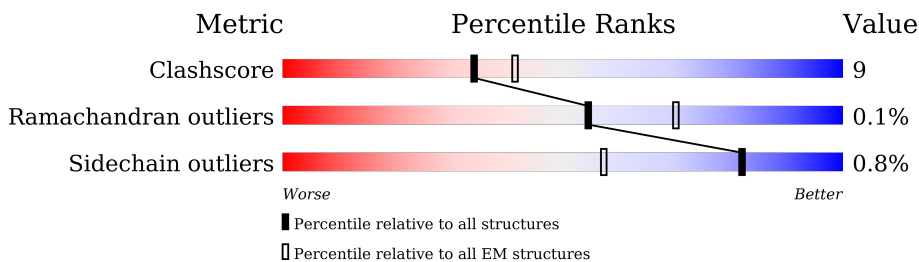
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.89 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  $\geq 3$ , 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	143	
6	F	227	
7	I	106	
8	J	41	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	K	160	
10	L	258	
11	1	248	
11	a	248	
12	3	298	
13	4	290	
14	5	274	
15	6	318	
16	7	241	
17	8	272	

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
18	CLA	1	601	X	-	-	-
18	CLA	1	602	X	-	-	-
18	CLA	1	603	X	-	-	-
18	CLA	1	604	X	-	-	-
18	CLA	1	606	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	1	616	X	-	-	-
18	CLA	3	602	X	-	-	-
18	CLA	3	603	X	-	-	-
18	CLA	3	604	X	-	-	-
18	CLA	3	606	X	-	-	-
18	CLA	3	607	X	-	-	-
18	CLA	3	608	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	3	609	X	-	-	-
18	CLA	3	610	X	-	-	-
18	CLA	3	611	X	-	-	-
18	CLA	3	612	X	-	-	-
18	CLA	3	613	X	-	-	-
18	CLA	3	614	X	-	-	-
18	CLA	3	615	X	-	-	-
18	CLA	3	617	X	-	-	-
18	CLA	4	602	X	-	-	-
18	CLA	4	603	X	-	-	-
18	CLA	4	604	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	613	X	-	-	-
18	CLA	4	614	X	-	-	-
18	CLA	4	616	X	-	-	-
18	CLA	4	618	X	-	-	-
18	CLA	5	601	X	-	-	-
18	CLA	5	602	X	-	-	-
18	CLA	5	603	X	-	-	-
18	CLA	5	604	X	-	-	-
18	CLA	5	606	X	-	-	-
18	CLA	5	607	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	616	X	-	-	-
18	CLA	5	617	X	-	-	-
18	CLA	5	618	X	-	-	-
18	CLA	6	601	X	-	-	-
18	CLA	6	602	X	-	-	-
18	CLA	6	603	X	-	-	-
18	CLA	6	604	X	-	-	-
18	CLA	6	606	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	6	607	X	-	-	-
18	CLA	6	608	X	-	-	-
18	CLA	6	609	X	-	-	-
18	CLA	6	610	X	-	-	-
18	CLA	6	611	X	-	-	-
18	CLA	6	612	X	-	-	-
18	CLA	6	613	X	-	-	-
18	CLA	6	614	X	-	-	-
18	CLA	6	616	X	-	-	-
18	CLA	6	617	X	-	-	-
18	CLA	6	618	X	-	-	-
18	CLA	6	620	X	-	-	-
18	CLA	7	602	X	-	-	-
18	CLA	7	603	X	-	-	-
18	CLA	7	604	X	-	-	-
18	CLA	7	606	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	613	X	-	-	-
18	CLA	7	614	X	-	-	-
18	CLA	7	615	X	-	-	-
18	CLA	7	616	X	-	-	-
18	CLA	8	601	X	-	-	-
18	CLA	8	602	X	-	-	-
18	CLA	8	603	X	-	-	-
18	CLA	8	604	X	-	-	-
18	CLA	8	606	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	613	X	-	-	-
18	CLA	8	614	X	-	-	-
18	CLA	A	801	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	842	X	-	-	-
18	CLA	A	843	X	-	-	-
18	CLA	A	845	X	-	-	-
18	CLA	A	854	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	F	301	X	-	-	-
18	CLA	F	304	X	-	-	-
18	CLA	J	101	X	-	-	-
18	CLA	K	201	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	K	203	X	-	-	-
18	CLA	K	204	X	-	-	-
18	CLA	K	206	X	-	-	-
18	CLA	L	302	X	-	-	-
18	CLA	L	303	X	-	-	-
18	CLA	L	304	X	-	-	-
18	CLA	a	601	X	-	-	-
18	CLA	a	602	X	-	-	-
18	CLA	a	603	X	-	-	-
18	CLA	a	604	X	-	-	-
18	CLA	a	606	X	-	-	-
18	CLA	a	607	X	-	-	-
18	CLA	a	608	X	-	-	-
18	CLA	a	609	X	-	-	-
18	CLA	a	610	X	-	-	-
18	CLA	a	611	X	-	-	-
18	CLA	a	612	X	-	-	-
18	CLA	a	613	X	-	-	-
18	CLA	a	614	X	-	-	-
18	CLA	a	616	X	-	-	-

## 2 Entry composition i

There are 28 unique types of molecules in this entry. The entry contains 44968 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	5819	3805	993	999	22	0	0

- Molecule 2 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	731	5812	3818	975	1001	18	0	0

- Molecule 3 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	600	369	103	116	12	0	0

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	144	1129	722	200	200	7	0	0

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	64	505	322	89	94	0	0

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	164	1254	811	209	231	3	0	0

- Molecule 7 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	32	242	166	34	41	1	0	0

- Molecule 8 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	41	337	231	47	58	1	0	0

- Molecule 9 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	85	578	368	99	109	2	0	0

- Molecule 10 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	105	761	502	122	135	2	0	0

- Molecule 11 is a protein called Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	1	193	1433	932	239	259	3	0	0
11	a	194	1444	941	240	260	3	0	0

- Molecule 12 is a protein called Lhca3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	3	221	1683	1099	271	305	8	0	0

- Molecule 13 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	4	210	1631	1071	263	292	5	0	0

- Molecule 14 is a protein called Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	5	226	1765	1149	295	313	8	0	0

- Molecule 15 is a protein called Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	6	230	1771	1167	293	305	6	0	0

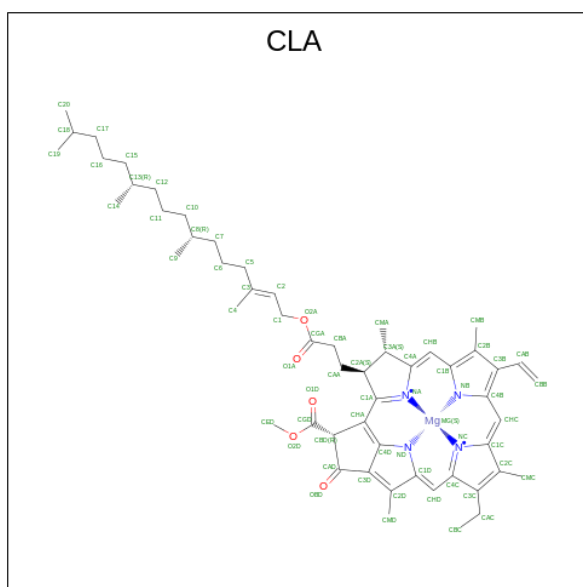
- Molecule 16 is a protein called Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	7	213	1649	1072	274	297	6	0	0

- Molecule 17 is a protein called Lhca8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	8	215	1630	1058	278	290	4	0	0

- Molecule 18 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0

Continued on next page...





*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	A	1	Total 2625	C 2181	Mg 45	N 180	O 219	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0
18	B	1	Total 2277	C 1888	Mg 40	N 160	O 189	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0
18	B	1	2277	1888	40	160	189	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
18	F	1	Total	C	Mg	N	O	0
			140	114	3	12	11	
18	F	1	Total	C	Mg	N	O	0
			140	114	3	12	11	
18	F	1	Total	C	Mg	N	O	0
			140	114	3	12	11	
18	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	K	1	Total	C	Mg	N	O	0
			201	161	4	16	20	
18	K	1	Total	C	Mg	N	O	0
			201	161	4	16	20	
18	K	1	Total	C	Mg	N	O	0
			201	161	4	16	20	
18	K	1	Total	C	Mg	N	O	0
			201	161	4	16	20	
18	L	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
18	L	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
18	L	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
18	1	1	Total	C	Mg	N	O	0
			675	546	14	56	59	
18	1	1	Total	C	Mg	N	O	0
			675	546	14	56	59	
18	1	1	Total	C	Mg	N	O	0
			675	546	14	56	59	
18	1	1	Total	C	Mg	N	O	0
			675	546	14	56	59	
18	1	1	Total	C	Mg	N	O	0
			675	546	14	56	59	
18	1	1	Total	C	Mg	N	O	0
			675	546	14	56	59	
18	1	1	Total	C	Mg	N	O	0
			675	546	14	56	59	
18	1	1	Total	C	Mg	N	O	0
			675	546	14	56	59	
18	1	1	Total	C	Mg	N	O	0
			675	546	14	56	59	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			675	546	14	56	59	
18	1	1	Total	C	Mg	N	O	0
			675	546	14	56	59	
18	1	1	Total	C	Mg	N	O	0
			675	546	14	56	59	
18	1	1	Total	C	Mg	N	O	0
			675	546	14	56	59	
18	a	1	Total	C	Mg	N	O	0
			722	586	14	56	66	
18	a	1	Total	C	Mg	N	O	0
			722	586	14	56	66	
18	a	1	Total	C	Mg	N	O	0
			722	586	14	56	66	
18	a	1	Total	C	Mg	N	O	0
			722	586	14	56	66	
18	a	1	Total	C	Mg	N	O	0
			722	586	14	56	66	
18	a	1	Total	C	Mg	N	O	0
			722	586	14	56	66	
18	a	1	Total	C	Mg	N	O	0
			722	586	14	56	66	
18	a	1	Total	C	Mg	N	O	0
			722	586	14	56	66	
18	a	1	Total	C	Mg	N	O	0
			722	586	14	56	66	
18	a	1	Total	C	Mg	N	O	0
			722	586	14	56	66	
18	a	1	Total	C	Mg	N	O	0
			722	586	14	56	66	
18	a	1	Total	C	Mg	N	O	0
			722	586	14	56	66	
18	a	1	Total	C	Mg	N	O	0
			722	586	14	56	66	
18	3	1	Total	C	Mg	N	O	0
			724	595	14	56	59	
18	3	1	Total	C	Mg	N	O	0
			724	595	14	56	59	
18	3	1	Total	C	Mg	N	O	0
			724	595	14	56	59	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	3	1	724	595	14	56	59	0
18	3	1	724	595	14	56	59	0
18	3	1	724	595	14	56	59	0
18	3	1	724	595	14	56	59	0
18	3	1	724	595	14	56	59	0
18	3	1	724	595	14	56	59	0
18	3	1	724	595	14	56	59	0
18	3	1	724	595	14	56	59	0
18	3	1	724	595	14	56	59	0
18	3	1	724	595	14	56	59	0
18	3	1	724	595	14	56	59	0
18	3	1	724	595	14	56	59	0
18	3	1	724	595	14	56	59	0
18	4	1	782	640	15	60	67	0
18	4	1	782	640	15	60	67	0
18	4	1	782	640	15	60	67	0
18	4	1	782	640	15	60	67	0
18	4	1	782	640	15	60	67	0
18	4	1	782	640	15	60	67	0
18	4	1	782	640	15	60	67	0
18	4	1	782	640	15	60	67	0
18	4	1	782	640	15	60	67	0
18	4	1	782	640	15	60	67	0
18	4	1	782	640	15	60	67	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
18	4	1	Total	C	Mg	N	O	0
			782	640	15	60	67	
18	4	1	Total	C	Mg	N	O	0
			782	640	15	60	67	
18	4	1	Total	C	Mg	N	O	0
			782	640	15	60	67	
18	4	1	Total	C	Mg	N	O	0
			782	640	15	60	67	
18	4	1	Total	C	Mg	N	O	0
			782	640	15	60	67	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	
18	5	1	Total	C	Mg	N	O	0
			878	718	17	68	75	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	5	1	Total 878	C 718	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	6	1	Total 893	C 733	Mg 17	N 68	O 75	0
18	7	1	Total 758	C 617	Mg 15	N 60	O 66	0
18	7	1	Total 758	C 617	Mg 15	N 60	O 66	0
18	7	1	Total 758	C 617	Mg 15	N 60	O 66	0

*Continued on next page...*



*Continued from previous page...*

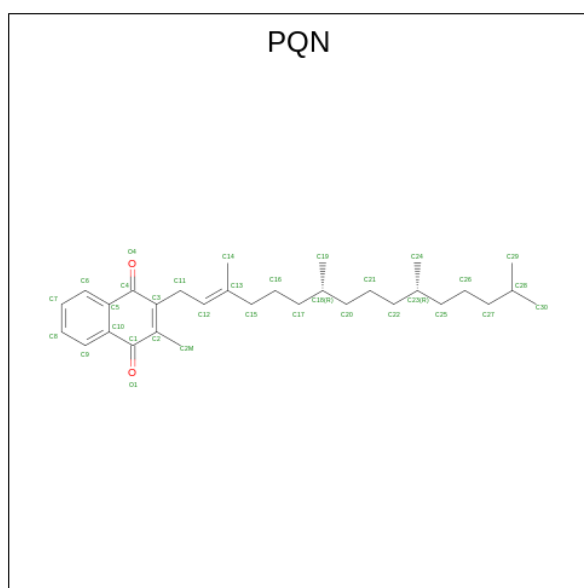
Mol	Chain	Residues	Atoms					AltConf
18	7	1	Total	C	Mg	N	O	0
			758	617	15	60	66	
18	7	1	Total	C	Mg	N	O	0
			758	617	15	60	66	
18	7	1	Total	C	Mg	N	O	0
			758	617	15	60	66	
18	7	1	Total	C	Mg	N	O	0
			758	617	15	60	66	
18	7	1	Total	C	Mg	N	O	0
			758	617	15	60	66	
18	7	1	Total	C	Mg	N	O	0
			758	617	15	60	66	
18	7	1	Total	C	Mg	N	O	0
			758	617	15	60	66	
18	7	1	Total	C	Mg	N	O	0
			758	617	15	60	66	
18	7	1	Total	C	Mg	N	O	0
			758	617	15	60	66	
18	7	1	Total	C	Mg	N	O	0
			758	617	15	60	66	
18	7	1	Total	C	Mg	N	O	0
			758	617	15	60	66	
18	7	1	Total	C	Mg	N	O	0
			758	617	15	60	66	
18	8	1	Total	C	Mg	N	O	0
			727	593	14	56	64	
18	8	1	Total	C	Mg	N	O	0
			727	593	14	56	64	
18	8	1	Total	C	Mg	N	O	0
			727	593	14	56	64	
18	8	1	Total	C	Mg	N	O	0
			727	593	14	56	64	
18	8	1	Total	C	Mg	N	O	0
			727	593	14	56	64	
18	8	1	Total	C	Mg	N	O	0
			727	593	14	56	64	
18	8	1	Total	C	Mg	N	O	0
			727	593	14	56	64	
18	8	1	Total	C	Mg	N	O	0
			727	593	14	56	64	

*Continued on next page...*

Continued from previous page...

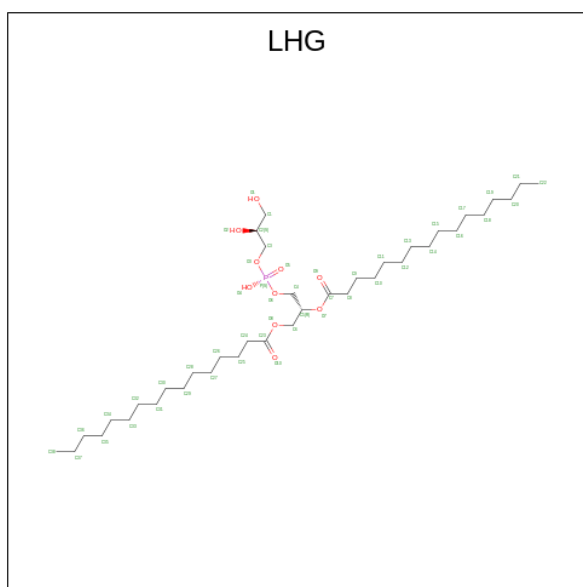
Mol	Chain	Residues	Atoms					AltConf
18	8	1	Total	C	Mg	N	O	0
			727	593	14	56	64	
18	8	1	Total	C	Mg	N	O	0
			727	593	14	56	64	
18	8	1	Total	C	Mg	N	O	0
			727	593	14	56	64	
18	8	1	Total	C	Mg	N	O	0
			727	593	14	56	64	
18	8	1	Total	C	Mg	N	O	0
			727	593	14	56	64	

- Molecule 19 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ).



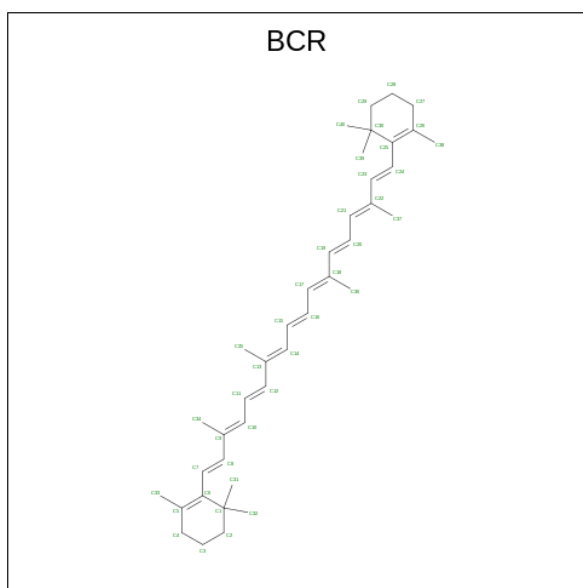
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			33	31	2	
19	B	1	Total	C	O	0
			33	31	2	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
20	A	1	79	57	20	2	0
20	A	1	79	57	20	2	0
20	B	1	36	26	9	1	0
20	1	1	49	38	10	1	0
20	a	1	49	38	10	1	0
20	3	1	94	72	20	2	0
20	3	1	94	72	20	2	0
20	4	1	49	38	10	1	0
20	5	1	98	76	20	2	0
20	5	1	98	76	20	2	0
20	6	1	48	37	10	1	0
20	7	1	37	26	10	1	0
20	8	1	98	76	20	2	0
20	8	1	98	76	20	2	0

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



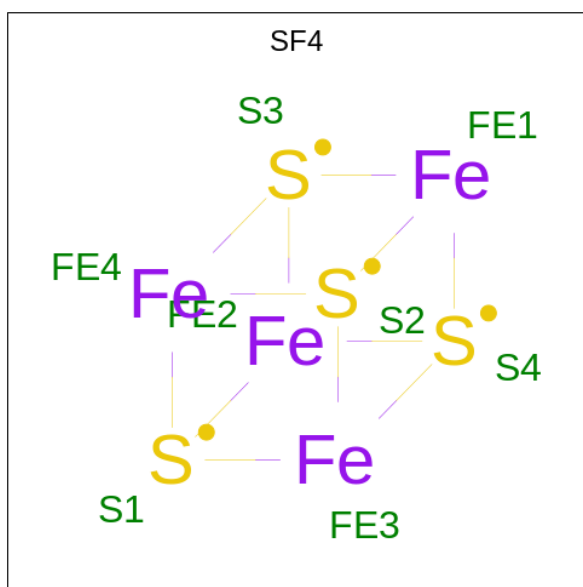
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 240 240	0
21	A	1	Total C 240 240	0
21	A	1	Total C 240 240	0
21	A	1	Total C 240 240	0
21	A	1	Total C 240 240	0
21	A	1	Total C 240 240	0
21	B	1	Total C 280 280	0
21	B	1	Total C 280 280	0
21	B	1	Total C 280 280	0
21	B	1	Total C 280 280	0
21	B	1	Total C 280 280	0
21	B	1	Total C 280 280	0
21	B	1	Total C 280 280	0

*Continued on next page...*

*Continued from previous page...*

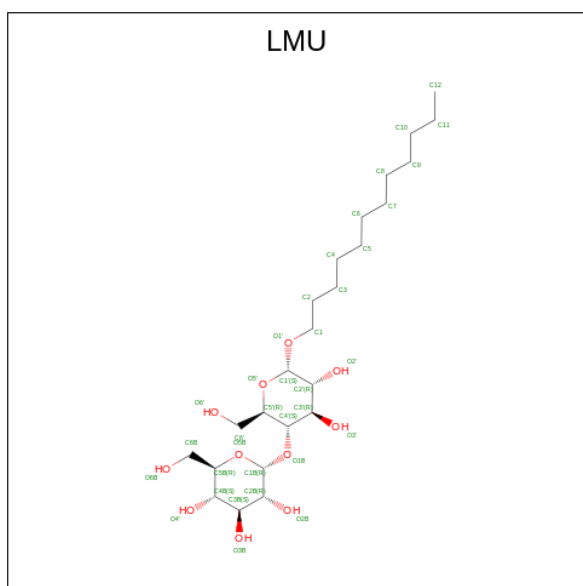
Mol	Chain	Residues	Atoms	AltConf
21	F	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	K	1	Total C 80 80	0
21	K	1	Total C 80 80	0
21	L	1	Total C 80 80	0
21	L	1	Total C 80 80	0
21	1	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	3	1	Total C 120 120	0
21	3	1	Total C 120 120	0
21	3	1	Total C 120 120	0
21	4	1	Total C 40 40	0
21	5	1	Total C 40 40	0
21	6	1	Total C 40 40	0
21	7	1	Total C 80 80	0
21	7	1	Total C 80 80	0
21	8	1	Total C 40 40	0

- Molecule 22 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



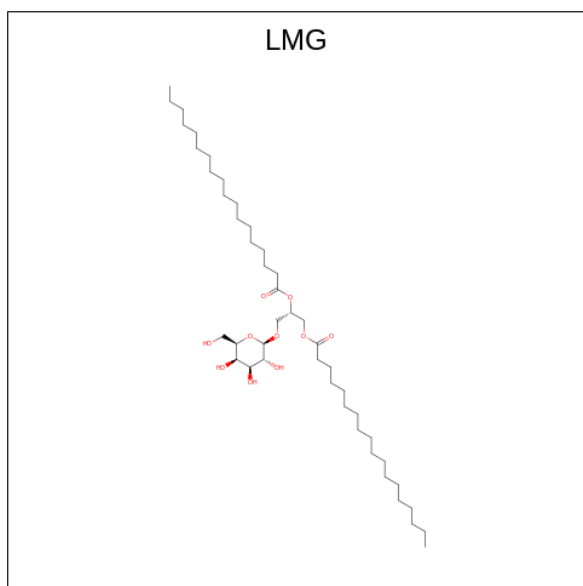
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total Fe S 8 4 4	0
22	C	1	Total Fe S 16 8 8	0
22	C	1	Total Fe S 16 8 8	0

- Molecule 23 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			101	71	30	
23	A	1	Total	C	O	0
			101	71	30	
23	A	1	Total	C	O	0
			101	71	30	
23	K	1	Total	C	O	0
			35	24	11	
23	5	1	Total	C	O	0
			33	22	11	
23	8	1	Total	C	O	0
			70	48	22	
23	8	1	Total	C	O	0
			70	48	22	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



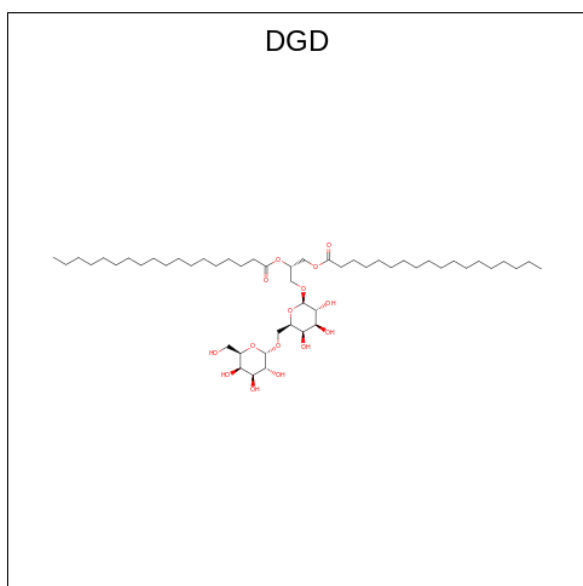
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			40	30	10	
24	J	1	Total	C	O	0
			40	30	10	
24	4	1	Total	C	O	0
			80	60	20	
24	4	1	Total	C	O	0
			80	60	20	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	5	1	80	60	20	0
24	5	1	80	60	20	0
24	7	1	44	34	10	0

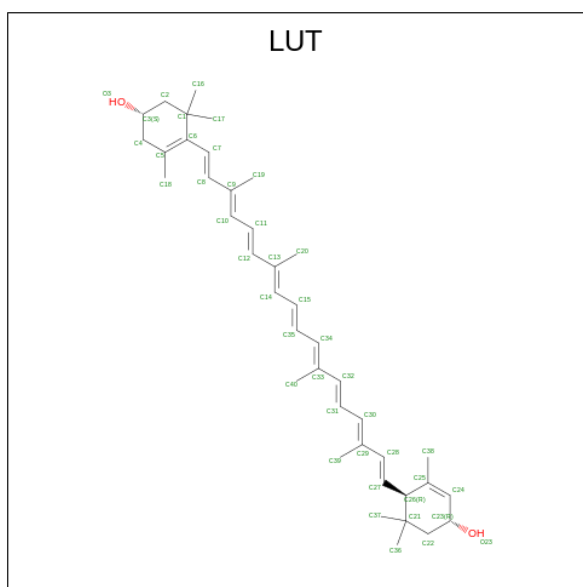
- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGD) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	B	1	62	47	15	0
25	J	1	58	43	15	0

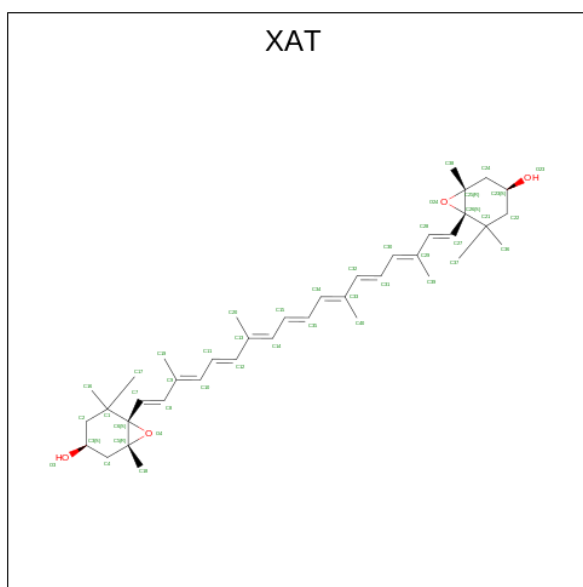
- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula:  $C_{40}H_{56}O_2$ ).





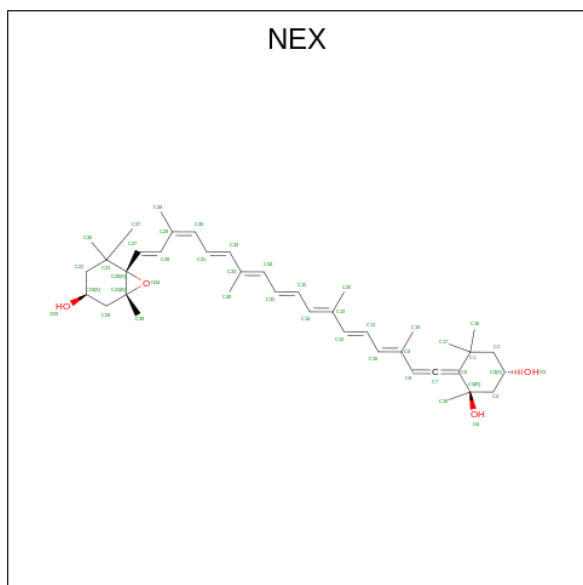
Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			42	40	2	
26	a	1	Total	C	O	0
			42	40	2	
26	3	1	Total	C	O	0
			42	40	2	
26	4	1	Total	C	O	0
			42	40	2	
26	5	1	Total	C	O	0
			42	40	2	
26	6	1	Total	C	O	0
			42	40	2	
26	7	1	Total	C	O	0
			42	40	2	
26	8	1	Total	C	O	0
			42	40	2	

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	a	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	
27	7	1	Total	C	O	0
			44	40	4	
27	8	1	Total	C	O	0
			44	40	4	

- Molecule 28 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).

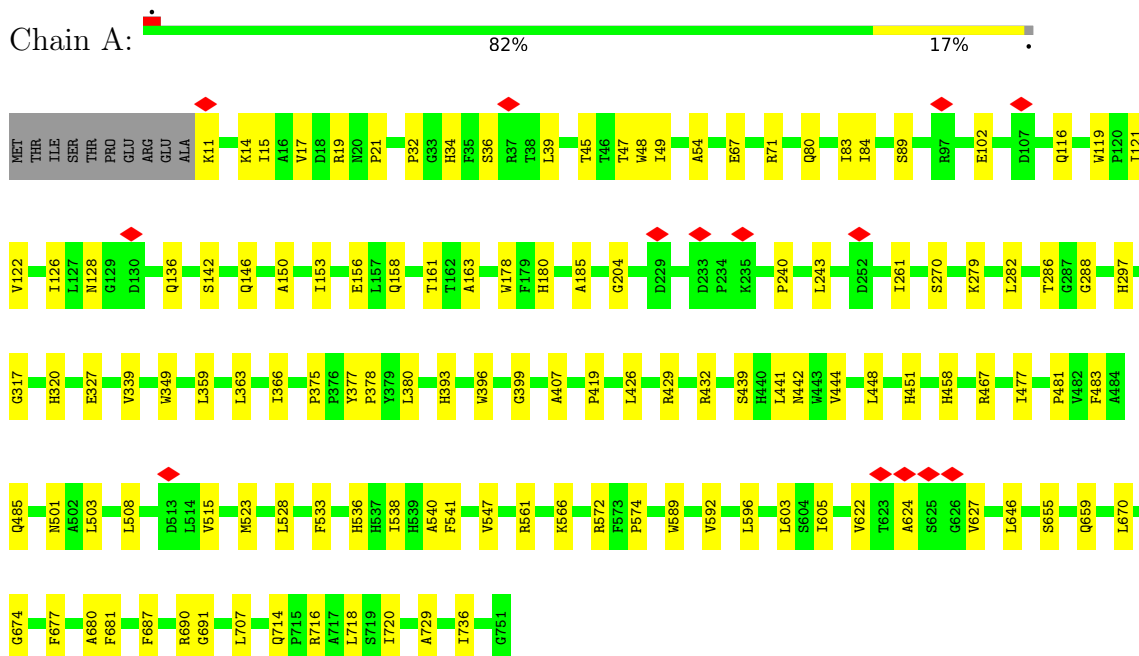


Mol	Chain	Residues	Atoms			AltConf
28	5	1	Total	C	O	0
			44	40	4	
28	6	1	Total	C	O	0
			44	40	4	

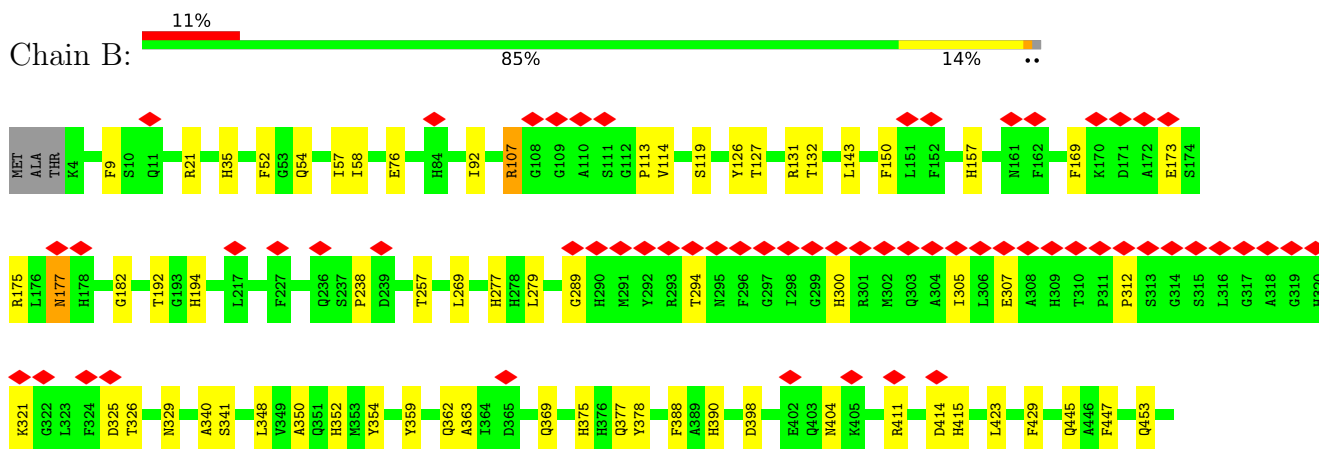
### 3 Residue-property plots

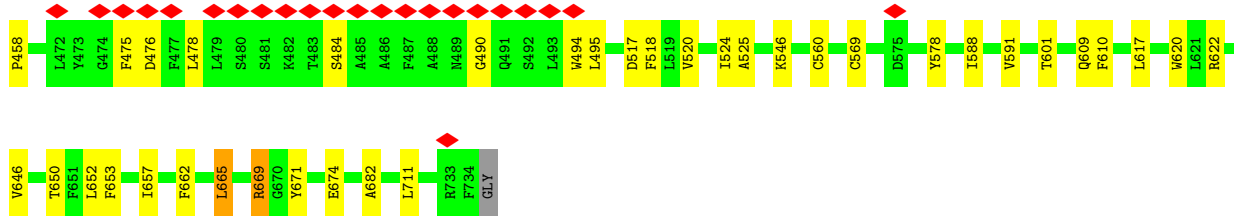
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

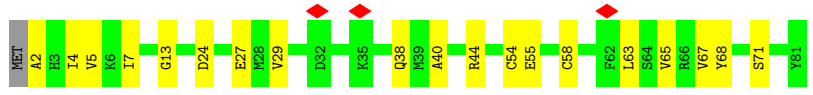
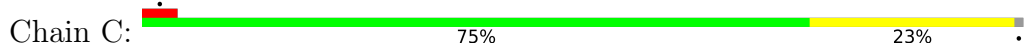


#### • Molecule 2: PsaB

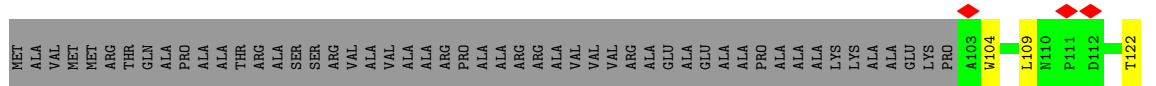




• Molecule 3: PsaC



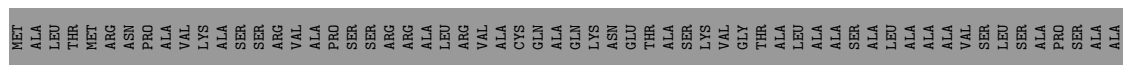
• Molecule 4: PsaD



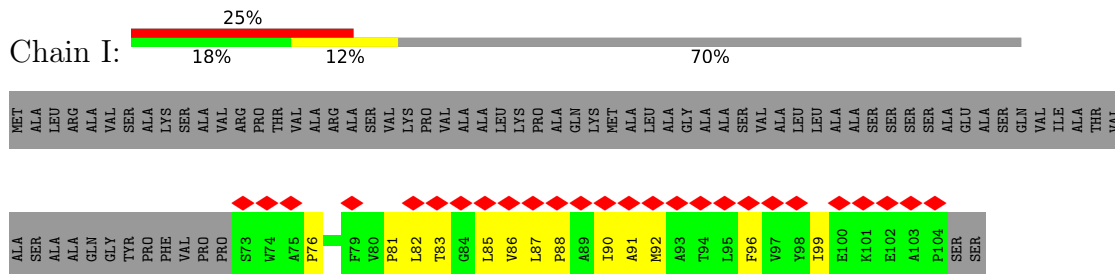
• Molecule 5: PsaE



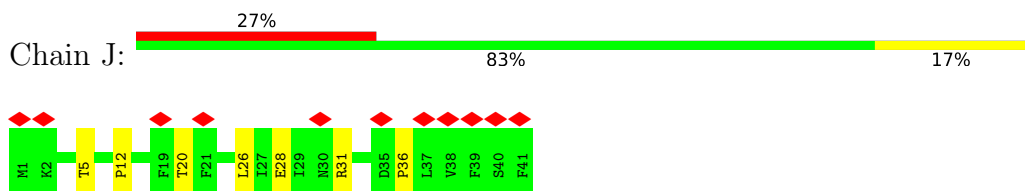
• Molecule 6: PsaF



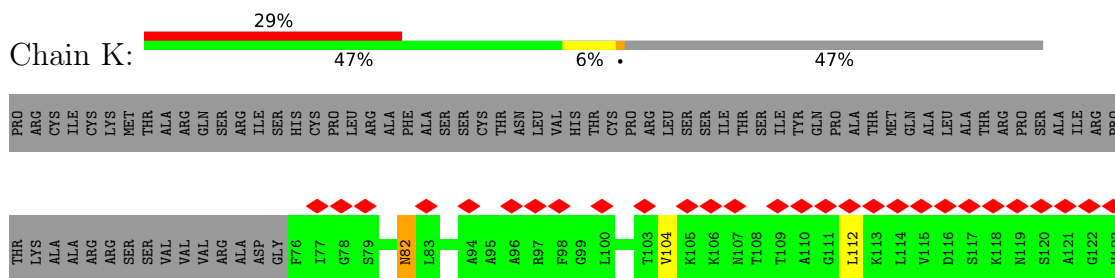
• Molecule 7: PsaI



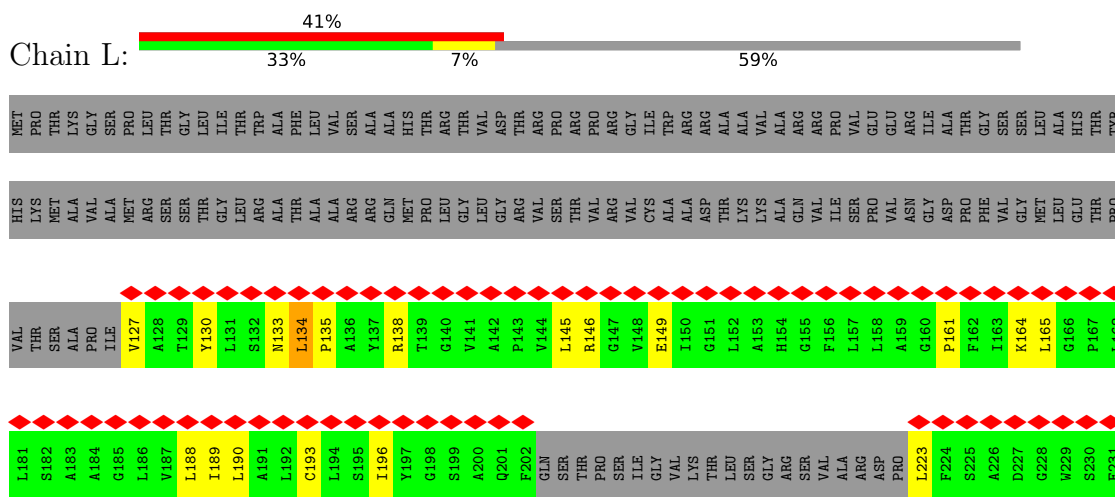
• Molecule 8: PsaJ



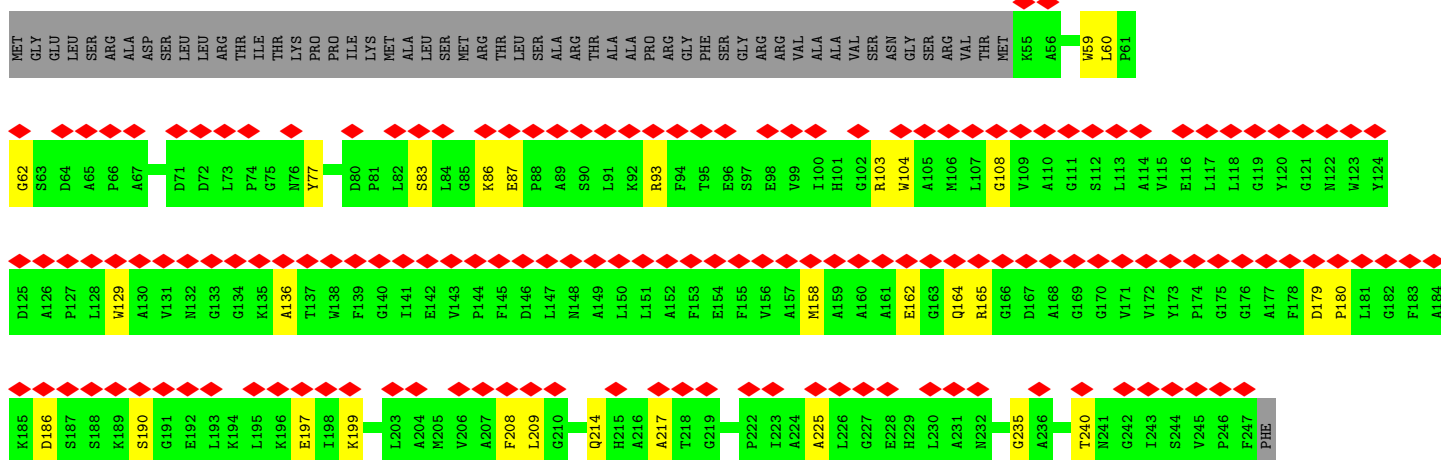
• Molecule 9: PsaK



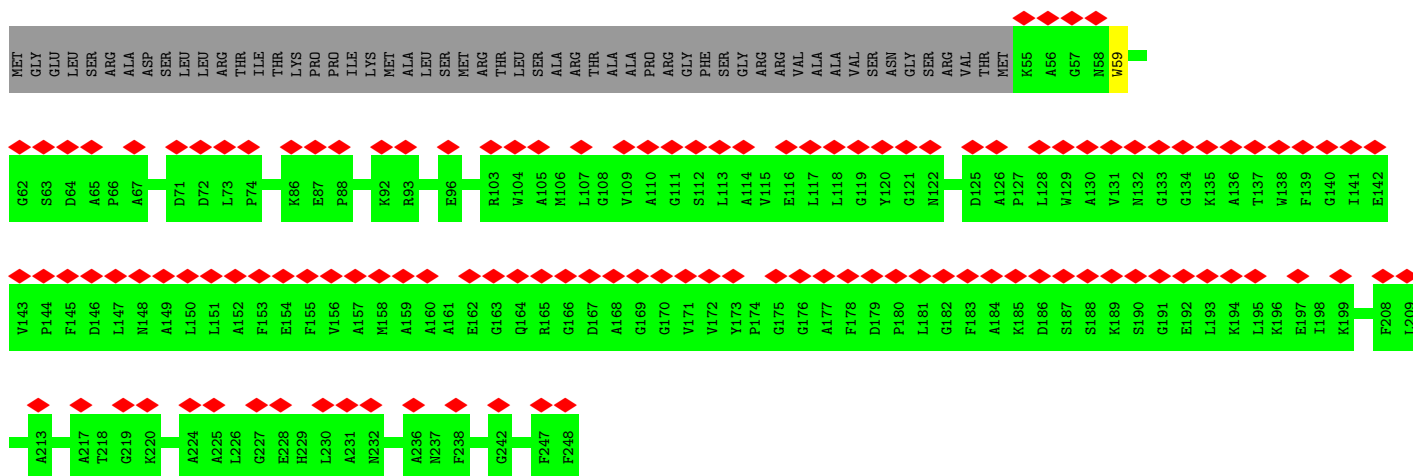
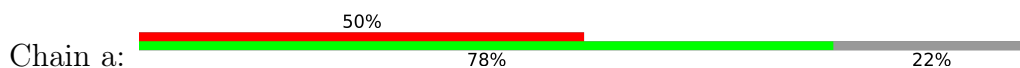
• Molecule 10: PsaL



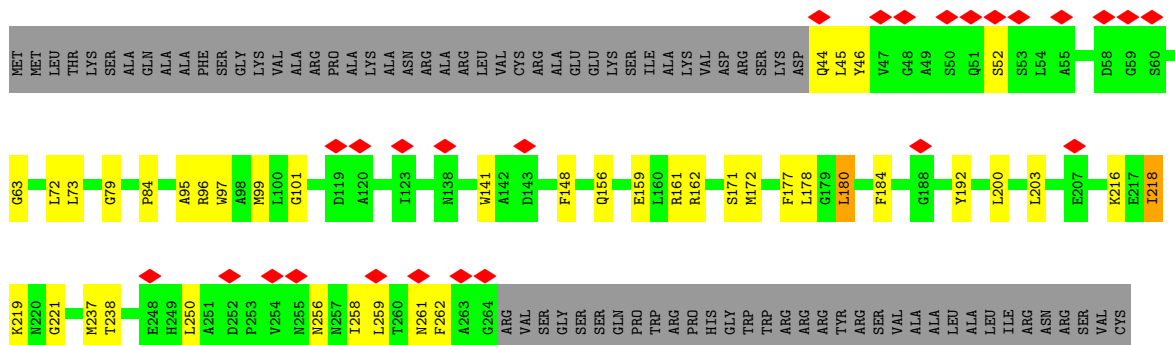
• Molecule 11: Lhca1



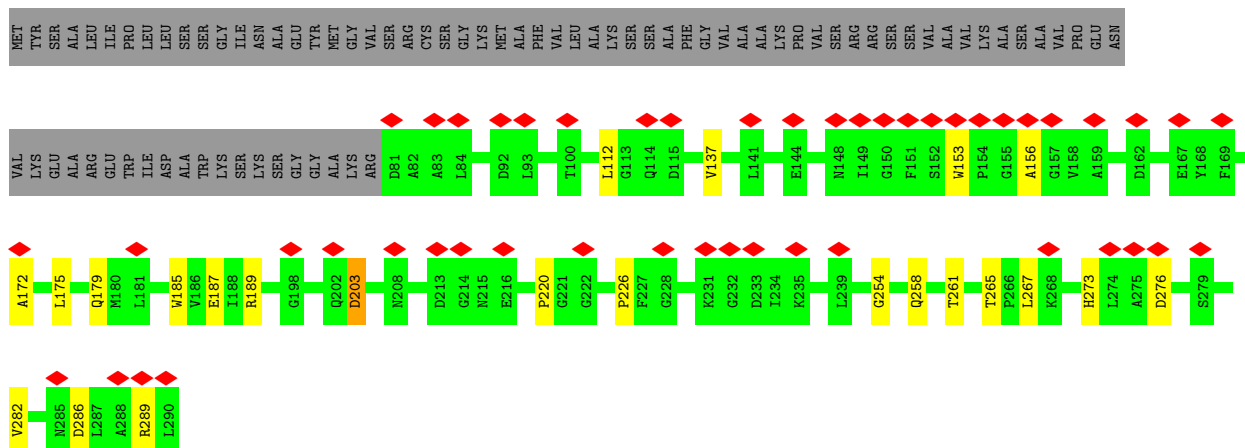
• Molecule 11: Lhca1



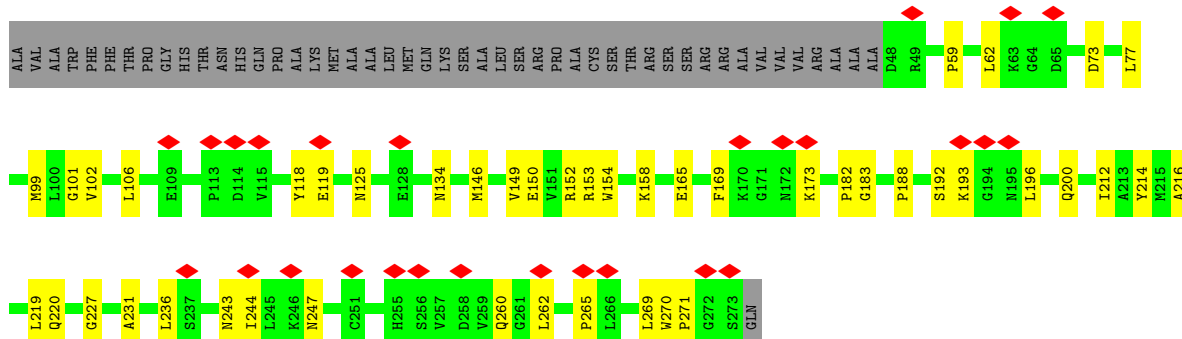
• Molecule 12: Lhca3



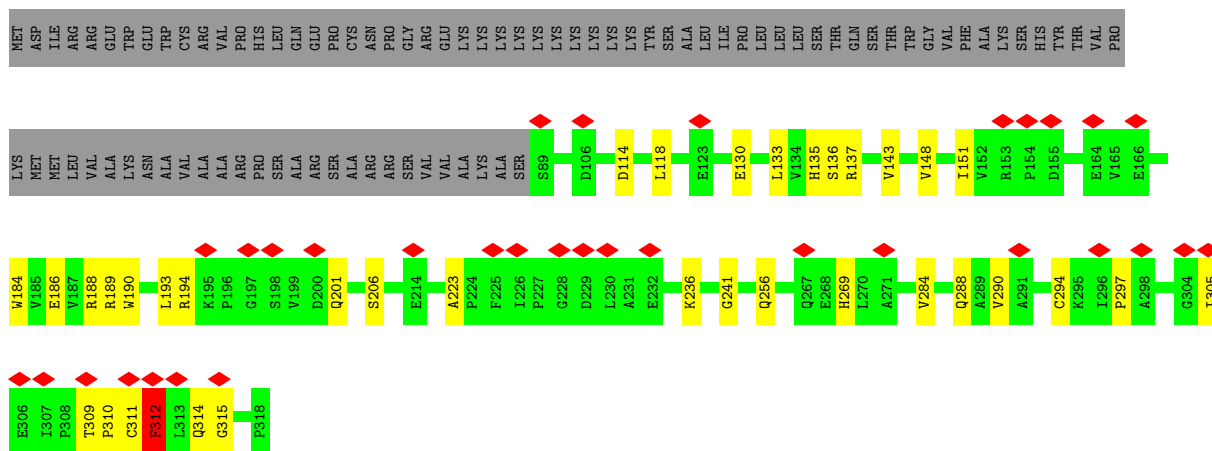
• Molecule 13: Lhca4



• Molecule 14: Lhca5



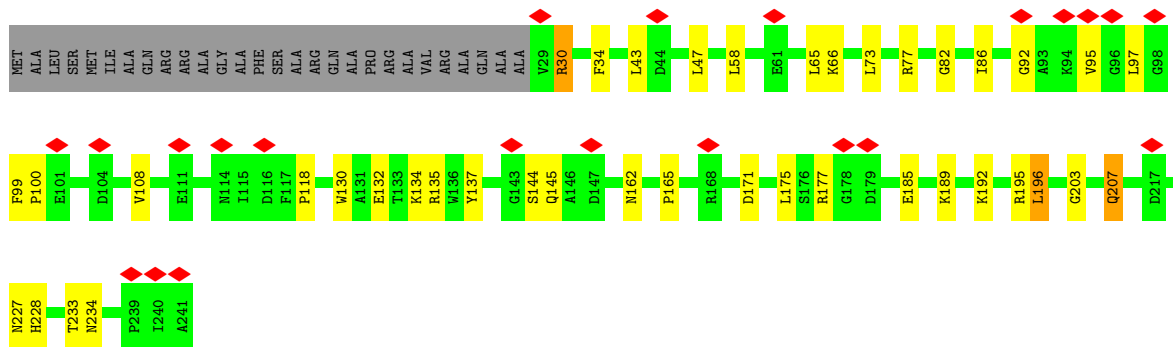
• Molecule 15: Lhca6



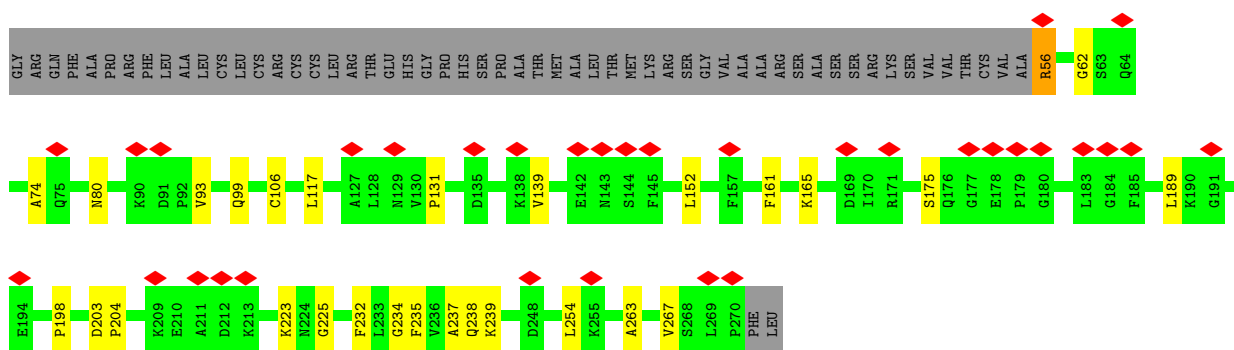
• Molecule 16: Lhca7







• Molecule 17: Lhca8



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58955	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.391	Depositor
Minimum map value	-0.159	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: LMG, LHG, LUT, SF4, BCR, XAT, PQN, DGD, NEX, LMU, CLA

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	0.42	0/6015	0.57	1/8201 (0.0%)
2	B	0.41	0/6024	0.58	3/8225 (0.0%)
3	C	0.42	0/610	0.65	0/826
4	D	0.38	0/1157	0.60	0/1563
5	E	0.38	0/515	0.53	0/700
6	F	0.35	0/1280	0.55	0/1733
7	I	0.32	0/250	0.58	0/345
8	J	0.36	0/349	0.56	0/478
9	K	0.30	0/583	0.65	0/790
10	L	0.30	0/779	0.61	1/1063 (0.1%)
11	1	0.32	0/1478	0.55	0/2012
11	a	0.32	0/1490	0.54	0/2028
12	3	0.39	0/1731	0.65	2/2349 (0.1%)
13	4	0.33	0/1686	0.53	0/2300
14	5	0.36	0/1820	0.58	1/2480 (0.0%)
15	6	0.35	0/1833	0.57	0/2505
16	7	0.38	0/1701	0.60	1/2310 (0.0%)
17	8	0.36	0/1680	0.63	0/2288
All	All	0.38	0/30981	0.58	9/42196 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	3	180	LEU	CA-CB-CG	6.97	131.34	115.30
2	B	665	LEU	CB-CG-CD2	-6.66	99.68	111.00
12	3	200	LEU	CA-CB-CG	6.59	130.46	115.30
16	7	196	LEU	CA-CB-CG	6.08	129.29	115.30
14	5	106	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	426	LEU	CA-CB-CG	5.59	128.15	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	134	LEU	CA-CB-CG	5.52	128.01	115.30
2	B	560	CYS	CA-CB-SG	-5.32	104.42	114.00
2	B	476	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5819	0	5672	100	0
2	B	5812	0	5569	83	0
3	C	600	0	589	12	0
4	D	1129	0	1144	33	0
5	E	505	0	504	4	0
6	F	1254	0	1288	14	0
7	I	242	0	252	9	0
8	J	337	0	336	7	0
9	K	578	0	617	9	0
10	L	761	0	768	18	0
11	1	1433	0	1387	25	0
11	a	1444	0	1396	0	0
12	3	1683	0	1641	33	0
13	4	1631	0	1587	21	0
14	5	1765	0	1738	39	0
15	6	1771	0	1772	27	0
16	7	1649	0	1589	35	0
17	8	1630	0	1609	25	0
18	1	675	0	541	23	0
18	3	724	0	628	22	0
18	4	782	0	686	23	0
18	5	878	0	758	36	0
18	6	893	0	809	25	0
18	7	758	0	641	20	0
18	8	727	0	635	17	0
18	A	2625	0	2614	122	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	B	2277	0	2218	91	0
18	F	140	0	113	5	0
18	J	42	0	31	0	0
18	K	201	0	171	5	0
18	L	135	0	99	8	0
18	a	722	0	618	0	0
19	A	33	0	46	3	0
19	B	33	0	46	2	0
20	1	49	0	74	2	0
20	3	94	0	137	6	0
20	4	49	0	74	4	0
20	5	98	0	148	5	0
20	6	48	0	69	1	0
20	7	37	0	44	5	0
20	8	98	0	148	9	0
20	A	79	0	104	3	0
20	B	36	0	41	1	0
20	a	49	0	74	0	0
21	1	40	0	56	2	0
21	3	120	0	168	13	0
21	4	40	0	56	3	0
21	5	40	0	56	3	0
21	6	40	0	56	4	0
21	7	80	0	112	5	0
21	8	40	0	56	2	0
21	A	240	0	336	24	0
21	B	280	0	392	20	0
21	F	40	0	56	6	0
21	J	40	0	56	2	0
21	K	80	0	112	6	0
21	L	80	0	112	8	0
21	a	40	0	56	0	0
22	A	8	0	0	0	0
22	C	16	0	0	0	0
23	5	33	0	39	0	0
23	8	70	0	92	1	0
23	A	101	0	130	6	0
23	K	35	0	46	0	0
24	4	80	0	100	1	0
24	5	80	0	100	3	0
24	7	44	0	61	0	0
24	A	40	0	50	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	J	40	0	50	4	0
25	B	62	0	85	3	0
25	J	58	0	77	3	0
26	1	42	0	56	3	0
26	3	42	0	56	2	0
26	4	42	0	56	6	0
26	5	42	0	56	4	0
26	6	42	0	56	2	0
26	7	42	0	56	3	0
26	8	42	0	56	5	0
26	a	42	0	56	0	0
27	1	44	0	56	3	0
27	3	44	0	56	2	0
27	4	44	0	56	2	0
27	5	44	0	56	6	0
27	6	44	0	56	2	0
27	7	44	0	56	4	0
27	8	44	0	56	2	0
27	a	44	0	56	0	0
28	5	44	0	56	4	0
28	6	44	0	56	4	0
All	All	44968	0	44543	755	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 9.

All (755) 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)
4:D:202:HIS:HB3	4:D:203:PRO:CD	1.63	1.28
4:D:202:HIS:CB	4:D:203:PRO:HD3	1.75	1.16
4:D:202:HIS:HB3	4:D:203:PRO:HD3	1.17	1.12
4:D:202:HIS:CG	4:D:203:PRO:HD3	1.95	1.01
12:3:46:TYR:OH	20:3:624:LHG:HC42	1.80	0.82
14:5:102:VAL:HG11	26:5:620:LUT:H12	1.62	0.82
4:D:104:TRP:CH2	4:D:204:ALA:O	2.34	0.81
18:A:830:CLA:H2	21:A:849:BCR:HC7	1.67	0.76
4:D:202:HIS:HB3	4:D:203:PRO:HD2	1.62	0.76
18:3:609:CLA:HBB1	18:3:617:CLA:HBB1	1.66	0.76
18:8:611:CLA:HBC3	20:8:622:LHG:HC62	1.68	0.74
16:7:192:LYS:HD2	20:7:622:LHG:HC61	1.69	0.74

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:104:TRP:HH2	4:D:204:ALA:O	1.69	0.74
12:3:46:TYR:OH	20:3:624:LHG:C4	2.36	0.73
9:K:127:ASP:OD1	18:K:201:CLA:NA	2.23	0.71
1:A:11:LYS:N	12:3:52:SER:HG	1.87	0.71
15:6:135:HIS:HE1	18:6:603:CLA:NA	1.88	0.70
18:7:611:CLA:NB	20:7:622:LHG:O4	2.24	0.70
3:C:4:ILE:HB	3:C:68:TYR:HB2	1.76	0.68
4:D:209:PRO:HA	4:D:216:ARG:HH22	1.59	0.68
11:1:77:TYR:OH	11:1:199:LYS:NZ	2.26	0.68
14:5:216:ALA:HB1	14:5:220:GLN:HE21	1.58	0.68
18:B:831:CLA:H2	21:F:305:BCR:H372	1.76	0.68
13:4:254:GLY:O	13:4:258:GLN:HB3	1.93	0.67
18:8:611:CLA:NB	20:8:622:LHG:O4	2.27	0.67
3:C:2:ALA:N	3:C:71:SER:HG	1.94	0.66
18:A:808:CLA:HMB3	18:A:809:CLA:H3A	1.78	0.66
2:B:177:ASN:ND2	2:B:289:GLY:O	2.29	0.66
18:8:613:CLA:H102	20:8:622:LHG:H301	1.78	0.66
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.78	0.65
4:D:200:TYR:HE2	4:D:203:PRO:O	1.80	0.65
15:6:143:VAL:HG11	26:6:619:LUT:H12	1.77	0.65
12:3:161:ARG:HB3	18:3:608:CLA:HMC3	1.76	0.64
1:A:17:VAL:HG11	18:A:811:CLA:HED3	1.78	0.64
1:A:153:ILE:O	1:A:158:GLN:NE2	2.30	0.64
1:A:707:LEU:O	6:F:168:ARG:NH1	2.31	0.64
4:D:200:TYR:CE2	4:D:203:PRO:O	2.50	0.64
14:5:220:GLN:OE1	18:5:613:CLA:NA	2.31	0.64
18:4:601:CLA:OBD	15:6:188:ARG:NH2	2.32	0.63
13:4:153:TRP:HB2	13:4:156:ALA:HB2	1.81	0.63
15:6:294:CYS:SG	15:6:314:GLN:NE2	2.71	0.63
18:B:825:CLA:HMA1	21:B:847:BCR:H14C	1.79	0.63
4:D:213:ASN:HB2	4:D:216:ARG:HH11	1.63	0.63
2:B:92:ILE:HB	2:B:113:PRO:HB2	1.80	0.63
2:B:414:ASP:HA	6:F:226:PRO:HB3	1.82	0.62
2:B:398:ASP:OD1	4:D:236:LYS:NZ	2.29	0.62
1:A:714:GLN:HE22	5:E:123:ASN:HA	1.65	0.62
18:A:811:CLA:HAB	18:A:814:CLA:H111	1.80	0.61
18:B:807:CLA:HHB	18:B:808:CLA:HHB	1.81	0.61
18:B:841:CLA:HBB2	18:1:602:CLA:H42	1.81	0.61
18:5:604:CLA:H2A	18:5:604:CLA:HED3	1.82	0.61
13:4:226:PRO:HD2	26:4:619:LUT:H23	1.81	0.61
1:A:441:LEU:HD22	18:A:840:CLA:HBB1	1.81	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ASN:HB2	18:A:837:CLA:HED3	1.82	0.61
14:5:188:PRO:HD2	26:5:620:LUT:H23	1.83	0.61
16:7:134:LYS:HB3	18:7:608:CLA:HMC3	1.83	0.61
1:A:467:ARG:NH2	18:A:835:CLA:O1D	2.34	0.61
4:D:146:ILE:HG12	4:D:156:ILE:HG22	1.83	0.61
18:B:808:CLA:H8	18:B:808:CLA:HBB1	1.83	0.61
16:7:118:PRO:HB2	17:8:263:ALA:HB1	1.83	0.61
18:A:807:CLA:H161	18:A:830:CLA:HBB2	1.81	0.60
3:C:58:CYS:HB3	3:C:63:LEU:HD12	1.83	0.60
10:L:138:ARG:O	10:L:146:ARG:NH2	2.34	0.60
18:A:827:CLA:H72	18:A:836:CLA:HAB	1.82	0.60
18:4:602:CLA:H2A	18:4:602:CLA:HED3	1.82	0.60
2:B:238:PRO:HB3	2:B:257:THR:HG21	1.83	0.60
18:B:813:CLA:H42	21:B:844:BCR:H21C	1.83	0.60
12:3:258:ILE:HG23	12:3:259:LEU:HD22	1.84	0.60
1:A:429:ARG:HG2	1:A:432:ARG:HH21	1.67	0.59
18:A:813:CLA:H43	12:3:72:LEU:HD21	1.84	0.59
18:B:808:CLA:HAB	18:B:809:CLA:HBA1	1.83	0.59
18:6:616:CLA:HBC3	18:6:620:CLA:HMC3	1.83	0.59
18:A:822:CLA:H101	21:A:851:BCR:H10C	1.84	0.59
11:1:103:ARG:NH1	11:1:197:GLU:OE2	2.34	0.59
11:1:93:ARG:NH1	18:1:603:CLA:O1A	2.35	0.59
18:A:824:CLA:HHB	18:A:845:CLA:HBC3	1.83	0.59
12:3:219:LYS:NZ	20:3:624:LHG:O5	2.31	0.59
11:1:162:GLU:OE1	11:1:165:ARG:NH2	2.31	0.59
17:8:56:ARG:NH1	17:8:80:ASN:O	2.36	0.59
17:8:238:GLN:OE1	18:8:613:CLA:NA	2.36	0.58
16:7:100:PRO:HG3	16:7:108:VAL:HG11	1.84	0.58
18:B:819:CLA:HBB1	18:B:824:CLA:H61	1.85	0.58
18:A:804:CLA:HBB1	21:A:856:BCR:H281	1.85	0.58
2:B:169:PHE:O	2:B:175:ARG:NH2	2.37	0.58
2:B:388:PHE:HZ	18:B:825:CLA:HAB	1.69	0.58
2:B:300:HIS:HE1	18:B:821:CLA:NA	2.01	0.58
18:4:609:CLA:HMB2	24:4:624:LMG:H162	1.85	0.57
11:1:162:GLU:OE2	18:1:609:CLA:NC	2.38	0.57
4:D:148:GLU:O	4:D:178:GLN:NE2	2.35	0.57
1:A:622:VAL:HG22	1:A:624:ALA:H	1.70	0.57
9:K:82:ASN:ND2	18:K:204:CLA:OBD	2.38	0.57
9:K:150:ILE:HG12	18:K:203:CLA:HAB	1.86	0.57
18:4:610:CLA:H52	26:4:619:LUT:H30	1.86	0.57
18:5:609:CLA:HBA1	18:5:619:CLA:HMD2	1.87	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLY:H	9:K:104:VAL:HG13	1.69	0.57
21:B:801:BCR:HC41	18:B:832:CLA:HBB2	1.87	0.57
12:3:250:LEU:HD21	18:3:614:CLA:HMC3	1.87	0.57
16:7:66:LYS:O	16:7:162:ASN:ND2	2.33	0.56
2:B:307:GLU:HG3	2:B:321:LYS:HA	1.87	0.56
2:B:669:ARG:HB2	19:B:842:PQN:H7	1.86	0.56
18:B:812:CLA:H2A	18:B:812:CLA:HED3	1.87	0.56
18:A:820:CLA:HAB	18:A:820:CLA:H8	1.87	0.56
2:B:157:HIS:HE1	18:B:811:CLA:NA	2.02	0.56
13:4:286:ASP:OD1	13:4:289:ARG:NH2	2.38	0.56
16:7:132:GLU:OE1	16:7:135:ARG:NH2	2.37	0.56
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.87	0.56
2:B:341:SER:HB3	18:B:824:CLA:H51	1.86	0.56
1:A:45:THR:HG23	1:A:716:ARG:HG3	1.87	0.56
2:B:157:HIS:CE1	18:B:811:CLA:NA	2.74	0.56
18:B:817:CLA:H61	18:B:834:CLA:HAA1	1.86	0.56
5:E:101:GLN:NE2	5:E:123:ASN:OD1	2.35	0.56
18:4:606:CLA:HAB	18:4:607:CLA:HMC3	1.86	0.56
2:B:126:TYR:O	2:B:131:ARG:NH1	2.38	0.56
2:B:423:LEU:HG	18:B:838:CLA:HBB1	1.87	0.56
2:B:300:HIS:HB3	2:B:305:ILE:HD11	1.87	0.56
18:B:837:CLA:H143	21:F:305:BCR:HC8	1.88	0.56
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.87	0.55
2:B:662:PHE:HA	2:B:665:LEU:HB2	1.88	0.55
1:A:34:HIS:NE2	18:A:812:CLA:O1A	2.39	0.55
18:B:827:CLA:HBC3	25:B:850:DGD:HBC3	1.88	0.55
18:B:828:CLA:H202	21:B:844:BCR:H352	1.88	0.55
13:4:189:ARG:HB3	18:4:608:CLA:HMC3	1.87	0.55
15:6:118:LEU:HD23	16:7:175:LEU:HD21	1.88	0.55
1:A:67:GLU:OE2	1:A:71:ARG:NH2	2.39	0.55
11:1:186:ASP:HA	11:1:190:SER:HB3	1.86	0.55
3:C:27:GLU:HB2	4:D:216:ARG:HH21	1.72	0.55
16:7:30:ARG:NH2	16:7:43:LEU:O	2.38	0.55
18:4:601:CLA:H2	20:4:622:LHG:H131	1.88	0.55
14:5:101:GLY:HA2	27:5:621:XAT:H181	1.88	0.55
18:6:601:CLA:H2	20:6:623:LHG:H142	1.89	0.55
1:A:396:TRP:HB3	18:A:829:CLA:HMC3	1.89	0.55
2:B:375:HIS:HE1	18:B:827:CLA:ND	2.05	0.55
18:A:811:CLA:H2	18:A:813:CLA:HBC2	1.88	0.54
18:B:808:CLA:H2	18:B:808:CLA:H102	1.89	0.54
10:L:135:PRO:HA	10:L:138:ARG:HE	1.72	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1:199:LYS:NZ	20:1:620:LHG:O5	2.40	0.54
11:1:214:GLN:HE21	11:1:225:ALA:HB3	1.70	0.54
21:7:621:BCR:HC31	20:8:622:LHG:HC81	1.89	0.54
1:A:605:ILE:HD12	18:A:801:CLA:H122	1.89	0.54
24:5:627:LMG:H131	27:6:621:XAT:H363	1.90	0.54
18:A:818:CLA:H93	21:K:207:BCR:HC21	1.88	0.54
2:B:390:HIS:HE1	18:B:829:CLA:NA	2.06	0.54
18:5:604:CLA:HMB3	27:5:621:XAT:H162	1.89	0.54
1:A:128:ASN:O	6:F:90:ARG:NH2	2.40	0.54
2:B:325:ASP:O	2:B:329:ASN:ND2	2.41	0.54
11:1:217:ALA:HB2	18:1:616:CLA:HED2	1.89	0.54
15:6:256:GLN:NE2	28:6:624:NEX:O23	2.40	0.54
6:F:212:ARG:HH12	17:8:93:VAL:HB	1.72	0.54
11:1:62:GLY:HA3	17:8:175:SER:HB3	1.88	0.54
13:4:265:THR:HG22	13:4:267:LEU:H	1.72	0.54
7:I:88:PRO:O	7:I:92:MET:N	2.39	0.54
3:C:29:VAL:HG22	4:D:216:ARG:HG3	1.90	0.54
11:1:108:GLY:HA2	27:1:618:XAT:H181	1.89	0.54
18:7:611:CLA:HBC1	20:7:622:LHG:H292	1.89	0.54
18:B:837:CLA:H111	18:B:837:CLA:H203	1.90	0.54
15:6:186:GLU:OE1	15:6:189:ARG:NH2	2.38	0.54
18:A:811:CLA:HBB2	18:A:814:CLA:HMA3	1.90	0.54
21:B:801:BCR:H10C	18:B:832:CLA:HMB2	1.90	0.54
18:F:303:CLA:HMB3	8:J:26:LEU:HD21	1.88	0.54
20:5:625:LHG:HC91	24:5:627:LMG:H311	1.90	0.53
1:A:327:GLU:HG2	1:A:339:VAL:HG22	1.91	0.53
15:6:223:ALA:HB2	18:6:610:CLA:HBD	1.89	0.53
16:7:134:LYS:HG3	18:7:608:CLA:HBB1	1.90	0.53
1:A:279:LYS:HG2	1:A:503:LEU:HD12	1.89	0.53
14:5:260:GLN:HB2	28:5:624:NEX:H8	1.89	0.53
1:A:32:PRO:HB2	1:A:48:TRP:HH2	1.73	0.53
1:A:116:GLN:NE2	18:A:810:CLA:OBD	2.36	0.53
1:A:121:ILE:HG12	1:A:122:VAL:HG13	1.89	0.53
18:6:610:CLA:HBB1	18:6:612:CLA:H3A	1.90	0.53
1:A:121:ILE:HB	21:A:856:BCR:H322	1.91	0.53
2:B:312:PRO:HB2	11:1:87:GLU:HG3	1.90	0.53
3:C:40:ALA:O	4:D:221:GLN:NE2	2.40	0.53
1:A:359:LEU:HD12	18:A:828:CLA:H43	1.90	0.53
1:A:540:ALA:HB1	18:A:839:CLA:HMB3	1.89	0.53
15:6:314:GLN:HG3	16:7:97:LEU:HD21	1.90	0.53
16:7:77:ARG:NH1	18:7:608:CLA:OBD	2.42	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ALA:HB2	20:A:846:LHG:HC82	1.90	0.53
2:B:650:THR:HA	2:B:653:PHE:HB3	1.90	0.53
4:D:191:ARG:HB2	4:D:201:LEU:HD22	1.91	0.53
14:5:152:ARG:NH2	18:6:601:CLA:OBD	2.41	0.53
1:A:119:TRP:HB3	21:A:856:BCR:H323	1.91	0.52
21:A:852:BCR:H362	18:A:854:CLA:H42	1.91	0.52
8:J:28:GLU:OE1	8:J:31:ARG:NH2	2.42	0.52
1:A:670:LEU:HB3	18:A:854:CLA:H62	1.91	0.52
21:B:801:BCR:H381	18:F:301:CLA:HMC2	1.91	0.52
14:5:236:LEU:HD21	18:5:614:CLA:HMC3	1.91	0.52
17:8:203:ASP:OD1	26:8:619:LUT:O23	2.26	0.52
18:B:803:CLA:H152	18:B:810:CLA:HBC1	1.91	0.52
18:B:841:CLA:H3A	20:B:851:LHG:H241	1.92	0.52
16:7:171:ASP:OD1	26:7:619:LUT:O23	2.26	0.52
18:A:828:CLA:H151	18:A:836:CLA:H112	1.91	0.52
1:A:19:ARG:HE	12:3:79:GLY:HA2	1.74	0.52
2:B:352:HIS:ND1	18:B:817:CLA:OBD	2.41	0.52
12:3:96:ARG:HA	12:3:99:MET:HG2	1.91	0.52
21:3:620:BCR:HC21	18:7:601:CLA:HMD2	1.91	0.52
15:6:148:VAL:HA	15:6:151:ILE:HG12	1.90	0.52
1:A:89:SER:OG	1:A:163:ALA:O	2.26	0.52
10:L:149:GLU:HG3	18:L:302:CLA:HMA3	1.91	0.52
13:4:172:ALA:HA	13:4:175:LEU:HD22	1.92	0.52
14:5:243:ASN:O	14:5:247:ASN:ND2	2.42	0.52
1:A:483:PHE:HB3	18:A:838:CLA:H11	1.90	0.51
2:B:119:SER:HA	18:B:827:CLA:HMA2	1.91	0.51
18:B:806:CLA:HBB	18:B:829:CLA:HAB	1.91	0.51
14:5:146:MET:HG3	18:5:609:CLA:HMC3	1.91	0.51
14:5:158:LYS:NZ	18:5:619:CLA:O1D	2.40	0.51
2:B:646:VAL:HG21	18:B:809:CLA:HMD2	1.93	0.51
18:4:601:CLA:HAB	20:4:622:LHG:H292	1.91	0.51
14:5:165:GLU:HG2	14:5:173:LYS:HG2	1.92	0.51
17:8:117:LEU:HD21	26:8:619:LUT:H10	1.92	0.51
1:A:180:HIS:CE1	18:A:811:CLA:NA	2.79	0.51
2:B:127:THR:HG21	2:B:359:TYR:HD1	1.75	0.51
2:B:175:ARG:HD2	18:B:824:CLA:HMD1	1.92	0.51
18:4:602:CLA:HAB	27:4:620:XAT:H32	1.92	0.51
17:8:239:LYS:HZ1	20:8:623:LHG:H222	1.75	0.51
1:A:270:SER:HA	18:A:818:CLA:HAA2	1.93	0.51
10:L:134:LEU:HD12	18:L:303:CLA:HBD	1.92	0.51
20:4:622:LHG:H172	18:6:617:CLA:HMA2	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:8:74:ALA:O	17:8:80:ASN:ND2	2.44	0.51
18:B:806:CLA:HMB2	18:B:829:CLA:HBB2	1.92	0.51
12:3:63:GLY:HA3	12:3:218:ILE:HG21	1.93	0.51
13:4:261:THR:HA	18:4:616:CLA:HED1	1.93	0.51
14:5:152:ARG:HB3	18:5:608:CLA:HMC3	1.92	0.51
1:A:161:THR:HG21	18:A:817:CLA:HAA2	1.92	0.51
18:5:610:CLA:H2	26:5:620:LUT:H373	1.93	0.51
12:3:46:TYR:OH	20:3:624:LHG:HC41	2.11	0.50
18:A:802:CLA:H203	18:A:854:CLA:H172	1.92	0.50
2:B:458:PRO:HG3	2:B:518:PHE:HB2	1.92	0.50
2:B:524:ILE:HG12	2:B:591:VAL:HG12	1.93	0.50
8:J:36:PRO:HB3	25:J:103:DGD:HG2	1.93	0.50
13:4:220:PRO:HB3	18:4:608:CLA:HBC2	1.92	0.50
18:A:806:CLA:H52	21:A:849:BCR:HC8	1.92	0.50
18:1:606:CLA:HMB1	18:1:609:CLA:HAC1	1.94	0.50
17:8:204:PRO:HD2	26:8:619:LUT:H23	1.92	0.50
1:A:142:SER:HA	18:A:829:CLA:HMA2	1.94	0.50
18:A:812:CLA:H192	18:A:812:CLA:H141	1.93	0.50
2:B:362:GLN:NE2	2:B:369:GLN:OE1	2.41	0.50
1:A:690:ARG:H	2:B:569:CYS:HB2	1.76	0.50
2:B:173:GLU:HG3	2:B:294:THR:HG22	1.92	0.50
2:B:445:GLN:OE1	2:B:453:GLN:NE2	2.45	0.50
18:B:825:CLA:HBB1	18:B:838:CLA:HBB	1.93	0.50
13:4:203:ASP:N	13:4:203:ASP:OD1	2.44	0.50
14:5:150:GLU:OE1	14:5:153:ARG:NH2	2.33	0.50
15:6:305:ILE:HG12	28:6:624:NEX:H161	1.93	0.50
20:5:625:LHG:H272	24:5:627:LMG:H352	1.93	0.50
18:3:617:CLA:HBB2	21:3:621:BCR:H312	1.94	0.50
2:B:620:TRP:HB3	18:B:802:CLA:H101	1.94	0.50
12:3:159:GLU:OE1	12:3:162:ARG:NH1	2.45	0.50
2:B:269:LEU:HD22	18:B:817:CLA:HBA1	1.94	0.49
21:A:848:BCR:H362	21:A:849:BCR:H21C	1.93	0.49
18:5:610:CLA:HBB1	18:5:612:CLA:H3A	1.95	0.49
18:7:613:CLA:H2	18:7:614:CLA:HMD1	1.95	0.49
18:B:837:CLA:HBC2	25:J:103:DGD:HAF1	1.92	0.49
4:D:136:VAL:HG12	4:D:165:LYS:HB3	1.93	0.49
15:6:184:TRP:CD1	21:6:622:BCR:H12C	2.48	0.49
17:8:117:LEU:HD23	17:8:235:PHE:HZ	1.77	0.49
1:A:282:LEU:HB2	1:A:515:VAL:HG21	1.94	0.49
10:L:190:LEU:HB3	21:L:305:BCR:H401	1.93	0.49
11:1:179:ASP:OD1	26:1:617:LUT:O23	2.31	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:620:BCR:HC42	20:7:622:LHG:HC92	1.93	0.49
1:A:574:PRO:HB3	1:A:720:ILE:HB	1.95	0.49
11:1:158:MET:HG2	18:1:609:CLA:HMC3	1.95	0.49
1:A:204:GLY:HA3	18:A:814:CLA:HBB1	1.94	0.49
18:B:806:CLA:H92	18:B:829:CLA:H102	1.95	0.49
18:8:610:CLA:H92	18:8:612:CLA:HMA1	1.94	0.49
2:B:194:HIS:CE1	18:B:814:CLA:NA	2.80	0.49
13:4:137:VAL:HG11	26:4:619:LUT:H10	1.93	0.49
18:7:610:CLA:HBB1	18:7:612:CLA:H3A	1.95	0.49
1:A:540:ALA:HB2	18:A:839:CLA:HMA1	1.94	0.49
1:A:377:TYR:HD2	1:A:380:LEU:HD22	1.78	0.49
18:A:801:CLA:HED3	18:A:801:CLA:HBD	1.76	0.49
1:A:718:LEU:HG	19:A:844:PQN:H143	1.94	0.48
18:A:829:CLA:H171	21:J:102:BCR:H17C	1.95	0.48
21:B:846:BCR:H321	18:1:603:CLA:H43	1.94	0.48
6:F:162:TYR:HE2	6:F:200:ALA:HA	1.78	0.48
7:I:87:LEU:HD13	7:I:90:ILE:HD12	1.95	0.48
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.96	0.48
2:B:57:ILE:HG21	18:B:806:CLA:HMD2	1.96	0.48
2:B:107:ARG:NH1	2:B:114:VAL:O	2.46	0.48
12:3:171:SER:OG	12:3:172:MET:N	2.46	0.48
18:5:606:CLA:HHC	18:5:606:CLA:HBB1	1.95	0.48
20:5:625:LHG:H181	18:6:620:CLA:HAB	1.95	0.48
16:7:165:PRO:HD3	18:7:608:CLA:HMD2	1.95	0.48
1:A:407:ALA:HA	1:A:592:VAL:HG11	1.94	0.48
1:A:441:LEU:HA	1:A:444:VAL:HG12	1.95	0.48
1:A:596:LEU:HD21	18:A:831:CLA:HBC1	1.95	0.48
10:L:149:GLU:OE2	18:L:302:CLA:ND	2.47	0.48
1:A:508:LEU:HD12	1:A:523:MET:HB3	1.95	0.48
4:D:179:LEU:HD22	4:D:185:LEU:HD12	1.95	0.48
12:3:101:GLY:HA2	27:3:619:XAT:H181	1.95	0.48
15:6:315:GLY:HA2	16:7:95:VAL:HG11	1.95	0.48
1:A:178:TRP:HB2	18:A:812:CLA:HMC3	1.94	0.48
18:A:836:CLA:H41	18:A:836:CLA:H62	1.55	0.48
1:A:21:PRO:HG2	1:A:185:ALA:HB3	1.95	0.48
10:L:193:CYS:SG	21:L:305:BCR:H19C	2.54	0.48
18:5:613:CLA:H111	20:5:623:LHG:H292	1.96	0.48
1:A:49:ILE:HD12	18:A:804:CLA:HBD	1.95	0.48
1:A:674:GLY:O	1:A:677:PHE:HB3	2.14	0.48
2:B:277:HIS:HE1	18:B:817:CLA:ND	2.09	0.48
18:3:609:CLA:HBA2	18:3:609:CLA:H3A	1.38	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:607:CLA:HBB2	18:5:609:CLA:HBC1	1.94	0.48
16:7:73:LEU:O	16:7:77:ARG:HG2	2.14	0.48
1:A:419:PRO:HG3	4:D:148:GLU:HB2	1.95	0.48
12:3:161:ARG:NE	12:3:172:MET:SD	2.80	0.48
17:8:237:ALA:HB1	18:8:616:CLA:HBA2	1.95	0.48
18:A:807:CLA:H13	18:A:807:CLA:H101	1.69	0.48
18:A:816:CLA:HMA2	23:A:857:LMU:H21	1.95	0.48
18:A:835:CLA:HAA2	10:L:165:LEU:HD12	1.96	0.48
18:B:840:CLA:H201	10:L:196:ILE:HD13	1.96	0.48
12:3:238:THR:OG1	12:3:261:ASN:ND2	2.45	0.48
18:A:802:CLA:H102	18:A:842:CLA:HMC2	1.96	0.47
2:B:326:THR:HG21	2:B:404:ASN:HD21	1.79	0.47
2:B:517:ASP:HA	2:B:520:VAL:HG12	1.95	0.47
13:4:254:GLY:O	13:4:258:GLN:CB	2.61	0.47
14:5:219:LEU:HD22	14:5:270:TRP:HZ3	1.79	0.47
15:6:190:TRP:CE2	15:6:194:ARG:HD2	2.49	0.47
15:6:297:PRO:O	15:6:309:THR:OG1	2.32	0.47
1:A:320:HIS:CE1	18:A:823:CLA:NA	2.81	0.47
18:A:828:CLA:H152	18:A:828:CLA:H111	1.69	0.47
2:B:354:TYR:HA	2:B:369:GLN:HE22	1.79	0.47
18:1:610:CLA:HBB1	18:1:612:CLA:H3A	1.95	0.47
18:3:606:CLA:HBA1	21:3:620:BCR:H19C	1.95	0.47
2:B:182:GLY:HA3	18:B:813:CLA:HBB1	1.96	0.47
2:B:546:LYS:NZ	5:E:96:SER:O	2.42	0.47
4:D:137:ILE:HD13	4:D:175:LEU:HD23	1.96	0.47
18:1:601:CLA:H11	17:8:161:PHE:HB2	1.96	0.47
18:6:607:CLA:HBB	28:6:624:NEX:H371	1.96	0.47
18:B:809:CLA:H101	18:B:829:CLA:H202	1.96	0.47
2:B:363:ALA:HA	2:B:369:GLN:HG3	1.97	0.47
6:F:189:VAL:H	24:J:104:LMG:HC61	1.79	0.47
2:B:671:TYR:OH	18:B:803:CLA:OBD	2.26	0.47
17:8:223:LYS:NZ	20:8:622:LHG:O6	2.32	0.47
1:A:477:ILE:HG12	23:A:859:LMU:H1B	1.97	0.47
18:A:809:CLA:HAA1	18:A:829:CLA:HED2	1.97	0.47
10:L:161:PRO:HG3	18:L:304:CLA:HAB	1.95	0.47
14:5:244:ILE:HB	18:5:613:CLA:H2	1.95	0.47
18:B:813:CLA:H71	18:B:813:CLA:H142	1.97	0.47
18:B:824:CLA:H71	18:B:826:CLA:H42	1.97	0.47
18:B:831:CLA:HAC1	18:B:838:CLA:HBC3	1.97	0.47
12:3:203:LEU:HB2	18:3:610:CLA:HBA1	1.97	0.47
1:A:261:ILE:HG13	12:3:262:PHE:HD1	1.79	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:CYS:SG	3:C:55:GLU:N	2.88	0.47
6:F:162:TYR:OH	6:F:196:ALA:O	2.27	0.47
9:K:126:ASN:HB2	18:K:201:CLA:HBA2	1.97	0.47
13:4:220:PRO:HD3	18:4:608:CLA:HMD2	1.97	0.47
1:A:572:ARG:HH21	20:A:846:LHG:HC32	1.80	0.46
21:A:856:BCR:H391	8:J:12:PRO:HB2	1.96	0.46
11:1:162:GLU:OE2	18:1:609:CLA:ND	2.48	0.46
18:4:610:CLA:HBB1	18:4:612:CLA:H3A	1.96	0.46
16:7:47:LEU:HD11	16:7:65:LEU:HD11	1.97	0.46
11:1:60:LEU:HD12	18:1:601:CLA:HMA3	1.97	0.46
18:4:614:CLA:H62	18:4:614:CLA:H41	1.66	0.46
18:5:604:CLA:H92	18:5:604:CLA:H61	1.83	0.46
18:7:604:CLA:HBB1	27:7:620:XAT:H192	1.97	0.46
2:B:525:ALA:HB2	18:B:837:CLA:HMA1	1.98	0.46
18:B:833:CLA:HMA1	25:J:103:DGD:HA71	1.97	0.46
4:D:104:TRP:HE3	4:D:104:TRP:O	1.98	0.46
13:4:112:LEU:HD13	18:4:602:CLA:H42	1.97	0.46
1:A:150:ALA:HB2	1:A:378:PRO:HD2	1.97	0.46
18:A:806:CLA:H203	18:A:814:CLA:H62	1.98	0.46
2:B:494:TRP:CH2	18:B:835:CLA:H2A	2.50	0.46
3:C:24:ASP:OD1	3:C:44:ARG:NH2	2.45	0.46
12:3:237:MET:HE2	12:3:261:ASN:HB3	1.96	0.46
1:A:485:GLN:NE2	1:A:528:LEU:O	2.46	0.46
17:8:223:LYS:HZ1	20:8:622:LHG:C4	2.25	0.46
1:A:153:ILE:HD13	18:A:815:CLA:HED3	1.97	0.46
1:A:297:HIS:HE2	18:A:820:CLA:C2B	2.29	0.46
18:A:801:CLA:H62	18:A:801:CLA:H102	1.77	0.46
18:A:830:CLA:H91	18:A:830:CLA:H111	1.80	0.46
18:B:813:CLA:H203	21:B:844:BCR:H381	1.98	0.46
14:5:265:PRO:HB2	18:5:607:CLA:H42	1.97	0.46
21:8:621:BCR:H15C	21:8:621:BCR:H351	1.76	0.46
3:C:13:GLY:O	3:C:38:GLN:NE2	2.48	0.46
21:3:621:BCR:H20C	21:3:621:BCR:H361	1.65	0.46
17:8:198:PRO:HB3	18:8:608:CLA:HBC2	1.96	0.46
18:A:814:CLA:H61	18:A:814:CLA:H41	1.64	0.46
19:A:844:PQN:H141	18:F:301:CLA:HBB2	1.97	0.46
18:B:829:CLA:HBC2	25:B:850:DGD:HB92	1.97	0.46
21:B:848:BCR:H20C	21:B:848:BCR:H361	1.77	0.46
25:B:850:DGD:O5D	25:B:850:DGD:O4D	2.32	0.46
13:4:137:VAL:HG11	26:4:619:LUT:H12	1.98	0.46
1:A:547:VAL:HG11	18:A:840:CLA:HMB3	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ALA:HB3	2:B:377:GLN:HE21	1.81	0.46
2:B:478:LEU:O	2:B:484:SER:OG	2.30	0.46
10:L:127:VAL:HG12	10:L:130:TYR:H	1.80	0.46
21:3:620:BCR:H11C	21:3:620:BCR:H341	1.76	0.46
15:6:269:HIS:CG	18:6:613:CLA:HAA2	2.51	0.46
1:A:102:GLU:OE2	1:A:156:GLU:N	2.48	0.46
18:A:802:CLA:CGA	18:A:802:CLA:H3A	2.46	0.46
18:A:818:CLA:H11	9:K:152:LEU:HD13	1.97	0.46
18:A:828:CLA:H2	18:A:836:CLA:H92	1.97	0.46
18:A:841:CLA:HBB1	18:F:301:CLA:HMD1	1.98	0.46
21:A:852:BCR:H391	18:B:832:CLA:HMA1	1.98	0.46
15:6:136:SER:HB2	15:6:241:GLY:HA3	1.97	0.46
15:6:188:ARG:HB3	18:6:608:CLA:HMC3	1.97	0.46
16:7:185:GLU:HG2	16:7:189:LYS:HD2	1.98	0.46
18:A:814:CLA:H43	21:A:849:BCR:H14C	1.98	0.45
18:A:831:CLA:H102	18:A:842:CLA:HAA2	1.98	0.45
21:3:622:BCR:H20C	21:3:622:BCR:H361	1.55	0.45
14:5:77:LEU:HD13	18:5:602:CLA:H42	1.98	0.45
2:B:340:ALA:HB2	21:B:847:BCR:H372	1.97	0.45
12:3:141:TRP:HB3	14:5:271:PRO:HB3	1.99	0.45
16:7:192:LYS:NZ	20:7:622:LHG:O5	2.42	0.45
18:A:854:CLA:H41	18:A:854:CLA:H61	1.56	0.45
17:8:131:PRO:HG3	17:8:139:VAL:HG21	1.97	0.45
1:A:561:ARG:NH1	4:D:122:THR:O	2.50	0.45
1:A:45:THR:HG22	1:A:47:THR:H	1.81	0.45
1:A:80:GLN:HE21	1:A:84:ILE:HG13	1.81	0.45
21:B:846:BCR:H24C	21:B:847:BCR:H21C	1.98	0.45
4:D:191:ARG:HB3	4:D:199:GLN:HB3	1.98	0.45
10:L:189:ILE:HD11	21:L:301:BCR:H272	1.98	0.45
18:A:854:CLA:H11	2:B:617:LEU:HD12	1.96	0.45
2:B:143:LEU:HG	21:B:845:BCR:H382	1.99	0.45
2:B:359:TYR:OH	18:B:828:CLA:OBD	2.23	0.45
2:B:657:ILE:HG12	18:B:840:CLA:HMB3	1.98	0.45
9:K:125:SER:HB2	9:K:132:THR:HG22	1.98	0.45
17:8:152:LEU:HD12	18:8:607:CLA:HBC3	1.97	0.45
18:A:809:CLA:HMC3	18:A:810:CLA:HMD2	1.98	0.45
21:B:801:BCR:H333	18:B:833:CLA:H11	1.99	0.45
4:D:137:ILE:HG21	4:D:175:LEU:HD23	1.98	0.45
26:4:619:LUT:H35	26:4:619:LUT:H401	1.81	0.45
18:7:602:CLA:H61	27:7:620:XAT:H28	1.97	0.45
2:B:494:TRP:HE1	18:B:834:CLA:HED1	1.82	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:807:CLA:O1A	7:I:83:THR:OG1	2.35	0.45
18:B:810:CLA:H172	10:L:188:LEU:HD23	1.99	0.45
11:1:209:LEU:HD23	18:1:603:CLA:HBB2	1.99	0.45
14:5:212:ILE:HD12	20:5:623:LHG:H261	1.98	0.45
18:5:612:CLA:HMC2	26:5:620:LUT:H11	1.98	0.45
4:D:104:TRP:O	4:D:104:TRP:CE3	2.70	0.45
6:F:195:LEU:HD13	6:F:195:LEU:HA	1.84	0.45
11:1:164:GLN:HG3	18:1:608:CLA:HMC3	1.98	0.45
16:7:203:GLY:O	16:7:207:GLN:NE2	2.50	0.45
1:A:481:PRO:HG3	1:A:533:PHE:HB2	1.97	0.45
2:B:375:HIS:HE2	18:B:828:CLA:C1B	2.29	0.45
18:B:805:CLA:HBA1	18:B:805:CLA:H3A	1.72	0.45
27:5:621:XAT:H15	27:5:621:XAT:H201	1.82	0.45
16:7:82:GLY:HA2	27:7:620:XAT:H181	1.99	0.45
1:A:14:LYS:NZ	1:A:15:ILE:O	2.42	0.44
18:A:801:CLA:HMB1	18:B:802:CLA:HAA1	1.98	0.44
18:A:829:CLA:H141	18:A:829:CLA:H193	1.99	0.44
4:D:139:TRP:HB3	4:D:187:PRO:HB3	1.98	0.44
18:1:608:CLA:HMB3	21:1:619:BCR:H362	1.98	0.44
12:3:177:PHE:CZ	18:3:608:CLA:HBB2	2.52	0.44
26:3:618:LUT:H15	26:3:618:LUT:H201	1.83	0.44
16:7:34:PHE:HD1	18:7:601:CLA:HMA3	1.82	0.44
16:7:130:TRP:CD1	21:7:621:BCR:H12C	2.52	0.44
18:A:820:CLA:H203	18:A:828:CLA:H3A	1.98	0.44
18:A:820:CLA:HBA2	18:A:820:CLA:H3A	1.64	0.44
18:A:825:CLA:H193	18:A:825:CLA:H162	1.83	0.44
2:B:578:TYR:HE1	2:B:711:LEU:HB2	1.82	0.44
21:L:305:BCR:H11C	21:L:305:BCR:H341	1.84	0.44
12:3:156:GLN:OE1	18:3:617:CLA:ND	2.51	0.44
14:5:119:GLU:O	14:5:125:ASN:ND2	2.39	0.44
18:6:611:CLA:HAC2	18:6:613:CLA:H192	1.98	0.44
16:7:58:LEU:HD13	18:7:602:CLA:H42	1.99	0.44
18:A:806:CLA:H2	18:A:806:CLA:H62	1.71	0.44
2:B:21:ARG:HH22	7:I:99:ILE:HG22	1.82	0.44
18:8:613:CLA:H52	18:8:614:CLA:HMD1	1.99	0.44
28:6:624:NEX:H15	28:6:624:NEX:H201	1.80	0.44
18:7:604:CLA:HAB	21:7:621:BCR:H393	1.98	0.44
1:A:36:SER:HB3	1:A:39:LEU:HB2	1.99	0.44
18:A:802:CLA:H171	18:A:842:CLA:H51	1.99	0.44
18:A:827:CLA:HAB	21:A:851:BCR:H311	2.00	0.44
2:B:54:GLN:HE21	2:B:58:ILE:HG13	1.83	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ARG:HB2	18:B:813:CLA:HBC2	1.99	0.44
2:B:475:PHE:HE1	6:F:139:LEU:HD21	1.82	0.44
21:B:845:BCR:H24C	21:B:845:BCR:H371	1.71	0.44
4:D:109:LEU:HB2	4:D:190:TYR:CE2	2.53	0.44
18:3:617:CLA:O1D	18:7:601:CLA:H3A	2.17	0.44
27:3:619:XAT:H15	27:3:619:XAT:H201	1.81	0.44
17:8:234:GLY:O	17:8:238:GLN:HG3	2.18	0.44
17:8:254:LEU:HD21	18:8:614:CLA:HMC3	1.99	0.44
1:A:622:VAL:HG23	1:A:627:VAL:HB	2.00	0.44
7:I:81:PRO:O	7:I:85:LEU:HB2	2.18	0.44
18:4:613:CLA:H143	18:4:613:CLA:H111	1.82	0.44
14:5:183:GLY:N	18:5:610:CLA:OBD	2.51	0.44
16:7:144:SER:OG	16:7:145:GLN:N	2.50	0.44
18:8:610:CLA:H51	26:8:619:LUT:H373	2.00	0.44
1:A:363:LEU:HD11	18:A:830:CLA:H202	2.00	0.44
21:A:848:BCR:H20C	21:A:848:BCR:H361	1.78	0.44
4:D:202:HIS:CG	4:D:203:PRO:CD	2.83	0.44
18:1:613:CLA:H121	20:1:620:LHG:H282	2.00	0.44
21:1:619:BCR:H20C	21:1:619:BCR:H361	1.83	0.44
18:3:606:CLA:HMB2	21:3:620:BCR:H373	1.99	0.44
14:5:169:PHE:HE2	18:5:618:CLA:H3A	1.82	0.44
14:5:219:LEU:HD21	14:5:269:LEU:HD23	1.99	0.44
19:A:844:PQN:H142	19:A:844:PQN:H112	1.87	0.44
21:B:843:BCR:H11C	21:B:843:BCR:H341	1.83	0.44
14:5:196:LEU:O	14:5:200:GLN:HB2	2.18	0.44
27:8:620:XAT:H15	27:8:620:XAT:H201	1.79	0.44
1:A:128:ASN:HB3	1:A:136:GLN:HB3	1.99	0.44
18:A:842:CLA:H3A	18:A:842:CLA:HBA2	1.57	0.44
18:B:832:CLA:H2	18:B:832:CLA:H62	1.74	0.44
18:1:611:CLA:H52	18:1:611:CLA:H12	1.83	0.44
18:3:609:CLA:H2A	18:3:609:CLA:HED2	1.98	0.44
14:5:214:TYR:CZ	27:5:621:XAT:H8	2.53	0.44
18:B:818:CLA:H3A	18:B:818:CLA:HBA2	1.58	0.43
14:5:73:ASP:HB2	18:5:602:CLA:HBA2	2.00	0.43
28:5:624:NEX:H11	28:5:624:NEX:H191	1.88	0.43
15:6:284:VAL:HB	18:6:616:CLA:C1C	2.48	0.43
1:A:80:GLN:HB2	18:A:806:CLA:HMB2	1.99	0.43
18:A:829:CLA:H143	18:A:829:CLA:H111	1.86	0.43
21:A:851:BCR:H20C	21:A:851:BCR:H361	1.85	0.43
12:3:192:TYR:HB3	18:3:610:CLA:HED2	1.99	0.43
20:4:622:LHG:H132	18:6:617:CLA:HED3	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:TYR:HB3	18:B:827:CLA:HMC3	1.99	0.43
21:B:846:BCR:H11C	21:B:846:BCR:H341	1.84	0.43
17:8:161:PHE:CD2	21:8:621:BCR:H12C	2.53	0.43
1:A:146:GLN:HB3	1:A:377:TYR:HB3	1.99	0.43
18:A:804:CLA:H72	18:A:804:CLA:H111	1.83	0.43
18:A:819:CLA:HBC1	18:A:828:CLA:H18	2.00	0.43
6:F:137:PRO:HB2	18:F:304:CLA:HBC3	2.00	0.43
21:L:301:BCR:H24C	21:L:301:BCR:H371	1.76	0.43
15:6:310:PRO:O	15:6:312:PHE:N	2.43	0.43
18:8:606:CLA:H151	18:8:608:CLA:HED2	1.99	0.43
1:A:83:ILE:HD11	18:A:812:CLA:H122	2.00	0.43
1:A:240:PRO:HA	1:A:243:LEU:HD12	2.01	0.43
1:A:680:ALA:HB3	18:A:802:CLA:HBB2	2.00	0.43
18:B:818:CLA:H93	18:B:818:CLA:H61	1.89	0.43
3:C:7:ILE:HG22	3:C:65:VAL:HG12	2.01	0.43
10:L:164:LYS:HD3	18:L:304:CLA:HMB2	2.00	0.43
20:3:624:LHG:HC61	20:3:624:LHG:H241	1.79	0.43
1:A:349:TRP:HB3	18:A:806:CLA:HAC1	2.00	0.43
11:1:180:PRO:HD2	26:1:617:LUT:H23	2.00	0.43
12:3:44:GLN:HB2	12:3:45:LEU:H	1.67	0.43
26:3:618:LUT:H35	26:3:618:LUT:H401	1.89	0.43
18:6:604:CLA:H93	18:6:604:CLA:H111	1.90	0.43
16:7:77:ARG:HD2	18:7:610:CLA:C4C	2.48	0.43
18:8:601:CLA:H93	18:8:613:CLA:H122	2.00	0.43
18:8:604:CLA:H3A	18:8:604:CLA:HBA2	1.73	0.43
5:E:84:LYS:HG2	5:E:87:SER:HB3	2.00	0.43
18:L:302:CLA:HBA2	18:L:302:CLA:H3A	1.43	0.43
21:4:621:BCR:H11C	21:4:621:BCR:H341	1.84	0.43
18:8:610:CLA:H41	18:8:610:CLA:H62	1.59	0.43
18:B:817:CLA:HBA2	18:B:817:CLA:H3A	1.38	0.43
13:4:179:GLN:HE21	18:4:609:CLA:HMC1	1.84	0.43
14:5:214:TYR:CE2	27:5:621:XAT:H10	2.54	0.43
18:6:604:CLA:H161	18:6:604:CLA:H141	1.81	0.43
21:7:623:BCR:H371	21:7:623:BCR:H24C	1.77	0.43
1:A:393:HIS:HE1	18:A:829:CLA:ND	2.12	0.43
1:A:538:ILE:HG23	18:A:801:CLA:H193	2.00	0.43
18:A:819:CLA:HBA2	18:A:819:CLA:H3A	1.66	0.43
18:A:834:CLA:HBB1	23:A:859:LMU:H41	2.01	0.43
12:3:184:PHE:CG	18:3:608:CLA:HMC2	2.54	0.43
16:7:137:TYR:HB3	17:8:62:GLY:HA3	2.01	0.43
1:A:366:ILE:HG21	18:A:820:CLA:H201	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:SER:HB2	2:B:682:ALA:HB2	2.00	0.43
18:A:821:CLA:H3A	18:A:821:CLA:HBA2	1.62	0.43
18:A:822:CLA:HMB2	18:A:826:CLA:HMA3	2.01	0.43
18:A:828:CLA:H202	18:A:828:CLA:H162	1.89	0.43
21:A:850:BCR:H11C	21:A:850:BCR:H341	1.84	0.43
21:A:850:BCR:H24C	21:A:850:BCR:H371	1.79	0.43
2:B:411:ARG:O	2:B:415:HIS:ND1	2.52	0.43
18:B:819:CLA:HMB2	18:B:824:CLA:HMA3	2.00	0.43
21:F:305:BCR:H20C	21:F:305:BCR:H361	1.77	0.43
8:J:5:THR:HB	24:J:104:LMG:HC71	2.00	0.43
12:3:216:LYS:HE2	18:3:612:CLA:HAA2	2.00	0.43
20:3:623:LHG:HC41	16:7:227:ASN:HD21	1.83	0.43
13:4:185:TRP:CD1	21:4:621:BCR:H12C	2.54	0.43
16:7:134:LYS:HE3	18:7:608:CLA:HMC3	2.00	0.43
18:8:613:CLA:H91	20:8:622:LHG:H321	2.00	0.43
1:A:547:VAL:HG21	18:A:840:CLA:HMA1	2.02	0.42
1:A:566:LYS:NZ	2:B:674:GLU:OE2	2.39	0.42
18:A:835:CLA:H52	21:L:301:BCR:H363	2.01	0.42
2:B:76:GLU:HG2	2:B:132:THR:HA	2.01	0.42
11:1:208:PHE:CD2	27:1:618:XAT:H12	2.54	0.42
18:1:603:CLA:H41	18:1:603:CLA:H61	1.83	0.42
13:4:276:ASP:OD1	13:4:276:ASP:N	2.52	0.42
14:5:99:MET:SD	18:5:610:CLA:HAB	2.59	0.42
18:5:609:CLA:H3A	18:5:609:CLA:HBA2	1.73	0.42
15:6:236:LYS:HD3	18:6:612:CLA:HBD	1.99	0.42
18:6:604:CLA:H171	21:6:622:BCR:H392	2.01	0.42
16:7:92:GLY:HA3	16:7:99:PHE:HD2	1.83	0.42
16:7:189:LYS:HE3	18:7:612:CLA:HAA2	2.01	0.42
18:A:828:CLA:H203	18:A:836:CLA:H71	2.01	0.42
18:A:834:CLA:H141	18:A:834:CLA:H161	1.76	0.42
3:C:55:GLU:HB2	3:C:63:LEU:HG	2.01	0.42
6:F:188:ASP:HA	24:J:104:LMG:HC61	2.01	0.42
21:3:622:BCR:H341	21:3:622:BCR:H11C	1.59	0.42
14:5:192:SER:OG	14:5:193:LYS:N	2.50	0.42
18:5:602:CLA:H2	27:5:621:XAT:H382	2.01	0.42
15:6:130:GLU:HG2	15:6:193:LEU:HD12	2.01	0.42
18:B:807:CLA:HMB1	18:B:808:CLA:H193	2.02	0.42
13:4:273:HIS:CG	18:4:613:CLA:HAA2	2.54	0.42
18:4:603:CLA:HBC3	27:4:620:XAT:H11	2.02	0.42
14:5:154:TRP:CG	18:5:617:CLA:HBC1	2.54	0.42
2:B:588:ILE:HA	2:B:591:VAL:HG22	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:VAL:HG22	3:C:67:VAL:HG22	1.99	0.42
10:L:133:ASN:HB3	18:L:302:CLA:HAC1	2.01	0.42
21:L:305:BCR:H15C	21:L:305:BCR:H351	1.88	0.42
18:1:603:CLA:H11	18:1:603:CLA:HMA2	2.01	0.42
21:4:621:BCR:H15C	21:4:621:BCR:H351	1.82	0.42
14:5:149:VAL:HG21	21:5:622:BCR:H362	2.01	0.42
18:6:601:CLA:H111	18:6:601:CLA:H152	1.93	0.42
16:7:165:PRO:HB3	18:7:608:CLA:HBC2	2.02	0.42
1:A:589:TRP:CD1	18:A:831:CLA:HMD1	2.55	0.42
2:B:429:PHE:CE2	18:B:837:CLA:HAB	2.55	0.42
14:5:59:PRO:HD2	14:5:62:LEU:HD12	2.02	0.42
15:6:133:LEU:HB3	15:6:137:ARG:NH2	2.34	0.42
17:8:165:LYS:HZ1	17:8:189:LEU:HD23	1.85	0.42
1:A:655:SER:O	1:A:659:GLN:NE2	2.52	0.42
18:1:602:CLA:H2A	18:1:602:CLA:HED2	2.01	0.42
18:4:610:CLA:HBB2	26:4:619:LUT:H34	2.01	0.42
14:5:227:GLY:O	14:5:231:ALA:N	2.45	0.42
15:6:201:GLN:NE2	15:6:206:SER:OG	2.53	0.42
18:A:842:CLA:H101	18:A:842:CLA:H62	1.86	0.42
21:A:856:BCR:H15C	8:J:20:THR:HG22	2.00	0.42
18:B:827:CLA:HBA2	18:B:827:CLA:H3A	1.75	0.42
18:5:609:CLA:H13	18:5:609:CLA:H101	1.91	0.42
18:A:841:CLA:H111	18:A:841:CLA:HHC	2.02	0.42
18:B:839:CLA:HMA2	7:I:96:PHE:HE1	1.84	0.42
21:B:847:BCR:H351	21:B:847:BCR:H15C	1.79	0.42
24:J:104:LMG:H182	24:J:104:LMG:H152	1.84	0.42
2:B:54:GLN:HB2	18:B:805:CLA:HMB2	2.02	0.42
18:B:807:CLA:HED2	7:I:76:PRO:HB3	2.02	0.42
7:I:82:LEU:HA	7:I:86:VAL:HB	2.02	0.42
21:3:620:BCR:H21C	21:3:620:BCR:H24C	1.86	0.42
21:5:622:BCR:H20C	21:5:622:BCR:H361	1.87	0.42
15:6:114:ASP:HB2	18:6:602:CLA:HBA2	2.02	0.42
18:8:610:CLA:H112	18:8:610:CLA:H91	1.76	0.42
1:A:691:GLY:N	2:B:569:CYS:O	2.48	0.42
2:B:490:GLY:HA3	2:B:495:LEU:HD13	2.00	0.42
4:D:136:VAL:HB	4:D:163:LEU:HD11	2.01	0.42
14:5:182:PRO:HD3	18:5:608:CLA:HMD2	2.02	0.42
14:5:262:LEU:HA	15:6:288:GLN:HE21	1.84	0.42
27:6:621:XAT:H15	27:6:621:XAT:H201	1.86	0.42
21:7:621:BCR:H15C	21:7:621:BCR:H351	1.84	0.42
26:8:619:LUT:H35	26:8:619:LUT:H401	1.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:808:CLA:H11	23:A:858:LMU:H21	2.01	0.41
21:F:305:BCR:H24C	21:F:305:BCR:H371	1.70	0.41
21:K:207:BCR:H20C	21:K:207:BCR:H361	1.84	0.41
10:L:146:ARG:HH11	10:L:223:LEU:HD22	1.84	0.41
13:4:282:VAL:N	18:4:613:CLA:O1A	2.53	0.41
18:6:616:CLA:H192	18:6:620:CLA:HBC1	2.01	0.41
21:A:849:BCR:H15C	21:A:849:BCR:H351	1.81	0.41
18:B:803:CLA:H111	18:B:803:CLA:H142	1.78	0.41
11:1:103:ARG:NE	18:1:608:CLA:OBD	2.53	0.41
14:5:219:LEU:HD11	18:5:616:CLA:HMB3	2.01	0.41
16:7:43:LEU:HD12	16:7:43:LEU:HA	1.88	0.41
16:7:82:GLY:O	16:7:86:ILE:HD12	2.20	0.41
16:7:228:HIS:HA	16:7:233:THR:HG21	2.01	0.41
26:7:619:LUT:H15	26:7:619:LUT:H201	1.82	0.41
27:7:620:XAT:H35	27:7:620:XAT:H401	1.85	0.41
18:A:811:CLA:H122	18:A:811:CLA:H162	1.88	0.41
18:A:812:CLA:H62	18:A:812:CLA:H41	1.96	0.41
18:A:839:CLA:HBB2	18:A:840:CLA:HBC3	2.02	0.41
2:B:478:LEU:HD23	2:B:478:LEU:HA	1.86	0.41
21:B:848:BCR:H351	21:B:848:BCR:H15C	1.82	0.41
18:1:603:CLA:HBB1	27:1:618:XAT:C35	2.50	0.41
18:3:604:CLA:HMC1	21:3:622:BCR:H21C	2.02	0.41
18:3:610:CLA:HBB1	18:3:610:CLA:H51	2.02	0.41
21:6:622:BCR:H24C	21:6:622:BCR:H371	1.94	0.41
18:A:822:CLA:H192	21:A:850:BCR:H272	2.01	0.41
18:A:830:CLA:HBD	18:A:830:CLA:H11	2.02	0.41
2:B:601:THR:HG21	2:B:610:PHE:HB2	2.02	0.41
21:B:843:BCR:H20C	21:B:843:BCR:H361	1.82	0.41
18:1:613:CLA:H3A	18:1:613:CLA:HBA2	1.84	0.41
12:3:95:ALA:HB1	12:3:221:GLY:HA3	2.02	0.41
13:4:187:GLU:OE2	18:4:609:CLA:ND	2.53	0.41
18:5:606:CLA:HBB2	18:5:607:CLA:CBB	2.50	0.41
20:8:623:LHG:H271	23:8:624:LMU:H81	2.02	0.41
1:A:126:ILE:HG21	2:B:447:PHE:HA	2.02	0.41
1:A:536:HIS:CG	18:A:839:CLA:HED3	2.55	0.41
11:1:235:GLY:HA2	11:1:240:THR:HG21	2.02	0.41
1:A:736:ILE:HG21	18:A:829:CLA:HMC2	2.02	0.41
18:A:814:CLA:H121	18:A:814:CLA:HMB3	2.02	0.41
2:B:348:LEU:HD23	18:B:818:CLA:H62	2.01	0.41
21:B:843:BCR:H24C	21:B:843:BCR:H371	1.92	0.41
4:D:128:LYS:HG2	4:D:132:GLU:HB2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:73:LEU:HG	12:3:84:PRO:HB3	2.01	0.41
12:3:178:LEU:HD12	18:5:619:CLA:HMB1	2.01	0.41
18:5:602:CLA:H162	18:5:602:CLA:H141	1.85	0.41
18:A:806:CLA:H112	18:A:806:CLA:H91	1.87	0.41
18:A:834:CLA:H152	19:B:842:PQN:H191	2.03	0.41
18:A:841:CLA:H162	18:A:841:CLA:H192	1.84	0.41
18:B:831:CLA:H13	18:B:831:CLA:H102	1.81	0.41
6:F:158:TYR:O	6:F:162:TYR:HB2	2.21	0.41
10:L:138:ARG:NH1	10:L:149:GLU:OE1	2.53	0.41
12:3:180:LEU:HD11	21:3:622:BCR:HC22	2.02	0.41
1:A:458:HIS:CE1	18:A:835:CLA:NA	2.89	0.41
1:A:681:PHE:HZ	18:A:842:CLA:HBC2	1.85	0.41
18:A:806:CLA:H161	18:A:806:CLA:H202	1.86	0.41
2:B:398:ASP:HA	4:D:233:ILE:HD13	2.02	0.41
18:B:829:CLA:H71	18:B:840:CLA:HED1	2.02	0.41
11:1:129:TRP:CE2	11:1:136:ALA:HB2	2.56	0.41
17:8:106:CYS:HB2	17:8:225:GLY:HA3	2.03	0.41
1:A:83:ILE:HG21	18:A:807:CLA:HMD2	2.02	0.41
1:A:646:LEU:HD22	2:B:652:LEU:HD21	2.03	0.41
18:A:803:CLA:H141	18:A:803:CLA:H161	1.84	0.41
18:A:825:CLA:H93	18:A:825:CLA:H111	1.88	0.41
18:A:825:CLA:H43	21:A:851:BCR:H16C	2.02	0.41
21:A:852:BCR:H371	21:A:852:BCR:H24C	1.81	0.41
18:B:806:CLA:H93	18:B:806:CLA:H61	1.88	0.41
18:B:818:CLA:H62	18:B:818:CLA:H41	1.80	0.41
18:B:830:CLA:HMB2	18:B:831:CLA:C3D	2.51	0.41
18:B:834:CLA:H61	18:B:834:CLA:H102	1.87	0.41
18:B:841:CLA:H3A	18:B:841:CLA:HBA1	1.82	0.41
10:L:145:LEU:HD21	18:L:302:CLA:HED3	2.03	0.41
12:3:97:TRP:CE2	18:3:608:CLA:HED2	2.55	0.41
18:5:607:CLA:H91	18:5:607:CLA:H111	1.93	0.41
28:5:624:NEX:H21	15:6:290:VAL:HG11	2.02	0.41
28:5:624:NEX:H30	18:6:616:CLA:H42	2.02	0.41
18:6:604:CLA:H71	21:6:622:BCR:H402	2.02	0.41
1:A:687:PHE:CG	2:B:665:LEU:HD22	2.56	0.41
18:A:818:CLA:CHD	18:A:819:CLA:HBB2	2.51	0.41
18:A:818:CLA:H91	18:A:818:CLA:H112	1.82	0.41
18:A:833:CLA:HMB1	18:A:843:CLA:HAA2	2.02	0.41
18:A:843:CLA:H202	18:A:843:CLA:H161	1.84	0.41
2:B:9:PHE:HB2	2:B:35:HIS:CG	2.56	0.41
18:B:831:CLA:H62	18:B:831:CLA:H41	1.97	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:137:PRO:HG2	21:F:305:BCR:H333	2.03	0.41
26:1:617:LUT:H35	26:1:617:LUT:H401	1.83	0.41
18:3:604:CLA:H11	18:3:615:CLA:HMB2	2.02	0.41
14:5:118:TYR:CD1	18:5:607:CLA:HMA2	2.56	0.41
18:5:602:CLA:H192	18:5:613:CLA:H162	2.02	0.41
18:5:608:CLA:HBB2	18:5:618:CLA:CHC	2.51	0.41
18:6:609:CLA:HBA1	18:6:609:CLA:H3A	1.93	0.41
18:7:610:CLA:H93	18:7:612:CLA:HMA1	2.01	0.41
18:A:841:CLA:H142	18:A:841:CLA:H112	1.87	0.40
21:A:848:BCR:H11C	21:A:848:BCR:H341	1.82	0.40
2:B:429:PHE:CD2	18:B:837:CLA:HAB	2.56	0.40
18:B:833:CLA:H41	18:B:833:CLA:H61	1.58	0.40
21:F:305:BCR:H16C	21:F:305:BCR:H19C	1.83	0.40
9:K:144:HIS:ND1	21:K:207:BCR:H12C	2.35	0.40
21:K:207:BCR:H11C	21:K:207:BCR:H341	1.94	0.40
11:1:83:SER:HB2	11:1:86:LYS:HE3	2.03	0.40
18:6:616:CLA:H91	18:6:616:CLA:H111	1.83	0.40
1:A:286:THR:HG23	1:A:288:GLY:H	1.86	0.40
1:A:729:ALA:HA	20:A:846:LHG:H341	2.03	0.40
21:A:850:BCR:H15C	21:A:850:BCR:H351	1.83	0.40
18:B:811:CLA:H41	18:B:811:CLA:H61	1.89	0.40
21:K:202:BCR:H11C	21:K:202:BCR:H341	1.86	0.40
18:3:607:CLA:H92	18:3:617:CLA:HMB2	2.01	0.40
18:3:610:CLA:H43	18:3:612:CLA:HBA1	2.03	0.40
18:4:601:CLA:H3A	18:4:601:CLA:HBA2	1.48	0.40
1:A:48:TRP:HE3	1:A:49:ILE:HG22	1.86	0.40
21:A:856:BCR:HC32	8:J:31:ARG:HH11	1.85	0.40
23:A:858:LMU:H122	23:A:858:LMU:H91	1.93	0.40
6:F:179:LYS:NZ	6:F:182:ASP:OD2	2.41	0.40
7:I:88:PRO:HA	7:I:91:ALA:HB3	2.04	0.40
21:3:621:BCR:H11C	21:3:621:BCR:H341	1.60	0.40
21:5:622:BCR:H24C	21:5:622:BCR:H371	1.92	0.40
26:6:619:LUT:H35	26:6:619:LUT:H401	1.86	0.40
16:7:196:LEU:HD12	26:7:619:LUT:H11	2.03	0.40
1:A:451:HIS:HB3	23:A:859:LMU:H92	2.03	0.40
18:B:810:CLA:HED1	21:L:301:BCR:H382	2.03	0.40
18:B:813:CLA:H141	18:B:813:CLA:H162	1.80	0.40
9:K:112:LEU:HG	18:K:206:CLA:HAA2	2.02	0.40
12:3:148:PHE:CG	18:3:607:CLA:HAA1	2.56	0.40
17:8:232:PHE:CD2	27:8:620:XAT:H12	2.57	0.40
18:A:829:CLA:H62	18:A:829:CLA:H101	1.88	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:PHE:HD1	2:B:150:PHE:HD1	1.69	0.40
21:J:102:BCR:H15C	21:J:102:BCR:H351	1.84	0.40
21:K:202:BCR:H15C	21:K:202:BCR:H351	1.80	0.40
11:1:104:TRP:CD1	18:1:609:CLA:HMD3	2.56	0.40
14:5:192:SER:HB2	18:5:610:CLA:HAA1	2.04	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	739/751 (98%)	708 (96%)	31 (4%)	0	100	100
2	B	729/735 (99%)	699 (96%)	30 (4%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	142/196 (72%)	131 (92%)	9 (6%)	2 (1%)	11	36
5	E	62/143 (43%)	58 (94%)	4 (6%)	0	100	100
6	F	162/227 (71%)	149 (92%)	13 (8%)	0	100	100
7	I	30/106 (28%)	28 (93%)	2 (7%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	83/160 (52%)	73 (88%)	10 (12%)	0	100	100
10	L	101/258 (39%)	98 (97%)	3 (3%)	0	100	100
11	1	191/248 (77%)	171 (90%)	19 (10%)	1 (0%)	29	61
11	a	192/248 (77%)	175 (91%)	16 (8%)	1 (0%)	29	61
12	3	219/298 (74%)	202 (92%)	17 (8%)	0	100	100
13	4	208/290 (72%)	196 (94%)	12 (6%)	0	100	100
14	5	224/274 (82%)	198 (88%)	26 (12%)	0	100	100
15	6	228/318 (72%)	206 (90%)	21 (9%)	1 (0%)	34	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	7	211/241 (88%)	193 (92%)	18 (8%)	0	100	100
17	8	213/272 (78%)	198 (93%)	15 (7%)	0	100	100
All	All	3851/4887 (79%)	3594 (93%)	252 (6%)	5 (0%)	54	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	202	HIS
4	D	203	PRO
15	6	312	PHE
11	1	59	TRP
11	a	59	TRP

### 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	601/610 (98%)	600 (100%)	1 (0%)	93	98
2	B	595/597 (100%)	590 (99%)	5 (1%)	81	94
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	120/152 (79%)	118 (98%)	2 (2%)	60	86
5	E	55/123 (45%)	54 (98%)	1 (2%)	59	85
6	F	126/169 (75%)	125 (99%)	1 (1%)	81	94
7	I	26/76 (34%)	26 (100%)	0	100	100
8	J	37/37 (100%)	37 (100%)	0	100	100
9	K	59/123 (48%)	58 (98%)	1 (2%)	60	86
10	L	74/198 (37%)	73 (99%)	1 (1%)	67	89
11	1	136/180 (76%)	136 (100%)	0	100	100
11	a	137/180 (76%)	137 (100%)	0	100	100
12	3	167/230 (73%)	165 (99%)	2 (1%)	71	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	4	165/226 (73%)	164 (99%)	1 (1%)	86	96
14	5	183/219 (84%)	182 (100%)	1 (0%)	88	96
15	6	184/260 (71%)	182 (99%)	2 (1%)	73	92
16	7	164/181 (91%)	159 (97%)	5 (3%)	41	75
17	8	161/207 (78%)	158 (98%)	3 (2%)	57	84
All	All	3059/3838 (80%)	3033 (99%)	26 (1%)	82	94

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	442	ASN
2	B	107	ARG
2	B	177	ASN
2	B	609	GLN
2	B	622	ARG
2	B	669	ARG
4	D	202	HIS
4	D	213	ASN
5	E	123	ASN
6	F	117	ASN
9	K	82	ASN
10	L	169	ARG
12	3	218	ILE
12	3	256	ASN
13	4	203	ASP
14	5	134	ASN
15	6	311	CYS
15	6	312	PHE
16	7	30	ARG
16	7	177	ARG
16	7	195	ARG
16	7	207	GLN
16	7	234	ASN
17	8	56	ARG
17	8	99	GLN
17	8	267	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	HIS
1	A	714	GLN
2	B	35	HIS
2	B	72	GLN
2	B	115	ASN
2	B	157	HIS
5	E	101	GLN
5	E	123	ASN
13	4	114	GLN
13	4	285	ASN
15	6	201	GLN
15	6	314	GLN
16	7	227	ASN
16	7	234	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

299 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	A	837	1	45,53,73	1.78	8 (17%)	52,89,113	1.74	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	a	601	11	53,62,73	1.62	8 (15%)	61,100,113	1.47	7 (11%)
18	CLA	A	825	-	65,73,73	1.42	8 (12%)	76,113,113	1.46	9 (11%)
18	CLA	B	829	-	65,73,73	1.51	9 (13%)	76,113,113	1.68	9 (11%)
18	CLA	B	836	-	50,58,73	1.62	7 (14%)	58,95,113	1.65	6 (10%)
18	CLA	4	612	13	40,49,73	1.84	7 (17%)	45,84,113	1.69	8 (17%)
18	CLA	1	616	11	43,51,73	1.91	8 (18%)	54,87,113	1.64	8 (14%)
18	CLA	A	818	-	60,68,73	1.48	7 (11%)	70,107,113	1.64	7 (10%)
18	CLA	L	303	-	45,53,73	1.76	5 (11%)	52,89,113	1.60	7 (13%)
18	CLA	4	601	13	65,73,73	1.50	10 (15%)	76,113,113	1.32	7 (9%)
18	CLA	A	828	-	64,72,73	1.42	7 (10%)	74,111,113	1.53	7 (9%)
18	CLA	B	817	-	59,67,73	1.54	9 (15%)	68,105,113	1.58	8 (11%)
18	CLA	4	613	13	65,73,73	1.47	7 (10%)	76,113,113	1.45	7 (9%)
18	CLA	6	603	-	54,62,73	1.64	8 (14%)	67,100,113	1.51	9 (13%)
19	PQN	A	844	-	34,34,34	2.87	11 (32%)	42,45,45	2.23	7 (16%)
20	LHG	8	623	-	48,48,48	0.61	0	51,54,54	1.26	6 (11%)
24	LMG	5	627	-	40,40,55	0.86	0	48,48,63	1.20	3 (6%)
18	CLA	5	603	-	54,62,73	1.68	9 (16%)	67,100,113	1.42	8 (11%)
24	LMG	4	623	-	40,40,55	0.89	1 (2%)	48,48,63	1.23	4 (8%)
18	CLA	5	607	-	65,73,73	1.45	8 (12%)	76,113,113	1.70	13 (17%)
18	CLA	8	613	17	65,73,73	1.45	8 (12%)	76,113,113	1.56	8 (10%)
21	BCR	4	621	-	41,41,41	0.68	0	56,56,56	1.94	16 (28%)
20	LHG	7	622	18	36,36,48	0.74	1 (2%)	39,42,54	1.28	4 (10%)
18	CLA	7	614	-	42,50,73	1.78	7 (16%)	48,85,113	1.67	8 (16%)
20	LHG	B	851	18	35,35,48	0.72	1 (2%)	38,40,54	1.33	5 (13%)
18	CLA	F	303	-	42,50,73	1.87	8 (19%)	48,85,113	1.65	7 (14%)
24	LMG	7	624	-	44,44,55	0.83	0	52,52,63	1.25	5 (9%)
18	CLA	3	615	-	39,48,73	1.90	8 (20%)	44,83,113	1.78	7 (15%)
18	CLA	7	616	16	43,51,73	1.85	7 (16%)	54,87,113	1.66	8 (14%)
18	CLA	B	802	-	65,73,73	1.46	9 (13%)	76,113,113	1.35	8 (10%)
18	CLA	4	604	-	54,62,73	1.67	8 (14%)	67,100,113	1.46	9 (13%)
18	CLA	4	611	20	42,50,73	1.78	7 (16%)	48,85,113	1.60	8 (16%)
21	BCR	L	305	-	41,41,41	0.68	0	56,56,56	1.77	12 (21%)
28	NEX	6	624	-	38,46,46	0.93	2 (5%)	50,70,70	2.28	16 (32%)
18	CLA	A	826	-	64,72,73	1.42	8 (12%)	74,111,113	1.55	8 (10%)
18	CLA	B	832	-	60,68,73	1.49	7 (11%)	70,107,113	1.61	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	LMU	8	625	-	36,36,36	1.19	2 (5%)	47,47,47	1.27	6 (12%)
21	BCR	7	623	-	41,41,41	0.71	0	56,56,56	1.81	13 (23%)
18	CLA	8	604	-	50,58,73	1.65	6 (12%)	58,95,113	1.63	7 (12%)
18	CLA	A	812	-	65,73,73	1.41	7 (10%)	76,113,113	1.50	8 (10%)
18	CLA	A	820	-	65,73,73	1.47	10 (15%)	76,113,113	1.65	11 (14%)
18	CLA	A	829	-	65,73,73	1.41	8 (12%)	76,113,113	1.54	7 (9%)
18	CLA	B	804	-	41,49,73	1.78	8 (19%)	47,84,113	1.78	8 (17%)
18	CLA	a	602	11	61,69,73	1.51	7 (11%)	71,108,113	1.43	7 (9%)
18	CLA	6	618	15	39,48,73	1.87	8 (20%)	48,83,113	1.84	9 (18%)
21	BCR	A	849	-	41,41,41	0.83	0	56,56,56	2.03	18 (32%)
18	CLA	7	607	-	42,50,73	1.79	7 (16%)	48,85,113	1.72	9 (18%)
21	BCR	A	856	-	41,41,41	0.72	0	56,56,56	1.96	17 (30%)
18	CLA	3	614	-	39,48,73	1.87	7 (17%)	44,83,113	1.66	7 (15%)
18	CLA	8	601	17	65,73,73	1.46	10 (15%)	76,113,113	1.44	10 (13%)
28	NEX	5	624	-	38,46,46	1.00	1 (2%)	50,70,70	2.18	16 (32%)
27	XAT	6	621	-	39,47,47	0.92	2 (5%)	54,74,74	2.72	20 (37%)
18	CLA	4	602	13	60,68,73	1.46	8 (13%)	70,107,113	1.62	8 (11%)
18	CLA	B	806	2	65,73,73	1.45	10 (15%)	76,113,113	1.45	9 (11%)
20	LHG	6	623	18	47,47,48	0.65	1 (2%)	50,53,54	1.27	6 (12%)
25	DGD	B	850	-	63,63,67	0.98	1 (1%)	77,77,81	1.42	11 (14%)
18	CLA	a	614	-	55,62,73	1.70	7 (12%)	60,99,113	1.50	7 (11%)
18	CLA	8	602	17	60,68,73	1.51	7 (11%)	70,107,113	1.50	8 (11%)
21	BCR	J	102	-	41,41,41	0.70	0	56,56,56	1.99	18 (32%)
18	CLA	B	822	-	42,50,73	1.85	5 (11%)	48,85,113	1.67	7 (14%)
18	CLA	3	607	12	56,64,73	1.61	7 (12%)	69,102,113	1.54	11 (15%)
18	CLA	4	609	13	61,69,73	1.51	7 (11%)	71,108,113	1.53	10 (14%)
18	CLA	3	612	12	43,51,73	1.79	7 (16%)	49,86,113	1.63	8 (16%)
18	CLA	A	805	-	52,60,73	1.61	8 (15%)	60,97,113	1.64	8 (13%)
18	CLA	A	808	-	50,58,73	1.61	7 (14%)	58,95,113	1.70	9 (15%)
18	CLA	3	608	-	55,63,73	1.64	11 (20%)	64,101,113	1.49	7 (10%)
18	CLA	A	839	-	55,63,73	1.57	9 (16%)	64,101,113	1.52	8 (12%)
18	CLA	A	823	-	42,50,73	1.77	9 (21%)	48,85,113	1.71	7 (14%)
18	CLA	B	810	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
18	CLA	3	611	20	37,46,73	1.95	7 (18%)	46,81,113	1.81	10 (21%)
21	BCR	K	207	-	41,41,41	0.75	0	56,56,56	1.78	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	8	609	17	45,53,73	1.73	7 (15%)	52,89,113	1.71	6 (11%)
18	CLA	6	616	15	65,73,73	1.45	6 (9%)	76,113,113	1.59	11 (14%)
24	LMG	4	624	-	40,40,55	0.91	1 (2%)	48,48,63	1.22	4 (8%)
18	CLA	a	608	-	43,52,73	1.81	6 (13%)	49,88,113	1.64	7 (14%)
18	CLA	B	834	-	60,68,73	1.55	8 (13%)	70,107,113	1.47	9 (12%)
18	CLA	1	606	11	37,47,73	1.92	6 (16%)	41,80,113	1.70	7 (17%)
18	CLA	A	809	1	65,73,73	1.40	7 (10%)	76,113,113	1.49	7 (9%)
18	CLA	6	620	-	45,53,73	1.74	10 (22%)	52,89,113	1.87	11 (21%)
18	CLA	1	610	11	38,47,73	1.93	7 (18%)	44,81,113	1.73	8 (18%)
18	CLA	L	304	-	45,53,73	1.79	5 (11%)	52,89,113	1.62	6 (11%)
18	CLA	A	819	-	59,67,73	1.58	10 (16%)	68,105,113	1.39	5 (7%)
18	CLA	4	603	13	44,52,73	1.83	8 (18%)	55,88,113	1.76	10 (18%)
18	CLA	8	608	-	51,59,73	1.69	8 (15%)	59,96,113	1.65	8 (13%)
18	CLA	3	617	12	39,48,73	1.84	9 (23%)	44,83,113	1.67	8 (18%)
18	CLA	A	832	-	50,58,73	1.64	8 (16%)	58,95,113	1.60	8 (13%)
18	CLA	A	840	-	52,60,73	1.62	7 (13%)	60,97,113	1.68	11 (18%)
18	CLA	B	833	-	65,73,73	1.47	7 (10%)	76,113,113	1.53	10 (13%)
18	CLA	K	203	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	10 (13%)
18	CLA	A	830	-	65,73,73	1.43	8 (12%)	76,113,113	1.53	10 (13%)
18	CLA	7	611	20	59,67,73	1.47	7 (11%)	68,105,113	1.58	7 (10%)
26	LUT	8	619	-	42,43,43	0.77	0	51,60,60	1.58	10 (19%)
18	CLA	5	618	14	39,48,73	1.92	8 (20%)	48,83,113	1.79	9 (18%)
18	CLA	8	607	-	41,49,73	1.86	8 (19%)	51,84,113	1.74	9 (17%)
27	XAT	1	618	-	39,47,47	0.86	1 (2%)	54,74,74	2.59	20 (37%)
18	CLA	7	610	16	65,73,73	1.43	9 (13%)	76,113,113	1.42	10 (13%)
18	CLA	1	614	-	37,45,73	2.08	8 (21%)	44,79,113	1.82	10 (22%)
18	CLA	5	611	20	42,50,73	1.78	6 (14%)	48,85,113	1.64	7 (14%)
18	CLA	5	614	-	45,52,73	1.91	7 (15%)	48,87,113	1.65	8 (16%)
18	CLA	A	831	-	65,73,73	1.53	10 (15%)	76,113,113	1.70	14 (18%)
18	CLA	1	607	-	39,48,73	1.87	7 (17%)	44,83,113	1.70	7 (15%)
23	LMU	5	628	-	34,34,36	1.26	2 (5%)	45,45,47	1.31	7 (15%)
18	CLA	A	804	-	65,73,73	1.46	8 (12%)	76,113,113	1.46	8 (10%)
18	CLA	5	610	14	54,62,73	1.60	7 (12%)	62,99,113	1.61	7 (11%)
18	CLA	B	827	-	62,70,73	1.46	8 (12%)	72,109,113	1.53	7 (9%)
24	LMG	A	860	-	40,40,55	0.93	2 (5%)	48,48,63	1.27	5 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	8	614	-	56,64,73	1.54	7 (12%)	65,102,113	1.58	9 (13%)
23	LMU	K	208	-	36,36,36	1.21	2 (5%)	47,47,47	1.33	5 (10%)
26	LUT	3	618	-	42,43,43	0.79	0	51,60,60	1.55	9 (17%)
18	CLA	B	841	20	44,52,73	1.82	5 (11%)	50,87,113	1.60	9 (18%)
18	CLA	3	613	12	52,61,73	1.61	8 (15%)	59,98,113	1.62	8 (13%)
18	CLA	5	616	14	41,50,73	1.89	9 (21%)	50,85,113	1.62	8 (16%)
18	CLA	B	816	-	55,63,73	1.56	7 (12%)	64,101,113	1.59	6 (9%)
18	CLA	7	606	-	41,49,73	1.84	8 (19%)	47,84,113	1.72	7 (14%)
18	CLA	B	824	-	65,73,73	1.54	7 (10%)	76,113,113	1.45	9 (11%)
18	CLA	A	807	1	65,73,73	1.48	10 (15%)	76,113,113	1.43	7 (9%)
18	CLA	F	304	-	41,49,73	1.82	6 (14%)	47,84,113	1.70	9 (19%)
18	CLA	1	611	20	65,73,73	1.44	6 (9%)	76,113,113	1.48	8 (10%)
18	CLA	a	606	11	43,52,73	1.79	6 (13%)	48,87,113	1.65	5 (10%)
18	CLA	1	608	-	43,52,73	1.85	5 (11%)	49,88,113	1.58	6 (12%)
18	CLA	5	608	-	50,58,73	1.63	8 (16%)	58,95,113	1.69	8 (13%)
18	CLA	5	619	-	43,51,73	1.85	8 (18%)	54,87,113	1.95	11 (20%)
25	DGD	J	103	-	59,59,67	0.99	3 (5%)	73,73,81	1.47	10 (13%)
18	CLA	3	609	12	60,68,73	1.52	8 (13%)	70,107,113	1.64	11 (15%)
21	BCR	L	301	-	41,41,41	0.75	0	56,56,56	1.84	15 (26%)
27	XAT	8	620	-	39,47,47	0.92	1 (2%)	54,74,74	2.67	19 (35%)
21	BCR	1	619	-	41,41,41	0.66	0	56,56,56	1.93	16 (28%)
18	CLA	8	612	17	40,49,73	1.80	7 (17%)	45,84,113	1.75	9 (20%)
18	CLA	6	617	-	45,53,73	1.75	7 (15%)	52,89,113	1.57	6 (11%)
18	CLA	1	603	-	53,62,73	1.65	6 (11%)	61,100,113	1.61	8 (13%)
18	CLA	7	609	16	45,53,73	1.67	6 (13%)	52,89,113	1.86	9 (17%)
18	CLA	a	607	-	45,53,73	1.75	6 (13%)	52,89,113	1.65	8 (15%)
23	LMU	A	858	-	34,35,36	1.29	2 (5%)	42,45,47	1.22	5 (11%)
18	CLA	a	609	11	65,73,73	1.49	6 (9%)	76,113,113	1.43	8 (10%)
21	BCR	6	622	-	41,41,41	0.72	0	56,56,56	1.95	17 (30%)
18	CLA	7	612	16	44,52,73	1.86	8 (18%)	51,88,113	1.53	9 (17%)
18	CLA	B	803	-	65,73,73	1.39	9 (13%)	76,113,113	1.92	13 (17%)
18	CLA	A	838	-	50,58,73	1.56	7 (14%)	58,95,113	1.78	8 (13%)
18	CLA	B	818	-	60,68,73	1.49	8 (13%)	70,107,113	1.61	8 (11%)
18	CLA	B	840	-	65,73,73	1.46	8 (12%)	76,113,113	1.52	6 (7%)
21	BCR	B	845	-	41,41,41	0.71	0	56,56,56	1.96	17 (30%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	B	821	-	46,54,73	1.80	6 (13%)	53,90,113	1.60	8 (15%)
23	LMU	A	859	-	35,35,36	1.27	3 (8%)	43,45,47	1.23	4 (9%)
18	CLA	B	819	-	55,63,73	1.63	7 (12%)	64,101,113	1.52	6 (9%)
18	CLA	A	854	-	65,73,73	1.46	9 (13%)	76,113,113	1.57	11 (14%)
18	CLA	3	606	-	53,62,73	1.63	7 (13%)	61,100,113	1.51	7 (11%)
20	LHG	3	624	18	48,48,48	0.63	0	51,54,54	1.22	6 (11%)
21	BCR	B	843	-	41,41,41	0.70	0	56,56,56	1.94	15 (26%)
18	CLA	6	610	15	65,73,73	1.44	7 (10%)	76,113,113	1.40	7 (9%)
18	CLA	B	807	-	52,60,73	1.64	9 (17%)	60,97,113	1.53	9 (15%)
18	CLA	B	839	-	65,73,73	1.43	8 (12%)	76,113,113	1.47	8 (10%)
18	CLA	5	604	-	63,71,73	1.53	8 (12%)	78,111,113	1.45	9 (11%)
18	CLA	4	616	13	43,51,73	1.85	8 (18%)	54,87,113	1.71	8 (14%)
18	CLA	3	610	12	65,73,73	1.45	9 (13%)	76,113,113	1.44	7 (9%)
18	CLA	1	612	11	45,53,73	1.77	6 (13%)	52,89,113	1.63	7 (13%)
18	CLA	5	617	-	50,58,73	1.66	8 (16%)	58,95,113	1.62	8 (13%)
18	CLA	8	611	20	42,50,73	1.78	7 (16%)	48,85,113	1.63	8 (16%)
20	LHG	A	847	18	29,29,48	0.83	1 (3%)	32,35,54	1.29	3 (9%)
18	CLA	A	803	-	65,73,73	1.46	10 (15%)	76,113,113	1.54	7 (9%)
27	XAT	5	621	-	39,47,47	0.93	0	54,74,74	2.78	21 (38%)
18	CLA	1	613	-	65,73,73	1.48	6 (9%)	76,113,113	1.45	8 (10%)
18	CLA	A	810	1	50,58,73	1.66	10 (20%)	58,95,113	1.52	10 (17%)
18	CLA	B	808	-	65,73,73	1.43	8 (12%)	76,113,113	1.64	10 (13%)
18	CLA	B	831	-	65,73,73	1.43	7 (10%)	76,113,113	1.50	6 (7%)
21	BCR	A	851	-	41,41,41	0.79	0	56,56,56	2.14	14 (25%)
18	CLA	6	614	-	60,68,73	1.52	7 (11%)	70,107,113	1.51	7 (10%)
27	XAT	3	619	-	39,47,47	0.93	2 (5%)	54,74,74	2.63	21 (38%)
21	BCR	3	620	-	41,41,41	0.72	0	56,56,56	2.06	19 (33%)
18	CLA	A	801	-	65,73,73	1.48	9 (13%)	76,113,113	1.40	7 (9%)
18	CLA	A	814	-	65,73,73	1.39	7 (10%)	76,113,113	1.58	10 (13%)
20	LHG	1	620	18	48,48,48	0.60	0	51,54,54	1.24	6 (11%)
18	CLA	7	615	-	38,47,73	1.91	7 (18%)	46,81,113	1.74	8 (17%)
26	LUT	6	619	-	42,43,43	0.76	0	51,60,60	1.57	12 (23%)
18	CLA	B	835	-	45,53,73	1.77	6 (13%)	52,89,113	1.82	9 (17%)
18	CLA	6	606	-	39,48,73	1.83	6 (15%)	44,83,113	1.75	8 (18%)
18	CLA	7	613	16	65,73,73	1.46	8 (12%)	76,113,113	1.43	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	XAT	a	618	-	39,47,47	0.87	1 (2%)	54,74,74	2.61	20 (37%)
22	SF4	C	102	-	0,12,12	-	-	-		
21	BCR	A	848	-	41,41,41	0.77	0	56,56,56	1.86	15 (26%)
26	LUT	1	617	-	42,43,43	0.74	0	51,60,60	1.66	14 (27%)
18	CLA	a	613	-	65,73,73	1.49	7 (10%)	76,113,113	1.49	8 (10%)
18	CLA	8	616	17	43,51,73	1.87	6 (13%)	54,87,113	1.82	12 (22%)
18	CLA	A	817	-	45,53,73	1.71	7 (15%)	52,89,113	1.97	11 (21%)
21	BCR	F	305	-	41,41,41	0.78	0	56,56,56	2.14	18 (32%)
22	SF4	C	101	-	0,12,12	-	-	-		
18	CLA	8	606	-	64,72,73	1.50	7 (10%)	75,112,113	1.35	6 (8%)
18	CLA	a	616	11	45,53,73	1.74	6 (13%)	52,89,113	1.55	7 (13%)
18	CLA	B	838	-	47,55,73	1.66	7 (14%)	54,91,113	1.64	7 (12%)
20	LHG	8	622	18	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
21	BCR	3	621	-	41,41,41	0.70	0	56,56,56	2.46	20 (35%)
21	BCR	A	850	-	41,41,41	0.75	0	56,56,56	1.95	15 (26%)
21	BCR	K	202	-	41,41,41	0.72	0	56,56,56	2.06	15 (26%)
18	CLA	8	603	-	44,52,73	1.80	8 (18%)	55,88,113	1.79	9 (16%)
18	CLA	A	842	-	65,73,73	1.44	8 (12%)	76,113,113	1.45	6 (7%)
21	BCR	B	846	-	41,41,41	0.73	0	56,56,56	2.05	16 (28%)
21	BCR	B	848	-	41,41,41	0.79	0	56,56,56	1.78	11 (19%)
18	CLA	1	602	11	61,69,73	1.49	7 (11%)	71,108,113	1.43	7 (9%)
18	CLA	5	602	14	65,73,73	1.44	7 (10%)	76,113,113	1.54	7 (9%)
18	CLA	A	802	-	65,73,73	1.39	8 (12%)	76,113,113	1.71	10 (13%)
26	LUT	a	617	-	42,43,43	0.74	0	51,60,60	1.58	12 (23%)
18	CLA	B	826	-	55,63,73	1.57	7 (12%)	64,101,113	1.69	6 (9%)
26	LUT	5	620	-	42,43,43	0.77	0	51,60,60	1.64	13 (25%)
18	CLA	1	609	11	40,48,73	1.96	6 (15%)	50,83,113	1.78	10 (20%)
23	LMU	8	624	-	36,36,36	1.20	2 (5%)	47,47,47	0.96	2 (4%)
26	LUT	7	619	-	42,43,43	0.89	2 (4%)	51,60,60	1.85	14 (27%)
18	CLA	A	821	-	53,61,73	1.59	8 (15%)	61,98,113	1.59	7 (11%)
18	CLA	B	811	-	54,62,73	1.63	7 (12%)	67,100,113	1.52	9 (13%)
18	CLA	A	836	-	65,73,73	1.46	9 (13%)	76,113,113	1.44	7 (9%)
18	CLA	B	815	-	43,51,73	1.73	7 (16%)	49,86,113	1.75	7 (14%)
21	BCR	5	622	-	41,41,41	0.69	0	56,56,56	2.11	20 (35%)
18	CLA	5	612	14	40,49,73	1.80	7 (17%)	45,84,113	1.75	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	A	822	-	65,73,73	1.47	8 (12%)	76,113,113	1.53	7 (9%)
18	CLA	6	601	15	65,73,73	1.43	8 (12%)	76,113,113	1.56	8 (10%)
21	BCR	3	622	-	41,41,41	0.71	0	56,56,56	2.61	21 (37%)
18	CLA	6	613	-	63,72,73	1.47	8 (12%)	73,112,113	1.49	9 (12%)
21	BCR	B	844	-	41,41,41	0.73	0	56,56,56	2.03	18 (32%)
20	LHG	A	846	-	48,48,48	0.71	1 (2%)	51,54,54	1.27	6 (11%)
20	LHG	5	623	18	48,48,48	0.62	1 (2%)	51,54,54	1.25	6 (11%)
18	CLA	B	828	-	65,73,73	1.43	9 (13%)	76,113,113	1.46	8 (10%)
18	CLA	3	602	12	60,68,73	1.45	9 (15%)	70,107,113	1.51	7 (10%)
18	CLA	4	606	-	39,48,73	1.83	7 (17%)	44,83,113	1.71	7 (15%)
18	CLA	5	613	14	64,72,73	1.45	7 (10%)	74,111,113	1.53	7 (9%)
18	CLA	7	602	16	65,73,73	1.44	9 (13%)	76,113,113	1.40	8 (10%)
20	LHG	3	623	-	44,44,48	0.60	0	47,50,54	1.26	6 (12%)
21	BCR	a	619	-	41,41,41	0.69	0	56,56,56	1.93	16 (28%)
18	CLA	B	830	-	43,51,73	1.82	9 (20%)	49,86,113	1.81	9 (18%)
18	CLA	4	610	13	61,69,73	1.48	7 (11%)	71,108,113	1.55	8 (11%)
18	CLA	B	812	-	43,51,73	1.80	6 (13%)	49,86,113	1.62	6 (12%)
18	CLA	F	301	-	57,65,73	1.59	9 (15%)	66,103,113	1.41	9 (13%)
18	CLA	B	837	-	65,73,73	1.46	7 (10%)	76,113,113	1.42	8 (10%)
18	CLA	A	835	-	61,69,73	1.47	9 (14%)	71,108,113	1.68	12 (16%)
18	CLA	4	607	-	45,53,73	1.75	7 (15%)	52,89,113	1.73	7 (13%)
18	CLA	8	610	17	60,68,73	1.44	7 (11%)	70,107,113	1.50	7 (10%)
18	CLA	1	601	11	53,62,73	1.62	8 (15%)	61,100,113	1.45	9 (14%)
18	CLA	B	820	-	50,58,73	1.70	6 (12%)	58,95,113	1.62	7 (12%)
18	CLA	K	206	9	45,53,73	1.77	7 (15%)	52,89,113	1.68	7 (13%)
18	CLA	6	604	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	7 (9%)
18	CLA	6	611	20	42,50,73	1.75	7 (16%)	48,85,113	1.61	7 (14%)
22	SF4	A	853	-	0,12,12	-	-	-	-	-
18	CLA	4	618	13	39,48,73	1.91	8 (20%)	48,83,113	1.79	10 (20%)
23	LMU	A	857	-	34,34,36	1.38	3 (8%)	44,44,47	1.26	4 (9%)
20	LHG	a	620	18	48,48,48	0.64	1 (2%)	51,54,54	1.25	6 (11%)
27	XAT	7	620	-	39,47,47	0.91	2 (5%)	54,74,74	2.67	20 (37%)
20	LHG	4	622	18	48,48,48	0.62	1 (2%)	51,54,54	1.25	7 (13%)
18	CLA	7	608	-	50,58,73	1.68	10 (20%)	58,95,113	1.56	9 (15%)
18	CLA	A	843	-	64,72,73	1.42	8 (12%)	74,111,113	1.44	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	A	806	-	65,73,73	1.47	9 (13%)	76,113,113	1.66	11 (14%)
18	CLA	4	614	-	56,64,73	1.60	8 (14%)	65,102,113	1.49	7 (10%)
18	CLA	A	811	-	65,73,73	1.43	7 (10%)	76,113,113	1.44	7 (9%)
18	CLA	3	603	-	55,63,73	1.62	8 (14%)	64,101,113	1.70	12 (18%)
21	BCR	A	852	-	41,41,41	0.78	1 (2%)	56,56,56	2.10	16 (28%)
21	BCR	B	801	-	41,41,41	0.71	0	56,56,56	2.01	13 (23%)
18	CLA	A	815	-	50,58,73	1.67	9 (18%)	58,95,113	1.56	9 (15%)
18	CLA	a	612	11	45,53,73	1.77	7 (15%)	52,89,113	1.62	7 (13%)
26	LUT	4	619	-	42,43,43	0.79	0	51,60,60	1.62	11 (21%)
18	CLA	a	611	20	37,46,73	1.96	7 (18%)	46,81,113	1.78	9 (19%)
18	CLA	7	603	-	43,52,73	1.79	8 (18%)	49,88,113	1.66	7 (14%)
18	CLA	J	101	8	42,50,73	1.82	6 (14%)	48,85,113	1.73	8 (16%)
18	CLA	7	601	16	60,68,73	1.50	8 (13%)	70,107,113	1.55	9 (12%)
19	PQN	B	842	-	34,34,34	2.90	11 (32%)	42,45,45	2.04	5 (11%)
21	BCR	8	621	-	41,41,41	0.71	0	56,56,56	1.94	18 (32%)
18	CLA	K	201	9	45,53,73	1.77	7 (15%)	52,89,113	1.87	12 (23%)
18	CLA	B	823	-	45,53,73	1.79	6 (13%)	52,89,113	1.58	6 (11%)
18	CLA	5	601	14	56,64,73	1.58	7 (12%)	65,102,113	1.48	6 (9%)
18	CLA	a	610	11	59,67,73	1.55	9 (15%)	69,106,113	1.40	7 (10%)
18	CLA	a	603	-	54,62,73	1.63	7 (12%)	62,99,113	1.57	8 (12%)
18	CLA	6	608	-	51,59,73	1.64	7 (13%)	59,96,113	1.60	6 (10%)
18	CLA	6	602	15	65,73,73	1.46	9 (13%)	76,113,113	1.45	8 (10%)
18	CLA	B	813	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	9 (11%)
18	CLA	1	604	-	49,57,73	1.69	6 (12%)	55,93,113	1.75	8 (14%)
18	CLA	A	813	-	54,62,73	1.53	7 (12%)	62,99,113	1.70	6 (9%)
18	CLA	4	608	-	65,73,73	1.44	7 (10%)	76,113,113	1.44	7 (9%)
18	CLA	5	606	-	39,48,73	1.91	7 (17%)	44,83,113	1.56	7 (15%)
21	BCR	7	621	-	41,41,41	0.73	0	56,56,56	2.02	22 (39%)
24	LMG	J	104	-	40,40,55	0.90	2 (5%)	48,48,63	1.22	4 (8%)
18	CLA	A	827	-	59,67,73	1.50	8 (13%)	68,105,113	1.59	10 (14%)
18	CLA	A	833	-	45,53,73	1.72	6 (13%)	52,89,113	1.77	6 (11%)
18	CLA	6	607	-	41,49,73	1.83	8 (19%)	51,84,113	1.87	10 (19%)
18	CLA	6	609	15	45,53,73	1.76	9 (20%)	52,89,113	1.67	8 (15%)
18	CLA	A	841	-	65,73,73	1.45	9 (13%)	76,113,113	1.42	7 (9%)
21	BCR	B	847	-	41,41,41	0.73	0	56,56,56	2.00	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	CLA	K	204	-	46,54,73	1.70	7 (15%)	53,90,113	1.65	6 (11%)
18	CLA	5	609	14	65,73,73	1.46	8 (12%)	76,113,113	1.46	9 (11%)
18	CLA	B	809	2	65,73,73	1.42	9 (13%)	76,113,113	1.49	6 (7%)
18	CLA	7	604	-	54,62,73	1.59	7 (12%)	63,100,113	1.62	8 (12%)
18	CLA	A	845	20	50,58,73	1.66	7 (14%)	58,95,113	1.59	6 (10%)
18	CLA	B	825	-	62,70,73	1.49	8 (12%)	72,109,113	1.39	8 (11%)
24	LMG	5	626	-	40,40,55	0.88	0	48,48,63	1.20	5 (10%)
18	CLA	L	302	10	45,53,73	1.80	5 (11%)	52,89,113	1.73	8 (15%)
18	CLA	A	824	-	41,49,73	1.82	6 (14%)	47,84,113	1.76	11 (23%)
18	CLA	a	604	-	49,57,73	1.68	7 (14%)	55,93,113	1.74	9 (16%)
18	CLA	A	834	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	7 (9%)
20	LHG	5	625	-	48,48,48	0.61	0	51,54,54	1.25	6 (11%)
27	XAT	4	620	-	39,47,47	0.89	1 (2%)	54,74,74	2.61	18 (33%)
18	CLA	B	814	-	64,72,73	1.43	8 (12%)	74,111,113	1.53	7 (9%)
18	CLA	6	612	15	40,49,73	1.83	7 (17%)	45,84,113	1.77	7 (15%)
18	CLA	3	604	-	65,73,73	1.47	7 (10%)	76,113,113	1.46	6 (7%)
18	CLA	A	816	-	45,53,73	1.72	7 (15%)	52,89,113	1.83	7 (13%)
18	CLA	B	805	-	65,73,73	1.39	8 (12%)	76,113,113	1.53	8 (10%)

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	A	837	1	1/1/11/20	8/13/91/115	-
18	CLA	a	601	11	1/1/13/20	6/23/101/115	-
18	CLA	A	825	-	1/1/15/20	20/37/115/115	-
18	CLA	B	829	-	1/1/15/20	10/37/115/115	-
18	CLA	B	836	-	1/1/12/20	6/19/97/115	-
18	CLA	7	602	16	1/1/15/20	13/37/115/115	-
18	CLA	1	616	11	1/1/11/20	4/11/87/115	-
18	CLA	A	818	-	1/1/14/20	13/31/109/115	-
18	CLA	L	303	-	1/1/11/20	6/13/91/115	-
18	CLA	6	603	-	1/1/13/20	7/25/101/115	-
18	CLA	A	828	-	1/1/14/20	10/35/113/115	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	817	-	1/1/13/20	10/30/108/115	-
18	CLA	4	613	13	1/1/15/20	13/37/115/115	-
18	CLA	4	601	13	-	16/37/115/115	-
19	PQN	A	844	-	-	7/23/43/43	0/2/2/2
20	LHG	8	623	-	-	33/53/53/53	-
24	LMG	5	627	-	-	15/35/55/70	0/1/1/1
18	CLA	5	603	-	1/1/13/20	7/25/101/115	-
24	LMG	4	623	-	-	12/35/55/70	0/1/1/1
18	CLA	5	607	-	1/1/15/20	15/37/115/115	-
18	CLA	8	613	17	1/1/15/20	19/37/115/115	-
21	BCR	4	621	-	-	4/29/63/63	0/2/2/2
20	LHG	7	622	18	-	24/41/41/53	-
18	CLA	7	614	-	1/1/10/20	4/10/88/115	-
20	LHG	B	851	18	-	19/39/39/53	-
18	CLA	F	303	-	-	5/10/88/115	-
24	LMG	7	624	-	-	15/39/59/70	0/1/1/1
18	CLA	3	615	-	1/1/10/20	1/6/84/115	-
18	CLA	7	616	16	1/1/11/20	7/11/87/115	-
18	CLA	B	802	-	1/1/15/20	18/37/115/115	-
18	CLA	4	604	-	1/1/13/20	10/25/101/115	-
18	CLA	4	611	20	1/1/10/20	4/10/88/115	-
21	BCR	L	305	-	-	10/29/63/63	0/2/2/2
28	NEX	6	624	-	-	4/27/83/83	0/3/3/3
18	CLA	A	826	-	1/1/14/20	13/35/113/115	-
18	CLA	B	832	-	1/1/14/20	8/31/109/115	-
23	LMU	8	625	-	-	11/21/61/61	0/2/2/2
21	BCR	7	623	-	-	3/29/63/63	0/2/2/2
18	CLA	8	604	-	1/1/12/20	11/19/97/115	-
18	CLA	A	812	-	1/1/15/20	15/37/115/115	-
18	CLA	A	820	-	1/1/15/20	16/37/115/115	-
18	CLA	A	829	-	1/1/15/20	8/37/115/115	-
18	CLA	B	804	-	1/1/10/20	3/8/86/115	-
18	CLA	a	602	11	1/1/14/20	6/33/111/115	-
18	CLA	6	618	15	1/1/10/20	2/8/84/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	A	849	-	-	2/29/63/63	0/2/2/2
18	CLA	7	607	-	1/1/10/20	6/10/88/115	-
21	BCR	A	856	-	-	7/29/63/63	0/2/2/2
18	CLA	3	614	-	1/1/10/20	0/6/84/115	-
18	CLA	8	601	17	1/1/15/20	16/37/115/115	-
28	NEX	5	624	-	-	2/27/83/83	0/3/3/3
27	XAT	6	621	-	-	2/31/93/93	0/4/4/4
18	CLA	4	602	13	1/1/14/20	7/31/109/115	-
18	CLA	B	806	2	1/1/15/20	11/37/115/115	-
20	LHG	6	623	18	-	26/52/52/53	-
25	DGD	B	850	-	-	23/51/91/95	0/2/2/2
18	CLA	a	614	-	1/1/12/20	7/25/99/115	-
18	CLA	8	602	17	1/1/14/20	7/31/109/115	-
21	BCR	J	102	-	-	7/29/63/63	0/2/2/2
18	CLA	B	822	-	1/1/10/20	2/10/88/115	-
18	CLA	3	607	12	1/1/13/20	6/28/104/115	-
18	CLA	4	609	13	1/1/14/20	6/33/111/115	-
18	CLA	3	612	12	1/1/10/20	3/11/89/115	-
18	CLA	A	805	-	1/1/12/20	3/22/100/115	-
18	CLA	A	808	-	1/1/12/20	4/19/97/115	-
18	CLA	3	608	-	1/1/13/20	7/25/103/115	-
18	CLA	A	839	-	1/1/13/20	4/25/103/115	-
18	CLA	A	823	-	1/1/10/20	2/10/88/115	-
18	CLA	B	810	-	1/1/15/20	12/37/115/115	-
18	CLA	3	611	20	1/1/10/20	0/4/80/115	-
21	BCR	K	207	-	-	4/29/63/63	0/2/2/2
18	CLA	8	609	17	1/1/11/20	4/13/91/115	-
18	CLA	6	616	15	1/1/15/20	18/37/115/115	-
24	LMG	4	624	-	-	13/35/55/70	0/1/1/1
18	CLA	a	608	-	1/1/11/20	2/11/89/115	-
18	CLA	B	834	-	1/1/14/20	11/31/109/115	-
18	CLA	1	606	11	1/1/8/20	1/5/79/115	-
18	CLA	A	809	1	1/1/15/20	10/37/115/115	-
18	CLA	6	620	-	1/1/11/20	7/13/91/115	-
18	CLA	1	610	11	1/1/9/20	0/6/80/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	L	304	-	1/1/11/20	7/13/91/115	-
18	CLA	A	819	-	1/1/13/20	8/30/108/115	-
18	CLA	4	603	13	1/1/11/20	5/13/89/115	-
18	CLA	8	608	-	1/1/12/20	9/21/99/115	-
18	CLA	3	617	12	1/1/10/20	2/6/84/115	-
18	CLA	A	832	-	1/1/12/20	4/19/97/115	-
18	CLA	A	840	-	1/1/12/20	4/22/100/115	-
18	CLA	B	833	-	1/1/15/20	16/37/115/115	-
18	CLA	K	203	-	1/1/15/20	10/37/115/115	-
18	CLA	A	830	-	1/1/15/20	18/37/115/115	-
18	CLA	7	611	20	1/1/13/20	12/29/107/115	-
26	LUT	8	619	-	-	2/29/67/67	0/2/2/2
18	CLA	5	618	14	1/1/10/20	0/8/84/115	-
18	CLA	8	607	-	1/1/10/20	5/10/86/115	-
27	XAT	1	618	-	-	1/31/93/93	0/4/4/4
18	CLA	7	610	16	1/1/15/20	8/37/115/115	-
18	CLA	1	614	-	1/1/9/20	0/4/76/115	-
18	CLA	5	611	20	1/1/10/20	5/10/88/115	-
18	CLA	5	614	-	1/1/10/20	7/13/87/115	-
18	CLA	A	831	-	1/1/15/20	9/37/115/115	-
18	CLA	1	607	-	1/1/10/20	0/6/84/115	-
23	LMU	5	628	-	-	12/19/59/61	0/2/2/2
18	CLA	A	804	-	1/1/15/20	14/37/115/115	-
18	CLA	5	610	14	1/1/12/20	3/24/102/115	-
18	CLA	B	827	-	1/1/14/20	17/34/112/115	-
24	LMG	A	860	-	-	14/35/55/70	0/1/1/1
18	CLA	8	614	-	1/1/13/20	8/27/105/115	-
23	LMU	K	208	-	-	12/21/61/61	0/2/2/2
26	LUT	3	618	-	-	2/29/67/67	0/2/2/2
18	CLA	B	841	20	1/1/10/20	5/12/90/115	-
18	CLA	3	613	12	1/1/12/20	5/21/99/115	-
18	CLA	5	616	14	1/1/10/20	4/8/84/115	-
18	CLA	B	816	-	1/1/13/20	10/25/103/115	-
18	CLA	7	606	-	1/1/10/20	2/8/86/115	-
18	CLA	B	824	-	1/1/15/20	12/37/115/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	807	1	1/1/15/20	13/37/115/115	-
18	CLA	F	304	-	1/1/10/20	4/8/86/115	-
18	CLA	1	611	20	1/1/15/20	11/37/115/115	-
18	CLA	a	606	11	1/1/10/20	4/10/88/115	-
18	CLA	1	608	-	1/1/11/20	0/11/89/115	-
18	CLA	5	608	-	1/1/12/20	7/19/97/115	-
18	CLA	5	619	-	-	7/11/87/115	-
25	DGD	J	103	-	-	26/47/87/95	0/2/2/2
18	CLA	3	609	12	1/1/14/20	20/31/109/115	-
21	BCR	L	301	-	-	5/29/63/63	0/2/2/2
27	XAT	8	620	-	-	2/31/93/93	0/4/4/4
21	BCR	1	619	-	-	0/29/63/63	0/2/2/2
18	CLA	8	612	17	-	2/8/86/115	-
18	CLA	6	617	-	1/1/11/20	5/13/91/115	-
18	CLA	1	603	-	1/1/13/20	13/23/101/115	-
18	CLA	7	609	16	1/1/11/20	6/13/91/115	-
18	CLA	a	607	-	1/1/11/20	5/13/91/115	-
23	LMU	A	858	-	-	7/21/57/61	0/2/2/2
18	CLA	a	609	11	1/1/15/20	20/37/115/115	-
21	BCR	6	622	-	-	6/29/63/63	0/2/2/2
18	CLA	7	612	16	-	5/11/89/115	-
18	CLA	B	803	-	1/1/15/20	12/37/115/115	-
18	CLA	A	838	-	1/1/12/20	7/19/97/115	-
18	CLA	B	818	-	1/1/14/20	15/31/109/115	-
18	CLA	B	840	-	1/1/15/20	7/37/115/115	-
21	BCR	B	845	-	-	4/29/63/63	0/2/2/2
18	CLA	B	821	-	1/1/11/20	7/14/92/115	-
23	LMU	A	859	-	-	9/21/57/61	0/2/2/2
18	CLA	B	819	-	1/1/13/20	6/25/103/115	-
18	CLA	A	854	-	1/1/15/20	14/37/115/115	-
18	CLA	3	606	-	1/1/13/20	8/23/101/115	-
20	LHG	3	624	18	-	27/53/53/53	-
21	BCR	B	843	-	-	5/29/63/63	0/2/2/2
18	CLA	6	610	15	1/1/15/20	10/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	807	-	1/1/12/20	5/22/100/115	-
18	CLA	B	839	-	1/1/15/20	9/37/115/115	-
18	CLA	5	604	-	1/1/15/20	15/35/111/115	-
18	CLA	4	616	13	1/1/11/20	7/11/87/115	-
18	CLA	3	610	12	1/1/15/20	6/37/115/115	-
18	CLA	1	612	11	1/1/11/20	7/13/91/115	-
18	CLA	5	617	-	1/1/12/20	8/19/97/115	-
18	CLA	8	611	20	1/1/10/20	4/10/88/115	-
20	LHG	A	847	18	-	17/34/34/53	-
18	CLA	A	803	-	1/1/15/20	7/37/115/115	-
27	XAT	5	621	-	-	2/31/93/93	0/4/4/4
18	CLA	1	613	-	1/1/15/20	9/37/115/115	-
18	CLA	A	810	1	1/1/12/20	5/19/97/115	-
18	CLA	B	808	-	1/1/15/20	14/37/115/115	-
18	CLA	B	831	-	1/1/15/20	10/37/115/115	-
21	BCR	A	851	-	-	5/29/63/63	0/2/2/2
18	CLA	6	614	-	1/1/14/20	11/31/109/115	-
27	XAT	3	619	-	-	2/31/93/93	0/4/4/4
21	BCR	3	620	-	-	5/29/63/63	0/2/2/2
18	CLA	A	801	-	1/1/15/20	9/37/115/115	-
18	CLA	A	814	-	1/1/15/20	18/37/115/115	-
20	LHG	1	620	18	-	17/53/53/53	-
18	CLA	7	615	-	1/1/9/20	2/5/81/115	-
26	LUT	6	619	-	-	2/29/67/67	0/2/2/2
18	CLA	B	835	-	1/1/11/20	7/13/91/115	-
18	CLA	6	606	-	1/1/10/20	4/6/84/115	-
18	CLA	7	613	16	1/1/15/20	12/37/115/115	-
27	XAT	a	618	-	-	1/31/93/93	0/4/4/4
22	SF4	C	102	-	-	-	0/6/5/5
21	BCR	A	848	-	-	4/29/63/63	0/2/2/2
26	LUT	1	617	-	-	4/29/67/67	0/2/2/2
18	CLA	a	613	-	1/1/15/20	11/37/115/115	-
18	CLA	8	616	17	-	11/11/87/115	-
18	CLA	A	817	-	1/1/11/20	4/13/91/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	F	305	-	-	2/29/63/63	0/2/2/2
22	SF4	C	101	-	-	-	0/6/5/5
18	CLA	8	606	-	1/1/15/20	9/35/113/115	-
18	CLA	a	616	11	1/1/11/20	4/13/91/115	-
18	CLA	B	838	-	1/1/11/20	6/16/94/115	-
20	LHG	8	622	18	-	25/53/53/53	-
21	BCR	3	621	-	-	6/29/63/63	0/2/2/2
21	BCR	A	850	-	-	0/29/63/63	0/2/2/2
21	BCR	K	202	-	-	4/29/63/63	0/2/2/2
18	CLA	8	603	-	1/1/11/20	7/13/89/115	-
18	CLA	A	842	-	1/1/15/20	10/37/115/115	-
21	BCR	B	846	-	-	2/29/63/63	0/2/2/2
21	BCR	B	848	-	-	4/29/63/63	0/2/2/2
18	CLA	1	602	11	1/1/14/20	7/33/111/115	-
18	CLA	5	602	14	1/1/15/20	5/37/115/115	-
18	CLA	A	802	-	1/1/15/20	11/37/115/115	-
26	LUT	a	617	-	-	5/29/67/67	0/2/2/2
18	CLA	B	826	-	1/1/13/20	6/25/103/115	-
26	LUT	5	620	-	-	2/29/67/67	0/2/2/2
18	CLA	1	609	11	1/1/10/20	3/8/84/115	-
23	LMU	8	624	-	-	10/21/61/61	0/2/2/2
26	LUT	7	619	-	-	2/29/67/67	0/2/2/2
18	CLA	A	821	-	1/1/12/20	11/23/101/115	-
18	CLA	B	811	-	1/1/13/20	9/25/101/115	-
18	CLA	A	836	-	1/1/15/20	13/37/115/115	-
18	CLA	B	815	-	1/1/10/20	4/11/89/115	-
21	BCR	5	622	-	-	6/29/63/63	0/2/2/2
18	CLA	5	612	14	1/1/10/20	2/8/86/115	-
18	CLA	A	822	-	1/1/15/20	11/37/115/115	-
18	CLA	6	601	15	1/1/15/20	16/37/115/115	-
21	BCR	3	622	-	-	8/29/63/63	0/2/2/2
18	CLA	6	613	-	1/1/15/20	14/35/113/115	-
21	BCR	B	844	-	-	9/29/63/63	0/2/2/2
20	LHG	A	846	-	-	34/53/53/53	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LHG	5	623	18	-	24/53/53/53	-
18	CLA	B	828	-	1/1/15/20	13/37/115/115	-
18	CLA	3	602	12	1/1/14/20	5/31/109/115	-
18	CLA	4	606	-	1/1/10/20	2/6/84/115	-
18	CLA	5	613	14	1/1/14/20	20/35/113/115	-
20	LHG	3	623	-	-	22/49/49/53	-
21	BCR	a	619	-	-	2/29/63/63	0/2/2/2
18	CLA	B	830	-	1/1/10/20	5/11/89/115	-
18	CLA	4	610	13	1/1/14/20	7/33/111/115	-
18	CLA	B	812	-	1/1/10/20	3/11/89/115	-
18	CLA	F	301	-	1/1/13/20	8/28/106/115	-
18	CLA	B	837	-	1/1/15/20	6/37/115/115	-
18	CLA	A	835	-	1/1/14/20	11/33/111/115	-
18	CLA	4	607	-	1/1/11/20	6/13/91/115	-
18	CLA	8	610	17	1/1/14/20	7/31/109/115	-
18	CLA	1	601	11	1/1/13/20	3/23/101/115	-
18	CLA	B	820	-	1/1/12/20	8/19/97/115	-
18	CLA	K	206	9	1/1/11/20	7/13/91/115	-
18	CLA	6	604	-	1/1/15/20	18/37/115/115	-
18	CLA	6	611	20	1/1/10/20	2/10/88/115	-
27	XAT	7	620	-	-	1/31/93/93	0/4/4/4
18	CLA	4	618	13	1/1/10/20	1/8/84/115	-
23	LMU	A	857	-	-	9/19/56/61	0/2/2/2
20	LHG	a	620	18	-	10/53/53/53	-
22	SF4	A	853	-	-	-	0/6/5/5
20	LHG	4	622	18	-	25/53/53/53	-
18	CLA	7	608	-	1/1/12/20	3/19/97/115	-
18	CLA	A	843	-	1/1/14/20	16/35/113/115	-
18	CLA	A	806	-	1/1/15/20	15/37/115/115	-
18	CLA	4	614	-	1/1/13/20	12/27/105/115	-
18	CLA	A	811	-	1/1/15/20	15/37/115/115	-
18	CLA	3	603	-	1/1/13/20	7/25/103/115	-
21	BCR	A	852	-	-	7/29/63/63	0/2/2/2
21	BCR	B	801	-	-	4/29/63/63	0/2/2/2
18	CLA	A	815	-	1/1/12/20	8/19/97/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	a	612	11	1/1/11/20	5/13/91/115	-
26	LUT	4	619	-	-	2/29/67/67	0/2/2/2
18	CLA	a	611	20	1/1/10/20	0/4/80/115	-
18	CLA	7	603	-	1/1/11/20	4/11/89/115	-
18	CLA	J	101	8	1/1/10/20	5/10/88/115	-
18	CLA	7	601	16	-	12/31/109/115	-
19	PQN	B	842	-	-	9/23/43/43	0/2/2/2
21	BCR	8	621	-	-	6/29/63/63	0/2/2/2
18	CLA	K	201	9	1/1/11/20	8/13/91/115	-
18	CLA	B	823	-	1/1/11/20	5/13/91/115	-
18	CLA	5	601	14	1/1/13/20	6/27/105/115	-
18	CLA	a	610	11	1/1/14/20	4/29/107/115	-
18	CLA	a	603	-	1/1/12/20	6/23/101/115	-
18	CLA	6	608	-	1/1/12/20	7/21/99/115	-
18	CLA	6	602	15	1/1/15/20	7/37/115/115	-
18	CLA	B	813	-	1/1/15/20	21/37/115/115	-
18	CLA	1	604	-	1/1/11/20	10/18/96/115	-
18	CLA	A	813	-	1/1/12/20	4/24/102/115	-
18	CLA	4	608	-	1/1/15/20	13/37/115/115	-
18	CLA	5	606	-	1/1/10/20	3/6/84/115	-
21	BCR	7	621	-	-	2/29/63/63	0/2/2/2
24	LMG	J	104	-	-	17/35/55/70	0/1/1/1
18	CLA	A	827	-	1/1/13/20	6/30/108/115	-
18	CLA	A	833	-	1/1/11/20	2/13/91/115	-
18	CLA	6	607	-	1/1/10/20	4/10/86/115	-
18	CLA	4	612	13	-	2/8/86/115	-
18	CLA	6	609	15	1/1/11/20	4/13/91/115	-
18	CLA	A	841	-	1/1/15/20	18/37/115/115	-
21	BCR	B	847	-	-	2/29/63/63	0/2/2/2
18	CLA	K	204	-	1/1/11/20	7/15/93/115	-
18	CLA	5	609	14	1/1/15/20	12/37/115/115	-
18	CLA	B	809	2	1/1/15/20	18/37/115/115	-
18	CLA	7	604	-	1/1/13/20	8/23/101/115	-
18	CLA	A	845	20	1/1/12/20	11/19/97/115	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	825	-	1/1/14/20	9/34/112/115	-
24	LMG	5	626	-	-	26/35/55/70	0/1/1/1
18	CLA	L	302	10	1/1/11/20	7/13/91/115	-
18	CLA	A	824	-	1/1/10/20	2/8/86/115	-
18	CLA	a	604	-	1/1/11/20	10/18/96/115	-
18	CLA	A	834	-	1/1/15/20	12/37/115/115	-
20	LHG	5	625	-	-	31/53/53/53	-
27	XAT	4	620	-	-	1/31/93/93	0/4/4/4
18	CLA	B	814	-	1/1/14/20	13/36/114/115	-
18	CLA	6	612	15	1/1/10/20	3/8/86/115	-
18	CLA	3	604	-	1/1/15/20	7/37/115/115	-
18	CLA	A	816	-	1/1/11/20	4/13/91/115	-
18	CLA	B	805	-	1/1/15/20	14/37/115/115	-

All (1701) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	842	PQN	C12-C13	8.68	1.53	1.33
19	A	844	PQN	C12-C13	8.32	1.52	1.33
18	7	612	CLA	C4B-NB	8.02	1.42	1.35
19	A	844	PQN	O1-C1	8.02	1.40	1.23
19	B	842	PQN	O1-C1	7.81	1.39	1.23
18	B	824	CLA	C4B-NB	7.78	1.42	1.35
18	1	609	CLA	C4B-NB	7.74	1.42	1.35
18	B	821	CLA	C4B-NB	7.71	1.42	1.35
18	5	606	CLA	C4B-NB	7.67	1.42	1.35
18	B	822	CLA	C4B-NB	7.67	1.42	1.35
18	1	616	CLA	C4B-NB	7.67	1.42	1.35
18	1	608	CLA	C4B-NB	7.66	1.42	1.35
18	F	303	CLA	C4B-NB	7.64	1.42	1.35
18	1	603	CLA	C4B-NB	7.57	1.42	1.35
18	L	302	CLA	C4B-NB	7.55	1.41	1.35
18	K	201	CLA	C4B-NB	7.54	1.41	1.35
19	B	842	PQN	O4-C4	7.53	1.39	1.23
18	B	823	CLA	C4B-NB	7.52	1.41	1.35
18	B	820	CLA	C4B-NB	7.51	1.41	1.35
18	a	603	CLA	C4B-NB	7.50	1.41	1.35
18	1	606	CLA	C4B-NB	7.47	1.41	1.35
18	a	612	CLA	C4B-NB	7.47	1.41	1.35
18	a	608	CLA	C4B-NB	7.46	1.41	1.35

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	610	CLA	C4B-NB	7.45	1.41	1.35
18	B	841	CLA	C4B-NB	7.45	1.41	1.35
18	B	812	CLA	C4B-NB	7.44	1.41	1.35
18	1	612	CLA	C4B-NB	7.43	1.41	1.35
18	L	304	CLA	C4B-NB	7.42	1.41	1.35
18	B	819	CLA	C4B-NB	7.41	1.41	1.35
18	3	615	CLA	C4B-NB	7.41	1.41	1.35
19	A	844	PQN	O4-C4	7.40	1.38	1.23
18	J	101	CLA	C4B-NB	7.40	1.41	1.35
18	a	601	CLA	C4B-NB	7.39	1.41	1.35
18	K	206	CLA	C4B-NB	7.39	1.41	1.35
18	8	608	CLA	C4B-NB	7.38	1.41	1.35
18	B	835	CLA	C4B-NB	7.37	1.41	1.35
18	4	612	CLA	C4B-NB	7.36	1.41	1.35
18	A	837	CLA	C4B-NB	7.36	1.41	1.35
18	a	609	CLA	C4B-NB	7.35	1.41	1.35
18	8	606	CLA	C4B-NB	7.34	1.41	1.35
18	K	203	CLA	C4B-NB	7.33	1.41	1.35
18	a	613	CLA	C4B-NB	7.33	1.41	1.35
18	L	303	CLA	C4B-NB	7.33	1.41	1.35
18	7	616	CLA	C4B-NB	7.33	1.41	1.35
18	1	604	CLA	C4B-NB	7.32	1.41	1.35
18	1	607	CLA	C4B-NB	7.32	1.41	1.35
18	3	611	CLA	C4B-NB	7.30	1.41	1.35
18	6	612	CLA	C4B-NB	7.30	1.41	1.35
18	8	604	CLA	C4B-NB	7.29	1.41	1.35
18	4	614	CLA	C4B-NB	7.29	1.41	1.35
18	3	606	CLA	C4B-NB	7.29	1.41	1.35
18	3	614	CLA	C4B-NB	7.29	1.41	1.35
18	3	612	CLA	C4B-NB	7.28	1.41	1.35
18	5	601	CLA	C4B-NB	7.28	1.41	1.35
18	A	845	CLA	C4B-NB	7.25	1.41	1.35
18	4	616	CLA	C4B-NB	7.24	1.41	1.35
18	a	607	CLA	C4B-NB	7.24	1.41	1.35
18	3	603	CLA	C4B-NB	7.23	1.41	1.35
18	7	607	CLA	C4B-NB	7.23	1.41	1.35
18	6	609	CLA	C4B-NB	7.22	1.41	1.35
18	6	603	CLA	C4B-NB	7.22	1.41	1.35
18	3	613	CLA	C4B-NB	7.22	1.41	1.35
18	5	618	CLA	C4B-NB	7.21	1.41	1.35
18	1	613	CLA	C4B-NB	7.19	1.41	1.35
18	4	603	CLA	C4B-NB	7.19	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	614	CLA	C4B-NB	7.19	1.41	1.35
18	B	811	CLA	C4B-NB	7.19	1.41	1.35
18	a	606	CLA	C4B-NB	7.19	1.41	1.35
18	F	304	CLA	C4B-NB	7.18	1.41	1.35
18	a	604	CLA	C4B-NB	7.18	1.41	1.35
18	6	617	CLA	C4B-NB	7.18	1.41	1.35
18	5	604	CLA	C4B-NB	7.17	1.41	1.35
18	6	613	CLA	C4B-NB	7.17	1.41	1.35
18	a	611	CLA	C4B-NB	7.17	1.41	1.35
18	5	616	CLA	C4B-NB	7.17	1.41	1.35
18	4	601	CLA	C4B-NB	7.17	1.41	1.35
18	5	614	CLA	C4B-NB	7.17	1.41	1.35
18	3	607	CLA	C4B-NB	7.17	1.41	1.35
18	5	611	CLA	C4B-NB	7.16	1.41	1.35
18	8	613	CLA	C4B-NB	7.15	1.41	1.35
18	1	601	CLA	C4B-NB	7.14	1.41	1.35
18	a	614	CLA	C4B-NB	7.14	1.41	1.35
18	7	606	CLA	C4B-NB	7.14	1.41	1.35
18	B	834	CLA	C4B-NB	7.13	1.41	1.35
18	4	618	CLA	C4B-NB	7.13	1.41	1.35
18	6	614	CLA	C4B-NB	7.11	1.41	1.35
18	A	823	CLA	C4B-NB	7.11	1.41	1.35
18	7	615	CLA	C4B-NB	7.11	1.41	1.35
18	8	603	CLA	C4B-NB	7.11	1.41	1.35
18	4	609	CLA	C4B-NB	7.10	1.41	1.35
18	6	618	CLA	C4B-NB	7.10	1.41	1.35
18	4	604	CLA	C4B-NB	7.10	1.41	1.35
18	8	607	CLA	C4B-NB	7.09	1.41	1.35
18	3	604	CLA	C4B-NB	7.09	1.41	1.35
18	A	815	CLA	C4B-NB	7.09	1.41	1.35
18	4	613	CLA	C4B-NB	7.08	1.41	1.35
18	a	616	CLA	C4B-NB	7.08	1.41	1.35
18	1	611	CLA	C4B-NB	7.07	1.41	1.35
18	B	833	CLA	C4B-NB	7.05	1.41	1.35
18	B	807	CLA	C4B-NB	7.05	1.41	1.35
18	7	604	CLA	C4B-NB	7.05	1.41	1.35
18	5	612	CLA	C4B-NB	7.04	1.41	1.35
18	6	616	CLA	C4B-NB	7.04	1.41	1.35
18	A	822	CLA	C4B-NB	7.03	1.41	1.35
18	A	816	CLA	C4B-NB	7.02	1.41	1.35
18	8	616	CLA	C4B-NB	7.02	1.41	1.35
18	6	608	CLA	C4B-NB	7.01	1.41	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	804	CLA	C4B-NB	7.00	1.41	1.35
18	B	810	CLA	C4B-NB	7.00	1.41	1.35
18	5	619	CLA	C4B-NB	7.00	1.41	1.35
18	A	824	CLA	C4B-NB	7.00	1.41	1.35
18	8	611	CLA	C4B-NB	7.00	1.41	1.35
18	5	610	CLA	C4B-NB	7.00	1.41	1.35
18	A	832	CLA	C4B-NB	7.00	1.41	1.35
18	A	841	CLA	C4B-NB	6.99	1.41	1.35
18	4	606	CLA	C4B-NB	6.99	1.41	1.35
18	5	609	CLA	C4B-NB	6.99	1.41	1.35
18	B	840	CLA	C4B-NB	6.99	1.41	1.35
18	B	830	CLA	C4B-NB	6.99	1.41	1.35
18	A	818	CLA	C4B-NB	6.99	1.41	1.35
18	7	614	CLA	C4B-NB	6.99	1.41	1.35
18	B	815	CLA	C4B-NB	6.98	1.41	1.35
18	a	602	CLA	C4B-NB	6.98	1.41	1.35
18	4	611	CLA	C4B-NB	6.98	1.41	1.35
18	8	612	CLA	C4B-NB	6.97	1.41	1.35
18	B	816	CLA	C4B-NB	6.97	1.41	1.35
18	4	608	CLA	C4B-NB	6.97	1.41	1.35
18	A	804	CLA	C4B-NB	6.96	1.41	1.35
18	6	611	CLA	C4B-NB	6.96	1.41	1.35
18	7	603	CLA	C4B-NB	6.96	1.41	1.35
18	6	606	CLA	C4B-NB	6.95	1.41	1.35
18	4	607	CLA	C4B-NB	6.94	1.41	1.35
18	7	608	CLA	C4B-NB	6.94	1.41	1.35
18	F	301	CLA	C4B-NB	6.93	1.41	1.35
18	B	837	CLA	C4B-NB	6.93	1.41	1.35
18	a	610	CLA	C4B-NB	6.92	1.41	1.35
18	B	826	CLA	C4B-NB	6.92	1.41	1.35
18	A	821	CLA	C4B-NB	6.91	1.41	1.35
18	7	613	CLA	C4B-NB	6.90	1.41	1.35
18	5	613	CLA	C4B-NB	6.90	1.41	1.35
18	3	617	CLA	C4B-NB	6.90	1.41	1.35
18	B	814	CLA	C4B-NB	6.88	1.41	1.35
18	A	842	CLA	C4B-NB	6.88	1.41	1.35
18	6	604	CLA	C4B-NB	6.88	1.41	1.35
18	A	819	CLA	C4B-NB	6.87	1.41	1.35
18	8	601	CLA	C4B-NB	6.86	1.41	1.35
18	K	204	CLA	C4B-NB	6.86	1.41	1.35
18	B	831	CLA	C4B-NB	6.86	1.41	1.35
18	6	620	CLA	C4B-NB	6.85	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	603	CLA	C4B-NB	6.85	1.41	1.35
18	B	836	CLA	C4B-NB	6.84	1.41	1.35
18	B	813	CLA	C4B-NB	6.84	1.41	1.35
18	8	609	CLA	C4B-NB	6.83	1.41	1.35
18	A	840	CLA	C4B-NB	6.82	1.41	1.35
18	A	854	CLA	C4B-NB	6.80	1.41	1.35
18	7	602	CLA	C4B-NB	6.79	1.41	1.35
18	6	602	CLA	C4B-NB	6.79	1.41	1.35
18	5	602	CLA	C4B-NB	6.79	1.41	1.35
18	A	833	CLA	C4B-NB	6.78	1.41	1.35
18	6	610	CLA	C4B-NB	6.78	1.41	1.35
18	8	614	CLA	C4B-NB	6.78	1.41	1.35
18	7	611	CLA	C4B-NB	6.77	1.41	1.35
18	8	602	CLA	C4B-NB	6.77	1.41	1.35
18	3	609	CLA	C4B-NB	6.77	1.41	1.35
18	B	818	CLA	C4B-NB	6.77	1.41	1.35
18	1	602	CLA	C4B-NB	6.76	1.41	1.35
18	A	811	CLA	C4B-NB	6.75	1.41	1.35
18	B	827	CLA	C4B-NB	6.75	1.41	1.35
18	A	806	CLA	C4B-NB	6.75	1.41	1.35
18	A	810	CLA	C4B-NB	6.75	1.41	1.35
18	5	617	CLA	C4B-NB	6.75	1.41	1.35
18	A	808	CLA	C4B-NB	6.74	1.41	1.35
18	A	817	CLA	C4B-NB	6.72	1.41	1.35
18	A	812	CLA	C4B-NB	6.71	1.41	1.35
18	A	801	CLA	C4B-NB	6.71	1.41	1.35
18	B	806	CLA	C4B-NB	6.71	1.41	1.35
18	7	601	CLA	C4B-NB	6.70	1.41	1.35
18	B	832	CLA	C4B-NB	6.70	1.41	1.35
18	B	817	CLA	C4B-NB	6.69	1.41	1.35
18	7	610	CLA	C4B-NB	6.68	1.41	1.35
18	A	834	CLA	C4B-NB	6.67	1.41	1.35
18	7	609	CLA	C4B-NB	6.67	1.41	1.35
18	A	805	CLA	C4B-NB	6.67	1.41	1.35
18	A	820	CLA	C4B-NB	6.67	1.41	1.35
18	6	601	CLA	C4B-NB	6.66	1.41	1.35
18	5	608	CLA	C4B-NB	6.66	1.41	1.35
18	B	838	CLA	C4B-NB	6.66	1.41	1.35
18	A	831	CLA	C4B-NB	6.65	1.41	1.35
18	6	607	CLA	C4B-NB	6.65	1.41	1.35
18	A	836	CLA	C4B-NB	6.63	1.41	1.35
18	3	610	CLA	C4B-NB	6.62	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	805	CLA	C4B-NB	6.62	1.41	1.35
18	A	835	CLA	C4B-NB	6.60	1.41	1.35
18	4	610	CLA	C4B-NB	6.58	1.41	1.35
18	A	807	CLA	C4B-NB	6.58	1.41	1.35
18	A	830	CLA	C4B-NB	6.55	1.41	1.35
18	A	826	CLA	C4B-NB	6.54	1.41	1.35
18	B	829	CLA	C4B-NB	6.54	1.41	1.35
18	A	829	CLA	C4B-NB	6.52	1.41	1.35
18	B	802	CLA	C4B-NB	6.52	1.41	1.35
18	B	808	CLA	C4B-NB	6.52	1.41	1.35
18	A	839	CLA	C4B-NB	6.51	1.41	1.35
18	B	809	CLA	C4B-NB	6.50	1.41	1.35
18	B	825	CLA	C4B-NB	6.49	1.41	1.35
18	A	813	CLA	C4B-NB	6.49	1.41	1.35
18	A	803	CLA	C4B-NB	6.48	1.41	1.35
18	3	608	CLA	C4B-NB	6.46	1.41	1.35
18	A	843	CLA	C4B-NB	6.45	1.41	1.35
18	B	839	CLA	C4B-NB	6.44	1.41	1.35
18	A	809	CLA	C4B-NB	6.42	1.40	1.35
18	8	610	CLA	C4B-NB	6.41	1.40	1.35
18	A	828	CLA	C4B-NB	6.40	1.40	1.35
18	A	827	CLA	C4B-NB	6.34	1.40	1.35
18	5	607	CLA	C4B-NB	6.32	1.40	1.35
18	B	828	CLA	C4B-NB	6.30	1.40	1.35
18	A	825	CLA	C4B-NB	6.29	1.40	1.35
18	A	802	CLA	C4B-NB	6.28	1.40	1.35
18	4	602	CLA	C4B-NB	6.19	1.40	1.35
18	A	814	CLA	C4B-NB	6.08	1.40	1.35
18	A	838	CLA	C4B-NB	5.95	1.40	1.35
18	3	602	CLA	C4B-NB	5.93	1.40	1.35
18	B	803	CLA	C4B-NB	5.78	1.40	1.35
18	5	614	CLA	CHB-C4A	4.96	1.38	1.34
18	a	614	CLA	CHB-C4A	4.42	1.38	1.34
18	A	831	CLA	CMB-C2B	-4.41	1.42	1.51
19	B	842	PQN	C2-C1	-4.34	1.38	1.48
18	1	609	CLA	C1D-ND	4.30	1.43	1.37
20	8	622	LHG	O8-C23	4.27	1.45	1.33
19	A	844	PQN	C2-C1	-4.25	1.38	1.48
18	5	603	CLA	CAB-C3B	-4.16	1.43	1.51
18	B	829	CLA	CMB-C2B	-4.12	1.43	1.51
18	1	614	CLA	CHB-C4A	4.11	1.38	1.34
20	8	622	LHG	O7-C7	4.09	1.45	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	609	CLA	C1D-ND	4.05	1.42	1.37
18	B	821	CLA	C1D-ND	4.04	1.42	1.37
18	B	822	CLA	C1D-ND	3.98	1.42	1.37
18	F	303	CLA	C1D-ND	3.98	1.42	1.37
18	3	608	CLA	C4D-ND	-3.97	1.32	1.37
18	B	830	CLA	C1D-ND	3.94	1.42	1.37
18	J	101	CLA	C1D-ND	3.91	1.42	1.37
18	B	820	CLA	C1D-ND	3.90	1.42	1.37
18	L	302	CLA	C1D-ND	3.90	1.42	1.37
18	B	841	CLA	C1D-ND	3.89	1.42	1.37
23	A	857	LMU	O5'-C1'	3.88	1.50	1.41
23	A	858	LMU	O5B-C1B	3.88	1.51	1.41
18	1	608	CLA	C1D-ND	3.88	1.42	1.37
23	5	628	LMU	O5B-C1B	3.86	1.51	1.41
18	4	604	CLA	CAB-C3B	-3.85	1.43	1.51
18	8	616	CLA	C1D-ND	3.84	1.42	1.37
18	a	606	CLA	C1D-ND	3.84	1.42	1.37
18	1	604	CLA	C1D-ND	3.83	1.42	1.37
18	1	603	CLA	C1D-ND	3.82	1.42	1.37
18	5	607	CLA	C1D-ND	3.82	1.42	1.37
18	3	609	CLA	C1D-ND	3.81	1.42	1.37
18	4	609	CLA	C1D-ND	3.81	1.42	1.37
18	1	610	CLA	C1D-ND	3.80	1.42	1.37
18	B	824	CLA	C1D-ND	3.79	1.42	1.37
18	1	607	CLA	C1D-ND	3.79	1.42	1.37
18	B	803	CLA	C4D-ND	-3.78	1.32	1.37
18	K	203	CLA	C1D-ND	3.78	1.42	1.37
18	a	610	CLA	C1D-ND	3.77	1.42	1.37
18	4	610	CLA	C1D-ND	3.77	1.42	1.37
18	K	206	CLA	C1D-ND	3.77	1.42	1.37
18	a	603	CLA	C1D-ND	3.76	1.42	1.37
18	4	616	CLA	C1D-ND	3.76	1.42	1.37
18	a	604	CLA	C1D-ND	3.76	1.42	1.37
18	5	610	CLA	C1D-ND	3.76	1.42	1.37
18	a	611	CLA	C1D-ND	3.75	1.42	1.37
23	K	208	LMU	O5'-C1'	3.75	1.51	1.41
18	L	304	CLA	C1D-ND	3.75	1.42	1.37
18	7	615	CLA	C1D-ND	3.74	1.42	1.37
18	a	608	CLA	C1D-ND	3.73	1.42	1.37
23	A	857	LMU	O5B-C1B	3.73	1.51	1.41
18	A	817	CLA	C1D-ND	3.72	1.42	1.37
18	5	619	CLA	CAB-C3B	-3.72	1.43	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	613	CLA	C1D-ND	3.72	1.42	1.37
18	5	613	CLA	C1D-ND	3.72	1.42	1.37
18	B	810	CLA	C1D-ND	3.71	1.42	1.37
23	8	624	LMU	O5B-C1B	3.71	1.51	1.41
18	4	607	CLA	C1D-ND	3.71	1.42	1.37
18	A	837	CLA	C1D-ND	3.71	1.42	1.37
18	B	812	CLA	C1D-ND	3.71	1.42	1.37
18	1	606	CLA	C1D-ND	3.70	1.42	1.37
23	A	859	LMU	O5'-C1'	3.70	1.51	1.42
18	6	618	CLA	CAB-C3B	-3.70	1.43	1.51
18	8	616	CLA	CAB-C3B	-3.70	1.43	1.51
18	a	613	CLA	C1D-ND	3.70	1.42	1.37
18	5	618	CLA	CAB-C3B	-3.69	1.44	1.51
18	3	615	CLA	C1D-ND	3.69	1.42	1.37
18	6	603	CLA	CAB-C3B	-3.69	1.44	1.51
18	B	813	CLA	C1D-ND	3.69	1.42	1.37
18	7	606	CLA	C1D-ND	3.69	1.42	1.37
18	A	831	CLA	C4D-ND	-3.67	1.32	1.37
18	8	603	CLA	CAB-C3B	-3.67	1.44	1.51
18	B	817	CLA	C1D-ND	3.67	1.42	1.37
18	K	204	CLA	C1D-ND	3.67	1.42	1.37
23	K	208	LMU	O5B-C1B	3.66	1.51	1.41
18	B	835	CLA	C1D-ND	3.66	1.42	1.37
18	5	616	CLA	CAB-C3B	-3.66	1.44	1.51
18	A	806	CLA	C4D-ND	-3.66	1.32	1.37
18	4	618	CLA	C1D-ND	3.66	1.42	1.37
18	8	609	CLA	C1D-ND	3.66	1.42	1.37
18	4	602	CLA	C1D-ND	3.65	1.42	1.37
18	8	607	CLA	CAB-C3B	-3.65	1.44	1.51
23	5	628	LMU	O5'-C1'	3.65	1.51	1.41
18	1	614	CLA	CAB-C3B	-3.65	1.44	1.51
18	4	614	CLA	C1D-ND	3.65	1.42	1.37
18	5	604	CLA	CAB-C3B	-3.65	1.44	1.51
18	B	819	CLA	C1D-ND	3.64	1.42	1.37
18	B	825	CLA	C4D-ND	-3.64	1.32	1.37
18	F	304	CLA	C1D-ND	3.64	1.42	1.37
18	A	835	CLA	C1D-ND	3.64	1.42	1.37
18	3	612	CLA	C1D-ND	3.64	1.42	1.37
18	B	823	CLA	C1D-ND	3.64	1.42	1.37
18	A	807	CLA	C4D-ND	-3.63	1.32	1.37
18	3	607	CLA	C1D-ND	3.63	1.42	1.37
18	B	828	CLA	C4D-ND	-3.63	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	612	CLA	C1D-ND	3.63	1.42	1.37
18	5	616	CLA	C1D-ND	3.63	1.42	1.37
18	8	606	CLA	C1D-ND	3.63	1.42	1.37
18	1	611	CLA	C1D-ND	3.63	1.42	1.37
18	B	834	CLA	C1D-ND	3.62	1.42	1.37
18	8	608	CLA	C1D-ND	3.62	1.42	1.37
18	3	603	CLA	C1D-ND	3.62	1.42	1.37
18	A	833	CLA	C1D-ND	3.61	1.42	1.37
18	A	812	CLA	C4D-ND	-3.61	1.32	1.37
18	A	839	CLA	C4D-ND	-3.61	1.32	1.37
18	7	613	CLA	C1D-ND	3.61	1.42	1.37
18	B	815	CLA	C1D-ND	3.61	1.42	1.37
18	a	611	CLA	CAB-C3B	-3.61	1.44	1.51
19	B	842	PQN	C3-C2	3.61	1.41	1.35
18	a	607	CLA	C1D-ND	3.60	1.42	1.37
18	6	607	CLA	CAB-C3B	-3.60	1.44	1.51
18	5	614	CLA	C1D-ND	3.59	1.42	1.37
18	3	614	CLA	C1D-ND	3.59	1.42	1.37
18	6	614	CLA	C1D-ND	3.58	1.42	1.37
18	4	603	CLA	CAB-C3B	-3.58	1.44	1.51
18	5	603	CLA	C4D-ND	-3.57	1.32	1.37
18	4	618	CLA	CAB-C3B	-3.57	1.44	1.51
18	7	615	CLA	CAB-C3B	-3.57	1.44	1.51
18	7	601	CLA	C4D-ND	-3.57	1.32	1.37
18	3	611	CLA	CAB-C3B	-3.57	1.44	1.51
18	A	833	CLA	C4D-ND	-3.56	1.32	1.37
18	3	606	CLA	C1D-ND	3.56	1.42	1.37
18	A	803	CLA	C4D-ND	-3.55	1.32	1.37
18	4	604	CLA	C1D-ND	3.55	1.42	1.37
18	1	601	CLA	C1D-ND	3.55	1.42	1.37
18	4	616	CLA	CAB-C3B	-3.55	1.44	1.51
18	A	814	CLA	C4D-ND	-3.55	1.32	1.37
18	B	829	CLA	C4D-ND	-3.54	1.32	1.37
18	4	611	CLA	C1D-ND	3.54	1.42	1.37
18	6	601	CLA	C1D-ND	3.54	1.42	1.37
18	7	611	CLA	C1D-ND	3.54	1.42	1.37
18	6	606	CLA	C1D-ND	3.54	1.42	1.37
18	5	611	CLA	C1D-ND	3.54	1.42	1.37
18	1	616	CLA	CAB-C3B	-3.54	1.44	1.51
18	4	608	CLA	C1D-ND	3.53	1.42	1.37
18	8	603	CLA	C1D-ND	3.53	1.42	1.37
18	7	608	CLA	C1D-ND	3.53	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	602	CLA	C1D-ND	3.53	1.42	1.37
18	B	811	CLA	CAB-C3B	-3.52	1.44	1.51
18	a	614	CLA	C1D-ND	3.52	1.42	1.37
18	7	616	CLA	CAB-C3B	-3.52	1.44	1.51
18	A	845	CLA	C1D-ND	3.52	1.42	1.37
18	6	611	CLA	C1D-ND	3.52	1.42	1.37
18	5	612	CLA	C1D-ND	3.52	1.42	1.37
18	A	829	CLA	C1D-ND	3.51	1.42	1.37
18	A	839	CLA	C1D-ND	3.51	1.42	1.37
18	5	619	CLA	C1D-ND	3.51	1.42	1.37
18	6	604	CLA	C1D-ND	3.51	1.42	1.37
18	A	825	CLA	C4D-ND	-3.51	1.32	1.37
18	A	819	CLA	C4D-ND	-3.51	1.32	1.37
18	4	602	CLA	C4D-ND	-3.50	1.32	1.37
18	B	832	CLA	C4D-ND	-3.50	1.32	1.37
18	A	834	CLA	C1D-ND	3.50	1.42	1.37
18	1	602	CLA	C1D-ND	3.50	1.42	1.37
18	B	805	CLA	C4D-ND	-3.50	1.32	1.37
18	7	603	CLA	C1D-ND	3.50	1.42	1.37
18	7	616	CLA	C1D-ND	3.50	1.42	1.37
18	3	607	CLA	CAB-C3B	-3.50	1.44	1.51
18	B	831	CLA	C1D-ND	3.50	1.42	1.37
18	A	825	CLA	C1D-ND	3.49	1.42	1.37
18	3	610	CLA	C4D-ND	-3.49	1.32	1.37
18	A	816	CLA	C1D-ND	3.49	1.42	1.37
18	4	603	CLA	C1D-ND	3.49	1.42	1.37
18	5	602	CLA	C4D-ND	-3.48	1.32	1.37
18	A	854	CLA	CHC-C1C	3.48	1.43	1.35
18	3	610	CLA	C1D-ND	3.48	1.42	1.37
18	A	824	CLA	C1D-ND	3.48	1.42	1.37
18	8	608	CLA	C4D-ND	-3.48	1.32	1.37
18	B	826	CLA	C1D-ND	3.48	1.42	1.37
18	5	609	CLA	C1D-ND	3.48	1.42	1.37
18	1	601	CLA	C4D-ND	-3.48	1.32	1.37
18	1	609	CLA	CAB-C3B	-3.48	1.44	1.51
18	B	807	CLA	C1D-ND	3.47	1.42	1.37
18	1	614	CLA	C1D-ND	3.47	1.42	1.37
18	B	838	CLA	C4D-ND	-3.47	1.32	1.37
23	8	625	LMU	O5'-C1'	3.47	1.50	1.41
18	B	833	CLA	C1D-ND	3.47	1.42	1.37
18	4	613	CLA	C1D-ND	3.47	1.42	1.37
18	5	601	CLA	C1D-ND	3.47	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	608	CLA	C1D-ND	3.47	1.42	1.37
18	a	602	CLA	C1D-ND	3.46	1.42	1.37
18	8	610	CLA	C1D-ND	3.46	1.42	1.37
18	3	617	CLA	C1D-ND	3.46	1.42	1.37
18	5	617	CLA	C1D-ND	3.46	1.42	1.37
18	A	838	CLA	C4D-ND	-3.46	1.32	1.37
18	3	603	CLA	C4D-ND	-3.46	1.32	1.37
18	3	604	CLA	C1D-ND	3.46	1.42	1.37
23	A	858	LMU	O5'-C1'	3.45	1.50	1.41
18	8	604	CLA	C1D-ND	3.45	1.42	1.37
18	7	614	CLA	C1D-ND	3.45	1.42	1.37
18	A	805	CLA	C4D-ND	-3.45	1.33	1.37
18	5	608	CLA	C1D-ND	3.45	1.42	1.37
18	6	617	CLA	C1D-ND	3.45	1.42	1.37
18	A	810	CLA	C4D-ND	-3.45	1.33	1.37
18	B	826	CLA	C4D-ND	-3.44	1.33	1.37
18	B	816	CLA	C1D-ND	3.44	1.42	1.37
18	B	806	CLA	C4D-ND	-3.44	1.33	1.37
18	8	614	CLA	C1D-ND	3.44	1.42	1.37
18	4	612	CLA	C1D-ND	3.43	1.42	1.37
18	A	802	CLA	C4D-ND	-3.43	1.33	1.37
18	7	604	CLA	C1D-ND	3.43	1.42	1.37
23	8	625	LMU	O5B-C1B	3.43	1.50	1.41
18	A	854	CLA	C4D-ND	-3.43	1.33	1.37
18	A	807	CLA	C1D-ND	3.43	1.42	1.37
18	5	618	CLA	C1D-ND	3.43	1.42	1.37
18	5	608	CLA	C4D-ND	-3.43	1.33	1.37
18	5	606	CLA	C1D-ND	3.42	1.42	1.37
18	A	836	CLA	C1D-ND	3.42	1.42	1.37
18	7	608	CLA	C4D-ND	-3.42	1.33	1.37
19	A	844	PQN	C3-C2	3.42	1.41	1.35
23	A	859	LMU	O5B-C1B	3.42	1.50	1.41
18	3	611	CLA	C1D-ND	3.42	1.42	1.37
18	B	807	CLA	C4D-ND	-3.41	1.33	1.37
18	A	801	CLA	C1D-ND	3.41	1.42	1.37
18	A	813	CLA	C4D-ND	-3.41	1.33	1.37
18	A	830	CLA	C4D-ND	-3.41	1.33	1.37
18	3	608	CLA	C1D-ND	3.41	1.42	1.37
18	6	616	CLA	C1D-ND	3.41	1.42	1.37
18	7	601	CLA	C1D-ND	3.41	1.42	1.37
18	B	818	CLA	C4D-ND	-3.41	1.33	1.37
18	a	612	CLA	C1D-ND	3.40	1.42	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	612	CLA	C1D-ND	3.40	1.42	1.37
18	B	833	CLA	C4D-ND	-3.40	1.33	1.37
18	B	837	CLA	C1D-ND	3.40	1.42	1.37
18	A	811	CLA	C4D-ND	-3.40	1.33	1.37
18	B	832	CLA	C1D-ND	3.40	1.42	1.37
18	3	602	CLA	C4D-ND	-3.40	1.33	1.37
18	6	610	CLA	C1D-ND	3.39	1.42	1.37
18	8	613	CLA	C1D-ND	3.39	1.42	1.37
18	B	811	CLA	C1D-ND	3.39	1.41	1.37
18	7	612	CLA	C4D-ND	-3.39	1.33	1.37
18	B	808	CLA	C1D-ND	3.39	1.41	1.37
18	5	604	CLA	C1D-ND	3.39	1.41	1.37
18	5	607	CLA	C4D-ND	-3.38	1.33	1.37
18	B	836	CLA	C1D-ND	3.38	1.41	1.37
18	8	612	CLA	C1D-ND	3.38	1.41	1.37
18	1	616	CLA	C1D-ND	3.38	1.41	1.37
18	B	841	CLA	CHC-C1C	3.38	1.43	1.35
18	A	808	CLA	C1D-ND	3.37	1.41	1.37
18	8	602	CLA	C4D-ND	-3.37	1.33	1.37
18	A	828	CLA	C1D-ND	3.37	1.41	1.37
18	B	840	CLA	C4D-ND	-3.36	1.33	1.37
18	4	613	CLA	C4D-ND	-3.36	1.33	1.37
18	B	823	CLA	CHC-C1C	3.36	1.43	1.35
18	A	814	CLA	C1D-ND	3.36	1.41	1.37
18	a	616	CLA	C1D-ND	3.36	1.41	1.37
19	B	842	PQN	C3-C4	-3.36	1.38	1.47
18	7	607	CLA	C1D-ND	3.36	1.41	1.37
18	8	614	CLA	C4D-ND	-3.36	1.33	1.37
18	A	842	CLA	C1D-ND	3.36	1.41	1.37
18	A	829	CLA	C4D-ND	-3.35	1.33	1.37
18	B	837	CLA	C4D-ND	-3.35	1.33	1.37
18	B	836	CLA	C4D-ND	-3.35	1.33	1.37
18	8	607	CLA	C1D-ND	3.35	1.41	1.37
18	A	820	CLA	C4D-ND	-3.35	1.33	1.37
18	A	840	CLA	C4D-ND	-3.35	1.33	1.37
18	7	602	CLA	C4D-ND	-3.35	1.33	1.37
18	4	606	CLA	C1D-ND	3.35	1.41	1.37
18	B	817	CLA	C4D-ND	-3.35	1.33	1.37
18	4	601	CLA	C4D-ND	-3.35	1.33	1.37
18	B	809	CLA	C4D-ND	-3.35	1.33	1.37
18	L	303	CLA	C1D-ND	3.35	1.41	1.37
18	7	602	CLA	C1D-ND	3.34	1.41	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	840	CLA	C1D-ND	3.34	1.41	1.37
23	8	624	LMU	O5'-C1'	3.34	1.50	1.41
18	A	823	CLA	C4D-ND	-3.33	1.33	1.37
18	A	827	CLA	C1D-ND	3.33	1.41	1.37
18	8	602	CLA	C1D-ND	3.33	1.41	1.37
18	7	612	CLA	C1D-ND	3.32	1.41	1.37
18	7	614	CLA	C4D-ND	-3.32	1.33	1.37
18	6	607	CLA	C4D-ND	-3.32	1.33	1.37
18	5	602	CLA	C1D-ND	3.32	1.41	1.37
18	6	607	CLA	C1D-ND	3.32	1.41	1.37
18	B	839	CLA	C4D-ND	-3.32	1.33	1.37
18	A	815	CLA	C4D-ND	-3.32	1.33	1.37
18	A	822	CLA	C4D-ND	-3.31	1.33	1.37
18	A	826	CLA	C4D-ND	-3.31	1.33	1.37
18	A	820	CLA	C1D-ND	3.31	1.41	1.37
18	B	825	CLA	C1D-ND	3.31	1.41	1.37
18	A	843	CLA	C1D-ND	3.31	1.41	1.37
18	8	611	CLA	C4D-ND	-3.31	1.33	1.37
18	1	602	CLA	C4D-ND	-3.30	1.33	1.37
18	a	602	CLA	C4D-ND	-3.30	1.33	1.37
18	A	805	CLA	C1D-ND	3.30	1.41	1.37
19	A	844	PQN	C3-C4	-3.30	1.38	1.47
18	6	602	CLA	C4D-ND	-3.30	1.33	1.37
18	3	602	CLA	C1D-ND	3.30	1.41	1.37
18	A	804	CLA	C1D-ND	3.30	1.41	1.37
18	B	818	CLA	C1D-ND	3.30	1.41	1.37
18	6	603	CLA	C1D-ND	3.29	1.41	1.37
18	F	301	CLA	C4D-ND	-3.29	1.33	1.37
18	F	301	CLA	CMB-C2B	-3.29	1.44	1.51
18	B	827	CLA	C4D-ND	-3.29	1.33	1.37
18	A	818	CLA	C4D-ND	-3.29	1.33	1.37
18	5	613	CLA	C4D-ND	-3.29	1.33	1.37
18	4	601	CLA	C1D-ND	3.28	1.41	1.37
18	3	604	CLA	C4D-ND	-3.28	1.33	1.37
18	B	839	CLA	C1D-ND	3.28	1.41	1.37
18	3	617	CLA	C4D-ND	-3.28	1.33	1.37
18	5	617	CLA	C4D-ND	-3.28	1.33	1.37
18	6	608	CLA	C4D-ND	-3.27	1.33	1.37
18	A	809	CLA	C4D-ND	-3.27	1.33	1.37
18	A	827	CLA	C4D-ND	-3.27	1.33	1.37
18	A	841	CLA	C4D-ND	-3.27	1.33	1.37
18	A	801	CLA	C4D-ND	-3.27	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	8	601	CLA	C1D-ND	3.27	1.41	1.37
18	A	820	CLA	CMB-C2B	-3.27	1.44	1.51
18	7	610	CLA	C4D-ND	-3.27	1.33	1.37
18	B	831	CLA	C4D-ND	-3.26	1.33	1.37
18	A	821	CLA	C4D-ND	-3.26	1.33	1.37
18	A	804	CLA	C4D-ND	-3.26	1.33	1.37
18	4	608	CLA	C4D-ND	-3.26	1.33	1.37
18	B	802	CLA	C4D-ND	-3.26	1.33	1.37
18	8	610	CLA	C4D-ND	-3.26	1.33	1.37
18	8	613	CLA	C4D-ND	-3.25	1.33	1.37
18	a	608	CLA	CHC-C1C	3.25	1.43	1.35
18	A	808	CLA	C4D-ND	-3.25	1.33	1.37
18	8	611	CLA	C1D-ND	3.25	1.41	1.37
18	A	828	CLA	C4D-ND	-3.25	1.33	1.37
18	B	824	CLA	CHC-C1C	3.25	1.43	1.35
18	a	601	CLA	C4D-ND	-3.25	1.33	1.37
18	A	834	CLA	C4D-ND	-3.24	1.33	1.37
18	3	612	CLA	C4D-ND	-3.24	1.33	1.37
18	4	614	CLA	C4D-ND	-3.24	1.33	1.37
18	B	803	CLA	CMC-C2C	-3.24	1.43	1.50
18	6	620	CLA	C4D-ND	-3.24	1.33	1.37
18	A	832	CLA	C4D-ND	-3.24	1.33	1.37
18	K	201	CLA	C1D-ND	3.23	1.41	1.37
18	A	824	CLA	C4D-ND	-3.23	1.33	1.37
18	7	603	CLA	C4D-ND	-3.23	1.33	1.37
18	B	804	CLA	CHC-C1C	3.23	1.43	1.35
18	B	806	CLA	C1D-ND	3.23	1.41	1.37
18	A	815	CLA	C1D-ND	3.23	1.41	1.37
18	A	805	CLA	CHC-C1C	3.22	1.43	1.35
18	8	601	CLA	C4D-ND	-3.22	1.33	1.37
18	A	803	CLA	CMB-C2B	-3.22	1.44	1.51
18	A	813	CLA	C1D-ND	3.21	1.41	1.37
18	A	826	CLA	C1D-ND	3.21	1.41	1.37
18	A	836	CLA	C4D-ND	-3.21	1.33	1.37
18	A	815	CLA	CHC-C1C	3.20	1.43	1.35
18	B	820	CLA	CHC-C1C	3.20	1.43	1.35
18	A	842	CLA	C4D-ND	-3.20	1.33	1.37
18	A	811	CLA	C1D-ND	3.20	1.41	1.37
18	1	608	CLA	CHC-C1C	3.19	1.43	1.35
18	3	607	CLA	C4D-ND	-3.19	1.33	1.37
18	4	604	CLA	C4D-ND	-3.19	1.33	1.37
18	B	840	CLA	C1D-ND	3.19	1.41	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	610	CLA	CHC-C1C	3.19	1.43	1.35
18	B	841	CLA	C4D-ND	-3.19	1.33	1.37
18	6	610	CLA	C4D-ND	-3.19	1.33	1.37
18	A	818	CLA	C1D-ND	3.19	1.41	1.37
18	6	603	CLA	C4D-ND	-3.19	1.33	1.37
18	6	617	CLA	C4D-ND	-3.19	1.33	1.37
18	5	604	CLA	C4D-ND	-3.18	1.33	1.37
18	A	843	CLA	C4D-ND	-3.18	1.33	1.37
18	6	618	CLA	C4D-ND	-3.18	1.33	1.37
18	A	819	CLA	C1D-ND	3.18	1.41	1.37
18	B	837	CLA	CHC-C1C	3.18	1.43	1.35
18	4	606	CLA	C4D-ND	-3.18	1.33	1.37
18	A	816	CLA	C4D-ND	-3.18	1.33	1.37
19	B	842	PQN	C11-C12	3.18	1.55	1.50
18	A	845	CLA	C4D-ND	-3.18	1.33	1.37
18	B	809	CLA	CMB-C2B	-3.17	1.45	1.51
18	6	609	CLA	C1D-ND	3.17	1.41	1.37
18	3	613	CLA	C4D-ND	-3.17	1.33	1.37
18	1	613	CLA	C4D-ND	-3.17	1.33	1.37
18	4	611	CLA	C4D-ND	-3.16	1.33	1.37
18	B	810	CLA	C4D-ND	-3.16	1.33	1.37
18	7	612	CLA	CHC-C1C	3.15	1.43	1.35
18	a	614	CLA	C4D-ND	-3.15	1.33	1.37
18	B	825	CLA	CHC-C1C	3.15	1.43	1.35
18	6	613	CLA	C1D-ND	3.15	1.41	1.37
18	A	841	CLA	C1D-ND	3.15	1.41	1.37
18	6	608	CLA	CHC-C1C	3.15	1.43	1.35
18	6	620	CLA	CHC-C1C	3.15	1.43	1.35
18	B	811	CLA	C4D-ND	-3.15	1.33	1.37
18	B	804	CLA	C4D-ND	-3.14	1.33	1.37
28	5	624	NEX	C7-C8	-3.14	1.26	1.32
18	a	610	CLA	C4D-ND	-3.14	1.33	1.37
18	B	812	CLA	CHC-C1C	3.14	1.43	1.35
18	6	616	CLA	CHC-C1C	3.14	1.43	1.35
18	A	836	CLA	CMB-C2B	-3.14	1.45	1.51
18	8	609	CLA	C4D-ND	-3.14	1.33	1.37
18	8	616	CLA	C4D-ND	-3.14	1.33	1.37
18	7	611	CLA	C4D-ND	-3.13	1.33	1.37
18	B	813	CLA	C4D-ND	-3.13	1.33	1.37
18	5	603	CLA	CHC-C1C	3.13	1.43	1.35
19	A	844	PQN	C11-C12	3.13	1.55	1.50
18	4	611	CLA	CHC-C1C	3.13	1.43	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	834	CLA	C4D-ND	-3.13	1.33	1.37
18	1	609	CLA	CHC-C1C	3.13	1.43	1.35
18	A	823	CLA	C1D-ND	3.13	1.41	1.37
18	6	606	CLA	C4D-ND	-3.13	1.33	1.37
18	8	607	CLA	C4D-ND	-3.13	1.33	1.37
18	A	835	CLA	C4D-ND	-3.12	1.33	1.37
18	1	614	CLA	CHC-C1C	3.12	1.43	1.35
18	4	607	CLA	C4D-ND	-3.12	1.33	1.37
18	B	814	CLA	CHC-C1C	3.12	1.43	1.35
18	B	808	CLA	C4D-ND	-3.12	1.33	1.37
18	B	828	CLA	C1D-ND	3.12	1.41	1.37
18	6	604	CLA	C4D-ND	-3.12	1.33	1.37
18	8	606	CLA	C4D-ND	-3.12	1.33	1.37
18	A	809	CLA	CHC-C1C	3.12	1.43	1.35
18	B	814	CLA	C4D-ND	-3.12	1.33	1.37
18	8	612	CLA	C4D-ND	-3.12	1.33	1.37
18	B	836	CLA	CHC-C1C	3.11	1.43	1.35
18	7	607	CLA	C4D-ND	-3.11	1.33	1.37
18	1	607	CLA	CHC-C1C	3.11	1.42	1.35
18	6	617	CLA	CHC-C1C	3.11	1.42	1.35
18	5	610	CLA	C4D-ND	-3.11	1.33	1.37
18	F	304	CLA	CHC-C1C	3.11	1.42	1.35
18	K	203	CLA	CHC-C1C	3.11	1.42	1.35
18	5	611	CLA	C4D-ND	-3.11	1.33	1.37
18	6	610	CLA	CHC-C1C	3.11	1.42	1.35
18	7	616	CLA	CHC-C1C	3.11	1.42	1.35
18	8	610	CLA	CHC-C1C	3.11	1.42	1.35
18	a	613	CLA	C4D-ND	-3.10	1.33	1.37
18	a	607	CLA	CHC-C1C	3.10	1.42	1.35
18	a	602	CLA	CHC-C1C	3.10	1.42	1.35
18	B	835	CLA	CHC-C1C	3.10	1.42	1.35
18	A	822	CLA	C1D-ND	3.10	1.41	1.37
18	a	612	CLA	CHC-C1C	3.10	1.42	1.35
18	6	612	CLA	CHC-C1C	3.10	1.42	1.35
18	5	616	CLA	C4D-ND	-3.10	1.33	1.37
18	A	838	CLA	C1D-ND	3.09	1.41	1.37
18	F	301	CLA	C1D-ND	3.09	1.41	1.37
18	7	602	CLA	CHC-C1C	3.09	1.42	1.35
18	4	604	CLA	CHC-C1C	3.09	1.42	1.35
18	a	610	CLA	CHC-C1C	3.09	1.42	1.35
18	3	608	CLA	CMB-C2B	-3.09	1.45	1.51
18	5	617	CLA	CMB-C2B	-3.09	1.45	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	610	CLA	C4D-ND	-3.08	1.33	1.37
18	A	806	CLA	C1D-ND	3.08	1.41	1.37
18	B	838	CLA	C1D-ND	3.08	1.41	1.37
18	a	601	CLA	CHC-C1C	3.08	1.42	1.35
18	1	614	CLA	C4D-ND	-3.08	1.33	1.37
18	3	606	CLA	C4D-ND	-3.08	1.33	1.37
18	1	606	CLA	CHC-C1C	3.08	1.42	1.35
18	a	607	CLA	C4D-ND	-3.08	1.33	1.37
18	A	819	CLA	C3B-C2B	-3.08	1.36	1.40
18	6	614	CLA	CHC-C1C	3.08	1.42	1.35
18	4	612	CLA	CHC-C1C	3.07	1.42	1.35
18	4	616	CLA	CHC-C1C	3.07	1.42	1.35
18	7	615	CLA	CHC-C1C	3.07	1.42	1.35
18	6	611	CLA	CHC-C1C	3.07	1.42	1.35
18	B	816	CLA	CHC-C1C	3.07	1.42	1.35
18	L	303	CLA	C4D-ND	-3.07	1.33	1.37
18	6	614	CLA	C4D-ND	-3.07	1.33	1.37
18	7	610	CLA	CHC-C1C	3.07	1.42	1.35
18	1	604	CLA	CHC-C1C	3.07	1.42	1.35
18	3	617	CLA	CHC-C1C	3.06	1.42	1.35
18	B	813	CLA	CHC-C1C	3.06	1.42	1.35
18	5	614	CLA	CHC-C1C	3.06	1.42	1.35
18	B	817	CLA	CHC-C1C	3.06	1.42	1.35
18	1	602	CLA	CHC-C1C	3.06	1.42	1.35
18	A	819	CLA	CMB-C2B	-3.06	1.45	1.51
18	A	802	CLA	CHC-C1C	3.06	1.42	1.35
18	3	611	CLA	C4D-ND	-3.06	1.33	1.37
18	B	807	CLA	CHC-C1C	3.06	1.42	1.35
18	5	618	CLA	C4D-ND	-3.06	1.33	1.37
18	8	608	CLA	CHC-C1C	3.06	1.42	1.35
18	K	206	CLA	CHC-C1C	3.05	1.42	1.35
18	L	303	CLA	CHC-C1C	3.05	1.42	1.35
18	L	304	CLA	CHC-C1C	3.05	1.42	1.35
18	7	610	CLA	C1D-ND	3.05	1.41	1.37
18	A	810	CLA	CHC-C1C	3.05	1.42	1.35
18	7	614	CLA	CHC-C1C	3.05	1.42	1.35
18	B	826	CLA	CHC-C1C	3.05	1.42	1.35
18	A	822	CLA	CMB-C2B	-3.05	1.45	1.51
18	K	204	CLA	C4D-ND	-3.05	1.33	1.37
18	B	805	CLA	C1D-ND	3.05	1.41	1.37
18	L	302	CLA	CHC-C1C	3.05	1.42	1.35
18	1	608	CLA	C4D-ND	-3.05	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	810	CLA	C1D-ND	3.05	1.41	1.37
18	a	601	CLA	C1D-ND	3.04	1.41	1.37
18	7	609	CLA	C1D-ND	3.04	1.41	1.37
18	3	611	CLA	CHC-C1C	3.04	1.42	1.35
18	5	607	CLA	CHC-C1C	3.04	1.42	1.35
18	6	618	CLA	CHC-C1C	3.04	1.42	1.35
18	B	804	CLA	C1D-ND	3.04	1.41	1.37
18	5	610	CLA	CHC-C1C	3.04	1.42	1.35
18	3	615	CLA	C4D-ND	-3.04	1.33	1.37
18	3	610	CLA	CHC-C1C	3.04	1.42	1.35
18	B	840	CLA	CMB-C2B	-3.03	1.45	1.51
18	B	833	CLA	CHC-C1C	3.03	1.42	1.35
18	4	603	CLA	C4D-ND	-3.03	1.33	1.37
18	5	603	CLA	C1D-ND	3.03	1.41	1.37
18	F	303	CLA	C4D-ND	-3.03	1.33	1.37
18	1	613	CLA	CHC-C1C	3.03	1.42	1.35
18	5	618	CLA	CHC-C1C	3.03	1.42	1.35
18	A	811	CLA	CHC-C1C	3.03	1.42	1.35
18	7	604	CLA	CHC-C1C	3.03	1.42	1.35
18	a	616	CLA	C4D-ND	-3.03	1.33	1.37
18	3	614	CLA	C4D-ND	-3.03	1.33	1.37
18	5	606	CLA	C4D-ND	-3.03	1.33	1.37
18	A	827	CLA	CHC-C1C	3.03	1.42	1.35
18	B	822	CLA	CHC-C1C	3.03	1.42	1.35
18	8	611	CLA	CHC-C1C	3.02	1.42	1.35
18	8	606	CLA	CHC-C1C	3.02	1.42	1.35
18	B	827	CLA	C1D-ND	3.02	1.41	1.37
18	7	609	CLA	CHC-C1C	3.02	1.42	1.35
18	B	819	CLA	C4D-ND	-3.02	1.33	1.37
18	A	833	CLA	CHC-C1C	3.02	1.42	1.35
18	B	834	CLA	CHC-C1C	3.02	1.42	1.35
18	6	602	CLA	CHC-C1C	3.02	1.42	1.35
18	7	613	CLA	CHC-C1C	3.02	1.42	1.35
18	8	614	CLA	CHC-C1C	3.01	1.42	1.35
18	F	303	CLA	CHC-C1C	3.01	1.42	1.35
18	5	619	CLA	C4D-ND	-3.01	1.33	1.37
18	7	615	CLA	C4D-ND	-3.01	1.33	1.37
18	4	607	CLA	CHC-C1C	3.01	1.42	1.35
18	3	613	CLA	C1D-ND	3.01	1.41	1.37
18	A	842	CLA	CHC-C1C	3.01	1.42	1.35
18	6	613	CLA	C4D-ND	-3.01	1.33	1.37
18	B	802	CLA	CMB-C2B	-3.01	1.45	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	612	CLA	CHC-C1C	3.00	1.42	1.35
18	3	607	CLA	CHC-C1C	3.00	1.42	1.35
18	A	816	CLA	CHC-C1C	3.00	1.42	1.35
18	a	611	CLA	CHC-C1C	3.00	1.42	1.35
18	4	601	CLA	CHC-C1C	3.00	1.42	1.35
18	4	616	CLA	C4D-ND	-3.00	1.33	1.37
18	B	815	CLA	C4D-ND	-3.00	1.33	1.37
18	7	616	CLA	C4D-ND	-3.00	1.33	1.37
18	a	604	CLA	CHC-C1C	3.00	1.42	1.35
18	A	837	CLA	C4D-ND	-3.00	1.33	1.37
18	4	613	CLA	CHC-C1C	3.00	1.42	1.35
18	5	609	CLA	CHC-C1C	3.00	1.42	1.35
18	3	614	CLA	CHC-C1C	3.00	1.42	1.35
18	a	612	CLA	C4D-ND	-2.99	1.33	1.37
18	1	616	CLA	CHC-C1C	2.99	1.42	1.35
18	8	604	CLA	CHC-C1C	2.99	1.42	1.35
18	B	830	CLA	CMB-C2B	-2.99	1.45	1.51
18	4	612	CLA	C4D-ND	-2.99	1.33	1.37
18	1	606	CLA	C4D-ND	-2.99	1.33	1.37
18	6	611	CLA	C4D-ND	-2.99	1.33	1.37
18	A	809	CLA	C1D-ND	2.99	1.41	1.37
18	B	811	CLA	CHC-C1C	2.99	1.42	1.35
18	a	614	CLA	CHC-C1C	2.99	1.42	1.35
18	5	609	CLA	C4D-ND	-2.99	1.33	1.37
18	6	604	CLA	CHC-C1C	2.98	1.42	1.35
18	a	613	CLA	CHC-C1C	2.98	1.42	1.35
18	A	837	CLA	CHC-C1C	2.98	1.42	1.35
18	a	606	CLA	CHC-C1C	2.98	1.42	1.35
18	5	604	CLA	CHC-C1C	2.98	1.42	1.35
18	A	813	CLA	CHC-C1C	2.98	1.42	1.35
18	B	820	CLA	C4D-ND	-2.98	1.33	1.37
18	4	618	CLA	C4D-ND	-2.97	1.33	1.37
18	7	609	CLA	C4D-ND	-2.97	1.33	1.37
18	4	602	CLA	CHC-C1C	2.97	1.42	1.35
18	6	613	CLA	CHC-C1C	2.97	1.42	1.35
18	6	601	CLA	C4D-ND	-2.97	1.33	1.37
18	5	612	CLA	C4D-ND	-2.97	1.33	1.37
18	5	614	CLA	C4D-ND	-2.97	1.33	1.37
18	6	612	CLA	C4D-ND	-2.97	1.33	1.37
18	1	612	CLA	CHC-C1C	2.97	1.42	1.35
18	6	620	CLA	C1D-ND	2.97	1.41	1.37
18	A	812	CLA	C1D-ND	2.96	1.41	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	7	604	CLA	C4D-ND	-2.96	1.33	1.37
18	4	608	CLA	CHC-C1C	2.96	1.42	1.35
18	A	812	CLA	CHC-C1C	2.96	1.42	1.35
18	A	823	CLA	CHC-C1C	2.96	1.42	1.35
18	A	821	CLA	CHC-C1C	2.96	1.42	1.35
18	5	608	CLA	CHC-C1C	2.96	1.42	1.35
18	6	601	CLA	CHC-C1C	2.96	1.42	1.35
18	8	612	CLA	CHC-C1C	2.96	1.42	1.35
18	5	601	CLA	C4D-ND	-2.96	1.33	1.37
18	8	604	CLA	C4D-ND	-2.96	1.33	1.37
18	A	822	CLA	CHC-C1C	2.96	1.42	1.35
18	B	835	CLA	C4D-ND	-2.96	1.33	1.37
18	4	614	CLA	CHC-C1C	2.96	1.42	1.35
18	B	823	CLA	C4D-ND	-2.95	1.33	1.37
18	8	616	CLA	CHC-C1C	2.95	1.42	1.35
18	a	616	CLA	CHC-C1C	2.95	1.42	1.35
18	5	602	CLA	CHC-C1C	2.95	1.42	1.35
18	A	803	CLA	C1D-ND	2.95	1.41	1.37
18	1	611	CLA	CHC-C1C	2.95	1.42	1.35
18	B	839	CLA	CHC-C1C	2.95	1.42	1.35
18	K	203	CLA	C4D-ND	-2.95	1.33	1.37
18	J	101	CLA	CHC-C1C	2.94	1.42	1.35
18	7	613	CLA	C4D-ND	-2.94	1.33	1.37
18	8	602	CLA	CHC-C1C	2.94	1.42	1.35
18	6	609	CLA	CHC-C1C	2.94	1.42	1.35
18	K	206	CLA	C4D-ND	-2.94	1.33	1.37
18	B	821	CLA	CHC-C1C	2.94	1.42	1.35
18	8	609	CLA	CHC-C1C	2.94	1.42	1.35
18	A	832	CLA	C1D-ND	2.94	1.41	1.37
18	a	609	CLA	CHC-C1C	2.94	1.42	1.35
18	7	608	CLA	CHC-C1C	2.94	1.42	1.35
18	A	824	CLA	CHC-C1C	2.94	1.42	1.35
18	6	603	CLA	CHC-C1C	2.93	1.42	1.35
18	7	606	CLA	CMB-C2B	-2.93	1.45	1.51
18	A	845	CLA	CHC-C1C	2.93	1.42	1.35
18	A	829	CLA	CHC-C1C	2.93	1.42	1.35
18	A	832	CLA	CHC-C1C	2.93	1.42	1.35
18	8	601	CLA	CHC-C1C	2.93	1.42	1.35
18	K	204	CLA	CHC-C1C	2.93	1.42	1.35
18	6	607	CLA	CHC-C1C	2.93	1.42	1.35
18	1	612	CLA	C4D-ND	-2.93	1.33	1.37
18	B	802	CLA	CHC-C1C	2.93	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	816	CLA	C4D-ND	-2.93	1.33	1.37
18	1	601	CLA	CHC-C1C	2.93	1.42	1.35
18	6	606	CLA	CHC-C1C	2.93	1.42	1.35
18	A	821	CLA	C1D-ND	2.92	1.41	1.37
18	B	803	CLA	CHC-C1C	2.92	1.42	1.35
18	B	812	CLA	C4D-ND	-2.92	1.33	1.37
18	3	603	CLA	CHC-C1C	2.92	1.42	1.35
18	5	619	CLA	CHC-C1C	2.92	1.42	1.35
18	5	616	CLA	CHC-C1C	2.92	1.42	1.35
28	6	624	NEX	C7-C8	-2.92	1.27	1.32
18	1	616	CLA	C4D-ND	-2.92	1.33	1.37
18	3	606	CLA	CHC-C1C	2.92	1.42	1.35
18	3	612	CLA	CHC-C1C	2.92	1.42	1.35
18	a	608	CLA	C4D-ND	-2.92	1.33	1.37
18	B	829	CLA	CMD-C2D	-2.91	1.44	1.50
18	B	832	CLA	CHC-C1C	2.91	1.42	1.35
18	A	841	CLA	CHC-C1C	2.91	1.42	1.35
18	5	601	CLA	CHC-C1C	2.91	1.42	1.35
18	7	603	CLA	CHC-C1C	2.91	1.42	1.35
18	B	831	CLA	CHC-C1C	2.91	1.42	1.35
18	7	606	CLA	C4D-ND	-2.91	1.33	1.37
18	a	611	CLA	C4D-ND	-2.91	1.33	1.37
18	7	607	CLA	CHC-C1C	2.91	1.42	1.35
18	B	827	CLA	CHC-C1C	2.90	1.42	1.35
18	6	618	CLA	C1D-ND	2.90	1.41	1.37
18	4	610	CLA	C4D-ND	-2.90	1.33	1.37
18	A	830	CLA	CHC-C1C	2.90	1.42	1.35
18	3	608	CLA	CHC-C1C	2.90	1.42	1.35
18	4	606	CLA	CHC-C1C	2.90	1.42	1.35
18	8	607	CLA	CHC-C1C	2.90	1.42	1.35
18	6	616	CLA	C4D-ND	-2.90	1.33	1.37
18	B	814	CLA	C1D-ND	2.90	1.41	1.37
18	A	819	CLA	CHC-C1C	2.90	1.42	1.35
18	A	802	CLA	CMD-C2D	-2.89	1.44	1.50
18	3	604	CLA	CHC-C1C	2.89	1.42	1.35
18	3	615	CLA	CHC-C1C	2.89	1.42	1.35
18	A	804	CLA	CHC-C1C	2.89	1.42	1.35
18	5	611	CLA	CHC-C1C	2.89	1.42	1.35
18	A	843	CLA	CMB-C2B	-2.89	1.45	1.51
18	6	609	CLA	C4D-ND	-2.89	1.33	1.37
18	7	606	CLA	CHC-C1C	2.88	1.42	1.35
18	a	606	CLA	C4D-ND	-2.88	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	609	CLA	CMB-C2B	-2.88	1.45	1.51
18	A	838	CLA	CHC-C1C	2.88	1.42	1.35
18	B	829	CLA	C1D-ND	2.88	1.41	1.37
18	A	818	CLA	CHC-C1C	2.87	1.42	1.35
18	A	840	CLA	CHC-C1C	2.87	1.42	1.35
18	8	603	CLA	C4D-ND	-2.87	1.33	1.37
18	3	602	CLA	CHC-C1C	2.87	1.42	1.35
18	B	809	CLA	C1D-ND	2.87	1.41	1.37
18	4	618	CLA	CHC-C1C	2.87	1.42	1.35
18	B	821	CLA	C4D-ND	-2.87	1.33	1.37
18	a	604	CLA	C4D-ND	-2.87	1.33	1.37
18	A	828	CLA	CHC-C1C	2.87	1.42	1.35
18	K	201	CLA	CHC-C1C	2.86	1.42	1.35
18	B	815	CLA	CHC-C1C	2.86	1.42	1.35
18	A	806	CLA	CHC-C1C	2.86	1.42	1.35
18	A	832	CLA	CMB-C2B	-2.86	1.45	1.51
18	B	802	CLA	C1D-ND	2.86	1.41	1.37
18	A	808	CLA	CHC-C1C	2.86	1.42	1.35
18	1	603	CLA	CHC-C1C	2.86	1.42	1.35
18	B	819	CLA	CHC-C1C	2.85	1.42	1.35
18	A	826	CLA	CHC-C1C	2.85	1.42	1.35
18	A	817	CLA	C4D-ND	-2.85	1.33	1.37
18	B	805	CLA	CHC-C1C	2.85	1.42	1.35
18	a	603	CLA	C4D-ND	-2.85	1.33	1.37
18	8	603	CLA	CHC-C1C	2.84	1.42	1.35
18	B	808	CLA	CHC-C1C	2.84	1.42	1.35
18	J	101	CLA	C4D-ND	-2.83	1.33	1.37
18	B	817	CLA	CMB-C2B	-2.83	1.45	1.51
18	A	820	CLA	CHC-C1C	2.82	1.42	1.35
18	B	822	CLA	C4D-ND	-2.82	1.33	1.37
19	B	842	PQN	C10-C1	-2.82	1.42	1.48
18	A	801	CLA	CMB-C2B	-2.82	1.45	1.51
20	A	846	LHG	O7-C5	-2.82	1.39	1.46
18	7	604	CLA	CMB-C2B	-2.82	1.45	1.51
18	1	607	CLA	C4D-ND	-2.82	1.33	1.37
18	1	616	CLA	CMB-C2B	-2.82	1.45	1.51
18	A	854	CLA	C1D-ND	2.82	1.41	1.37
18	A	835	CLA	CHC-C1C	2.81	1.42	1.35
18	3	613	CLA	CMB-C2B	-2.80	1.45	1.51
18	A	803	CLA	CHC-C1C	2.80	1.42	1.35
18	5	603	CLA	CMB-C2B	-2.80	1.45	1.51
18	4	603	CLA	CHC-C1C	2.80	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	304	CLA	C4D-ND	-2.80	1.33	1.37
18	4	609	CLA	C4D-ND	-2.80	1.33	1.37
18	4	610	CLA	CHC-C1C	2.80	1.42	1.35
18	5	606	CLA	CHC-C1C	2.80	1.42	1.35
19	A	844	PQN	C11-C3	2.80	1.56	1.51
18	5	604	CLA	CMB-C2B	-2.79	1.45	1.51
18	A	801	CLA	CHC-C1C	2.79	1.42	1.35
18	7	611	CLA	CHC-C1C	2.79	1.42	1.35
18	A	839	CLA	CHC-C1C	2.79	1.42	1.35
18	4	604	CLA	CMB-C2B	-2.79	1.45	1.51
18	B	810	CLA	CHC-C1C	2.79	1.42	1.35
18	B	828	CLA	CMB-C2B	-2.79	1.45	1.51
18	4	609	CLA	CHC-C1C	2.79	1.42	1.35
18	A	830	CLA	C1D-ND	2.79	1.41	1.37
18	7	601	CLA	CHC-C1C	2.78	1.42	1.35
18	a	603	CLA	CHC-C1C	2.78	1.42	1.35
18	A	836	CLA	CHC-C1C	2.78	1.42	1.35
18	A	839	CLA	CMB-C2B	-2.78	1.45	1.51
18	A	843	CLA	CHC-C1C	2.78	1.42	1.35
18	B	838	CLA	CMB-C2B	-2.78	1.45	1.51
18	5	619	CLA	CMB-C2B	-2.78	1.45	1.51
18	3	609	CLA	CMB-C2B	-2.78	1.45	1.51
18	1	604	CLA	C4D-ND	-2.77	1.33	1.37
18	B	818	CLA	CHC-C1C	2.77	1.42	1.35
18	B	838	CLA	CHC-C1C	2.77	1.42	1.35
18	B	819	CLA	CMB-C2B	-2.77	1.45	1.51
18	1	611	CLA	C4D-ND	-2.77	1.33	1.37
18	B	818	CLA	CMB-C2B	-2.77	1.45	1.51
18	B	826	CLA	CMC-C2C	-2.77	1.44	1.50
18	B	806	CLA	CHC-C1C	2.76	1.42	1.35
18	3	604	CLA	CMB-C2B	-2.76	1.45	1.51
18	L	302	CLA	C4D-ND	-2.76	1.33	1.37
18	A	817	CLA	CHC-C1C	2.76	1.42	1.35
18	7	608	CLA	CMB-C2B	-2.76	1.45	1.51
18	B	830	CLA	CHC-C1C	2.76	1.42	1.35
18	8	613	CLA	CHC-C1C	2.76	1.42	1.35
18	6	607	CLA	CMC-C2C	-2.75	1.45	1.50
18	5	602	CLA	CMB-C2B	-2.74	1.45	1.51
18	5	607	CLA	CMC-C2C	-2.74	1.45	1.50
18	3	615	CLA	CMB-C2B	-2.74	1.45	1.51
18	A	814	CLA	CHC-C1C	2.74	1.42	1.35
18	L	304	CLA	C4D-ND	-2.74	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	609	CLA	C4D-ND	-2.74	1.33	1.37
18	B	824	CLA	C4D-ND	-2.74	1.33	1.37
18	6	604	CLA	CMB-C2B	-2.73	1.46	1.51
18	F	301	CLA	CMD-C2D	-2.73	1.45	1.50
18	6	602	CLA	CMB-C2B	-2.73	1.46	1.51
23	A	857	LMU	O5'-C5'	2.72	1.48	1.43
18	A	807	CLA	CHC-C1C	2.72	1.41	1.35
18	A	807	CLA	CMB-C2B	-2.72	1.46	1.51
18	B	834	CLA	CMB-C2B	-2.72	1.46	1.51
18	8	613	CLA	CMB-C2B	-2.72	1.46	1.51
18	A	831	CLA	CMD-C2D	-2.71	1.45	1.50
18	5	613	CLA	CHC-C1C	2.71	1.41	1.35
18	3	609	CLA	CHC-C1C	2.71	1.41	1.35
18	B	828	CLA	CMD-C2D	-2.71	1.45	1.50
18	4	601	CLA	CMB-C2B	-2.71	1.46	1.51
18	a	609	CLA	C4D-ND	-2.70	1.34	1.37
18	F	301	CLA	CHC-C1C	2.70	1.41	1.35
18	B	808	CLA	CMC-C2C	-2.70	1.45	1.50
18	A	817	CLA	CMB-C2B	-2.70	1.46	1.51
18	B	827	CLA	CMB-C2B	-2.70	1.46	1.51
18	A	811	CLA	CMB-C2B	-2.70	1.46	1.51
18	A	834	CLA	CHC-C1C	2.70	1.41	1.35
18	A	825	CLA	CMB-C2B	-2.70	1.46	1.51
18	A	828	CLA	CMB-C2B	-2.70	1.46	1.51
18	7	613	CLA	CMB-C2B	-2.69	1.46	1.51
18	A	830	CLA	CMD-C2D	-2.69	1.45	1.50
18	3	603	CLA	CMB-C2B	-2.69	1.46	1.51
18	A	801	CLA	CMD-C2D	-2.69	1.45	1.50
18	1	609	CLA	C4D-ND	-2.69	1.34	1.37
18	B	828	CLA	CHC-C1C	2.68	1.41	1.35
18	A	809	CLA	CMB-C2B	-2.68	1.46	1.51
18	1	603	CLA	C4D-ND	-2.68	1.34	1.37
18	8	611	CLA	CMB-C2B	-2.68	1.46	1.51
18	a	610	CLA	CMB-C2B	-2.68	1.46	1.51
18	3	613	CLA	CHC-C1C	2.68	1.41	1.35
18	A	834	CLA	CMB-C2B	-2.68	1.46	1.51
18	A	841	CLA	CMB-C2B	-2.68	1.46	1.51
18	5	606	CLA	CMB-C2B	-2.67	1.46	1.51
18	a	604	CLA	CMB-C2B	-2.67	1.46	1.51
18	A	825	CLA	CHC-C1C	2.66	1.41	1.35
18	1	610	CLA	CMB-C2B	-2.66	1.46	1.51
18	A	821	CLA	CMB-C2B	-2.66	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	303	CLA	CMB-C2B	-2.66	1.46	1.51
18	A	810	CLA	CMD-C2D	-2.64	1.45	1.50
18	6	616	CLA	CMB-C2B	-2.64	1.46	1.51
18	A	810	CLA	CMB-C2B	-2.64	1.46	1.51
18	8	607	CLA	CMB-C2B	-2.64	1.46	1.51
18	A	842	CLA	CMB-C2B	-2.64	1.46	1.51
18	B	810	CLA	CMB-C2B	-2.64	1.46	1.51
18	B	837	CLA	CMB-C2B	-2.64	1.46	1.51
18	5	618	CLA	CMB-C2B	-2.64	1.46	1.51
18	7	610	CLA	CMB-C2B	-2.63	1.46	1.51
18	8	606	CLA	CMB-C2B	-2.63	1.46	1.51
18	K	201	CLA	C4D-ND	-2.63	1.34	1.37
18	B	806	CLA	CMB-C2B	-2.63	1.46	1.51
18	7	614	CLA	CMB-C2B	-2.63	1.46	1.51
18	8	601	CLA	CMB-C2B	-2.63	1.46	1.51
18	B	808	CLA	CMB-C2B	-2.63	1.46	1.51
18	B	840	CLA	CHC-C1C	2.62	1.41	1.35
18	A	840	CLA	CMB-C2B	-2.62	1.46	1.51
18	A	845	CLA	CMB-C2B	-2.62	1.46	1.51
18	B	809	CLA	CHC-C1C	2.62	1.41	1.35
18	A	820	CLA	CMC-C2C	-2.62	1.45	1.50
18	B	824	CLA	CMB-C2B	-2.62	1.46	1.51
18	8	608	CLA	CMB-C2B	-2.62	1.46	1.51
18	B	839	CLA	CMB-C2B	-2.61	1.46	1.51
18	A	805	CLA	CMB-C2B	-2.61	1.46	1.51
18	B	824	CLA	CMD-C2D	-2.61	1.45	1.50
18	A	826	CLA	CMB-C2B	-2.61	1.46	1.51
18	8	603	CLA	CMB-C2B	-2.61	1.46	1.51
18	7	603	CLA	CMB-C2B	-2.61	1.46	1.51
18	A	832	CLA	CMD-C2D	-2.61	1.45	1.50
18	6	608	CLA	CMB-C2B	-2.60	1.46	1.51
18	5	617	CLA	CHC-C1C	2.60	1.41	1.35
18	B	807	CLA	CMB-C2B	-2.60	1.46	1.51
18	4	603	CLA	CMB-C2B	-2.60	1.46	1.51
18	A	806	CLA	CMB-C2B	-2.60	1.46	1.51
18	1	604	CLA	CMB-C2B	-2.60	1.46	1.51
18	4	613	CLA	CMB-C2B	-2.60	1.46	1.51
18	6	606	CLA	CMB-C2B	-2.60	1.46	1.51
18	B	825	CLA	CMD-C2D	-2.60	1.45	1.50
18	3	608	CLA	C3B-C2B	-2.60	1.36	1.40
18	A	819	CLA	C3B-CAB	-2.60	1.42	1.47
18	4	606	CLA	CMB-C2B	-2.59	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	831	CLA	MG-ND	-2.59	2.00	2.05
18	5	609	CLA	CMB-C2B	-2.59	1.46	1.51
18	6	603	CLA	CMB-C2B	-2.59	1.46	1.51
18	8	604	CLA	CMB-C2B	-2.59	1.46	1.51
18	4	610	CLA	CMB-C2B	-2.58	1.46	1.51
18	8	602	CLA	CMB-C2B	-2.58	1.46	1.51
18	A	804	CLA	CMB-C2B	-2.58	1.46	1.51
18	A	823	CLA	CMB-C2B	-2.58	1.46	1.51
18	A	808	CLA	CMB-C2B	-2.58	1.46	1.51
18	7	612	CLA	CMB-C2B	-2.58	1.46	1.51
18	B	833	CLA	CMB-C2B	-2.58	1.46	1.51
18	A	806	CLA	CMD-C2D	-2.58	1.45	1.50
18	K	201	CLA	CMD-C2D	-2.58	1.45	1.50
19	A	844	PQN	C10-C5	-2.58	1.36	1.40
18	a	603	CLA	CMB-C2B	-2.58	1.46	1.51
18	B	829	CLA	CHC-C1C	2.58	1.41	1.35
18	A	835	CLA	CMB-C2B	-2.58	1.46	1.51
18	B	802	CLA	CMD-C2D	-2.57	1.45	1.50
18	6	613	CLA	CMB-C2B	-2.57	1.46	1.51
18	A	830	CLA	CMB-C2B	-2.57	1.46	1.51
18	3	612	CLA	CMB-C2B	-2.57	1.46	1.51
18	A	815	CLA	CMB-C2B	-2.56	1.46	1.51
18	7	601	CLA	CMB-C2B	-2.56	1.46	1.51
25	J	103	DGD	C4E-C3E	2.56	1.58	1.52
18	A	802	CLA	MG-ND	-2.56	2.00	2.05
18	6	607	CLA	CMB-C2B	-2.56	1.46	1.51
18	A	854	CLA	CMC-C2C	-2.55	1.45	1.50
18	a	616	CLA	CMD-C2D	-2.55	1.45	1.50
18	5	616	CLA	CMB-C2B	-2.55	1.46	1.51
18	A	803	CLA	MG-ND	-2.55	2.00	2.05
18	B	804	CLA	CMB-C2B	-2.55	1.46	1.51
18	6	620	CLA	CMB-C2B	-2.55	1.46	1.51
18	4	609	CLA	CMB-C2B	-2.55	1.46	1.51
18	4	601	CLA	C3B-C2B	-2.54	1.36	1.40
18	4	618	CLA	CMB-C2B	-2.54	1.46	1.51
18	3	607	CLA	CMB-C2B	-2.54	1.46	1.51
18	4	616	CLA	CMB-C2B	-2.54	1.46	1.51
18	B	836	CLA	CMB-C2B	-2.54	1.46	1.51
18	8	614	CLA	CMB-C2B	-2.54	1.46	1.51
18	B	816	CLA	CMB-C2B	-2.54	1.46	1.51
18	1	601	CLA	CMB-C2B	-2.53	1.46	1.51
18	a	602	CLA	CMB-C2B	-2.53	1.46	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	J	103	DGD	C4E-C5E	2.53	1.58	1.53
18	A	813	CLA	CMB-C2B	-2.53	1.46	1.51
18	A	827	CLA	CMB-C2B	-2.53	1.46	1.51
18	3	617	CLA	CMB-C2B	-2.53	1.46	1.51
18	7	602	CLA	CMB-C2B	-2.53	1.46	1.51
18	B	830	CLA	C4D-ND	-2.53	1.34	1.37
18	6	611	CLA	CMB-C2B	-2.53	1.46	1.51
18	5	613	CLA	CMB-C2B	-2.53	1.46	1.51
18	F	304	CLA	CMB-C2B	-2.53	1.46	1.51
18	5	601	CLA	CMB-C2B	-2.53	1.46	1.51
18	A	806	CLA	CMC-C2C	-2.53	1.45	1.50
18	5	611	CLA	CMB-C2B	-2.53	1.46	1.51
18	4	614	CLA	CMB-C2B	-2.53	1.46	1.51
18	B	829	CLA	MG-ND	-2.52	2.00	2.05
18	B	811	CLA	CMB-C2B	-2.52	1.46	1.51
18	K	203	CLA	CMB-C2B	-2.52	1.46	1.51
19	A	844	PQN	C5-C4	-2.52	1.43	1.48
18	5	608	CLA	CMB-C2B	-2.52	1.46	1.51
18	7	616	CLA	CMD-C2D	-2.52	1.45	1.50
18	B	831	CLA	CMB-C2B	-2.52	1.46	1.51
18	3	614	CLA	CMB-C2B	-2.52	1.46	1.51
18	3	610	CLA	CMB-C2B	-2.52	1.46	1.51
18	A	818	CLA	CMB-C2B	-2.52	1.46	1.51
18	6	612	CLA	CMB-C2B	-2.51	1.46	1.51
20	6	623	LHG	O7-C5	-2.51	1.40	1.46
18	1	606	CLA	CMB-C2B	-2.51	1.46	1.51
18	3	606	CLA	CMB-C2B	-2.51	1.46	1.51
18	F	301	CLA	C3B-C2B	-2.51	1.36	1.40
18	8	616	CLA	CMB-C2B	-2.51	1.46	1.51
18	a	606	CLA	CMB-C2B	-2.51	1.46	1.51
18	5	601	CLA	CMD-C2D	-2.51	1.45	1.50
18	1	611	CLA	CMB-C2B	-2.51	1.46	1.51
18	7	607	CLA	CMB-C2B	-2.51	1.46	1.51
18	B	813	CLA	CMB-C2B	-2.50	1.46	1.51
18	A	824	CLA	CMB-C2B	-2.50	1.46	1.51
18	5	610	CLA	CMB-C2B	-2.50	1.46	1.51
18	a	613	CLA	CMB-C2B	-2.50	1.46	1.51
18	B	814	CLA	CMD-C2D	-2.50	1.45	1.50
18	B	835	CLA	CMB-C2B	-2.50	1.46	1.51
18	a	609	CLA	CMB-C2B	-2.50	1.46	1.51
18	B	808	CLA	CMD-C2D	-2.50	1.45	1.50
18	a	611	CLA	CMB-C2B	-2.50	1.46	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	612	CLA	CMB-C2B	-2.50	1.46	1.51
18	K	206	CLA	CMB-C2B	-2.49	1.46	1.51
18	4	611	CLA	CMB-C2B	-2.49	1.46	1.51
18	1	603	CLA	CMB-C2B	-2.49	1.46	1.51
18	6	610	CLA	CMB-C2B	-2.49	1.46	1.51
18	A	833	CLA	CMB-C2B	-2.49	1.46	1.51
18	A	830	CLA	CMC-C2C	-2.49	1.45	1.50
18	B	839	CLA	CMD-C2D	-2.49	1.45	1.50
18	B	822	CLA	CMB-C2B	-2.49	1.46	1.51
18	A	837	CLA	CMB-C2B	-2.49	1.46	1.51
18	4	607	CLA	CMB-C2B	-2.49	1.46	1.51
18	3	602	CLA	CMB-C2B	-2.49	1.46	1.51
18	B	815	CLA	CMB-C2B	-2.49	1.46	1.51
18	8	609	CLA	CMB-C2B	-2.49	1.46	1.51
18	K	204	CLA	CMB-C2B	-2.49	1.46	1.51
18	A	854	CLA	CMB-C2B	-2.49	1.46	1.51
18	6	618	CLA	CMB-C2B	-2.48	1.46	1.51
19	A	844	PQN	C10-C1	-2.48	1.43	1.48
18	6	617	CLA	CMB-C2B	-2.48	1.46	1.51
18	L	304	CLA	CMB-C2B	-2.48	1.46	1.51
18	B	832	CLA	CMB-C2B	-2.48	1.46	1.51
18	B	828	CLA	MG-ND	-2.48	2.00	2.05
18	A	831	CLA	C3B-C2B	-2.48	1.36	1.40
18	A	814	CLA	CMB-C2B	-2.48	1.46	1.51
18	1	614	CLA	CMB-C2B	-2.47	1.46	1.51
20	7	622	LHG	O7-C5	-2.47	1.40	1.46
18	6	614	CLA	CMB-C2B	-2.47	1.46	1.51
23	A	859	LMU	C2'-C3'	-2.47	1.48	1.52
18	J	101	CLA	CMB-C2B	-2.47	1.46	1.51
18	1	613	CLA	CMB-C2B	-2.47	1.46	1.51
18	6	601	CLA	CMB-C2B	-2.47	1.46	1.51
20	5	623	LHG	O7-C5	-2.47	1.40	1.46
18	7	611	CLA	CMD-C2D	-2.47	1.45	1.50
18	A	838	CLA	CMB-C2B	-2.47	1.46	1.51
18	B	812	CLA	CMB-C2B	-2.47	1.46	1.51
18	8	612	CLA	CMB-C2B	-2.46	1.46	1.51
18	a	614	CLA	CMB-C2B	-2.46	1.46	1.51
18	A	829	CLA	CMB-C2B	-2.46	1.46	1.51
18	B	821	CLA	CMB-C2B	-2.46	1.46	1.51
18	3	611	CLA	CMB-C2B	-2.46	1.46	1.51
18	A	839	CLA	C3B-C2B	-2.46	1.37	1.40
18	B	823	CLA	CMB-C2B	-2.46	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	602	CLA	CMB-C2B	-2.46	1.46	1.51
18	7	611	CLA	CMB-C2B	-2.46	1.46	1.51
18	B	802	CLA	C3B-C2B	-2.46	1.37	1.40
18	B	825	CLA	CMB-C2B	-2.46	1.46	1.51
18	B	817	CLA	CMC-C2C	-2.45	1.45	1.50
18	1	616	CLA	CMD-C2D	-2.45	1.45	1.50
18	L	303	CLA	CMB-C2B	-2.45	1.46	1.51
25	J	103	DGD	O1G-C1G	-2.45	1.39	1.45
18	5	614	CLA	CMB-C2B	-2.45	1.46	1.51
18	A	821	CLA	CMD-C2D	-2.45	1.45	1.50
18	a	601	CLA	CMB-C2B	-2.45	1.46	1.51
18	3	610	CLA	CMC-C2C	-2.45	1.45	1.50
19	B	842	PQN	C5-C4	-2.45	1.43	1.48
18	8	601	CLA	CMD-C2D	-2.45	1.45	1.50
18	B	803	CLA	CMB-C2B	-2.45	1.46	1.51
18	a	616	CLA	CMB-C2B	-2.45	1.46	1.51
18	7	616	CLA	CMB-C2B	-2.45	1.46	1.51
26	7	619	LUT	C22-C21	-2.45	1.51	1.54
18	A	836	CLA	C3B-C2B	-2.45	1.37	1.40
18	4	612	CLA	CMB-C2B	-2.44	1.46	1.51
18	A	816	CLA	CMB-C2B	-2.44	1.46	1.51
18	5	606	CLA	C3B-C2B	-2.43	1.37	1.40
18	A	831	CLA	C1D-ND	2.43	1.40	1.37
18	4	608	CLA	CMB-C2B	-2.43	1.46	1.51
18	B	803	CLA	MG-ND	-2.43	2.01	2.05
18	A	826	CLA	CMD-C2D	-2.42	1.45	1.50
18	A	831	CLA	CMC-C2C	-2.42	1.45	1.50
18	5	617	CLA	C3B-C2B	-2.42	1.37	1.40
18	3	602	CLA	CMD-C2D	-2.42	1.45	1.50
18	1	609	CLA	CMB-C2B	-2.42	1.46	1.51
18	K	201	CLA	CMB-C2B	-2.42	1.46	1.51
18	5	617	CLA	CMC-C2C	-2.42	1.45	1.50
18	1	607	CLA	CMB-C2B	-2.42	1.46	1.51
18	B	833	CLA	CMC-C2C	-2.42	1.45	1.50
18	3	602	CLA	CMC-C2C	-2.42	1.45	1.50
18	7	613	CLA	CMD-C2D	-2.41	1.45	1.50
21	A	852	BCR	C30-C25	-2.41	1.50	1.53
18	7	615	CLA	CMB-C2B	-2.41	1.46	1.51
19	B	842	PQN	C10-C5	-2.41	1.36	1.40
18	A	807	CLA	C3B-C2B	-2.41	1.37	1.40
18	A	827	CLA	CMD-C2D	-2.41	1.45	1.50
18	A	824	CLA	CMD-C2D	-2.41	1.45	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	842	PQN	C11-C3	2.40	1.55	1.51
18	B	829	CLA	C3B-C2B	-2.40	1.37	1.40
18	A	802	CLA	CMB-C2B	-2.40	1.46	1.51
18	A	812	CLA	CMB-C2B	-2.40	1.46	1.51
18	L	302	CLA	CMB-C2B	-2.40	1.46	1.51
18	a	607	CLA	CMB-C2B	-2.40	1.46	1.51
18	B	840	CLA	C3B-C2B	-2.40	1.37	1.40
18	B	814	CLA	CMB-C2B	-2.40	1.46	1.51
18	3	608	CLA	MG-ND	-2.40	2.01	2.05
18	B	820	CLA	CMB-C2B	-2.40	1.46	1.51
18	A	838	CLA	CMD-C2D	-2.40	1.45	1.50
18	A	831	CLA	C4B-CHC	-2.39	1.34	1.41
18	a	612	CLA	CMB-C2B	-2.39	1.46	1.51
18	6	609	CLA	CMD-C2D	-2.39	1.45	1.50
18	A	801	CLA	C3B-C2B	-2.38	1.37	1.40
18	3	613	CLA	CMD-C2D	-2.38	1.45	1.50
18	A	810	CLA	C3B-C2B	-2.38	1.37	1.40
18	a	608	CLA	CMB-C2B	-2.38	1.46	1.51
20	A	847	LHG	O7-C5	-2.37	1.40	1.46
18	A	831	CLA	CHC-C1C	2.37	1.41	1.35
18	1	608	CLA	CMB-C2B	-2.37	1.46	1.51
18	3	603	CLA	CMD-C2D	-2.36	1.45	1.50
18	A	803	CLA	CMD-C2D	-2.36	1.45	1.50
18	B	805	CLA	CMB-C2B	-2.36	1.46	1.51
18	B	841	CLA	CMB-C2B	-2.36	1.46	1.51
18	4	607	CLA	CMC-C2C	-2.36	1.45	1.50
18	B	826	CLA	CMB-C2B	-2.35	1.46	1.51
18	6	607	CLA	CMD-C2D	-2.35	1.45	1.50
27	3	619	XAT	O4-C5	-2.35	1.42	1.46
18	A	828	CLA	CMC-C2C	-2.35	1.45	1.50
18	5	607	CLA	CMB-C2B	-2.35	1.46	1.51
18	A	818	CLA	CMC-C2C	-2.35	1.45	1.50
18	1	612	CLA	CMB-C2B	-2.35	1.46	1.51
18	4	602	CLA	CMB-C2B	-2.35	1.46	1.51
18	4	601	CLA	CMD-C2D	-2.35	1.45	1.50
18	7	609	CLA	CMB-C2B	-2.34	1.46	1.51
18	3	610	CLA	C3B-C2B	-2.34	1.37	1.40
18	A	812	CLA	CMD-C2D	-2.34	1.45	1.50
18	5	610	CLA	CMC-C2C	-2.34	1.45	1.50
18	3	606	CLA	CMD-C2D	-2.34	1.45	1.50
18	8	607	CLA	CMD-C2D	-2.34	1.45	1.50
18	A	807	CLA	CMC-C2C	-2.33	1.45	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	607	CLA	CMD-C2D	-2.33	1.45	1.50
18	B	805	CLA	CMD-C2D	-2.33	1.45	1.50
18	A	809	CLA	CMD-C2D	-2.33	1.45	1.50
18	A	836	CLA	CMD-C2D	-2.33	1.45	1.50
18	B	834	CLA	CMD-C2D	-2.33	1.45	1.50
18	a	601	CLA	CMD-C2D	-2.33	1.45	1.50
18	A	815	CLA	CMD-C2D	-2.32	1.45	1.50
18	B	809	CLA	CMD-C2D	-2.32	1.45	1.50
18	7	613	CLA	C3B-C2B	-2.32	1.37	1.40
18	F	301	CLA	MG-ND	-2.31	2.01	2.05
18	A	814	CLA	CMC-C2C	-2.31	1.45	1.50
18	3	606	CLA	CMC-C2C	-2.31	1.45	1.50
18	A	803	CLA	C3B-C2B	-2.31	1.37	1.40
18	4	609	CLA	C3B-C2B	-2.31	1.37	1.40
18	A	841	CLA	C3B-C2B	-2.31	1.37	1.40
18	7	608	CLA	CMD-C2D	-2.30	1.45	1.50
18	A	826	CLA	MG-ND	-2.30	2.01	2.05
18	A	813	CLA	CMC-C2C	-2.30	1.45	1.50
18	B	815	CLA	CMC-C2C	-2.30	1.45	1.50
18	B	803	CLA	CMD-C2D	-2.29	1.45	1.50
18	5	608	CLA	CMC-C2C	-2.29	1.45	1.50
18	B	840	CLA	CMD-C2D	-2.29	1.45	1.50
18	5	603	CLA	CMD-C2D	-2.29	1.45	1.50
18	B	830	CLA	C3B-C2B	-2.29	1.37	1.40
18	A	825	CLA	MG-ND	-2.29	2.01	2.05
18	A	804	CLA	CMD-C2D	-2.29	1.46	1.50
18	8	601	CLA	CMC-C2C	-2.29	1.46	1.50
18	B	838	CLA	CMD-C2D	-2.29	1.46	1.50
18	8	608	CLA	CMC-C2C	-2.28	1.46	1.50
18	5	618	CLA	CMD-C2D	-2.28	1.46	1.50
18	4	603	CLA	CMD-C2D	-2.28	1.46	1.50
18	7	612	CLA	CMC-C2C	-2.28	1.46	1.50
18	A	810	CLA	MG-ND	-2.28	2.01	2.05
18	A	840	CLA	CMD-C2D	-2.28	1.46	1.50
18	A	819	CLA	CMC-C2C	-2.28	1.46	1.50
18	B	802	CLA	CMC-C2C	-2.28	1.46	1.50
18	a	610	CLA	C3B-CAB	-2.27	1.43	1.47
18	5	607	CLA	C3B-CAB	-2.27	1.43	1.47
18	A	830	CLA	MG-ND	-2.27	2.01	2.05
18	A	812	CLA	CMC-C2C	-2.27	1.46	1.50
18	A	807	CLA	CMD-C2D	-2.27	1.46	1.50
18	3	608	CLA	CMC-C2C	-2.27	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	842	CLA	CMD-C2D	-2.27	1.46	1.50
18	A	817	CLA	CMD-C2D	-2.27	1.46	1.50
18	3	608	CLA	CMD-C2D	-2.27	1.46	1.50
18	7	614	CLA	CMD-C2D	-2.26	1.46	1.50
18	A	814	CLA	CMD-C2D	-2.26	1.46	1.50
18	B	819	CLA	CMD-C2D	-2.26	1.46	1.50
18	8	613	CLA	CMD-C2D	-2.26	1.46	1.50
18	A	804	CLA	CMC-C2C	-2.26	1.46	1.50
18	A	819	CLA	CMD-C2D	-2.26	1.46	1.50
26	7	619	LUT	C30-C29	-2.25	1.32	1.35
18	5	618	CLA	CMC-C2C	-2.25	1.46	1.50
18	B	806	CLA	MG-ND	-2.25	2.01	2.05
20	a	620	LHG	O7-C5	-2.25	1.41	1.46
18	7	610	CLA	CMC-C2C	-2.25	1.46	1.50
18	1	613	CLA	CMD-C2D	-2.25	1.46	1.50
18	6	610	CLA	CMD-C2D	-2.25	1.46	1.50
18	B	839	CLA	C3B-CAB	-2.25	1.43	1.47
18	A	815	CLA	C3B-C2B	-2.25	1.37	1.40
18	A	805	CLA	C3B-CAB	-2.25	1.43	1.47
18	3	608	CLA	C3B-CAB	-2.25	1.43	1.47
18	A	836	CLA	C3B-CAB	-2.24	1.43	1.47
18	A	838	CLA	MG-ND	-2.24	2.01	2.05
18	7	608	CLA	C3B-C2B	-2.24	1.37	1.40
18	A	829	CLA	CMD-C2D	-2.24	1.46	1.50
18	8	610	CLA	CMB-C2B	-2.24	1.47	1.51
18	8	612	CLA	CMD-C2D	-2.24	1.46	1.50
18	A	810	CLA	C3B-CAB	-2.24	1.43	1.47
27	7	620	XAT	O24-C25	-2.24	1.43	1.46
18	7	601	CLA	CMD-C2D	-2.24	1.46	1.50
18	B	802	CLA	C3B-CAB	-2.23	1.43	1.47
18	A	822	CLA	CMD-C2D	-2.23	1.46	1.50
18	B	804	CLA	CMD-C2D	-2.23	1.46	1.50
18	6	614	CLA	CMD-C2D	-2.23	1.46	1.50
18	5	604	CLA	CMD-C2D	-2.23	1.46	1.50
18	A	810	CLA	CMC-C2C	-2.23	1.46	1.50
18	B	828	CLA	CMC-C2C	-2.23	1.46	1.50
18	4	618	CLA	CMC-C2C	-2.23	1.46	1.50
18	5	603	CLA	MG-ND	-2.23	2.01	2.05
18	7	602	CLA	CMC-C2C	-2.23	1.46	1.50
18	A	854	CLA	CMD-C2D	-2.23	1.46	1.50
18	5	603	CLA	CMC-C2C	-2.23	1.46	1.50
18	7	601	CLA	CMC-C2C	-2.22	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	827	CLA	CMD-C2D	-2.22	1.46	1.50
18	B	830	CLA	CMD-C2D	-2.22	1.46	1.50
18	5	612	CLA	CMC-C2C	-2.22	1.46	1.50
18	4	614	CLA	CMD-C2D	-2.22	1.46	1.50
18	6	620	CLA	CMC-C2C	-2.22	1.46	1.50
18	B	813	CLA	CMD-C2D	-2.22	1.46	1.50
18	B	815	CLA	CMD-C2D	-2.22	1.46	1.50
18	6	602	CLA	CMC-C2C	-2.22	1.46	1.50
18	7	602	CLA	C3B-C2B	-2.22	1.37	1.40
18	A	805	CLA	CMC-C2C	-2.22	1.46	1.50
18	6	618	CLA	CMC-C2C	-2.22	1.46	1.50
18	3	603	CLA	MG-ND	-2.22	2.01	2.05
27	6	621	XAT	O24-C25	-2.22	1.43	1.46
18	5	606	CLA	CMD-C2D	-2.21	1.46	1.50
18	A	839	CLA	CMC-C2C	-2.21	1.46	1.50
18	6	610	CLA	CMC-C2C	-2.21	1.46	1.50
18	A	816	CLA	CMC-C2C	-2.21	1.46	1.50
18	A	832	CLA	MG-ND	-2.21	2.01	2.05
18	A	802	CLA	CMC-C2C	-2.21	1.46	1.50
18	4	610	CLA	CMC-C2C	-2.21	1.46	1.50
18	3	609	CLA	C3B-CAB	-2.21	1.43	1.47
18	B	837	CLA	CMD-C2D	-2.21	1.46	1.50
18	A	826	CLA	CMC-C2C	-2.21	1.46	1.50
18	6	620	CLA	CMD-C2D	-2.20	1.46	1.50
18	8	610	CLA	CMC-C2C	-2.20	1.46	1.50
18	4	602	CLA	CMD-C2D	-2.20	1.46	1.50
18	5	612	CLA	CMD-C2D	-2.20	1.46	1.50
18	8	603	CLA	CMC-C2C	-2.20	1.46	1.50
18	B	806	CLA	CMD-C2D	-2.20	1.46	1.50
18	4	608	CLA	CMD-C2D	-2.20	1.46	1.50
18	B	826	CLA	CMD-C2D	-2.20	1.46	1.50
18	B	829	CLA	C4B-CHC	-2.20	1.34	1.41
18	A	833	CLA	CMD-C2D	-2.20	1.46	1.50
18	B	813	CLA	CMC-C2C	-2.20	1.46	1.50
18	3	609	CLA	CMD-C2D	-2.20	1.46	1.50
18	B	808	CLA	C3B-C2B	-2.20	1.37	1.40
18	6	604	CLA	CMD-C2D	-2.19	1.46	1.50
18	A	816	CLA	CMD-C2D	-2.19	1.46	1.50
18	A	821	CLA	C3B-C2B	-2.19	1.37	1.40
18	5	602	CLA	CMC-C2C	-2.19	1.46	1.50
18	6	613	CLA	CMD-C2D	-2.19	1.46	1.50
18	F	304	CLA	CMD-C2D	-2.19	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	610	CLA	C3B-CAB	-2.19	1.43	1.47
18	B	807	CLA	CMD-C2D	-2.19	1.46	1.50
18	6	617	CLA	CMD-C2D	-2.19	1.46	1.50
18	3	610	CLA	CMD-C2D	-2.19	1.46	1.50
18	6	608	CLA	CMC-C2C	-2.19	1.46	1.50
18	7	603	CLA	C3B-C2B	-2.18	1.37	1.40
18	B	838	CLA	C3B-C2B	-2.18	1.37	1.40
27	7	620	XAT	O4-C5	-2.18	1.43	1.46
18	5	602	CLA	CMD-C2D	-2.18	1.46	1.50
18	B	836	CLA	CMD-C2D	-2.18	1.46	1.50
18	A	842	CLA	C3B-C2B	-2.18	1.37	1.40
18	6	620	CLA	C3B-C2B	-2.18	1.37	1.40
18	8	601	CLA	MG-ND	-2.18	2.01	2.05
18	A	820	CLA	CMD-C2D	-2.18	1.46	1.50
18	B	832	CLA	CMD-C2D	-2.18	1.46	1.50
18	8	609	CLA	CMD-C2D	-2.18	1.46	1.50
18	A	820	CLA	C3B-C2B	-2.18	1.37	1.40
18	7	612	CLA	CMD-C2D	-2.18	1.46	1.50
18	5	608	CLA	CMD-C2D	-2.18	1.46	1.50
18	A	818	CLA	CMD-C2D	-2.18	1.46	1.50
18	B	817	CLA	C3B-C2B	-2.17	1.37	1.40
18	8	607	CLA	CMC-C2C	-2.17	1.46	1.50
27	6	621	XAT	O4-C5	-2.17	1.43	1.46
18	A	828	CLA	CMD-C2D	-2.17	1.46	1.50
18	K	204	CLA	CMD-C2D	-2.17	1.46	1.50
18	K	201	CLA	MG-ND	-2.17	2.01	2.05
18	6	603	CLA	CMD-C2D	-2.17	1.46	1.50
18	8	602	CLA	CMC-C2C	-2.17	1.46	1.50
18	a	603	CLA	CMD-C2D	-2.17	1.46	1.50
18	A	829	CLA	CMC-C2C	-2.17	1.46	1.50
18	1	602	CLA	CMC-C2C	-2.17	1.46	1.50
18	5	611	CLA	CMD-C2D	-2.17	1.46	1.50
18	5	619	CLA	CMD-C2D	-2.17	1.46	1.50
18	7	603	CLA	CMD-C2D	-2.17	1.46	1.50
18	A	845	CLA	CMC-C2C	-2.16	1.46	1.50
18	3	611	CLA	CMD-C2D	-2.16	1.46	1.50
18	8	611	CLA	CMD-C2D	-2.16	1.46	1.50
18	4	610	CLA	CMD-C2D	-2.16	1.46	1.50
18	6	617	CLA	CMC-C2C	-2.16	1.46	1.50
18	A	813	CLA	CMD-C2D	-2.16	1.46	1.50
18	B	803	CLA	C1D-ND	2.16	1.40	1.37
18	B	812	CLA	CMD-C2D	-2.16	1.46	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	8	601	CLA	C3B-CAB	-2.16	1.43	1.47
18	B	805	CLA	MG-ND	-2.16	2.01	2.05
24	A	860	LMG	C4-C3	2.16	1.57	1.52
18	4	611	CLA	CMC-C2C	-2.16	1.46	1.50
18	A	803	CLA	CMC-C2C	-2.16	1.46	1.50
18	B	809	CLA	MG-ND	-2.15	2.01	2.05
18	6	612	CLA	CMD-C2D	-2.15	1.46	1.50
18	6	609	CLA	C3B-C2B	-2.15	1.37	1.40
18	B	804	CLA	CMC-C2C	-2.15	1.46	1.50
18	5	610	CLA	CMD-C2D	-2.15	1.46	1.50
18	7	609	CLA	CMD-C2D	-2.15	1.46	1.50
18	4	601	CLA	C3B-CAB	-2.15	1.43	1.47
18	6	620	CLA	C3B-CAB	-2.15	1.43	1.47
18	8	612	CLA	CMC-C2C	-2.15	1.46	1.50
18	A	801	CLA	CMC-C2C	-2.15	1.46	1.50
18	5	616	CLA	CMD-C2D	-2.15	1.46	1.50
18	B	833	CLA	CMD-C2D	-2.15	1.46	1.50
18	A	803	CLA	C3B-CAB	-2.15	1.43	1.47
18	8	604	CLA	CMD-C2D	-2.15	1.46	1.50
18	6	613	CLA	CMC-C2C	-2.15	1.46	1.50
18	6	616	CLA	CMD-C2D	-2.15	1.46	1.50
18	F	301	CLA	C3B-CAB	-2.15	1.43	1.47
18	B	817	CLA	C3B-CAB	-2.15	1.43	1.47
18	A	834	CLA	CMD-C2D	-2.14	1.46	1.50
18	6	614	CLA	CMC-C2C	-2.14	1.46	1.50
18	A	841	CLA	CMD-C2D	-2.14	1.46	1.50
18	7	613	CLA	CMC-C2C	-2.14	1.46	1.50
18	a	602	CLA	CMC-C2C	-2.14	1.46	1.50
18	3	604	CLA	CMD-C2D	-2.14	1.46	1.50
18	A	805	CLA	CMD-C2D	-2.13	1.46	1.50
18	3	617	CLA	CMD-C2D	-2.13	1.46	1.50
18	B	832	CLA	CMC-C2C	-2.13	1.46	1.50
18	A	843	CLA	CMD-C2D	-2.13	1.46	1.50
18	7	610	CLA	C3B-C2B	-2.13	1.37	1.40
18	A	842	CLA	CMC-C2C	-2.13	1.46	1.50
18	A	804	CLA	C3B-C2B	-2.13	1.37	1.40
18	a	602	CLA	CMD-C2D	-2.13	1.46	1.50
18	8	603	CLA	CMD-C2D	-2.13	1.46	1.50
18	3	614	CLA	CMC-C2C	-2.13	1.46	1.50
24	A	860	LMG	O7-C8	-2.13	1.41	1.46
18	B	818	CLA	CMD-C2D	-2.13	1.46	1.50
18	4	612	CLA	CMD-C2D	-2.13	1.46	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	7	604	CLA	CMD-C2D	-2.13	1.46	1.50
18	A	823	CLA	CMD-C2D	-2.13	1.46	1.50
18	A	807	CLA	MG-ND	-2.13	2.01	2.05
18	5	607	CLA	CMD-C2D	-2.13	1.46	1.50
18	8	611	CLA	CMC-C2C	-2.13	1.46	1.50
18	B	835	CLA	CMD-C2D	-2.13	1.46	1.50
18	B	814	CLA	MG-ND	-2.13	2.01	2.05
18	A	807	CLA	C3B-CAB	-2.13	1.43	1.47
18	A	839	CLA	C3B-CAB	-2.13	1.43	1.47
18	7	603	CLA	CMC-C2C	-2.13	1.46	1.50
18	4	603	CLA	CMC-C2C	-2.12	1.46	1.50
18	B	806	CLA	CMC-C2C	-2.12	1.46	1.50
18	8	602	CLA	CMD-C2D	-2.12	1.46	1.50
18	B	807	CLA	C3B-CAB	-2.12	1.43	1.47
18	6	602	CLA	C3B-CAB	-2.12	1.43	1.47
18	B	827	CLA	CMC-C2C	-2.12	1.46	1.50
18	3	612	CLA	CMD-C2D	-2.12	1.46	1.50
18	7	610	CLA	CMD-C2D	-2.12	1.46	1.50
18	4	602	CLA	CMC-C2C	-2.12	1.46	1.50
18	B	825	CLA	CMC-C2C	-2.12	1.46	1.50
18	1	603	CLA	CMD-C2D	-2.12	1.46	1.50
18	7	608	CLA	CAC-C3C	-2.12	1.45	1.51
18	6	608	CLA	CMD-C2D	-2.12	1.46	1.50
18	6	612	CLA	CMC-C2C	-2.12	1.46	1.50
18	B	817	CLA	CMD-C2D	-2.11	1.46	1.50
18	a	614	CLA	CMD-C2D	-2.11	1.46	1.50
18	J	101	CLA	CMD-C2D	-2.11	1.46	1.50
18	7	612	CLA	C3B-C2B	-2.11	1.37	1.40
18	B	837	CLA	CMC-C2C	-2.11	1.46	1.50
18	A	854	CLA	MG-ND	-2.11	2.01	2.05
18	A	822	CLA	C3B-C2B	-2.11	1.37	1.40
18	B	831	CLA	CMC-C2C	-2.11	1.46	1.50
18	1	604	CLA	CMD-C2D	-2.11	1.46	1.50
18	a	604	CLA	CMD-C2D	-2.11	1.46	1.50
18	7	606	CLA	CMD-C2D	-2.11	1.46	1.50
18	A	825	CLA	C3B-C2B	-2.11	1.37	1.40
18	A	820	CLA	C4B-CHC	-2.11	1.35	1.41
18	A	839	CLA	CMD-C2D	-2.11	1.46	1.50
18	B	830	CLA	C3C-C2C	2.11	1.41	1.36
18	B	816	CLA	CMD-C2D	-2.11	1.46	1.50
18	7	607	CLA	CMD-C2D	-2.11	1.46	1.50
18	A	815	CLA	C3B-CAB	-2.11	1.43	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	606	CLA	CMD-C2D	-2.11	1.46	1.50
24	J	104	LMG	O7-C8	-2.11	1.41	1.46
18	A	843	CLA	MG-ND	-2.11	2.01	2.05
27	3	619	XAT	O24-C25	-2.11	1.43	1.46
18	a	612	CLA	CMD-C2D	-2.11	1.46	1.50
18	6	602	CLA	CMD-C2D	-2.11	1.46	1.50
18	6	604	CLA	CMC-C2C	-2.11	1.46	1.50
18	B	806	CLA	C3B-C2B	-2.11	1.37	1.40
18	1	601	CLA	CMD-C2D	-2.11	1.46	1.50
18	B	834	CLA	C3B-CAB	-2.10	1.43	1.47
18	4	609	CLA	CMD-C2D	-2.10	1.46	1.50
18	4	613	CLA	CMD-C2D	-2.10	1.46	1.50
18	A	811	CLA	CMD-C2D	-2.10	1.46	1.50
18	5	617	CLA	C4B-CHC	-2.10	1.35	1.41
18	6	606	CLA	CMD-C2D	-2.10	1.46	1.50
18	8	601	CLA	C3B-C2B	-2.10	1.37	1.40
18	B	836	CLA	CMC-C2C	-2.10	1.46	1.50
24	4	624	LMG	C4-C5	2.10	1.57	1.53
18	5	608	CLA	MG-ND	-2.10	2.01	2.05
18	8	606	CLA	CMD-C2D	-2.10	1.46	1.50
18	6	613	CLA	C3B-C2B	-2.10	1.37	1.40
18	A	806	CLA	MG-ND	-2.10	2.01	2.05
18	4	614	CLA	C3B-C2B	-2.10	1.37	1.40
18	A	854	CLA	C3B-CAB	-2.10	1.43	1.47
18	A	801	CLA	C3B-CAB	-2.10	1.43	1.47
18	B	805	CLA	CMC-C2C	-2.09	1.46	1.50
18	6	601	CLA	CMD-C2D	-2.09	1.46	1.50
18	A	808	CLA	CMC-C2C	-2.09	1.46	1.50
20	4	622	LHG	O7-C5	-2.09	1.41	1.46
18	B	831	CLA	CMD-C2D	-2.09	1.46	1.50
18	8	614	CLA	CMD-C2D	-2.09	1.46	1.50
18	4	616	CLA	CMD-C2D	-2.09	1.46	1.50
18	A	819	CLA	MG-ND	-2.09	2.01	2.05
18	6	620	CLA	O2A-CGA	2.09	1.37	1.30
18	4	612	CLA	CMC-C2C	-2.09	1.46	1.50
18	B	818	CLA	CMC-C2C	-2.09	1.46	1.50
18	3	612	CLA	CMC-C2C	-2.09	1.46	1.50
18	7	606	CLA	CMC-C2C	-2.09	1.46	1.50
18	A	821	CLA	CMC-C2C	-2.09	1.46	1.50
18	A	837	CLA	CMD-C2D	-2.09	1.46	1.50
18	7	608	CLA	CMC-C2C	-2.09	1.46	1.50
18	4	606	CLA	CMC-C2C	-2.09	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	6	604	CLA	MG-ND	-2.09	2.01	2.05
18	A	827	CLA	MG-ND	-2.09	2.01	2.05
27	a	618	XAT	O4-C5	-2.09	1.43	1.46
18	8	613	CLA	CMC-C2C	-2.09	1.46	1.50
18	F	303	CLA	C3B-C2B	-2.09	1.37	1.40
18	K	204	CLA	CMC-C2C	-2.09	1.46	1.50
18	a	610	CLA	C3B-C2B	-2.09	1.37	1.40
18	A	802	CLA	C3B-CAB	-2.08	1.43	1.47
27	8	620	XAT	O4-C5	-2.08	1.43	1.46
18	1	602	CLA	CMD-C2D	-2.08	1.46	1.50
18	7	604	CLA	CMC-C2C	-2.08	1.46	1.50
18	3	614	CLA	CMD-C2D	-2.08	1.46	1.50
18	8	606	CLA	CMC-C2C	-2.08	1.46	1.50
18	a	603	CLA	C3B-C2B	-2.08	1.37	1.40
18	a	613	CLA	CMC-C2C	-2.08	1.46	1.50
18	B	816	CLA	CMC-C2C	-2.08	1.46	1.50
18	8	608	CLA	CMD-C2D	-2.08	1.46	1.50
18	A	820	CLA	MG-ND	-2.08	2.01	2.05
18	6	611	CLA	CMC-C2C	-2.08	1.46	1.50
18	A	845	CLA	CMD-C2D	-2.08	1.46	1.50
18	K	206	CLA	CMC-C2C	-2.08	1.46	1.50
18	7	602	CLA	CMD-C2D	-2.08	1.46	1.50
18	A	841	CLA	CMC-C2C	-2.08	1.46	1.50
18	B	828	CLA	C4B-CHC	-2.08	1.35	1.41
18	1	614	CLA	CMD-C2D	-2.08	1.46	1.50
18	a	601	CLA	MG-ND	-2.08	2.01	2.05
18	3	617	CLA	CMC-C2C	-2.08	1.46	1.50
18	K	206	CLA	CMD-C2D	-2.07	1.46	1.50
18	a	608	CLA	CMD-C2D	-2.07	1.46	1.50
18	6	611	CLA	CMD-C2D	-2.07	1.46	1.50
25	B	850	DGD	O2G-C2G	-2.07	1.41	1.46
18	A	806	CLA	CAC-C3C	-2.07	1.45	1.51
18	K	203	CLA	CMD-C2D	-2.07	1.46	1.50
18	8	608	CLA	C3B-C2B	-2.07	1.37	1.40
18	3	604	CLA	C3B-C2B	-2.07	1.37	1.40
18	3	607	CLA	CMD-C2D	-2.07	1.46	1.50
18	8	613	CLA	C3B-C2B	-2.07	1.37	1.40
18	4	611	CLA	CMD-C2D	-2.07	1.46	1.50
18	4	616	CLA	CMC-C2C	-2.07	1.46	1.50
18	A	841	CLA	C3B-CAB	-2.07	1.43	1.47
18	A	843	CLA	CMC-C2C	-2.07	1.46	1.50
18	F	303	CLA	CMC-C2C	-2.07	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	5	619	CLA	MG-ND	-2.07	2.01	2.05
18	A	823	CLA	C3B-CAB	-2.07	1.43	1.47
18	B	809	CLA	CMC-C2C	-2.07	1.46	1.50
18	1	610	CLA	CMD-C2D	-2.07	1.46	1.50
18	B	806	CLA	C3B-CAB	-2.07	1.43	1.47
18	3	613	CLA	CMC-C2C	-2.07	1.46	1.50
18	6	609	CLA	MG-ND	-2.07	2.01	2.05
18	7	607	CLA	CMC-C2C	-2.07	1.46	1.50
18	7	615	CLA	CMD-C2D	-2.07	1.46	1.50
24	J	104	LMG	O4-C4	-2.07	1.38	1.43
18	A	834	CLA	C3B-C2B	-2.07	1.37	1.40
18	B	811	CLA	CMD-C2D	-2.06	1.46	1.50
18	a	601	CLA	CMC-C2C	-2.06	1.46	1.50
18	B	824	CLA	CMC-C2C	-2.06	1.46	1.50
18	7	606	CLA	CAC-C3C	-2.06	1.46	1.50
18	5	614	CLA	CMD-C2D	-2.06	1.46	1.50
18	A	835	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	810	CLA	CMD-C2D	-2.06	1.46	1.50
18	3	615	CLA	C3B-C2B	-2.06	1.37	1.40
18	A	835	CLA	CMC-C2C	-2.06	1.46	1.50
18	1	607	CLA	CMD-C2D	-2.06	1.46	1.50
18	a	610	CLA	CMC-C2C	-2.06	1.46	1.50
18	1	612	CLA	CMD-C2D	-2.06	1.46	1.50
20	B	851	LHG	O7-C5	-2.06	1.41	1.46
18	B	809	CLA	C4B-CHC	-2.06	1.35	1.41
18	A	835	CLA	C3B-C2B	-2.06	1.37	1.40
18	5	609	CLA	CMD-C2D	-2.06	1.46	1.50
18	1	616	CLA	MG-ND	-2.06	2.01	2.05
18	a	611	CLA	CMD-C2D	-2.06	1.46	1.50
18	B	834	CLA	C3B-C2B	-2.05	1.37	1.40
18	4	602	CLA	C3B-CAB	-2.05	1.43	1.47
18	B	814	CLA	CMC-C2C	-2.05	1.46	1.50
18	8	610	CLA	CMD-C2D	-2.05	1.46	1.50
18	B	820	CLA	CMD-C2D	-2.05	1.46	1.50
18	a	610	CLA	CMD-C2D	-2.05	1.46	1.50
18	7	611	CLA	CMC-C2C	-2.05	1.46	1.50
18	7	614	CLA	C3B-C2B	-2.05	1.37	1.40
18	3	603	CLA	CMC-C2C	-2.05	1.46	1.50
18	A	811	CLA	C3B-C2B	-2.05	1.37	1.40
18	A	808	CLA	CMD-C2D	-2.05	1.46	1.50
18	4	601	CLA	CMC-C2C	-2.05	1.46	1.50
18	A	827	CLA	CMC-C2C	-2.05	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	6	624	NEX	O24-C25	-2.05	1.43	1.46
18	6	603	CLA	CMC-C2C	-2.05	1.46	1.50
18	4	613	CLA	CMC-C2C	-2.05	1.46	1.50
18	B	807	CLA	CMC-C2C	-2.04	1.46	1.50
18	4	618	CLA	CMD-C2D	-2.04	1.46	1.50
18	3	613	CLA	MG-ND	-2.04	2.01	2.05
18	6	601	CLA	CMC-C2C	-2.04	1.46	1.50
18	B	807	CLA	C3B-C2B	-2.04	1.37	1.40
18	a	609	CLA	CMD-C2D	-2.04	1.46	1.50
18	3	608	CLA	CAC-C3C	-2.04	1.45	1.51
18	4	604	CLA	CMC-C2C	-2.04	1.46	1.50
18	B	840	CLA	CMC-C2C	-2.04	1.46	1.50
18	B	819	CLA	CMC-C2C	-2.04	1.46	1.50
18	B	804	CLA	C3B-CAB	-2.04	1.43	1.47
18	a	604	CLA	CMC-C2C	-2.04	1.46	1.50
18	1	611	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	823	CLA	CMC-C2C	-2.04	1.46	1.50
18	A	829	CLA	C3B-CAB	-2.04	1.43	1.47
18	1	610	CLA	C3B-CAB	-2.04	1.43	1.47
18	a	613	CLA	CMD-C2D	-2.04	1.46	1.50
18	A	822	CLA	CMC-C2C	-2.04	1.46	1.50
18	A	837	CLA	C3B-C2B	-2.03	1.37	1.40
18	7	601	CLA	C3B-CAB	-2.03	1.43	1.47
18	B	839	CLA	CMC-C2C	-2.03	1.46	1.50
18	B	830	CLA	C4B-CHC	-2.03	1.35	1.41
18	B	823	CLA	CMC-C2C	-2.03	1.46	1.50
18	3	615	CLA	CMC-C2C	-2.03	1.46	1.50
18	4	604	CLA	CMD-C2D	-2.03	1.46	1.50
18	6	609	CLA	C3B-CAB	-2.03	1.43	1.47
18	A	832	CLA	CMC-C2C	-2.03	1.46	1.50
18	A	825	CLA	CMD-C2D	-2.03	1.46	1.50
18	3	602	CLA	C3B-CAB	-2.03	1.43	1.47
18	A	837	CLA	CMC-C2C	-2.03	1.46	1.50
18	8	609	CLA	CMC-C2C	-2.03	1.46	1.50
18	A	815	CLA	CMC-C2C	-2.02	1.46	1.50
18	6	618	CLA	CMD-C2D	-2.02	1.46	1.50
18	F	303	CLA	CMD-C2D	-2.02	1.46	1.50
18	4	606	CLA	CMD-C2D	-2.02	1.46	1.50
18	6	604	CLA	C3B-CAB	-2.02	1.43	1.47
18	B	825	CLA	MG-ND	-2.02	2.01	2.05
18	5	613	CLA	CMD-C2D	-2.02	1.46	1.50
18	5	609	CLA	C3B-CAB	-2.02	1.43	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	818	CLA	MG-ND	-2.02	2.01	2.05
18	A	836	CLA	MG-ND	-2.02	2.01	2.05
18	5	616	CLA	MG-ND	-2.02	2.01	2.05
24	4	623	LMG	C4-C5	2.02	1.57	1.53
18	A	817	CLA	CMC-C2C	-2.02	1.46	1.50
18	4	614	CLA	CMC-C2C	-2.02	1.46	1.50
27	4	620	XAT	O24-C25	-2.02	1.43	1.46
18	1	607	CLA	CMC-C2C	-2.02	1.46	1.50
18	A	840	CLA	C3B-CAB	-2.01	1.43	1.47
18	4	601	CLA	MG-ND	-2.01	2.01	2.05
18	7	610	CLA	C3B-CAB	-2.01	1.43	1.47
18	a	612	CLA	CMC-C2C	-2.01	1.46	1.50
18	8	614	CLA	CMC-C2C	-2.01	1.46	1.50
27	1	618	XAT	O4-C5	-2.01	1.43	1.46
18	5	604	CLA	CMC-C2C	-2.01	1.46	1.50
18	5	601	CLA	MG-ND	-2.01	2.01	2.05
18	5	616	CLA	CMC-C2C	-2.01	1.46	1.50
18	5	609	CLA	C3B-C2B	-2.01	1.37	1.40
18	A	823	CLA	C3B-C2B	-2.01	1.37	1.40
18	B	827	CLA	C3B-CAB	-2.01	1.43	1.47
18	1	601	CLA	MG-ND	-2.01	2.01	2.05
18	6	602	CLA	C3B-C2B	-2.01	1.37	1.40
18	A	809	CLA	MG-ND	-2.01	2.01	2.05
18	7	608	CLA	MG-ND	-2.01	2.01	2.05
18	3	615	CLA	CMD-C2D	-2.01	1.46	1.50
18	4	608	CLA	CMC-C2C	-2.01	1.46	1.50
18	7	602	CLA	C3B-CAB	-2.01	1.43	1.47
18	3	602	CLA	CMA-C3A	-2.01	1.48	1.53
18	3	617	CLA	C3B-C2B	-2.00	1.37	1.40
18	3	609	CLA	MG-ND	-2.00	2.01	2.05
18	1	601	CLA	CMC-C2C	-2.00	1.46	1.50
18	6	601	CLA	C3B-CAB	-2.00	1.43	1.47
18	B	821	CLA	CMD-C2D	-2.00	1.46	1.50
18	1	606	CLA	CMD-C2D	-2.00	1.46	1.50
18	a	607	CLA	CMD-C2D	-2.00	1.46	1.50
18	A	835	CLA	C4B-CHC	-2.00	1.35	1.41
18	B	803	CLA	C3B-CAB	-2.00	1.43	1.47
18	3	617	CLA	C3B-CAB	-2.00	1.43	1.47
18	A	834	CLA	CMC-C2C	-2.00	1.46	1.50
18	5	613	CLA	C3B-CAB	-2.00	1.43	1.47

All (2702) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	621	XAT	O24-C25-C24	11.52	122.04	113.38
18	B	803	CLA	C4A-NA-C1A	9.21	110.84	106.71
18	8	613	CLA	C4A-NA-C1A	9.08	110.79	106.71
27	6	621	XAT	O24-C25-C24	8.96	120.11	113.38
27	8	620	XAT	O24-C25-C24	8.87	120.04	113.38
19	A	844	PQN	C11-C12-C13	-8.68	112.35	126.79
18	5	613	CLA	C4A-NA-C1A	8.61	110.58	106.71
18	A	813	CLA	C4A-NA-C1A	8.56	110.55	106.71
27	7	620	XAT	O24-C25-C24	8.55	119.81	113.38
18	3	613	CLA	C4A-NA-C1A	8.55	110.55	106.71
27	1	618	XAT	O4-C5-C4	8.51	119.78	113.38
18	B	840	CLA	C4A-NA-C1A	8.31	110.44	106.71
18	B	808	CLA	C4A-NA-C1A	8.30	110.44	106.71
18	K	201	CLA	C4A-NA-C1A	8.28	110.43	106.71
18	A	817	CLA	C4A-NA-C1A	8.16	110.37	106.71
18	8	608	CLA	C4A-NA-C1A	8.12	110.36	106.71
18	A	808	CLA	C4A-NA-C1A	7.98	110.29	106.71
18	3	615	CLA	C4A-NA-C1A	7.89	110.25	106.71
18	A	837	CLA	C4A-NA-C1A	7.81	110.22	106.71
18	A	842	CLA	C4A-NA-C1A	7.81	110.22	106.71
18	6	607	CLA	C4A-NA-C1A	7.80	110.21	106.71
18	L	302	CLA	C4A-NA-C1A	7.77	110.20	106.71
18	6	618	CLA	C4A-NA-C1A	7.75	110.19	106.71
18	8	607	CLA	C4A-NA-C1A	7.72	110.18	106.71
18	7	611	CLA	C4A-NA-C1A	7.71	110.17	106.71
18	8	609	CLA	C4A-NA-C1A	7.71	110.17	106.71
18	8	616	CLA	C4A-NA-C1A	7.69	110.16	106.71
18	5	607	CLA	C4A-NA-C1A	7.67	110.16	106.71
18	B	826	CLA	C4A-NA-C1A	7.66	110.15	106.71
18	A	818	CLA	C4A-NA-C1A	7.64	110.14	106.71
18	8	603	CLA	C4A-NA-C1A	7.62	110.13	106.71
18	A	845	CLA	C4A-NA-C1A	7.60	110.12	106.71
18	5	617	CLA	C4A-NA-C1A	7.59	110.12	106.71
18	B	805	CLA	C4A-NA-C1A	7.56	110.11	106.71
18	B	815	CLA	C4A-NA-C1A	7.56	110.11	106.71
18	J	101	CLA	C4A-NA-C1A	7.56	110.10	106.71
18	a	613	CLA	C4A-NA-C1A	7.55	110.10	106.71
18	A	821	CLA	C4A-NA-C1A	7.53	110.09	106.71
18	1	603	CLA	C4A-NA-C1A	7.48	110.07	106.71
18	B	818	CLA	C4A-NA-C1A	7.48	110.07	106.71
27	1	618	XAT	O24-C25-C24	7.48	119.00	113.38
18	6	613	CLA	C4A-NA-C1A	7.48	110.07	106.71
18	B	820	CLA	C4A-NA-C1A	7.47	110.06	106.71

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	616	CLA	C4A-NA-C1A	7.46	110.06	106.71
18	4	613	CLA	C4A-NA-C1A	7.44	110.05	106.71
18	K	206	CLA	C4A-NA-C1A	7.43	110.05	106.71
18	6	609	CLA	C4A-NA-C1A	7.41	110.04	106.71
18	B	831	CLA	C4A-NA-C1A	7.40	110.03	106.71
18	A	816	CLA	C4A-NA-C1A	7.40	110.03	106.71
18	A	807	CLA	C4A-NA-C1A	7.39	110.03	106.71
21	B	801	BCR	C24-C23-C22	-7.38	115.09	126.23
18	A	835	CLA	C4A-NA-C1A	7.37	110.02	106.71
18	B	838	CLA	C4A-NA-C1A	7.36	110.01	106.71
18	B	809	CLA	C4A-NA-C1A	7.35	110.01	106.71
18	A	806	CLA	C4A-NA-C1A	7.34	110.01	106.71
18	1	613	CLA	C4A-NA-C1A	7.33	110.00	106.71
18	A	826	CLA	C4A-NA-C1A	7.32	110.00	106.71
18	B	819	CLA	C4A-NA-C1A	7.32	110.00	106.71
18	3	611	CLA	C4A-NA-C1A	7.30	109.99	106.71
18	5	602	CLA	C4A-NA-C1A	7.30	109.99	106.71
18	A	804	CLA	C4A-NA-C1A	7.29	109.98	106.71
18	A	823	CLA	C4A-NA-C1A	7.27	109.97	106.71
18	L	304	CLA	C4A-NA-C1A	7.27	109.97	106.71
18	A	839	CLA	C4A-NA-C1A	7.25	109.97	106.71
18	B	827	CLA	C4A-NA-C1A	7.25	109.97	106.71
18	A	836	CLA	C4A-NA-C1A	7.24	109.96	106.71
18	B	835	CLA	C4A-NA-C1A	7.24	109.96	106.71
18	8	614	CLA	C4A-NA-C1A	7.24	109.96	106.71
18	4	609	CLA	C4A-NA-C1A	7.22	109.95	106.71
18	A	814	CLA	C4A-NA-C1A	7.22	109.95	106.71
18	5	619	CLA	C4A-NA-C1A	7.22	109.95	106.71
18	8	601	CLA	C4A-NA-C1A	7.21	109.95	106.71
19	B	842	PQN	C15-C13-C12	-7.21	106.52	121.12
18	A	828	CLA	C4A-NA-C1A	7.21	109.95	106.71
18	A	809	CLA	C4A-NA-C1A	7.21	109.95	106.71
18	3	602	CLA	C4A-NA-C1A	7.20	109.94	106.71
18	8	604	CLA	C4A-NA-C1A	7.20	109.94	106.71
18	A	843	CLA	C4A-NA-C1A	7.18	109.93	106.71
18	B	816	CLA	C4A-NA-C1A	7.17	109.93	106.71
18	4	610	CLA	C4A-NA-C1A	7.17	109.93	106.71
18	B	812	CLA	C4A-NA-C1A	7.16	109.92	106.71
18	a	609	CLA	C4A-NA-C1A	7.15	109.92	106.71
18	A	841	CLA	C4A-NA-C1A	7.15	109.92	106.71
18	4	607	CLA	C4A-NA-C1A	7.15	109.92	106.71
27	7	620	XAT	O4-C5-C4	7.15	118.75	113.38

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	829	CLA	C4A-NA-C1A	7.14	109.92	106.71
18	B	807	CLA	C4A-NA-C1A	7.14	109.92	106.71
18	7	613	CLA	C4A-NA-C1A	7.14	109.91	106.71
18	K	204	CLA	C4A-NA-C1A	7.12	109.91	106.71
18	1	611	CLA	C4A-NA-C1A	7.11	109.90	106.71
19	A	844	PQN	C15-C13-C12	-7.11	106.74	121.12
18	3	603	CLA	C4A-NA-C1A	7.10	109.90	106.71
27	a	618	XAT	O4-C5-C4	7.10	118.72	113.38
18	6	601	CLA	C4A-NA-C1A	7.10	109.90	106.71
18	4	602	CLA	C4A-NA-C1A	7.10	109.90	106.71
18	4	608	CLA	C4A-NA-C1A	7.09	109.89	106.71
18	A	811	CLA	C4A-NA-C1A	7.09	109.89	106.71
18	B	829	CLA	CMB-C2B-C1B	-7.08	117.58	128.46
18	B	832	CLA	C4A-NA-C1A	7.07	109.89	106.71
21	A	851	BCR	C24-C23-C22	-7.05	115.58	126.23
18	6	614	CLA	C4A-NA-C1A	7.04	109.87	106.71
18	a	607	CLA	C4A-NA-C1A	7.04	109.87	106.71
18	A	838	CLA	C4A-NA-C1A	7.03	109.87	106.71
18	A	822	CLA	C4A-NA-C1A	7.01	109.86	106.71
18	5	618	CLA	C4A-NA-C1A	6.99	109.85	106.71
18	8	602	CLA	C4A-NA-C1A	6.99	109.85	106.71
18	A	825	CLA	C4A-NA-C1A	6.98	109.84	106.71
18	A	802	CLA	C4A-NA-C1A	6.96	109.84	106.71
18	5	608	CLA	C4A-NA-C1A	6.96	109.83	106.71
18	7	603	CLA	C4A-NA-C1A	6.96	109.83	106.71
18	B	802	CLA	C4A-NA-C1A	6.95	109.83	106.71
18	6	604	CLA	C4A-NA-C1A	6.95	109.83	106.71
27	4	620	XAT	O4-C5-C4	6.94	118.60	113.38
18	L	303	CLA	C4A-NA-C1A	6.94	109.83	106.71
18	4	603	CLA	C4A-NA-C1A	6.93	109.82	106.71
18	A	801	CLA	C4A-NA-C1A	6.92	109.82	106.71
18	4	614	CLA	C4A-NA-C1A	6.92	109.82	106.71
18	6	620	CLA	C4A-NA-C1A	6.92	109.81	106.71
18	A	812	CLA	C4A-NA-C1A	6.91	109.81	106.71
18	8	610	CLA	C4A-NA-C1A	6.91	109.81	106.71
18	B	821	CLA	C4A-NA-C1A	6.89	109.81	106.71
18	3	606	CLA	C4A-NA-C1A	6.89	109.80	106.71
18	B	814	CLA	C4A-NA-C1A	6.88	109.80	106.71
18	3	604	CLA	C4A-NA-C1A	6.88	109.80	106.71
18	5	604	CLA	C4A-NA-C1A	6.88	109.80	106.71
18	B	822	CLA	C4A-NA-C1A	6.87	109.80	106.71
18	B	830	CLA	C4A-NA-C1A	6.85	109.79	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	603	CLA	C4A-NA-C1A	6.85	109.78	106.71
18	7	602	CLA	C4A-NA-C1A	6.85	109.78	106.71
18	B	811	CLA	C4A-NA-C1A	6.84	109.78	106.71
18	A	831	CLA	CMB-C2B-C1B	-6.84	117.96	128.46
18	4	606	CLA	C4A-NA-C1A	6.83	109.78	106.71
18	a	604	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	7	604	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	7	615	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	A	819	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	5	611	CLA	C4A-NA-C1A	6.82	109.77	106.71
18	A	840	CLA	C4A-NA-C1A	6.79	109.76	106.71
18	3	608	CLA	C4A-NA-C1A	6.79	109.76	106.71
18	7	607	CLA	C4A-NA-C1A	6.78	109.75	106.71
18	a	601	CLA	C4A-NA-C1A	6.77	109.75	106.71
21	3	622	BCR	C11-C10-C9	-6.74	117.69	127.31
27	a	618	XAT	O24-C25-C24	6.74	118.44	113.38
18	7	616	CLA	C4A-NA-C1A	6.73	109.73	106.71
18	A	830	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	A	820	CLA	C4A-NA-C1A	6.72	109.73	106.71
18	A	831	CLA	C4A-NA-C1A	6.71	109.72	106.71
18	a	606	CLA	C4A-NA-C1A	6.71	109.72	106.71
18	1	608	CLA	C4A-NA-C1A	6.71	109.72	106.71
18	6	612	CLA	C4A-NA-C1A	6.71	109.72	106.71
18	3	610	CLA	C4A-NA-C1A	6.71	109.72	106.71
18	B	833	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	B	842	PQN	C11-C12-C13	-6.70	115.64	126.79
18	K	203	CLA	C4A-NA-C1A	6.68	109.71	106.71
18	F	303	CLA	C4A-NA-C1A	6.67	109.71	106.71
18	4	618	CLA	C4A-NA-C1A	6.66	109.70	106.71
18	6	602	CLA	C4A-NA-C1A	6.64	109.69	106.71
18	6	606	CLA	C4A-NA-C1A	6.63	109.69	106.71
18	7	614	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	A	834	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	5	610	CLA	C4A-NA-C1A	6.62	109.68	106.71
18	5	601	CLA	C4A-NA-C1A	6.61	109.68	106.71
18	B	834	CLA	C4A-NA-C1A	6.59	109.67	106.71
18	1	612	CLA	C4A-NA-C1A	6.59	109.67	106.71
18	B	806	CLA	C4A-NA-C1A	6.59	109.67	106.71
21	J	102	BCR	C28-C27-C26	-6.58	102.32	114.08
18	5	609	CLA	C4A-NA-C1A	6.58	109.67	106.71
18	1	602	CLA	C4A-NA-C1A	6.58	109.66	106.71
18	B	813	CLA	C4A-NA-C1A	6.58	109.66	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	610	CLA	C4A-NA-C1A	6.55	109.65	106.71
18	B	810	CLA	C4A-NA-C1A	6.55	109.65	106.71
27	3	619	XAT	O24-C25-C24	6.54	118.30	113.38
18	1	609	CLA	C4A-NA-C1A	6.54	109.65	106.71
27	4	620	XAT	O24-C25-C24	6.53	118.29	113.38
18	7	609	CLA	C4A-NA-C1A	6.53	109.64	106.71
21	3	621	BCR	C11-C10-C9	-6.52	118.00	127.31
27	5	621	XAT	O4-C5-C4	6.49	118.26	113.38
18	A	832	CLA	C4A-NA-C1A	6.48	109.62	106.71
18	a	614	CLA	C4A-NA-C1A	6.47	109.61	106.71
18	B	839	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	1	607	CLA	C4A-NA-C1A	6.44	109.60	106.71
18	6	603	CLA	C4A-NA-C1A	6.43	109.60	106.71
21	A	852	BCR	C20-C21-C22	-6.43	118.14	127.31
18	3	609	CLA	C4A-NA-C1A	6.42	109.59	106.71
18	4	601	CLA	C4A-NA-C1A	6.41	109.59	106.71
18	1	616	CLA	C4A-NA-C1A	6.40	109.58	106.71
18	7	608	CLA	C4A-NA-C1A	6.39	109.58	106.71
18	1	601	CLA	C4A-NA-C1A	6.38	109.57	106.71
18	1	604	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	8	612	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	a	616	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	a	608	CLA	C4A-NA-C1A	6.37	109.57	106.71
18	B	823	CLA	C4A-NA-C1A	6.36	109.57	106.71
18	5	612	CLA	C4A-NA-C1A	6.35	109.56	106.71
18	F	304	CLA	C4A-NA-C1A	6.34	109.56	106.71
18	a	611	CLA	C4A-NA-C1A	6.33	109.55	106.71
18	6	608	CLA	C4A-NA-C1A	6.33	109.55	106.71
18	A	824	CLA	C4A-NA-C1A	6.30	109.54	106.71
18	5	616	CLA	C4A-NA-C1A	6.30	109.54	106.71
18	7	610	CLA	C4A-NA-C1A	6.29	109.53	106.71
18	a	612	CLA	C4A-NA-C1A	6.29	109.53	106.71
18	4	604	CLA	C4A-NA-C1A	6.27	109.53	106.71
19	A	844	PQN	C14-C13-C12	-6.25	107.65	123.68
18	F	301	CLA	C4A-NA-C1A	6.23	109.51	106.71
21	3	622	BCR	C20-C21-C22	-6.22	118.43	127.31
18	A	833	CLA	C4A-NA-C1A	6.22	109.50	106.71
27	8	620	XAT	O4-C5-C4	6.21	118.05	113.38
18	B	817	CLA	C4A-NA-C1A	6.21	109.50	106.71
18	A	810	CLA	C4A-NA-C1A	6.18	109.48	106.71
21	3	621	BCR	C7-C8-C9	-6.17	116.91	126.23
18	A	854	CLA	C4A-NA-C1A	6.15	109.47	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	606	CLA	C4A-NA-C1A	6.15	109.47	106.71
18	A	827	CLA	C4A-NA-C1A	6.14	109.47	106.71
27	6	621	XAT	O4-C5-C4	6.14	117.99	113.38
18	5	603	CLA	C4A-NA-C1A	6.12	109.46	106.71
18	5	614	CLA	C4A-NA-C1A	6.12	109.46	106.71
18	6	611	CLA	C4A-NA-C1A	6.11	109.45	106.71
21	F	305	BCR	C16-C17-C18	-6.09	118.62	127.31
18	4	612	CLA	C4A-NA-C1A	6.08	109.44	106.71
18	7	606	CLA	C4A-NA-C1A	6.07	109.44	106.71
18	B	837	CLA	C4A-NA-C1A	6.07	109.44	106.71
18	8	611	CLA	C4A-NA-C1A	6.05	109.43	106.71
27	3	619	XAT	O4-C5-C4	6.05	117.93	113.38
18	B	804	CLA	C4A-NA-C1A	6.05	109.43	106.71
18	3	612	CLA	C4A-NA-C1A	5.95	109.38	106.71
18	B	824	CLA	C4A-NA-C1A	5.93	109.37	106.71
18	3	614	CLA	C4A-NA-C1A	5.92	109.37	106.71
18	B	825	CLA	C4A-NA-C1A	5.91	109.36	106.71
18	a	602	CLA	C4A-NA-C1A	5.90	109.36	106.71
18	A	802	CLA	CMB-C2B-C1B	-5.90	119.39	128.46
18	3	617	CLA	C4A-NA-C1A	5.90	109.36	106.71
18	a	610	CLA	C4A-NA-C1A	5.89	109.35	106.71
18	B	803	CLA	CAC-C3C-C4C	5.86	132.42	124.81
18	3	607	CLA	C4A-NA-C1A	5.82	109.32	106.71
18	4	611	CLA	C4A-NA-C1A	5.80	109.31	106.71
18	5	606	CLA	C4A-NA-C1A	5.80	109.31	106.71
18	B	828	CLA	C4A-NA-C1A	5.76	109.30	106.71
18	1	614	CLA	C4A-NA-C1A	5.74	109.29	106.71
18	6	617	CLA	C4A-NA-C1A	5.73	109.28	106.71
18	B	829	CLA	C4A-NA-C1A	5.72	109.28	106.71
27	3	619	XAT	C38-C25-C26	-5.71	112.69	122.26
27	6	621	XAT	C26-C27-C28	-5.70	113.95	125.99
21	A	852	BCR	C7-C8-C9	-5.68	117.65	126.23
27	4	620	XAT	C38-C25-C26	-5.68	112.74	122.26
21	B	844	BCR	C7-C8-C9	-5.66	117.67	126.23
27	3	619	XAT	C6-C7-C8	-5.65	114.04	125.99
18	A	820	CLA	CMB-C2B-C1B	-5.64	119.79	128.46
21	B	848	BCR	C24-C23-C22	-5.62	117.75	126.23
21	F	305	BCR	C20-C21-C22	-5.61	119.30	127.31
18	B	841	CLA	C4A-NA-C1A	5.57	109.21	106.71
18	B	836	CLA	CMB-C2B-C1B	-5.56	119.92	128.46
18	A	803	CLA	CMB-C2B-C1B	-5.56	119.92	128.46
18	8	606	CLA	C4A-NA-C1A	5.56	109.20	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	620	XAT	C26-C27-C28	-5.54	114.28	125.99
18	A	833	CLA	CMB-C2B-C1B	-5.49	120.02	128.46
27	8	620	XAT	C6-C7-C8	-5.47	114.42	125.99
18	A	815	CLA	C4A-NA-C1A	5.44	109.15	106.71
18	6	616	CLA	C4A-NA-C1A	5.44	109.15	106.71
28	6	624	NEX	C38-C25-C26	-5.44	113.15	122.26
18	6	616	CLA	CMB-C2B-C1B	-5.42	120.14	128.46
18	B	836	CLA	C4A-NA-C1A	5.42	109.14	106.71
21	A	851	BCR	C20-C21-C22	-5.41	119.59	127.31
21	3	622	BCR	C7-C8-C9	-5.39	118.09	126.23
27	a	618	XAT	C38-C25-C26	-5.37	113.26	122.26
21	7	621	BCR	C28-C27-C26	-5.37	104.49	114.08
18	A	803	CLA	C4A-NA-C1A	5.37	109.12	106.71
28	5	624	NEX	C38-C25-C26	-5.36	113.28	122.26
21	5	622	BCR	C28-C27-C26	-5.35	104.53	114.08
27	7	620	XAT	C26-C27-C28	-5.34	114.69	125.99
18	7	601	CLA	C4A-NA-C1A	5.33	109.10	106.71
18	A	805	CLA	C4A-NA-C1A	5.33	109.10	106.71
27	5	621	XAT	O4-C5-C18	5.30	121.41	115.06
27	5	621	XAT	C6-C7-C8	-5.30	114.78	125.99
18	A	802	CLA	CMB-C2B-C3B	5.30	134.60	124.68
27	8	620	XAT	C38-C25-C26	-5.29	113.40	122.26
27	6	621	XAT	C6-C7-C8	-5.28	114.82	125.99
27	6	621	XAT	C38-C25-C26	-5.28	113.42	122.26
27	a	618	XAT	C6-C7-C8	-5.27	114.85	125.99
27	4	620	XAT	C6-C7-C8	-5.27	114.86	125.99
18	A	818	CLA	CMB-C2B-C1B	-5.25	120.39	128.46
27	6	621	XAT	C18-C5-C6	-5.25	113.47	122.26
28	5	624	NEX	O24-C25-C38	5.22	121.31	115.06
28	6	624	NEX	O24-C25-C24	5.21	117.30	113.38
21	3	622	BCR	C24-C23-C22	-5.20	118.37	126.23
21	3	621	BCR	C20-C21-C22	-5.19	119.90	127.31
18	1	610	CLA	C4A-NA-C1A	5.18	109.03	106.71
21	5	622	BCR	C15-C14-C13	-5.17	119.93	127.31
27	8	620	XAT	C18-C5-C6	-5.17	113.59	122.26
28	6	624	NEX	O24-C25-C38	5.17	121.25	115.06
19	B	842	PQN	C14-C13-C12	-5.17	110.42	123.68
21	A	852	BCR	C16-C17-C18	-5.14	119.98	127.31
21	B	843	BCR	C28-C27-C26	-5.14	104.91	114.08
18	A	805	CLA	CMB-C2B-C1B	-5.13	120.58	128.46
18	3	609	CLA	CMB-C2B-C1B	-5.12	120.60	128.46
18	7	604	CLA	CMB-C2B-C1B	-5.11	120.61	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	845	BCR	C7-C8-C9	-5.11	118.52	126.23
21	3	621	BCR	C35-C13-C14	-5.07	115.81	122.92
21	3	622	BCR	C36-C18-C17	-5.07	115.83	122.92
27	3	619	XAT	C18-C5-C6	-5.06	113.78	122.26
21	K	202	BCR	C28-C27-C26	-5.05	105.06	114.08
18	B	826	CLA	CMB-C2B-C1B	-5.03	120.74	128.46
18	4	602	CLA	CMB-C2B-C1B	-5.01	120.76	128.46
18	A	826	CLA	CMB-C2B-C1B	-5.01	120.77	128.46
21	A	856	BCR	C15-C16-C17	-5.01	113.22	123.47
27	7	620	XAT	C6-C7-C8	-4.99	115.44	125.99
27	a	618	XAT	C18-C5-C6	-4.99	113.90	122.26
28	5	624	NEX	O24-C25-C24	4.98	117.12	113.38
21	B	844	BCR	C30-C25-C26	-4.97	115.61	122.61
18	7	601	CLA	O2D-CGD-O1D	-4.97	114.11	123.84
18	A	822	CLA	CMB-C2B-C1B	-4.97	120.83	128.46
21	B	843	BCR	C16-C17-C18	-4.97	120.22	127.31
18	B	832	CLA	CMB-C2B-C1B	-4.97	120.83	128.46
21	3	620	BCR	C3-C4-C5	-4.97	105.21	114.08
21	A	848	BCR	C16-C17-C18	-4.94	120.27	127.31
27	7	620	XAT	C38-C25-C26	-4.93	113.99	122.26
21	B	845	BCR	C24-C23-C22	-4.93	118.79	126.23
18	A	829	CLA	CMB-C2B-C1B	-4.91	120.91	128.46
18	B	827	CLA	CMB-C2B-C1B	-4.91	120.92	128.46
27	5	621	XAT	C18-C5-C6	-4.90	114.05	122.26
18	7	611	CLA	CMB-C2B-C1B	-4.90	120.93	128.46
18	A	838	CLA	CMB-C2B-C1B	-4.90	120.94	128.46
21	8	621	BCR	C15-C14-C13	-4.90	120.32	127.31
27	a	618	XAT	O24-C25-C38	4.89	120.92	115.06
18	3	603	CLA	CMB-C2B-C1B	-4.89	120.95	128.46
27	8	620	XAT	C26-C27-C28	-4.89	115.66	125.99
18	5	602	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
27	4	620	XAT	C18-C5-C6	-4.88	114.08	122.26
27	5	621	XAT	C26-C27-C28	-4.87	115.70	125.99
18	6	608	CLA	CMB-C2B-C1B	-4.85	121.01	128.46
18	A	854	CLA	CMB-C2B-C1B	-4.85	121.01	128.46
18	A	816	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
21	A	852	BCR	C24-C23-C22	-4.83	118.93	126.23
25	J	103	DGD	O3G-C3G-C2G	-4.83	99.26	110.90
27	4	620	XAT	O24-C25-C38	4.82	120.83	115.06
18	5	608	CLA	CMB-C2B-C1B	-4.81	121.08	128.46
18	A	806	CLA	CAA-C2A-C3A	-4.81	99.62	112.78
18	B	803	CLA	CMB-C2B-C1B	-4.77	121.12	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	622	BCR	C16-C17-C18	-4.77	120.50	127.31
21	a	619	BCR	C28-C27-C26	-4.77	105.56	114.08
21	A	850	BCR	C28-C27-C26	-4.77	105.56	114.08
21	5	622	BCR	C3-C4-C5	-4.77	105.56	114.08
18	8	610	CLA	CMB-C2B-C1B	-4.76	121.14	128.46
21	1	619	BCR	C16-C17-C18	-4.76	120.52	127.31
18	B	814	CLA	CMB-C2B-C1B	-4.75	121.16	128.46
27	7	620	XAT	C18-C5-C6	-4.75	114.30	122.26
27	1	618	XAT	C26-C27-C28	-4.75	115.95	125.99
21	3	620	BCR	C28-C27-C26	-4.75	105.60	114.08
18	B	804	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
18	7	609	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
27	1	618	XAT	C18-C5-C6	-4.73	114.33	122.26
18	7	612	CLA	C4A-NA-C1A	4.73	108.83	106.71
27	a	618	XAT	C26-C27-C28	-4.72	116.01	125.99
18	A	817	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
18	B	828	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
28	5	624	NEX	C26-C27-C28	-4.70	116.05	125.99
21	4	621	BCR	C28-C27-C26	-4.70	105.69	114.08
18	B	818	CLA	CMB-C2B-C1B	-4.70	121.25	128.46
21	3	622	BCR	C35-C13-C14	-4.69	116.36	122.92
21	B	848	BCR	C20-C21-C22	-4.67	120.64	127.31
18	B	836	CLA	CMB-C2B-C3B	4.67	133.42	124.68
21	6	622	BCR	C3-C4-C5	-4.67	105.74	114.08
21	F	305	BCR	C24-C23-C22	-4.66	119.19	126.23
27	1	618	XAT	C38-C25-C26	-4.66	114.45	122.26
21	B	846	BCR	C11-C10-C9	-4.65	120.67	127.31
21	B	846	BCR	C38-C26-C25	-4.65	119.31	124.53
18	A	827	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
18	5	619	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
18	A	813	CLA	CMB-C2B-C1B	-4.64	121.34	128.46
18	A	833	CLA	CMB-C2B-C3B	4.64	133.35	124.68
21	3	621	BCR	C24-C23-C22	-4.64	119.23	126.23
18	B	829	CLA	CMB-C2B-C3B	4.63	133.33	124.68
21	A	850	BCR	C7-C8-C9	-4.62	119.25	126.23
21	A	851	BCR	C28-C27-C26	-4.61	105.84	114.08
18	4	602	CLA	CMB-C2B-C3B	4.61	133.30	124.68
18	A	832	CLA	CMB-C2B-C1B	-4.60	121.39	128.46
18	B	831	CLA	CMB-C2B-C1B	-4.60	121.39	128.46
18	5	612	CLA	CMB-C2B-C1B	-4.60	121.40	128.46
21	A	849	BCR	C24-C23-C22	-4.59	119.29	126.23
18	B	805	CLA	CMB-C2B-C1B	-4.59	121.41	128.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	849	BCR	C20-C21-C22	-4.59	120.76	127.31
18	A	805	CLA	CMB-C2B-C3B	4.59	133.26	124.68
18	6	612	CLA	CMB-C2B-C1B	-4.58	121.42	128.46
21	8	621	BCR	C28-C27-C26	-4.58	105.90	114.08
18	B	817	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
27	8	620	XAT	C15-C14-C13	-4.57	120.78	127.31
18	a	604	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
18	B	835	CLA	CMB-C2B-C1B	-4.56	121.46	128.46
18	B	816	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
21	J	102	BCR	C3-C4-C5	-4.54	105.96	114.08
18	7	606	CLA	CMB-C2B-C1B	-4.54	121.48	128.46
21	a	619	BCR	C16-C17-C18	-4.54	120.83	127.31
18	1	604	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
18	6	616	CLA	CMB-C2B-C3B	4.52	133.13	124.68
18	5	619	CLA	CAB-C3B-C4B	-4.52	121.52	128.46
18	5	607	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
18	6	606	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
18	B	839	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
21	K	202	BCR	C11-C10-C9	-4.50	120.88	127.31
21	K	202	BCR	C16-C17-C18	-4.50	120.89	127.31
27	3	619	XAT	O4-C5-C18	4.49	120.44	115.06
18	A	838	CLA	CMB-C2B-C3B	4.49	133.08	124.68
18	A	835	CLA	O2D-CGD-O1D	-4.49	115.06	123.84
18	a	612	CLA	CMB-C2B-C1B	-4.48	121.57	128.46
21	B	801	BCR	C16-C17-C18	-4.48	120.92	127.31
21	B	844	BCR	C24-C23-C22	-4.47	119.47	126.23
18	1	610	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
18	5	609	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
18	5	610	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
18	A	803	CLA	CMB-C2B-C3B	4.46	133.03	124.68
21	L	305	BCR	C7-C8-C9	-4.46	119.50	126.23
27	6	621	XAT	O4-C5-C18	4.45	120.39	115.06
21	A	851	BCR	C16-C17-C18	-4.44	120.97	127.31
21	1	619	BCR	C28-C27-C26	-4.44	106.15	114.08
21	3	622	BCR	C28-C27-C26	-4.42	106.18	114.08
28	6	624	NEX	C26-C27-C28	-4.42	116.64	125.99
18	A	854	CLA	CMB-C2B-C3B	4.42	132.94	124.68
18	A	829	CLA	CMB-C2B-C3B	4.42	132.94	124.68
21	A	851	BCR	C15-C14-C13	-4.42	121.01	127.31
18	8	604	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
21	3	621	BCR	C28-C27-C26	-4.40	106.22	114.08
21	B	801	BCR	C20-C21-C22	-4.40	121.03	127.31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	856	BCR	C20-C21-C22	-4.39	121.04	127.31
27	3	619	XAT	C26-C27-C28	-4.39	116.70	125.99
21	K	202	BCR	C24-C23-C22	-4.39	119.60	126.23
18	7	601	CLA	O2D-CGD-CBD	4.39	119.06	111.27
21	A	849	BCR	C11-C10-C9	-4.38	121.05	127.31
28	5	624	NEX	C31-C30-C29	-4.38	121.06	127.31
18	A	818	CLA	CMB-C2B-C3B	4.38	132.87	124.68
21	L	305	BCR	C16-C17-C18	-4.38	121.07	127.31
18	5	607	CLA	CMB-C2B-C3B	4.37	132.85	124.68
21	B	846	BCR	C7-C8-C9	-4.37	119.64	126.23
18	B	832	CLA	CMB-C2B-C3B	4.36	132.84	124.68
18	B	809	CLA	CMB-C2B-C1B	-4.35	121.77	128.46
19	B	842	PQN	C14-C13-C15	-4.34	107.96	115.27
18	a	608	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
21	L	301	BCR	C7-C8-C9	-4.34	119.67	126.23
21	4	621	BCR	C15-C14-C13	-4.34	121.11	127.31
18	A	820	CLA	CMB-C2B-C3B	4.33	132.78	124.68
21	B	847	BCR	C15-C14-C13	-4.33	121.13	127.31
20	5	623	LHG	O4-P-O5	4.33	133.64	112.24
28	6	624	NEX	C31-C30-C29	-4.33	121.13	127.31
20	A	847	LHG	O4-P-O5	4.33	133.63	112.24
18	7	609	CLA	CMB-C2B-C3B	4.32	132.76	124.68
20	4	622	LHG	O4-P-O5	4.32	133.57	112.24
26	5	620	LUT	C35-C34-C33	-4.31	121.16	127.31
21	5	622	BCR	C16-C17-C18	-4.29	121.18	127.31
27	1	618	XAT	C6-C7-C8	-4.29	116.91	125.99
21	A	856	BCR	C3-C4-C5	-4.29	106.41	114.08
20	7	622	LHG	O4-P-O5	4.28	133.38	112.24
18	B	815	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
18	6	620	CLA	O2D-CGD-O1D	-4.25	115.52	123.84
18	7	611	CLA	CMB-C2B-C3B	4.25	132.63	124.68
20	6	623	LHG	O4-P-O5	4.25	133.26	112.24
18	3	609	CLA	CMB-C2B-C3B	4.25	132.62	124.68
18	A	806	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
18	8	612	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
18	A	814	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
21	B	843	BCR	C16-C15-C14	-4.24	114.79	123.47
18	B	826	CLA	CMB-C2B-C3B	4.23	132.60	124.68
18	A	828	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
18	4	612	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
21	K	202	BCR	C15-C14-C13	-4.23	121.27	127.31
21	B	846	BCR	C15-C14-C13	-4.23	121.27	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	301	BCR	C15-C14-C13	-4.23	121.28	127.31
27	3	619	XAT	O24-C25-C38	4.23	120.12	115.06
18	B	827	CLA	CMB-C2B-C3B	4.22	132.58	124.68
20	1	620	LHG	O4-P-O5	4.22	133.12	112.24
18	A	812	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
18	A	809	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
21	L	301	BCR	C24-C23-C22	-4.22	119.86	126.23
20	a	620	LHG	O4-P-O5	4.21	133.07	112.24
21	7	621	BCR	C16-C17-C18	-4.21	121.30	127.31
18	A	826	CLA	CMB-C2B-C3B	4.21	132.56	124.68
18	8	610	CLA	CMB-C2B-C3B	4.20	132.54	124.68
20	3	623	LHG	O4-P-O5	4.20	133.00	112.24
18	6	601	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
21	K	207	BCR	C20-C21-C22	-4.20	121.32	127.31
18	B	837	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
18	3	604	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
18	B	824	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
21	7	623	BCR	C20-C21-C22	-4.18	121.34	127.31
21	K	202	BCR	C3-C4-C5	-4.18	106.61	114.08
20	A	846	LHG	O4-P-O5	4.18	132.90	112.24
18	B	803	CLA	CMB-C2B-C3B	4.18	132.50	124.68
21	7	623	BCR	C15-C14-C13	-4.17	121.36	127.31
20	8	623	LHG	O4-P-O5	4.17	132.85	112.24
20	B	851	LHG	O4-P-O5	4.17	132.84	112.24
21	6	622	BCR	C15-C14-C13	-4.16	121.37	127.31
21	3	620	BCR	C20-C21-C22	-4.15	121.39	127.31
18	B	814	CLA	CMB-C2B-C3B	4.15	132.44	124.68
21	B	847	BCR	C11-C10-C9	-4.15	121.39	127.31
21	3	620	BCR	C16-C17-C18	-4.14	121.40	127.31
20	3	624	LHG	O4-P-O5	4.14	132.72	112.24
20	5	625	LHG	O4-P-O5	4.14	132.71	112.24
27	a	618	XAT	O4-C5-C18	4.14	120.02	115.06
18	A	816	CLA	CMB-C2B-C3B	4.14	132.42	124.68
18	B	804	CLA	CMB-C2B-C3B	4.11	132.38	124.68
21	3	622	BCR	C38-C26-C25	-4.11	119.92	124.53
18	A	830	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
18	8	603	CLA	CAB-C3B-C4B	-4.09	122.17	128.46
18	5	608	CLA	CMB-C2B-C3B	4.09	132.34	124.68
18	1	604	CLA	O2D-CGD-O1D	-4.09	115.85	123.84
21	B	801	BCR	C28-C27-C26	-4.08	106.78	114.08
18	6	610	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
18	6	608	CLA	CMB-C2B-C3B	4.08	132.32	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	618	LUT	C15-C14-C13	-4.08	121.49	127.31
26	4	619	LUT	C35-C34-C33	-4.07	121.50	127.31
21	A	852	BCR	C20-C19-C18	-4.07	114.98	126.42
26	5	620	LUT	C35-C15-C14	-4.07	115.14	123.47
21	K	207	BCR	C16-C17-C18	-4.06	121.51	127.31
28	5	624	NEX	C15-C14-C13	-4.06	121.51	127.31
21	A	849	BCR	C15-C14-C13	-4.06	121.51	127.31
18	6	618	CLA	CAB-C3B-C4B	-4.05	122.23	128.46
21	K	207	BCR	C15-C14-C13	-4.05	121.53	127.31
21	3	622	BCR	C19-C18-C17	4.04	125.15	118.94
18	3	602	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
21	4	621	BCR	C16-C17-C18	-4.04	121.54	127.31
21	6	622	BCR	C16-C15-C14	-4.04	115.19	123.47
18	7	604	CLA	CMB-C2B-C3B	4.04	132.23	124.68
18	B	841	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
20	8	622	LHG	O7-C7-C8	4.03	120.19	111.50
18	B	805	CLA	CMB-C2B-C3B	4.03	132.22	124.68
27	4	620	XAT	O4-C5-C18	4.03	119.88	115.06
18	A	827	CLA	CMB-C2B-C3B	4.03	132.21	124.68
21	B	845	BCR	C33-C5-C6	-4.02	120.02	124.53
21	3	621	BCR	C36-C18-C17	-4.01	117.31	122.92
21	A	856	BCR	C28-C27-C26	-4.00	106.94	114.08
21	A	851	BCR	C7-C8-C9	-4.00	120.20	126.23
18	A	831	CLA	CMB-C2B-C3B	3.99	132.15	124.68
18	4	610	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
18	7	610	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
21	A	850	BCR	C24-C23-C22	-3.99	120.21	126.23
27	8	620	XAT	O4-C5-C18	3.99	119.83	115.06
18	A	813	CLA	CMB-C2B-C3B	3.98	132.12	124.68
18	6	602	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
18	a	607	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
21	3	621	BCR	C12-C13-C14	3.97	125.03	118.94
21	A	849	BCR	C7-C8-C9	-3.97	120.24	126.23
18	a	610	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
26	1	617	LUT	C35-C34-C33	-3.96	121.66	127.31
18	B	833	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
18	1	612	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
18	5	618	CLA	CAB-C3B-C4B	-3.95	122.39	128.46
18	B	813	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
18	4	616	CLA	CAB-C3B-C4B	-3.93	122.42	128.46
18	8	606	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
18	B	831	CLA	CMB-C2B-C3B	3.92	132.01	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	607	CLA	CAB-C3B-C4B	-3.92	122.44	128.46
21	8	621	BCR	C3-C4-C5	-3.92	107.08	114.08
28	6	624	NEX	C15-C14-C13	-3.91	121.72	127.31
18	a	609	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
18	B	839	CLA	CMB-C2B-C3B	3.91	131.99	124.68
18	A	840	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
18	4	606	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
18	1	611	CLA	O2D-CGD-O1D	-3.91	116.20	123.84
18	6	614	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
18	B	816	CLA	CMB-C2B-C3B	3.90	131.98	124.68
26	7	619	LUT	C35-C34-C33	-3.90	121.75	127.31
18	7	615	CLA	CAB-C3B-C4B	-3.89	122.48	128.46
18	A	817	CLA	CMB-C2B-C3B	3.89	131.96	124.68
21	7	621	BCR	C3-C4-C5	-3.89	107.13	114.08
26	7	619	LUT	C7-C8-C9	-3.89	120.36	126.23
18	3	603	CLA	CMB-C2B-C3B	3.89	131.96	124.68
21	7	623	BCR	C24-C23-C22	-3.88	120.36	126.23
21	B	847	BCR	C23-C24-C25	-3.88	116.30	127.20
18	5	609	CLA	CMB-C2B-C3B	3.88	131.94	124.68
18	3	612	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
18	4	608	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
18	a	606	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
21	3	620	BCR	C11-C10-C9	-3.88	121.78	127.31
21	B	847	BCR	C7-C8-C9	-3.88	120.38	126.23
18	6	617	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
26	7	619	LUT	C15-C14-C13	-3.87	121.78	127.31
21	B	845	BCR	C16-C17-C18	-3.87	121.78	127.31
21	7	621	BCR	C15-C14-C13	-3.87	121.79	127.31
18	A	815	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
21	A	848	BCR	C7-C8-C9	-3.86	120.41	126.23
18	A	811	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
27	3	619	XAT	C24-C23-C22	-3.85	103.34	110.77
18	5	619	CLA	C2A-C1A-CHA	3.84	130.58	123.86
21	3	622	BCR	C11-C12-C13	-3.84	115.62	126.42
18	7	612	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
18	B	838	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
18	B	828	CLA	CMB-C2B-C3B	3.83	131.85	124.68
18	3	610	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
21	3	621	BCR	C33-C5-C6	-3.83	120.22	124.53
28	6	624	NEX	C24-C23-C22	-3.83	103.37	110.77
21	7	623	BCR	C16-C17-C18	-3.83	121.85	127.31
18	B	817	CLA	CMB-C2B-C3B	3.82	131.83	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	5	612	CLA	CMB-C2B-C3B	3.82	131.82	124.68
18	B	804	CLA	CAA-C2A-C3A	-3.82	107.19	116.10
18	1	601	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
21	1	619	BCR	C20-C21-C22	-3.82	121.86	127.31
21	8	621	BCR	C7-C8-C9	-3.81	120.47	126.23
18	A	834	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
21	B	848	BCR	C16-C17-C18	-3.81	121.87	127.31
21	3	620	BCR	C24-C23-C22	-3.81	120.47	126.23
18	5	610	CLA	CMB-C2B-C3B	3.81	131.80	124.68
26	8	619	LUT	C35-C34-C33	-3.81	121.88	127.31
18	4	603	CLA	CAB-C3B-C4B	-3.81	122.61	128.46
18	a	612	CLA	CMB-C2B-C3B	3.81	131.80	124.68
18	1	606	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
18	3	607	CLA	CAB-C3B-C4B	-3.80	122.62	128.46
21	J	102	BCR	C16-C17-C18	-3.80	121.89	127.31
18	A	808	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
21	A	848	BCR	C38-C26-C25	-3.80	120.26	124.53
18	B	822	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
21	3	622	BCR	C20-C19-C18	-3.79	115.76	126.42
18	a	602	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
18	B	818	CLA	CMB-C2B-C3B	3.79	131.77	124.68
18	A	814	CLA	CMB-C2B-C3B	3.79	131.77	124.68
18	1	616	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
27	3	619	XAT	C15-C14-C13	-3.79	121.90	127.31
18	5	619	CLA	CMB-C2B-C3B	3.79	132.11	124.69
18	B	835	CLA	CMB-C2B-C3B	3.79	131.76	124.68
18	3	602	CLA	CMB-C2B-C3B	3.78	131.76	124.68
21	B	844	BCR	C15-C14-C13	-3.78	121.91	127.31
21	J	102	BCR	C15-C14-C13	-3.78	121.91	127.31
25	B	850	DGD	O3G-C3G-C2G	-3.78	101.77	110.90
18	4	618	CLA	CAB-C3B-C4B	-3.78	122.65	128.46
18	F	304	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
18	1	611	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
21	K	207	BCR	C24-C23-C22	-3.77	120.54	126.23
25	J	103	DGD	O6D-C1D-O3G	-3.77	101.06	109.97
21	B	843	BCR	C11-C10-C9	-3.76	121.94	127.31
18	A	802	CLA	CHB-C4A-NA	3.76	129.71	124.51
27	7	620	XAT	C35-C34-C33	-3.76	121.94	127.31
18	1	604	CLA	CMB-C2B-C3B	3.75	131.69	124.68
18	4	613	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
18	4	607	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
18	B	806	CLA	CMB-C2B-C1B	-3.74	122.72	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	5	602	CLA	CMB-C2B-C3B	3.74	131.67	124.68
18	8	616	CLA	CAB-C3B-C4B	-3.73	122.72	128.46
21	1	619	BCR	C24-C23-C22	-3.73	120.60	126.23
21	3	622	BCR	C38-C26-C27	3.72	120.77	113.62
21	A	848	BCR	C24-C23-C22	-3.72	120.61	126.23
21	a	619	BCR	C33-C5-C6	-3.72	120.35	124.53
18	3	607	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
21	A	852	BCR	C34-C9-C10	-3.72	117.71	122.92
18	1	609	CLA	CAB-C3B-C4B	-3.72	122.75	128.46
18	a	604	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
18	6	612	CLA	CMB-C2B-C3B	3.71	131.63	124.68
18	1	609	CLA	CAA-C2A-C3A	-3.71	107.43	116.10
18	6	601	CLA	CMB-C2B-C3B	3.71	131.62	124.68
18	6	609	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
21	L	305	BCR	C11-C10-C9	-3.71	122.02	127.31
21	7	623	BCR	C33-C5-C6	-3.71	120.36	124.53
18	6	606	CLA	CMB-C2B-C3B	3.71	131.61	124.68
18	A	822	CLA	CMB-C2B-C3B	3.70	131.61	124.68
18	8	614	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
18	5	616	CLA	CAB-C3B-C4B	-3.70	122.78	128.46
18	1	614	CLA	C2A-C3A-C4A	-3.70	102.19	106.26
27	6	621	XAT	C15-C14-C13	-3.69	122.04	127.31
18	7	616	CLA	CAB-C3B-C4B	-3.69	122.79	128.46
21	3	621	BCR	C11-C12-C13	-3.69	116.05	126.42
18	3	606	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
27	8	620	XAT	C10-C11-C12	-3.68	111.72	123.22
18	1	610	CLA	CMB-C2B-C3B	3.68	131.56	124.68
23	A	857	LMU	C1B-O1B-C4'	-3.68	109.64	115.33
21	B	844	BCR	C33-C5-C6	-3.68	120.40	124.53
18	A	823	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
18	5	618	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
18	A	845	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
21	A	848	BCR	C20-C21-C22	-3.68	122.06	127.31
27	7	620	XAT	O24-C25-C38	3.68	119.46	115.06
18	A	824	CLA	CMA-C3A-C2A	-3.68	107.52	116.10
18	3	614	CLA	CAA-C2A-C3A	-3.67	107.53	116.10
18	A	843	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
18	a	608	CLA	CMB-C2B-C3B	3.67	131.55	124.68
21	1	619	BCR	C7-C8-C9	-3.67	120.69	126.23
18	B	823	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
28	6	624	NEX	C17-C1-C6	-3.66	107.19	110.47
21	B	845	BCR	C15-C14-C13	-3.66	122.08	127.31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	614	CLA	CAB-C3B-C4B	-3.66	122.84	128.46
18	B	825	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
18	4	611	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
18	a	604	CLA	CMB-C2B-C3B	3.65	131.51	124.68
18	8	607	CLA	CAB-C3B-C4B	-3.65	122.85	128.46
18	A	835	CLA	O2D-CGD-CBD	3.65	117.75	111.27
18	A	854	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
27	7	620	XAT	C15-C14-C13	-3.65	122.10	127.31
18	A	834	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
27	1	618	XAT	C35-C34-C33	-3.64	122.12	127.31
27	5	621	XAT	C15-C14-C13	-3.64	122.12	127.31
18	3	611	CLA	CAB-C3B-C4B	-3.63	122.89	128.46
18	1	608	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
27	1	618	XAT	O24-C25-C38	3.62	119.40	115.06
26	6	619	LUT	C35-C34-C33	-3.62	122.14	127.31
18	8	611	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
18	4	601	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
18	B	840	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
18	6	613	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
18	5	607	CLA	CHB-C4A-NA	3.62	129.52	124.51
18	A	832	CLA	CMB-C2B-C3B	3.62	131.45	124.68
18	1	613	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
18	6	616	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
18	7	602	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
18	6	611	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
18	1	614	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
18	B	808	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
18	8	612	CLA	CMB-C2B-C3B	3.61	131.42	124.68
18	8	601	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
18	6	601	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
18	B	829	CLA	C2D-C1D-ND	-3.60	107.45	110.10
21	8	621	BCR	C16-C17-C18	-3.60	122.18	127.31
18	B	820	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
18	7	606	CLA	CMB-C2B-C3B	3.59	131.40	124.68
21	3	621	BCR	C16-C15-C14	-3.59	116.13	123.47
21	B	846	BCR	C38-C26-C27	3.58	120.50	113.62
18	A	806	CLA	CMB-C2B-C3B	3.58	131.38	124.68
18	8	614	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
18	5	614	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
18	4	612	CLA	CMB-C2B-C3B	3.57	131.36	124.68
27	6	621	XAT	O24-C25-C38	3.57	119.33	115.06
18	B	802	CLA	O2D-CGD-O1D	-3.57	116.86	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	620	XAT	O4-C5-C18	3.57	119.33	115.06
18	5	601	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
21	4	621	BCR	C11-C10-C9	-3.56	122.22	127.31
18	A	809	CLA	CMB-C2B-C3B	3.56	131.35	124.68
18	A	821	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
18	6	604	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
18	6	603	CLA	CAB-C3B-C4B	-3.56	123.00	128.46
27	6	621	XAT	C4-C3-C2	-3.56	103.90	110.77
18	1	609	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
18	7	615	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
26	a	617	LUT	C35-C34-C33	-3.55	122.25	127.31
18	A	830	CLA	CMB-C2B-C3B	3.55	131.32	124.68
18	A	835	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
18	8	609	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
27	5	621	XAT	C10-C11-C12	-3.54	112.16	123.22
18	B	837	CLA	CMB-C2B-C3B	3.54	131.30	124.68
21	A	848	BCR	C11-C10-C9	-3.54	122.26	127.31
18	7	601	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
18	7	616	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
18	A	812	CLA	CMB-C2B-C3B	3.53	131.28	124.68
18	6	620	CLA	CAA-C2A-C3A	-3.53	103.11	112.78
18	B	841	CLA	CMB-C2B-C3B	3.53	131.28	124.68
18	B	807	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
18	8	604	CLA	CMB-C2B-C3B	3.52	131.27	124.68
18	a	611	CLA	CAB-C3B-C4B	-3.52	123.05	128.46
18	K	201	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
18	a	613	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
21	B	843	BCR	C20-C21-C22	-3.52	122.29	127.31
18	8	602	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
23	5	628	LMU	C2'-C3'-C4'	3.51	117.70	109.68
18	5	604	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
21	L	301	BCR	C11-C10-C9	-3.51	122.30	127.31
18	K	203	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
18	K	206	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
18	a	601	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
21	1	619	BCR	C33-C5-C6	-3.51	120.59	124.53
18	B	811	CLA	CAB-C3B-C4B	-3.50	123.08	128.46
18	6	610	CLA	CMB-C2B-C3B	3.50	131.22	124.68
27	1	618	XAT	O4-C5-C18	3.50	119.25	115.06
26	1	617	LUT	C35-C15-C14	-3.49	116.32	123.47
18	B	810	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
18	5	611	CLA	CMB-C2B-C1B	-3.49	123.10	128.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	801	BCR	C16-C15-C14	-3.49	116.32	123.47
21	4	621	BCR	C3-C4-C5	-3.48	107.86	114.08
18	A	837	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
18	6	620	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
26	a	617	LUT	C35-C15-C14	-3.48	116.34	123.47
21	F	305	BCR	C38-C26-C25	-3.48	120.62	124.53
21	A	850	BCR	C33-C5-C6	-3.48	120.62	124.53
21	A	850	BCR	C11-C10-C9	-3.48	122.35	127.31
18	7	614	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
18	A	825	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
18	B	824	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
21	A	849	BCR	C16-C17-C18	-3.47	122.36	127.31
21	F	305	BCR	C16-C15-C14	-3.47	116.37	123.47
18	L	302	CLA	CHB-C4A-NA	3.47	129.31	124.51
18	A	831	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
18	A	828	CLA	CMB-C2B-C3B	3.46	131.16	124.68
21	6	622	BCR	C38-C26-C25	-3.46	120.64	124.53
18	A	840	CLA	CMB-C2B-C3B	3.46	131.15	124.68
18	B	819	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
18	5	604	CLA	CAB-C3B-C4B	-3.46	123.15	128.46
18	4	609	CLA	CHB-C4A-NA	3.45	129.29	124.51
18	7	604	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
18	K	204	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
18	B	815	CLA	CMB-C2B-C3B	3.45	131.13	124.68
18	4	616	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
21	3	622	BCR	C12-C13-C14	3.45	124.23	118.94
21	4	621	BCR	C33-C5-C6	-3.45	120.66	124.53
21	A	850	BCR	C15-C14-C13	-3.44	122.40	127.31
21	7	623	BCR	C11-C10-C9	-3.44	122.40	127.31
23	K	208	LMU	C1'-C2'-C3'	3.43	117.15	110.00
21	A	850	BCR	C16-C17-C18	-3.43	122.41	127.31
21	a	619	BCR	C11-C10-C9	-3.43	122.41	127.31
18	B	824	CLA	CMB-C2B-C3B	3.43	131.10	124.68
27	7	620	XAT	C24-C23-C22	-3.43	104.16	110.77
18	a	611	CLA	CAA-C2A-C3A	-3.42	108.11	116.10
18	A	809	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
18	F	301	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
18	1	616	CLA	CAB-C3B-C4B	-3.41	123.22	128.46
21	L	305	BCR	C28-C27-C26	-3.41	107.98	114.08
18	7	613	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
18	5	619	CLA	CAB-C3B-C2B	3.41	131.37	124.69
18	a	614	CLA	CMB-C2B-C1B	-3.40	123.23	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K	207	BCR	C7-C8-C9	-3.40	121.10	126.23
28	6	624	NEX	C11-C10-C9	-3.40	122.46	127.31
18	B	834	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
21	B	847	BCR	C20-C21-C22	-3.40	122.46	127.31
18	6	618	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
27	5	621	XAT	C4-C3-C2	-3.40	104.21	110.77
18	4	609	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
18	a	610	CLA	CMB-C2B-C3B	3.39	131.03	124.68
18	A	842	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
27	5	621	XAT	C38-C25-C26	-3.39	116.58	122.26
18	B	813	CLA	CMB-C2B-C3B	3.39	131.02	124.68
26	4	619	LUT	C35-C15-C14	-3.39	116.54	123.47
18	B	840	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
18	6	614	CLA	CMB-C2B-C3B	3.38	131.01	124.68
26	6	619	LUT	C35-C15-C14	-3.38	116.55	123.47
18	A	817	CLA	CHB-C4A-NA	3.38	129.19	124.51
18	7	608	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
18	B	810	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
18	3	614	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
18	4	618	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
18	A	841	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
18	a	616	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
18	6	607	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
18	6	602	CLA	CMB-C2B-C3B	3.37	130.98	124.68
27	a	618	XAT	C10-C11-C12	-3.37	112.70	123.22
18	a	602	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
27	8	620	XAT	O24-C25-C38	3.37	119.09	115.06
18	1	607	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
18	7	607	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
27	3	619	XAT	C4-C3-C2	-3.36	104.28	110.77
18	a	611	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
18	4	608	CLA	CMB-C2B-C3B	3.35	130.95	124.68
18	a	607	CLA	CMB-C2B-C3B	3.35	130.95	124.68
18	A	820	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
18	L	302	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
21	A	849	BCR	C3-C4-C5	-3.35	108.10	114.08
21	B	847	BCR	C15-C16-C17	-3.34	116.62	123.47
21	8	621	BCR	C21-C20-C19	-3.34	112.78	123.22
21	A	851	BCR	C11-C10-C9	-3.34	122.54	127.31
18	3	617	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
18	1	612	CLA	CMB-C2B-C3B	3.34	130.92	124.68
21	3	621	BCR	C20-C19-C18	-3.34	117.05	126.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	821	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
21	B	848	BCR	C15-C14-C13	-3.33	122.56	127.31
18	7	610	CLA	CMB-C2B-C3B	3.33	130.91	124.68
18	4	610	CLA	CMB-C2B-C3B	3.33	130.91	124.68
18	B	811	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
18	1	606	CLA	CBD-CHA-C1A	3.32	131.58	128.06
21	7	621	BCR	C21-C20-C19	-3.32	112.84	123.22
18	B	821	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
18	B	833	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
21	1	619	BCR	C11-C10-C9	-3.32	122.58	127.31
26	8	619	LUT	C35-C15-C14	-3.32	116.68	123.47
18	8	616	CLA	CHB-C4A-NA	3.31	129.09	124.51
21	B	847	BCR	C24-C23-C22	-3.31	121.23	126.23
21	a	619	BCR	C20-C21-C22	-3.31	122.58	127.31
18	4	614	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
18	L	303	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
26	4	619	LUT	C10-C11-C12	-3.30	112.91	123.22
18	5	606	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
21	B	846	BCR	C3-C4-C5	-3.29	108.19	114.08
18	4	606	CLA	CMB-C2B-C3B	3.29	130.84	124.68
18	A	842	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
21	F	305	BCR	C10-C11-C12	-3.29	112.95	123.22
18	5	619	CLA	CHB-C4A-NA	3.29	129.06	124.51
18	3	611	CLA	CAA-C2A-C3A	-3.29	108.42	116.10
18	3	604	CLA	CMB-C2B-C3B	3.29	130.82	124.68
18	5	613	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
21	B	847	BCR	C3-C4-C5	-3.28	108.22	114.08
27	4	620	XAT	C15-C14-C13	-3.28	122.63	127.31
21	B	847	BCR	C16-C17-C18	-3.28	122.63	127.31
18	3	610	CLA	CMB-C2B-C3B	3.28	130.81	124.68
23	A	859	LMU	C1'-O5'-C5'	3.28	118.12	113.03
21	B	801	BCR	C29-C30-C25	3.27	115.52	110.48
18	A	829	CLA	C1B-CHB-C4A	-3.27	123.64	130.12
18	8	608	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
18	F	303	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
18	3	611	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
18	A	837	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
18	a	609	CLA	CMB-C2B-C3B	3.27	130.79	124.68
18	A	826	CLA	C2A-C1A-CHA	3.26	129.57	123.86
18	7	614	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
27	4	620	XAT	C35-C34-C33	-3.26	122.66	127.31
18	7	609	CLA	O2D-CGD-O1D	-3.26	117.47	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	305	BCR	C15-C14-C13	-3.26	122.66	127.31
18	A	815	CLA	CMB-C2B-C3B	3.26	130.77	124.68
21	a	619	BCR	C15-C14-C13	-3.25	122.67	127.31
18	1	602	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
18	1	601	CLA	CMB-C2B-C3B	3.25	130.77	124.68
18	F	304	CLA	CMB-C2B-C3B	3.25	130.76	124.68
18	A	824	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
18	A	815	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
21	L	305	BCR	C21-C20-C19	-3.25	113.09	123.22
21	B	845	BCR	C11-C10-C9	-3.24	122.69	127.31
18	B	812	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
18	8	611	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
18	A	811	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
21	B	843	BCR	C29-C30-C25	3.23	115.45	110.48
18	4	604	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
18	K	201	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
18	1	607	CLA	CAA-C2A-C3A	-3.22	108.58	116.10
18	B	833	CLA	CMB-C2B-C3B	3.22	130.70	124.68
27	3	619	XAT	C31-C30-C29	-3.22	122.72	127.31
23	A	857	LMU	C5'-C4'-C3'	3.22	114.21	109.40
18	B	835	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
18	6	601	CLA	CHB-C4A-NA	3.21	128.96	124.51
18	a	606	CLA	CMB-C2B-C3B	3.21	130.69	124.68
21	3	620	BCR	C15-C14-C13	-3.21	122.73	127.31
18	6	617	CLA	CMB-C2B-C3B	3.21	130.68	124.68
18	B	808	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
18	B	817	CLA	CHB-C4A-NA	3.21	128.95	124.51
21	4	621	BCR	C7-C8-C9	-3.21	121.39	126.23
18	A	840	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
18	3	609	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
18	3	613	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
27	a	618	XAT	C35-C34-C33	-3.20	122.74	127.31
18	A	817	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
18	B	814	CLA	CHB-C4A-NA	3.20	128.94	124.51
18	B	806	CLA	CMB-C2B-C3B	3.20	130.66	124.68
18	1	603	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
18	J	101	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
26	1	617	LUT	C10-C11-C12	-3.20	113.24	123.22
21	4	621	BCR	C33-C5-C4	3.19	119.75	113.62
18	a	614	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
28	5	624	NEX	C27-C28-C29	-3.19	120.58	125.53
18	a	603	CLA	CMB-C2B-C1B	-3.19	123.56	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	834	CLA	CMB-C2B-C3B	3.19	130.65	124.68
18	A	813	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
18	B	803	CLA	CBC-CAC-C3C	3.19	121.22	112.43
18	4	607	CLA	CMB-C2B-C3B	3.19	130.64	124.68
21	3	621	BCR	C19-C18-C17	3.19	123.83	118.94
18	K	203	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
21	B	844	BCR	C34-C9-C10	-3.19	118.46	122.92
18	B	809	CLA	CMB-C2B-C3B	3.18	130.63	124.68
18	B	825	CLA	CMB-C2B-C3B	3.18	130.63	124.68
18	4	611	CLA	CMB-C2B-C3B	3.18	130.62	124.68
18	A	808	CLA	CMB-C2B-C3B	3.18	130.62	124.68
18	B	838	CLA	CMB-C2B-C3B	3.17	130.62	124.68
18	3	612	CLA	CMB-C2B-C3B	3.17	130.62	124.68
18	a	602	CLA	CMB-C2B-C3B	3.17	130.61	124.68
21	6	622	BCR	C21-C20-C19	-3.17	113.32	123.22
21	F	305	BCR	C3-C4-C5	-3.17	108.42	114.08
21	L	301	BCR	C38-C26-C25	-3.17	120.97	124.53
18	A	835	CLA	CMB-C2B-C3B	3.17	130.60	124.68
18	6	603	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
18	8	614	CLA	CMB-C2B-C3B	3.17	130.60	124.68
18	A	810	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
18	B	805	CLA	CHB-C4A-NA	3.16	128.89	124.51
18	A	803	CLA	C1B-CHB-C4A	-3.16	123.85	130.12
21	K	202	BCR	C38-C26-C27	3.16	119.69	113.62
18	7	609	CLA	CHB-C4A-NA	3.16	128.88	124.51
18	1	606	CLA	CMB-C2B-C3B	3.16	130.59	124.68
18	B	841	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
21	K	202	BCR	C27-C26-C25	-3.16	118.15	122.73
18	6	617	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
18	A	828	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
26	7	619	LUT	C35-C15-C14	-3.15	117.02	123.47
18	B	803	CLA	CHB-C4A-NA	3.15	128.87	124.51
21	6	622	BCR	C11-C10-C9	-3.15	122.81	127.31
18	B	829	CLA	C1B-CHB-C4A	-3.15	123.88	130.12
27	a	618	XAT	C31-C30-C29	-3.15	122.82	127.31
18	B	808	CLA	CMB-C2B-C3B	3.15	130.57	124.68
18	A	811	CLA	CMB-C2B-C3B	3.14	130.56	124.68
18	6	620	CLA	CMB-C2B-C3B	3.14	130.56	124.68
18	A	854	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
18	B	818	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
21	3	622	BCR	C33-C5-C6	-3.14	121.00	124.53
18	7	603	CLA	CMB-C2B-C1B	-3.14	123.64	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	6	624	NEX	C35-C34-C33	-3.13	122.84	127.31
18	3	608	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
26	7	619	LUT	C30-C31-C32	-3.13	113.45	123.22
25	B	850	DGD	O5D-C6D-C5D	-3.13	103.26	109.05
18	5	607	CLA	C1B-CHB-C4A	-3.13	123.93	130.12
18	A	804	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
18	K	201	CLA	CHB-C4A-NA	3.12	128.83	124.51
18	B	816	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
21	B	845	BCR	C20-C21-C22	-3.12	122.85	127.31
28	5	624	NEX	C24-C23-C22	-3.12	104.75	110.77
21	B	848	BCR	C10-C11-C12	-3.12	113.48	123.22
21	1	619	BCR	C16-C15-C14	-3.12	117.09	123.47
26	4	619	LUT	C30-C31-C32	-3.11	113.50	123.22
18	A	813	CLA	CHB-C4A-NA	3.11	128.82	124.51
18	A	825	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
21	K	207	BCR	C33-C5-C6	-3.11	121.03	124.53
18	B	835	CLA	CHB-C4A-NA	3.11	128.81	124.51
27	4	620	XAT	C24-C23-C22	-3.11	104.77	110.77
18	1	610	CLA	CBD-CHA-C1A	3.11	132.16	128.50
18	A	821	CLA	CHB-C4A-NA	3.11	128.81	124.51
18	6	604	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
18	8	609	CLA	CMB-C2B-C3B	3.11	130.49	124.68
18	1	611	CLA	CMB-C2B-C3B	3.11	130.49	124.68
18	8	603	CLA	CAB-C3B-C2B	3.10	130.77	124.69
21	A	848	BCR	C33-C5-C6	-3.10	121.04	124.53
18	A	804	CLA	CHB-C4A-NA	3.10	128.80	124.51
18	A	836	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
25	B	850	DGD	O6D-C1D-O3G	-3.10	102.63	109.97
18	5	611	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
21	5	622	BCR	C4-C5-C6	-3.10	118.23	122.73
18	6	603	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
18	6	607	CLA	CAB-C3B-C2B	3.10	130.75	124.69
18	3	606	CLA	CMB-C2B-C3B	3.09	130.47	124.68
18	J	101	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
18	A	824	CLA	CAA-C2A-C3A	-3.09	108.89	116.10
18	1	608	CLA	CMB-C2B-C3B	3.09	130.46	124.68
18	A	805	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
18	J	101	CLA	CHB-C4A-NA	3.09	128.78	124.51
18	8	601	CLA	CMB-C2B-C3B	3.09	130.45	124.68
21	8	621	BCR	C4-C5-C6	-3.08	118.25	122.73
27	6	621	XAT	C35-C34-C33	-3.08	122.91	127.31
18	a	611	CLA	O2D-CGD-O1D	-3.08	117.09	124.09

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	8	616	CLA	C2A-C1A-CHA	3.08	129.25	123.86
18	1	602	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
18	B	826	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
27	6	621	XAT	C24-C23-C22	-3.08	104.82	110.77
27	1	618	XAT	C10-C11-C12	-3.08	113.61	123.22
18	B	830	CLA	CMC-C2C-C1C	-3.08	120.35	125.04
18	B	830	CLA	C2D-C1D-ND	-3.08	107.84	110.10
18	A	807	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
26	8	619	LUT	C15-C14-C13	-3.07	122.93	127.31
18	B	823	CLA	CMB-C2B-C3B	3.07	130.42	124.68
18	4	613	CLA	CMB-C2B-C3B	3.06	130.41	124.68
18	5	608	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
18	5	613	CLA	CHB-C4A-NA	3.06	128.75	124.51
18	4	604	CLA	CAB-C3B-C4B	-3.06	123.76	128.46
21	4	621	BCR	C21-C20-C19	-3.06	113.66	123.22
18	4	609	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
18	7	616	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
18	B	803	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
18	6	620	CLA	CHB-C4A-NA	3.06	128.74	124.51
18	3	612	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
18	B	832	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
27	4	620	XAT	C10-C11-C12	-3.05	113.68	123.22
18	A	823	CLA	CMB-C2B-C3B	3.05	130.39	124.68
18	3	607	CLA	CMB-C2B-C3B	3.05	130.66	124.69
18	4	604	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
18	3	617	CLA	CAA-C2A-C3A	-3.05	108.98	116.10
18	F	304	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
18	B	820	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
26	3	618	LUT	C10-C11-C12	-3.05	113.71	123.22
18	B	822	CLA	CMB-C2B-C3B	3.04	130.37	124.68
21	5	622	BCR	C8-C7-C6	-3.04	118.66	127.20
18	a	613	CLA	CHB-C4A-NA	3.04	128.72	124.51
18	B	808	CLA	O2A-CGA-O1A	-3.04	115.92	123.59
18	A	808	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
21	A	856	BCR	C10-C11-C12	-3.04	113.73	123.22
18	5	604	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
27	a	618	XAT	C15-C14-C13	-3.04	122.98	127.31
27	7	620	XAT	C4-C3-C2	-3.03	104.91	110.77
18	1	603	CLA	CHB-C4A-NA	3.03	128.71	124.51
18	4	602	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
21	B	846	BCR	C16-C17-C18	-3.03	122.98	127.31
21	B	846	BCR	C33-C5-C6	-3.03	121.12	124.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	807	CLA	CMB-C2B-C3B	3.03	130.34	124.68
18	3	610	CLA	CHB-C4A-NA	3.03	128.70	124.51
18	A	829	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
18	B	820	CLA	CMB-C2B-C3B	3.02	130.34	124.68
21	A	850	BCR	C1-C6-C5	-3.02	118.36	122.61
23	A	857	LMU	C2'-C3'-C4'	3.02	115.63	110.24
21	a	619	BCR	C7-C8-C9	-3.02	121.68	126.23
18	3	607	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	4	618	CLA	CAB-C3B-C2B	3.01	130.59	124.69
18	5	616	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
18	8	602	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	6	602	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	A	825	CLA	CHB-C4A-NA	3.01	128.67	124.51
18	8	611	CLA	CMB-C2B-C3B	3.01	130.31	124.68
18	7	607	CLA	CAA-C2A-C3A	-3.01	106.74	114.26
18	A	838	CLA	CHB-C4A-NA	3.01	128.67	124.51
18	5	613	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
18	B	829	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
18	A	804	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
18	K	206	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
18	8	609	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
18	B	808	CLA	CBA-CAA-C2A	3.00	122.73	113.86
18	B	808	CLA	CHB-C4A-NA	3.00	128.66	124.51
18	1	614	CLA	CMB-C2B-C3B	3.00	130.56	124.69
21	A	848	BCR	C15-C14-C13	-3.00	123.03	127.31
18	L	304	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
18	5	614	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
18	4	603	CLA	CHB-C4A-NA	3.00	128.66	124.51
18	8	603	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
18	8	613	CLA	CHB-C4A-NA	2.99	128.65	124.51
18	6	608	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
18	B	833	CLA	CAA-C2A-C3A	-2.99	104.58	112.78
21	5	622	BCR	C33-C5-C4	2.99	119.36	113.62
18	4	603	CLA	CAB-C3B-C2B	2.99	130.54	124.69
18	a	614	CLA	CMB-C2B-C3B	2.99	130.27	124.68
18	4	603	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
18	B	836	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
18	A	843	CLA	CMB-C2B-C3B	2.99	130.26	124.68
21	5	622	BCR	C20-C21-C22	-2.98	123.05	127.31
21	a	619	BCR	C24-C23-C22	-2.98	121.73	126.23
27	5	621	XAT	C24-C23-C22	-2.98	105.01	110.77
18	B	803	CLA	O2D-CGD-O1D	-2.98	118.01	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	619	LUT	C20-C13-C12	2.98	122.78	118.08
21	B	843	BCR	C7-C8-C9	-2.98	121.73	126.23
18	6	611	CLA	CMB-C2B-C3B	2.98	130.25	124.68
18	K	204	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
18	3	609	CLA	CHB-C4A-NA	2.98	128.63	124.51
18	1	613	CLA	CMB-C2B-C3B	2.98	130.25	124.68
18	A	806	CLA	CHB-C4A-NA	2.98	128.63	124.51
18	8	608	CLA	CHB-C4A-NA	2.98	128.63	124.51
18	6	613	CLA	CMB-C2B-C3B	2.97	130.24	124.68
27	8	620	XAT	C4-C3-C2	-2.97	105.03	110.77
18	A	814	CLA	CHB-C4A-NA	2.97	128.62	124.51
18	7	614	CLA	CMB-C2B-C3B	2.97	130.24	124.68
23	8	625	LMU	C3B-C4B-C5B	2.97	115.54	110.24
21	L	305	BCR	C16-C15-C14	-2.97	117.39	123.47
18	a	603	CLA	CHB-C4A-NA	2.97	128.62	124.51
18	4	608	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
18	L	304	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
18	A	825	CLA	CMB-C2B-C3B	2.97	130.23	124.68
18	K	204	CLA	CMB-C2B-C3B	2.97	130.23	124.68
18	7	609	CLA	O2D-CGD-CBD	2.96	116.54	111.27
18	8	607	CLA	CHB-C4A-NA	2.96	128.61	124.51
18	A	806	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
18	6	618	CLA	CAB-C3B-C2B	2.96	130.49	124.69
18	7	610	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
18	B	816	CLA	CHB-C4A-NA	2.96	128.61	124.51
18	5	603	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
18	A	840	CLA	CHB-C4A-NA	2.96	128.60	124.51
18	8	609	CLA	CHB-C4A-NA	2.96	128.60	124.51
21	L	301	BCR	C33-C5-C6	-2.96	121.21	124.53
21	B	843	BCR	C27-C26-C25	-2.96	118.44	122.73
23	K	208	LMU	C2'-C3'-C4'	2.95	116.42	109.68
18	A	839	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
18	B	806	CLA	CHB-C4A-NA	2.95	128.59	124.51
21	B	845	BCR	C33-C5-C4	2.95	119.29	113.62
18	7	601	CLA	CMB-C2B-C3B	2.95	130.20	124.68
21	A	856	BCR	C15-C14-C13	-2.95	123.10	127.31
18	4	607	CLA	CHB-C4A-NA	2.95	128.59	124.51
21	B	846	BCR	C24-C23-C22	-2.95	121.78	126.23
18	5	603	CLA	CAB-C3B-C4B	-2.95	123.93	128.46
18	B	815	CLA	CHB-C4A-NA	2.95	128.59	124.51
21	6	622	BCR	C7-C8-C9	-2.95	121.78	126.23
18	4	603	CLA	O2D-CGD-O1D	-2.95	118.07	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	816	CLA	CHB-C4A-NA	2.95	128.59	124.51
18	A	835	CLA	CHB-C4A-NA	2.95	128.59	124.51
21	3	622	BCR	C16-C15-C14	-2.95	117.44	123.47
18	5	618	CLA	CAB-C3B-C2B	2.95	130.46	124.69
18	B	834	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
18	A	828	CLA	CHB-C4A-NA	2.94	128.58	124.51
18	7	607	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
23	8	625	LMU	O5'-C1'-C2'	2.94	116.58	110.35
18	A	822	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
18	B	825	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
27	4	620	XAT	C19-C9-C8	2.94	122.71	118.08
18	7	615	CLA	CAB-C3B-C2B	2.94	130.44	124.69
18	8	602	CLA	CMB-C2B-C3B	2.94	130.18	124.68
18	K	203	CLA	CMB-C2B-C3B	2.94	130.17	124.68
18	8	604	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
21	L	305	BCR	C29-C30-C25	2.94	115.00	110.48
18	3	615	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
21	A	849	BCR	C38-C26-C27	2.93	119.25	113.62
18	A	818	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
18	6	609	CLA	CMB-C2B-C3B	2.93	130.16	124.68
21	A	851	BCR	C10-C11-C12	-2.93	114.06	123.22
18	K	204	CLA	CHB-C4A-NA	2.93	128.57	124.51
18	8	603	CLA	CHB-C4A-NA	2.93	128.57	124.51
23	A	858	LMU	C6B-C5B-C4B	-2.93	109.45	113.54
18	5	614	CLA	CMB-C2B-C3B	2.93	130.16	124.68
18	B	832	CLA	CHB-C4A-NA	2.93	128.56	124.51
23	8	625	LMU	C1'-C2'-C3'	2.93	116.10	110.00
18	B	824	CLA	O2D-CGD-CBD	2.93	116.47	111.27
18	6	614	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
18	B	840	CLA	CHB-C4A-NA	2.93	128.56	124.51
21	A	850	BCR	C33-C5-C4	2.93	119.24	113.62
18	6	604	CLA	CMB-C2B-C3B	2.93	130.16	124.68
18	A	809	CLA	CHB-C4A-NA	2.93	128.56	124.51
18	4	616	CLA	CAB-C3B-C2B	2.92	130.41	124.69
27	1	618	XAT	C24-C23-C22	-2.92	105.13	110.77
18	B	830	CLA	CHB-C4A-NA	2.92	128.55	124.51
21	B	801	BCR	C3-C4-C5	-2.92	108.87	114.08
18	a	609	CLA	CHB-C4A-NA	2.92	128.55	124.51
21	L	301	BCR	C28-C27-C26	-2.92	108.87	114.08
18	a	601	CLA	CMB-C2B-C3B	2.92	130.14	124.68
21	a	619	BCR	C33-C5-C4	2.92	119.22	113.62
18	6	607	CLA	CHB-C4A-NA	2.92	128.54	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	824	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
18	B	819	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
18	3	604	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
18	K	206	CLA	CMB-C2B-C3B	2.91	130.13	124.68
18	A	838	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
18	B	839	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
18	A	808	CLA	CHB-C4A-NA	2.91	128.54	124.51
18	a	610	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
24	A	860	LMG	O1-C7-C8	-2.91	103.88	110.90
18	A	836	CLA	CHB-C4A-NA	2.91	128.53	124.51
18	3	604	CLA	CHB-C4A-NA	2.91	128.53	124.51
18	4	610	CLA	CHB-C4A-NA	2.91	128.53	124.51
18	a	613	CLA	CMB-C2B-C3B	2.90	130.11	124.68
18	3	607	CLA	CAB-C3B-C2B	2.90	130.38	124.69
18	A	845	CLA	CMB-C2B-C3B	2.90	130.11	124.68
21	3	620	BCR	C33-C5-C4	2.90	119.19	113.62
21	B	844	BCR	C3-C4-C5	-2.90	108.90	114.08
21	A	850	BCR	C20-C21-C22	-2.90	123.17	127.31
18	8	606	CLA	CMB-C2B-C3B	2.90	130.10	124.68
28	5	624	NEX	C15-C35-C34	-2.90	117.54	123.47
21	5	622	BCR	C16-C15-C14	-2.90	117.54	123.47
18	B	832	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
18	A	822	CLA	CHB-C4A-NA	2.89	128.51	124.51
18	B	808	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
18	A	807	CLA	CHB-C4A-NA	2.89	128.51	124.51
18	a	616	CLA	CMB-C2B-C3B	2.89	130.09	124.68
18	7	608	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
18	A	805	CLA	CHB-C4A-NA	2.89	128.51	124.51
18	B	838	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
18	7	602	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
18	3	615	CLA	CHB-C4A-NA	2.89	128.51	124.51
18	B	839	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
18	5	603	CLA	CMB-C2B-C1B	-2.89	124.03	128.46
18	A	837	CLA	CHB-C4A-NA	2.89	128.50	124.51
18	L	304	CLA	CHB-C4A-NA	2.89	128.50	124.51
18	B	812	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
18	L	302	CLA	CMB-C2B-C3B	2.88	130.07	124.68
18	A	805	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
21	K	202	BCR	C20-C21-C22	-2.88	123.20	127.31
21	B	846	BCR	C21-C20-C19	-2.88	114.24	123.22
18	8	601	CLA	CHB-C4A-NA	2.88	128.49	124.51
18	6	618	CLA	CHB-C4A-NA	2.88	128.49	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	847	LHG	O8-C23-C24	2.88	120.93	111.91
18	3	608	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
18	5	601	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
21	A	849	BCR	C15-C16-C17	-2.87	117.59	123.47
18	B	805	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
18	F	303	CLA	CAA-C2A-C3A	-2.87	107.09	114.26
21	B	845	BCR	C34-C9-C10	-2.87	118.90	122.92
21	K	202	BCR	C30-C25-C26	-2.87	118.57	122.61
21	A	851	BCR	C33-C5-C6	-2.87	121.31	124.53
27	4	620	XAT	C35-C15-C14	-2.87	117.60	123.47
18	A	820	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
21	L	305	BCR	C15-C14-C13	-2.87	123.22	127.31
18	4	610	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
18	B	826	CLA	CHB-C4A-NA	2.87	128.47	124.51
18	7	615	CLA	CMB-C2B-C3B	2.87	130.30	124.69
18	A	821	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	B	834	CLA	CMB-C2B-C3B	2.86	130.04	124.68
18	B	809	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
18	5	602	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
26	7	619	LUT	C10-C11-C12	-2.86	114.28	123.22
18	A	819	CLA	CHB-C4A-NA	2.86	128.47	124.51
27	8	620	XAT	C19-C9-C8	2.86	122.58	118.08
18	4	614	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
18	A	823	CLA	CAA-C2A-C3A	-2.86	107.11	114.26
18	B	837	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
18	5	610	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
18	7	611	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
18	B	834	CLA	CHB-C4A-NA	2.86	128.46	124.51
18	8	601	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	J	103	DGD	O6E-C5E-C4E	2.85	114.88	109.69
18	4	616	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
18	A	839	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
18	B	810	CLA	CMB-C2B-C3B	2.85	130.01	124.68
20	A	846	LHG	O8-C23-C24	2.85	120.86	111.91
18	A	826	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
18	a	604	CLA	CHB-C4A-NA	2.85	128.45	124.51
27	8	620	XAT	C35-C34-C33	-2.85	123.24	127.31
21	7	621	BCR	C24-C23-C22	-2.85	121.93	126.23
18	5	618	CLA	CMB-C2B-C3B	2.85	130.27	124.69
27	1	618	XAT	C35-C15-C14	-2.85	117.64	123.47
21	B	847	BCR	C33-C5-C4	2.85	119.09	113.62
18	6	620	CLA	CAA-CBA-CGA	-2.85	104.95	112.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	609	CLA	CAB-C3B-C2B	2.85	130.26	124.69
18	7	612	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	3	610	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
18	1	611	CLA	CHB-C4A-NA	2.85	128.45	124.51
18	7	613	CLA	CHB-C4A-NA	2.85	128.45	124.51
18	8	613	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
18	1	604	CLA	O2D-CGD-CBD	2.85	116.33	111.27
18	6	609	CLA	CHB-C4A-NA	2.85	128.45	124.51
18	a	613	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
18	6	611	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
27	7	620	XAT	C31-C30-C29	-2.84	123.25	127.31
27	4	620	XAT	C8-C9-C10	-2.84	114.58	118.94
18	6	614	CLA	CHB-C4A-NA	2.84	128.44	124.51
18	B	813	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
18	B	827	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
21	A	856	BCR	C11-C10-C9	-2.84	123.26	127.31
18	8	602	CLA	CHB-C4A-NA	2.84	128.44	124.51
26	5	620	LUT	C30-C31-C32	-2.84	114.36	123.22
18	6	610	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
18	1	607	CLA	CMB-C2B-C3B	2.84	129.99	124.68
18	6	612	CLA	CHB-C4A-NA	2.84	128.43	124.51
18	A	801	CLA	C1D-ND-C4D	-2.84	104.32	106.33
18	7	602	CLA	CHB-C4A-NA	2.83	128.43	124.51
21	L	301	BCR	C15-C16-C17	-2.83	117.67	123.47
21	8	621	BCR	C29-C30-C25	2.83	114.84	110.48
18	A	821	CLA	CMB-C2B-C3B	2.83	129.98	124.68
21	1	619	BCR	C15-C14-C13	-2.83	123.27	127.31
18	6	616	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
21	3	622	BCR	C30-C25-C26	-2.83	118.63	122.61
18	B	807	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
18	5	617	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
26	8	619	LUT	C10-C11-C12	-2.83	114.39	123.22
26	3	618	LUT	C35-C34-C33	-2.83	123.28	127.31
18	8	616	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
18	K	206	CLA	CHB-C4A-NA	2.83	128.42	124.51
18	8	603	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
18	A	819	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	A	802	CLA	C1B-CHB-C4A	-2.82	124.52	130.12
18	L	302	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	3	607	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
18	A	833	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	6	610	CLA	CHB-C4A-NA	2.82	128.41	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	7	613	CLA	CMB-C2B-C3B	2.82	129.96	124.68
18	F	303	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
18	1	604	CLA	CHB-C4A-NA	2.82	128.41	124.51
18	3	606	CLA	CHB-C4A-NA	2.82	128.41	124.51
18	A	834	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
21	F	305	BCR	C36-C18-C17	-2.82	118.97	122.92
26	6	619	LUT	C10-C11-C12	-2.82	114.42	123.22
18	6	613	CLA	CHB-C4A-NA	2.82	128.41	124.51
18	3	603	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
18	4	618	CLA	CAA-C2A-C3A	-2.81	107.23	114.26
18	3	613	CLA	CHB-C4A-NA	2.81	128.40	124.51
18	5	618	CLA	CHB-C4A-NA	2.81	128.40	124.51
18	7	603	CLA	O2D-CGD-O1D	-2.81	117.70	124.09
18	4	614	CLA	CMB-C2B-C3B	2.81	129.94	124.68
18	A	809	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
18	L	303	CLA	CMB-C2B-C3B	2.81	129.94	124.68
18	4	610	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
18	7	612	CLA	CMB-C2B-C3B	2.81	129.93	124.68
18	4	602	CLA	CHB-C4A-NA	2.81	128.40	124.51
21	K	202	BCR	C2-C1-C6	2.81	114.80	110.48
18	8	608	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
21	L	305	BCR	C3-C4-C5	-2.81	109.06	114.08
18	A	841	CLA	CHB-C4A-NA	2.81	128.39	124.51
18	A	837	CLA	O2D-CGD-CBD	2.80	116.25	111.27
18	8	607	CLA	CMB-C2B-C1B	-2.80	124.15	128.46
20	3	623	LHG	O8-C23-C24	2.80	120.71	111.91
18	6	620	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
18	A	842	CLA	CHB-C4A-NA	2.80	128.39	124.51
27	4	620	XAT	C4-C3-C2	-2.80	105.36	110.77
18	5	601	CLA	CMB-C2B-C3B	2.80	129.92	124.68
18	4	607	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
18	7	616	CLA	CAB-C3B-C2B	2.80	130.17	124.69
21	F	305	BCR	C38-C26-C27	2.80	118.99	113.62
18	A	803	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
18	6	602	CLA	CHB-C4A-NA	2.79	128.38	124.51
21	3	620	BCR	C7-C8-C9	-2.79	122.02	126.23
18	B	806	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	A	811	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
18	1	616	CLA	CMB-C2B-C3B	2.79	130.15	124.69
18	B	807	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	8	613	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
18	6	607	CLA	CMB-C2B-C3B	2.79	130.15	124.69

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	824	CLA	CHB-C4A-NA	2.79	128.37	124.51
18	3	617	CLA	CMA-C3A-C2A	-2.79	109.60	116.10
18	3	602	CLA	CHB-C4A-NA	2.78	128.36	124.51
21	K	207	BCR	C38-C26-C25	-2.78	121.40	124.53
18	3	617	CLA	CMB-C2B-C3B	2.78	129.89	124.68
21	J	102	BCR	C20-C21-C22	-2.78	123.34	127.31
18	7	611	CLA	CHB-C4A-NA	2.78	128.36	124.51
18	B	818	CLA	C4-C3-C5	2.78	119.95	115.27
18	3	614	CLA	CMB-C2B-C3B	2.78	129.88	124.68
21	6	622	BCR	C20-C21-C22	-2.78	123.34	127.31
18	A	836	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
18	A	842	CLA	CMB-C2B-C3B	2.78	129.88	124.68
18	1	609	CLA	CMB-C2B-C3B	2.78	130.13	124.69
18	B	827	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
18	1	613	CLA	CHB-C4A-NA	2.78	128.36	124.51
18	5	611	CLA	CMB-C2B-C3B	2.78	129.88	124.68
25	B	850	DGD	CDB-CCB-CBB	-2.78	100.32	114.42
18	B	811	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
18	A	841	CLA	CMB-C2B-C3B	2.78	129.88	124.68
18	B	812	CLA	CHB-C4A-NA	2.78	128.35	124.51
18	B	825	CLA	CAA-C2A-C1A	-2.78	102.88	111.97
18	4	611	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
26	7	619	LUT	C22-C23-C24	-2.77	108.58	111.74
27	7	620	XAT	C10-C11-C12	-2.77	114.56	123.22
18	6	604	CLA	CHB-C4A-NA	2.77	128.35	124.51
18	8	610	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
18	4	609	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
21	3	621	BCR	C29-C30-C25	2.77	114.75	110.48
18	1	616	CLA	CAB-C3B-C2B	2.77	130.11	124.69
18	B	818	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
18	A	845	CLA	CHB-C4A-NA	2.77	128.34	124.51
18	8	612	CLA	CHB-C4A-NA	2.77	128.34	124.51
27	a	618	XAT	C4-C3-C2	-2.77	105.43	110.77
18	5	610	CLA	CHB-C4A-NA	2.77	128.34	124.51
21	3	620	BCR	C4-C5-C6	-2.77	118.71	122.73
28	5	624	NEX	C11-C10-C9	-2.77	123.36	127.31
18	B	830	CLA	CMC-C2C-C3C	2.76	133.62	126.12
18	7	610	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
18	3	611	CLA	O2D-CGD-O1D	-2.76	117.82	124.09
18	3	602	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
18	1	609	CLA	CHB-C4A-NA	2.76	128.33	124.51
18	B	812	CLA	CMB-C2B-C3B	2.76	129.84	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	814	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
18	6	601	CLA	O2D-CGD-CBD	2.76	116.17	111.27
18	a	606	CLA	CHB-C4A-NA	2.76	128.33	124.51
18	5	617	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	A	858	LMU	O5B-C1B-C2B	2.76	116.24	111.31
18	A	802	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
28	6	624	NEX	C27-C28-C29	-2.75	121.26	125.53
18	A	834	CLA	CHB-C4A-NA	2.75	128.32	124.51
21	J	102	BCR	C20-C19-C18	-2.75	118.68	126.42
18	B	839	CLA	CHB-C4A-NA	2.75	128.32	124.51
18	7	616	CLA	CMB-C2B-C3B	2.75	130.08	124.69
18	B	823	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
18	K	203	CLA	CHB-C4A-NA	2.75	128.32	124.51
27	5	621	XAT	C35-C34-C33	-2.75	123.38	127.31
18	8	607	CLA	CAB-C3B-C2B	2.75	130.07	124.69
18	7	612	CLA	CHB-C4A-NA	2.75	128.31	124.51
27	8	620	XAT	C31-C30-C29	-2.75	123.39	127.31
27	3	619	XAT	C10-C11-C12	-2.75	114.64	123.22
18	B	820	CLA	CHB-C4A-NA	2.75	128.31	124.51
18	K	201	CLA	C2A-C1A-CHA	2.75	128.66	123.86
27	8	620	XAT	C24-C23-C22	-2.75	105.47	110.77
24	5	627	LMG	O6-C1-O1	-2.74	103.47	109.97
18	5	609	CLA	CHB-C4A-NA	2.74	128.31	124.51
18	3	609	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
21	J	102	BCR	C27-C26-C25	-2.74	118.75	122.73
18	6	618	CLA	O2D-CGD-O1D	-2.74	117.86	124.09
18	B	830	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
18	a	603	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
18	1	610	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
18	5	610	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
21	A	852	BCR	C8-C9-C10	2.74	123.15	118.94
21	B	844	BCR	C28-C27-C26	-2.74	109.18	114.08
18	4	612	CLA	CHB-C4A-NA	2.74	128.30	124.51
18	3	611	CLA	CAB-C3B-C2B	2.74	130.05	124.69
26	7	619	LUT	C38-C25-C24	-2.74	117.70	123.56
18	B	817	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
21	B	847	BCR	C33-C5-C6	-2.74	121.45	124.53
21	A	852	BCR	C27-C26-C25	-2.74	118.76	122.73
18	A	832	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
18	1	614	CLA	CAB-C3B-C2B	2.74	130.05	124.69
21	6	622	BCR	C33-C5-C4	2.74	118.87	113.62
26	1	617	LUT	C30-C31-C32	-2.73	114.68	123.22

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	621	BCR	C11-C10-C9	-2.73	123.41	127.31
21	L	301	BCR	C16-C17-C18	-2.73	123.41	127.31
18	a	601	CLA	CHB-C4A-NA	2.73	128.29	124.51
18	A	824	CLA	CMB-C2B-C3B	2.73	129.79	124.68
21	B	846	BCR	C28-C27-C26	-2.73	109.20	114.08
18	8	612	CLA	O2D-CGD-O1D	-2.73	117.89	124.09
18	B	802	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
27	a	618	XAT	C24-C23-C22	-2.73	105.50	110.77
18	B	803	CLA	CAC-C3C-C2C	-2.73	122.86	127.53
18	6	609	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
18	7	607	CLA	CMB-C2B-C3B	2.73	129.78	124.68
18	8	616	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
18	A	801	CLA	CMB-C2B-C1B	-2.73	124.28	128.46
18	1	609	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
18	4	608	CLA	CHB-C4A-NA	2.72	128.28	124.51
18	A	843	CLA	CHB-C4A-NA	2.72	128.28	124.51
18	B	840	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
18	a	610	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
21	B	844	BCR	C8-C9-C10	2.72	123.11	118.94
21	a	619	BCR	C16-C15-C14	-2.72	117.91	123.47
18	B	828	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
18	A	837	CLA	CMB-C2B-C3B	2.72	129.76	124.68
18	A	830	CLA	CHB-C4A-NA	2.72	128.27	124.51
18	4	613	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
18	6	618	CLA	CMB-C2B-C3B	2.72	130.01	124.69
18	a	601	CLA	O2D-CGD-O1D	-2.72	117.92	124.09
18	A	820	CLA	CHB-C4A-NA	2.72	128.27	124.51
18	8	612	CLA	CAA-C2A-C3A	-2.72	107.47	114.26
26	3	618	LUT	C38-C25-C24	-2.71	117.75	123.56
18	5	604	CLA	CAB-C3B-C2B	2.71	130.00	124.69
18	B	818	CLA	CHB-C4A-NA	2.71	128.27	124.51
18	A	810	CLA	CMB-C2B-C3B	2.71	129.76	124.68
18	7	609	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
21	J	102	BCR	C24-C23-C22	-2.71	122.14	126.23
27	7	620	XAT	C35-C15-C14	-2.71	117.92	123.47
18	5	612	CLA	CHB-C4A-NA	2.71	128.26	124.51
18	5	606	CLA	O2D-CGD-O1D	-2.71	117.93	124.09
21	F	305	BCR	C20-C19-C18	-2.71	118.80	126.42
18	1	612	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
18	B	811	CLA	CHB-C4A-NA	2.71	128.26	124.51
21	L	301	BCR	C39-C30-C25	-2.71	105.90	110.30
18	B	822	CLA	O2D-CGD-O1D	-2.71	118.54	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	621	BCR	C15-C16-C17	-2.71	117.92	123.47
18	8	604	CLA	CHB-C4A-NA	2.71	128.26	124.51
18	B	821	CLA	CMB-C2B-C3B	2.71	129.74	124.68
18	1	602	CLA	CMB-C2B-C3B	2.71	129.74	124.68
21	B	845	BCR	C37-C22-C21	-2.70	119.13	122.92
18	B	838	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
18	A	845	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
20	a	620	LHG	O8-C23-C24	2.70	120.39	111.91
18	6	611	CLA	CAA-C2A-C3A	-2.70	107.51	114.26
21	A	848	BCR	C16-C15-C14	-2.70	117.94	123.47
18	F	304	CLA	CAA-C2A-C3A	-2.70	109.80	116.10
21	L	301	BCR	C20-C21-C22	-2.70	123.46	127.31
18	5	601	CLA	CHB-C4A-NA	2.70	128.24	124.51
18	4	616	CLA	CHB-C4A-NA	2.70	128.24	124.51
18	B	811	CLA	CAB-C3B-C2B	2.70	129.97	124.69
18	A	807	CLA	CMB-C2B-C3B	2.70	129.72	124.68
18	A	822	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
18	B	830	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
18	A	823	CLA	CHB-C4A-NA	2.69	128.23	124.51
18	B	837	CLA	CHB-C4A-NA	2.69	128.23	124.51
18	4	613	CLA	CHB-C4A-NA	2.69	128.23	124.51
26	5	620	LUT	C10-C11-C12	-2.69	114.83	123.22
26	4	619	LUT	C15-C14-C13	-2.69	123.47	127.31
18	6	606	CLA	CAA-C2A-C3A	-2.69	107.54	114.26
18	4	601	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
18	a	610	CLA	CHB-C4A-NA	2.69	128.23	124.51
18	7	604	CLA	CHB-C4A-NA	2.69	128.23	124.51
18	8	616	CLA	CAB-C3B-C2B	2.69	129.95	124.69
18	8	609	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
18	K	201	CLA	CMB-C2B-C3B	2.69	129.71	124.68
21	A	848	BCR	C38-C26-C27	2.69	118.78	113.62
21	7	623	BCR	C28-C27-C26	-2.69	109.28	114.08
18	5	616	CLA	CAB-C3B-C2B	2.69	129.95	124.69
18	7	601	CLA	CHD-C1D-ND	-2.69	121.99	124.45
18	8	613	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
18	8	616	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
18	6	603	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	B	805	CLA	O2A-CGA-O1A	-2.68	116.83	123.59
21	B	847	BCR	C21-C20-C19	-2.68	114.85	123.22
18	5	613	CLA	CMB-C2B-C3B	2.68	129.69	124.68
18	7	615	CLA	CHB-C4A-NA	2.68	128.22	124.51
18	8	610	CLA	CHB-C4A-NA	2.68	128.22	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	620	CLA	O2D-CGD-CBD	2.68	116.03	111.27
18	A	812	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
20	8	623	LHG	O8-C23-C24	2.68	120.31	111.91
18	a	611	CLA	CMB-C2B-C3B	2.68	129.93	124.69
18	a	614	CLA	C1B-CHB-C4A	-2.68	124.82	130.12
18	1	612	CLA	CHB-C4A-NA	2.67	128.21	124.51
18	8	611	CLA	O2D-CGD-CBD	2.67	116.02	111.27
18	B	804	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
21	A	849	BCR	C10-C11-C12	-2.67	114.88	123.22
18	A	843	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	A	860	LMG	O6-C1-O1	-2.67	103.65	109.97
18	B	817	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
27	6	621	XAT	C19-C9-C8	2.67	122.28	118.08
18	A	802	CLA	CMD-C2D-C1D	-2.67	120.01	124.71
27	5	621	XAT	O24-C25-C38	2.67	118.25	115.06
18	A	841	CLA	C1B-CHB-C4A	-2.67	124.84	130.12
18	4	616	CLA	CMB-C2B-C3B	2.67	129.91	124.69
20	a	620	LHG	C11-C10-C9	-2.67	100.89	114.42
18	3	613	CLA	O2D-CGD-O1D	-2.67	118.04	124.09
20	B	851	LHG	O8-C23-C24	2.66	120.27	111.91
18	A	827	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
18	A	831	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
18	3	612	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	B	819	CLA	CHB-C4A-NA	2.66	128.19	124.51
18	B	831	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
18	A	816	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
18	a	608	CLA	O2D-CGD-O1D	-2.65	118.07	124.09
18	4	611	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
21	J	102	BCR	C38-C26-C27	2.65	118.71	113.62
18	3	615	CLA	O2D-CGD-O1D	-2.65	118.07	124.09
18	5	609	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
18	A	818	CLA	CHB-C4A-NA	2.65	128.17	124.51
18	A	830	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
18	7	603	CLA	CHB-C4A-NA	2.65	128.17	124.51
18	B	832	CLA	O2D-CGD-CBD	2.65	115.97	111.27
18	1	602	CLA	CHB-C4A-NA	2.65	128.17	124.51
18	6	613	CLA	O2D-CGD-O1D	-2.65	118.08	124.09
21	4	621	BCR	C8-C7-C6	-2.64	119.77	127.20
18	3	603	CLA	CHB-C4A-NA	2.64	128.17	124.51
18	1	616	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
18	8	614	CLA	CHB-C4A-NA	2.64	128.17	124.51
18	4	604	CLA	C1B-CHB-C4A	-2.64	124.88	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	841	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
20	8	622	LHG	O8-C23-C24	2.64	120.20	111.91
21	K	207	BCR	C10-C11-C12	-2.64	114.98	123.22
18	7	609	CLA	CAC-C3C-C4C	2.64	128.24	124.81
21	A	856	BCR	C33-C5-C6	-2.64	121.56	124.53
21	L	305	BCR	C38-C26-C25	-2.64	121.56	124.53
18	7	603	CLA	CMB-C2B-C3B	2.64	129.62	124.68
20	5	623	LHG	O8-C23-C24	2.64	120.19	111.91
18	a	607	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	3	604	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
18	B	813	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	5	602	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	7	610	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	A	840	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
18	7	601	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
18	a	611	CLA	CAB-C3B-C2B	2.64	129.85	124.69
18	1	603	CLA	CMB-C2B-C3B	2.64	129.61	124.68
18	4	618	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	5	608	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	1	611	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
18	a	616	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
26	8	619	LUT	C30-C31-C32	-2.63	115.00	123.22
18	5	619	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
18	7	608	CLA	CMB-C2B-C3B	2.63	129.60	124.68
18	A	807	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
20	5	623	LHG	C11-C10-C9	-2.63	101.07	114.42
21	K	207	BCR	C30-C25-C26	-2.63	118.91	122.61
18	A	827	CLA	CAA-C2A-C1A	-2.63	103.36	111.97
18	B	840	CLA	CMB-C2B-C3B	2.63	129.60	124.68
23	8	625	LMU	O5B-C5B-C4B	2.63	114.47	109.69
18	A	839	CLA	CHB-C4A-NA	2.63	128.14	124.51
27	1	618	XAT	C4-C3-C2	-2.63	105.70	110.77
18	B	819	CLA	CMB-C2B-C3B	2.63	129.59	124.68
18	7	608	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
18	1	611	CLA	O2D-CGD-CBD	2.62	115.93	111.27
18	B	815	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
18	1	601	CLA	CHB-C4A-NA	2.62	128.14	124.51
18	6	603	CLA	CAB-C3B-C2B	2.62	129.82	124.69
28	6	624	NEX	C15-C35-C34	-2.62	118.11	123.47
18	B	827	CLA	CHB-C4A-NA	2.62	128.13	124.51
20	3	624	LHG	O8-C23-C24	2.62	120.12	111.91
26	3	618	LUT	C35-C15-C14	-2.62	118.11	123.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	610	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
18	4	609	CLA	CMB-C2B-C3B	2.61	129.57	124.68
18	A	802	CLA	C1-C2-C3	-2.61	121.52	126.04
18	J	101	CLA	CMB-C2B-C3B	2.61	129.57	124.68
18	L	303	CLA	CHB-C4A-NA	2.61	128.13	124.51
21	7	623	BCR	C15-C16-C17	-2.61	118.12	123.47
27	6	621	XAT	C31-C30-C29	-2.61	123.58	127.31
18	B	822	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
18	B	833	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
21	L	305	BCR	C20-C21-C22	-2.61	123.58	127.31
18	5	617	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	A	825	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
18	5	618	CLA	O2D-CGD-O1D	-2.61	118.16	124.09
21	1	619	BCR	C33-C5-C4	2.61	118.63	113.62
18	5	606	CLA	CAA-C2A-C3A	-2.61	107.74	114.26
18	F	303	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	4	602	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
18	1	607	CLA	CHB-C4A-NA	2.61	128.12	124.51
18	7	614	CLA	O2D-CGD-CBD	2.61	115.90	111.27
21	a	619	BCR	C29-C30-C25	2.61	114.49	110.48
18	A	811	CLA	CHB-C4A-NA	2.60	128.11	124.51
18	F	304	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
27	a	618	XAT	C19-C9-C8	2.60	122.18	118.08
21	J	102	BCR	C2-C1-C6	2.60	114.48	110.48
18	A	836	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
18	K	201	CLA	CMD-C2D-C1D	-2.60	120.13	124.71
24	7	624	LMG	O1-C7-C8	-2.60	104.63	110.90
18	4	618	CLA	CMB-C2B-C3B	2.60	129.78	124.69
18	A	827	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
18	4	614	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
21	A	849	BCR	C27-C26-C25	-2.60	118.96	122.73
18	6	616	CLA	CHB-C4A-NA	2.60	128.10	124.51
18	3	617	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
21	B	846	BCR	C23-C24-C25	-2.60	119.91	127.20
20	6	623	LHG	C11-C10-C9	-2.59	101.26	114.42
26	8	619	LUT	C31-C30-C29	-2.59	123.61	127.31
18	8	616	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
18	3	606	CLA	O2D-CGD-O1D	-2.59	118.20	124.09
18	B	834	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
18	1	609	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
21	F	305	BCR	C7-C8-C9	-2.59	122.32	126.23
18	a	611	CLA	CHB-C4A-NA	2.59	128.09	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	811	CLA	CMB-C2B-C3B	2.59	129.76	124.69
18	7	606	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
18	a	603	CLA	CMB-C2B-C3B	2.59	129.52	124.68
18	7	613	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
18	1	613	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
18	B	822	CLA	CHB-C4A-NA	2.59	128.09	124.51
18	1	613	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
18	A	803	CLA	C4D-C3D-CAD	-2.59	105.05	108.10
18	A	810	CLA	CHB-C4A-NA	2.59	128.09	124.51
18	8	608	CLA	CMB-C2B-C3B	2.59	129.52	124.68
18	1	614	CLA	C1B-CHB-C4A	-2.59	125.00	130.12
21	3	620	BCR	C1-C6-C5	-2.59	118.97	122.61
18	A	835	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
27	6	621	XAT	C35-C15-C14	-2.58	118.18	123.47
27	5	621	XAT	C19-C9-C8	2.58	122.15	118.08
21	B	846	BCR	C30-C25-C24	2.58	123.08	115.78
26	4	619	LUT	C39-C29-C28	2.58	122.15	118.08
18	B	833	CLA	CHB-C4A-NA	2.58	128.08	124.51
26	4	619	LUT	C7-C8-C9	-2.58	122.33	126.23
18	5	604	CLA	CMB-C2B-C3B	2.58	129.74	124.69
18	5	609	CLA	CHD-C1D-ND	-2.58	122.08	124.45
18	7	616	CLA	CHB-C4A-NA	2.58	128.08	124.51
21	B	846	BCR	C30-C25-C26	-2.58	118.98	122.61
18	3	611	CLA	CHB-C4A-NA	2.58	128.07	124.51
18	A	812	CLA	CHB-C4A-NA	2.58	128.07	124.51
18	4	612	CLA	CAA-C2A-C3A	-2.57	107.83	114.26
18	8	607	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
18	a	609	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
18	B	831	CLA	CHB-C4A-NA	2.57	128.07	124.51
18	4	604	CLA	CHB-C4A-NA	2.57	128.07	124.51
21	A	852	BCR	C10-C11-C12	-2.57	115.19	123.22
18	B	838	CLA	CHB-C4A-NA	2.57	128.07	124.51
26	6	619	LUT	C30-C31-C32	-2.57	115.20	123.22
18	8	614	CLA	O2D-CGD-CBD	2.57	115.83	111.27
18	6	611	CLA	CHB-C4A-NA	2.57	128.06	124.51
18	7	602	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
21	5	622	BCR	C23-C24-C25	-2.57	119.99	127.20
18	A	854	CLA	CHB-C4A-NA	2.57	128.06	124.51
27	3	619	XAT	C38-C25-C24	2.57	117.17	114.28
27	3	619	XAT	C35-C34-C33	-2.57	123.65	127.31
18	6	608	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
18	4	604	CLA	CMB-C2B-C3B	2.56	129.71	124.69

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	858	LMU	O5'-C5'-C4'	2.56	115.16	109.75
26	7	619	LUT	C39-C29-C28	2.56	122.12	118.08
21	3	622	BCR	C1-C6-C7	2.56	123.03	115.78
18	A	806	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
24	4	623	LMG	O6-C1-O1	-2.56	103.91	109.97
18	A	823	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
18	5	616	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
18	A	801	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
18	1	601	CLA	O2D-CGD-O1D	-2.56	118.28	124.09
26	a	617	LUT	C10-C11-C12	-2.56	115.23	123.22
18	A	808	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
18	7	612	CLA	O2A-CGA-O1A	-2.56	116.92	123.30
18	B	836	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	B	851	LHG	C11-C10-C9	-2.55	101.45	114.42
27	3	619	XAT	C19-C9-C8	2.55	122.10	118.08
20	5	625	LHG	O8-C23-C24	2.55	119.92	111.91
21	K	207	BCR	C11-C10-C9	-2.55	123.67	127.31
18	3	615	CLA	CAA-C2A-C3A	-2.55	107.88	114.26
18	B	828	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
18	5	612	CLA	O2D-CGD-O1D	-2.55	118.29	124.09
18	B	831	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
21	B	848	BCR	C39-C30-C25	-2.55	106.16	110.30
18	J	101	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
18	3	617	CLA	O2D-CGD-O1D	-2.55	118.30	124.09
18	A	818	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
18	a	611	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
18	6	606	CLA	CHB-C4A-NA	2.55	128.03	124.51
18	8	606	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
18	F	303	CLA	CMB-C2B-C3B	2.55	129.44	124.68
18	F	304	CLA	CHB-C4A-NA	2.55	128.03	124.51
18	A	804	CLA	CMB-C2B-C3B	2.55	129.44	124.68
26	a	617	LUT	C19-C9-C8	2.55	122.09	118.08
21	7	621	BCR	C38-C26-C27	2.54	118.50	113.62
21	6	622	BCR	C8-C7-C6	-2.54	120.06	127.20
18	3	609	CLA	C2A-C1A-CHA	2.54	128.31	123.86
21	8	621	BCR	C33-C5-C4	2.54	118.50	113.62
21	B	843	BCR	C38-C26-C27	2.54	118.50	113.62
18	6	612	CLA	O2D-CGD-O1D	-2.54	118.31	124.09
18	F	303	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
18	4	606	CLA	O2D-CGD-O1D	-2.54	118.32	124.09
18	A	826	CLA	CHB-C4A-NA	2.54	128.03	124.51
21	B	844	BCR	C38-C26-C27	2.54	118.50	113.62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	829	CLA	CHB-C4A-NA	2.54	128.02	124.51
21	7	621	BCR	C33-C5-C4	2.54	118.49	113.62
21	A	856	BCR	C29-C30-C25	2.54	114.39	110.48
18	B	823	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	5	619	CLA	CAA-C2A-C1A	2.54	120.29	111.97
18	a	608	CLA	CHB-C4A-NA	2.54	128.02	124.51
18	A	816	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
18	6	612	CLA	CAA-C2A-C3A	-2.54	107.92	114.26
18	7	607	CLA	CHB-C4A-NA	2.54	128.02	124.51
21	B	801	BCR	C7-C8-C9	-2.54	122.40	126.23
18	5	616	CLA	CHB-C4A-NA	2.53	128.02	124.51
18	B	824	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
18	A	839	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
23	5	628	LMU	C1B-O1B-C4'	-2.53	111.70	117.96
18	6	607	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
18	B	810	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
18	4	601	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
21	7	621	BCR	C7-C8-C9	-2.53	122.42	126.23
18	6	607	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
20	A	847	LHG	C11-C10-C9	-2.53	101.61	114.42
18	1	608	CLA	O2D-CGD-O1D	-2.53	118.36	124.09
18	a	607	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
18	B	837	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
18	1	614	CLA	O2D-CGD-O1D	-2.52	118.36	124.09
28	5	624	NEX	C38-C25-C24	2.52	117.12	114.28
18	3	608	CLA	CHB-C4A-NA	2.52	128.00	124.51
18	6	614	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
18	7	614	CLA	CAA-C2A-C3A	-2.52	107.96	114.26
20	8	623	LHG	C20-C19-C18	-2.52	101.63	114.42
21	a	619	BCR	C1-C6-C5	-2.52	119.07	122.61
18	5	618	CLA	CAA-C2A-C3A	-2.52	107.97	114.26
18	A	838	CLA	C1-C2-C3	-2.52	122.68	126.75
21	7	623	BCR	C38-C26-C25	-2.52	121.70	124.53
20	1	620	LHG	C11-C10-C9	-2.52	101.65	114.42
18	B	821	CLA	CHB-C4A-NA	2.51	127.99	124.51
18	4	601	CLA	CHB-C4A-NA	2.51	127.99	124.51
18	B	804	CLA	CHB-C4A-NA	2.51	127.99	124.51
18	B	813	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
18	B	828	CLA	C2D-C1D-ND	-2.51	108.25	110.10
23	A	858	LMU	C6'-C5'-C4'	-2.51	106.02	113.33
18	7	602	CLA	CMB-C2B-C3B	2.51	129.38	124.68
18	3	614	CLA	O2D-CGD-O1D	-2.51	118.39	124.09

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	621	XAT	C15-C35-C34	-2.51	118.33	123.47
18	F	301	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
21	4	621	BCR	C29-C30-C25	2.51	114.34	110.48
18	a	604	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
18	B	821	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
18	B	834	CLA	CHD-C1D-ND	-2.51	122.15	124.45
18	B	812	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
18	7	614	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	B	814	CLA	CAC-C3C-C4C	2.51	128.06	124.81
21	A	852	BCR	C38-C26-C27	2.51	118.43	113.62
21	3	621	BCR	C33-C5-C4	2.51	118.43	113.62
18	3	606	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
18	A	806	CLA	CAC-C3C-C4C	2.50	128.06	124.81
18	A	814	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
18	7	603	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
26	8	619	LUT	C38-C25-C24	-2.50	118.21	123.56
20	5	625	LHG	C20-C19-C18	-2.50	101.73	114.42
18	A	833	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	a	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	7	612	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
18	3	617	CLA	CHB-C4A-NA	2.50	127.97	124.51
18	3	603	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
21	A	852	BCR	C33-C5-C6	-2.50	121.73	124.53
18	4	606	CLA	CHB-C4A-NA	2.49	127.96	124.51
18	6	606	CLA	O2D-CGD-O1D	-2.49	118.42	124.09
21	7	623	BCR	C7-C8-C9	-2.49	122.47	126.23
18	A	824	CLA	CHB-C4A-NA	2.49	127.96	124.51
18	7	614	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
18	3	611	CLA	CMB-C2B-C3B	2.49	129.57	124.69
18	8	611	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
21	A	849	BCR	C38-C26-C25	-2.49	121.73	124.53
21	A	852	BCR	C16-C15-C14	-2.49	118.37	123.47
21	B	844	BCR	C20-C21-C22	-2.49	123.76	127.31
18	1	608	CLA	CHB-C4A-NA	2.49	127.95	124.51
21	B	848	BCR	C15-C16-C17	-2.49	118.38	123.47
18	1	607	CLA	O2D-CGD-O1D	-2.49	118.44	124.09
18	L	303	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
18	6	602	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
21	A	856	BCR	C16-C17-C18	-2.48	123.77	127.31
18	A	812	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
18	K	201	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
21	7	621	BCR	C33-C5-C6	-2.48	121.74	124.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	610	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
18	B	808	CLA	C1-C2-C3	-2.48	121.75	126.04
18	1	612	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
21	K	207	BCR	C38-C26-C27	2.48	118.38	113.62
18	3	608	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
18	4	612	CLA	O2D-CGD-O1D	-2.48	118.46	124.09
18	4	614	CLA	CHB-C4A-NA	2.48	127.94	124.51
18	A	828	CLA	CBA-CAA-C2A	-2.48	109.83	114.28
21	5	622	BCR	C21-C20-C19	-2.48	115.48	123.22
18	A	804	CLA	O2D-CGD-CBD	2.48	115.67	111.27
18	A	819	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
18	6	603	CLA	CMB-C2B-C3B	2.48	129.54	124.69
25	B	850	DGD	C3G-C2G-C1G	-2.48	105.93	111.79
18	a	612	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
26	1	617	LUT	C39-C29-C28	2.48	121.98	118.08
23	K	208	LMU	C4B-C3B-C2B	2.47	115.14	110.82
18	4	616	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
26	5	620	LUT	C21-C26-C27	-2.47	109.58	112.70
18	B	811	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
18	L	304	CLA	CMB-C2B-C3B	2.47	129.30	124.68
27	6	621	XAT	C39-C29-C28	2.47	121.97	118.08
18	3	614	CLA	CHB-C4A-NA	2.47	127.93	124.51
18	B	808	CLA	O2D-CGD-CBD	2.47	115.65	111.27
21	J	102	BCR	C10-C11-C12	-2.47	115.52	123.22
21	7	621	BCR	C23-C24-C25	-2.47	120.27	127.20
18	1	603	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
18	5	611	CLA	CHB-C4A-NA	2.47	127.92	124.51
18	7	608	CLA	CHB-C4A-NA	2.47	127.92	124.51
18	B	825	CLA	CHB-C4A-NA	2.47	127.92	124.51
18	4	613	CLA	C1B-CHB-C4A	-2.46	125.23	130.12
25	B	850	DGD	CFB-CEB-CDB	-2.46	101.91	114.42
21	3	620	BCR	C38-C26-C25	-2.46	121.76	124.53
27	1	618	XAT	C31-C30-C29	-2.46	123.80	127.31
18	1	616	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
18	5	606	CLA	CHB-C4A-NA	2.46	127.91	124.51
18	3	607	CLA	O2D-CGD-CBD	2.46	115.64	111.27
18	5	609	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
18	A	808	CLA	CHD-C1D-ND	-2.46	122.19	124.45
18	1	603	CLA	O2D-CGD-O1D	-2.46	118.50	124.09
18	B	807	CLA	CHB-C4A-NA	2.46	127.91	124.51
27	3	619	XAT	C30-C31-C32	-2.46	115.55	123.22
21	B	846	BCR	C15-C16-C17	-2.46	118.44	123.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	621	BCR	C27-C26-C25	-2.46	119.17	122.73
21	B	844	BCR	C33-C5-C4	2.45	118.33	113.62
18	B	832	CLA	CHD-C1D-ND	-2.45	122.20	124.45
21	7	621	BCR	C8-C7-C6	-2.45	120.31	127.20
18	5	602	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	A	844	PQN	C2M-C2-C3	-2.45	120.40	124.40
21	B	847	BCR	C8-C7-C6	-2.45	120.32	127.20
21	K	202	BCR	C15-C16-C17	-2.45	118.45	123.47
21	3	620	BCR	C1-C6-C7	2.45	122.71	115.78
27	7	620	XAT	C11-C10-C9	-2.45	123.81	127.31
21	F	305	BCR	C35-C13-C12	2.45	121.94	118.08
18	A	801	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
21	B	844	BCR	C16-C17-C18	-2.45	123.81	127.31
21	B	843	BCR	C30-C25-C26	-2.45	119.16	122.61
18	B	841	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
18	B	803	CLA	CHC-C1C-NC	2.45	127.92	124.20
18	A	823	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
18	6	616	CLA	O2D-CGD-CBD	2.45	115.62	111.27
18	L	303	CLA	CHD-C1D-ND	-2.45	122.21	124.45
18	A	826	CLA	CHA-C1A-NA	-2.45	120.80	126.40
18	B	835	CLA	C2A-C1A-CHA	2.45	128.14	123.86
18	7	604	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
21	A	849	BCR	C30-C25-C26	-2.45	119.17	122.61
18	A	831	CLA	CHC-C1C-NC	2.45	127.91	124.20
27	6	621	XAT	C10-C11-C12	-2.45	115.59	123.22
18	B	841	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	a	612	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	A	851	BCR	C38-C26-C25	-2.44	121.78	124.53
18	B	810	CLA	CHB-C4A-NA	2.44	127.89	124.51
18	A	815	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
18	a	616	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	5	622	BCR	C2-C1-C6	2.44	114.24	110.48
21	A	848	BCR	C30-C25-C26	-2.44	119.18	122.61
18	5	606	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
23	K	208	LMU	O5'-C1'-C2'	2.44	115.51	110.35
21	5	622	BCR	C11-C10-C9	-2.44	123.83	127.31
28	5	624	NEX	C4-C3-C2	-2.44	106.07	110.77
18	4	611	CLA	CHB-C4A-NA	2.44	127.88	124.51
26	1	617	LUT	C7-C8-C9	-2.44	122.55	126.23
26	a	617	LUT	C39-C29-C28	2.44	121.92	118.08
21	B	844	BCR	C30-C25-C24	2.44	122.67	115.78
18	4	603	CLA	C1B-CHB-C4A	-2.43	125.30	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	809	CLA	O2D-CGD-CBD	2.43	115.59	111.27
18	6	609	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
18	8	616	CLA	CMB-C2B-C3B	2.43	129.45	124.69
18	A	854	CLA	O2D-CGD-CBD	2.43	115.59	111.27
18	A	817	CLA	O2D-CGD-CBD	2.43	115.59	111.27
18	A	814	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
18	A	805	CLA	O2D-CGD-CBD	2.43	115.59	111.27
21	A	848	BCR	C23-C24-C25	-2.43	120.38	127.20
27	3	619	XAT	C15-C35-C34	-2.43	118.50	123.47
18	8	603	CLA	CMB-C2B-C3B	2.43	129.44	124.69
18	7	609	CLA	CHD-C1D-ND	-2.43	122.22	124.45
18	3	607	CLA	CHB-C4A-NA	2.43	127.87	124.51
18	B	829	CLA	CHB-C4A-NA	2.43	127.87	124.51
18	A	824	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
18	A	810	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
25	B	850	DGD	CBB-CAB-C9B	-2.43	102.11	114.42
18	4	612	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
18	A	830	CLA	CMC-C2C-C1C	-2.42	121.35	125.04
21	B	845	BCR	C1-C6-C5	-2.42	119.20	122.61
21	J	102	BCR	C29-C30-C25	2.42	114.21	110.48
26	3	618	LUT	C19-C9-C8	2.42	121.90	118.08
27	1	618	XAT	C19-C9-C8	2.42	121.90	118.08
18	B	809	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
21	A	849	BCR	C8-C7-C6	-2.42	120.40	127.20
27	5	621	XAT	C31-C32-C33	-2.42	119.61	126.42
18	7	607	CLA	CAC-C3C-C4C	2.42	127.95	124.81
18	5	607	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
21	A	856	BCR	C23-C24-C25	-2.42	120.41	127.20
20	5	625	LHG	C11-C10-C9	-2.42	102.15	114.42
18	A	826	CLA	CBA-CAA-C2A	2.42	118.63	114.28
27	3	619	XAT	C27-C28-C29	-2.42	121.78	125.53
26	5	620	LUT	C18-C5-C6	-2.42	121.81	124.53
18	7	611	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
18	5	611	CLA	CAA-C2A-C3A	-2.42	108.22	114.26
18	3	612	CLA	C1B-CHB-C4A	-2.41	125.33	130.12
20	A	846	LHG	C20-C19-C18	-2.41	102.17	114.42
26	a	617	LUT	C30-C31-C32	-2.41	115.69	123.22
18	B	833	CLA	CAA-C2A-C1A	-2.41	104.07	111.97
18	6	611	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
18	8	601	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
21	6	622	BCR	C4-C5-C6	-2.41	119.23	122.73
21	8	621	BCR	C38-C26-C27	2.41	118.24	113.62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	832	CLA	CHB-C4A-NA	2.41	127.84	124.51
18	A	843	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
18	B	835	CLA	O2D-CGD-CBD	2.41	115.54	111.27
18	B	823	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
18	B	836	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
18	B	809	CLA	CHB-C4A-NA	2.40	127.84	124.51
21	8	621	BCR	C1-C6-C5	-2.40	119.23	122.61
18	B	837	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
18	5	608	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
18	B	828	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	6	601	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
18	5	603	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	3	623	LHG	C11-C10-C9	-2.40	102.24	114.42
18	6	608	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	A	831	CLA	CMC-C2C-C1C	-2.40	121.39	125.04
18	B	816	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
18	B	825	CLA	O1D-CGD-CBD	2.40	129.39	124.48
23	5	628	LMU	O5'-C1'-C2'	2.40	115.42	110.35
21	8	621	BCR	C11-C10-C9	-2.40	123.89	127.31
21	A	848	BCR	C28-C27-C26	-2.40	109.80	114.08
18	A	817	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	5	628	LMU	C1'-O5'-C5'	2.39	118.39	113.69
26	5	620	LUT	C28-C29-C30	-2.39	115.27	118.94
21	3	622	BCR	C27-C26-C25	-2.39	119.26	122.73
18	A	831	CLA	CMD-C2D-C1D	-2.39	120.50	124.71
18	A	816	CLA	CHD-C1D-ND	-2.39	122.26	124.45
27	6	621	XAT	C8-C9-C10	-2.39	115.27	118.94
18	A	836	CLA	CMB-C2B-C3B	2.39	129.15	124.68
18	B	835	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
20	3	623	LHG	C20-C19-C18	-2.39	102.31	114.42
18	8	610	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
18	4	602	CLA	O2D-CGD-CBD	2.39	115.51	111.27
18	a	616	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
18	4	606	CLA	CAA-C2A-C3A	-2.39	108.30	114.26
18	a	603	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
18	A	815	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
18	8	611	CLA	CAA-C2A-C3A	-2.38	108.30	114.26
18	7	606	CLA	CHB-C4A-NA	2.38	127.81	124.51
18	8	611	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	A	859	LMU	C4B-C3B-C2B	2.38	114.98	110.82
28	6	624	NEX	C2-C1-C6	2.38	111.53	109.21
21	B	848	BCR	C35-C13-C12	2.38	121.83	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	840	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
18	B	821	CLA	O2D-CGD-CBD	2.38	115.50	111.27
21	6	622	BCR	C33-C5-C6	-2.38	121.86	124.53
18	B	815	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
18	8	612	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
26	1	617	LUT	C38-C25-C24	-2.38	118.47	123.56
18	7	613	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
21	3	620	BCR	C34-C9-C10	-2.38	119.59	122.92
18	A	841	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
21	a	619	BCR	C8-C7-C6	-2.38	120.53	127.20
18	7	608	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
24	J	104	LMG	O2-C2-C1	-2.37	104.28	110.05
21	A	856	BCR	C21-C20-C19	-2.37	115.81	123.22
18	1	608	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
21	F	305	BCR	C30-C25-C26	-2.37	119.27	122.61
24	4	624	LMG	O6-C1-O1	-2.37	104.35	109.97
18	A	814	CLA	C16-C15-C13	-2.37	108.25	115.92
21	B	847	BCR	C38-C26-C27	2.37	118.17	113.62
18	A	840	CLA	O2D-CGD-CBD	2.37	115.48	111.27
18	B	814	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
18	5	604	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
23	5	628	LMU	O5B-C1B-C2B	2.37	115.37	110.35
20	8	622	LHG	C5-O7-C7	-2.37	111.95	117.79
18	a	609	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
26	5	620	LUT	C39-C29-C28	2.37	121.81	118.08
21	3	620	BCR	C38-C26-C27	2.37	118.17	113.62
21	B	844	BCR	C38-C26-C25	-2.37	121.87	124.53
18	A	827	CLA	C2D-C1D-ND	-2.37	108.36	110.10
18	6	604	CLA	O2D-CGD-CBD	2.37	115.47	111.27
18	5	603	CLA	CMB-C2B-C3B	2.37	129.32	124.69
18	5	606	CLA	CMB-C2B-C3B	2.37	129.10	124.68
18	A	828	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
18	B	830	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
26	7	619	LUT	C3-C4-C5	-2.36	107.14	111.85
18	A	830	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
18	5	610	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
18	3	613	CLA	C1-C2-C3	-2.36	121.96	126.04
18	7	604	CLA	O2D-CGD-CBD	2.36	115.47	111.27
25	J	103	DGD	O5D-C6D-C5D	-2.36	104.67	109.05
18	5	616	CLA	CMB-C2B-C3B	2.36	129.31	124.69
18	3	608	CLA	CMB-C2B-C3B	2.36	129.10	124.68
18	K	201	CLA	CMD-C2D-C3D	2.36	133.05	127.61

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	8	614	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
21	A	851	BCR	C16-C15-C14	-2.36	118.64	123.47
27	3	619	XAT	O4-C5-C6	-2.36	57.00	58.96
18	1	602	CLA	O1D-CGD-CBD	2.36	129.31	124.48
26	3	618	LUT	C30-C31-C32	-2.36	115.85	123.22
18	5	607	CLA	C2D-C1D-ND	-2.36	108.37	110.10
20	4	622	LHG	C11-C10-C9	-2.36	102.45	114.42
26	1	617	LUT	C19-C9-C8	2.36	121.79	118.08
20	8	623	LHG	C11-C10-C9	-2.36	102.46	114.42
18	A	827	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	6	619	LUT	C38-C25-C24	-2.36	118.52	123.56
18	4	618	CLA	O2D-CGD-O1D	-2.36	118.74	124.09
18	5	619	CLA	CHA-C1A-NA	-2.36	121.00	126.40
20	7	622	LHG	C11-C10-C9	-2.36	102.47	114.42
18	K	206	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
18	7	606	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
18	A	839	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
18	F	301	CLA	C2D-C1D-ND	-2.35	108.37	110.10
18	A	802	CLA	CMD-C2D-C3D	2.35	133.02	127.61
20	3	624	LHG	C20-C19-C18	-2.35	102.49	114.42
18	1	604	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
23	A	857	LMU	O5B-C5B-C4B	2.35	113.96	109.69
18	B	803	CLA	C1C-C2C-C3C	2.35	109.42	106.96
18	L	302	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
18	B	824	CLA	C2D-C1D-ND	-2.35	108.37	110.10
21	B	843	BCR	C15-C14-C13	-2.35	123.96	127.31
18	B	833	CLA	CHD-C1D-ND	-2.35	122.30	124.45
18	8	606	CLA	CHB-C4A-NA	2.35	127.76	124.51
21	B	845	BCR	C28-C27-C26	-2.35	109.89	114.08
21	J	102	BCR	C11-C10-C9	-2.35	123.96	127.31
21	A	856	BCR	C35-C13-C12	2.35	121.77	118.08
21	A	850	BCR	C38-C26-C27	2.35	118.12	113.62
18	B	834	CLA	C2D-C1D-ND	-2.34	108.38	110.10
21	A	851	BCR	C20-C19-C18	-2.34	119.83	126.42
27	6	621	XAT	C31-C32-C33	-2.34	119.83	126.42
27	5	621	XAT	C8-C9-C10	-2.34	115.34	118.94
24	A	860	LMG	O3-C3-C2	-2.34	104.93	110.35
18	7	601	CLA	CHB-C4A-NA	2.34	127.75	124.51
18	a	608	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
18	5	611	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
21	5	622	BCR	C34-C9-C8	2.34	121.77	118.08
18	6	612	CLA	C1B-CHB-C4A	-2.34	125.48	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	813	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
21	B	801	BCR	C10-C11-C12	-2.34	115.92	123.22
18	1	606	CLA	CHB-C4A-NA	2.34	127.75	124.51
18	a	613	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
20	A	846	LHG	C18-C17-C16	-2.34	102.56	114.42
21	F	305	BCR	C33-C5-C6	-2.34	121.90	124.53
18	5	601	CLA	C2D-C1D-ND	-2.34	108.38	110.10
18	a	606	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
21	K	207	BCR	C15-C16-C17	-2.33	118.69	123.47
21	8	621	BCR	C24-C23-C22	-2.33	122.71	126.23
18	5	613	CLA	O2D-CGD-CBD	2.33	115.41	111.27
18	5	614	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
21	F	305	BCR	C34-C9-C8	2.33	121.75	118.08
25	J	103	DGD	C2G-O2G-C1B	2.33	123.53	117.79
18	a	601	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
18	A	806	CLA	CHD-C1D-ND	-2.33	122.31	124.45
18	a	609	CLA	C2A-C1A-CHA	2.33	127.93	123.86
21	3	620	BCR	C16-C15-C14	-2.33	118.70	123.47
18	8	610	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
18	6	617	CLA	CHB-C4A-NA	2.33	127.73	124.51
18	A	839	CLA	CMB-C2B-C3B	2.33	129.03	124.68
18	3	611	CLA	CMA-C3A-C2A	-2.33	110.67	116.10
21	3	622	BCR	C7-C6-C5	-2.32	115.83	121.46
18	3	602	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
18	A	833	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
18	L	304	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	5	619	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	6	617	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
26	a	617	LUT	C8-C7-C6	-2.32	120.68	127.20
18	K	203	CLA	C2A-C1A-CHA	2.32	127.92	123.86
18	a	613	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	5	609	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	6	610	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
18	A	837	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
18	B	822	CLA	CAA-C2A-C3A	-2.32	108.46	114.26
21	5	622	BCR	C29-C30-C25	2.32	114.05	110.48
26	5	620	LUT	C16-C1-C6	-2.32	106.54	110.30
27	7	620	XAT	C19-C9-C8	2.32	121.73	118.08
18	B	807	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
18	A	835	CLA	CHD-C1D-ND	-2.32	122.32	124.45
18	F	301	CLA	CMB-C2B-C3B	2.32	129.02	124.68
18	A	810	CLA	C1B-CHB-C4A	-2.32	125.53	130.12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	621	BCR	C1-C6-C5	-2.32	119.35	122.61
21	A	850	BCR	C27-C26-C25	-2.32	119.37	122.73
18	4	607	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
18	1	602	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
25	J	103	DGD	C5B-C4B-C3B	-2.32	102.67	114.42
18	6	604	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
18	F	301	CLA	CHB-C4A-NA	2.32	127.71	124.51
21	K	207	BCR	C23-C24-C25	-2.32	120.70	127.20
21	B	843	BCR	C1-C6-C5	-2.31	119.35	122.61
21	7	621	BCR	C34-C9-C8	2.31	121.72	118.08
21	K	202	BCR	C10-C11-C12	-2.31	116.00	123.22
18	1	606	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
18	5	613	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
18	1	613	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
18	a	612	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
20	6	623	LHG	C18-C17-C16	-2.31	102.70	114.42
18	4	611	CLA	O2D-CGD-CBD	2.31	115.37	111.27
20	6	623	LHG	O8-C23-C24	2.31	119.15	111.91
21	L	305	BCR	C23-C24-C25	-2.31	120.72	127.20
18	6	601	CLA	CAA-CBA-CGA	-2.31	106.51	113.25
18	A	820	CLA	CMC-C2C-C1C	-2.31	121.53	125.04
18	A	804	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
18	5	604	CLA	CHB-C4A-NA	2.31	127.70	124.51
21	A	856	BCR	C2-C1-C6	2.31	114.03	110.48
27	5	621	XAT	C28-C29-C30	-2.30	115.40	118.94
18	A	824	CLA	O2D-CGD-CBD	2.30	115.36	111.27
24	4	624	LMG	O3-C3-C2	-2.30	105.02	110.35
18	8	602	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
18	5	607	CLA	CMC-C2C-C1C	-2.30	121.53	125.04
18	A	842	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
21	B	843	BCR	C24-C23-C22	-2.30	122.76	126.23
28	6	624	NEX	C16-C1-C6	2.30	112.53	110.47
18	3	615	CLA	CMB-C2B-C3B	2.30	128.98	124.68
18	1	610	CLA	CHB-C4A-NA	2.30	127.69	124.51
18	a	601	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
18	3	613	CLA	CMB-C2B-C3B	2.30	128.97	124.68
20	3	624	LHG	C11-C10-C9	-2.30	102.77	114.42
18	8	608	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
18	A	832	CLA	C1-C2-C3	-2.29	123.04	126.75
18	B	805	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
26	5	620	LUT	C38-C25-C24	-2.29	118.65	123.56
18	B	802	CLA	CMB-C2B-C1B	-2.29	124.94	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	620	LHG	C20-C19-C18	-2.29	102.80	114.42
21	L	301	BCR	C34-C9-C10	-2.29	119.72	122.92
25	J	103	DGD	C3G-C2G-C1G	-2.29	106.37	111.79
18	3	613	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
20	7	622	LHG	O8-C23-O10	-2.29	117.82	123.59
18	A	808	CLA	O2D-CGD-CBD	2.29	115.33	111.27
20	5	623	LHG	C20-C19-C18	-2.29	102.82	114.42
18	a	602	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
18	6	616	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
18	A	807	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
21	7	621	BCR	C27-C26-C25	-2.28	119.42	122.73
18	7	615	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
18	4	603	CLA	CMB-C2B-C3B	2.28	129.16	124.69
18	A	817	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
18	J	101	CLA	O2D-CGD-CBD	2.28	115.32	111.27
18	B	839	CLA	C2D-C1D-ND	-2.28	108.42	110.10
18	1	601	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
28	5	624	NEX	C35-C34-C33	-2.28	124.06	127.31
18	A	827	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
18	3	603	CLA	CBC-CAC-C3C	-2.28	106.15	112.43
23	A	858	LMU	C1B-O5B-C5B	2.28	118.16	113.69
18	7	607	CLA	CHD-C1D-ND	-2.28	122.36	124.45
18	A	838	CLA	C2A-C1A-CHA	2.28	127.84	123.86
18	8	604	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
21	F	305	BCR	C8-C7-C6	-2.28	120.81	127.20
26	a	617	LUT	C16-C1-C6	-2.28	106.61	110.30
20	A	846	LHG	C11-C10-C9	-2.28	102.87	114.42
24	J	104	LMG	O1-C7-C8	-2.28	105.41	110.90
18	A	839	CLA	CHD-C1D-ND	-2.28	122.36	124.45
26	6	619	LUT	C39-C29-C28	2.28	121.66	118.08
18	1	614	CLA	CAA-C2A-C3A	-2.27	107.85	114.44
18	6	609	CLA	O2D-CGD-CBD	2.27	115.31	111.27
20	4	622	LHG	C20-C19-C18	-2.27	102.89	114.42
25	B	850	DGD	O3D-C3D-C4D	-2.27	105.10	110.35
18	B	829	CLA	C3C-C4C-NC	-2.27	108.02	110.57
21	B	847	BCR	C4-C5-C6	-2.27	119.43	122.73
18	A	815	CLA	CHB-C4A-NA	2.27	127.65	124.51
18	1	616	CLA	CHB-C4A-NA	2.27	127.65	124.51
18	1	603	CLA	C2A-C1A-CHA	2.27	127.83	123.86
18	4	608	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
18	7	610	CLA	C1-C2-C3	-2.27	122.12	126.04
23	8	625	LMU	C2'-C3'-C4'	2.26	114.85	109.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	619	LUT	C28-C29-C30	-2.26	115.47	118.94
18	A	835	CLA	C2D-C1D-ND	-2.26	108.44	110.10
18	B	819	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
18	4	601	CLA	O2D-CGD-CBD	2.26	115.29	111.27
27	1	618	XAT	C38-C25-C24	2.26	116.82	114.28
18	3	603	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
26	1	617	LUT	C11-C10-C9	-2.26	124.09	127.31
21	B	845	BCR	C15-C16-C17	-2.25	118.86	123.47
18	1	607	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
18	3	606	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
18	1	603	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
18	A	818	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
18	8	613	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
24	J	104	LMG	O6-C1-O1	-2.25	104.64	109.97
20	4	622	LHG	O8-C23-C24	2.25	118.97	111.91
21	B	848	BCR	C20-C19-C18	-2.25	120.09	126.42
18	7	610	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
18	A	837	CLA	C2A-C1A-CHA	2.25	127.80	123.86
20	1	620	LHG	C20-C19-C18	-2.25	103.00	114.42
18	3	609	CLA	CMC-C2C-C1C	-2.25	121.61	125.04
20	5	625	LHG	C18-C17-C16	-2.25	103.01	114.42
18	A	805	CLA	CHD-C1D-ND	-2.25	122.39	124.45
18	6	606	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
18	A	808	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
18	B	828	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
18	B	804	CLA	CMA-C3A-C2A	-2.25	110.86	116.10
21	B	847	BCR	C38-C26-C25	-2.25	122.01	124.53
18	K	204	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
18	5	603	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
27	1	618	XAT	C20-C13-C12	2.24	121.61	118.08
26	6	619	LUT	C16-C1-C6	-2.24	106.66	110.30
20	3	624	LHG	C18-C17-C16	-2.24	103.03	114.42
26	1	617	LUT	C31-C30-C29	-2.24	124.11	127.31
18	5	614	CLA	C3A-C4A-CHB	-2.24	120.20	124.24
20	B	851	LHG	O3-C3-C2	-2.24	100.11	109.69
20	1	620	LHG	O8-C23-C24	2.24	118.94	111.91
18	A	834	CLA	O2D-CGD-CBD	2.24	115.25	111.27
26	7	619	LUT	C28-C29-C30	-2.24	115.51	118.94
18	A	815	CLA	CHD-C1D-ND	-2.24	122.40	124.45
18	4	607	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
18	B	804	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
18	A	821	CLA	C1B-CHB-C4A	-2.24	125.69	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	619	LUT	C36-C21-C26	2.24	112.93	109.55
18	A	806	CLA	C3C-C4C-NC	-2.24	108.06	110.57
23	K	208	LMU	O5'-C5'-C4'	2.23	114.46	109.75
21	1	619	BCR	C1-C6-C5	-2.23	119.47	122.61
18	3	610	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
18	5	607	CLA	C2A-C1A-CHA	2.23	127.77	123.86
18	A	820	CLA	CHC-C1C-NC	2.23	127.59	124.20
18	8	608	CLA	C4-C3-C5	2.23	118.53	115.98
26	8	619	LUT	C39-C29-C28	2.23	121.59	118.08
18	A	825	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
18	A	817	CLA	C3C-C4C-NC	-2.23	108.07	110.57
18	6	613	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
18	3	603	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
18	K	201	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
18	B	813	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
18	a	607	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
18	B	817	CLA	CHD-C1D-ND	-2.23	122.41	124.45
27	8	620	XAT	O4-C5-C6	-2.23	57.12	58.96
18	6	616	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
18	A	840	CLA	CAA-CBA-CGA	-2.22	106.75	113.25
18	4	602	CLA	CHD-C1D-ND	-2.22	122.41	124.45
21	7	621	BCR	C10-C11-C12	-2.22	116.28	123.22
18	A	820	CLA	C2D-C1D-ND	-2.22	108.47	110.10
18	A	835	CLA	CMC-C2C-C1C	-2.22	121.66	125.04
18	A	801	CLA	C2A-C1A-CHA	2.22	127.74	123.86
21	A	851	BCR	C15-C16-C17	-2.22	118.93	123.47
27	7	620	XAT	C39-C29-C28	2.22	121.58	118.08
18	8	601	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
18	7	616	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
18	A	838	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
24	A	860	LMG	O2-C2-C1	-2.22	104.66	110.05
18	3	612	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
24	J	104	LMG	O3-C3-C2	-2.22	105.22	110.35
18	A	819	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
21	6	622	BCR	C24-C23-C22	-2.22	122.89	126.23
18	A	810	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
23	A	859	LMU	O5B-C5B-C4B	2.22	113.72	109.69
18	5	603	CLA	CAA-C2A-C3A	-2.22	106.71	112.78
18	8	602	CLA	CHD-C1D-ND	-2.21	122.42	124.45
27	1	618	XAT	O24-C25-C26	-2.21	57.13	58.96
18	3	602	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
18	1	612	CLA	C2A-C1A-CHA	2.21	127.73	123.86

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	609	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
18	B	841	CLA	C2A-C1A-CHA	2.21	127.73	123.86
20	7	622	LHG	C27-C26-C25	-2.21	103.20	114.42
18	B	806	CLA	C2D-C1D-ND	-2.21	108.47	110.10
18	a	610	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
24	4	624	LMG	O2-C2-C1	-2.21	104.68	110.05
18	a	602	CLA	O1D-CGD-CBD	2.21	129.00	124.48
21	3	620	BCR	C33-C5-C6	-2.21	122.05	124.53
18	a	612	CLA	C2A-C1A-CHA	2.21	127.72	123.86
18	5	612	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
18	L	303	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
24	5	626	LMG	O6-C1-O1	-2.21	104.75	109.97
18	5	617	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
18	7	612	CLA	CHA-C1A-NA	-2.21	121.35	126.40
18	6	602	CLA	O2D-CGD-CBD	2.20	115.19	111.27
18	A	843	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
21	7	621	BCR	C38-C26-C25	-2.20	122.05	124.53
18	3	615	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
18	4	603	CLA	C2D-C1D-ND	-2.20	108.48	110.10
21	B	844	BCR	C15-C16-C17	-2.20	118.96	123.47
21	5	622	BCR	C38-C26-C27	2.20	117.85	113.62
21	J	102	BCR	C15-C16-C17	-2.20	118.97	123.47
27	5	621	XAT	C39-C29-C28	2.20	121.55	118.08
18	7	613	CLA	C2D-C1D-ND	-2.20	108.48	110.10
18	a	604	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
18	a	604	CLA	O2D-CGD-CBD	2.20	115.18	111.27
21	K	202	BCR	C38-C26-C25	-2.20	122.06	124.53
27	7	620	XAT	O4-C5-C6	-2.20	57.14	58.96
18	A	845	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
21	A	848	BCR	C20-C19-C18	-2.20	120.24	126.42
18	6	613	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
18	B	834	CLA	C3C-C4C-NC	-2.20	108.11	110.57
18	A	831	CLA	C2D-C1D-ND	-2.20	108.49	110.10
21	B	845	BCR	C3-C4-C5	-2.20	110.16	114.08
26	6	619	LUT	C19-C9-C8	2.19	121.53	118.08
18	6	620	CLA	CAC-C3C-C4C	2.19	127.66	124.81
18	5	614	CLA	CHB-C4A-NA	2.19	127.70	124.34
21	L	301	BCR	C30-C25-C26	-2.19	119.53	122.61
18	A	814	CLA	C11-C10-C8	-2.19	108.83	115.92
18	4	618	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
18	6	613	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
21	5	622	BCR	C11-C12-C13	-2.19	120.26	126.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	8	616	CLA	CHA-C1A-NA	-2.19	121.38	126.40
18	A	822	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
18	1	610	CLA	CMA-C3A-C2A	-2.19	108.09	114.44
18	A	811	CLA	O1D-CGD-CBD	2.19	128.96	124.48
26	4	619	LUT	C3-C4-C5	-2.19	107.50	111.85
18	8	603	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
21	4	621	BCR	C1-C6-C7	2.19	121.96	115.78
18	7	603	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
18	6	618	CLA	CAA-C2A-C3A	-2.18	108.80	114.26
18	5	609	CLA	C2A-C1A-CHA	2.18	127.68	123.86
21	4	621	BCR	C16-C15-C14	-2.18	119.00	123.47
21	8	621	BCR	C37-C22-C23	2.18	121.52	118.08
24	4	623	LMG	O1-C7-C8	-2.18	105.63	110.90
18	A	812	CLA	CHD-C1D-ND	-2.18	122.45	124.45
18	A	830	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
18	A	831	CLA	CMD-C2D-C3D	2.18	132.63	127.61
21	7	621	BCR	C16-C15-C14	-2.18	119.01	123.47
18	4	609	CLA	CMC-C2C-C3C	2.18	132.04	126.12
18	a	614	CLA	CHB-C4A-NA	2.18	127.68	124.34
18	F	301	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
18	A	817	CLA	C2D-C1D-ND	-2.18	108.50	110.10
21	3	621	BCR	C16-C17-C18	-2.18	124.20	127.31
26	5	620	LUT	C1-C2-C3	2.18	118.56	113.64
18	K	203	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
18	8	604	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
20	6	623	LHG	C5-O7-C7	-2.18	112.43	117.79
27	8	620	XAT	C18-C5-C4	2.18	116.73	114.28
27	1	618	XAT	C11-C10-C9	-2.18	124.20	127.31
18	3	609	CLA	CMC-C2C-C3C	2.18	132.03	126.12
21	6	622	BCR	C37-C22-C23	2.18	121.51	118.08
20	3	623	LHG	C27-C26-C25	-2.18	103.38	114.42
21	4	621	BCR	C4-C5-C6	-2.17	119.57	122.73
24	5	626	LMG	O3-C3-C2	-2.17	105.32	110.35
27	a	618	XAT	O24-C25-C26	-2.17	57.16	58.96
18	5	607	CLA	CHC-C1C-NC	2.17	127.50	124.20
18	B	826	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
18	3	607	CLA	CHD-C1D-ND	-2.17	122.46	124.45
18	A	802	CLA	C3C-C4C-NC	-2.17	108.14	110.57
20	1	620	LHG	C27-C26-C25	-2.17	103.40	114.42
21	B	845	BCR	C29-C30-C25	2.17	113.82	110.48
21	3	622	BCR	C15-C16-C17	-2.17	119.03	123.47
18	B	806	CLA	C2A-C1A-CHA	2.17	127.65	123.86

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	841	CLA	CHA-C1A-NA	-2.17	121.43	126.40
28	6	624	NEX	C38-C25-C24	2.17	116.72	114.28
20	3	623	LHG	C18-C17-C16	-2.17	103.41	114.42
18	B	813	CLA	C16-C15-C13	-2.17	108.91	115.92
20	5	625	LHG	C27-C26-C25	-2.17	103.42	114.42
27	7	620	XAT	O24-C25-C26	-2.17	57.16	58.96
18	B	820	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
21	3	620	BCR	C29-C30-C25	2.17	113.82	110.48
20	B	851	LHG	C27-C26-C25	-2.17	103.43	114.42
18	4	606	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
18	B	841	CLA	O2D-CGD-CBD	2.16	115.11	111.27
18	A	832	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
18	4	612	CLA	C2A-C1A-CHA	2.16	127.64	123.86
21	B	847	BCR	C11-C12-C13	-2.16	120.34	126.42
18	A	804	CLA	CAA-CBA-CGA	-2.16	106.93	113.25
21	B	801	BCR	C20-C19-C18	-2.16	120.34	126.42
24	5	626	LMG	O7-C10-O9	-2.16	118.47	123.70
18	5	602	CLA	C16-C15-C13	-2.16	108.93	115.92
21	A	850	BCR	C3-C4-C5	-2.16	110.22	114.08
18	7	613	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
20	8	623	LHG	C27-C26-C25	-2.16	103.46	114.42
18	B	806	CLA	CHA-C1A-NA	-2.16	121.45	126.40
18	A	817	CLA	CHD-C1D-ND	-2.16	122.47	124.45
18	5	608	CLA	C2A-C1A-CHA	2.16	127.64	123.86
27	a	618	XAT	C20-C13-C12	2.16	121.48	118.08
21	A	852	BCR	C33-C5-C4	2.16	117.76	113.62
18	A	832	CLA	C2D-C1D-ND	-2.16	108.51	110.10
21	6	622	BCR	C11-C12-C13	-2.16	120.36	126.42
21	1	619	BCR	C38-C26-C25	-2.16	122.11	124.53
18	8	603	CLA	O2A-CGA-O1A	-2.16	117.93	123.30
20	1	620	LHG	C18-C17-C16	-2.15	103.48	114.42
18	A	824	CLA	C2D-C1D-ND	-2.15	108.52	110.10
18	5	618	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
18	6	614	CLA	CHD-C1D-ND	-2.15	122.47	124.45
26	7	619	LUT	C15-C35-C34	-2.15	119.06	123.47
18	8	616	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
20	a	620	LHG	C18-C17-C16	-2.15	103.50	114.42
18	7	607	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
18	4	604	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	K	201	CLA	O2A-CGA-O1A	-2.15	117.94	123.30
18	A	810	CLA	C2D-C1D-ND	-2.15	108.52	110.10
19	A	844	PQN	C14-C13-C15	-2.15	111.65	115.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	807	CLA	CHD-C1D-ND	-2.15	122.48	124.45
18	4	604	CLA	CAB-C3B-C2B	2.15	128.90	124.69
24	5	626	LMG	O2-C2-C1	-2.15	104.82	110.05
20	4	622	LHG	C18-C17-C16	-2.15	103.51	114.42
18	4	601	CLA	CMB-C2B-C3B	2.15	128.70	124.68
21	J	102	BCR	C23-C24-C25	-2.15	121.17	127.20
18	6	607	CLA	CHC-C1C-NC	2.15	127.46	124.20
21	A	852	BCR	C1-C6-C5	-2.15	119.59	122.61
18	A	820	CLA	O2D-CGD-CBD	2.15	115.08	111.27
20	8	623	LHG	C18-C17-C16	-2.15	103.52	114.42
18	5	616	CLA	O2A-CGA-O1A	-2.15	117.95	123.30
21	A	852	BCR	C23-C24-C25	-2.15	121.17	127.20
21	A	848	BCR	C10-C11-C12	-2.15	116.52	123.22
23	8	624	LMU	O5B-C5B-C4B	2.15	113.59	109.69
21	B	848	BCR	C34-C9-C8	2.15	121.46	118.08
21	1	619	BCR	C29-C30-C25	2.14	113.78	110.48
18	A	831	CLA	CMC-C2C-C3C	2.14	131.94	126.12
18	8	606	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
18	3	608	CLA	CHA-C4D-ND	2.14	136.98	132.50
18	7	602	CLA	CHD-C1D-ND	-2.14	122.48	124.45
18	A	854	CLA	C6-C7-C8	-2.14	109.00	115.92
20	6	623	LHG	C27-C26-C25	-2.14	103.55	114.42
21	A	856	BCR	C7-C8-C9	-2.14	123.00	126.23
18	B	830	CLA	CBC-CAC-C3C	2.14	118.33	112.43
20	a	620	LHG	C27-C26-C25	-2.14	103.56	114.42
18	6	603	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
18	8	607	CLA	CMB-C2B-C3B	2.14	128.88	124.69
21	B	844	BCR	C27-C26-C25	-2.14	119.62	122.73
18	6	616	CLA	CAC-C3C-C4C	2.14	127.59	124.81
18	4	618	CLA	CHD-C1D-ND	-2.14	122.49	124.45
27	4	620	XAT	C39-C29-C28	2.14	121.44	118.08
21	J	102	BCR	C34-C9-C8	2.14	121.44	118.08
18	A	814	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
18	A	821	CLA	CAC-C3C-C4C	2.14	127.58	124.81
21	B	844	BCR	C21-C20-C19	-2.14	116.55	123.22
18	A	814	CLA	C11-C12-C13	-2.14	109.02	115.92
18	7	610	CLA	O2D-CGD-CBD	2.14	115.06	111.27
18	A	830	CLA	C2D-C1D-ND	-2.13	108.53	110.10
18	5	607	CLA	CHD-C1D-ND	-2.13	122.49	124.45
18	A	810	CLA	C2A-C1A-CHA	2.13	127.59	123.86
18	7	612	CLA	O1D-CGD-CBD	2.13	128.85	124.48
18	1	606	CLA	CHD-C1D-ND	-2.13	122.50	124.45

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	619	LUT	C38-C25-C24	-2.13	119.00	123.56
25	B	850	DGD	C5B-C4B-C3B	-2.13	103.61	114.42
28	5	624	NEX	C25-C24-C23	-2.13	108.53	112.75
18	K	203	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
18	F	301	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
18	A	840	CLA	C2D-C1D-ND	-2.13	108.53	110.10
18	4	610	CLA	C1-C2-C3	-2.13	122.36	126.04
21	7	621	BCR	C29-C30-C25	2.13	113.76	110.48
23	8	625	LMU	O1B-C4'-C3'	2.13	112.94	107.28
24	4	624	LMG	O1-C7-C8	-2.13	105.77	110.90
18	B	832	CLA	C1-C2-C3	-2.13	122.37	126.04
18	a	603	CLA	C2D-C1D-ND	-2.13	108.54	110.10
18	8	601	CLA	O2D-CGD-CBD	2.12	115.04	111.27
21	A	851	BCR	C38-C26-C27	2.12	117.70	113.62
18	5	604	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
26	3	618	LUT	C16-C1-C6	-2.12	106.85	110.30
26	1	617	LUT	C8-C7-C6	-2.12	121.24	127.20
24	7	624	LMG	O2-C2-C1	-2.12	104.89	110.05
18	5	612	CLA	CAA-C2A-C3A	-2.12	108.95	114.26
18	6	602	CLA	CHD-C1D-ND	-2.12	122.50	124.45
18	8	614	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
27	5	621	XAT	O4-C5-C6	-2.12	57.20	58.96
18	4	610	CLA	CMC-C2C-C1C	-2.12	121.81	125.04
18	B	802	CLA	CHB-C4A-NA	2.12	127.45	124.51
25	J	103	DGD	O2D-C2D-C1D	-2.12	104.89	110.05
21	3	622	BCR	C3-C4-C5	-2.12	110.29	114.08
18	A	835	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
18	B	833	CLA	O2D-CGD-CBD	2.12	115.03	111.27
21	8	621	BCR	C23-C24-C25	-2.12	121.25	127.20
21	A	850	BCR	C21-C20-C19	-2.12	116.61	123.22
18	6	616	CLA	C2D-C1D-ND	-2.12	108.54	110.10
21	3	621	BCR	C34-C9-C10	-2.12	119.96	122.92
18	A	829	CLA	CHD-C1D-ND	-2.12	122.51	124.45
21	3	621	BCR	C31-C1-C6	-2.12	106.86	110.30
18	1	601	CLA	C2A-C1A-CHA	2.12	127.56	123.86
18	3	614	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
21	B	801	BCR	C1-C6-C5	-2.12	119.63	122.61
20	4	622	LHG	O8-C23-O10	-2.12	118.25	123.59
21	1	619	BCR	C8-C7-C6	-2.11	121.26	127.20
18	1	614	CLA	CHB-C4A-NA	2.11	127.58	124.34
18	7	611	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
18	7	602	CLA	O2D-CGD-CBD	2.11	115.02	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	617	LUT	C12-C13-C14	-2.11	115.70	118.94
18	a	603	CLA	CBA-CAA-C2A	-2.11	110.49	114.28
27	8	620	XAT	O24-C25-C26	-2.11	57.21	58.96
18	5	617	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
18	5	607	CLA	C3C-C4C-NC	-2.11	108.20	110.57
18	5	608	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
18	3	603	CLA	C1-C2-C3	-2.11	122.39	126.04
24	5	627	LMG	O2-C2-C1	-2.11	104.92	110.05
18	a	614	CLA	O2D-CGD-CBD	2.11	115.02	111.27
26	1	617	LUT	C21-C26-C27	-2.11	110.04	112.70
18	B	810	CLA	O1D-CGD-CBD	2.11	128.80	124.48
18	6	607	CLA	CAA-C2A-C1A	-2.11	107.47	112.14
23	8	624	LMU	C1B-O5B-C5B	2.11	117.82	113.69
18	B	802	CLA	C1-C2-C3	-2.10	122.41	126.04
24	A	860	LMG	O7-C10-O9	-2.10	118.62	123.70
18	8	613	CLA	C3A-C2A-C1A	2.10	104.49	101.34
18	A	807	CLA	CHD-C1D-ND	-2.10	122.52	124.45
18	a	613	CLA	C1-C2-C3	-2.10	122.41	126.04
18	6	613	CLA	C16-C15-C13	-2.10	109.12	115.92
18	a	609	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
18	L	302	CLA	C2A-C1A-CHA	2.10	127.53	123.86
18	4	611	CLA	CAA-C2A-C3A	-2.10	109.01	114.26
18	B	818	CLA	O2D-CGD-CBD	2.10	115.00	111.27
18	B	805	CLA	O2A-C1-C2	-2.10	103.11	108.64
27	a	618	XAT	C35-C15-C14	-2.10	119.17	123.47
18	B	811	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
18	B	824	CLA	C2A-C1A-CHA	2.10	127.53	123.86
21	8	621	BCR	C15-C16-C17	-2.10	119.17	123.47
27	1	618	XAT	C12-C13-C14	-2.10	115.72	118.94
18	6	609	CLA	O2A-CGA-O1A	-2.10	118.07	123.30
18	3	613	CLA	CMD-C2D-C3D	2.10	132.44	127.61
18	1	609	CLA	C2A-C1A-CHA	2.10	127.51	123.85
21	a	619	BCR	C38-C26-C27	2.10	117.64	113.62
18	A	825	CLA	O1D-CGD-CBD	2.10	128.77	124.48
21	B	845	BCR	C10-C11-C12	-2.10	116.68	123.22
21	6	622	BCR	C23-C24-C25	-2.10	121.32	127.20
18	B	807	CLA	O2D-CGD-CBD	2.10	114.99	111.27
21	5	622	BCR	C37-C22-C23	2.10	121.38	118.08
18	B	825	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
21	A	852	BCR	C15-C14-C13	-2.09	124.32	127.31
21	L	301	BCR	C21-C20-C19	-2.09	116.68	123.22
21	J	102	BCR	C36-C18-C19	2.09	121.38	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	806	CLA	CHC-C1C-NC	2.09	127.37	124.20
18	a	616	CLA	C2D-C1D-ND	-2.09	108.56	110.10
18	B	835	CLA	C3A-C2A-C1A	2.09	104.47	101.34
28	5	624	NEX	C30-C31-C32	-2.09	116.70	123.22
20	3	624	LHG	C27-C26-C25	-2.09	103.83	114.42
18	4	609	CLA	CHD-C1D-ND	-2.09	122.54	124.45
18	B	802	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
18	A	812	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
21	7	621	BCR	C1-C6-C5	-2.09	119.68	122.61
18	B	827	CLA	CHD-C1D-ND	-2.08	122.54	124.45
26	5	620	LUT	C7-C8-C9	-2.08	123.08	126.23
18	7	601	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
18	B	838	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
18	3	607	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
26	6	619	LUT	C20-C13-C12	2.08	121.36	118.08
21	A	849	BCR	C33-C5-C4	2.08	117.61	113.62
21	1	619	BCR	C38-C26-C27	2.08	117.61	113.62
18	3	611	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
18	A	854	CLA	C1-C2-C3	-2.08	122.44	126.04
18	A	840	CLA	C2A-C1A-CHA	2.08	127.50	123.86
27	8	620	XAT	C15-C35-C34	-2.08	119.22	123.47
18	5	617	CLA	C1-C2-C3	-2.08	123.39	126.75
26	5	620	LUT	C8-C7-C6	-2.08	121.36	127.20
18	B	839	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
27	5	621	XAT	O24-C25-C26	-2.08	57.24	58.96
21	K	202	BCR	C8-C7-C6	-2.08	121.37	127.20
18	B	837	CLA	CHD-C1D-ND	-2.08	122.55	124.45
23	5	628	LMU	C1B-C2B-C3B	2.08	114.32	110.00
21	K	207	BCR	C20-C19-C18	-2.08	120.58	126.42
28	6	624	NEX	O24-C25-C26	-2.08	57.24	58.96
18	A	801	CLA	CBA-CAA-C2A	-2.07	107.74	113.86
26	6	619	LUT	C31-C30-C29	-2.07	124.35	127.31
18	K	206	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
18	a	607	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
18	7	608	CLA	O2D-CGD-CBD	2.07	114.95	111.27
26	a	617	LUT	C28-C29-C30	-2.07	115.76	118.94
18	5	612	CLA	C2A-C1A-CHA	2.07	127.48	123.86
18	5	617	CLA	C2A-C1A-CHA	2.07	127.48	123.86
18	8	612	CLA	C2A-C1A-CHA	2.07	127.48	123.86
18	8	612	CLA	CBA-CAA-C2A	-2.07	108.85	113.47
26	6	619	LUT	C1-C2-C3	2.07	118.32	113.64
18	A	827	CLA	CAA-C2A-C3A	-2.07	107.11	112.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	846	BCR	C33-C5-C4	2.07	117.59	113.62
18	A	835	CLA	CMC-C2C-C3C	2.07	131.74	126.12
18	8	607	CLA	C2A-C1A-CHA	2.07	127.48	123.86
18	7	608	CLA	C1-C2-C3	-2.07	123.40	126.75
21	5	622	BCR	C39-C30-C25	-2.07	106.94	110.30
24	4	623	LMG	O3-C3-C2	-2.07	105.57	110.35
20	A	846	LHG	C27-C26-C25	-2.07	103.93	114.42
18	8	602	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
18	8	607	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
21	3	621	BCR	C1-C6-C5	-2.07	119.70	122.61
26	8	619	LUT	C7-C8-C9	-2.06	123.11	126.23
21	7	623	BCR	C8-C7-C6	-2.06	121.40	127.20
18	5	614	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
18	4	609	CLA	CMC-C2C-C1C	-2.06	121.90	125.04
21	7	621	BCR	C4-C5-C6	-2.06	119.74	122.73
18	6	618	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
21	A	856	BCR	C36-C18-C19	2.06	121.33	118.08
18	3	603	CLA	C2D-C1D-ND	-2.06	108.58	110.10
18	1	613	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
18	K	203	CLA	O2D-CGD-CBD	2.06	114.93	111.27
18	3	612	CLA	O1D-CGD-CBD	2.06	128.70	124.48
18	8	601	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
18	7	606	CLA	CAA-C2A-C3A	-2.06	109.11	114.26
21	B	801	BCR	C15-C14-C13	-2.06	124.37	127.31
18	4	614	CLA	CHD-C1D-ND	-2.06	122.56	124.45
21	A	849	BCR	C28-C27-C26	-2.06	110.41	114.08
18	A	825	CLA	C2D-C1D-ND	-2.06	108.59	110.10
18	6	603	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
18	B	806	CLA	C1B-CHB-C4A	-2.06	126.05	130.12
26	1	617	LUT	C20-C13-C12	2.06	121.31	118.08
26	a	617	LUT	C38-C25-C24	-2.05	119.16	123.56
18	5	607	CLA	O2D-CGD-CBD	2.05	114.92	111.27
18	a	607	CLA	CHD-C1D-ND	-2.05	122.57	124.45
18	8	608	CLA	C2A-C1A-CHA	2.05	127.45	123.86
21	L	301	BCR	C10-C11-C12	-2.05	116.81	123.22
18	A	836	CLA	C2D-C1D-ND	-2.05	108.59	110.10
18	6	620	CLA	CAA-C2A-C1A	-2.05	105.25	111.97
21	1	619	BCR	C10-C11-C12	-2.05	116.82	123.22
18	K	201	CLA	O2D-CGD-CBD	2.05	114.91	111.27
18	a	604	CLA	C2D-C1D-ND	-2.05	108.59	110.10
18	1	611	CLA	C2A-C1A-CHA	2.05	127.44	123.86
19	A	844	PQN	C16-C17-C18	-2.05	109.30	115.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	5	623	LHG	C18-C17-C16	-2.05	104.03	114.42
18	3	603	CLA	CHA-C4D-ND	2.05	136.78	132.50
18	6	606	CLA	CHD-C1D-ND	-2.05	122.57	124.45
27	a	618	XAT	C15-C35-C34	-2.05	119.28	123.47
18	A	837	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
26	6	619	LUT	C15-C14-C13	-2.05	124.39	127.31
21	B	843	BCR	C35-C13-C12	2.05	121.30	118.08
18	A	831	CLA	CHB-C4A-NA	2.05	127.34	124.51
26	8	619	LUT	C21-C26-C27	-2.05	110.11	112.70
18	3	609	CLA	CHA-C1A-NA	-2.04	121.72	126.40
21	5	622	BCR	C24-C23-C22	-2.04	123.15	126.23
18	B	817	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
20	5	623	LHG	C27-C26-C25	-2.04	104.06	114.42
21	a	619	BCR	C38-C26-C25	-2.04	122.24	124.53
18	A	803	CLA	C2A-C1A-CHA	2.04	127.43	123.86
18	B	802	CLA	O1D-CGD-CBD	2.04	128.66	124.48
18	B	803	CLA	CMC-C2C-C1C	-2.04	121.93	125.04
18	7	615	CLA	CAA-C2A-C3A	-2.04	109.17	114.26
18	A	824	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	A	850	BCR	C39-C30-C25	-2.04	107.00	110.30
26	4	619	LUT	C21-C26-C27	-2.03	110.13	112.70
21	3	620	BCR	C37-C22-C21	-2.03	120.07	122.92
21	A	849	BCR	C21-C20-C19	-2.03	116.87	123.22
21	A	849	BCR	C36-C18-C19	2.03	121.28	118.08
27	6	621	XAT	C28-C29-C30	-2.03	115.82	118.94
21	F	305	BCR	C37-C22-C21	-2.03	120.08	122.92
18	A	815	CLA	O2D-CGD-CBD	2.03	114.88	111.27
27	3	619	XAT	O24-C25-C26	-2.03	57.28	58.96
18	8	613	CLA	CMB-C2B-C3B	2.03	128.47	124.68
26	3	618	LUT	C15-C35-C34	-2.03	119.32	123.47
24	5	627	LMG	O3-C3-C2	-2.03	105.66	110.35
18	K	203	CLA	CHA-C1A-NA	-2.03	121.75	126.40
18	F	304	CLA	C2D-C1D-ND	-2.03	108.61	110.10
18	A	831	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
21	3	621	BCR	C38-C26-C25	-2.03	122.25	124.53
18	A	837	CLA	C3A-C2A-C1A	2.03	104.37	101.34
28	5	624	NEX	C10-C11-C12	-2.03	116.89	123.22
21	A	856	BCR	C33-C5-C4	2.03	117.51	113.62
21	B	848	BCR	C33-C5-C6	-2.03	122.25	124.53
18	4	608	CLA	O2D-CGD-CBD	2.03	114.87	111.27
18	7	604	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
19	B	842	PQN	C9-C10-C5	2.02	121.51	119.26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	6	610	CLA	CHD-C1D-ND	-2.02	122.59	124.45
25	B	850	DGD	C7B-C6B-C5B	-2.02	104.15	114.42
27	4	620	XAT	O24-C25-C26	-2.02	57.28	58.96
21	4	621	BCR	C24-C23-C22	-2.02	123.18	126.23
19	A	844	PQN	C2M-C2-C1	2.02	119.62	116.27
18	1	601	CLA	CHA-C1A-NA	-2.02	121.77	126.40
18	1	604	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
18	4	609	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
18	B	829	CLA	O1D-CGD-CBD	2.02	128.62	124.48
20	4	622	LHG	C27-C26-C25	-2.02	104.17	114.42
18	B	815	CLA	C2A-C1A-CHA	2.02	127.39	123.86
24	7	624	LMG	O3-C3-C2	-2.02	105.69	110.35
18	8	601	CLA	C2D-C1D-ND	-2.02	108.62	110.10
18	8	614	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	A	859	LMU	O5'-C1'-C2'	2.02	113.91	110.87
18	B	813	CLA	C1-C2-C3	-2.02	122.56	126.04
18	F	301	CLA	CAA-C2A-C3A	-2.02	107.26	112.78
18	4	613	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
18	7	610	CLA	CHD-C1D-ND	-2.01	122.60	124.45
21	8	621	BCR	C34-C9-C8	2.01	121.25	118.08
21	7	623	BCR	C34-C9-C8	2.01	121.25	118.08
18	A	854	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
21	B	801	BCR	C4-C5-C6	-2.01	119.81	122.73
21	B	843	BCR	C3-C4-C5	-2.01	110.49	114.08
18	A	810	CLA	CHA-C1A-NA	-2.01	121.79	126.40
21	a	619	BCR	C3-C4-C5	-2.01	110.49	114.08
21	B	847	BCR	C27-C26-C25	-2.01	119.81	122.73
18	A	854	CLA	C2A-C1A-CHA	2.01	127.37	123.86
26	a	617	LUT	C1-C2-C3	2.01	118.18	113.64
26	a	617	LUT	C11-C10-C9	-2.01	124.44	127.31
27	a	618	XAT	C11-C10-C9	-2.01	124.44	127.31
21	7	623	BCR	C38-C26-C27	2.01	117.47	113.62
21	B	845	BCR	C1-C6-C7	2.01	121.46	115.78
18	A	820	CLA	C2A-C1A-CHA	2.01	127.37	123.86
18	A	831	CLA	CHC-C1C-C2C	-2.01	121.17	126.72
18	B	803	CLA	CMD-C2D-C3D	2.01	132.23	127.61
18	B	821	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
18	A	830	CLA	CMD-C2D-C1D	-2.01	121.18	124.71
24	7	624	LMG	C1-C2-C3	-2.01	105.82	110.00
18	L	302	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
18	7	613	CLA	O2A-C1-C2	-2.01	103.36	108.64
18	4	603	CLA	CAA-C2A-C3A	-2.01	107.29	112.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	623	LMG	C1-C2-C3	-2.00	105.82	110.00
18	F	304	CLA	O2D-CGD-CBD	2.00	114.83	111.27
21	J	102	BCR	C7-C8-C9	-2.00	123.21	126.23
18	a	608	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
24	7	624	LMG	O6-C1-O1	-2.00	105.23	109.97
25	B	850	DGD	O3E-C3E-C2E	-2.00	105.72	110.35
23	5	628	LMU	C3'-C4'-C5'	2.00	115.52	110.93
25	J	103	DGD	O6D-C5D-C6D	-2.00	102.62	106.67
25	J	103	DGD	O3G-C1D-C2D	-2.00	105.18	108.30
18	B	820	CLA	O2D-CGD-CBD	2.00	114.83	111.27
18	J	101	CLA	C2A-C1A-CHA	2.00	127.36	123.86
24	5	626	LMG	O8-C28-O10	-2.00	118.54	123.59
18	1	601	CLA	CAA-C2A-C3A	-2.00	107.30	112.78

All (208) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	801	CLA	ND
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
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

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
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	842	CLA	ND
18	A	843	CLA	ND
18	A	845	CLA	ND
18	A	854	CLA	ND
18	B	802	CLA	ND
18	B	803	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
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

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
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	F	301	CLA	ND
18	F	304	CLA	ND
18	J	101	CLA	ND
18	K	201	CLA	ND
18	K	203	CLA	ND
18	K	204	CLA	ND
18	K	206	CLA	ND
18	L	302	CLA	ND
18	L	303	CLA	ND
18	L	304	CLA	ND
18	1	601	CLA	ND
18	1	602	CLA	ND
18	1	603	CLA	ND
18	1	604	CLA	ND
18	1	606	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	1	616	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
18	a	601	CLA	ND
18	a	602	CLA	ND
18	a	603	CLA	ND
18	a	604	CLA	ND
18	a	606	CLA	ND
18	a	607	CLA	ND
18	a	608	CLA	ND
18	a	609	CLA	ND
18	a	610	CLA	ND
18	a	611	CLA	ND
18	a	612	CLA	ND
18	a	613	CLA	ND
18	a	614	CLA	ND
18	a	616	CLA	ND
18	3	602	CLA	ND
18	3	603	CLA	ND
18	3	604	CLA	ND
18	3	606	CLA	ND
18	3	607	CLA	ND
18	3	608	CLA	ND
18	3	609	CLA	ND
18	3	610	CLA	ND
18	3	611	CLA	ND
18	3	612	CLA	ND
18	3	613	CLA	ND
18	3	614	CLA	ND
18	3	615	CLA	ND
18	3	617	CLA	ND
18	4	602	CLA	ND
18	4	603	CLA	ND
18	4	604	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	613	CLA	ND
18	4	614	CLA	ND
18	4	616	CLA	ND
18	4	618	CLA	ND
18	5	601	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
18	5	602	CLA	ND
18	5	603	CLA	ND
18	5	604	CLA	ND
18	5	606	CLA	ND
18	5	607	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	616	CLA	ND
18	5	617	CLA	ND
18	5	618	CLA	ND
18	6	601	CLA	ND
18	6	602	CLA	ND
18	6	603	CLA	ND
18	6	604	CLA	ND
18	6	606	CLA	ND
18	6	607	CLA	ND
18	6	608	CLA	ND
18	6	609	CLA	ND
18	6	610	CLA	ND
18	6	611	CLA	ND
18	6	612	CLA	ND
18	6	613	CLA	ND
18	6	614	CLA	ND
18	6	616	CLA	ND
18	6	617	CLA	ND
18	6	618	CLA	ND
18	6	620	CLA	ND
18	7	602	CLA	ND
18	7	603	CLA	ND
18	7	604	CLA	ND
18	7	606	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	613	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
18	7	614	CLA	ND
18	7	615	CLA	ND
18	7	616	CLA	ND
18	8	601	CLA	ND
18	8	602	CLA	ND
18	8	603	CLA	ND
18	8	604	CLA	ND
18	8	606	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	613	CLA	ND
18	8	614	CLA	ND

All (2486) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	801	CLA	CBD-CGD-O2D-CED
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	C3A-C2A-CAA-CBA
18	A	805	CLA	C1A-C2A-CAA-CBA
18	A	805	CLA	C3A-C2A-CAA-CBA
18	A	805	CLA	C3-C5-C6-C7
18	A	806	CLA	C1A-C2A-CAA-CBA
18	A	806	CLA	CHA-CBD-CGD-O1D
18	A	806	CLA	CHA-CBD-CGD-O2D
18	A	806	CLA	CAD-CBD-CGD-O1D
18	A	806	CLA	CAD-CBD-CGD-O2D
18	A	812	CLA	C2-C3-C5-C6
18	A	812	CLA	C4-C3-C5-C6
18	A	814	CLA	C2-C3-C5-C6
18	A	814	CLA	C4-C3-C5-C6
18	A	815	CLA	CBD-CGD-O2D-CED
18	A	817	CLA	CHA-CBD-CGD-O1D
18	A	817	CLA	CHA-CBD-CGD-O2D
18	A	819	CLA	C3A-C2A-CAA-CBA
18	A	820	CLA	C1A-C2A-CAA-CBA
18	A	820	CLA	C3A-C2A-CAA-CBA
18	A	820	CLA	CHA-CBD-CGD-O1D
18	A	820	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	821	CLA	C1A-C2A-CAA-CBA
18	A	821	CLA	C3A-C2A-CAA-CBA
18	A	825	CLA	C1A-C2A-CAA-CBA
18	A	825	CLA	C3A-C2A-CAA-CBA
18	A	826	CLA	C1A-C2A-CAA-CBA
18	A	826	CLA	C3A-C2A-CAA-CBA
18	A	828	CLA	CHA-CBD-CGD-O1D
18	A	828	CLA	CHA-CBD-CGD-O2D
18	A	829	CLA	CBD-CGD-O2D-CED
18	A	837	CLA	C1A-C2A-CAA-CBA
18	A	837	CLA	CBD-CGD-O2D-CED
18	A	840	CLA	CHA-CBD-CGD-O1D
18	A	840	CLA	CHA-CBD-CGD-O2D
18	A	841	CLA	CHA-CBD-CGD-O1D
18	A	841	CLA	CHA-CBD-CGD-O2D
18	A	842	CLA	C1A-C2A-CAA-CBA
18	A	842	CLA	C3A-C2A-CAA-CBA
18	A	845	CLA	C1A-C2A-CAA-CBA
18	A	845	CLA	CHA-CBD-CGD-O1D
18	A	845	CLA	CHA-CBD-CGD-O2D
18	A	854	CLA	C4-C3-C5-C6
18	B	802	CLA	CHA-CBD-CGD-O1D
18	B	802	CLA	CHA-CBD-CGD-O2D
18	B	802	CLA	CBD-CGD-O2D-CED
18	B	802	CLA	C12-C13-C15-C16
18	B	803	CLA	C3A-C2A-CAA-CBA
18	B	803	CLA	CBD-CGD-O2D-CED
18	B	804	CLA	CBD-CGD-O2D-CED
18	B	805	CLA	C1A-C2A-CAA-CBA
18	B	805	CLA	C3A-C2A-CAA-CBA
18	B	805	CLA	C14-C13-C15-C16
18	B	807	CLA	CHA-CBD-CGD-O1D
18	B	807	CLA	CHA-CBD-CGD-O2D
18	B	808	CLA	CHA-CBD-CGD-O1D
18	B	808	CLA	CHA-CBD-CGD-O2D
18	B	810	CLA	C1A-C2A-CAA-CBA
18	B	811	CLA	CBD-CGD-O2D-CED
18	B	812	CLA	CBD-CGD-O2D-CED
18	B	813	CLA	C1A-C2A-CAA-CBA
18	B	813	CLA	C3A-C2A-CAA-CBA
18	B	813	CLA	CBD-CGD-O2D-CED
18	B	814	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	817	CLA	C1A-C2A-CAA-CBA
18	B	817	CLA	C3A-C2A-CAA-CBA
18	B	818	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	CBD-CGD-O2D-CED
18	B	830	CLA	CBD-CGD-O2D-CED
18	B	831	CLA	C2A-CAA-CBA-CGA
18	B	833	CLA	C1A-C2A-CAA-CBA
18	B	833	CLA	C2-C3-C5-C6
18	B	833	CLA	C4-C3-C5-C6
18	B	835	CLA	CBD-CGD-O2D-CED
18	B	840	CLA	C1A-C2A-CAA-CBA
18	B	840	CLA	C3A-C2A-CAA-CBA
18	B	840	CLA	CBD-CGD-O2D-CED
18	F	301	CLA	C1A-C2A-CAA-CBA
18	F	301	CLA	CBD-CGD-O2D-CED
18	F	303	CLA	C1A-C2A-CAA-CBA
18	F	303	CLA	CBD-CGD-O2D-CED
18	F	304	CLA	CBD-CGD-O2D-CED
18	J	101	CLA	C1A-C2A-CAA-CBA
18	J	101	CLA	CBD-CGD-O2D-CED
18	K	201	CLA	C1A-C2A-CAA-CBA
18	K	201	CLA	C3A-C2A-CAA-CBA
18	K	201	CLA	CBD-CGD-O2D-CED
18	K	204	CLA	CBA-CGA-O2A-C1
18	L	302	CLA	C3A-C2A-CAA-CBA
18	L	303	CLA	CHA-CBD-CGD-O1D
18	1	602	CLA	CBD-CGD-O2D-CED
18	1	603	CLA	O1A-CGA-O2A-C1
18	1	604	CLA	CAD-CBD-CGD-O1D
18	1	604	CLA	CAD-CBD-CGD-O2D
18	1	609	CLA	CBD-CGD-O2D-CED
18	1	612	CLA	CBD-CGD-O2D-CED
18	a	602	CLA	CBD-CGD-O2D-CED
18	a	604	CLA	CHA-CBD-CGD-O1D
18	a	604	CLA	CHA-CBD-CGD-O2D
18	a	604	CLA	CAD-CBD-CGD-O1D
18	a	604	CLA	CBD-CGD-O2D-CED
18	a	609	CLA	C1A-C2A-CAA-CBA
18	a	609	CLA	C3A-C2A-CAA-CBA
18	a	612	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	a	614	CLA	C1A-C2A-CAA-CBA
18	a	614	CLA	CBD-CGD-O2D-CED
18	3	603	CLA	C1A-C2A-CAA-CBA
18	3	606	CLA	CHA-CBD-CGD-O2D
18	3	609	CLA	C1A-C2A-CAA-CBA
18	3	609	CLA	C3A-C2A-CAA-CBA
18	3	610	CLA	C1A-C2A-CAA-CBA
18	3	610	CLA	C3A-C2A-CAA-CBA
18	3	612	CLA	CBD-CGD-O2D-CED
18	4	601	CLA	C1A-C2A-CAA-CBA
18	4	601	CLA	C3A-C2A-CAA-CBA
18	4	606	CLA	C1A-C2A-CAA-CBA
18	4	606	CLA	C3A-C2A-CAA-CBA
18	4	608	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C3A-C2A-CAA-CBA
18	4	609	CLA	C12-C13-C15-C16
18	4	611	CLA	C1A-C2A-CAA-CBA
18	4	611	CLA	C3A-C2A-CAA-CBA
18	4	612	CLA	C1A-C2A-CAA-CBA
18	4	613	CLA	CBD-CGD-O2D-CED
18	4	614	CLA	C2-C3-C5-C6
18	4	614	CLA	C4-C3-C5-C6
18	5	601	CLA	C1A-C2A-CAA-CBA
18	5	606	CLA	C1A-C2A-CAA-CBA
18	5	606	CLA	C3A-C2A-CAA-CBA
18	5	607	CLA	CBD-CGD-O2D-CED
18	5	608	CLA	C1A-C2A-CAA-CBA
18	5	609	CLA	C1A-C2A-CAA-CBA
18	5	609	CLA	C3A-C2A-CAA-CBA
18	5	611	CLA	C1A-C2A-CAA-CBA
18	5	611	CLA	C3A-C2A-CAA-CBA
18	5	612	CLA	C1A-C2A-CAA-CBA
18	5	612	CLA	C3A-C2A-CAA-CBA
18	5	613	CLA	CHA-CBD-CGD-O1D
18	5	613	CLA	CHA-CBD-CGD-O2D
18	5	614	CLA	C1A-C2A-CAA-CBA
18	5	614	CLA	C3A-C2A-CAA-CBA
18	5	614	CLA	CBD-CGD-O2D-CED
18	5	619	CLA	C1A-C2A-CAA-CBA
18	6	601	CLA	CHA-CBD-CGD-O1D
18	6	601	CLA	CHA-CBD-CGD-O2D
18	6	606	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	6	606	CLA	C3A-C2A-CAA-CBA
18	6	607	CLA	C1A-C2A-CAA-CBA
18	6	607	CLA	C3A-C2A-CAA-CBA
18	6	607	CLA	CHA-CBD-CGD-O1D
18	6	607	CLA	CHA-CBD-CGD-O2D
18	6	608	CLA	C2-C3-C5-C6
18	6	609	CLA	C1A-C2A-CAA-CBA
18	6	609	CLA	C3A-C2A-CAA-CBA
18	6	611	CLA	C1A-C2A-CAA-CBA
18	6	611	CLA	C3A-C2A-CAA-CBA
18	6	612	CLA	C1A-C2A-CAA-CBA
18	6	612	CLA	C3A-C2A-CAA-CBA
18	6	617	CLA	CBD-CGD-O2D-CED
18	6	618	CLA	C1A-C2A-CAA-CBA
18	6	618	CLA	C3A-C2A-CAA-CBA
18	6	620	CLA	C1A-C2A-CAA-CBA
18	7	606	CLA	C1A-C2A-CAA-CBA
18	7	606	CLA	C3A-C2A-CAA-CBA
18	7	607	CLA	C1A-C2A-CAA-CBA
18	7	607	CLA	CHA-CBD-CGD-O1D
18	7	607	CLA	CBD-CGD-O2D-CED
18	7	609	CLA	C3A-C2A-CAA-CBA
18	7	610	CLA	C6-C7-C8-C10
18	7	613	CLA	CHA-CBD-CGD-O1D
18	7	613	CLA	CHA-CBD-CGD-O2D
18	7	614	CLA	C1A-C2A-CAA-CBA
18	7	615	CLA	C1A-C2A-CAA-CBA
18	7	616	CLA	CHA-CBD-CGD-O1D
18	7	616	CLA	CHA-CBD-CGD-O2D
18	7	616	CLA	CAD-CBD-CGD-O1D
18	8	601	CLA	CHA-CBD-CGD-O1D
18	8	601	CLA	CHA-CBD-CGD-O2D
18	8	602	CLA	CBD-CGD-O2D-CED
18	8	603	CLA	C2A-CAA-CBA-CGA
18	8	604	CLA	C1A-C2A-CAA-CBA
18	8	604	CLA	CBD-CGD-O2D-CED
18	8	607	CLA	C1A-C2A-CAA-CBA
18	8	607	CLA	C3A-C2A-CAA-CBA
18	8	607	CLA	CBD-CGD-O2D-CED
18	8	608	CLA	CBD-CGD-O2D-CED
18	8	608	CLA	C2-C3-C5-C6
18	8	608	CLA	C4-C3-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	8	609	CLA	C1A-C2A-CAA-CBA
18	8	609	CLA	C3A-C2A-CAA-CBA
18	8	611	CLA	C1A-C2A-CAA-CBA
18	8	611	CLA	C3A-C2A-CAA-CBA
18	8	613	CLA	CHA-CBD-CGD-O1D
18	8	613	CLA	CHA-CBD-CGD-O2D
18	8	616	CLA	C1A-C2A-CAA-CBA
18	8	616	CLA	CAD-CBD-CGD-O1D
18	8	616	CLA	CAD-CBD-CGD-O2D
19	B	842	PQN	C11-C12-C13-C14
19	B	842	PQN	C19-C18-C20-C21
20	A	846	LHG	O1-C1-C2-C3
20	A	846	LHG	C3-O3-P-O4
20	A	847	LHG	C3-O3-P-O4
20	A	847	LHG	C3-O3-P-O5
20	A	847	LHG	C3-O3-P-O6
20	B	851	LHG	C4-O6-P-O5
20	1	620	LHG	C1-C2-C3-O3
20	3	623	LHG	O1-C1-C2-C3
20	3	623	LHG	C3-O3-P-O4
20	3	623	LHG	C3-O3-P-O5
20	3	623	LHG	C3-O3-P-O6
20	3	624	LHG	C3-O3-P-O5
20	3	624	LHG	C4-O6-P-O5
20	3	624	LHG	C24-C23-O8-C6
20	5	623	LHG	O1-C1-C2-C3
20	5	623	LHG	C4-O6-P-O5
20	5	625	LHG	C3-O3-P-O4
20	6	623	LHG	C3-O3-P-O4
20	7	622	LHG	C3-O3-P-O4
20	7	622	LHG	C3-O3-P-O6
20	7	622	LHG	C4-O6-P-O3
20	7	622	LHG	C4-O6-P-O4
20	7	622	LHG	C4-O6-P-O5
20	8	623	LHG	C1-C2-C3-O3
20	8	623	LHG	C2-C3-O3-P
20	8	623	LHG	C3-O3-P-O4
20	8	623	LHG	C4-O6-P-O3
20	8	623	LHG	C4-O6-P-O4
20	8	623	LHG	C4-O6-P-O5
20	8	623	LHG	O7-C5-C6-O8
21	A	848	BCR	C21-C22-C23-C24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	A	848	BCR	C37-C22-C23-C24
21	A	851	BCR	C21-C22-C23-C24
21	A	851	BCR	C37-C22-C23-C24
21	A	852	BCR	C17-C18-C19-C20
21	A	852	BCR	C36-C18-C19-C20
21	A	856	BCR	C21-C22-C23-C24
21	A	856	BCR	C37-C22-C23-C24
21	B	843	BCR	C7-C8-C9-C10
21	B	843	BCR	C7-C8-C9-C34
21	B	844	BCR	C7-C8-C9-C34
21	B	844	BCR	C21-C22-C23-C24
21	B	844	BCR	C37-C22-C23-C24
21	B	844	BCR	C23-C24-C25-C30
21	B	848	BCR	C21-C22-C23-C24
21	B	848	BCR	C37-C22-C23-C24
21	J	102	BCR	C21-C22-C23-C24
21	J	102	BCR	C37-C22-C23-C24
21	K	202	BCR	C7-C8-C9-C10
21	K	202	BCR	C7-C8-C9-C34
21	K	207	BCR	C21-C22-C23-C24
21	K	207	BCR	C37-C22-C23-C24
21	L	305	BCR	C7-C8-C9-C10
21	L	305	BCR	C7-C8-C9-C34
21	3	620	BCR	C21-C22-C23-C24
21	3	620	BCR	C37-C22-C23-C24
21	3	620	BCR	C23-C24-C25-C30
21	3	622	BCR	C1-C6-C7-C8
21	3	622	BCR	C5-C6-C7-C8
21	3	622	BCR	C21-C22-C23-C24
21	3	622	BCR	C37-C22-C23-C24
21	5	622	BCR	C23-C24-C25-C30
21	8	621	BCR	C7-C8-C9-C10
21	8	621	BCR	C7-C8-C9-C34
23	K	208	LMU	O5'-C1'-O1'-C1
23	5	628	LMU	O5'-C1'-O1'-C1
23	5	628	LMU	C2-C1-O1'-C1'
24	A	860	LMG	C11-C10-O7-C8
24	J	104	LMG	C11-C10-O7-C8
25	B	850	DGD	O1B-C1B-O2G-C2G
25	B	850	DGD	O2G-C2G-C3G-O3G
25	J	103	DGD	C2B-C1B-O2G-C2G
25	J	103	DGD	O6E-C1E-O5D-C6D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	1	617	LUT	C27-C28-C29-C39
26	a	617	LUT	C1-C6-C7-C8
26	4	619	LUT	C1-C6-C7-C8
26	5	620	LUT	C1-C6-C7-C8
26	6	619	LUT	C1-C6-C7-C8
27	5	621	XAT	C27-C28-C29-C30
27	5	621	XAT	C27-C28-C29-C39
27	6	621	XAT	O4-C6-C7-C8
18	B	822	CLA	O1D-CGD-O2D-CED
18	F	303	CLA	O1D-CGD-O2D-CED
18	7	608	CLA	O1D-CGD-O2D-CED
18	7	616	CLA	O1D-CGD-O2D-CED
18	A	801	CLA	O1D-CGD-O2D-CED
18	A	811	CLA	O1D-CGD-O2D-CED
18	A	817	CLA	O1D-CGD-O2D-CED
18	A	829	CLA	O1D-CGD-O2D-CED
18	B	803	CLA	O1D-CGD-O2D-CED
18	B	811	CLA	O1D-CGD-O2D-CED
18	B	835	CLA	O1D-CGD-O2D-CED
18	F	301	CLA	O1D-CGD-O2D-CED
18	F	304	CLA	O1D-CGD-O2D-CED
18	J	101	CLA	O1D-CGD-O2D-CED
18	1	609	CLA	O1D-CGD-O2D-CED
18	5	607	CLA	O1D-CGD-O2D-CED
18	7	607	CLA	O1D-CGD-O2D-CED
18	8	604	CLA	O1D-CGD-O2D-CED
18	8	608	CLA	O1D-CGD-O2D-CED
18	A	811	CLA	CBD-CGD-O2D-CED
18	A	817	CLA	CBD-CGD-O2D-CED
18	A	825	CLA	CBD-CGD-O2D-CED
18	A	834	CLA	CBD-CGD-O2D-CED
18	A	835	CLA	CBD-CGD-O2D-CED
18	B	810	CLA	CBD-CGD-O2D-CED
18	B	814	CLA	CBD-CGD-O2D-CED
18	B	815	CLA	CBD-CGD-O2D-CED
18	B	820	CLA	CBD-CGD-O2D-CED
18	B	822	CLA	CBD-CGD-O2D-CED
18	B	823	CLA	CBD-CGD-O2D-CED
18	B	829	CLA	CBD-CGD-O2D-CED
18	B	831	CLA	CBD-CGD-O2D-CED
18	B	832	CLA	CBD-CGD-O2D-CED
18	L	302	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	1	604	CLA	CBD-CGD-O2D-CED
18	a	607	CLA	CBD-CGD-O2D-CED
18	3	602	CLA	CBD-CGD-O2D-CED
18	3	603	CLA	CBD-CGD-O2D-CED
18	3	608	CLA	CBD-CGD-O2D-CED
18	4	601	CLA	CBD-CGD-O2D-CED
18	4	604	CLA	CBD-CGD-O2D-CED
18	4	607	CLA	CBD-CGD-O2D-CED
18	4	608	CLA	CBD-CGD-O2D-CED
18	4	609	CLA	CBD-CGD-O2D-CED
18	4	611	CLA	CBD-CGD-O2D-CED
18	4	614	CLA	CBD-CGD-O2D-CED
18	4	616	CLA	CBD-CGD-O2D-CED
18	5	604	CLA	CBD-CGD-O2D-CED
18	5	608	CLA	CBD-CGD-O2D-CED
18	5	617	CLA	CBD-CGD-O2D-CED
18	6	603	CLA	CBD-CGD-O2D-CED
18	6	620	CLA	CBD-CGD-O2D-CED
18	7	602	CLA	CBD-CGD-O2D-CED
18	7	604	CLA	CBD-CGD-O2D-CED
18	7	608	CLA	CBD-CGD-O2D-CED
18	7	614	CLA	CBD-CGD-O2D-CED
18	7	616	CLA	CBD-CGD-O2D-CED
18	8	611	CLA	CBD-CGD-O2D-CED
18	8	614	CLA	CBD-CGD-O2D-CED
18	8	616	CLA	CBD-CGD-O2D-CED
18	A	834	CLA	O1A-CGA-O2A-C1
18	8	613	CLA	O1A-CGA-O2A-C1
20	3	624	LHG	O10-C23-O8-C6
24	J	104	LMG	O10-C28-O8-C9
23	K	208	LMU	O5B-C1B-O1B-C4'
18	A	825	CLA	O1D-CGD-O2D-CED
18	A	834	CLA	O1D-CGD-O2D-CED
18	B	823	CLA	O1D-CGD-O2D-CED
18	L	302	CLA	O1D-CGD-O2D-CED
18	a	607	CLA	O1D-CGD-O2D-CED
18	3	603	CLA	O1D-CGD-O2D-CED
18	4	607	CLA	O1D-CGD-O2D-CED
18	4	611	CLA	O1D-CGD-O2D-CED
18	5	608	CLA	O1D-CGD-O2D-CED
18	7	604	CLA	O1D-CGD-O2D-CED
18	B	802	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	810	CLA	O1D-CGD-O2D-CED
18	B	827	CLA	O1D-CGD-O2D-CED
18	B	830	CLA	O1D-CGD-O2D-CED
18	K	201	CLA	O1D-CGD-O2D-CED
18	1	612	CLA	O1D-CGD-O2D-CED
18	a	604	CLA	O1D-CGD-O2D-CED
18	8	602	CLA	O1D-CGD-O2D-CED
18	8	611	CLA	O1D-CGD-O2D-CED
18	A	813	CLA	CBD-CGD-O2D-CED
18	A	818	CLA	CBD-CGD-O2D-CED
18	A	824	CLA	CBD-CGD-O2D-CED
18	A	838	CLA	CBD-CGD-O2D-CED
18	B	818	CLA	CBD-CGD-O2D-CED
18	B	819	CLA	CBD-CGD-O2D-CED
18	B	821	CLA	CBD-CGD-O2D-CED
18	B	833	CLA	CBD-CGD-O2D-CED
18	B	834	CLA	CBD-CGD-O2D-CED
18	K	206	CLA	CBD-CGD-O2D-CED
18	L	304	CLA	CBD-CGD-O2D-CED
18	1	611	CLA	CBD-CGD-O2D-CED
18	3	609	CLA	CBD-CGD-O2D-CED
18	4	602	CLA	CBD-CGD-O2D-CED
18	5	611	CLA	CBD-CGD-O2D-CED
18	6	602	CLA	CBD-CGD-O2D-CED
18	6	608	CLA	CBD-CGD-O2D-CED
18	6	614	CLA	CBD-CGD-O2D-CED
18	7	612	CLA	CBD-CGD-O2D-CED
18	A	818	CLA	O1A-CGA-O2A-C1
18	A	822	CLA	O1A-CGA-O2A-C1
18	B	816	CLA	O1A-CGA-O2A-C1
18	B	820	CLA	O1A-CGA-O2A-C1
18	B	821	CLA	O1A-CGA-O2A-C1
18	4	609	CLA	O1A-CGA-O2A-C1
18	5	603	CLA	O1A-CGA-O2A-C1
18	7	604	CLA	O1A-CGA-O2A-C1
18	8	604	CLA	O1A-CGA-O2A-C1
20	A	847	LHG	O10-C23-O8-C6
20	B	851	LHG	O10-C23-O8-C6
18	K	204	CLA	O1A-CGA-O2A-C1
18	B	813	CLA	O1D-CGD-O2D-CED
18	1	602	CLA	O1D-CGD-O2D-CED
18	a	612	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	a	614	CLA	O1D-CGD-O2D-CED
18	4	613	CLA	O1D-CGD-O2D-CED
18	5	614	CLA	O1D-CGD-O2D-CED
18	B	804	CLA	O1D-CGD-O2D-CED
18	B	812	CLA	O1D-CGD-O2D-CED
18	B	840	CLA	O1D-CGD-O2D-CED
18	a	602	CLA	O1D-CGD-O2D-CED
18	3	612	CLA	O1D-CGD-O2D-CED
18	8	607	CLA	O1D-CGD-O2D-CED
18	A	854	CLA	CBD-CGD-O2D-CED
18	B	806	CLA	CBD-CGD-O2D-CED
18	B	839	CLA	CBD-CGD-O2D-CED
18	1	613	CLA	CBD-CGD-O2D-CED
18	a	613	CLA	CBD-CGD-O2D-CED
18	3	604	CLA	CBD-CGD-O2D-CED
18	8	613	CLA	CBD-CGD-O2D-CED
18	A	837	CLA	O1D-CGD-O2D-CED
18	3	602	CLA	O1D-CGD-O2D-CED
20	5	625	LHG	O9-C7-O7-C5
24	J	104	LMG	O9-C10-O7-C8
25	J	103	DGD	O1B-C1B-O2G-C2G
18	3	610	CLA	O1A-CGA-O2A-C1
18	5	607	CLA	O1A-CGA-O2A-C1
18	A	836	CLA	C3-C5-C6-C7
18	A	854	CLA	C3-C5-C6-C7
18	B	806	CLA	C3-C5-C6-C7
18	B	808	CLA	C3-C5-C6-C7
18	B	809	CLA	C3-C5-C6-C7
18	1	611	CLA	C3-C5-C6-C7
18	3	607	CLA	C3-C5-C6-C7
18	4	604	CLA	C3-C5-C6-C7
18	5	607	CLA	C3-C5-C6-C7
18	6	603	CLA	C3-C5-C6-C7
18	6	616	CLA	C3-C5-C6-C7
18	7	613	CLA	C3-C5-C6-C7
19	A	844	PQN	C13-C15-C16-C17
18	A	818	CLA	CBA-CGA-O2A-C1
18	A	834	CLA	CBA-CGA-O2A-C1
18	B	816	CLA	CBA-CGA-O2A-C1
18	B	820	CLA	CBA-CGA-O2A-C1
18	B	821	CLA	CBA-CGA-O2A-C1
18	1	603	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	a	604	CLA	CBA-CGA-O2A-C1
18	4	604	CLA	CBA-CGA-O2A-C1
18	4	609	CLA	CBA-CGA-O2A-C1
18	5	603	CLA	CBA-CGA-O2A-C1
18	8	613	CLA	CBA-CGA-O2A-C1
20	A	847	LHG	C24-C23-O8-C6
20	B	851	LHG	C24-C23-O8-C6
18	B	803	CLA	C2C-C3C-CAC-CBC
23	A	858	LMU	O5B-C5B-C6B-O6B
25	B	850	DGD	C2B-C1B-O2G-C2G
18	4	604	CLA	O1D-CGD-O2D-CED
18	6	617	CLA	O1D-CGD-O2D-CED
18	A	840	CLA	CBD-CGD-O2D-CED
25	J	103	DGD	C4D-C5D-C6D-O5D
23	8	624	LMU	O5B-C1B-O1B-C4'
18	5	613	CLA	C4-C3-C5-C6
18	7	601	CLA	C4-C3-C5-C6
18	8	606	CLA	C4-C3-C5-C6
18	A	854	CLA	C2-C3-C5-C6
18	7	601	CLA	C2-C3-C5-C6
18	8	606	CLA	C2-C3-C5-C6
18	A	820	CLA	CBD-CGD-O2D-CED
18	B	817	CLA	CBD-CGD-O2D-CED
18	6	604	CLA	CBD-CGD-O2D-CED
18	A	837	CLA	C2A-CAA-CBA-CGA
18	B	809	CLA	C2A-CAA-CBA-CGA
18	B	839	CLA	C2A-CAA-CBA-CGA
18	K	206	CLA	C2A-CAA-CBA-CGA
18	a	616	CLA	C2A-CAA-CBA-CGA
18	4	601	CLA	C2A-CAA-CBA-CGA
18	4	607	CLA	C2A-CAA-CBA-CGA
24	4	624	LMG	O10-C28-O8-C9
18	A	835	CLA	O1D-CGD-O2D-CED
18	4	608	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	C3-C5-C6-C7
18	A	818	CLA	C3-C5-C6-C7
18	A	821	CLA	C3-C5-C6-C7
18	B	829	CLA	C3-C5-C6-C7
18	4	601	CLA	C3-C5-C6-C7
18	7	601	CLA	C3-C5-C6-C7
18	8	601	CLA	C3-C5-C6-C7
18	A	820	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	822	CLA	CBA-CGA-O2A-C1
18	B	810	CLA	CBA-CGA-O2A-C1
18	B	818	CLA	CBA-CGA-O2A-C1
18	B	831	CLA	CBA-CGA-O2A-C1
18	1	611	CLA	CBA-CGA-O2A-C1
18	3	603	CLA	CBA-CGA-O2A-C1
18	3	610	CLA	CBA-CGA-O2A-C1
18	4	613	CLA	CBA-CGA-O2A-C1
18	5	607	CLA	CBA-CGA-O2A-C1
18	6	608	CLA	CBA-CGA-O2A-C1
18	7	604	CLA	CBA-CGA-O2A-C1
18	8	604	CLA	CBA-CGA-O2A-C1
23	A	859	LMU	C3'-C4'-O1B-C1B
25	J	103	DGD	O6D-C5D-C6D-O5D
18	A	815	CLA	O1D-CGD-O2D-CED
18	B	831	CLA	O1D-CGD-O2D-CED
18	4	614	CLA	O1D-CGD-O2D-CED
18	5	604	CLA	O1D-CGD-O2D-CED
18	7	614	CLA	O1D-CGD-O2D-CED
19	A	844	PQN	C11-C12-C13-C14
18	B	824	CLA	CBD-CGD-O2D-CED
18	B	820	CLA	O1D-CGD-O2D-CED
18	A	820	CLA	O1A-CGA-O2A-C1
18	B	810	CLA	O1A-CGA-O2A-C1
18	B	818	CLA	O1A-CGA-O2A-C1
18	B	831	CLA	O1A-CGA-O2A-C1
18	4	604	CLA	O1A-CGA-O2A-C1
18	4	613	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	O1D-CGD-O2D-CED
18	8	616	CLA	O1D-CGD-O2D-CED
23	8	624	LMU	O5'-C5'-C6'-O6'
24	A	860	LMG	O6-C5-C6-O5
18	A	809	CLA	CBD-CGD-O2D-CED
18	A	821	CLA	CBD-CGD-O2D-CED
18	A	830	CLA	CBD-CGD-O2D-CED
18	A	831	CLA	CBD-CGD-O2D-CED
18	B	809	CLA	CBD-CGD-O2D-CED
18	5	613	CLA	CBD-CGD-O2D-CED
18	B	832	CLA	O1D-CGD-O2D-CED
20	1	620	LHG	O2-C2-C3-O3
18	A	807	CLA	C3-C5-C6-C7
18	A	829	CLA	C3-C5-C6-C7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	832	CLA	C3-C5-C6-C7
18	F	301	CLA	C3-C5-C6-C7
18	7	602	CLA	C3-C5-C6-C7
18	B	819	CLA	CBA-CGA-O2A-C1
18	1	604	CLA	CBA-CGA-O2A-C1
18	a	614	CLA	CBA-CGA-O2A-C1
18	6	614	CLA	CBA-CGA-O2A-C1
24	J	104	LMG	C29-C28-O8-C9
24	4	623	LMG	C29-C28-O8-C9
18	A	839	CLA	O1A-CGA-O2A-C1
18	1	604	CLA	O1A-CGA-O2A-C1
18	a	604	CLA	O1A-CGA-O2A-C1
18	6	608	CLA	O1A-CGA-O2A-C1
23	A	857	LMU	O5B-C5B-C6B-O6B
24	4	623	LMG	O6-C5-C6-O5
24	A	860	LMG	C4-C5-C6-O5
18	4	609	CLA	O1D-CGD-O2D-CED
18	5	617	CLA	O1D-CGD-O2D-CED
24	5	626	LMG	C11-C10-O7-C8
18	B	829	CLA	O1D-CGD-O2D-CED
18	A	845	CLA	CBD-CGD-O2D-CED
18	B	816	CLA	CBD-CGD-O2D-CED
18	B	828	CLA	CBD-CGD-O2D-CED
18	6	601	CLA	CBD-CGD-O2D-CED
23	K	208	LMU	O5'-C5'-C6'-O6'
23	K	208	LMU	C4'-C5'-C6'-O6'
23	8	625	LMU	C3'-C4'-O1B-C1B
18	1	611	CLA	O1A-CGA-O2A-C1
18	B	815	CLA	O1D-CGD-O2D-CED
18	4	601	CLA	O1D-CGD-O2D-CED
18	8	603	CLA	CBD-CGD-O2D-CED
18	6	613	CLA	C3-C5-C6-C7
18	A	839	CLA	CBA-CGA-O2A-C1
18	a	614	CLA	O1A-CGA-O2A-C1
18	3	603	CLA	O1A-CGA-O2A-C1
18	A	836	CLA	C4-C3-C5-C6
18	B	818	CLA	C4-C3-C5-C6
18	8	610	CLA	C4-C3-C5-C6
24	4	623	LMG	C4-C5-C6-O5
18	A	836	CLA	C2-C3-C5-C6
18	B	818	CLA	C2-C3-C5-C6
18	8	610	CLA	C2-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	843	CLA	C2A-CAA-CBA-CGA
18	K	201	CLA	C2A-CAA-CBA-CGA
18	5	616	CLA	C2A-CAA-CBA-CGA
18	8	616	CLA	C2A-CAA-CBA-CGA
18	3	608	CLA	O1D-CGD-O2D-CED
18	6	620	CLA	O1D-CGD-O2D-CED
18	8	614	CLA	O1D-CGD-O2D-CED
23	8	625	LMU	O5B-C5B-C6B-O6B
18	B	819	CLA	O1A-CGA-O2A-C1
24	4	623	LMG	O10-C28-O8-C9
24	7	624	LMG	O6-C1-O1-C7
18	A	801	CLA	CBA-CGA-O2A-C1
18	A	821	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	CBA-CGA-O2A-C1
18	A	845	CLA	CBA-CGA-O2A-C1
18	B	811	CLA	CBA-CGA-O2A-C1
20	A	846	LHG	C24-C23-O8-C6
20	8	622	LHG	C24-C23-O8-C6
18	B	821	CLA	O1D-CGD-O2D-CED
23	A	858	LMU	C4B-C5B-C6B-O6B
18	4	616	CLA	O1D-CGD-O2D-CED
18	6	603	CLA	O1D-CGD-O2D-CED
18	6	614	CLA	O1A-CGA-O2A-C1
23	A	857	LMU	C4B-C5B-C6B-O6B
18	A	818	CLA	O1D-CGD-O2D-CED
18	B	819	CLA	O1D-CGD-O2D-CED
18	B	833	CLA	O1D-CGD-O2D-CED
18	K	206	CLA	O1D-CGD-O2D-CED
18	1	604	CLA	O1D-CGD-O2D-CED
18	1	611	CLA	O1D-CGD-O2D-CED
18	3	609	CLA	O1D-CGD-O2D-CED
18	7	602	CLA	O1D-CGD-O2D-CED
18	7	612	CLA	O1D-CGD-O2D-CED
18	6	608	CLA	O1D-CGD-O2D-CED
20	A	846	LHG	C1-C2-C3-O3
20	A	847	LHG	C1-C2-C3-O3
23	8	625	LMU	C4B-C5B-C6B-O6B
18	A	801	CLA	O1A-CGA-O2A-C1
18	A	821	CLA	O1A-CGA-O2A-C1
18	B	811	CLA	O1A-CGA-O2A-C1
18	B	833	CLA	C3-C5-C6-C7
18	A	835	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	843	CLA	CBA-CGA-O2A-C1
18	B	824	CLA	CBA-CGA-O2A-C1
18	a	613	CLA	CBA-CGA-O2A-C1
18	4	614	CLA	CBA-CGA-O2A-C1
18	6	604	CLA	CBA-CGA-O2A-C1
18	6	616	CLA	CBA-CGA-O2A-C1
18	7	613	CLA	CBA-CGA-O2A-C1
20	7	622	LHG	C24-C23-O8-C6
24	4	624	LMG	C29-C28-O8-C9
24	7	624	LMG	C29-C28-O8-C9
18	4	603	CLA	CBD-CGD-O2D-CED
18	B	803	CLA	C4C-C3C-CAC-CBC
23	5	628	LMU	O5B-C1B-O1B-C4'
18	A	814	CLA	C13-C15-C16-C17
18	4	601	CLA	C15-C16-C17-C18
23	K	208	LMU	O1'-C1-C2-C3
18	6	614	CLA	O1D-CGD-O2D-CED
18	A	825	CLA	C15-C16-C17-C18
18	B	828	CLA	C13-C15-C16-C17
19	B	842	PQN	C25-C26-C27-C28
20	A	846	LHG	O2-C2-C3-O3
20	8	623	LHG	O2-C2-C3-O3
18	A	841	CLA	C3-C5-C6-C7
20	6	623	LHG	C23-C24-C25-C26
23	5	628	LMU	C2'-C1'-O1'-C1
24	J	104	LMG	C2-C1-O1-C7
24	7	624	LMG	C2-C1-O1-C7
24	4	624	LMG	O7-C8-C9-O8
20	B	851	LHG	C29-C30-C31-C32
18	A	835	CLA	O1A-CGA-O2A-C1
18	4	614	CLA	O1A-CGA-O2A-C1
24	5	626	LMG	O10-C28-O8-C9
18	5	613	CLA	C2-C3-C5-C6
18	A	829	CLA	C14-C13-C15-C16
18	B	808	CLA	C11-C12-C13-C14
18	B	818	CLA	C6-C7-C8-C9
18	B	828	CLA	C14-C13-C15-C16
18	6	604	CLA	C6-C7-C8-C9
18	B	818	CLA	O1D-CGD-O2D-CED
18	6	602	CLA	O1D-CGD-O2D-CED
18	7	611	CLA	C10-C11-C12-C13
18	A	821	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	854	CLA	C2A-CAA-CBA-CGA
18	3	609	CLA	C2A-CAA-CBA-CGA
18	5	609	CLA	C2A-CAA-CBA-CGA
21	B	801	BCR	C37-C22-C23-C24
21	B	847	BCR	C37-C22-C23-C24
21	J	102	BCR	C11-C12-C13-C35
21	J	102	BCR	C36-C18-C19-C20
21	K	202	BCR	C37-C22-C23-C24
21	L	305	BCR	C36-C18-C19-C20
21	6	622	BCR	C11-C12-C13-C35
27	8	620	XAT	C27-C28-C29-C39
28	6	624	NEX	C11-C12-C13-C20
21	J	102	BCR	C17-C18-C19-C20
21	K	202	BCR	C21-C22-C23-C24
23	8	624	LMU	O5B-C5B-C6B-O6B
20	5	625	LHG	C8-C7-O7-C5
20	B	851	LHG	C23-C24-C25-C26
20	7	622	LHG	C23-C24-C25-C26
18	A	843	CLA	O1A-CGA-O2A-C1
18	a	613	CLA	O1A-CGA-O2A-C1
18	A	803	CLA	C15-C16-C17-C18
18	A	811	CLA	C5-C6-C7-C8
18	B	825	CLA	C10-C11-C12-C13
18	B	837	CLA	C15-C16-C17-C18
18	a	613	CLA	C10-C11-C12-C13
18	3	607	CLA	C5-C6-C7-C8
18	5	602	CLA	C10-C11-C12-C13
18	A	824	CLA	O1D-CGD-O2D-CED
18	B	834	CLA	O1D-CGD-O2D-CED
24	5	626	LMG	O6-C5-C6-O5
23	8	624	LMU	C4'-C5'-C6'-O6'
18	1	601	CLA	CBA-CGA-O2A-C1
18	5	604	CLA	CBA-CGA-O2A-C1
18	A	822	CLA	C13-C15-C16-C17
18	a	601	CLA	C5-C6-C7-C8
18	a	603	CLA	C5-C6-C7-C8
18	3	604	CLA	C5-C6-C7-C8
18	5	607	CLA	C8-C10-C11-C12
18	6	601	CLA	C15-C16-C17-C18
18	7	601	CLA	C5-C6-C7-C8
19	A	844	PQN	C18-C20-C21-C22
20	4	622	LHG	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	5	623	LHG	C23-C24-C25-C26
18	A	813	CLA	O1D-CGD-O2D-CED
18	6	616	CLA	O1A-CGA-O2A-C1
24	J	104	LMG	O6-C5-C6-O5
18	A	804	CLA	C13-C15-C16-C17
18	A	806	CLA	C5-C6-C7-C8
18	A	812	CLA	C8-C10-C11-C12
18	A	834	CLA	C10-C11-C12-C13
18	B	833	CLA	C5-C6-C7-C8
18	B	833	CLA	C13-C15-C16-C17
18	1	603	CLA	C5-C6-C7-C8
18	1	613	CLA	C10-C11-C12-C13
18	3	609	CLA	C5-C6-C7-C8
18	3	609	CLA	C10-C11-C12-C13
18	4	601	CLA	C13-C15-C16-C17
18	5	602	CLA	C8-C10-C11-C12
18	5	603	CLA	C5-C6-C7-C8
18	5	604	CLA	C5-C6-C7-C8
18	5	609	CLA	C15-C16-C17-C18
18	6	601	CLA	C5-C6-C7-C8
18	6	613	CLA	C5-C6-C7-C8
18	L	304	CLA	O1D-CGD-O2D-CED
20	3	623	LHG	O1-C1-C2-O2
20	5	623	LHG	O1-C1-C2-O2
20	7	622	LHG	O1-C1-C2-O2
18	6	604	CLA	O1A-CGA-O2A-C1
20	3	623	LHG	C7-C8-C9-C10
20	5	625	LHG	C23-C24-C25-C26
24	7	624	LMG	C10-C11-C12-C13
25	B	850	DGD	C1B-C2B-C3B-C4B
18	K	204	CLA	CBD-CGD-O2D-CED
18	L	303	CLA	CBD-CGD-O2D-CED
18	A	834	CLA	C15-C16-C17-C18
18	B	806	CLA	C5-C6-C7-C8
18	1	601	CLA	C5-C6-C7-C8
18	3	610	CLA	C13-C15-C16-C17
18	5	604	CLA	C13-C15-C16-C17
18	6	616	CLA	C10-C11-C12-C13
18	7	610	CLA	C5-C6-C7-C8
18	B	803	CLA	CBA-CGA-O2A-C1
18	B	805	CLA	CBA-CGA-O2A-C1
18	A	838	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	8	625	LMU	O5'-C5'-C6'-O6'
18	A	843	CLA	C2-C1-O2A-CGA
18	A	812	CLA	C15-C16-C17-C18
18	A	836	CLA	C13-C15-C16-C17
18	B	824	CLA	C10-C11-C12-C13
18	B	831	CLA	C15-C16-C17-C18
18	1	611	CLA	C8-C10-C11-C12
18	A	833	CLA	CBD-CGD-O2D-CED
18	A	841	CLA	CBD-CGD-O2D-CED
18	a	609	CLA	CBD-CGD-O2D-CED
18	B	812	CLA	C2A-CAA-CBA-CGA
18	B	825	CLA	C13-C15-C16-C17
18	B	827	CLA	C13-C15-C16-C17
18	B	824	CLA	C13-C15-C16-C17
18	6	610	CLA	C15-C16-C17-C18
18	8	601	CLA	C8-C10-C11-C12
18	B	806	CLA	O1D-CGD-O2D-CED
18	8	613	CLA	O1D-CGD-O2D-CED
18	a	609	CLA	C11-C12-C13-C15
18	8	613	CLA	C11-C10-C8-C7
18	8	610	CLA	C3-C5-C6-C7
18	7	613	CLA	O1A-CGA-O2A-C1
18	3	613	CLA	CAA-CBA-CGA-O2A
18	A	830	CLA	C2A-CAA-CBA-CGA
18	B	813	CLA	C2A-CAA-CBA-CGA
18	4	613	CLA	C2A-CAA-CBA-CGA
18	1	613	CLA	O1D-CGD-O2D-CED
18	4	602	CLA	O1D-CGD-O2D-CED
18	5	611	CLA	O1D-CGD-O2D-CED
18	B	808	CLA	C5-C6-C7-C8
18	B	814	CLA	C8-C10-C11-C12
18	6	613	CLA	C10-C11-C12-C13
18	6	614	CLA	C5-C6-C7-C8
18	8	601	CLA	C13-C15-C16-C17
18	8	606	CLA	C8-C10-C11-C12
18	B	824	CLA	O1A-CGA-O2A-C1
18	6	604	CLA	C5-C6-C7-C8
18	7	613	CLA	C15-C16-C17-C18
18	a	613	CLA	O1D-CGD-O2D-CED
20	A	847	LHG	O2-C2-C3-O3
20	6	623	LHG	O2-C2-C3-O3
24	A	860	LMG	O9-C10-O7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	806	CLA	C13-C15-C16-C17
18	A	812	CLA	C13-C15-C16-C17
18	B	834	CLA	C8-C10-C11-C12
18	B	837	CLA	C5-C6-C7-C8
18	A	808	CLA	CBA-CGA-O2A-C1
20	4	622	LHG	C24-C23-O8-C6
18	A	854	CLA	O1D-CGD-O2D-CED
18	B	839	CLA	O1D-CGD-O2D-CED
18	A	830	CLA	O1A-CGA-O2A-C1
18	A	845	CLA	O1A-CGA-O2A-C1
18	1	601	CLA	O1A-CGA-O2A-C1
18	5	604	CLA	O1A-CGA-O2A-C1
20	8	622	LHG	O10-C23-O8-C6
18	A	807	CLA	C15-C16-C17-C18
18	A	812	CLA	C5-C6-C7-C8
18	A	830	CLA	C8-C10-C11-C12
18	B	814	CLA	C13-C15-C16-C17
18	K	203	CLA	C5-C6-C7-C8
18	3	609	CLA	C8-C10-C11-C12
18	6	601	CLA	C13-C15-C16-C17
18	7	611	CLA	C5-C6-C7-C8
18	7	613	CLA	C13-C15-C16-C17
18	8	613	CLA	C15-C16-C17-C18
18	A	842	CLA	C10-C11-C12-C13
18	B	805	CLA	C13-C15-C16-C17
18	B	813	CLA	C5-C6-C7-C8
18	5	601	CLA	C5-C6-C7-C8
18	5	609	CLA	C13-C15-C16-C17
18	6	613	CLA	C15-C16-C17-C18
18	6	616	CLA	C13-C15-C16-C17
20	a	620	LHG	C3-O3-P-O6
20	5	625	LHG	C3-O3-P-O6
20	6	623	LHG	C3-O3-P-O6
20	8	622	LHG	C4-O6-P-O3
20	8	623	LHG	C3-O3-P-O6
24	5	627	LMG	C10-C11-C12-C13
18	A	825	CLA	C3-C5-C6-C7
18	5	603	CLA	C3-C5-C6-C7
18	A	838	CLA	CBA-CGA-O2A-C1
18	1	613	CLA	CBA-CGA-O2A-C1
18	A	840	CLA	O1D-CGD-O2D-CED
24	5	627	LMG	C28-C29-C30-C31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	817	CLA	O1D-CGD-O2D-CED
18	3	604	CLA	O1D-CGD-O2D-CED
18	B	829	CLA	C4-C3-C5-C6
18	A	828	CLA	CAA-CBA-CGA-O2A
18	a	609	CLA	C8-C10-C11-C12
18	3	602	CLA	C8-C10-C11-C12
18	B	830	CLA	C2C-C3C-CAC-CBC
18	A	818	CLA	C2A-CAA-CBA-CGA
18	B	827	CLA	C2A-CAA-CBA-CGA
18	A	801	CLA	C3-C5-C6-C7
18	1	603	CLA	C3-C5-C6-C7
18	B	813	CLA	CBA-CGA-O2A-C1
18	A	841	CLA	C5-C6-C7-C8
18	B	802	CLA	C10-C11-C12-C13
20	3	624	LHG	C26-C27-C28-C29
20	3	624	LHG	C33-C34-C35-C36
20	8	623	LHG	C32-C33-C34-C35
20	6	623	LHG	C8-C7-O7-C5
24	4	623	LMG	C11-C10-O7-C8
18	5	613	CLA	C2A-CAA-CBA-CGA
20	A	846	LHG	C32-C33-C34-C35
20	5	625	LHG	C15-C16-C17-C18
20	8	622	LHG	C11-C10-C9-C8
20	8	622	LHG	C31-C32-C33-C34
25	J	103	DGD	C3A-C4A-C5A-C6A
18	A	822	CLA	C16-C17-C18-C20
18	B	809	CLA	C16-C17-C18-C19
18	B	826	CLA	C6-C7-C8-C10
18	1	603	CLA	C6-C7-C8-C9
18	5	613	CLA	C16-C17-C18-C20
18	7	601	CLA	C11-C12-C13-C15
18	7	602	CLA	C16-C17-C18-C20
18	B	809	CLA	CBA-CGA-O2A-C1
20	1	620	LHG	C25-C26-C27-C28
20	5	625	LHG	C13-C14-C15-C16
20	8	623	LHG	C15-C16-C17-C18
23	8	625	LMU	C2-C3-C4-C5
25	J	103	DGD	C6A-C7A-C8A-C9A
25	J	103	DGD	C4B-C5B-C6B-C7B
18	A	827	CLA	CBD-CGD-O2D-CED
20	A	846	LHG	C31-C32-C33-C34
20	3	623	LHG	C11-C10-C9-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	5	623	LHG	C16-C17-C18-C19
20	6	623	LHG	C27-C28-C29-C30
24	J	104	LMG	C31-C32-C33-C34
24	5	626	LMG	C30-C31-C32-C33
18	A	820	CLA	O1D-CGD-O2D-CED
18	6	604	CLA	O1D-CGD-O2D-CED
20	8	622	LHG	C2-C3-O3-P
20	5	623	LHG	C12-C13-C14-C15
20	5	625	LHG	C30-C31-C32-C33
24	A	860	LMG	C17-C18-C19-C20
24	J	104	LMG	C17-C18-C19-C20
18	B	809	CLA	O1D-CGD-O2D-CED
20	3	623	LHG	O2-C2-C3-O3
20	1	620	LHG	C23-C24-C25-C26
18	A	830	CLA	O1D-CGD-O2D-CED
23	A	859	LMU	O5'-C1'-O1'-C1
23	8	624	LMU	C2'-C1'-O1'-C1
25	J	103	DGD	C2D-C1D-O3G-C3G
18	a	609	CLA	CBA-CGA-O2A-C1
24	5	626	LMG	C29-C28-O8-C9
20	3	624	LHG	C12-C13-C14-C15
18	5	613	CLA	C10-C11-C12-C13
18	B	805	CLA	O1A-CGA-O2A-C1
18	A	812	CLA	C16-C17-C18-C20
18	a	609	CLA	C16-C17-C18-C20
18	4	602	CLA	C11-C12-C13-C14
18	5	603	CLA	C6-C7-C8-C10
18	A	809	CLA	O1D-CGD-O2D-CED
18	A	821	CLA	O1D-CGD-O2D-CED
18	B	807	CLA	C4-C3-C5-C6
18	B	814	CLA	C4-C3-C5-C6
20	3	624	LHG	C28-C29-C30-C31
20	8	623	LHG	C10-C11-C12-C13
20	8	623	LHG	C27-C28-C29-C30
23	8	625	LMU	C7-C8-C9-C10
25	J	103	DGD	C5B-C6B-C7B-C8B
18	A	807	CLA	C11-C10-C8-C9
18	A	828	CLA	C11-C10-C8-C9
18	K	203	CLA	C11-C10-C8-C9
18	4	608	CLA	C11-C12-C13-C14
18	A	843	CLA	C8-C10-C11-C12
20	1	620	LHG	C27-C28-C29-C30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	3	624	LHG	C24-C25-C26-C27
20	5	623	LHG	C15-C16-C17-C18
20	8	622	LHG	C32-C33-C34-C35
23	A	858	LMU	C6-C7-C8-C9
24	5	627	LMG	C32-C33-C34-C35
25	B	850	DGD	C6A-C7A-C8A-C9A
25	J	103	DGD	C7A-C8A-C9A-CAA
25	J	103	DGD	C3B-C4B-C5B-C6B
18	A	820	CLA	C15-C16-C17-C18
18	A	854	CLA	C8-C10-C11-C12
18	A	822	CLA	C2A-CAA-CBA-CGA
18	B	820	CLA	C2A-CAA-CBA-CGA
18	1	604	CLA	C2A-CAA-CBA-CGA
18	a	609	CLA	C2A-CAA-CBA-CGA
18	3	608	CLA	C2A-CAA-CBA-CGA
18	4	608	CLA	C2A-CAA-CBA-CGA
18	5	608	CLA	C2A-CAA-CBA-CGA
18	A	808	CLA	O1A-CGA-O2A-C1
18	B	803	CLA	O1A-CGA-O2A-C1
21	L	305	BCR	C37-C22-C23-C24
20	A	847	LHG	C11-C10-C9-C8
20	3	624	LHG	C9-C10-C11-C12
20	6	623	LHG	C31-C32-C33-C34
25	J	103	DGD	C4A-C5A-C6A-C7A
25	J	103	DGD	C9A-CAA-CBA-CCA
20	4	622	LHG	O1-C1-C2-C3
20	5	625	LHG	O1-C1-C2-C3
20	7	622	LHG	O1-C1-C2-C3
21	B	801	BCR	C21-C22-C23-C24
21	B	844	BCR	C7-C8-C9-C10
21	L	305	BCR	C21-C22-C23-C24
18	A	814	CLA	C3-C5-C6-C7
18	B	805	CLA	C3-C5-C6-C7
18	B	827	CLA	C3-C5-C6-C7
20	A	846	LHG	O9-C7-O7-C5
18	B	818	CLA	C5-C6-C7-C8
24	A	860	LMG	C11-C12-C13-C14
24	4	623	LMG	C17-C18-C19-C20
24	5	626	LMG	C16-C17-C18-C19
24	5	626	LMG	C28-C29-C30-C31
20	3	623	LHG	C29-C30-C31-C32
20	5	625	LHG	C34-C35-C36-C37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	8	622	LHG	C28-C29-C30-C31
20	8	623	LHG	C14-C15-C16-C17
24	A	860	LMG	C32-C33-C34-C35
24	5	626	LMG	C32-C33-C34-C35
24	5	627	LMG	C17-C18-C19-C20
18	B	809	CLA	C16-C17-C18-C20
18	B	816	CLA	C6-C7-C8-C9
18	B	816	CLA	C6-C7-C8-C10
18	B	832	CLA	C11-C12-C13-C14
18	B	832	CLA	C11-C12-C13-C15
18	1	603	CLA	C6-C7-C8-C10
18	1	611	CLA	C16-C17-C18-C19
23	8	624	LMU	O5'-C1'-O1'-C1
25	J	103	DGD	O6D-C1D-O3G-C3G
18	A	836	CLA	C8-C10-C11-C12
20	3	623	LHG	C28-C29-C30-C31
20	5	623	LHG	C11-C12-C13-C14
20	5	625	LHG	C27-C28-C29-C30
20	8	623	LHG	C17-C18-C19-C20
24	7	624	LMG	C30-C31-C32-C33
18	A	831	CLA	O1D-CGD-O2D-CED
18	B	828	CLA	O1D-CGD-O2D-CED
20	a	620	LHG	C27-C28-C29-C30
20	8	622	LHG	C18-C19-C20-C21
20	8	622	LHG	C30-C31-C32-C33
20	8	623	LHG	C33-C34-C35-C36
23	8	624	LMU	C4-C5-C6-C7
24	7	624	LMG	C17-C18-C19-C20
20	A	847	LHG	C23-C24-C25-C26
20	3	623	LHG	C17-C18-C19-C20
20	4	622	LHG	C29-C30-C31-C32
20	8	622	LHG	C33-C34-C35-C36
24	4	624	LMG	C32-C33-C34-C35
18	B	824	CLA	O1D-CGD-O2D-CED
25	B	850	DGD	O6E-C5E-C6E-O5E
20	7	622	LHG	C29-C30-C31-C32
18	A	828	CLA	C3A-C2A-CAA-CBA
18	B	809	CLA	C3A-C2A-CAA-CBA
18	B	810	CLA	C3A-C2A-CAA-CBA
18	B	826	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C3A-C2A-CAA-CBA
18	B	833	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	F	301	CLA	C3A-C2A-CAA-CBA
18	a	606	CLA	C3A-C2A-CAA-CBA
18	3	603	CLA	C3A-C2A-CAA-CBA
18	5	601	CLA	C3A-C2A-CAA-CBA
18	5	619	CLA	C3A-C2A-CAA-CBA
18	6	616	CLA	C3A-C2A-CAA-CBA
18	7	615	CLA	CBD-CGD-O2D-CED
18	8	616	CLA	C3A-C2A-CAA-CBA
18	A	834	CLA	C13-C15-C16-C17
18	B	828	CLA	C8-C10-C11-C12
18	3	602	CLA	C10-C11-C12-C13
23	A	857	LMU	C2-C1-O1'-C1'
23	8	625	LMU	C2-C1-O1'-C1'
20	A	846	LHG	C25-C26-C27-C28
24	7	624	LMG	C20-C21-C22-C23
25	B	850	DGD	CEB-CFB-CGB-CHB
18	1	613	CLA	O1A-CGA-O2A-C1
18	A	812	CLA	C16-C17-C18-C19
18	1	611	CLA	C16-C17-C18-C20
18	a	609	CLA	C16-C17-C18-C19
18	5	613	CLA	C16-C17-C18-C19
18	7	601	CLA	C11-C12-C13-C14
20	B	851	LHG	C24-C25-C26-C27
18	5	613	CLA	O1D-CGD-O2D-CED
20	5	623	LHG	C32-C33-C34-C35
18	a	610	CLA	C5-C6-C7-C8
18	4	610	CLA	C10-C11-C12-C13
18	4	613	CLA	C13-C15-C16-C17
18	3	608	CLA	C4-C3-C5-C6
19	B	842	PQN	C14-C13-C15-C16
18	4	601	CLA	CBA-CGA-O2A-C1
18	3	608	CLA	C2-C3-C5-C6
20	A	846	LHG	O1-C1-C2-O2
20	4	622	LHG	O1-C1-C2-O2
20	5	625	LHG	O1-C1-C2-O2
23	A	858	LMU	C3'-C4'-O1B-C1B
23	A	858	LMU	C5'-C4'-O1B-C1B
24	4	623	LMG	C16-C17-C18-C19
24	5	626	LMG	C15-C16-C17-C18
18	7	611	CLA	C3-C5-C6-C7
18	A	838	CLA	O1A-CGA-O2A-C1
24	A	860	LMG	C10-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	822	CLA	C16-C17-C18-C19
18	B	826	CLA	C6-C7-C8-C9
23	8	625	LMU	C11-C10-C9-C8
18	A	843	CLA	C3-C5-C6-C7
20	A	846	LHG	C17-C18-C19-C20
20	8	623	LHG	C29-C30-C31-C32
18	B	813	CLA	O1A-CGA-O2A-C1
18	A	829	CLA	C13-C15-C16-C17
18	6	613	CLA	C8-C10-C11-C12
18	6	601	CLA	O1D-CGD-O2D-CED
24	5	626	LMG	C14-C15-C16-C17
20	3	623	LHG	C30-C31-C32-C33
23	K	208	LMU	C5-C6-C7-C8
18	B	810	CLA	C10-C11-C12-C13
18	B	809	CLA	O1A-CGA-O2A-C1
24	7	624	LMG	O10-C28-O8-C9
20	4	622	LHG	C12-C13-C14-C15
18	5	603	CLA	C6-C7-C8-C9
18	A	806	CLA	C3-C5-C6-C7
18	4	614	CLA	C3-C5-C6-C7
21	A	848	BCR	C1-C6-C7-C8
21	A	848	BCR	C5-C6-C7-C8
21	A	851	BCR	C23-C24-C25-C26
21	A	851	BCR	C23-C24-C25-C30
21	A	856	BCR	C1-C6-C7-C8
21	A	856	BCR	C5-C6-C7-C8
21	A	856	BCR	C23-C24-C25-C26
21	A	856	BCR	C23-C24-C25-C30
21	B	843	BCR	C1-C6-C7-C8
21	B	843	BCR	C5-C6-C7-C8
21	B	844	BCR	C23-C24-C25-C26
21	B	848	BCR	C5-C6-C7-C8
21	L	301	BCR	C1-C6-C7-C8
21	L	301	BCR	C5-C6-C7-C8
21	L	305	BCR	C5-C6-C7-C8
21	L	305	BCR	C23-C24-C25-C26
21	L	305	BCR	C23-C24-C25-C30
21	3	620	BCR	C23-C24-C25-C26
21	5	622	BCR	C23-C24-C25-C26
21	6	622	BCR	C23-C24-C25-C26
21	6	622	BCR	C23-C24-C25-C30
21	8	621	BCR	C1-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	8	621	BCR	C5-C6-C7-C8
26	1	617	LUT	C1-C6-C7-C8
26	1	617	LUT	C5-C6-C7-C8
26	a	617	LUT	C5-C6-C7-C8
26	4	619	LUT	C5-C6-C7-C8
26	5	620	LUT	C5-C6-C7-C8
26	6	619	LUT	C5-C6-C7-C8
26	8	619	LUT	C1-C6-C7-C8
26	8	619	LUT	C5-C6-C7-C8
24	4	624	LMG	O6-C5-C6-O5
20	3	623	LHG	C9-C10-C11-C12
20	5	625	LHG	C14-C15-C16-C17
20	5	625	LHG	C32-C33-C34-C35
23	8	624	LMU	O1'-C1-C2-C3
20	6	623	LHG	C24-C23-O8-C6
24	5	627	LMG	C29-C28-O8-C9
18	B	809	CLA	C10-C11-C12-C13
18	B	827	CLA	C5-C6-C7-C8
18	4	608	CLA	C5-C6-C7-C8
18	8	613	CLA	C5-C6-C7-C8
20	8	623	LHG	C8-C7-O7-C5
18	a	609	CLA	O1A-CGA-O2A-C1
24	5	626	LMG	C17-C18-C19-C20
23	A	858	LMU	C1-C2-C3-C4
18	A	825	CLA	C13-C15-C16-C17
18	5	613	CLA	C13-C15-C16-C17
20	A	846	LHG	C13-C14-C15-C16
20	4	622	LHG	C31-C32-C33-C34
18	B	808	CLA	C4-C3-C5-C6
18	A	826	CLA	C11-C10-C8-C7
18	A	828	CLA	C11-C10-C8-C7
18	A	836	CLA	C11-C12-C13-C15
18	B	803	CLA	C11-C10-C8-C7
18	B	808	CLA	C2-C3-C5-C6
18	B	809	CLA	C12-C13-C15-C16
18	B	814	CLA	C2-C3-C5-C6
18	B	818	CLA	C6-C7-C8-C10
18	B	832	CLA	C2-C3-C5-C6
18	K	203	CLA	C11-C10-C8-C7
18	4	608	CLA	C11-C12-C13-C15
18	4	608	CLA	C12-C13-C15-C16
18	6	614	CLA	C11-C10-C8-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	8	613	CLA	C12-C13-C15-C16
19	B	842	PQN	C21-C22-C23-C25
18	4	601	CLA	O1A-CGA-O2A-C1
18	B	830	CLA	C4C-C3C-CAC-CBC
20	A	846	LHG	C27-C28-C29-C30
18	8	606	CLA	C13-C15-C16-C17
24	5	626	LMG	O9-C10-O7-C8
18	A	804	CLA	CBA-CGA-O2A-C1
18	A	807	CLA	CBA-CGA-O2A-C1
18	8	602	CLA	CBA-CGA-O2A-C1
18	A	803	CLA	C2A-CAA-CBA-CGA
18	A	819	CLA	C2A-CAA-CBA-CGA
18	A	841	CLA	C2A-CAA-CBA-CGA
18	B	828	CLA	C2A-CAA-CBA-CGA
18	6	610	CLA	C2A-CAA-CBA-CGA
18	A	825	CLA	C8-C10-C11-C12
18	B	829	CLA	C10-C11-C12-C13
18	5	607	CLA	C5-C6-C7-C8
18	6	616	CLA	C15-C16-C17-C18
18	A	826	CLA	C2A-CAA-CBA-CGA
20	8	623	LHG	C25-C26-C27-C28
23	A	857	LMU	O5B-C1B-O1B-C4'
18	A	845	CLA	O1D-CGD-O2D-CED
20	3	624	LHG	C31-C32-C33-C34
23	K	208	LMU	C4-C5-C6-C7
18	B	816	CLA	O1D-CGD-O2D-CED
18	B	838	CLA	CBD-CGD-O2D-CED
18	3	607	CLA	CBA-CGA-O2A-C1
18	A	806	CLA	C8-C10-C11-C12
18	A	806	CLA	C15-C16-C17-C18
20	4	622	LHG	C32-C33-C34-C35
20	B	851	LHG	C8-C7-O7-C5
20	8	622	LHG	C8-C7-O7-C5
24	7	624	LMG	C11-C10-O7-C8
20	8	622	LHG	C25-C26-C27-C28
18	4	601	CLA	C5-C6-C7-C8
18	B	841	CLA	CBD-CGD-O2D-CED
20	6	623	LHG	O9-C7-O7-C5
20	8	622	LHG	O9-C7-O7-C5
20	8	623	LHG	O9-C7-O7-C5
24	4	623	LMG	O9-C10-O7-C8
18	B	818	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	5	623	LHG	C13-C14-C15-C16
23	A	859	LMU	C3-C4-C5-C6
24	5	627	LMG	C30-C31-C32-C33
25	J	103	DGD	C2E-C1E-O5D-C6D
20	A	846	LHG	O7-C5-C6-O8
24	5	626	LMG	O1-C7-C8-O7
23	5	628	LMU	O5'-C5'-C6'-O6'
18	A	843	CLA	C5-C6-C7-C8
20	5	623	LHG	C30-C31-C32-C33
25	B	850	DGD	C4A-C5A-C6A-C7A
18	B	814	CLA	C15-C16-C17-C18
24	7	624	LMG	C18-C19-C20-C21
18	8	603	CLA	O1D-CGD-O2D-CED
18	B	832	CLA	C4-C3-C5-C6
18	B	807	CLA	C2-C3-C5-C6
18	B	829	CLA	C2-C3-C5-C6
20	A	846	LHG	C30-C31-C32-C33
18	A	809	CLA	C14-C13-C15-C16
18	A	826	CLA	C11-C10-C8-C9
18	A	836	CLA	C11-C12-C13-C14
18	B	802	CLA	C11-C10-C8-C9
18	B	805	CLA	C11-C12-C13-C14
18	B	809	CLA	C14-C13-C15-C16
18	a	609	CLA	C11-C12-C13-C14
18	4	608	CLA	C14-C13-C15-C16
18	5	604	CLA	C6-C7-C8-C9
18	5	604	CLA	C11-C10-C8-C9
18	6	614	CLA	C11-C10-C8-C9
18	8	602	CLA	C11-C10-C8-C9
19	A	844	PQN	C21-C22-C23-C24
18	B	811	CLA	C3-C5-C6-C7
18	A	809	CLA	C2A-CAA-CBA-CGA
18	A	829	CLA	C2A-CAA-CBA-CGA
18	1	616	CLA	C2A-CAA-CBA-CGA
18	5	602	CLA	C2A-CAA-CBA-CGA
18	8	602	CLA	C2A-CAA-CBA-CGA
20	4	622	LHG	C13-C14-C15-C16
20	5	625	LHG	C29-C30-C31-C32
24	A	860	LMG	C16-C17-C18-C19
25	J	103	DGD	CEA-CFA-CGA-CHA
26	a	617	LUT	C27-C28-C29-C39
18	A	804	CLA	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	A	846	LHG	O10-C23-O8-C6
18	A	809	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	C1A-C2A-CAA-CBA
18	A	811	CLA	C1A-C2A-CAA-CBA
18	A	812	CLA	C1A-C2A-CAA-CBA
18	A	819	CLA	C1A-C2A-CAA-CBA
18	A	828	CLA	C1A-C2A-CAA-CBA
18	A	836	CLA	C1A-C2A-CAA-CBA
18	B	803	CLA	C1A-C2A-CAA-CBA
18	B	809	CLA	C1A-C2A-CAA-CBA
18	B	811	CLA	C1A-C2A-CAA-CBA
18	B	823	CLA	C1A-C2A-CAA-CBA
18	B	826	CLA	C1A-C2A-CAA-CBA
18	B	828	CLA	C1A-C2A-CAA-CBA
18	B	834	CLA	C1A-C2A-CAA-CBA
18	B	835	CLA	C1A-C2A-CAA-CBA
18	L	302	CLA	C1A-C2A-CAA-CBA
18	L	303	CLA	C1A-C2A-CAA-CBA
18	1	602	CLA	C1A-C2A-CAA-CBA
18	1	616	CLA	C1A-C2A-CAA-CBA
18	a	606	CLA	C1A-C2A-CAA-CBA
18	a	610	CLA	C1A-C2A-CAA-CBA
18	3	607	CLA	C1A-C2A-CAA-CBA
18	4	610	CLA	C1A-C2A-CAA-CBA
18	4	616	CLA	C1A-C2A-CAA-CBA
18	5	610	CLA	C1A-C2A-CAA-CBA
18	5	617	CLA	C1A-C2A-CAA-CBA
18	6	610	CLA	C1A-C2A-CAA-CBA
18	6	616	CLA	C1A-C2A-CAA-CBA
18	7	609	CLA	C1A-C2A-CAA-CBA
18	8	614	CLA	C1A-C2A-CAA-CBA
18	4	602	CLA	C11-C12-C13-C15
20	A	846	LHG	C8-C7-O7-C5
18	7	611	CLA	C2-C3-C5-C6
21	A	849	BCR	C9-C10-C11-C12
18	B	803	CLA	C8-C10-C11-C12
18	B	803	CLA	C10-C11-C12-C13
20	B	851	LHG	C4-O6-P-O3
20	3	623	LHG	C24-C25-C26-C27
18	A	834	CLA	C3-C5-C6-C7
23	5	628	LMU	C4B-C5B-C6B-O6B
24	4	624	LMG	C17-C18-C19-C20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	807	CLA	O1A-CGA-O2A-C1
18	B	839	CLA	C5-C6-C7-C8
20	7	622	LHG	O6-C4-C5-C6
23	8	625	LMU	C1-C2-C3-C4
18	7	602	CLA	C16-C17-C18-C19
18	A	836	CLA	C15-C16-C17-C18
20	6	623	LHG	C7-C8-C9-C10
24	J	104	LMG	C28-C29-C30-C31
18	F	303	CLA	C3A-C2A-CAA-CBA
18	4	612	CLA	C3A-C2A-CAA-CBA
18	7	607	CLA	C3A-C2A-CAA-CBA
20	3	624	LHG	C11-C10-C9-C8
18	B	829	CLA	C13-C15-C16-C17
18	3	607	CLA	O1A-CGA-O2A-C1
24	J	104	LMG	C30-C31-C32-C33
18	a	608	CLA	C2A-CAA-CBA-CGA
18	6	616	CLA	C2A-CAA-CBA-CGA
18	7	610	CLA	C3-C5-C6-C7
20	A	846	LHG	C4-C5-C6-O8
20	A	846	LHG	C12-C13-C14-C15
20	5	623	LHG	C29-C30-C31-C32
20	6	623	LHG	C4-C5-C6-O8
20	8	623	LHG	C4-C5-C6-O8
24	J	104	LMG	O1-C7-C8-C9
24	5	626	LMG	O1-C7-C8-C9
24	5	626	LMG	C31-C32-C33-C34
24	7	624	LMG	C7-C8-C9-O8
25	J	103	DGD	O1G-C1G-C2G-C3G
24	4	623	LMG	C8-C7-O1-C1
20	1	620	LHG	C31-C32-C33-C34
20	a	620	LHG	C25-C26-C27-C28
18	a	609	CLA	O1D-CGD-O2D-CED
18	B	810	CLA	C13-C15-C16-C17
18	5	604	CLA	C15-C16-C17-C18
20	5	623	LHG	C35-C36-C37-C38
20	8	622	LHG	C17-C18-C19-C20
24	4	623	LMG	C33-C34-C35-C36
18	A	819	CLA	C10-C11-C12-C13
20	3	623	LHG	C15-C16-C17-C18
24	4	624	LMG	C15-C16-C17-C18
24	J	104	LMG	O6-C1-O1-C7
18	A	822	CLA	C15-C16-C17-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	7	622	LHG	C25-C26-C27-C28
23	5	628	LMU	C4-C5-C6-C7
18	A	843	CLA	C15-C16-C17-C18
23	A	859	LMU	C2'-C1'-O1'-C1
20	B	851	LHG	C11-C10-C9-C8
20	6	623	LHG	C32-C33-C34-C35
20	B	851	LHG	C27-C28-C29-C30
18	4	603	CLA	O1D-CGD-O2D-CED
18	A	825	CLA	C10-C11-C12-C13
18	3	613	CLA	C2A-CAA-CBA-CGA
18	A	807	CLA	C4-C3-C5-C6
18	A	820	CLA	C4-C3-C5-C6
18	8	613	CLA	C16-C17-C18-C20
18	B	802	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	CBA-CGA-O2A-C1
18	3	604	CLA	CBA-CGA-O2A-C1
18	7	601	CLA	CBA-CGA-O2A-C1
20	5	625	LHG	C24-C23-O8-C6
18	A	843	CLA	C13-C15-C16-C17
18	8	613	CLA	C8-C10-C11-C12
18	8	614	CLA	C5-C6-C7-C8
18	B	817	CLA	C11-C12-C13-C14
25	J	103	DGD	C3G-C2G-O2G-C1B
18	B	816	CLA	C2A-CAA-CBA-CGA
18	B	829	CLA	C2A-CAA-CBA-CGA
18	4	604	CLA	C2A-CAA-CBA-CGA
18	B	841	CLA	CAA-CBA-CGA-O2A
23	5	628	LMU	C3'-C4'-O1B-C1B
25	B	850	DGD	C8A-C9A-CAA-CBA
18	L	303	CLA	O1D-CGD-O2D-CED
20	4	622	LHG	C27-C28-C29-C30
20	8	623	LHG	C9-C10-C11-C12
24	5	627	LMG	C13-C14-C15-C16
18	A	815	CLA	CBA-CGA-O2A-C1
18	B	817	CLA	CBA-CGA-O2A-C1
20	A	846	LHG	O6-C4-C5-O7
18	K	204	CLA	O1D-CGD-O2D-CED
18	5	607	CLA	C16-C17-C18-C19
18	5	607	CLA	C16-C17-C18-C20
20	B	851	LHG	C10-C11-C12-C13
18	8	602	CLA	O1A-CGA-O2A-C1
18	a	609	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	A	846	LHG	C23-C24-C25-C26
18	A	804	CLA	C15-C16-C17-C18
18	A	818	CLA	C10-C11-C12-C13
18	B	806	CLA	C13-C15-C16-C17
20	6	623	LHG	O7-C5-C6-O8
20	3	624	LHG	C16-C17-C18-C19
20	4	622	LHG	C30-C31-C32-C33
23	K	208	LMU	C3-C4-C5-C6
24	5	626	LMG	C11-C12-C13-C14
24	J	104	LMG	C18-C19-C20-C21
24	5	626	LMG	C12-C13-C14-C15
18	A	826	CLA	C2-C1-O2A-CGA
18	5	613	CLA	C2-C1-O2A-CGA
25	B	850	DGD	C7B-C8B-C9B-CAB
18	A	804	CLA	C12-C13-C15-C16
18	A	809	CLA	C11-C12-C13-C15
18	A	809	CLA	C12-C13-C15-C16
18	A	814	CLA	C11-C10-C8-C7
18	A	825	CLA	C6-C7-C8-C10
18	A	825	CLA	C11-C12-C13-C15
18	A	830	CLA	C6-C7-C8-C10
18	B	802	CLA	C11-C10-C8-C7
18	B	805	CLA	C11-C12-C13-C15
18	B	806	CLA	C11-C12-C13-C15
18	B	806	CLA	C12-C13-C15-C16
18	B	828	CLA	C12-C13-C15-C16
18	B	834	CLA	C6-C7-C8-C10
18	B	834	CLA	C11-C10-C8-C7
18	B	840	CLA	C6-C7-C8-C10
18	1	613	CLA	C6-C7-C8-C10
18	a	609	CLA	C12-C13-C15-C16
18	a	613	CLA	C6-C7-C8-C10
18	5	604	CLA	C11-C10-C8-C7
18	6	604	CLA	C6-C7-C8-C10
18	6	613	CLA	C11-C10-C8-C7
18	6	616	CLA	C6-C7-C8-C10
18	7	602	CLA	C11-C10-C8-C7
18	8	602	CLA	C11-C10-C8-C7
19	A	844	PQN	C21-C22-C23-C25
19	B	842	PQN	C17-C18-C20-C21
18	3	609	CLA	C3-C5-C6-C7
24	A	860	LMG	O10-C28-O8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	803	CLA	C14-C13-C15-C16
18	A	809	CLA	C11-C12-C13-C14
18	A	811	CLA	C11-C10-C8-C9
18	A	814	CLA	C11-C10-C8-C9
18	A	820	CLA	C11-C10-C8-C9
18	A	825	CLA	C6-C7-C8-C9
18	A	825	CLA	C11-C12-C13-C14
18	A	826	CLA	C14-C13-C15-C16
18	A	830	CLA	C6-C7-C8-C9
18	A	831	CLA	C14-C13-C15-C16
18	A	836	CLA	C11-C10-C8-C9
18	A	841	CLA	C11-C10-C8-C9
18	A	854	CLA	C14-C13-C15-C16
18	B	802	CLA	C6-C7-C8-C9
18	B	806	CLA	C11-C12-C13-C14
18	B	806	CLA	C14-C13-C15-C16
18	B	813	CLA	C11-C12-C13-C14
18	B	817	CLA	C6-C7-C8-C9
18	B	828	CLA	C11-C10-C8-C9
18	B	834	CLA	C11-C10-C8-C9
18	B	837	CLA	C14-C13-C15-C16
18	1	613	CLA	C6-C7-C8-C9
18	a	609	CLA	C14-C13-C15-C16
18	a	610	CLA	C11-C10-C8-C9
18	a	613	CLA	C6-C7-C8-C9
18	4	608	CLA	C11-C10-C8-C9
18	4	613	CLA	C11-C10-C8-C9
18	4	614	CLA	C6-C7-C8-C9
18	5	607	CLA	C14-C13-C15-C16
18	5	609	CLA	C11-C10-C8-C9
18	6	604	CLA	C11-C12-C13-C14
18	6	613	CLA	C6-C7-C8-C9
18	7	602	CLA	C6-C7-C8-C9
18	8	601	CLA	C11-C12-C13-C14
18	8	613	CLA	C14-C13-C15-C16
27	1	618	XAT	C29-C30-C31-C32
18	K	203	CLA	CBA-CGA-O2A-C1
18	a	601	CLA	CBA-CGA-O2A-C1
18	8	601	CLA	CBA-CGA-O2A-C1
18	8	614	CLA	CBA-CGA-O2A-C1
18	4	602	CLA	C2A-CAA-CBA-CGA
18	6	602	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	7	601	CLA	O1A-CGA-O2A-C1
21	4	621	BCR	C36-C18-C19-C20
18	A	842	CLA	C16-C17-C18-C20
18	a	603	CLA	C6-C7-C8-C9
20	A	847	LHG	O1-C1-C2-C3
18	A	841	CLA	O1D-CGD-O2D-CED
20	6	623	LHG	C12-C13-C14-C15
24	A	860	LMG	C33-C34-C35-C36
18	B	825	CLA	C3-C5-C6-C7
18	A	833	CLA	O1D-CGD-O2D-CED
18	B	817	CLA	C8-C10-C11-C12
20	A	846	LHG	C14-C15-C16-C17
18	B	825	CLA	CBA-CGA-O2A-C1
18	B	828	CLA	CBA-CGA-O2A-C1
23	8	624	LMU	C1-C2-C3-C4
20	1	620	LHG	C28-C29-C30-C31
20	5	625	LHG	C9-C10-C11-C12
18	B	836	CLA	CBD-CGD-O2D-CED
20	5	623	LHG	C11-C10-C9-C8
18	8	613	CLA	C16-C17-C18-C19
20	A	847	LHG	O6-C4-C5-C6
20	5	625	LHG	O6-C4-C5-C6
20	8	623	LHG	O6-C4-C5-C6
18	A	828	CLA	C15-C16-C17-C18
18	A	839	CLA	C5-C6-C7-C8
18	6	604	CLA	C10-C11-C12-C13
18	A	820	CLA	C2-C3-C5-C6
18	4	609	CLA	C14-C13-C15-C16
20	A	846	LHG	C34-C35-C36-C37
18	B	824	CLA	C16-C17-C18-C19
20	A	847	LHG	C10-C11-C12-C13
25	J	103	DGD	C2B-C3B-C4B-C5B
18	8	606	CLA	C15-C16-C17-C18
18	A	827	CLA	O1D-CGD-O2D-CED
18	5	604	CLA	C2A-CAA-CBA-CGA
18	7	611	CLA	C2A-CAA-CBA-CGA
18	A	810	CLA	CBA-CGA-O2A-C1
18	A	819	CLA	CBA-CGA-O2A-C1
18	A	837	CLA	C3A-C2A-CAA-CBA
18	A	845	CLA	C3A-C2A-CAA-CBA
18	B	828	CLA	C3A-C2A-CAA-CBA
18	1	606	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	a	606	CLA	CBD-CGD-O2D-CED
18	5	608	CLA	C3A-C2A-CAA-CBA
18	5	616	CLA	CBD-CGD-O2D-CED
18	8	604	CLA	C3A-C2A-CAA-CBA
18	B	809	CLA	C8-C10-C11-C12
18	K	203	CLA	C15-C16-C17-C18
20	a	620	LHG	C31-C32-C33-C34
27	a	618	XAT	C29-C30-C31-C32
23	A	858	LMU	C2-C1-O1'-C1'
20	1	620	LHG	C35-C36-C37-C38
20	8	622	LHG	C9-C10-C11-C12
25	B	850	DGD	C4B-C5B-C6B-C7B
18	B	808	CLA	C15-C16-C17-C18
20	3	623	LHG	C16-C17-C18-C19
25	J	103	DGD	CFA-CGA-CHA-CIA
18	B	818	CLA	C8-C10-C11-C12
24	4	624	LMG	C7-C8-C9-O8
24	5	626	LMG	C7-C8-C9-O8
24	5	627	LMG	C7-C8-C9-O8
25	B	850	DGD	O1G-C1G-C2G-C3G
25	B	850	DGD	C1G-C2G-C3G-O3G
23	8	625	LMU	C4'-C5'-C6'-O6'
24	A	860	LMG	C18-C19-C20-C21
24	4	624	LMG	C33-C34-C35-C36
24	5	626	LMG	C18-C19-C20-C21
18	4	613	CLA	C15-C16-C17-C18
20	a	620	LHG	C34-C35-C36-C37
18	B	840	CLA	C3-C5-C6-C7
18	A	822	CLA	C4-C3-C5-C6
24	7	624	LMG	C29-C30-C31-C32
20	6	623	LHG	C11-C10-C9-C8
20	6	623	LHG	C30-C31-C32-C33
18	A	806	CLA	C10-C11-C12-C13
20	A	846	LHG	C4-O6-P-O3
18	A	815	CLA	O1A-CGA-O2A-C1
18	a	601	CLA	O1A-CGA-O2A-C1
18	B	810	CLA	C2A-CAA-CBA-CGA
18	a	614	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	C13-C15-C16-C17
18	B	808	CLA	C8-C10-C11-C12
18	4	613	CLA	C10-C11-C12-C13
20	5	625	LHG	O6-C4-C5-O7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
23	A	857	LMU	C1-C2-C3-C4
18	A	832	CLA	CBA-CGA-O2A-C1
18	B	808	CLA	CBA-CGA-O2A-C1
20	4	622	LHG	C35-C36-C37-C38
18	B	817	CLA	O1A-CGA-O2A-C1
18	3	604	CLA	O1A-CGA-O2A-C1
18	B	824	CLA	C16-C17-C18-C20
18	A	807	CLA	C10-C11-C12-C13
18	A	842	CLA	CAA-CBA-CGA-O2A
20	A	847	LHG	C24-C25-C26-C27
23	A	859	LMU	C4-C5-C6-C7
18	6	604	CLA	C13-C15-C16-C17
18	B	802	CLA	O1A-CGA-O2A-C1
18	K	203	CLA	O1A-CGA-O2A-C1
20	A	847	LHG	C11-C12-C13-C14
18	a	603	CLA	C6-C7-C8-C10
18	A	819	CLA	C11-C12-C13-C14
20	6	623	LHG	C10-C11-C12-C13
24	4	624	LMG	O6-C1-O1-C7
18	7	613	CLA	CBD-CGD-O2D-CED
20	8	622	LHG	C11-C12-C13-C14
18	A	826	CLA	C4-C3-C5-C6
18	A	827	CLA	C2-C1-O2A-CGA
18	A	835	CLA	C2-C1-O2A-CGA
18	B	839	CLA	C2-C1-O2A-CGA
18	5	609	CLA	C2-C1-O2A-CGA
18	B	824	CLA	C15-C16-C17-C18
18	A	804	CLA	C11-C12-C13-C14
18	A	811	CLA	C6-C7-C8-C9
18	A	820	CLA	C6-C7-C8-C9
18	A	831	CLA	C11-C10-C8-C9
18	A	843	CLA	C14-C13-C15-C16
18	B	802	CLA	C14-C13-C15-C16
18	B	814	CLA	C14-C13-C15-C16
18	B	833	CLA	C11-C10-C8-C9
18	4	601	CLA	C11-C12-C13-C14
18	4	604	CLA	C6-C7-C8-C9
18	7	601	CLA	C6-C7-C8-C9
18	7	602	CLA	C11-C10-C8-C9
18	7	610	CLA	C6-C7-C8-C9
18	8	601	CLA	C14-C13-C15-C16
24	4	623	LMG	C18-C19-C20-C21

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	854	CLA	C5-C6-C7-C8
18	1	611	CLA	C5-C6-C7-C8
18	a	613	CLA	C5-C6-C7-C8
23	A	857	LMU	C7-C8-C9-C10
18	8	613	CLA	C2A-CAA-CBA-CGA
18	A	842	CLA	C16-C17-C18-C19
21	B	848	BCR	C1-C6-C7-C8
21	K	207	BCR	C5-C6-C7-C8
21	L	305	BCR	C1-C6-C7-C8
21	3	621	BCR	C23-C24-C25-C26
21	7	621	BCR	C23-C24-C25-C26
21	7	621	BCR	C23-C24-C25-C30
21	7	623	BCR	C1-C6-C7-C8
21	7	623	BCR	C5-C6-C7-C8
21	8	621	BCR	C23-C24-C25-C26
21	8	621	BCR	C23-C24-C25-C30
26	3	618	LUT	C1-C6-C7-C8
26	3	618	LUT	C5-C6-C7-C8
26	7	619	LUT	C1-C6-C7-C8
18	5	607	CLA	C15-C16-C17-C18
20	5	623	LHG	C27-C28-C29-C30
18	3	612	CLA	C2A-CAA-CBA-CGA
18	A	823	CLA	C1A-C2A-CAA-CBA
18	3	615	CLA	C1A-C2A-CAA-CBA
18	8	612	CLA	C1A-C2A-CAA-CBA
21	L	305	BCR	C17-C18-C19-C20
21	6	622	BCR	C11-C12-C13-C14
26	1	617	LUT	C27-C28-C29-C30
18	6	610	CLA	C8-C10-C11-C12
18	B	838	CLA	O1D-CGD-O2D-CED
18	A	831	CLA	C8-C10-C11-C12
18	B	814	CLA	C5-C6-C7-C8
18	6	604	CLA	C8-C10-C11-C12
18	8	601	CLA	O1A-CGA-O2A-C1
18	8	614	CLA	O1A-CGA-O2A-C1
20	A	846	LHG	O6-C4-C5-C6
18	A	804	CLA	C11-C12-C13-C15
18	A	811	CLA	C6-C7-C8-C10
18	A	811	CLA	C11-C10-C8-C7
18	A	811	CLA	C11-C12-C13-C15
18	A	820	CLA	C6-C7-C8-C10
18	A	820	CLA	C11-C10-C8-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	825	CLA	C12-C13-C15-C16
18	A	831	CLA	C11-C10-C8-C7
18	A	831	CLA	C12-C13-C15-C16
18	A	836	CLA	C11-C10-C8-C7
18	A	841	CLA	C11-C10-C8-C7
18	A	843	CLA	C12-C13-C15-C16
18	A	854	CLA	C12-C13-C15-C16
18	B	802	CLA	C6-C7-C8-C10
18	B	805	CLA	C12-C13-C15-C16
18	B	808	CLA	C11-C12-C13-C15
18	B	808	CLA	C12-C13-C15-C16
18	B	809	CLA	C11-C12-C13-C15
18	B	813	CLA	C11-C10-C8-C7
18	B	813	CLA	C11-C12-C13-C15
18	B	814	CLA	C12-C13-C15-C16
18	B	817	CLA	C6-C7-C8-C10
18	B	827	CLA	C12-C13-C15-C16
18	B	828	CLA	C11-C10-C8-C7
18	B	831	CLA	C12-C13-C15-C16
18	B	833	CLA	C11-C10-C8-C7
18	B	837	CLA	C12-C13-C15-C16
18	a	610	CLA	C11-C10-C8-C7
18	4	601	CLA	C11-C12-C13-C15
18	4	604	CLA	C6-C7-C8-C10
18	4	608	CLA	C11-C10-C8-C7
18	4	610	CLA	C6-C7-C8-C10
18	4	613	CLA	C6-C7-C8-C10
18	4	613	CLA	C11-C10-C8-C7
18	4	614	CLA	C6-C7-C8-C10
18	5	604	CLA	C12-C13-C15-C16
18	5	607	CLA	C12-C13-C15-C16
18	5	609	CLA	C11-C10-C8-C7
18	6	601	CLA	C12-C13-C15-C16
18	6	604	CLA	C11-C12-C13-C15
18	7	602	CLA	C6-C7-C8-C10
18	8	601	CLA	C11-C12-C13-C15
18	8	614	CLA	C6-C7-C8-C10
20	1	620	LHG	C16-C17-C18-C19
20	3	624	LHG	C30-C31-C32-C33
27	4	620	XAT	C29-C30-C31-C32
20	6	623	LHG	C15-C16-C17-C18
18	B	825	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	837	CLA	O1A-CGA-O2A-C1
18	a	604	CLA	C2A-CAA-CBA-CGA
18	B	824	CLA	C5-C6-C7-C8
23	8	625	LMU	C5'-C4'-O1B-C1B
18	A	825	CLA	C5-C6-C7-C8
18	A	818	CLA	CAD-CBD-CGD-O2D
18	A	837	CLA	CAD-CBD-CGD-O2D
18	B	804	CLA	CAD-CBD-CGD-O2D
18	B	814	CLA	CAD-CBD-CGD-O2D
18	B	830	CLA	CAD-CBD-CGD-O2D
18	B	834	CLA	CAD-CBD-CGD-O2D
18	B	838	CLA	CAD-CBD-CGD-O2D
18	B	839	CLA	CAD-CBD-CGD-O2D
18	1	612	CLA	CAD-CBD-CGD-O2D
18	a	604	CLA	CAD-CBD-CGD-O2D
18	a	612	CLA	CAD-CBD-CGD-O2D
18	3	610	CLA	CAD-CBD-CGD-O2D
18	4	603	CLA	CAD-CBD-CGD-O2D
18	4	610	CLA	CAD-CBD-CGD-O2D
18	5	610	CLA	CAD-CBD-CGD-O2D
18	5	611	CLA	CAD-CBD-CGD-O2D
18	5	614	CLA	CAD-CBD-CGD-O2D
18	6	614	CLA	CAD-CBD-CGD-O2D
18	6	617	CLA	CAD-CBD-CGD-O2D
18	7	601	CLA	CAD-CBD-CGD-O2D
18	7	612	CLA	CAD-CBD-CGD-O2D
18	7	614	CLA	CAD-CBD-CGD-O2D
18	8	607	CLA	CAD-CBD-CGD-O2D
23	5	628	LMU	C5'-C4'-O1B-C1B
18	B	828	CLA	O1A-CGA-O2A-C1
18	7	611	CLA	CBA-CGA-O2A-C1
18	B	827	CLA	C2-C3-C5-C6
20	8	622	LHG	C24-C25-C26-C27
20	4	622	LHG	C4-C5-C6-O8
20	5	625	LHG	C2-C3-O3-P
20	A	847	LHG	O6-C4-C5-O7
20	3	624	LHG	O6-C4-C5-O7
20	7	622	LHG	O6-C4-C5-O7
18	B	825	CLA	C8-C10-C11-C12
18	B	827	CLA	CAA-CBA-CGA-O2A
18	A	842	CLA	C2A-CAA-CBA-CGA
18	L	302	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	3	607	CLA	C2A-CAA-CBA-CGA
20	3	624	LHG	C34-C35-C36-C37
20	8	622	LHG	C12-C13-C14-C15
24	5	626	LMG	C13-C14-C15-C16
20	3	624	LHG	C11-C12-C13-C14
18	A	804	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O2D
18	A	815	CLA	CHA-CBD-CGD-O1D
18	A	825	CLA	CHA-CBD-CGD-O1D
18	B	805	CLA	CHA-CBD-CGD-O1D
18	B	813	CLA	CHA-CBD-CGD-O1D
18	B	820	CLA	CHA-CBD-CGD-O1D
18	B	820	CLA	CHA-CBD-CGD-O2D
18	B	821	CLA	CHA-CBD-CGD-O1D
18	B	821	CLA	CHA-CBD-CGD-O2D
18	B	824	CLA	CHA-CBD-CGD-O1D
18	B	824	CLA	CHA-CBD-CGD-O2D
18	B	827	CLA	CHA-CBD-CGD-O1D
18	F	304	CLA	CHA-CBD-CGD-O1D
18	F	304	CLA	CHA-CBD-CGD-O2D
18	J	101	CLA	CHA-CBD-CGD-O1D
18	J	101	CLA	CHA-CBD-CGD-O2D
18	K	204	CLA	CHA-CBD-CGD-O1D
18	K	206	CLA	CHA-CBD-CGD-O1D
18	K	206	CLA	CHA-CBD-CGD-O2D
18	L	303	CLA	CHA-CBD-CGD-O2D
18	1	604	CLA	CHA-CBD-CGD-O1D
18	3	609	CLA	CHA-CBD-CGD-O1D
18	3	609	CLA	CHA-CBD-CGD-O2D
18	5	601	CLA	CHA-CBD-CGD-O1D
18	5	617	CLA	CHA-CBD-CGD-O1D
18	5	617	CLA	CHA-CBD-CGD-O2D
18	6	604	CLA	CHA-CBD-CGD-O1D
18	6	604	CLA	CHA-CBD-CGD-O2D
18	6	616	CLA	CHA-CBD-CGD-O1D
18	6	616	CLA	CHA-CBD-CGD-O2D
18	7	602	CLA	CHA-CBD-CGD-O1D
18	7	602	CLA	CHA-CBD-CGD-O2D
18	7	604	CLA	CHA-CBD-CGD-O1D
18	7	604	CLA	CHA-CBD-CGD-O2D
18	7	607	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	828	CLA	C3-C5-C6-C7
18	6	604	CLA	C3-C5-C6-C7
18	6	614	CLA	C3-C5-C6-C7
18	A	810	CLA	O1A-CGA-O2A-C1
20	3	624	LHG	C35-C36-C37-C38
20	1	620	LHG	C11-C10-C9-C8
20	1	620	LHG	C10-C11-C12-C13
20	4	622	LHG	C34-C35-C36-C37
20	A	847	LHG	O7-C5-C6-O8
20	4	622	LHG	O7-C5-C6-O8
24	J	104	LMG	O1-C7-C8-O7
24	5	626	LMG	O7-C8-C9-O8
25	B	850	DGD	O1G-C1G-C2G-O2G
25	J	103	DGD	O1G-C1G-C2G-O2G
20	5	623	LHG	C28-C29-C30-C31
18	A	819	CLA	O1A-CGA-O2A-C1
20	3	624	LHG	C29-C30-C31-C32
18	A	807	CLA	C16-C17-C18-C20
20	8	623	LHG	O1-C1-C2-O2
24	4	624	LMG	C16-C17-C18-C19
18	B	827	CLA	C4-C3-C5-C6
20	8	623	LHG	C11-C12-C13-C14
18	A	832	CLA	O1A-CGA-O2A-C1
24	5	627	LMG	O10-C28-O8-C9
18	A	807	CLA	C2-C3-C5-C6
18	A	822	CLA	C2-C3-C5-C6
25	B	850	DGD	CFB-CGB-CHB-CIB
18	A	811	CLA	C11-C12-C13-C14
18	A	825	CLA	C14-C13-C15-C16
18	B	809	CLA	C11-C12-C13-C14
18	B	827	CLA	C14-C13-C15-C16
18	4	613	CLA	C6-C7-C8-C9
18	6	614	CLA	C6-C7-C8-C9
18	3	606	CLA	O1A-CGA-O2A-C1
20	3	624	LHG	C23-C24-C25-C26
18	6	610	CLA	C13-C15-C16-C17
18	L	304	CLA	C2A-CAA-CBA-CGA
18	7	610	CLA	CBD-CGD-O2D-CED
18	8	608	CLA	CBA-CGA-O2A-C1
21	5	622	BCR	C11-C12-C13-C35
21	B	847	BCR	C21-C22-C23-C24
26	a	617	LUT	C27-C28-C29-C30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	a	620	LHG	C24-C25-C26-C27
18	A	816	CLA	C1A-C2A-CAA-CBA
18	A	831	CLA	C1A-C2A-CAA-CBA
18	A	832	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	C1A-C2A-CAA-CBA
18	B	838	CLA	C1A-C2A-CAA-CBA
18	K	203	CLA	C1A-C2A-CAA-CBA
18	a	616	CLA	C1A-C2A-CAA-CBA
18	3	617	CLA	CHA-CBD-CGD-O2D
18	4	607	CLA	C1A-C2A-CAA-CBA
18	7	601	CLA	C1A-C2A-CAA-CBA
18	7	603	CLA	CHA-CBD-CGD-O2D
18	7	610	CLA	C1A-C2A-CAA-CBA
18	8	610	CLA	C1A-C2A-CAA-CBA
18	A	811	CLA	C10-C11-C12-C13
18	B	809	CLA	C2-C1-O2A-CGA
18	3	606	CLA	CBA-CGA-O2A-C1
20	A	846	LHG	C3-O3-P-O6
20	8	623	LHG	C16-C17-C18-C19
20	7	622	LHG	O2-C2-C3-O3
20	1	620	LHG	C30-C31-C32-C33
18	A	802	CLA	C4-C3-C5-C6
18	F	301	CLA	C4-C3-C5-C6
20	3	624	LHG	C2-C3-O3-P
24	5	627	LMG	C15-C16-C17-C18
18	7	611	CLA	O1A-CGA-O2A-C1
20	A	846	LHG	C4-O6-P-O4
20	a	620	LHG	C3-O3-P-O5
20	5	625	LHG	C3-O3-P-O5
20	8	622	LHG	C4-O6-P-O4
20	8	622	LHG	C4-O6-P-O5
20	8	623	LHG	C19-C20-C21-C22
24	A	860	LMG	O6-C1-O1-C7
18	A	818	CLA	C8-C10-C11-C12
18	A	812	CLA	CBA-CGA-O2A-C1
20	3	624	LHG	O6-C4-C5-C6
18	5	610	CLA	C6-C7-C8-C9
24	5	627	LMG	C33-C34-C35-C36
20	5	623	LHG	C24-C25-C26-C27
18	1	602	CLA	C2A-CAA-CBA-CGA
18	3	608	CLA	C3-C5-C6-C7
25	J	103	DGD	CCA-CDA-CEA-CFA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
24	5	627	LMG	C11-C10-O7-C8
18	A	807	CLA	C16-C17-C18-C19
18	5	604	CLA	C16-C17-C18-C20
18	A	815	CLA	CAD-CBD-CGD-O1D
18	A	825	CLA	CAD-CBD-CGD-O1D
18	A	828	CLA	CAD-CBD-CGD-O1D
18	A	845	CLA	CAD-CBD-CGD-O1D
18	A	854	CLA	CAD-CBD-CGD-O1D
18	B	805	CLA	CAD-CBD-CGD-O1D
18	B	813	CLA	CAD-CBD-CGD-O1D
18	K	204	CLA	CAD-CBD-CGD-O1D
18	5	617	CLA	CAD-CBD-CGD-O1D
18	6	601	CLA	CAD-CBD-CGD-O1D
18	6	620	CLA	CAD-CBD-CGD-O1D
18	7	602	CLA	CAD-CBD-CGD-O1D
18	8	601	CLA	CAD-CBD-CGD-O1D
18	5	617	CLA	CAA-CBA-CGA-O2A
18	8	608	CLA	O1A-CGA-O2A-C1
18	B	813	CLA	C3-C5-C6-C7
18	6	616	CLA	C5-C6-C7-C8
20	A	847	LHG	C7-C8-C9-C10
20	5	625	LHG	C7-C8-C9-C10
18	8	613	CLA	C13-C15-C16-C17
18	7	609	CLA	C2C-C3C-CAC-CBC
18	A	812	CLA	C12-C13-C15-C16
18	A	818	CLA	C6-C7-C8-C10
18	A	829	CLA	C12-C13-C15-C16
18	A	830	CLA	C12-C13-C15-C16
18	A	841	CLA	C12-C13-C15-C16
18	a	606	CLA	CHA-CBD-CGD-O2D
18	3	604	CLA	C6-C7-C8-C10
18	4	618	CLA	C3A-C2A-CAA-CBA
18	5	613	CLA	C11-C12-C13-C15
18	6	602	CLA	C11-C12-C13-C15
18	6	610	CLA	C6-C7-C8-C10
18	6	614	CLA	C6-C7-C8-C10
18	7	611	CLA	C6-C7-C8-C10
18	8	612	CLA	C3A-C2A-CAA-CBA
20	B	851	LHG	C7-C8-C9-C10
20	8	623	LHG	O6-C4-C5-O7
18	4	608	CLA	C3-C5-C6-C7
21	6	622	BCR	C9-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	4	622	LHG	C9-C10-C11-C12
18	7	613	CLA	O1D-CGD-O2D-CED
20	7	622	LHG	C26-C27-C28-C29
23	8	624	LMU	C4B-C5B-C6B-O6B
24	5	627	LMG	O7-C8-C9-O8
20	8	622	LHG	C13-C14-C15-C16
23	A	859	LMU	C5'-C4'-O1B-C1B
18	A	814	CLA	C8-C10-C11-C12
18	A	826	CLA	C10-C11-C12-C13
20	1	620	LHG	C29-C30-C31-C32
20	5	623	LHG	C9-C10-C11-C12
24	4	624	LMG	C8-C7-O1-C1
18	3	608	CLA	C5-C6-C7-C8
18	7	610	CLA	O1D-CGD-O2D-CED
20	A	846	LHG	C2-C3-O3-P
18	3	613	CLA	C4-C3-C5-C6
18	A	827	CLA	CBA-CGA-O2A-C1
24	A	860	LMG	C29-C28-O8-C9
18	A	826	CLA	C2-C3-C5-C6
18	B	808	CLA	C14-C13-C15-C16
18	B	813	CLA	C11-C10-C8-C9
18	B	818	CLA	C11-C10-C8-C9
18	5	604	CLA	C14-C13-C15-C16
18	5	613	CLA	C11-C12-C13-C14
18	6	601	CLA	C14-C13-C15-C16
18	8	613	CLA	C11-C10-C8-C9
18	8	614	CLA	C6-C7-C8-C9
18	A	812	CLA	O1A-CGA-O2A-C1
18	6	603	CLA	O1A-CGA-O2A-C1
18	7	602	CLA	C2A-CAA-CBA-CGA
20	5	623	LHG	C33-C34-C35-C36
27	7	620	XAT	C29-C30-C31-C32
20	8	623	LHG	C30-C31-C32-C33
20	B	851	LHG	C11-C12-C13-C14
25	B	850	DGD	C8B-C9B-CAB-CBB
20	3	623	LHG	C23-C24-C25-C26
23	K	208	LMU	O5B-C5B-C6B-O6B
18	A	827	CLA	O1A-CGA-O2A-C1
18	A	814	CLA	C10-C11-C12-C13
18	A	830	CLA	C5-C6-C7-C8
19	B	842	PQN	C23-C25-C26-C27
18	5	609	CLA	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	B	809	CLA	C15-C16-C17-C18
18	a	609	CLA	C13-C15-C16-C17
24	7	624	LMG	C13-C14-C15-C16
18	6	616	CLA	C8-C10-C11-C12
18	1	604	CLA	C1-C2-C3-C4
18	a	604	CLA	C1-C2-C3-C4
18	B	841	CLA	O1D-CGD-O2D-CED
23	K	208	LMU	C1-C2-C3-C4
18	A	813	CLA	C2A-CAA-CBA-CGA
18	A	814	CLA	C2A-CAA-CBA-CGA
18	6	613	CLA	C2A-CAA-CBA-CGA
18	7	613	CLA	C2A-CAA-CBA-CGA
18	A	834	CLA	C5-C6-C7-C8
18	A	841	CLA	C2-C1-O2A-CGA
18	3	606	CLA	C2-C1-O2A-CGA
18	6	616	CLA	C2-C1-O2A-CGA
18	8	610	CLA	C2-C1-O2A-CGA
20	3	623	LHG	C11-C12-C13-C14
20	7	622	LHG	C12-C13-C14-C15
18	B	836	CLA	O1D-CGD-O2D-CED
18	1	602	CLA	C3-C5-C6-C7
23	A	857	LMU	C2B-C1B-O1B-C4'
18	6	603	CLA	CBA-CGA-O2A-C1
18	B	808	CLA	O1A-CGA-O2A-C1
18	B	816	CLA	C5-C6-C7-C8
18	1	603	CLA	C4-C3-C5-C6
21	K	207	BCR	C1-C6-C7-C8
26	7	619	LUT	C5-C6-C7-C8
20	7	622	LHG	O10-C23-O8-C6
18	B	832	CLA	CAA-CBA-CGA-O2A
20	B	851	LHG	C12-C13-C14-C15
20	8	623	LHG	C28-C29-C30-C31
20	6	623	LHG	C17-C18-C19-C20
20	7	622	LHG	C8-C7-O7-C5
18	B	821	CLA	C2A-CAA-CBA-CGA
18	8	608	CLA	C2A-CAA-CBA-CGA
24	7	624	LMG	O7-C8-C9-O8
20	1	620	LHG	C3-O3-P-O6
20	3	624	LHG	C4-O6-P-O3
20	4	622	LHG	C3-O3-P-O6
20	5	623	LHG	C3-O3-P-O6
20	5	625	LHG	C4-O6-P-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	8	622	LHG	C3-O3-P-O6
18	5	613	CLA	C15-C16-C17-C18
23	A	859	LMU	C11-C10-C9-C8
18	B	813	CLA	C6-C7-C8-C10
18	3	613	CLA	C2-C3-C5-C6
18	6	613	CLA	C6-C7-C8-C10
18	8	601	CLA	C12-C13-C15-C16
18	A	804	CLA	C14-C13-C15-C16
18	B	831	CLA	C14-C13-C15-C16
18	B	840	CLA	C6-C7-C8-C9
18	4	610	CLA	C6-C7-C8-C9
18	6	613	CLA	C11-C10-C8-C9
18	A	842	CLA	C13-C15-C16-C17
18	B	829	CLA	C5-C6-C7-C8
21	L	301	BCR	C13-C14-C15-C16
21	5	622	BCR	C13-C14-C15-C16
18	5	604	CLA	C16-C17-C18-C19
20	a	620	LHG	C11-C10-C9-C8
24	5	626	LMG	C10-C11-C12-C13
25	B	850	DGD	C3B-C4B-C5B-C6B
18	5	619	CLA	C2A-CAA-CBA-CGA
18	A	826	CLA	CBA-CGA-O2A-C1
18	6	601	CLA	O1A-CGA-O2A-C1
21	B	801	BCR	C7-C8-C9-C34
18	6	601	CLA	CBA-CGA-O2A-C1
20	a	620	LHG	C2-C3-O3-P
20	3	623	LHG	C2-C3-O3-P
20	4	622	LHG	C2-C3-O3-P
20	5	625	LHG	C5-C4-O6-P
20	7	622	LHG	C2-C3-O3-P
28	6	624	NEX	C11-C12-C13-C14
20	5	625	LHG	C18-C19-C20-C21
18	3	602	CLA	C3-C5-C6-C7
18	A	819	CLA	CAA-CBA-CGA-O2A
20	5	625	LHG	C17-C18-C19-C20
18	A	814	CLA	CBA-CGA-O2A-C1
18	B	836	CLA	CBA-CGA-O2A-C1
18	5	609	CLA	CBA-CGA-O2A-C1
20	5	625	LHG	C24-C25-C26-C27
18	B	802	CLA	CAA-CBA-CGA-O2A
18	1	613	CLA	C5-C6-C7-C8
18	8	606	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	5	602	CLA	CBA-CGA-O2A-C1
18	6	613	CLA	CBA-CGA-O2A-C1
21	A	856	BCR	C13-C14-C15-C16
21	6	622	BCR	C13-C14-C15-C16
27	3	619	XAT	C29-C30-C31-C32
20	3	624	LHG	C27-C28-C29-C30
18	6	601	CLA	C8-C10-C11-C12
20	8	623	LHG	C31-C32-C33-C34
18	B	816	CLA	C3-C5-C6-C7
18	8	613	CLA	C4-C3-C5-C6
20	7	622	LHG	C10-C11-C12-C13
18	A	826	CLA	C8-C10-C11-C12
20	6	623	LHG	C9-C10-C11-C12
18	A	808	CLA	C2-C1-O2A-CGA
18	B	831	CLA	C2-C1-O2A-CGA
18	B	836	CLA	C2-C1-O2A-CGA
18	a	609	CLA	C2-C1-O2A-CGA
18	5	617	CLA	C2-C1-O2A-CGA
18	A	826	CLA	C13-C15-C16-C17
18	7	603	CLA	CAA-CBA-CGA-O1A
18	B	835	CLA	C2A-CAA-CBA-CGA
18	a	601	CLA	C2A-CAA-CBA-CGA
18	a	602	CLA	C2A-CAA-CBA-CGA
18	6	620	CLA	C2A-CAA-CBA-CGA
20	3	623	LHG	C27-C28-C29-C30
25	J	103	DGD	C8A-C9A-CAA-CBA
18	B	839	CLA	CBA-CGA-O2A-C1
20	6	623	LHG	C14-C15-C16-C17
18	A	803	CLA	C3A-C2A-CAA-CBA
18	A	806	CLA	C3A-C2A-CAA-CBA
18	L	304	CLA	C3A-C2A-CAA-CBA
23	A	859	LMU	C5-C6-C7-C8
26	a	617	LUT	C29-C30-C31-C32
18	5	613	CLA	CBA-CGA-O2A-C1
20	6	623	LHG	C28-C29-C30-C31
18	B	835	CLA	CAA-CBA-CGA-O2A
18	7	609	CLA	CAA-CBA-CGA-O1A
23	A	857	LMU	C3-C4-C5-C6
18	A	802	CLA	C2-C3-C5-C6
18	F	301	CLA	C2-C3-C5-C6
25	B	850	DGD	C9A-CAA-CBA-CCA
18	A	818	CLA	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	1	611	CLA	C6-C7-C8-C9
18	3	604	CLA	C6-C7-C8-C9
18	8	601	CLA	C6-C7-C8-C9
25	J	103	DGD	C5A-C6A-C7A-C8A
18	7	611	CLA	C8-C10-C11-C12
18	8	601	CLA	C10-C11-C12-C13
20	5	625	LHG	C4-C5-C6-O8
21	A	852	BCR	C11-C10-C9-C34
21	A	852	BCR	C16-C17-C18-C36
21	B	844	BCR	C11-C10-C9-C34
21	B	845	BCR	C11-C10-C9-C34
21	B	845	BCR	C20-C21-C22-C37
21	F	305	BCR	C16-C17-C18-C36
21	L	301	BCR	C11-C10-C9-C34
21	3	621	BCR	C35-C13-C14-C15
21	3	621	BCR	C16-C17-C18-C36
21	3	622	BCR	C35-C13-C14-C15
21	3	622	BCR	C16-C17-C18-C36
28	5	624	NEX	C39-C29-C30-C31
28	6	624	NEX	C39-C29-C30-C31
18	5	614	CLA	CAA-CBA-CGA-O1A
18	A	825	CLA	C2A-CAA-CBA-CGA
18	B	836	CLA	O1A-CGA-O2A-C1
18	B	803	CLA	O2A-C1-C2-C3
18	6	617	CLA	CAA-CBA-CGA-O2A
21	A	849	BCR	C7-C8-C9-C34
18	L	302	CLA	CAA-CBA-CGA-O1A
18	A	803	CLA	C1A-C2A-CAA-CBA
18	A	838	CLA	C1A-C2A-CAA-CBA
18	B	839	CLA	C1A-C2A-CAA-CBA
18	L	304	CLA	C1A-C2A-CAA-CBA
18	1	603	CLA	C1A-C2A-CAA-CBA
18	1	612	CLA	C1A-C2A-CAA-CBA
18	a	607	CLA	C1A-C2A-CAA-CBA
18	4	614	CLA	C1A-C2A-CAA-CBA
18	6	608	CLA	C1A-C2A-CAA-CBA
18	7	608	CLA	C1A-C2A-CAA-CBA
18	8	603	CLA	C1A-C2A-CAA-CBA
18	8	606	CLA	C1A-C2A-CAA-CBA
18	A	806	CLA	C6-C7-C8-C10
18	A	814	CLA	C11-C12-C13-C15
18	B	825	CLA	C6-C7-C8-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	4	601	CLA	C6-C7-C8-C10
18	7	601	CLA	C6-C7-C8-C10
18	A	811	CLA	C15-C16-C17-C18
18	A	841	CLA	O1A-CGA-O2A-C1
18	6	617	CLA	CAA-CBA-CGA-O1A
20	8	622	LHG	C35-C36-C37-C38
20	1	620	LHG	C24-C23-O8-C6
18	B	835	CLA	CAA-CBA-CGA-O1A
18	a	612	CLA	CAA-CBA-CGA-O2A
18	A	820	CLA	C5-C6-C7-C8
18	3	609	CLA	C11-C12-C13-C14
18	A	802	CLA	C2A-CAA-CBA-CGA
18	L	303	CLA	C2A-CAA-CBA-CGA
18	3	606	CLA	C5-C6-C7-C8
18	4	613	CLA	C8-C10-C11-C12
18	6	603	CLA	C5-C6-C7-C8
18	4	603	CLA	CAA-CBA-CGA-O2A
18	5	614	CLA	CAA-CBA-CGA-O2A
18	7	603	CLA	CAA-CBA-CGA-O2A
24	7	624	LMG	C11-C12-C13-C14
18	5	613	CLA	C5-C6-C7-C8
18	a	609	CLA	C4-C3-C5-C6
18	A	835	CLA	C8-C10-C11-C12
18	a	612	CLA	CAA-CBA-CGA-O1A
18	B	802	CLA	C13-C15-C16-C17
21	A	852	BCR	C11-C10-C9-C8
21	A	852	BCR	C16-C17-C18-C19
21	B	844	BCR	C11-C10-C9-C8
21	B	845	BCR	C11-C10-C9-C8
21	B	845	BCR	C20-C21-C22-C23
21	F	305	BCR	C16-C17-C18-C19
21	L	301	BCR	C11-C10-C9-C8
21	3	621	BCR	C12-C13-C14-C15
21	3	621	BCR	C16-C17-C18-C19
21	3	622	BCR	C12-C13-C14-C15
21	3	622	BCR	C16-C17-C18-C19
23	K	208	LMU	C2'-C1'-O1'-C1
28	5	624	NEX	C28-C29-C30-C31
28	6	624	NEX	C28-C29-C30-C31
18	5	609	CLA	C8-C10-C11-C12
19	B	842	PQN	C15-C16-C17-C18
18	4	603	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	5	619	CLA	CAA-CBA-CGA-O1A
18	6	613	CLA	O1A-CGA-O2A-C1
20	5	625	LHG	O7-C5-C6-O8
20	7	622	LHG	O7-C5-C6-O8
27	6	621	XAT	C29-C30-C31-C32
18	5	619	CLA	CAA-CBA-CGA-O2A
18	7	609	CLA	CAA-CBA-CGA-O2A
18	B	802	CLA	C4-C3-C5-C6
19	A	844	PQN	C14-C13-C15-C16
18	A	802	CLA	C2-C1-O2A-CGA
18	B	816	CLA	C2-C1-O2A-CGA
18	3	603	CLA	C2-C1-O2A-CGA
18	6	608	CLA	C2-C1-O2A-CGA
18	7	604	CLA	C2-C1-O2A-CGA
18	B	833	CLA	O1A-CGA-O2A-C1
18	B	839	CLA	O1A-CGA-O2A-C1
18	L	302	CLA	CAA-CBA-CGA-O2A
18	a	603	CLA	C2A-CAA-CBA-CGA
18	A	830	CLA	C11-C12-C13-C14
18	6	601	CLA	C11-C10-C8-C9
18	A	814	CLA	O1A-CGA-O2A-C1
18	8	601	CLA	CAA-CBA-CGA-O2A
18	5	602	CLA	O1A-CGA-O2A-C1
18	7	604	CLA	C5-C6-C7-C8
18	8	604	CLA	C2A-CAA-CBA-CGA
21	B	846	BCR	C1-C6-C7-C8
21	B	846	BCR	C5-C6-C7-C8
21	J	102	BCR	C1-C6-C7-C8
21	a	619	BCR	C23-C24-C25-C30
21	3	621	BCR	C23-C24-C25-C30
21	4	621	BCR	C23-C24-C25-C26
21	4	621	BCR	C23-C24-C25-C30
21	A	852	BCR	C19-C20-C21-C22
18	B	813	CLA	C4-C3-C5-C6
18	6	613	CLA	C4-C3-C5-C6
21	J	102	BCR	C11-C12-C13-C14
21	5	622	BCR	C11-C12-C13-C14
18	A	835	CLA	C5-C6-C7-C8
18	6	620	CLA	CAA-CBA-CGA-O2A
18	7	612	CLA	CAA-CBA-CGA-O2A
18	A	801	CLA	CAA-CBA-CGA-O2A
23	A	859	LMU	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	842	CLA	C15-C16-C17-C18
23	5	628	LMU	O5B-C5B-C6B-O6B
18	B	819	CLA	C2A-CAA-CBA-CGA
18	A	806	CLA	CAA-CBA-CGA-O2A
18	A	841	CLA	CBA-CGA-O2A-C1
20	B	851	LHG	C30-C31-C32-C33
18	B	802	CLA	C3-C5-C6-C7
18	5	616	CLA	CAA-CBA-CGA-O2A
18	B	831	CLA	C4-C3-C5-C6
18	6	604	CLA	C4-C3-C5-C6
18	6	601	CLA	C11-C10-C8-C7
18	6	616	CLA	C12-C13-C15-C16
18	B	833	CLA	CBA-CGA-O2A-C1
20	3	623	LHG	C10-C11-C12-C13
20	a	620	LHG	C10-C11-C12-C13
24	5	626	LMG	C29-C30-C31-C32
18	6	620	CLA	CAA-CBA-CGA-O1A
20	4	622	LHG	C1-C2-C3-O3
20	6	623	LHG	C1-C2-C3-O3
18	4	602	CLA	C5-C6-C7-C8
18	B	823	CLA	CAA-CBA-CGA-O2A
18	7	612	CLA	CAA-CBA-CGA-O1A
18	7	611	CLA	O2A-C1-C2-C3
25	B	850	DGD	CBB-CCB-CDB-CEB
18	1	612	CLA	CAA-CBA-CGA-O2A
18	1	616	CLA	CAA-CBA-CGA-O2A
18	8	609	CLA	CAA-CBA-CGA-O2A
18	A	854	CLA	CBA-CGA-O2A-C1
18	5	608	CLA	CBA-CGA-O2A-C1
18	1	603	CLA	CAA-CBA-CGA-O2A
18	6	616	CLA	CAA-CBA-CGA-O2A
20	4	622	LHG	O8-C23-C24-C25
18	A	803	CLA	C4-C3-C5-C6
18	B	834	CLA	C4-C3-C5-C6
18	A	811	CLA	C13-C15-C16-C17
20	4	622	LHG	C11-C12-C13-C14
20	B	851	LHG	C3-O3-P-O6
18	A	841	CLA	CAA-CBA-CGA-O2A
20	7	622	LHG	C9-C10-C11-C12
18	A	806	CLA	C6-C7-C8-C9
18	A	812	CLA	C14-C13-C15-C16
18	A	814	CLA	C11-C12-C13-C14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	830	CLA	C14-C13-C15-C16
18	A	841	CLA	C11-C12-C13-C14
18	A	841	CLA	C14-C13-C15-C16
18	6	602	CLA	C11-C12-C13-C14
18	6	610	CLA	C6-C7-C8-C9
18	7	611	CLA	C6-C7-C8-C9
18	7	611	CLA	C11-C10-C8-C9
18	7	613	CLA	C11-C10-C8-C9
20	1	620	LHG	C34-C35-C36-C37
18	8	606	CLA	C3A-C2A-CAA-CBA
18	A	854	CLA	O1A-CGA-O2A-C1
18	3	609	CLA	O1A-CGA-O2A-C1
18	5	608	CLA	O1A-CGA-O2A-C1
18	A	810	CLA	CAA-CBA-CGA-O2A
20	6	623	LHG	O8-C23-C24-C25
25	J	103	DGD	CBA-CCA-CDA-CEA
18	1	612	CLA	CAA-CBA-CGA-O1A
18	7	616	CLA	CAA-CBA-CGA-O2A
18	8	603	CLA	CAA-CBA-CGA-O2A
18	A	808	CLA	CAD-CBD-CGD-O2D
18	A	823	CLA	CAD-CBD-CGD-O2D
18	A	827	CLA	CAD-CBD-CGD-O2D
18	A	831	CLA	CAD-CBD-CGD-O2D
18	A	834	CLA	CAD-CBD-CGD-O2D
18	A	838	CLA	CAD-CBD-CGD-O2D
18	B	825	CLA	CAD-CBD-CGD-O2D
18	B	829	CLA	CAD-CBD-CGD-O2D
18	B	833	CLA	CAD-CBD-CGD-O2D
18	B	835	CLA	CAD-CBD-CGD-O2D
18	B	836	CLA	CAD-CBD-CGD-O2D
18	F	301	CLA	CAD-CBD-CGD-O2D
18	F	303	CLA	CAD-CBD-CGD-O2D
18	K	201	CLA	CAD-CBD-CGD-O2D
18	1	609	CLA	CAD-CBD-CGD-O2D
18	1	613	CLA	CAD-CBD-CGD-O2D
18	a	614	CLA	CAD-CBD-CGD-O2D
18	4	604	CLA	CAD-CBD-CGD-O2D
18	4	614	CLA	CAD-CBD-CGD-O2D
18	A	801	CLA	C16-C17-C18-C19
20	B	851	LHG	O9-C7-O7-C5
18	6	604	CLA	C15-C16-C17-C18
18	A	816	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	a	607	CLA	CAA-CBA-CGA-O2A
18	3	609	CLA	C4-C3-C5-C6
18	a	616	CLA	CAA-CBA-CGA-O2A
18	B	802	CLA	C2-C3-C5-C6
18	6	613	CLA	C2-C3-C5-C6
18	B	813	CLA	CAA-CBA-CGA-O2A
18	B	838	CLA	CAA-CBA-CGA-O2A
24	4	623	LMG	O8-C28-C29-C30
24	5	626	LMG	O8-C28-C29-C30
21	B	801	BCR	C7-C8-C9-C10
21	4	621	BCR	C17-C18-C19-C20
27	8	620	XAT	C27-C28-C29-C30
24	J	104	LMG	C7-C8-C9-O8
27	3	619	XAT	O24-C26-C27-C28
18	B	823	CLA	CAA-CBA-CGA-O1A
18	5	616	CLA	CAA-CBA-CGA-O1A
18	A	843	CLA	C6-C7-C8-C10
18	A	821	CLA	CAA-CBA-CGA-O2A
18	3	609	CLA	CAA-CBA-CGA-O2A
24	5	627	LMG	O7-C10-C11-C12
20	3	623	LHG	C31-C32-C33-C34
20	4	622	LHG	C17-C18-C19-C20
18	a	616	CLA	CAA-CBA-CGA-O1A
18	4	607	CLA	CAA-CBA-CGA-O1A
18	4	607	CLA	CAA-CBA-CGA-O2A
18	4	616	CLA	CAA-CBA-CGA-O2A
18	A	804	CLA	O2A-C1-C2-C3
18	A	811	CLA	O2A-C1-C2-C3
18	B	807	CLA	C2A-CAA-CBA-CGA
18	a	613	CLA	C2A-CAA-CBA-CGA
18	4	610	CLA	C2A-CAA-CBA-CGA
18	A	854	CLA	C13-C15-C16-C17
18	4	604	CLA	C5-C6-C7-C8
25	B	850	DGD	C4E-C5E-C6E-O5E
18	A	842	CLA	CAA-CBA-CGA-O1A
18	1	616	CLA	CAA-CBA-CGA-O1A
18	8	603	CLA	CAA-CBA-CGA-O1A
20	8	623	LHG	C18-C19-C20-C21
18	4	601	CLA	C16-C17-C18-C19
18	8	606	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	CHA-CBD-CGD-O1D
18	A	802	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	804	CLA	CHA-CBD-CGD-O2D
18	A	814	CLA	CHA-CBD-CGD-O1D
18	A	815	CLA	CHA-CBD-CGD-O2D
18	A	816	CLA	CHA-CBD-CGD-O2D
18	A	821	CLA	CHA-CBD-CGD-O1D
18	A	825	CLA	CHA-CBD-CGD-O2D
18	A	830	CLA	CHA-CBD-CGD-O1D
18	A	830	CLA	CHA-CBD-CGD-O2D
18	A	835	CLA	CHA-CBD-CGD-O2D
18	A	843	CLA	CHA-CBD-CGD-O1D
18	A	843	CLA	CHA-CBD-CGD-O2D
18	B	805	CLA	CHA-CBD-CGD-O2D
18	B	810	CLA	CHA-CBD-CGD-O2D
18	B	811	CLA	CHA-CBD-CGD-O1D
18	B	811	CLA	CHA-CBD-CGD-O2D
18	B	813	CLA	CHA-CBD-CGD-O2D
18	B	815	CLA	CHA-CBD-CGD-O1D
18	B	827	CLA	CHA-CBD-CGD-O2D
18	B	841	CLA	CHA-CBD-CGD-O1D
18	K	204	CLA	CHA-CBD-CGD-O2D
18	L	304	CLA	CHA-CBD-CGD-O1D
18	L	304	CLA	CHA-CBD-CGD-O2D
18	1	602	CLA	CHA-CBD-CGD-O1D
18	1	604	CLA	CHA-CBD-CGD-O2D
18	a	602	CLA	CHA-CBD-CGD-O2D
18	a	603	CLA	CHA-CBD-CGD-O1D
18	a	603	CLA	CHA-CBD-CGD-O2D
18	4	602	CLA	CHA-CBD-CGD-O2D
18	4	616	CLA	CHA-CBD-CGD-O1D
18	5	601	CLA	CHA-CBD-CGD-O2D
18	5	603	CLA	CHA-CBD-CGD-O1D
18	5	607	CLA	CHA-CBD-CGD-O1D
18	5	607	CLA	CHA-CBD-CGD-O2D
18	5	619	CLA	CHA-CBD-CGD-O1D
18	5	619	CLA	CHA-CBD-CGD-O2D
18	6	603	CLA	CHA-CBD-CGD-O1D
18	8	604	CLA	CHA-CBD-CGD-O1D
18	8	604	CLA	CHA-CBD-CGD-O2D
18	8	616	CLA	CHA-CBD-CGD-O1D
18	8	616	CLA	CHA-CBD-CGD-O2D
21	A	851	BCR	C19-C20-C21-C22
18	7	616	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	8	609	CLA	CAA-CBA-CGA-O1A
18	B	813	CLA	C2-C3-C5-C6
20	4	622	LHG	C18-C19-C20-C21
23	5	628	LMU	C2B-C1B-O1B-C4'
20	5	625	LHG	C35-C36-C37-C38
18	A	816	CLA	CAA-CBA-CGA-O1A
18	4	616	CLA	CAA-CBA-CGA-O1A
18	3	609	CLA	C11-C12-C13-C15
18	A	807	CLA	CAA-CBA-CGA-O2A
18	A	818	CLA	CAA-CBA-CGA-O2A
18	A	830	CLA	CAA-CBA-CGA-O2A
18	B	810	CLA	CAA-CBA-CGA-O2A
18	8	608	CLA	CAA-CBA-CGA-O2A
20	3	624	LHG	O7-C5-C6-O8
18	4	610	CLA	C8-C10-C11-C12
18	A	813	CLA	C6-C7-C8-C9
18	A	835	CLA	CAA-CBA-CGA-O2A
18	B	834	CLA	CAA-CBA-CGA-O2A
18	8	604	CLA	CAA-CBA-CGA-O2A
18	6	609	CLA	CAA-CBA-CGA-O2A
20	B	851	LHG	O2-C2-C3-O3
18	B	819	CLA	C3-C5-C6-C7
18	A	845	CLA	CAA-CBA-CGA-O2A
18	7	609	CLA	CBD-CGD-O2D-CED
20	4	622	LHG	O10-C23-O8-C6
18	a	609	CLA	C5-C6-C7-C8
18	A	802	CLA	C12-C13-C15-C16
18	A	830	CLA	C11-C12-C13-C15
18	K	203	CLA	C6-C7-C8-C10
18	1	603	CLA	C2-C3-C5-C6
18	3	609	CLA	C2-C3-C5-C6
20	7	622	LHG	C5-C4-O6-P
24	5	626	LMG	C4-C5-C6-O5
24	5	626	LMG	O6-C1-O1-C7
18	B	833	CLA	CAA-CBA-CGA-O2A
18	a	607	CLA	CAA-CBA-CGA-O1A
18	A	802	CLA	C11-C10-C8-C9
18	A	812	CLA	C6-C7-C8-C9
18	B	825	CLA	C6-C7-C8-C9
18	K	203	CLA	C6-C7-C8-C9
18	5	613	CLA	C14-C13-C15-C16
19	B	842	PQN	C21-C22-C23-C24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	3	620	BCR	C13-C14-C15-C16
18	B	826	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	C16-C17-C18-C19
18	3	609	CLA	CBA-CGA-O2A-C1
18	3	606	CLA	CAA-CBA-CGA-O2A
18	A	802	CLA	C10-C11-C12-C13
18	3	609	CLA	C4C-C3C-CAC-CBC
20	A	846	LHG	C29-C30-C31-C32
18	B	838	CLA	CAA-CBA-CGA-O1A
18	1	603	CLA	CAA-CBA-CGA-O1A
18	B	805	CLA	C4-C3-C5-C6
20	8	623	LHG	O1-C1-C2-C3
18	8	613	CLA	C2-C3-C5-C6
20	A	846	LHG	O10-C23-C24-C25
18	B	826	CLA	CBA-CGA-O2A-C1
18	A	814	CLA	C1A-C2A-CAA-CBA
18	A	815	CLA	C1A-C2A-CAA-CBA
18	A	835	CLA	C1A-C2A-CAA-CBA
18	A	843	CLA	C1A-C2A-CAA-CBA
18	1	603	CLA	CHA-CBD-CGD-O2D
18	a	608	CLA	C1A-C2A-CAA-CBA
18	a	613	CLA	C1A-C2A-CAA-CBA
18	5	606	CLA	CHA-CBD-CGD-O2D
18	6	612	CLA	CHA-CBD-CGD-O2D
20	A	846	LHG	C11-C10-C9-C8
18	A	843	CLA	C16-C17-C18-C20
18	4	601	CLA	C16-C17-C18-C20
24	J	104	LMG	O10-C28-C29-C30
18	8	610	CLA	O1A-CGA-O2A-C1
18	A	810	CLA	CAA-CBA-CGA-O1A
18	A	845	CLA	CAA-CBA-CGA-O1A
18	3	609	CLA	CAA-CBA-CGA-O1A
18	A	839	CLA	C2A-CAA-CBA-CGA
18	a	601	CLA	C6-C7-C8-C10
18	6	616	CLA	CAA-CBA-CGA-O1A
18	8	601	CLA	C5-C6-C7-C8
23	5	628	LMU	C2-C3-C4-C5
20	6	623	LHG	C33-C34-C35-C36
18	A	841	CLA	CAA-CBA-CGA-O1A
24	5	627	LMG	O9-C10-C11-C12
18	A	837	CLA	CAA-CBA-CGA-O2A
24	4	624	LMG	C2-C1-O1-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	A	846	LHG	C3-O3-P-O5
20	A	846	LHG	C4-O6-P-O5
20	B	851	LHG	C3-O3-P-O5
20	1	620	LHG	C3-O3-P-O5
20	4	622	LHG	C3-O3-P-O5
20	5	623	LHG	C3-O3-P-O5
20	5	625	LHG	C4-O6-P-O5
18	A	830	CLA	CAA-CBA-CGA-O1A
25	B	850	DGD	O1B-C1B-C2B-C3B
18	a	613	CLA	C15-C16-C17-C18
21	B	844	BCR	C5-C6-C7-C8
21	a	619	BCR	C23-C24-C25-C26
18	A	829	CLA	C15-C16-C17-C18
18	A	818	CLA	CAA-CBA-CGA-O1A
18	A	821	CLA	CAA-CBA-CGA-O1A
24	J	104	LMG	O8-C28-C29-C30
18	6	609	CLA	CAA-CBA-CGA-O1A
18	8	616	CLA	CAA-CBA-CGA-O2A
18	A	835	CLA	CAA-CBA-CGA-O1A
18	3	606	CLA	CAA-CBA-CGA-O1A
20	5	623	LHG	C10-C11-C12-C13
18	A	811	CLA	CAD-CBD-CGD-O1D
18	A	814	CLA	CAD-CBD-CGD-O1D
18	A	830	CLA	CAD-CBD-CGD-O1D
18	A	832	CLA	CAD-CBD-CGD-O1D
18	B	815	CLA	CAD-CBD-CGD-O1D
18	B	827	CLA	CAD-CBD-CGD-O1D
18	B	841	CLA	CAD-CBD-CGD-O1D
18	K	201	CLA	CAD-CBD-CGD-O1D
18	4	616	CLA	CAD-CBD-CGD-O1D
18	5	601	CLA	CAD-CBD-CGD-O1D
18	5	607	CLA	CAD-CBD-CGD-O1D
18	B	833	CLA	CAA-CBA-CGA-O1A
18	8	608	CLA	CAA-CBA-CGA-O1A
23	A	857	LMU	C6-C7-C8-C9
18	A	804	CLA	C10-C11-C12-C13
18	A	814	CLA	C6-C7-C8-C9
18	A	822	CLA	C6-C7-C8-C9
18	A	834	CLA	C11-C12-C13-C14
18	B	813	CLA	C6-C7-C8-C9
18	6	610	CLA	C11-C12-C13-C14
19	A	844	PQN	C16-C17-C18-C19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	7	622	LHG	C30-C31-C32-C33
18	B	827	CLA	CAA-CBA-CGA-O1A
18	8	604	CLA	CAA-CBA-CGA-O1A
20	5	623	LHG	O10-C23-C24-C25
18	5	613	CLA	CAA-CBA-CGA-O2A
18	A	801	CLA	C16-C17-C18-C20
18	1	602	CLA	CAA-CBA-CGA-O2A
18	a	602	CLA	CAA-CBA-CGA-O2A
18	A	841	CLA	C15-C16-C17-C18
18	A	837	CLA	CAA-CBA-CGA-O1A
18	K	206	CLA	CAA-CBA-CGA-O1A
18	3	613	CLA	CBA-CGA-O2A-C1
18	5	609	CLA	CAA-CBA-CGA-O2A
18	6	602	CLA	CAA-CBA-CGA-O2A
18	6	610	CLA	CAA-CBA-CGA-O2A
20	A	846	LHG	O8-C23-C24-C25
20	3	624	LHG	C1-C2-C3-O3
18	A	801	CLA	C5-C6-C7-C8
18	7	613	CLA	C10-C11-C12-C13
18	B	810	CLA	CAA-CBA-CGA-O1A
18	7	610	CLA	C4-C3-C5-C6
18	4	614	CLA	C5-C6-C7-C8
18	A	802	CLA	C11-C10-C8-C7
18	A	807	CLA	C12-C13-C15-C16
18	A	812	CLA	C6-C7-C8-C10
18	A	814	CLA	C6-C7-C8-C10
18	A	822	CLA	C6-C7-C8-C10
18	A	834	CLA	C11-C12-C13-C15
18	A	838	CLA	C3A-C2A-CAA-CBA
18	B	818	CLA	C11-C10-C8-C7
18	1	603	CLA	C3A-C2A-CAA-CBA
18	1	612	CLA	C3A-C2A-CAA-CBA
18	a	601	CLA	CAD-CBD-CGD-O2D
18	a	602	CLA	C11-C12-C13-C15
18	a	609	CLA	C2-C3-C5-C6
18	3	606	CLA	CHA-CBD-CGD-O1D
18	3	617	CLA	CAD-CBD-CGD-O2D
18	5	613	CLA	C12-C13-C15-C16
18	6	604	CLA	C11-C10-C8-C7
18	6	606	CLA	CHA-CBD-CGD-O1D
18	6	606	CLA	CAD-CBD-CGD-O2D
18	7	603	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	8	603	CLA	C3A-C2A-CAA-CBA
18	A	807	CLA	CAA-CBA-CGA-O1A
18	A	836	CLA	CAA-CBA-CGA-O2A
18	B	806	CLA	CAA-CBA-CGA-O2A
20	8	622	LHG	O7-C7-C8-C9
21	B	843	BCR	C11-C12-C13-C14
21	7	623	BCR	C17-C18-C19-C20
18	6	610	CLA	CAA-CBA-CGA-O1A
20	6	623	LHG	O10-C23-C24-C25
21	5	622	BCR	C9-C10-C11-C12
23	K	208	LMU	C2-C1-O1'-C1'
18	K	203	CLA	CAA-CBA-CGA-O2A
25	B	850	DGD	O2G-C1B-C2B-C3B
25	B	850	DGD	C5B-C6B-C7B-C8B
18	B	806	CLA	CAA-CBA-CGA-O1A
18	B	834	CLA	CAA-CBA-CGA-O1A
18	6	602	CLA	CAA-CBA-CGA-O1A
18	8	610	CLA	CBA-CGA-O2A-C1
18	1	611	CLA	C15-C16-C17-C18
18	6	601	CLA	CAA-CBA-CGA-O2A
20	3	624	LHG	O8-C23-C24-C25
18	A	836	CLA	CAA-CBA-CGA-O1A
18	B	811	CLA	C2A-CAA-CBA-CGA
18	8	616	CLA	CAA-CBA-CGA-O1A
20	5	623	LHG	O9-C7-C8-C9
18	K	201	CLA	CAA-CBA-CGA-O2A
18	K	206	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

235 monomers are involved in 528 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	837	CLA	1	0
18	A	825	CLA	3	0
18	B	829	CLA	7	0
18	4	612	CLA	1	0
18	1	616	CLA	1	0
18	A	818	CLA	5	0
18	L	303	CLA	1	0
18	4	601	CLA	4	0
18	A	828	CLA	8	0
18	B	817	CLA	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	4	613	CLA	3	0
18	6	603	CLA	1	0
19	A	844	PQN	3	0
20	8	623	LHG	2	0
24	5	627	LMG	3	0
18	5	607	CLA	5	0
18	8	613	CLA	5	0
21	4	621	BCR	3	0
20	7	622	LHG	5	0
18	7	614	CLA	1	0
20	B	851	LHG	1	0
18	F	303	CLA	1	0
18	3	615	CLA	1	0
18	B	802	CLA	2	0
21	L	305	BCR	4	0
28	6	624	NEX	4	0
18	A	826	CLA	1	0
18	B	832	CLA	4	0
21	7	623	BCR	1	0
18	8	604	CLA	1	0
18	A	812	CLA	5	0
18	A	820	CLA	5	0
18	A	829	CLA	9	0
21	A	849	BCR	5	0
21	A	856	BCR	6	0
18	3	614	CLA	1	0
18	8	601	CLA	1	0
28	5	624	NEX	4	0
27	6	621	XAT	2	0
18	4	602	CLA	3	0
18	B	806	CLA	5	0
20	6	623	LHG	1	0
25	B	850	DGD	3	0
21	J	102	BCR	2	0
18	3	607	CLA	2	0
18	4	609	CLA	3	0
18	3	612	CLA	2	0
18	A	808	CLA	2	0
18	3	608	CLA	4	0
18	A	839	CLA	4	0
18	A	823	CLA	1	0
18	B	810	CLA	3	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	K	207	BCR	4	0
18	6	616	CLA	5	0
24	4	624	LMG	1	0
18	B	834	CLA	3	0
18	1	606	CLA	1	0
18	A	809	CLA	3	0
18	6	620	CLA	3	0
18	1	610	CLA	1	0
18	L	304	CLA	2	0
18	A	819	CLA	3	0
18	4	603	CLA	1	0
18	8	608	CLA	2	0
18	3	617	CLA	5	0
18	A	840	CLA	4	0
18	B	833	CLA	3	0
18	K	203	CLA	1	0
18	A	830	CLA	5	0
18	7	611	CLA	2	0
26	8	619	LUT	5	0
18	5	618	CLA	2	0
18	8	607	CLA	1	0
27	1	618	XAT	3	0
18	7	610	CLA	3	0
18	5	614	CLA	1	0
18	A	831	CLA	3	0
18	A	804	CLA	3	0
18	5	610	CLA	5	0
18	B	827	CLA	5	0
18	8	614	CLA	2	0
26	3	618	LUT	2	0
18	B	841	CLA	3	0
18	5	616	CLA	1	0
18	B	824	CLA	5	0
18	A	807	CLA	3	0
18	F	304	CLA	1	0
18	1	611	CLA	1	0
18	1	608	CLA	3	0
18	5	608	CLA	3	0
18	5	619	CLA	3	0
25	J	103	DGD	3	0
18	3	609	CLA	3	0
21	L	301	BCR	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	8	620	XAT	2	0
21	1	619	BCR	2	0
18	8	612	CLA	1	0
18	6	617	CLA	2	0
18	1	603	CLA	6	0
23	A	858	LMU	2	0
21	6	622	BCR	4	0
18	7	612	CLA	3	0
18	B	803	CLA	3	0
18	A	838	CLA	1	0
18	B	818	CLA	4	0
18	B	840	CLA	3	0
21	B	845	BCR	2	0
18	B	821	CLA	1	0
23	A	859	LMU	3	0
18	B	819	CLA	2	0
18	A	854	CLA	5	0
18	3	606	CLA	2	0
20	3	624	LHG	5	0
21	B	843	BCR	3	0
18	6	610	CLA	2	0
18	B	807	CLA	4	0
18	B	839	CLA	1	0
18	5	604	CLA	3	0
18	4	616	CLA	1	0
18	3	610	CLA	4	0
18	1	612	CLA	1	0
18	5	617	CLA	1	0
18	8	611	CLA	2	0
18	A	803	CLA	1	0
27	5	621	XAT	6	0
18	1	613	CLA	2	0
18	A	810	CLA	2	0
18	B	808	CLA	5	0
18	B	831	CLA	5	0
21	A	851	BCR	4	0
27	3	619	XAT	2	0
21	3	620	BCR	6	0
18	A	801	CLA	5	0
18	A	814	CLA	7	0
20	1	620	LHG	2	0
26	6	619	LUT	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	835	CLA	1	0
18	7	613	CLA	1	0
21	A	848	BCR	3	0
26	1	617	LUT	3	0
18	8	616	CLA	1	0
18	A	817	CLA	1	0
21	F	305	BCR	6	0
18	8	606	CLA	1	0
18	B	838	CLA	3	0
20	8	622	LHG	7	0
21	3	621	BCR	3	0
21	A	850	BCR	4	0
21	K	202	BCR	2	0
18	A	842	CLA	6	0
21	B	846	BCR	3	0
21	B	848	BCR	2	0
18	1	602	CLA	2	0
18	5	602	CLA	5	0
18	A	802	CLA	5	0
18	B	826	CLA	1	0
26	5	620	LUT	4	0
18	1	609	CLA	5	0
23	8	624	LMU	1	0
26	7	619	LUT	3	0
18	A	821	CLA	1	0
18	B	811	CLA	3	0
18	A	836	CLA	5	0
21	5	622	BCR	3	0
18	5	612	CLA	2	0
18	A	822	CLA	3	0
18	6	601	CLA	3	0
21	3	622	BCR	4	0
18	6	613	CLA	2	0
21	B	844	BCR	3	0
20	A	846	LHG	3	0
20	5	623	LHG	2	0
18	B	828	CLA	3	0
18	4	606	CLA	1	0
18	5	613	CLA	4	0
18	7	602	CLA	2	0
20	3	623	LHG	1	0
18	B	830	CLA	1	0

*Continued on next page...*

*Continued from previous page...*

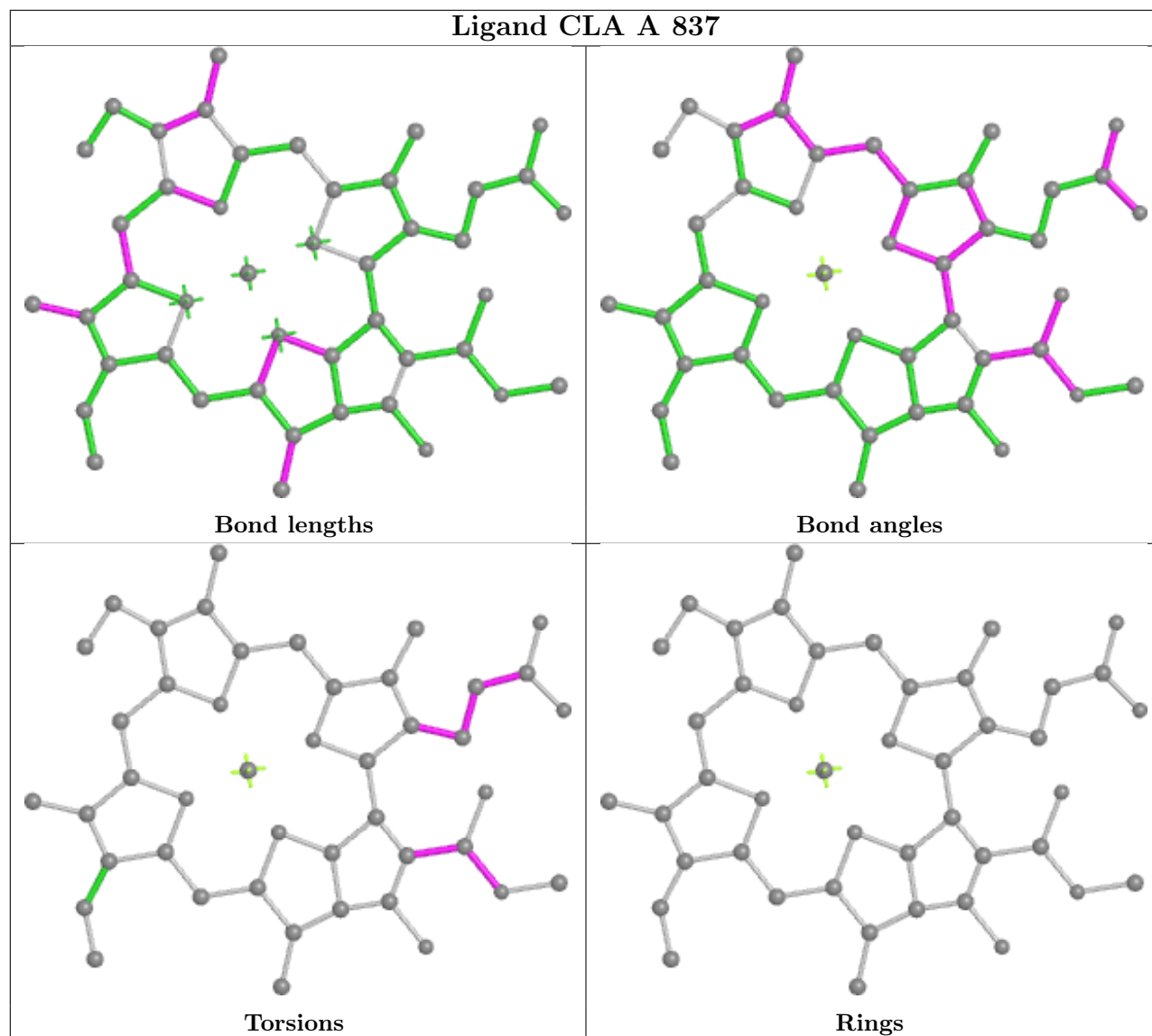
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	4	610	CLA	3	0
18	B	812	CLA	1	0
18	F	301	CLA	3	0
18	B	837	CLA	6	0
18	A	835	CLA	4	0
18	4	607	CLA	1	0
18	8	610	CLA	4	0
18	1	601	CLA	2	0
18	K	206	CLA	1	0
18	6	604	CLA	4	0
18	6	611	CLA	1	0
23	A	857	LMU	1	0
27	7	620	XAT	4	0
20	4	622	LHG	4	0
18	7	608	CLA	6	0
18	A	843	CLA	2	0
18	A	806	CLA	7	0
18	4	614	CLA	1	0
18	A	811	CLA	6	0
21	A	852	BCR	3	0
21	B	801	BCR	4	0
18	A	815	CLA	1	0
26	4	619	LUT	6	0
18	7	601	CLA	3	0
19	B	842	PQN	2	0
21	8	621	BCR	2	0
18	K	201	CLA	2	0
18	6	608	CLA	1	0
18	6	602	CLA	1	0
18	B	813	CLA	6	0
18	A	813	CLA	2	0
18	4	608	CLA	3	0
18	5	606	CLA	2	0
21	7	621	BCR	4	0
24	J	104	LMG	4	0
18	A	827	CLA	2	0
18	A	833	CLA	1	0
18	6	607	CLA	1	0
18	6	609	CLA	1	0
18	A	841	CLA	4	0
21	B	847	BCR	4	0
18	K	204	CLA	1	0

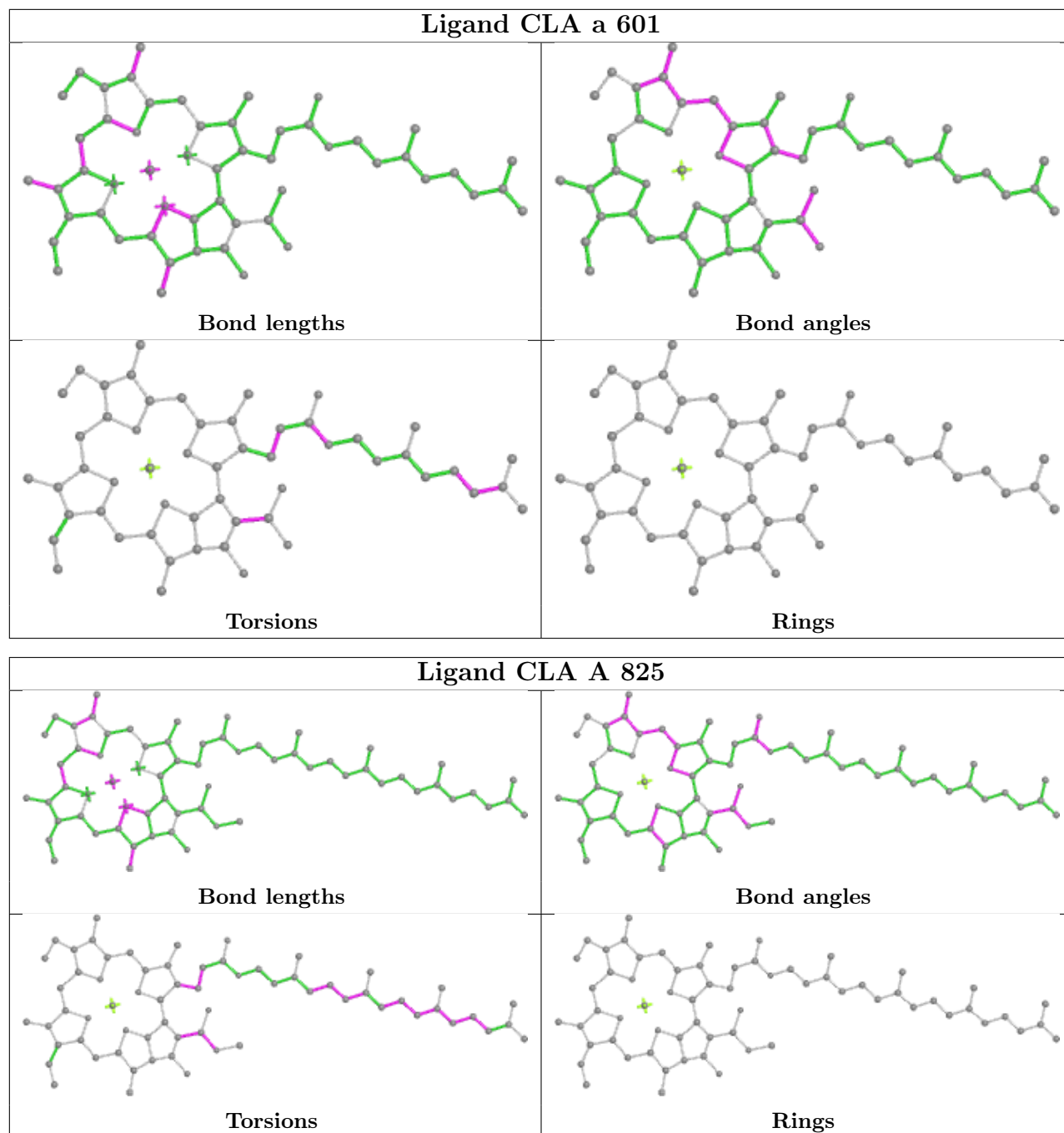
*Continued on next page...*

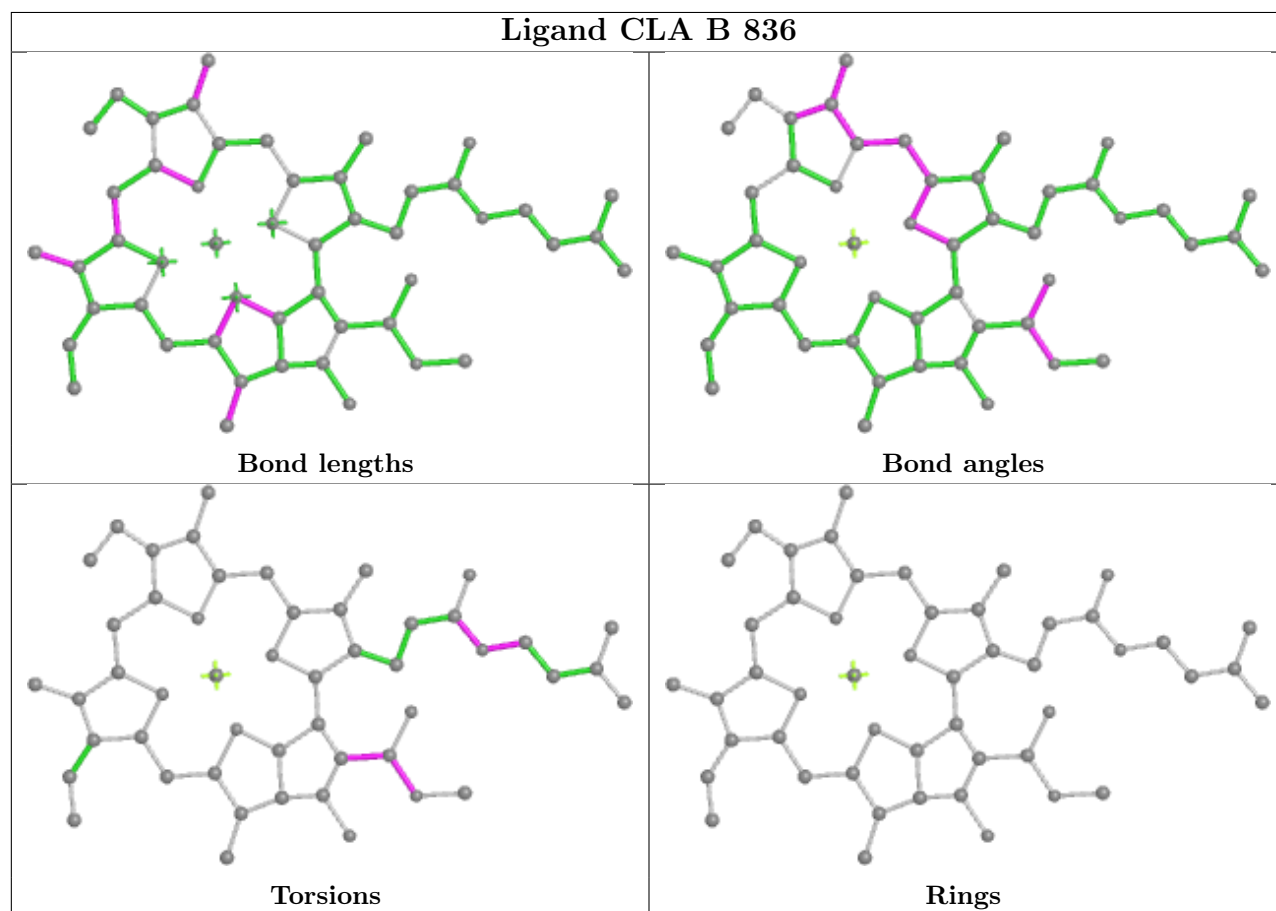
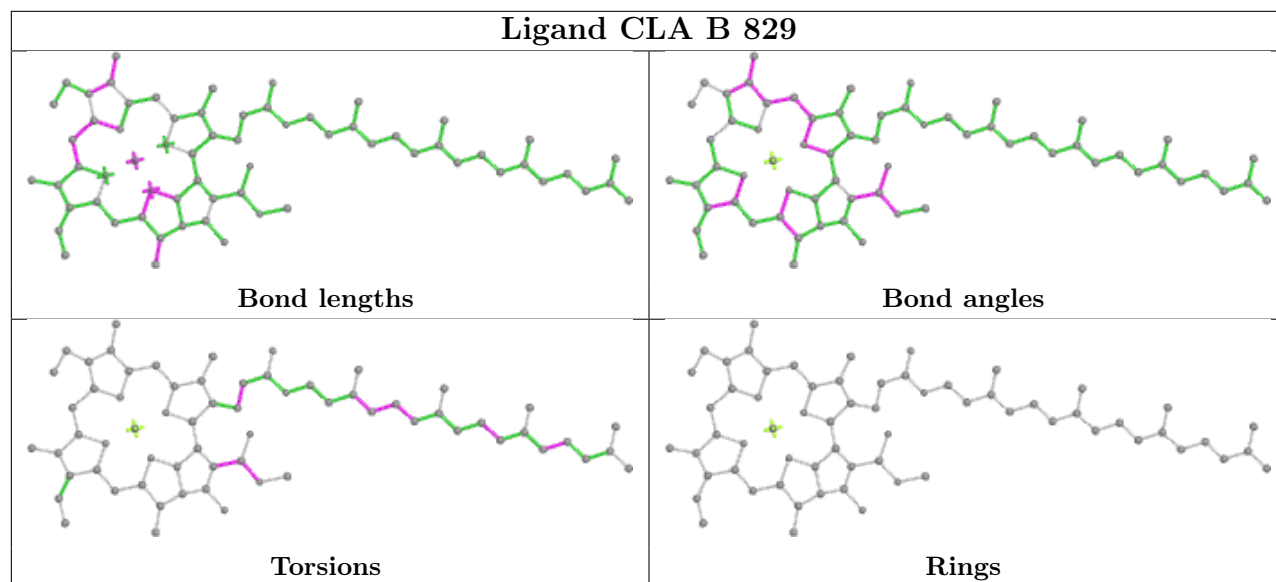
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	5	609	CLA	5	0
18	B	809	CLA	3	0
18	7	604	CLA	2	0
18	A	845	CLA	1	0
18	B	825	CLA	3	0
18	L	302	CLA	5	0
18	A	824	CLA	1	0
18	A	834	CLA	3	0
20	5	625	LHG	3	0
27	4	620	XAT	2	0
18	B	814	CLA	1	0
18	6	612	CLA	2	0
18	3	604	CLA	2	0
18	A	816	CLA	1	0
18	B	805	CLA	2	0

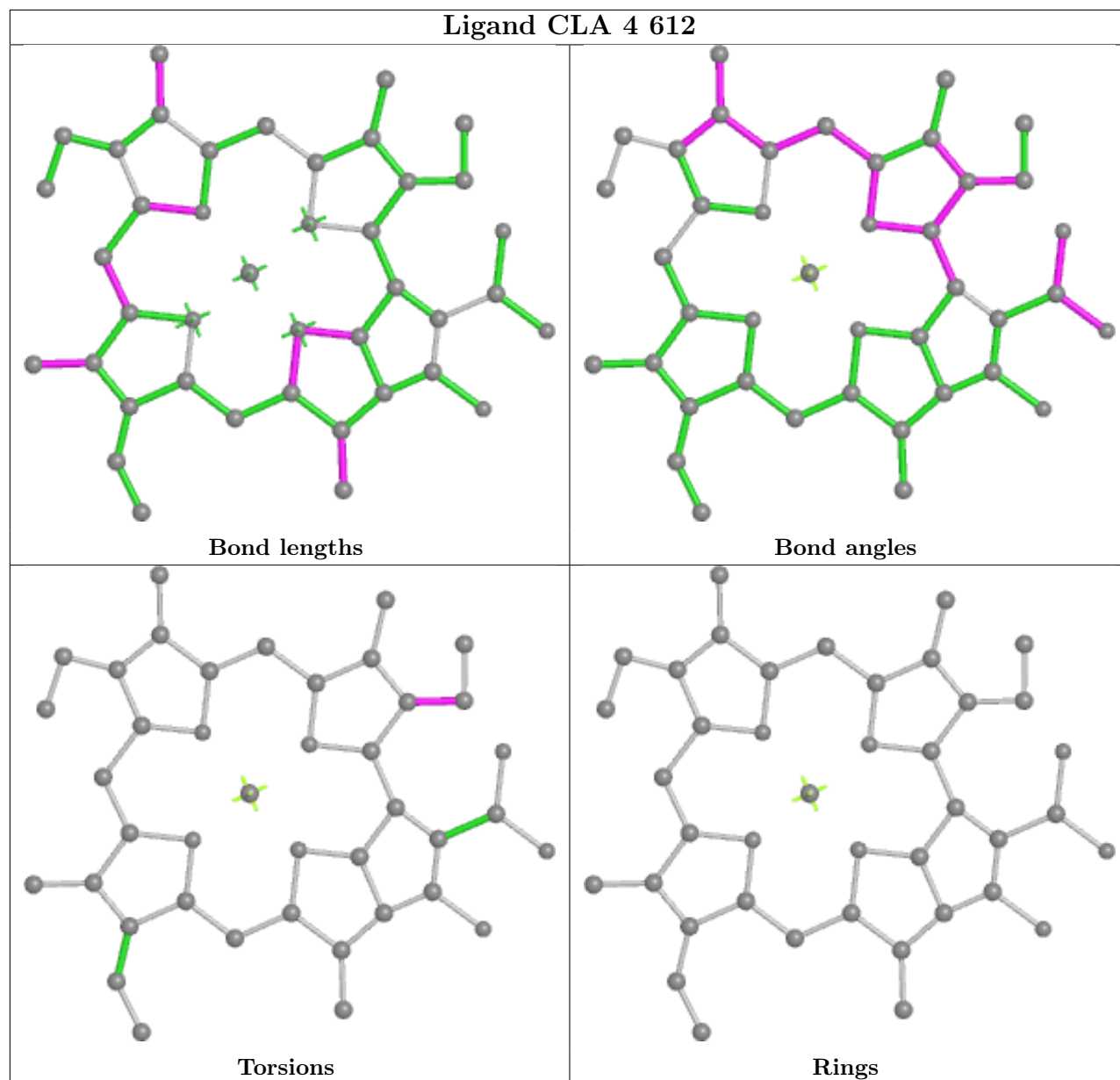
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

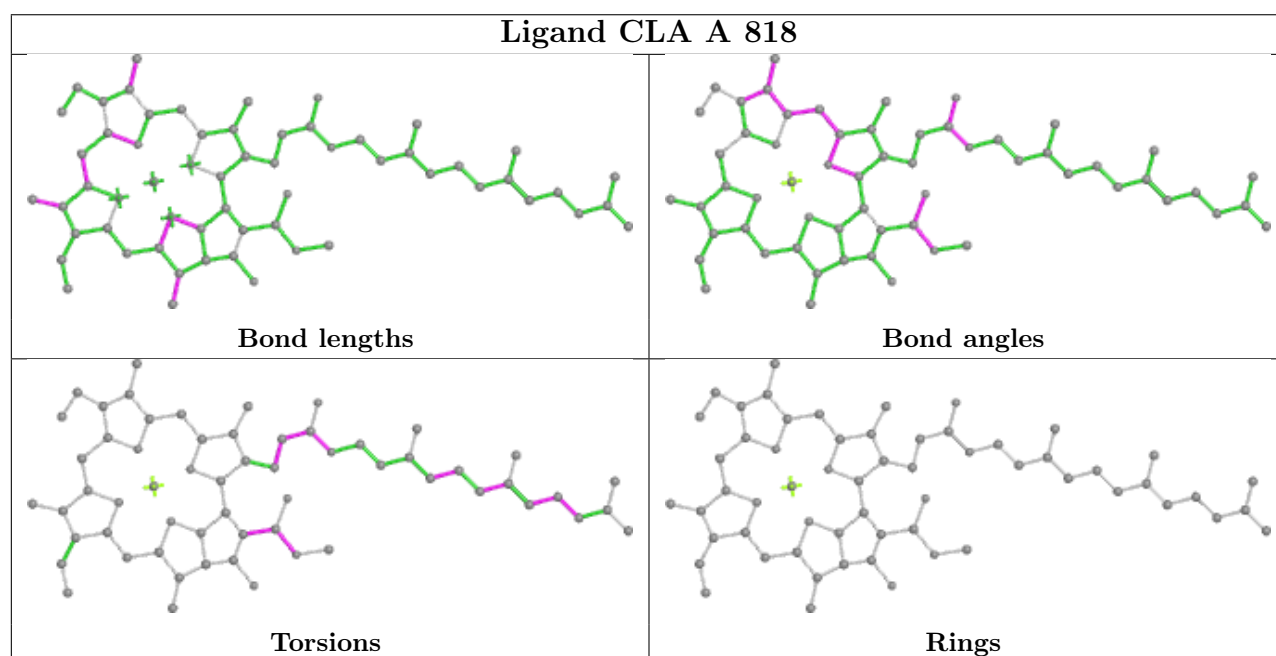
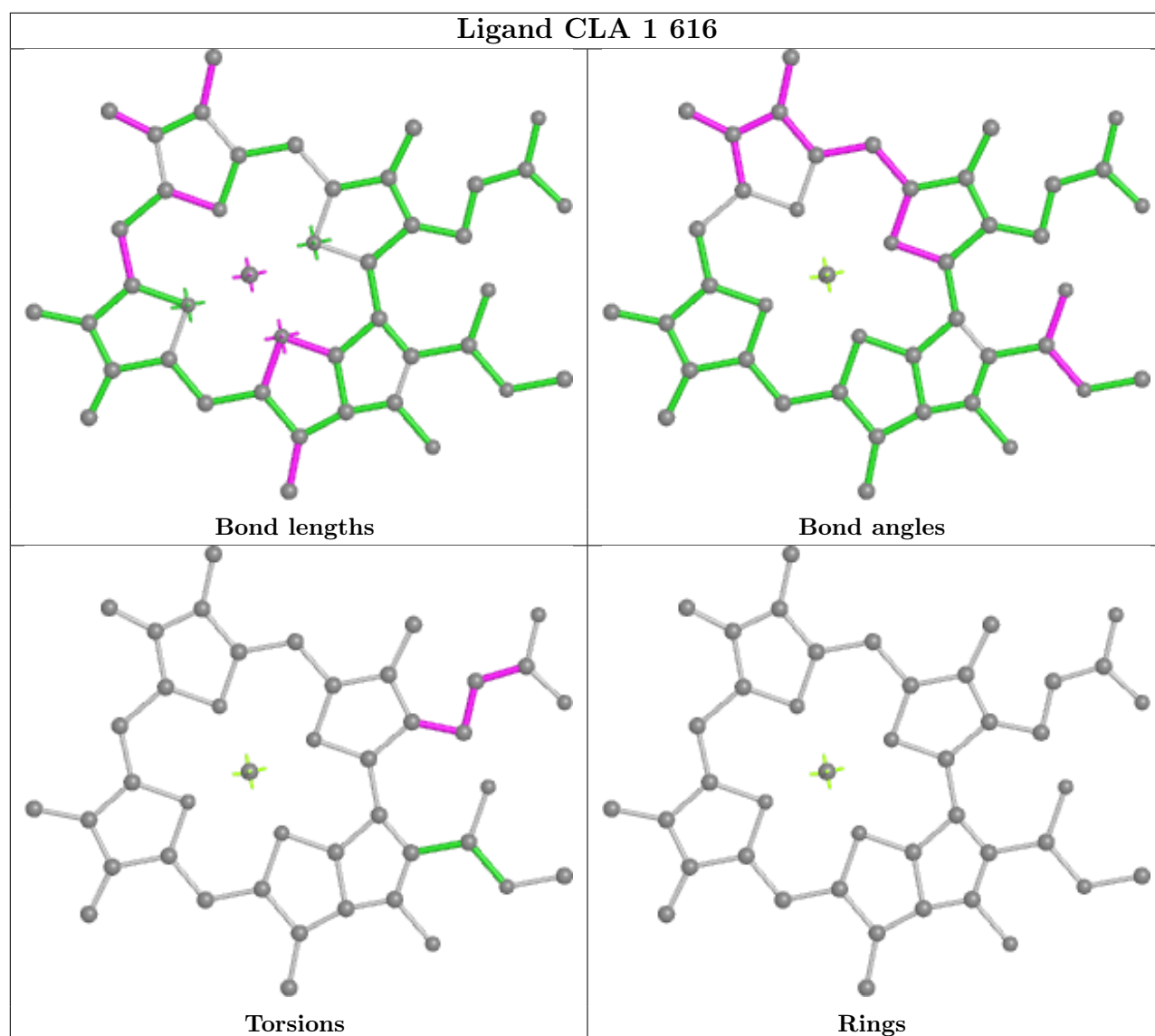


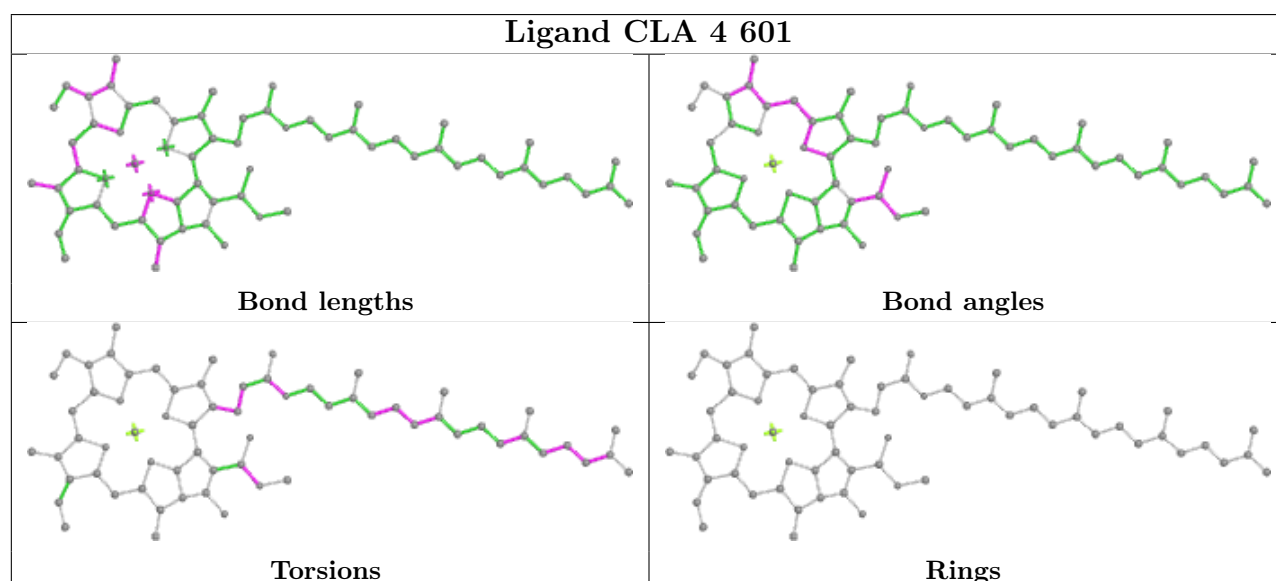
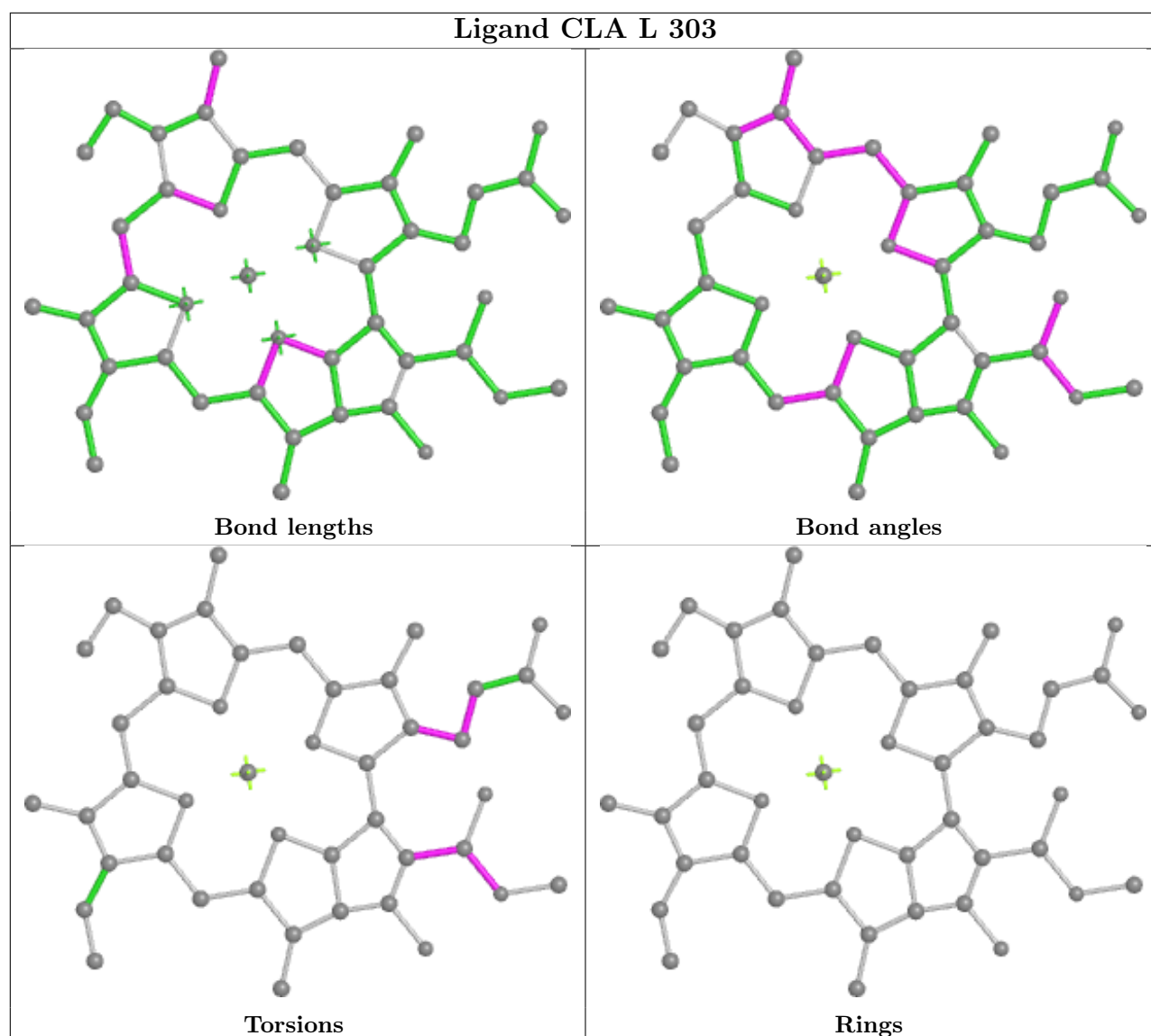


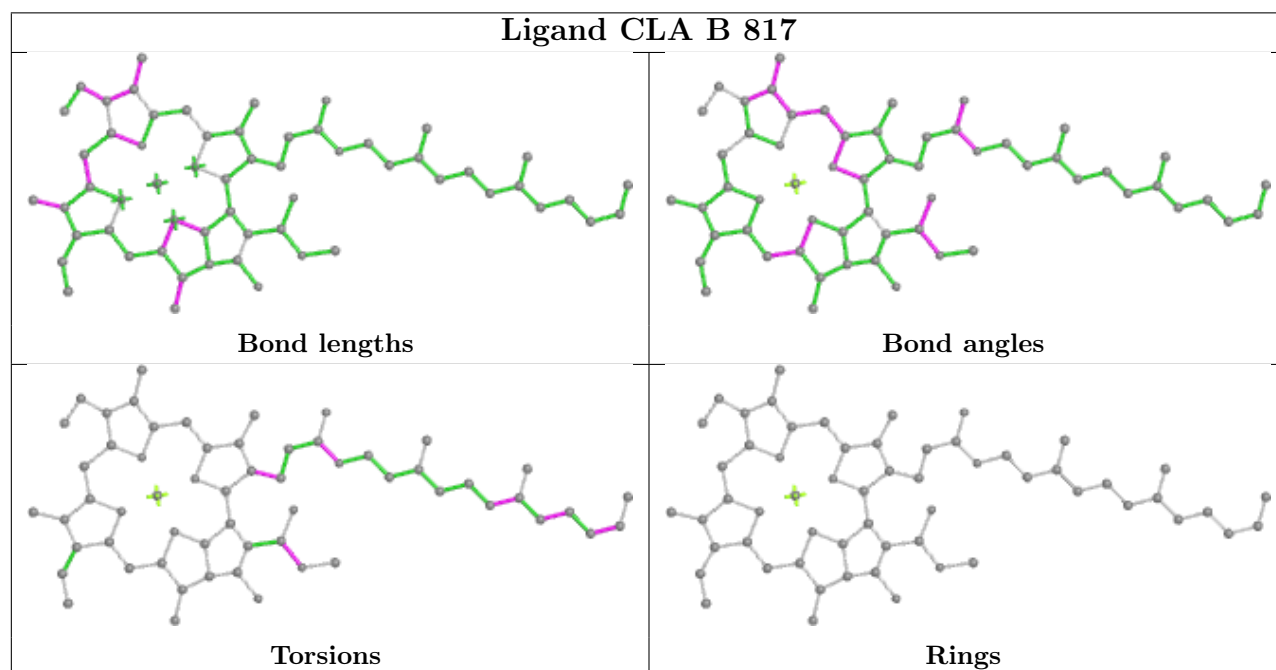
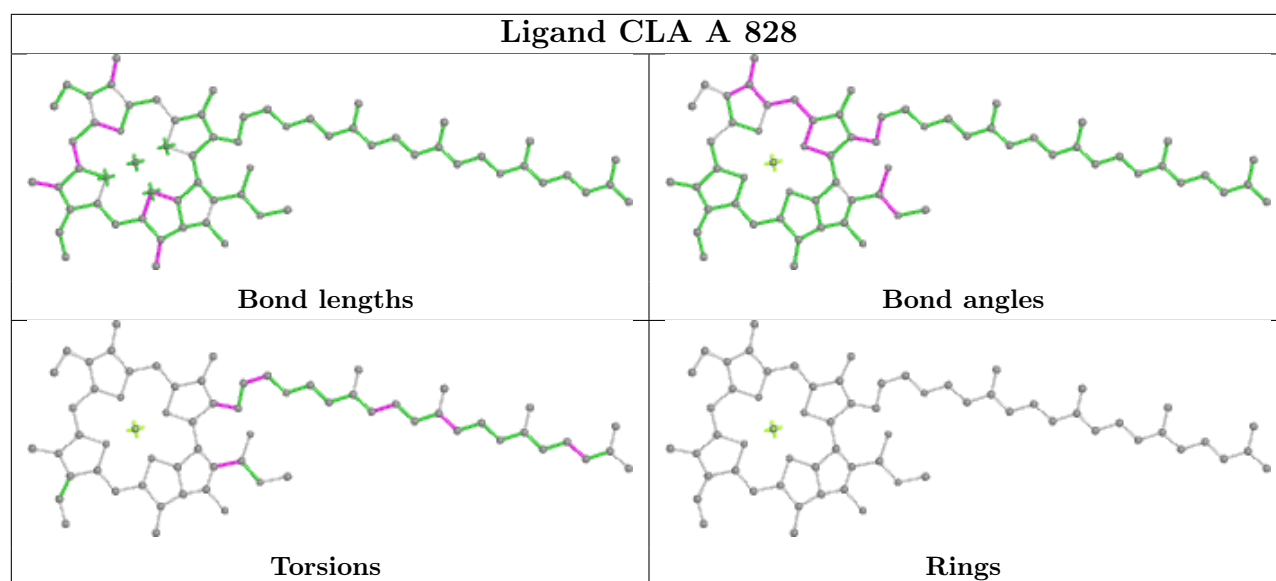


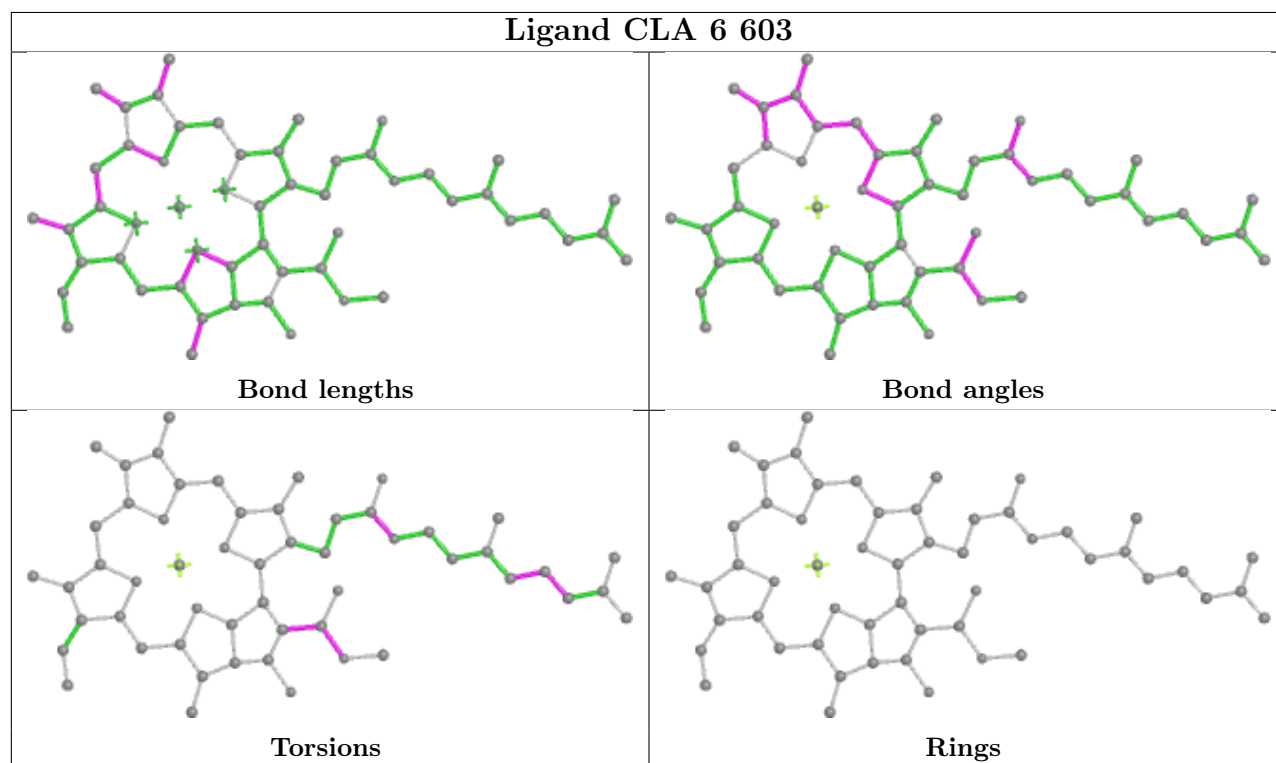
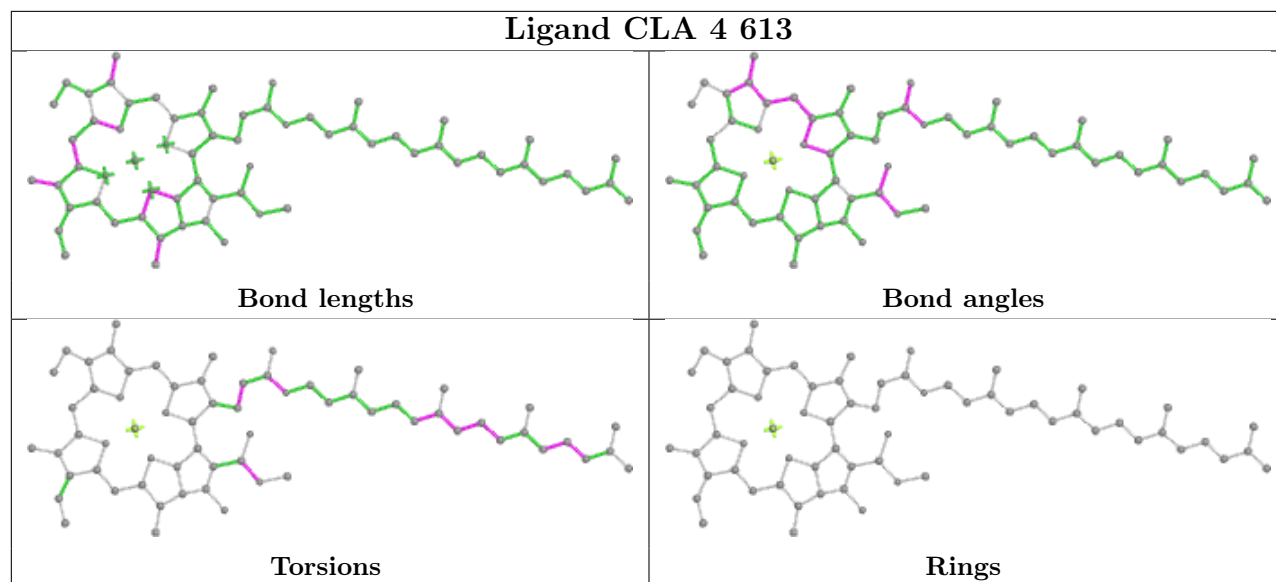


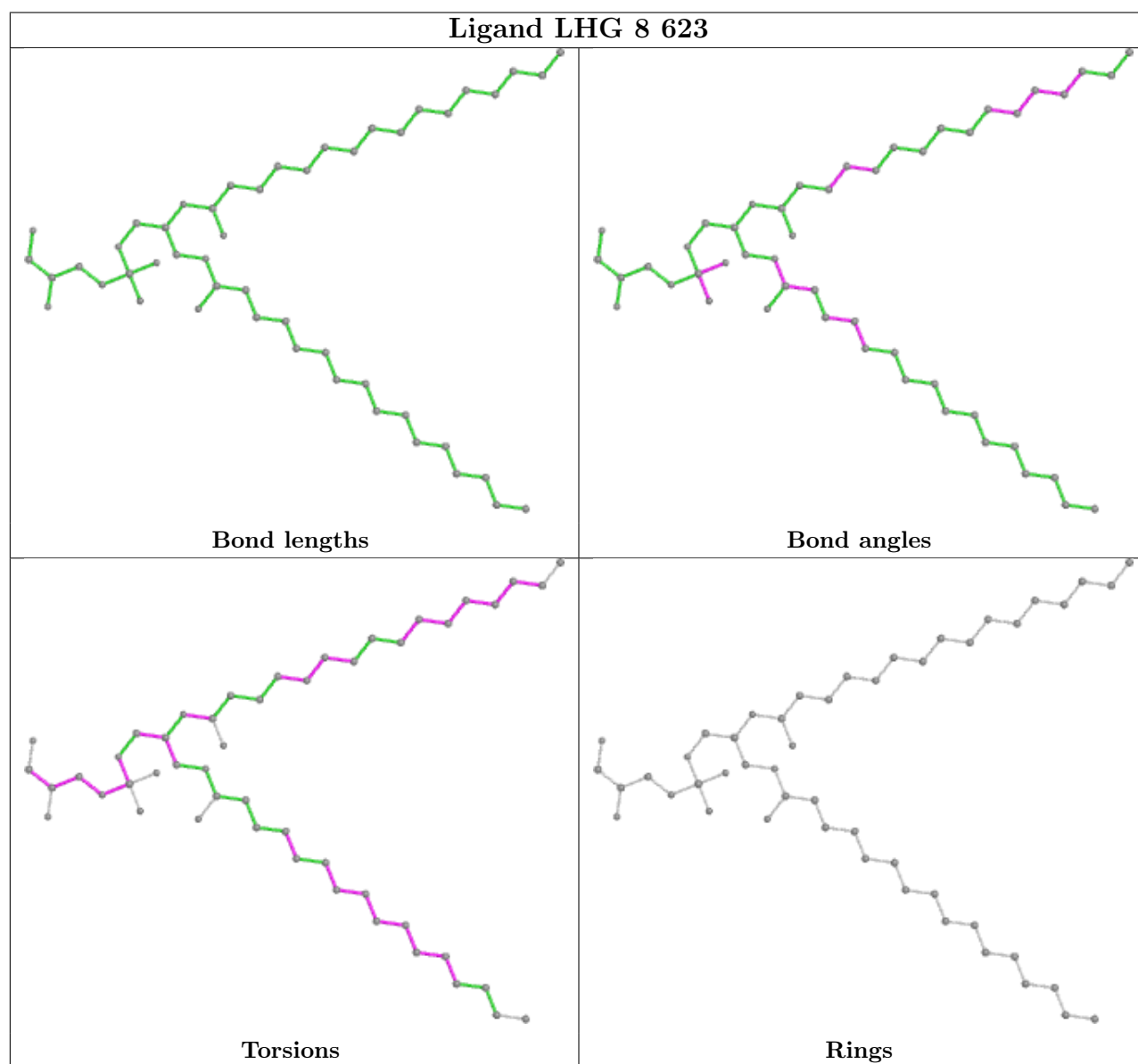
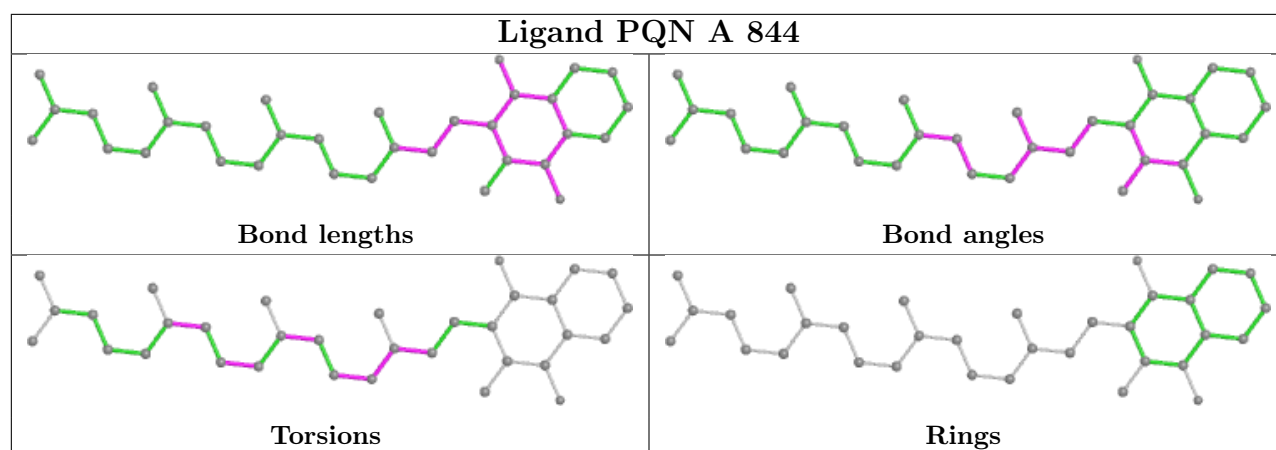


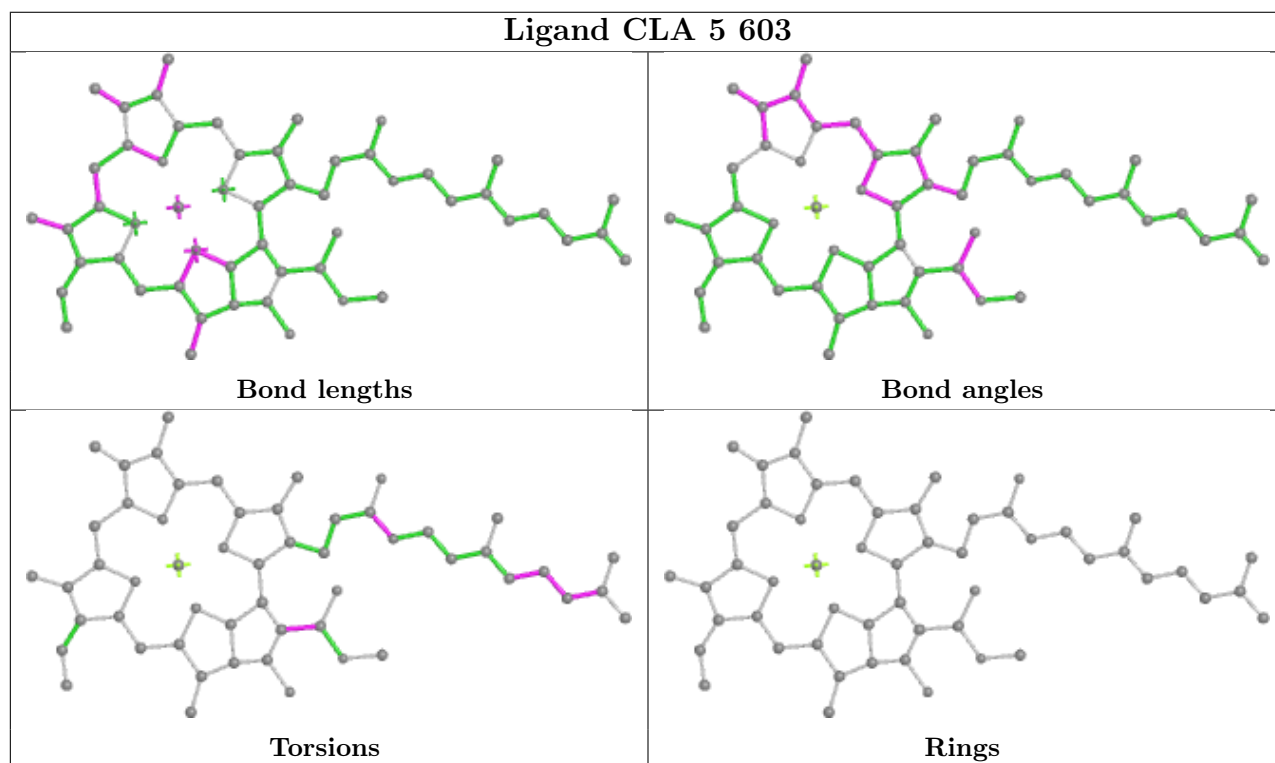
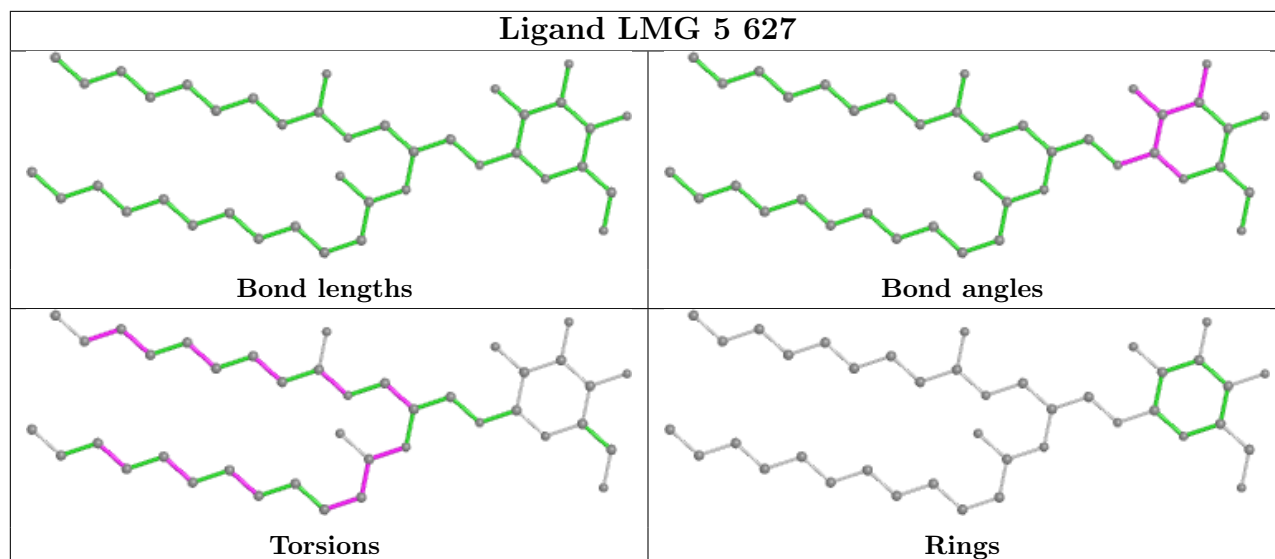


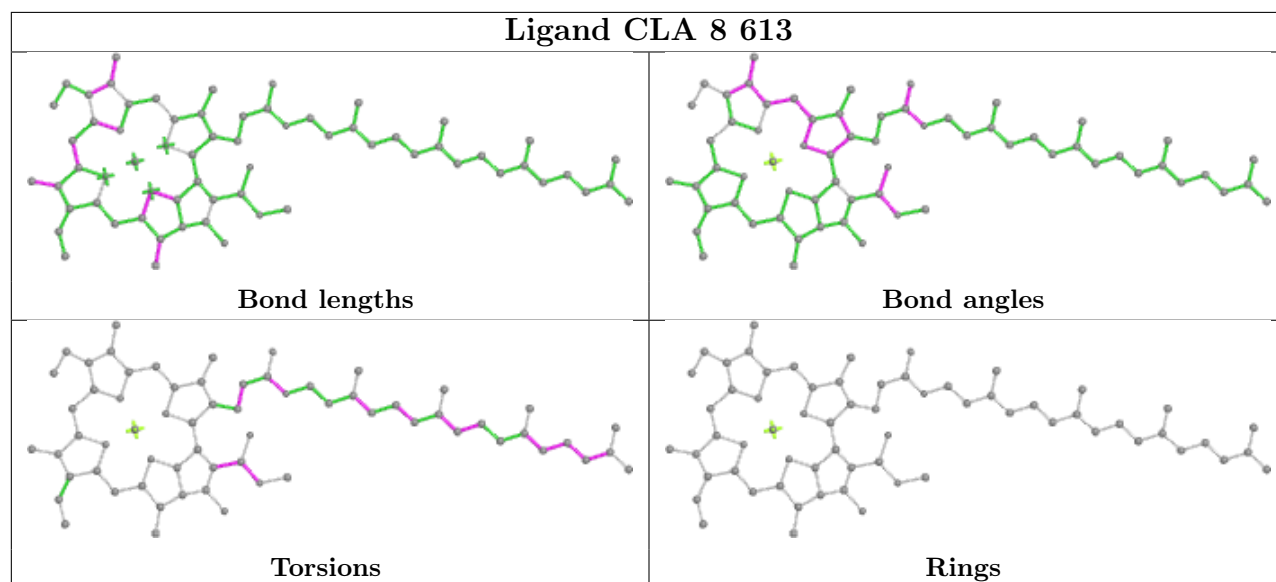
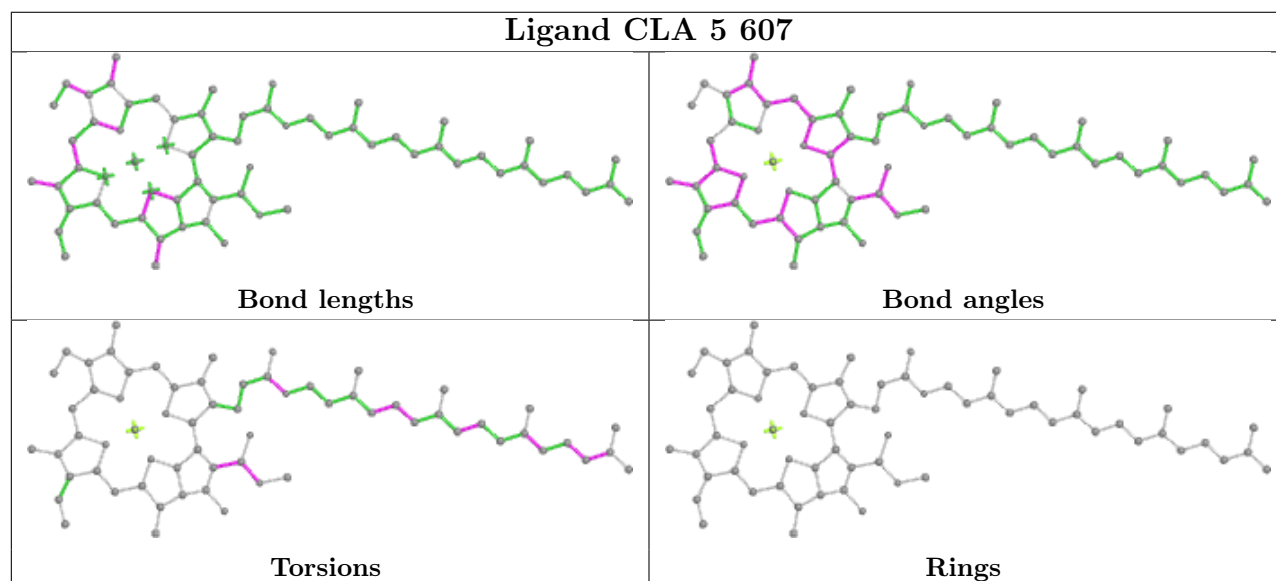
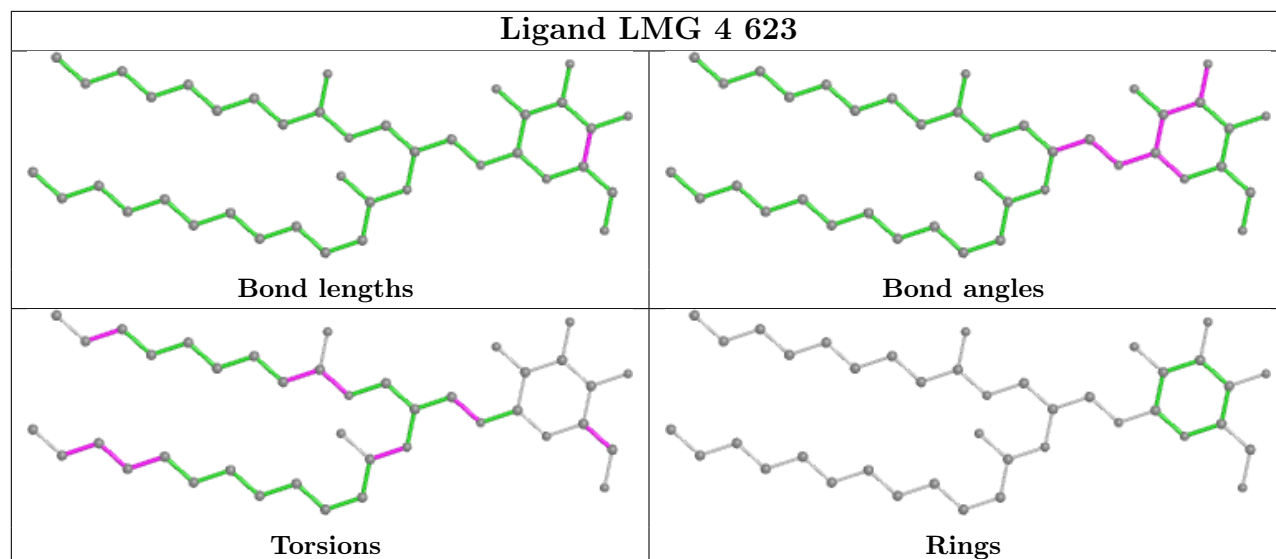




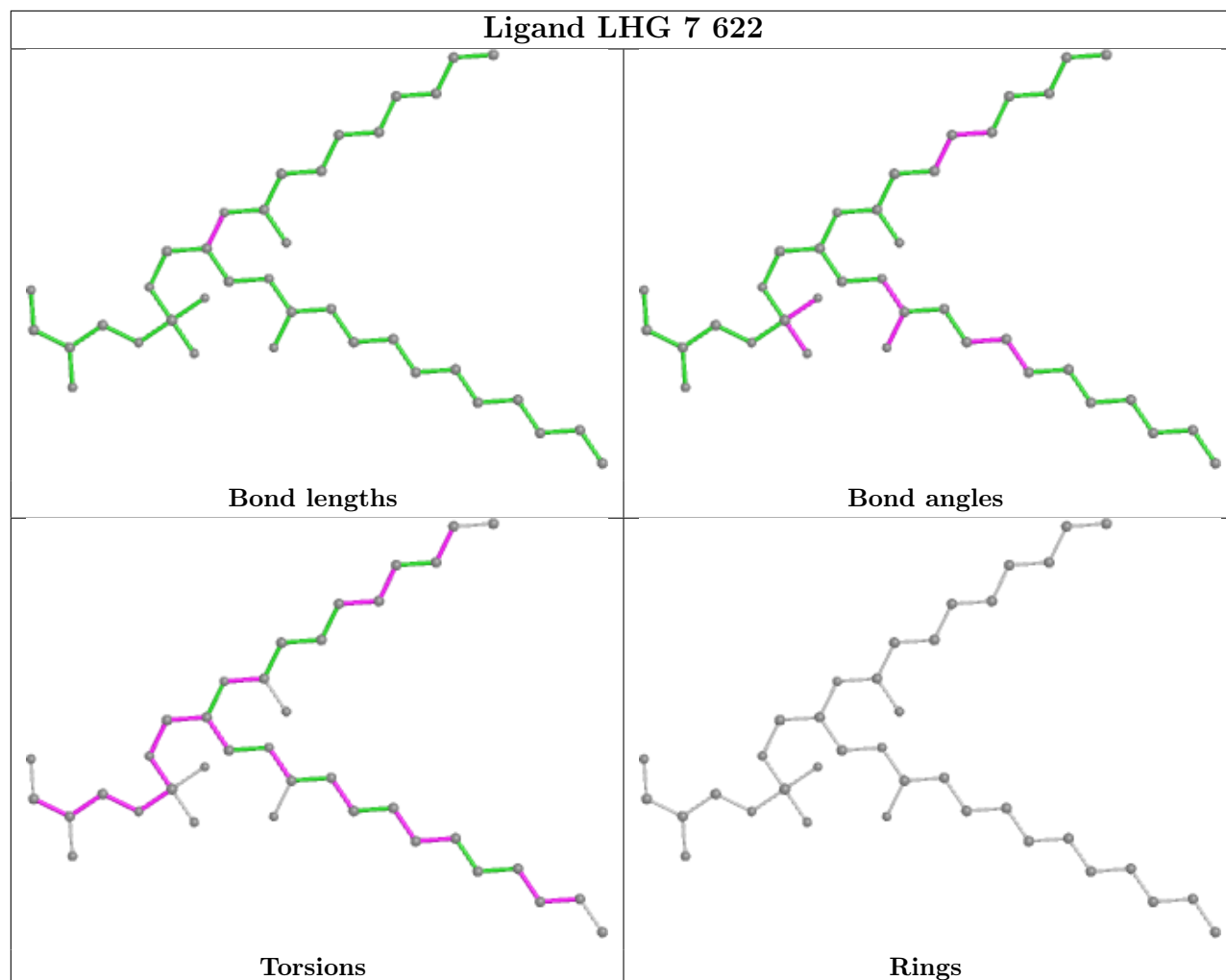
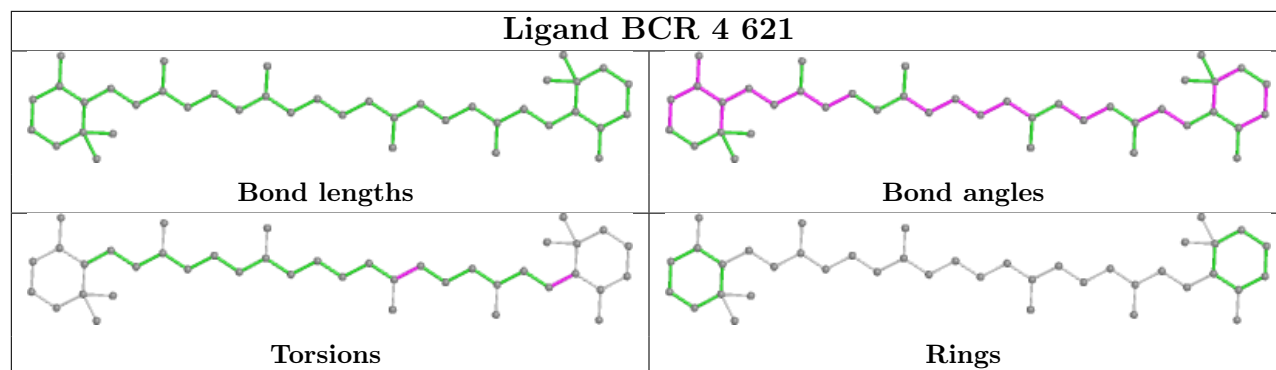


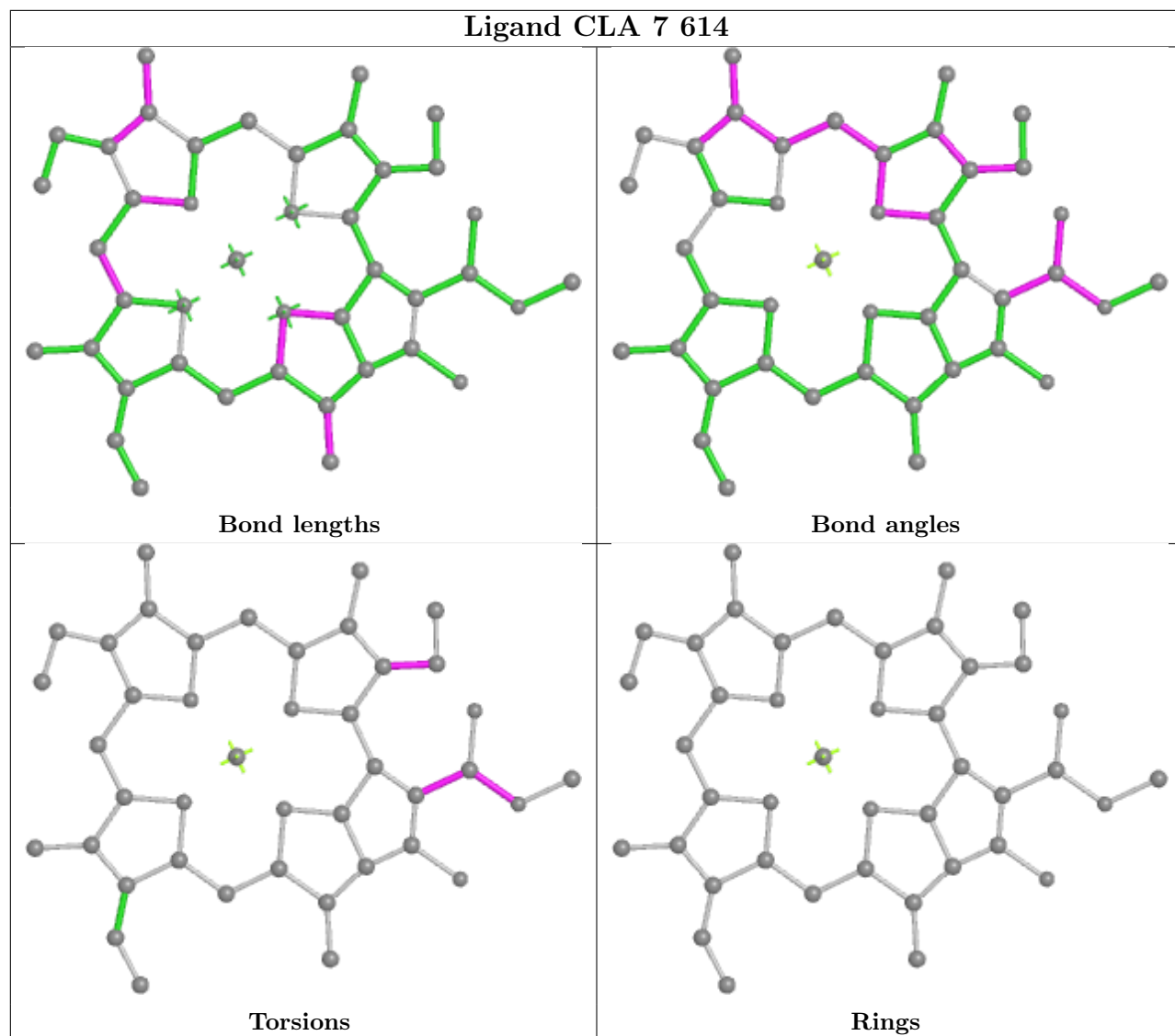


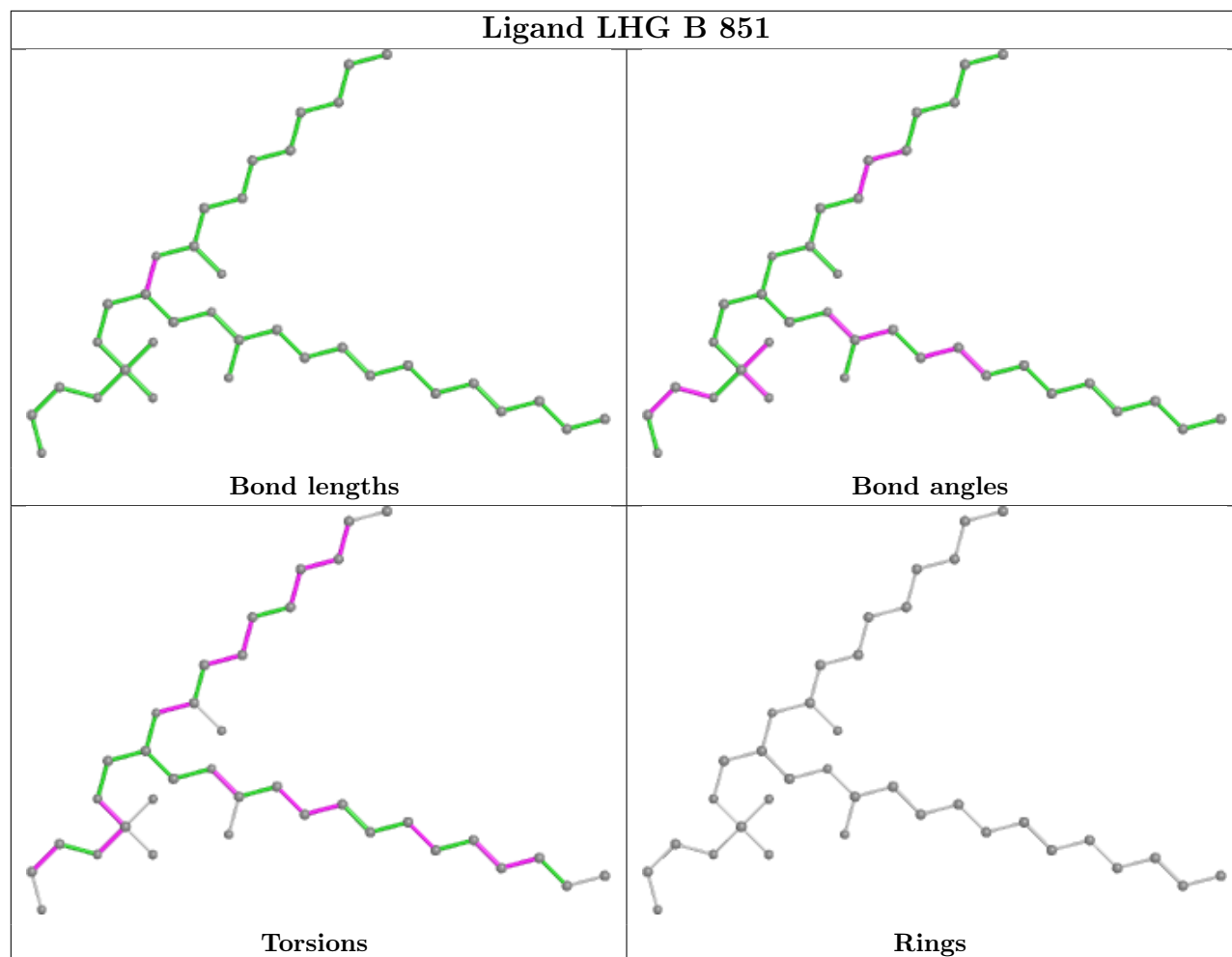


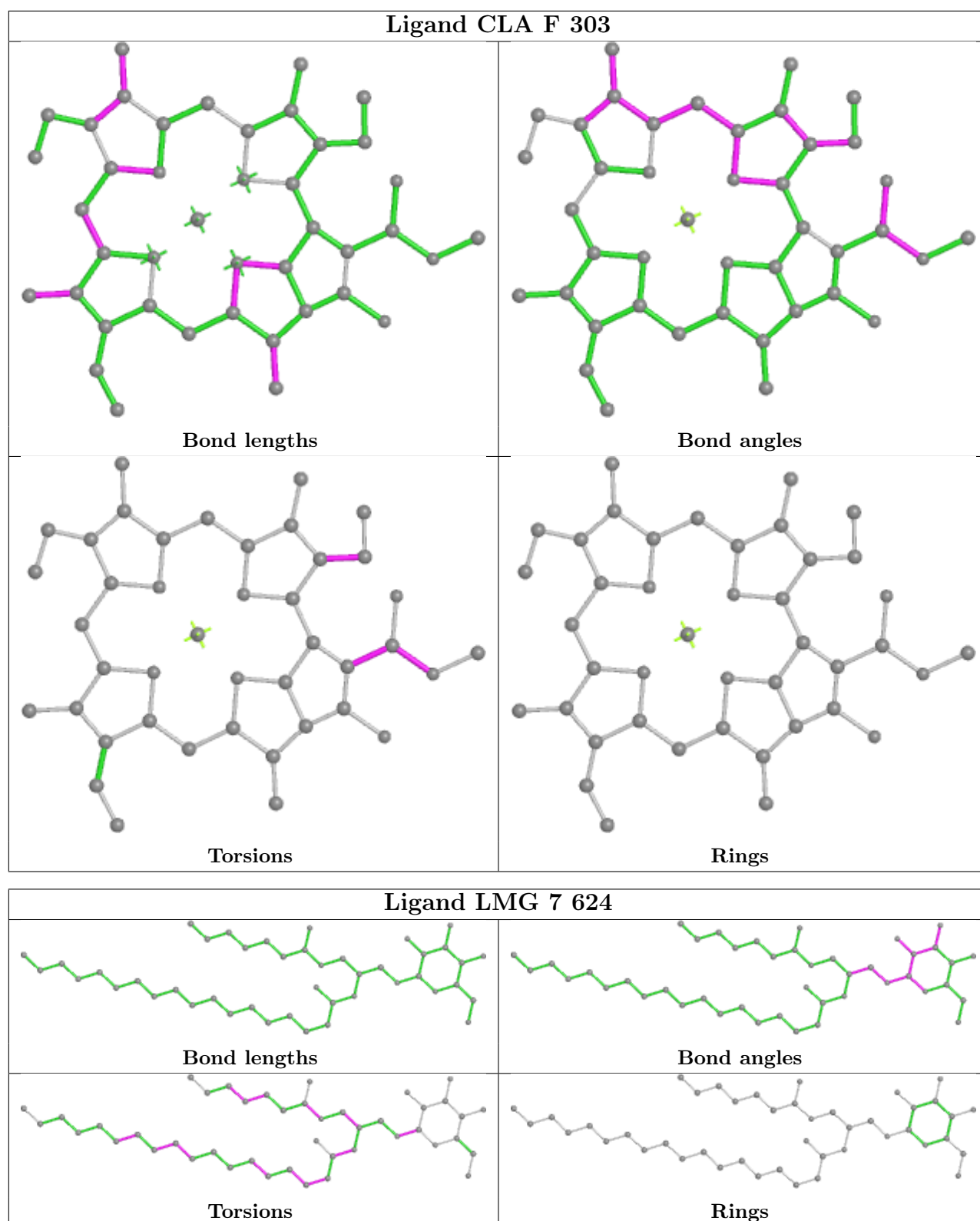


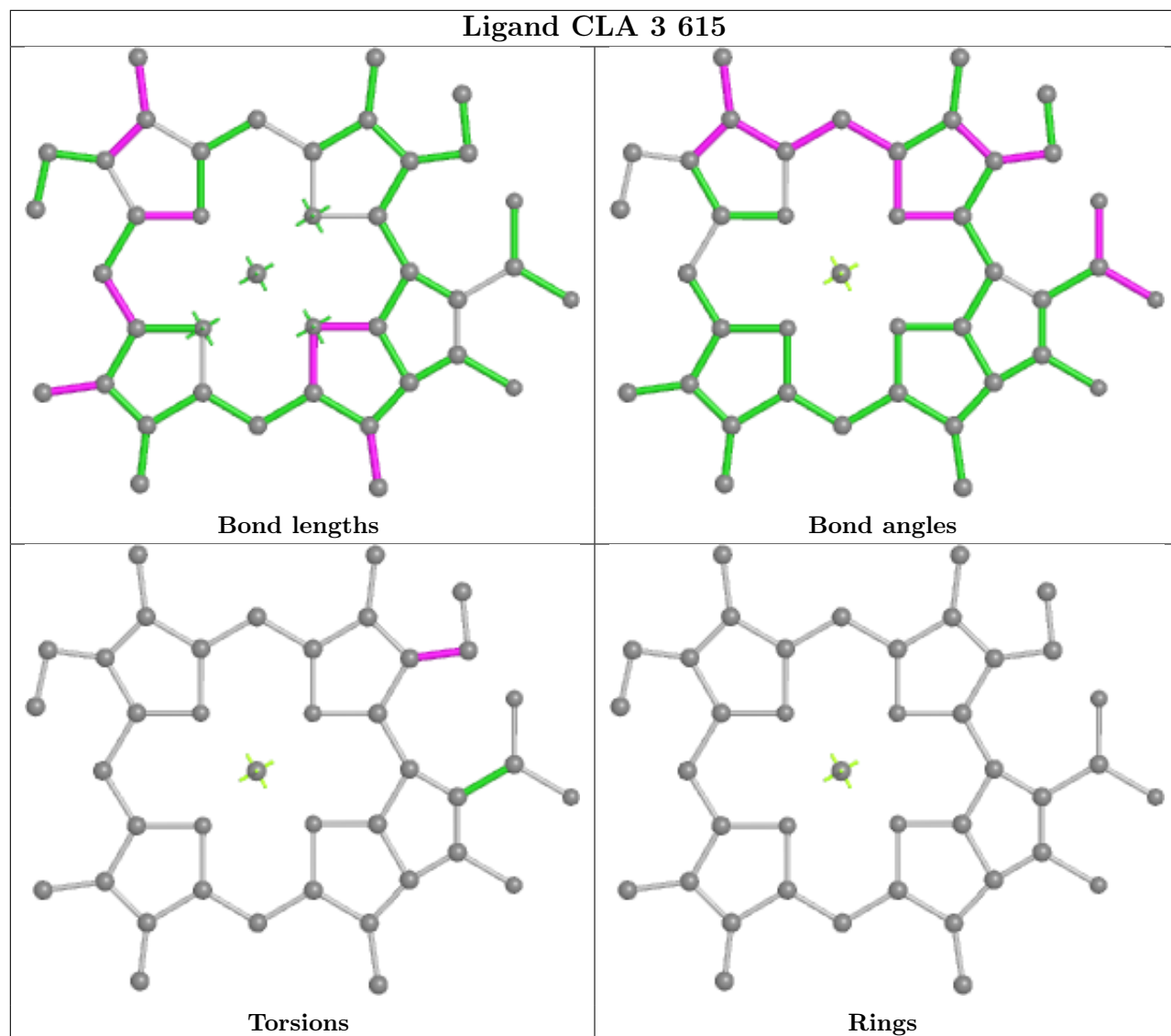


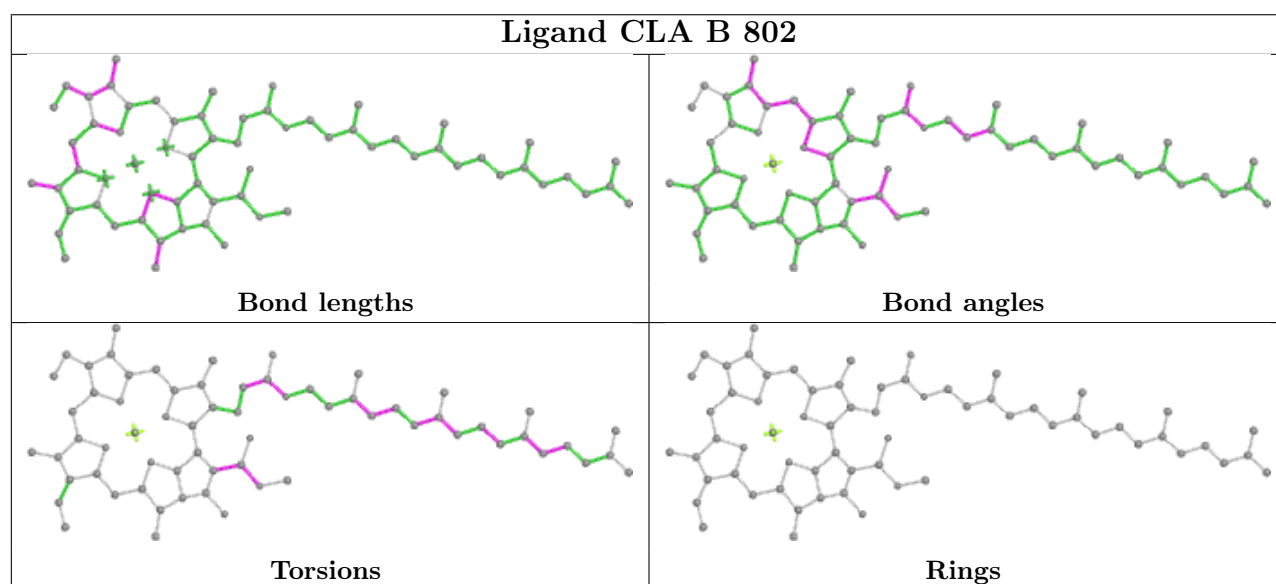
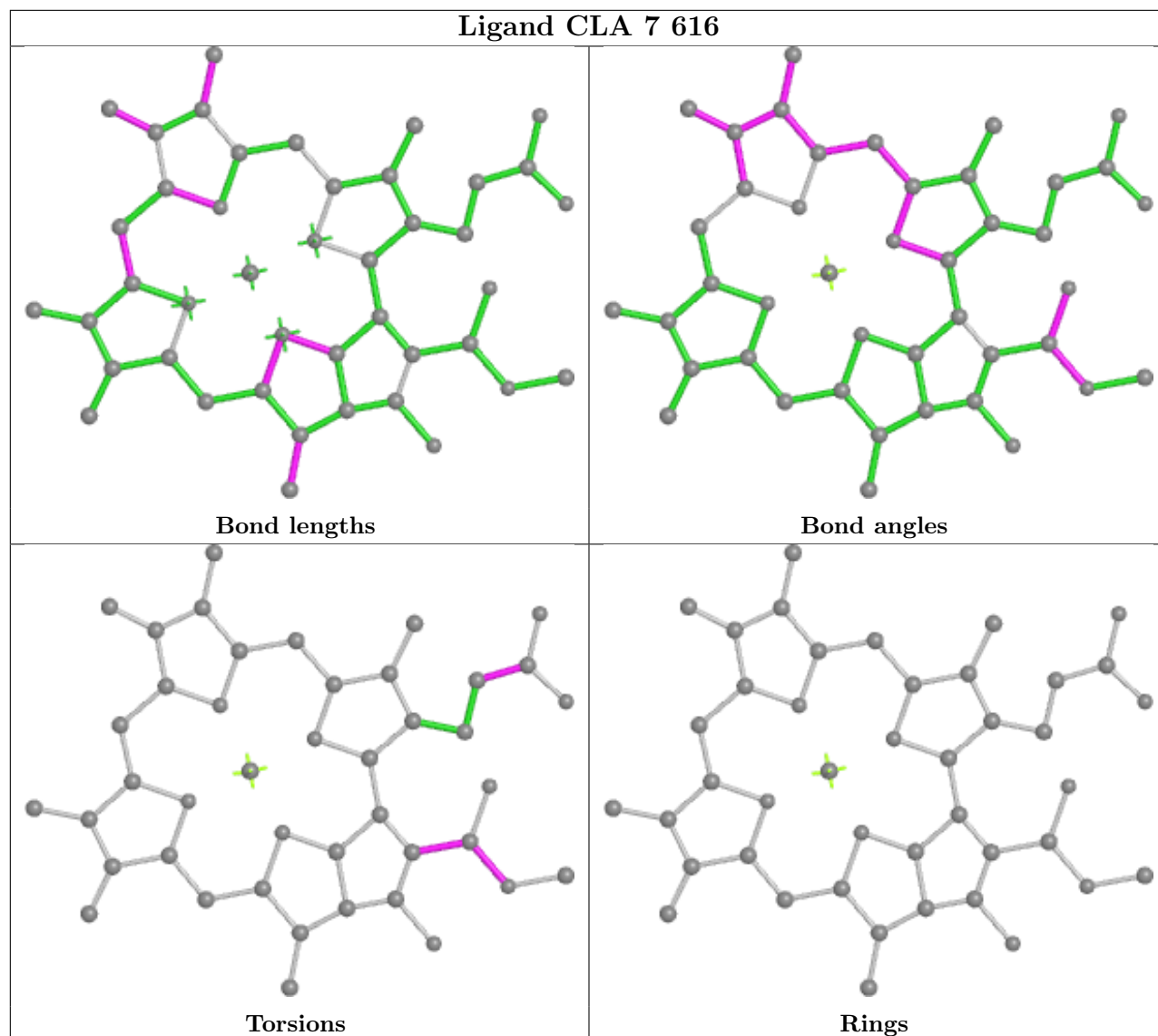


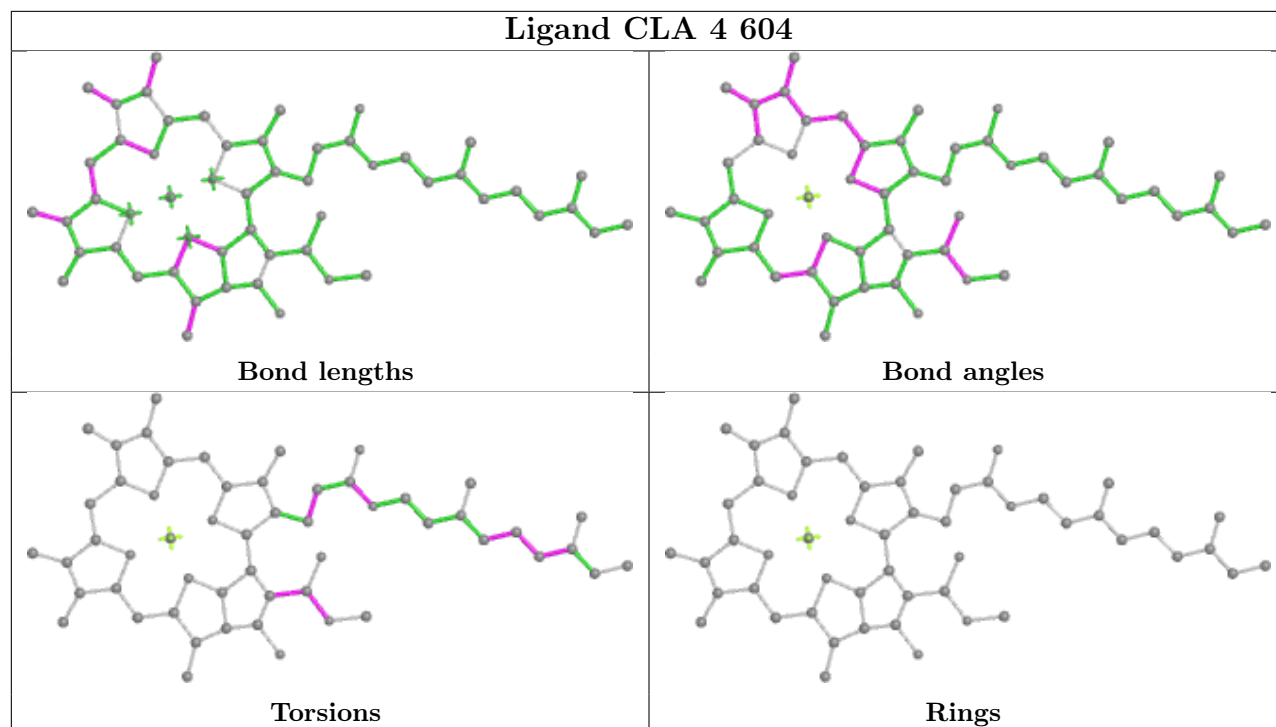


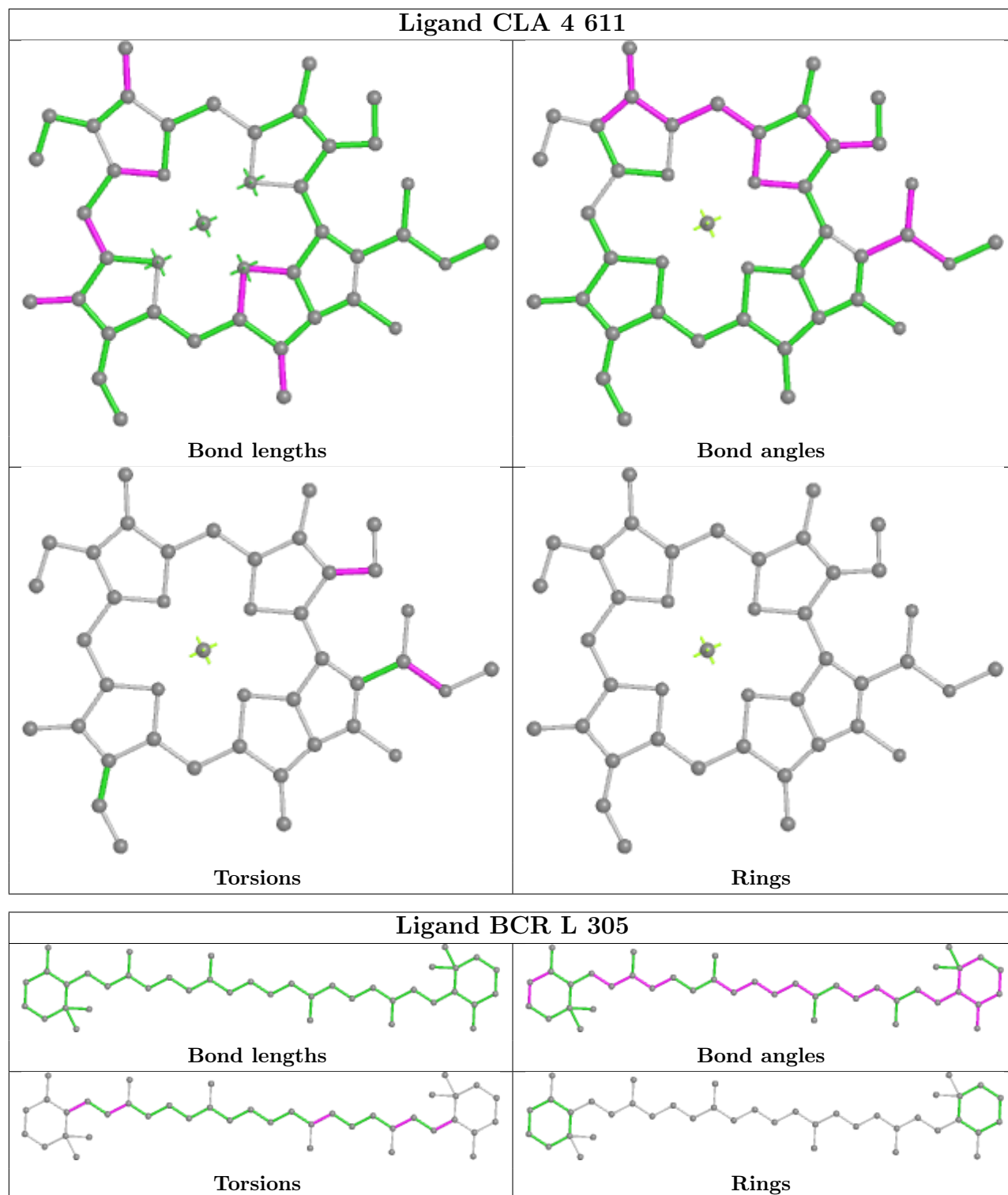




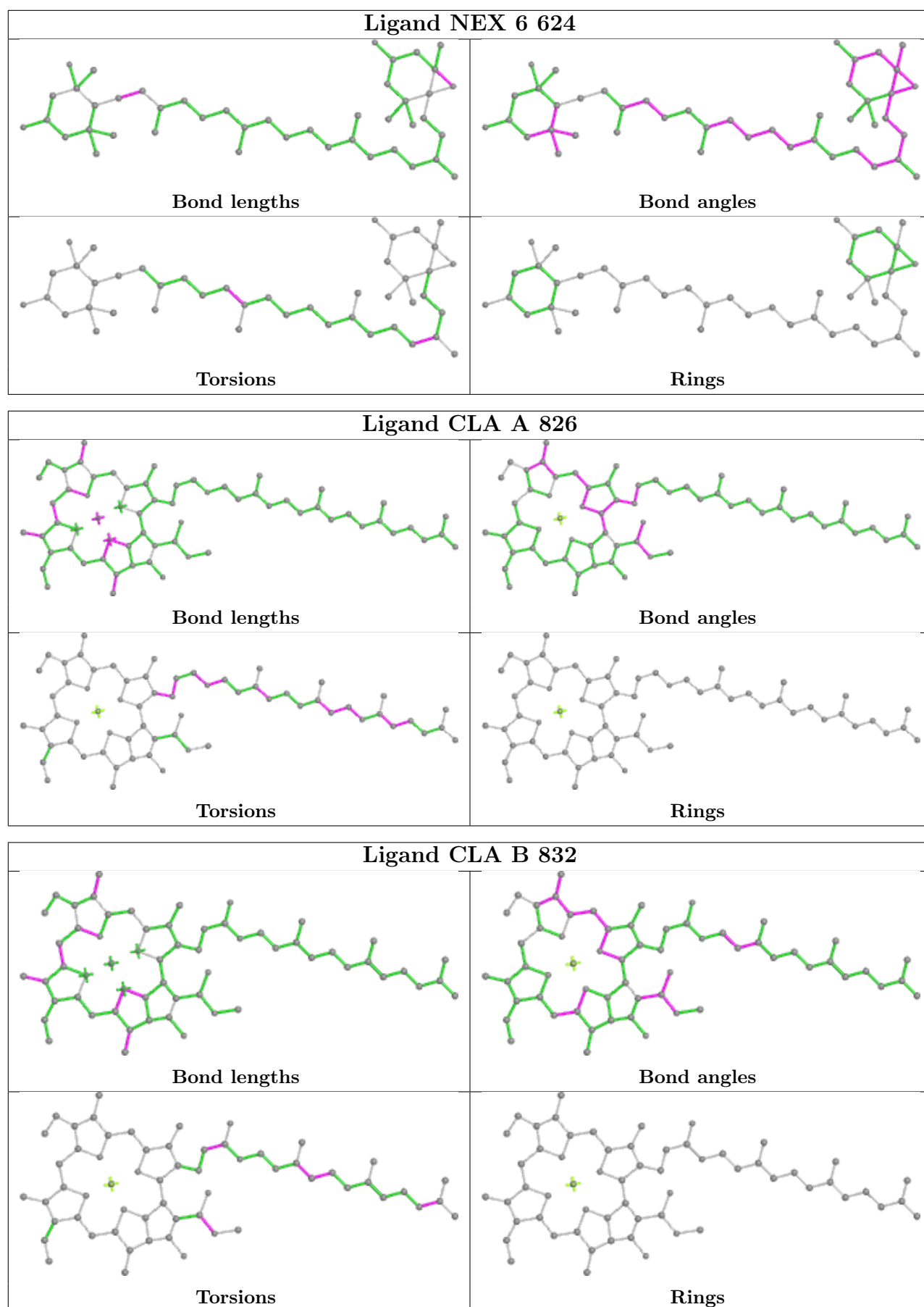


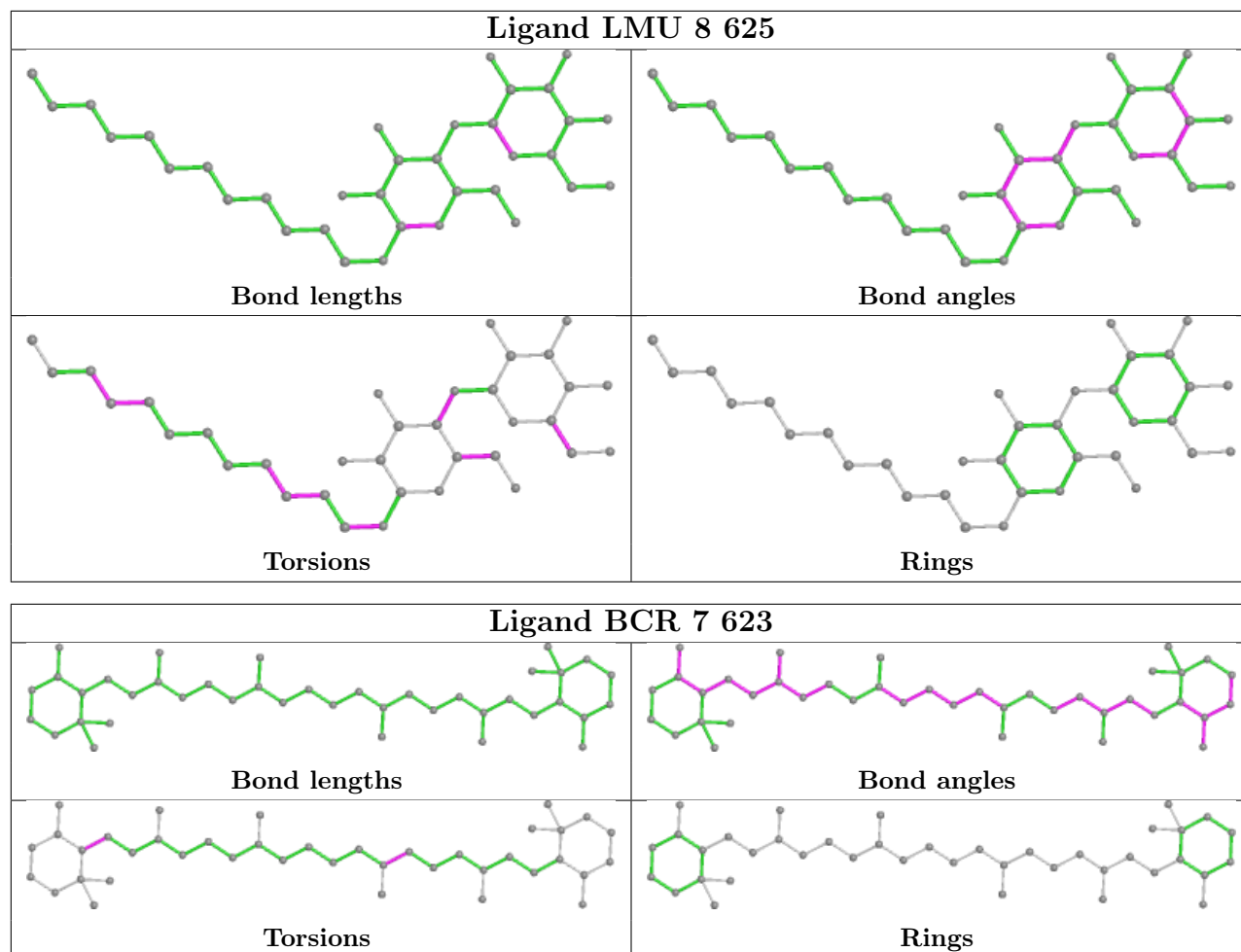


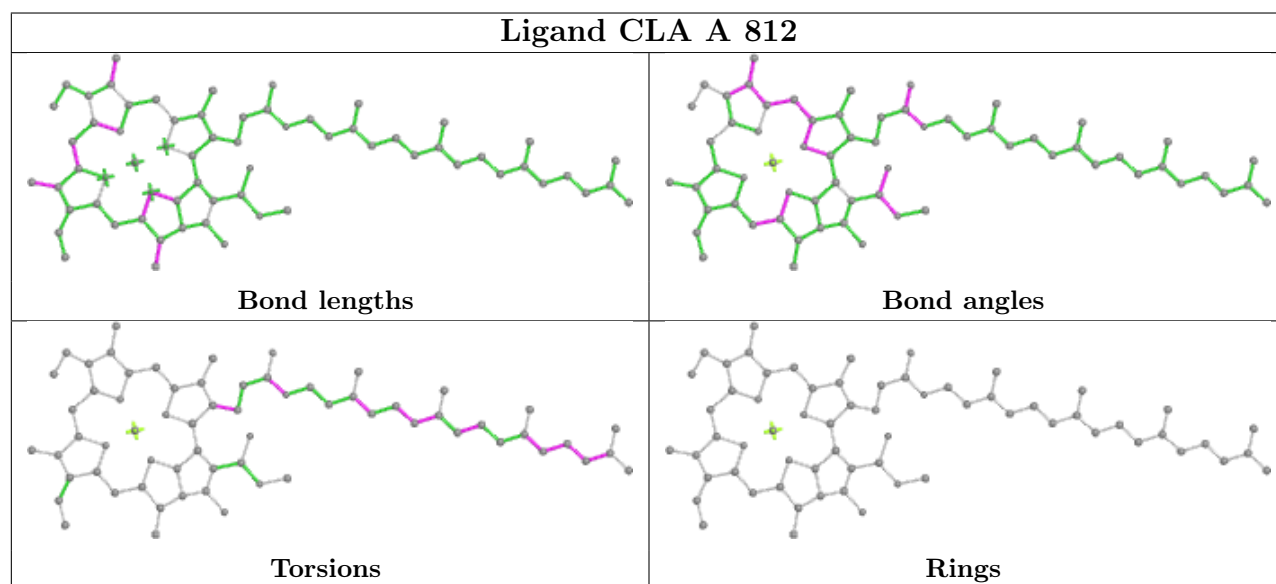
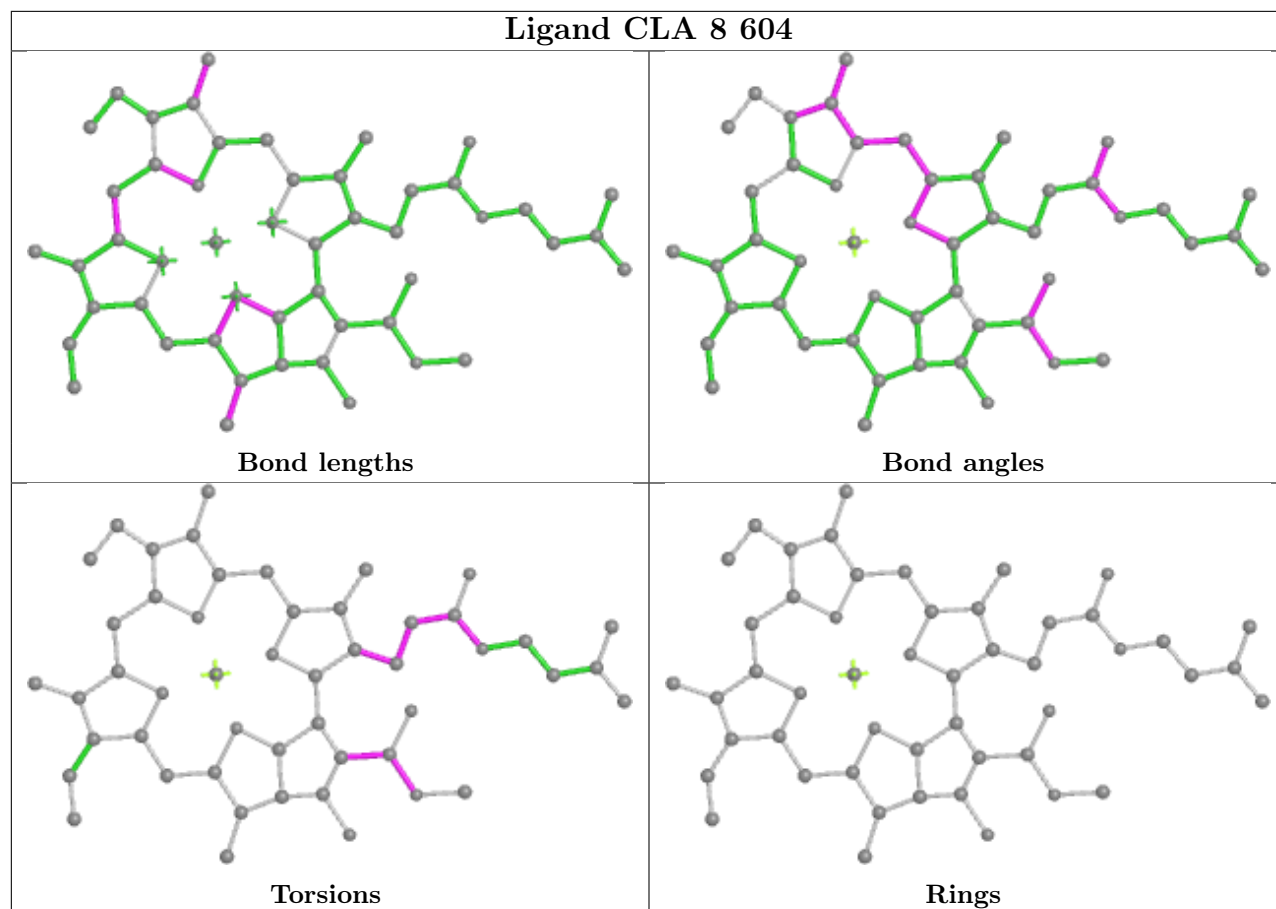


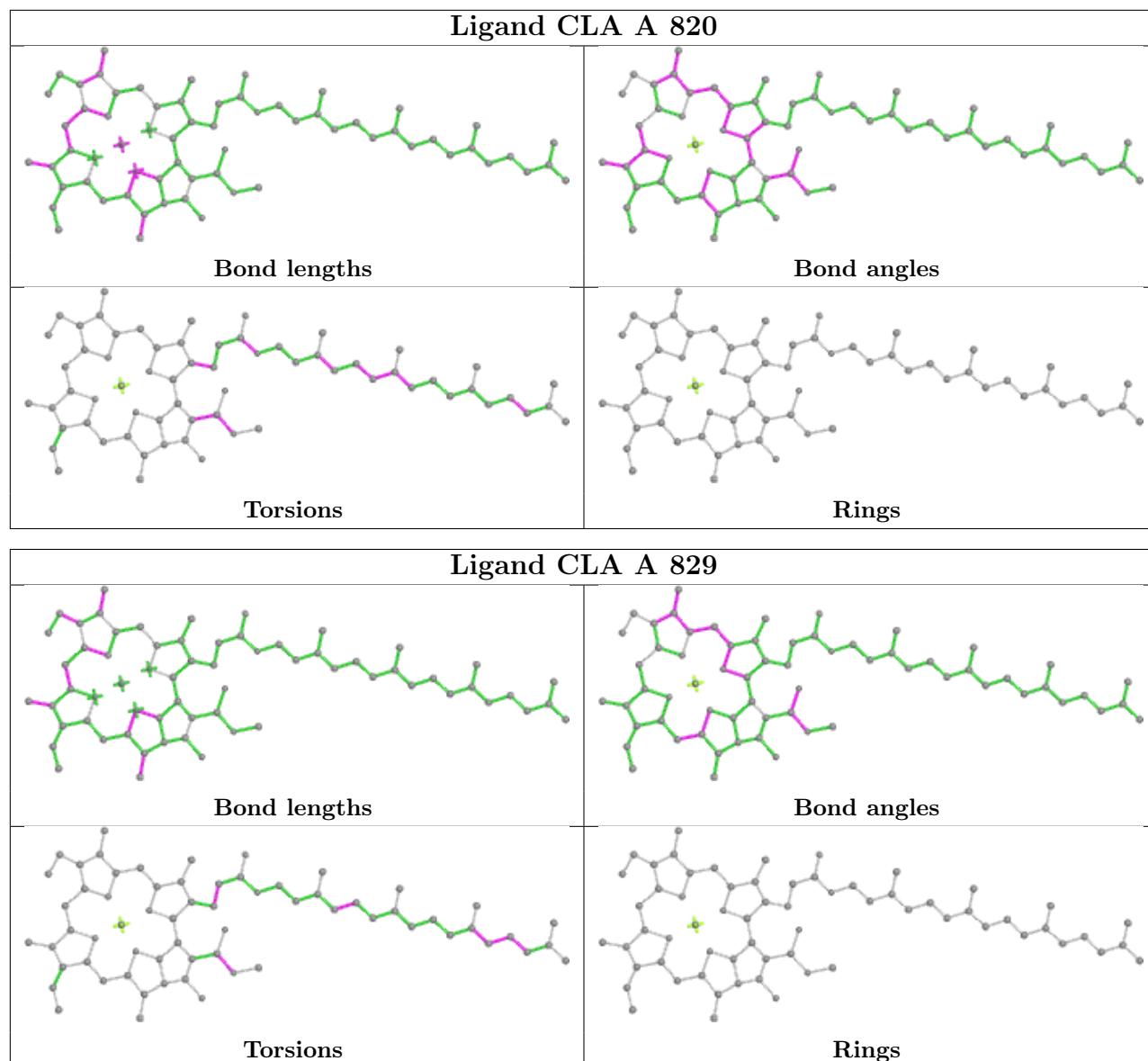


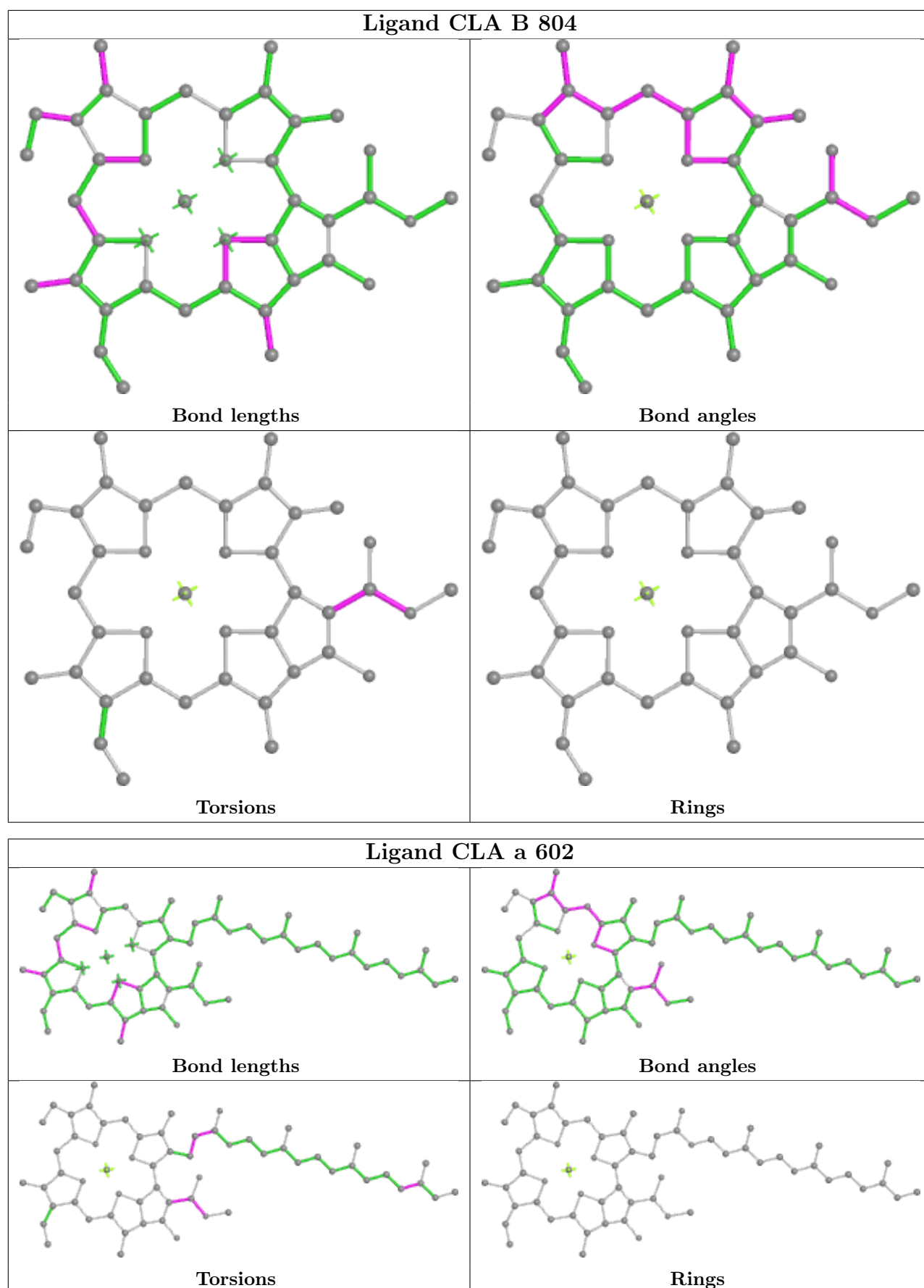


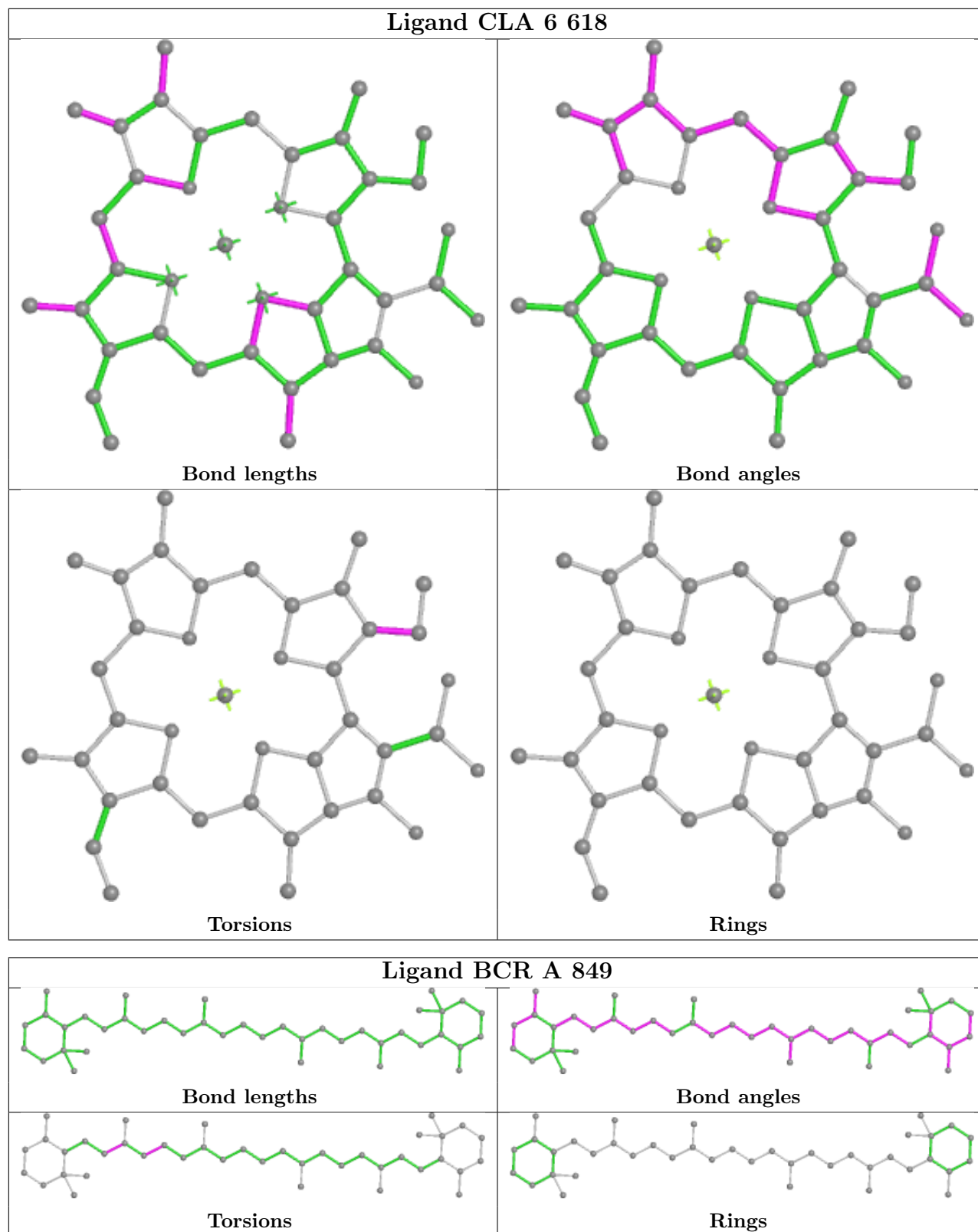


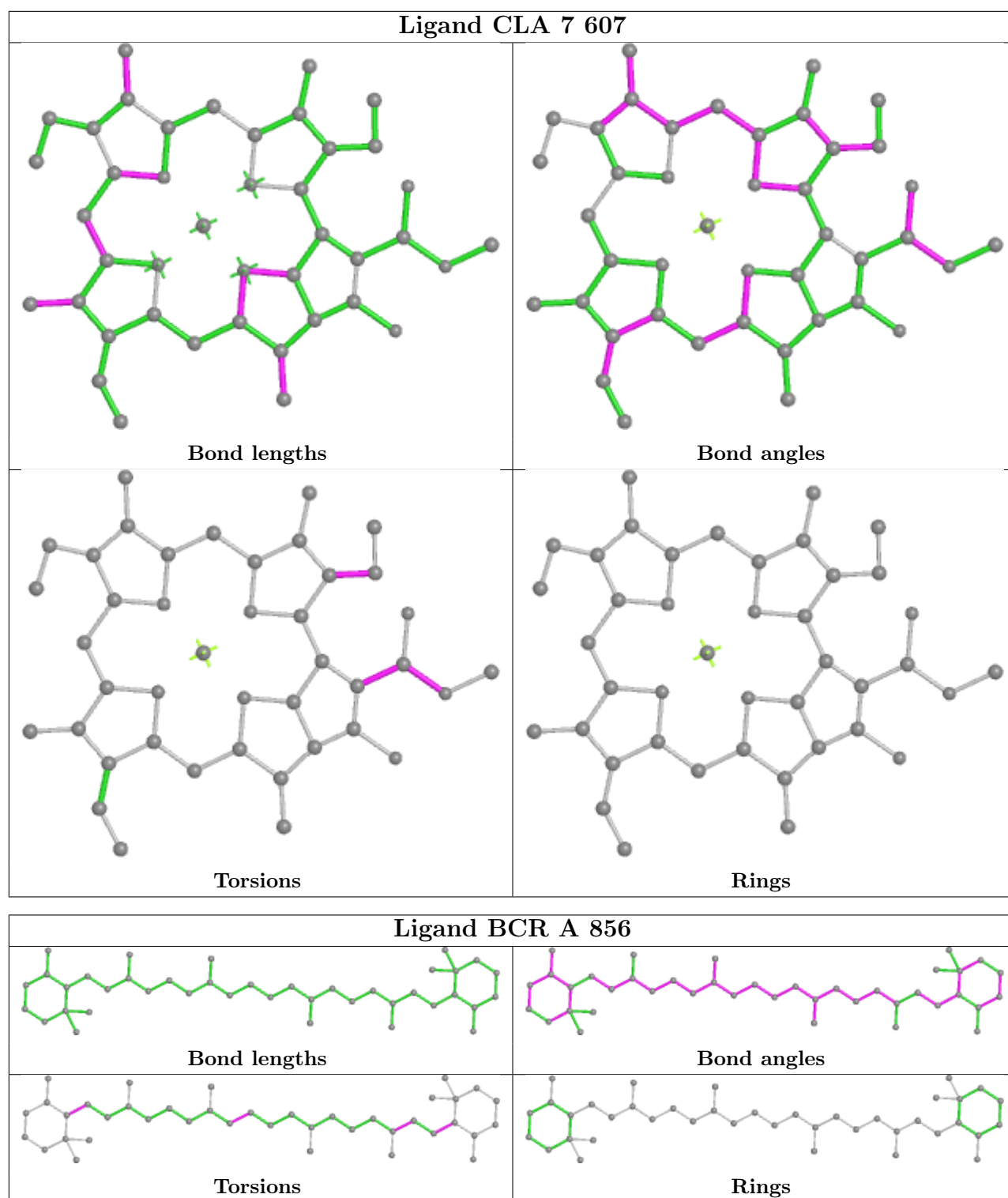


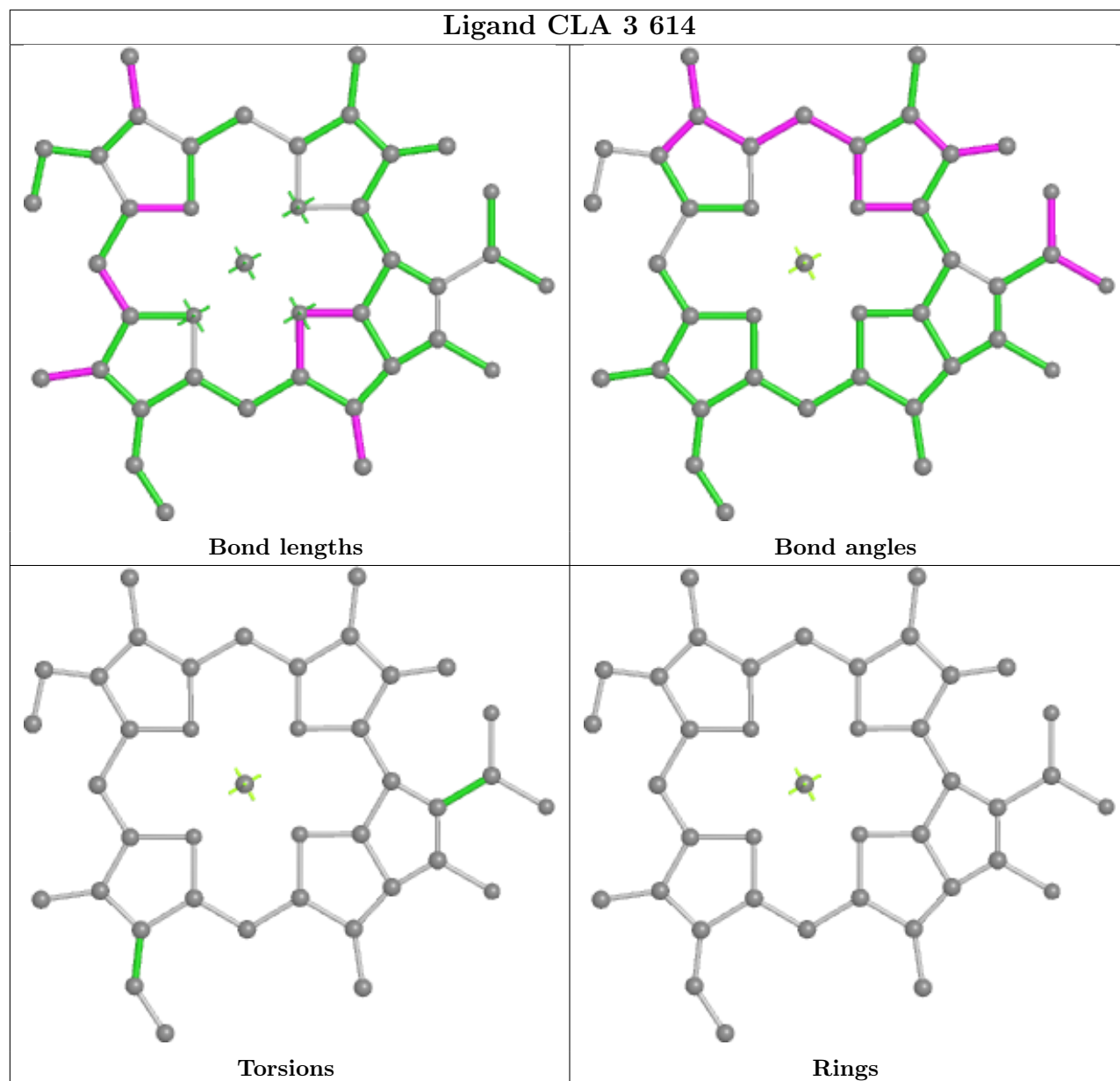




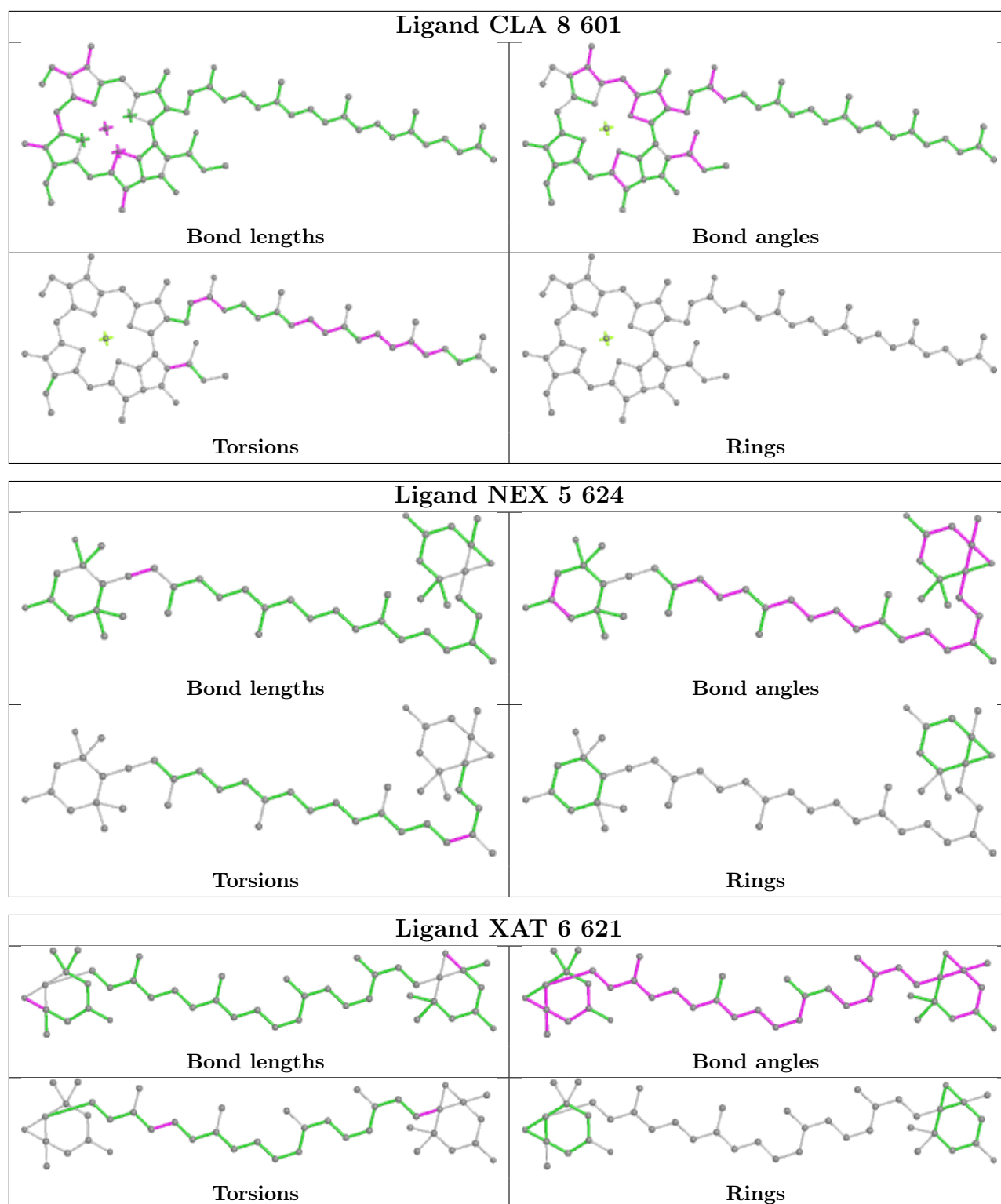


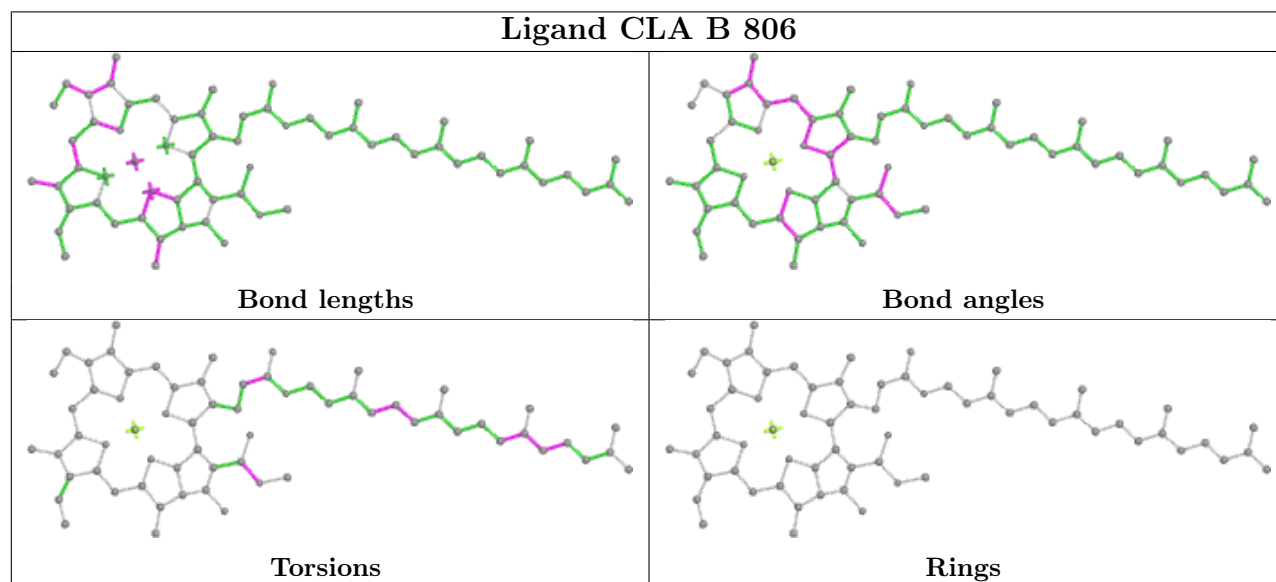
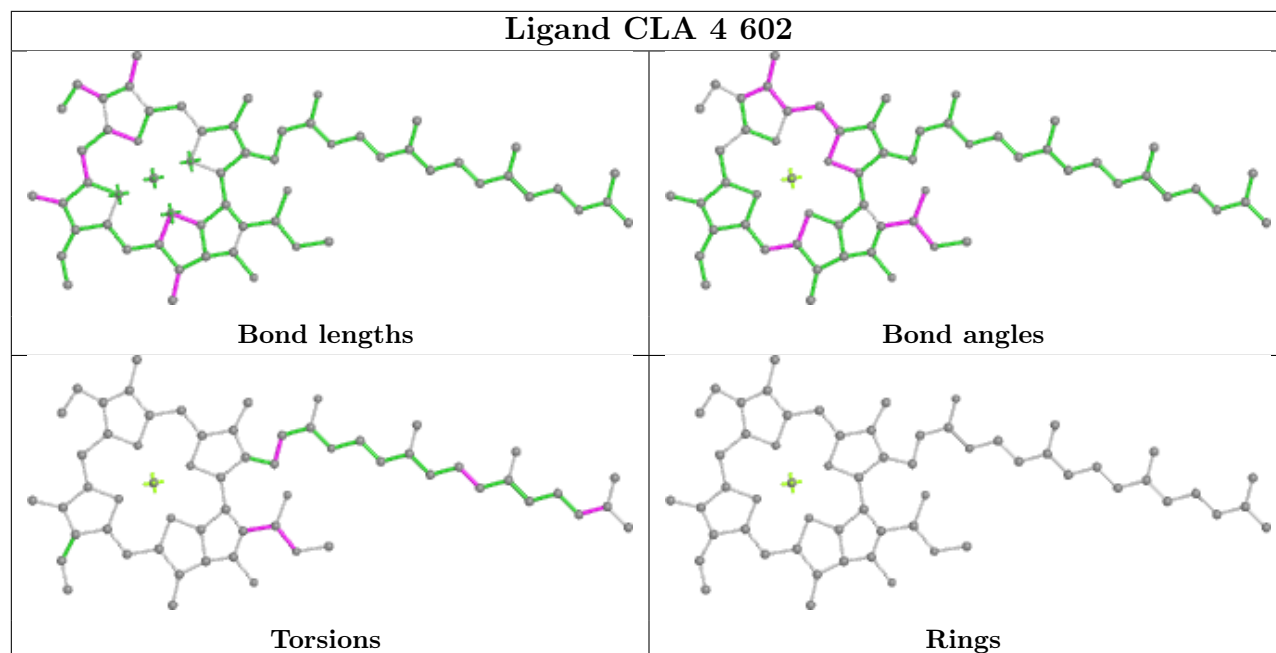


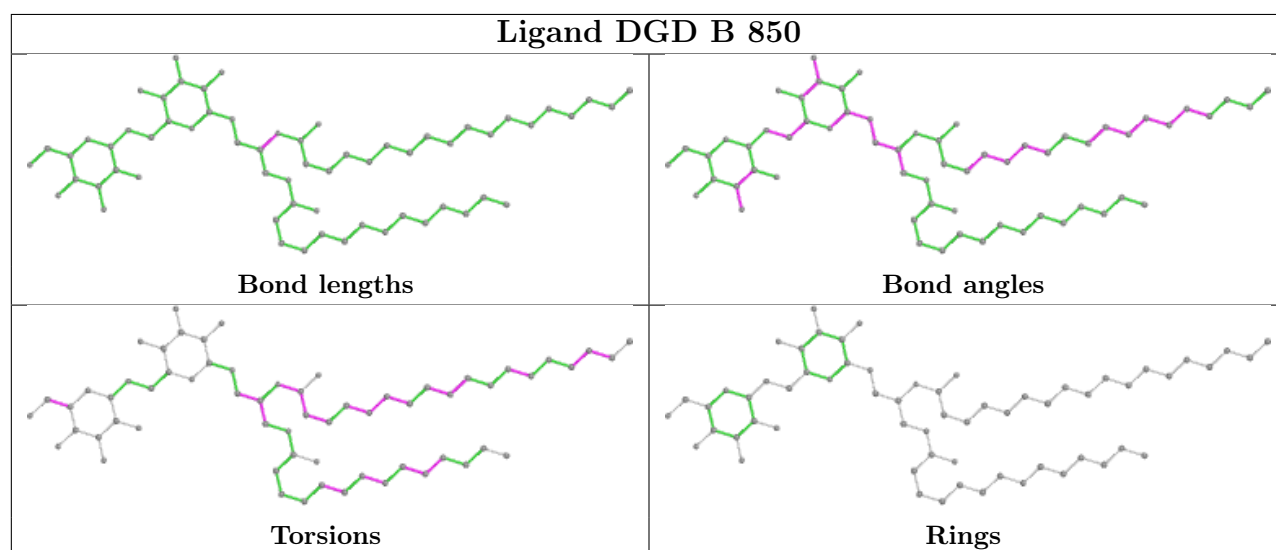
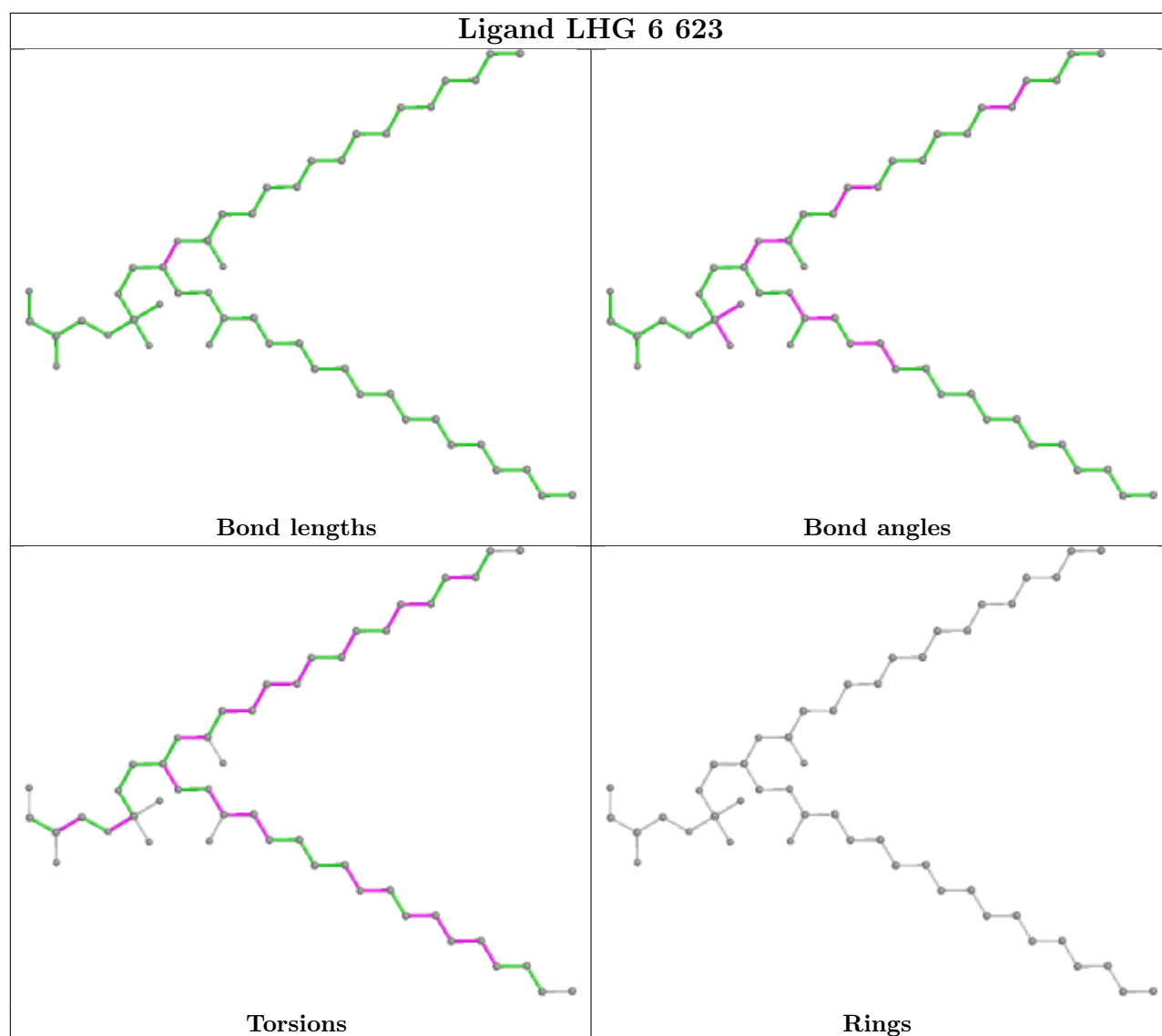


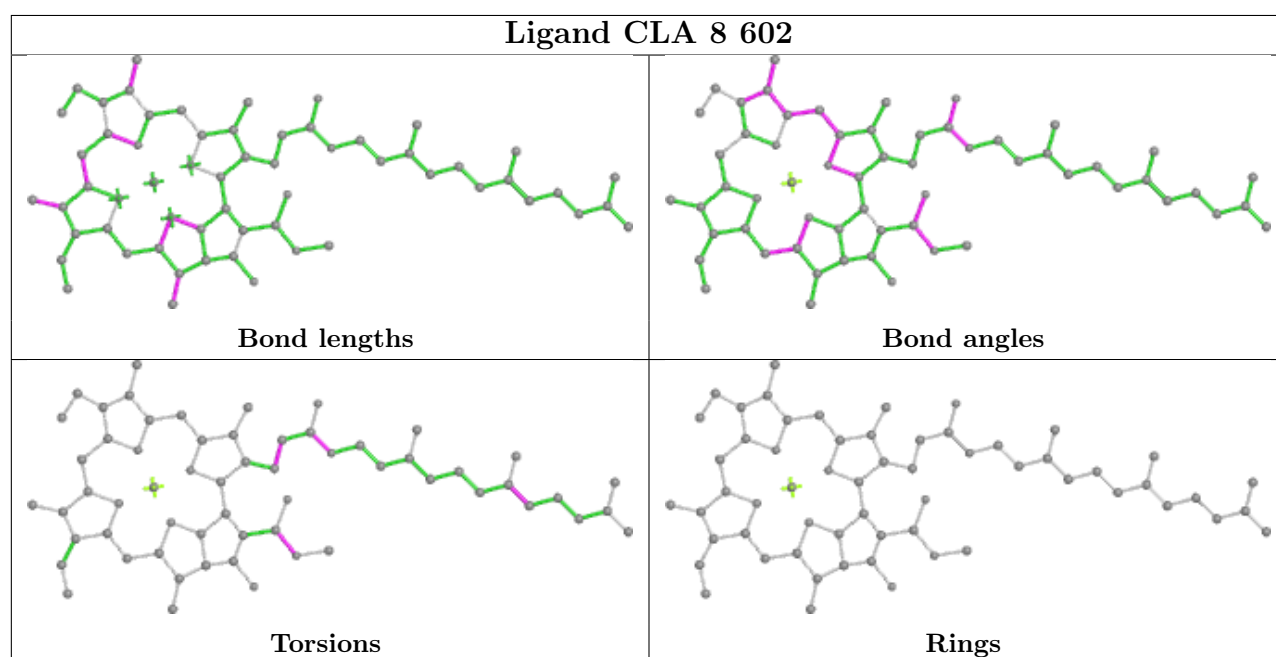
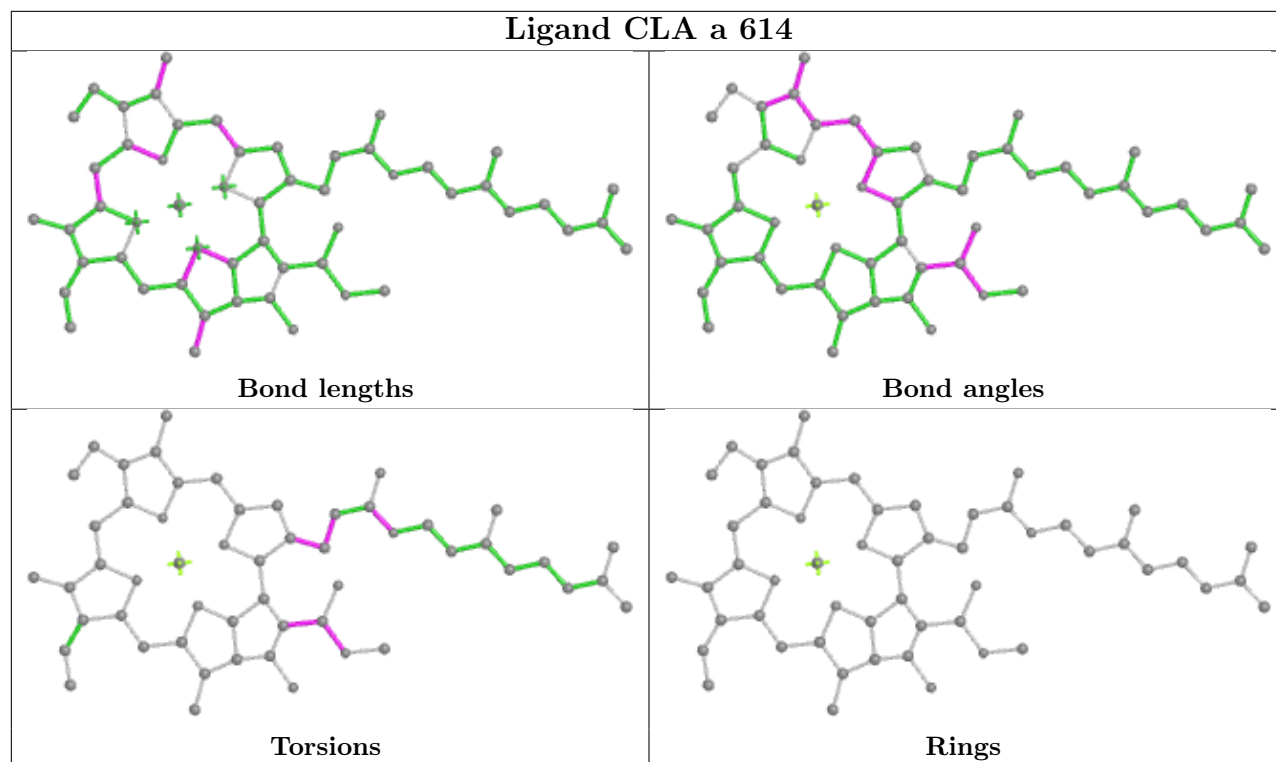


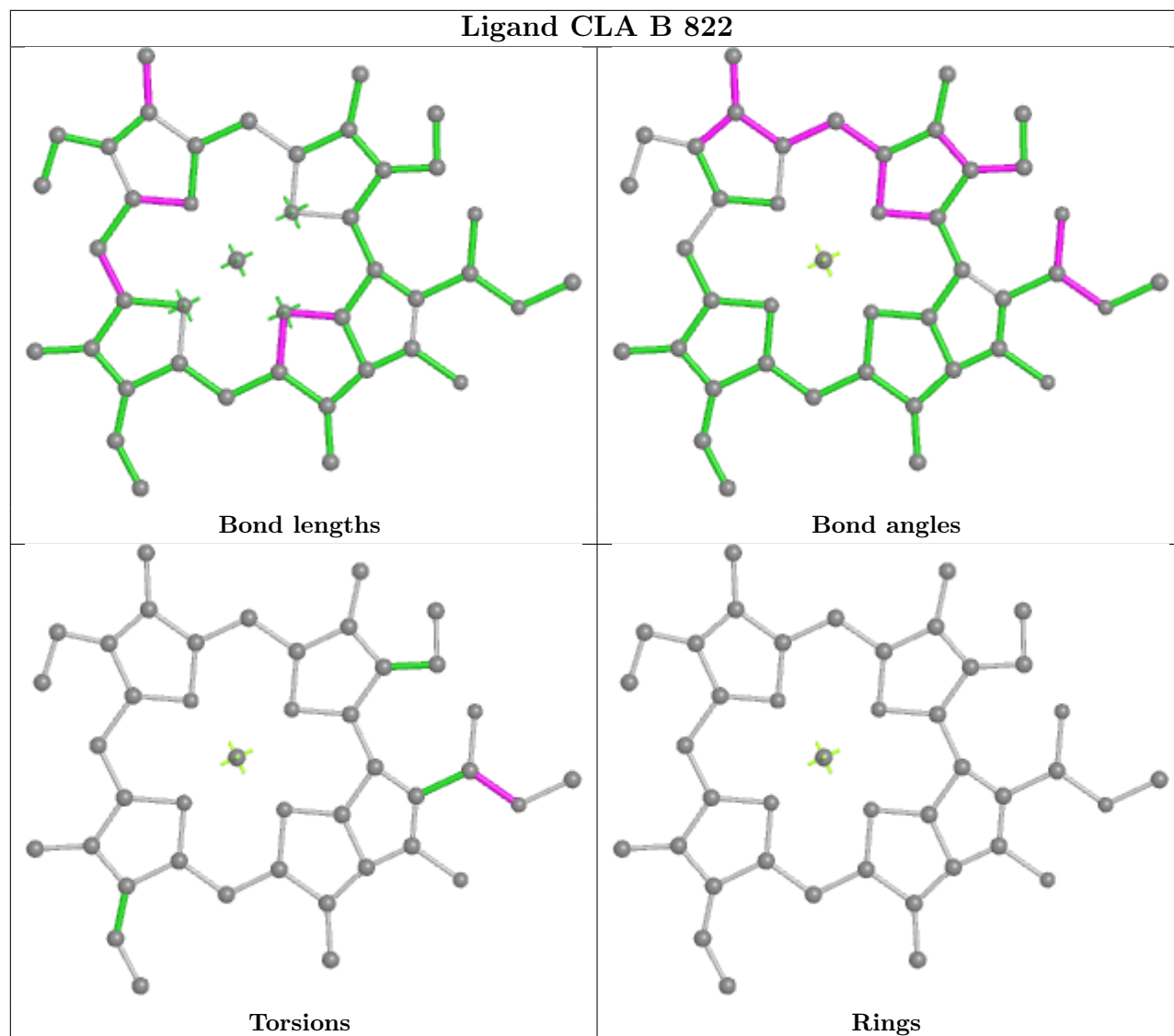
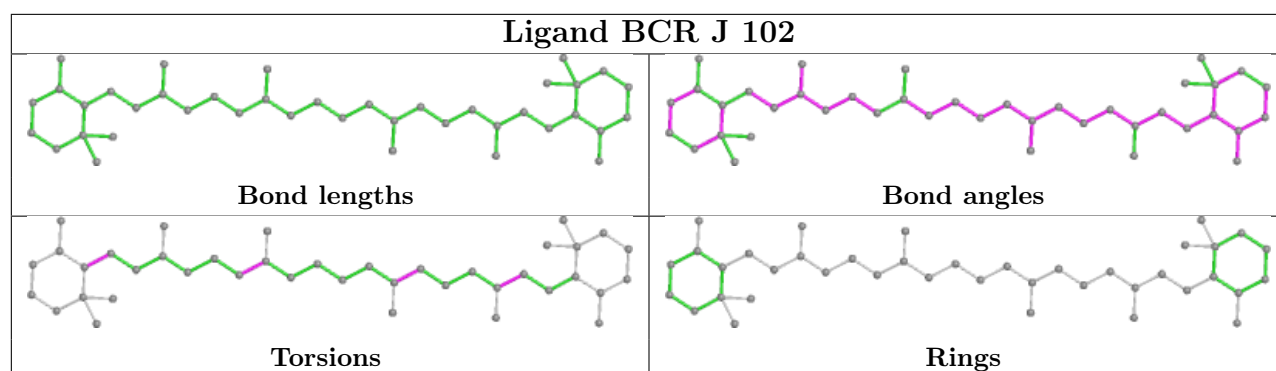


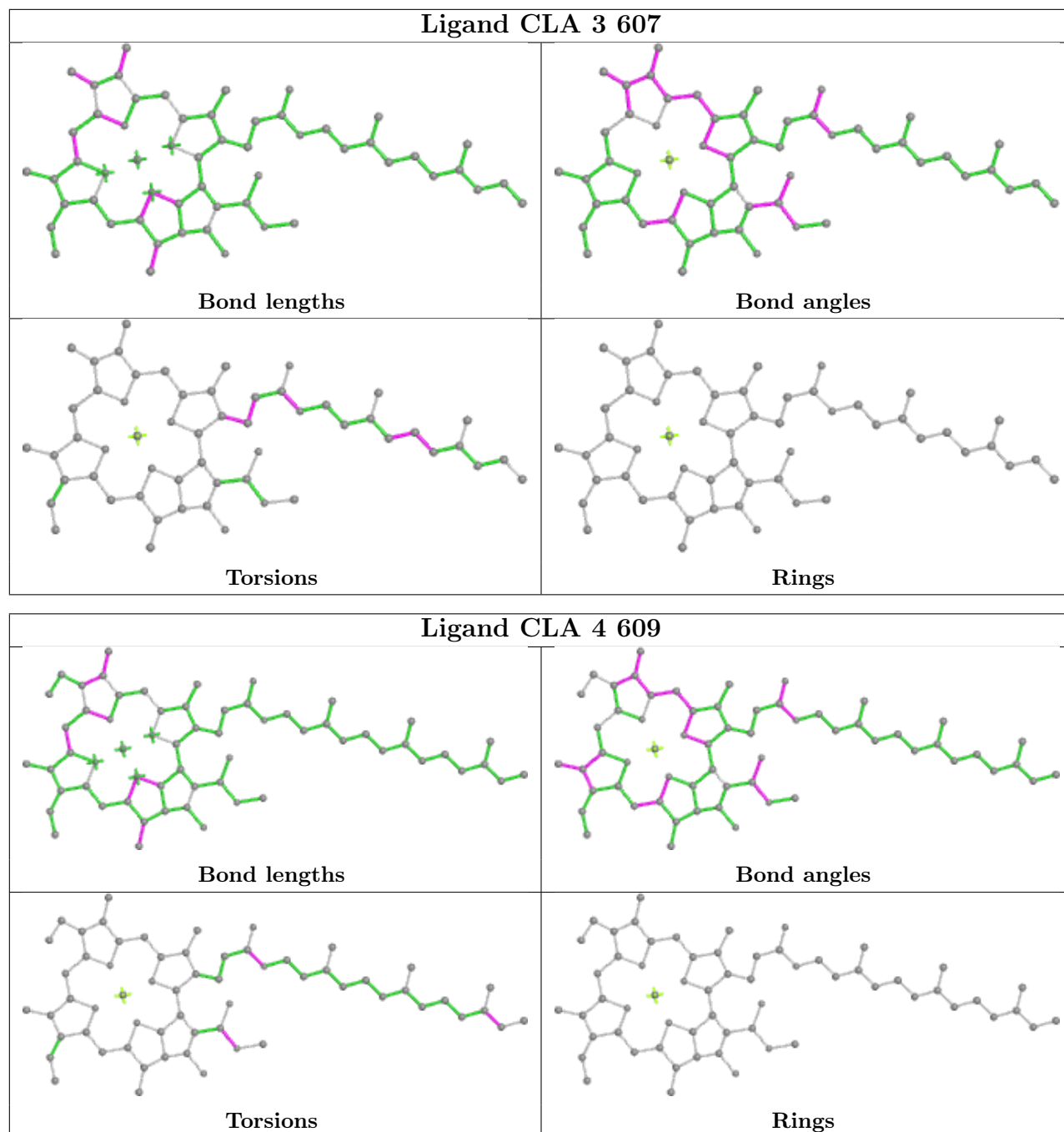


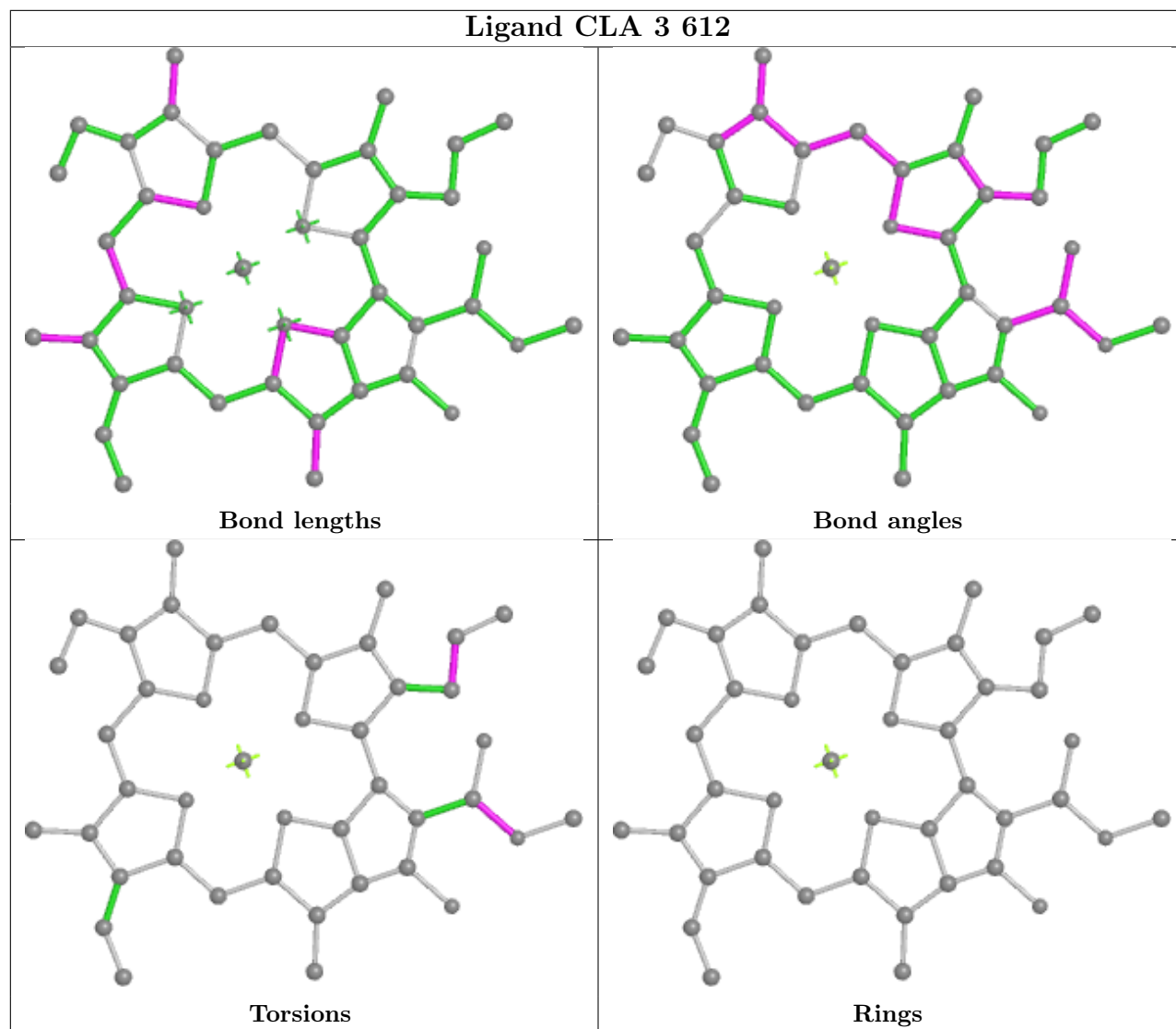


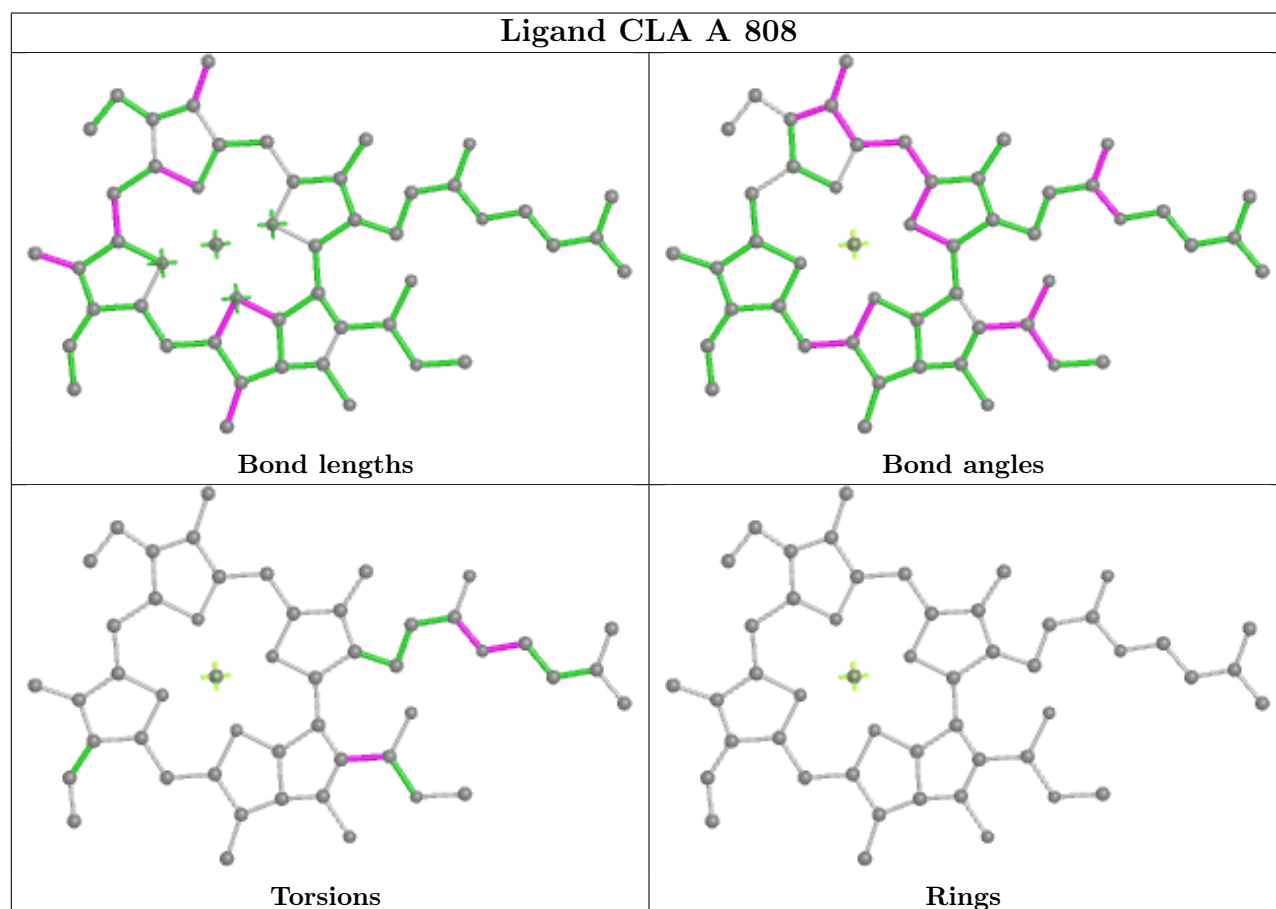
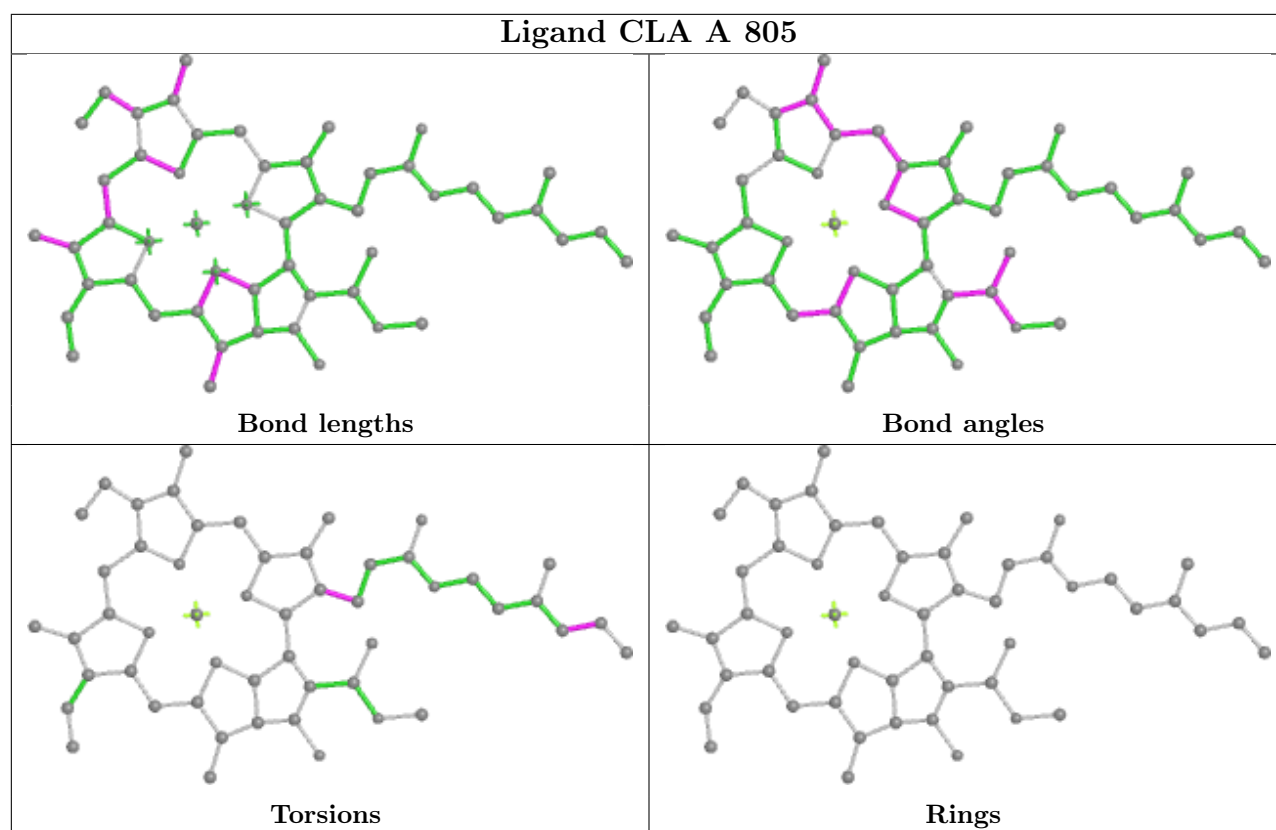




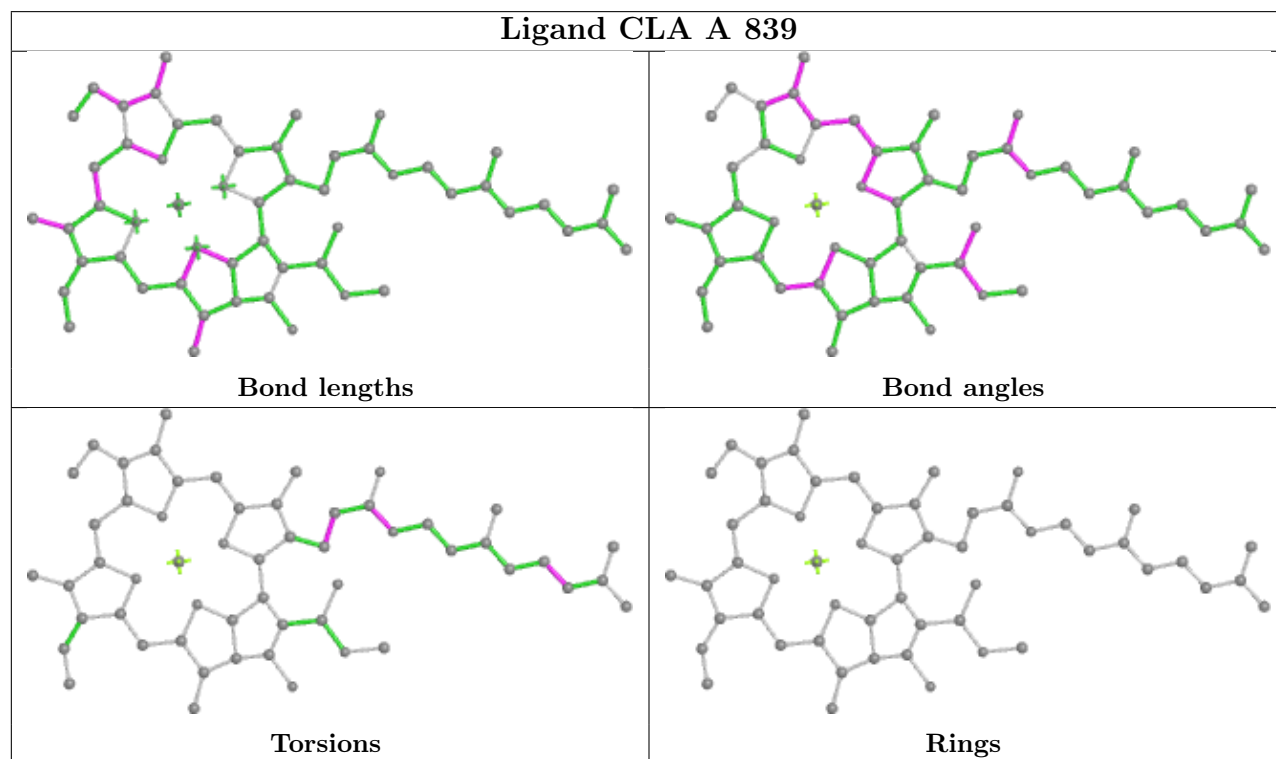
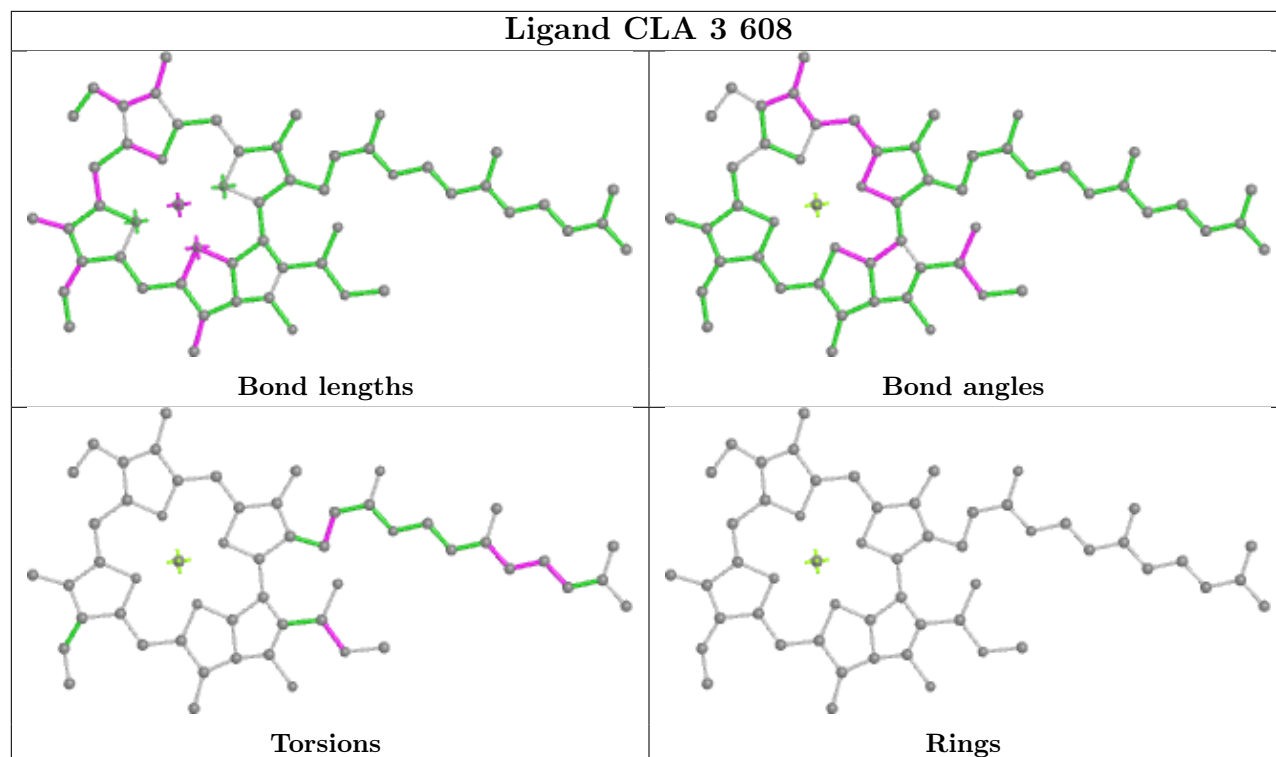


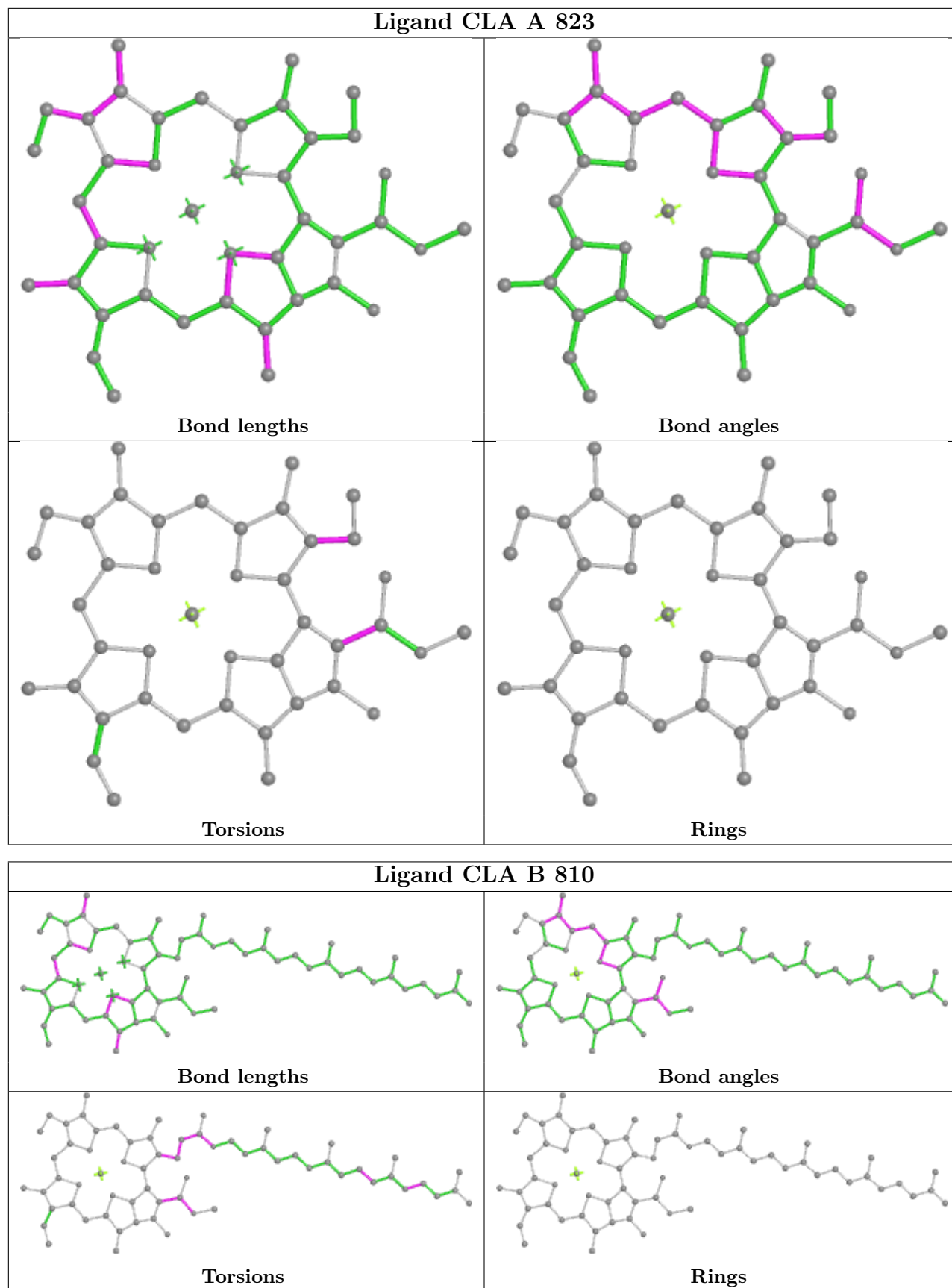


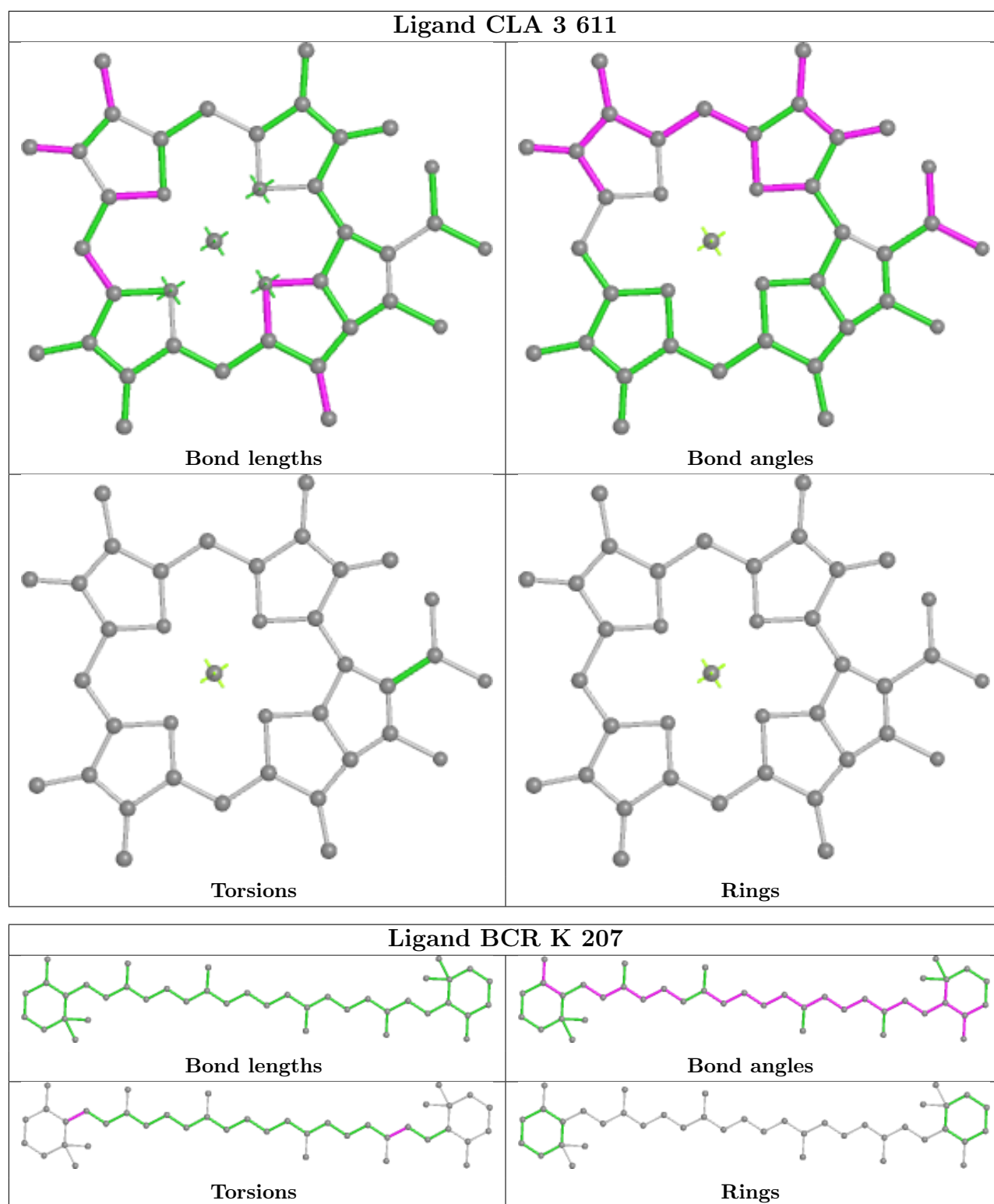


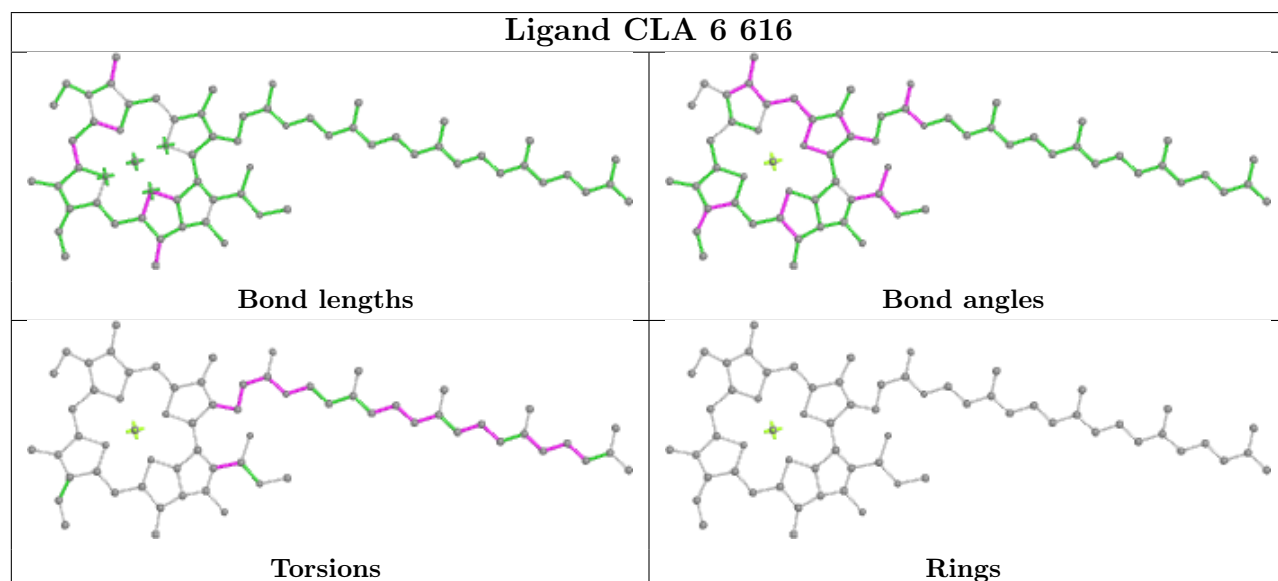
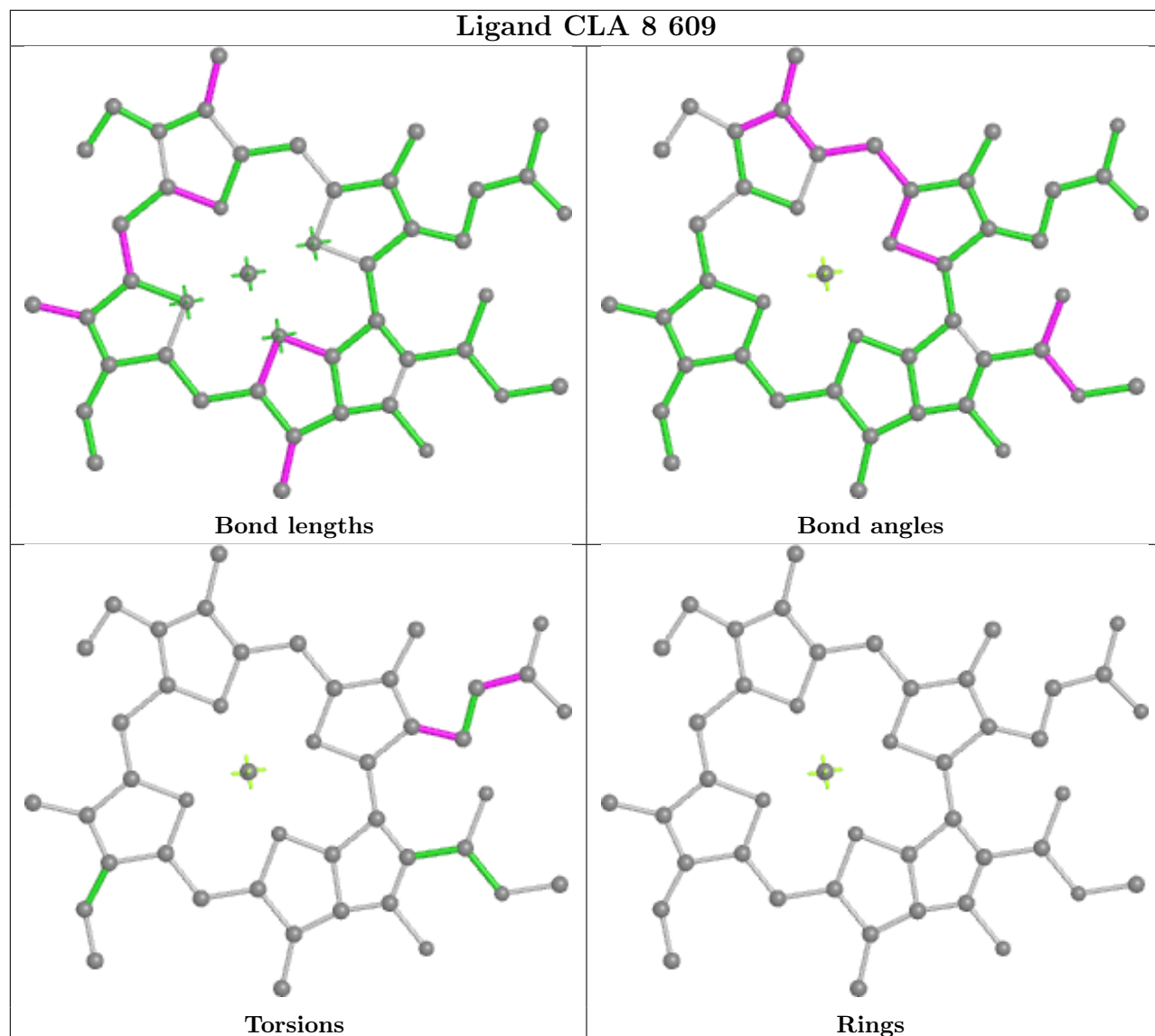


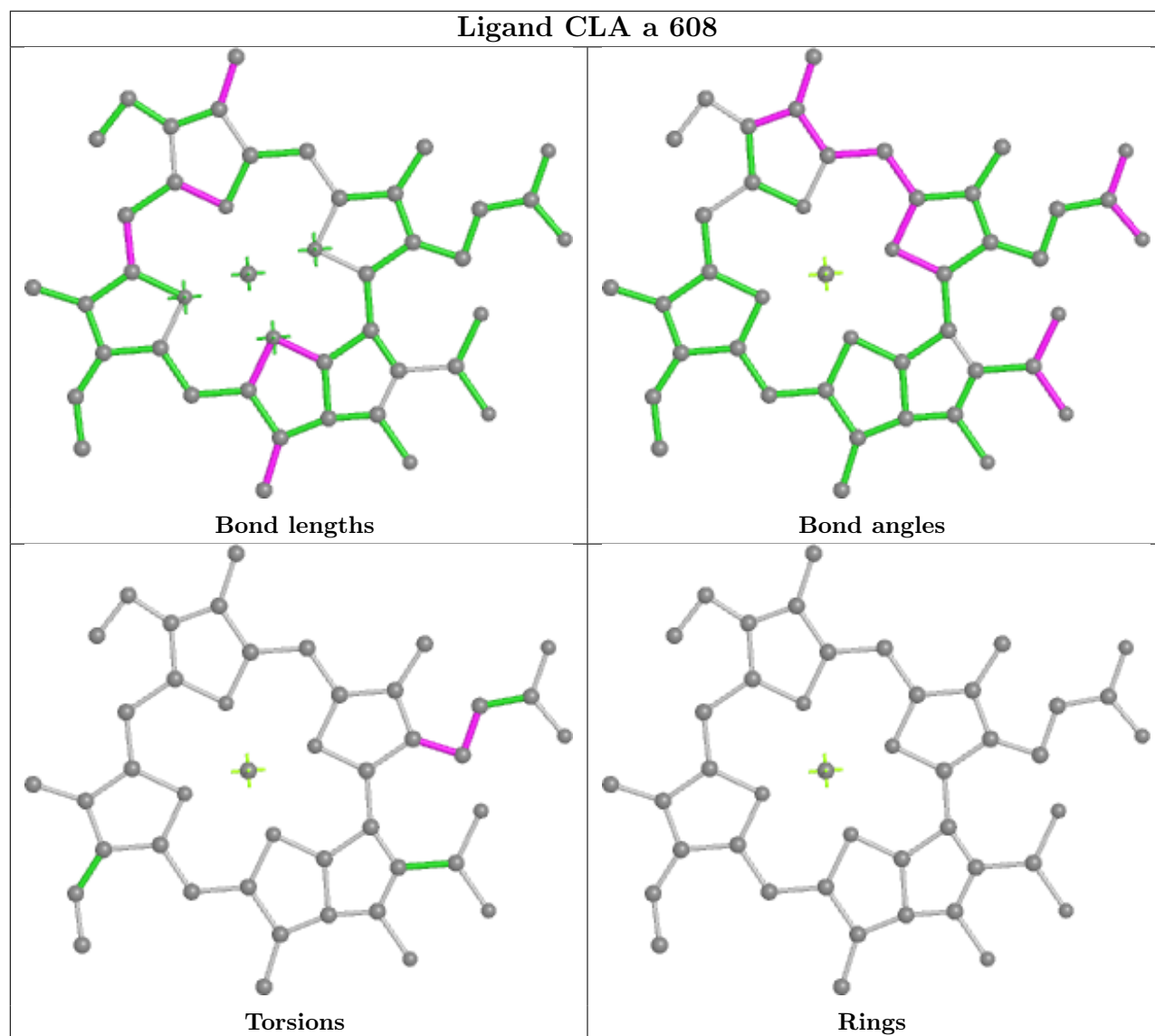
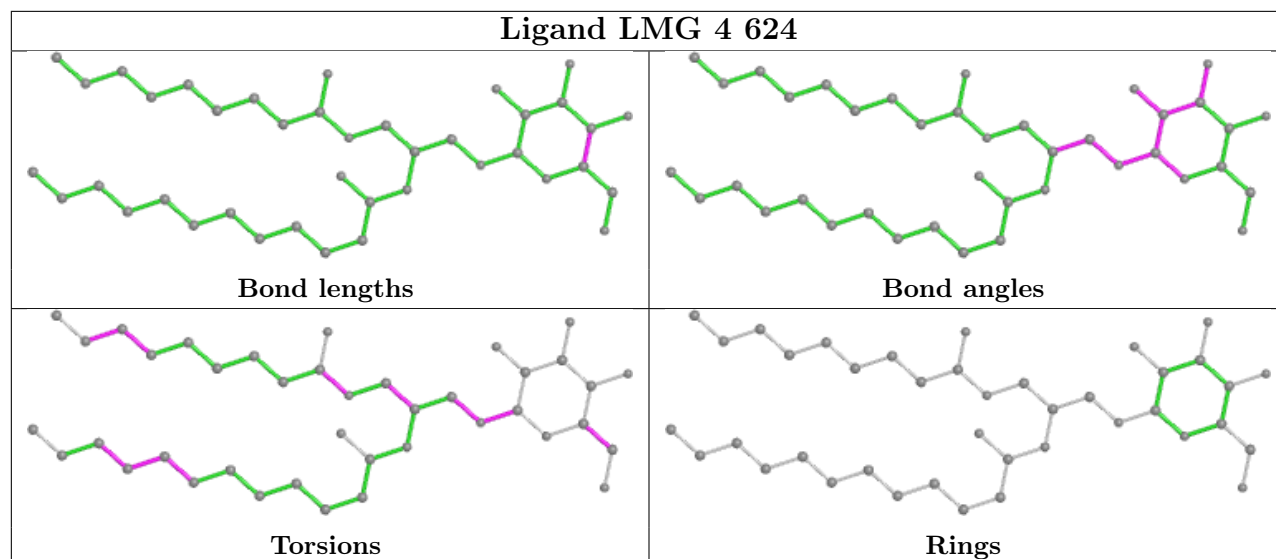


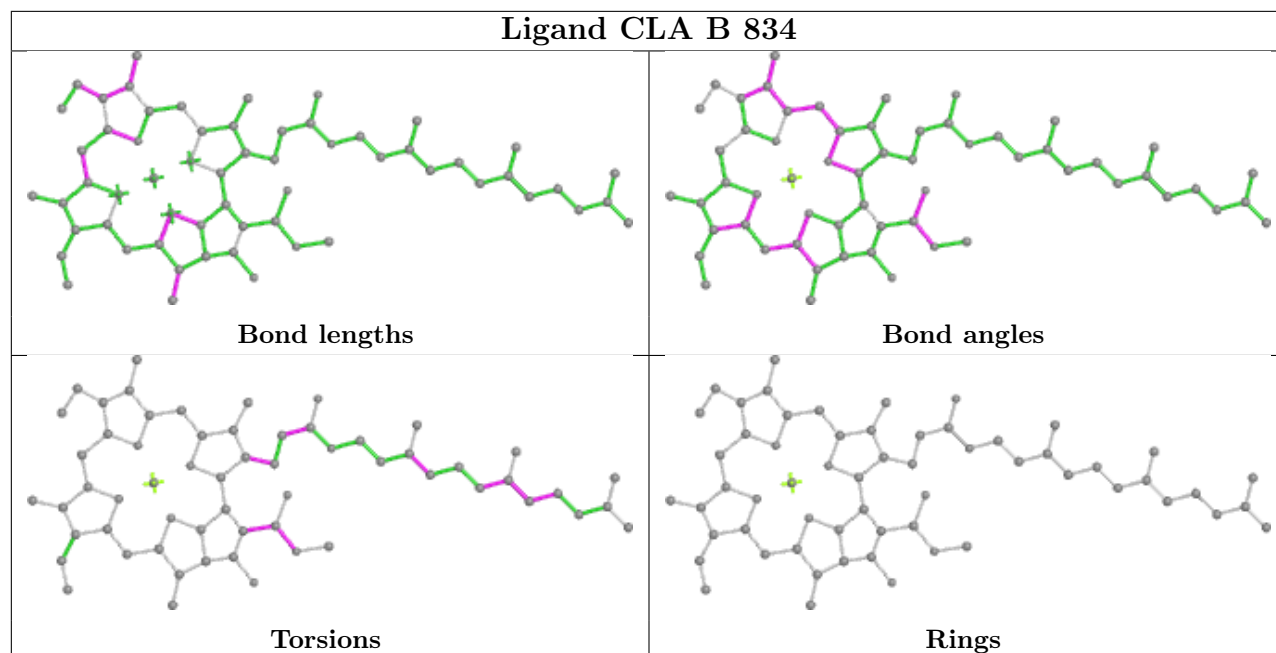


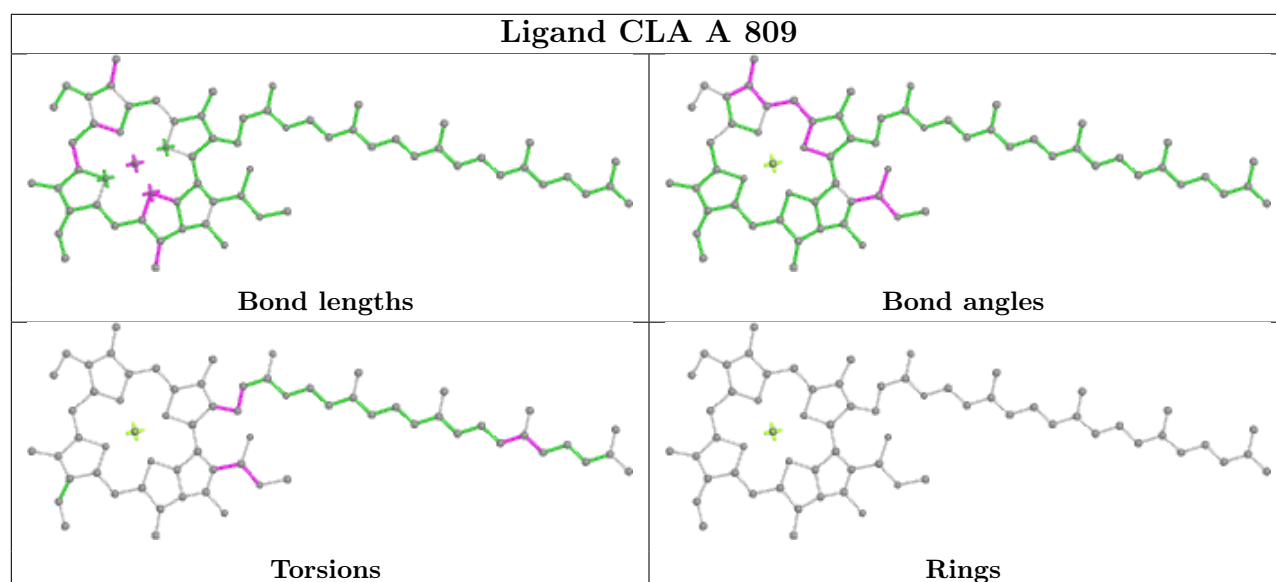
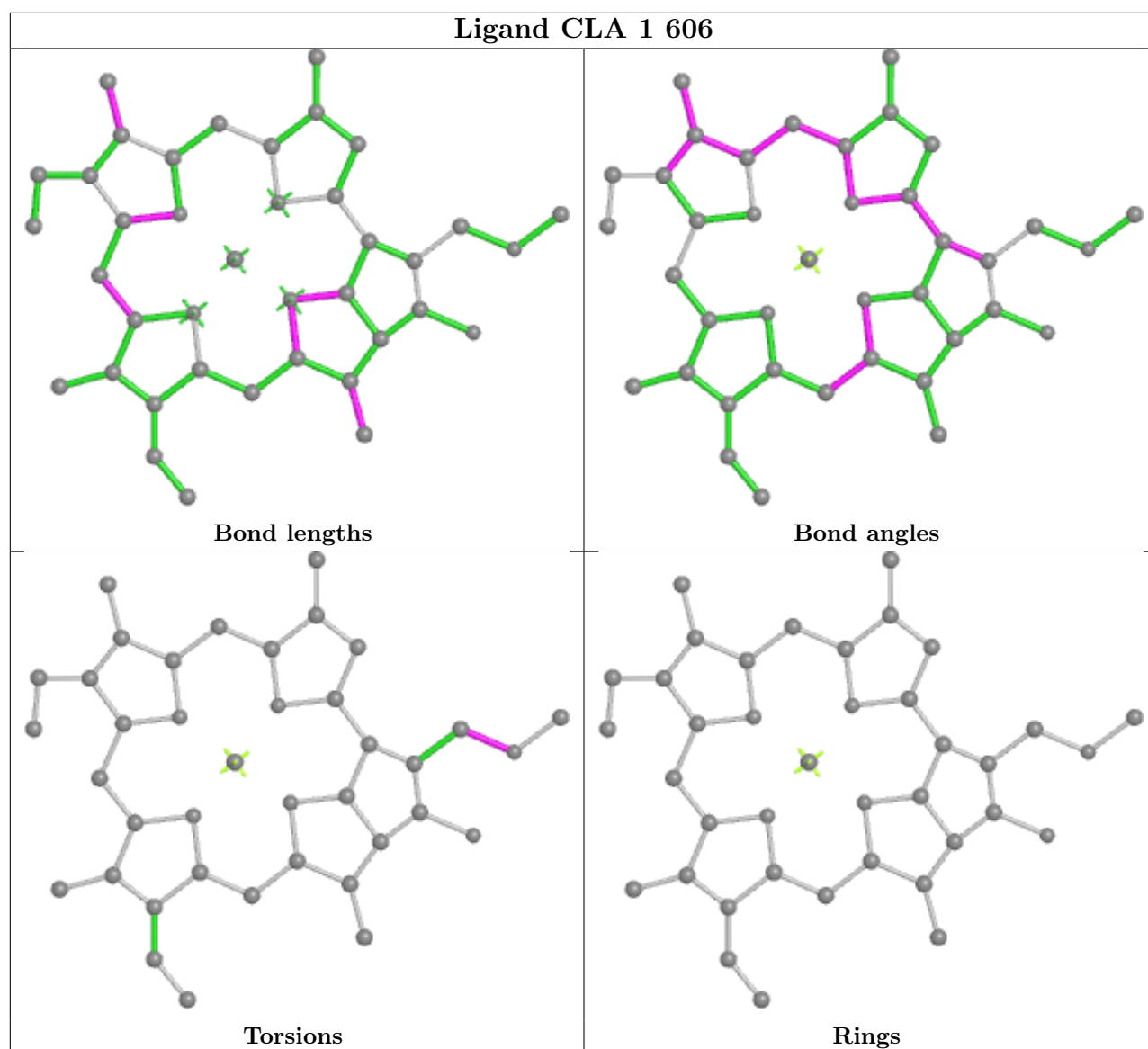


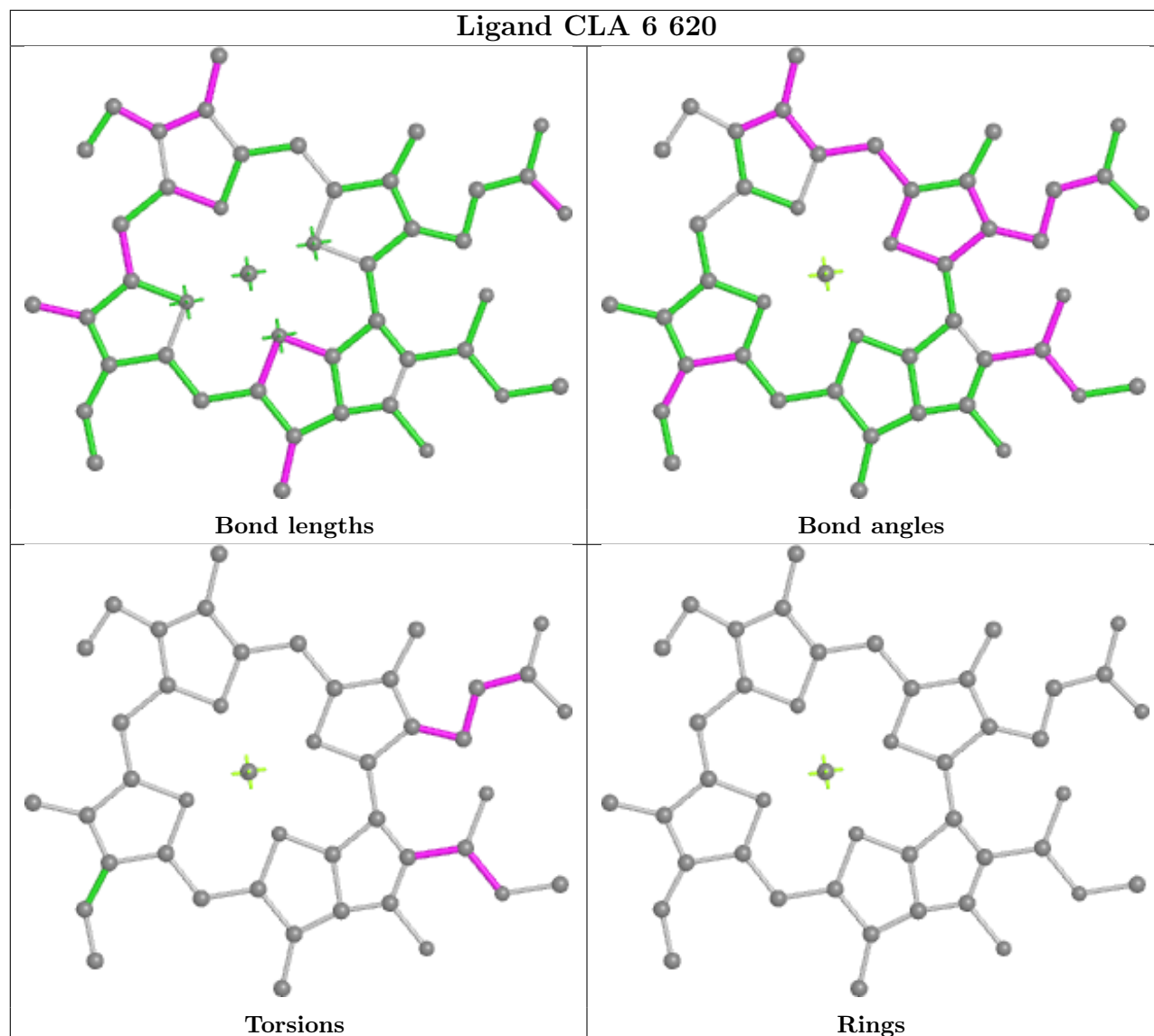




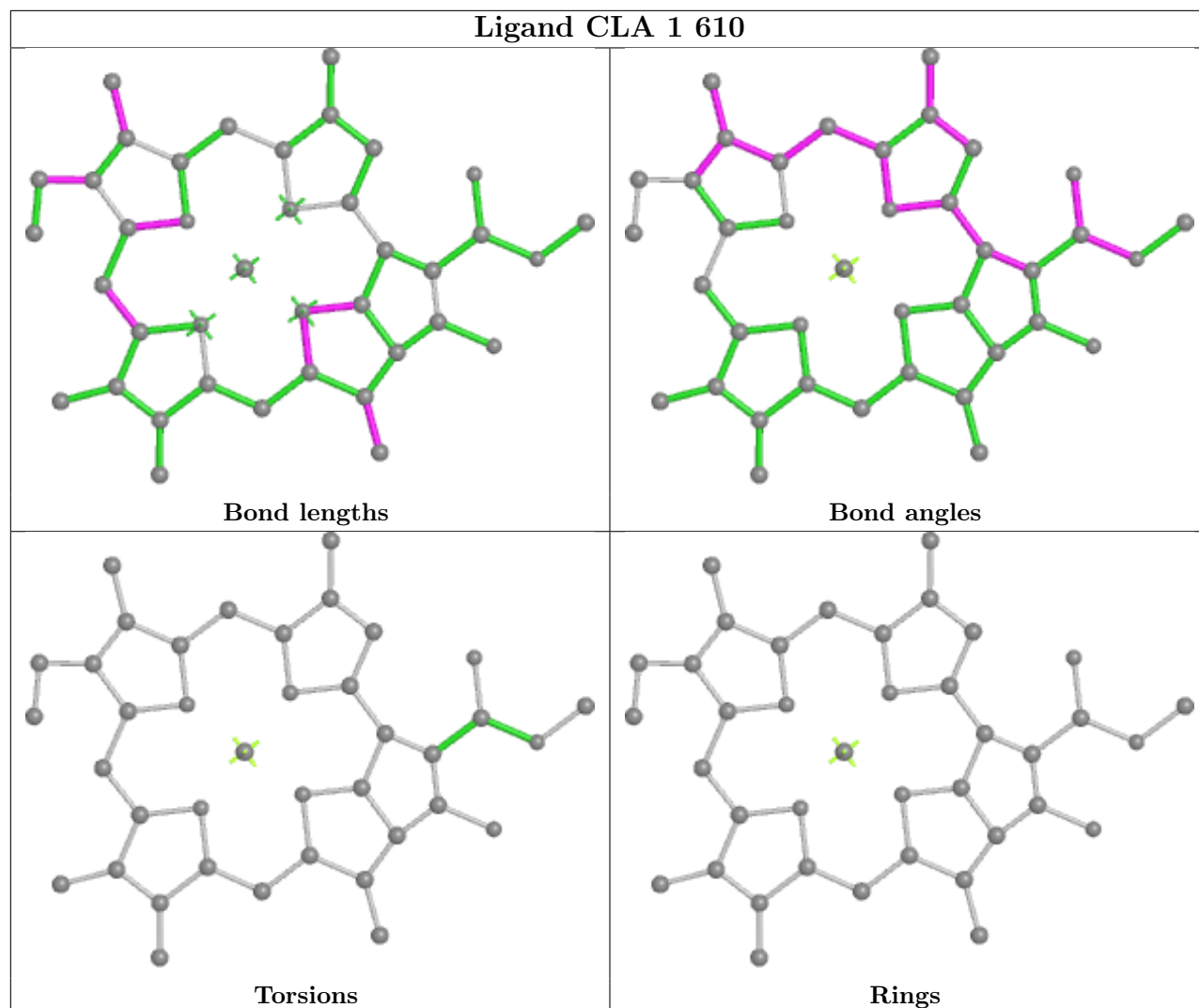


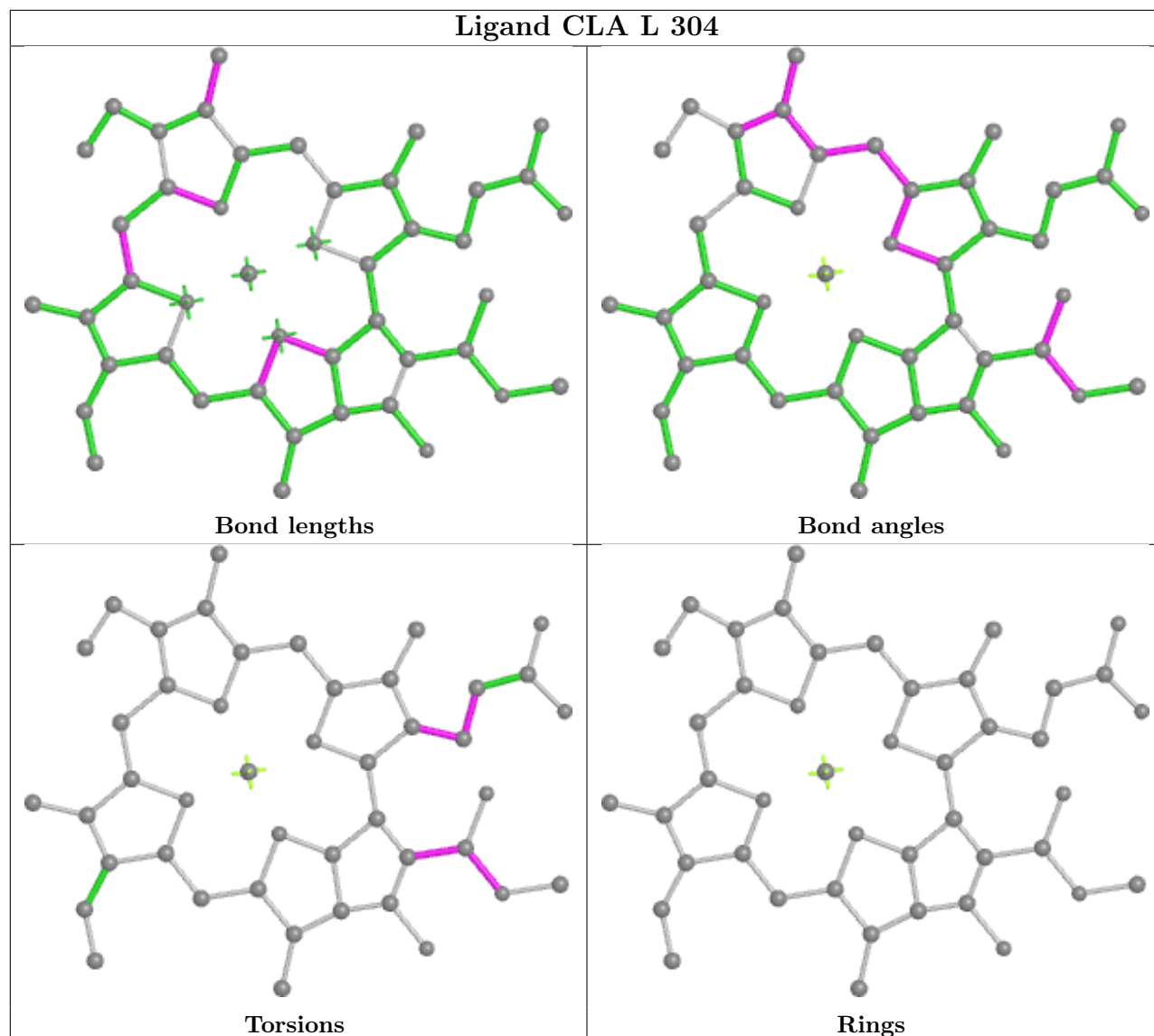


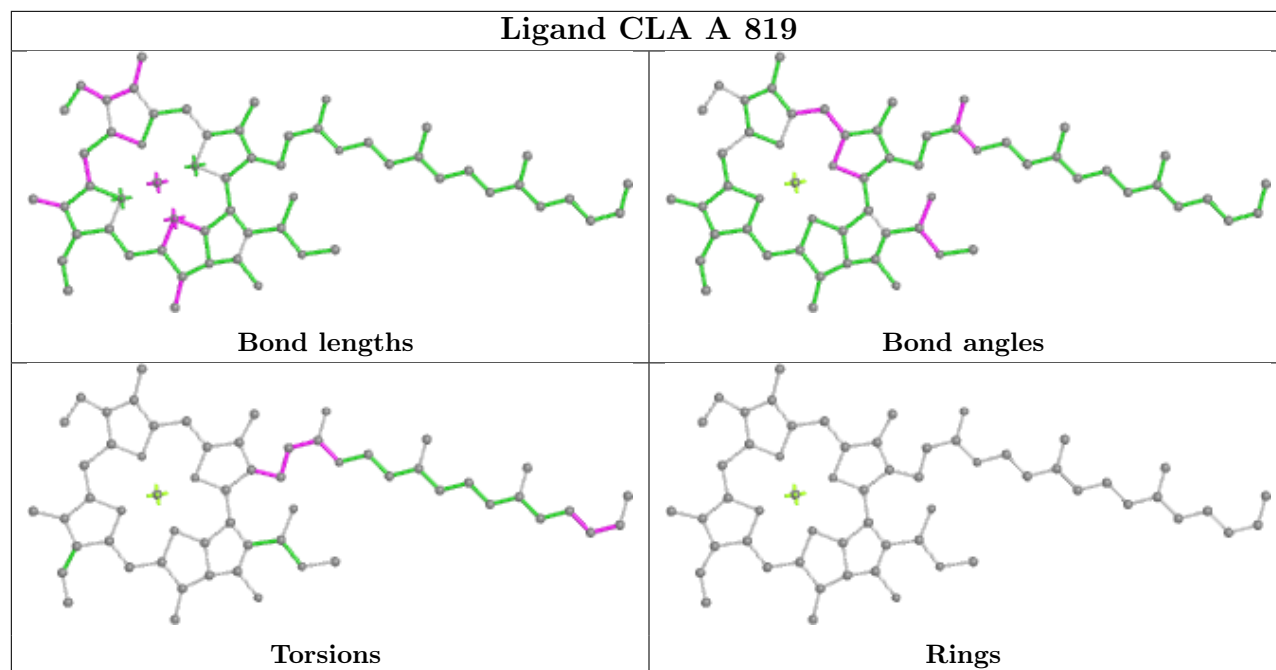


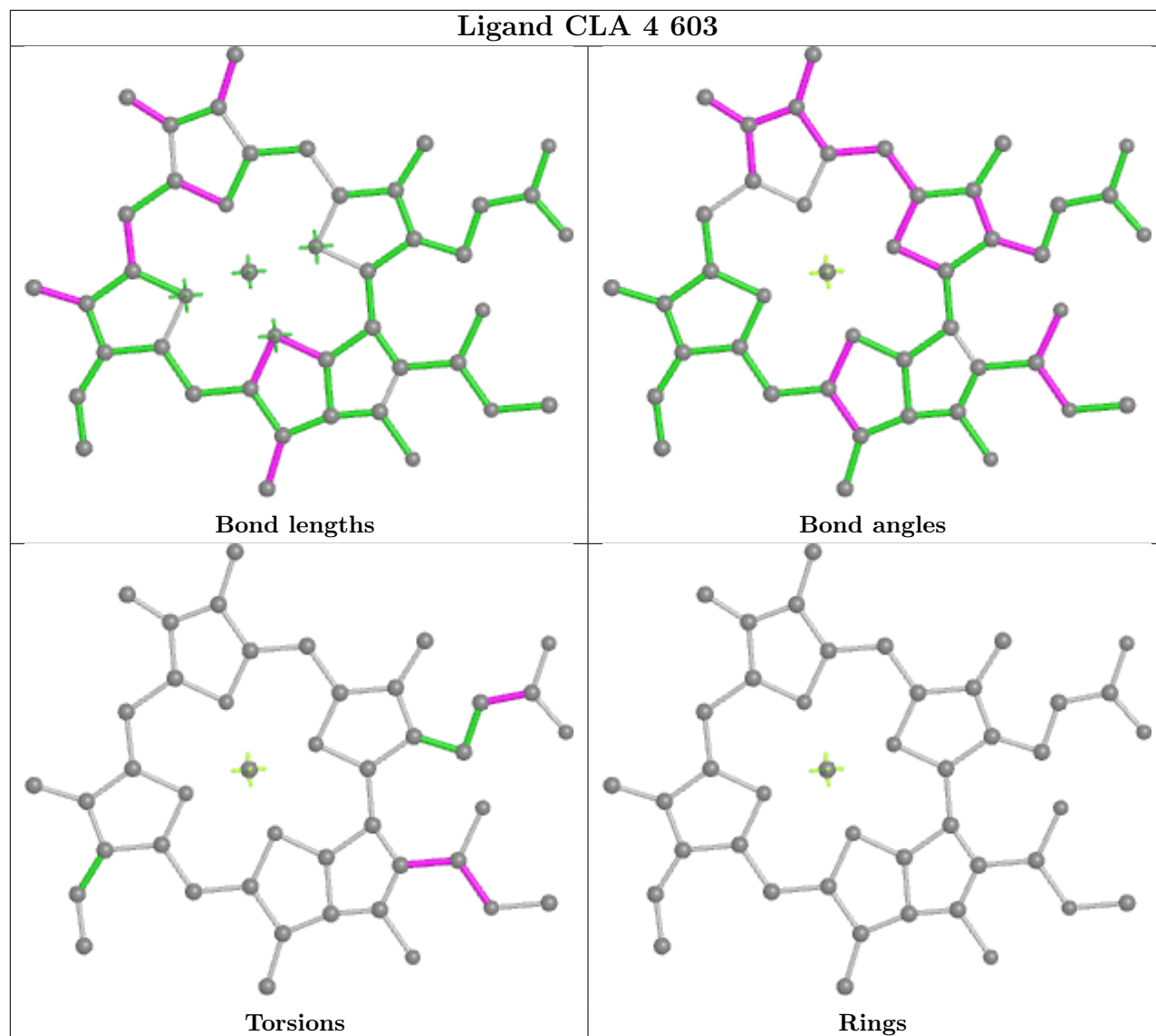


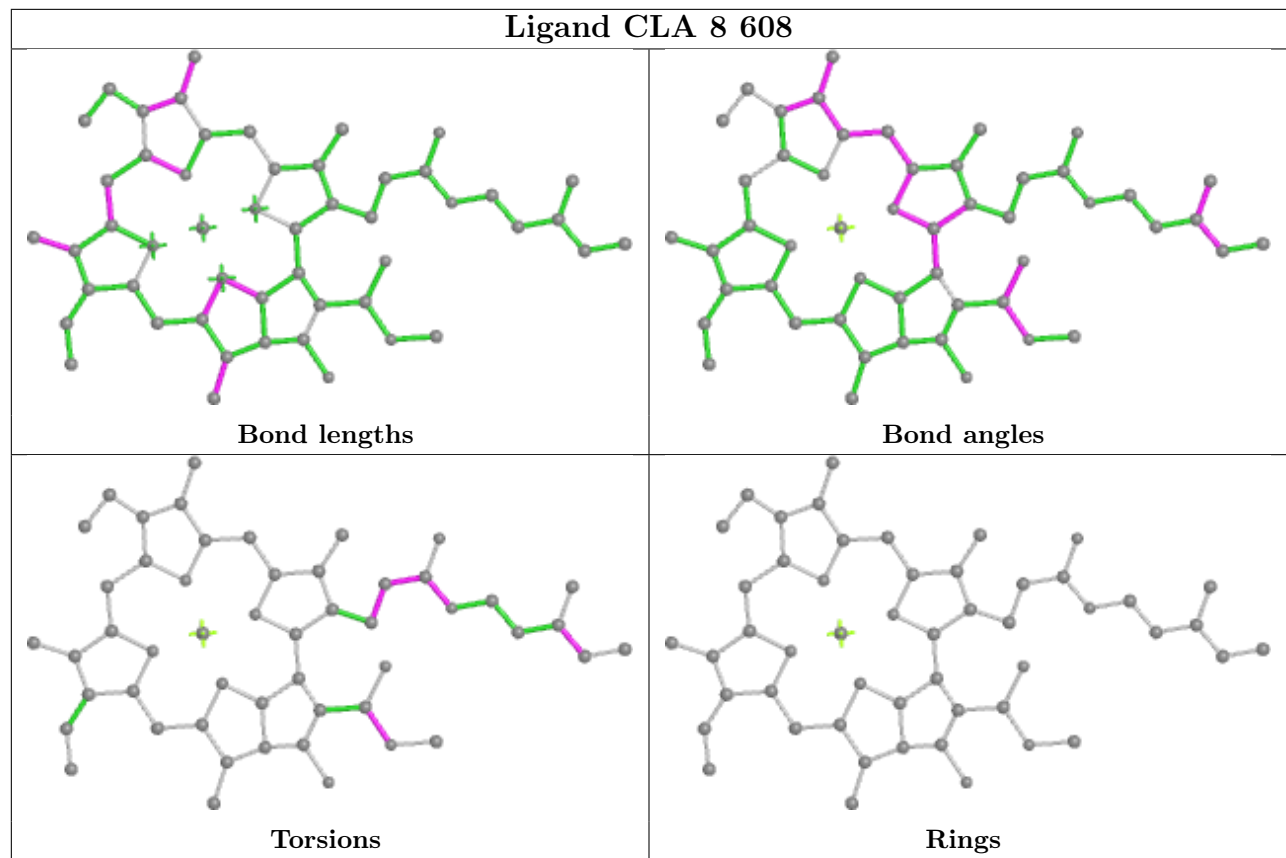


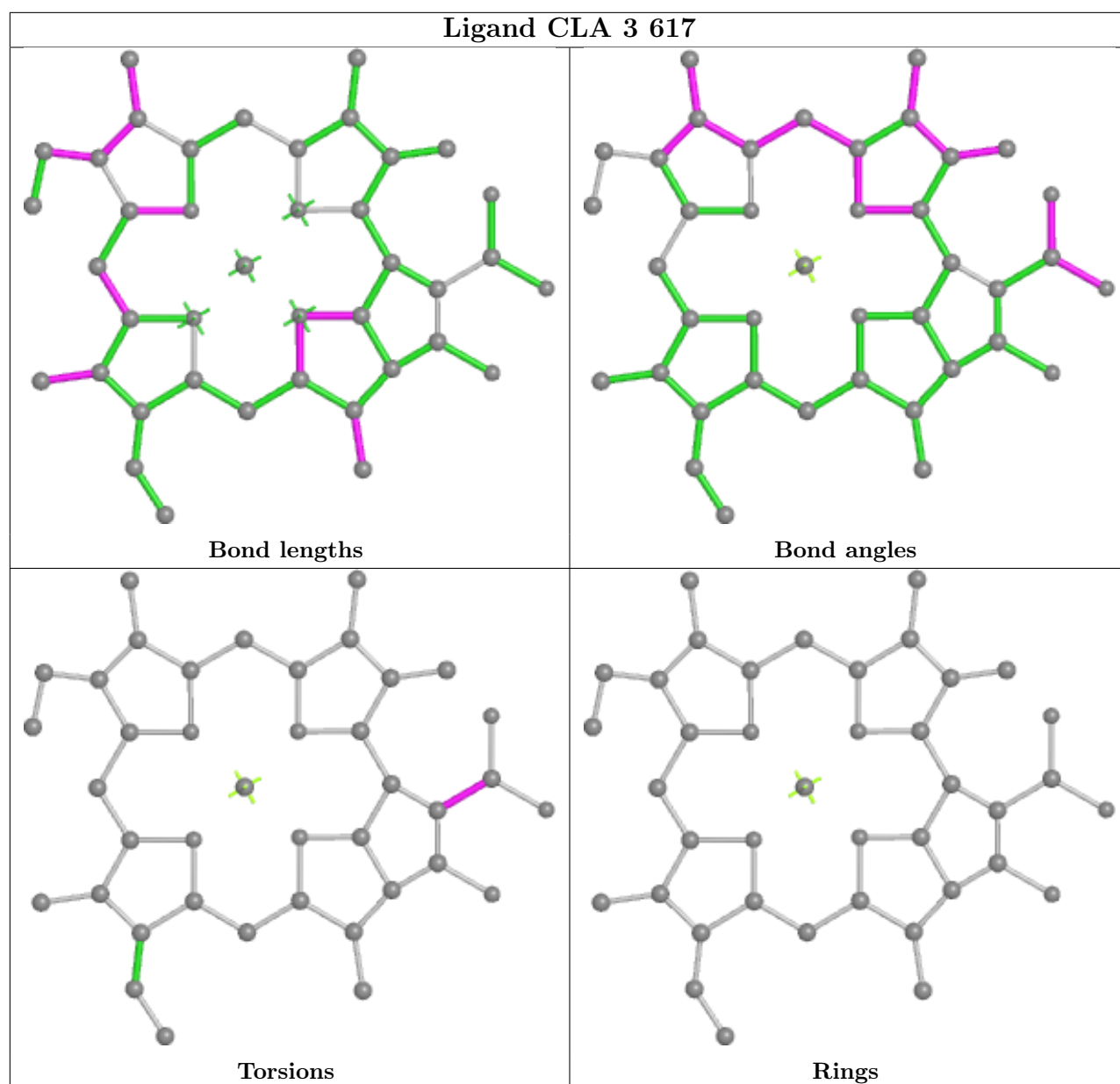


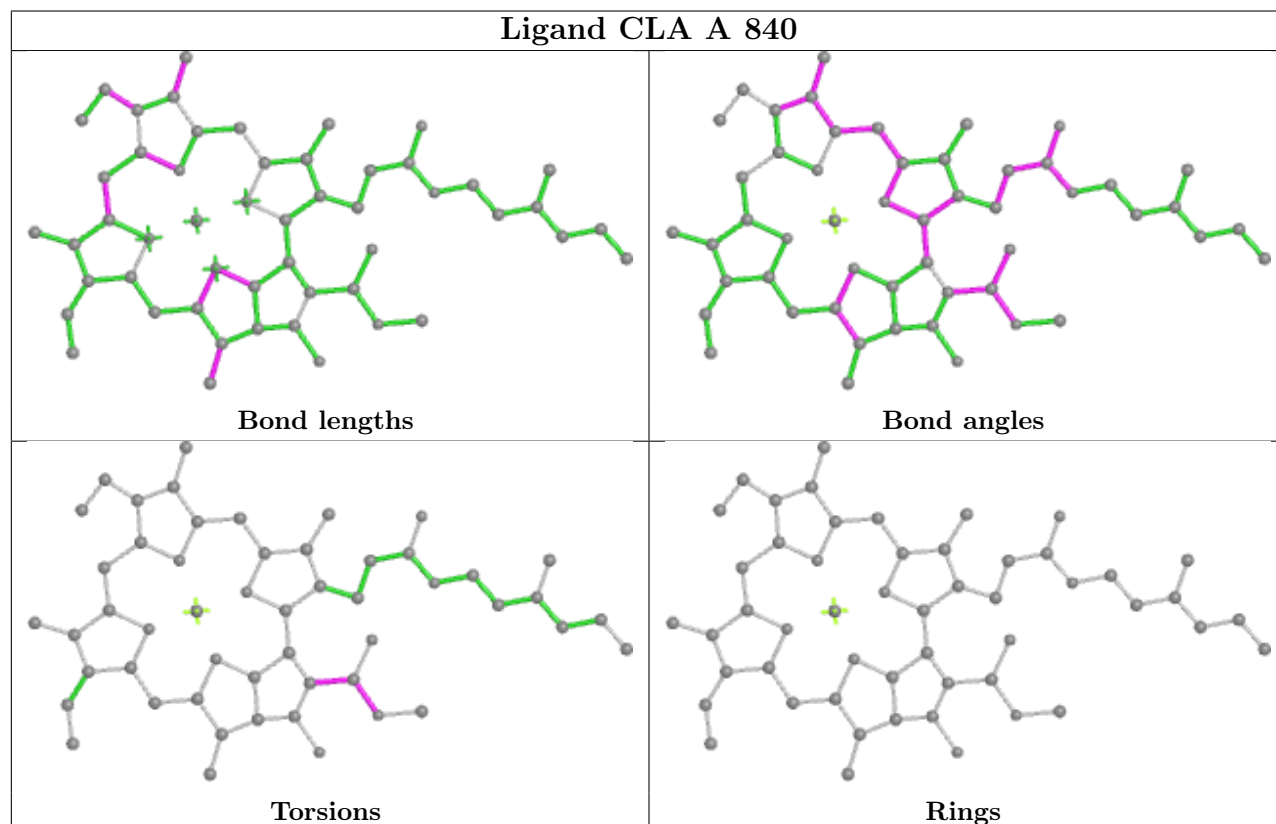
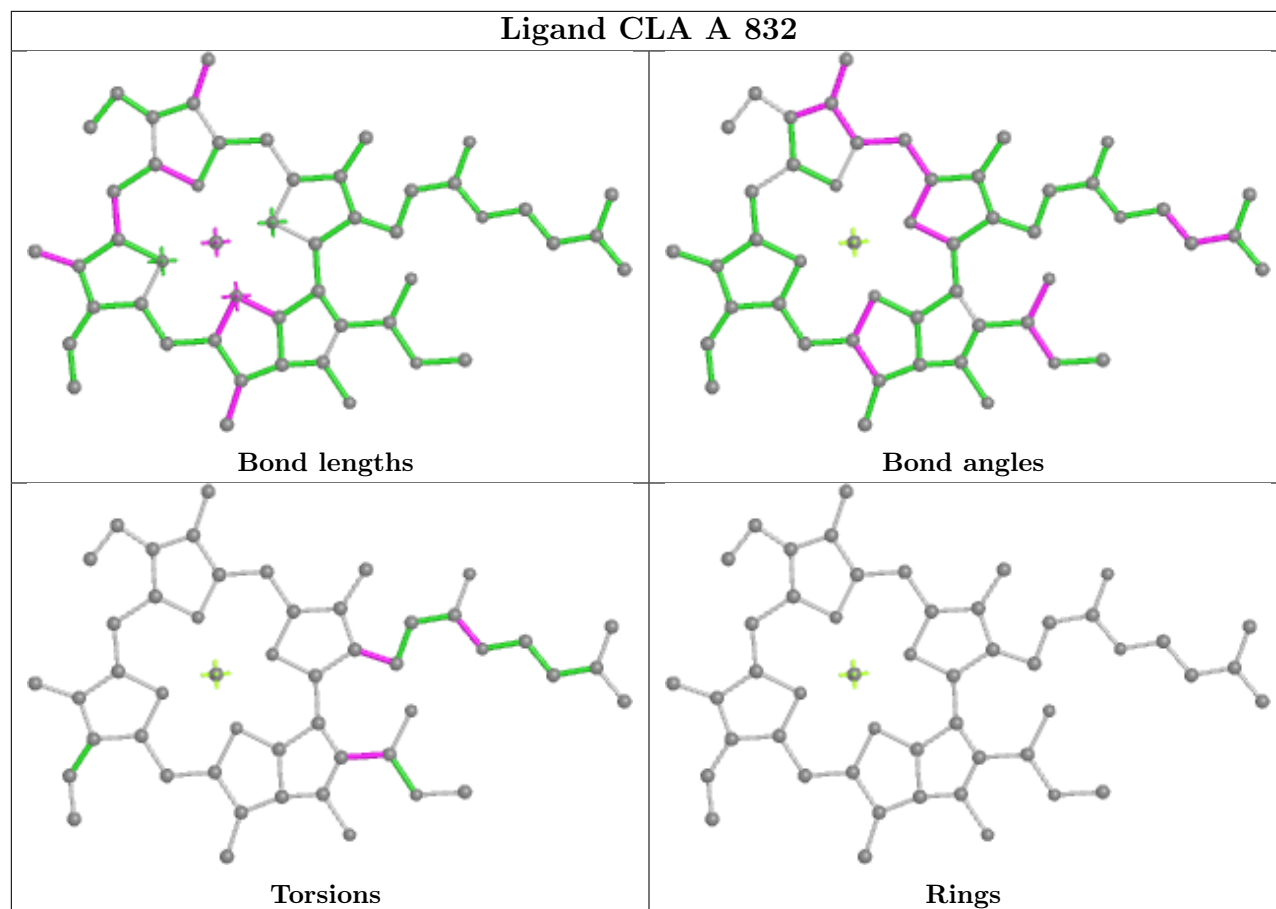


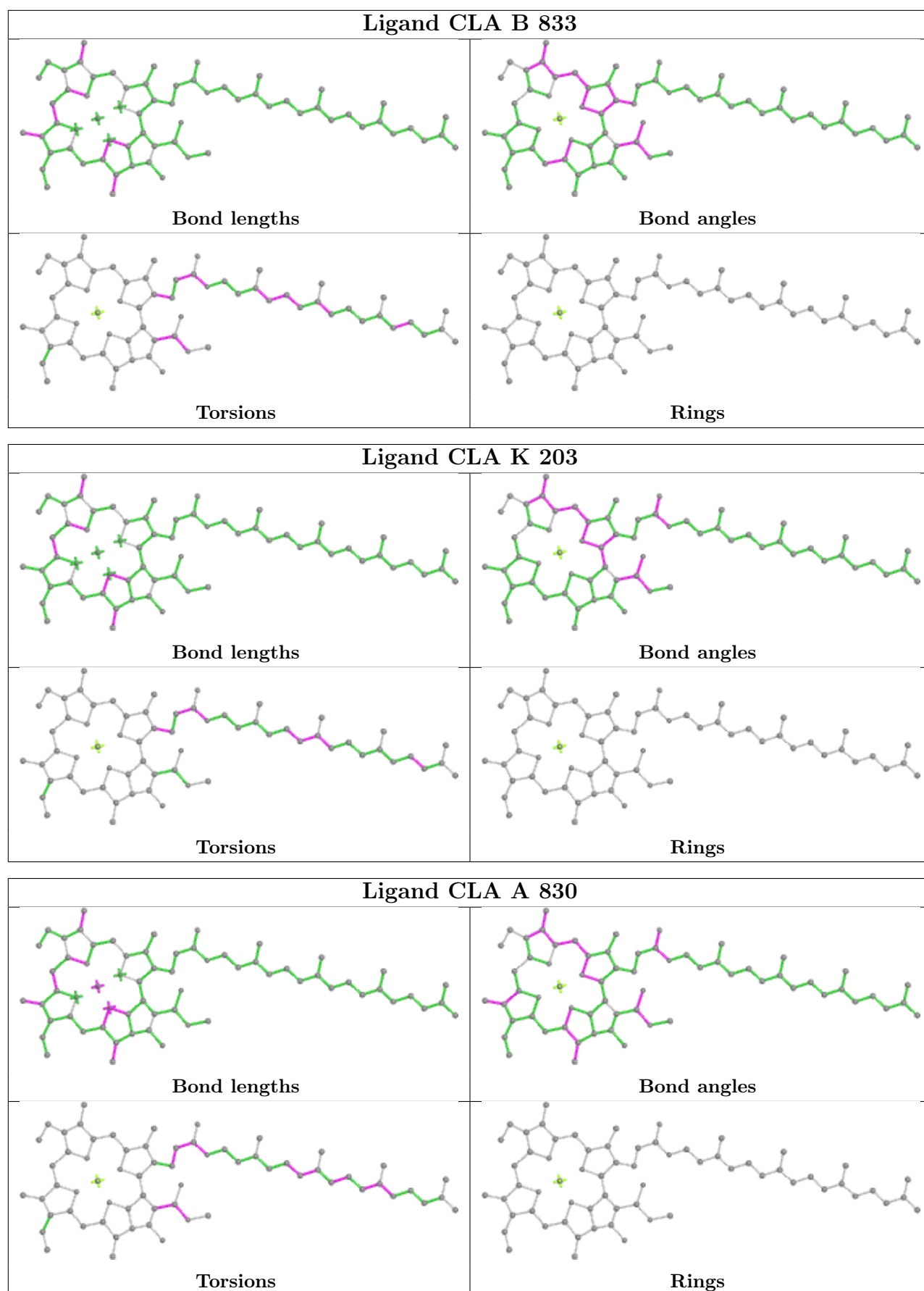




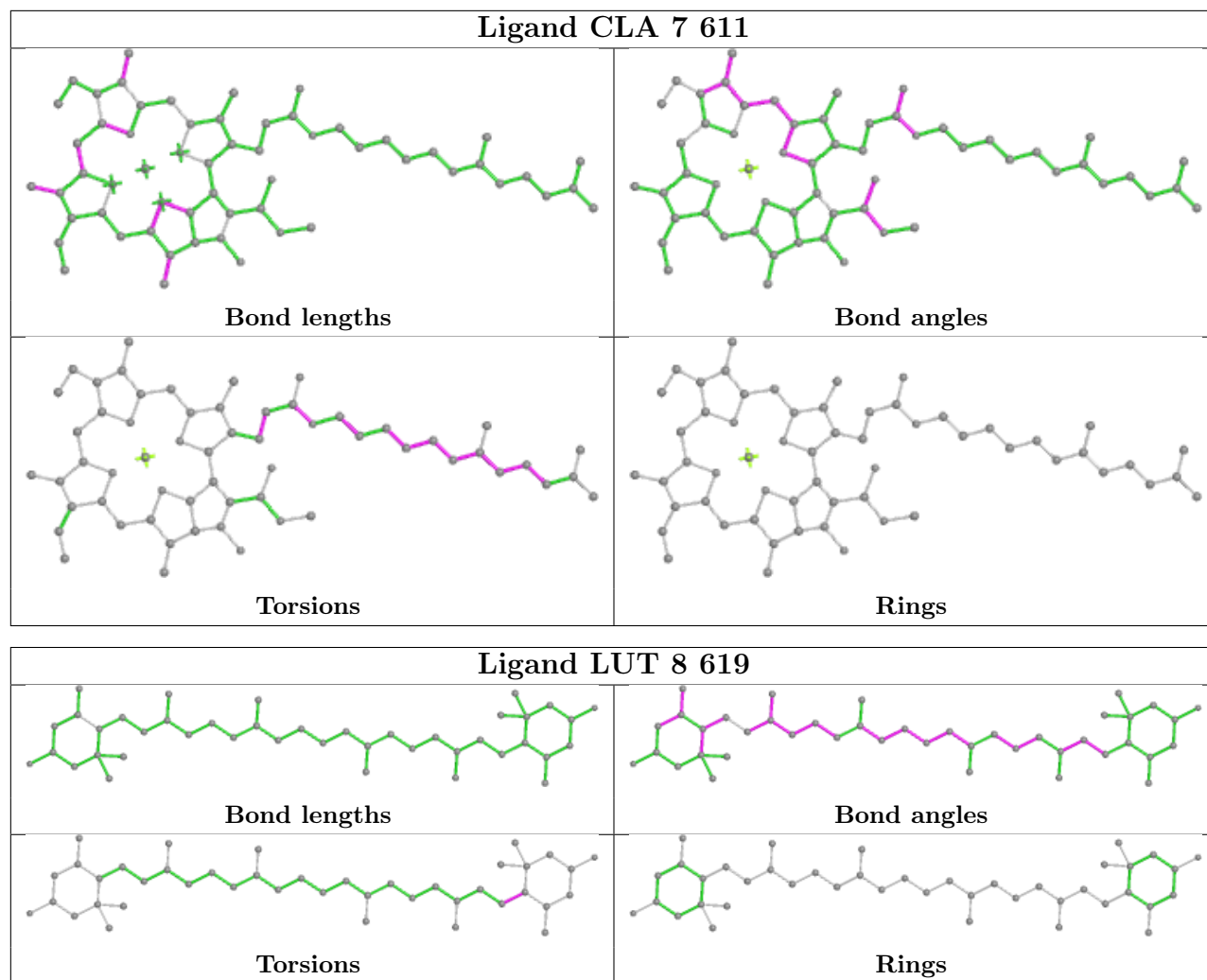


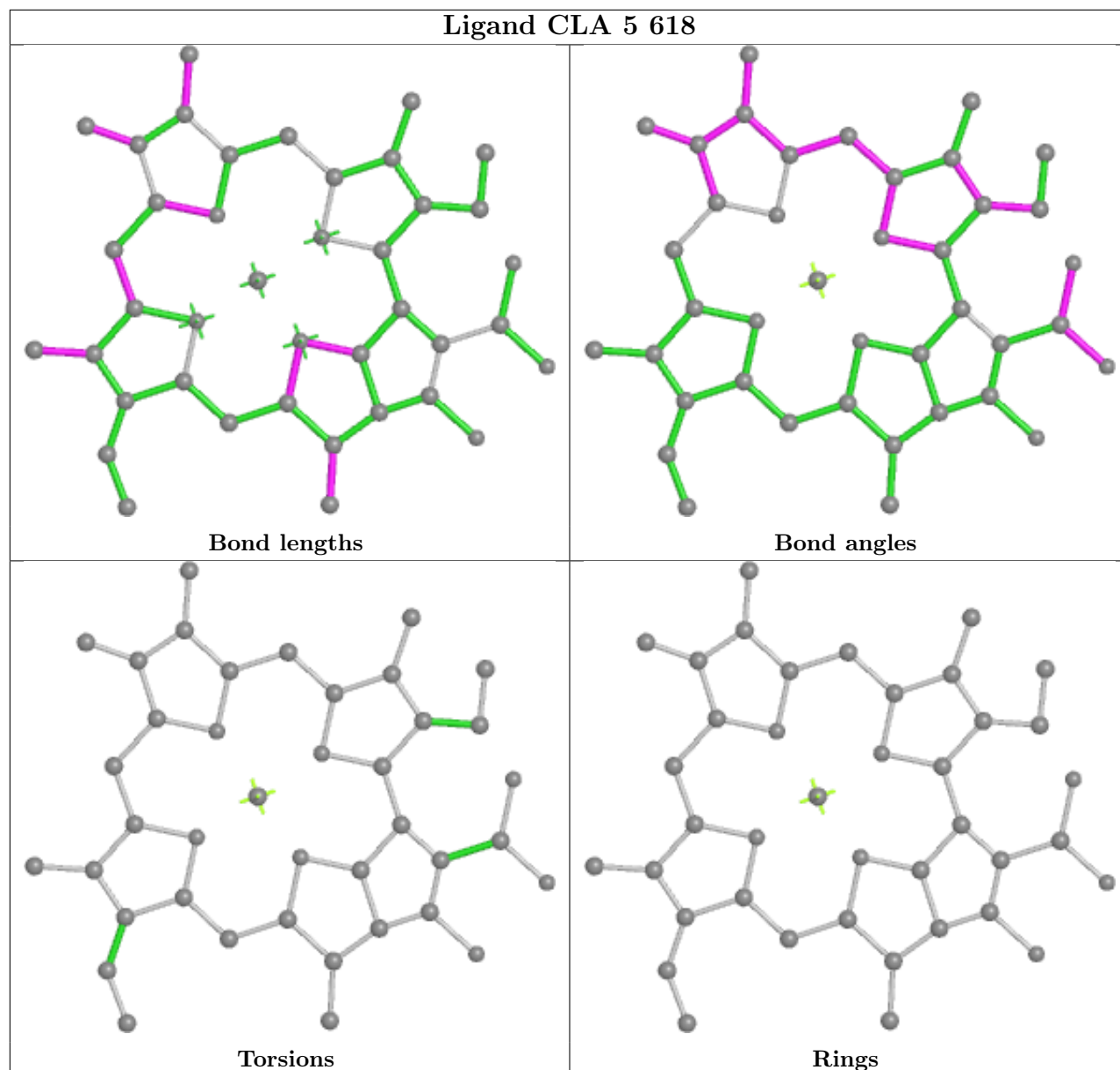


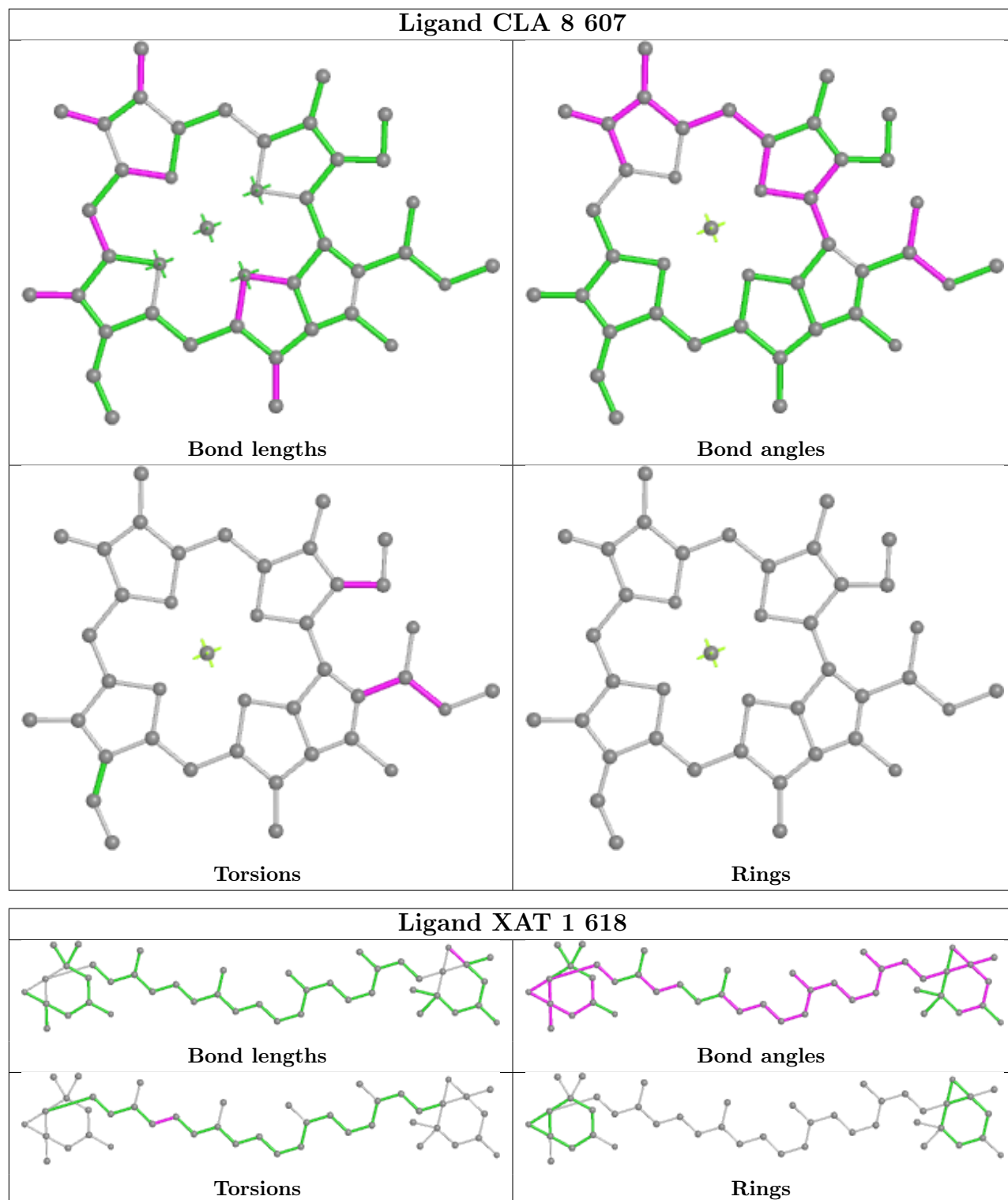


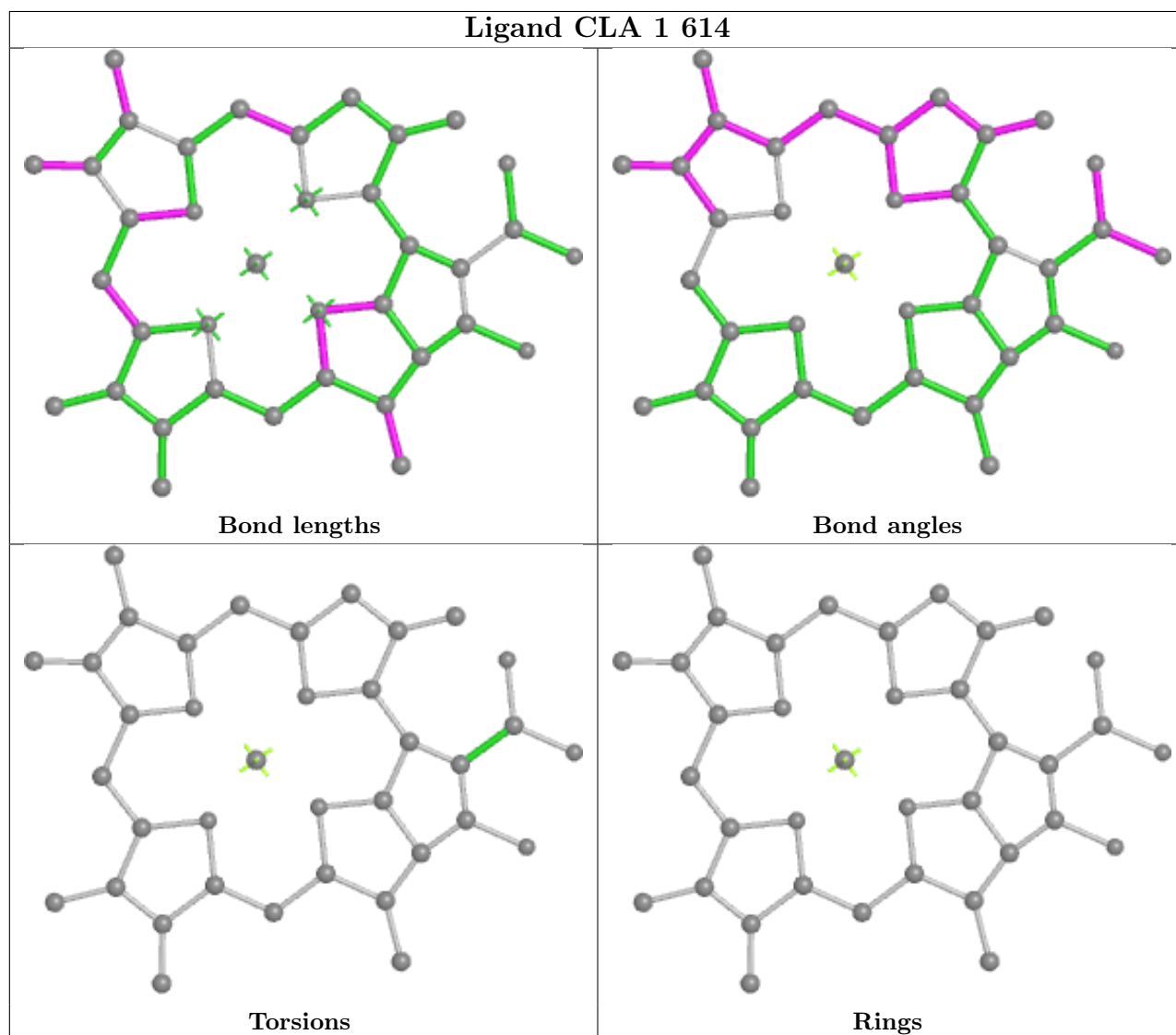
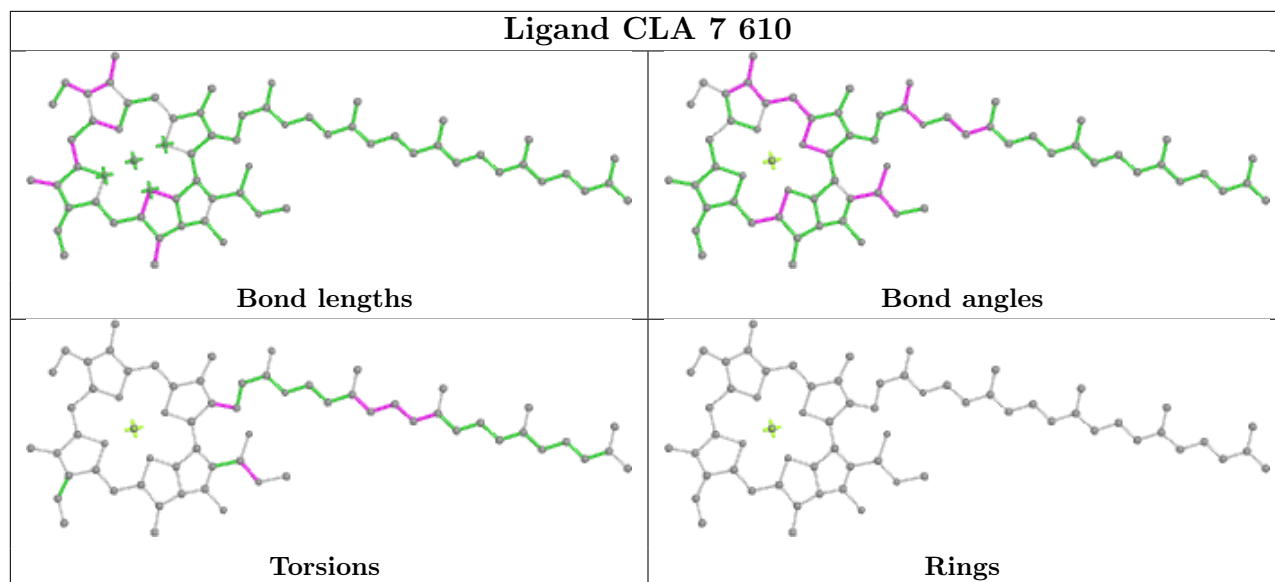


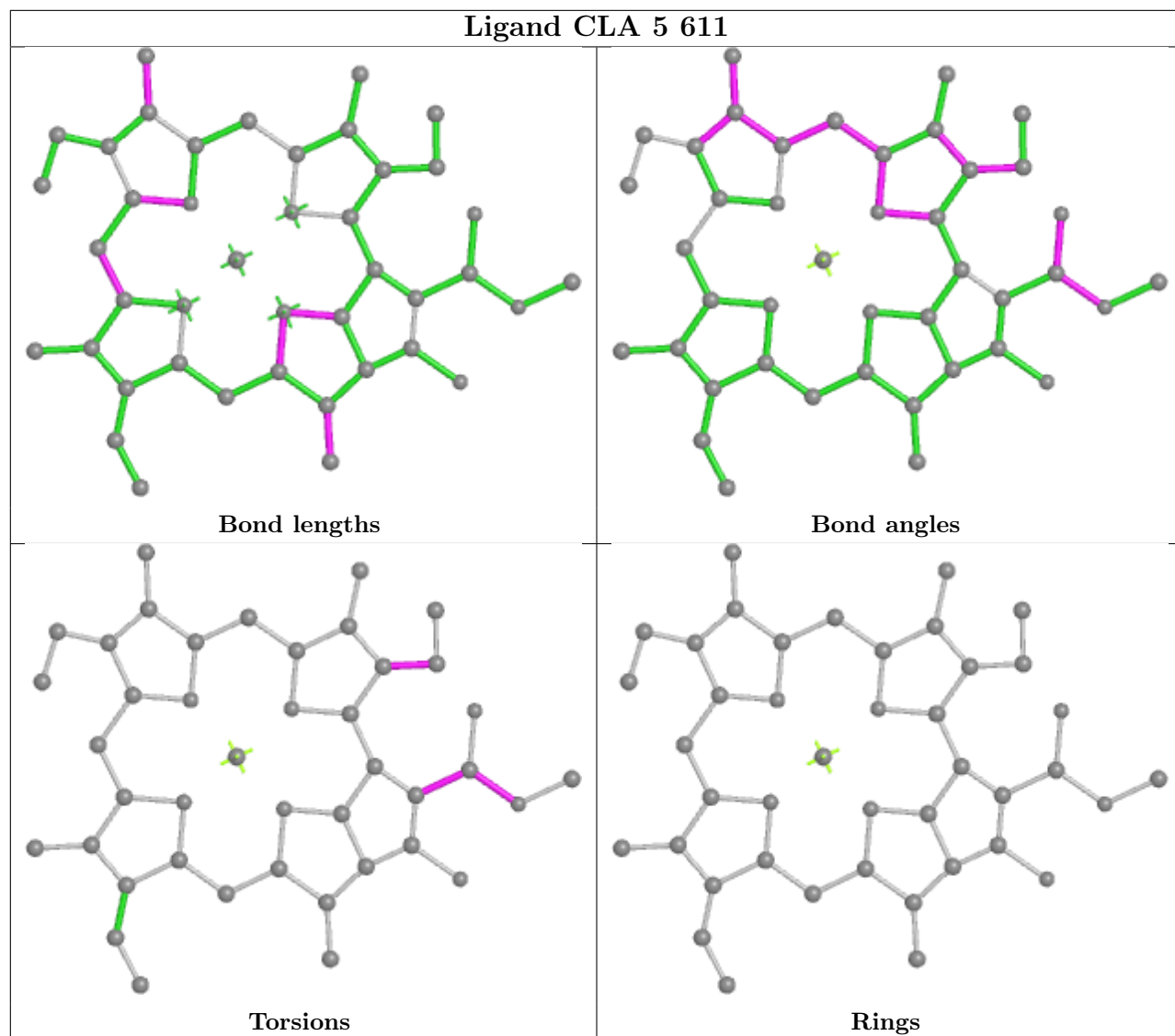




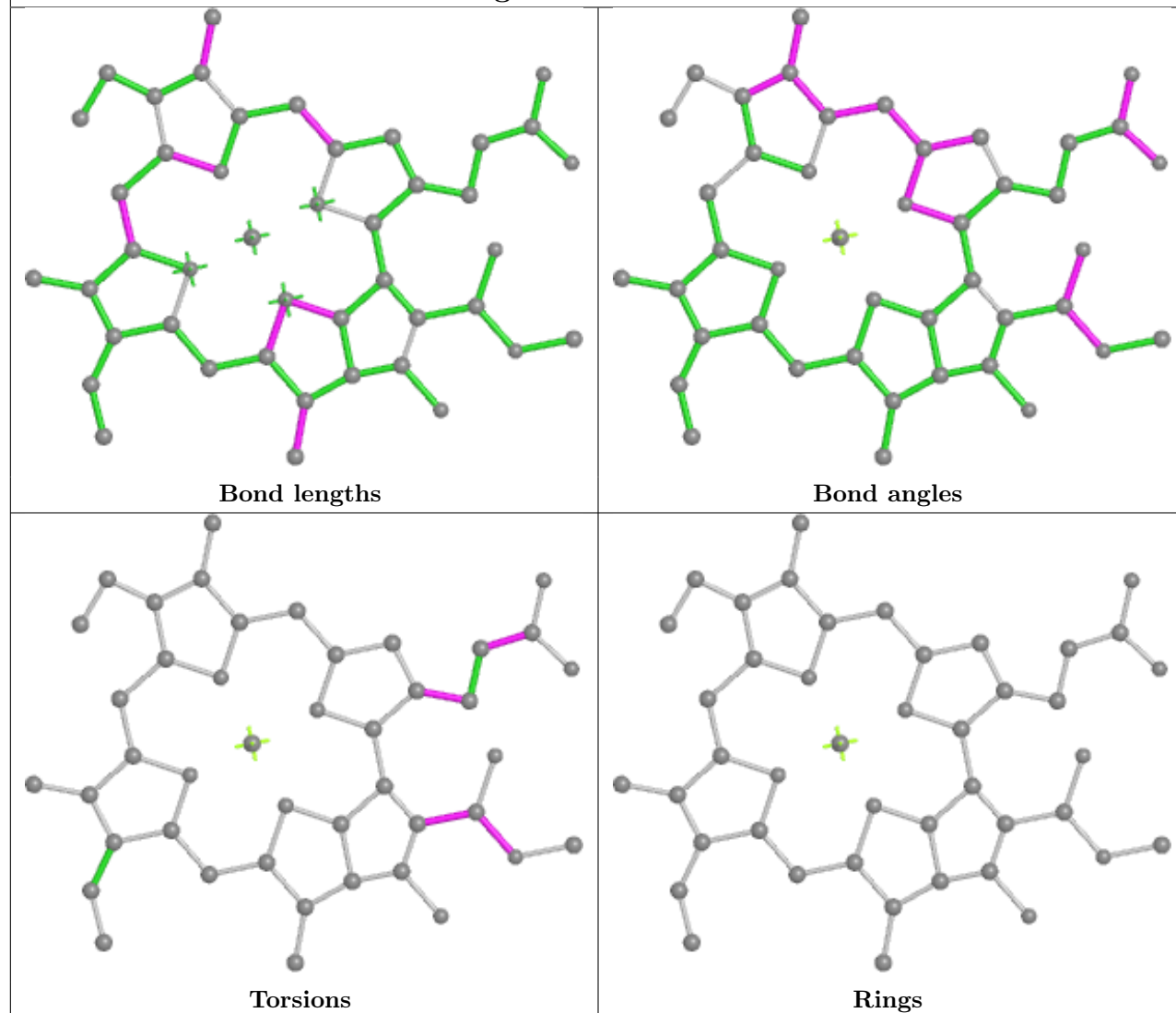




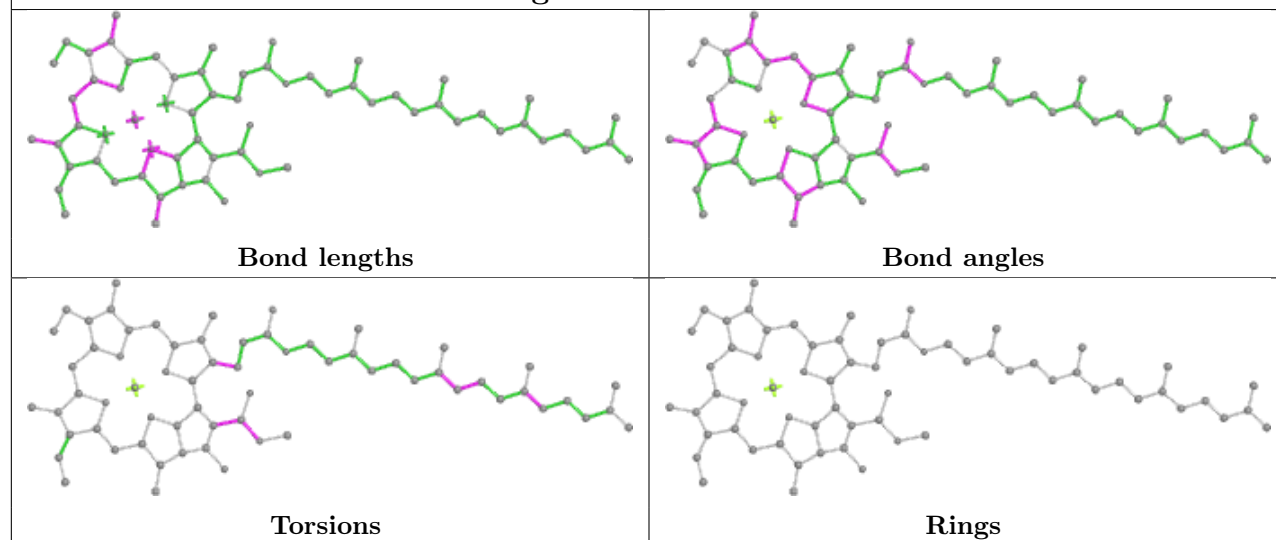


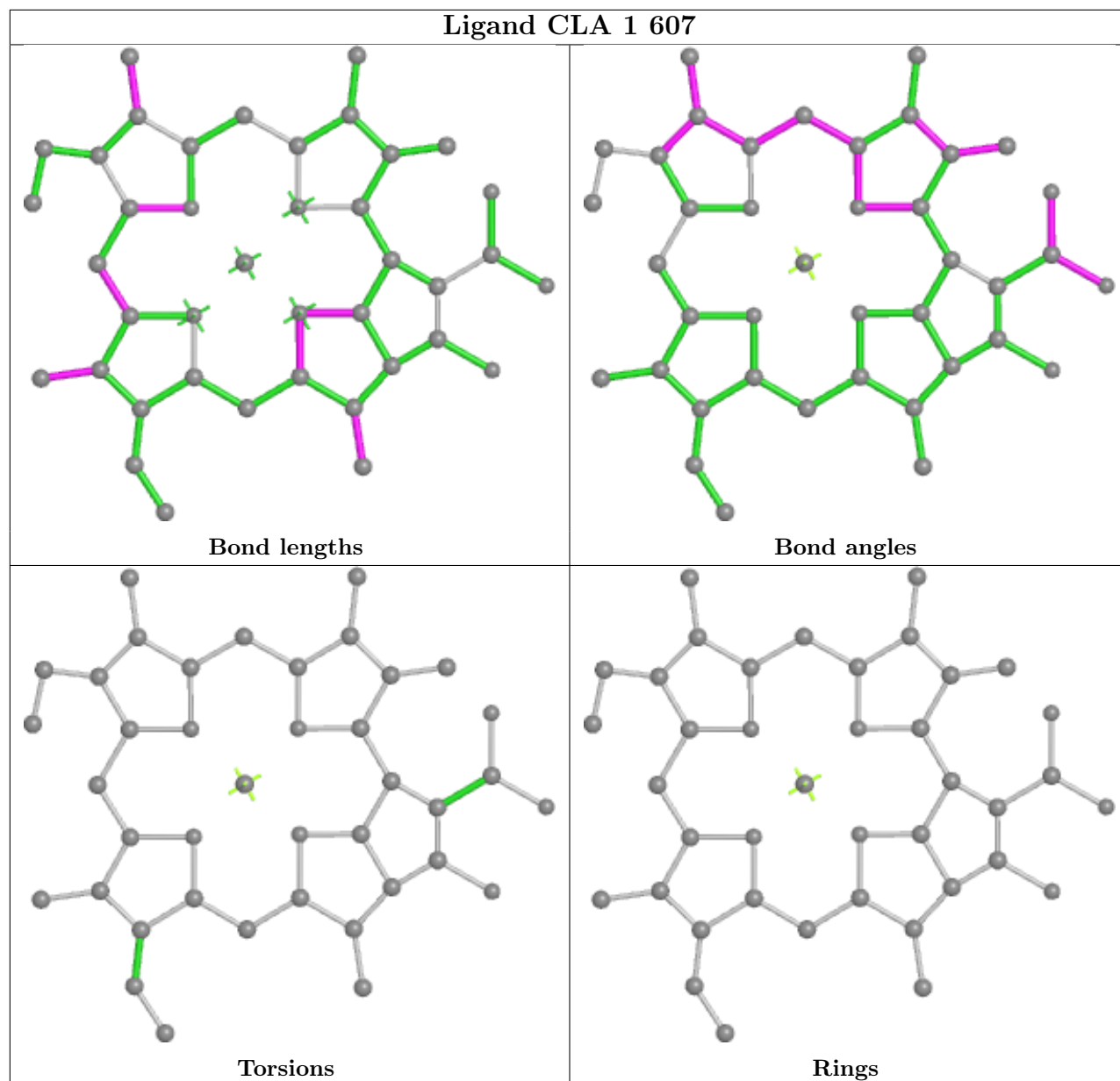


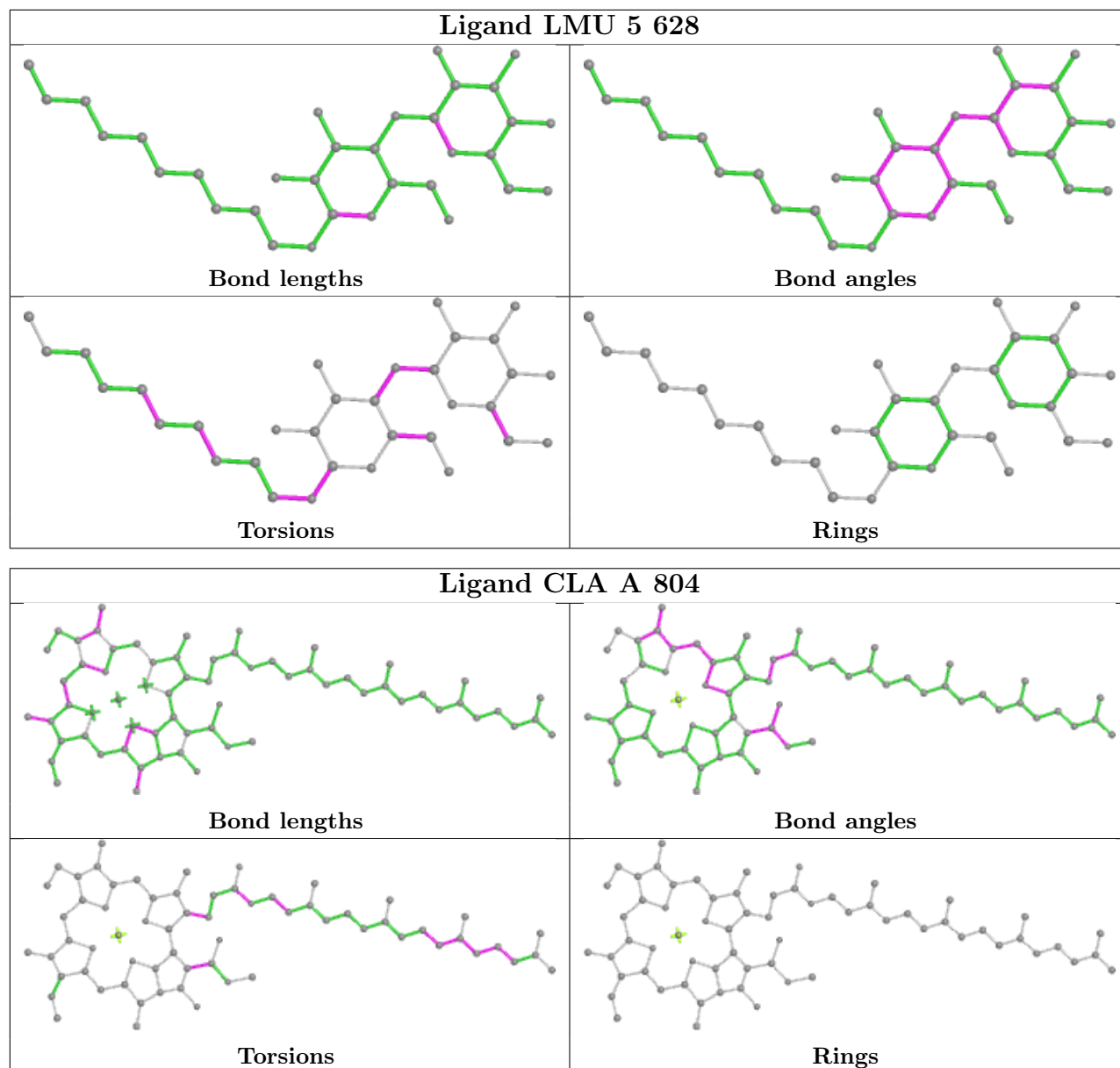
## Ligand CLA 5 614



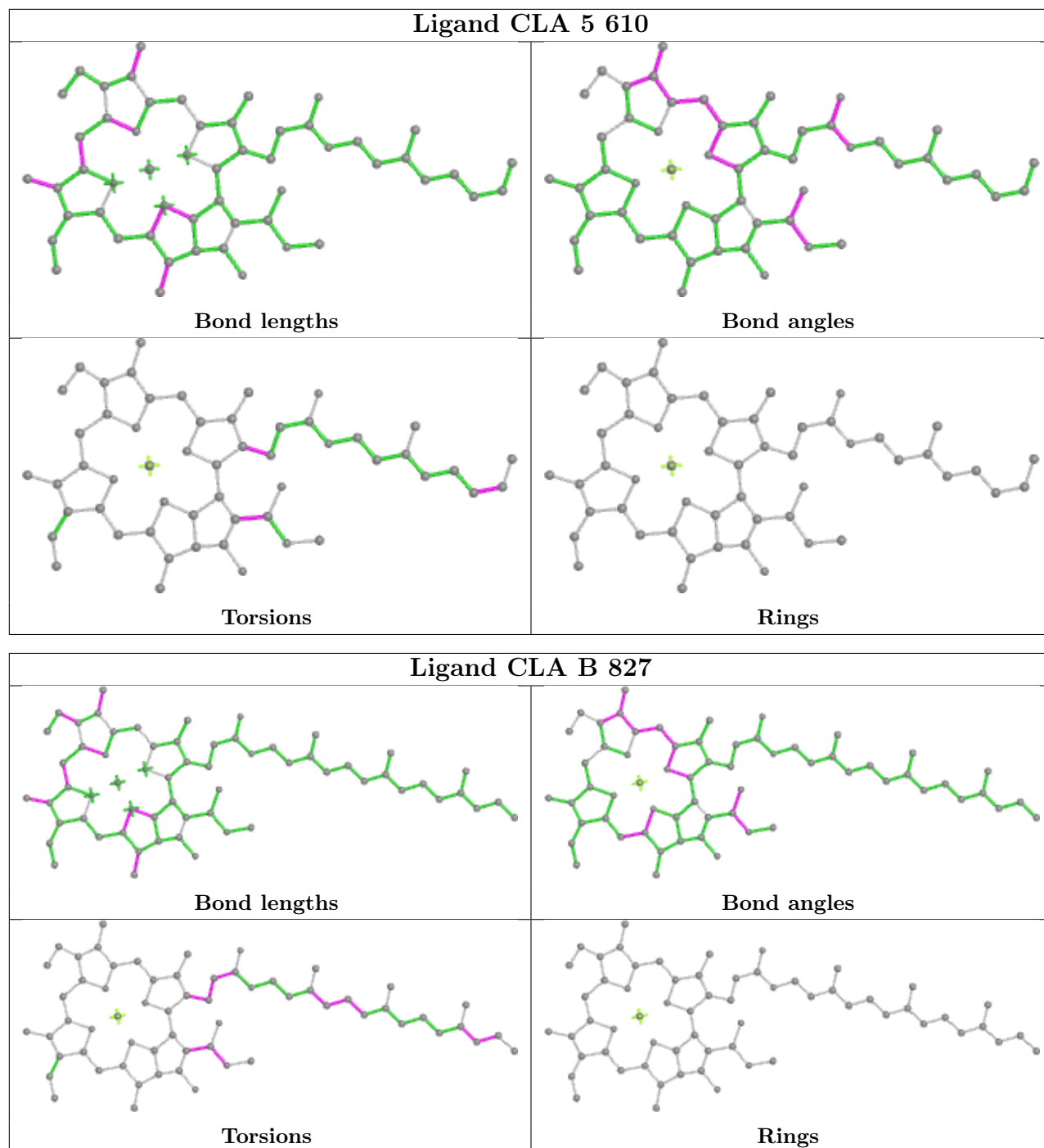
## Ligand CLA A 831

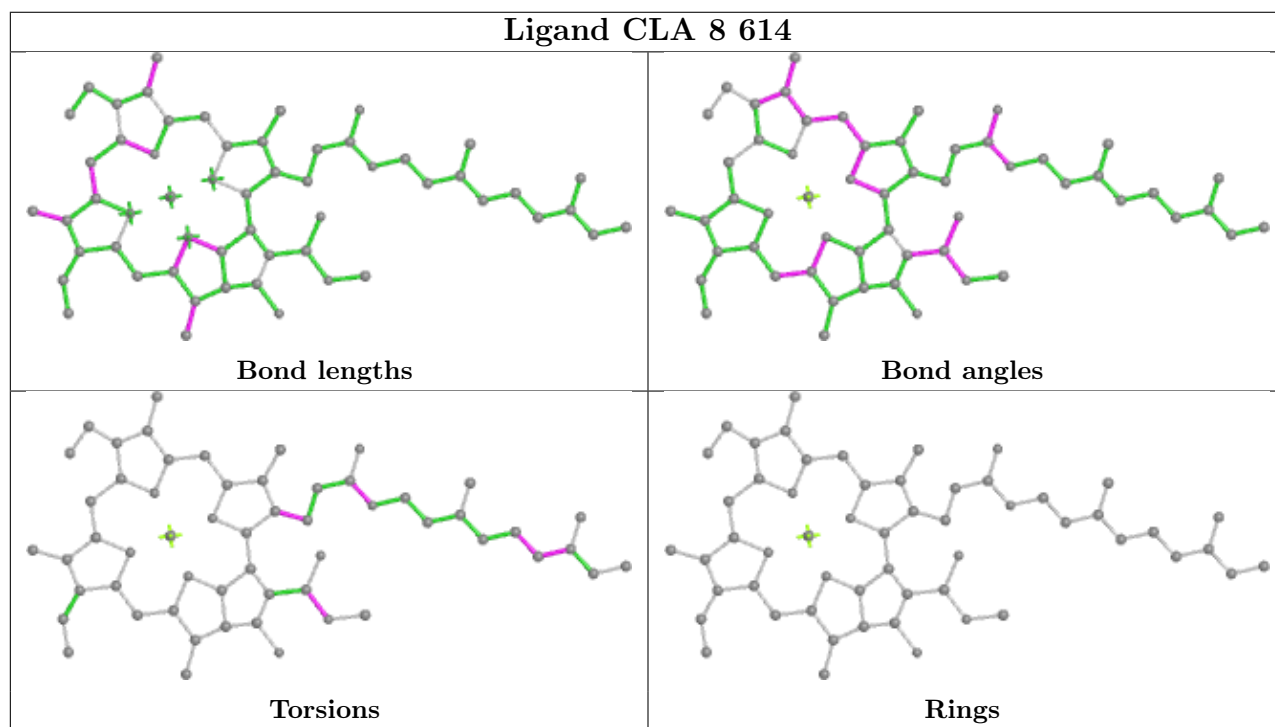
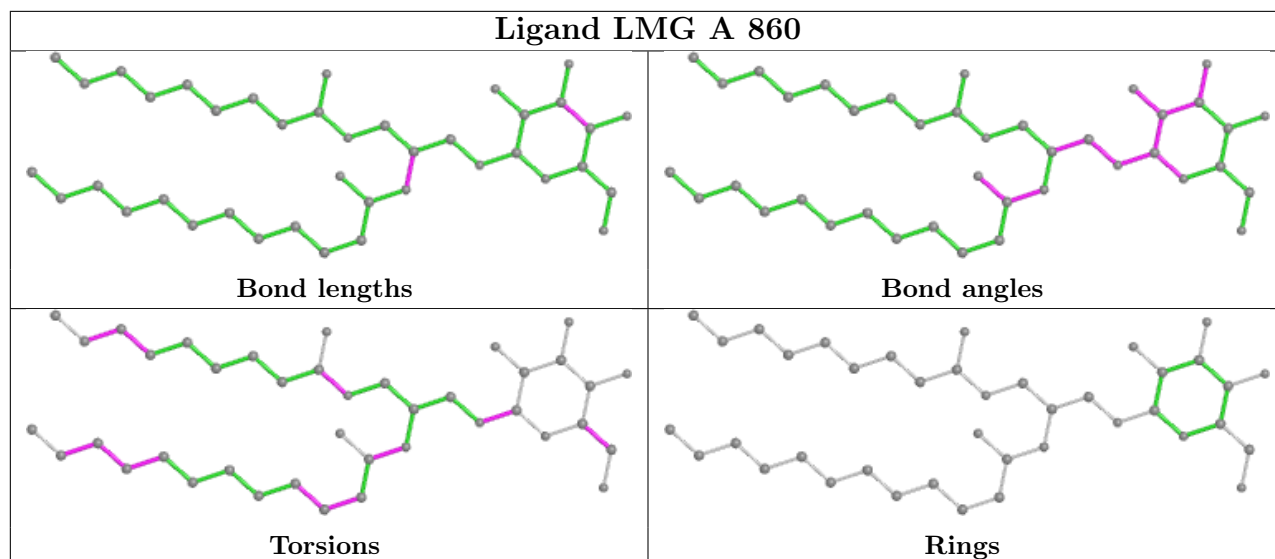


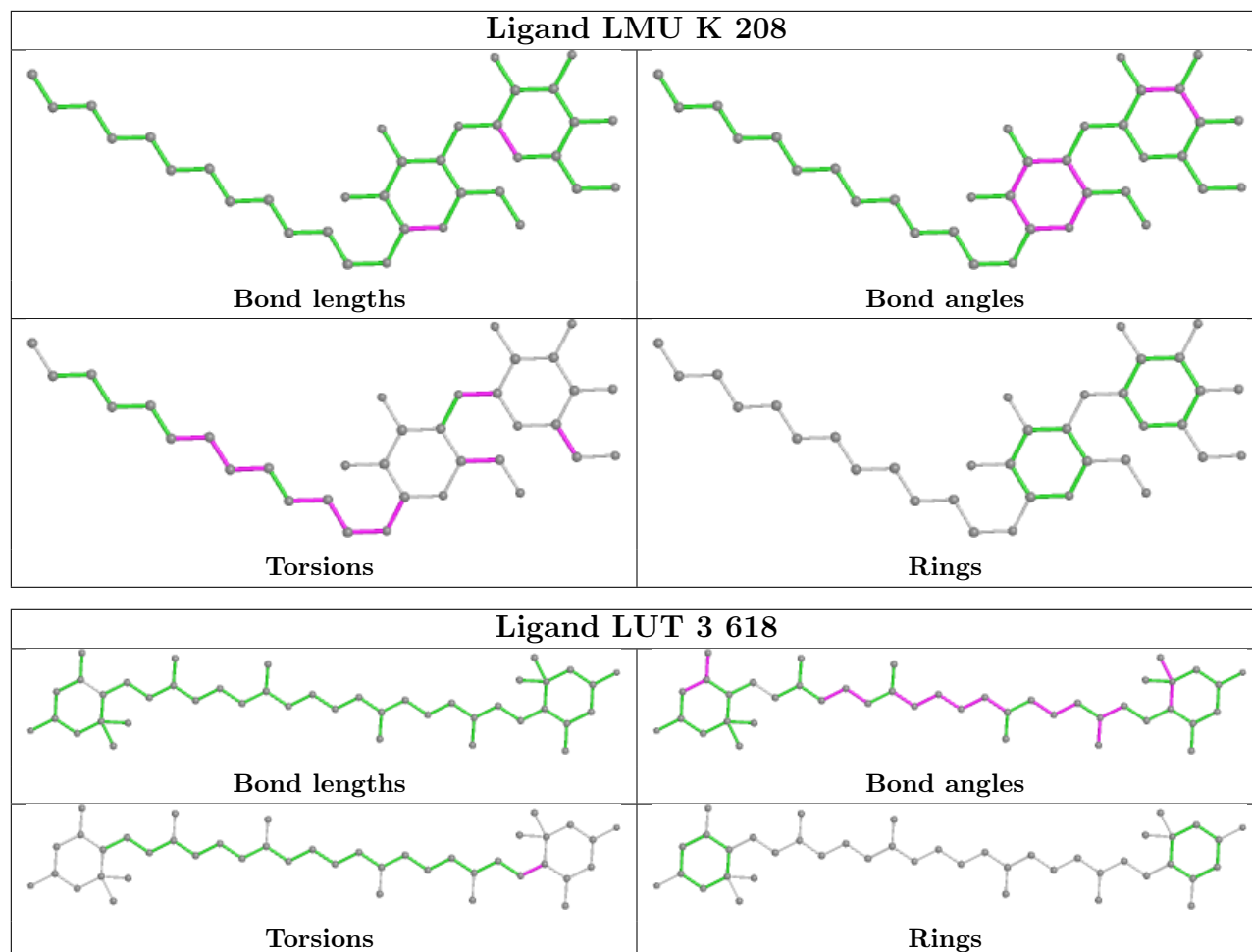


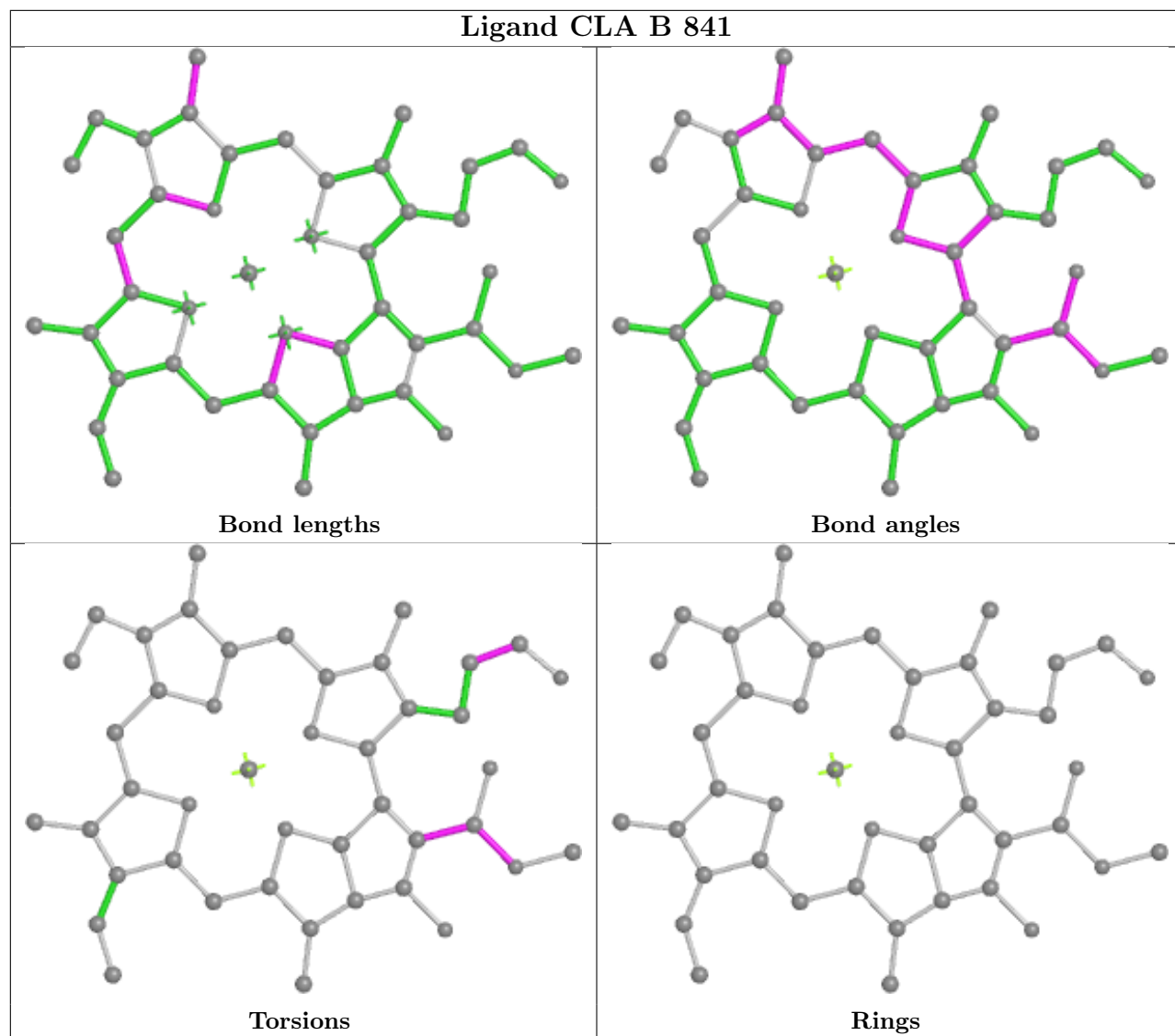


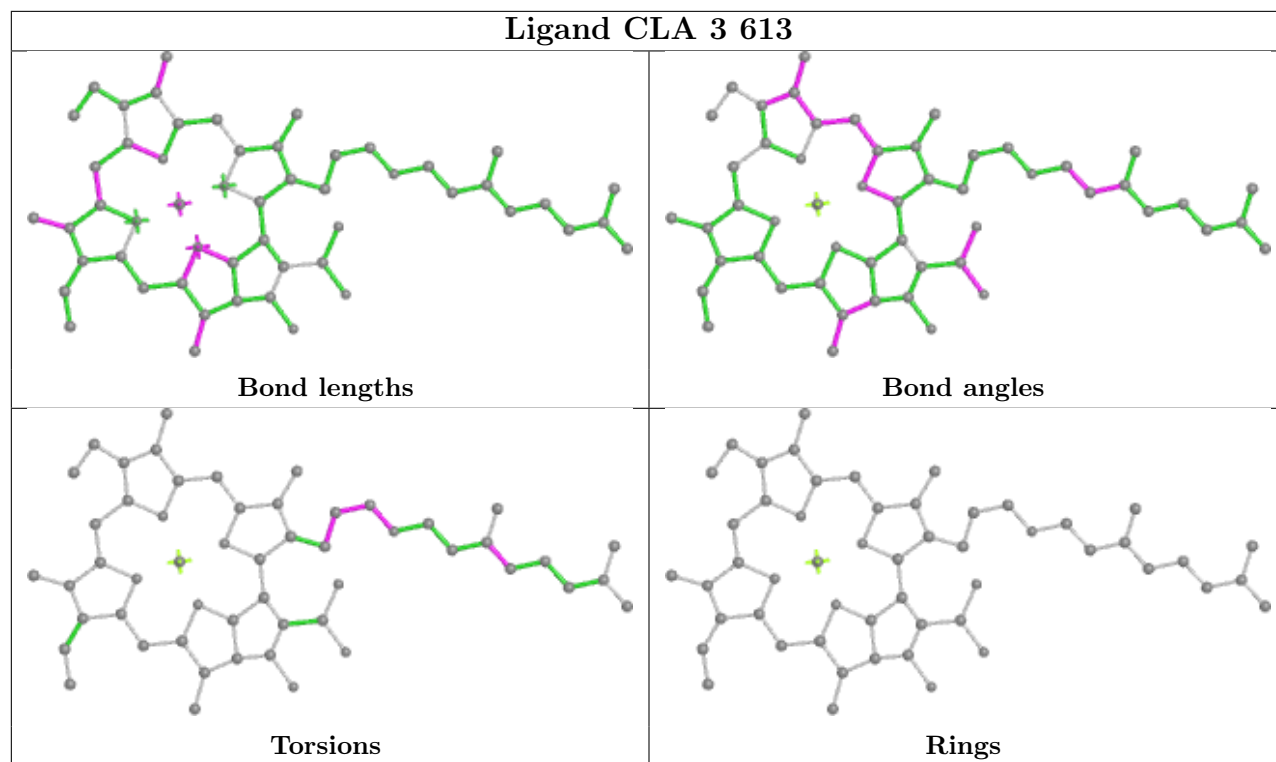


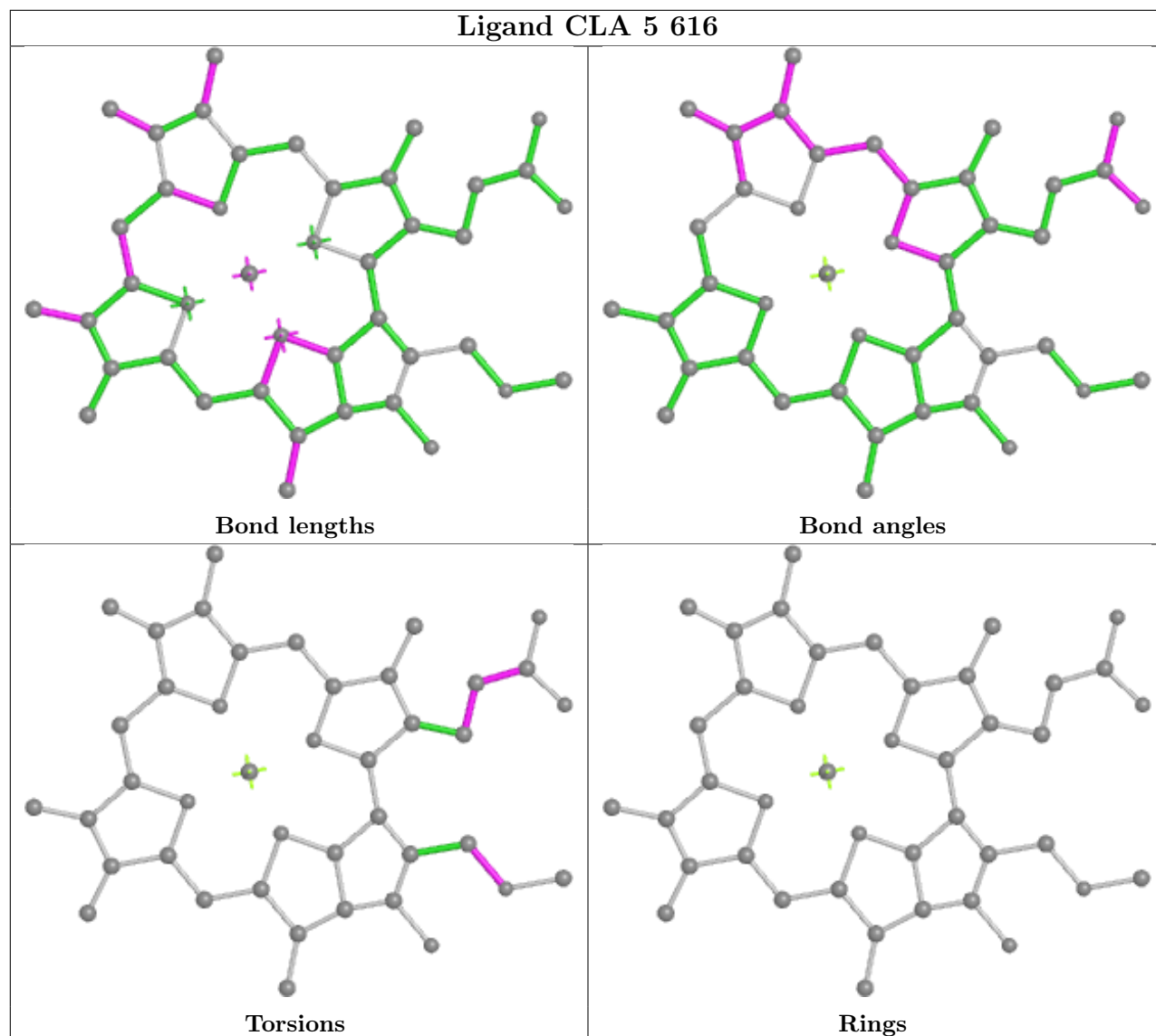


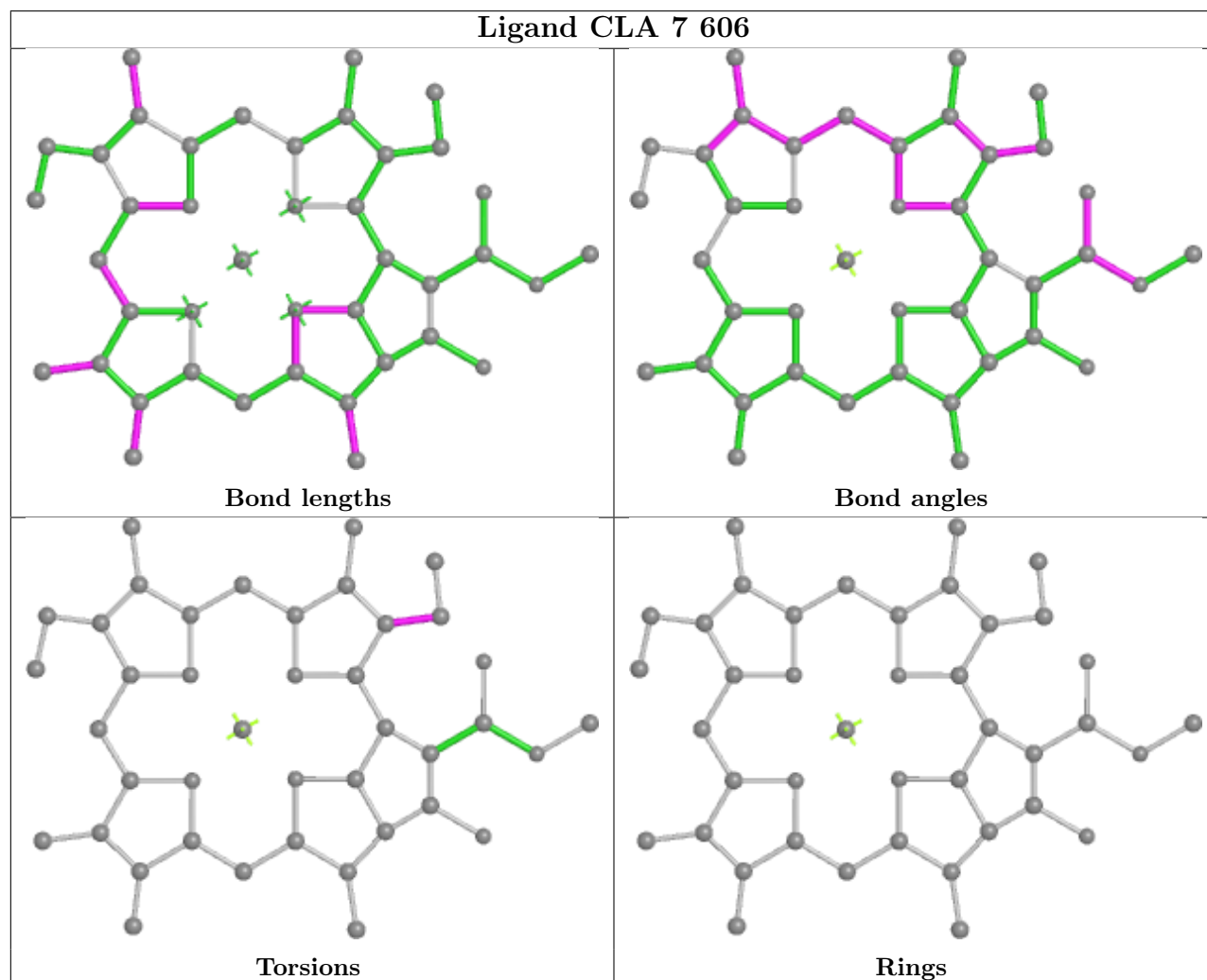
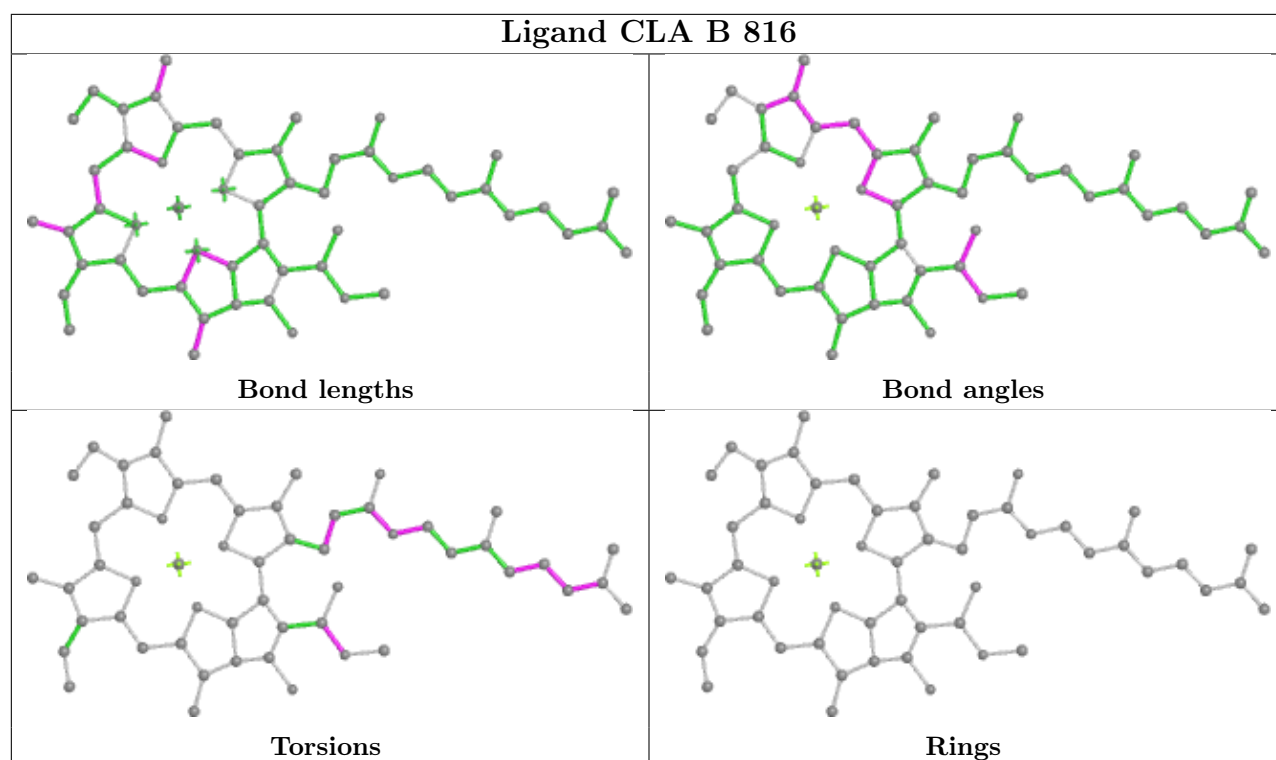


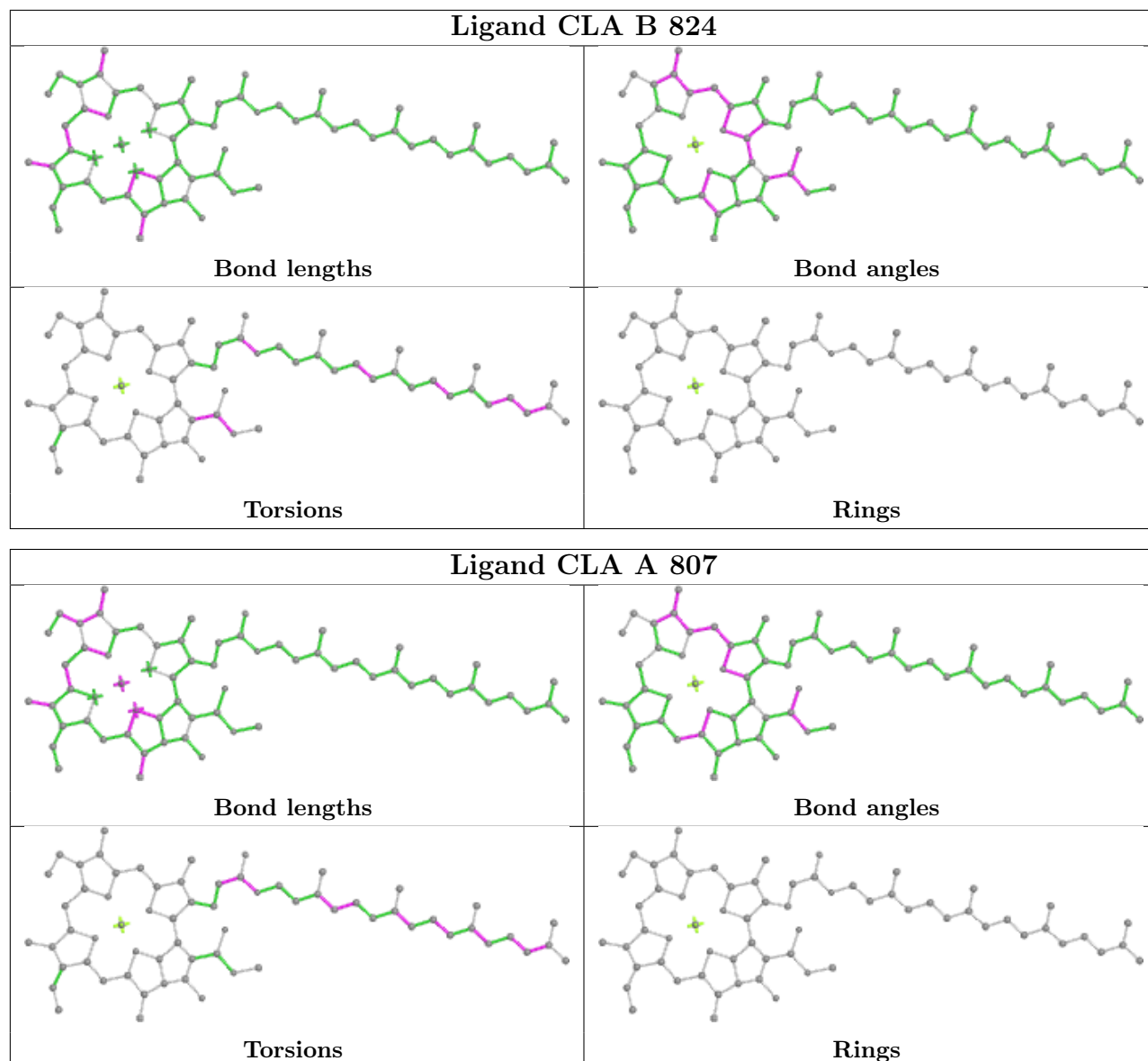




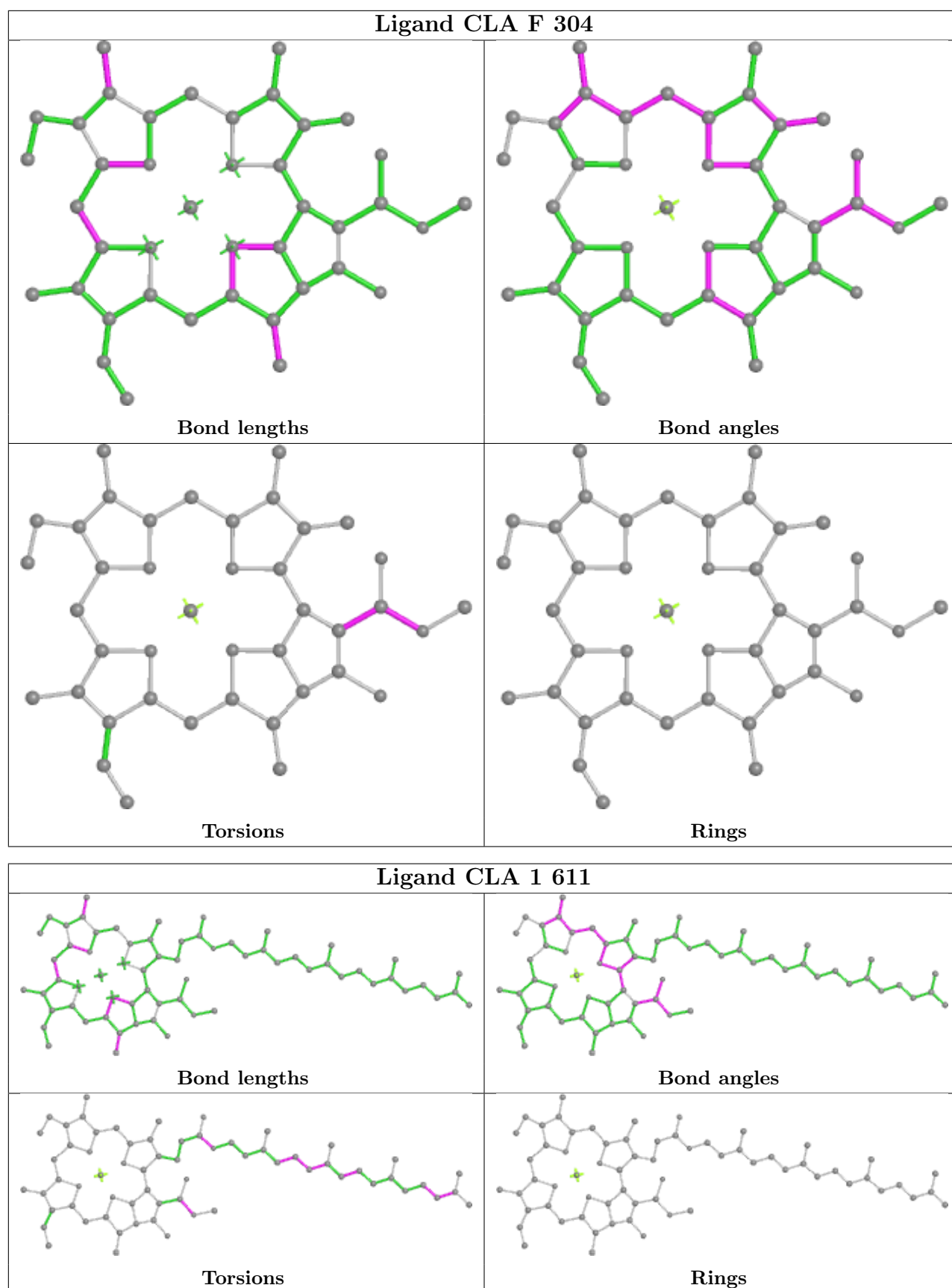


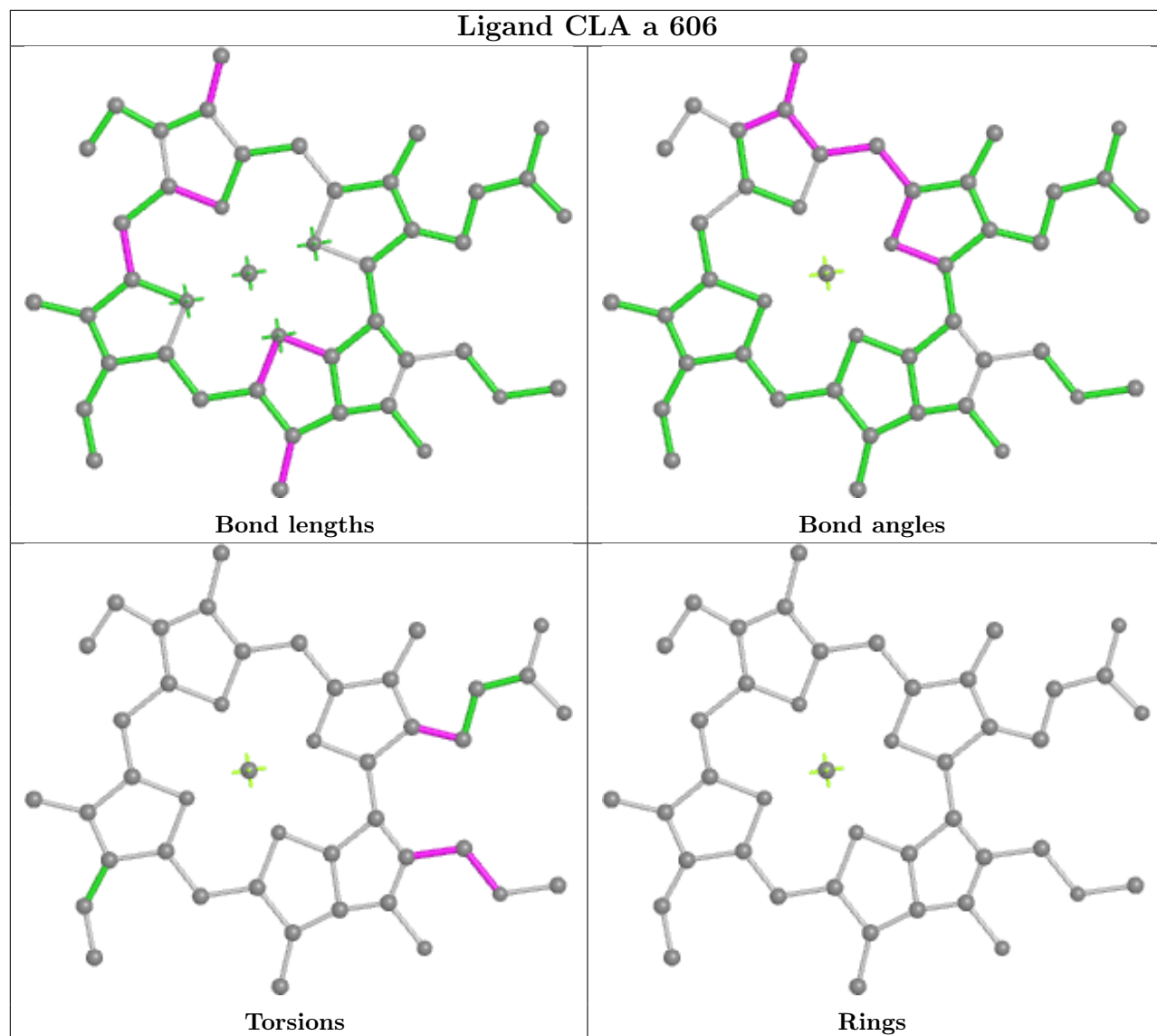


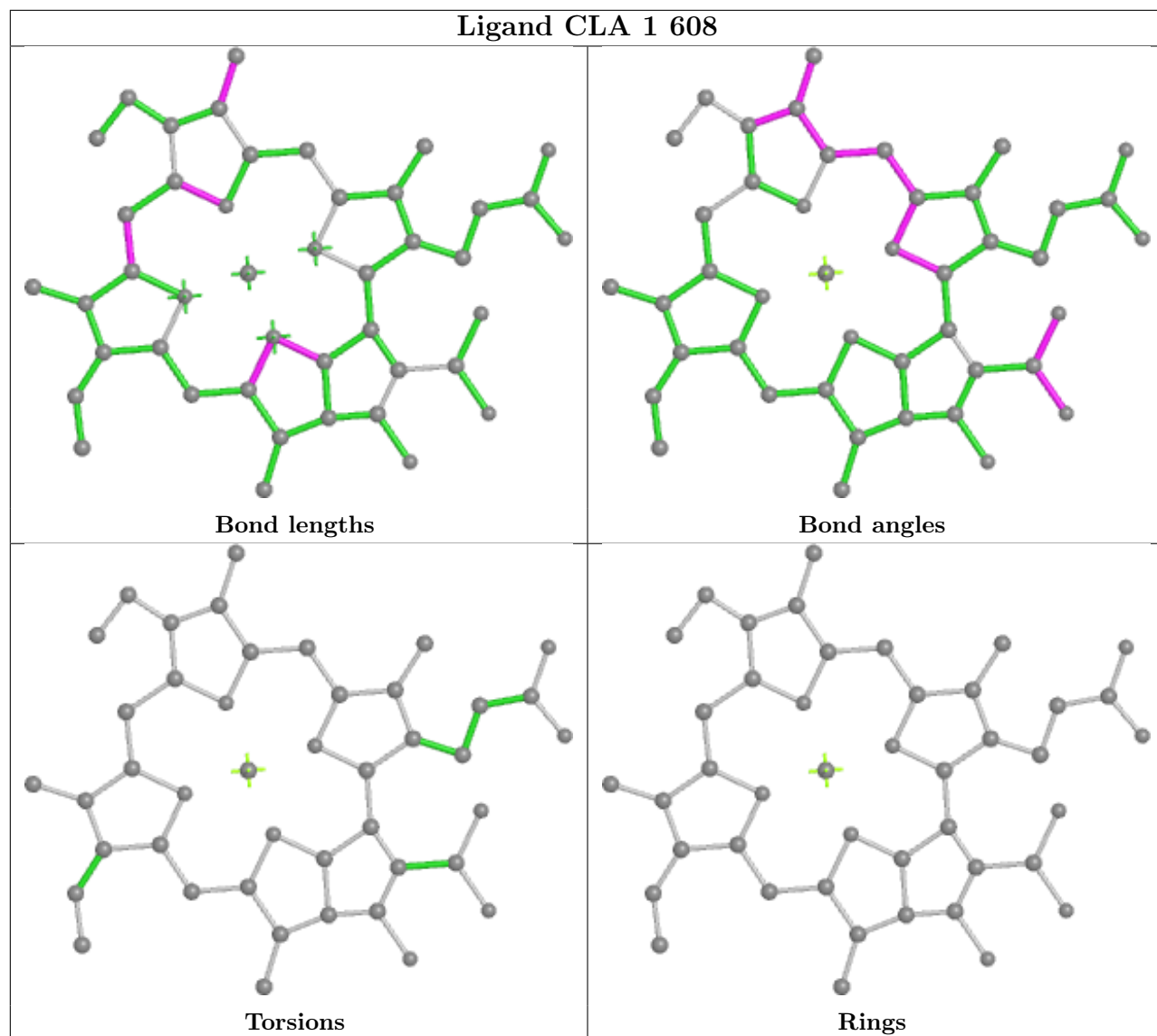


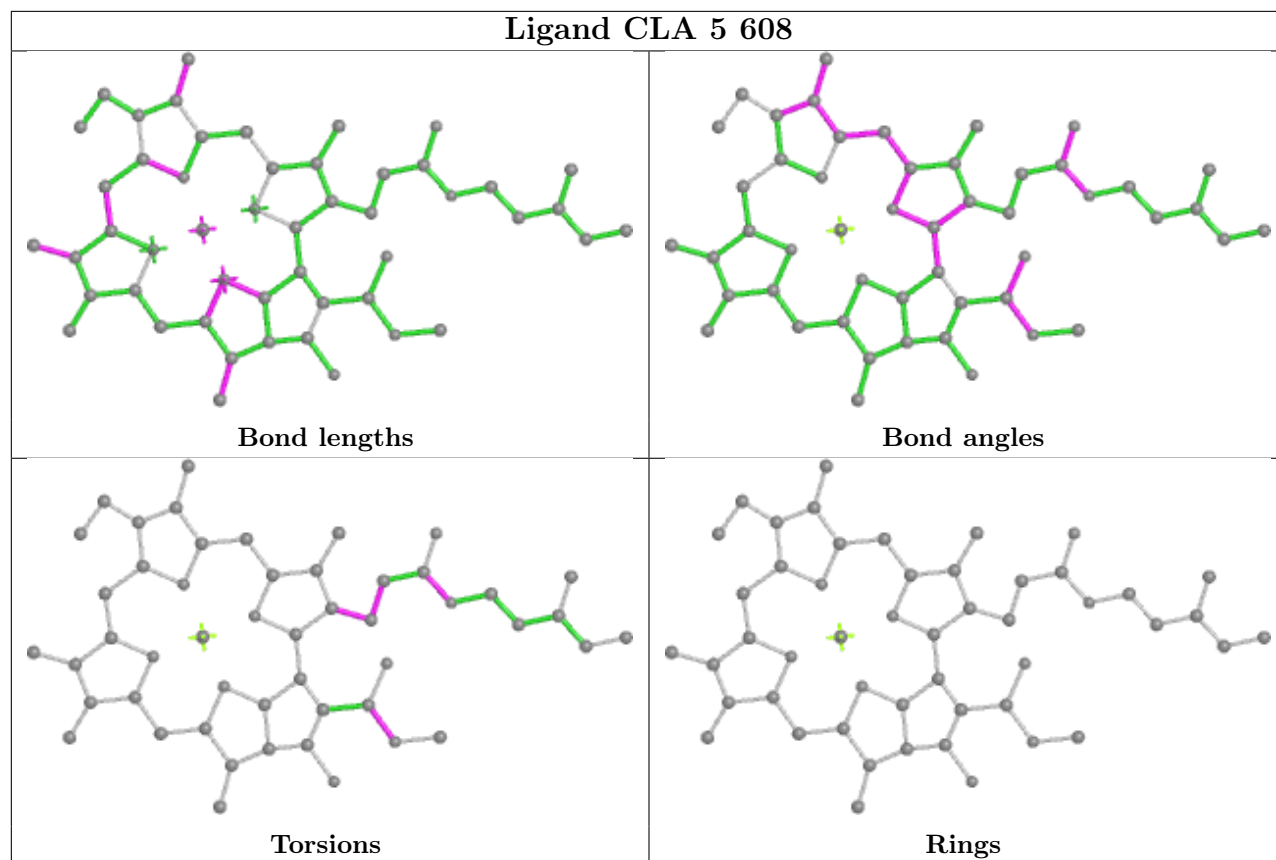


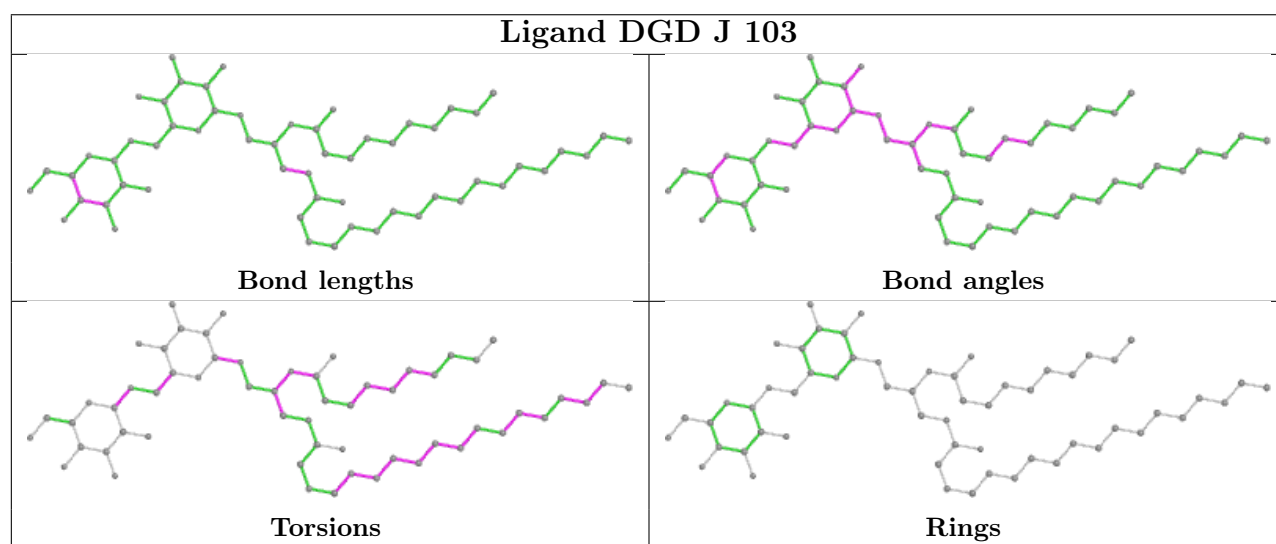
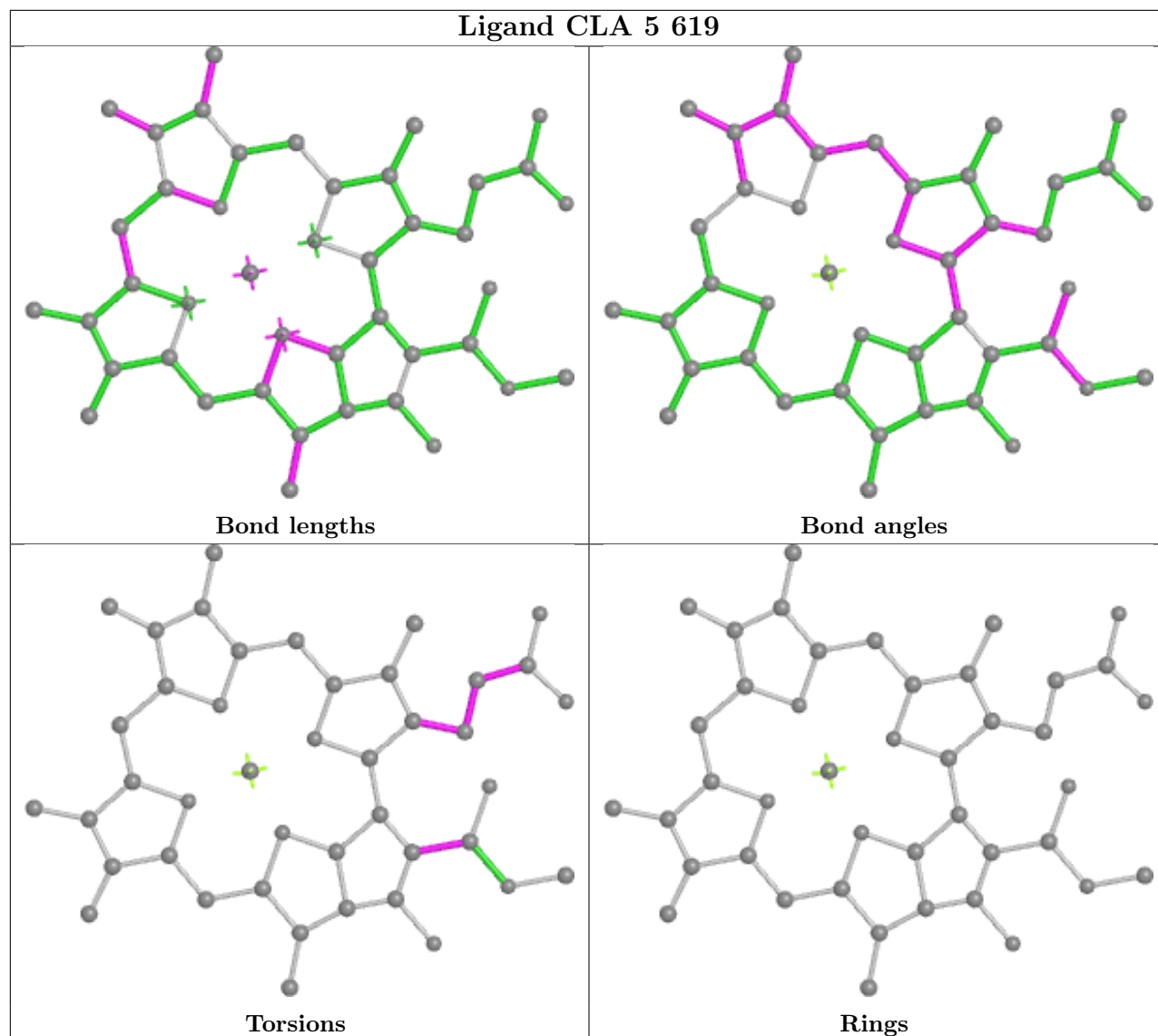


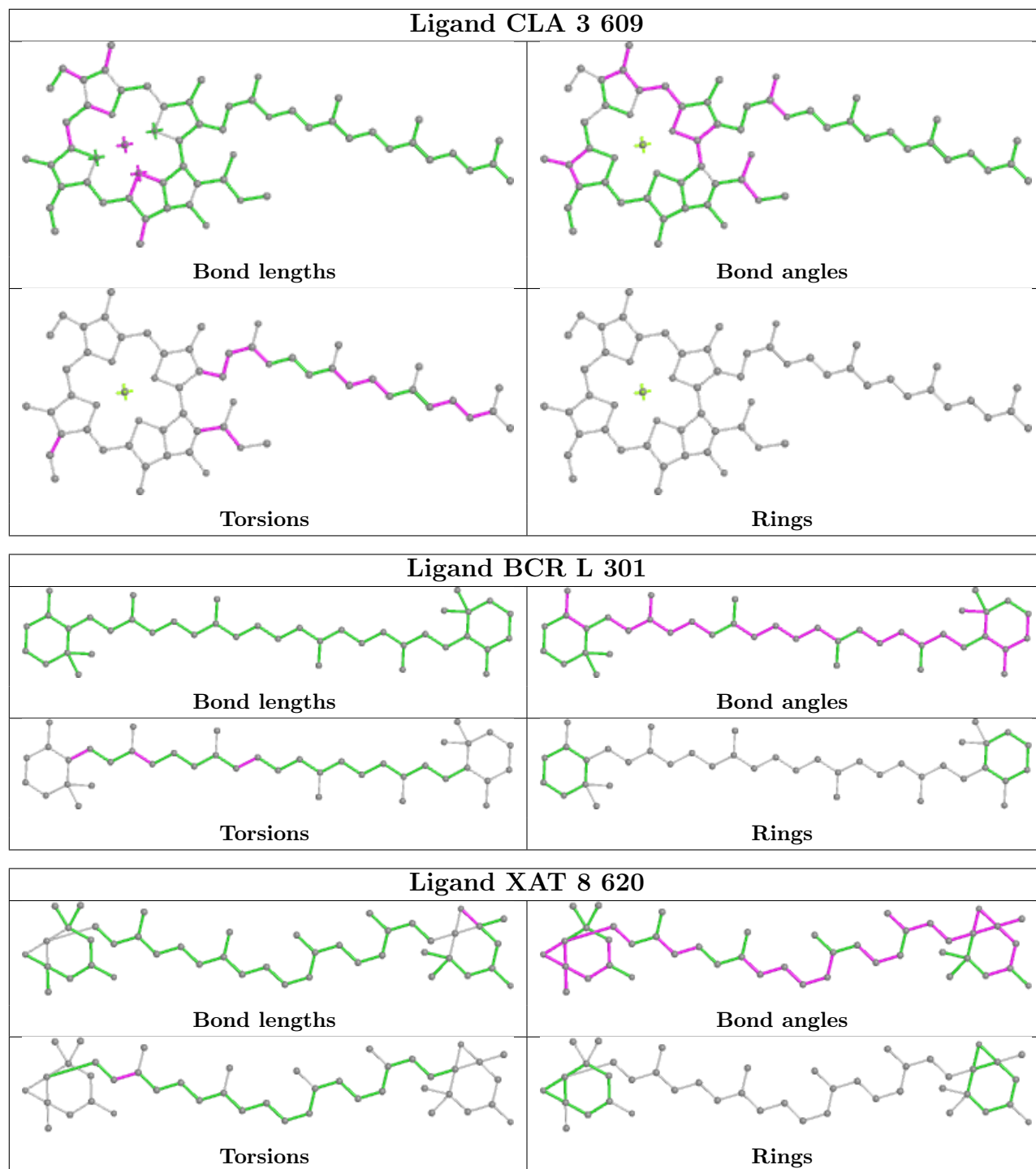


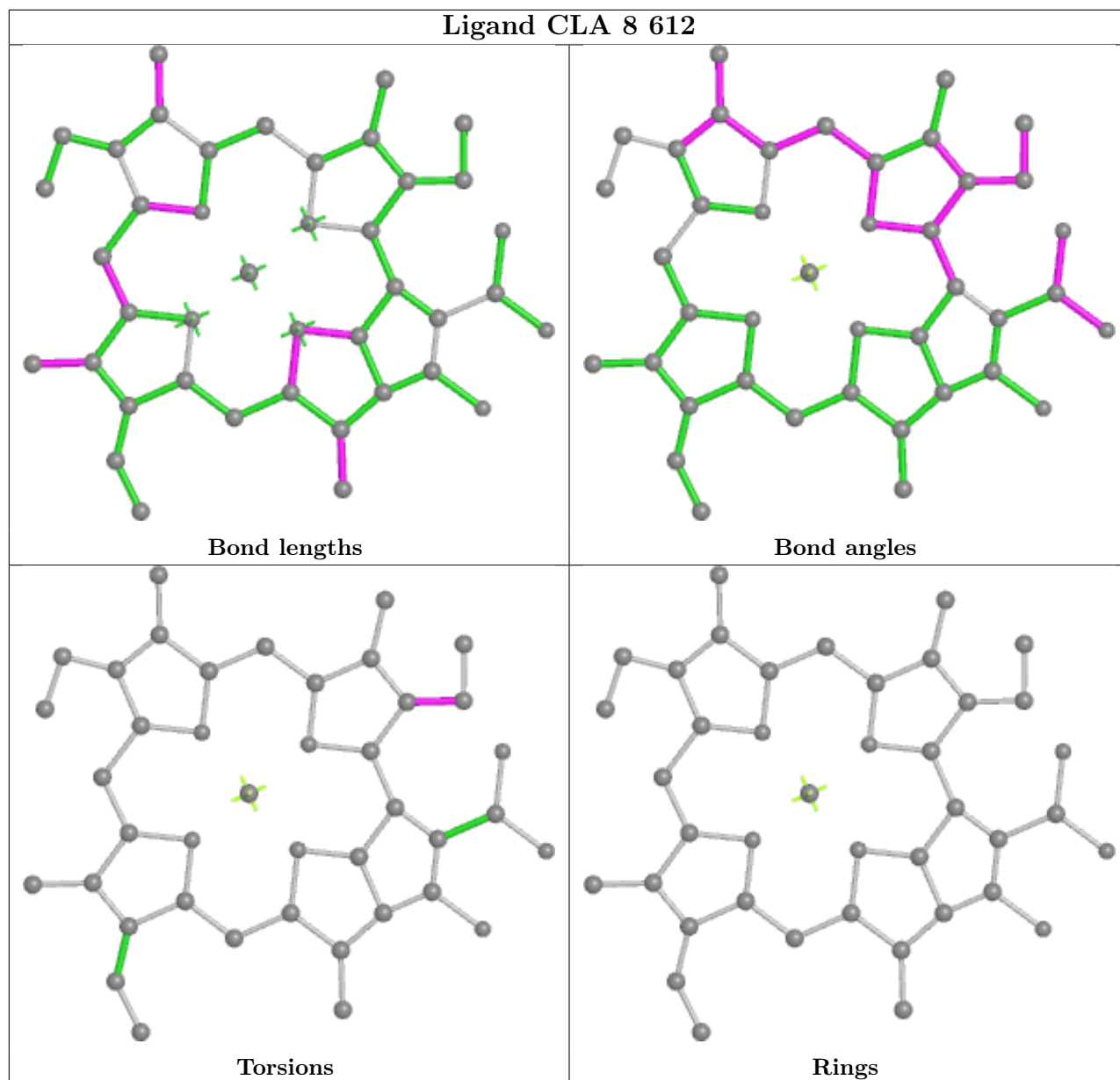
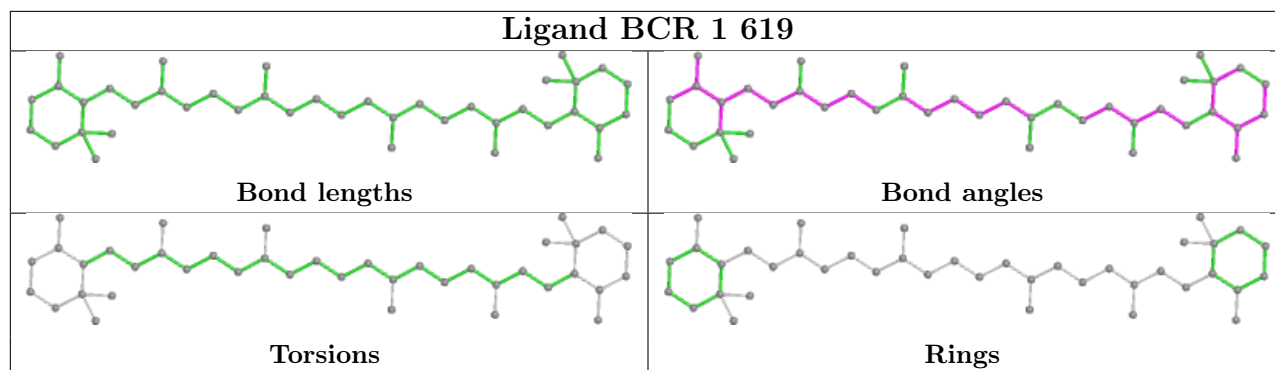


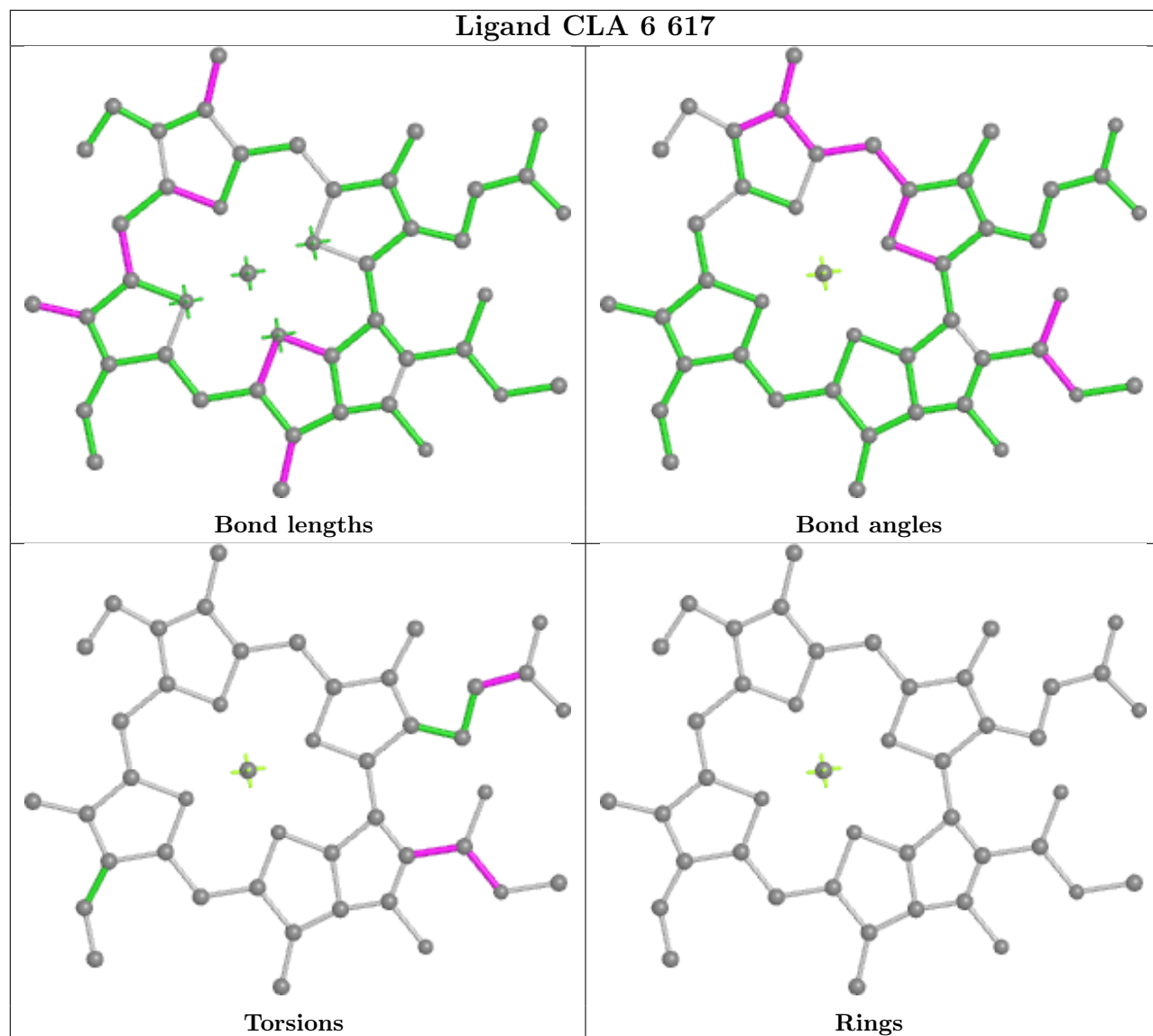




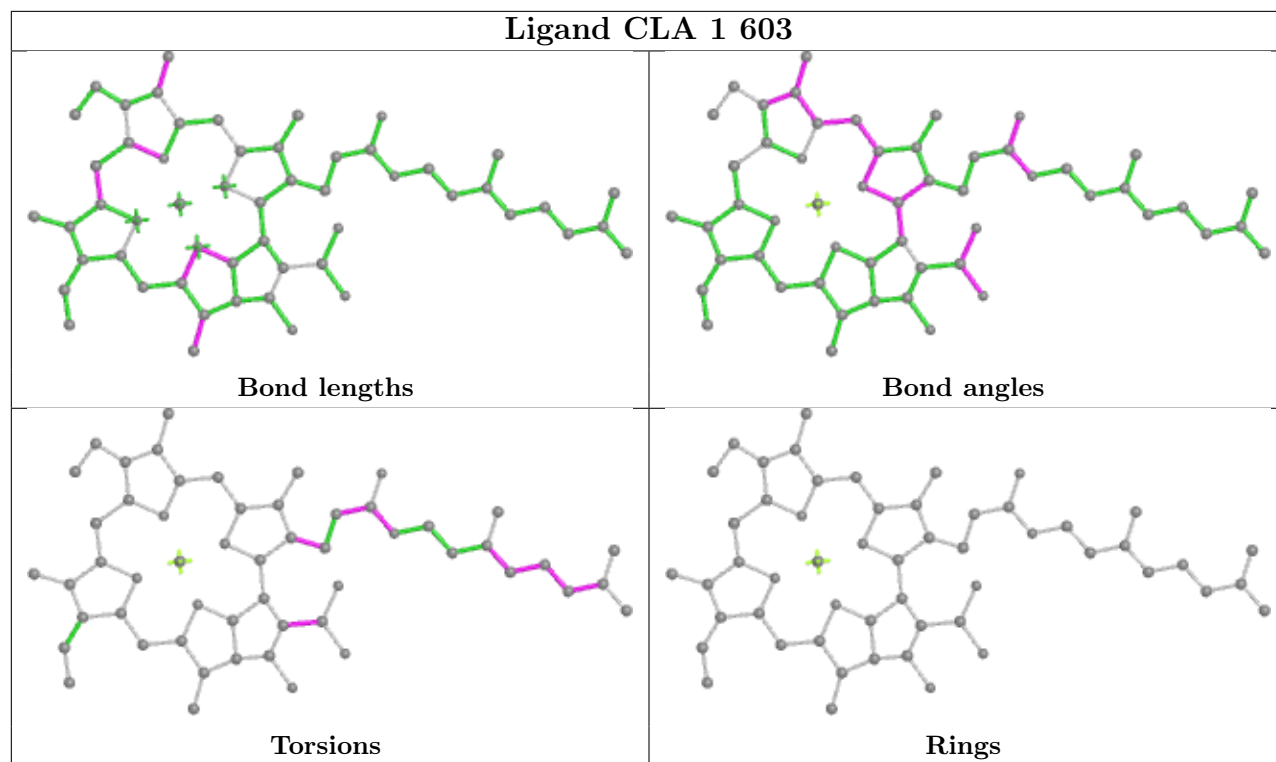


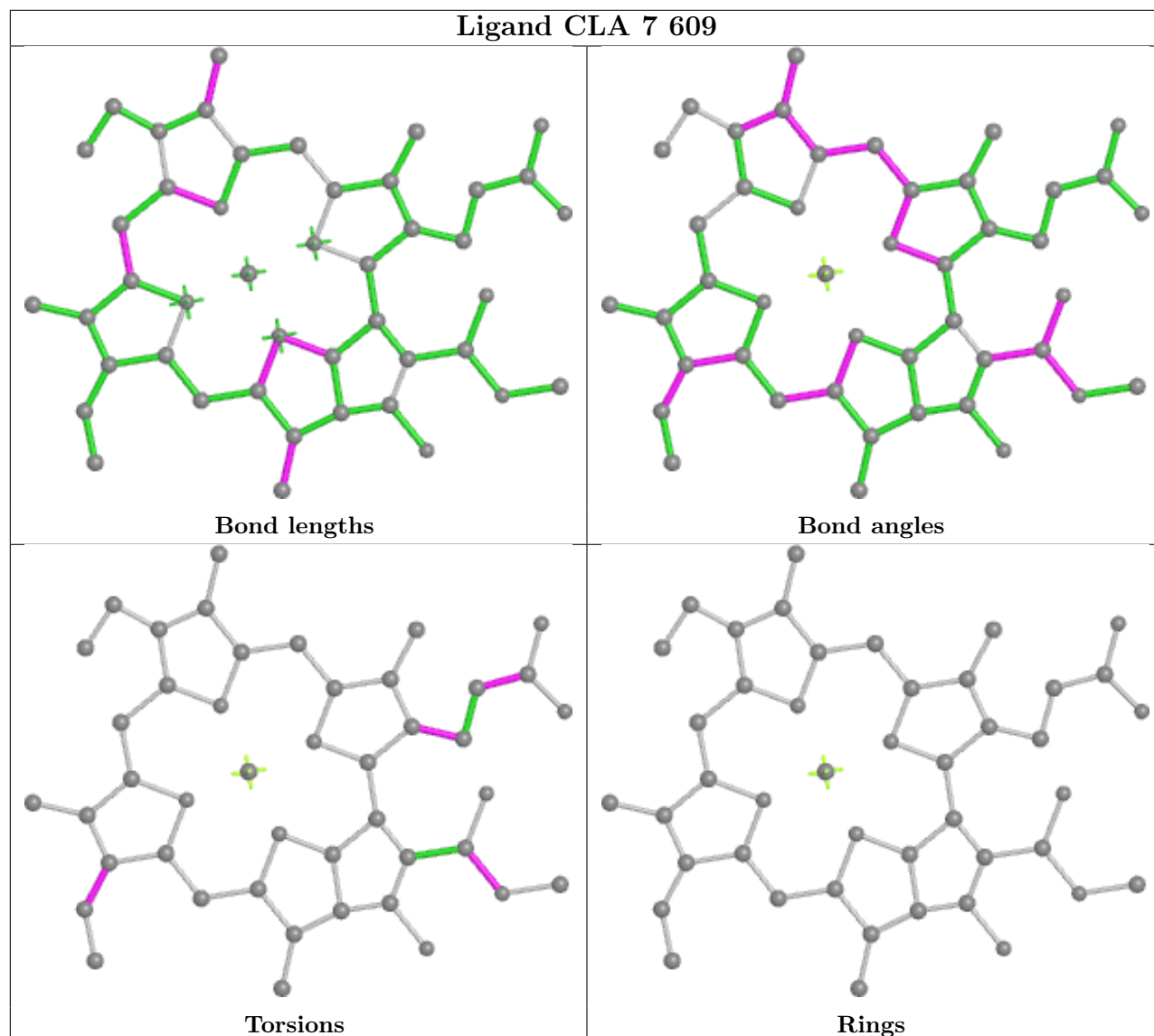


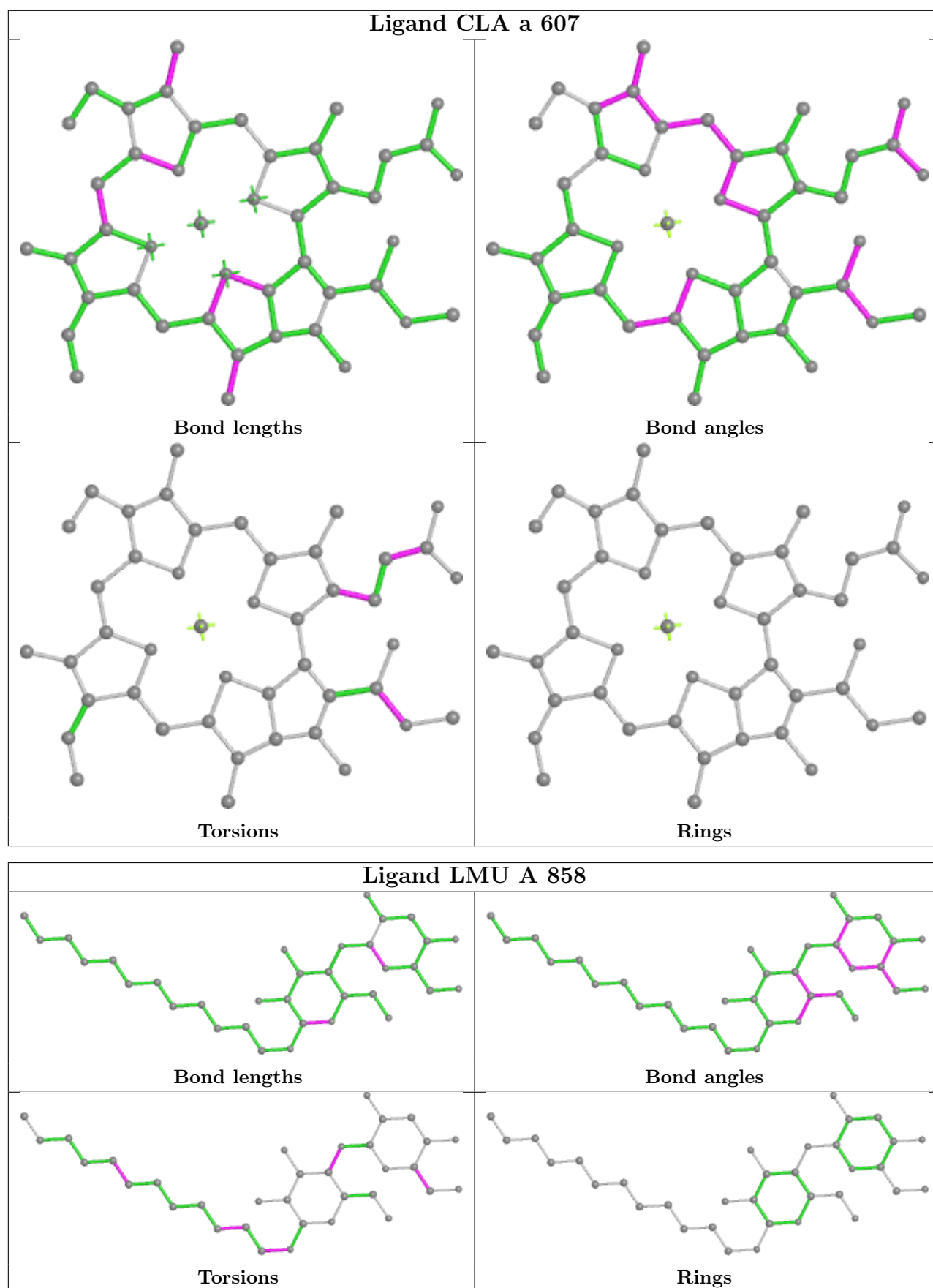


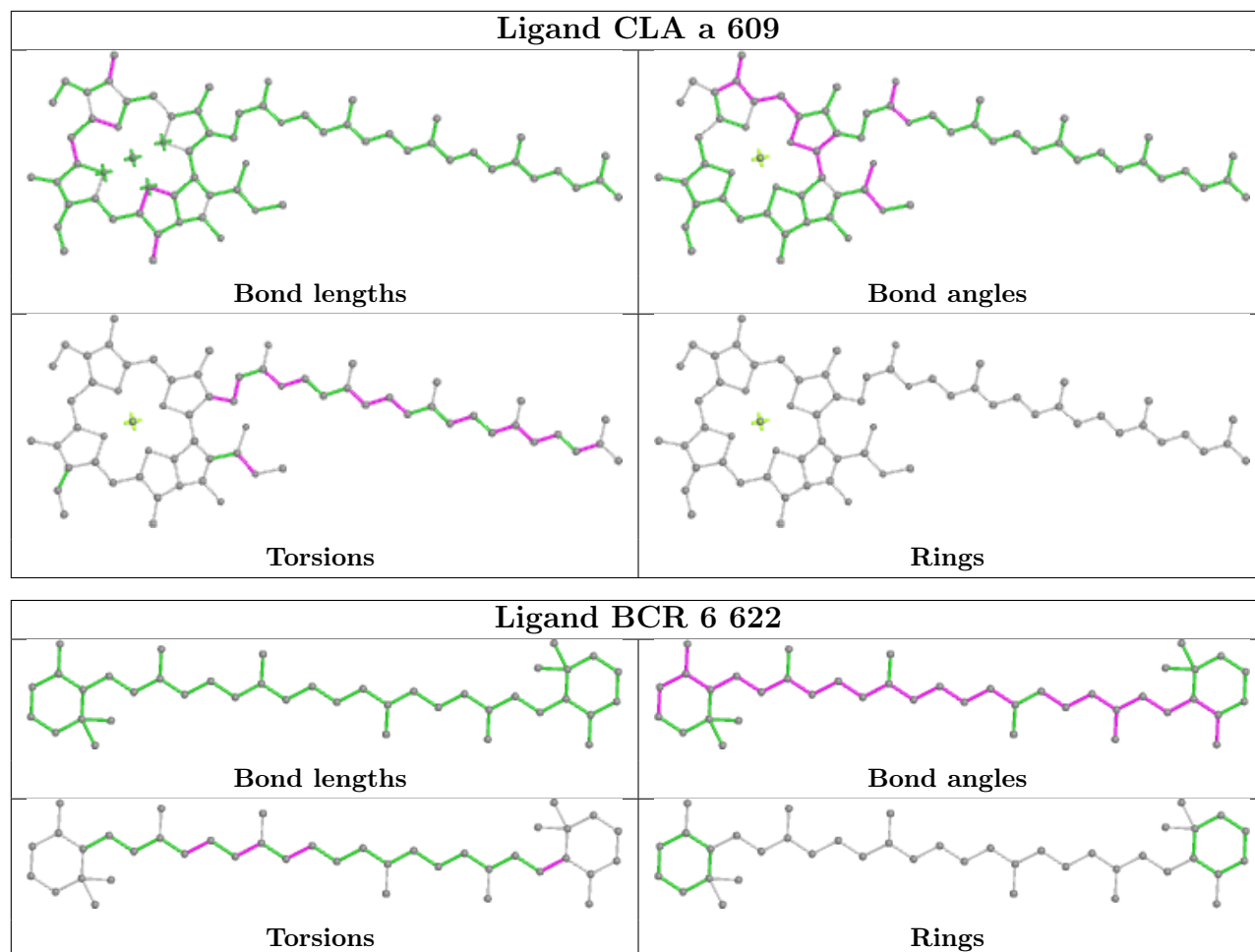




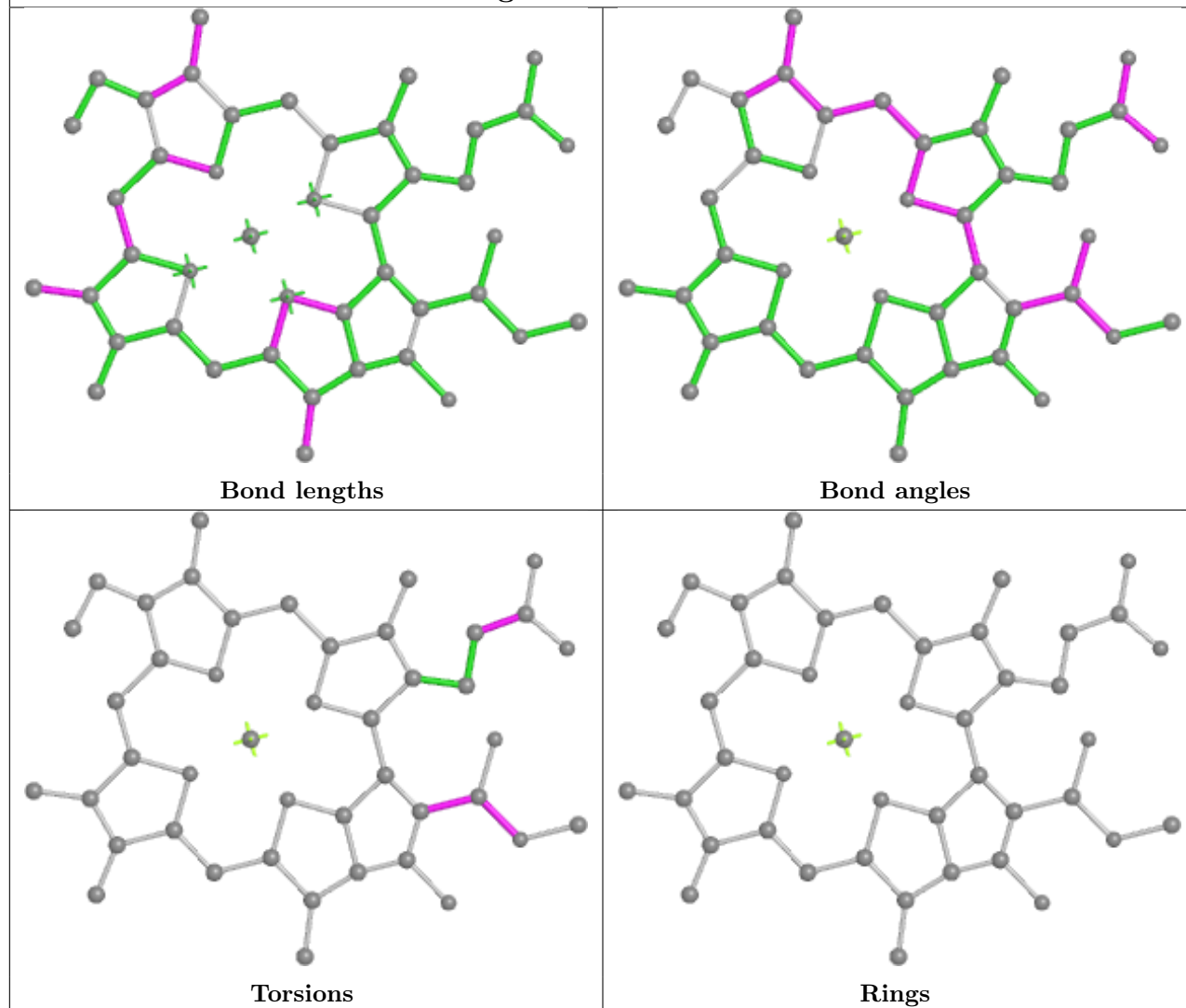




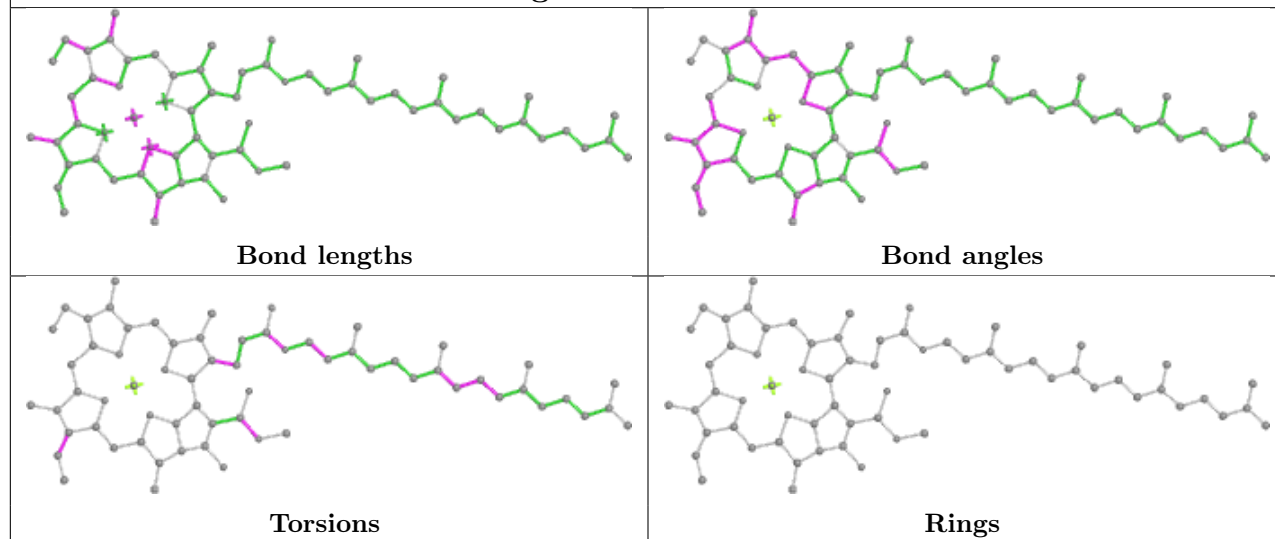


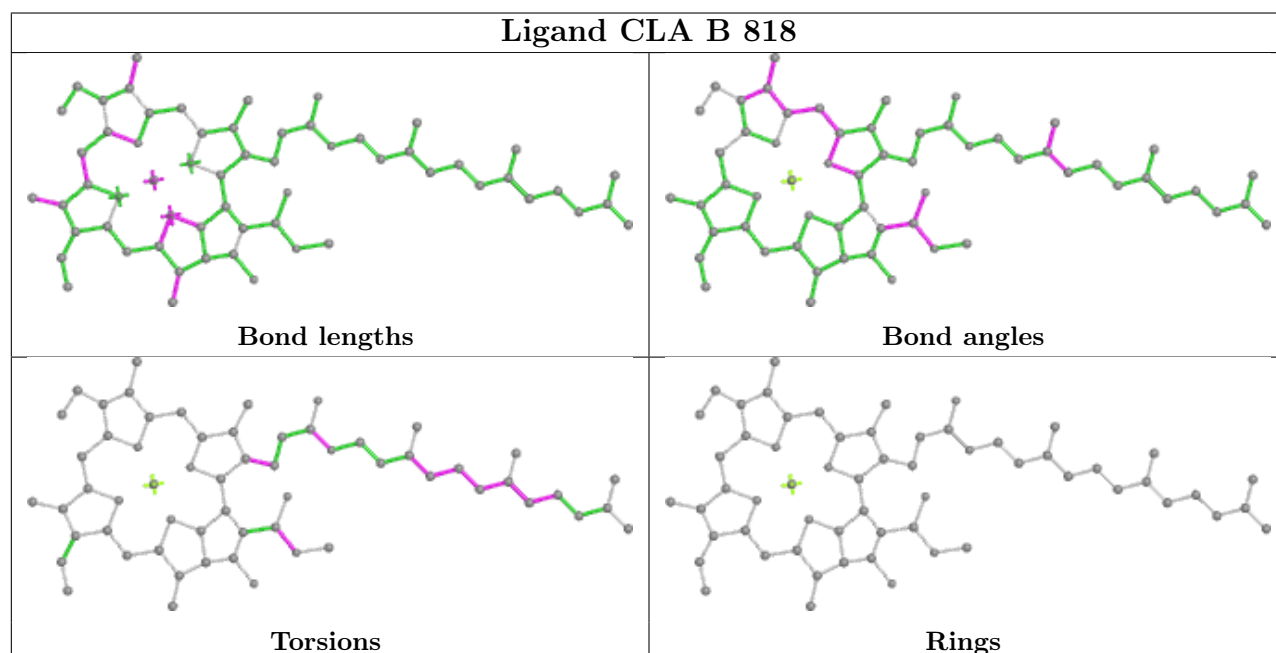
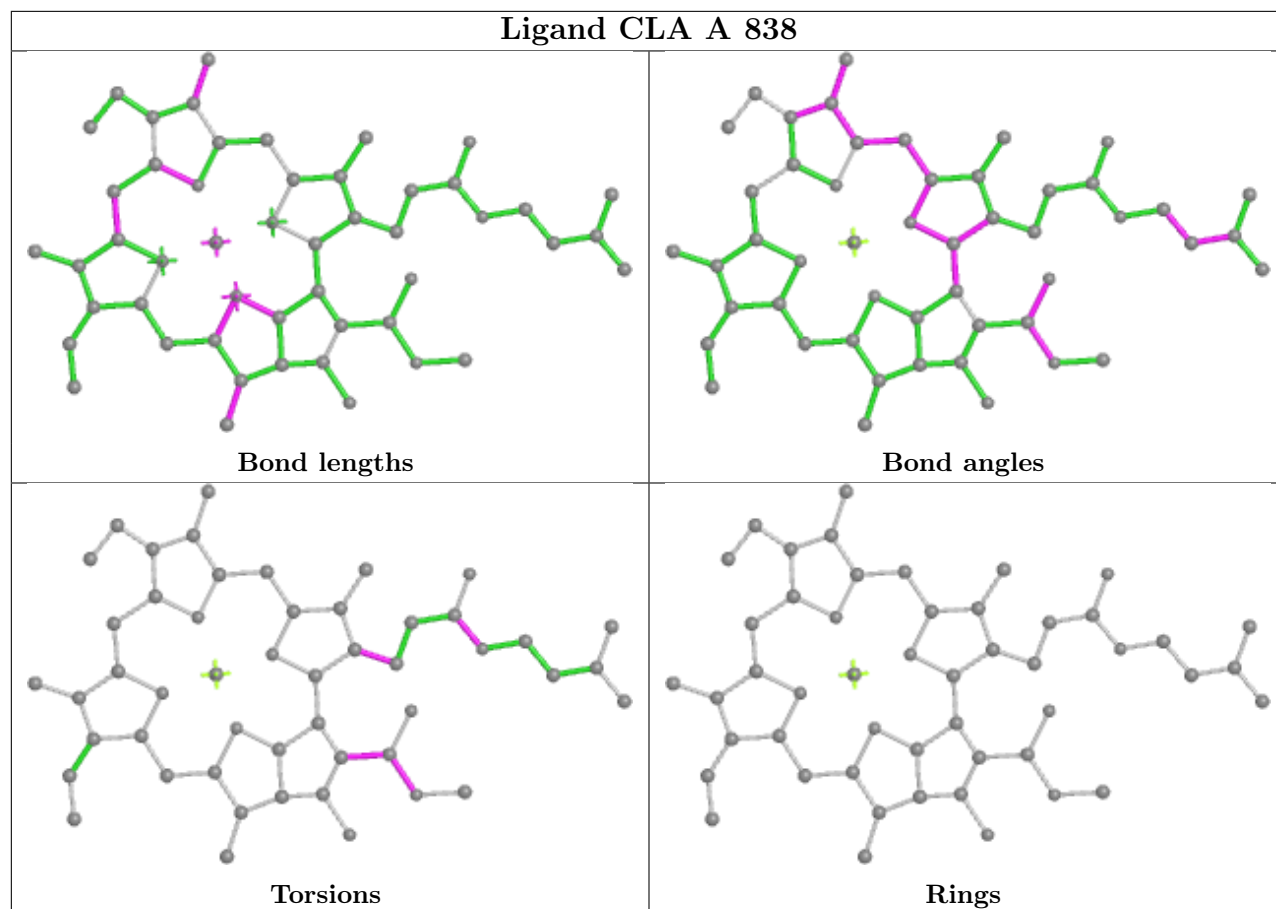


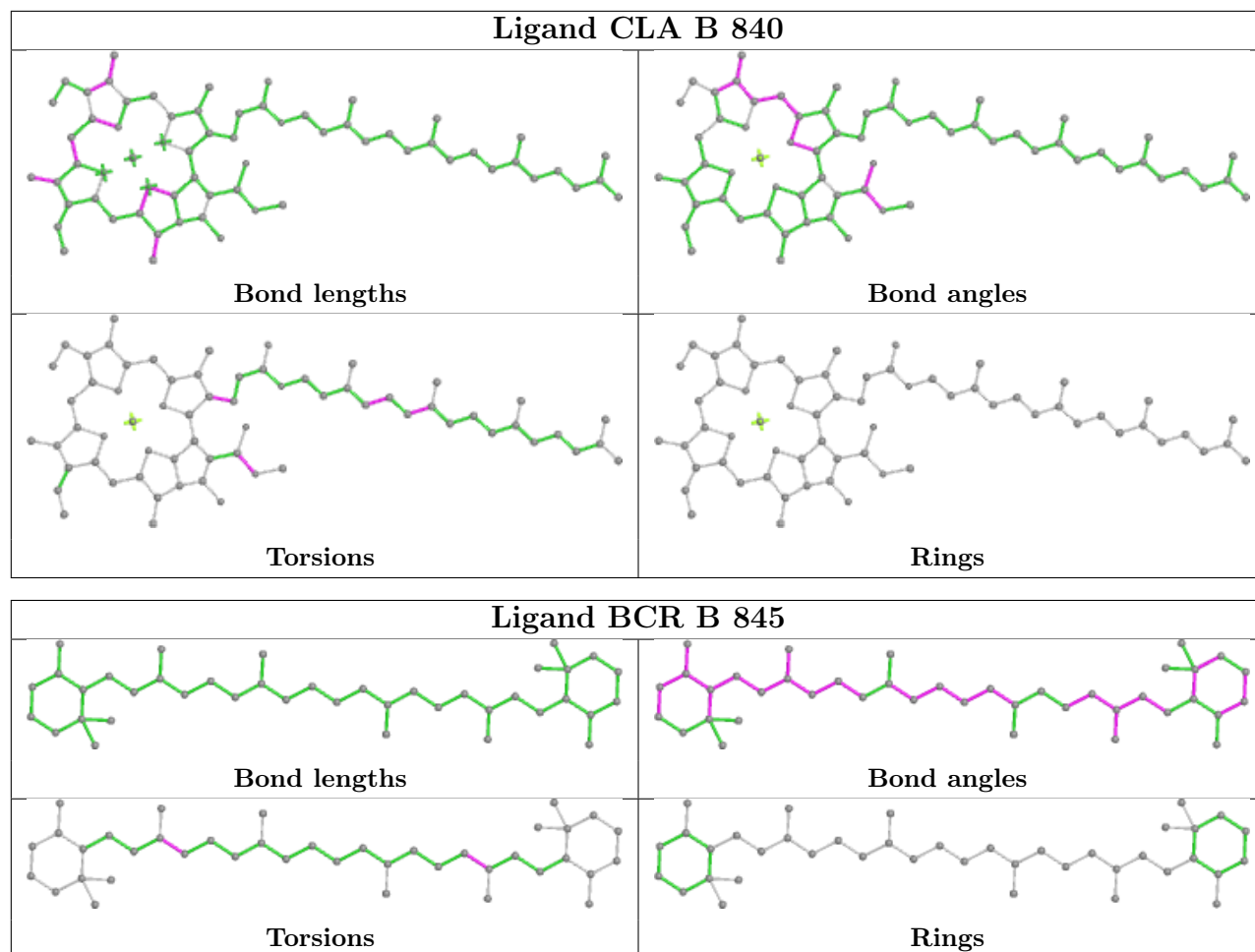
## Ligand CLA 7 612

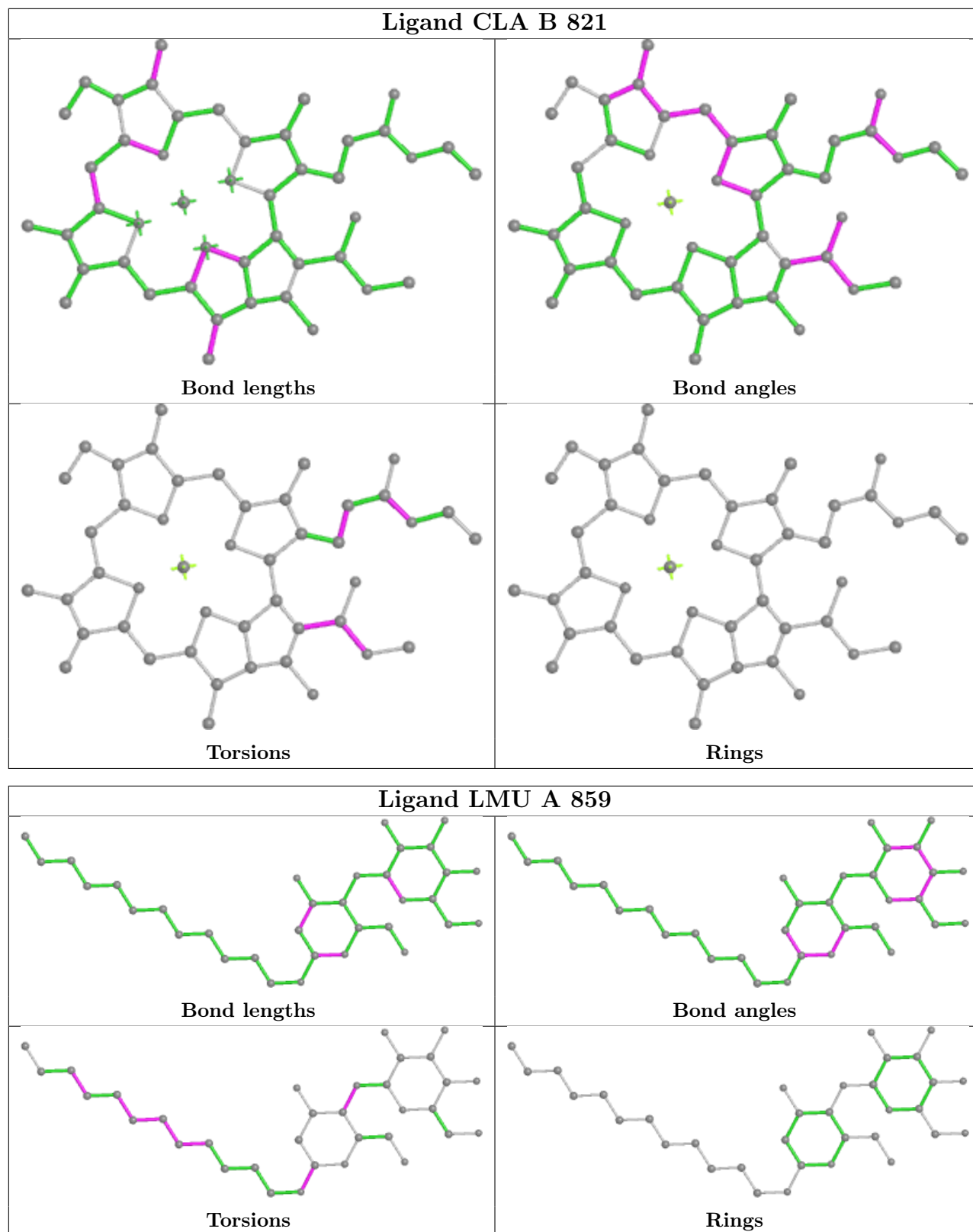


## Ligand CLA B 803

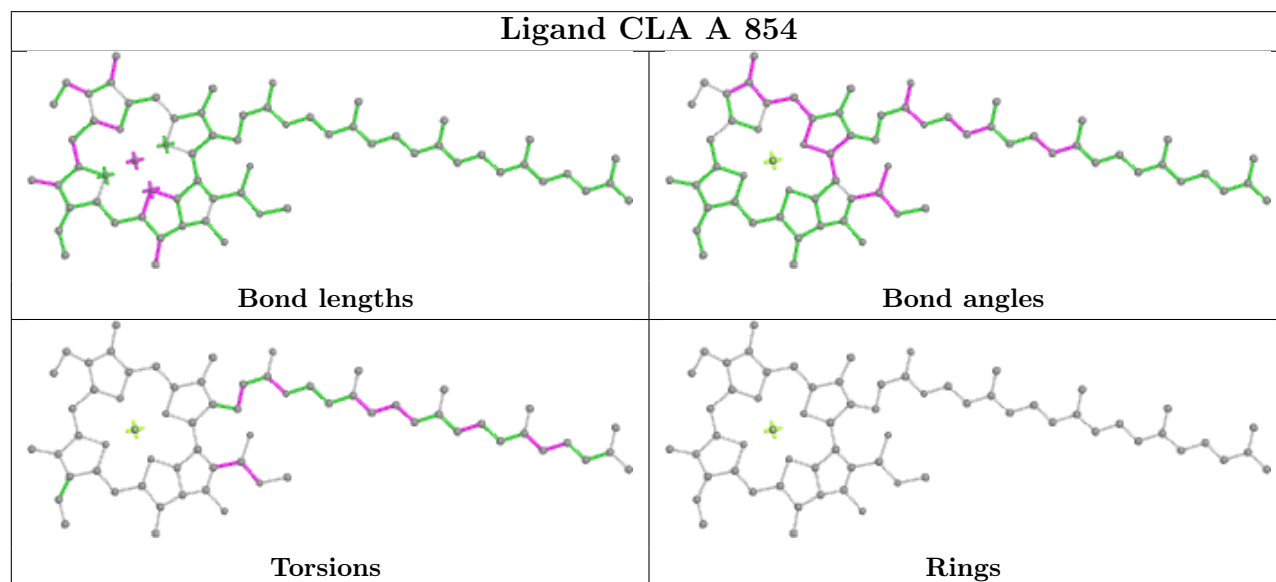
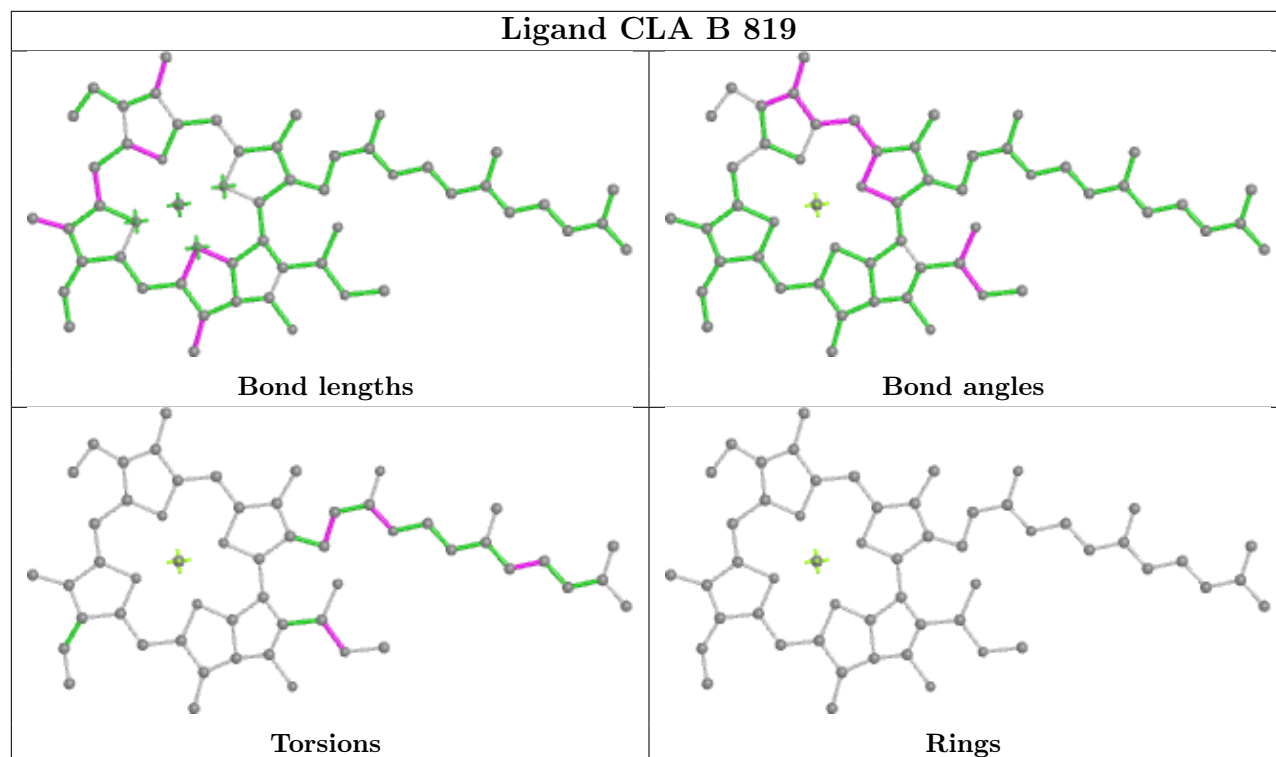


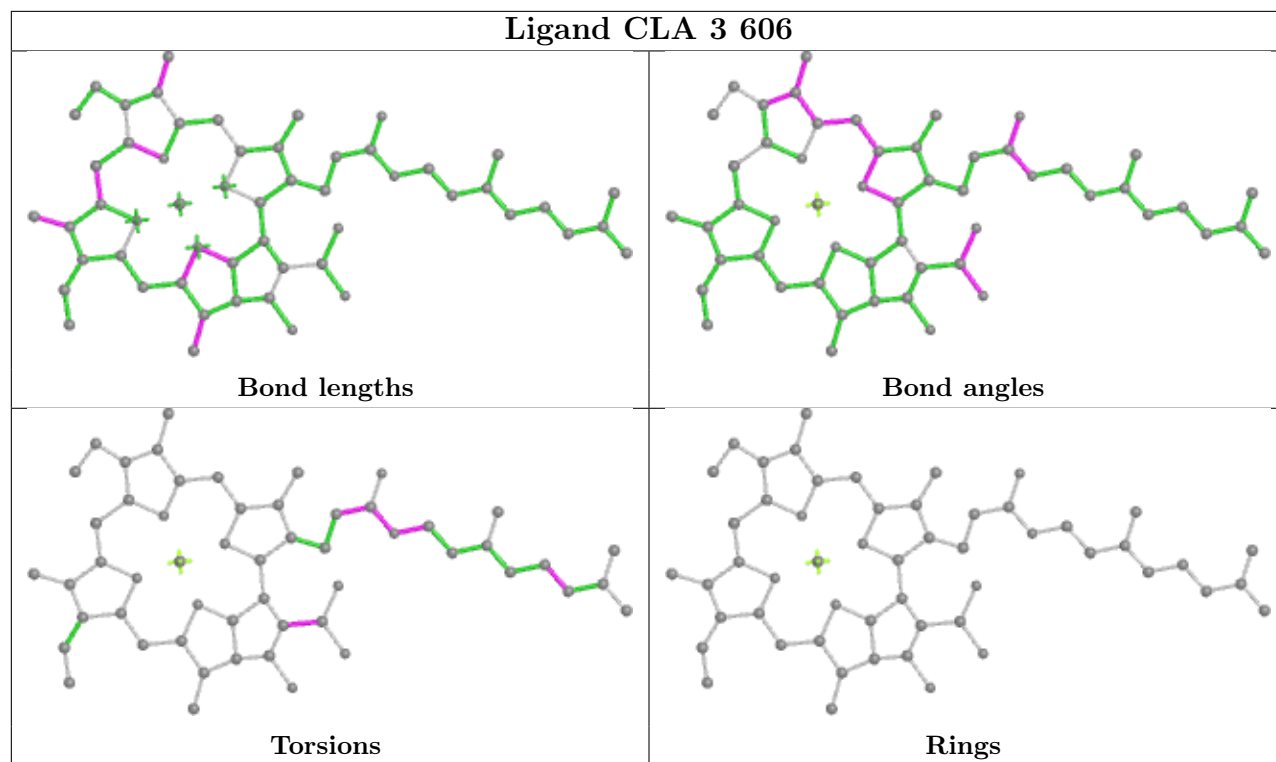


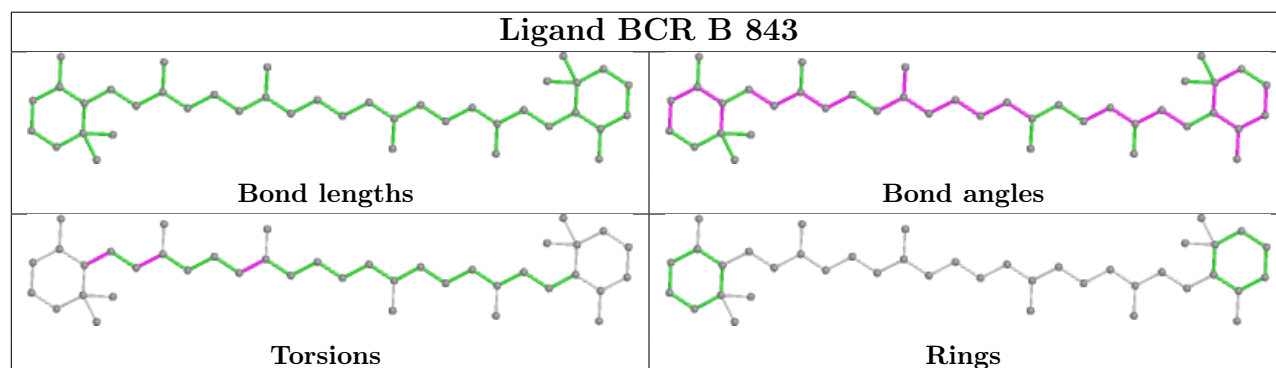
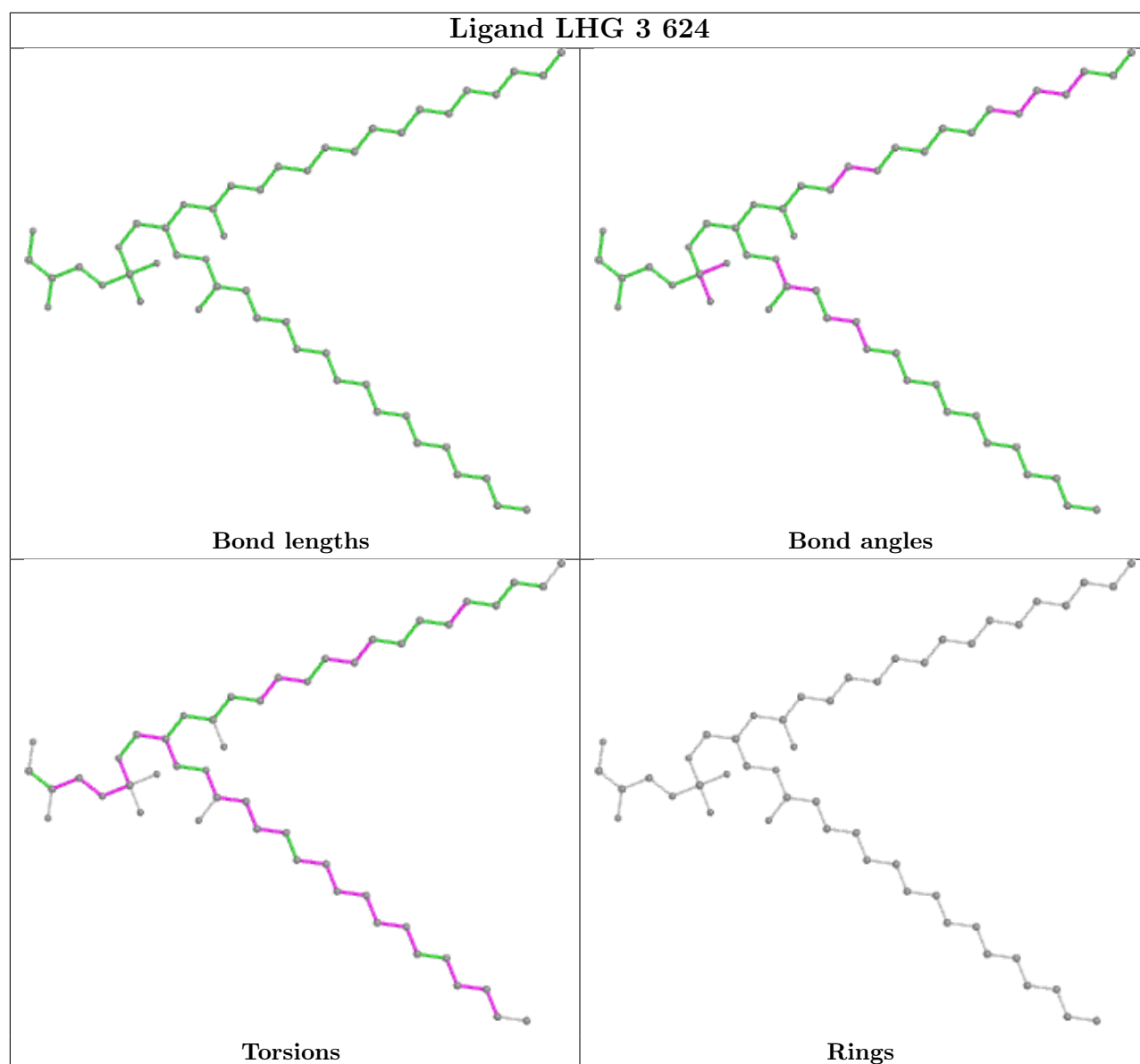


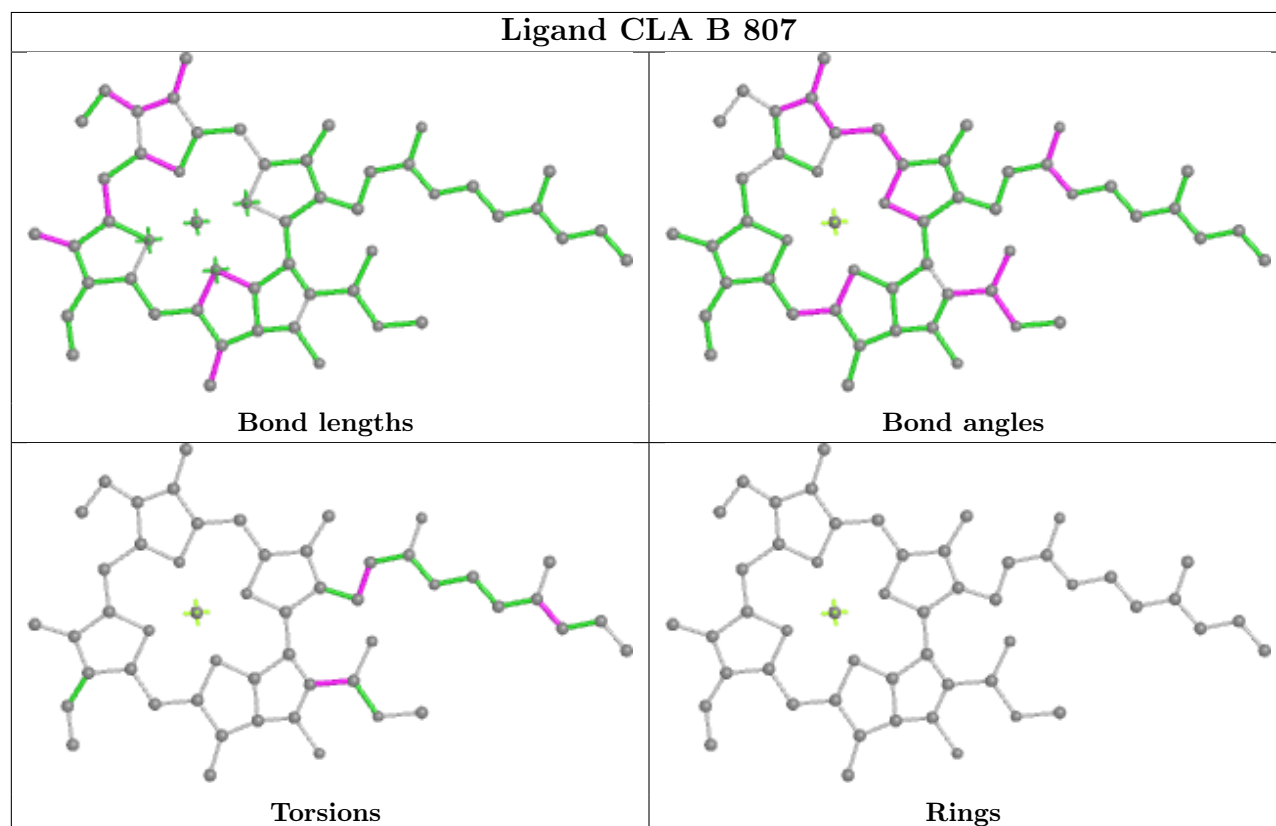
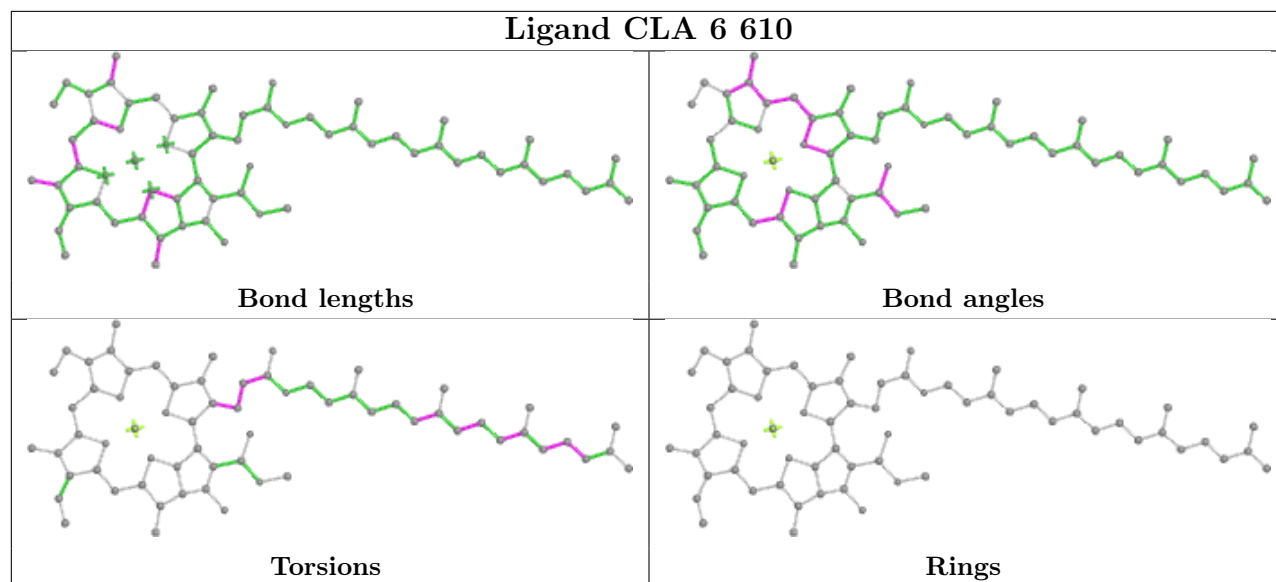


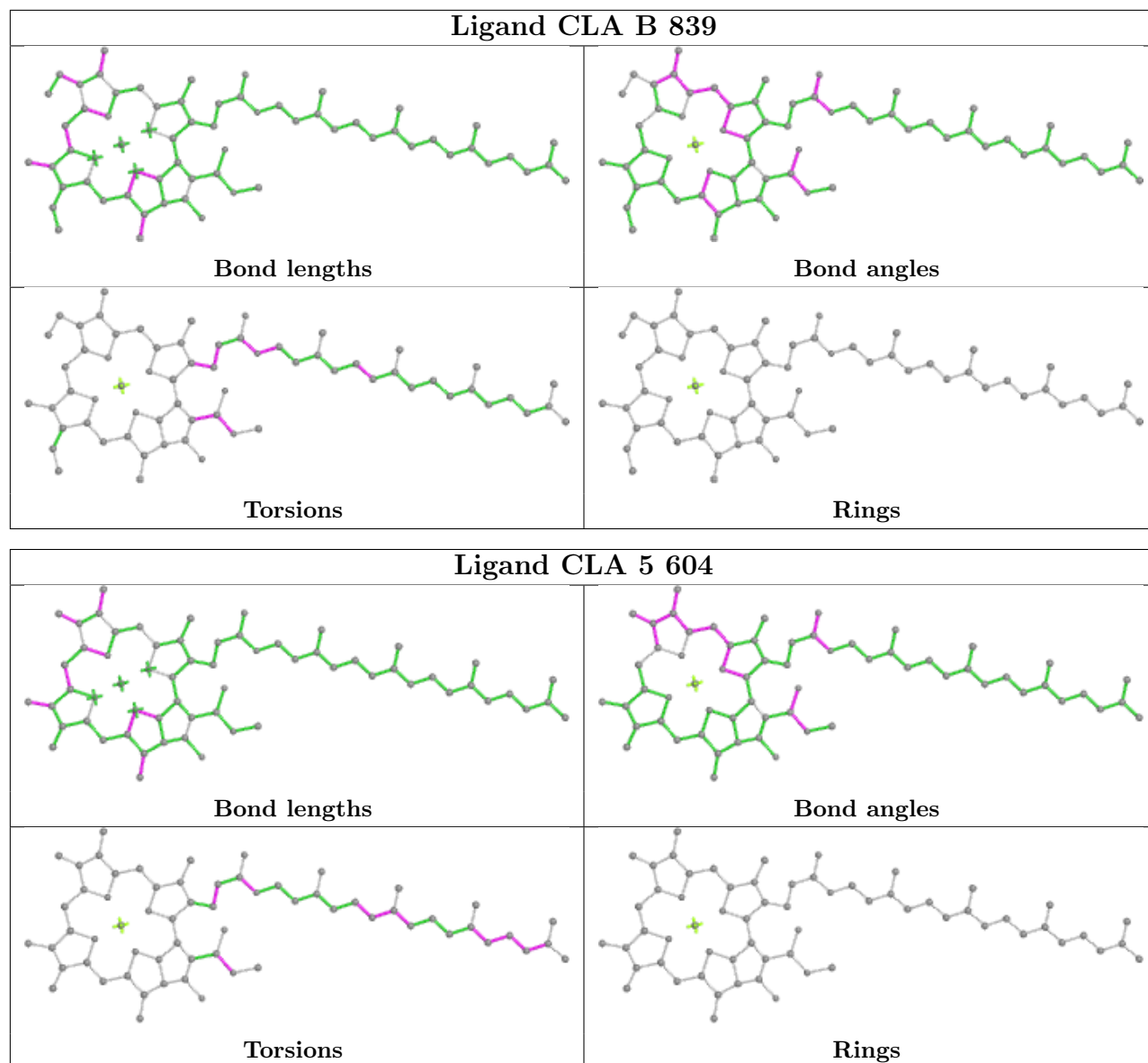


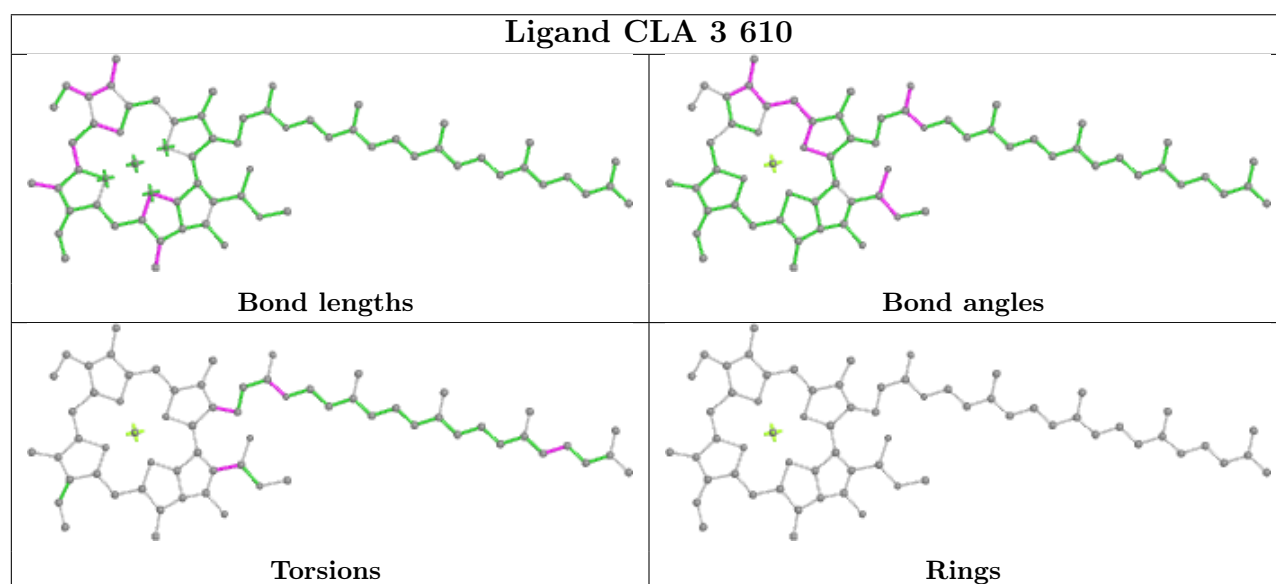
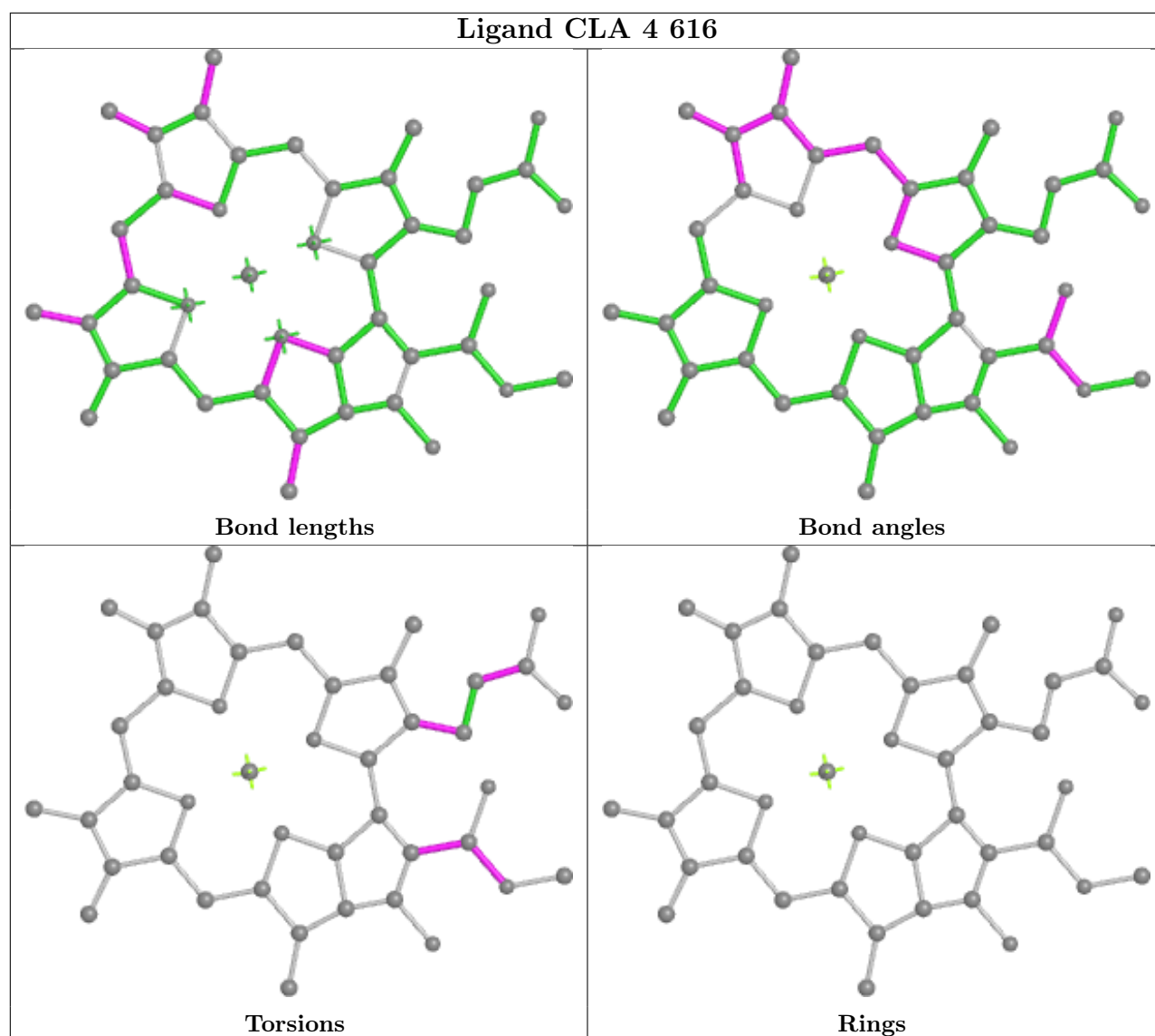


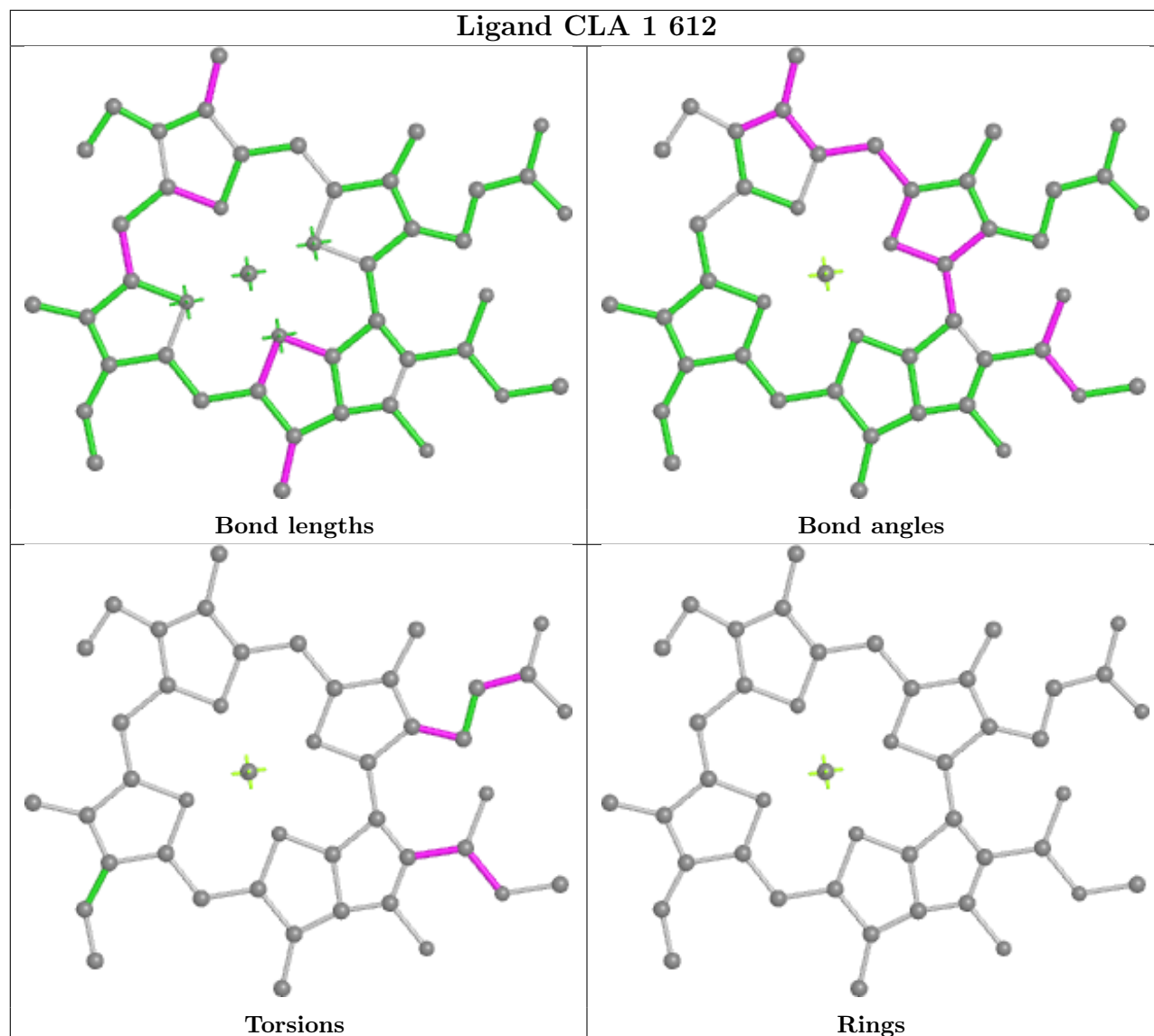


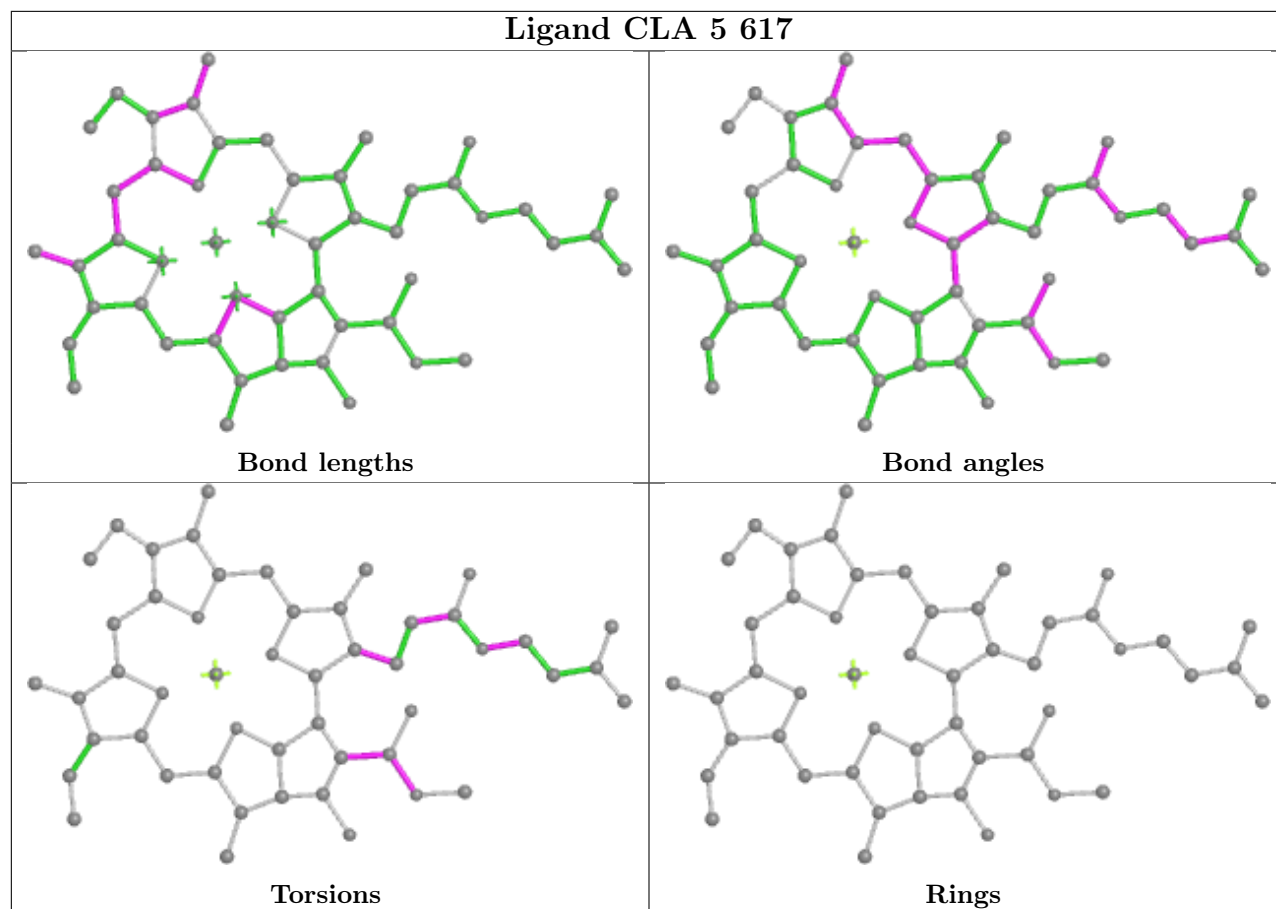




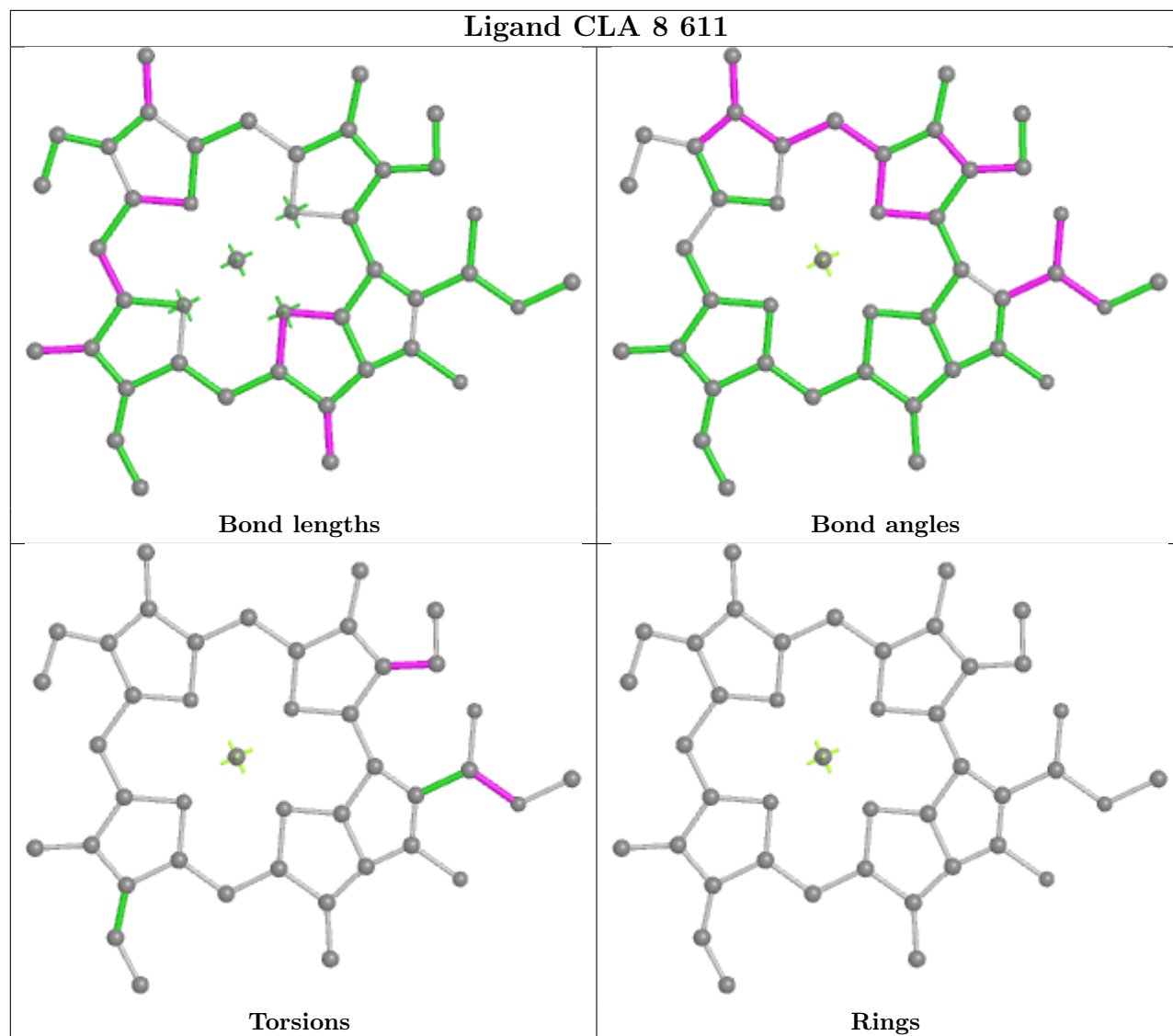


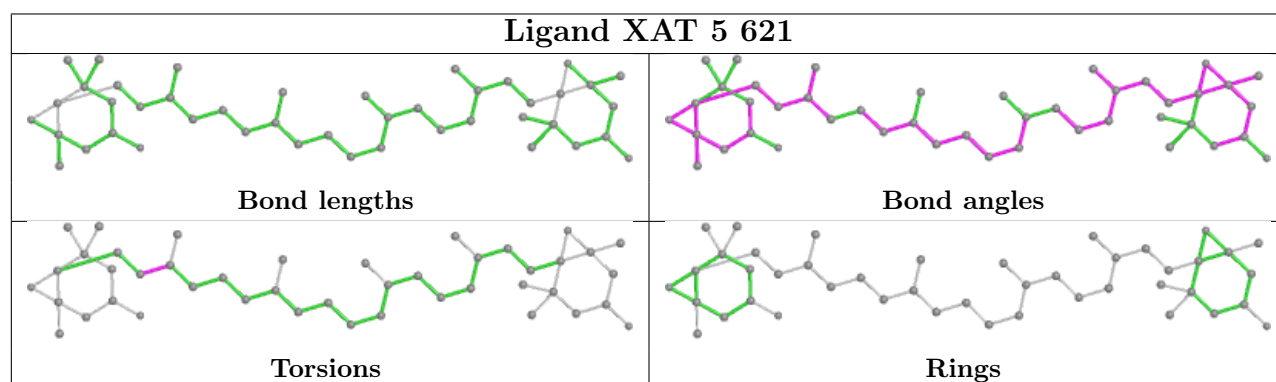
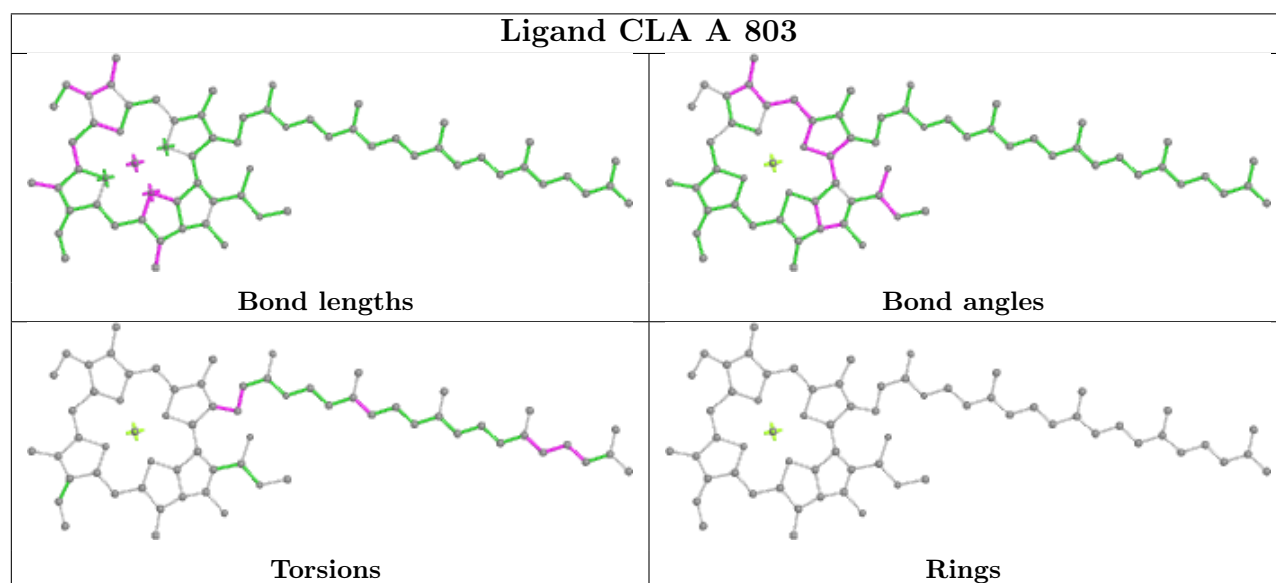
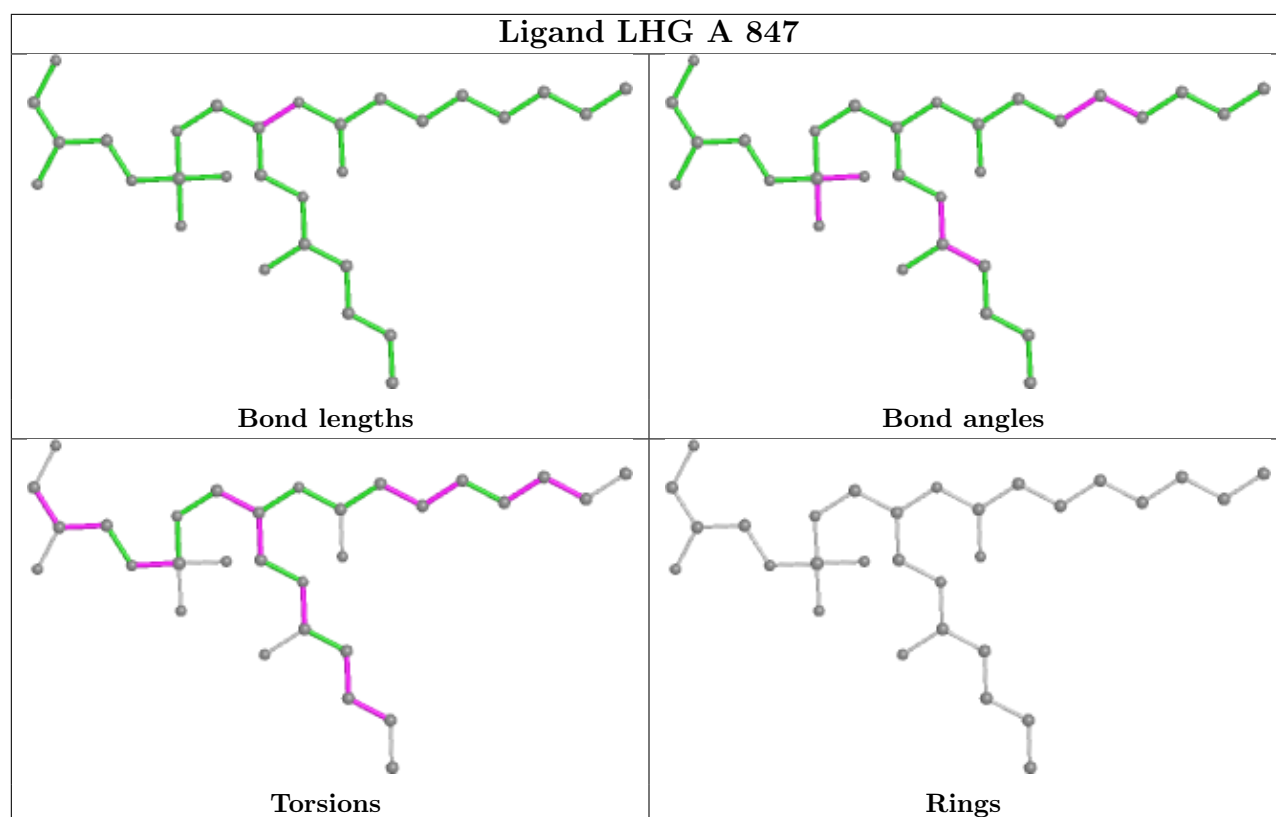


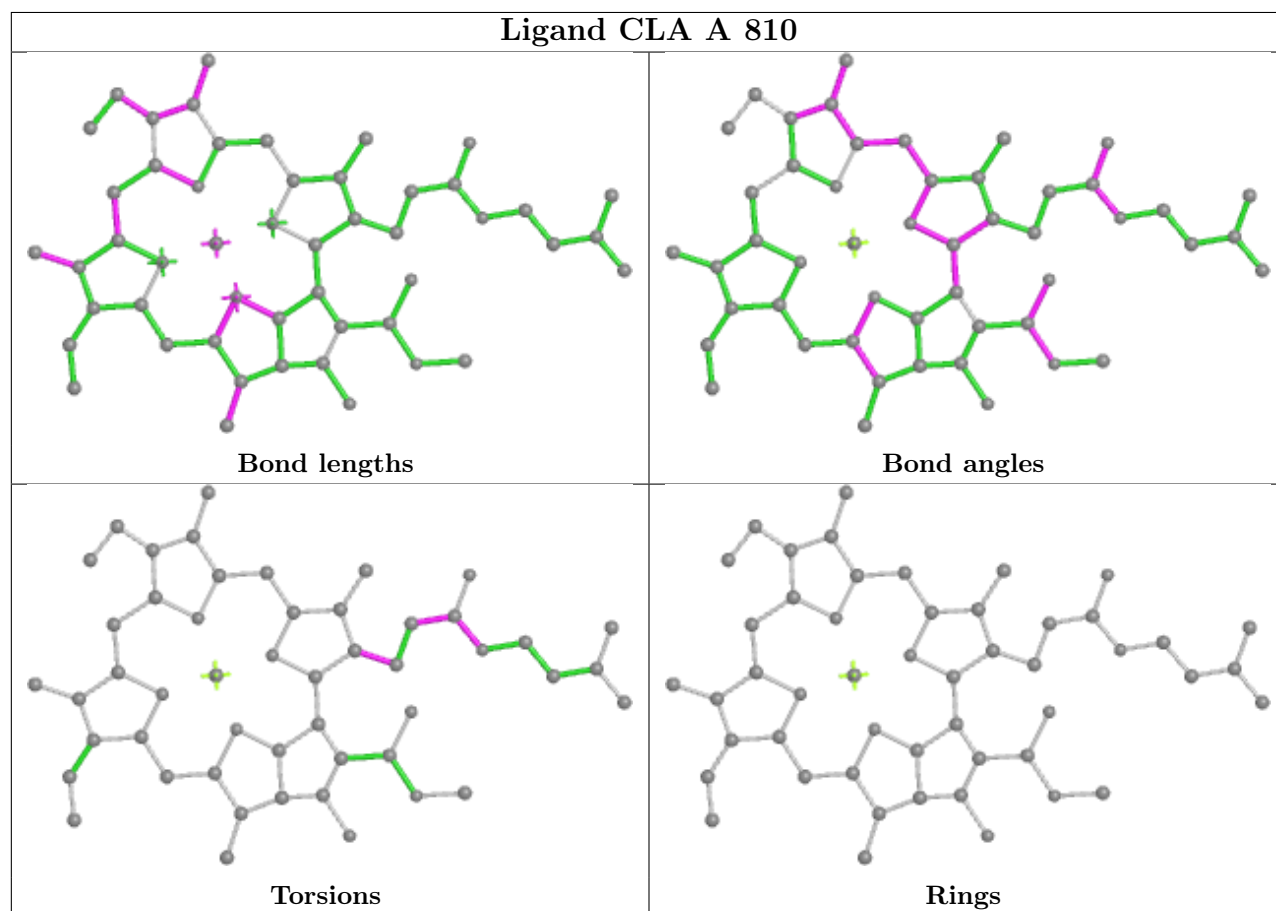
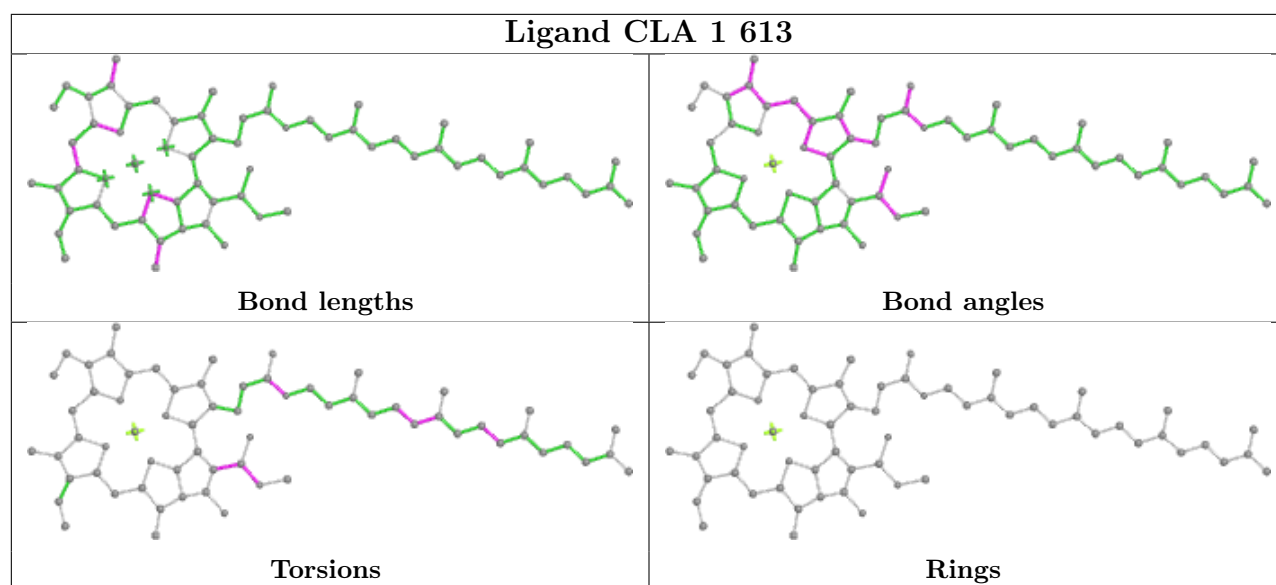


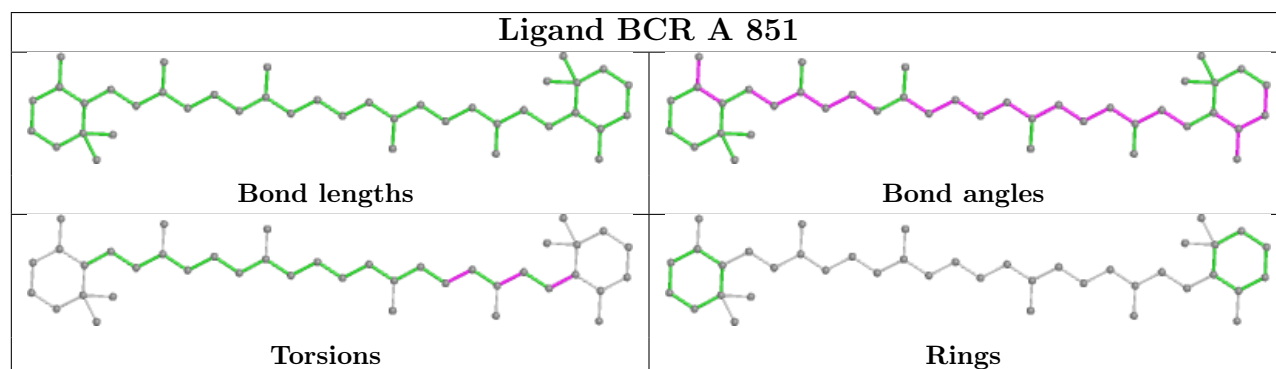
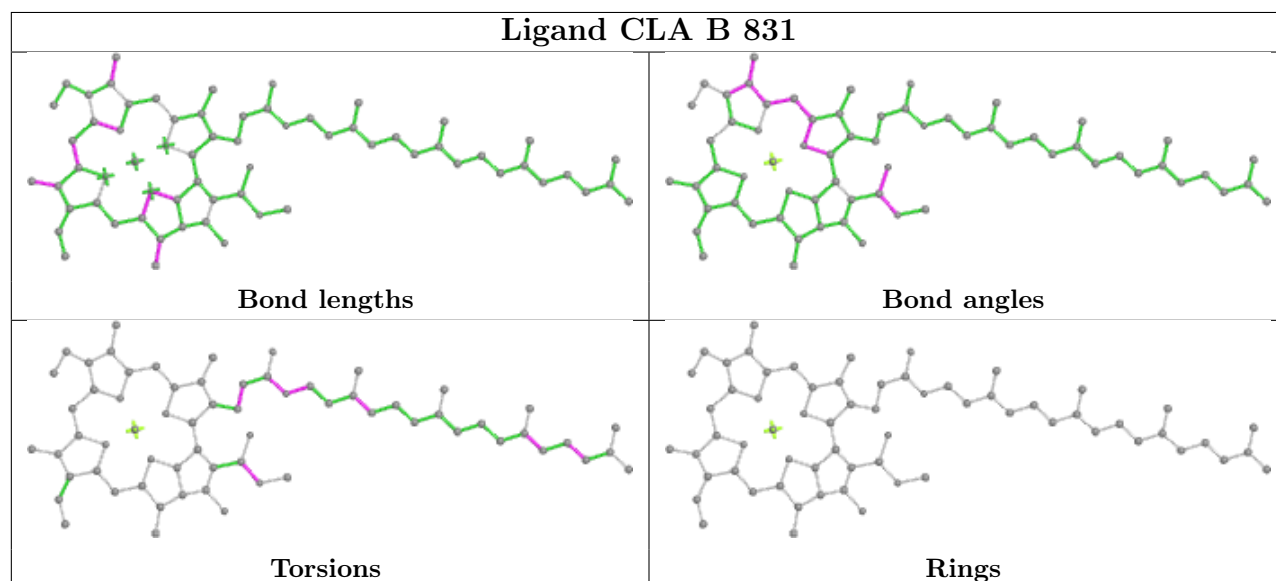
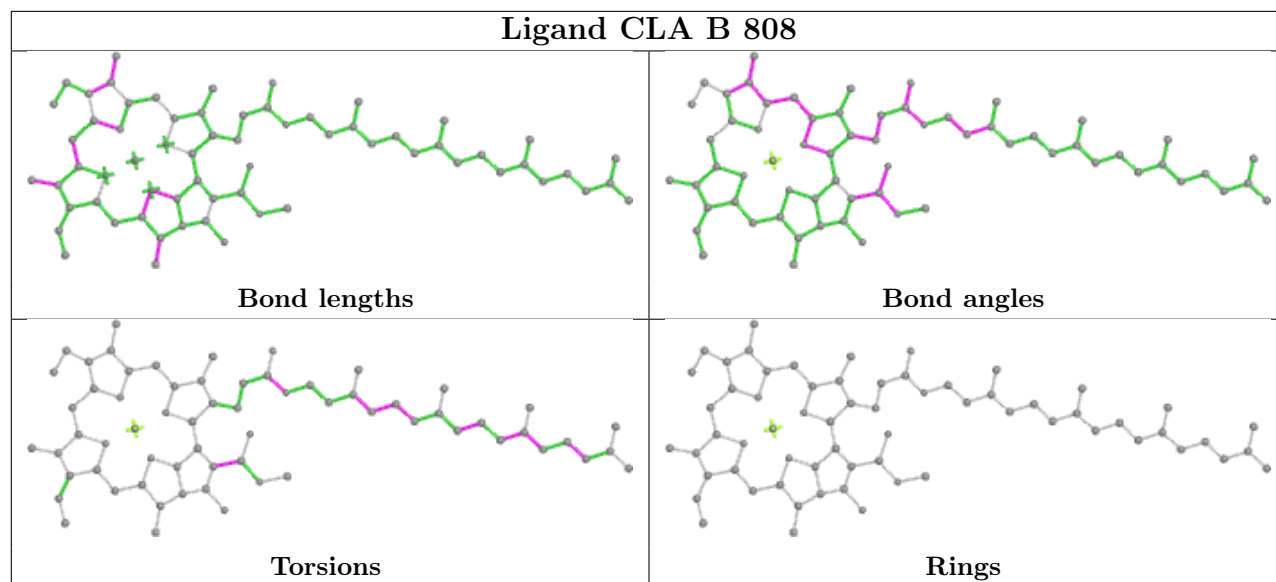


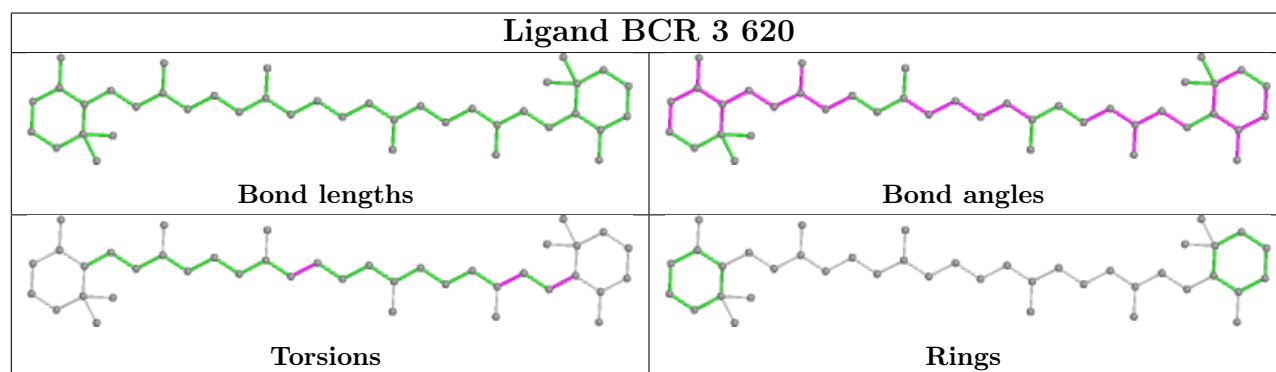
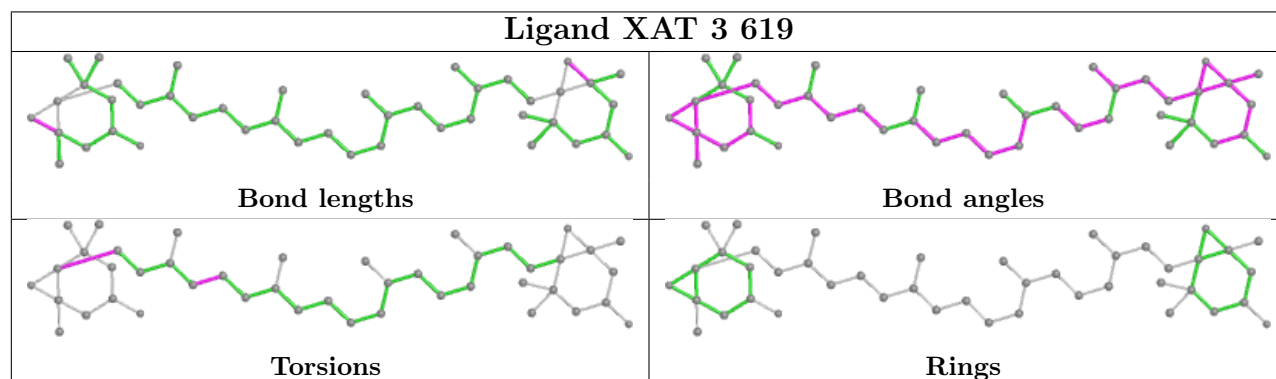
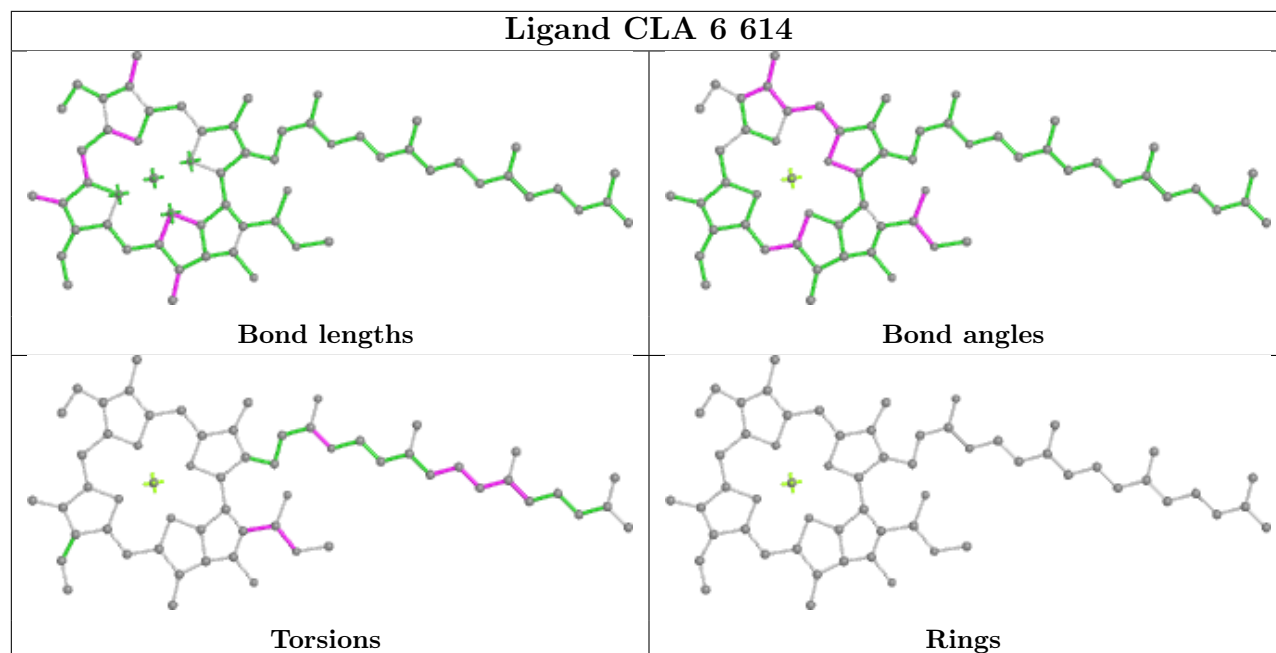


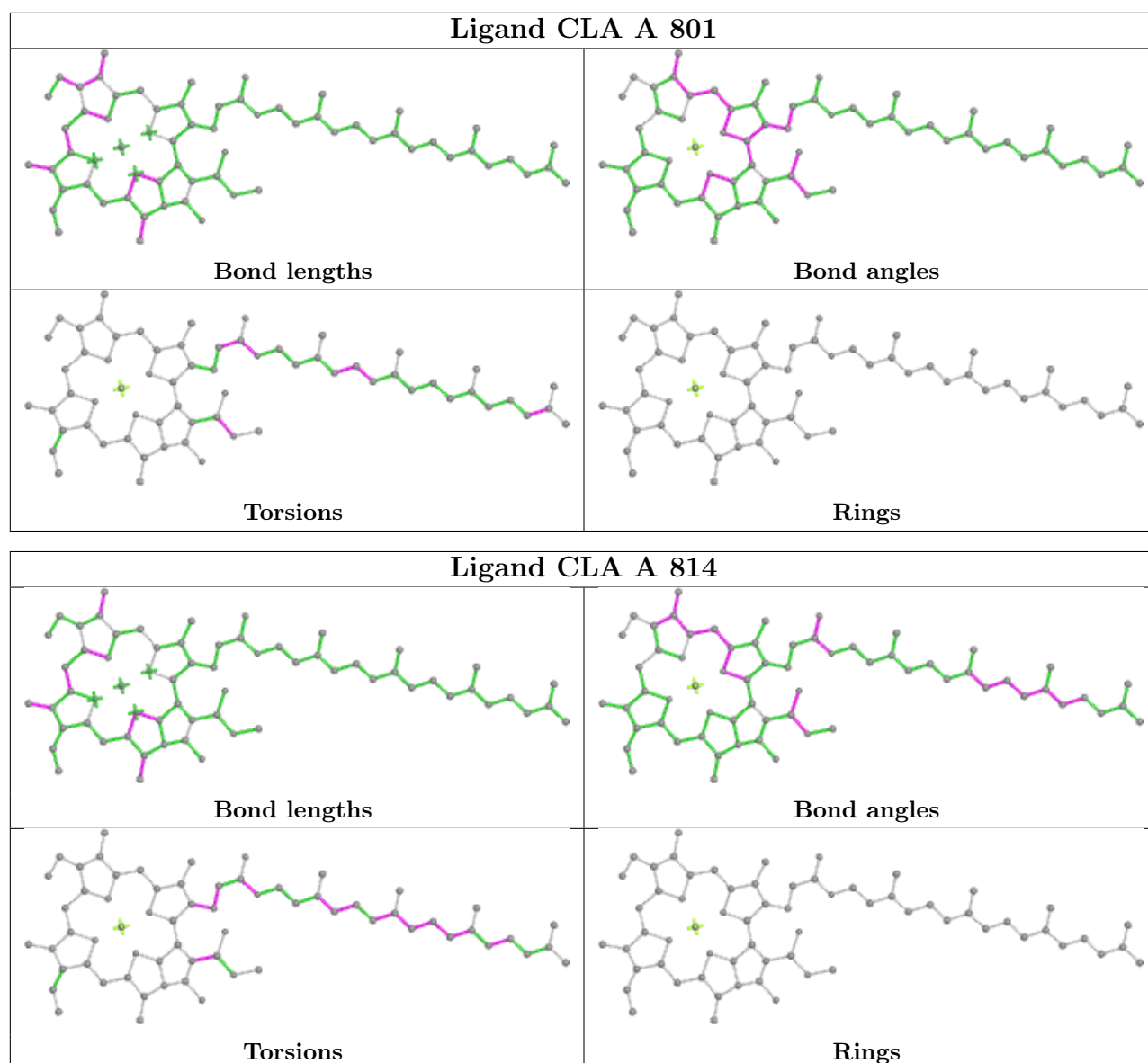


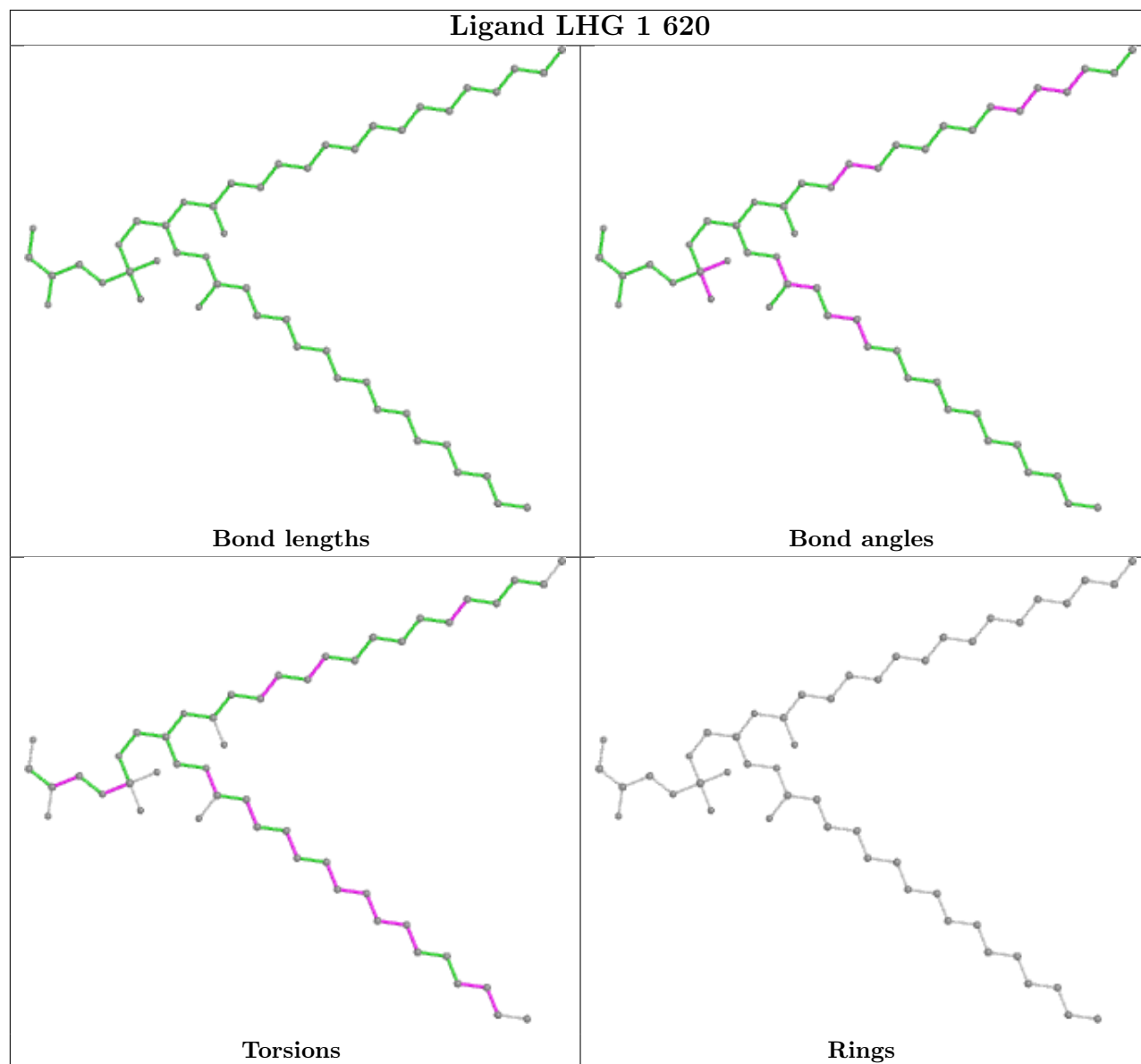


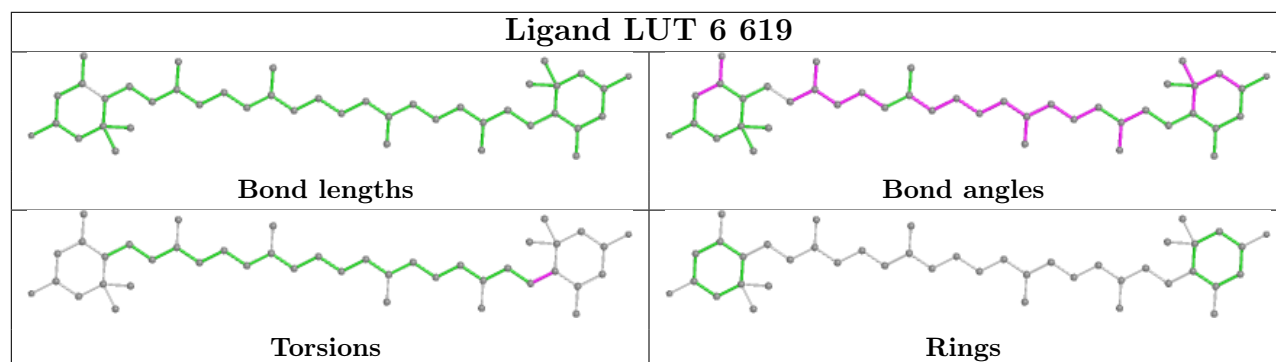
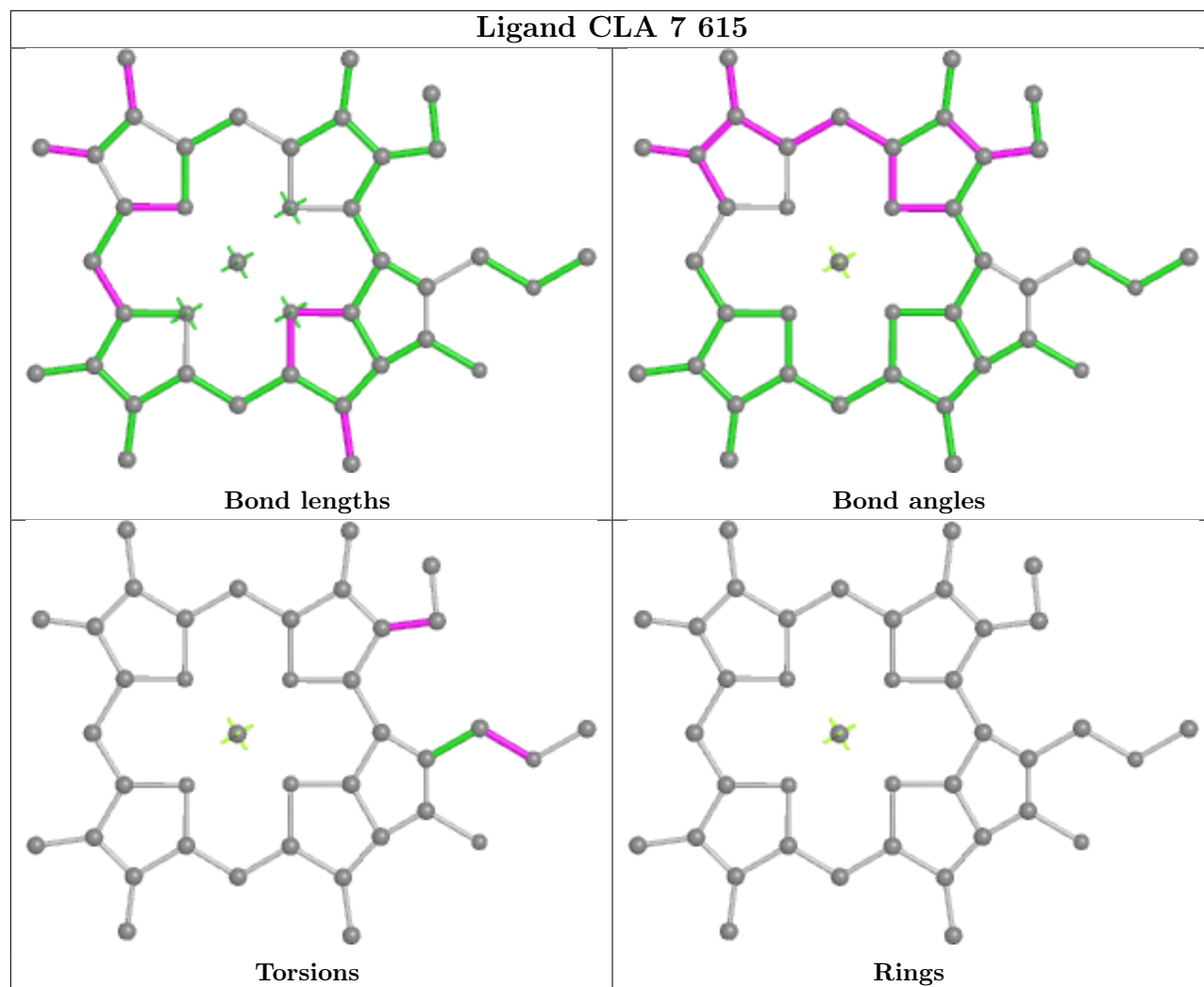




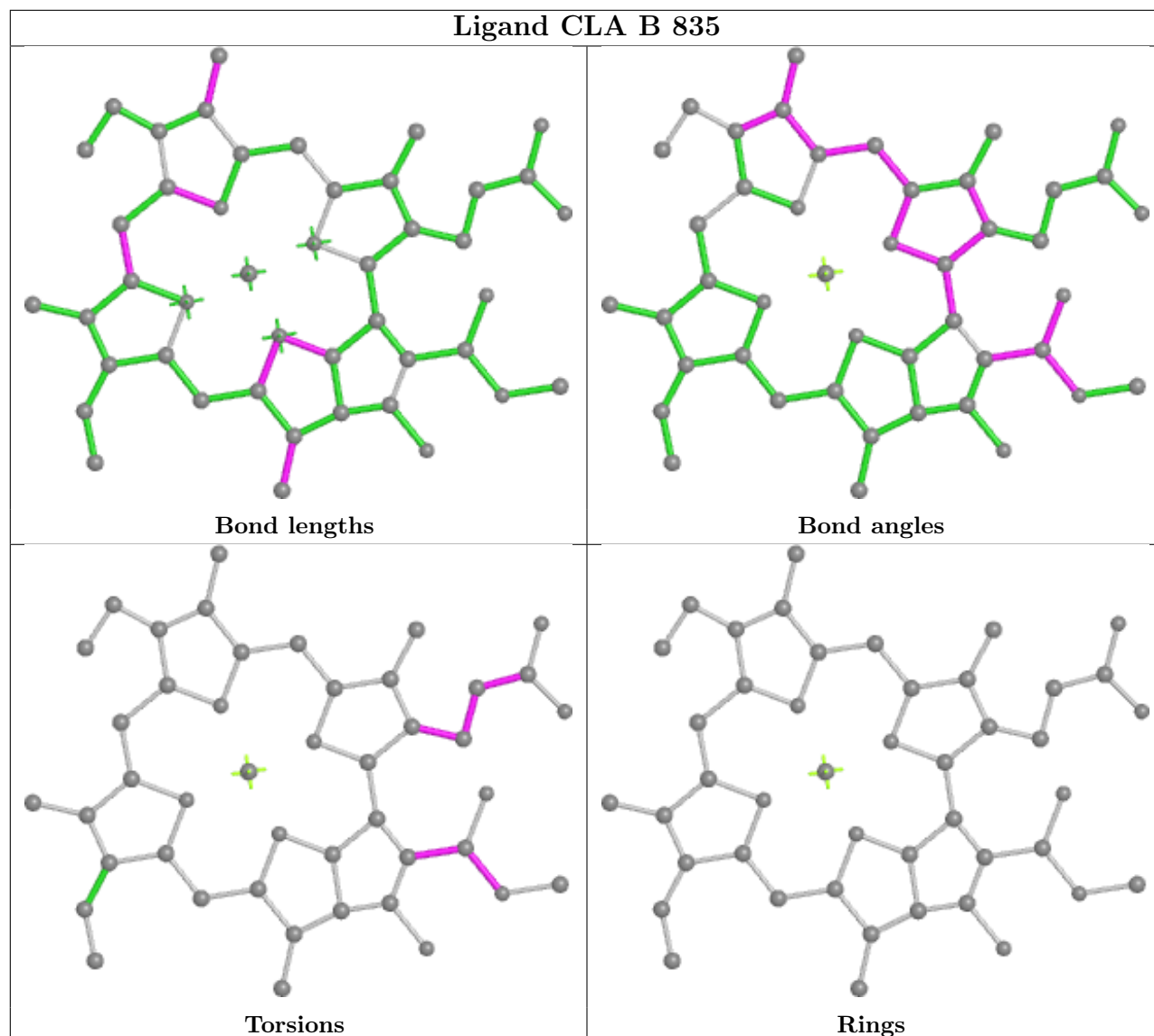


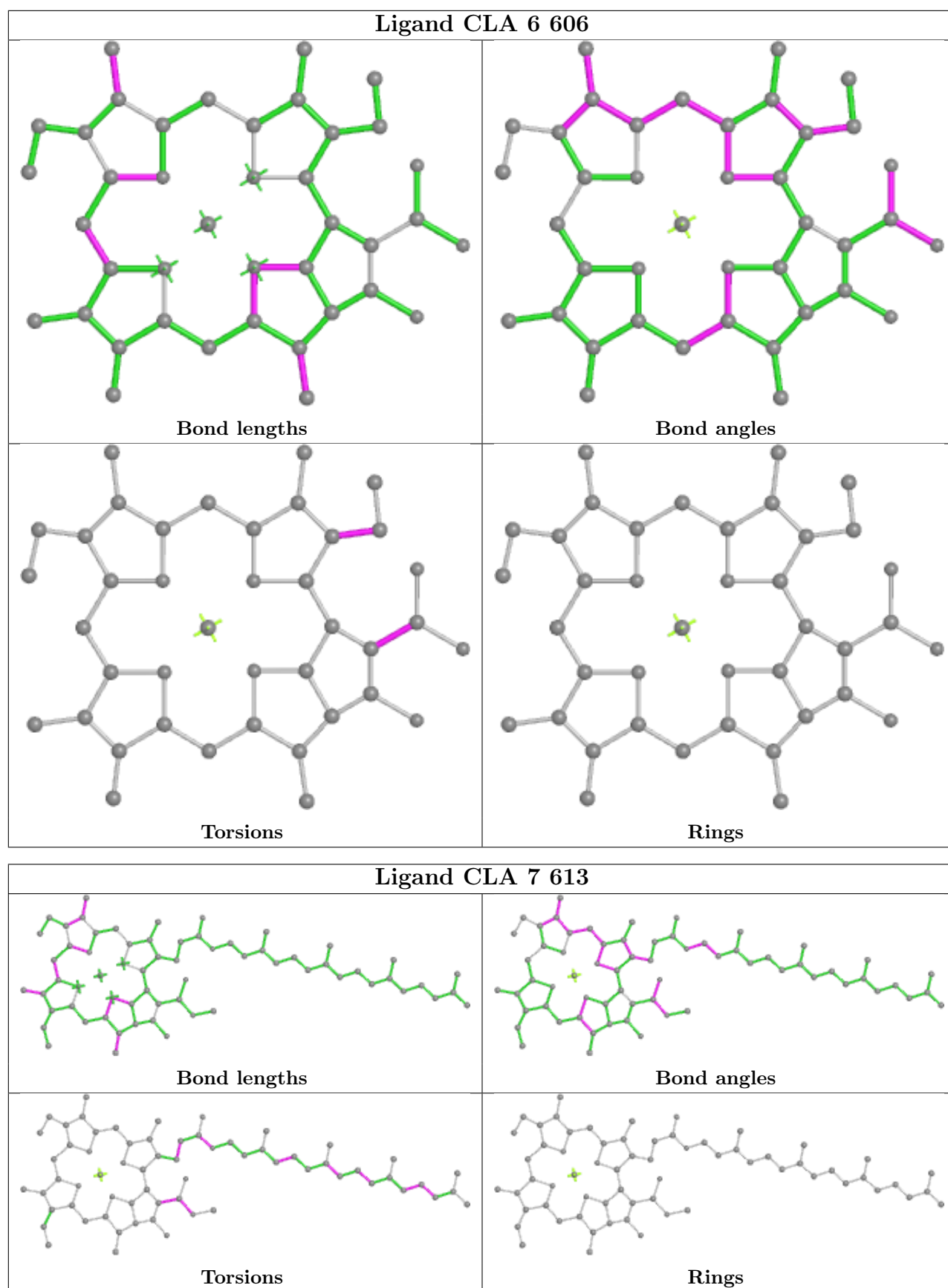


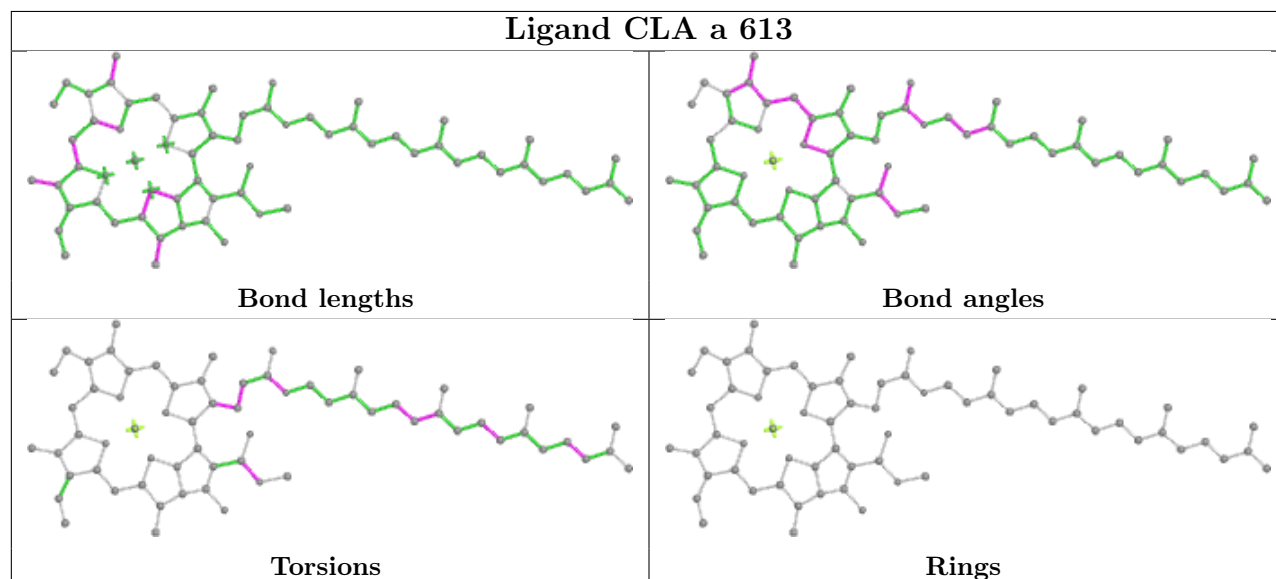
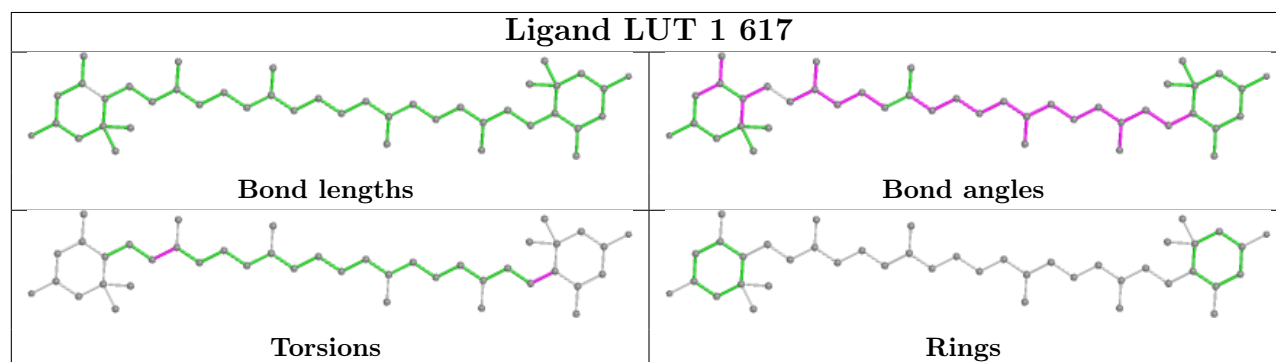
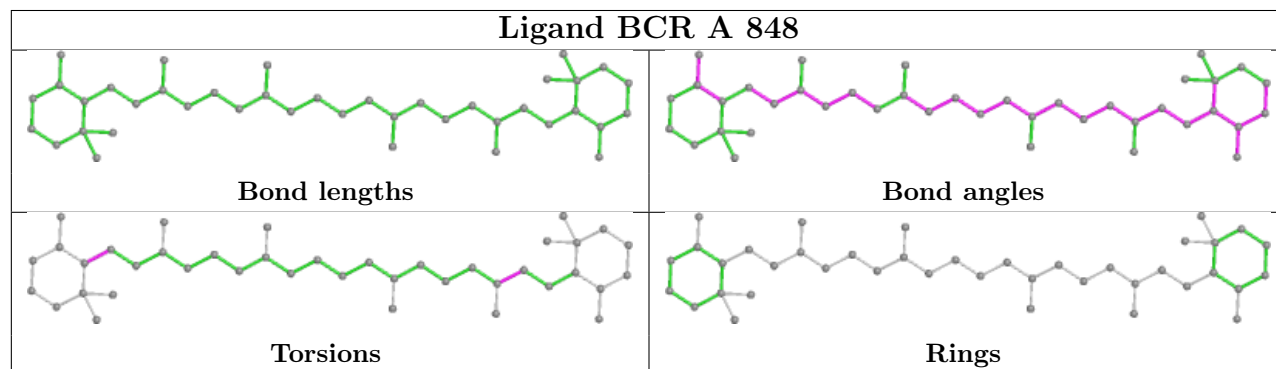
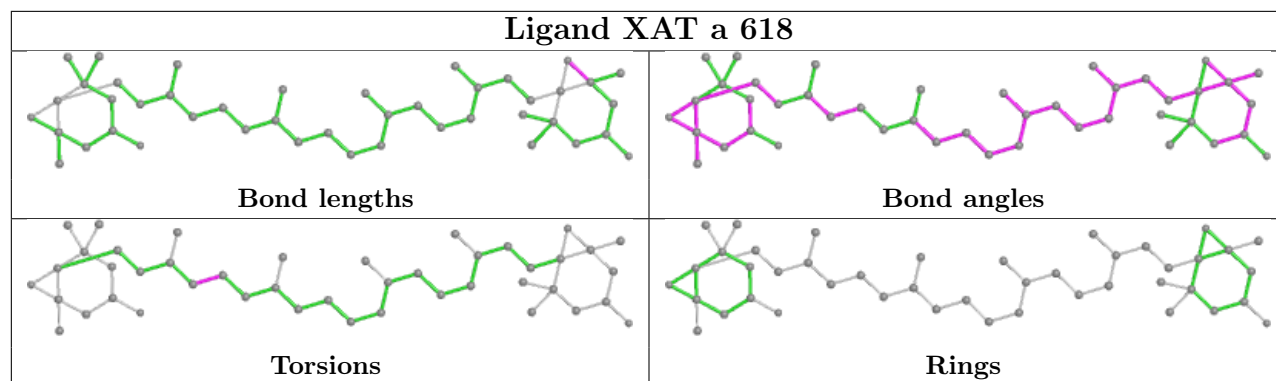


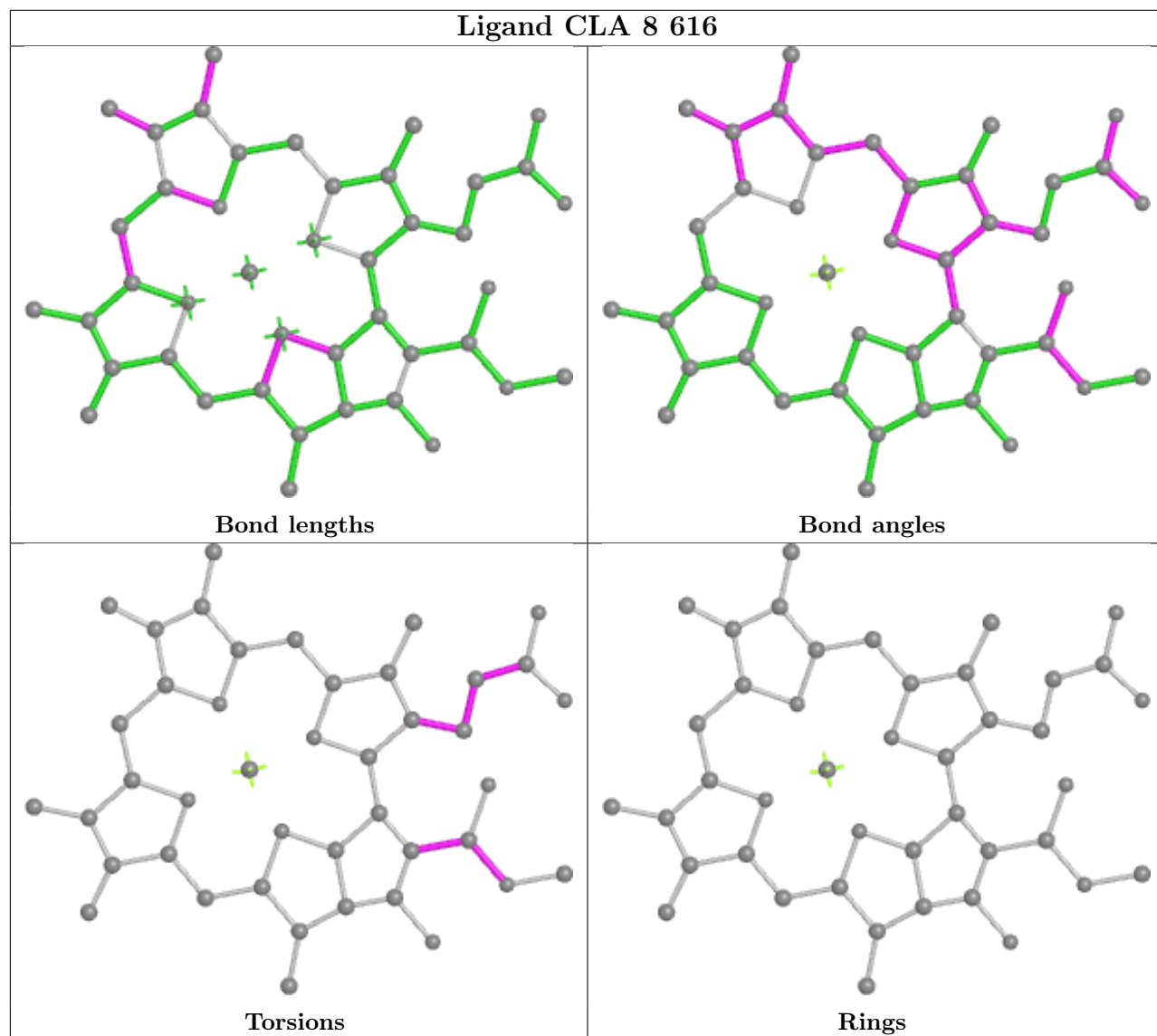


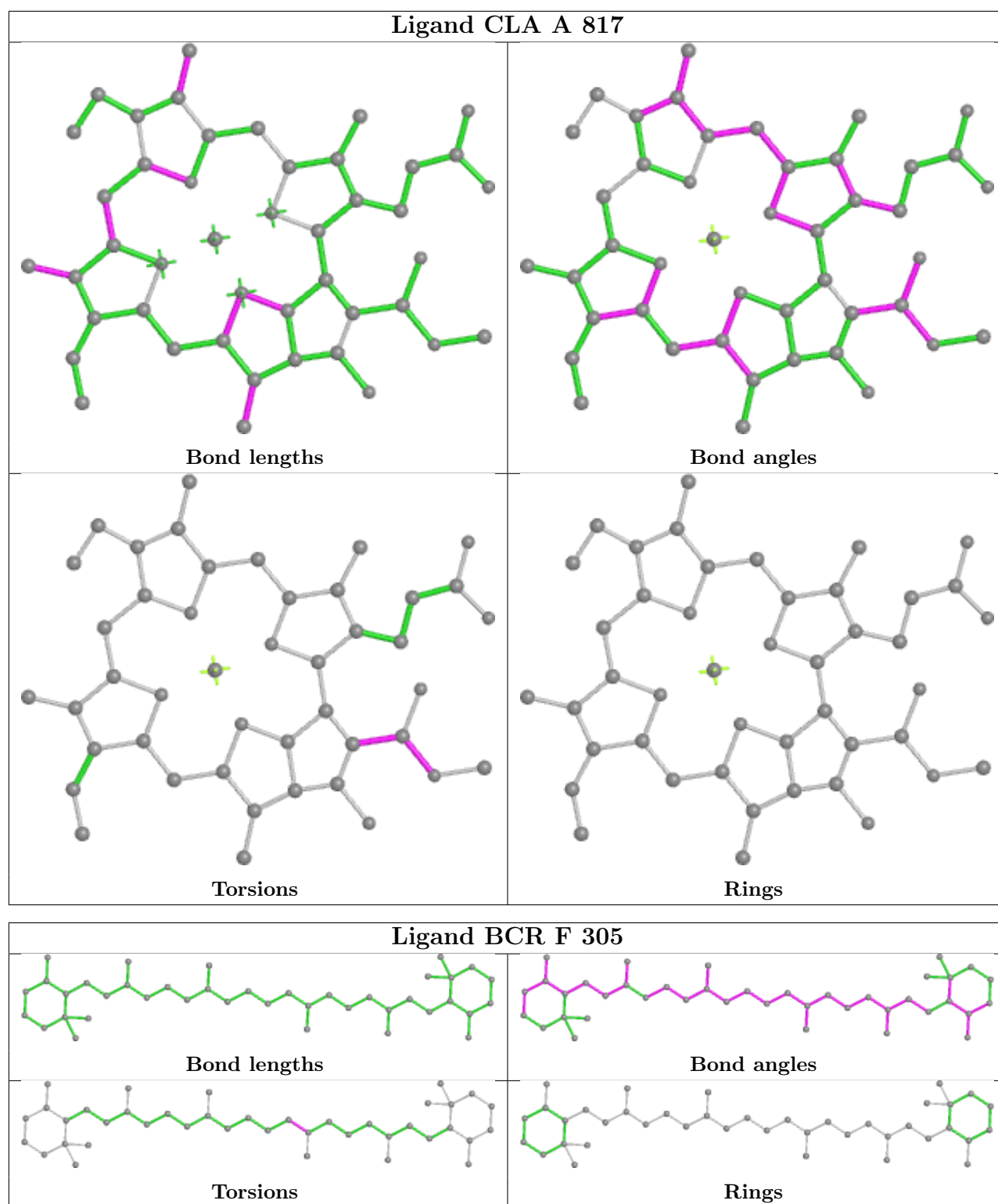


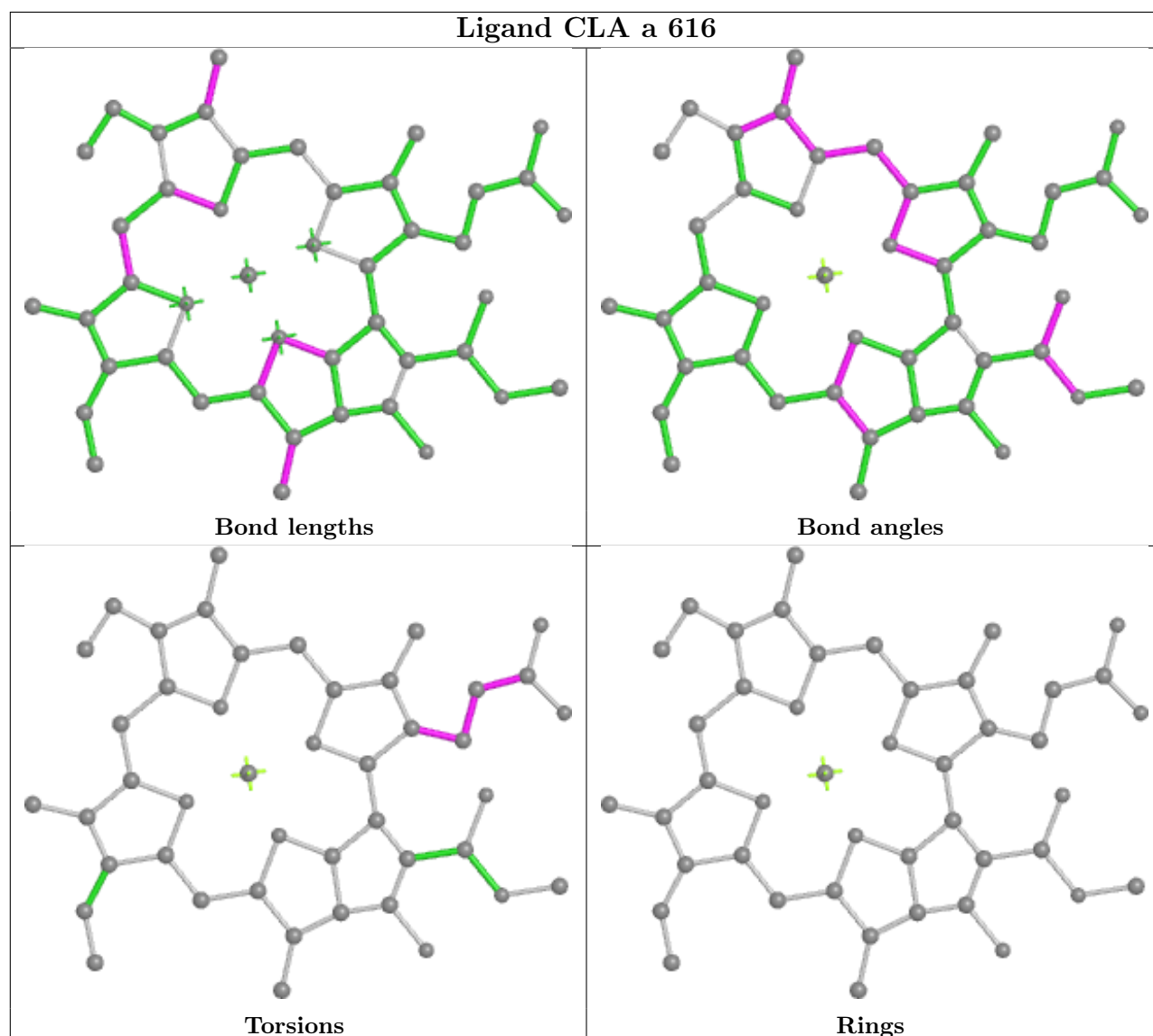
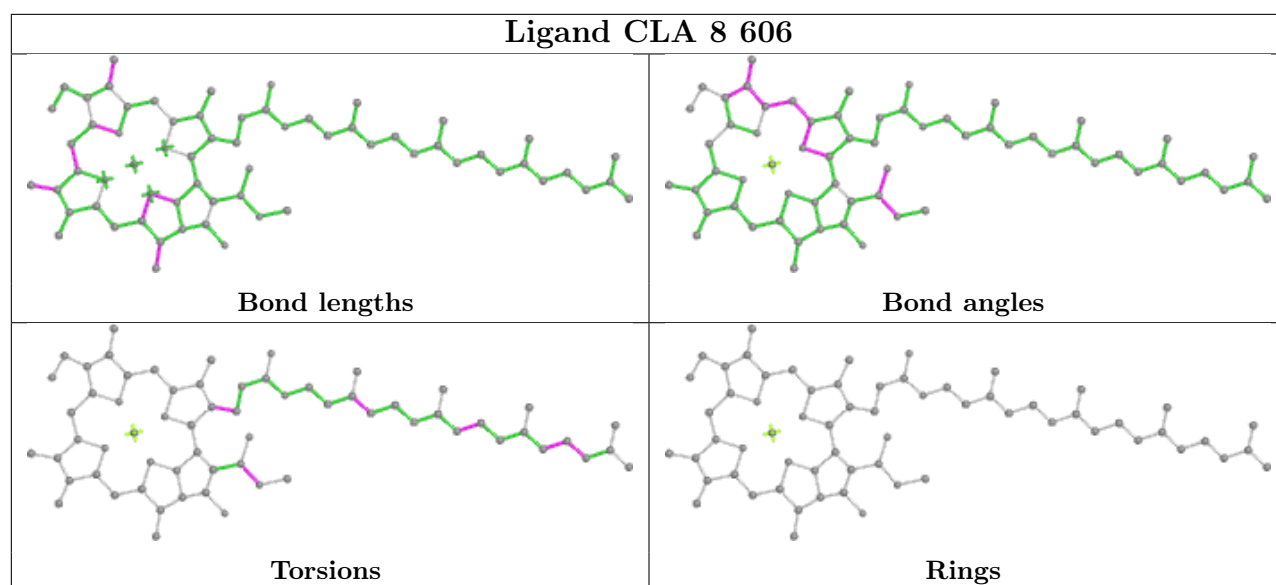


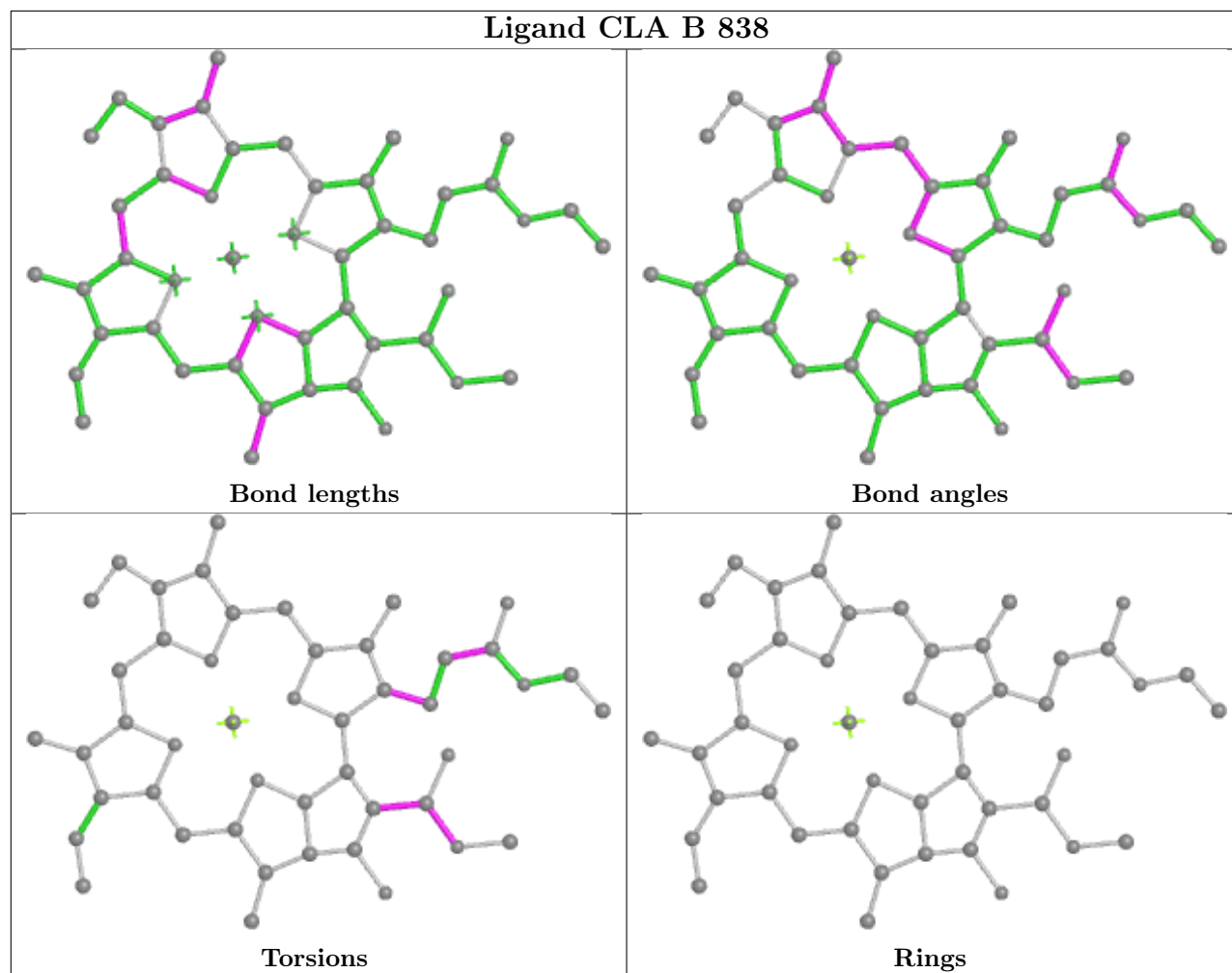


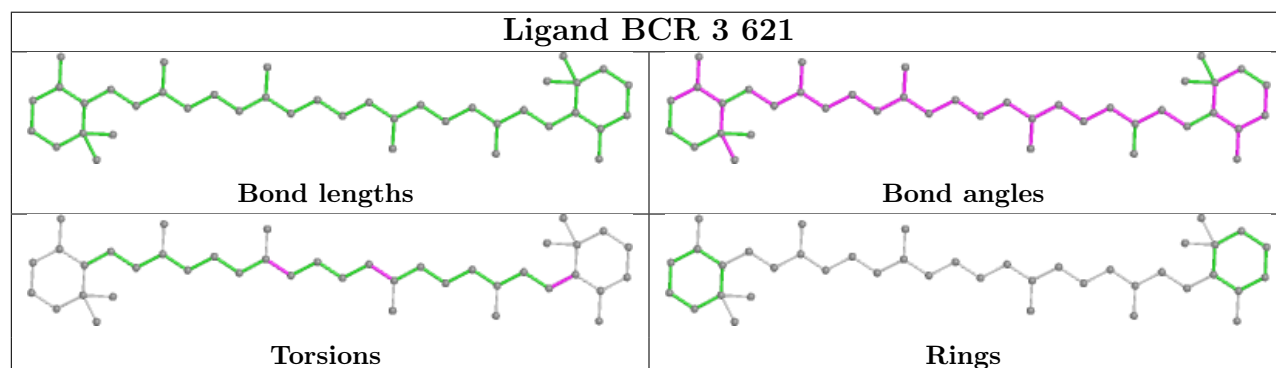
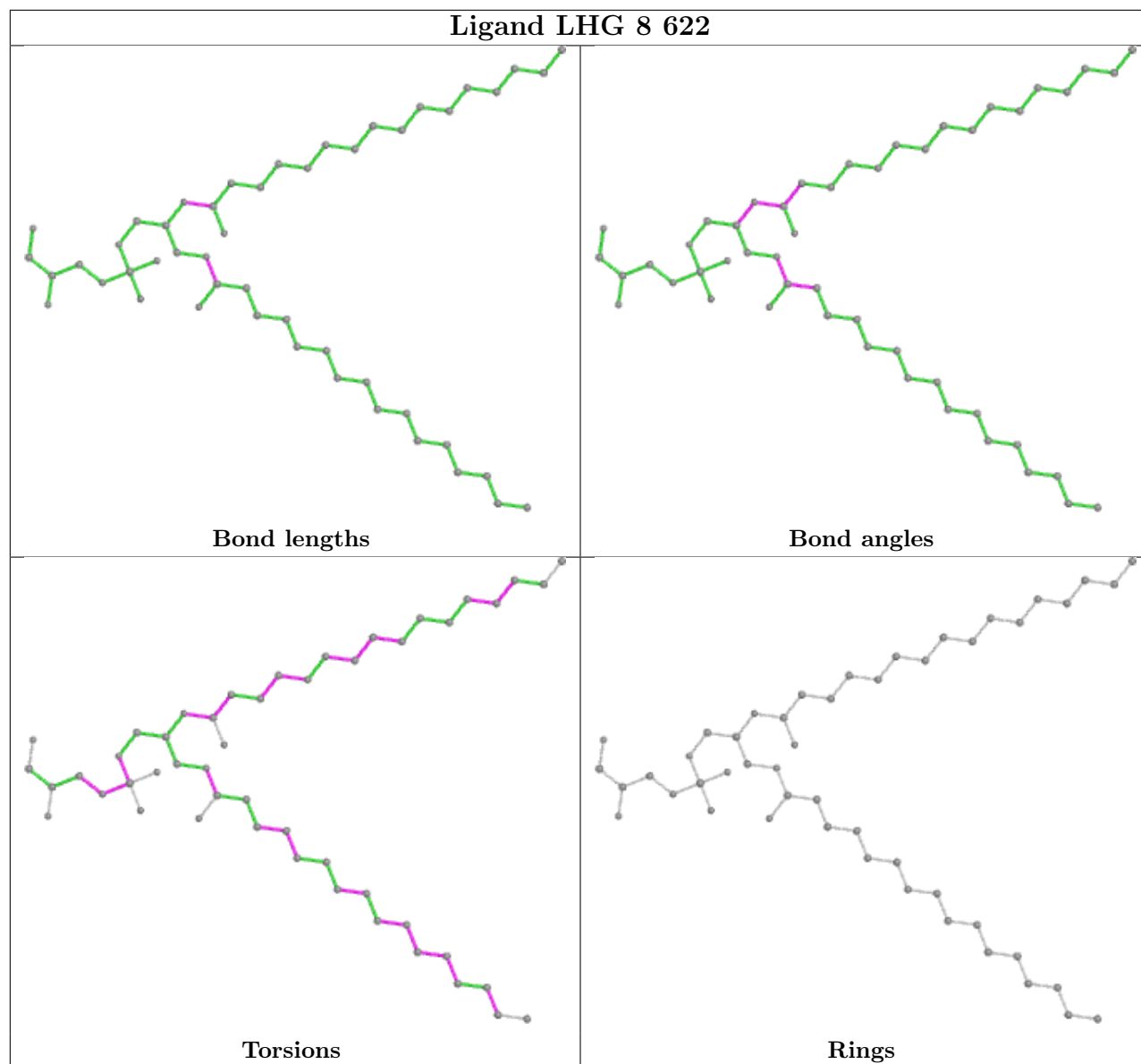




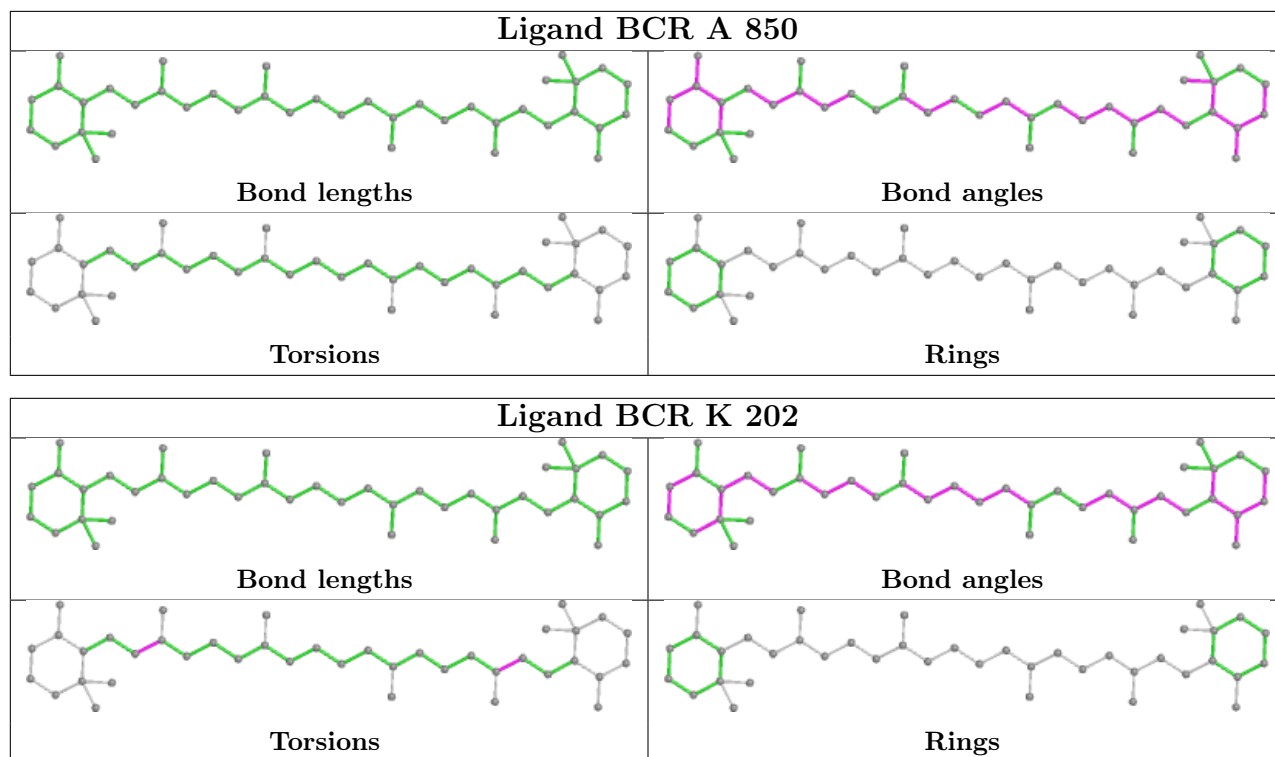




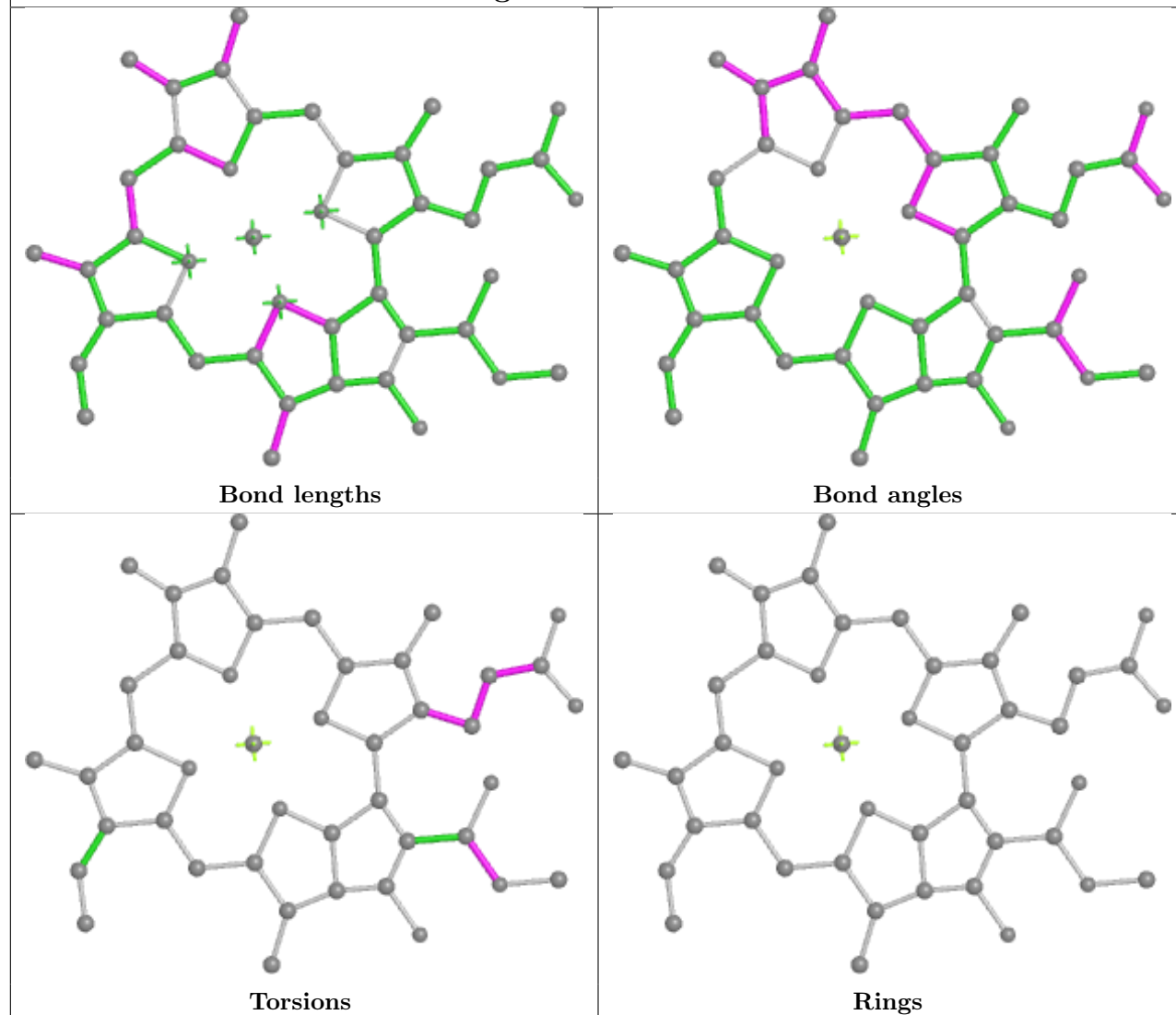




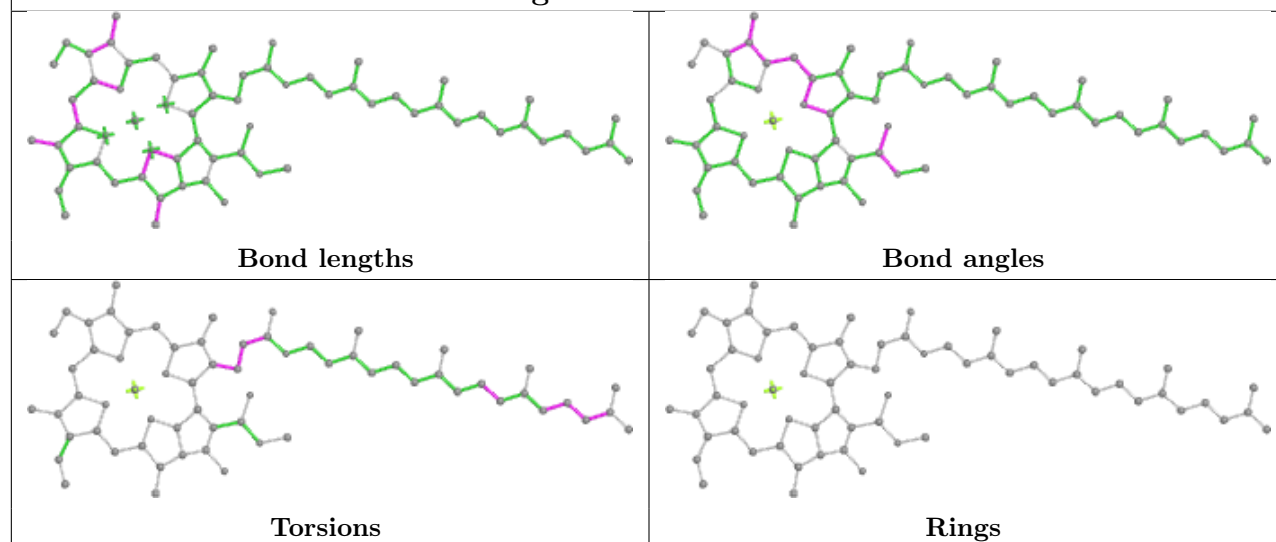


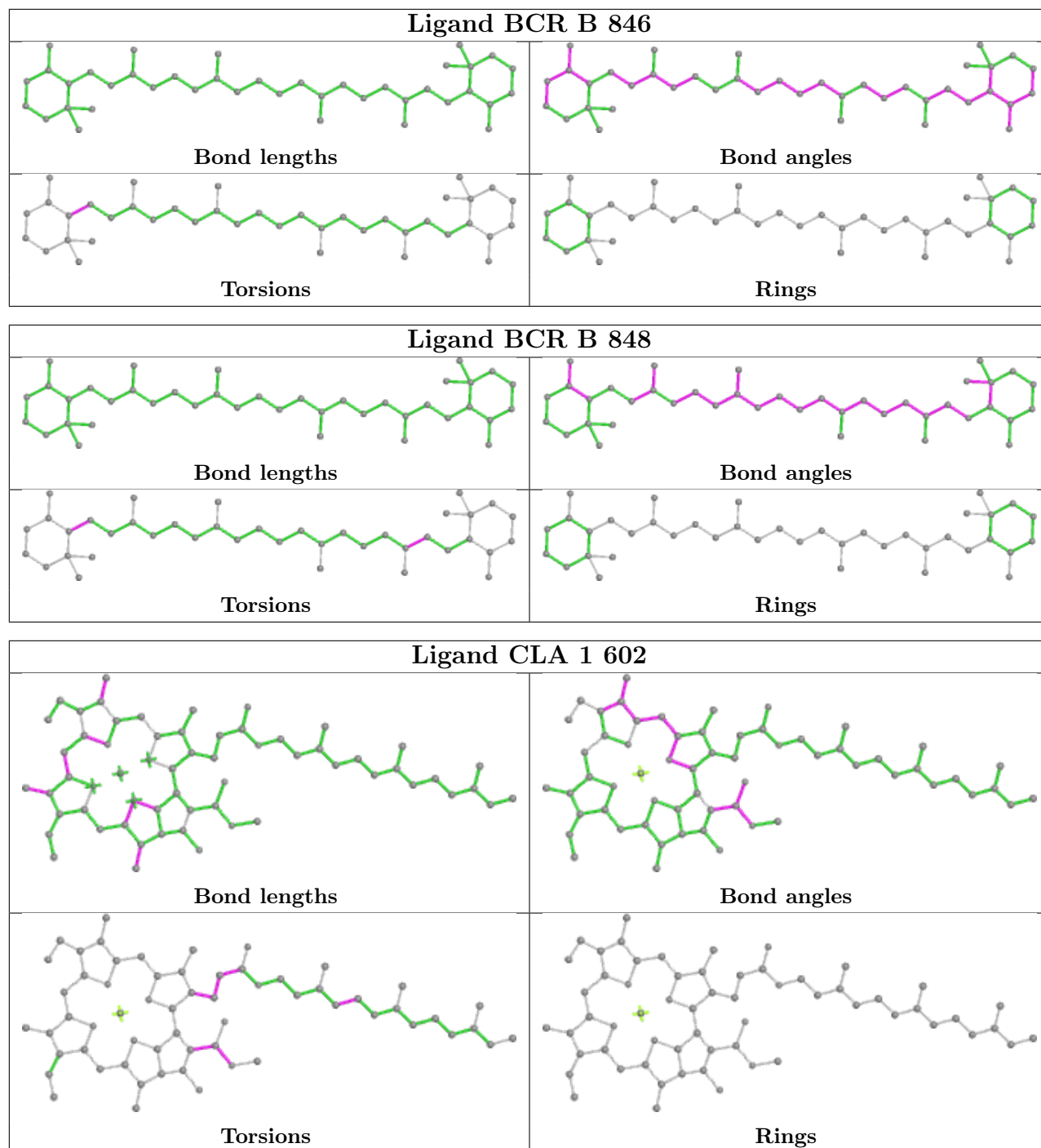


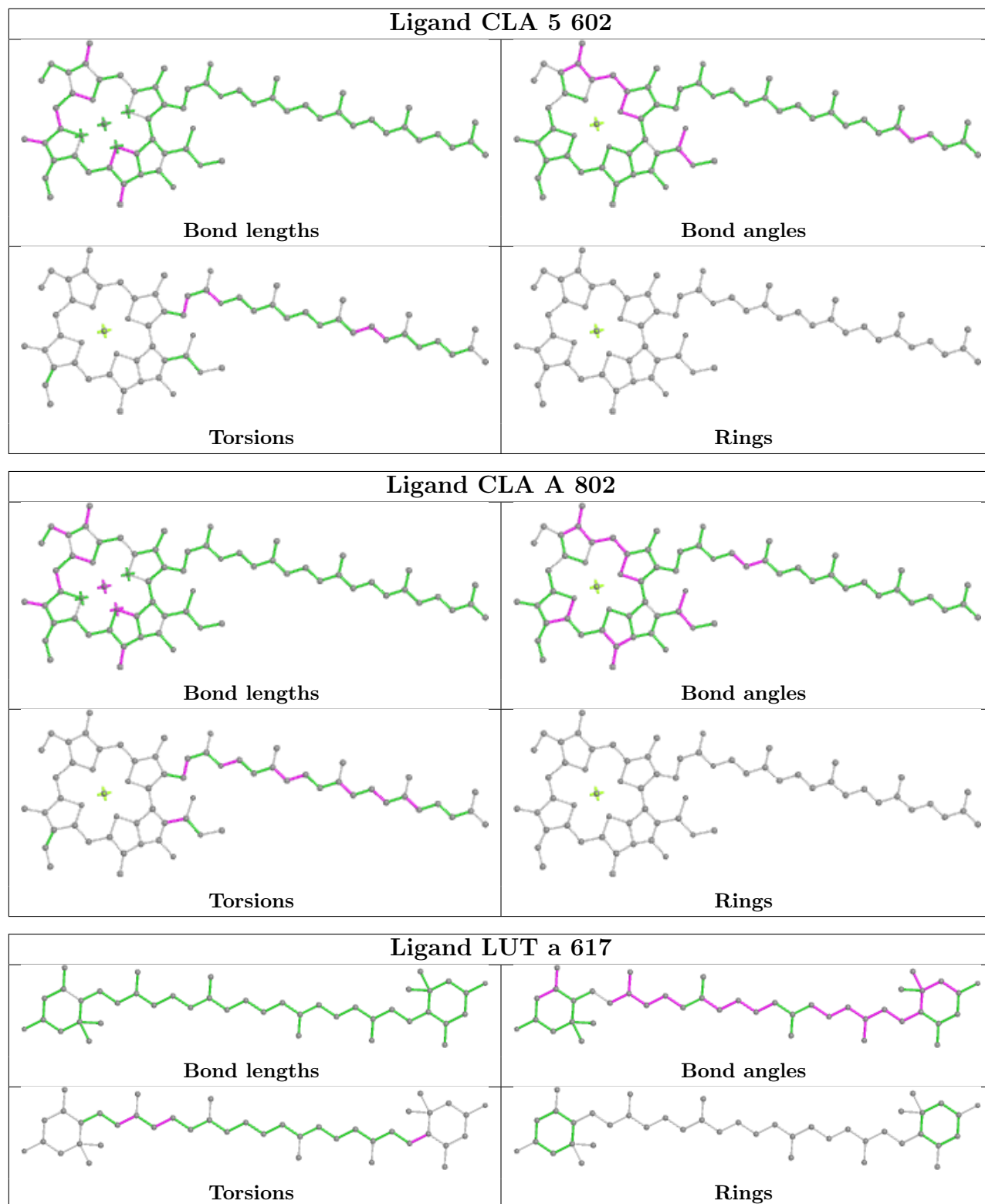
## Ligand CLA 8 603

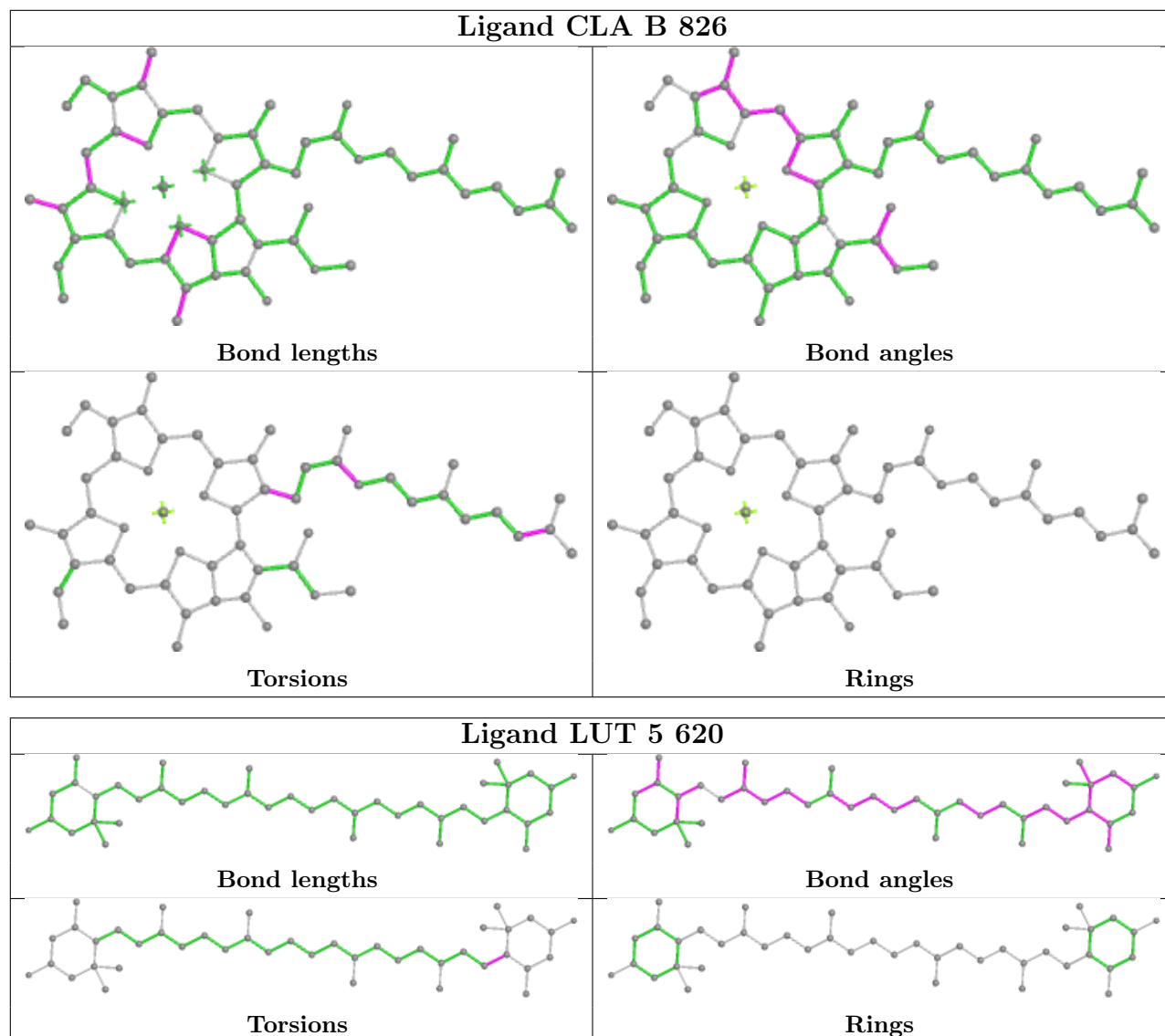


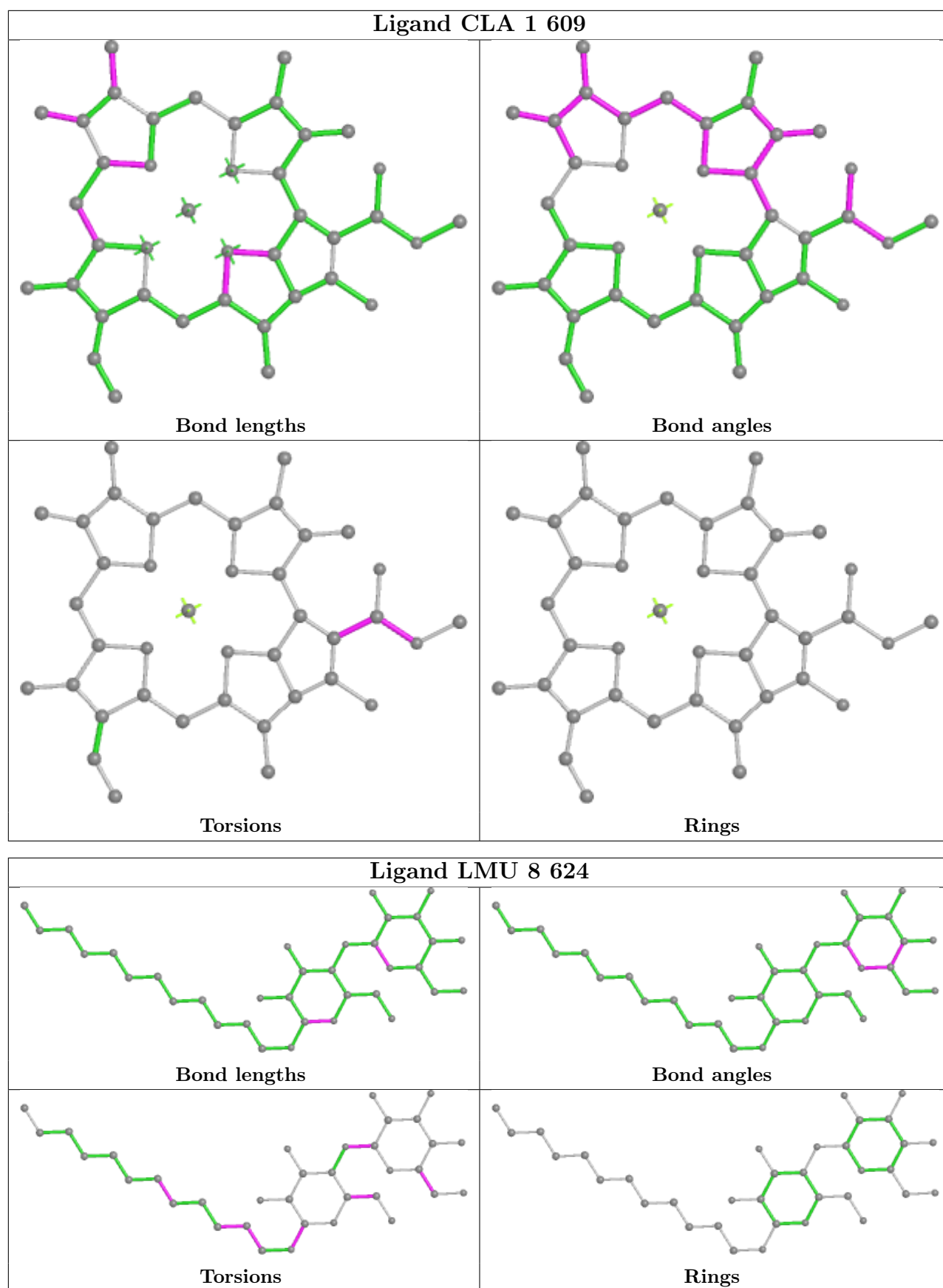
## Ligand CLA A 842

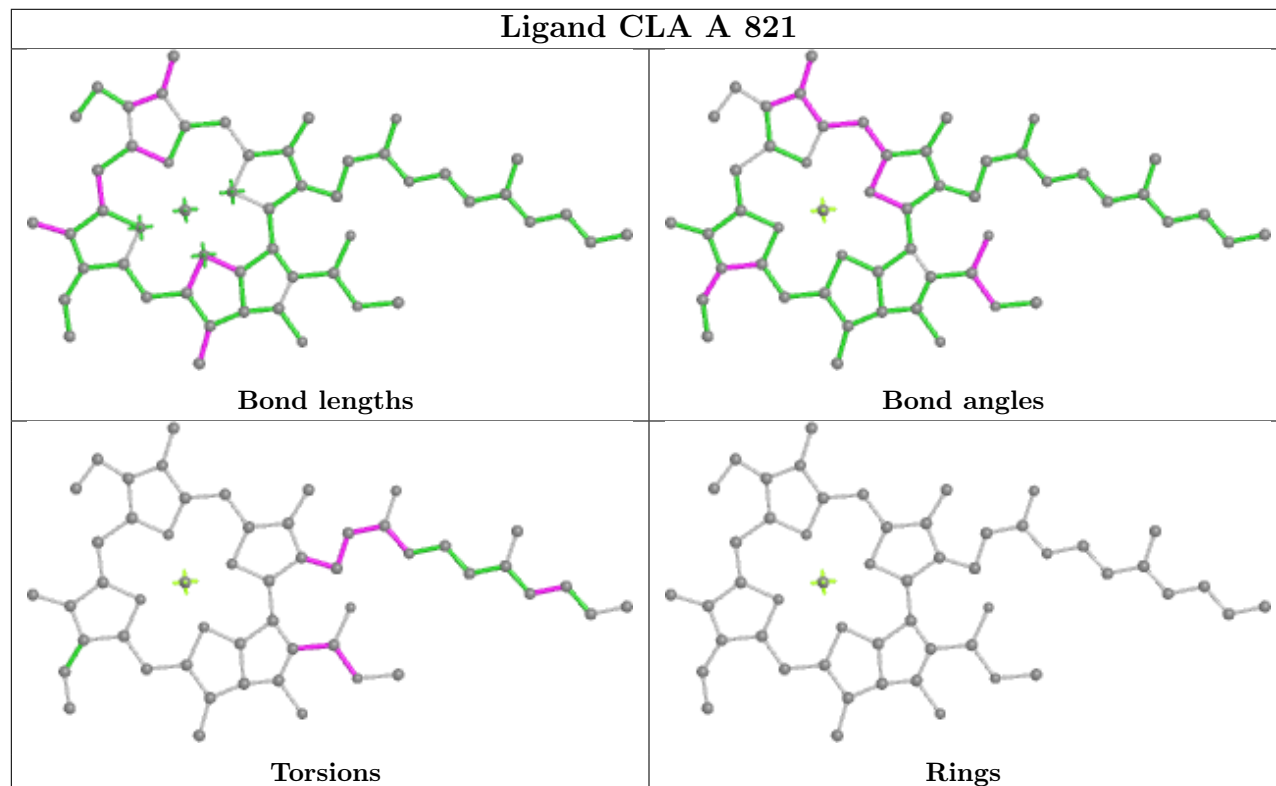
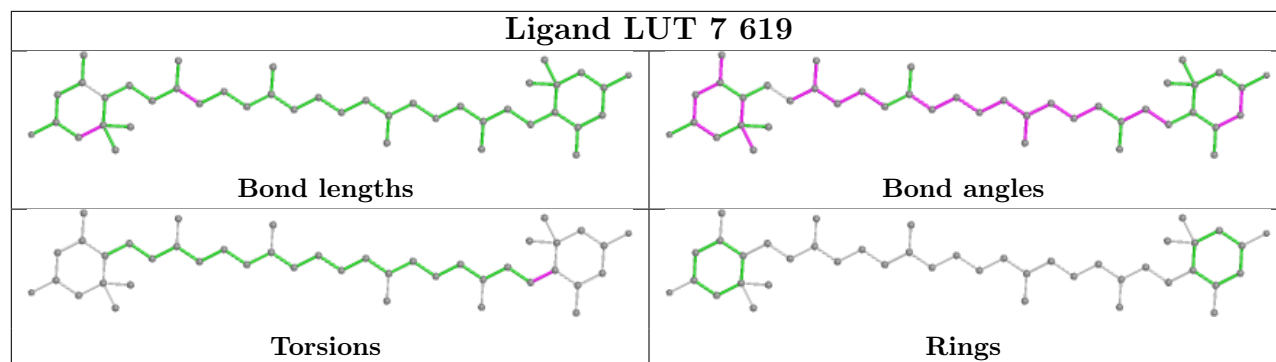


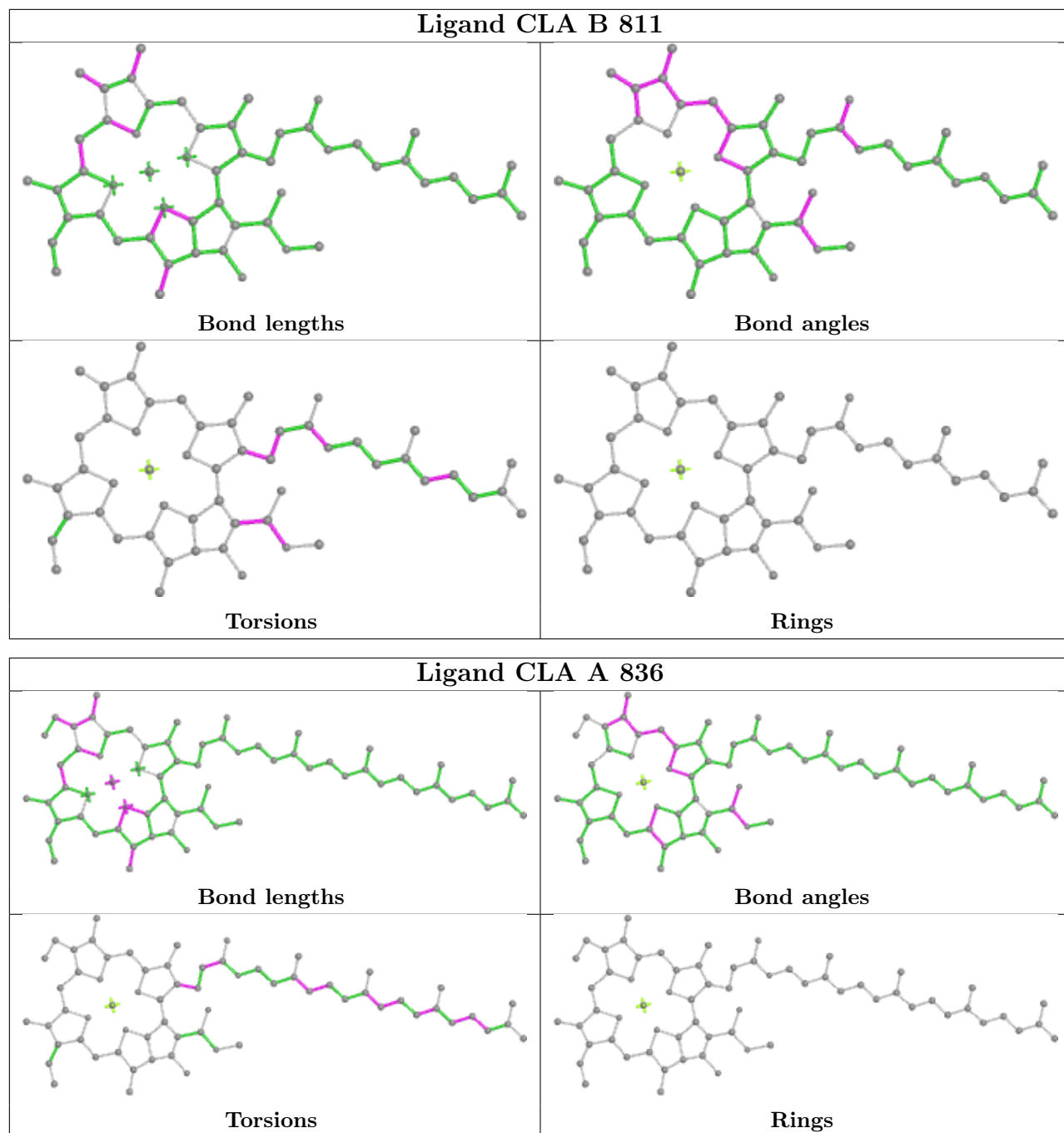




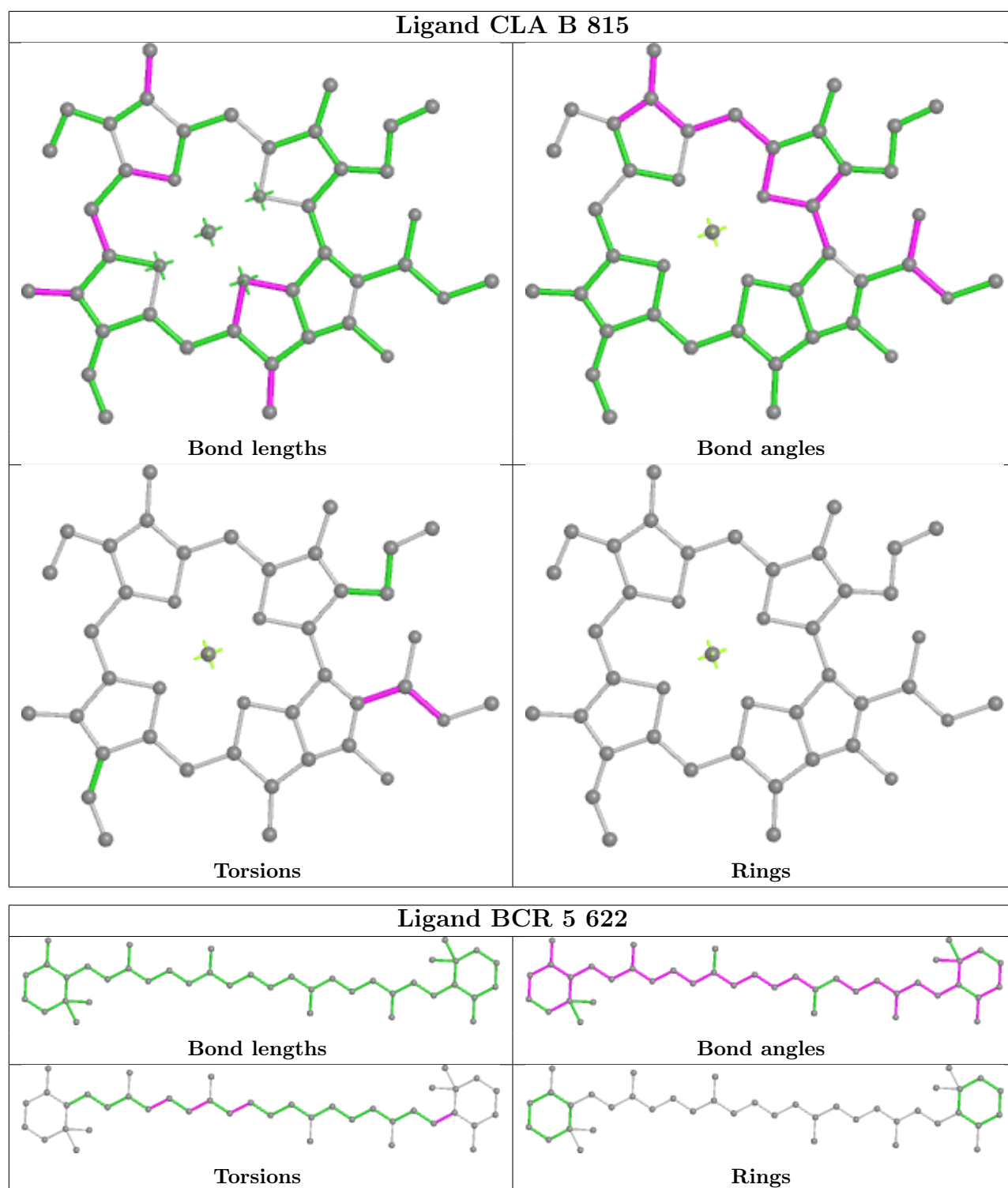


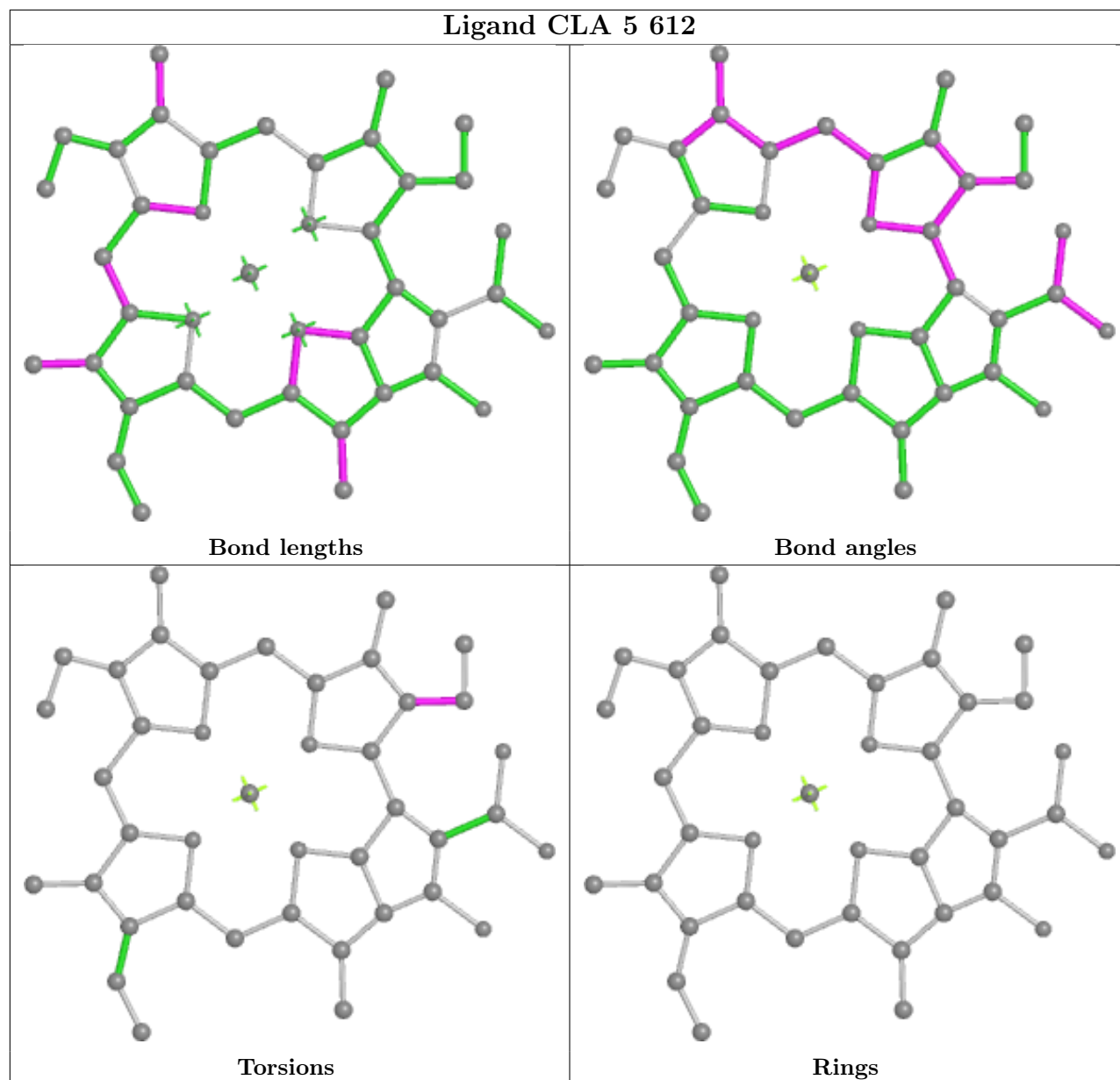


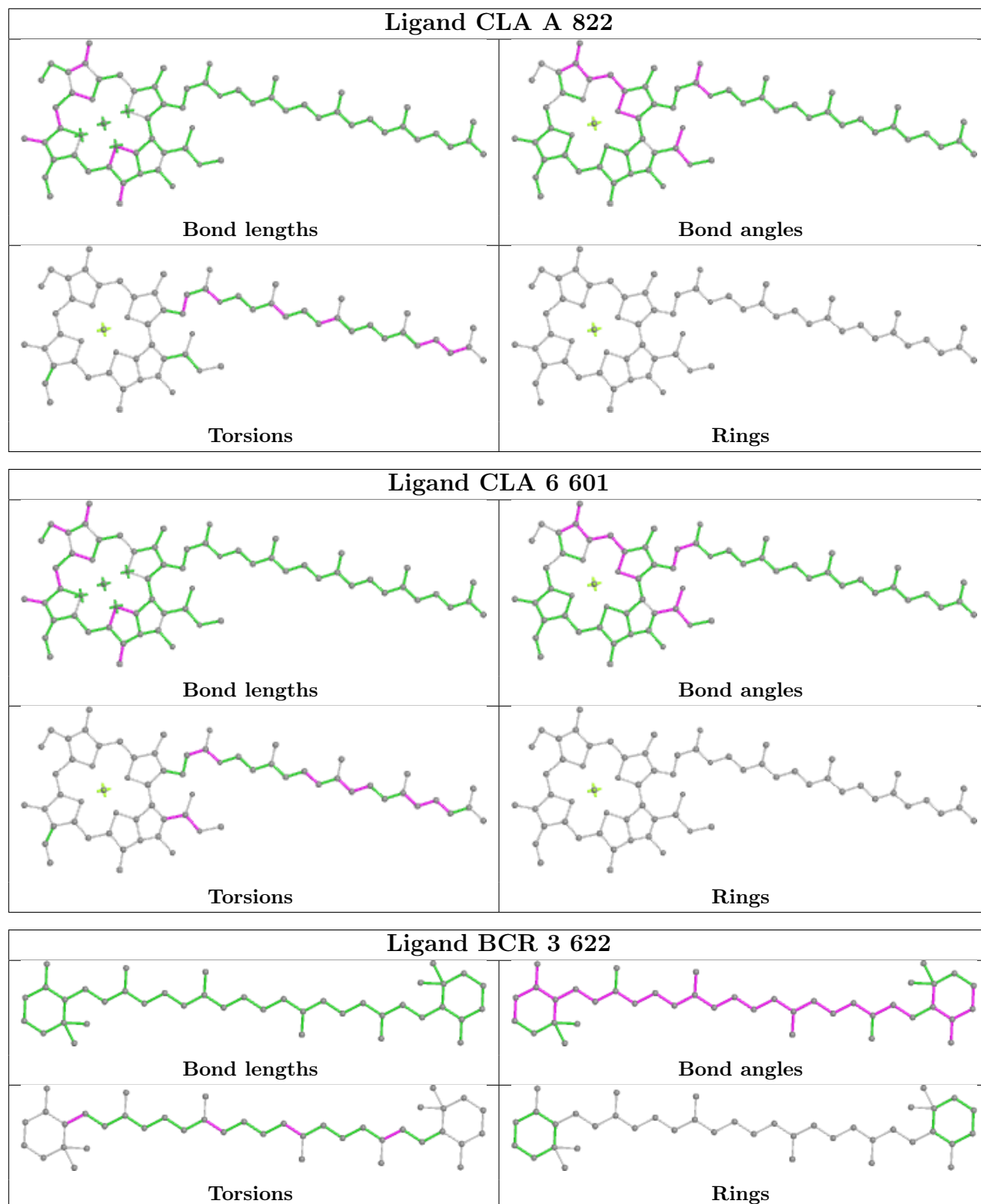


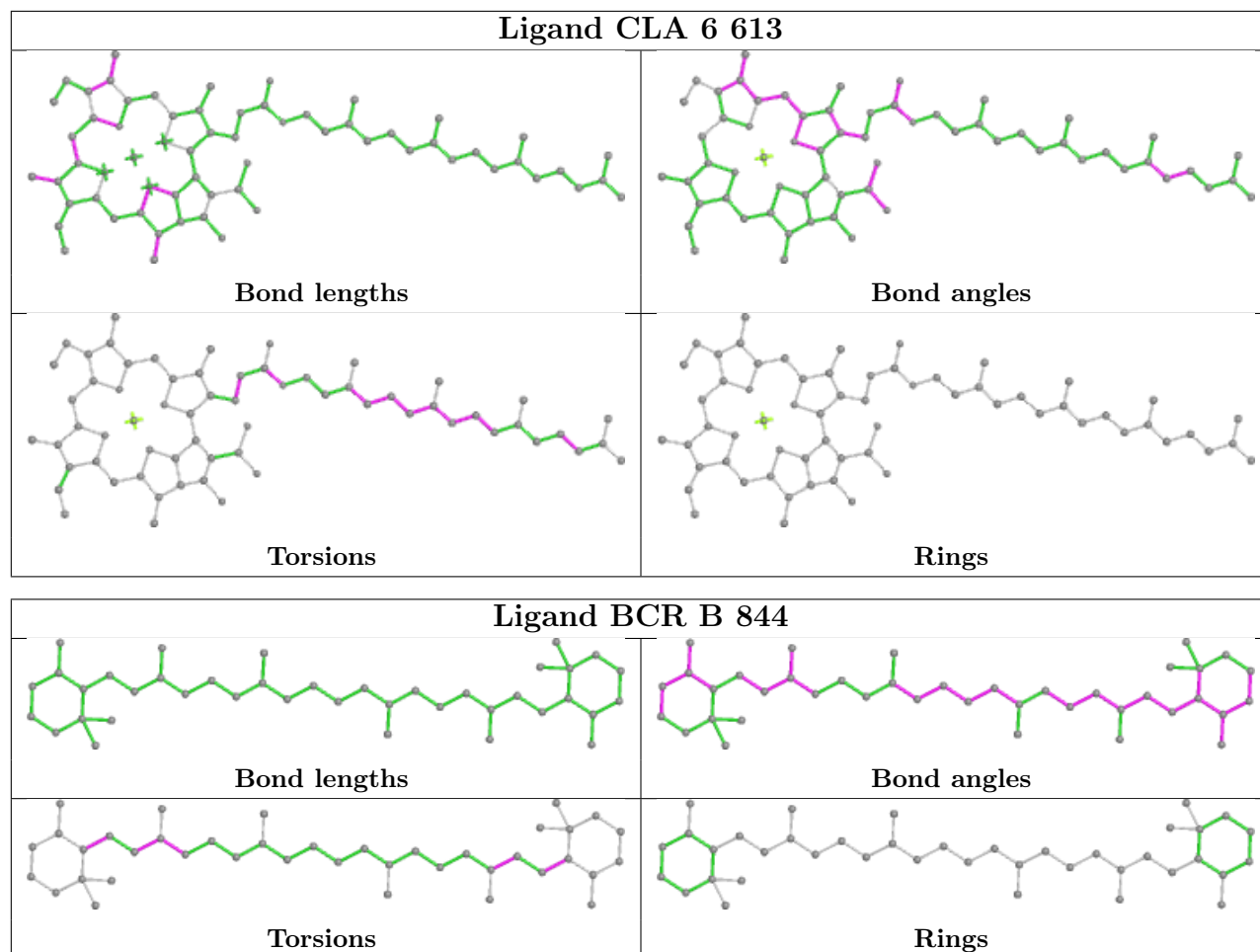


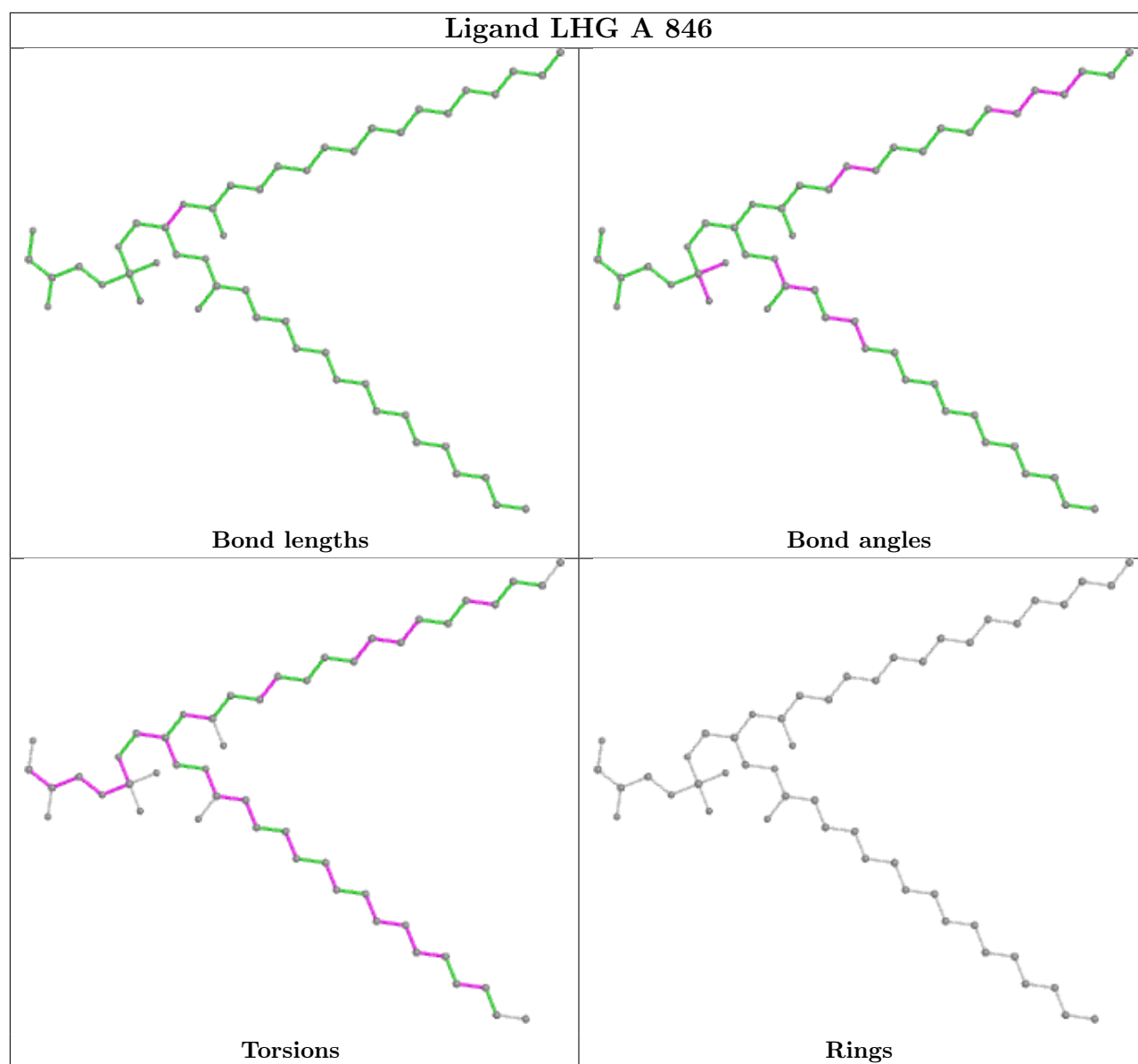


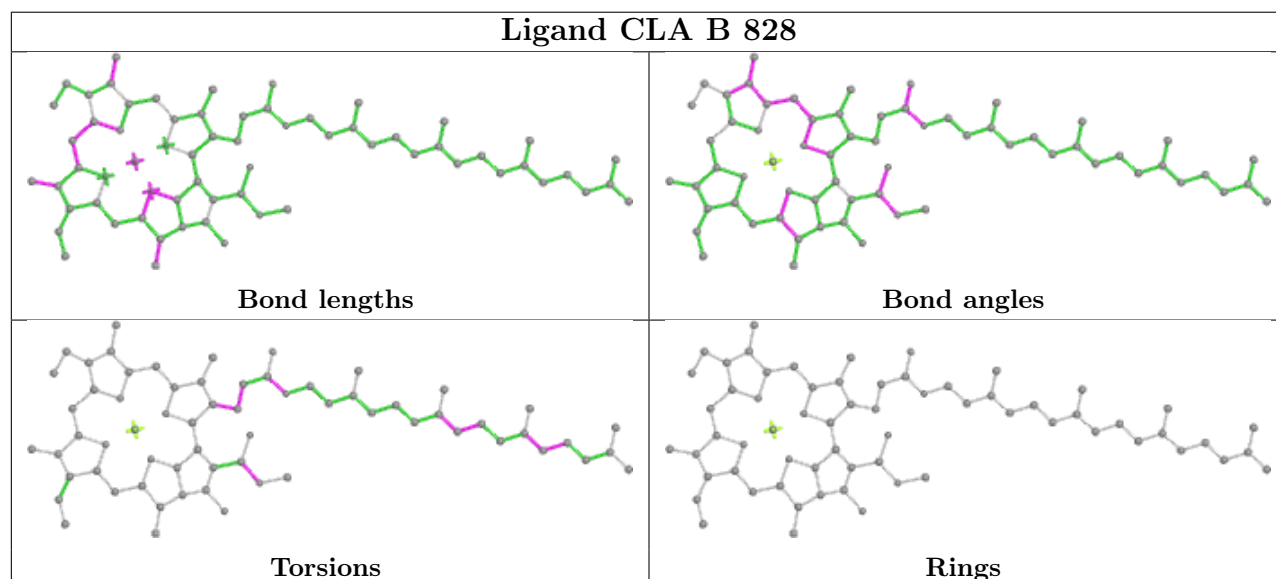
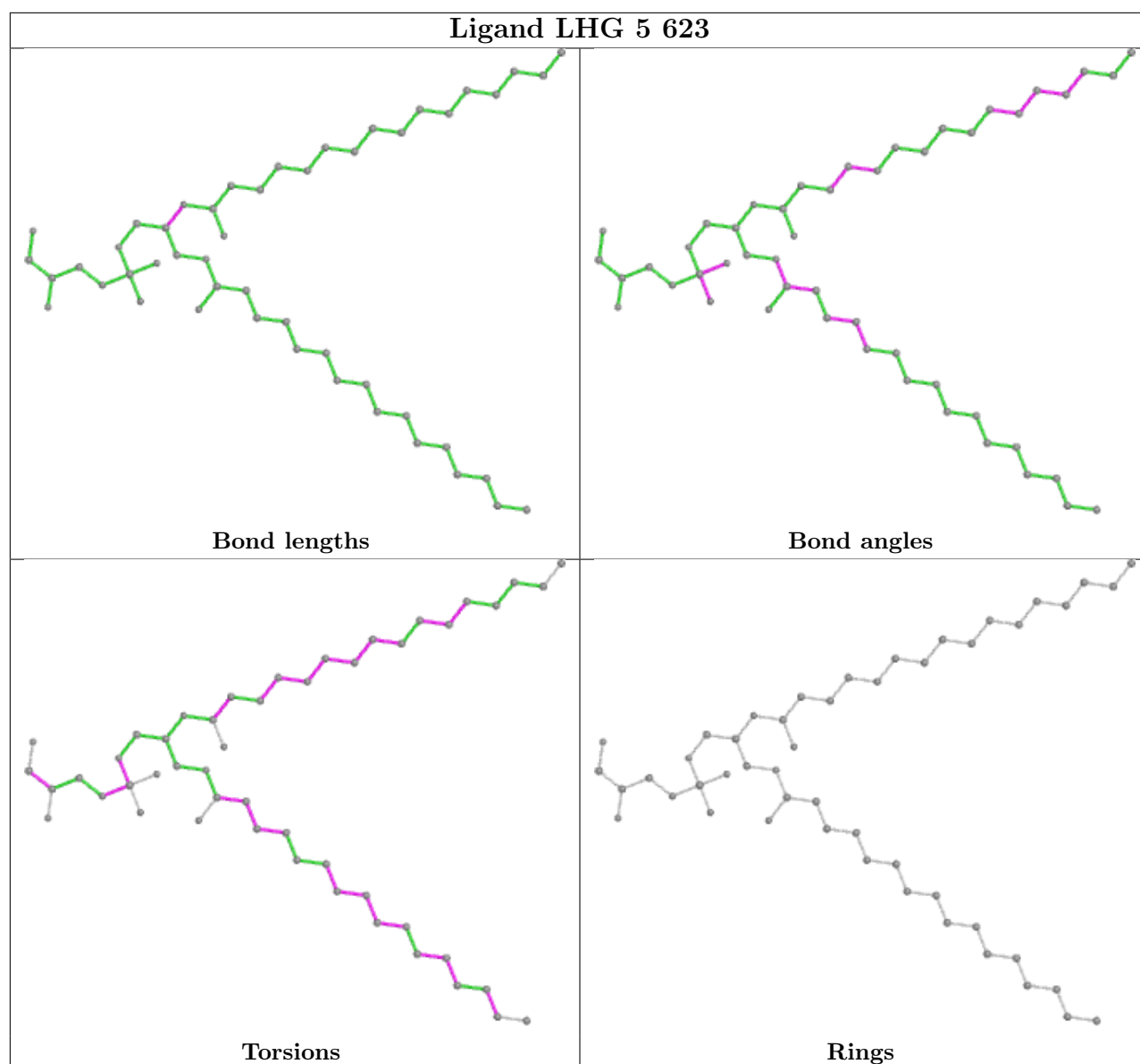


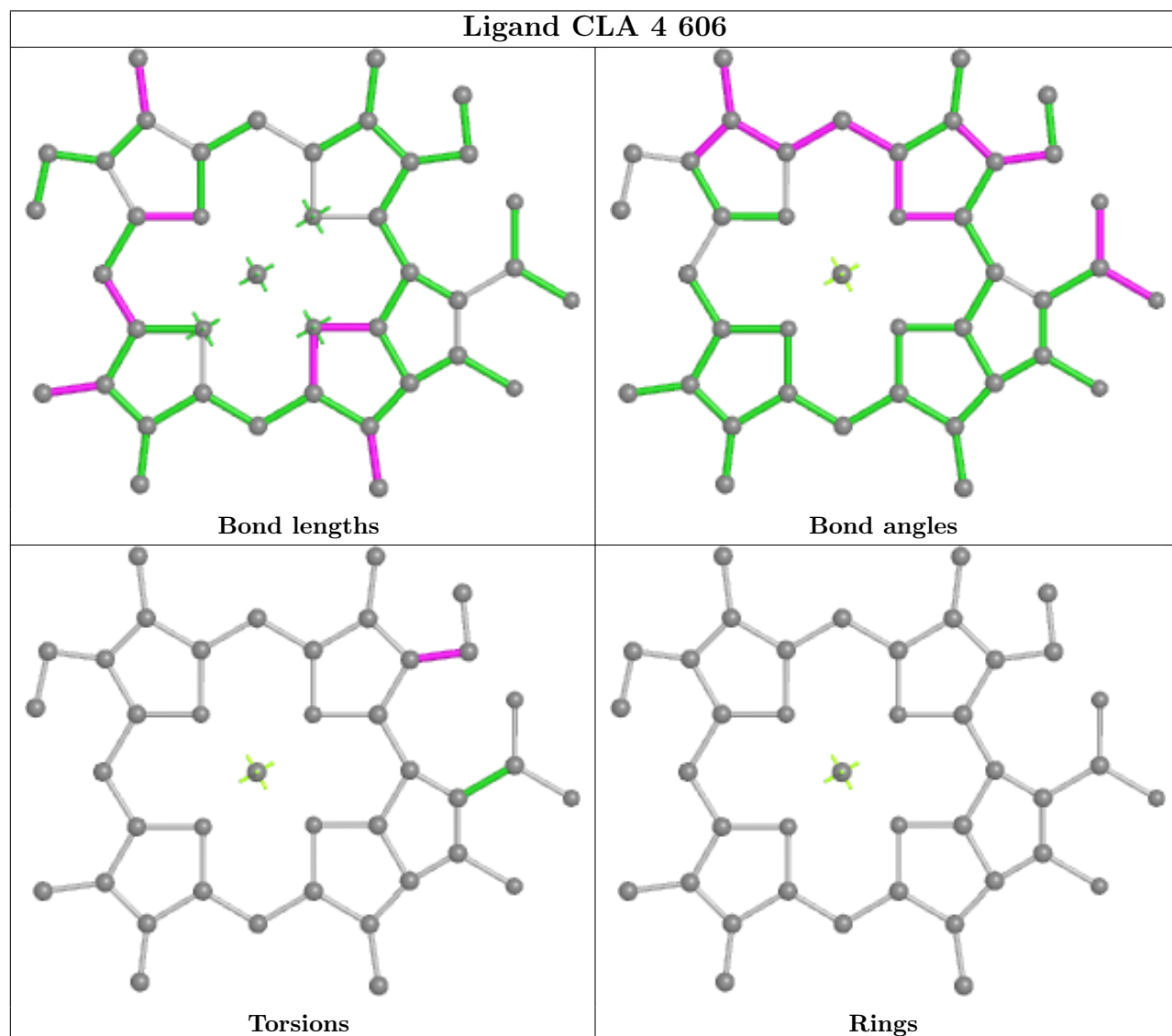
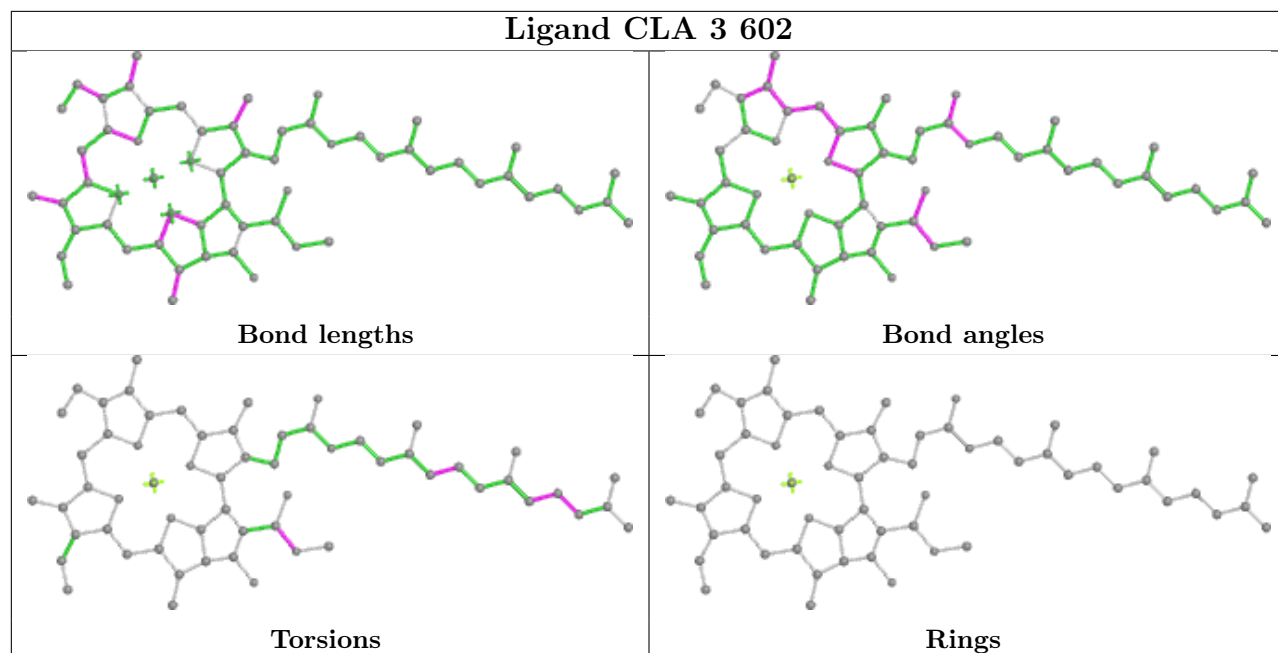


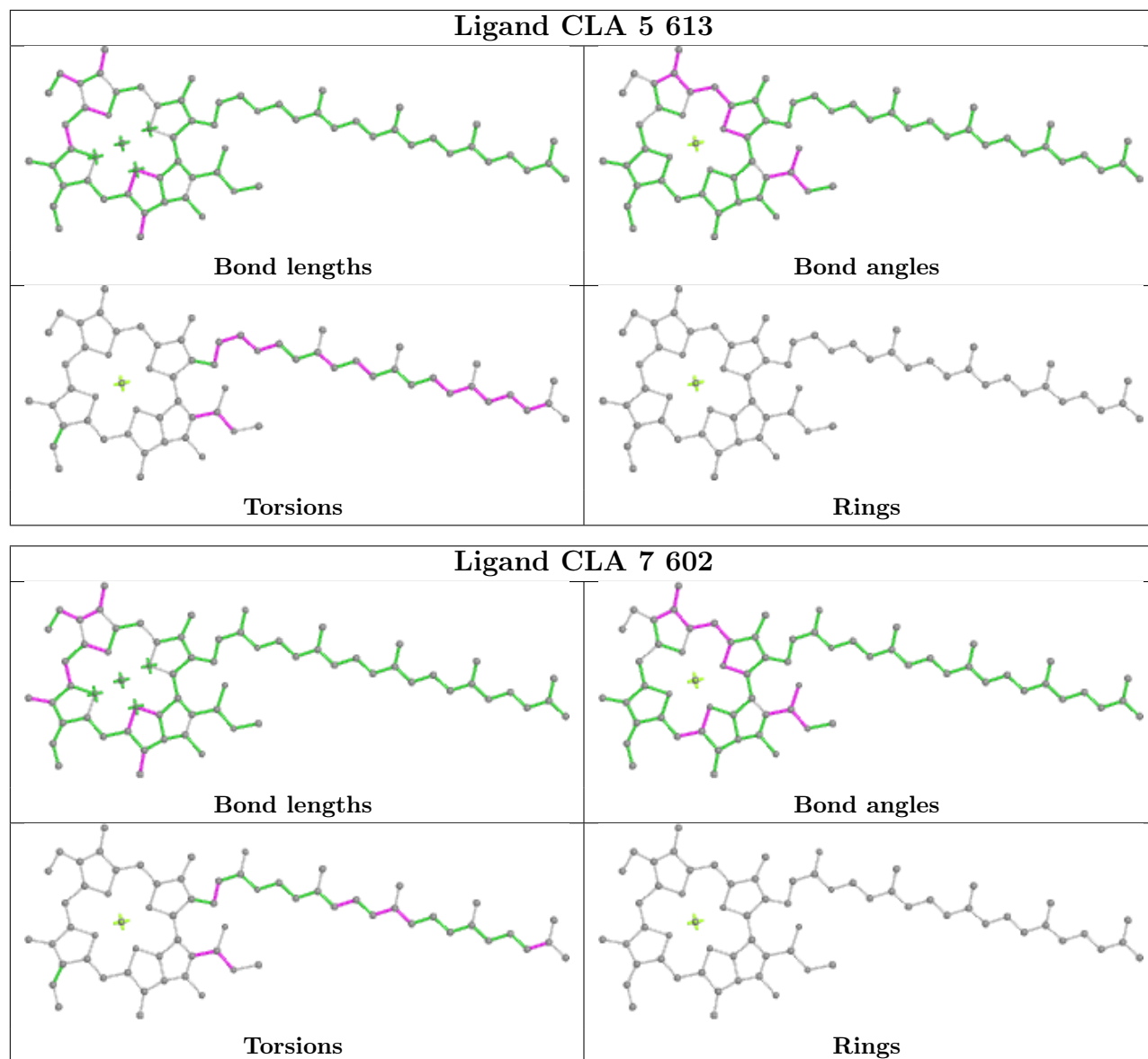




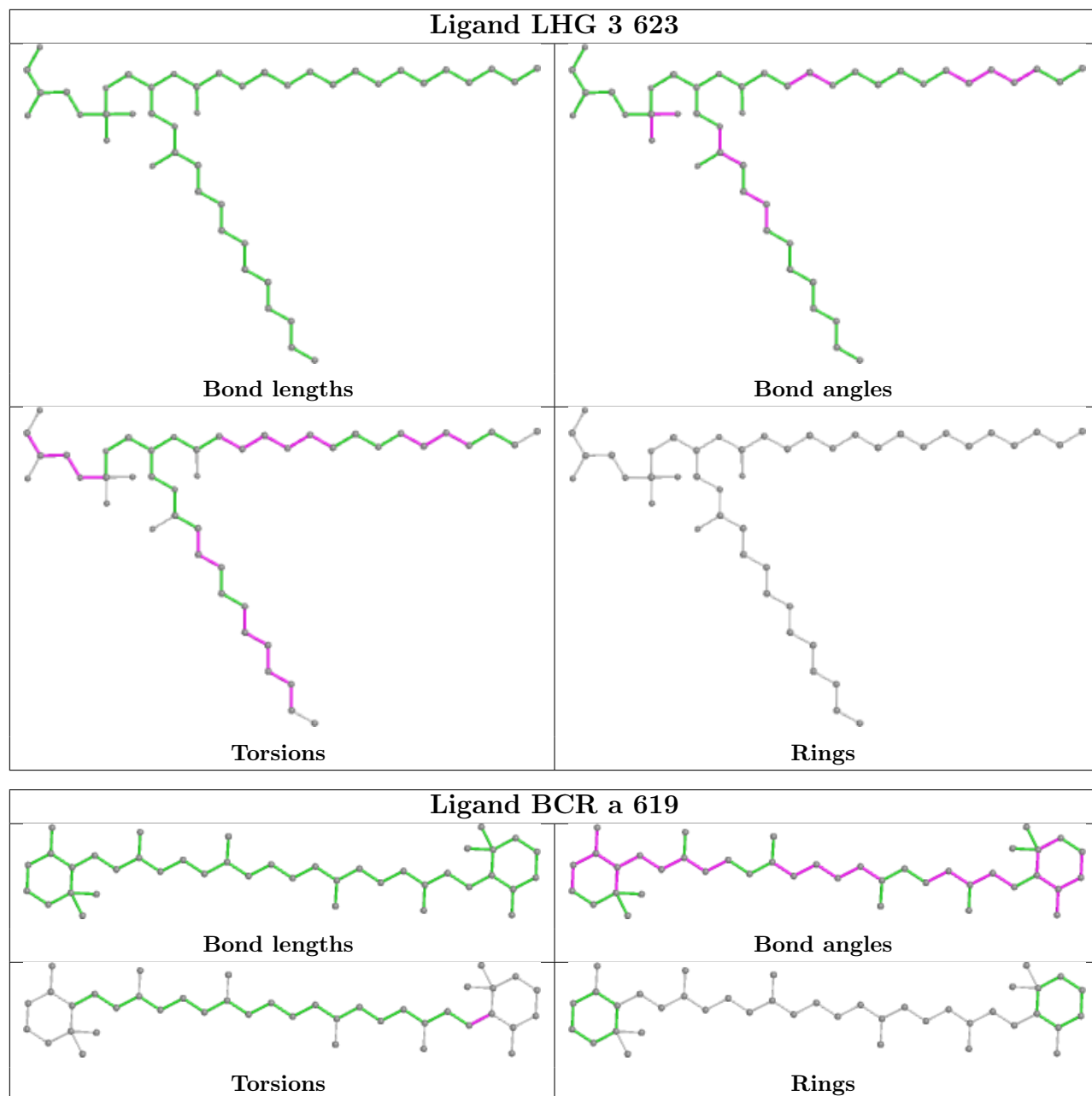


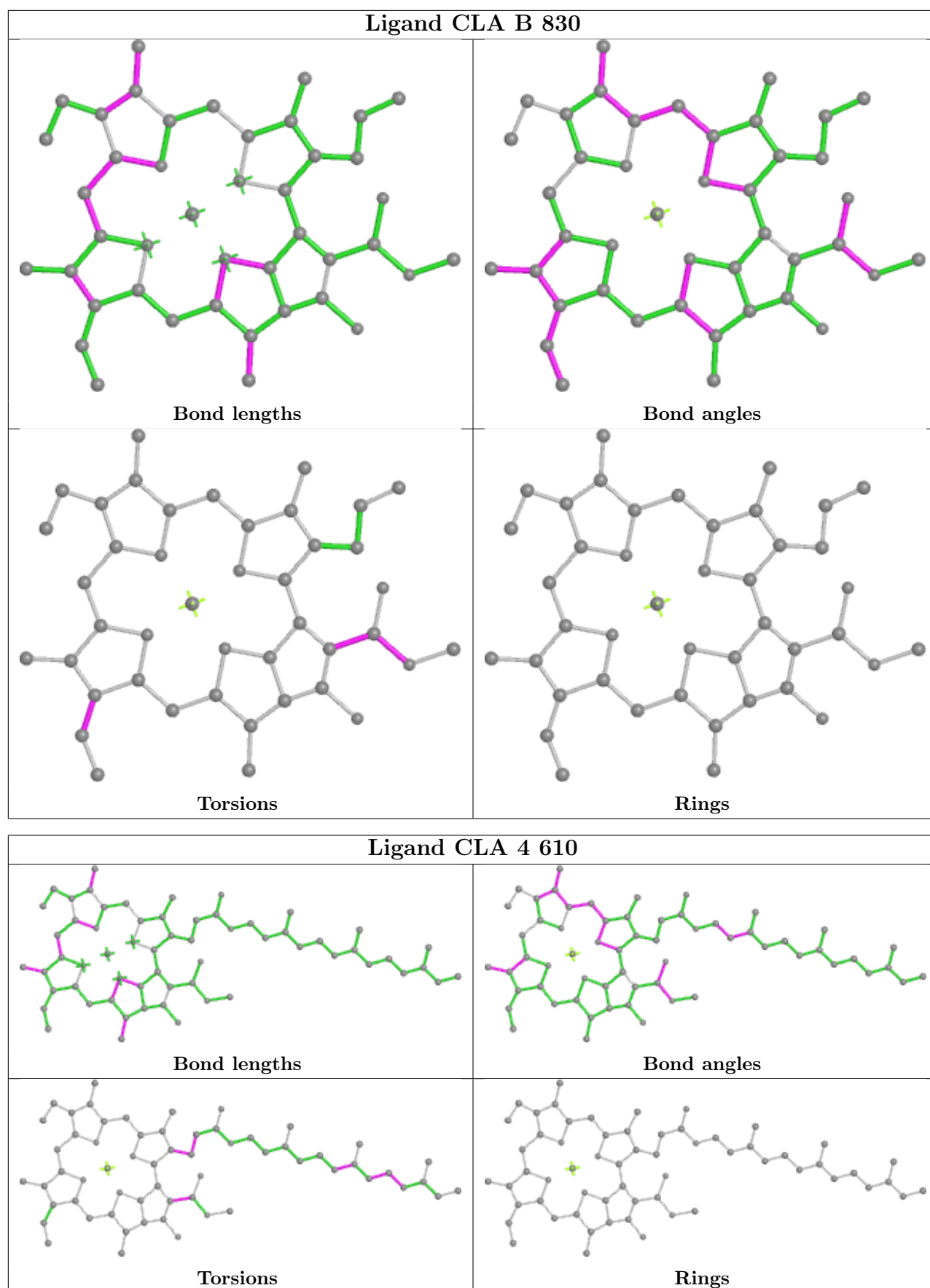


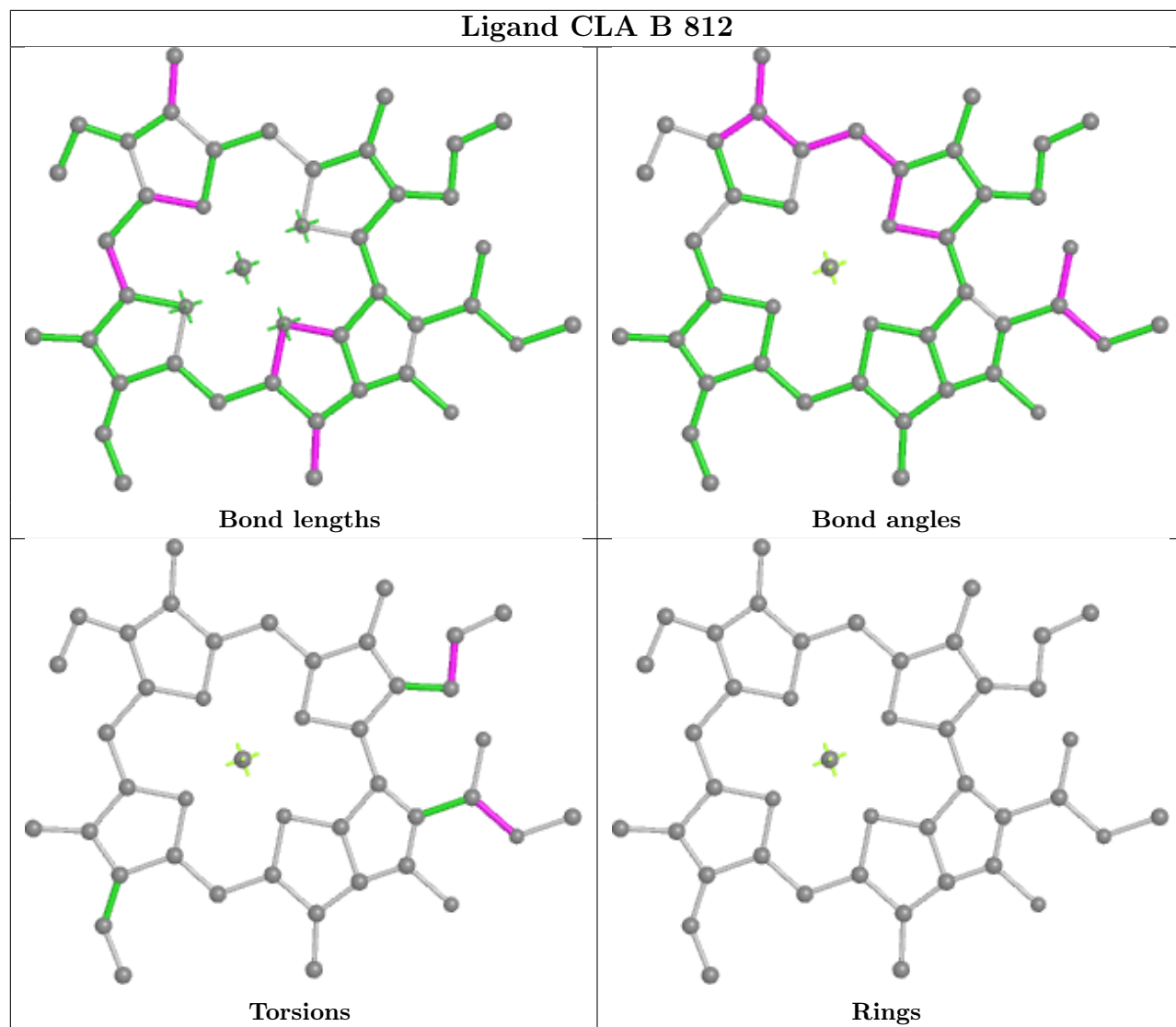


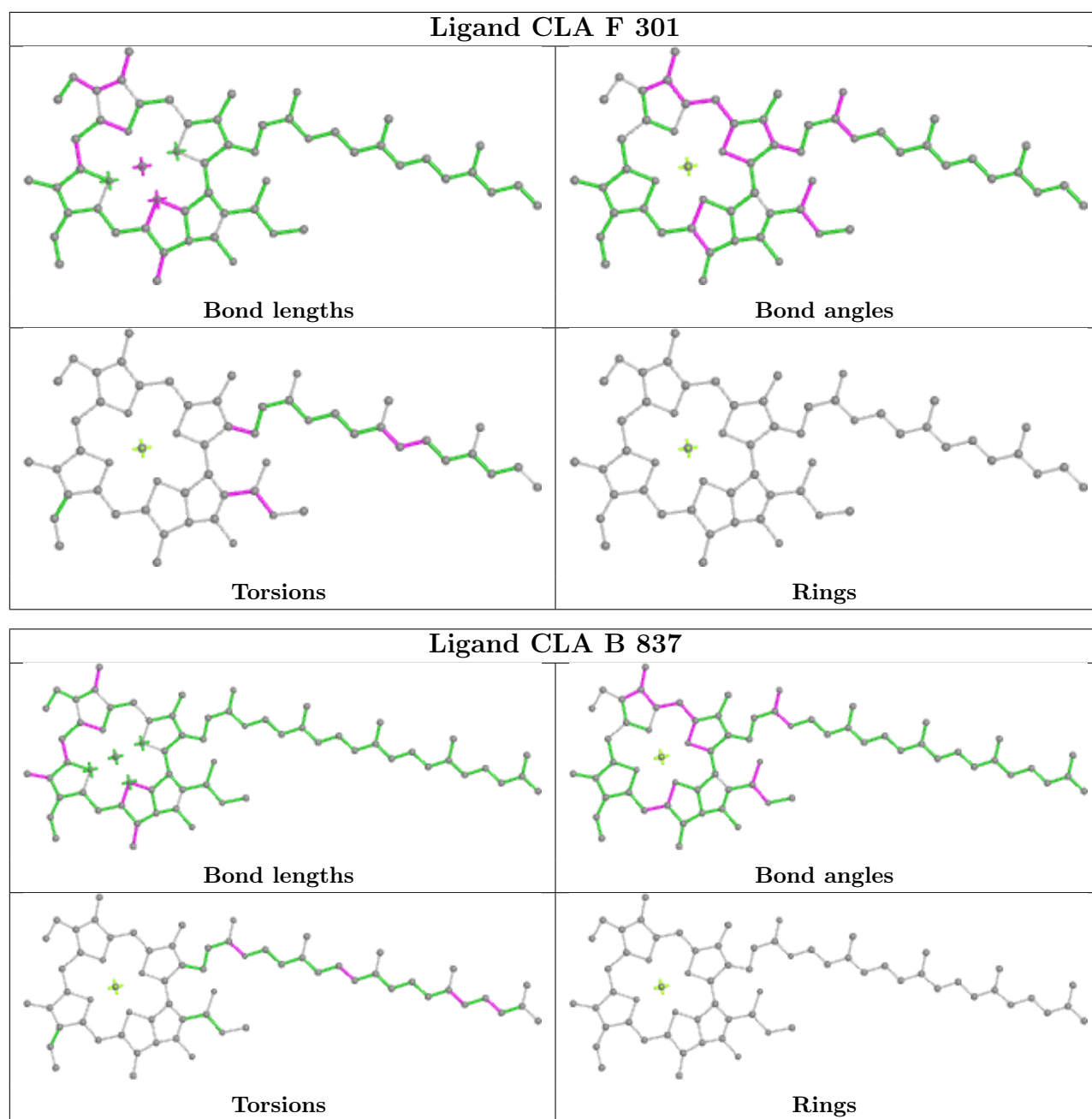


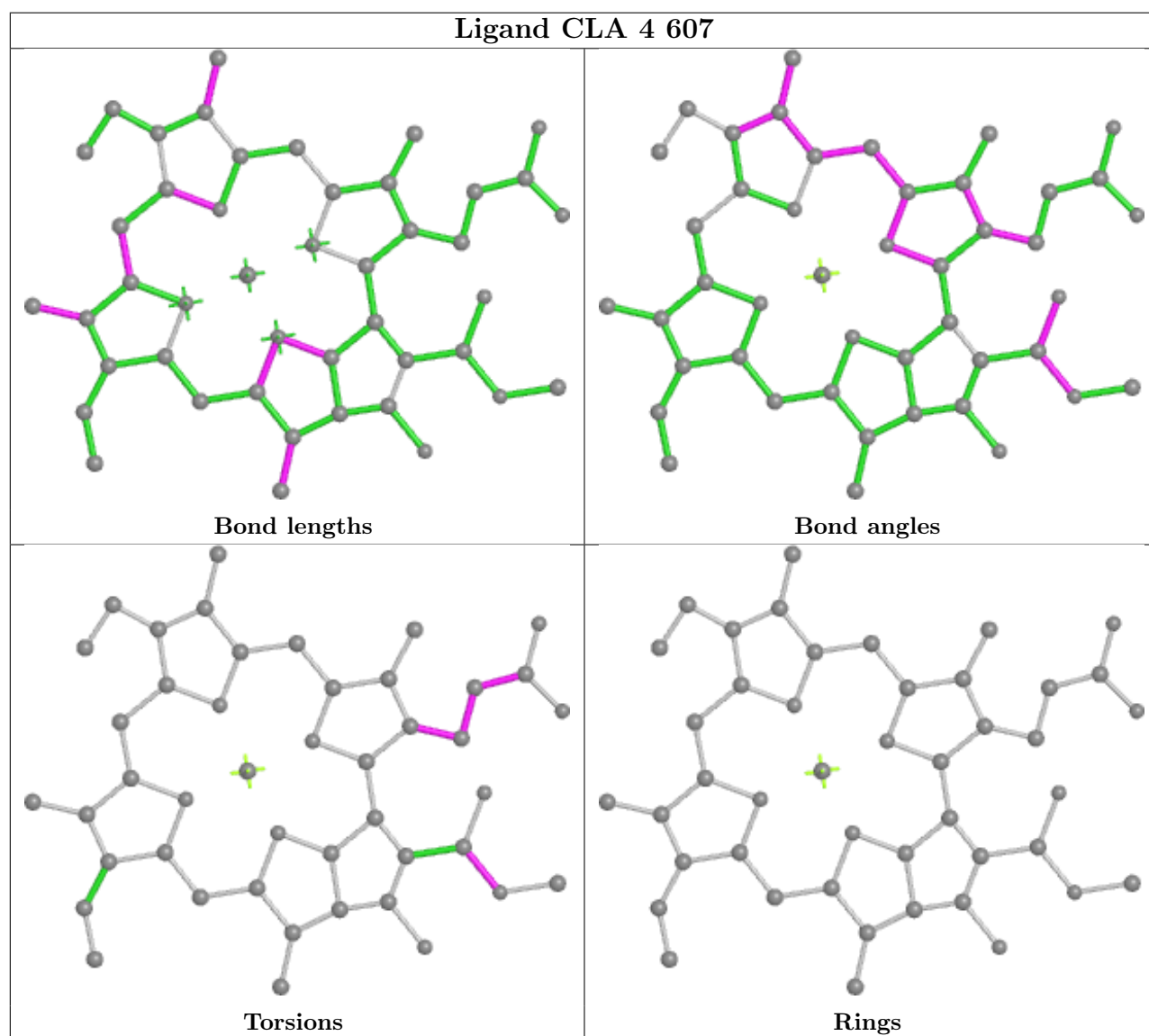
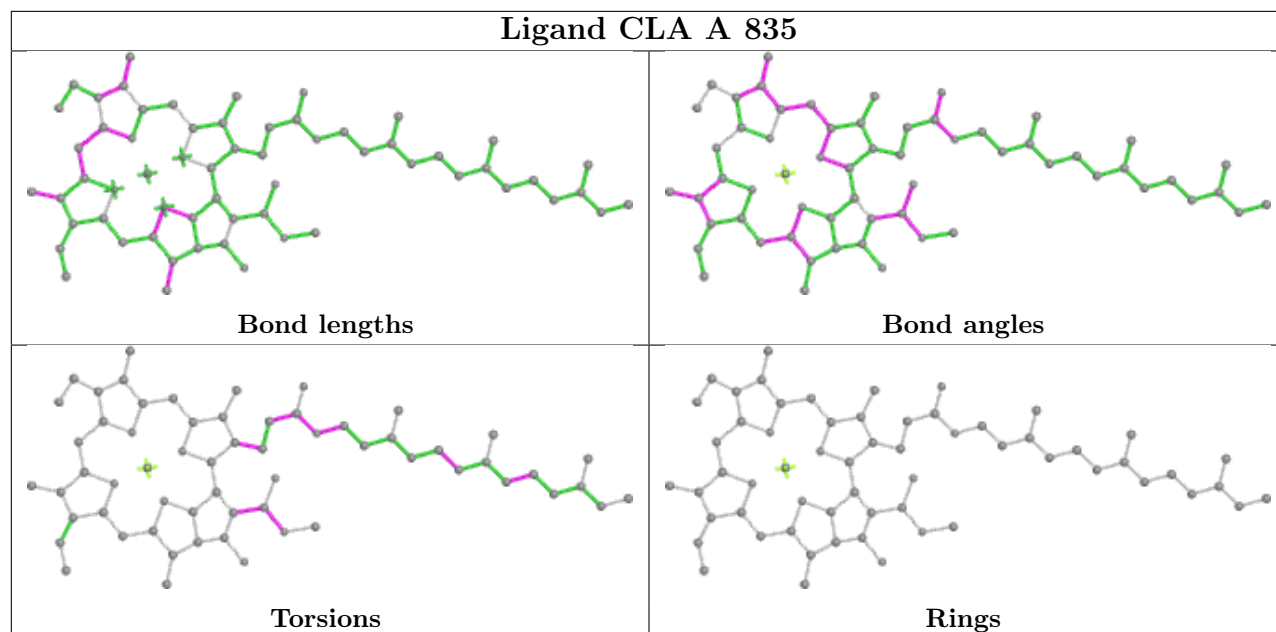


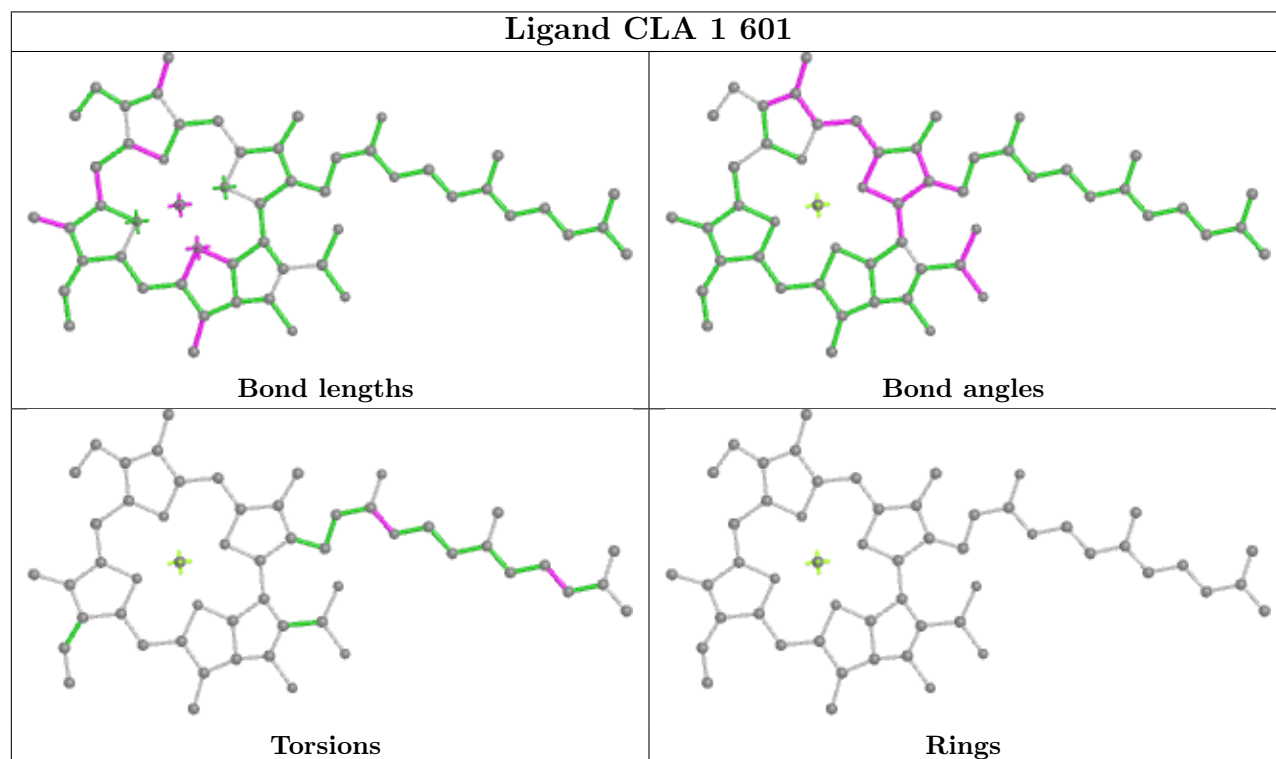
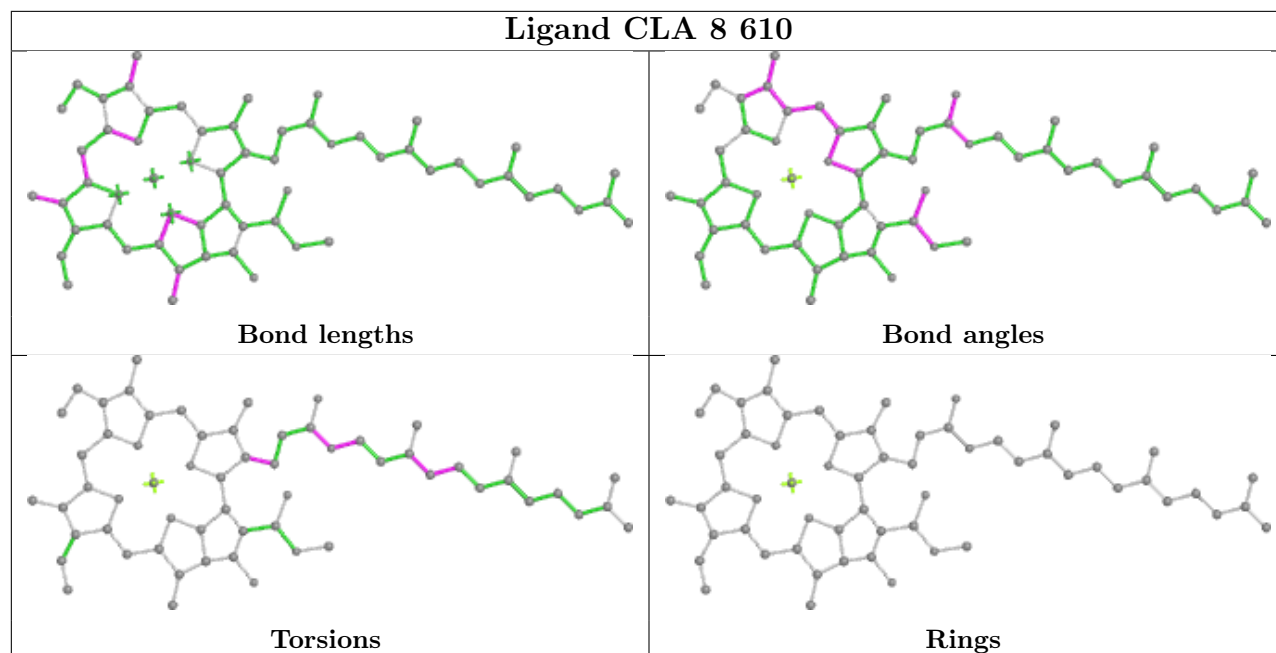


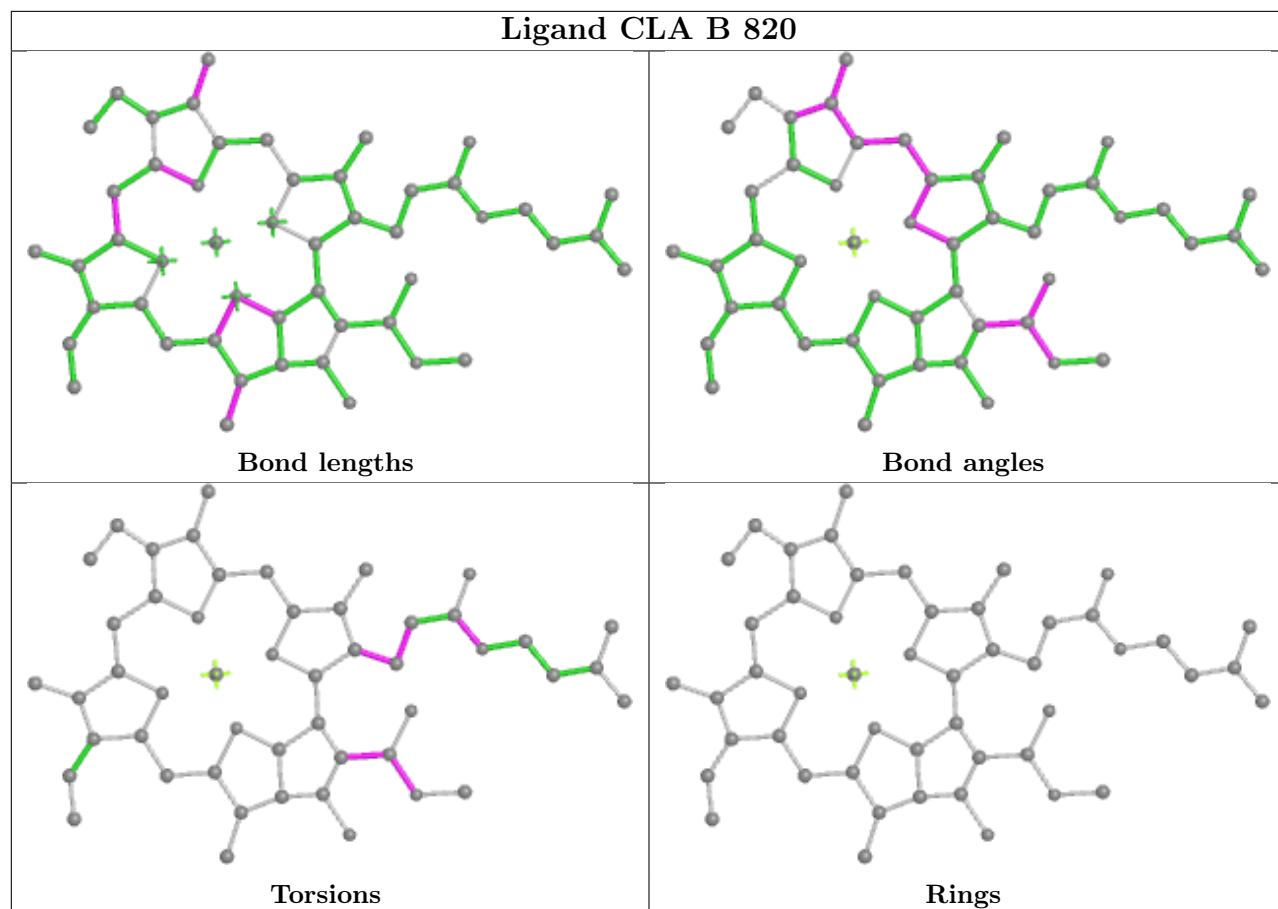


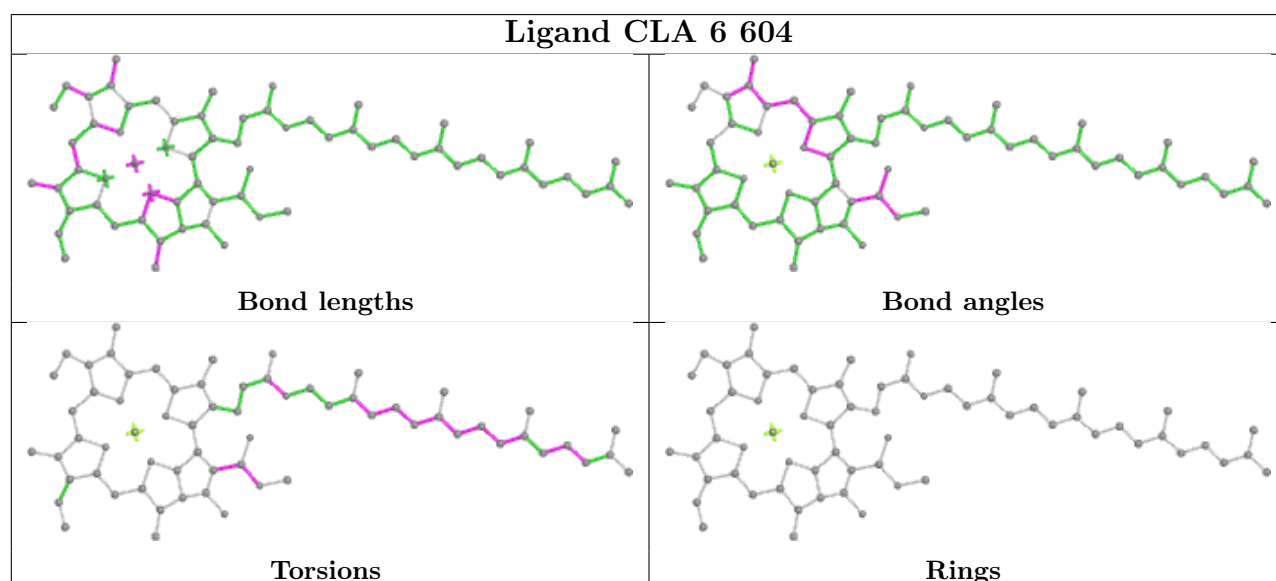
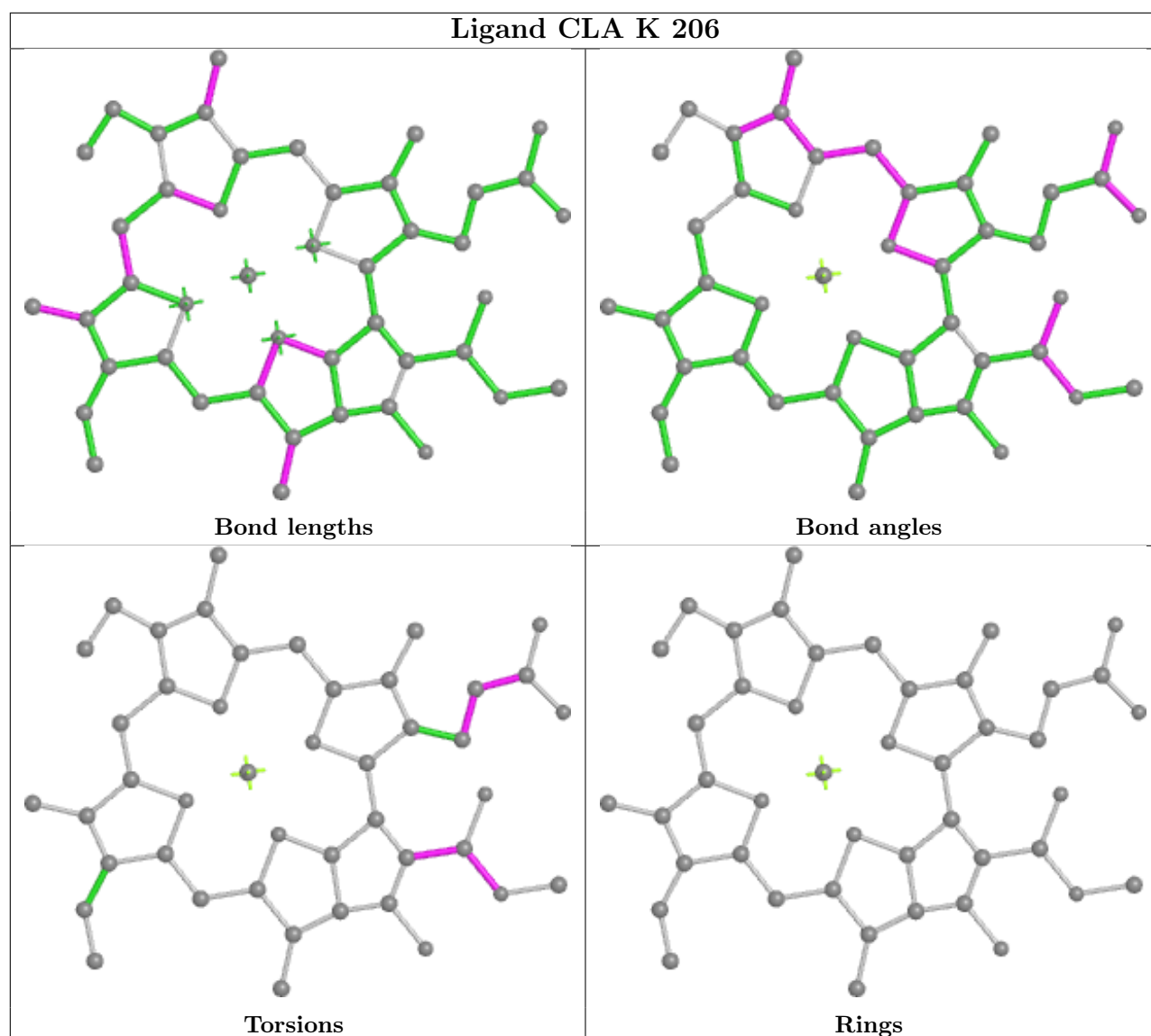






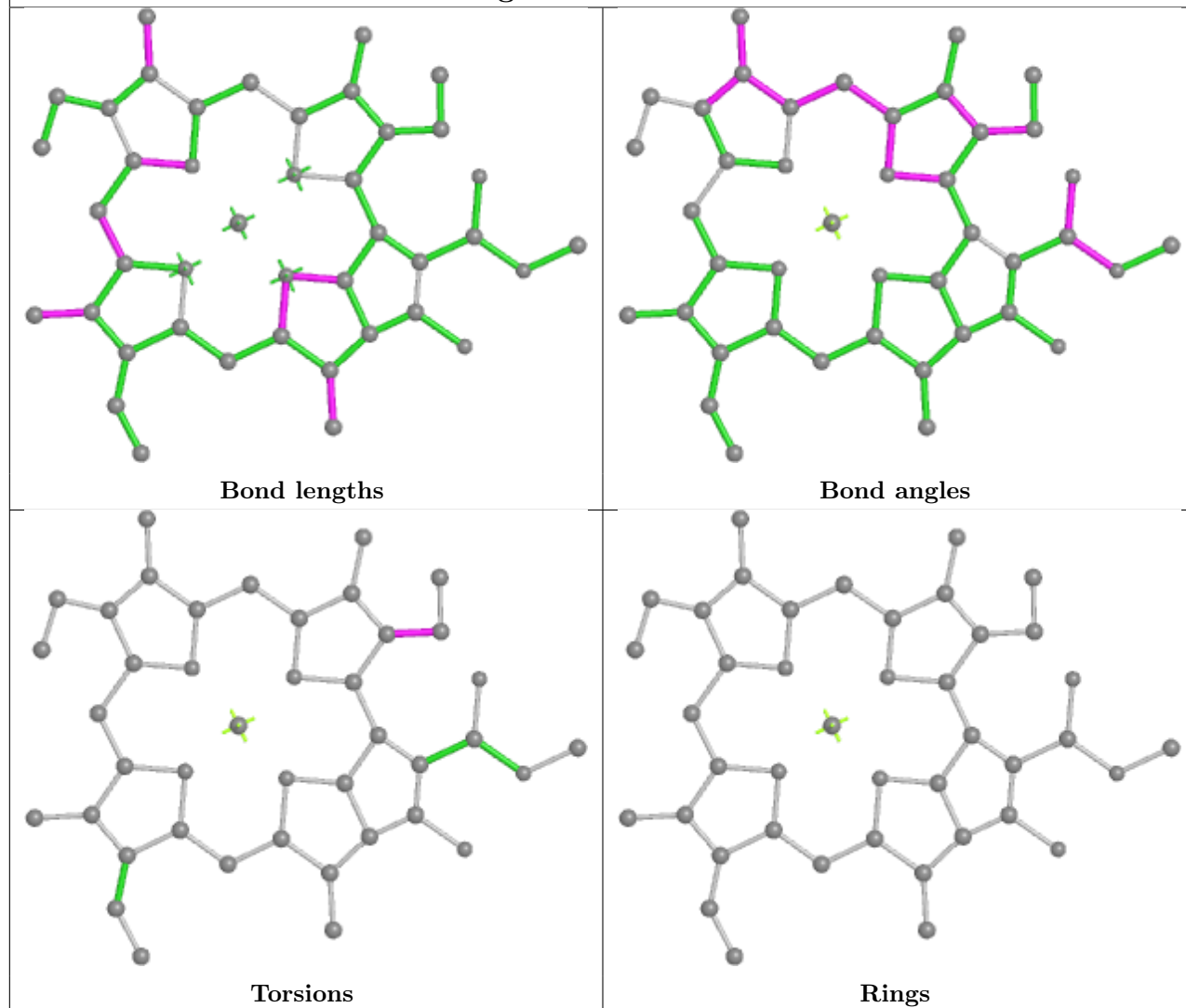


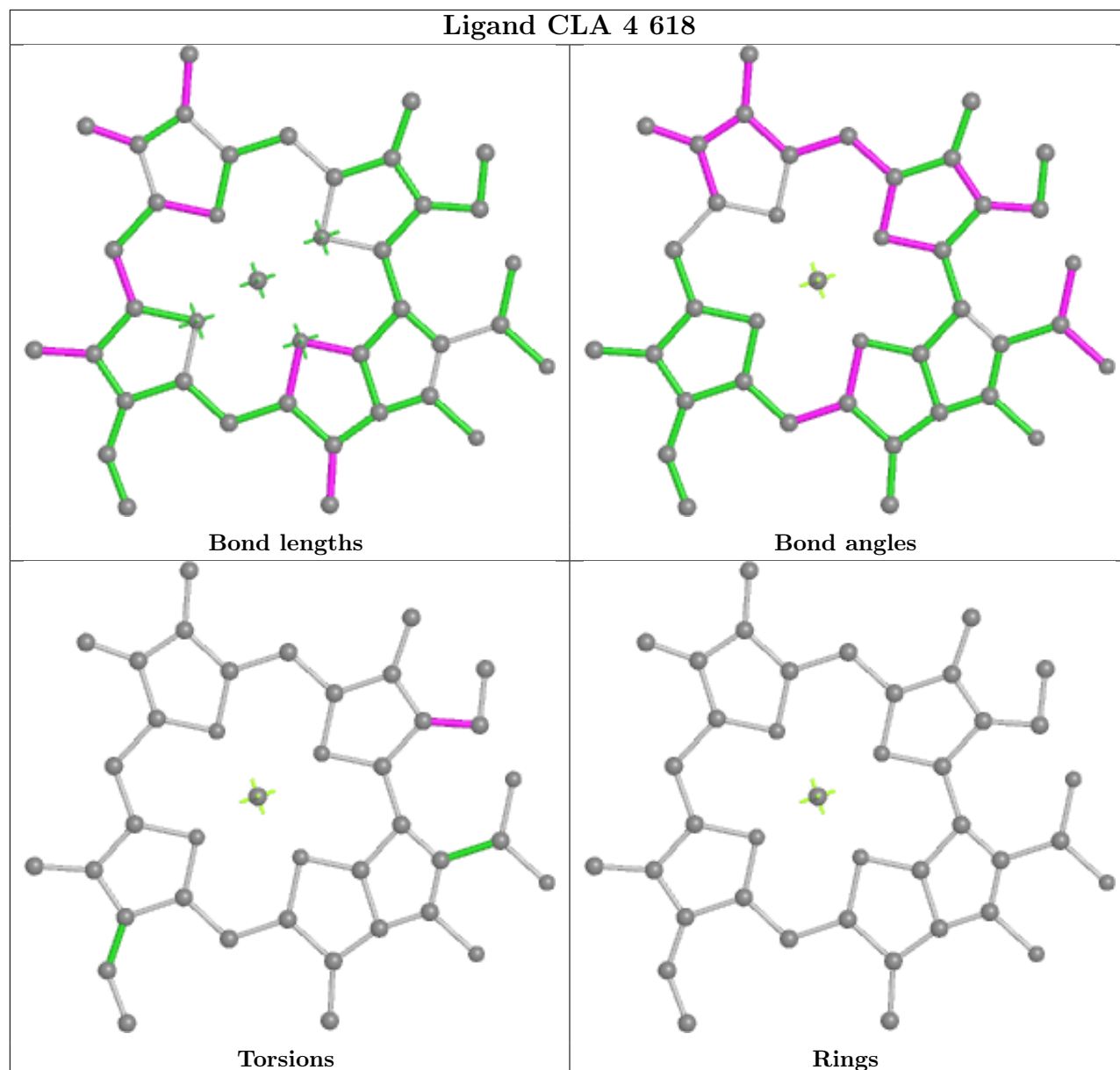


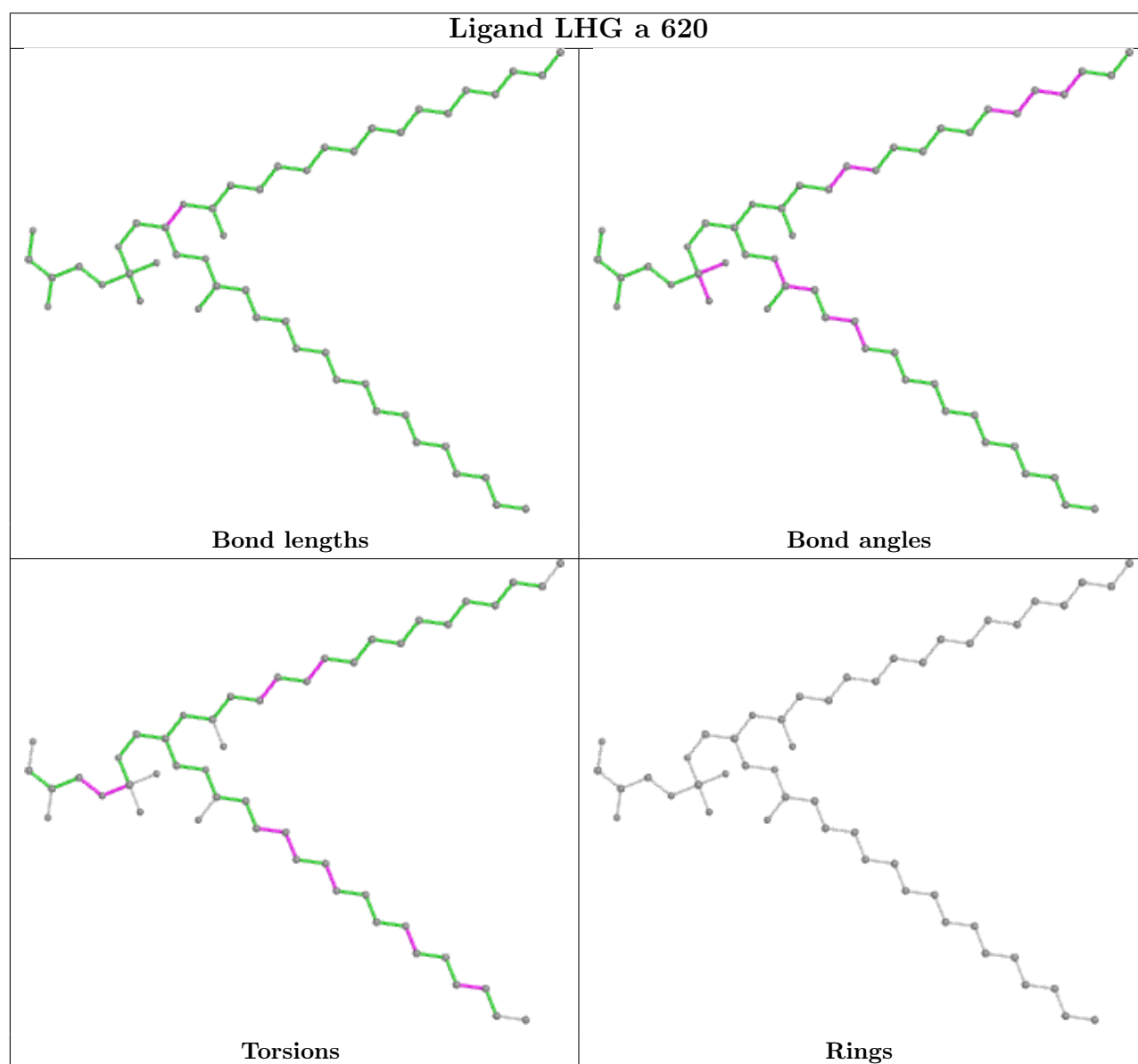
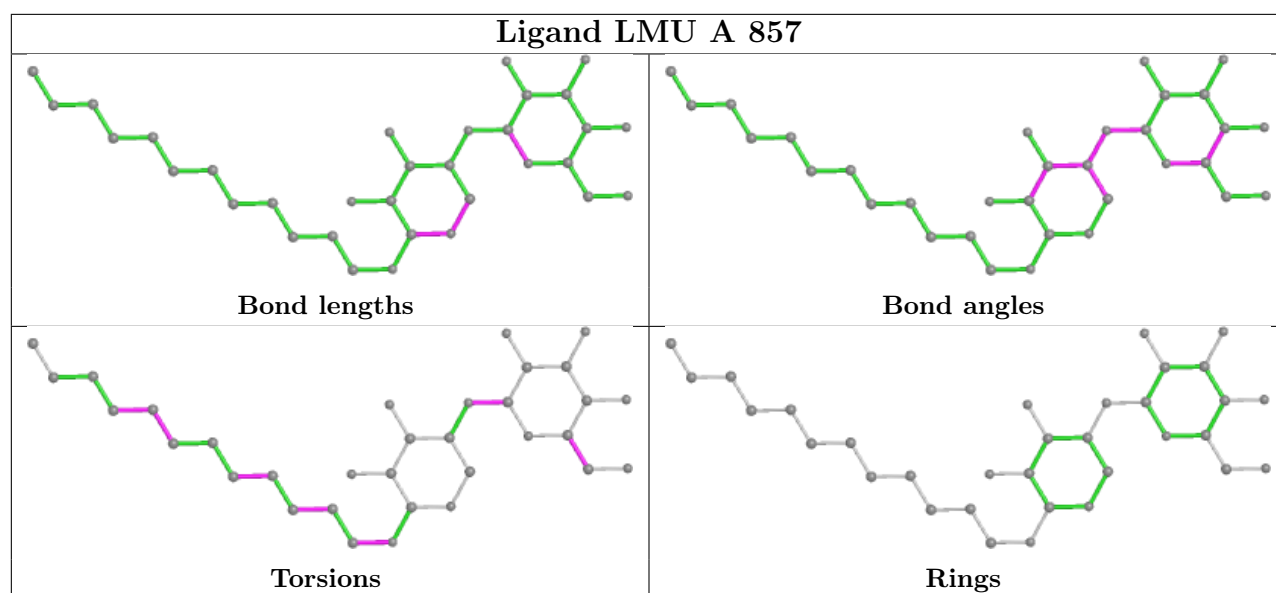


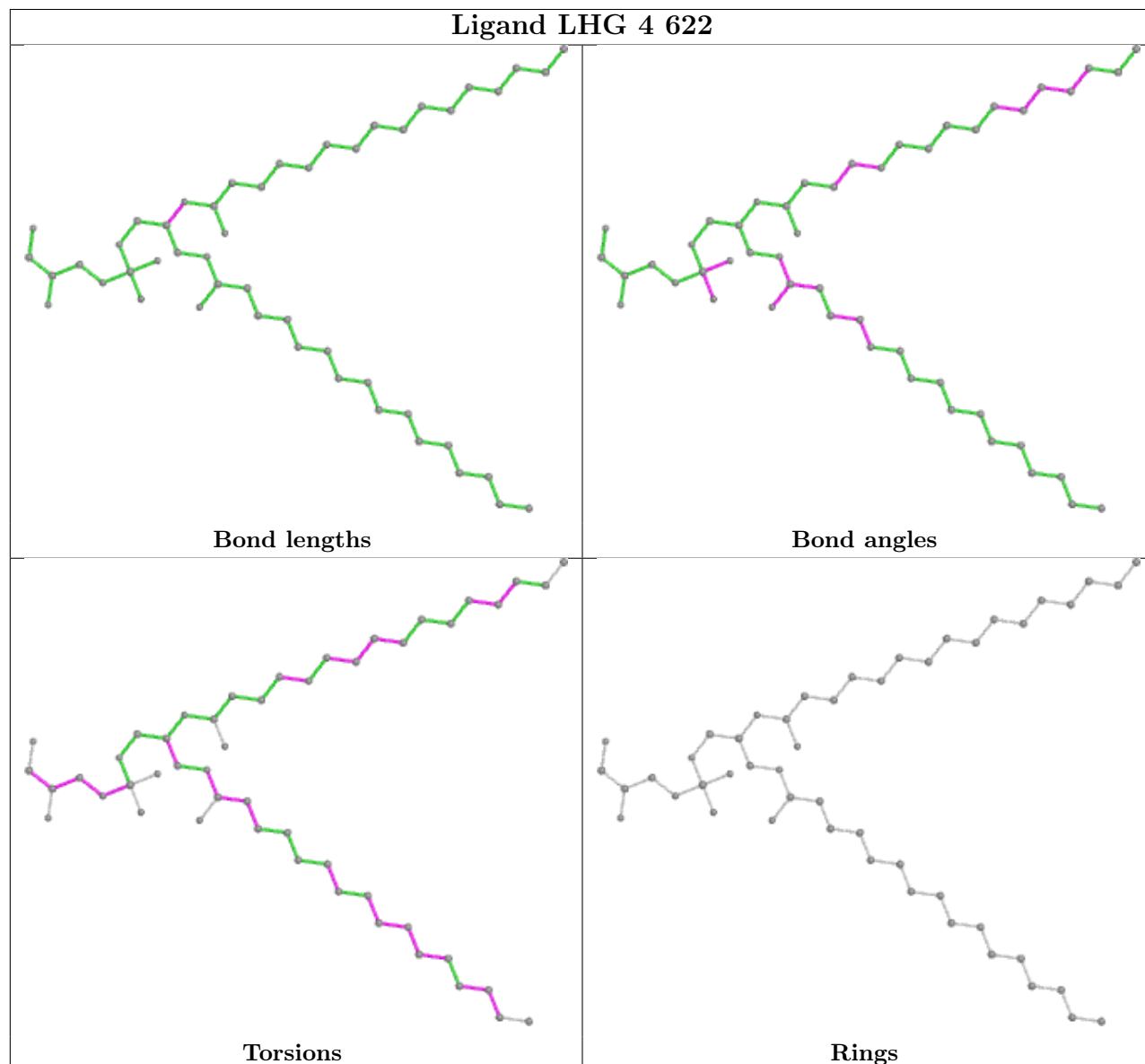
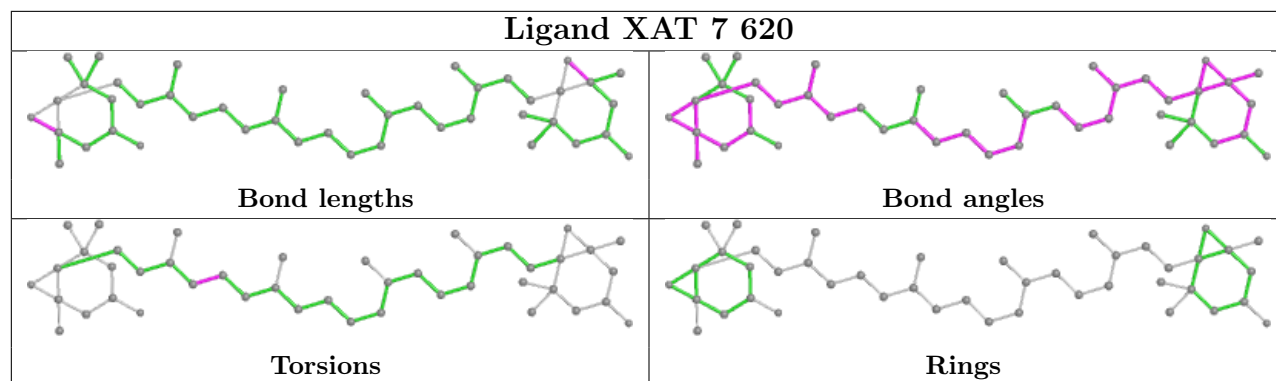


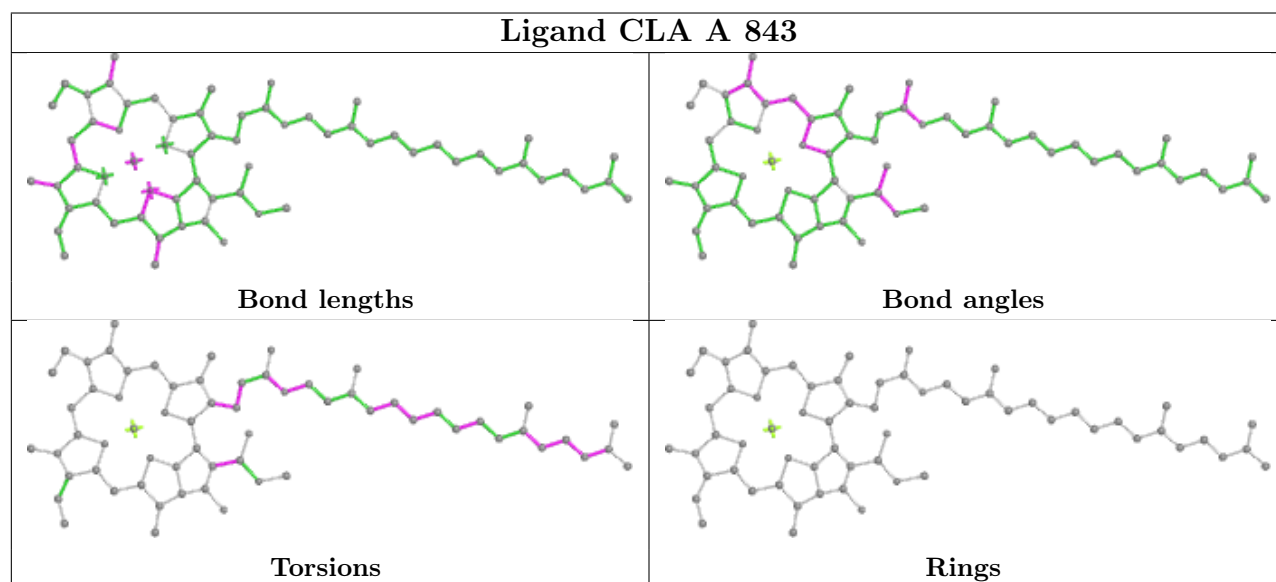
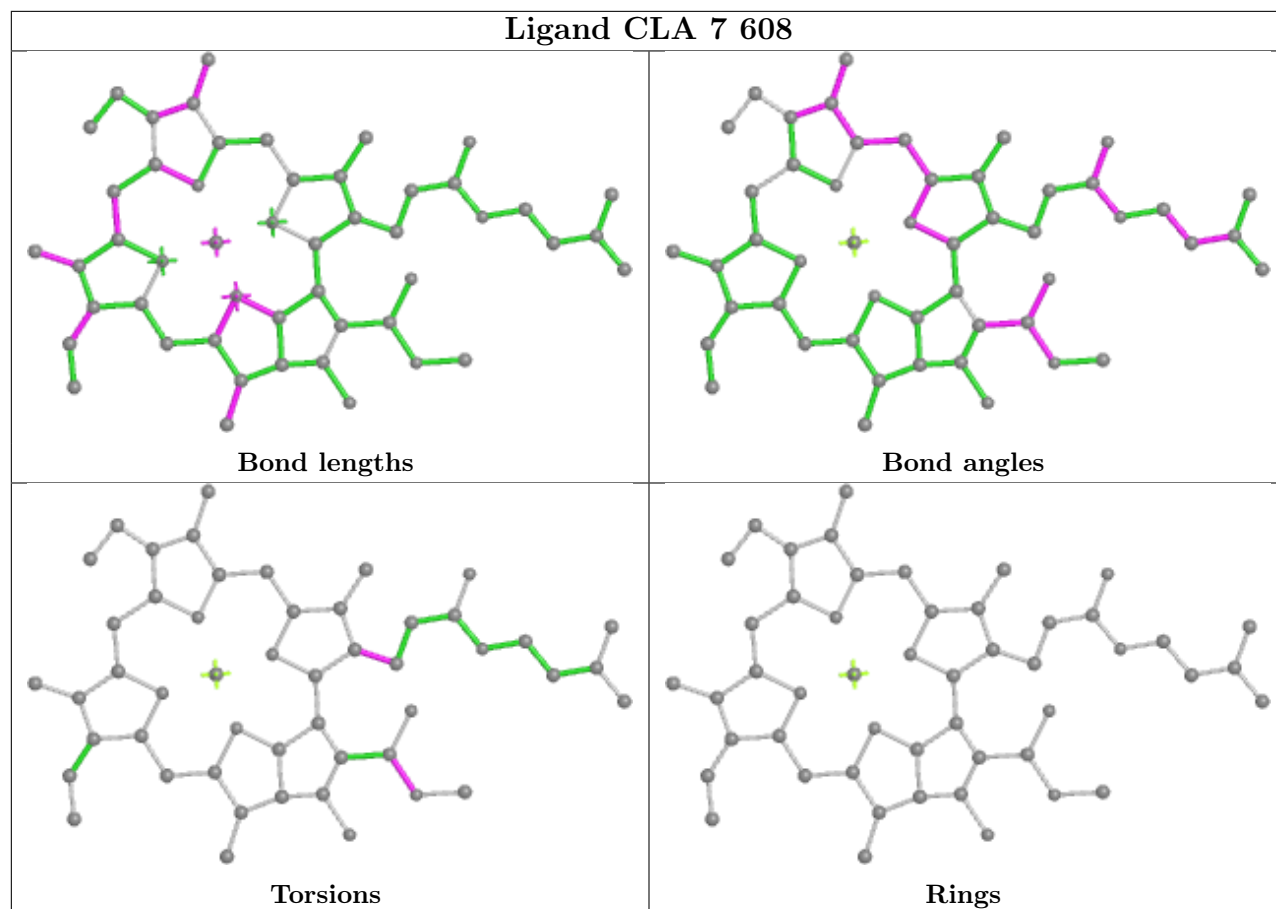
## Ligand CLA 6 611

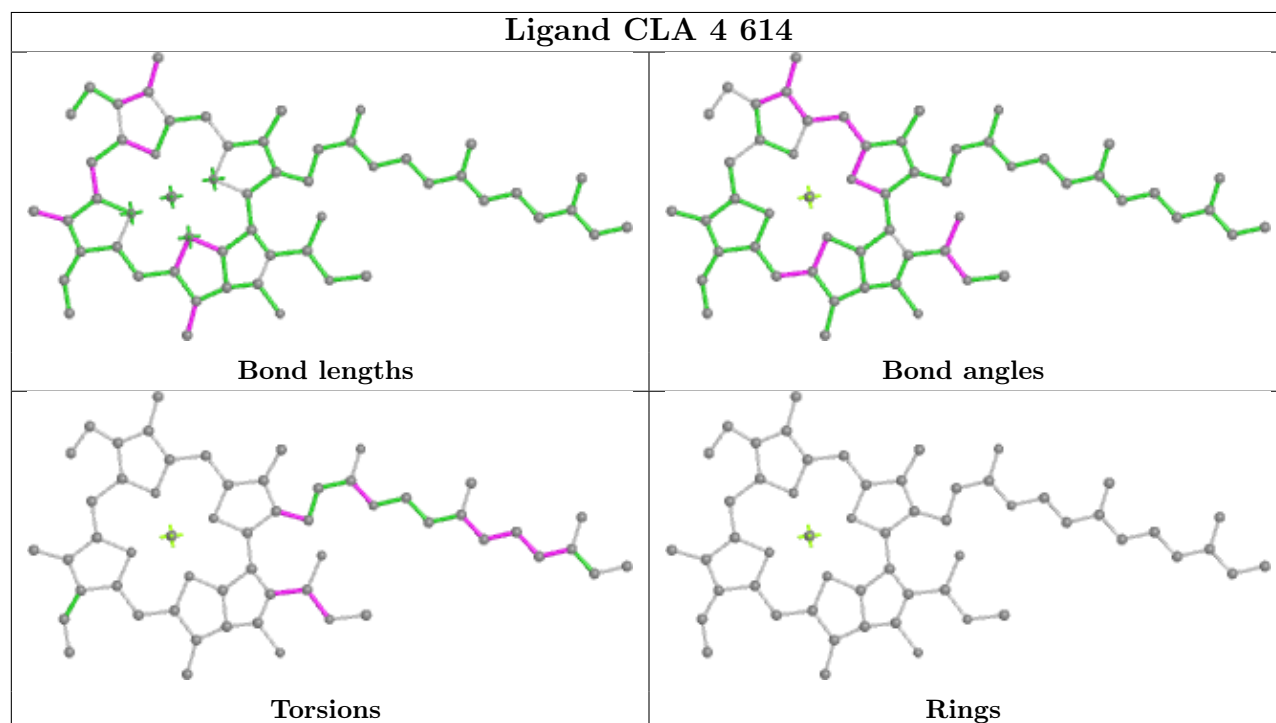
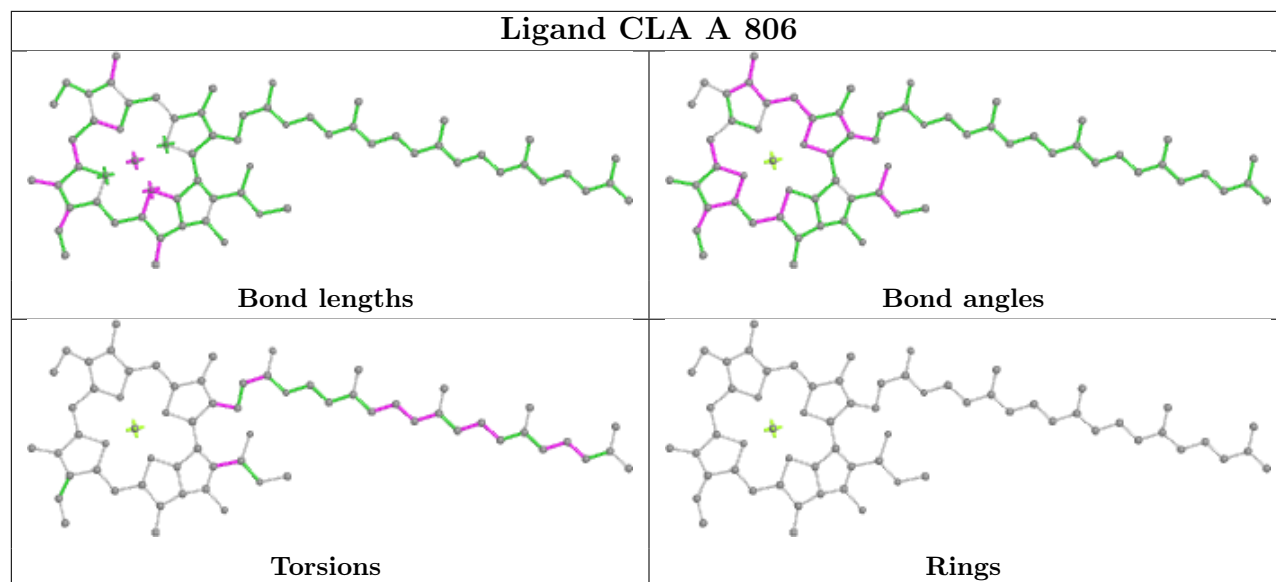


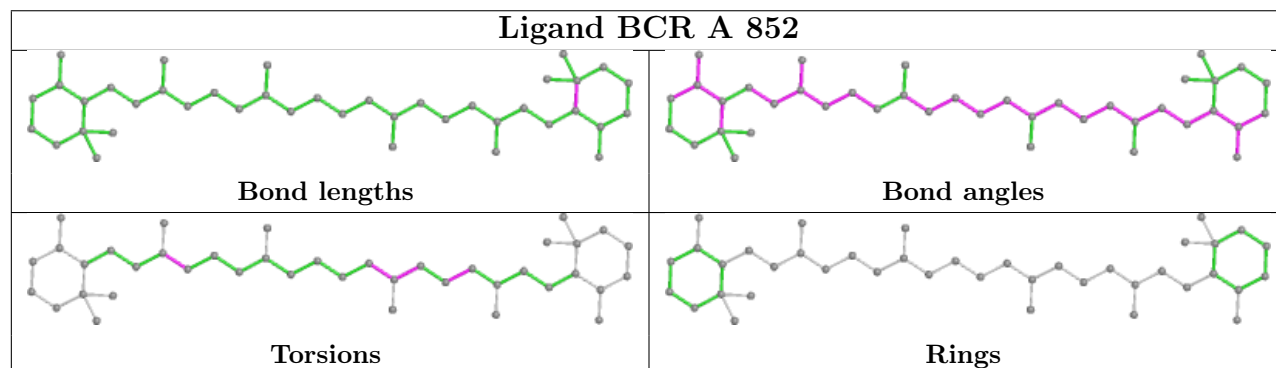
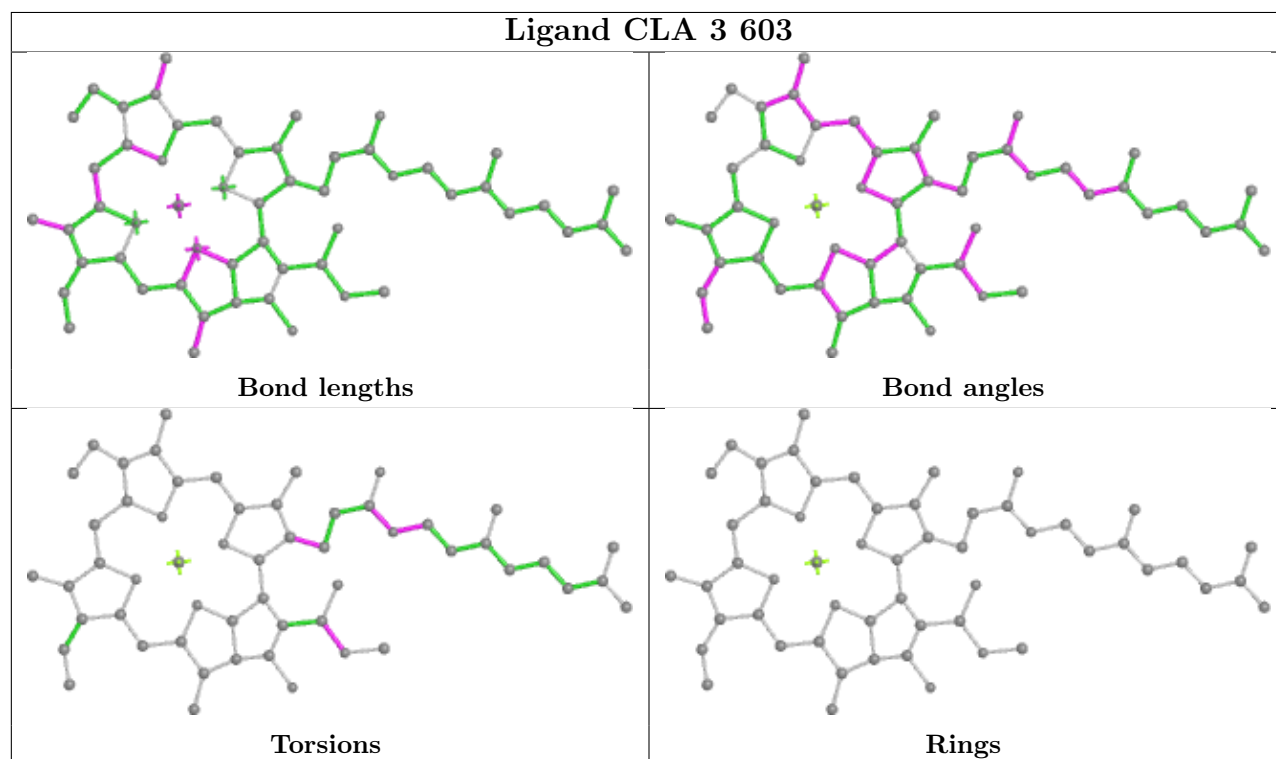
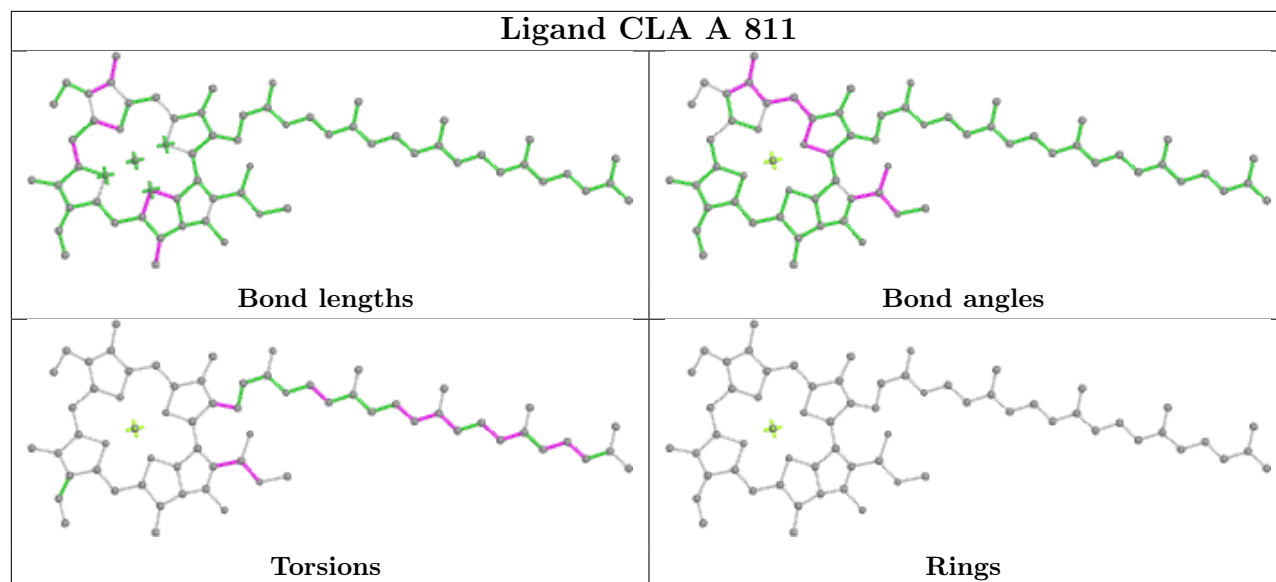


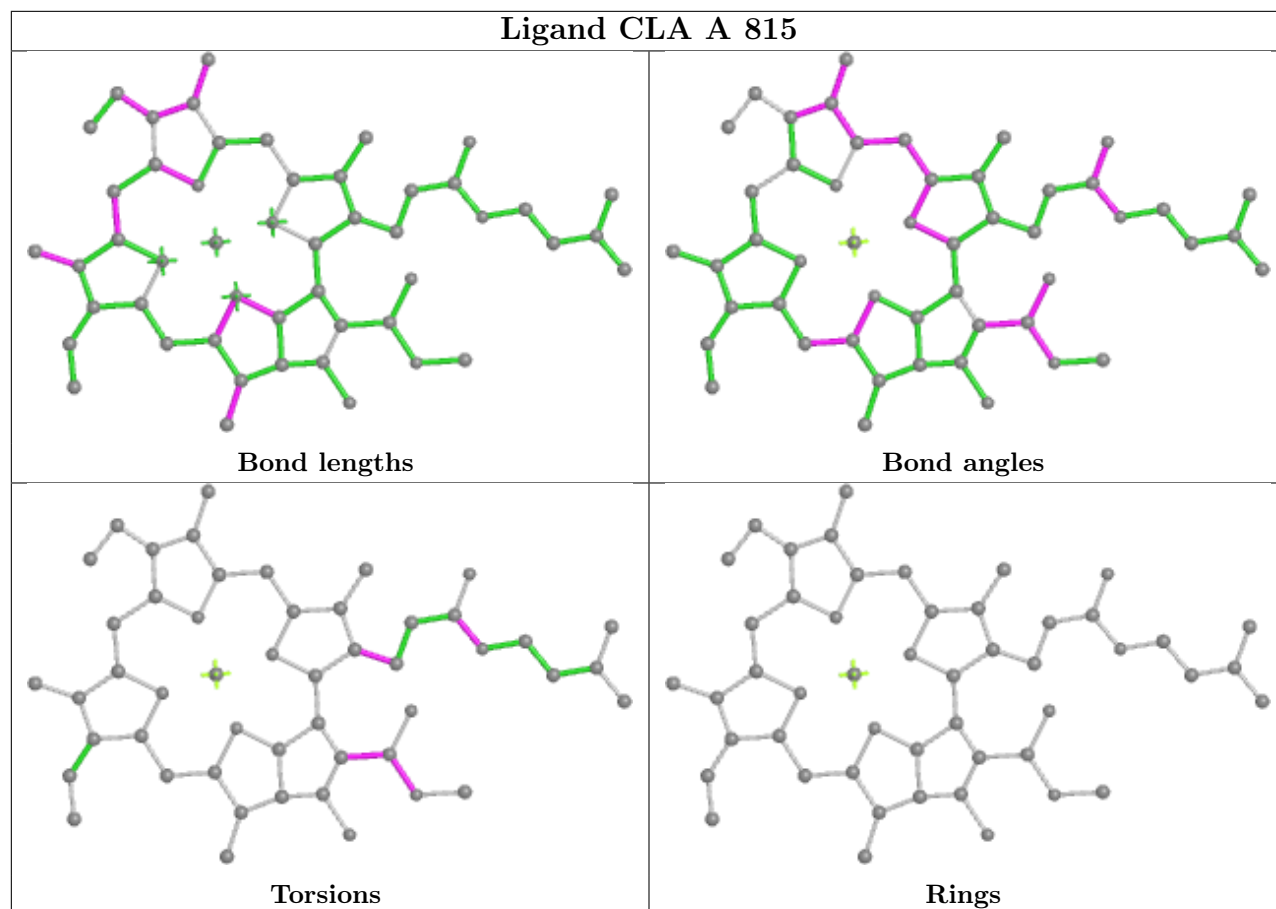
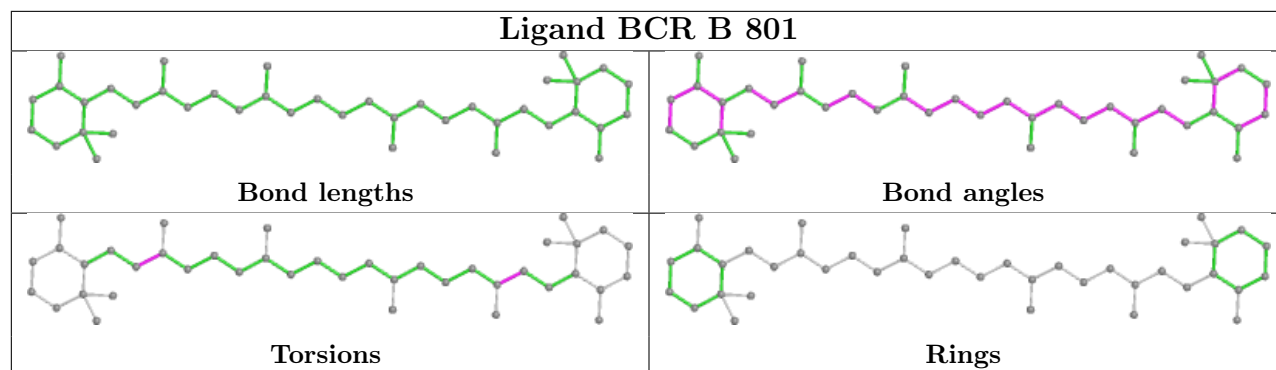




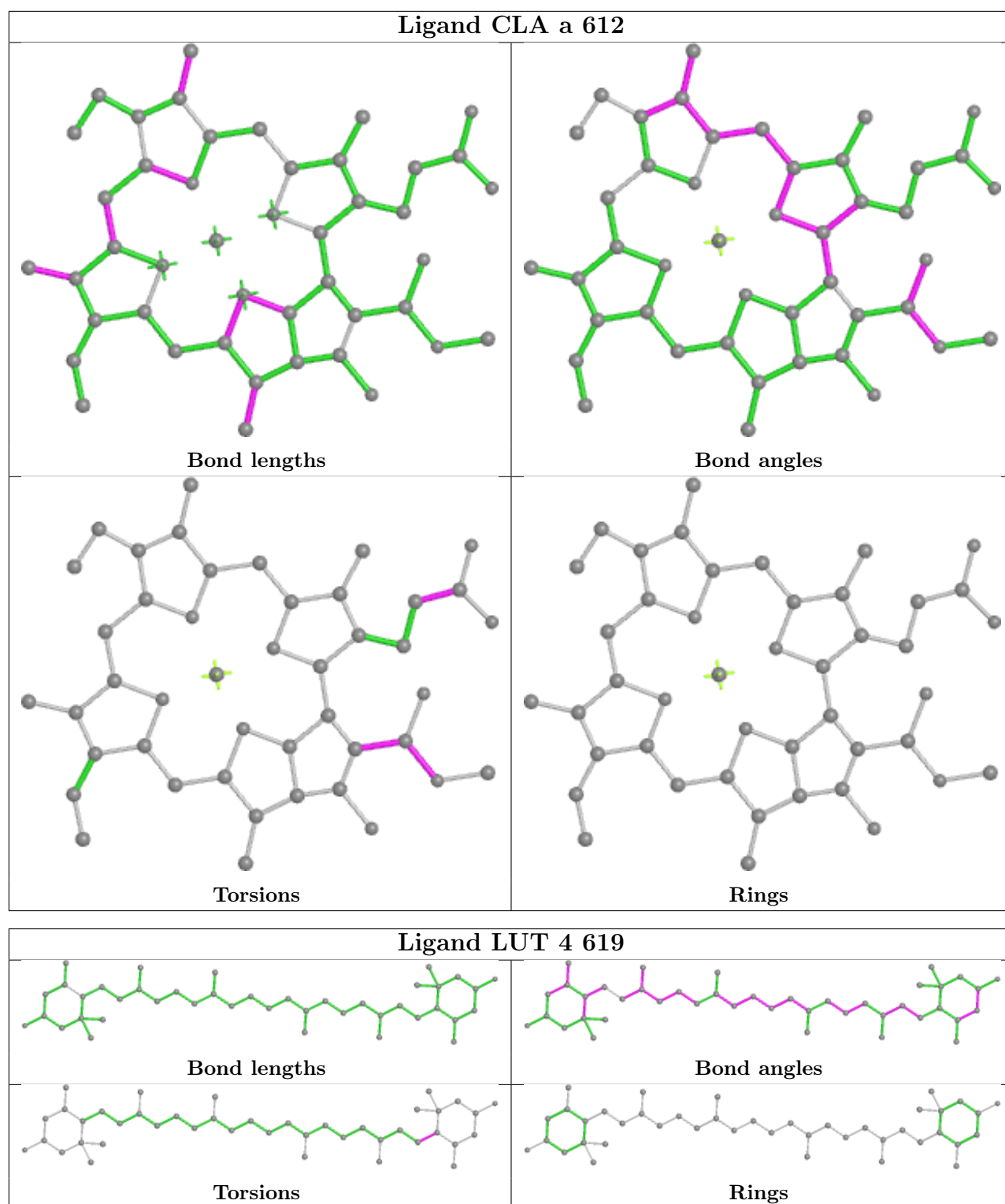


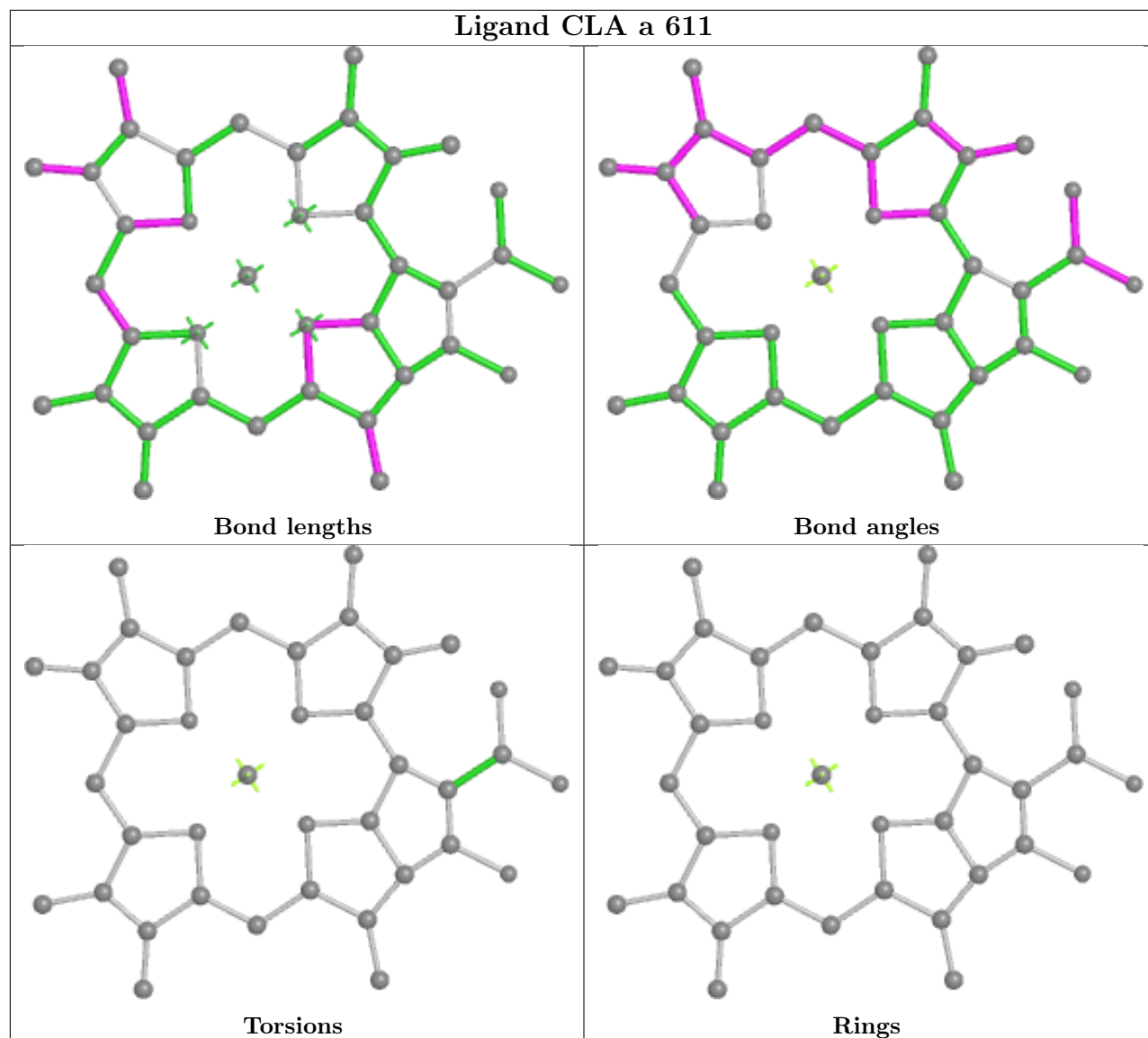


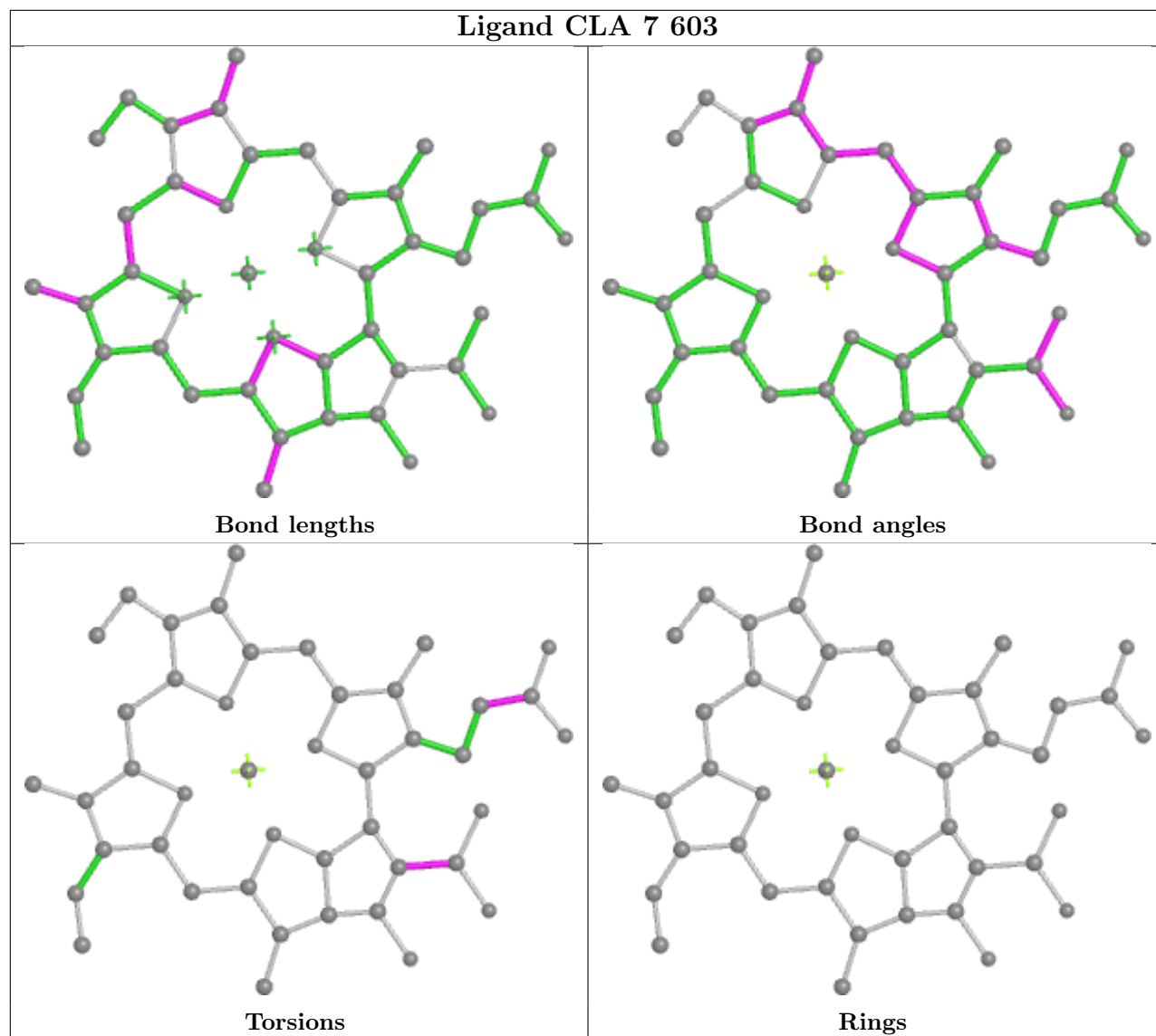


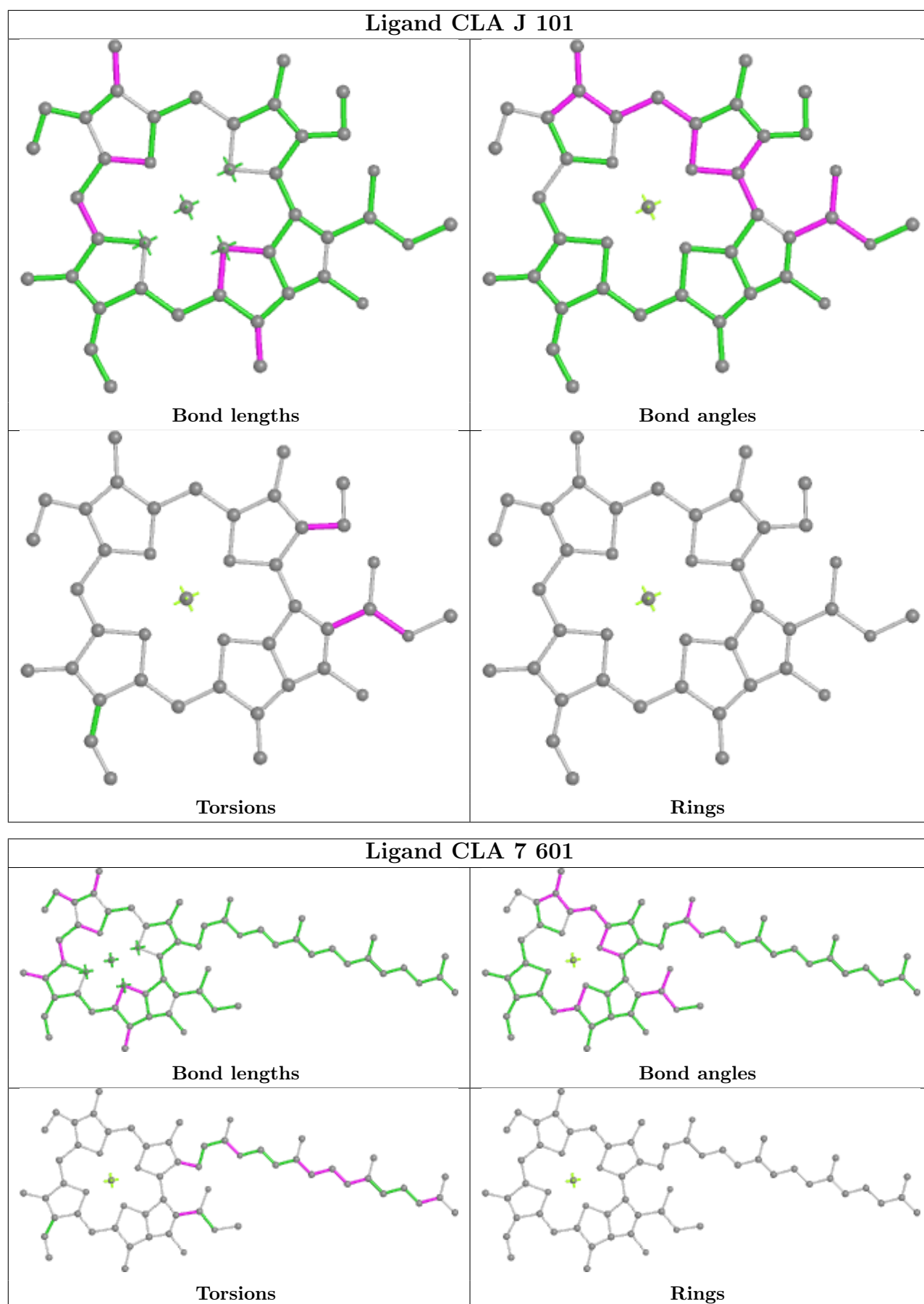


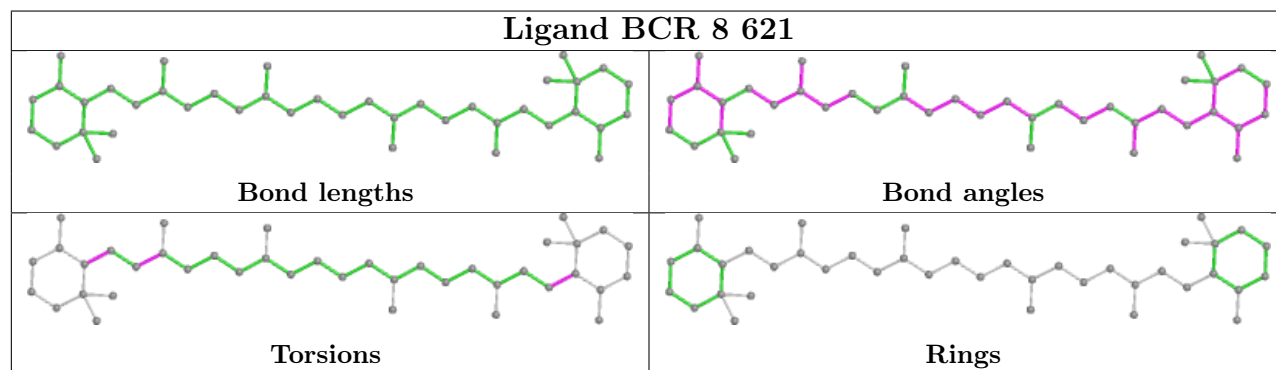
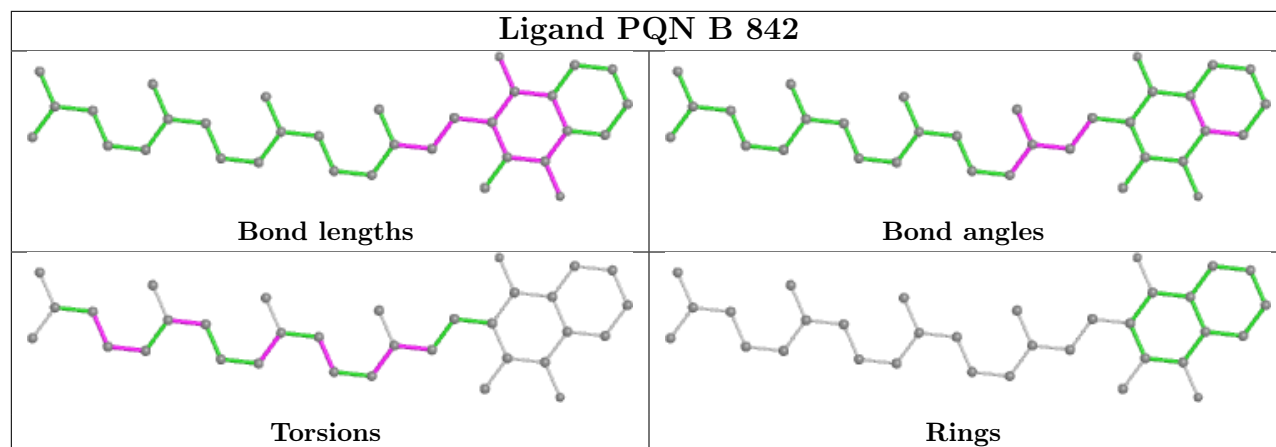


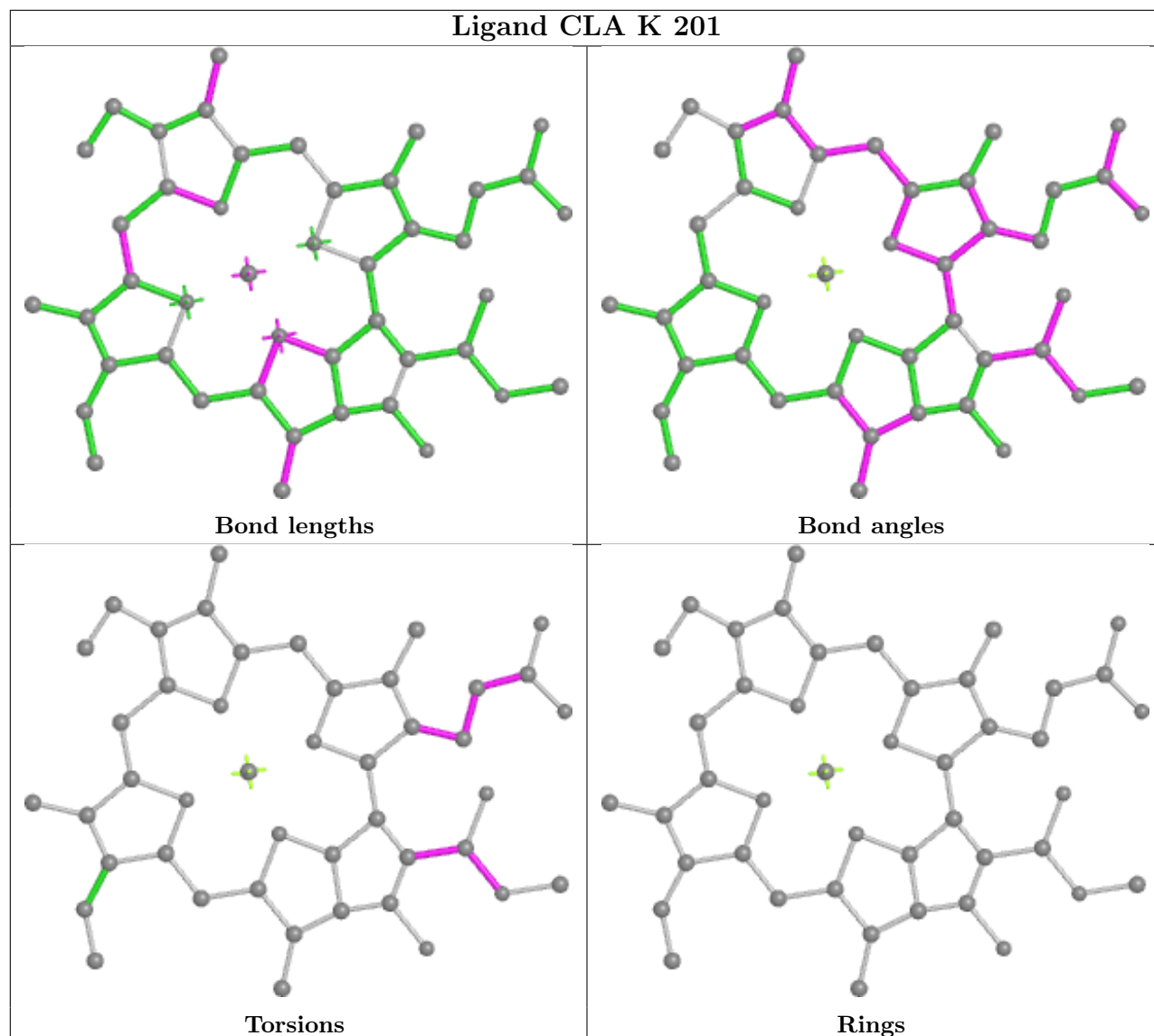


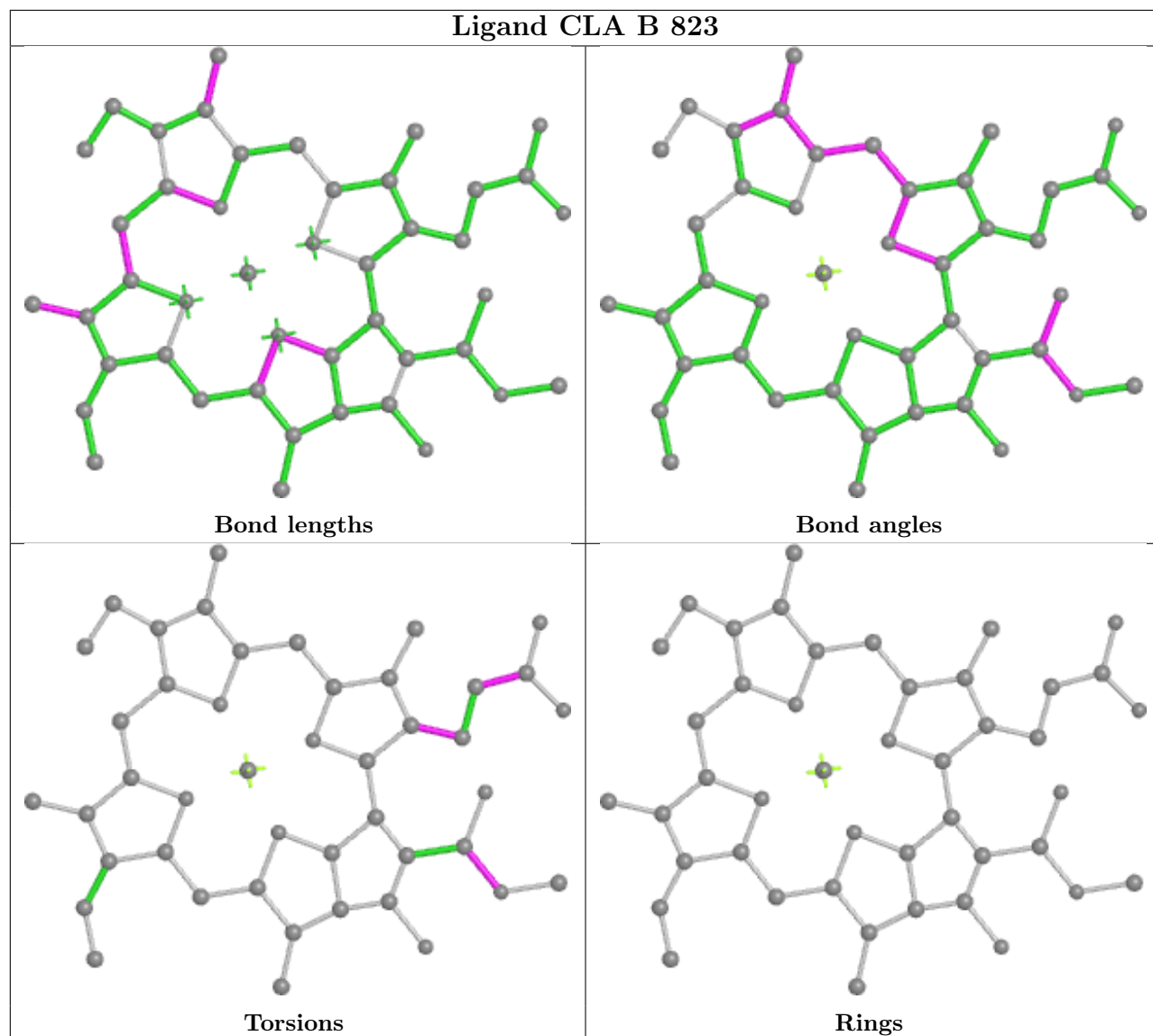


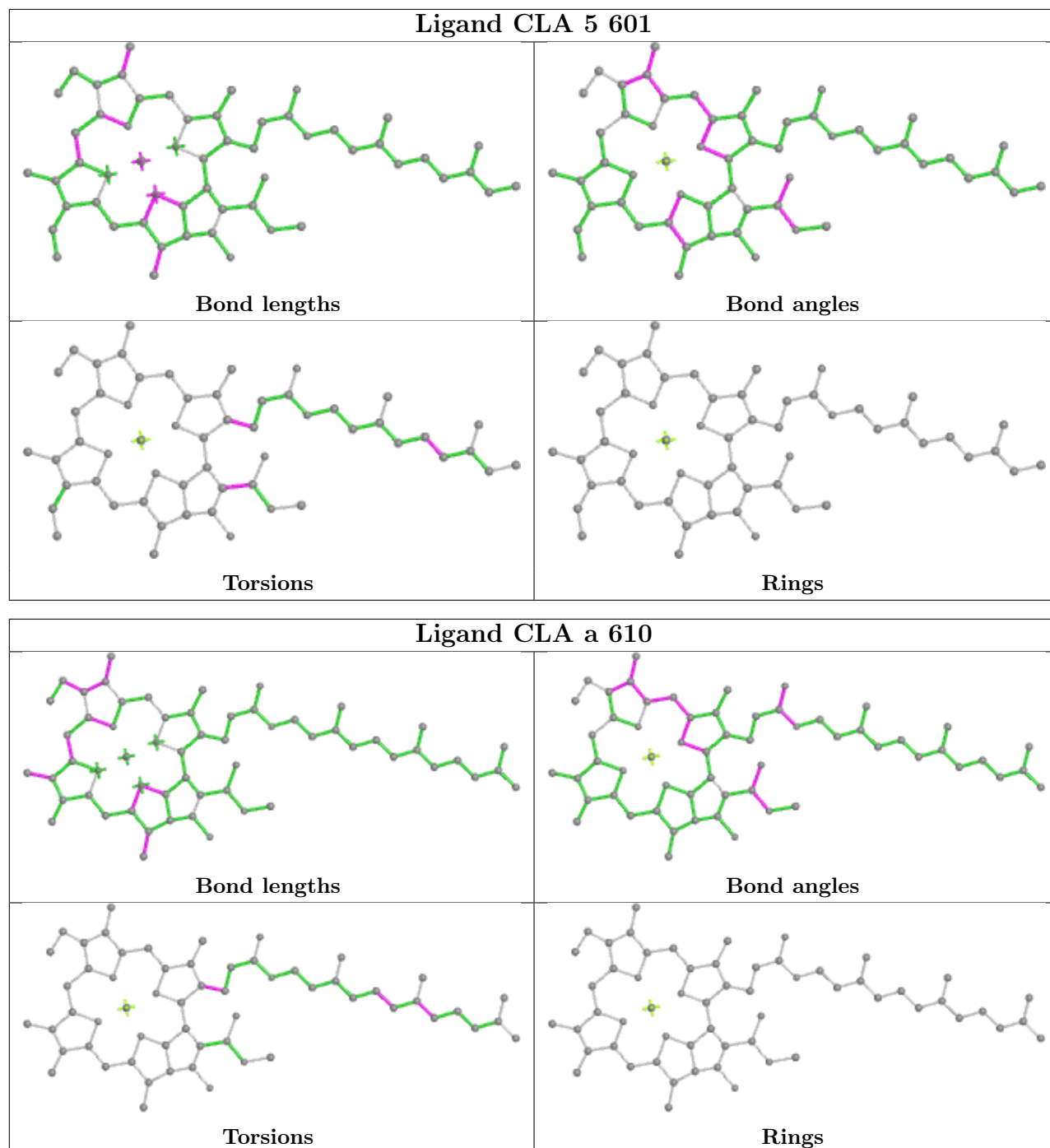




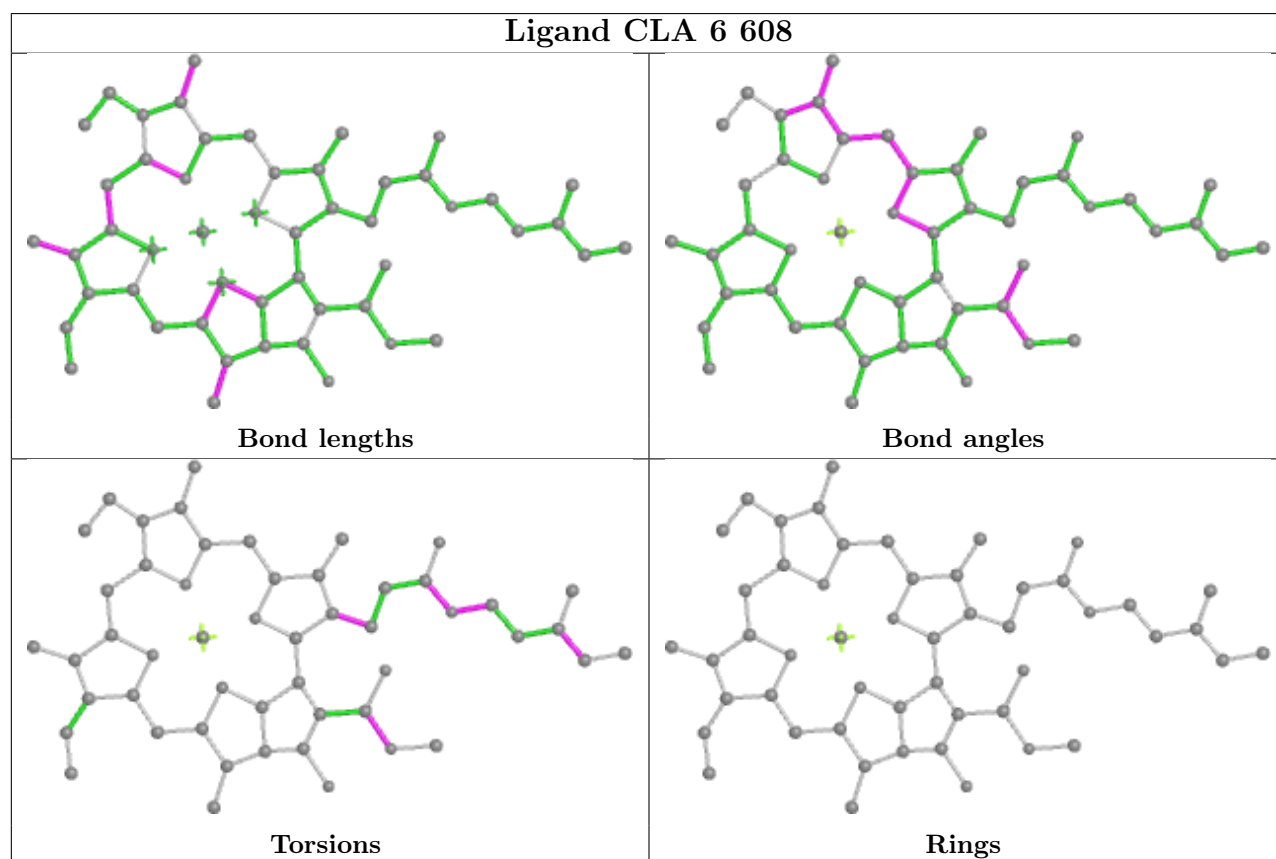
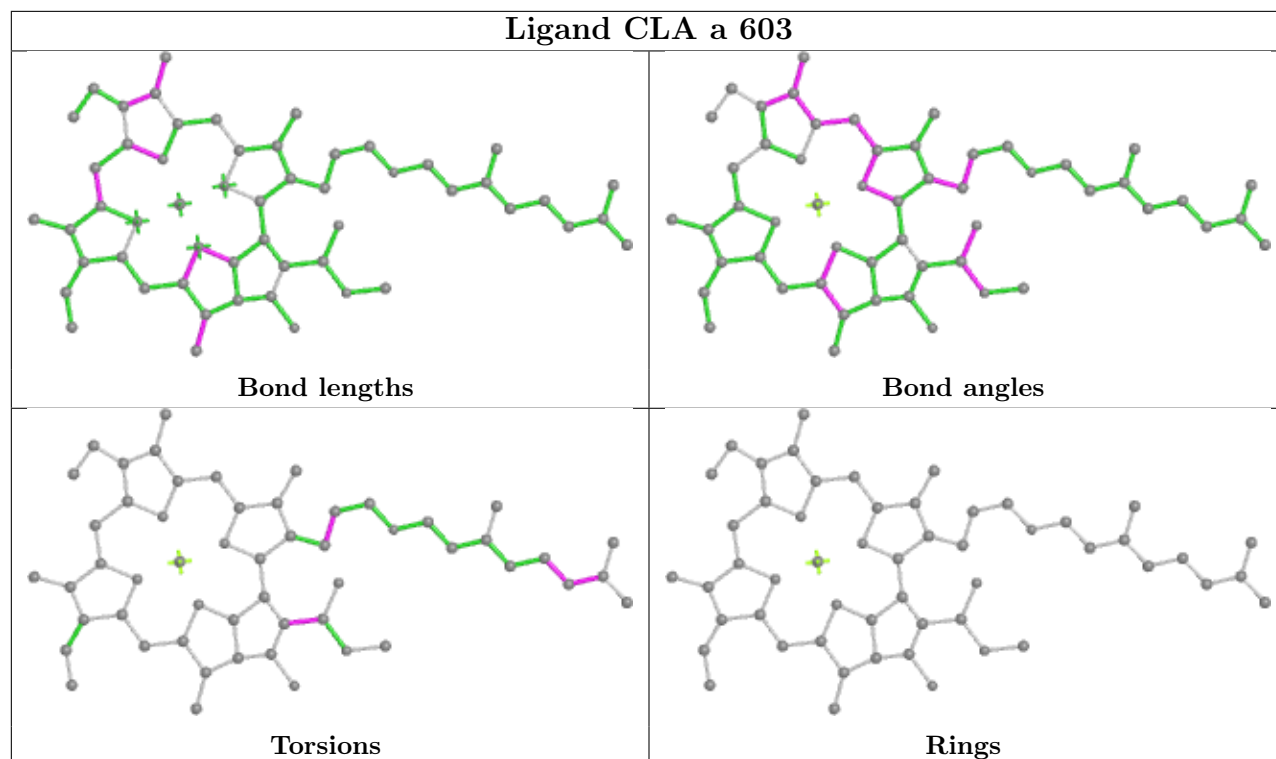


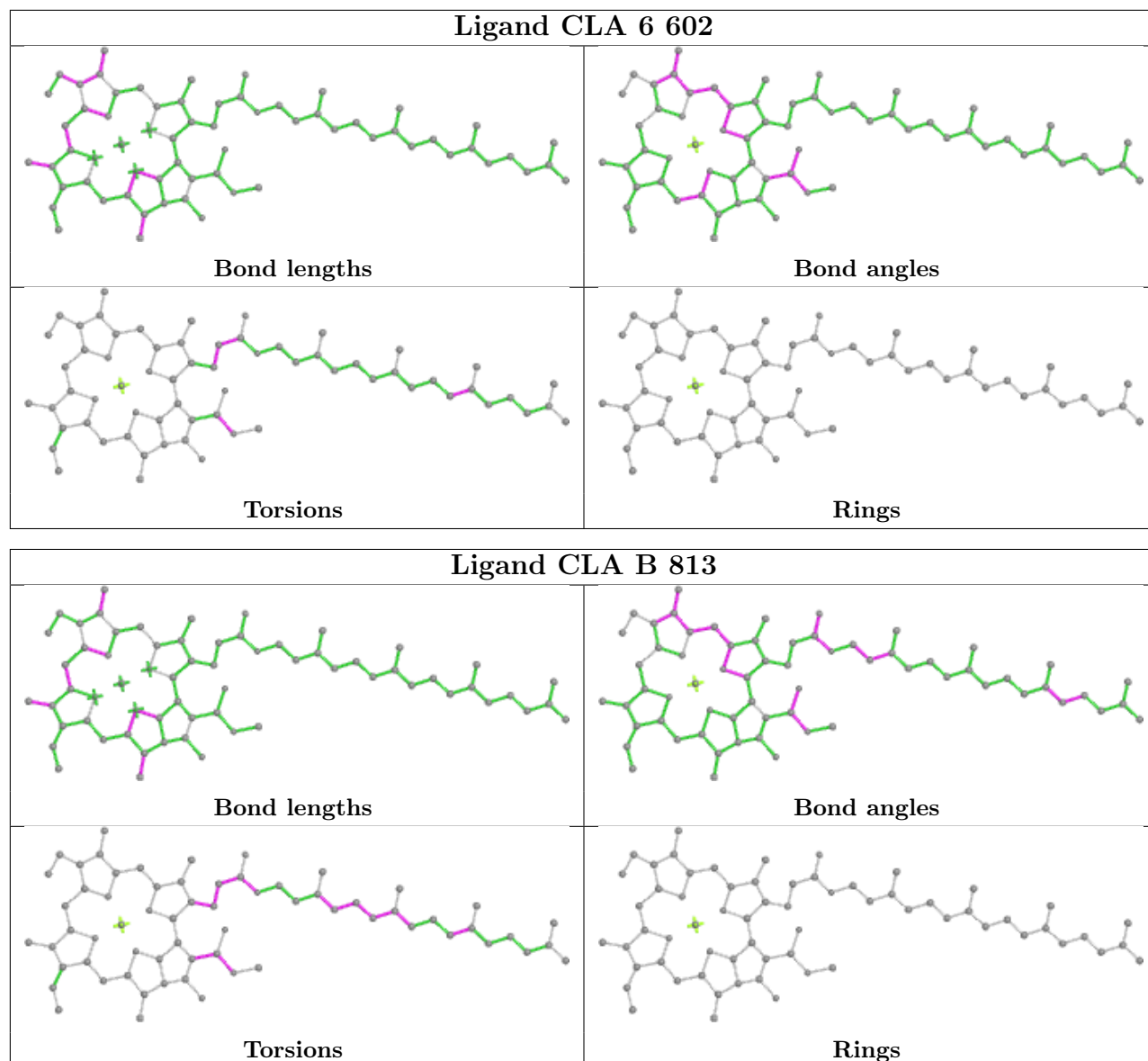


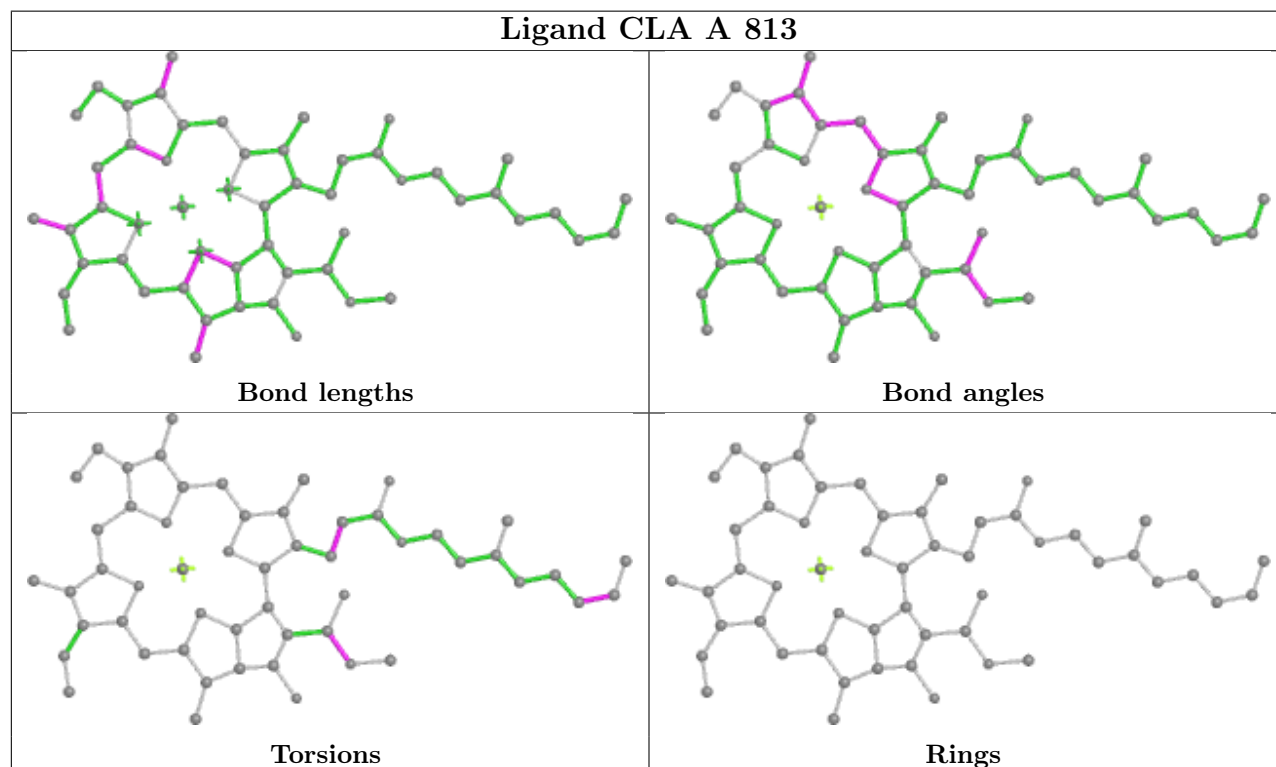
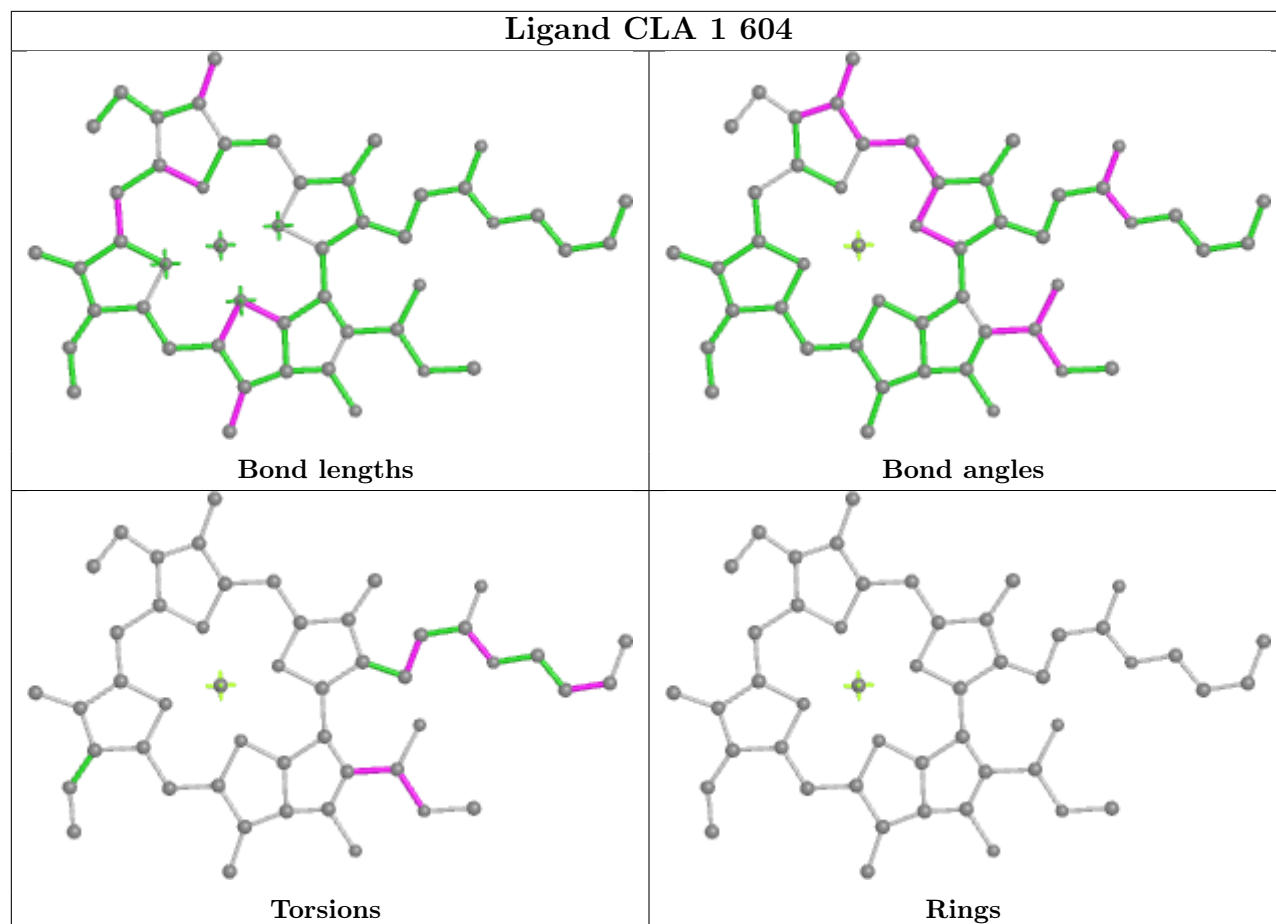


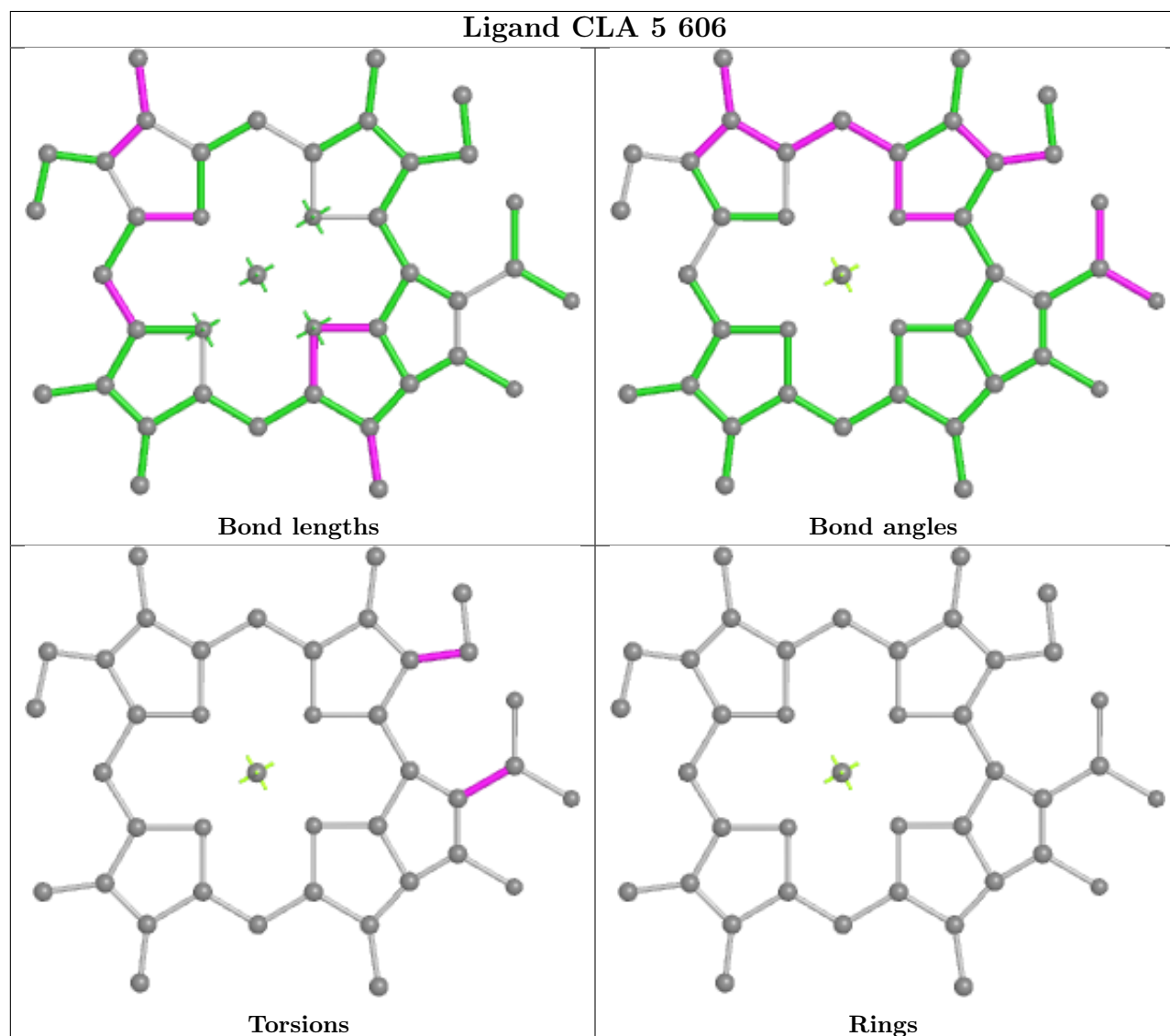
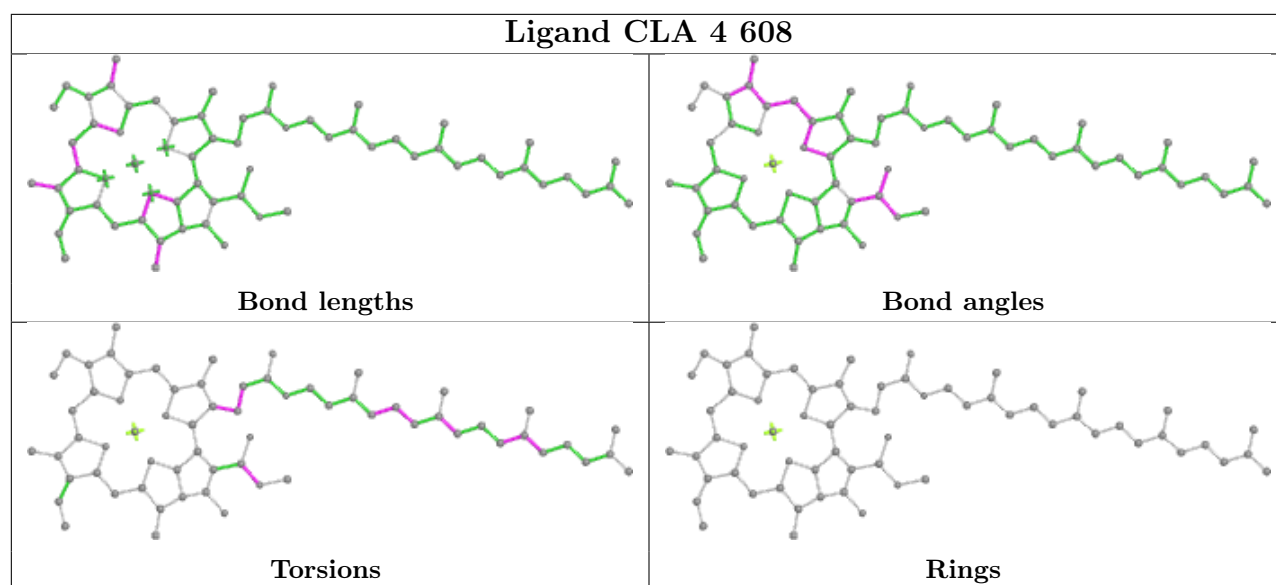


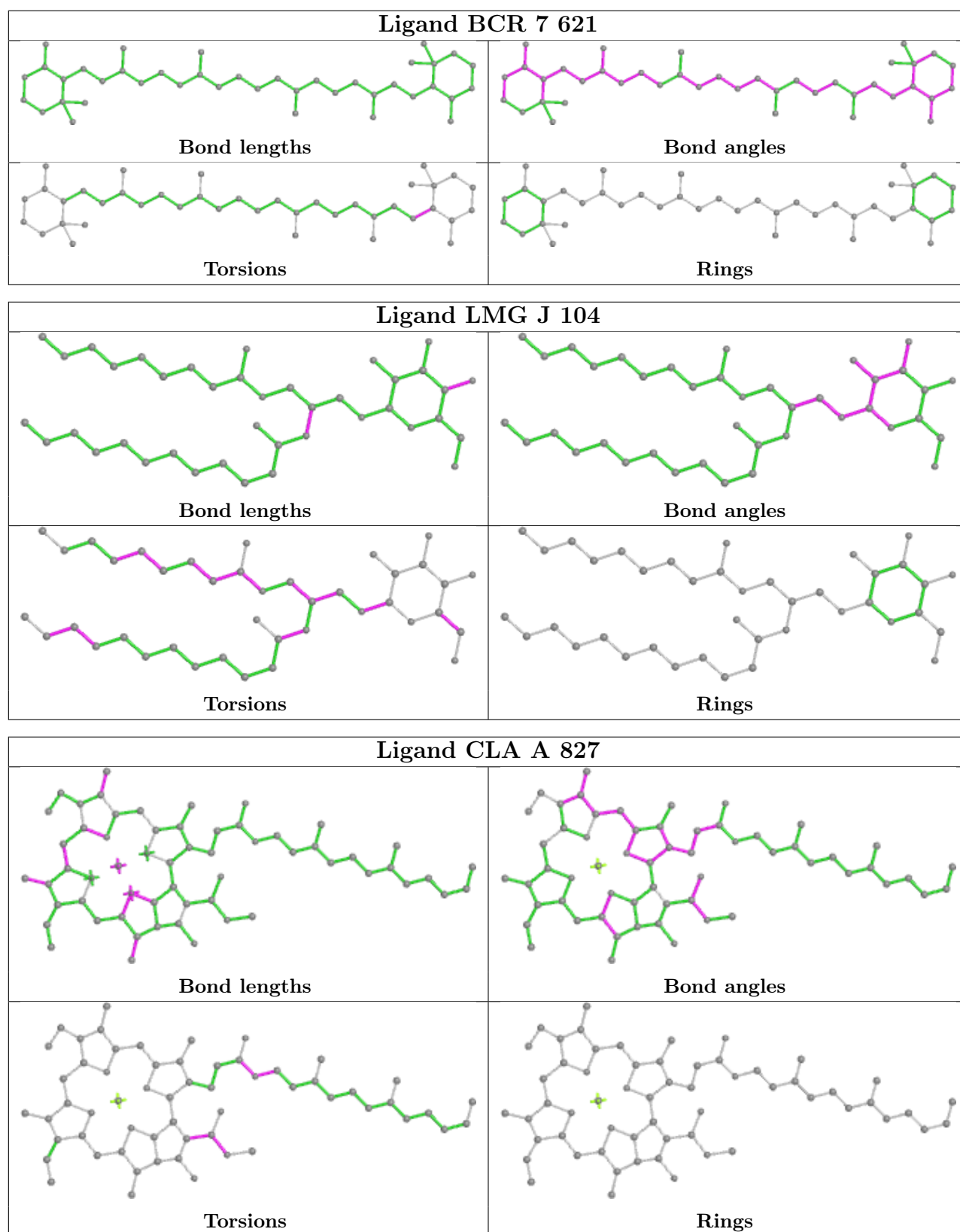


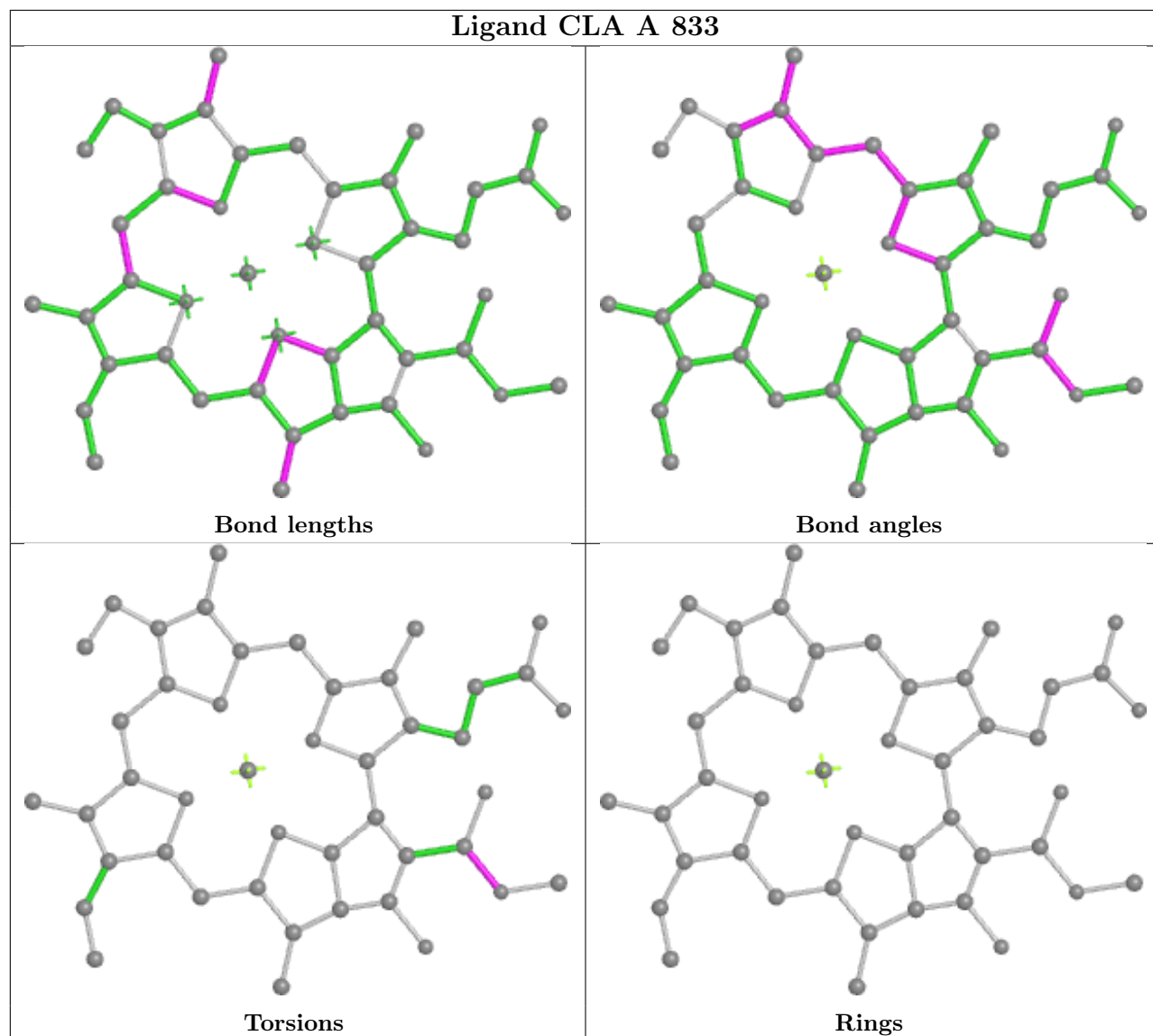


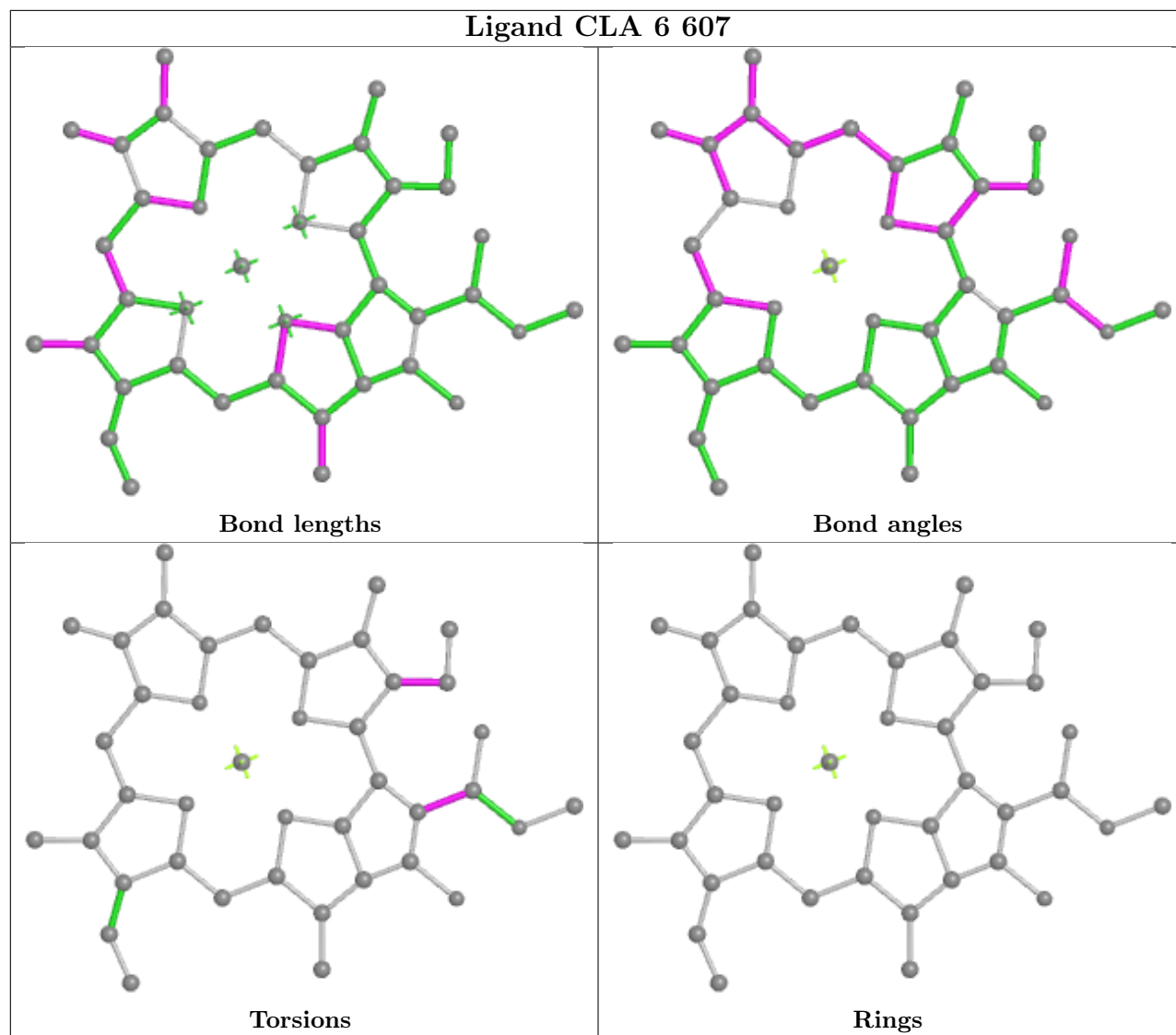


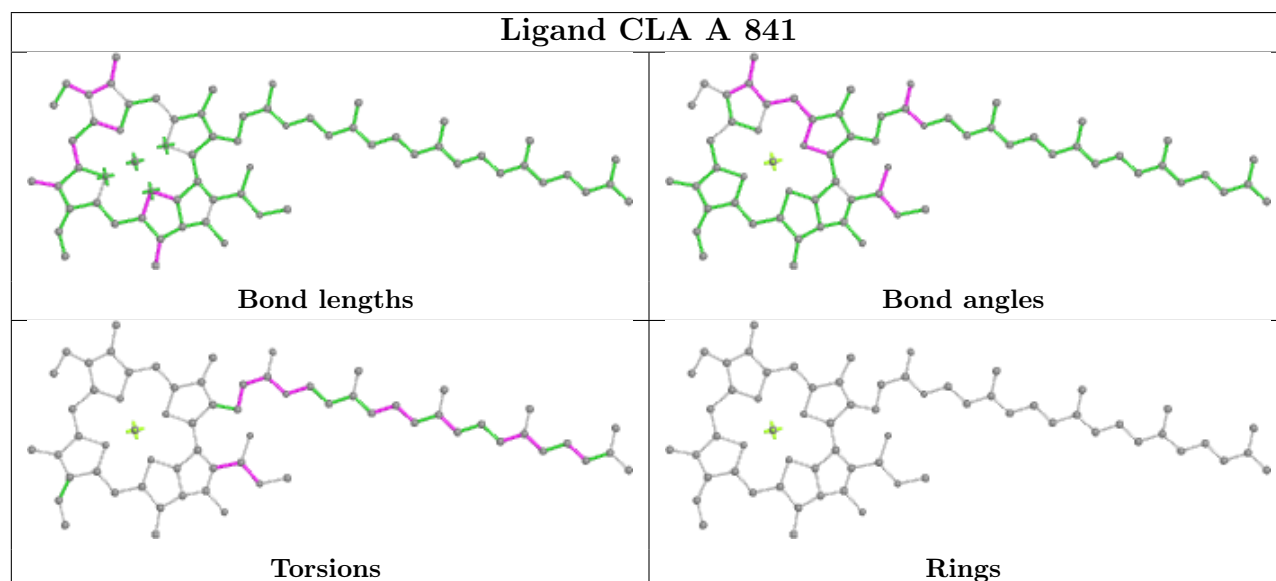
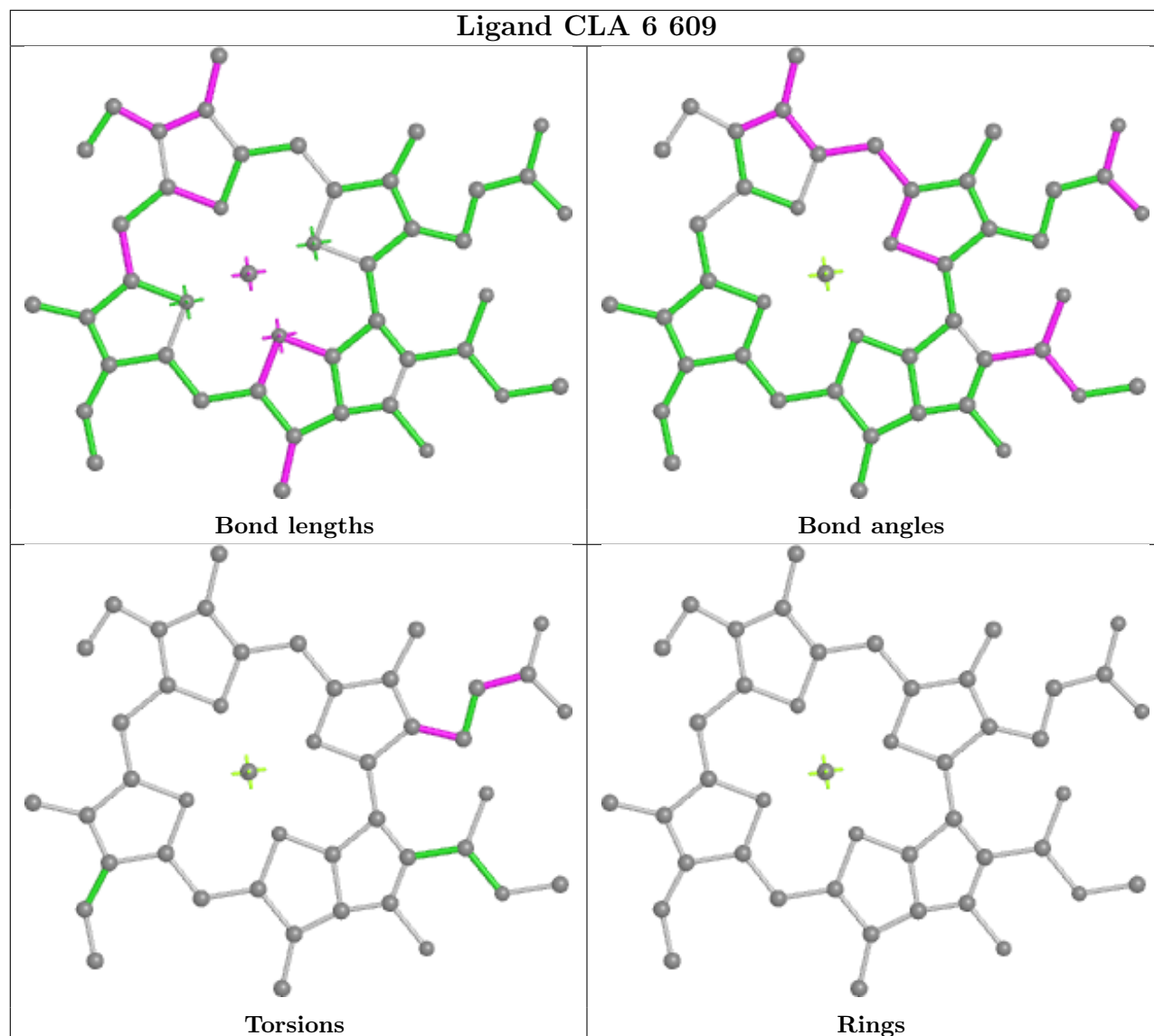




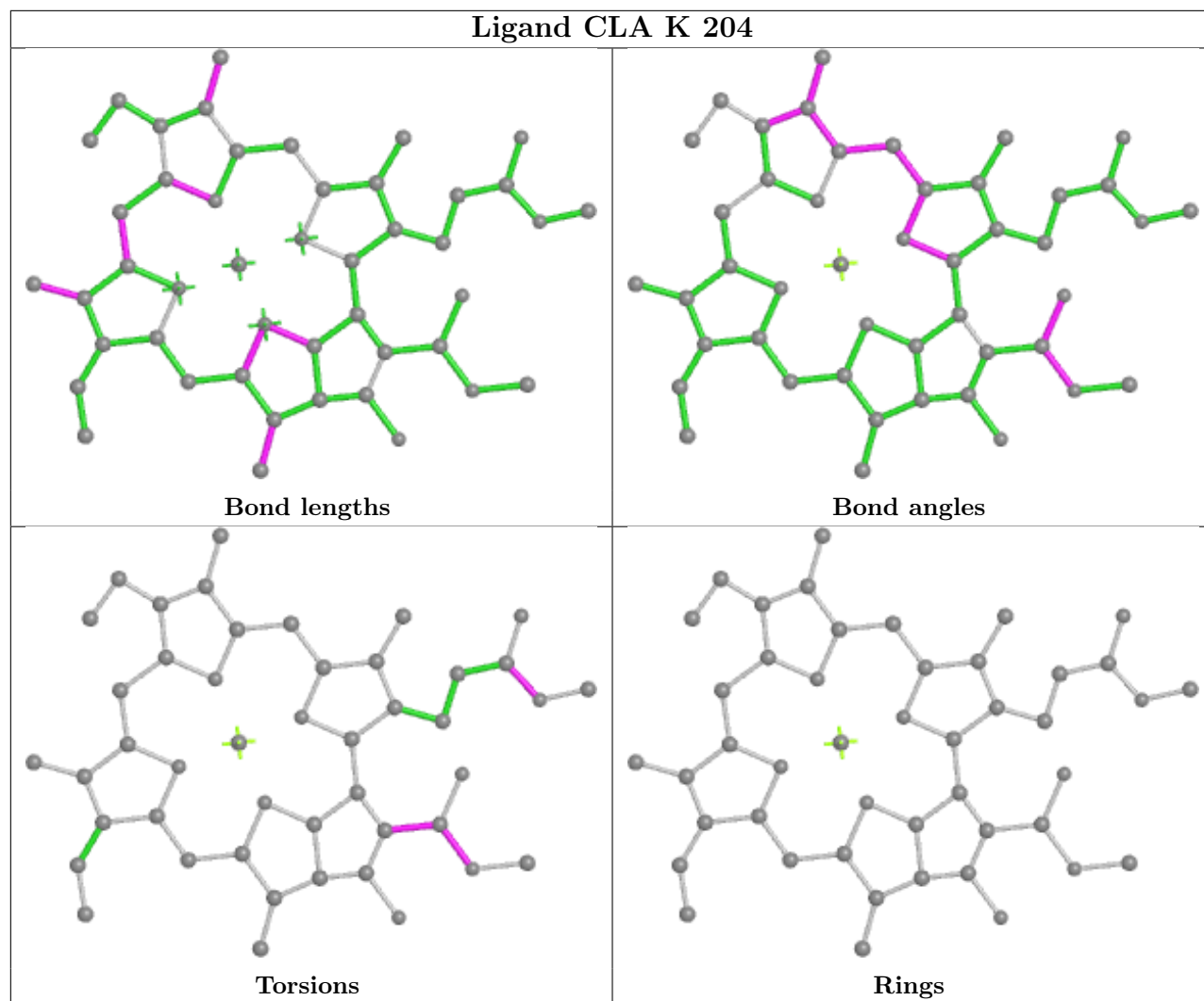
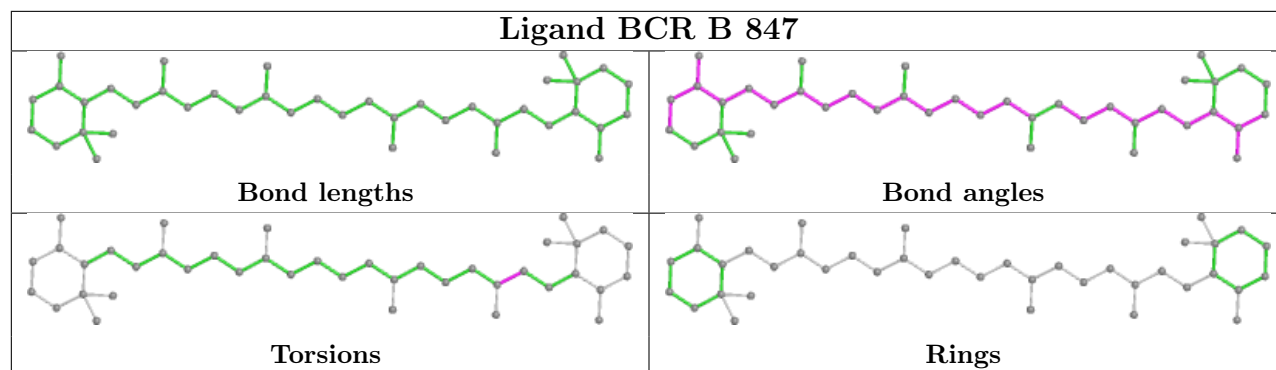


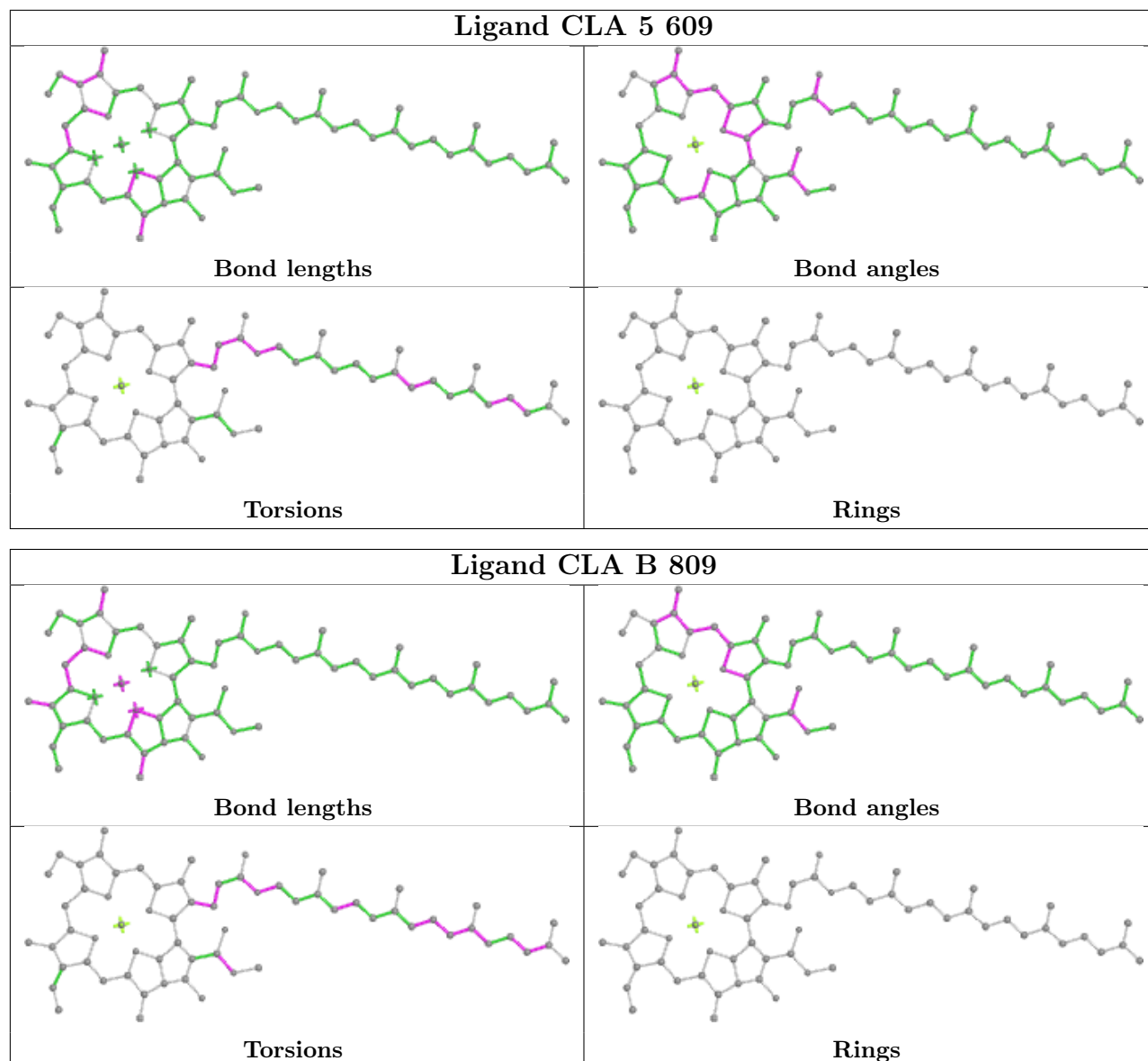


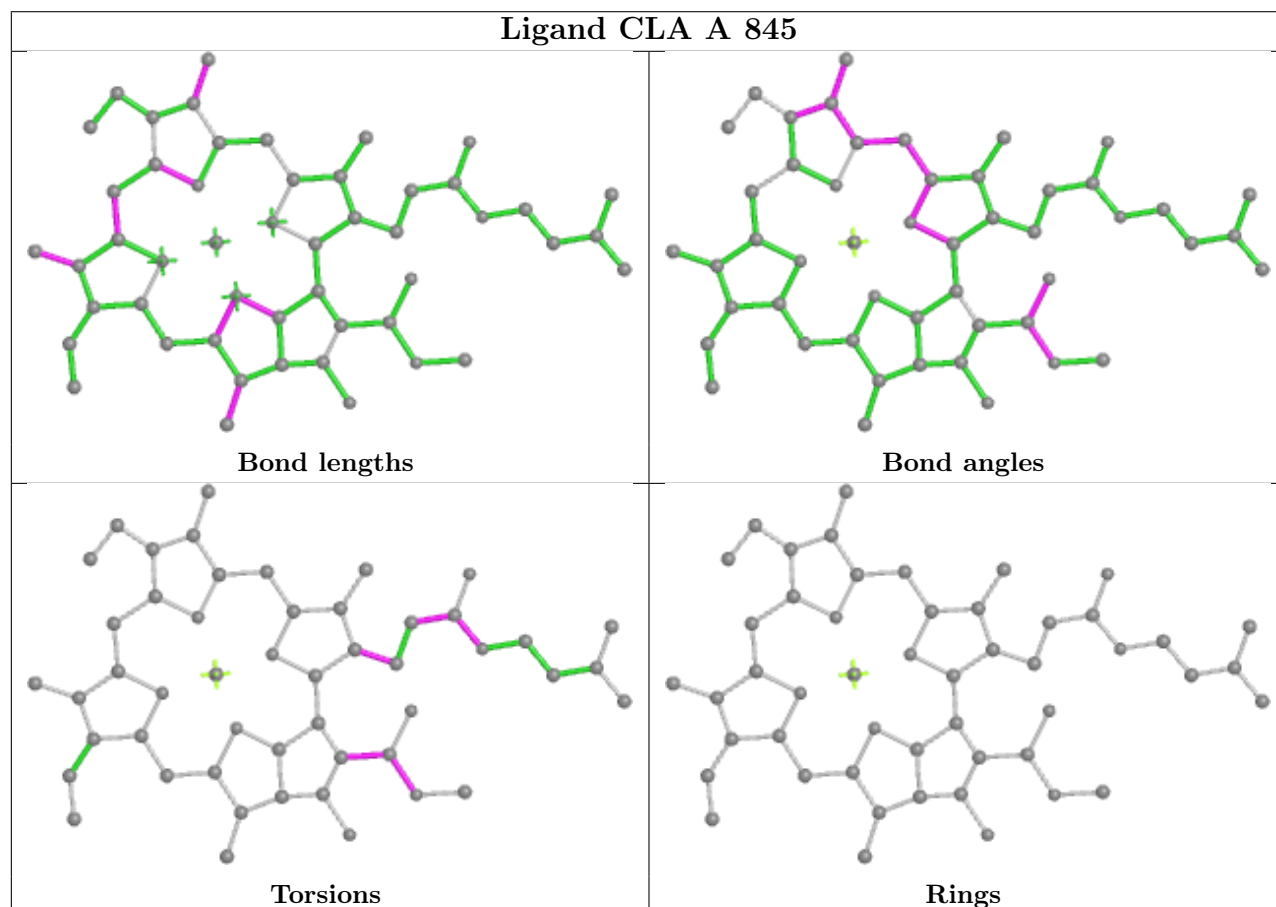
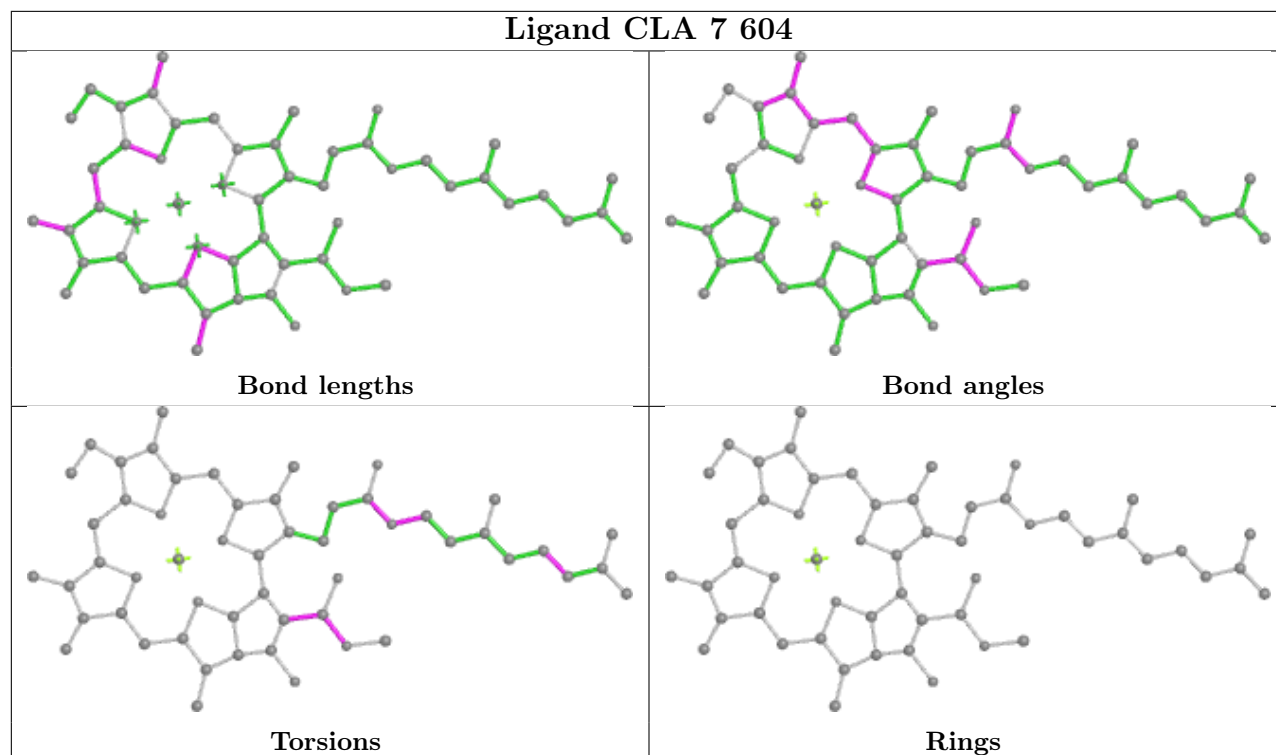


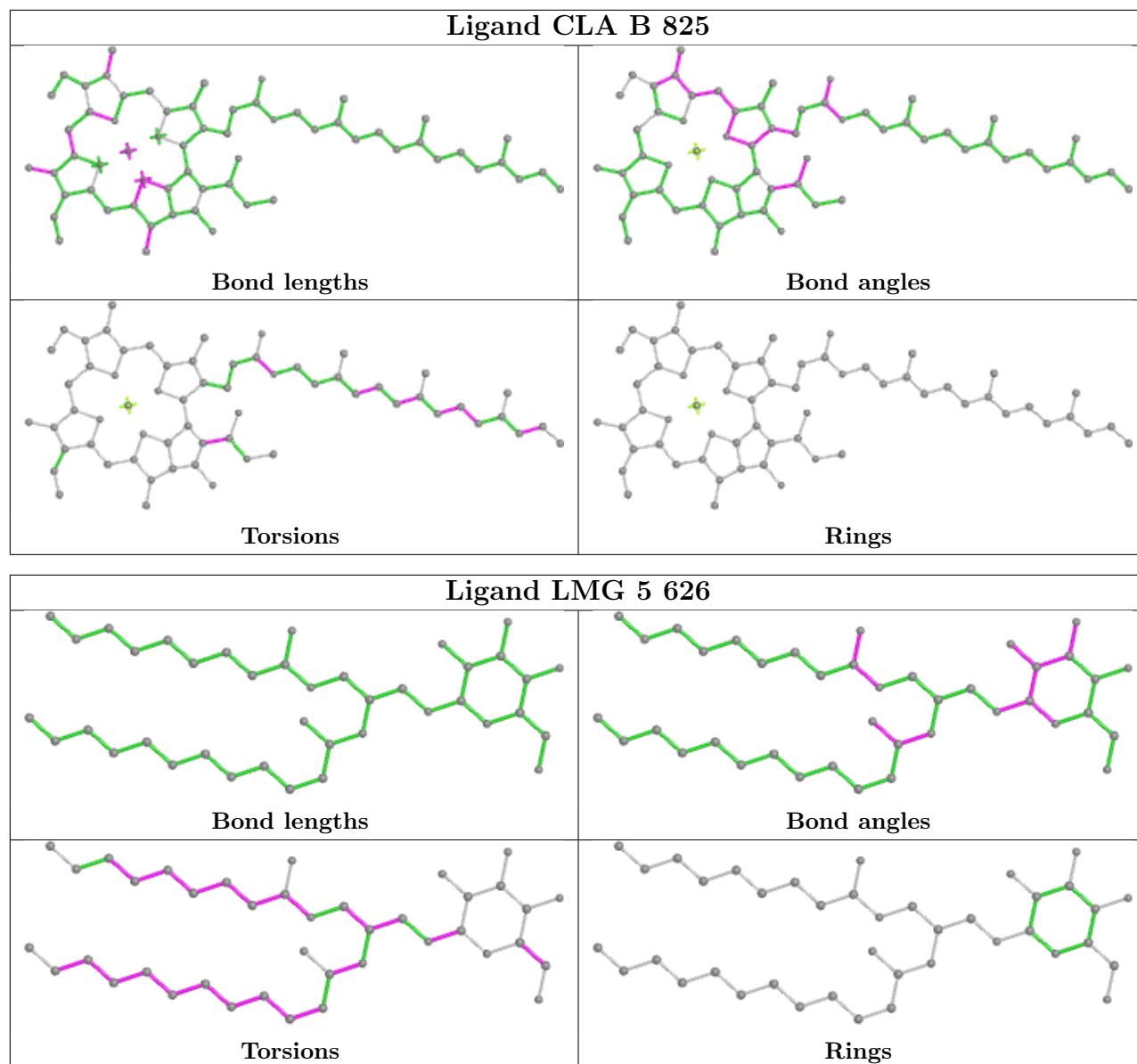


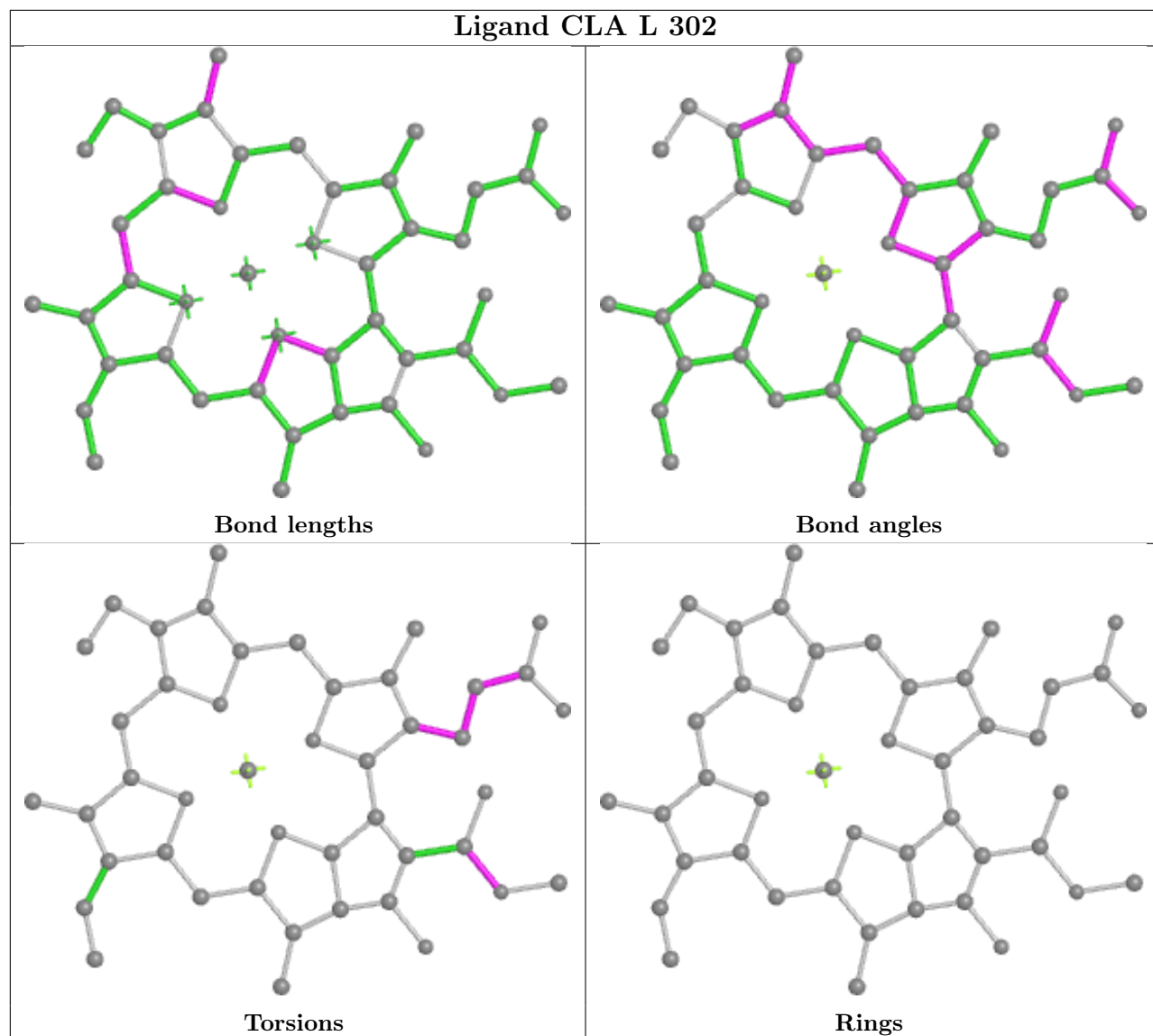


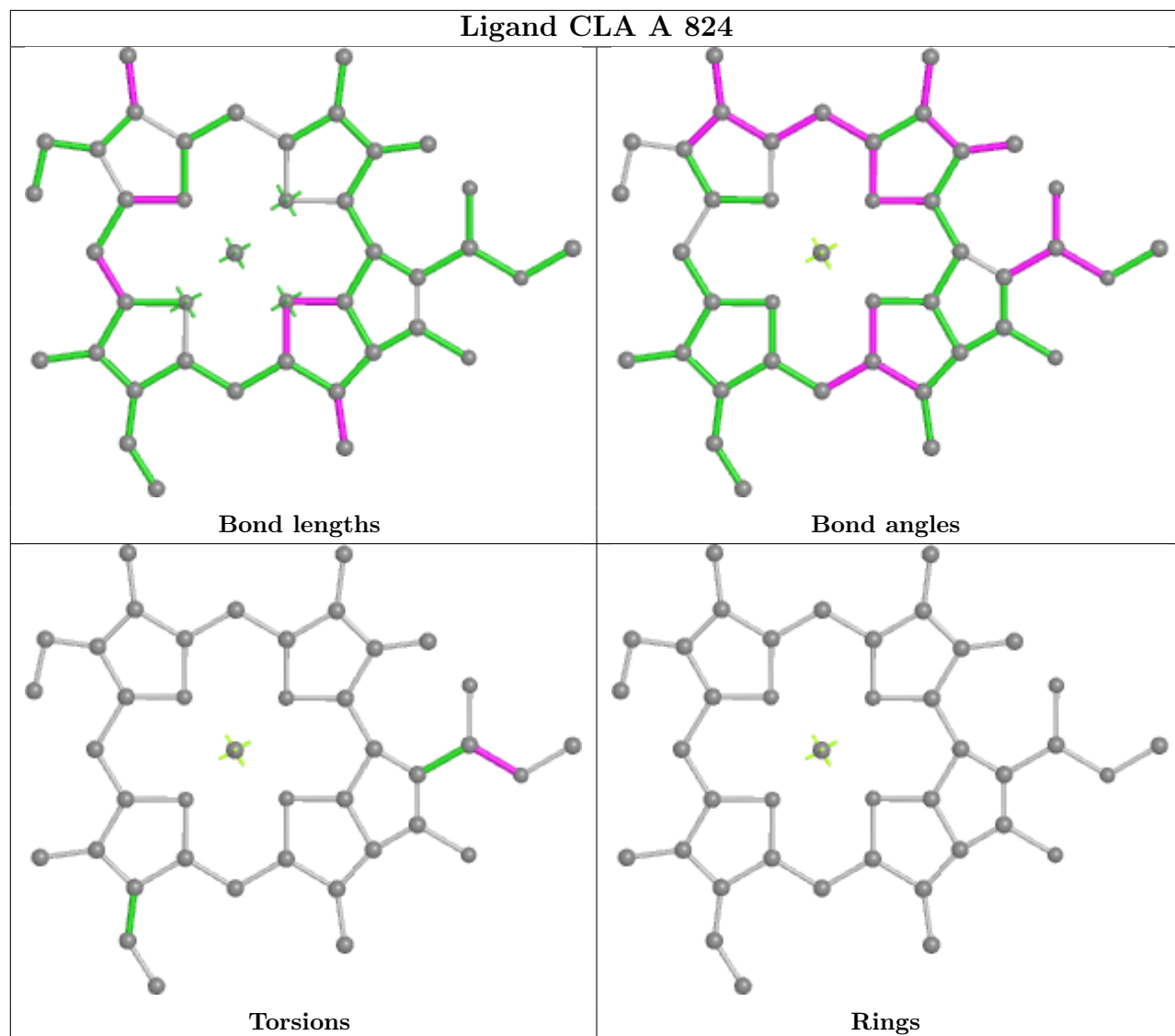


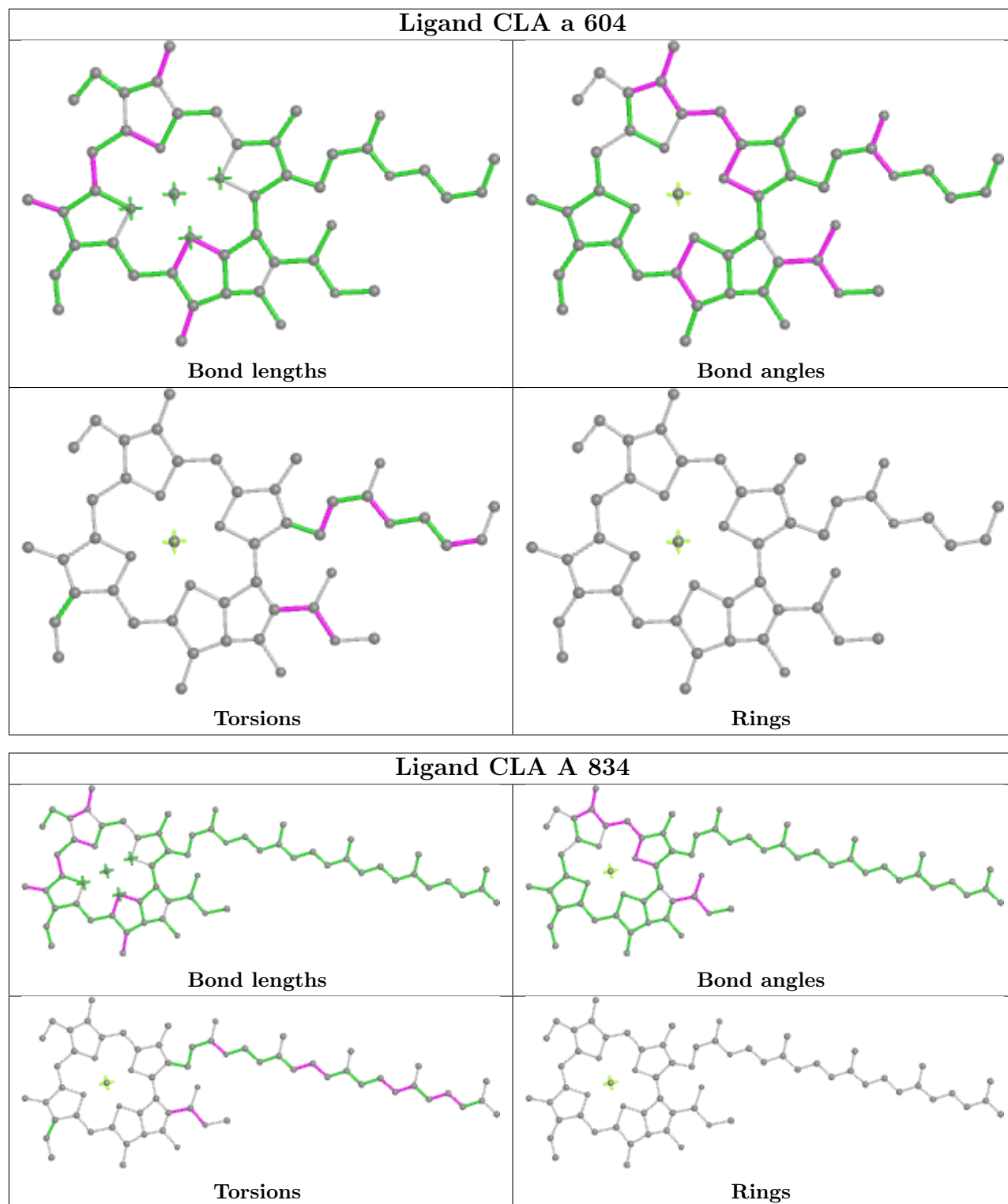


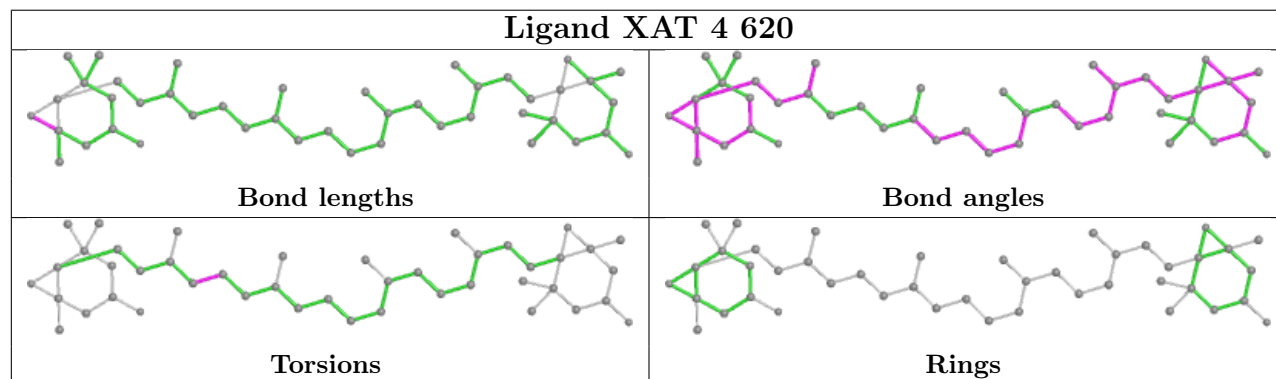
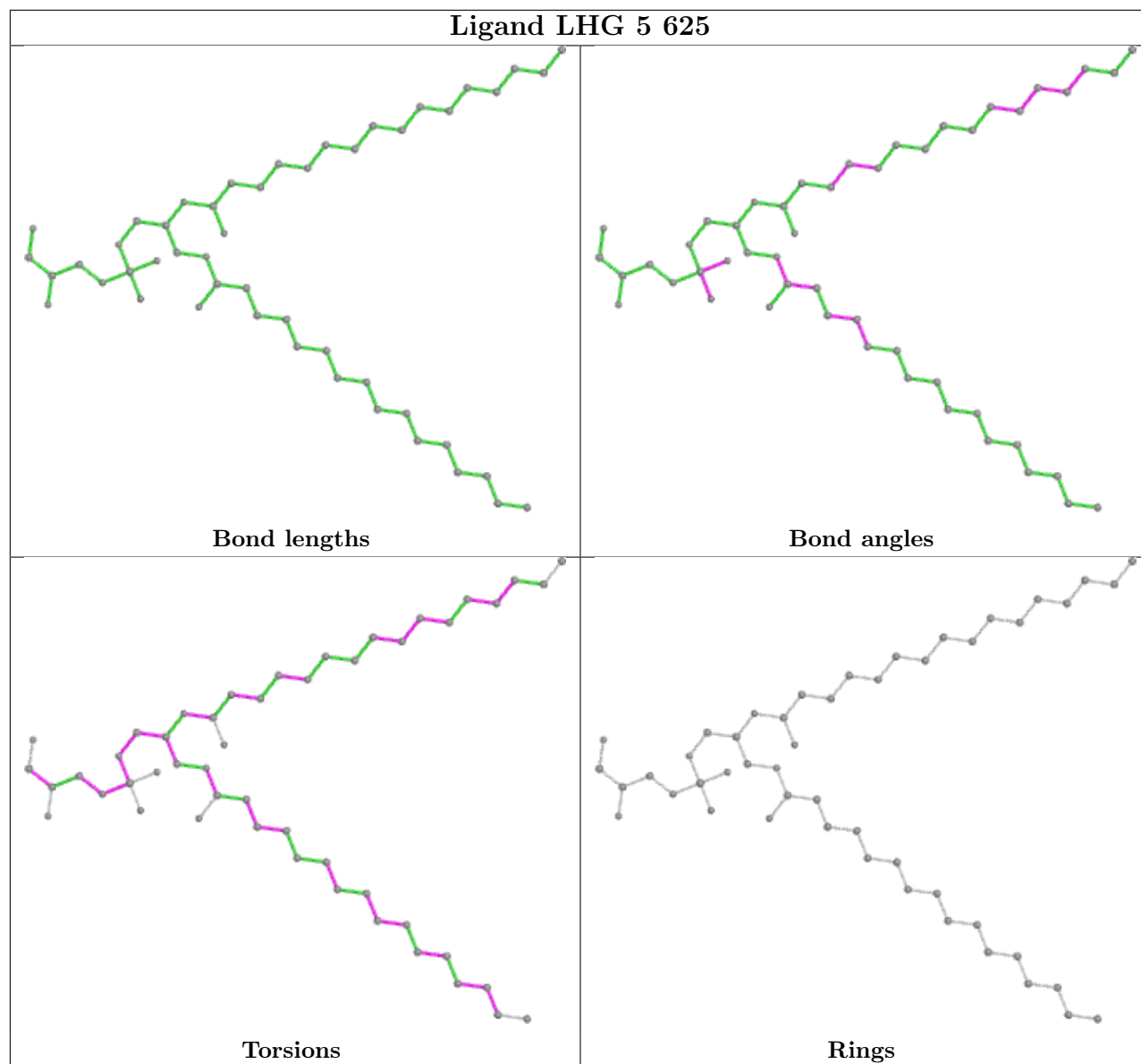




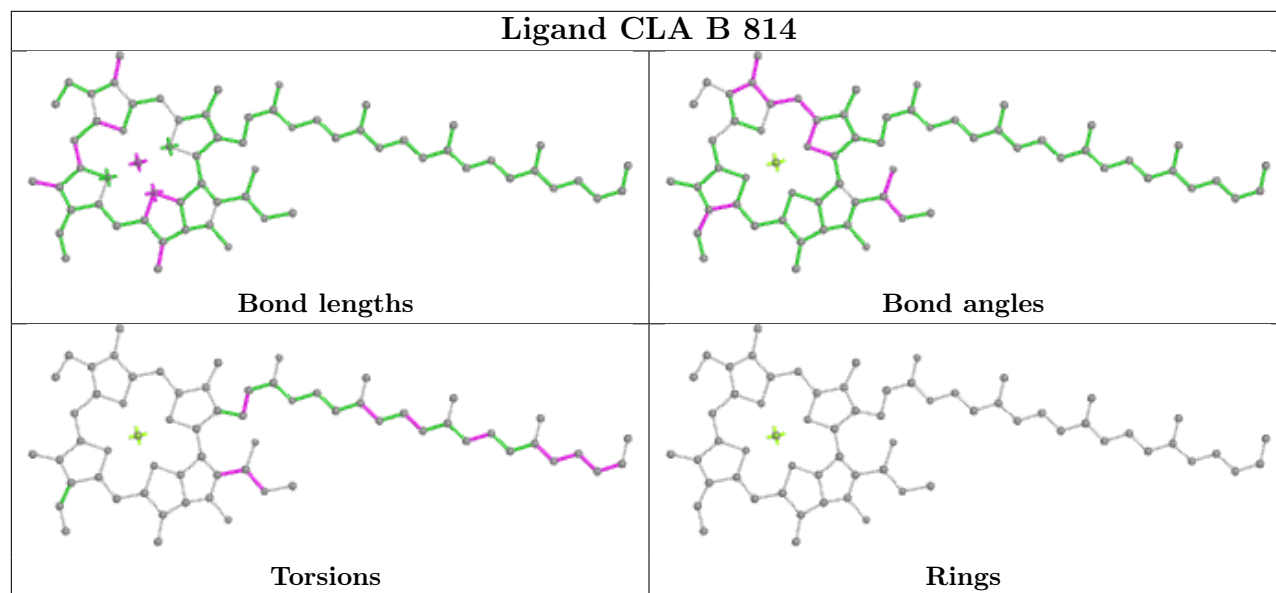


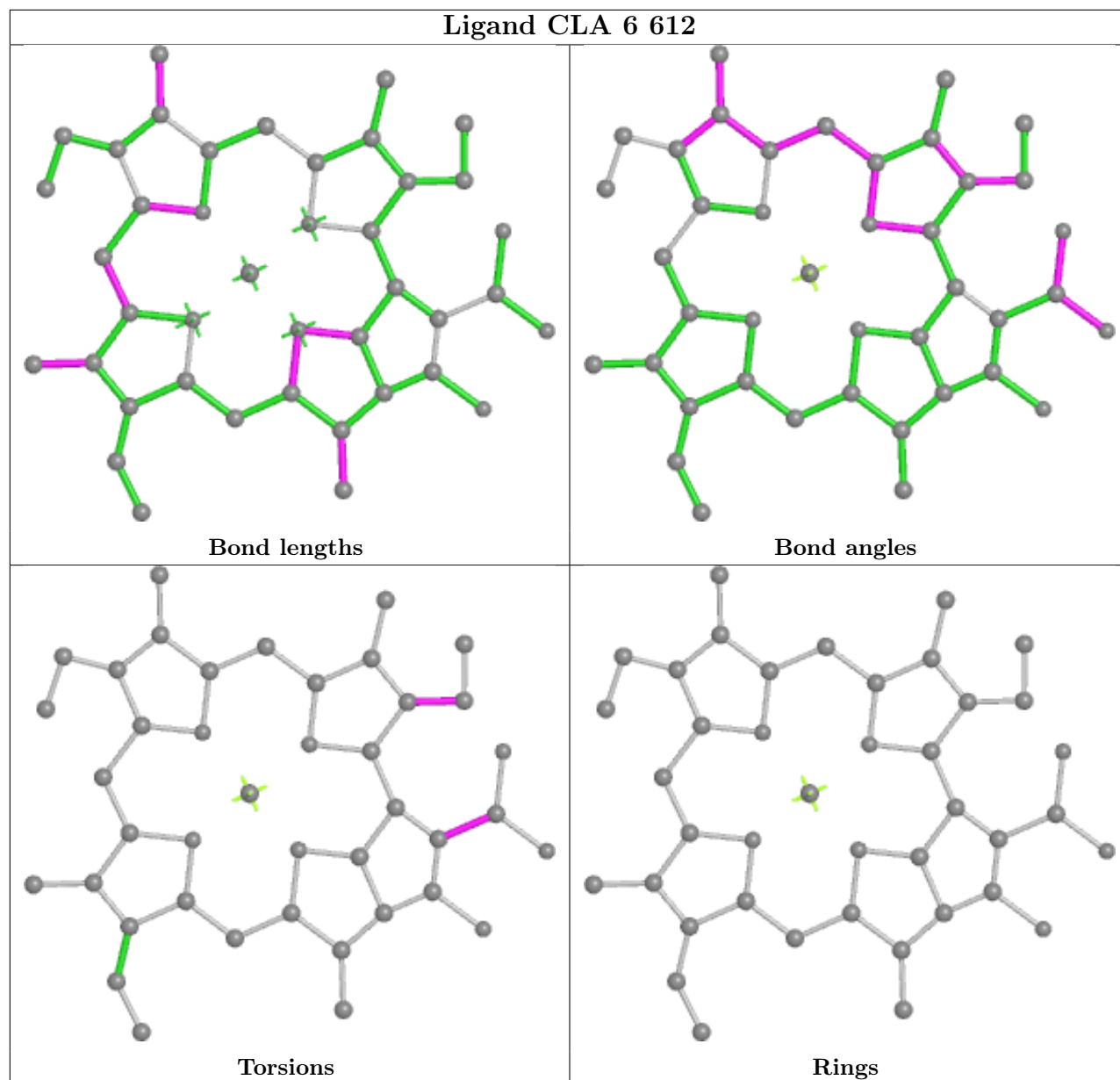


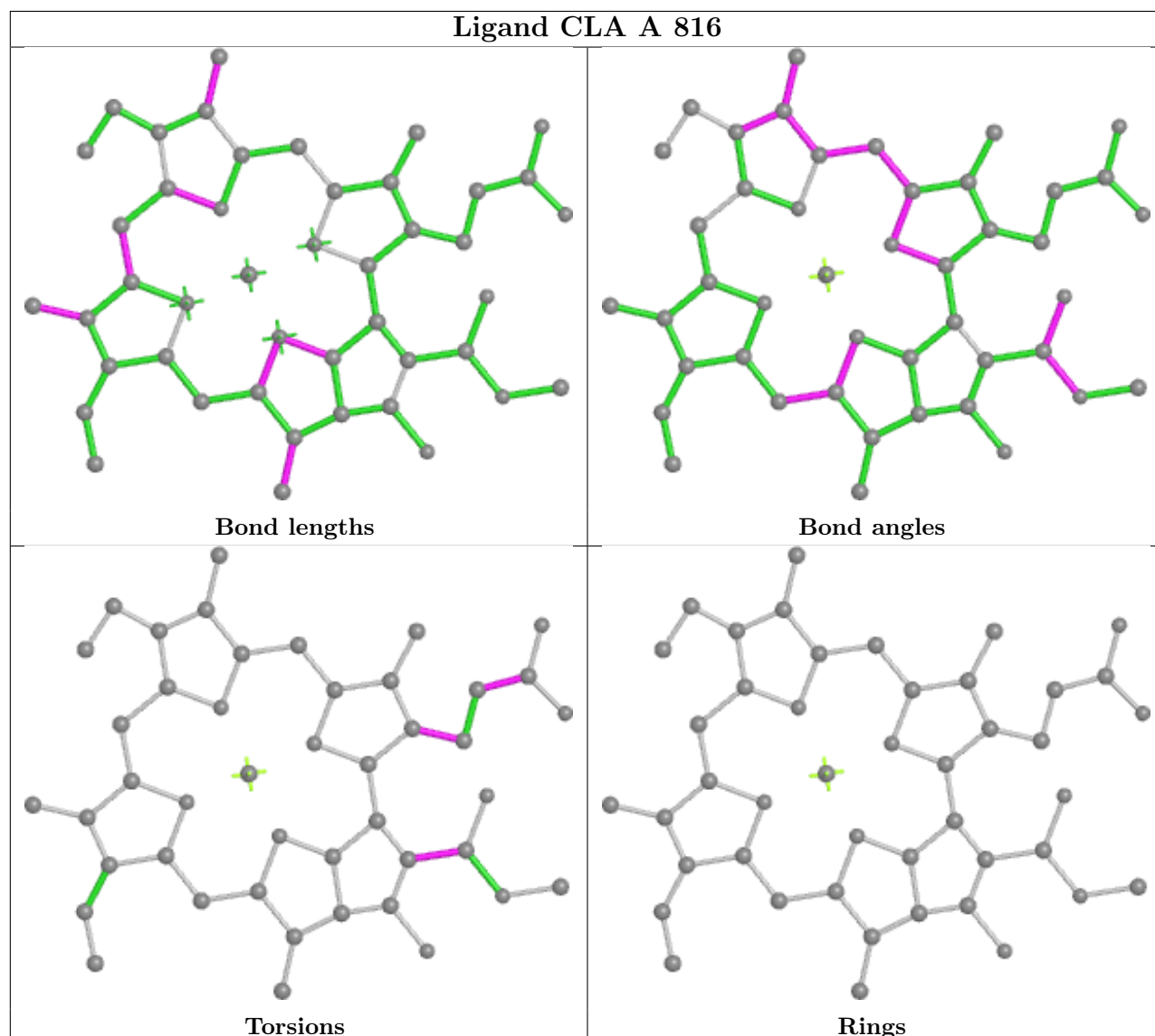
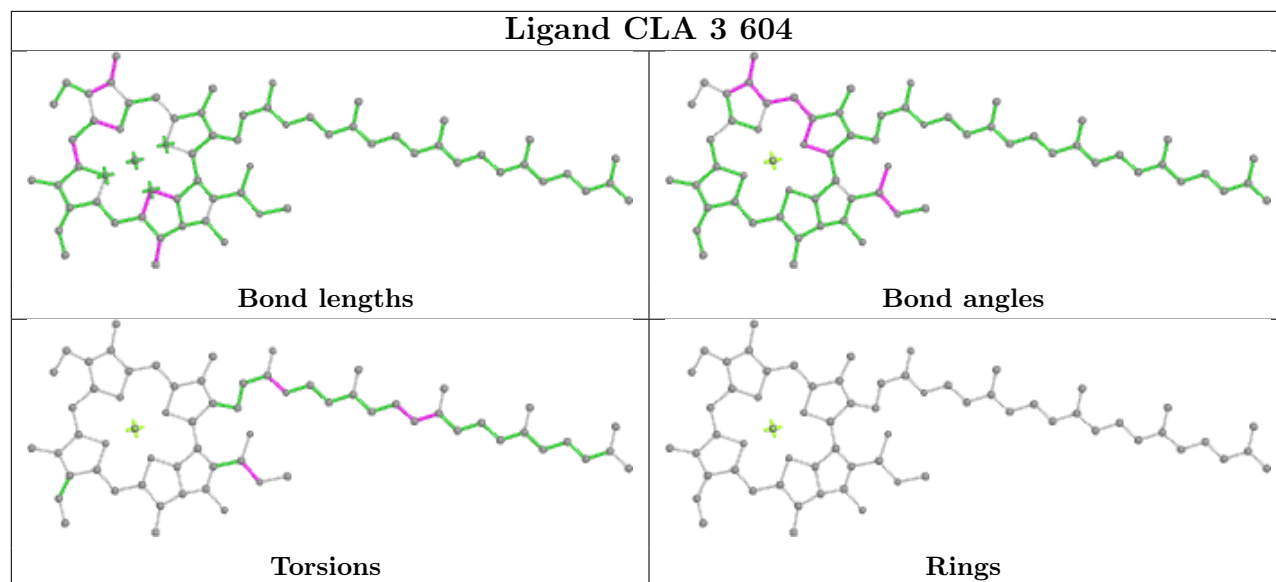


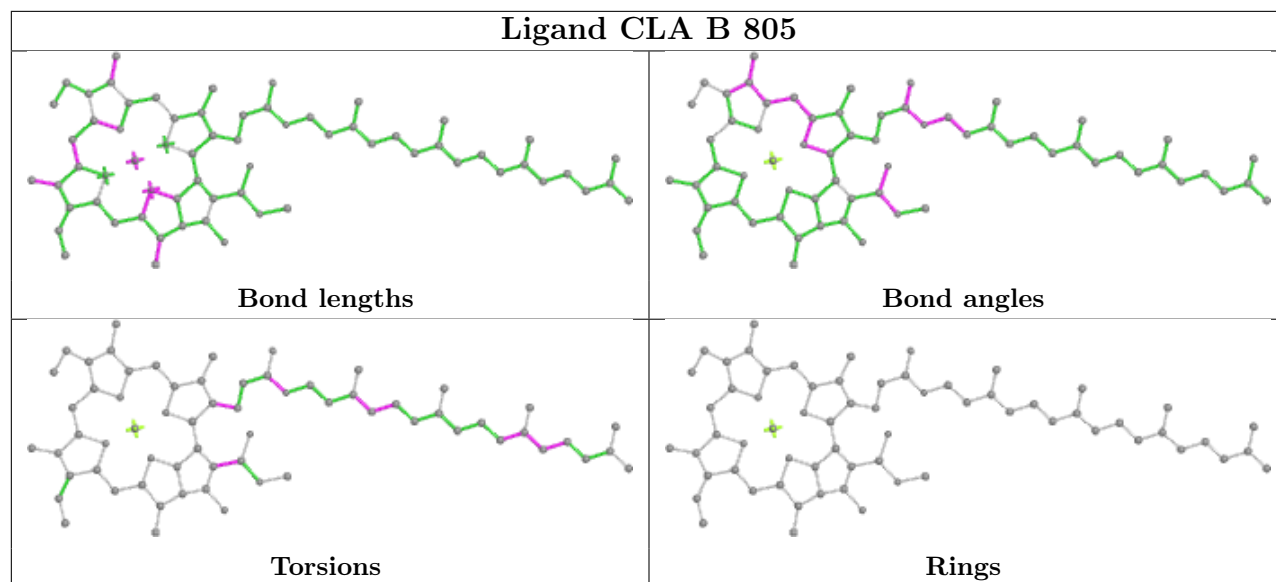












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

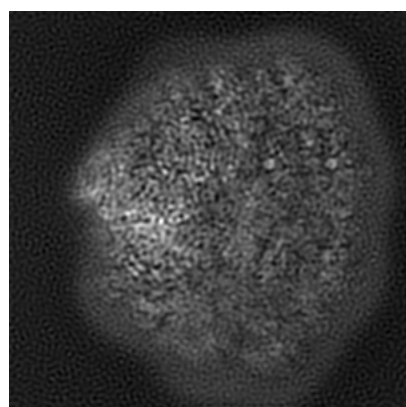
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9678. These allow visual inspection of the internal detail of the map and identification of artifacts.

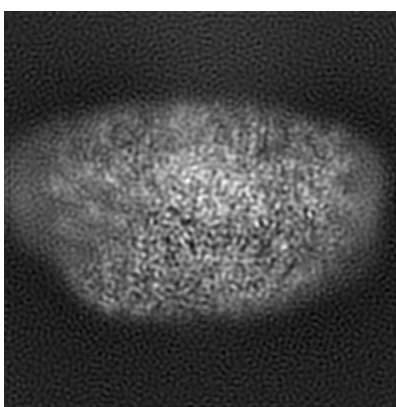
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

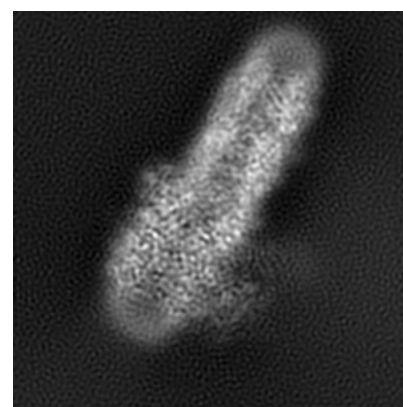
#### 6.1.1 Primary map



X



Y

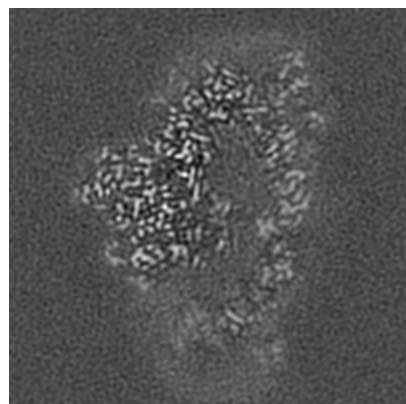


Z

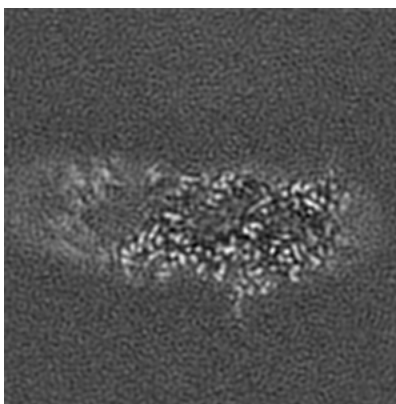
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

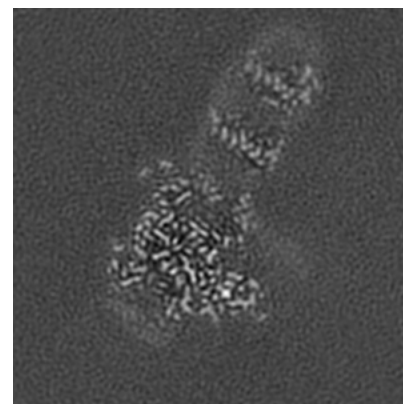
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

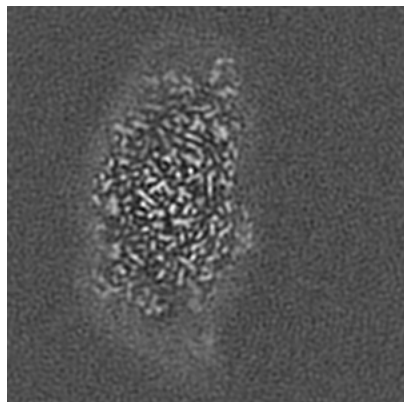


Z Index: 100

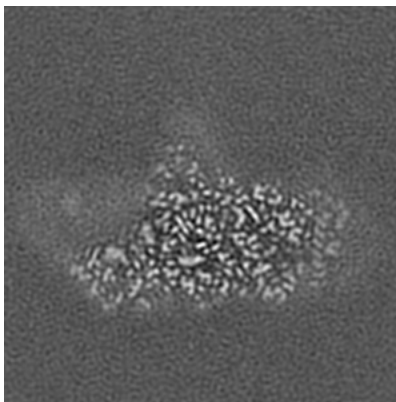
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

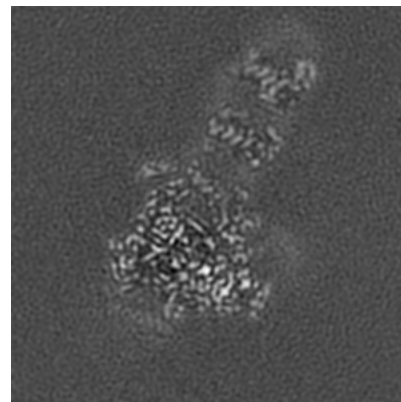
### 6.3.1 Primary map



X Index: 80



Y Index: 82



Z Index: 98

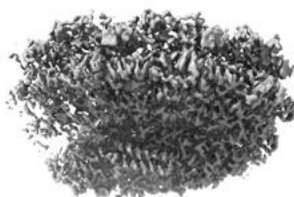
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

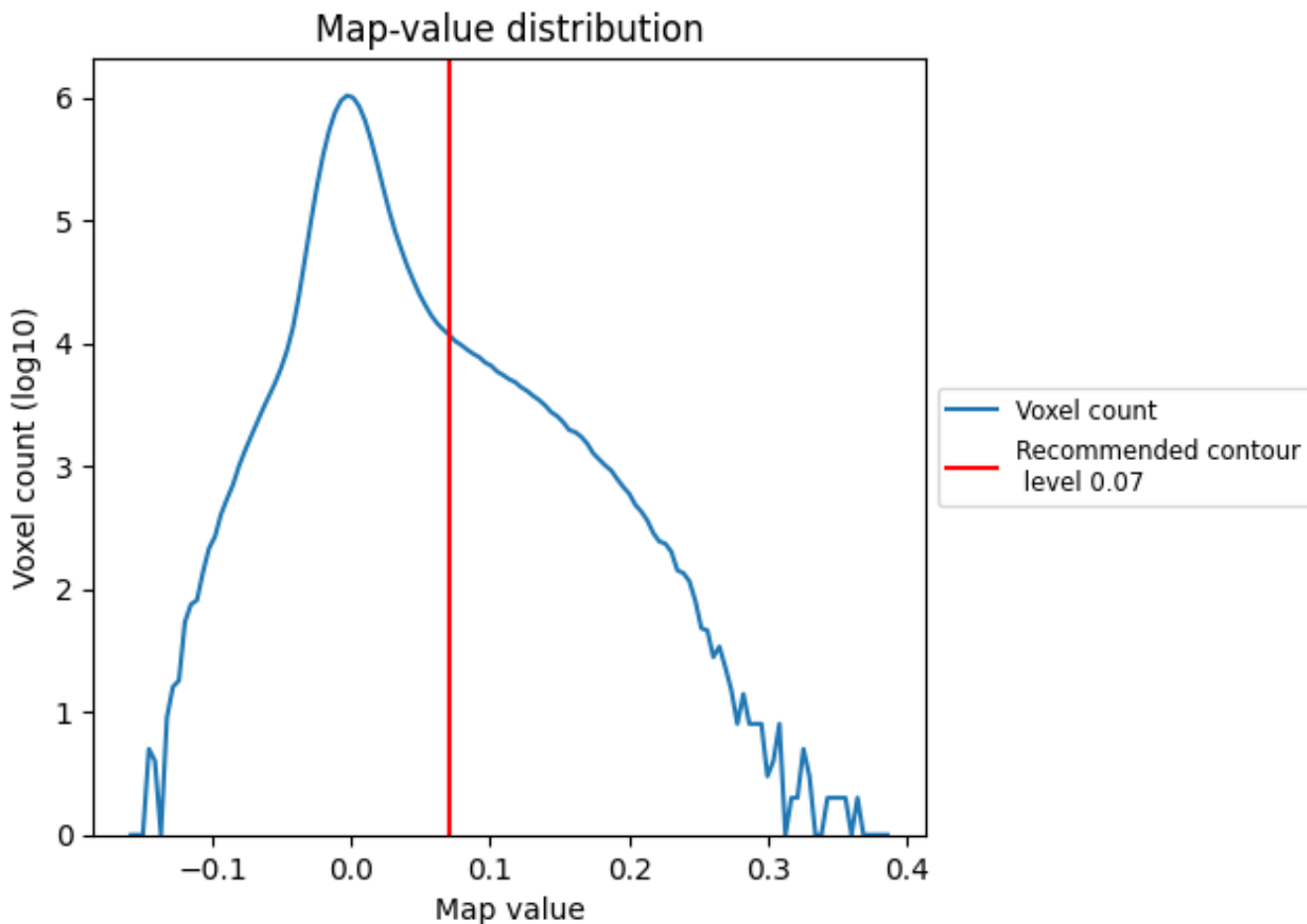
## 6.5 Mask visualisation

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.

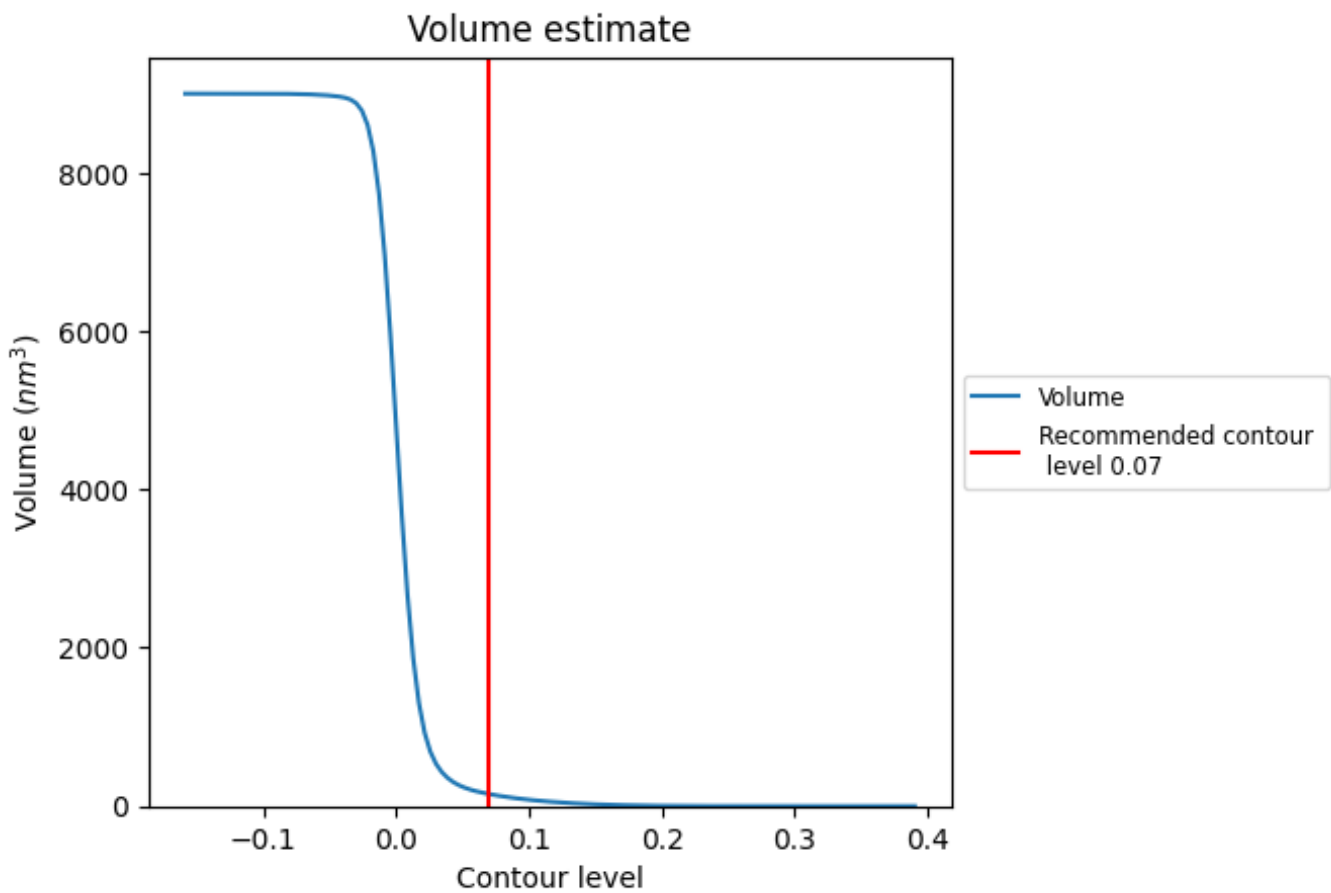
### 7.1 Map-value distribution [i](#)



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.



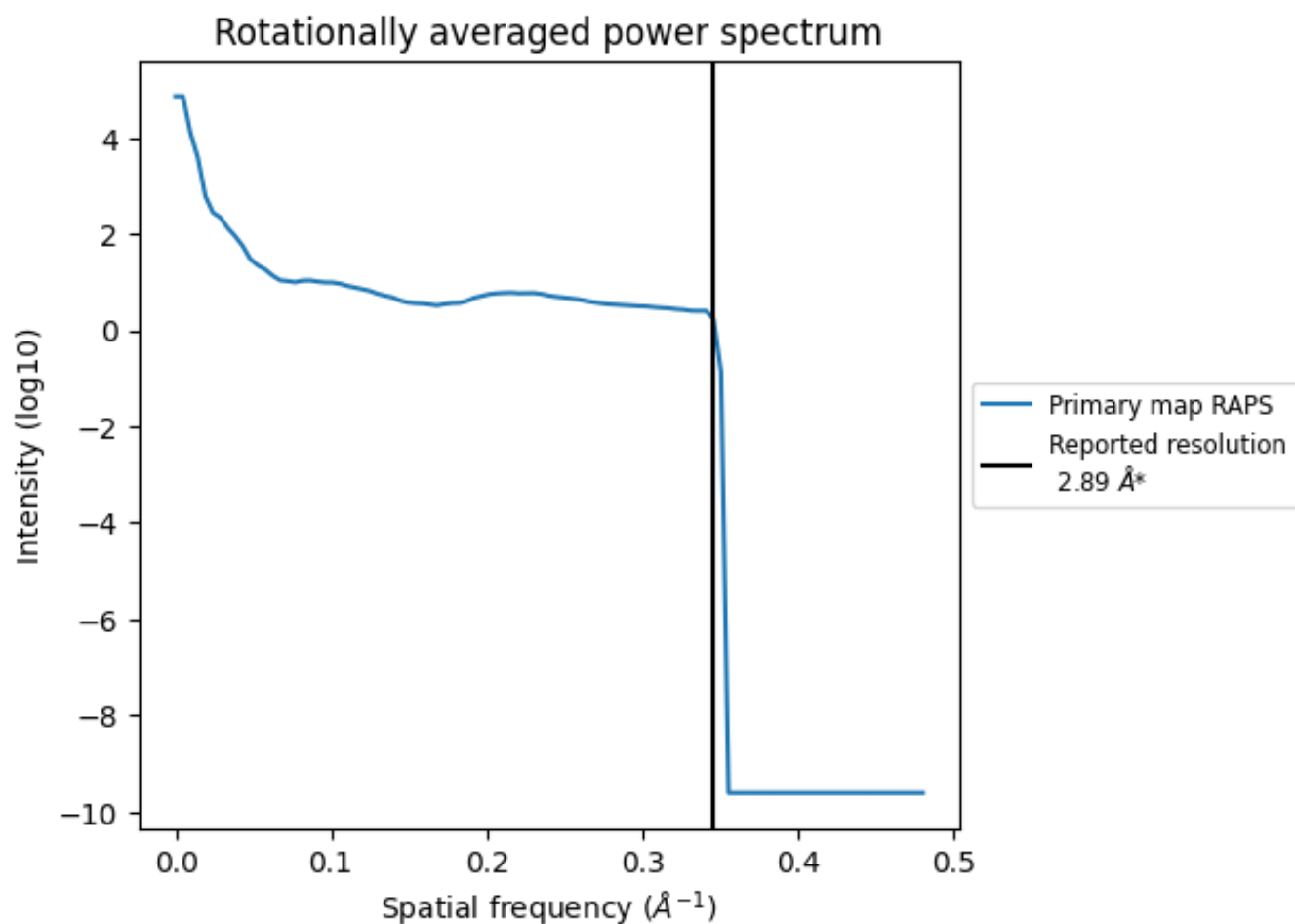
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $153 \text{ nm}^3$ ; this corresponds to an approximate mass of 138 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 0.346 Å<sup>-1</sup>

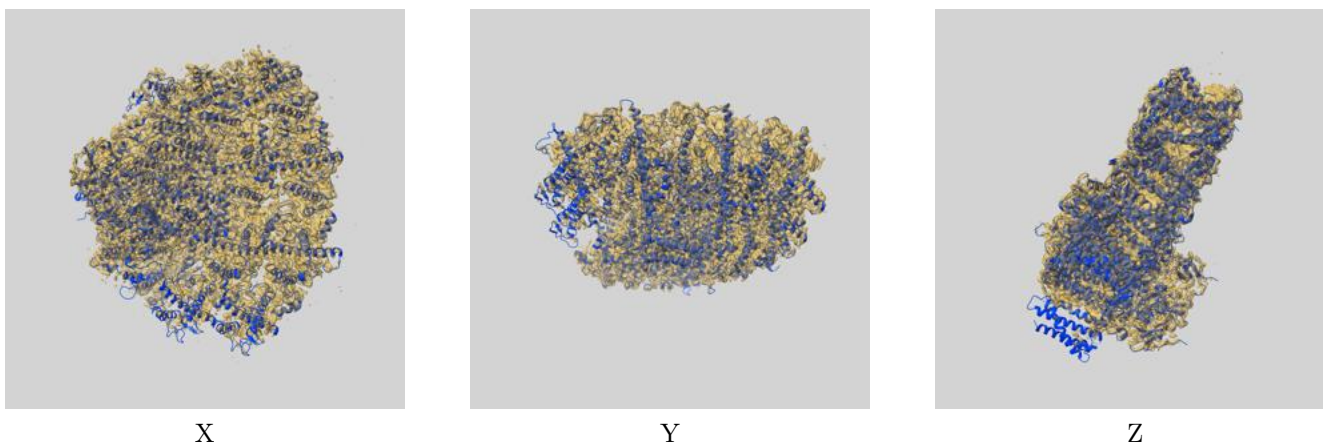
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

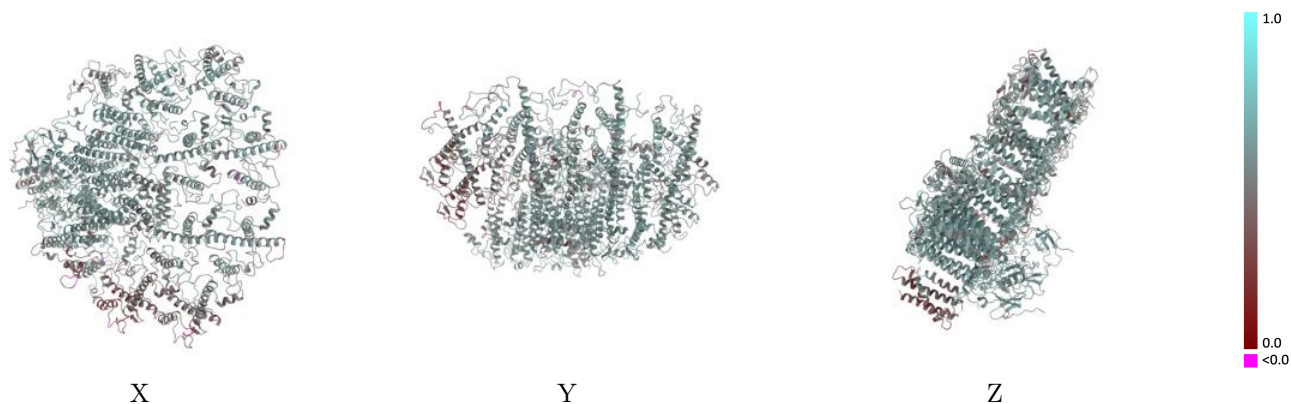
This section contains information regarding the fit between EMDB map EMD-9678 and PDB model 6IJJ. Per-residue inclusion information can be found in section [3](#) on page [32](#).

### 9.1 Map-model overlay [i](#)



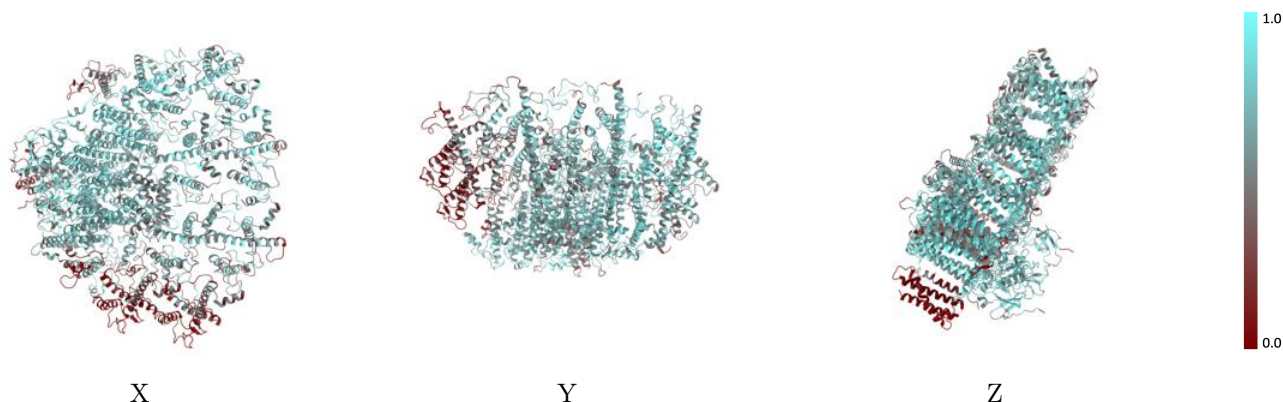
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



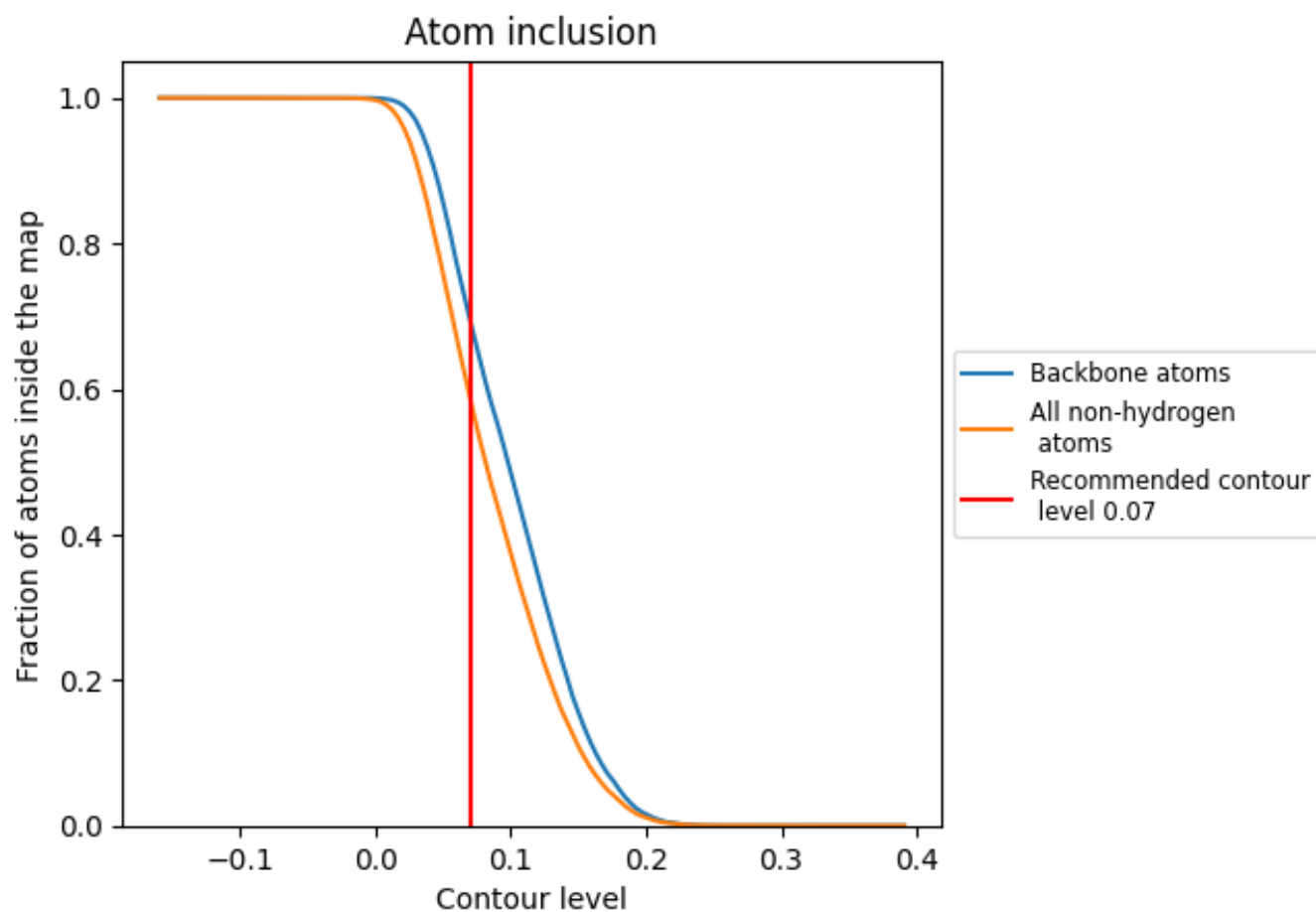
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 59% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5896	 0.5370
1	 0.2228	 0.3740
3	 0.6650	 0.5730
4	 0.5480	 0.5270
5	 0.5936	 0.5430
6	 0.6173	 0.5440
7	 0.6347	 0.5530
8	 0.5856	 0.5300
A	 0.7669	 0.6020
B	 0.6295	 0.5440
C	 0.7907	 0.5640
D	 0.6829	 0.5550
E	 0.6789	 0.5520
F	 0.5243	 0.5090
I	 0.2083	 0.4660
J	 0.3886	 0.5120
K	 0.3664	 0.5030
L	 0.0221	 0.3540
a	 0.3297	 0.4660

