



## Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 03:46 AM JST

PDB ID : 6K61  
EMDB ID : EMD-9918  
Title : Cryo-EM structure of the tetrameric photosystem I from a heterocyst-forming cyanobacterium *Anabaena* sp. PCC7120  
Authors : Zheng, L.; Li, Y.; Li, X.; Zhong, Q.; Li, N.; Zhang, K.; Zhang, Y.; Chu, H.; Ma, C.; Li, G.; Zhao, J.; Gao, N.  
Deposited on : 2019-05-31  
Resolution : 2.37 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

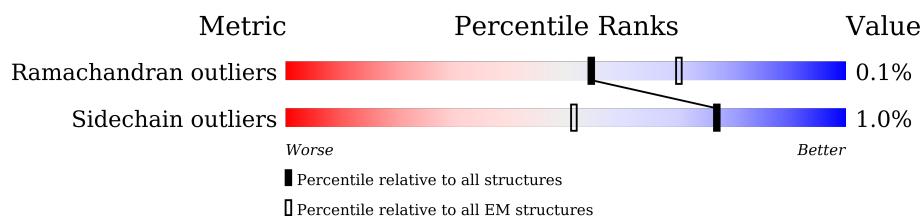
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

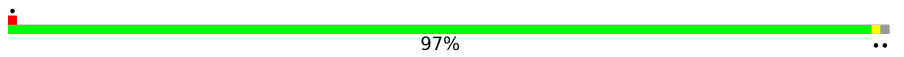
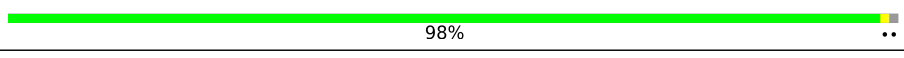


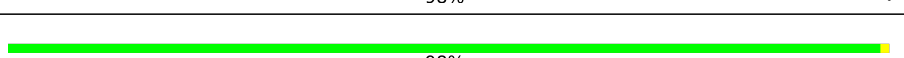
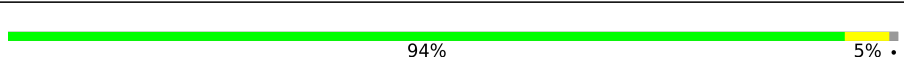
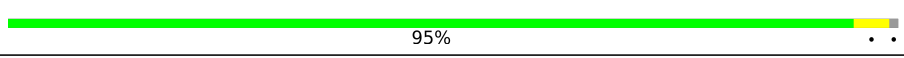
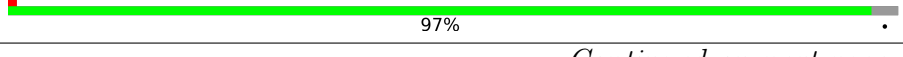

The reported resolution of this entry is 2.37 Å.

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)
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	752	
1	a	752	
2	X	44	
2	x	44	
3	B	741	
3	b	741	
4	C	81	
4	c	81	
5	D	139	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	d	139	
6	E	70	
6	e	70	
7	F	164	
7	f	164	
8	J	49	
8	j	49	
9	K	86	
9	k	86	
10	I	46	
10	i	46	
11	L	172	
11	l	172	
12	M	32	
12	m	32	

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
13	CL0	A	801	X	-	-	-
13	CL0	a	801	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	802	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	823	X	-	-	-
14	CLA	B	824	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	B	841	X	-	-	-
14	CLA	B	842	X	-	-	-
14	CLA	B	843	X	-	-	-
14	CLA	F	202	X	-	-	-
14	CLA	F	204	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	102	X	-	-	-
14	CLA	L	1501	X	-	-	-
14	CLA	L	1503	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	a	802	X	-	-	-
14	CLA	a	803	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	804	X	-	-	-
14	CLA	a	805	X	-	-	-
14	CLA	a	806	X	-	-	-
14	CLA	a	807	X	-	-	-
14	CLA	a	808	X	-	-	-
14	CLA	a	809	X	-	-	-
14	CLA	a	810	X	-	-	-
14	CLA	a	811	X	-	-	-
14	CLA	a	812	X	-	-	-
14	CLA	a	813	X	-	-	-
14	CLA	a	814	X	-	-	-
14	CLA	a	815	X	-	-	-
14	CLA	a	816	X	-	-	-
14	CLA	a	817	X	-	-	-
14	CLA	a	818	X	-	-	-
14	CLA	a	819	X	-	-	-
14	CLA	a	820	X	-	-	-
14	CLA	a	821	X	-	-	-
14	CLA	a	822	X	-	-	-
14	CLA	a	823	X	-	-	-
14	CLA	a	824	X	-	-	-
14	CLA	a	825	X	-	-	-
14	CLA	a	827	X	-	-	-
14	CLA	a	828	X	-	-	-
14	CLA	a	829	X	-	-	-
14	CLA	a	830	X	-	-	-
14	CLA	a	831	X	-	-	-
14	CLA	a	832	X	-	-	-
14	CLA	a	833	X	-	-	-
14	CLA	a	834	X	-	-	-
14	CLA	a	835	X	-	-	-
14	CLA	a	836	X	-	-	-
14	CLA	a	837	X	-	-	-
14	CLA	a	838	X	-	-	-
14	CLA	a	839	X	-	-	-
14	CLA	a	840	X	-	-	-
14	CLA	a	841	X	-	-	-
14	CLA	b	802	X	-	-	-
14	CLA	b	803	X	-	-	-
14	CLA	b	804	X	-	-	-
14	CLA	b	805	X	-	-	-
14	CLA	b	806	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	807	X	-	-	-
14	CLA	b	808	X	-	-	-
14	CLA	b	809	X	-	-	-
14	CLA	b	810	X	-	-	-
14	CLA	b	811	X	-	-	-
14	CLA	b	812	X	-	-	-
14	CLA	b	813	X	-	-	-
14	CLA	b	814	X	-	-	-
14	CLA	b	815	X	-	-	-
14	CLA	b	817	X	-	-	-
14	CLA	b	818	X	-	-	-
14	CLA	b	819	X	-	-	-
14	CLA	b	820	X	-	-	-
14	CLA	b	821	X	-	-	-
14	CLA	b	822	X	-	-	-
14	CLA	b	823	X	-	-	-
14	CLA	b	824	X	-	-	-
14	CLA	b	825	X	-	-	-
14	CLA	b	826	X	-	-	-
14	CLA	b	828	X	-	-	-
14	CLA	b	829	X	-	-	-
14	CLA	b	830	X	-	-	-
14	CLA	b	831	X	-	-	-
14	CLA	b	832	X	-	-	-
14	CLA	b	833	X	-	-	-
14	CLA	b	834	X	-	-	-
14	CLA	b	835	X	-	-	-
14	CLA	b	836	X	-	-	-
14	CLA	b	837	X	-	-	-
14	CLA	b	838	X	-	-	-
14	CLA	b	839	X	-	-	-
14	CLA	b	840	X	-	-	-
14	CLA	b	841	X	-	-	-
14	CLA	b	842	X	-	-	-
14	CLA	f	201	X	-	-	-
14	CLA	f	203	X	-	-	-
14	CLA	j	101	X	-	-	-
14	CLA	j	102	X	-	-	-
14	CLA	j	103	X	-	-	-
14	CLA	k	101	X	-	-	-
14	CLA	k	102	X	-	-	-
14	CLA	l	203	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	l	205	X	-	-	-
14	CLA	m	1201	X	-	-	-
14	CLA	x	1701	X	-	-	-

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49283 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5823	3820	1003	979	21		
1	a	742	Total	C	N	O	S	0	0
			5823	3820	1003	979	21		

- Molecule 2 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	X	31	Total	C	N	O	0	0
			257	179	40	38		
2	x	31	Total	C	N	O	0	0
			257	179	40	38		

- Molecule 3 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	740	Total	C	N	O	S	0	0
			5918	3905	991	1004	18		
3	b	740	Total	C	N	O	S	0	0
			5918	3905	991	1004	18		

- Molecule 4 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
4	c	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	135	Total	C	N	O	S	0	0
			1040	666	179	194	1		
5	d	136	Total	C	N	O	S	0	0
			1047	670	180	196	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	61	Total	C	N	O	S	0	0
			490	313	84	93			
6	e	61	Total	C	N	O	S	0	0
			490	313	84	93			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		
7	f	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	45	Total	C	N	O	S	0	0
			359	244	54	61			
8	j	45	Total	C	N	O	S	0	0
			359	244	54	61			

- Molecule 9 is a protein called Photosystem I reaction center subunit Psak 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	73	Total	C	N	O	S	0	0
			537	357	89	90	1		
9	k	78	Total	C	N	O	S	0	0
			568	376	94	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	34	Total	C	N	O	S	0	0
			275	189	38	48			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
10	i	34	Total	C	N	O	0	0
			275	189	38	48		

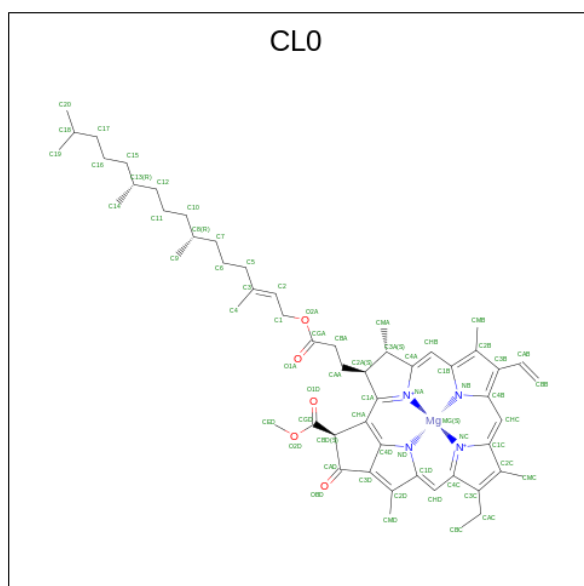
- Molecule 11 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	155	Total	C	N	O	S	0	0
			1163	763	197	202	1		
11	l	155	Total	C	N	O	S	0	0
			1163	763	197	202	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	31	Total	C	N	O	0	0
			241	160	37	44		
12	m	31	Total	C	N	O	0	0
			241	160	37	44		

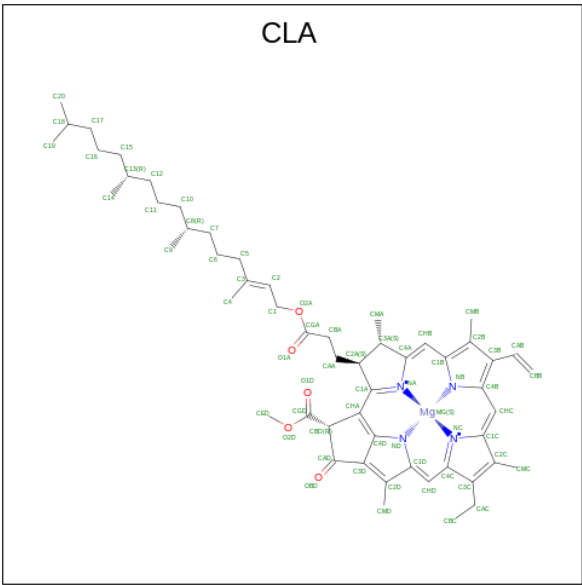
- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Continued from previous page...

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

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	X	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	F	1	Total 110	C 90	Mg 2	N 8	O 10	0
14	F	1	Total 110	C 90	Mg 2	N 8	O 10	0
14	J	1	Total 82	C 66	Mg 2	N 8	O 6	0
14	J	1	Total 82	C 66	Mg 2	N 8	O 6	0
14	K	1	Total 90	C 72	Mg 2	N 8	O 8	0
14	K	1	Total 90	C 72	Mg 2	N 8	O 8	0
14	L	1	Total 156	C 126	Mg 3	N 12	O 15	0
14	L	1	Total 156	C 126	Mg 3	N 12	O 15	0
14	L	1	Total 156	C 126	Mg 3	N 12	O 15	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	a	1	Total	C	Mg	N	O	0
			2342	1942	40	160	200	
14	x	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	f	1	Total	C	Mg	N	O	0
			104	84	2	8	10	

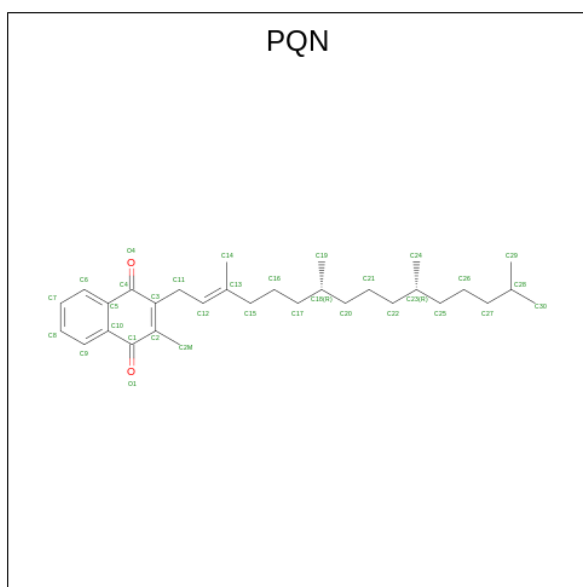
*Continued on next page...*



Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	f	1	Total	C	Mg	N	O	0
			104	84	2	8	10	
14	j	1	Total	C	Mg	N	O	0
			140	114	3	12	11	
14	j	1	Total	C	Mg	N	O	0
			140	114	3	12	11	
14	j	1	Total	C	Mg	N	O	0
			140	114	3	12	11	
14	k	1	Total	C	Mg	N	O	0
			90	72	2	8	8	
14	k	1	Total	C	Mg	N	O	0
			90	72	2	8	8	
14	l	1	Total	C	Mg	N	O	0
			150	120	3	12	15	
14	l	1	Total	C	Mg	N	O	0
			150	120	3	12	15	
14	l	1	Total	C	Mg	N	O	0
			150	120	3	12	15	
14	m	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



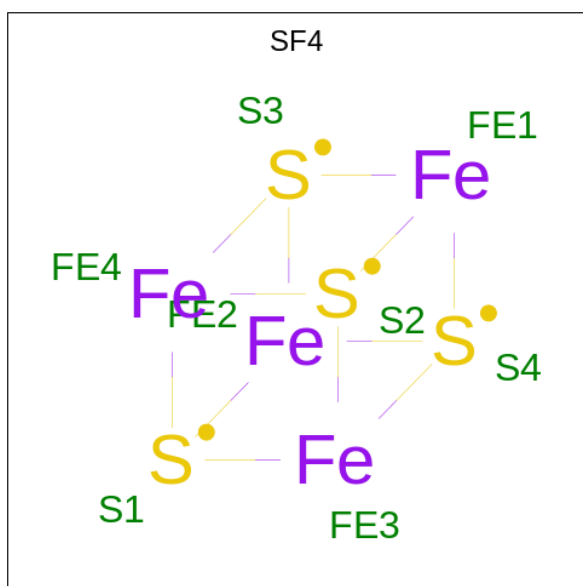
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	

Continued on next page...

Continued from previous page...

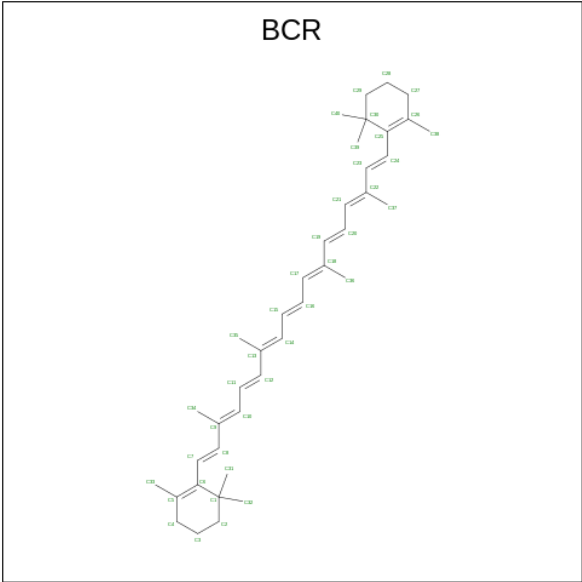
Mol	Chain	Residues	Atoms			AltConf
15	B	1	Total	C	O	0
			33	31	2	
15	a	1	Total	C	O	0
			33	31	2	
15	b	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula:  $\text{C}_{40}\text{H}_{56}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	C	0
			240	240	
17	A	1	Total	C	0
			240	240	
17	A	1	Total	C	0
			240	240	
17	A	1	Total	C	0
			240	240	
17	A	1	Total	C	0
			240	240	
17	A	1	Total	C	0
			240	240	
17	B	1	Total	C	0
			240	240	
17	B	1	Total	C	0
			240	240	
17	B	1	Total	C	0
			240	240	
17	B	1	Total	C	0
			240	240	
17	B	1	Total	C	0
			240	240	
17	F	1	Total	C	0
			80	80	
17	F	1	Total	C	0
			80	80	

Continued on next page...

*Continued from previous page...*

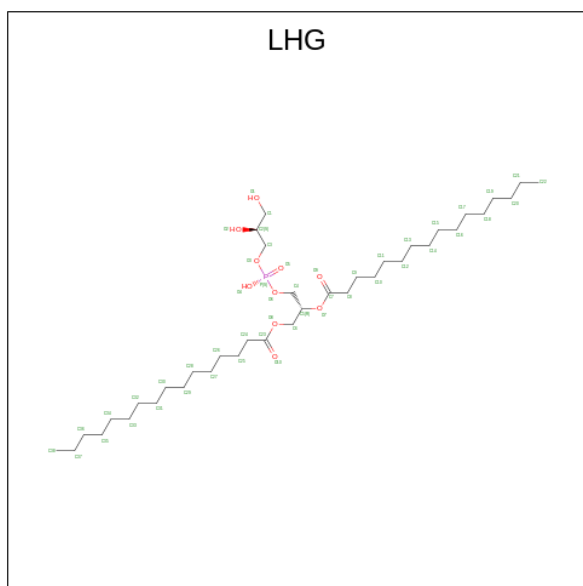
Mol	Chain	Residues	Atoms		AltConf
17	J	1	Total 120	C 120	0
17	J	1	Total 120	C 120	0
17	J	1	Total 120	C 120	0
17	K	1	Total 40	C 40	0
17	I	1	Total 80	C 80	0
17	I	1	Total 80	C 80	0
17	L	1	Total 40	C 40	0
17	M	1	Total 40	C 40	0
17	a	1	Total 240	C 240	0
17	a	1	Total 240	C 240	0
17	a	1	Total 240	C 240	0
17	a	1	Total 240	C 240	0
17	a	1	Total 240	C 240	0
17	a	1	Total 240	C 240	0
17	b	1	Total 240	C 240	0
17	b	1	Total 240	C 240	0
17	b	1	Total 240	C 240	0
17	b	1	Total 240	C 240	0
17	b	1	Total 240	C 240	0
17	b	1	Total 240	C 240	0
17	f	1	Total 80	C 80	0

*Continued on next page...*

*Continued from previous page...*

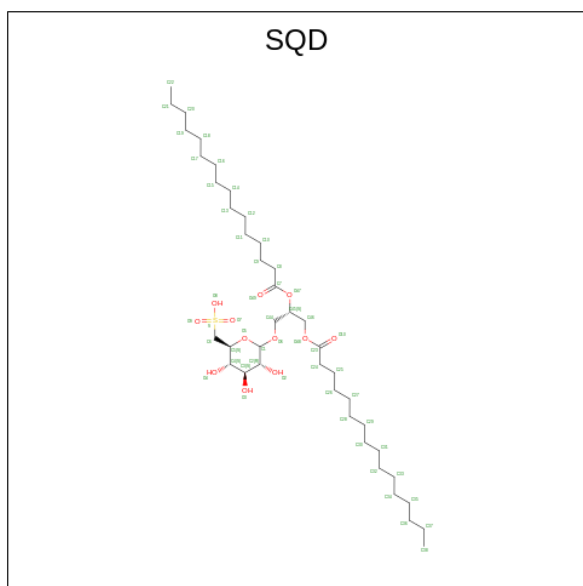
Mol	Chain	Residues	Atoms		AltConf
17	f	1	Total	C	0
			80	80	
17	j	1	Total	C	0
			120	120	
17	j	1	Total	C	0
			120	120	
17	j	1	Total	C	0
			120	120	
17	k	1	Total	C	0
			40	40	
17	i	1	Total	C	0
			80	80	
17	i	1	Total	C	0
			80	80	
17	l	1	Total	C	0
			120	120	
17	l	1	Total	C	0
			120	120	
17	l	1	Total	C	0
			120	120	
17	m	1	Total	C	0
			40	40	

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			98	76	20	2	
18	A	1	Total	C	O	P	0
			98	76	20	2	
18	F	1	Total	C	O	P	0
			43	32	10	1	
18	a	1	Total	C	O	P	0
			98	76	20	2	
18	a	1	Total	C	O	P	0
			98	76	20	2	
18	i	1	Total	C	O	P	0
			43	32	10	1	

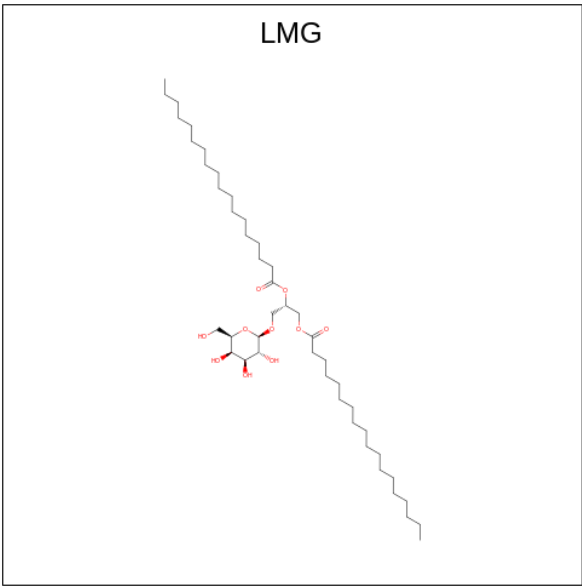
- Molecule 19 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
19	X	1	Total	C	O	S	0
			54	41	12	1	
19	x	1	Total	C	O	S	0
			54	41	12	1	
19	b	1	Total	C	O	S	0
			54	41	12	1	
19	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter

code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).

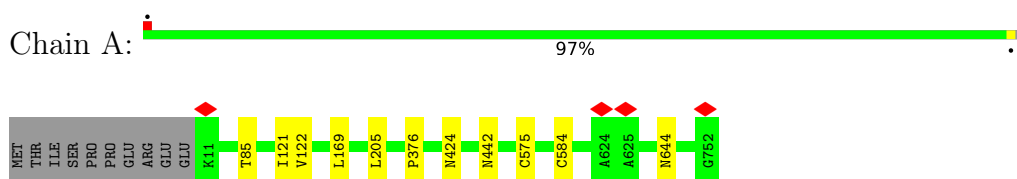


Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total	C	O	0
			90	70	20	
20	B	1	Total	C	O	0
			90	70	20	
20	b	1	Total	C	O	0
			55	45	10	

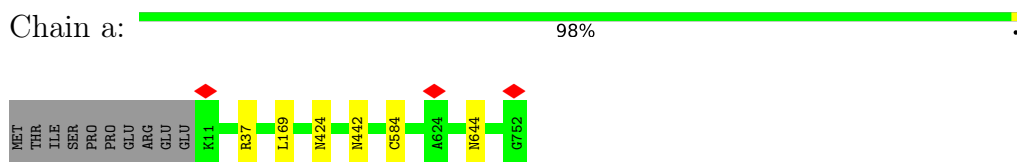
### 3 Residue-property plots [i](#)

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

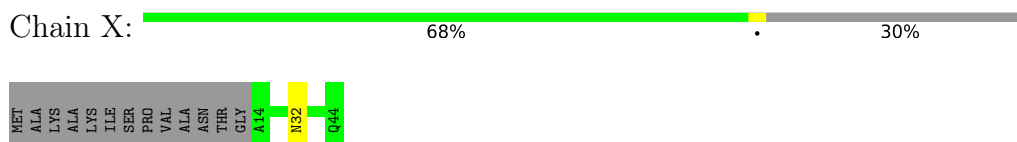
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



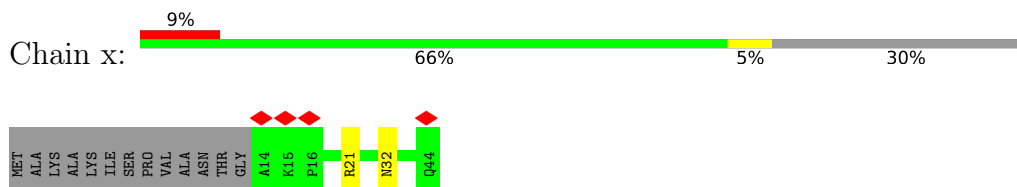
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



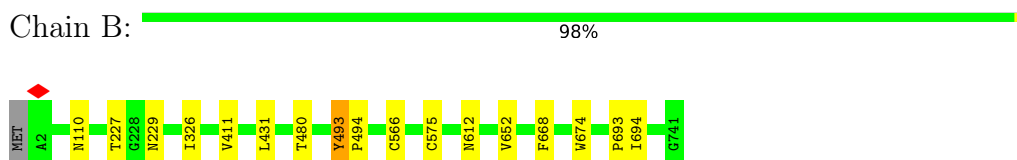
- Molecule 2: Photosystem I 4.8 kDa protein



- Molecule 2: Photosystem I 4.8 kDa protein



- Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2 1





- Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain b:  98%



- Molecule 4: Photosystem I iron-sulfur center

Chain C:  94%



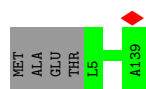
- Molecule 4: Photosystem I iron-sulfur center

Chain c:  95%



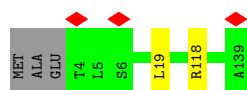
- Molecule 5: Photosystem I reaction center subunit II

Chain D:  97%




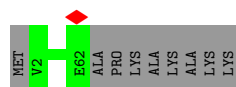
- Molecule 5: Photosystem I reaction center subunit II

Chain d:  96%




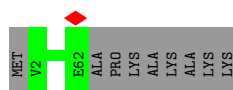
- Molecule 6: Photosystem I reaction center subunit IV

Chain E:  87%



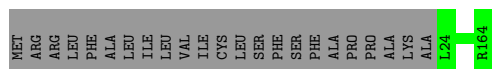
- Molecule 6: Photosystem I reaction center subunit IV

Chain e:  87%



- Molecule 7: Photosystem I reaction center subunit III

Chain F: 86% 14%



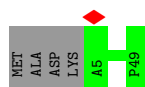
- Molecule 7: Photosystem I reaction center subunit III

Chain f: 85% 14%



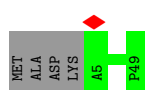
- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 92% 8%



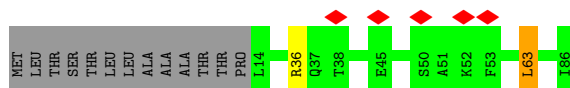
- Molecule 8: Photosystem I reaction center subunit IX

Chain j: 92% 8%



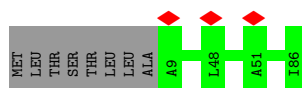
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K: 6% 83% 15%



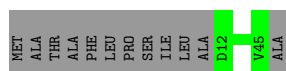
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain k: 91% 9%



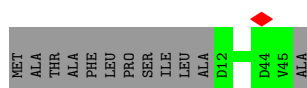
- Molecule 10: Photosystem I reaction center subunit VIII

Chain I:  74% 26%




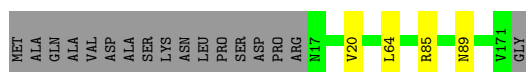
- Molecule 10: Photosystem I reaction center subunit VIII

Chain i:  74% 26%




- Molecule 11: Photosystem I reaction center subunit XI

Chain L:  88% 10%



- Molecule 11: Photosystem I reaction center subunit XI

Chain l:  89% 10%



- Molecule 12: Photosystem I reaction center subunit XII

Chain M:  97%



- Molecule 12: Photosystem I reaction center subunit XII

Chain m:  97%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	71600	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 ( $e^-/\text{\AA}^2$ )	58	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	0.173	Depositor
Minimum map value	-0.073	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.019	Depositor
Map size ( $\text{\AA}$ )	420.80002, 420.80002, 420.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.052, 1.052, 1.052	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, PQN, SQD, CLA, BCR, LHG, LMG, CLO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.49	1/6022 (0.0%)	0.59	3/8214 (0.0%)
1	a	0.50	0/6022	0.58	1/8214 (0.0%)
2	X	0.41	0/267	0.54	0/366
2	x	0.34	0/267	0.48	0/366
3	B	0.54	2/6142 (0.0%)	0.71	5/8396 (0.1%)
3	b	0.54	2/6142 (0.0%)	0.62	4/8396 (0.0%)
4	C	0.52	0/608	0.68	0/825
4	c	0.55	0/608	0.65	0/825
5	D	0.45	0/1064	0.62	0/1436
5	d	0.45	0/1071	0.62	1/1446 (0.1%)
6	E	0.43	0/499	0.48	0/677
6	e	0.41	0/499	0.46	0/677
7	F	0.38	0/1104	0.57	0/1500
7	f	0.40	0/1104	0.54	0/1500
8	J	0.38	0/371	0.52	0/509
8	j	0.36	0/371	0.51	0/509
9	K	0.35	0/551	0.67	1/750 (0.1%)
9	k	0.41	0/583	0.58	0/796
10	I	0.43	0/284	0.54	0/388
10	i	0.53	0/284	0.59	0/388
11	L	0.48	0/1198	0.64	1/1642 (0.1%)
11	l	0.50	0/1198	0.60	0/1642
12	M	0.44	0/245	0.57	0/334
12	m	0.46	0/245	0.59	0/334
All	All	0.49	5/36749 (0.0%)	0.61	16/50130 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	B	0	4
3	b	0	2
4	c	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	411	VAL	CB-CG1	-8.36	1.35	1.52
3	B	652	VAL	CB-CG2	-6.76	1.38	1.52
3	b	411	VAL	CB-CG1	-6.03	1.40	1.52
3	b	652	VAL	CB-CG2	-5.68	1.41	1.52
1	A	376	PRO	C-N	-5.04	1.22	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	493	TYR	C-N-CD	-20.83	74.77	120.60
3	B	493	TYR	C-N-CA	13.79	179.94	122.00
3	b	431	LEU	CA-CB-CG	7.55	132.66	115.30
5	d	19	LEU	CA-CB-CG	7.06	131.54	115.30
3	b	155	LEU	CA-CB-CG	6.75	130.83	115.30
9	K	63	LEU	CA-CB-CG	6.40	130.03	115.30
1	A	169	LEU	CA-CB-CG	6.36	129.93	115.30
3	B	431	LEU	CA-CB-CG	6.25	129.66	115.30
11	L	64	LEU	CA-CB-CG	5.92	128.91	115.30
3	B	668	PHE	CB-CG-CD2	-5.88	116.68	120.80
3	b	668	PHE	CB-CG-CD2	-5.72	116.79	120.80
1	A	575	CYS	CA-CB-SG	-5.53	104.05	114.00
1	a	169	LEU	CA-CB-CG	5.43	127.78	115.30
3	B	566	CYS	CA-CB-SG	-5.41	104.26	114.00
3	b	475	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	205	LEU	CA-CB-CG	5.24	127.34	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ILE	Peptide
3	B	480	THR	Peptide
3	B	493	TYR	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
3	B	674	TRP	Peptide
3	B	693	PRO	Peptide
3	b	674	TRP	Peptide
3	b	693	PRO	Peptide
4	c	62	PHE	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	740/752 (98%)	709 (96%)	30 (4%)	1 (0%)	51	67
1	a	740/752 (98%)	710 (96%)	30 (4%)	0	100	100
2	X	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
2	x	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
3	B	738/741 (100%)	715 (97%)	21 (3%)	2 (0%)	41	53
3	b	738/741 (100%)	721 (98%)	16 (2%)	1 (0%)	51	67
4	C	78/81 (96%)	73 (94%)	3 (4%)	2 (3%)	5	4
4	c	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
5	D	133/139 (96%)	130 (98%)	3 (2%)	0	100	100
5	d	134/139 (96%)	131 (98%)	3 (2%)	0	100	100
6	E	59/70 (84%)	57 (97%)	2 (3%)	0	100	100
6	e	59/70 (84%)	57 (97%)	2 (3%)	0	100	100
7	F	139/164 (85%)	131 (94%)	8 (6%)	0	100	100
7	f	139/164 (85%)	135 (97%)	4 (3%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	43/49 (88%)	43 (100%)	0	0	100	100
8	j	43/49 (88%)	43 (100%)	0	0	100	100
9	K	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
9	k	76/86 (88%)	74 (97%)	2 (3%)	0	100	100
10	I	32/46 (70%)	31 (97%)	1 (3%)	0	100	100
10	i	32/46 (70%)	31 (97%)	1 (3%)	0	100	100
11	L	153/172 (89%)	152 (99%)	1 (1%)	0	100	100
11	l	153/172 (89%)	151 (99%)	2 (1%)	0	100	100
12	M	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
12	m	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
All	All	4494/4752 (95%)	4347 (97%)	141 (3%)	6 (0%)	54	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
3	B	494	PRO
3	B	694	ILE
3	b	694	ILE
4	C	63	LEU
4	C	62	PHE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	595/605 (98%)	590 (99%)	5 (1%)	81	91
1	a	595/605 (98%)	590 (99%)	5 (1%)	81	91
2	X	25/34 (74%)	24 (96%)	1 (4%)	31	47
2	x	25/34 (74%)	23 (92%)	2 (8%)	12	17
3	B	600/602 (100%)	594 (99%)	6 (1%)	76	87

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	b	600/602 (100%)	596 (99%)	4 (1%)	84	92
4	C	67/69 (97%)	65 (97%)	2 (3%)	41	59
4	c	67/69 (97%)	65 (97%)	2 (3%)	41	59
5	D	107/110 (97%)	107 (100%)	0	100	100
5	d	108/110 (98%)	107 (99%)	1 (1%)	78	89
6	E	54/60 (90%)	54 (100%)	0	100	100
6	e	54/60 (90%)	54 (100%)	0	100	100
7	F	110/129 (85%)	110 (100%)	0	100	100
7	f	110/129 (85%)	109 (99%)	1 (1%)	78	89
8	J	39/42 (93%)	39 (100%)	0	100	100
8	j	39/42 (93%)	39 (100%)	0	100	100
9	K	54/64 (84%)	52 (96%)	2 (4%)	34	50
9	k	57/64 (89%)	57 (100%)	0	100	100
10	I	31/39 (80%)	31 (100%)	0	100	100
10	i	31/39 (80%)	31 (100%)	0	100	100
11	L	118/131 (90%)	115 (98%)	3 (2%)	47	65
11	l	118/131 (90%)	116 (98%)	2 (2%)	60	76
12	M	26/27 (96%)	26 (100%)	0	100	100
12	m	26/27 (96%)	26 (100%)	0	100	100
All	All	3656/3824 (96%)	3620 (99%)	36 (1%)	77	87

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	THR
1	A	424	ASN
1	A	442	ASN
1	A	584	CYS
1	A	644	ASN
2	X	32	ASN
3	B	110	ASN
3	B	227	THR
3	B	229	ASN
3	B	326	ILE
3	B	575	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	B	612	ASN
4	C	39	VAL
4	C	44	ARG
9	K	36	ARG
9	K	63	LEU
11	L	20	VAL
11	L	85	ARG
11	L	89	ASN
1	a	37	ARG
1	a	424	ASN
1	a	442	ASN
1	a	584	CYS
1	a	644	ASN
2	x	21	ARG
2	x	32	ASN
3	b	110	ASN
3	b	309	THR
3	b	431	LEU
3	b	612	ASN
4	c	39	VAL
4	c	44	ARG
5	d	118	ARG
7	f	34	ASN
11	l	50	LEU
11	l	141	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	297	HIS
1	A	338	HIS
1	A	350	HIS
1	A	352	GLN
1	A	356	ASN
1	A	424	ASN
1	A	539	HIS
1	A	568	ASN
1	A	644	ASN
1	A	745	HIS
1	A	747	HIS
2	X	32	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	B	110	ASN
3	B	229	ASN
3	B	262	HIS
3	B	299	HIS
3	B	341	HIS
3	B	407	ASN
3	B	456	GLN
3	B	612	ASN
3	B	615	GLN
3	B	640	ASN
3	B	679	GLN
3	B	689	HIS
5	D	96	HIS
5	D	125	ASN
5	D	128	GLN
8	J	7	GLN
8	J	37	ASN
11	L	89	ASN
11	L	134	GLN
1	a	34	HIS
1	a	146	GLN
1	a	271	GLN
1	a	297	HIS
1	a	350	HIS
1	a	352	GLN
1	a	356	ASN
1	a	369	HIS
1	a	424	ASN
1	a	539	HIS
1	a	568	ASN
1	a	644	ASN
1	a	745	HIS
1	a	747	HIS
2	x	32	ASN
3	b	50	HIS
3	b	95	HIS
3	b	110	ASN
3	b	158	GLN
3	b	262	HIS
3	b	341	HIS
3	b	354	GLN
3	b	380	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	b	407	ASN
3	b	456	GLN
3	b	612	ASN
3	b	615	GLN
3	b	640	ASN
3	b	679	GLN
3	b	689	HIS
5	d	72	GLN
5	d	96	HIS
7	f	34	ASN
7	f	46	ASN
8	j	7	GLN
9	k	81	HIS
11	l	114	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](#)

259 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
14	CLA	a	829	-	65,73,73	1.50	9 (13%)	76,113,113	1.81	13 (17%)
14	CLA	J	101	-	45,53,73	1.73	8 (17%)	52,89,113	1.71	8 (15%)
17	BCR	A	851	-	41,41,41	1.19	3 (7%)	56,56,56	1.22	4 (7%)
17	BCR	M	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.32	9 (16%)
14	CLA	B	830	3	65,73,73	1.46	8 (12%)	76,113,113	1.54	11 (14%)
20	LMG	B	851	-	55,55,55	0.91	2 (3%)	63,63,63	1.44	8 (12%)
14	CLA	A	804	-	54,62,73	1.55	8 (14%)	62,99,113	1.70	7 (11%)
14	CLA	A	813	-	60,68,73	1.52	9 (15%)	70,107,113	1.53	12 (17%)
14	CLA	a	830	1	54,62,73	1.53	9 (16%)	62,99,113	1.43	9 (14%)
14	CLA	A	828	-	65,73,73	1.34	7 (10%)	76,113,113	1.64	11 (14%)
14	CLA	A	811	-	65,73,73	1.50	8 (12%)	76,113,113	1.66	12 (15%)
14	CLA	A	806	1	65,73,73	1.42	9 (13%)	76,113,113	1.58	10 (13%)
14	CLA	B	819	-	45,53,73	1.70	8 (17%)	52,89,113	1.62	9 (17%)
14	CLA	B	835	-	58,66,73	1.52	9 (15%)	67,104,113	1.51	7 (10%)
14	CLA	a	831	1	65,73,73	1.42	9 (13%)	76,113,113	1.57	11 (14%)
14	CLA	a	818	-	65,73,73	1.36	7 (10%)	76,113,113	1.73	13 (17%)
17	BCR	A	847	-	41,41,41	1.09	3 (7%)	56,56,56	1.28	6 (10%)
17	BCR	B	847	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	9 (16%)
17	BCR	l	207	-	41,41,41	1.11	2 (4%)	56,56,56	1.44	7 (12%)
19	SQD	b	801	-	53,54,54	0.97	6 (11%)	62,65,65	1.73	11 (17%)
14	CLA	B	814	3	54,62,73	1.48	7 (12%)	62,99,113	1.81	11 (17%)
14	CLA	B	841	3	47,55,73	1.73	8 (17%)	54,91,113	1.57	8 (14%)
14	CLA	f	203	-	45,53,73	1.72	8 (17%)	52,89,113	1.69	6 (11%)
14	CLA	B	815	3	54,62,73	1.58	7 (12%)	62,99,113	1.57	9 (14%)
14	CLA	A	830	1	65,73,73	1.57	9 (13%)	76,113,113	1.72	10 (13%)
14	CLA	A	820	-	54,62,73	1.58	8 (14%)	62,99,113	1.61	10 (16%)
14	CLA	A	821	-	65,73,73	1.56	7 (10%)	76,113,113	1.35	10 (13%)
17	BCR	m	1202	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	10 (17%)
14	CLA	a	817	-	60,68,73	1.56	10 (16%)	70,107,113	1.52	10 (14%)
18	LHG	A	853	14	48,48,48	0.77	2 (4%)	51,54,54	1.21	6 (11%)
14	CLA	A	808	1	65,73,73	1.38	7 (10%)	76,113,113	1.57	10 (13%)
17	BCR	b	848	-	41,41,41	1.15	2 (4%)	56,56,56	1.45	5 (8%)
16	SF4	C	101	-	0,12,12	-	-	-	-	-
14	CLA	B	811	3	65,73,73	1.47	10 (15%)	76,113,113	1.86	14 (18%)
14	CLA	b	833	-	54,62,73	1.61	10 (18%)	62,99,113	1.53	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	J	102	-	38,45,73	1.87	7 (18%)	43,78,113	1.71	7 (16%)
14	CLA	A	814	1	54,62,73	1.55	7 (12%)	62,99,113	1.80	9 (14%)
14	CLA	B	804	-	65,73,73	1.39	7 (10%)	76,113,113	1.53	12 (15%)
14	CLA	b	829	-	65,73,73	1.42	8 (12%)	76,113,113	1.61	9 (11%)
14	CLA	A	840	-	59,67,73	1.50	9 (15%)	68,105,113	1.35	7 (10%)
14	CLA	a	832	1	65,73,73	1.36	7 (10%)	76,113,113	1.54	11 (14%)
14	CLA	b	827	3	65,73,73	1.36	8 (12%)	76,113,113	1.55	12 (15%)
14	CLA	B	806	-	65,73,73	1.46	8 (12%)	76,113,113	2.08	13 (17%)
14	CLA	B	809	3	65,73,73	1.40	9 (13%)	76,113,113	1.59	10 (13%)
14	CLA	b	828	-	65,73,73	1.40	5 (7%)	76,113,113	1.74	14 (18%)
14	CLA	a	811	-	59,67,73	1.53	7 (11%)	68,105,113	1.50	8 (11%)
14	CLA	A	835	1	54,62,73	1.61	8 (14%)	62,99,113	1.54	8 (12%)
14	CLA	F	204	-	45,53,73	1.74	7 (15%)	52,89,113	1.64	10 (19%)
14	CLA	b	806	3	65,73,73	1.39	9 (13%)	76,113,113	1.54	8 (10%)
14	CLA	b	809	3	65,73,73	1.37	8 (12%)	76,113,113	1.54	9 (11%)
14	CLA	B	818	3	49,57,73	1.52	7 (14%)	55,93,113	1.69	9 (16%)
14	CLA	A	823	1	54,62,73	1.52	7 (12%)	62,99,113	1.72	10 (16%)
14	CLA	j	103	-	38,45,73	1.86	9 (23%)	43,78,113	1.69	7 (16%)
17	BCR	b	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.41	10 (17%)
14	CLA	a	819	-	54,62,73	1.58	7 (12%)	62,99,113	1.66	8 (12%)
14	CLA	b	818	-	49,57,73	1.62	9 (18%)	55,93,113	1.71	8 (14%)
17	BCR	b	849	-	41,41,41	1.21	4 (9%)	56,56,56	1.42	8 (14%)
18	LHG	F	201	-	42,42,48	0.73	1 (2%)	45,48,54	1.18	4 (8%)
14	CLA	b	831	-	65,73,73	1.31	9 (13%)	76,113,113	1.48	5 (6%)
14	CLA	B	838	-	45,53,73	1.83	8 (17%)	52,89,113	1.57	9 (17%)
14	CLA	b	821	3	65,73,73	1.35	9 (13%)	76,113,113	1.56	13 (17%)
14	CLA	m	1201	3	55,63,73	1.53	9 (16%)	64,101,113	1.60	9 (14%)
15	PQN	b	844	-	34,34,34	1.41	2 (5%)	42,45,45	1.38	7 (16%)
14	CLA	L	1503	-	45,53,73	1.65	6 (13%)	52,89,113	1.88	9 (17%)
14	CLA	a	815	-	45,53,73	1.73	7 (15%)	52,89,113	1.75	6 (11%)
14	CLA	B	837	-	45,53,73	1.68	7 (15%)	52,89,113	1.96	11 (21%)
14	CLA	a	824	-	65,73,73	1.39	6 (9%)	76,113,113	1.65	10 (13%)
17	BCR	j	105	-	41,41,41	1.17	2 (4%)	56,56,56	1.32	7 (12%)
14	CLA	x	1701	2	49,57,73	1.66	8 (16%)	55,93,113	1.54	6 (10%)
14	CLA	a	810	-	65,73,73	1.45	9 (13%)	76,113,113	1.59	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	a	835	1	45,53,73	1.69	7 (15%)	52,89,113	1.73	7 (13%)
14	CLA	b	803	-	65,73,73	1.44	10 (15%)	76,113,113	1.58	13 (17%)
19	SQD	l	202	-	53,54,54	0.97	6 (11%)	62,65,65	2.03	14 (22%)
14	CLA	A	819	-	65,73,73	1.44	7 (10%)	76,113,113	1.65	10 (13%)
14	CLA	a	837	1	65,73,73	1.38	10 (15%)	76,113,113	1.69	11 (14%)
17	BCR	B	850	-	41,41,41	1.16	3 (7%)	56,56,56	1.19	3 (5%)
14	CLA	b	843	3	65,73,73	1.47	9 (13%)	76,113,113	1.94	15 (19%)
14	CLA	A	809	1	65,73,73	1.42	6 (9%)	76,113,113	1.58	10 (13%)
14	CLA	b	807	-	65,73,73	1.42	10 (15%)	76,113,113	1.91	12 (15%)
17	BCR	I	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.30	8 (14%)
20	LMG	B	803	-	35,35,55	0.94	1 (2%)	43,43,63	1.24	4 (9%)
17	BCR	J	104	-	41,41,41	1.18	3 (7%)	56,56,56	1.39	9 (16%)
14	CLA	b	841	3	47,55,73	1.65	9 (19%)	54,91,113	1.59	9 (16%)
16	SF4	c	101	-	0,12,12	-	-	-	-	-
14	CLA	A	812	-	59,67,73	1.53	7 (11%)	68,105,113	1.47	7 (10%)
14	CLA	A	827	1	65,73,73	1.42	6 (9%)	76,113,113	1.52	7 (9%)
17	BCR	j	106	-	41,41,41	1.15	2 (4%)	56,56,56	1.37	6 (10%)
14	CLA	B	836	3	54,62,73	1.43	7 (12%)	62,99,113	1.83	12 (19%)
14	CLA	a	813	-	54,62,73	1.55	7 (12%)	62,99,113	1.65	7 (11%)
14	CLA	A	831	1	54,62,73	1.54	8 (14%)	62,99,113	1.62	10 (16%)
14	CLA	b	805	-	65,73,73	1.43	7 (10%)	76,113,113	1.57	11 (14%)
14	CLA	b	830	-	65,73,73	1.39	8 (12%)	76,113,113	1.49	10 (13%)
14	CLA	a	833	1	65,73,73	1.44	7 (10%)	76,113,113	1.83	17 (22%)
14	CLA	b	822	-	65,73,73	1.49	7 (10%)	76,113,113	1.64	9 (11%)
17	BCR	K	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	8 (14%)
14	CLA	b	836	3	54,62,73	1.54	8 (14%)	62,99,113	1.78	13 (20%)
14	CLA	b	816	-	65,73,73	1.45	8 (12%)	76,113,113	1.50	10 (13%)
17	BCR	A	848	-	41,41,41	1.13	1 (2%)	56,56,56	1.46	9 (16%)
17	BCR	b	846	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	7 (12%)
14	CLA	B	832	3	65,73,73	1.57	10 (15%)	76,113,113	1.76	11 (14%)
14	CLA	b	838	-	45,53,73	1.74	7 (15%)	52,89,113	1.60	6 (11%)
20	LMG	b	851	-	55,55,55	0.92	2 (3%)	63,63,63	1.49	11 (17%)
17	BCR	A	850	-	41,41,41	1.15	3 (7%)	56,56,56	1.25	7 (12%)
19	SQD	X	1702	-	53,54,54	0.98	5 (9%)	62,65,65	1.74	12 (19%)
14	CLA	B	813	-	60,68,73	1.52	9 (15%)	70,107,113	1.41	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	a	836	-	51,59,73	1.54	9 (17%)	59,96,113	1.71	11 (18%)
14	CLA	B	840	3	65,73,73	1.40	8 (12%)	76,113,113	1.60	12 (15%)
14	CLA	B	842	-	65,73,73	1.38	7 (10%)	76,113,113	1.49	9 (11%)
14	CLA	a	808	1	65,73,73	1.41	8 (12%)	76,113,113	1.59	10 (13%)
14	CLA	b	814	-	54,62,73	1.54	7 (12%)	62,99,113	1.66	9 (14%)
14	CLA	b	840	3	65,73,73	1.34	7 (10%)	76,113,113	1.61	10 (13%)
17	BCR	a	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.28	7 (12%)
14	CLA	X	1701	2	49,57,73	1.63	8 (16%)	55,93,113	1.73	10 (18%)
14	CLA	L	1502	11	60,68,73	1.45	8 (13%)	70,107,113	1.67	10 (14%)
14	CLA	A	807	-	60,68,73	1.51	8 (13%)	70,107,113	5.15	11 (15%)
14	CLA	A	826	-	54,62,73	1.51	7 (12%)	62,99,113	1.68	12 (19%)
17	BCR	a	845	-	41,41,41	1.09	2 (4%)	56,56,56	1.28	3 (5%)
17	BCR	a	849	-	41,41,41	1.21	3 (7%)	56,56,56	1.29	4 (7%)
14	CLA	A	841	1	65,73,73	1.44	9 (13%)	76,113,113	1.48	10 (13%)
14	CLA	b	835	3	65,73,73	1.48	8 (12%)	76,113,113	1.37	11 (14%)
14	CLA	B	828	-	65,73,73	1.37	5 (7%)	76,113,113	1.74	19 (25%)
17	BCR	I	102	-	41,41,41	1.20	4 (9%)	56,56,56	1.46	8 (14%)
14	CLA	l	203	11	45,53,73	1.68	7 (15%)	52,89,113	1.93	11 (21%)
14	CLA	a	814	-	45,53,73	1.69	7 (15%)	52,89,113	1.86	7 (13%)
14	CLA	a	821	1	45,53,73	1.73	8 (17%)	52,89,113	1.80	11 (21%)
14	CLA	A	805	1	65,73,73	1.36	7 (10%)	76,113,113	1.76	15 (19%)
14	CLA	a	803	-	54,62,73	1.56	6 (11%)	62,99,113	1.65	6 (9%)
14	CLA	a	840	1	65,73,73	1.47	9 (13%)	76,113,113	1.52	8 (10%)
14	CLA	A	836	1	45,53,73	1.68	7 (15%)	52,89,113	1.84	8 (15%)
14	CLA	B	831	-	65,73,73	1.37	8 (12%)	76,113,113	1.48	6 (7%)
17	BCR	A	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.27	7 (12%)
14	CLA	b	839	-	60,68,73	1.56	9 (15%)	70,107,113	1.47	11 (15%)
17	BCR	a	847	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	6 (10%)
14	CLA	l	204	11	60,68,73	1.46	8 (13%)	70,107,113	1.64	9 (12%)
17	BCR	F	205	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	7 (12%)
14	CLA	a	838	-	65,73,73	1.43	8 (12%)	76,113,113	1.40	7 (9%)
14	CLA	B	833	3	54,62,73	1.57	8 (14%)	62,99,113	1.51	7 (11%)
14	CLA	a	827	-	65,73,73	1.36	6 (9%)	76,113,113	1.63	11 (14%)
14	CLA	a	807	-	65,73,73	1.45	9 (13%)	76,113,113	1.54	10 (13%)
14	CLA	l	205	-	45,53,73	1.68	7 (15%)	52,89,113	1.92	9 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	K	101	-	42,49,73	1.77	7 (16%)	48,83,113	1.55	7 (14%)
14	CLA	b	804	-	65,73,73	1.47	8 (12%)	76,113,113	1.53	10 (13%)
14	CLA	B	805	-	65,73,73	1.36	8 (12%)	76,113,113	1.47	6 (7%)
14	CLA	B	829	3	65,73,73	1.50	7 (10%)	76,113,113	1.69	10 (13%)
14	CLA	B	824	3	45,53,73	1.69	7 (15%)	52,89,113	1.74	8 (15%)
14	CLA	A	816	-	45,53,73	1.73	7 (15%)	52,89,113	1.72	8 (15%)
14	CLA	A	842	-	65,73,73	1.46	9 (13%)	76,113,113	1.66	10 (13%)
14	CLA	b	819	-	45,53,73	1.67	7 (15%)	52,89,113	1.80	8 (15%)
14	CLA	b	824	3	45,53,73	1.69	7 (15%)	52,89,113	1.68	7 (13%)
14	CLA	j	101	-	58,66,73	1.55	9 (15%)	67,104,113	1.59	10 (14%)
14	CLA	b	825	-	55,63,73	1.54	7 (12%)	64,101,113	1.57	7 (10%)
14	CLA	a	834	1	54,62,73	1.59	9 (16%)	62,99,113	1.58	6 (9%)
14	CLA	a	812	-	60,68,73	1.54	9 (15%)	70,107,113	1.41	7 (10%)
18	LHG	i	103	-	42,42,48	0.64	0	45,48,54	1.26	6 (13%)
14	CLA	A	802	-	65,73,73	1.47	9 (13%)	76,113,113	1.52	11 (14%)
14	CLA	A	834	-	65,73,73	1.37	7 (10%)	76,113,113	1.69	14 (18%)
16	SF4	a	843	-	0,12,12	-	-	-	-	-
18	LHG	a	850	-	48,48,48	0.76	1 (2%)	51,54,54	1.33	6 (11%)
14	CLA	B	834	-	60,68,73	1.43	7 (11%)	70,107,113	1.61	6 (8%)
17	BCR	B	849	-	41,41,41	1.21	6 (14%)	56,56,56	1.46	7 (12%)
17	BCR	k	103	-	41,41,41	1.06	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	A	829	-	65,73,73	1.36	8 (12%)	76,113,113	1.61	13 (17%)
14	CLA	a	828	-	65,73,73	1.39	8 (12%)	76,113,113	1.53	8 (10%)
18	LHG	a	851	14	48,48,48	0.93	5 (10%)	51,54,54	0.98	2 (3%)
14	CLA	b	834	-	60,68,73	1.48	8 (13%)	70,107,113	1.54	8 (11%)
14	CLA	B	821	3	65,73,73	1.44	8 (12%)	76,113,113	1.36	7 (9%)
14	CLA	b	808	-	65,73,73	1.36	10 (15%)	76,113,113	1.76	11 (14%)
15	PQN	B	844	-	34,34,34	1.50	2 (5%)	42,45,45	1.26	4 (9%)
17	BCR	b	850	-	41,41,41	1.10	3 (7%)	56,56,56	1.10	3 (5%)
14	CLA	B	817	-	50,58,73	1.57	7 (14%)	58,95,113	1.62	9 (15%)
14	CLA	B	826	-	65,73,73	1.37	6 (9%)	76,113,113	1.60	10 (13%)
17	BCR	B	845	-	41,41,41	1.12	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	B	823	3	45,53,73	1.68	9 (20%)	52,89,113	1.99	14 (26%)
14	CLA	b	817	3	50,58,73	1.65	8 (16%)	58,95,113	1.69	8 (13%)
14	CLA	a	820	-	65,73,73	1.45	7 (10%)	76,113,113	1.64	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	a	816	-	59,67,73	1.49	10 (16%)	68,105,113	1.57	11 (16%)
14	CLA	b	823	3	45,53,73	1.72	9 (20%)	52,89,113	1.64	7 (13%)
17	BCR	b	845	-	41,41,41	1.12	2 (4%)	56,56,56	1.17	3 (5%)
17	BCR	a	844	-	41,41,41	1.18	4 (9%)	56,56,56	1.32	8 (14%)
14	CLA	b	815	-	54,62,73	1.61	7 (12%)	62,99,113	1.70	10 (16%)
17	BCR	f	202	-	41,41,41	1.20	3 (7%)	56,56,56	1.25	5 (8%)
14	CLA	A	839	-	65,73,73	1.41	8 (12%)	76,113,113	1.51	10 (13%)
14	CLA	A	824	1	45,53,73	1.69	8 (17%)	52,89,113	1.70	8 (15%)
17	BCR	i	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.43	9 (16%)
13	CL0	a	801	1	65,73,73	2.36	18 (27%)	76,113,113	2.61	22 (28%)
14	CLA	a	823	1	45,53,73	1.64	6 (13%)	52,89,113	1.83	9 (17%)
16	SF4	C	102	-	0,12,12	-	-	-	-	-
14	CLA	B	843	3	65,73,73	1.39	9 (13%)	76,113,113	1.63	14 (18%)
14	CLA	b	832	3	65,73,73	1.51	9 (13%)	76,113,113	1.71	15 (19%)
14	CLA	A	837	-	51,59,73	1.49	7 (13%)	59,96,113	1.89	10 (16%)
15	PQN	A	844	-	34,34,34	1.50	2 (5%)	42,45,45	1.08	4 (9%)
17	BCR	l	206	-	41,41,41	1.09	1 (2%)	56,56,56	1.56	12 (21%)
14	CLA	B	802	1	65,73,73	1.40	9 (13%)	76,113,113	1.48	9 (11%)
14	CLA	b	802	-	65,73,73	1.28	7 (10%)	76,113,113	1.67	7 (9%)
17	BCR	A	849	-	41,41,41	1.17	3 (7%)	56,56,56	1.44	8 (14%)
14	CLA	B	827	3	65,73,73	1.40	8 (12%)	76,113,113	1.72	13 (17%)
14	CLA	a	826	-	65,73,73	1.39	9 (13%)	76,113,113	1.59	8 (10%)
17	BCR	B	848	-	41,41,41	1.09	3 (7%)	56,56,56	1.30	5 (8%)
17	BCR	L	1504	-	41,41,41	1.07	3 (7%)	56,56,56	1.32	7 (12%)
14	CLA	B	801	-	65,73,73	1.38	7 (10%)	76,113,113	1.71	11 (14%)
14	CLA	B	816	-	65,73,73	1.42	9 (13%)	76,113,113	1.48	8 (10%)
14	CLA	a	841	18	45,53,73	1.61	7 (15%)	52,89,113	4.16	9 (17%)
14	CLA	A	803	-	65,73,73	1.39	7 (10%)	76,113,113	1.62	8 (10%)
17	BCR	B	846	-	41,41,41	1.10	3 (7%)	56,56,56	1.33	9 (16%)
14	CLA	A	817	-	59,67,73	1.56	8 (13%)	68,105,113	1.57	9 (13%)
14	CLA	a	822	1	54,62,73	1.61	8 (14%)	62,99,113	1.47	12 (19%)
17	BCR	i	102	-	41,41,41	1.20	3 (7%)	56,56,56	1.32	8 (14%)
14	CLA	a	805	1	65,73,73	1.40	8 (12%)	76,113,113	1.53	8 (10%)
14	CLA	B	812	-	65,73,73	1.39	8 (12%)	76,113,113	1.69	13 (17%)
14	CLA	b	811	-	65,73,73	1.42	11 (16%)	76,113,113	1.71	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	BCR	J	103	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	6 (10%)
17	BCR	a	846	-	41,41,41	1.13	2 (4%)	56,56,56	1.45	9 (16%)
14	CLA	A	838	1	65,73,73	1.35	7 (10%)	76,113,113	1.62	10 (13%)
14	CLA	b	812	3	65,73,73	1.51	9 (13%)	76,113,113	1.65	10 (13%)
14	CLA	B	810	3	65,73,73	1.31	7 (10%)	76,113,113	1.46	7 (9%)
14	CLA	b	842	-	65,73,73	1.44	6 (9%)	76,113,113	1.47	8 (10%)
14	CLA	k	101	-	42,49,73	1.78	7 (16%)	48,83,113	1.62	5 (10%)
16	SF4	A	845	-	0,12,12	-	-	-	-	-
14	CLA	A	832	1	65,73,73	1.38	8 (12%)	76,113,113	1.62	7 (9%)
14	CLA	A	843	18	45,53,73	1.73	8 (17%)	52,89,113	1.73	9 (17%)
17	BCR	l	201	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	8 (14%)
14	CLA	b	810	3	65,73,73	1.34	7 (10%)	76,113,113	1.57	9 (11%)
14	CLA	B	808	-	65,73,73	1.51	10 (15%)	76,113,113	2.02	20 (26%)
16	SF4	c	102	-	0,12,12	-	-	-	-	-
19	SQD	x	1702	-	53,54,54	0.97	5 (9%)	62,65,65	1.76	9 (14%)
14	CLA	B	807	3	55,63,73	1.50	7 (12%)	64,101,113	1.61	8 (12%)
14	CLA	B	825	-	55,63,73	1.54	6 (10%)	64,101,113	1.64	7 (10%)
18	LHG	A	852	-	48,48,48	0.83	3 (6%)	51,54,54	1.33	7 (13%)
14	CLA	b	837	-	45,53,73	1.70	7 (15%)	52,89,113	1.79	10 (19%)
14	CLA	j	102	-	45,53,73	1.72	7 (15%)	52,89,113	1.67	7 (13%)
15	PQN	a	842	-	34,34,34	1.47	2 (5%)	42,45,45	1.27	5 (11%)
13	CL0	A	801	-	65,73,73	2.35	18 (27%)	76,113,113	2.61	22 (28%)
14	CLA	A	815	-	45,53,73	1.66	7 (15%)	52,89,113	1.92	6 (11%)
14	CLA	A	822	-	45,53,73	1.68	7 (15%)	52,89,113	1.69	8 (15%)
14	CLA	a	825	-	54,62,73	1.54	7 (12%)	62,99,113	1.60	9 (14%)
14	CLA	B	839	3	60,68,73	1.53	10 (16%)	70,107,113	1.45	11 (15%)
14	CLA	K	102	-	49,57,73	1.65	6 (12%)	55,93,113	1.69	8 (14%)
14	CLA	b	813	-	60,68,73	1.58	9 (15%)	70,107,113	1.49	13 (18%)
14	CLA	k	102	-	49,57,73	1.67	8 (16%)	55,93,113	1.74	10 (18%)
17	BCR	F	203	-	41,41,41	1.17	2 (4%)	56,56,56	1.35	8 (14%)
14	CLA	A	825	-	65,73,73	1.38	8 (12%)	76,113,113	1.55	9 (11%)
17	BCR	J	105	-	41,41,41	1.12	2 (4%)	56,56,56	1.33	9 (16%)
14	CLA	a	804	1	65,73,73	1.37	7 (10%)	76,113,113	1.67	14 (18%)
17	BCR	f	204	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	8 (14%)
14	CLA	a	839	1	65,73,73	1.40	9 (13%)	76,113,113	1.49	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	B	820	3	65,73,73	1.43	9 (13%)	76,113,113	1.54	7 (9%)
14	CLA	F	202	3	65,73,73	1.46	7 (10%)	76,113,113	1.52	9 (11%)
14	CLA	A	818	1	60,68,73	1.54	10 (16%)	70,107,113	1.46	7 (10%)
14	CLA	a	806	-	60,68,73	1.50	10 (16%)	70,107,113	1.49	9 (12%)
14	CLA	A	810	1	45,53,73	1.70	7 (15%)	52,89,113	1.73	7 (13%)
14	CLA	B	822	-	65,73,73	1.43	7 (10%)	76,113,113	1.55	8 (10%)
14	CLA	a	809	1	45,53,73	1.68	7 (15%)	52,89,113	1.80	5 (9%)
14	CLA	f	201	-	59,67,73	1.55	8 (13%)	68,105,113	1.35	7 (10%)
14	CLA	a	802	1	65,73,73	1.42	7 (10%)	76,113,113	1.53	8 (10%)
14	CLA	L	1501	11	51,59,73	1.76	9 (17%)	59,96,113	1.60	10 (16%)
17	BCR	j	104	-	41,41,41	1.15	3 (7%)	56,56,56	1.33	7 (12%)
14	CLA	b	820	-	65,73,73	1.44	10 (15%)	76,113,113	1.43	8 (10%)
14	CLA	b	826	-	65,73,73	1.35	6 (9%)	76,113,113	1.56	10 (13%)
14	CLA	A	833	1	65,73,73	1.45	8 (12%)	76,113,113	1.46	9 (11%)

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
14	CLA	a	829	-	1/1/15/20	11/37/115/115	-
14	CLA	J	101	-	1/1/11/20	8/13/91/115	-
17	BCR	A	851	-	-	16/29/63/63	0/2/2/2
17	BCR	M	101	-	-	12/29/63/63	0/2/2/2
14	CLA	B	830	3	1/1/15/20	12/37/115/115	-
20	LMG	B	851	-	-	28/50/70/70	0/1/1/1
14	CLA	A	804	-	1/1/12/20	4/24/102/115	-
14	CLA	A	813	-	1/1/14/20	14/31/109/115	-
14	CLA	a	830	1	1/1/12/20	7/24/102/115	-
14	CLA	A	828	-	1/1/15/20	16/37/115/115	-
14	CLA	A	811	-	1/1/15/20	10/37/115/115	-
14	CLA	A	806	1	1/1/15/20	14/37/115/115	-
14	CLA	B	819	-	1/1/11/20	1/13/91/115	-
14	CLA	B	835	-	1/1/13/20	12/29/107/115	-
14	CLA	a	831	1	1/1/15/20	15/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	818	-	1/1/15/20	13/37/115/115	-
17	BCR	A	847	-	-	10/29/63/63	0/2/2/2
17	BCR	B	847	-	-	13/29/63/63	0/2/2/2
17	BCR	l	207	-	-	6/29/63/63	0/2/2/2
19	SQD	b	801	-	-	22/49/69/69	0/1/1/1
14	CLA	B	814	3	1/1/12/20	9/24/102/115	-
14	CLA	B	841	3	1/1/11/20	3/16/94/115	-
14	CLA	f	203	-	1/1/11/20	5/13/91/115	-
14	CLA	B	815	3	1/1/12/20	5/24/102/115	-
14	CLA	A	830	1	1/1/15/20	9/37/115/115	-
14	CLA	A	820	-	1/1/12/20	9/24/102/115	-
14	CLA	A	821	-	1/1/15/20	12/37/115/115	-
17	BCR	m	1202	-	-	11/29/63/63	0/2/2/2
14	CLA	a	817	-	1/1/14/20	13/31/109/115	-
18	LHG	A	853	14	-	21/53/53/53	-
14	CLA	A	808	1	1/1/15/20	21/37/115/115	-
17	BCR	b	848	-	-	15/29/63/63	0/2/2/2
16	SF4	C	101	-	-	-	0/6/5/5
14	CLA	B	811	3	1/1/15/20	7/37/115/115	-
14	CLA	b	833	-	1/1/12/20	7/24/102/115	-
14	CLA	J	102	-	1/1/8/20	0/2/76/115	-
14	CLA	A	814	1	1/1/12/20	5/24/102/115	-
14	CLA	B	804	-	1/1/15/20	15/37/115/115	-
14	CLA	b	829	-	1/1/15/20	10/37/115/115	-
14	CLA	A	840	-	1/1/13/20	7/30/108/115	-
14	CLA	a	832	1	1/1/15/20	8/37/115/115	-
14	CLA	b	827	3	-	13/37/115/115	-
14	CLA	B	806	-	1/1/15/20	12/37/115/115	-
14	CLA	B	809	3	1/1/15/20	16/37/115/115	-
14	CLA	b	828	-	1/1/15/20	15/37/115/115	-
14	CLA	a	811	-	1/1/13/20	11/30/108/115	-
14	CLA	A	835	1	1/1/12/20	8/24/102/115	-
14	CLA	F	204	-	1/1/11/20	1/13/91/115	-
14	CLA	b	806	3	1/1/15/20	9/37/115/115	-
14	CLA	b	809	3	1/1/15/20	20/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	818	3	1/1/11/20	5/18/96/115	-
14	CLA	A	823	1	1/1/12/20	9/24/102/115	-
14	CLA	j	103	-	1/1/8/20	0/2/76/115	-
17	BCR	b	847	-	-	10/29/63/63	0/2/2/2
14	CLA	a	819	-	1/1/12/20	9/24/102/115	-
14	CLA	b	818	-	1/1/11/20	5/18/96/115	-
17	BCR	b	849	-	-	8/29/63/63	0/2/2/2
18	LHG	F	201	-	-	27/47/47/53	-
14	CLA	b	831	-	1/1/15/20	12/37/115/115	-
14	CLA	B	838	-	1/1/11/20	6/13/91/115	-
14	CLA	b	821	3	1/1/15/20	9/37/115/115	-
14	CLA	m	1201	3	1/1/13/20	9/25/103/115	-
15	PQN	b	844	-	-	5/23/43/43	0/2/2/2
14	CLA	L	1503	-	1/1/11/20	6/13/91/115	-
14	CLA	a	815	-	1/1/11/20	0/13/91/115	-
14	CLA	B	837	-	1/1/11/20	2/13/91/115	-
14	CLA	a	824	-	1/1/15/20	13/37/115/115	-
17	BCR	j	105	-	-	11/29/63/63	0/2/2/2
14	CLA	x	1701	2	1/1/11/20	7/18/96/115	-
14	CLA	a	810	-	1/1/15/20	7/37/115/115	-
14	CLA	a	835	1	1/1/11/20	7/13/91/115	-
14	CLA	b	803	-	1/1/15/20	9/37/115/115	-
19	SQD	l	202	-	-	25/49/69/69	0/1/1/1
14	CLA	A	819	-	1/1/15/20	12/37/115/115	-
14	CLA	a	837	1	1/1/15/20	16/37/115/115	-
17	BCR	B	850	-	-	9/29/63/63	0/2/2/2
14	CLA	b	843	3	-	12/37/115/115	-
14	CLA	A	809	1	1/1/15/20	12/37/115/115	-
14	CLA	b	807	-	1/1/15/20	12/37/115/115	-
17	BCR	I	101	-	-	11/29/63/63	0/2/2/2
20	LMG	B	803	-	-	12/30/50/70	0/1/1/1
17	BCR	J	104	-	-	13/29/63/63	0/2/2/2
14	CLA	b	841	3	1/1/11/20	7/16/94/115	-
16	SF4	c	101	-	-	-	0/6/5/5
14	CLA	A	812	-	1/1/13/20	7/30/108/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	827	1	1/1/15/20	14/37/115/115	-
17	BCR	j	106	-	-	15/29/63/63	0/2/2/2
14	CLA	B	836	3	1/1/12/20	11/24/102/115	-
14	CLA	a	813	-	1/1/12/20	2/24/102/115	-
14	CLA	A	831	1	1/1/12/20	6/24/102/115	-
14	CLA	b	805	-	1/1/15/20	18/37/115/115	-
14	CLA	b	830	-	1/1/15/20	16/37/115/115	-
14	CLA	a	833	1	1/1/15/20	16/37/115/115	-
14	CLA	b	822	-	1/1/15/20	9/37/115/115	-
17	BCR	K	103	-	-	12/29/63/63	0/2/2/2
14	CLA	b	836	3	1/1/12/20	8/24/102/115	-
14	CLA	b	816	-	-	16/37/115/115	-
17	BCR	A	848	-	-	12/29/63/63	0/2/2/2
17	BCR	b	846	-	-	12/29/63/63	0/2/2/2
14	CLA	B	832	3	1/1/15/20	9/37/115/115	-
14	CLA	b	838	-	1/1/11/20	5/13/91/115	-
20	LMG	b	851	-	-	23/50/70/70	0/1/1/1
17	BCR	A	850	-	-	13/29/63/63	0/2/2/2
19	SQD	X	1702	-	-	17/49/69/69	0/1/1/1
14	CLA	B	813	-	1/1/14/20	13/31/109/115	-
14	CLA	a	836	-	1/1/12/20	8/21/99/115	-
14	CLA	B	840	3	1/1/15/20	9/37/115/115	-
14	CLA	B	842	-	1/1/15/20	5/37/115/115	-
14	CLA	a	808	1	1/1/15/20	13/37/115/115	-
14	CLA	b	814	-	1/1/12/20	11/24/102/115	-
14	CLA	b	840	3	1/1/15/20	9/37/115/115	-
17	BCR	a	848	-	-	9/29/63/63	0/2/2/2
14	CLA	X	1701	2	1/1/11/20	9/18/96/115	-
14	CLA	L	1502	11	-	8/31/109/115	-
14	CLA	A	807	-	1/1/14/20	17/31/109/115	-
14	CLA	A	826	-	1/1/12/20	6/24/102/115	-
17	BCR	a	845	-	-	7/29/63/63	0/2/2/2
17	BCR	a	849	-	-	15/29/63/63	0/2/2/2
14	CLA	A	841	1	1/1/15/20	21/37/115/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	835	3	1/1/15/20	15/37/115/115	-
14	CLA	B	828	-	1/1/15/20	12/37/115/115	-
17	BCR	I	102	-	-	11/29/63/63	0/2/2/2
14	CLA	l	203	11	1/1/11/20	8/13/91/115	-
14	CLA	a	814	-	1/1/11/20	6/13/91/115	-
14	CLA	a	821	1	1/1/11/20	4/13/91/115	-
14	CLA	A	805	1	1/1/15/20	16/37/115/115	-
14	CLA	a	803	-	1/1/12/20	5/24/102/115	-
14	CLA	a	840	1	1/1/15/20	6/37/115/115	-
14	CLA	A	836	1	1/1/11/20	3/13/91/115	-
14	CLA	B	831	-	1/1/15/20	11/37/115/115	-
17	BCR	A	846	-	-	10/29/63/63	0/2/2/2
14	CLA	b	839	-	1/1/14/20	8/31/109/115	-
17	BCR	a	847	-	-	17/29/63/63	0/2/2/2
14	CLA	l	204	11	-	9/31/109/115	-
17	BCR	F	205	-	-	10/29/63/63	0/2/2/2
14	CLA	a	838	-	1/1/15/20	11/37/115/115	-
14	CLA	B	833	3	1/1/12/20	6/24/102/115	-
14	CLA	a	827	-	1/1/15/20	9/37/115/115	-
14	CLA	a	807	-	1/1/15/20	20/37/115/115	-
14	CLA	l	205	-	1/1/11/20	4/13/91/115	-
14	CLA	K	101	-	1/1/9/20	5/7/81/115	-
14	CLA	b	804	-	1/1/15/20	21/37/115/115	-
14	CLA	B	805	-	1/1/15/20	12/37/115/115	-
14	CLA	B	829	3	1/1/15/20	10/37/115/115	-
14	CLA	B	824	3	1/1/11/20	2/13/91/115	-
14	CLA	A	816	-	1/1/11/20	0/13/91/115	-
14	CLA	A	842	-	1/1/15/20	20/37/115/115	-
14	CLA	b	819	-	1/1/11/20	2/13/91/115	-
14	CLA	b	824	3	1/1/11/20	2/13/91/115	-
14	CLA	j	101	-	1/1/13/20	10/29/107/115	-
14	CLA	b	825	-	1/1/13/20	13/25/103/115	-
14	CLA	a	834	1	1/1/12/20	4/24/102/115	-
14	CLA	a	812	-	1/1/14/20	15/31/109/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	i	103	-	-	28/47/47/53	-
14	CLA	A	802	-	1/1/15/20	8/37/115/115	-
14	CLA	A	834	-	1/1/15/20	13/37/115/115	-
18	LHG	a	850	-	-	17/53/53/53	-
16	SF4	a	843	-	-	-	0/6/5/5
14	CLA	B	834	-	1/1/14/20	16/31/109/115	-
17	BCR	B	849	-	-	12/29/63/63	0/2/2/2
17	BCR	k	103	-	-	7/29/63/63	0/2/2/2
14	CLA	A	829	-	1/1/15/20	10/37/115/115	-
14	CLA	a	828	-	1/1/15/20	15/37/115/115	-
18	LHG	a	851	14	-	24/53/53/53	-
14	CLA	b	834	-	1/1/14/20	16/31/109/115	-
14	CLA	B	821	3	1/1/15/20	11/37/115/115	-
14	CLA	b	808	-	1/1/15/20	13/37/115/115	-
15	PQN	B	844	-	-	4/23/43/43	0/2/2/2
17	BCR	b	850	-	-	10/29/63/63	0/2/2/2
14	CLA	B	817	-	1/1/12/20	2/19/97/115	-
14	CLA	B	826	-	1/1/15/20	9/37/115/115	-
17	BCR	B	845	-	-	12/29/63/63	0/2/2/2
14	CLA	B	823	3	1/1/11/20	7/13/91/115	-
14	CLA	b	817	3	1/1/12/20	3/19/97/115	-
14	CLA	a	820	-	1/1/15/20	16/37/115/115	-
14	CLA	a	816	-	1/1/13/20	9/30/108/115	-
14	CLA	b	823	3	1/1/11/20	6/13/91/115	-
17	BCR	b	845	-	-	12/29/63/63	0/2/2/2
17	BCR	a	844	-	-	11/29/63/63	0/2/2/2
14	CLA	b	815	-	1/1/12/20	9/24/102/115	-
17	BCR	f	202	-	-	16/29/63/63	0/2/2/2
14	CLA	A	839	-	-	16/37/115/115	-
14	CLA	A	824	1	1/1/11/20	2/13/91/115	-
17	BCR	i	101	-	-	14/29/63/63	0/2/2/2
13	CL0	a	801	1	3/3/20/25	4/37/135/135	-
14	CLA	a	823	1	1/1/11/20	4/13/91/115	-
16	SF4	C	102	-	-	-	0/6/5/5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	843	3	1/1/15/20	15/37/115/115	-
14	CLA	b	832	3	1/1/15/20	11/37/115/115	-
14	CLA	A	837	-	1/1/12/20	11/21/99/115	-
15	PQN	A	844	-	-	5/23/43/43	0/2/2/2
17	BCR	l	206	-	-	10/29/63/63	0/2/2/2
14	CLA	B	802	1	1/1/15/20	12/37/115/115	-
14	CLA	b	802	-	1/1/15/20	10/37/115/115	-
17	BCR	A	849	-	-	15/29/63/63	0/2/2/2
14	CLA	B	827	3	1/1/15/20	7/37/115/115	-
14	CLA	a	826	-	-	7/37/115/115	-
17	BCR	B	848	-	-	12/29/63/63	0/2/2/2
17	BCR	L	1504	-	-	13/29/63/63	0/2/2/2
14	CLA	B	801	-	1/1/15/20	10/37/115/115	-
14	CLA	B	816	-	1/1/15/20	13/37/115/115	-
14	CLA	a	841	18	1/1/11/20	8/13/91/115	-
14	CLA	A	803	-	1/1/15/20	9/37/115/115	-
17	BCR	B	846	-	-	9/29/63/63	0/2/2/2
14	CLA	A	817	-	1/1/13/20	6/30/108/115	-
14	CLA	a	822	1	1/1/12/20	9/24/102/115	-
17	BCR	i	102	-	-	12/29/63/63	0/2/2/2
14	CLA	a	805	1	1/1/15/20	16/37/115/115	-
14	CLA	B	812	-	1/1/15/20	13/37/115/115	-
14	CLA	b	811	-	1/1/15/20	7/37/115/115	-
17	BCR	J	103	-	-	12/29/63/63	0/2/2/2
17	BCR	a	846	-	-	15/29/63/63	0/2/2/2
14	CLA	A	838	1	1/1/15/20	13/37/115/115	-
14	CLA	b	812	3	1/1/15/20	19/37/115/115	-
14	CLA	B	810	3	1/1/15/20	9/37/115/115	-
14	CLA	b	842	-	1/1/15/20	6/37/115/115	-
14	CLA	k	101	-	1/1/9/20	2/7/81/115	-
16	SF4	A	845	-	-	-	0/6/5/5
14	CLA	A	832	1	1/1/15/20	18/37/115/115	-
14	CLA	A	843	18	1/1/11/20	7/13/91/115	-
17	BCR	l	201	-	-	9/29/63/63	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	810	3	1/1/15/20	7/37/115/115	-
14	CLA	B	808	-	1/1/15/20	17/37/115/115	-
19	SQD	x	1702	-	-	14/49/69/69	0/1/1/1
16	SF4	c	102	-	-	-	0/6/5/5
14	CLA	B	807	3	1/1/13/20	6/25/103/115	-
14	CLA	B	825	-	1/1/13/20	11/25/103/115	-
18	LHG	A	852	-	-	21/53/53/53	-
14	CLA	b	837	-	1/1/11/20	2/13/91/115	-
14	CLA	j	102	-	1/1/11/20	9/13/91/115	-
15	PQN	a	842	-	-	5/23/43/43	0/2/2/2
13	CL0	A	801	-	3/3/20/25	4/37/135/135	-
14	CLA	A	815	-	1/1/11/20	3/13/91/115	-
14	CLA	A	822	-	1/1/11/20	6/13/91/115	-
14	CLA	a	825	-	1/1/12/20	6/24/102/115	-
14	CLA	B	839	3	1/1/14/20	7/31/109/115	-
14	CLA	K	102	-	1/1/11/20	2/18/96/115	-
14	CLA	b	813	-	1/1/14/20	16/31/109/115	-
14	CLA	k	102	-	1/1/11/20	4/18/96/115	-
17	BCR	F	203	-	-	14/29/63/63	0/2/2/2
14	CLA	A	825	-	1/1/15/20	16/37/115/115	-
17	BCR	J	105	-	-	9/29/63/63	0/2/2/2
14	CLA	a	804	1	1/1/15/20	17/37/115/115	-
17	BCR	f	204	-	-	15/29/63/63	0/2/2/2
14	CLA	a	839	1	1/1/15/20	5/37/115/115	-
14	CLA	B	820	3	1/1/15/20	15/37/115/115	-
14	CLA	F	202	3	1/1/15/20	17/37/115/115	-
14	CLA	A	818	1	1/1/14/20	8/31/109/115	-
14	CLA	a	806	-	1/1/14/20	8/31/109/115	-
14	CLA	A	810	1	1/1/11/20	3/13/91/115	-
14	CLA	B	822	-	1/1/15/20	10/37/115/115	-
14	CLA	a	809	1	1/1/11/20	7/13/91/115	-
14	CLA	f	201	-	1/1/13/20	7/30/108/115	-
14	CLA	a	802	1	1/1/15/20	10/37/115/115	-
14	CLA	L	1501	11	1/1/12/20	5/21/99/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	j	104	-	-	14/29/63/63	0/2/2/2
14	CLA	b	820	-	1/1/15/20	5/37/115/115	-
14	CLA	b	826	-	1/1/15/20	8/37/115/115	-
14	CLA	A	833	1	1/1/15/20	10/37/115/115	-

All (1676) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	801	CL0	MG-NA	9.30	2.28	2.06
13	A	801	CL0	MG-NA	9.30	2.28	2.06
14	A	821	CLA	C4B-NB	7.66	1.42	1.35
14	B	838	CLA	C4B-NB	7.58	1.42	1.35
14	A	811	CLA	C4B-NB	7.57	1.42	1.35
14	A	830	CLA	C4B-NB	7.54	1.41	1.35
15	B	844	PQN	C3-C2	7.53	1.49	1.35
15	A	844	PQN	C3-C2	7.44	1.48	1.35
14	J	102	CLA	C4B-NB	7.31	1.41	1.35
14	b	822	CLA	C4B-NB	7.26	1.41	1.35
14	A	817	CLA	C4B-NB	7.21	1.41	1.35
14	b	835	CLA	C4B-NB	7.20	1.41	1.35
14	L	1501	CLA	C4B-NB	7.19	1.41	1.35
14	a	840	CLA	C4B-NB	7.19	1.41	1.35
14	b	813	CLA	C4B-NB	7.16	1.41	1.35
14	B	841	CLA	C4B-NB	7.15	1.41	1.35
14	a	811	CLA	C4B-NB	7.15	1.41	1.35
14	B	808	CLA	C4B-NB	7.11	1.41	1.35
14	A	812	CLA	C4B-NB	7.11	1.41	1.35
14	B	813	CLA	C4B-NB	7.10	1.41	1.35
14	F	202	CLA	C4B-NB	7.10	1.41	1.35
14	A	807	CLA	C4B-NB	7.06	1.41	1.35
14	x	1701	CLA	C4B-NB	7.06	1.41	1.35
14	a	833	CLA	C4B-NB	7.05	1.41	1.35
14	b	815	CLA	C4B-NB	7.05	1.41	1.35
14	j	103	CLA	C4B-NB	7.05	1.41	1.35
14	a	810	CLA	C4B-NB	7.04	1.41	1.35
14	b	838	CLA	C4B-NB	7.02	1.41	1.35
15	a	842	PQN	C3-C2	7.01	1.48	1.35
14	a	819	CLA	C4B-NB	6.96	1.41	1.35
14	B	822	CLA	C4B-NB	6.95	1.41	1.35
14	A	843	CLA	C4B-NB	6.94	1.41	1.35
14	K	102	CLA	C4B-NB	6.93	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	204	CLA	C4B-NB	6.93	1.41	1.35
14	J	101	CLA	C4B-NB	6.92	1.41	1.35
14	b	823	CLA	C4B-NB	6.90	1.41	1.35
14	A	814	CLA	C4B-NB	6.89	1.41	1.35
14	j	102	CLA	C4B-NB	6.89	1.41	1.35
14	A	841	CLA	C4B-NB	6.89	1.41	1.35
14	b	833	CLA	C4B-NB	6.89	1.41	1.35
14	a	813	CLA	C4B-NB	6.88	1.41	1.35
14	k	101	CLA	C4B-NB	6.87	1.41	1.35
14	B	815	CLA	C4B-NB	6.87	1.41	1.35
14	B	829	CLA	C4B-NB	6.86	1.41	1.35
14	a	812	CLA	C4B-NB	6.86	1.41	1.35
14	B	811	CLA	C4B-NB	6.86	1.41	1.35
14	f	201	CLA	C4B-NB	6.85	1.41	1.35
14	a	807	CLA	C4B-NB	6.85	1.41	1.35
14	b	842	CLA	C4B-NB	6.84	1.41	1.35
14	b	817	CLA	C4B-NB	6.83	1.41	1.35
14	a	835	CLA	C4B-NB	6.82	1.41	1.35
14	k	102	CLA	C4B-NB	6.82	1.41	1.35
14	A	842	CLA	C4B-NB	6.82	1.41	1.35
14	b	832	CLA	C4B-NB	6.81	1.41	1.35
14	a	806	CLA	C4B-NB	6.79	1.41	1.35
14	a	820	CLA	C4B-NB	6.79	1.41	1.35
14	b	839	CLA	C4B-NB	6.77	1.41	1.35
14	a	803	CLA	C4B-NB	6.77	1.41	1.35
14	A	810	CLA	C4B-NB	6.76	1.41	1.35
14	B	819	CLA	C4B-NB	6.76	1.41	1.35
14	A	820	CLA	C4B-NB	6.73	1.41	1.35
14	a	829	CLA	C4B-NB	6.73	1.41	1.35
14	A	816	CLA	C4B-NB	6.73	1.41	1.35
14	b	837	CLA	C4B-NB	6.72	1.41	1.35
14	a	815	CLA	C4B-NB	6.71	1.41	1.35
14	A	819	CLA	C4B-NB	6.70	1.41	1.35
14	b	834	CLA	C4B-NB	6.70	1.41	1.35
15	b	844	PQN	C3-C2	6.70	1.47	1.35
14	K	101	CLA	C4B-NB	6.69	1.41	1.35
14	b	824	CLA	C4B-NB	6.69	1.41	1.35
14	a	809	CLA	C4B-NB	6.68	1.41	1.35
14	f	203	CLA	C4B-NB	6.67	1.41	1.35
14	b	804	CLA	C4B-NB	6.67	1.41	1.35
14	b	825	CLA	C4B-NB	6.65	1.41	1.35
14	A	835	CLA	C4B-NB	6.63	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	805	CLA	C4B-NB	6.63	1.41	1.35
14	B	825	CLA	C4B-NB	6.63	1.41	1.35
14	A	813	CLA	C4B-NB	6.62	1.41	1.35
14	B	802	CLA	C4B-NB	6.61	1.41	1.35
14	A	836	CLA	C4B-NB	6.60	1.41	1.35
14	X	1701	CLA	C4B-NB	6.58	1.41	1.35
14	B	824	CLA	C4B-NB	6.58	1.41	1.35
14	B	832	CLA	C4B-NB	6.58	1.41	1.35
14	A	802	CLA	C4B-NB	6.57	1.41	1.35
14	a	821	CLA	C4B-NB	6.56	1.41	1.35
14	A	804	CLA	C4B-NB	6.55	1.41	1.35
14	A	809	CLA	C4B-NB	6.55	1.41	1.35
14	a	802	CLA	C4B-NB	6.53	1.41	1.35
14	A	818	CLA	C4B-NB	6.53	1.41	1.35
14	a	838	CLA	C4B-NB	6.51	1.41	1.35
14	b	843	CLA	C4B-NB	6.50	1.41	1.35
14	a	822	CLA	C4B-NB	6.49	1.41	1.35
14	B	833	CLA	C4B-NB	6.49	1.41	1.35
14	l	203	CLA	C4B-NB	6.49	1.41	1.35
14	b	814	CLA	C4B-NB	6.48	1.41	1.35
14	a	814	CLA	C4B-NB	6.47	1.41	1.35
14	a	808	CLA	C4B-NB	6.47	1.41	1.35
14	B	821	CLA	C4B-NB	6.46	1.41	1.35
14	j	101	CLA	C4B-NB	6.46	1.41	1.35
14	B	806	CLA	C4B-NB	6.46	1.41	1.35
14	B	835	CLA	C4B-NB	6.46	1.41	1.35
14	A	840	CLA	C4B-NB	6.45	1.41	1.35
14	b	819	CLA	C4B-NB	6.45	1.41	1.35
14	A	823	CLA	C4B-NB	6.43	1.40	1.35
14	a	817	CLA	C4B-NB	6.43	1.40	1.35
14	B	837	CLA	C4B-NB	6.43	1.40	1.35
14	A	806	CLA	C4B-NB	6.42	1.40	1.35
14	A	822	CLA	C4B-NB	6.41	1.40	1.35
14	b	829	CLA	C4B-NB	6.39	1.40	1.35
14	A	815	CLA	C4B-NB	6.38	1.40	1.35
14	A	826	CLA	C4B-NB	6.37	1.40	1.35
14	b	820	CLA	C4B-NB	6.34	1.40	1.35
14	L	1502	CLA	C4B-NB	6.33	1.40	1.35
14	A	827	CLA	C4B-NB	6.32	1.40	1.35
14	A	805	CLA	C4B-NB	6.31	1.40	1.35
14	B	807	CLA	C4B-NB	6.31	1.40	1.35
14	B	834	CLA	C4B-NB	6.31	1.40	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	816	CLA	C4B-NB	6.30	1.40	1.35
14	l	205	CLA	C4B-NB	6.28	1.40	1.35
14	a	839	CLA	C4B-NB	6.28	1.40	1.35
14	b	818	CLA	C4B-NB	6.27	1.40	1.35
14	a	831	CLA	C4B-NB	6.26	1.40	1.35
14	B	839	CLA	C4B-NB	6.26	1.40	1.35
14	A	833	CLA	C4B-NB	6.24	1.40	1.35
14	A	808	CLA	C4B-NB	6.24	1.40	1.35
14	b	841	CLA	C4B-NB	6.22	1.40	1.35
14	a	834	CLA	C4B-NB	6.21	1.40	1.35
14	A	831	CLA	C4B-NB	6.21	1.40	1.35
14	b	836	CLA	C4B-NB	6.18	1.40	1.35
14	B	810	CLA	C4B-NB	6.18	1.40	1.35
14	a	827	CLA	C4B-NB	6.17	1.40	1.35
14	a	805	CLA	C4B-NB	6.17	1.40	1.35
14	A	824	CLA	C4B-NB	6.16	1.40	1.35
14	B	830	CLA	C4B-NB	6.15	1.40	1.35
14	B	823	CLA	C4B-NB	6.15	1.40	1.35
14	m	1201	CLA	C4B-NB	6.15	1.40	1.35
14	A	825	CLA	C4B-NB	6.14	1.40	1.35
14	A	803	CLA	C4B-NB	6.14	1.40	1.35
14	b	812	CLA	C4B-NB	6.12	1.40	1.35
14	B	840	CLA	C4B-NB	6.11	1.40	1.35
14	a	824	CLA	C4B-NB	6.11	1.40	1.35
14	A	839	CLA	C4B-NB	6.10	1.40	1.35
14	B	804	CLA	C4B-NB	6.10	1.40	1.35
14	B	820	CLA	C4B-NB	6.09	1.40	1.35
14	b	816	CLA	C4B-NB	6.09	1.40	1.35
14	B	828	CLA	C4B-NB	6.04	1.40	1.35
14	L	1503	CLA	C4B-NB	6.03	1.40	1.35
14	B	827	CLA	C4B-NB	6.03	1.40	1.35
14	a	804	CLA	C4B-NB	6.03	1.40	1.35
14	a	841	CLA	C4B-NB	6.03	1.40	1.35
14	l	204	CLA	C4B-NB	6.02	1.40	1.35
14	B	817	CLA	C4B-NB	6.01	1.40	1.35
14	a	826	CLA	C4B-NB	6.01	1.40	1.35
14	B	842	CLA	C4B-NB	6.00	1.40	1.35
14	b	828	CLA	C4B-NB	5.96	1.40	1.35
14	a	823	CLA	C4B-NB	5.95	1.40	1.35
14	B	818	CLA	C4B-NB	5.94	1.40	1.35
14	A	828	CLA	C4B-NB	5.91	1.40	1.35
14	B	814	CLA	C4B-NB	5.90	1.40	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	834	CLA	C4B-NB	5.88	1.40	1.35
14	a	818	CLA	C4B-NB	5.86	1.40	1.35
14	A	832	CLA	C4B-NB	5.85	1.40	1.35
14	b	810	CLA	C4B-NB	5.85	1.40	1.35
14	B	831	CLA	C4B-NB	5.84	1.40	1.35
14	a	828	CLA	C4B-NB	5.80	1.40	1.35
14	b	808	CLA	C4B-NB	5.80	1.40	1.35
14	a	825	CLA	C4B-NB	5.76	1.40	1.35
14	B	805	CLA	C4B-NB	5.74	1.40	1.35
14	B	826	CLA	C4B-NB	5.72	1.40	1.35
14	b	826	CLA	C4B-NB	5.70	1.40	1.35
14	B	801	CLA	C4B-NB	5.70	1.40	1.35
14	b	811	CLA	C4B-NB	5.69	1.40	1.35
14	A	829	CLA	C4B-NB	5.68	1.40	1.35
14	a	832	CLA	C4B-NB	5.67	1.40	1.35
14	b	806	CLA	C4B-NB	5.63	1.40	1.35
14	B	812	CLA	C4B-NB	5.63	1.40	1.35
14	a	830	CLA	C4B-NB	5.57	1.40	1.35
14	b	821	CLA	C4B-NB	5.56	1.40	1.35
14	B	843	CLA	C4B-NB	5.55	1.40	1.35
14	B	816	CLA	C4B-NB	5.52	1.40	1.35
14	b	809	CLA	C4B-NB	5.52	1.40	1.35
14	A	838	CLA	C4B-NB	5.52	1.40	1.35
14	b	840	CLA	C4B-NB	5.49	1.40	1.35
14	A	837	CLA	C4B-NB	5.46	1.40	1.35
14	a	837	CLA	C4B-NB	5.42	1.40	1.35
14	B	836	CLA	C4B-NB	5.41	1.40	1.35
14	b	830	CLA	C4B-NB	5.39	1.40	1.35
14	b	827	CLA	C4B-NB	5.35	1.40	1.35
13	A	801	CL0	O2A-C1	5.25	1.60	1.46
13	a	801	CL0	O2A-C1	5.23	1.60	1.46
13	A	801	CL0	O2D-CGD	5.18	1.45	1.33
13	a	801	CL0	O2D-CGD	5.18	1.45	1.33
14	B	809	CLA	C4B-NB	5.14	1.39	1.35
13	a	801	CL0	CHC-C1C	5.11	1.48	1.35
13	A	801	CL0	CHC-C1C	5.11	1.48	1.35
14	b	807	CLA	C4B-NB	5.08	1.39	1.35
14	b	802	CLA	C4B-NB	4.90	1.39	1.35
14	b	803	CLA	C4B-NB	4.88	1.39	1.35
14	B	830	CLA	C4D-ND	-4.85	1.31	1.37
14	a	836	CLA	C4B-NB	4.79	1.39	1.35
14	B	832	CLA	CMB-C2B	-4.71	1.41	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	831	CLA	C4B-NB	4.60	1.39	1.35
13	A	801	CL0	C3C-C2C	4.59	1.46	1.36
13	a	801	CL0	C3C-C2C	4.59	1.46	1.36
13	a	801	CL0	CHD-C1D	4.56	1.47	1.38
13	A	801	CL0	CHD-C1D	4.56	1.47	1.38
15	a	842	PQN	C10-C5	4.53	1.48	1.40
15	b	844	PQN	C10-C5	4.45	1.48	1.40
14	b	803	CLA	C4D-ND	-4.40	1.31	1.37
14	b	807	CLA	C4D-ND	-4.30	1.31	1.37
13	a	801	CL0	C3B-C2B	4.29	1.46	1.40
14	B	839	CLA	C4D-ND	-4.29	1.31	1.37
13	A	801	CL0	C3D-C4D	-4.28	1.34	1.44
13	a	801	CL0	C3D-C4D	-4.27	1.34	1.44
14	B	806	CLA	C4D-ND	-4.27	1.31	1.37
14	A	830	CLA	CMB-C2B	-4.26	1.42	1.51
13	A	801	CL0	C3B-C2B	4.25	1.46	1.40
14	b	816	CLA	C4D-ND	-4.25	1.31	1.37
14	b	812	CLA	CMB-C2B	-4.20	1.42	1.51
14	a	836	CLA	C4D-ND	-4.19	1.31	1.37
14	a	825	CLA	C4D-ND	-4.18	1.32	1.37
14	B	829	CLA	C4D-ND	-4.18	1.32	1.37
14	B	809	CLA	C4D-ND	-4.12	1.32	1.37
14	b	806	CLA	C4D-ND	-4.12	1.32	1.37
15	A	844	PQN	C10-C5	4.10	1.47	1.40
15	B	844	PQN	C10-C5	4.09	1.47	1.40
14	B	801	CLA	C4D-ND	-4.07	1.32	1.37
14	b	842	CLA	C4D-ND	-4.06	1.32	1.37
14	B	832	CLA	C4D-ND	-4.04	1.32	1.37
14	B	816	CLA	C4D-ND	-4.00	1.32	1.37
14	A	827	CLA	C4D-ND	-4.00	1.32	1.37
14	b	829	CLA	C4D-ND	-3.97	1.32	1.37
14	B	812	CLA	C4D-ND	-3.96	1.32	1.37
14	a	812	CLA	C4D-ND	-3.92	1.32	1.37
14	L	1501	CLA	C3B-C2B	-3.92	1.34	1.40
14	a	832	CLA	C4D-ND	-3.92	1.32	1.37
14	B	820	CLA	C4D-ND	-3.91	1.32	1.37
14	B	843	CLA	C4D-ND	-3.90	1.32	1.37
14	b	830	CLA	C4D-ND	-3.90	1.32	1.37
14	A	818	CLA	C4D-ND	-3.89	1.32	1.37
14	B	842	CLA	C4D-ND	-3.84	1.32	1.37
14	b	831	CLA	C4D-ND	-3.84	1.32	1.37
14	A	816	CLA	C1D-ND	3.83	1.42	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	830	CLA	C4D-ND	-3.82	1.32	1.37
14	a	826	CLA	C4D-ND	-3.81	1.32	1.37
14	a	834	CLA	C4D-ND	-3.80	1.32	1.37
14	a	837	CLA	C4D-ND	-3.80	1.32	1.37
14	b	809	CLA	C4D-ND	-3.78	1.32	1.37
13	a	801	CL0	OBD-CAD	3.77	1.29	1.22
14	A	833	CLA	C4D-ND	-3.77	1.32	1.37
14	b	828	CLA	C4D-ND	-3.75	1.32	1.37
14	b	805	CLA	C4D-ND	-3.75	1.32	1.37
13	A	801	CL0	OBD-CAD	3.74	1.28	1.22
13	a	801	CL0	CHD-C4C	3.74	1.47	1.39
13	A	801	CL0	CHD-C4C	3.74	1.47	1.39
14	A	839	CLA	C4D-ND	-3.73	1.32	1.37
14	A	842	CLA	C4D-ND	-3.72	1.32	1.37
14	a	838	CLA	C4D-ND	-3.72	1.32	1.37
14	A	806	CLA	C4D-ND	-3.72	1.32	1.37
14	b	813	CLA	C4D-ND	-3.72	1.32	1.37
14	a	815	CLA	C1D-ND	3.72	1.42	1.37
14	B	806	CLA	CMC-C2C	-3.70	1.43	1.50
13	a	801	CL0	MG-NC	3.70	2.15	2.06
13	A	801	CL0	MG-NC	3.69	2.15	2.06
17	i	102	BCR	C1-C6	-3.69	1.48	1.53
14	b	832	CLA	C4D-ND	-3.69	1.32	1.37
14	J	102	CLA	C1D-ND	3.69	1.42	1.37
14	b	804	CLA	C4D-ND	-3.69	1.32	1.37
14	b	820	CLA	C4D-ND	-3.69	1.32	1.37
14	A	826	CLA	C4D-ND	-3.68	1.32	1.37
14	B	824	CLA	C4D-ND	-3.68	1.32	1.37
14	B	825	CLA	C4D-ND	-3.68	1.32	1.37
14	B	808	CLA	OBD-CAD	3.67	1.28	1.22
14	b	810	CLA	C4D-ND	-3.67	1.32	1.37
14	A	832	CLA	C4D-ND	-3.67	1.32	1.37
14	a	817	CLA	C4D-ND	-3.67	1.32	1.37
17	A	851	BCR	C1-C6	-3.67	1.48	1.53
14	K	101	CLA	C1D-ND	3.67	1.42	1.37
14	b	817	CLA	C4D-ND	-3.65	1.32	1.37
14	a	822	CLA	C1D-ND	3.65	1.42	1.37
14	j	103	CLA	C1D-ND	3.64	1.42	1.37
14	A	813	CLA	C4D-ND	-3.64	1.32	1.37
14	a	824	CLA	C4D-ND	-3.64	1.32	1.37
14	b	811	CLA	C4D-ND	-3.64	1.32	1.37
14	b	827	CLA	C4D-ND	-3.64	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	840	CLA	C4D-ND	-3.64	1.32	1.37
14	k	102	CLA	C1D-ND	3.63	1.42	1.37
14	b	839	CLA	C4D-ND	-3.62	1.32	1.37
14	l	205	CLA	C4D-ND	-3.62	1.32	1.37
14	A	824	CLA	C1D-ND	3.62	1.42	1.37
14	L	1502	CLA	C4D-ND	-3.62	1.32	1.37
14	A	821	CLA	C4D-ND	-3.60	1.32	1.37
14	a	831	CLA	C4D-ND	-3.59	1.32	1.37
14	b	840	CLA	C4D-ND	-3.59	1.32	1.37
14	B	841	CLA	C1D-ND	3.59	1.42	1.37
14	a	841	CLA	C4D-ND	-3.59	1.32	1.37
14	b	843	CLA	C4D-ND	-3.59	1.32	1.37
14	A	830	CLA	C4D-ND	-3.59	1.32	1.37
14	b	822	CLA	C1D-ND	3.58	1.42	1.37
14	A	819	CLA	C4D-ND	-3.58	1.32	1.37
14	B	811	CLA	C1D-ND	3.58	1.42	1.37
14	B	825	CLA	C1D-ND	3.58	1.42	1.37
14	b	802	CLA	C4D-ND	-3.58	1.32	1.37
14	L	1501	CLA	C4D-ND	-3.57	1.32	1.37
14	A	843	CLA	C4D-ND	-3.57	1.32	1.37
14	B	804	CLA	C4D-ND	-3.57	1.32	1.37
14	b	812	CLA	C4D-ND	-3.57	1.32	1.37
14	B	821	CLA	C4D-ND	-3.57	1.32	1.37
14	A	838	CLA	C1D-ND	3.56	1.42	1.37
14	a	823	CLA	C4D-ND	-3.56	1.32	1.37
14	B	827	CLA	C4D-ND	-3.55	1.32	1.37
14	A	822	CLA	C4D-ND	-3.55	1.32	1.37
14	a	829	CLA	CMB-C2B	-3.55	1.44	1.51
14	A	810	CLA	C1D-ND	3.54	1.42	1.37
14	A	815	CLA	C1D-ND	3.54	1.42	1.37
14	a	803	CLA	C4D-ND	-3.54	1.32	1.37
14	B	840	CLA	C4D-ND	-3.54	1.32	1.37
14	b	815	CLA	C4D-ND	-3.54	1.32	1.37
14	a	829	CLA	C4D-ND	-3.53	1.32	1.37
14	a	814	CLA	C1D-ND	3.53	1.42	1.37
14	A	802	CLA	C4D-ND	-3.53	1.32	1.37
14	l	204	CLA	C4D-ND	-3.53	1.32	1.37
14	b	838	CLA	C1D-ND	3.53	1.42	1.37
14	k	101	CLA	C1D-ND	3.53	1.42	1.37
14	b	813	CLA	C1D-ND	3.53	1.42	1.37
14	A	803	CLA	C1D-ND	3.53	1.42	1.37
14	B	807	CLA	C4D-ND	-3.52	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	X	1701	CLA	C4D-ND	-3.52	1.32	1.37
14	a	827	CLA	C4D-ND	-3.52	1.32	1.37
14	B	835	CLA	C4D-ND	-3.50	1.32	1.37
14	m	1201	CLA	C4D-ND	-3.50	1.32	1.37
14	B	838	CLA	C1D-ND	3.50	1.42	1.37
14	a	825	CLA	C1D-ND	3.50	1.42	1.37
14	A	817	CLA	C4D-ND	-3.50	1.32	1.37
14	b	825	CLA	C1D-ND	3.49	1.42	1.37
14	f	201	CLA	C4D-ND	-3.49	1.32	1.37
14	A	836	CLA	C1D-ND	3.49	1.42	1.37
14	A	841	CLA	C4D-ND	-3.49	1.32	1.37
14	B	823	CLA	C1D-ND	3.48	1.42	1.37
14	b	821	CLA	C4D-ND	-3.48	1.32	1.37
14	b	826	CLA	C4D-ND	-3.48	1.32	1.37
14	B	829	CLA	C1D-ND	3.48	1.42	1.37
14	b	819	CLA	C4D-ND	-3.48	1.32	1.37
14	k	102	CLA	C4D-ND	-3.48	1.32	1.37
14	A	811	CLA	C4D-ND	-3.48	1.32	1.37
14	A	838	CLA	C4D-ND	-3.47	1.32	1.37
14	J	101	CLA	C1D-ND	3.46	1.42	1.37
14	a	802	CLA	C1D-ND	3.46	1.42	1.37
14	B	837	CLA	C1D-ND	3.45	1.42	1.37
14	A	831	CLA	C4D-ND	-3.45	1.32	1.37
14	a	807	CLA	C4D-ND	-3.45	1.33	1.37
14	A	825	CLA	C1D-ND	3.45	1.42	1.37
14	b	824	CLA	C1D-ND	3.44	1.42	1.37
14	a	816	CLA	C4D-ND	-3.44	1.33	1.37
14	A	821	CLA	CHC-C1C	3.44	1.43	1.35
14	l	204	CLA	CHC-C1C	3.44	1.43	1.35
14	A	829	CLA	C4D-ND	-3.44	1.33	1.37
14	a	820	CLA	C4D-ND	-3.44	1.33	1.37
14	j	101	CLA	C1D-ND	3.43	1.42	1.37
14	b	841	CLA	C4D-ND	-3.43	1.33	1.37
14	f	203	CLA	C4D-ND	-3.43	1.33	1.37
14	F	204	CLA	C4D-ND	-3.43	1.33	1.37
14	A	820	CLA	C1D-ND	3.43	1.42	1.37
14	B	817	CLA	C4D-ND	-3.42	1.33	1.37
14	a	817	CLA	C1D-ND	3.42	1.42	1.37
14	B	820	CLA	CMB-C2B	-3.42	1.44	1.51
14	L	1503	CLA	C4D-ND	-3.42	1.33	1.37
14	a	839	CLA	C4D-ND	-3.41	1.33	1.37
14	b	832	CLA	CMB-C2B	-3.41	1.44	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	836	CLA	C1D-ND	3.41	1.42	1.37
14	F	202	CLA	CHC-C1C	3.41	1.43	1.35
14	B	826	CLA	C4D-ND	-3.40	1.33	1.37
14	F	202	CLA	C4D-ND	-3.40	1.33	1.37
14	A	837	CLA	C4D-ND	-3.40	1.33	1.37
14	j	101	CLA	C4D-ND	-3.40	1.33	1.37
14	A	823	CLA	C1D-ND	3.40	1.42	1.37
14	b	814	CLA	C4D-ND	-3.40	1.33	1.37
14	A	839	CLA	C1D-ND	3.40	1.42	1.37
17	A	846	BCR	C1-C6	-3.39	1.49	1.53
14	a	802	CLA	C4D-ND	-3.39	1.33	1.37
14	b	822	CLA	C4D-ND	-3.39	1.33	1.37
14	a	823	CLA	C1D-ND	3.38	1.41	1.37
14	a	828	CLA	C4D-ND	-3.38	1.33	1.37
14	A	803	CLA	C4D-ND	-3.38	1.33	1.37
14	B	822	CLA	C4D-ND	-3.38	1.33	1.37
14	A	828	CLA	C4D-ND	-3.38	1.33	1.37
14	j	102	CLA	C1D-ND	3.37	1.41	1.37
14	b	804	CLA	C3B-C2B	-3.37	1.35	1.40
14	l	203	CLA	CHC-C1C	3.37	1.43	1.35
14	A	812	CLA	C1D-ND	3.37	1.41	1.37
14	A	804	CLA	C4D-ND	-3.37	1.33	1.37
14	B	833	CLA	C4D-ND	-3.37	1.33	1.37
14	a	822	CLA	C4D-ND	-3.37	1.33	1.37
14	b	818	CLA	C4D-ND	-3.37	1.33	1.37
14	a	833	CLA	C1D-ND	3.36	1.41	1.37
14	a	805	CLA	C4D-ND	-3.36	1.33	1.37
14	a	840	CLA	C4D-ND	-3.36	1.33	1.37
14	a	821	CLA	C4D-ND	-3.36	1.33	1.37
14	F	204	CLA	C1D-ND	3.35	1.41	1.37
14	a	819	CLA	C1D-ND	3.35	1.41	1.37
14	K	102	CLA	C4D-ND	-3.34	1.33	1.37
14	B	828	CLA	C1D-ND	3.34	1.41	1.37
14	A	832	CLA	C1D-ND	3.34	1.41	1.37
14	b	834	CLA	C1D-ND	3.34	1.41	1.37
14	a	809	CLA	C4D-ND	-3.33	1.33	1.37
14	B	815	CLA	C4D-ND	-3.33	1.33	1.37
14	x	1701	CLA	C4D-ND	-3.32	1.33	1.37
14	A	832	CLA	CHC-C1C	3.32	1.43	1.35
14	a	805	CLA	C1D-ND	3.32	1.41	1.37
14	a	806	CLA	C1D-ND	3.32	1.41	1.37
14	a	811	CLA	C1D-ND	3.32	1.41	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	804	CLA	CMB-C2B	-3.31	1.44	1.51
17	A	849	BCR	C1-C6	-3.31	1.49	1.53
14	K	102	CLA	C1D-ND	3.31	1.41	1.37
14	B	820	CLA	C1D-ND	3.31	1.41	1.37
14	A	811	CLA	C1D-ND	3.31	1.41	1.37
14	b	837	CLA	C1D-ND	3.30	1.41	1.37
14	A	807	CLA	C1D-ND	3.30	1.41	1.37
14	a	821	CLA	C1D-ND	3.30	1.41	1.37
14	B	813	CLA	C4D-ND	-3.30	1.33	1.37
14	A	834	CLA	C4D-ND	-3.30	1.33	1.37
14	b	834	CLA	C4D-ND	-3.30	1.33	1.37
14	A	823	CLA	C4D-ND	-3.30	1.33	1.37
14	b	807	CLA	CMC-C2C	-3.30	1.43	1.50
14	X	1701	CLA	C1D-ND	3.30	1.41	1.37
14	b	843	CLA	C1D-ND	3.29	1.41	1.37
14	b	815	CLA	CHC-C1C	3.29	1.43	1.35
14	B	823	CLA	C4D-ND	-3.29	1.33	1.37
14	f	203	CLA	C1D-ND	3.29	1.41	1.37
14	a	824	CLA	C1D-ND	3.29	1.41	1.37
14	b	808	CLA	C4D-ND	-3.29	1.33	1.37
14	A	833	CLA	C1D-ND	3.28	1.41	1.37
14	A	807	CLA	C4D-ND	-3.28	1.33	1.37
14	a	818	CLA	C4D-ND	-3.28	1.33	1.37
14	b	832	CLA	CMD-C2D	-3.28	1.43	1.50
14	a	833	CLA	C4D-ND	-3.28	1.33	1.37
14	B	819	CLA	CHC-C1C	3.28	1.43	1.35
14	A	824	CLA	C4D-ND	-3.27	1.33	1.37
14	A	820	CLA	C4D-ND	-3.27	1.33	1.37
17	m	1202	BCR	C1-C6	-3.26	1.49	1.53
14	B	825	CLA	CHC-C1C	3.26	1.43	1.35
14	B	838	CLA	C4D-ND	-3.26	1.33	1.37
14	b	828	CLA	C1D-ND	3.26	1.41	1.37
14	L	1502	CLA	CHC-C1C	3.25	1.43	1.35
14	b	835	CLA	CHC-C1C	3.25	1.43	1.35
14	A	836	CLA	C4D-ND	-3.25	1.33	1.37
14	x	1701	CLA	C1D-ND	3.24	1.41	1.37
14	a	811	CLA	C4D-ND	-3.24	1.33	1.37
14	A	809	CLA	C1D-ND	3.24	1.41	1.37
14	B	835	CLA	C1D-ND	3.24	1.41	1.37
14	b	841	CLA	C1D-ND	3.24	1.41	1.37
14	b	835	CLA	C4D-ND	-3.24	1.33	1.37
14	a	806	CLA	C4D-ND	-3.23	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	814	CLA	C4D-ND	-3.23	1.33	1.37
14	b	825	CLA	C4D-ND	-3.23	1.33	1.37
14	A	808	CLA	C4D-ND	-3.23	1.33	1.37
14	A	835	CLA	C4D-ND	-3.23	1.33	1.37
14	B	831	CLA	C4D-ND	-3.23	1.33	1.37
14	a	803	CLA	C1D-ND	3.23	1.41	1.37
14	A	819	CLA	CHC-C1C	3.22	1.43	1.35
14	l	205	CLA	C1D-ND	3.22	1.41	1.37
14	B	818	CLA	C4D-ND	-3.22	1.33	1.37
14	A	802	CLA	C1D-ND	3.22	1.41	1.37
17	B	850	BCR	C30-C25	-3.22	1.49	1.53
17	a	844	BCR	C1-C6	-3.22	1.49	1.53
14	A	804	CLA	C1D-ND	3.21	1.41	1.37
14	k	101	CLA	C4D-ND	-3.21	1.33	1.37
14	A	825	CLA	C4D-ND	-3.21	1.33	1.37
14	a	819	CLA	C4D-ND	-3.21	1.33	1.37
14	f	201	CLA	CHC-C1C	3.21	1.43	1.35
14	B	814	CLA	C4D-ND	-3.20	1.33	1.37
14	f	201	CLA	C1D-ND	3.20	1.41	1.37
14	a	828	CLA	CHC-C1C	3.20	1.43	1.35
14	B	814	CLA	C1D-ND	3.20	1.41	1.37
14	a	835	CLA	C1D-ND	3.20	1.41	1.37
14	B	834	CLA	C4D-ND	-3.20	1.33	1.37
14	a	835	CLA	C4D-ND	-3.20	1.33	1.37
17	b	849	BCR	C30-C25	-3.20	1.49	1.53
14	A	813	CLA	C1D-ND	3.19	1.41	1.37
14	K	101	CLA	C4D-ND	-3.19	1.33	1.37
14	A	814	CLA	C1D-ND	3.18	1.41	1.37
14	B	813	CLA	CHC-C1C	3.18	1.43	1.35
14	B	828	CLA	CHC-C1C	3.18	1.43	1.35
14	a	813	CLA	C1D-ND	3.18	1.41	1.37
14	b	811	CLA	CMB-C2B	-3.18	1.45	1.51
14	B	821	CLA	C1D-ND	3.17	1.41	1.37
14	L	1501	CLA	CMB-C2B	-3.17	1.45	1.51
14	a	837	CLA	CMB-C2B	-3.17	1.45	1.51
14	B	804	CLA	CHC-C1C	3.17	1.43	1.35
14	A	821	CLA	C1D-ND	3.17	1.41	1.37
14	A	827	CLA	C1D-ND	3.17	1.41	1.37
14	a	809	CLA	C1D-ND	3.17	1.41	1.37
14	B	828	CLA	C4D-ND	-3.16	1.33	1.37
14	B	807	CLA	CHC-C1C	3.16	1.43	1.35
14	B	807	CLA	C1D-ND	3.16	1.41	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	833	CLA	CHC-C1C	3.16	1.43	1.35
14	a	808	CLA	C4D-ND	-3.16	1.33	1.37
14	b	823	CLA	C4D-ND	-3.16	1.33	1.37
14	a	807	CLA	C1D-ND	3.16	1.41	1.37
14	B	812	CLA	CMB-C2B	-3.15	1.45	1.51
14	b	813	CLA	CHC-C1C	3.15	1.43	1.35
14	a	828	CLA	C1D-ND	3.15	1.41	1.37
17	a	849	BCR	C1-C6	-3.15	1.49	1.53
14	B	809	CLA	C1D-ND	3.15	1.41	1.37
14	m	1201	CLA	CHC-C1C	3.15	1.43	1.35
14	b	803	CLA	CMB-C2B	-3.15	1.45	1.51
14	B	805	CLA	CHC-C1C	3.15	1.43	1.35
14	A	817	CLA	C1D-ND	3.14	1.41	1.37
14	a	812	CLA	C1D-ND	3.14	1.41	1.37
14	K	102	CLA	CHC-C1C	3.14	1.43	1.35
14	A	821	CLA	C3B-C2B	-3.14	1.36	1.40
14	B	802	CLA	C4D-ND	-3.14	1.33	1.37
14	b	840	CLA	C1D-ND	3.14	1.41	1.37
14	B	826	CLA	CHC-C1C	3.14	1.43	1.35
14	A	835	CLA	CMB-C2B	-3.13	1.45	1.51
14	a	807	CLA	CHC-C1C	3.13	1.43	1.35
14	b	843	CLA	CMB-C2B	-3.13	1.45	1.51
14	b	826	CLA	CHC-C1C	3.13	1.43	1.35
17	b	845	BCR	C1-C6	-3.13	1.49	1.53
14	B	818	CLA	C1D-ND	3.13	1.41	1.37
14	b	814	CLA	C1D-ND	3.13	1.41	1.37
14	a	818	CLA	C1D-ND	3.13	1.41	1.37
14	b	833	CLA	C4D-ND	-3.12	1.33	1.37
14	J	102	CLA	CHC-C1C	3.12	1.43	1.35
17	a	847	BCR	C1-C6	-3.12	1.49	1.53
14	B	840	CLA	CHC-C1C	3.12	1.43	1.35
14	a	820	CLA	CHC-C1C	3.12	1.43	1.35
14	L	1503	CLA	C1D-ND	3.12	1.41	1.37
14	a	834	CLA	CMB-C2B	-3.11	1.45	1.51
14	A	815	CLA	C4D-ND	-3.11	1.33	1.37
13	a	801	CL0	C1D-ND	-3.11	1.34	1.37
14	a	810	CLA	C1D-ND	3.11	1.41	1.37
14	B	805	CLA	C4D-ND	-3.11	1.33	1.37
17	J	104	BCR	C1-C6	-3.11	1.49	1.53
14	A	834	CLA	C1D-ND	3.11	1.41	1.37
14	b	839	CLA	CMB-C2B	-3.11	1.45	1.51
14	A	827	CLA	CMC-C2C	-3.11	1.44	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	840	CLA	C1D-ND	3.11	1.41	1.37
14	A	822	CLA	C1D-ND	3.10	1.41	1.37
14	b	827	CLA	C1D-ND	3.10	1.41	1.37
20	B	851	LMG	O7-C8	-3.10	1.38	1.46
14	a	835	CLA	CHC-C1C	3.10	1.42	1.35
17	f	202	BCR	C1-C6	-3.10	1.49	1.53
17	A	850	BCR	C30-C25	-3.10	1.49	1.53
13	A	801	CL0	C1D-ND	-3.09	1.34	1.37
14	B	837	CLA	C4D-ND	-3.09	1.33	1.37
14	B	802	CLA	C1D-ND	3.09	1.41	1.37
14	b	822	CLA	CMB-C2B	-3.09	1.45	1.51
14	B	841	CLA	C4D-ND	-3.09	1.33	1.37
14	A	828	CLA	CHC-C1C	3.09	1.42	1.35
14	b	810	CLA	C1D-ND	3.09	1.41	1.37
14	b	836	CLA	CHC-C1C	3.08	1.42	1.35
14	a	810	CLA	C4D-ND	-3.08	1.33	1.37
14	B	818	CLA	CHC-C1C	3.08	1.42	1.35
14	B	838	CLA	CHC-C1C	3.08	1.42	1.35
14	b	833	CLA	CMB-C2B	-3.08	1.45	1.51
14	A	817	CLA	CHC-C1C	3.08	1.42	1.35
14	B	832	CLA	C3B-C2B	-3.08	1.36	1.40
14	B	824	CLA	C1D-ND	3.08	1.41	1.37
14	b	837	CLA	C4D-ND	-3.08	1.33	1.37
14	B	834	CLA	CHC-C1C	3.08	1.42	1.35
14	a	820	CLA	CMB-C2B	-3.08	1.45	1.51
14	A	805	CLA	C4D-ND	-3.07	1.33	1.37
14	B	819	CLA	C4D-ND	-3.07	1.33	1.37
14	b	819	CLA	C1D-ND	3.07	1.41	1.37
14	j	102	CLA	C4D-ND	-3.07	1.33	1.37
14	b	824	CLA	C4D-ND	-3.07	1.33	1.37
14	a	803	CLA	CHC-C1C	3.07	1.42	1.35
14	a	804	CLA	C4D-ND	-3.06	1.33	1.37
14	B	801	CLA	CHC-C1C	3.06	1.42	1.35
14	L	1501	CLA	CHC-C1C	3.06	1.42	1.35
14	b	816	CLA	CHC-C1C	3.06	1.42	1.35
17	I	102	BCR	C1-C6	-3.06	1.49	1.53
14	A	809	CLA	C4D-ND	-3.06	1.33	1.37
14	b	823	CLA	C1D-ND	3.06	1.41	1.37
14	B	830	CLA	CMB-C2B	-3.06	1.45	1.51
14	A	818	CLA	C1D-ND	3.06	1.41	1.37
14	B	829	CLA	CHC-C1C	3.06	1.42	1.35
14	B	834	CLA	C1D-ND	3.06	1.41	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	837	CLA	CHC-C1C	3.06	1.42	1.35
14	b	815	CLA	C1D-ND	3.06	1.41	1.37
14	b	812	CLA	C1D-ND	3.05	1.41	1.37
14	B	812	CLA	CHC-C1C	3.05	1.42	1.35
14	B	811	CLA	C4D-ND	-3.05	1.33	1.37
14	b	818	CLA	C1D-ND	3.05	1.41	1.37
14	B	808	CLA	C4D-ND	-3.05	1.33	1.37
14	J	101	CLA	C4D-ND	-3.05	1.33	1.37
14	A	806	CLA	CHC-C1C	3.05	1.42	1.35
14	A	843	CLA	CHC-C1C	3.05	1.42	1.35
14	B	831	CLA	CHC-C1C	3.05	1.42	1.35
14	b	839	CLA	C1D-ND	3.05	1.41	1.37
14	A	842	CLA	CMB-C2B	-3.04	1.45	1.51
14	b	825	CLA	CHC-C1C	3.04	1.42	1.35
14	B	816	CLA	C1D-ND	3.04	1.41	1.37
14	B	827	CLA	CHC-C1C	3.04	1.42	1.35
17	B	847	BCR	C1-C6	-3.04	1.49	1.53
14	A	816	CLA	C4D-ND	-3.04	1.33	1.37
14	B	841	CLA	CHC-C1C	3.04	1.42	1.35
14	b	842	CLA	CHC-C1C	3.04	1.42	1.35
14	A	812	CLA	C4D-ND	-3.03	1.33	1.37
14	b	830	CLA	CHC-C1C	3.03	1.42	1.35
14	J	101	CLA	CHC-C1C	3.03	1.42	1.35
14	a	806	CLA	CHC-C1C	3.03	1.42	1.35
14	B	832	CLA	CMD-C2D	-3.03	1.44	1.50
14	B	817	CLA	C1D-ND	3.03	1.41	1.37
14	a	821	CLA	CHC-C1C	3.02	1.42	1.35
14	a	813	CLA	C4D-ND	-3.02	1.33	1.37
14	b	838	CLA	C4D-ND	-3.02	1.33	1.37
14	A	835	CLA	C1D-ND	3.02	1.41	1.37
14	A	814	CLA	CHC-C1C	3.02	1.42	1.35
14	j	101	CLA	CHC-C1C	3.02	1.42	1.35
14	B	842	CLA	CMD-C2D	-3.02	1.44	1.50
14	l	203	CLA	C4D-ND	-3.02	1.33	1.37
14	j	103	CLA	CHC-C1C	3.01	1.42	1.35
14	A	808	CLA	C1D-ND	3.01	1.41	1.37
14	b	821	CLA	C1D-ND	3.01	1.41	1.37
14	A	804	CLA	CHC-C1C	3.01	1.42	1.35
14	L	1503	CLA	CHC-C1C	3.01	1.42	1.35
14	A	822	CLA	CHC-C1C	3.01	1.42	1.35
14	B	833	CLA	CMD-C2D	-3.01	1.44	1.50
14	b	826	CLA	C1D-ND	3.01	1.41	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	828	CLA	C1D-ND	3.00	1.41	1.37
14	A	819	CLA	CMB-C2B	-3.00	1.45	1.51
14	A	835	CLA	CHC-C1C	3.00	1.42	1.35
14	B	843	CLA	C1D-ND	3.00	1.41	1.37
14	a	829	CLA	CHC-C1C	3.00	1.42	1.35
14	a	815	CLA	C4D-ND	-3.00	1.33	1.37
14	b	839	CLA	C3B-C2B	-3.00	1.36	1.40
14	B	819	CLA	C1D-ND	3.00	1.41	1.37
14	b	833	CLA	C1D-ND	2.99	1.41	1.37
14	b	838	CLA	CHC-C1C	2.99	1.42	1.35
14	j	102	CLA	CHC-C1C	2.99	1.42	1.35
17	j	104	BCR	C1-C6	-2.99	1.49	1.53
14	A	823	CLA	CHC-C1C	2.99	1.42	1.35
14	b	807	CLA	C3B-CAB	-2.99	1.41	1.47
14	a	811	CLA	CHC-C1C	2.99	1.42	1.35
17	a	849	BCR	C30-C25	-2.99	1.49	1.53
14	A	843	CLA	C1D-ND	2.99	1.41	1.37
17	J	103	BCR	C1-C6	-2.99	1.49	1.53
14	a	808	CLA	C1D-ND	2.99	1.41	1.37
14	m	1201	CLA	C1D-ND	2.98	1.41	1.37
14	b	833	CLA	CHC-C1C	2.98	1.42	1.35
14	b	839	CLA	CHC-C1C	2.98	1.42	1.35
14	a	834	CLA	C1D-ND	2.98	1.41	1.37
19	X	1702	SQD	O47-C7	2.98	1.42	1.34
14	K	101	CLA	CHC-C1C	2.97	1.42	1.35
14	B	838	CLA	CMB-C2B	-2.97	1.45	1.51
14	b	824	CLA	CHC-C1C	2.97	1.42	1.35
14	k	101	CLA	CHC-C1C	2.97	1.42	1.35
14	a	804	CLA	CHC-C1C	2.97	1.42	1.35
14	A	818	CLA	CHC-C1C	2.97	1.42	1.35
14	B	830	CLA	CHC-C1C	2.97	1.42	1.35
14	B	840	CLA	C1D-ND	2.97	1.41	1.37
14	b	830	CLA	C1D-ND	2.96	1.41	1.37
14	a	827	CLA	C1D-ND	2.96	1.41	1.37
14	A	825	CLA	CHC-C1C	2.96	1.42	1.35
14	b	805	CLA	CHC-C1C	2.96	1.42	1.35
14	B	801	CLA	CMB-C2B	-2.96	1.45	1.51
14	A	802	CLA	CMB-C2B	-2.96	1.45	1.51
14	A	812	CLA	CHC-C1C	2.96	1.42	1.35
14	b	829	CLA	C1D-ND	2.96	1.41	1.37
20	b	851	LMG	O1-C7	-2.96	1.38	1.43
14	b	817	CLA	CHC-C1C	2.96	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	807	CLA	CHC-C1C	2.96	1.42	1.35
14	B	824	CLA	CHC-C1C	2.96	1.42	1.35
14	A	810	CLA	C4D-ND	-2.96	1.33	1.37
14	b	831	CLA	C1D-ND	2.96	1.41	1.37
18	A	852	LHG	O7-C5	-2.95	1.39	1.46
14	B	839	CLA	CHC-C1C	2.95	1.42	1.35
14	B	821	CLA	C3B-C2B	-2.95	1.36	1.40
14	a	837	CLA	CHC-C1C	2.95	1.42	1.35
14	b	805	CLA	C1D-ND	2.95	1.41	1.37
14	B	822	CLA	C1D-ND	2.95	1.41	1.37
14	a	810	CLA	CHC-C1C	2.95	1.42	1.35
14	B	829	CLA	CMC-C2C	-2.95	1.44	1.50
14	B	839	CLA	C1D-ND	2.95	1.41	1.37
14	b	837	CLA	CHC-C1C	2.95	1.42	1.35
14	L	1501	CLA	C1D-ND	2.95	1.41	1.37
14	X	1701	CLA	CHC-C1C	2.94	1.42	1.35
14	b	817	CLA	C1D-ND	2.94	1.41	1.37
14	A	824	CLA	CHC-C1C	2.94	1.42	1.35
14	x	1701	CLA	CHC-C1C	2.94	1.42	1.35
14	A	840	CLA	C1D-ND	2.94	1.41	1.37
14	a	841	CLA	C1D-ND	2.94	1.41	1.37
17	j	106	BCR	C30-C25	-2.94	1.49	1.53
14	a	822	CLA	CHC-C1C	2.93	1.42	1.35
14	a	827	CLA	CHC-C1C	2.93	1.42	1.35
14	B	814	CLA	CHC-C1C	2.93	1.42	1.35
14	a	838	CLA	CHC-C1C	2.93	1.42	1.35
14	b	834	CLA	CHC-C1C	2.93	1.42	1.35
14	A	814	CLA	C4D-ND	-2.93	1.33	1.37
14	a	839	CLA	C1D-ND	2.93	1.41	1.37
14	b	814	CLA	CHC-C1C	2.93	1.42	1.35
14	a	817	CLA	CMB-C2B	-2.93	1.45	1.51
14	a	830	CLA	CMB-C2B	-2.93	1.45	1.51
14	a	804	CLA	C1D-ND	2.93	1.41	1.37
14	b	820	CLA	CHC-C1C	2.93	1.42	1.35
17	j	105	BCR	C1-C6	-2.93	1.49	1.53
14	B	802	CLA	CHC-C1C	2.92	1.42	1.35
14	a	839	CLA	CHC-C1C	2.92	1.42	1.35
14	A	809	CLA	CHC-C1C	2.92	1.42	1.35
14	a	813	CLA	CHC-C1C	2.92	1.42	1.35
14	B	835	CLA	CHC-C1C	2.92	1.42	1.35
14	a	831	CLA	CMB-C2B	-2.92	1.45	1.51
14	b	804	CLA	CHC-C1C	2.92	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	811	CLA	C3B-C2B	-2.92	1.36	1.40
14	F	202	CLA	C3B-C2B	-2.92	1.36	1.40
19	x	1702	SQD	O48-C23	2.91	1.41	1.33
14	B	822	CLA	CMB-C2B	-2.91	1.45	1.51
13	a	801	CL0	C3D-C2D	2.91	1.47	1.39
14	b	819	CLA	CHC-C1C	2.91	1.42	1.35
14	A	831	CLA	C1D-ND	2.91	1.41	1.37
14	b	831	CLA	CHC-C1C	2.91	1.42	1.35
17	b	847	BCR	C30-C25	-2.91	1.49	1.53
14	b	811	CLA	CMC-C2C	-2.91	1.44	1.50
13	A	801	CL0	C3D-C2D	2.91	1.47	1.39
14	a	817	CLA	CHC-C1C	2.91	1.42	1.35
14	b	807	CLA	CHC-C1C	2.91	1.42	1.35
14	b	816	CLA	C1D-ND	2.91	1.41	1.37
14	b	827	CLA	CHC-C1C	2.90	1.42	1.35
14	A	827	CLA	CHC-C1C	2.90	1.42	1.35
14	A	805	CLA	CHC-C1C	2.90	1.42	1.35
14	l	205	CLA	CHC-C1C	2.90	1.42	1.35
14	B	833	CLA	CMB-C2B	-2.90	1.45	1.51
14	b	841	CLA	CHC-C1C	2.90	1.42	1.35
13	A	801	CL0	C4D-CHA	2.90	1.48	1.38
14	j	103	CLA	C4D-ND	-2.90	1.33	1.37
14	B	831	CLA	C1D-ND	2.90	1.41	1.37
14	b	803	CLA	CHC-C1C	2.90	1.42	1.35
14	B	820	CLA	CHC-C1C	2.90	1.42	1.35
14	a	814	CLA	CHC-C1C	2.90	1.42	1.35
14	B	810	CLA	C1D-ND	2.89	1.41	1.37
13	a	801	CL0	C4D-CHA	2.89	1.48	1.38
14	a	838	CLA	C1D-ND	2.89	1.41	1.37
14	b	812	CLA	CHC-C1C	2.89	1.42	1.35
14	B	842	CLA	CHC-C1C	2.89	1.42	1.35
14	A	806	CLA	C1D-ND	2.89	1.41	1.37
14	f	203	CLA	CHC-C1C	2.89	1.42	1.35
14	A	841	CLA	CHC-C1C	2.89	1.42	1.35
17	J	105	BCR	C30-C25	-2.89	1.49	1.53
14	J	102	CLA	C4D-ND	-2.89	1.33	1.37
14	B	836	CLA	C1D-ND	2.88	1.41	1.37
14	B	843	CLA	CMB-C2B	-2.88	1.45	1.51
14	b	828	CLA	CHC-C1C	2.88	1.42	1.35
14	a	819	CLA	CHC-C1C	2.88	1.42	1.35
14	a	836	CLA	C1D-ND	2.88	1.41	1.37
17	B	845	BCR	C1-C6	-2.88	1.49	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	840	CLA	CHC-C1C	2.88	1.42	1.35
14	B	826	CLA	C1D-ND	2.88	1.41	1.37
14	a	832	CLA	C1D-ND	2.88	1.41	1.37
14	b	836	CLA	C4D-ND	-2.88	1.33	1.37
14	A	836	CLA	CHC-C1C	2.87	1.42	1.35
14	F	204	CLA	CHC-C1C	2.87	1.42	1.35
14	a	808	CLA	CMD-C2D	-2.87	1.44	1.50
14	b	803	CLA	C1D-ND	2.87	1.41	1.37
14	B	841	CLA	C3B-C2B	-2.87	1.36	1.40
14	A	826	CLA	CHC-C1C	2.87	1.42	1.35
19	x	1702	SQD	O47-C7	2.87	1.42	1.34
14	b	818	CLA	CHC-C1C	2.87	1.42	1.35
14	A	819	CLA	C1D-ND	2.87	1.41	1.37
14	a	817	CLA	CMC-C2C	-2.87	1.44	1.50
14	A	831	CLA	CHC-C1C	2.87	1.42	1.35
14	a	830	CLA	CHC-C1C	2.87	1.42	1.35
14	A	810	CLA	CHC-C1C	2.86	1.42	1.35
14	b	802	CLA	CMC-C2C	-2.86	1.44	1.50
14	b	809	CLA	CHC-C1C	2.86	1.42	1.35
14	B	809	CLA	CMB-C2B	-2.86	1.45	1.51
14	A	815	CLA	CHC-C1C	2.86	1.42	1.35
14	b	840	CLA	CHC-C1C	2.86	1.42	1.35
14	A	821	CLA	CMB-C2B	-2.86	1.45	1.51
14	B	831	CLA	CMB-C2B	-2.86	1.45	1.51
14	A	802	CLA	CHC-C1C	2.86	1.42	1.35
14	a	809	CLA	CHC-C1C	2.86	1.42	1.35
14	b	808	CLA	OBD-CAD	2.86	1.27	1.22
14	a	818	CLA	CHC-C1C	2.86	1.42	1.35
14	b	842	CLA	CMB-C2B	-2.85	1.45	1.51
14	B	815	CLA	CHC-C1C	2.85	1.42	1.35
14	B	821	CLA	CHC-C1C	2.85	1.42	1.35
14	l	203	CLA	C1D-ND	2.85	1.41	1.37
17	F	205	BCR	C1-C6	-2.85	1.49	1.53
14	a	802	CLA	CHC-C1C	2.85	1.42	1.35
14	b	820	CLA	CMB-C2B	-2.85	1.45	1.51
14	A	808	CLA	CHC-C1C	2.85	1.42	1.35
14	a	812	CLA	CHC-C1C	2.84	1.42	1.35
14	j	101	CLA	C3B-C2B	-2.84	1.36	1.40
14	a	816	CLA	CMB-C2B	-2.84	1.45	1.51
14	B	810	CLA	C4D-ND	-2.84	1.33	1.37
19	X	1702	SQD	O48-C23	2.84	1.41	1.33
14	b	830	CLA	CMB-C2B	-2.84	1.45	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	l	204	CLA	C1D-ND	2.84	1.41	1.37
14	B	805	CLA	CMD-C2D	-2.84	1.44	1.50
14	a	837	CLA	C1D-ND	2.83	1.41	1.37
14	B	808	CLA	CMD-C2D	-2.83	1.44	1.50
14	B	815	CLA	C1D-ND	2.83	1.41	1.37
14	B	809	CLA	CHC-C1C	2.83	1.42	1.35
14	b	823	CLA	CHC-C1C	2.83	1.42	1.35
14	a	820	CLA	C1D-ND	2.83	1.41	1.37
17	b	848	BCR	C1-C6	-2.83	1.49	1.53
14	b	835	CLA	C3B-C2B	-2.83	1.36	1.40
17	a	848	BCR	C30-C25	-2.83	1.49	1.53
14	b	803	CLA	C3B-C2B	-2.82	1.36	1.40
14	b	816	CLA	CMB-C2B	-2.82	1.45	1.51
14	A	803	CLA	CHC-C1C	2.82	1.42	1.35
14	B	817	CLA	CHC-C1C	2.82	1.42	1.35
18	a	850	LHG	O7-C5	-2.81	1.39	1.46
14	a	816	CLA	C1D-ND	2.81	1.41	1.37
14	a	805	CLA	CHC-C1C	2.81	1.42	1.35
14	a	815	CLA	CHC-C1C	2.81	1.42	1.35
14	A	840	CLA	CHC-C1C	2.81	1.42	1.35
14	k	102	CLA	CHC-C1C	2.81	1.42	1.35
14	b	835	CLA	C1D-ND	2.81	1.41	1.37
14	A	808	CLA	CMB-C2B	-2.81	1.45	1.51
19	b	801	SQD	O48-C23	2.81	1.41	1.33
14	B	816	CLA	CHC-C1C	2.80	1.42	1.35
14	a	828	CLA	CMB-C2B	-2.80	1.45	1.51
14	B	834	CLA	CMB-C2B	-2.80	1.45	1.51
14	A	830	CLA	CHC-C1C	2.80	1.42	1.35
14	b	822	CLA	CMC-C2C	-2.80	1.44	1.50
14	A	841	CLA	C1D-ND	2.80	1.41	1.37
14	A	829	CLA	C1D-ND	2.80	1.41	1.37
14	B	813	CLA	CMD-C2D	-2.80	1.44	1.50
14	B	833	CLA	C1D-ND	2.80	1.41	1.37
14	A	842	CLA	CHC-C1C	2.80	1.42	1.35
14	a	834	CLA	CHC-C1C	2.80	1.42	1.35
14	A	838	CLA	CMB-C2B	-2.79	1.45	1.51
14	b	815	CLA	CMB-C2B	-2.79	1.45	1.51
14	a	815	CLA	CMB-C2B	-2.79	1.45	1.51
14	F	202	CLA	C1D-ND	2.79	1.41	1.37
14	b	828	CLA	CMB-C2B	-2.79	1.45	1.51
14	b	807	CLA	CMB-C2B	-2.78	1.45	1.51
14	B	837	CLA	CHC-C1C	2.78	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	850	BCR	C30-C25	-2.78	1.49	1.53
14	A	838	CLA	CHC-C1C	2.78	1.42	1.35
14	A	811	CLA	CHC-C1C	2.78	1.42	1.35
14	a	830	CLA	C1D-ND	2.78	1.41	1.37
14	B	804	CLA	C1D-ND	2.78	1.41	1.37
14	B	839	CLA	CMB-C2B	-2.78	1.45	1.51
14	B	805	CLA	C1D-ND	2.78	1.41	1.37
14	a	841	CLA	CHC-C1C	2.77	1.42	1.35
14	A	820	CLA	CMB-C2B	-2.77	1.45	1.51
14	B	829	CLA	CMB-C2B	-2.76	1.45	1.51
14	a	838	CLA	CMB-C2B	-2.76	1.45	1.51
14	j	101	CLA	CMB-C2B	-2.76	1.45	1.51
20	b	851	LMG	O7-C8	-2.76	1.39	1.46
14	a	810	CLA	CMB-C2B	-2.76	1.45	1.51
14	b	843	CLA	C3B-C2B	-2.76	1.36	1.40
14	A	818	CLA	CMB-C2B	-2.75	1.45	1.51
19	l	202	SQD	O48-C23	2.75	1.41	1.33
14	A	841	CLA	CMB-C2B	-2.75	1.45	1.51
14	a	840	CLA	CMB-C2B	-2.75	1.45	1.51
14	A	812	CLA	CMB-C2B	-2.75	1.45	1.51
14	a	829	CLA	C1D-ND	2.75	1.41	1.37
14	a	831	CLA	C1D-ND	2.74	1.41	1.37
14	A	826	CLA	C1D-ND	2.74	1.41	1.37
14	b	809	CLA	CMB-C2B	-2.74	1.45	1.51
14	a	826	CLA	C1D-ND	2.74	1.41	1.37
14	A	820	CLA	CHC-C1C	2.74	1.42	1.35
14	B	810	CLA	CHC-C1C	2.74	1.42	1.35
14	B	839	CLA	C3B-C2B	-2.74	1.36	1.40
17	f	202	BCR	C30-C25	-2.74	1.50	1.53
14	A	829	CLA	CHC-C1C	2.73	1.42	1.35
14	b	817	CLA	CMD-C2D	-2.73	1.45	1.50
14	f	201	CLA	CMB-C2B	-2.73	1.46	1.51
14	L	1502	CLA	CMB-C2B	-2.73	1.46	1.51
14	A	833	CLA	CHC-C1C	2.73	1.42	1.35
14	F	202	CLA	CMB-C2B	-2.73	1.46	1.51
14	a	822	CLA	C3B-C2B	-2.73	1.36	1.40
14	a	832	CLA	CHC-C1C	2.73	1.42	1.35
17	b	848	BCR	C30-C25	-2.73	1.50	1.53
14	B	808	CLA	CMB-C2B	-2.72	1.46	1.51
14	B	832	CLA	CHC-C1C	2.72	1.41	1.35
14	b	816	CLA	CMC-C2C	-2.72	1.45	1.50
14	A	839	CLA	C3B-C2B	-2.72	1.36	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	834	CLA	CHC-C1C	2.72	1.41	1.35
14	B	821	CLA	CMB-C2B	-2.72	1.46	1.51
14	A	811	CLA	CMB-C2B	-2.72	1.46	1.51
14	A	816	CLA	CMB-C2B	-2.72	1.46	1.51
14	a	812	CLA	CMB-C2B	-2.72	1.46	1.51
14	b	823	CLA	CMB-C2B	-2.72	1.46	1.51
14	b	835	CLA	CMB-C2B	-2.72	1.46	1.51
14	B	816	CLA	CMC-C2C	-2.72	1.45	1.50
14	b	809	CLA	C1D-ND	2.71	1.41	1.37
14	b	802	CLA	CHC-C1C	2.71	1.41	1.35
14	B	805	CLA	CMB-C2B	-2.71	1.46	1.51
14	a	811	CLA	CMB-C2B	-2.71	1.46	1.51
14	B	836	CLA	CHC-C1C	2.71	1.41	1.35
14	a	831	CLA	CHC-C1C	2.71	1.41	1.35
14	a	826	CLA	CMC-C2C	-2.70	1.45	1.50
17	j	105	BCR	C30-C25	-2.70	1.50	1.53
14	b	829	CLA	CHC-C1C	2.70	1.41	1.35
14	b	833	CLA	CMD-C2D	-2.70	1.45	1.50
17	F	203	BCR	C1-C6	-2.70	1.50	1.53
14	b	820	CLA	C1D-ND	2.70	1.41	1.37
14	B	823	CLA	CMB-C2B	-2.70	1.46	1.51
17	M	101	BCR	C1-C6	-2.70	1.50	1.53
14	a	823	CLA	CHC-C1C	2.70	1.41	1.35
14	a	825	CLA	CHC-C1C	2.70	1.41	1.35
14	B	841	CLA	CMB-C2B	-2.70	1.46	1.51
14	b	812	CLA	C3B-C2B	-2.69	1.36	1.40
14	A	829	CLA	CMB-C2B	-2.69	1.46	1.51
14	a	822	CLA	CMB-C2B	-2.69	1.46	1.51
14	A	817	CLA	CMB-C2B	-2.69	1.46	1.51
14	A	817	CLA	C3B-C2B	-2.69	1.36	1.40
14	k	102	CLA	CMB-C2B	-2.69	1.46	1.51
17	A	851	BCR	C30-C25	-2.69	1.50	1.53
14	L	1503	CLA	CMB-C2B	-2.69	1.46	1.51
17	f	204	BCR	C1-C6	-2.69	1.50	1.53
14	a	816	CLA	CHC-C1C	2.69	1.41	1.35
14	b	807	CLA	CMD-C2D	-2.69	1.45	1.50
14	A	813	CLA	CHC-C1C	2.69	1.41	1.35
14	B	815	CLA	C3B-C2B	-2.68	1.36	1.40
14	A	805	CLA	CMD-C2D	-2.68	1.45	1.50
14	B	816	CLA	CMB-C2B	-2.68	1.46	1.51
14	b	818	CLA	CMB-C2B	-2.68	1.46	1.51
14	b	836	CLA	CMB-C2B	-2.68	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	821	CLA	CMB-C2B	-2.67	1.46	1.51
14	b	821	CLA	CMB-C2B	-2.67	1.46	1.51
14	B	826	CLA	CMB-C2B	-2.67	1.46	1.51
14	a	808	CLA	CMB-C2B	-2.67	1.46	1.51
14	B	827	CLA	C1D-ND	2.67	1.41	1.37
17	B	850	BCR	C1-C6	-2.67	1.50	1.53
14	A	835	CLA	C3B-C2B	-2.67	1.36	1.40
14	A	833	CLA	C3B-C2B	-2.67	1.36	1.40
14	B	816	CLA	CMD-C2D	-2.66	1.45	1.50
14	f	203	CLA	CMB-C2B	-2.66	1.46	1.51
14	a	816	CLA	CMC-C2C	-2.66	1.45	1.50
14	a	833	CLA	CHC-C1C	2.66	1.41	1.35
14	b	806	CLA	CMB-C2B	-2.66	1.46	1.51
14	B	836	CLA	C4D-ND	-2.66	1.34	1.37
14	a	806	CLA	CMB-C2B	-2.66	1.46	1.51
14	a	817	CLA	C3B-C2B	-2.65	1.36	1.40
14	b	802	CLA	CMB-C2B	-2.65	1.46	1.51
17	b	847	BCR	C1-C6	-2.65	1.50	1.53
17	b	845	BCR	C30-C25	-2.65	1.50	1.53
14	b	811	CLA	C1D-ND	2.65	1.41	1.37
14	A	831	CLA	CMB-C2B	-2.65	1.46	1.51
17	F	203	BCR	C30-C25	-2.65	1.50	1.53
14	b	831	CLA	CMD-C2D	-2.65	1.45	1.50
14	a	824	CLA	CHC-C1C	2.65	1.41	1.35
14	A	839	CLA	CMB-C2B	-2.65	1.46	1.51
14	a	836	CLA	CMB-C2B	-2.65	1.46	1.51
14	B	830	CLA	C1D-ND	2.65	1.41	1.37
14	A	813	CLA	CMB-C2B	-2.64	1.46	1.51
14	b	841	CLA	CMB-C2B	-2.64	1.46	1.51
14	A	841	CLA	CMD-C2D	-2.64	1.45	1.50
14	F	204	CLA	CMB-C2B	-2.64	1.46	1.51
14	b	811	CLA	C3B-C2B	-2.64	1.36	1.40
14	A	833	CLA	CMB-C2B	-2.64	1.46	1.51
14	a	826	CLA	CHC-C1C	2.64	1.41	1.35
14	B	811	CLA	CMB-C2B	-2.64	1.46	1.51
14	a	830	CLA	C3B-CAB	-2.63	1.42	1.47
14	A	842	CLA	C1D-ND	2.63	1.41	1.37
14	A	840	CLA	CMB-C2B	-2.63	1.46	1.51
14	a	834	CLA	C3B-CAB	-2.63	1.42	1.47
14	a	804	CLA	CMC-C2C	-2.63	1.45	1.50
17	I	101	BCR	C1-C6	-2.63	1.50	1.53
14	x	1701	CLA	CMB-C2B	-2.63	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	848	BCR	C30-C25	-2.63	1.50	1.53
19	l	202	SQD	O47-C7	2.63	1.41	1.34
14	a	813	CLA	CMB-C2B	-2.63	1.46	1.51
17	I	102	BCR	C30-C25	-2.63	1.50	1.53
14	a	808	CLA	CHC-C1C	2.62	1.41	1.35
17	K	103	BCR	C1-C6	-2.62	1.50	1.53
14	A	816	CLA	CHC-C1C	2.62	1.41	1.35
14	B	831	CLA	CMD-C2D	-2.62	1.45	1.50
14	a	804	CLA	CMB-C2B	-2.62	1.46	1.51
14	b	821	CLA	CHC-C1C	2.62	1.41	1.35
14	a	819	CLA	CMB-C2B	-2.62	1.46	1.51
14	A	809	CLA	CMD-C2D	-2.62	1.45	1.50
14	a	836	CLA	CHC-C1C	2.62	1.41	1.35
14	A	830	CLA	CMC-C2C	-2.62	1.45	1.50
14	a	825	CLA	CMD-C2D	-2.62	1.45	1.50
14	B	811	CLA	CMD-C2D	-2.62	1.45	1.50
14	a	835	CLA	CMB-C2B	-2.62	1.46	1.51
14	b	834	CLA	CMB-C2B	-2.61	1.46	1.51
14	L	1503	CLA	CMD-C2D	-2.61	1.45	1.50
14	b	826	CLA	CMB-C2B	-2.61	1.46	1.51
14	B	802	CLA	CMB-C2B	-2.61	1.46	1.51
14	b	814	CLA	CMB-C2B	-2.61	1.46	1.51
17	B	848	BCR	C1-C6	-2.61	1.50	1.53
14	A	804	CLA	CMB-C2B	-2.61	1.46	1.51
14	B	806	CLA	CHC-C1C	2.61	1.41	1.35
14	a	834	CLA	C3B-C2B	-2.61	1.36	1.40
14	b	822	CLA	CHC-C1C	2.61	1.41	1.35
14	b	840	CLA	CMB-C2B	-2.60	1.46	1.51
14	a	836	CLA	MG-ND	-2.60	2.00	2.05
14	B	827	CLA	CMC-C2C	-2.60	1.45	1.50
14	B	811	CLA	CHC-C1C	2.60	1.41	1.35
14	A	843	CLA	CMB-C2B	-2.60	1.46	1.51
14	b	817	CLA	CMB-C2B	-2.60	1.46	1.51
14	B	809	CLA	CMD-C2D	-2.60	1.45	1.50
14	B	815	CLA	CMB-C2B	-2.60	1.46	1.51
14	A	834	CLA	CMB-C2B	-2.60	1.46	1.51
17	A	850	BCR	C1-C6	-2.60	1.50	1.53
14	l	205	CLA	CMB-C2B	-2.60	1.46	1.51
14	b	810	CLA	CHC-C1C	2.60	1.41	1.35
17	a	848	BCR	C1-C6	-2.60	1.50	1.53
14	B	812	CLA	C1D-ND	2.60	1.41	1.37
14	K	101	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)
14	a	802	CLA	CMB-C2B	-2.59	1.46	1.51
14	A	807	CLA	CMB-C2B	-2.59	1.46	1.51
14	B	828	CLA	CMB-C2B	-2.59	1.46	1.51
14	a	832	CLA	CMB-C2B	-2.59	1.46	1.51
14	m	1201	CLA	CMB-C2B	-2.59	1.46	1.51
14	b	805	CLA	CMB-C2B	-2.58	1.46	1.51
14	a	839	CLA	CMB-C2B	-2.58	1.46	1.51
14	b	837	CLA	CMB-C2B	-2.58	1.46	1.51
14	j	103	CLA	CMB-C2B	-2.58	1.46	1.51
14	b	832	CLA	CHC-C1C	2.58	1.41	1.35
14	A	840	CLA	CMD-C2D	-2.58	1.45	1.50
14	b	804	CLA	C1D-ND	2.58	1.41	1.37
14	A	817	CLA	CMC-C2C	-2.58	1.45	1.50
14	B	836	CLA	CMB-C2B	-2.58	1.46	1.51
14	b	806	CLA	C3B-C2B	-2.58	1.36	1.40
14	b	811	CLA	CHC-C1C	2.58	1.41	1.35
14	b	838	CLA	CMB-C2B	-2.57	1.46	1.51
17	J	104	BCR	C30-C25	-2.57	1.50	1.53
14	B	827	CLA	CMD-C2D	-2.57	1.45	1.50
14	a	826	CLA	CMB-C2B	-2.57	1.46	1.51
14	a	836	CLA	CMD-C2D	-2.56	1.45	1.50
14	a	814	CLA	CMB-C2B	-2.56	1.46	1.51
14	a	825	CLA	CMB-C2B	-2.56	1.46	1.51
14	B	837	CLA	CMB-C2B	-2.56	1.46	1.51
14	b	808	CLA	CHC-C1C	2.56	1.41	1.35
14	b	827	CLA	CMD-C2D	-2.56	1.45	1.50
14	l	205	CLA	CMD-C2D	-2.56	1.45	1.50
14	A	819	CLA	CMC-C2C	-2.56	1.45	1.50
14	J	102	CLA	CMB-C2B	-2.56	1.46	1.51
14	B	822	CLA	CMD-C2D	-2.56	1.45	1.50
17	j	106	BCR	C1-C6	-2.55	1.50	1.53
14	B	813	CLA	CMB-C2B	-2.55	1.46	1.51
17	A	847	BCR	C1-C6	-2.55	1.50	1.53
14	B	827	CLA	CMB-C2B	-2.55	1.46	1.51
18	a	851	LHG	O2-C2	-2.55	1.35	1.43
14	A	837	CLA	CMD-C2D	-2.55	1.45	1.50
14	A	806	CLA	CMB-C2B	-2.55	1.46	1.51
14	J	101	CLA	CMB-C2B	-2.55	1.46	1.51
14	b	803	CLA	CMD-C2D	-2.54	1.45	1.50
14	b	811	CLA	CMD-C2D	-2.54	1.45	1.50
14	B	842	CLA	C1D-ND	2.54	1.40	1.37
14	a	823	CLA	CMB-C2B	-2.54	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	824	CLA	CMB-C2B	-2.54	1.46	1.51
14	j	102	CLA	CMB-C2B	-2.54	1.46	1.51
14	A	835	CLA	CMD-C2D	-2.54	1.45	1.50
14	b	832	CLA	MG-ND	-2.54	2.00	2.05
14	B	814	CLA	CMB-C2B	-2.54	1.46	1.51
14	a	802	CLA	CMC-C2C	-2.53	1.45	1.50
14	A	815	CLA	CMB-C2B	-2.53	1.46	1.51
14	A	805	CLA	CMB-C2B	-2.53	1.46	1.51
14	k	101	CLA	CMB-C2B	-2.53	1.46	1.51
14	B	817	CLA	CMB-C2B	-2.53	1.46	1.51
14	B	808	CLA	CHC-C1C	2.53	1.41	1.35
14	A	810	CLA	CMB-C2B	-2.53	1.46	1.51
14	X	1701	CLA	CMB-C2B	-2.53	1.46	1.51
14	B	822	CLA	CHC-C1C	2.53	1.41	1.35
14	b	813	CLA	CMD-C2D	-2.52	1.45	1.50
14	B	835	CLA	CMB-C2B	-2.52	1.46	1.51
14	a	818	CLA	CMB-C2B	-2.52	1.46	1.51
14	a	827	CLA	CMB-C2B	-2.52	1.46	1.51
14	a	817	CLA	C3B-CAB	-2.51	1.42	1.47
14	A	814	CLA	CMB-C2B	-2.51	1.46	1.51
14	A	826	CLA	CMB-C2B	-2.51	1.46	1.51
14	A	839	CLA	CHC-C1C	2.51	1.41	1.35
17	B	846	BCR	C1-C6	-2.51	1.50	1.53
14	B	838	CLA	C3B-C2B	-2.51	1.36	1.40
14	a	809	CLA	CMB-C2B	-2.51	1.46	1.51
14	B	817	CLA	CMD-C2D	-2.51	1.45	1.50
14	B	813	CLA	C1D-ND	2.51	1.40	1.37
14	K	102	CLA	CMB-C2B	-2.51	1.46	1.51
14	b	820	CLA	C3B-C2B	-2.51	1.36	1.40
14	b	841	CLA	C3B-C2B	-2.51	1.36	1.40
13	A	801	CL0	C4B-CHC	2.51	1.48	1.41
19	b	801	SQD	O47-C45	-2.51	1.40	1.46
14	b	806	CLA	CHC-C1C	2.50	1.41	1.35
14	B	832	CLA	MG-ND	-2.50	2.00	2.05
14	b	808	CLA	CMD-C2D	-2.50	1.45	1.50
14	A	830	CLA	C3B-C2B	-2.50	1.36	1.40
14	A	823	CLA	CMB-C2B	-2.50	1.46	1.51
14	A	837	CLA	CMB-C2B	-2.50	1.46	1.51
14	A	830	CLA	MG-ND	-2.50	2.00	2.05
14	A	829	CLA	CMD-C2D	-2.50	1.45	1.50
13	a	801	CL0	C4B-CHC	2.50	1.47	1.41
14	A	837	CLA	C1D-ND	2.49	1.40	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	827	CLA	CMC-C2C	-2.49	1.45	1.50
14	a	805	CLA	CMB-C2B	-2.49	1.46	1.51
14	B	812	CLA	CMD-C2D	-2.49	1.45	1.50
14	a	841	CLA	CMB-C2B	-2.49	1.46	1.51
14	a	830	CLA	C3B-C2B	-2.49	1.36	1.40
14	B	840	CLA	CMD-C2D	-2.49	1.45	1.50
14	b	803	CLA	C3B-CAB	-2.49	1.42	1.47
14	a	805	CLA	CMC-C2C	-2.49	1.45	1.50
14	B	842	CLA	CMB-C2B	-2.49	1.46	1.51
14	B	824	CLA	CMB-C2B	-2.49	1.46	1.51
14	b	819	CLA	CMB-C2B	-2.49	1.46	1.51
14	m	1201	CLA	CMD-C2D	-2.49	1.45	1.50
14	A	822	CLA	CMB-C2B	-2.49	1.46	1.51
17	a	846	BCR	C1-C6	-2.49	1.50	1.53
14	b	813	CLA	CMB-C2B	-2.48	1.46	1.51
14	A	813	CLA	CMC-C2C	-2.48	1.45	1.50
14	B	826	CLA	CMD-C2D	-2.48	1.45	1.50
19	l	202	SQD	O3-C3	-2.47	1.37	1.43
14	A	836	CLA	CMB-C2B	-2.47	1.46	1.51
14	a	827	CLA	CMD-C2D	-2.47	1.45	1.50
13	A	801	CL0	C1C-NC	-2.47	1.34	1.37
14	a	807	CLA	CMB-C2B	-2.47	1.46	1.51
13	a	801	CL0	C1C-NC	-2.47	1.34	1.37
14	a	833	CLA	CMB-C2B	-2.47	1.46	1.51
14	b	830	CLA	MG-ND	-2.47	2.00	2.05
17	B	849	BCR	C30-C25	-2.47	1.50	1.53
14	a	824	CLA	CMB-C2B	-2.47	1.46	1.51
14	B	804	CLA	CMB-C2B	-2.47	1.46	1.51
14	m	1201	CLA	CMC-C2C	-2.47	1.45	1.50
14	b	842	CLA	C1D-ND	2.46	1.40	1.37
14	A	824	CLA	CMB-C2B	-2.46	1.46	1.51
14	b	810	CLA	CMB-C2B	-2.46	1.46	1.51
17	B	849	BCR	C1-C6	-2.46	1.50	1.53
14	A	831	CLA	C3B-CAB	-2.46	1.42	1.47
14	a	838	CLA	C3B-C2B	-2.46	1.37	1.40
14	B	810	CLA	CMB-C2B	-2.46	1.46	1.51
14	b	833	CLA	C3B-C2B	-2.46	1.37	1.40
14	a	803	CLA	CMB-C2B	-2.45	1.46	1.51
14	A	805	CLA	C1D-ND	2.45	1.40	1.37
14	b	829	CLA	CMB-C2B	-2.45	1.46	1.51
14	A	825	CLA	CMD-C2D	-2.45	1.45	1.50
17	f	204	BCR	C30-C25	-2.45	1.50	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	820	CLA	CMD-C2D	-2.45	1.45	1.50
17	a	844	BCR	C30-C25	-2.45	1.50	1.53
14	B	839	CLA	CMD-C2D	-2.45	1.45	1.50
14	B	816	CLA	MG-ND	-2.45	2.00	2.05
14	A	809	CLA	CMB-C2B	-2.45	1.46	1.51
14	A	841	CLA	C3B-C2B	-2.45	1.37	1.40
14	A	811	CLA	C3B-C2B	-2.45	1.37	1.40
17	b	849	BCR	C1-C6	-2.44	1.50	1.53
14	L	1502	CLA	C3B-C2B	-2.44	1.37	1.40
14	a	818	CLA	CMD-C2D	-2.44	1.45	1.50
14	b	808	CLA	C1D-ND	2.44	1.40	1.37
14	A	818	CLA	CMD-C2D	-2.44	1.45	1.50
19	b	801	SQD	O2-C2	-2.44	1.37	1.43
14	A	825	CLA	CMB-C2B	-2.43	1.46	1.51
14	a	817	CLA	CMD-C2D	-2.43	1.45	1.50
14	a	812	CLA	CMD-C2D	-2.43	1.45	1.50
14	b	811	CLA	C3B-CAB	-2.43	1.43	1.47
14	a	840	CLA	CMD-C2D	-2.43	1.45	1.50
18	A	852	LHG	C8-C7	-2.43	1.43	1.50
17	m	1202	BCR	C30-C25	-2.43	1.50	1.53
14	A	827	CLA	CMB-C2B	-2.43	1.46	1.51
14	A	832	CLA	CMD-C2D	-2.42	1.45	1.50
14	A	842	CLA	C3B-C2B	-2.42	1.37	1.40
14	b	837	CLA	CMD-C2D	-2.42	1.45	1.50
14	b	825	CLA	CMB-C2B	-2.42	1.46	1.51
14	A	831	CLA	C3B-C2B	-2.42	1.37	1.40
14	A	835	CLA	CMC-C2C	-2.42	1.45	1.50
19	x	1702	SQD	O2-C2	-2.42	1.37	1.43
14	b	829	CLA	CMC-C2C	-2.42	1.45	1.50
17	B	845	BCR	C30-C25	-2.42	1.50	1.53
14	A	818	CLA	C3B-CAB	-2.41	1.43	1.47
14	B	832	CLA	C4B-CHC	-2.41	1.34	1.41
19	X	1702	SQD	O2-C2	-2.41	1.37	1.43
14	a	829	CLA	C3B-C2B	-2.41	1.37	1.40
13	a	801	CL0	C1B-CHB	2.41	1.47	1.41
17	J	103	BCR	C30-C25	-2.41	1.50	1.53
14	b	842	CLA	C3B-C2B	-2.41	1.37	1.40
14	b	821	CLA	CMC-C2C	-2.41	1.45	1.50
14	A	832	CLA	CMB-C2B	-2.41	1.46	1.51
17	A	848	BCR	C1-C6	-2.41	1.50	1.53
13	A	801	CL0	C1B-CHB	2.41	1.47	1.41
14	B	835	CLA	CMC-C2C	-2.41	1.45	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	805	CLA	CMC-C2C	-2.41	1.45	1.50
19	l	202	SQD	O2-C2	-2.40	1.37	1.43
14	B	823	CLA	CHC-C1C	2.40	1.41	1.35
14	B	840	CLA	CMB-C2B	-2.40	1.46	1.51
14	A	828	CLA	CMB-C2B	-2.40	1.46	1.51
14	a	828	CLA	CMC-C2C	-2.40	1.45	1.50
17	A	851	BCR	C33-C5	-2.40	1.47	1.50
14	B	807	CLA	CMD-C2D	-2.40	1.45	1.50
14	b	816	CLA	CMD-C2D	-2.40	1.45	1.50
14	a	829	CLA	CMD-C2D	-2.40	1.45	1.50
14	j	101	CLA	CMC-C2C	-2.40	1.45	1.50
14	b	830	CLA	CMD-C2D	-2.40	1.45	1.50
14	A	819	CLA	CMD-C2D	-2.40	1.45	1.50
14	B	801	CLA	CMC-C2C	-2.40	1.45	1.50
14	l	203	CLA	CMB-C2B	-2.39	1.46	1.51
14	A	813	CLA	MG-ND	-2.39	2.01	2.05
14	a	806	CLA	CMD-C2D	-2.39	1.45	1.50
17	L	1504	BCR	C1-C6	-2.39	1.50	1.53
14	A	813	CLA	CMD-C2D	-2.39	1.45	1.50
14	l	204	CLA	CMB-C2B	-2.38	1.46	1.51
14	B	834	CLA	CMD-C2D	-2.38	1.45	1.50
17	b	846	BCR	C1-C6	-2.38	1.50	1.53
17	l	206	BCR	C1-C6	-2.38	1.50	1.53
14	B	804	CLA	CMD-C2D	-2.38	1.45	1.50
14	B	843	CLA	C1C-NC	-2.38	1.34	1.37
14	A	824	CLA	CMD-C2D	-2.37	1.45	1.50
14	b	832	CLA	C1D-ND	2.37	1.40	1.37
17	j	104	BCR	C30-C25	-2.37	1.50	1.53
14	a	810	CLA	CMD-C2D	-2.37	1.45	1.50
14	b	821	CLA	CMD-C2D	-2.37	1.45	1.50
14	a	811	CLA	C3B-C2B	-2.36	1.37	1.40
14	l	203	CLA	CMC-C2C	-2.36	1.45	1.50
14	b	806	CLA	CMD-C2D	-2.36	1.45	1.50
14	B	819	CLA	CMB-C2B	-2.36	1.46	1.51
14	A	806	CLA	CMC-C2C	-2.36	1.45	1.50
14	K	101	CLA	CMD-C2D	-2.36	1.45	1.50
14	b	841	CLA	CMD-C2D	-2.36	1.45	1.50
14	A	804	CLA	CMC-C2C	-2.36	1.45	1.50
14	A	818	CLA	CMC-C2C	-2.36	1.45	1.50
14	a	830	CLA	CMD-C2D	-2.36	1.45	1.50
14	A	803	CLA	CMC-C2C	-2.35	1.45	1.50
14	a	816	CLA	C3B-CAB	-2.35	1.43	1.47

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	851	LHG	O8-C6	-2.35	1.39	1.45
14	b	835	CLA	CMD-C2D	-2.35	1.45	1.50
14	b	823	CLA	CMD-C2D	-2.35	1.45	1.50
14	b	836	CLA	CMD-C2D	-2.35	1.45	1.50
14	b	812	CLA	CMD-C2D	-2.35	1.45	1.50
14	b	820	CLA	MG-ND	-2.35	2.01	2.05
14	a	831	CLA	CMD-C2D	-2.35	1.45	1.50
19	X	1702	SQD	O3-C3	-2.35	1.37	1.43
14	k	101	CLA	CMD-C2D	-2.34	1.45	1.50
14	B	802	CLA	CMC-C2C	-2.34	1.45	1.50
17	a	845	BCR	C1-C6	-2.34	1.50	1.53
17	i	102	BCR	C33-C5	-2.34	1.47	1.50
14	a	812	CLA	CMC-C2C	-2.34	1.45	1.50
14	f	203	CLA	CMD-C2D	-2.34	1.45	1.50
14	B	819	CLA	CMC-C2C	-2.34	1.45	1.50
14	A	803	CLA	CMB-C2B	-2.33	1.46	1.51
14	b	833	CLA	C3B-CAB	-2.33	1.43	1.47
14	b	818	CLA	C3B-C2B	-2.33	1.37	1.40
14	l	204	CLA	C3B-C2B	-2.33	1.37	1.40
14	A	807	CLA	CMD-C2D	-2.33	1.45	1.50
14	a	828	CLA	CMD-C2D	-2.33	1.45	1.50
14	B	818	CLA	CMB-C2B	-2.33	1.46	1.51
14	A	821	CLA	CMC-C2C	-2.32	1.45	1.50
14	b	818	CLA	CMD-C2D	-2.32	1.45	1.50
14	b	813	CLA	C3B-C2B	-2.32	1.37	1.40
14	b	809	CLA	CMD-C2D	-2.32	1.45	1.50
14	b	809	CLA	MG-ND	-2.32	2.01	2.05
19	b	801	SQD	O47-C7	2.32	1.40	1.34
14	B	804	CLA	CMC-C2C	-2.32	1.45	1.50
19	X	1702	SQD	O4-C4	-2.32	1.37	1.43
14	B	815	CLA	CMD-C2D	-2.32	1.45	1.50
14	a	826	CLA	MG-ND	-2.31	2.01	2.05
17	a	846	BCR	C30-C25	-2.31	1.50	1.53
14	b	843	CLA	C3C-C2C	2.31	1.41	1.36
14	A	804	CLA	CMD-C2D	-2.31	1.45	1.50
14	b	822	CLA	CMD-C2D	-2.31	1.45	1.50
14	B	823	CLA	C4B-CHC	-2.31	1.34	1.41
14	A	803	CLA	CMD-C2D	-2.31	1.45	1.50
17	B	846	BCR	C30-C25	-2.31	1.50	1.53
14	b	829	CLA	CMD-C2D	-2.31	1.45	1.50
14	b	831	CLA	CMB-C2B	-2.31	1.46	1.51
14	b	839	CLA	CMD-C2D	-2.31	1.45	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	832	CLA	C3B-C2B	-2.31	1.37	1.40
14	a	820	CLA	CMC-C2C	-2.30	1.45	1.50
17	F	205	BCR	C30-C25	-2.30	1.50	1.53
14	a	822	CLA	CMD-C2D	-2.30	1.45	1.50
14	A	812	CLA	C3B-C2B	-2.30	1.37	1.40
14	A	843	CLA	C3B-C2B	-2.30	1.37	1.40
14	A	842	CLA	CMD-C2D	-2.30	1.45	1.50
14	B	806	CLA	CMB-C2B	-2.30	1.46	1.51
14	B	806	CLA	C1D-ND	2.30	1.40	1.37
14	b	806	CLA	C1D-ND	2.30	1.40	1.37
14	B	830	CLA	CMC-C2C	-2.30	1.45	1.50
14	a	823	CLA	CMD-C2D	-2.30	1.45	1.50
14	b	808	CLA	CMB-C2B	-2.30	1.46	1.51
17	B	847	BCR	C30-C25	-2.30	1.50	1.53
14	B	832	CLA	CMC-C2C	-2.30	1.45	1.50
14	b	813	CLA	C3B-CAB	-2.30	1.43	1.47
14	F	204	CLA	CMD-C2D	-2.30	1.45	1.50
14	b	831	CLA	CMC-C2C	-2.30	1.45	1.50
14	a	821	CLA	CMD-C2D	-2.29	1.45	1.50
17	A	846	BCR	C30-C25	-2.29	1.50	1.53
17	k	103	BCR	C1-C6	-2.29	1.50	1.53
14	B	830	CLA	CMD-C2D	-2.29	1.45	1.50
14	b	841	CLA	C3B-CAB	-2.29	1.43	1.47
14	a	805	CLA	CMD-C2D	-2.29	1.45	1.50
14	b	816	CLA	MG-ND	-2.29	2.01	2.05
19	b	801	SQD	O3-C3	-2.29	1.37	1.43
14	a	839	CLA	CMC-C2C	-2.29	1.46	1.50
14	B	825	CLA	CMB-C2B	-2.29	1.46	1.51
14	A	833	CLA	CMC-C2C	-2.29	1.46	1.50
17	M	101	BCR	C30-C25	-2.29	1.50	1.53
17	J	105	BCR	C1-C6	-2.28	1.50	1.53
14	a	833	CLA	CMD-C2D	-2.28	1.46	1.50
14	L	1502	CLA	C1D-ND	2.28	1.40	1.37
14	b	818	CLA	C3B-CAB	-2.28	1.43	1.47
17	a	849	BCR	C33-C5	-2.28	1.47	1.50
14	a	810	CLA	C3B-C2B	-2.28	1.37	1.40
17	l	207	BCR	C30-C25	-2.28	1.50	1.53
14	B	836	CLA	CMD-C2D	-2.28	1.46	1.50
14	k	102	CLA	CMC-C2C	-2.28	1.46	1.50
14	B	801	CLA	CMD-C2D	-2.28	1.46	1.50
14	a	835	CLA	CMD-C2D	-2.28	1.46	1.50
19	l	202	SQD	O4-C4	-2.27	1.37	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	812	CLA	MG-ND	-2.27	2.01	2.05
14	A	828	CLA	CMC-C2C	-2.27	1.46	1.50
14	b	812	CLA	CMC-C2C	-2.27	1.46	1.50
14	B	823	CLA	C3B-C2B	-2.27	1.37	1.40
14	L	1501	CLA	C3B-CAB	-2.27	1.43	1.47
14	B	813	CLA	C3B-C2B	-2.27	1.37	1.40
14	A	828	CLA	CMD-C2D	-2.27	1.46	1.50
14	b	806	CLA	C3B-CAB	-2.27	1.43	1.47
14	a	820	CLA	CMD-C2D	-2.27	1.46	1.50
17	l	201	BCR	C1-C6	-2.27	1.50	1.53
14	b	831	CLA	MG-ND	-2.27	2.01	2.05
14	b	803	CLA	CMC-C2C	-2.27	1.46	1.50
14	b	827	CLA	MG-ND	-2.26	2.01	2.05
14	b	843	CLA	CHC-C1C	2.26	1.40	1.35
14	B	838	CLA	CMD-C2D	-2.26	1.46	1.50
14	A	833	CLA	C3B-CAB	-2.26	1.43	1.47
14	a	807	CLA	CMC-C2C	-2.26	1.46	1.50
14	A	802	CLA	C3B-C2B	-2.26	1.37	1.40
17	a	845	BCR	C30-C25	-2.26	1.50	1.53
14	B	841	CLA	CMD-C2D	-2.26	1.46	1.50
14	a	809	CLA	CMD-C2D	-2.26	1.46	1.50
14	K	102	CLA	CMC-C2C	-2.26	1.46	1.50
14	B	829	CLA	CMD-C2D	-2.26	1.46	1.50
14	B	819	CLA	CMD-C2D	-2.26	1.46	1.50
14	a	838	CLA	CMD-C2D	-2.26	1.46	1.50
14	a	837	CLA	CMC-C2C	-2.26	1.46	1.50
14	b	819	CLA	CMD-C2D	-2.26	1.46	1.50
14	B	802	CLA	C3B-C2B	-2.26	1.37	1.40
14	b	803	CLA	MG-ND	-2.26	2.01	2.05
14	a	804	CLA	CMD-C2D	-2.25	1.46	1.50
14	a	816	CLA	CMD-C2D	-2.25	1.46	1.50
14	A	808	CLA	CMC-C2C	-2.25	1.46	1.50
19	l	202	SQD	O47-C45	-2.25	1.41	1.46
14	B	819	CLA	C3B-C2B	-2.25	1.37	1.40
14	b	840	CLA	CMD-C2D	-2.25	1.46	1.50
14	B	823	CLA	CMD-C2D	-2.25	1.46	1.50
14	B	837	CLA	CMD-C2D	-2.25	1.46	1.50
17	i	102	BCR	C30-C25	-2.25	1.50	1.53
14	B	835	CLA	C3B-C2B	-2.25	1.37	1.40
14	b	820	CLA	C3B-CAB	-2.24	1.43	1.47
14	a	840	CLA	C3B-C2B	-2.24	1.37	1.40
14	b	805	CLA	MG-ND	-2.24	2.01	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	838	CLA	CMD-C2D	-2.24	1.46	1.50
14	a	839	CLA	C3B-CAB	-2.24	1.43	1.47
14	B	836	CLA	CMC-C2C	-2.24	1.46	1.50
14	A	829	CLA	CMC-C2C	-2.24	1.46	1.50
14	B	807	CLA	CMB-C2B	-2.24	1.47	1.51
14	A	818	CLA	MG-ND	-2.23	2.01	2.05
14	a	807	CLA	CMD-C2D	-2.23	1.46	1.50
14	a	818	CLA	CMC-C2C	-2.23	1.46	1.50
14	l	204	CLA	C3B-CAB	-2.23	1.43	1.47
14	l	203	CLA	CMD-C2D	-2.23	1.46	1.50
14	A	808	CLA	CMD-C2D	-2.23	1.46	1.50
18	F	201	LHG	O7-C5	-2.23	1.41	1.46
14	b	825	CLA	CMD-C2D	-2.23	1.46	1.50
19	x	1702	SQD	O3-C3	-2.23	1.37	1.43
14	A	814	CLA	CMD-C2D	-2.23	1.46	1.50
14	a	824	CLA	CMD-C2D	-2.23	1.46	1.50
17	A	847	BCR	C30-C25	-2.22	1.50	1.53
14	a	812	CLA	MG-ND	-2.22	2.01	2.05
14	a	836	CLA	C4B-CHC	-2.22	1.34	1.41
14	b	811	CLA	C1C-NC	-2.22	1.34	1.37
14	j	101	CLA	CMD-C2D	-2.22	1.46	1.50
14	A	802	CLA	C4B-CHC	-2.22	1.34	1.41
14	A	826	CLA	CMD-C2D	-2.22	1.46	1.50
14	b	815	CLA	CMD-C2D	-2.22	1.46	1.50
14	b	839	CLA	MG-ND	-2.22	2.01	2.05
14	a	832	CLA	CMD-C2D	-2.22	1.46	1.50
14	a	840	CLA	CMC-C2C	-2.22	1.46	1.50
14	b	804	CLA	CMD-C2D	-2.22	1.46	1.50
14	b	808	CLA	CMC-C2C	-2.22	1.46	1.50
14	X	1701	CLA	C3B-C2B	-2.21	1.37	1.40
14	B	843	CLA	CHC-C1C	2.21	1.40	1.35
14	B	811	CLA	CMC-C2C	-2.21	1.46	1.50
14	A	818	CLA	C3B-C2B	-2.21	1.37	1.40
14	a	841	CLA	CMC-C2C	-2.21	1.46	1.50
14	a	831	CLA	C3B-C2B	-2.21	1.37	1.40
14	b	807	CLA	C3B-C2B	-2.21	1.37	1.40
14	b	821	CLA	CAC-C3C	-2.21	1.45	1.51
19	b	801	SQD	O4-C4	-2.21	1.37	1.43
14	B	805	CLA	CMC-C2C	-2.21	1.46	1.50
14	A	830	CLA	CMD-C2D	-2.21	1.46	1.50
14	B	838	CLA	CMC-C2C	-2.21	1.46	1.50
14	f	201	CLA	C3B-C2B	-2.21	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	810	CLA	MG-ND	-2.21	2.01	2.05
14	A	836	CLA	CMD-C2D	-2.21	1.46	1.50
14	B	835	CLA	C3B-CAB	-2.21	1.43	1.47
14	a	837	CLA	CMD-C2D	-2.20	1.46	1.50
14	B	808	CLA	C4B-CHC	-2.20	1.34	1.41
14	B	813	CLA	CMC-C2C	-2.20	1.46	1.50
14	b	843	CLA	C4B-CHC	-2.20	1.34	1.41
14	A	811	CLA	CMC-C2C	-2.20	1.46	1.50
14	A	811	CLA	CMD-C2D	-2.20	1.46	1.50
14	b	843	CLA	CMD-C2D	-2.20	1.46	1.50
14	B	839	CLA	C3B-CAB	-2.20	1.43	1.47
14	a	807	CLA	C3B-C2B	-2.20	1.37	1.40
14	b	840	CLA	CMC-C2C	-2.20	1.46	1.50
14	A	817	CLA	CMD-C2D	-2.19	1.46	1.50
14	a	831	CLA	MG-ND	-2.19	2.01	2.05
17	b	847	BCR	C38-C26	-2.19	1.47	1.50
14	A	834	CLA	CMD-C2D	-2.19	1.46	1.50
14	a	816	CLA	C3B-C2B	-2.19	1.37	1.40
14	b	833	CLA	MG-ND	-2.19	2.01	2.05
14	A	813	CLA	C3B-C2B	-2.19	1.37	1.40
17	K	103	BCR	C30-C25	-2.19	1.50	1.53
14	A	834	CLA	CMC-C2C	-2.19	1.46	1.50
14	A	816	CLA	CMD-C2D	-2.19	1.46	1.50
14	B	808	CLA	C3D-C4D	2.19	1.49	1.44
14	B	835	CLA	CMD-C2D	-2.19	1.46	1.50
14	B	833	CLA	C3B-C2B	-2.19	1.37	1.40
14	a	831	CLA	CMC-C2C	-2.19	1.46	1.50
14	b	807	CLA	MG-ND	-2.19	2.01	2.05
17	b	846	BCR	C30-C25	-2.19	1.50	1.53
14	b	834	CLA	CMD-C2D	-2.19	1.46	1.50
14	j	103	CLA	C3B-C2B	-2.19	1.37	1.40
19	x	1702	SQD	O4-C4	-2.19	1.37	1.43
14	b	804	CLA	CMC-C2C	-2.18	1.46	1.50
14	A	829	CLA	MG-ND	-2.18	2.01	2.05
17	B	849	BCR	C36-C18	-2.18	1.46	1.50
14	a	802	CLA	CMD-C2D	-2.18	1.46	1.50
14	x	1701	CLA	CMD-C2D	-2.18	1.46	1.50
14	l	204	CLA	CMC-C2C	-2.18	1.46	1.50
14	b	809	CLA	CMC-C2C	-2.18	1.46	1.50
14	a	832	CLA	CMC-C2C	-2.18	1.46	1.50
14	A	830	CLA	C1D-ND	2.18	1.40	1.37
14	a	841	CLA	CMD-C2D	-2.18	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	831	CLA	C3B-CAB	-2.18	1.43	1.47
14	a	803	CLA	CMD-C2D	-2.18	1.46	1.50
14	f	201	CLA	CMC-C2C	-2.18	1.46	1.50
14	A	822	CLA	CMD-C2D	-2.18	1.46	1.50
14	a	838	CLA	CMC-C2C	-2.18	1.46	1.50
14	a	829	CLA	MG-ND	-2.18	2.01	2.05
14	x	1701	CLA	C3B-C2B	-2.17	1.37	1.40
14	A	820	CLA	CMD-C2D	-2.17	1.46	1.50
14	a	829	CLA	CMC-C2C	-2.17	1.46	1.50
14	l	205	CLA	CMC-C2C	-2.17	1.46	1.50
14	a	813	CLA	CMD-C2D	-2.17	1.46	1.50
14	a	836	CLA	CMC-C2C	-2.17	1.46	1.50
14	b	829	CLA	MG-ND	-2.17	2.01	2.05
14	b	817	CLA	CMC-C2C	-2.17	1.46	1.50
14	a	821	CLA	C3B-CAB	-2.17	1.43	1.47
14	A	824	CLA	C3B-C2B	-2.17	1.37	1.40
14	b	814	CLA	CMD-C2D	-2.17	1.46	1.50
14	A	823	CLA	CMD-C2D	-2.17	1.46	1.50
17	k	103	BCR	C30-C25	-2.17	1.50	1.53
14	a	834	CLA	MG-ND	-2.17	2.01	2.05
14	A	814	CLA	CMC-C2C	-2.16	1.46	1.50
14	B	843	CLA	CMD-C2D	-2.16	1.46	1.50
14	A	839	CLA	CMD-C2D	-2.16	1.46	1.50
18	A	853	LHG	P-O4	-2.16	1.45	1.55
14	j	101	CLA	C3B-CAB	-2.16	1.43	1.47
14	L	1502	CLA	C3B-CAB	-2.16	1.43	1.47
14	m	1201	CLA	C3B-C2B	-2.16	1.37	1.40
14	B	843	CLA	C4B-CHC	-2.16	1.35	1.41
13	A	801	CL0	C1D-C2D	2.16	1.49	1.45
14	a	810	CLA	CMC-C2C	-2.16	1.46	1.50
14	a	834	CLA	CMD-C2D	-2.16	1.46	1.50
14	a	822	CLA	CMC-C2C	-2.16	1.46	1.50
20	B	851	LMG	O1-C7	-2.16	1.39	1.43
14	a	817	CLA	MG-ND	-2.15	2.01	2.05
14	A	842	CLA	C3B-CAB	-2.15	1.43	1.47
14	A	807	CLA	C3B-C2B	-2.15	1.37	1.40
14	b	810	CLA	CMC-C2C	-2.15	1.46	1.50
14	b	814	CLA	C3B-C2B	-2.15	1.37	1.40
14	b	820	CLA	CMC-C2C	-2.15	1.46	1.50
14	b	806	CLA	CMC-C2C	-2.15	1.46	1.50
14	A	825	CLA	CMC-C2C	-2.15	1.46	1.50
14	b	815	CLA	C3B-C2B	-2.15	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	806	CLA	C3B-C2B	-2.14	1.37	1.40
17	B	849	BCR	C17-C18	-2.14	1.32	1.35
14	f	203	CLA	CMC-C2C	-2.14	1.46	1.50
14	a	814	CLA	CMD-C2D	-2.14	1.46	1.50
18	A	853	LHG	O8-C6	-2.14	1.40	1.45
14	B	809	CLA	CMC-C2C	-2.14	1.46	1.50
14	A	840	CLA	MG-ND	-2.14	2.01	2.05
14	a	807	CLA	C3B-CAB	-2.14	1.43	1.47
14	A	825	CLA	MG-ND	-2.14	2.01	2.05
14	A	806	CLA	CMD-C2D	-2.14	1.46	1.50
14	A	832	CLA	CMC-C2C	-2.14	1.46	1.50
14	B	814	CLA	CMC-C2C	-2.14	1.46	1.50
14	k	102	CLA	CMD-C2D	-2.13	1.46	1.50
14	B	806	CLA	CMD-C2D	-2.13	1.46	1.50
14	b	838	CLA	CMD-C2D	-2.13	1.46	1.50
14	a	815	CLA	CMD-C2D	-2.13	1.46	1.50
14	J	102	CLA	CMD-C2D	-2.13	1.46	1.50
14	B	825	CLA	CMC-C2C	-2.13	1.46	1.50
13	a	801	CL0	C1D-C2D	2.13	1.49	1.45
14	A	838	CLA	CMC-C2C	-2.13	1.46	1.50
14	B	810	CLA	CMD-C2D	-2.13	1.46	1.50
17	i	101	BCR	C1-C6	-2.12	1.50	1.53
17	b	850	BCR	C1-C6	-2.12	1.50	1.53
14	B	824	CLA	CMD-C2D	-2.12	1.46	1.50
14	a	819	CLA	CMD-C2D	-2.12	1.46	1.50
14	B	813	CLA	C3B-CAB	-2.12	1.43	1.47
14	A	810	CLA	CMD-C2D	-2.12	1.46	1.50
14	J	101	CLA	C3B-CAB	-2.12	1.43	1.47
14	j	103	CLA	CMD-C2D	-2.12	1.46	1.50
14	B	805	CLA	C3B-CAB	-2.12	1.43	1.47
14	B	809	CLA	C3B-C2B	-2.12	1.37	1.40
14	B	808	CLA	CMC-C2C	-2.12	1.46	1.50
18	A	852	LHG	O6-C4	-2.12	1.36	1.44
14	B	830	CLA	MG-ND	-2.12	2.01	2.05
14	A	812	CLA	CMD-C2D	-2.12	1.46	1.50
14	b	823	CLA	C3B-C2B	-2.12	1.37	1.40
14	a	837	CLA	C3B-CAB	-2.12	1.43	1.47
14	B	822	CLA	C3B-C2B	-2.12	1.37	1.40
17	L	1504	BCR	C30-C25	-2.11	1.50	1.53
14	b	834	CLA	CMC-C2C	-2.11	1.46	1.50
14	B	821	CLA	CMD-C2D	-2.11	1.46	1.50
17	L	1504	BCR	C38-C26	-2.11	1.47	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	201	CLA	CMD-C2D	-2.11	1.46	1.50
14	A	843	CLA	CMC-C2C	-2.11	1.46	1.50
18	a	851	LHG	O6-C4	-2.11	1.36	1.44
14	a	833	CLA	CMC-C2C	-2.11	1.46	1.50
14	A	806	CLA	C3B-CAB	-2.11	1.43	1.47
20	B	803	LMG	O8-C9	-2.11	1.40	1.45
14	A	802	CLA	CMD-C2D	-2.11	1.46	1.50
14	b	827	CLA	CMB-C2B	-2.11	1.47	1.51
14	b	808	CLA	MG-ND	-2.11	2.01	2.05
14	A	806	CLA	MG-ND	-2.10	2.01	2.05
14	a	839	CLA	MG-ND	-2.10	2.01	2.05
14	B	807	CLA	CMC-C2C	-2.10	1.46	1.50
14	a	837	CLA	MG-ND	-2.10	2.01	2.05
14	b	826	CLA	CMD-C2D	-2.10	1.46	1.50
14	B	824	CLA	CMC-C2C	-2.10	1.46	1.50
14	b	835	CLA	CMC-C2C	-2.10	1.46	1.50
14	b	836	CLA	CMC-C2C	-2.10	1.46	1.50
14	B	801	CLA	C3B-CAB	-2.10	1.43	1.47
14	j	102	CLA	CMD-C2D	-2.10	1.46	1.50
14	A	842	CLA	CMC-C2C	-2.10	1.46	1.50
14	B	840	CLA	CMC-C2C	-2.10	1.46	1.50
14	a	811	CLA	CMD-C2D	-2.10	1.46	1.50
14	b	824	CLA	CMD-C2D	-2.10	1.46	1.50
14	A	843	CLA	CMD-C2D	-2.10	1.46	1.50
14	B	812	CLA	CMC-C2C	-2.10	1.46	1.50
14	A	804	CLA	MG-ND	-2.09	2.01	2.05
17	B	849	BCR	C4-C5	-2.09	1.46	1.51
14	B	818	CLA	C3B-CAB	-2.09	1.43	1.47
14	B	820	CLA	C3B-CAB	-2.09	1.43	1.47
14	A	802	CLA	CMC-C2C	-2.09	1.46	1.50
14	K	101	CLA	CMC-C2C	-2.09	1.46	1.50
17	a	844	BCR	C33-C5	-2.09	1.47	1.50
14	b	833	CLA	CMC-C2C	-2.09	1.46	1.50
14	k	101	CLA	CMC-C2C	-2.09	1.46	1.50
14	a	810	CLA	C3B-CAB	-2.09	1.43	1.47
14	B	840	CLA	C3B-CAB	-2.09	1.43	1.47
14	B	814	CLA	CMD-C2D	-2.09	1.46	1.50
14	B	811	CLA	C3B-CAB	-2.09	1.43	1.47
14	a	839	CLA	CMD-C2D	-2.09	1.46	1.50
17	J	104	BCR	C33-C5	-2.09	1.47	1.50
18	a	851	LHG	O3-C3	-2.09	1.36	1.44
17	B	850	BCR	C38-C26	-2.09	1.47	1.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	814	CLA	CMC-C2C	-2.09	1.46	1.50
14	a	830	CLA	MG-ND	-2.09	2.01	2.05
14	b	817	CLA	C3B-CAB	-2.09	1.43	1.47
14	b	808	CLA	C4B-CHC	-2.09	1.35	1.41
14	a	813	CLA	CMC-C2C	-2.08	1.46	1.50
14	A	841	CLA	CMC-C2C	-2.08	1.46	1.50
18	a	851	LHG	O7-C5	-2.08	1.41	1.46
14	B	802	CLA	CMD-C2D	-2.08	1.46	1.50
14	x	1701	CLA	CMC-C2C	-2.08	1.46	1.50
14	B	843	CLA	C3B-C2B	-2.08	1.37	1.40
14	B	802	CLA	C3B-CAB	-2.08	1.43	1.47
14	B	841	CLA	CMC-C2C	-2.08	1.46	1.50
14	F	204	CLA	CMC-C2C	-2.08	1.46	1.50
14	a	828	CLA	MG-ND	-2.08	2.01	2.05
14	B	832	CLA	C1D-ND	2.08	1.40	1.37
14	A	840	CLA	C3B-CAB	-2.08	1.43	1.47
14	b	807	CLA	C4B-CHC	-2.07	1.35	1.41
14	B	821	CLA	CMC-C2C	-2.07	1.46	1.50
14	a	825	CLA	CMC-C2C	-2.07	1.46	1.50
14	B	806	CLA	C4B-CHC	-2.07	1.35	1.41
14	A	824	CLA	C3B-CAB	-2.07	1.43	1.47
14	b	823	CLA	MG-ND	-2.07	2.01	2.05
14	A	815	CLA	CMD-C2D	-2.07	1.46	1.50
14	B	834	CLA	CMC-C2C	-2.07	1.46	1.50
14	a	821	CLA	CMC-C2C	-2.07	1.46	1.50
14	j	102	CLA	CMC-C2C	-2.07	1.46	1.50
14	A	841	CLA	MG-ND	-2.07	2.01	2.05
14	A	836	CLA	CMC-C2C	-2.07	1.46	1.50
14	a	819	CLA	CMC-C2C	-2.07	1.46	1.50
14	b	821	CLA	MG-ND	-2.07	2.01	2.05
14	b	838	CLA	CMC-C2C	-2.07	1.46	1.50
17	b	849	BCR	C36-C18	-2.07	1.46	1.50
14	a	806	CLA	C3B-CAB	-2.07	1.43	1.47
14	B	837	CLA	CMC-C2C	-2.07	1.46	1.50
14	A	810	CLA	CMC-C2C	-2.07	1.46	1.50
14	a	812	CLA	C3B-C2B	-2.07	1.37	1.40
14	B	808	CLA	C3B-C2B	-2.06	1.37	1.40
14	X	1701	CLA	CMC-C2C	-2.06	1.46	1.50
17	A	847	BCR	C38-C26	-2.06	1.47	1.50
14	B	842	CLA	CMC-C2C	-2.06	1.46	1.50
14	k	102	CLA	C3B-C2B	-2.06	1.37	1.40
14	L	1502	CLA	CMD-C2D	-2.06	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	849	BCR	C33-C5	-2.06	1.47	1.50
14	A	822	CLA	CMC-C2C	-2.06	1.46	1.50
14	F	202	CLA	CMC-C2C	-2.06	1.46	1.50
14	B	827	CLA	C4B-CHC	-2.06	1.35	1.41
14	B	839	CLA	CMC-C2C	-2.06	1.46	1.50
14	J	101	CLA	CMD-C2D	-2.06	1.46	1.50
14	A	840	CLA	C3B-C2B	-2.06	1.37	1.40
17	A	849	BCR	C30-C25	-2.06	1.50	1.53
14	a	808	CLA	CMC-C2C	-2.06	1.46	1.50
14	a	837	CLA	C3B-C2B	-2.06	1.37	1.40
17	a	847	BCR	C33-C5	-2.06	1.47	1.50
14	L	1501	CLA	CMD-C2D	-2.06	1.46	1.50
14	b	813	CLA	CMC-C2C	-2.05	1.46	1.50
14	b	805	CLA	CMD-C2D	-2.05	1.46	1.50
14	a	808	CLA	C4B-CHC	-2.05	1.35	1.41
17	J	103	BCR	C33-C5	-2.05	1.47	1.50
14	A	826	CLA	MG-ND	-2.05	2.01	2.05
14	a	816	CLA	MG-ND	-2.05	2.01	2.05
14	b	839	CLA	C3B-CAB	-2.05	1.43	1.47
14	a	826	CLA	C4B-CHC	-2.05	1.35	1.41
14	a	806	CLA	CMC-C2C	-2.05	1.46	1.50
14	b	802	CLA	MG-ND	-2.05	2.01	2.05
17	l	201	BCR	C30-C25	-2.05	1.51	1.53
14	j	103	CLA	CMC-C2C	-2.04	1.46	1.50
14	j	103	CLA	C3B-CAB	-2.04	1.43	1.47
14	a	809	CLA	CMC-C2C	-2.04	1.46	1.50
14	b	811	CLA	C4B-CHC	-2.04	1.35	1.41
17	a	844	BCR	C36-C18	-2.04	1.46	1.50
17	B	846	BCR	C38-C26	-2.04	1.47	1.50
14	a	840	CLA	MG-ND	-2.04	2.01	2.05
14	A	820	CLA	CMC-C2C	-2.04	1.46	1.50
17	j	104	BCR	C33-C5	-2.04	1.47	1.50
14	A	815	CLA	CMC-C2C	-2.04	1.46	1.50
14	b	819	CLA	MG-ND	-2.04	2.01	2.05
14	f	203	CLA	C3B-CAB	-2.04	1.43	1.47
14	a	835	CLA	CMC-C2C	-2.04	1.46	1.50
14	A	832	CLA	MG-ND	-2.04	2.01	2.05
14	b	825	CLA	CMC-C2C	-2.03	1.46	1.50
14	B	810	CLA	CMC-C2C	-2.03	1.46	1.50
14	A	837	CLA	MG-ND	-2.03	2.01	2.05
14	J	101	CLA	CMC-C2C	-2.03	1.46	1.50
14	a	806	CLA	MG-ND	-2.03	2.01	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	818	CLA	CMC-C2C	-2.03	1.46	1.50
14	A	820	CLA	C3B-C2B	-2.03	1.37	1.40
14	A	831	CLA	CMD-C2D	-2.03	1.46	1.50
14	b	818	CLA	CMC-C2C	-2.03	1.46	1.50
14	b	836	CLA	C3B-C2B	-2.03	1.37	1.40
17	I	102	BCR	C38-C26	-2.03	1.47	1.50
14	J	102	CLA	CMC-C2C	-2.03	1.46	1.50
14	b	802	CLA	CMD-C2D	-2.03	1.46	1.50
14	B	833	CLA	C3B-CAB	-2.03	1.43	1.47
14	X	1701	CLA	CMD-C2D	-2.03	1.46	1.50
14	A	823	CLA	CMC-C2C	-2.03	1.46	1.50
14	B	817	CLA	C4B-CHC	-2.03	1.35	1.41
14	a	826	CLA	CMD-C2D	-2.03	1.46	1.50
17	A	849	BCR	C33-C5	-2.02	1.47	1.50
14	B	809	CLA	MG-ND	-2.02	2.01	2.05
17	B	848	BCR	C38-C26	-2.02	1.47	1.50
14	B	820	CLA	CMC-C2C	-2.02	1.46	1.50
17	l	207	BCR	C1-C6	-2.02	1.51	1.53
14	A	816	CLA	C3B-C2B	-2.02	1.37	1.40
14	B	820	CLA	MG-ND	-2.02	2.01	2.05
14	B	831	CLA	CMC-C2C	-2.02	1.46	1.50
14	L	1501	CLA	CMC-C2C	-2.02	1.46	1.50
14	b	830	CLA	C3B-CAB	-2.02	1.43	1.47
14	b	832	CLA	C4B-CHC	-2.02	1.35	1.41
17	I	102	BCR	C33-C5	-2.02	1.47	1.50
14	B	823	CLA	C3B-CAB	-2.02	1.43	1.47
14	b	824	CLA	CMC-C2C	-2.02	1.46	1.50
14	B	811	CLA	CAC-C3C	-2.02	1.45	1.51
17	A	850	BCR	C33-C5	-2.02	1.47	1.50
17	b	850	BCR	C38-C26	-2.02	1.47	1.50
14	m	1201	CLA	CMA-C3A	-2.02	1.48	1.53
14	b	823	CLA	CMC-C2C	-2.01	1.46	1.50
14	b	834	CLA	C3B-C2B	-2.01	1.37	1.40
17	B	845	BCR	C33-C5	-2.01	1.47	1.50
14	b	841	CLA	CMC-C2C	-2.01	1.46	1.50
14	B	812	CLA	C3B-C2B	-2.01	1.37	1.40
14	a	815	CLA	C3B-C2B	-2.01	1.37	1.40
17	b	849	BCR	C38-C26	-2.01	1.47	1.50
14	b	837	CLA	CMC-C2C	-2.01	1.46	1.50
14	B	820	CLA	C3B-C2B	-2.01	1.37	1.40
14	B	839	CLA	MG-ND	-2.01	2.01	2.05
14	A	839	CLA	CMC-C2C	-2.01	1.46	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	807	CLA	C3B-CAB	-2.01	1.43	1.47
14	B	816	CLA	C3B-CAB	-2.00	1.43	1.47
14	B	831	CLA	C3B-CAB	-2.00	1.43	1.47
17	f	202	BCR	C33-C5	-2.00	1.47	1.50
14	a	805	CLA	C4B-CHC	-2.00	1.35	1.41

All (2279) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	807	CLA	O2D-CGD-CBD	25.81	157.13	111.27
14	A	807	CLA	O2D-CGD-O1D	-24.58	75.78	123.84
14	A	807	CLA	O1D-CGD-CBD	-21.05	81.42	124.48
14	a	841	CLA	O2A-CGA-O1A	-20.37	72.52	123.30
14	a	841	CLA	O2A-CGA-CBA	13.87	158.58	114.03
14	a	841	CLA	O1A-CGA-CBA	-11.49	86.16	123.08
14	B	806	CLA	C4A-NA-C1A	10.60	111.47	106.71
14	b	808	CLA	C4A-NA-C1A	10.10	111.25	106.71
14	b	811	CLA	C4A-NA-C1A	9.83	111.13	106.71
14	B	808	CLA	C4A-NA-C1A	9.70	111.07	106.71
14	b	822	CLA	C4A-NA-C1A	9.50	110.98	106.71
14	b	807	CLA	C4A-NA-C1A	9.31	110.89	106.71
14	B	811	CLA	C4A-NA-C1A	9.28	110.88	106.71
14	B	822	CLA	C4A-NA-C1A	9.00	110.75	106.71
14	B	829	CLA	C4A-NA-C1A	8.82	110.67	106.71
14	b	843	CLA	C4A-NA-C1A	8.80	110.66	106.71
14	l	205	CLA	C4A-NA-C1A	8.73	110.63	106.71
14	a	826	CLA	C4A-NA-C1A	8.66	110.60	106.71
14	B	827	CLA	C4A-NA-C1A	8.66	110.60	106.71
14	a	809	CLA	C4A-NA-C1A	8.56	110.56	106.71
14	A	811	CLA	C4A-NA-C1A	8.55	110.55	106.71
14	a	804	CLA	C4A-NA-C1A	8.49	110.52	106.71
14	a	810	CLA	C4A-NA-C1A	8.41	110.49	106.71
14	a	841	CLA	C4A-NA-C1A	8.39	110.48	106.71
14	B	823	CLA	C4A-NA-C1A	8.38	110.47	106.71
14	a	808	CLA	C4A-NA-C1A	8.37	110.47	106.71
14	A	842	CLA	C4A-NA-C1A	8.34	110.46	106.71
14	a	824	CLA	C4A-NA-C1A	8.31	110.44	106.71
14	A	839	CLA	C4A-NA-C1A	8.24	110.41	106.71
14	A	808	CLA	C4A-NA-C1A	8.17	110.38	106.71
14	A	836	CLA	C4A-NA-C1A	8.15	110.37	106.71
14	b	829	CLA	C4A-NA-C1A	8.10	110.35	106.71
19	l	202	SQD	O6-C1-C2	8.08	120.92	108.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	805	CLA	C4A-NA-C1A	8.08	110.34	106.71
14	A	805	CLA	C4A-NA-C1A	7.95	110.28	106.71
14	B	837	CLA	C4A-NA-C1A	7.92	110.27	106.71
14	B	843	CLA	C4A-NA-C1A	7.92	110.27	106.71
14	a	819	CLA	C4A-NA-C1A	7.91	110.26	106.71
13	a	801	CL0	CMD-C2D-C1D	7.88	138.59	124.71
13	A	801	CL0	CMD-C2D-C1D	7.87	138.59	124.71
14	A	806	CLA	C4A-NA-C1A	7.87	110.24	106.71
14	b	840	CLA	C4A-NA-C1A	7.86	110.24	106.71
14	b	842	CLA	C4A-NA-C1A	7.86	110.24	106.71
14	B	832	CLA	C4A-NA-C1A	7.86	110.24	106.71
14	a	829	CLA	CMB-C2B-C1B	-7.85	116.41	128.46
14	A	838	CLA	C4A-NA-C1A	7.82	110.22	106.71
14	A	827	CLA	C4A-NA-C1A	7.81	110.22	106.71
14	b	806	CLA	C4A-NA-C1A	7.80	110.21	106.71
14	L	1502	CLA	C4A-NA-C1A	7.71	110.17	106.71
14	A	828	CLA	C4A-NA-C1A	7.69	110.16	106.71
14	B	804	CLA	C4A-NA-C1A	7.69	110.16	106.71
14	a	840	CLA	C4A-NA-C1A	7.67	110.16	106.71
14	B	809	CLA	C4A-NA-C1A	7.66	110.15	106.71
14	X	1701	CLA	C4A-NA-C1A	7.66	110.15	106.71
14	b	817	CLA	C4A-NA-C1A	7.64	110.14	106.71
14	a	836	CLA	C4A-NA-C1A	7.63	110.14	106.71
14	b	809	CLA	C4A-NA-C1A	7.63	110.14	106.71
14	B	814	CLA	C4A-NA-C1A	7.56	110.11	106.71
14	x	1701	CLA	C4A-NA-C1A	7.56	110.11	106.71
14	a	815	CLA	C4A-NA-C1A	7.56	110.10	106.71
14	k	102	CLA	C4A-NA-C1A	7.55	110.10	106.71
14	B	830	CLA	C4A-NA-C1A	7.55	110.10	106.71
14	A	832	CLA	C4A-NA-C1A	7.54	110.10	106.71
14	A	815	CLA	C4A-NA-C1A	7.52	110.09	106.71
14	A	830	CLA	CMB-C2B-C1B	-7.49	116.94	128.46
14	B	824	CLA	C4A-NA-C1A	7.49	110.07	106.71
14	B	801	CLA	C4A-NA-C1A	7.48	110.07	106.71
14	A	804	CLA	C4A-NA-C1A	7.48	110.07	106.71
14	B	836	CLA	C4A-NA-C1A	7.46	110.06	106.71
14	j	101	CLA	C4A-NA-C1A	7.44	110.05	106.71
14	m	1201	CLA	C4A-NA-C1A	7.43	110.05	106.71
14	A	814	CLA	C4A-NA-C1A	7.42	110.04	106.71
14	F	202	CLA	C4A-NA-C1A	7.41	110.04	106.71
14	k	101	CLA	C4A-NA-C1A	7.41	110.04	106.71
14	A	816	CLA	C4A-NA-C1A	7.36	110.01	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	810	CLA	C4A-NA-C1A	7.34	110.00	106.71
14	B	805	CLA	C4A-NA-C1A	7.34	110.00	106.71
14	b	823	CLA	C4A-NA-C1A	7.34	110.00	106.71
14	B	802	CLA	C4A-NA-C1A	7.30	109.99	106.71
14	l	204	CLA	C4A-NA-C1A	7.30	109.99	106.71
14	A	843	CLA	C4A-NA-C1A	7.30	109.99	106.71
14	a	802	CLA	C4A-NA-C1A	7.27	109.98	106.71
14	a	827	CLA	C4A-NA-C1A	7.26	109.97	106.71
14	a	807	CLA	C4A-NA-C1A	7.26	109.97	106.71
14	B	807	CLA	C4A-NA-C1A	7.21	109.95	106.71
14	B	835	CLA	C4A-NA-C1A	7.18	109.93	106.71
14	b	828	CLA	C4A-NA-C1A	7.17	109.93	106.71
14	A	825	CLA	C4A-NA-C1A	7.15	109.92	106.71
14	A	817	CLA	C4A-NA-C1A	7.14	109.92	106.71
14	A	823	CLA	C4A-NA-C1A	7.12	109.91	106.71
14	J	101	CLA	C4A-NA-C1A	7.11	109.90	106.71
14	A	809	CLA	C4A-NA-C1A	7.10	109.90	106.71
14	A	820	CLA	C4A-NA-C1A	7.07	109.89	106.71
14	L	1503	CLA	C4A-NA-C1A	7.06	109.88	106.71
14	a	838	CLA	C4A-NA-C1A	7.04	109.87	106.71
14	b	824	CLA	C4A-NA-C1A	7.03	109.87	106.71
14	A	833	CLA	C4A-NA-C1A	7.03	109.87	106.71
14	a	813	CLA	C4A-NA-C1A	6.99	109.85	106.71
14	B	838	CLA	C4A-NA-C1A	6.94	109.83	106.71
14	b	831	CLA	C4A-NA-C1A	6.93	109.82	106.71
14	a	825	CLA	C4A-NA-C1A	6.92	109.82	106.71
14	A	803	CLA	C4A-NA-C1A	6.91	109.81	106.71
14	A	841	CLA	C4A-NA-C1A	6.90	109.81	106.71
13	a	801	CL0	C2C-C1C-NC	6.90	116.44	109.97
14	B	820	CLA	C4A-NA-C1A	6.90	109.81	106.71
13	A	801	CL0	C2C-C1C-NC	6.89	116.43	109.97
14	j	102	CLA	C4A-NA-C1A	6.89	109.81	106.71
14	a	814	CLA	C4A-NA-C1A	6.86	109.79	106.71
14	B	832	CLA	CMB-C2B-C1B	-6.86	117.92	128.46
14	B	810	CLA	C4A-NA-C1A	6.85	109.79	106.71
14	j	103	CLA	C4A-NA-C1A	6.85	109.78	106.71
14	K	101	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	b	830	CLA	C4A-NA-C1A	6.82	109.77	106.71
14	B	841	CLA	C4A-NA-C1A	6.81	109.77	106.71
14	B	826	CLA	C4A-NA-C1A	6.77	109.75	106.71
14	B	831	CLA	C4A-NA-C1A	6.77	109.75	106.71
14	a	834	CLA	C4A-NA-C1A	6.77	109.75	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	819	CLA	C4A-NA-C1A	6.77	109.75	106.71
14	b	832	CLA	CMB-C2B-C1B	-6.76	118.07	128.46
14	B	825	CLA	C4A-NA-C1A	6.76	109.75	106.71
14	b	814	CLA	C4A-NA-C1A	6.72	109.72	106.71
14	b	825	CLA	C4A-NA-C1A	6.72	109.72	106.71
14	A	824	CLA	C4A-NA-C1A	6.68	109.71	106.71
14	A	819	CLA	C4A-NA-C1A	6.68	109.71	106.71
14	A	837	CLA	C4A-NA-C1A	6.67	109.70	106.71
14	b	802	CLA	CMB-C2B-C1B	-6.67	118.22	128.46
14	a	821	CLA	C4A-NA-C1A	6.66	109.70	106.71
14	b	802	CLA	C4A-NA-C1A	6.65	109.70	106.71
13	a	801	CL0	C2D-C1D-ND	6.65	115.01	110.10
14	A	835	CLA	C4A-NA-C1A	6.65	109.70	106.71
14	b	826	CLA	C4A-NA-C1A	6.64	109.69	106.71
13	A	801	CL0	C4A-NA-C1A	6.64	109.69	106.71
13	a	801	CL0	C4A-NA-C1A	6.64	109.69	106.71
14	b	836	CLA	C4A-NA-C1A	6.64	109.69	106.71
14	B	812	CLA	C4A-NA-C1A	6.62	109.68	106.71
14	A	834	CLA	C4A-NA-C1A	6.62	109.68	106.71
14	B	840	CLA	C4A-NA-C1A	6.62	109.68	106.71
13	A	801	CL0	C2D-C1D-ND	6.62	114.98	110.10
14	b	812	CLA	CMB-C2B-C1B	-6.61	118.30	128.46
14	b	810	CLA	C4A-NA-C1A	6.60	109.67	106.71
14	a	803	CLA	C4A-NA-C1A	6.59	109.67	106.71
14	A	802	CLA	C4A-NA-C1A	6.58	109.66	106.71
14	a	837	CLA	C4A-NA-C1A	6.56	109.66	106.71
14	A	822	CLA	C4A-NA-C1A	6.54	109.65	106.71
14	b	837	CLA	C4A-NA-C1A	6.51	109.63	106.71
14	a	820	CLA	C4A-NA-C1A	6.51	109.63	106.71
14	b	838	CLA	C4A-NA-C1A	6.50	109.63	106.71
14	A	831	CLA	C4A-NA-C1A	6.49	109.62	106.71
14	b	812	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	X	1702	SQD	O6-C1-C2	6.45	118.37	108.30
14	a	835	CLA	C4A-NA-C1A	6.44	109.60	106.71
14	A	807	CLA	C4A-NA-C1A	6.43	109.60	106.71
14	b	834	CLA	C4A-NA-C1A	6.43	109.60	106.71
14	a	823	CLA	C4A-NA-C1A	6.43	109.60	106.71
14	a	820	CLA	CMB-C2B-C1B	-6.42	118.59	128.46
14	A	829	CLA	C4A-NA-C1A	6.42	109.59	106.71
14	K	102	CLA	C4A-NA-C1A	6.42	109.59	106.71
14	b	818	CLA	C4A-NA-C1A	6.40	109.58	106.71
14	B	806	CLA	CMB-C2B-C1B	-6.40	118.63	128.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	804	CLA	C4A-NA-C1A	6.39	109.58	106.71
14	L	1501	CLA	C4A-NA-C1A	6.38	109.58	106.71
14	A	826	CLA	C4A-NA-C1A	6.38	109.57	106.71
14	b	827	CLA	C4A-NA-C1A	6.38	109.57	106.71
14	A	818	CLA	C4A-NA-C1A	6.37	109.57	106.71
14	B	834	CLA	C4A-NA-C1A	6.35	109.56	106.71
14	F	204	CLA	C4A-NA-C1A	6.35	109.56	106.71
14	J	102	CLA	C4A-NA-C1A	6.35	109.56	106.71
14	a	828	CLA	C4A-NA-C1A	6.33	109.55	106.71
14	A	819	CLA	CMB-C2B-C1B	-6.33	118.74	128.46
14	B	801	CLA	CMB-C2B-C1B	-6.32	118.74	128.46
14	A	840	CLA	C4A-NA-C1A	6.26	109.52	106.71
14	a	816	CLA	C4A-NA-C1A	6.23	109.51	106.71
14	a	811	CLA	C4A-NA-C1A	6.23	109.51	106.71
14	f	203	CLA	C4A-NA-C1A	6.23	109.51	106.71
14	a	833	CLA	C4A-NA-C1A	6.21	109.50	106.71
14	a	818	CLA	C4A-NA-C1A	6.20	109.49	106.71
14	A	812	CLA	C4A-NA-C1A	6.19	109.49	106.71
14	l	203	CLA	C4A-NA-C1A	6.19	109.49	106.71
14	a	832	CLA	C4A-NA-C1A	6.18	109.48	106.71
14	a	829	CLA	C4A-NA-C1A	6.17	109.48	106.71
14	a	839	CLA	C4A-NA-C1A	6.15	109.47	106.71
14	B	828	CLA	C4A-NA-C1A	6.12	109.46	106.71
14	b	833	CLA	C4A-NA-C1A	6.10	109.45	106.71
14	B	818	CLA	C4A-NA-C1A	6.10	109.45	106.71
14	B	839	CLA	C4A-NA-C1A	6.08	109.44	106.71
14	a	806	CLA	C4A-NA-C1A	6.08	109.44	106.71
14	a	817	CLA	C4A-NA-C1A	6.07	109.44	106.71
14	b	835	CLA	C4A-NA-C1A	6.06	109.43	106.71
14	a	831	CLA	C4A-NA-C1A	6.05	109.42	106.71
14	b	815	CLA	C4A-NA-C1A	6.01	109.41	106.71
19	x	1702	SQD	O6-C1-C2	6.01	117.68	108.30
14	B	842	CLA	C4A-NA-C1A	5.99	109.40	106.71
14	B	834	CLA	CMB-C2B-C1B	-5.97	119.28	128.46
19	b	801	SQD	O9-S-C6	5.97	114.03	106.94
14	b	841	CLA	C4A-NA-C1A	5.95	109.38	106.71
14	B	833	CLA	C4A-NA-C1A	5.95	109.38	106.71
14	A	832	CLA	CMB-C2B-C1B	-5.92	119.37	128.46
14	b	843	CLA	CAC-C3C-C4C	-5.82	117.26	124.81
14	A	830	CLA	C4A-NA-C1A	5.81	109.32	106.71
13	a	801	CL0	C1C-C2C-C3C	-5.81	100.85	106.96
14	l	203	CLA	CMB-C2B-C1B	-5.76	119.61	128.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	814	CLA	CMB-C2B-C1B	-5.76	119.61	128.46
13	A	801	CL0	C1C-C2C-C3C	-5.76	100.91	106.96
14	b	839	CLA	C4A-NA-C1A	5.73	109.28	106.71
14	a	833	CLA	O2D-CGD-O1D	-5.73	112.64	123.84
14	a	827	CLA	CMB-C2B-C1B	-5.73	119.66	128.46
13	A	801	CL0	O2D-CGD-CBD	5.68	121.36	111.27
14	B	815	CLA	C4A-NA-C1A	5.68	109.26	106.71
13	a	801	CL0	O2D-CGD-CBD	5.68	121.36	111.27
14	a	818	CLA	CMB-C2B-C1B	-5.66	119.76	128.46
14	B	819	CLA	C4A-NA-C1A	5.60	109.22	106.71
14	b	802	CLA	CMB-C2B-C3B	5.60	135.16	124.68
14	B	813	CLA	C4A-NA-C1A	5.59	109.22	106.71
14	a	835	CLA	CMB-C2B-C1B	-5.59	119.88	128.46
14	f	201	CLA	C4A-NA-C1A	5.57	109.21	106.71
14	B	821	CLA	C4A-NA-C1A	5.56	109.21	106.71
14	b	820	CLA	C4A-NA-C1A	5.55	109.20	106.71
14	A	823	CLA	CMB-C2B-C1B	-5.54	119.95	128.46
14	B	825	CLA	CMB-C2B-C1B	-5.52	119.98	128.46
14	a	822	CLA	C4A-NA-C1A	5.51	109.19	106.71
14	b	805	CLA	CMB-C2B-C1B	-5.51	120.00	128.46
14	b	803	CLA	CMB-C2B-C1B	-5.50	120.01	128.46
14	A	803	CLA	CMB-C2B-C1B	-5.47	120.05	128.46
14	a	829	CLA	CMB-C2B-C3B	5.47	134.91	124.68
14	A	815	CLA	CMB-C2B-C1B	-5.46	120.08	128.46
14	B	837	CLA	CMB-C2B-C1B	-5.45	120.09	128.46
14	b	837	CLA	CMB-C2B-C1B	-5.44	120.11	128.46
14	b	821	CLA	CMB-C2B-C1B	-5.42	120.14	128.46
14	a	831	CLA	CMB-C2B-C1B	-5.41	120.15	128.46
14	a	823	CLA	CMB-C2B-C1B	-5.39	120.18	128.46
14	B	814	CLA	CMB-C2B-C1B	-5.38	120.19	128.46
14	B	812	CLA	CMB-C2B-C1B	-5.38	120.19	128.46
14	A	804	CLA	CMB-C2B-C1B	-5.36	120.22	128.46
14	b	816	CLA	CMB-C2B-C1B	-5.36	120.23	128.46
14	B	816	CLA	C4A-NA-C1A	5.35	109.11	106.71
14	b	805	CLA	C4A-NA-C1A	5.31	109.09	106.71
14	b	819	CLA	CMB-C2B-C1B	-5.28	120.35	128.46
14	B	828	CLA	CMB-C2B-C1B	-5.25	120.40	128.46
14	a	830	CLA	C4A-NA-C1A	5.22	109.05	106.71
14	A	813	CLA	C4A-NA-C1A	5.22	109.05	106.71
14	A	837	CLA	CMB-C2B-C1B	-5.17	120.52	128.46
14	b	821	CLA	C4A-NA-C1A	5.15	109.02	106.71
14	B	817	CLA	C4A-NA-C1A	5.15	109.02	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	814	CLA	CMB-C2B-C1B	-5.14	120.56	128.46
14	b	831	CLA	CMB-C2B-C1B	-5.14	120.57	128.46
14	b	830	CLA	CMB-C2B-C1B	-5.13	120.58	128.46
14	B	820	CLA	CMB-C2B-C1B	-5.12	120.60	128.46
14	A	825	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
14	a	803	CLA	CMB-C2B-C1B	-5.09	120.65	128.46
14	B	801	CLA	CMB-C2B-C3B	5.08	134.19	124.68
17	I	102	BCR	C15-C16-C17	-5.08	113.07	123.47
19	l	202	SQD	O8-S-C6	5.07	113.83	105.74
14	a	813	CLA	CMB-C2B-C1B	-5.06	120.68	128.46
14	b	826	CLA	CMB-C2B-C1B	-5.05	120.70	128.46
14	A	829	CLA	CMB-C2B-C1B	-5.04	120.71	128.46
14	a	821	CLA	CMB-C2B-C1B	-5.04	120.71	128.46
14	b	816	CLA	C4A-NA-C1A	5.02	108.96	106.71
14	b	832	CLA	C4A-NA-C1A	5.02	108.96	106.71
14	b	809	CLA	CMB-C2B-C1B	-4.97	120.82	128.46
14	B	829	CLA	CMB-C2B-C1B	-4.96	120.84	128.46
14	a	826	CLA	CMB-C2B-C1B	-4.94	120.86	128.46
14	A	832	CLA	CMB-C2B-C3B	4.93	133.91	124.68
14	b	807	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
14	A	806	CLA	CMB-C2B-C1B	-4.91	120.92	128.46
14	B	818	CLA	CMB-C2B-C1B	-4.91	120.92	128.46
13	A	801	CL0	C3D-C2D-C1D	-4.90	99.14	105.83
14	A	802	CLA	CMB-C2B-C1B	-4.90	120.93	128.46
13	a	801	CL0	C3D-C2D-C1D	-4.90	99.15	105.83
14	a	818	CLA	CMB-C2B-C3B	4.89	133.83	124.68
14	b	803	CLA	C4A-NA-C1A	4.89	108.90	106.71
13	A	801	CL0	O2A-CGA-O1A	-4.88	111.27	123.59
13	a	801	CL0	O2A-CGA-O1A	-4.87	111.31	123.59
14	A	836	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
19	b	801	SQD	O6-C1-C2	4.87	115.90	108.30
14	a	837	CLA	CMB-C2B-C1B	-4.86	120.99	128.46
14	b	805	CLA	CMB-C2B-C3B	4.86	133.77	124.68
14	f	203	CLA	CMB-C2B-C1B	-4.85	121.00	128.46
14	b	831	CLA	CMB-C2B-C3B	4.85	133.76	124.68
14	B	826	CLA	CMB-C2B-C1B	-4.85	121.02	128.46
14	B	828	CLA	CMB-C2B-C3B	4.83	133.72	124.68
14	B	811	CLA	O2D-CGD-O1D	-4.82	114.41	123.84
14	a	812	CLA	C4A-NA-C1A	4.82	108.87	106.71
14	l	203	CLA	CMB-C2B-C3B	4.81	133.68	124.68
14	B	842	CLA	CMB-C2B-C1B	-4.80	121.08	128.46
14	A	803	CLA	CMB-C2B-C3B	4.80	133.66	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	819	CLA	CMB-C2B-C3B	4.77	133.61	124.68
14	B	834	CLA	CMB-C2B-C3B	4.77	133.60	124.68
14	B	808	CLA	CMB-C2B-C1B	-4.76	121.14	128.46
14	a	820	CLA	CMB-C2B-C3B	4.76	133.58	124.68
19	b	801	SQD	O7-S-C6	4.75	112.59	106.94
14	B	810	CLA	CMB-C2B-C1B	-4.75	121.16	128.46
14	A	805	CLA	CMB-C2B-C1B	-4.74	121.17	128.46
14	B	836	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
14	L	1503	CLA	CMB-C2B-C1B	-4.74	121.19	128.46
14	A	814	CLA	CMB-C2B-C3B	4.73	133.54	124.68
14	A	838	CLA	CMB-C2B-C1B	-4.73	121.19	128.46
14	b	803	CLA	CMB-C2B-C3B	4.71	133.49	124.68
14	A	821	CLA	C4A-NA-C1A	4.70	108.82	106.71
14	A	815	CLA	CMB-C2B-C3B	4.70	133.47	124.68
14	B	806	CLA	CMB-C2B-C3B	4.70	133.47	124.68
14	b	827	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
13	a	801	CL0	C1D-ND-C4D	-4.66	103.03	106.33
14	A	830	CLA	CMB-C2B-C3B	4.66	133.39	124.68
19	x	1702	SQD	O7-S-C6	4.65	112.47	106.94
14	B	816	CLA	CMB-C2B-C1B	-4.65	121.31	128.46
14	a	827	CLA	CMB-C2B-C3B	4.65	133.37	124.68
13	A	801	CL0	C1D-ND-C4D	-4.65	103.03	106.33
13	A	801	CL0	O2A-C1-C2	4.64	120.83	108.64
13	a	801	CL0	O2A-C1-C2	4.64	120.83	108.64
14	a	802	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
14	a	828	CLA	CMB-C2B-C1B	-4.63	121.34	128.46
14	B	825	CLA	CMB-C2B-C3B	4.63	133.34	124.68
14	b	828	CLA	CMB-C2B-C1B	-4.63	121.35	128.46
14	B	837	CLA	CMB-C2B-C3B	4.62	133.33	124.68
14	B	830	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
14	b	843	CLA	CAC-C3C-C2C	4.61	135.41	127.53
14	b	821	CLA	CMB-C2B-C3B	4.60	133.29	124.68
14	A	842	CLA	CMB-C2B-C1B	-4.59	121.41	128.46
14	A	826	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
14	b	827	CLA	CMB-C2B-C3B	4.57	133.22	124.68
14	B	840	CLA	CMB-C2B-C1B	-4.56	121.45	128.46
14	B	831	CLA	CMB-C2B-C1B	-4.56	121.46	128.46
14	A	837	CLA	CMB-C2B-C3B	4.55	133.20	124.68
14	A	804	CLA	CMB-C2B-C3B	4.55	133.18	124.68
14	b	837	CLA	CMB-C2B-C3B	4.55	133.18	124.68
14	b	829	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
14	B	827	CLA	CMB-C2B-C1B	-4.52	121.51	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	809	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
14	b	840	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
14	L	1502	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
14	B	818	CLA	CMB-C2B-C3B	4.49	133.09	124.68
14	b	807	CLA	CMB-C2B-C3B	4.49	133.08	124.68
14	b	819	CLA	CMB-C2B-C3B	4.49	133.07	124.68
14	b	825	CLA	CMB-C2B-C1B	-4.48	121.57	128.46
17	B	849	BCR	C15-C16-C17	-4.48	114.30	123.47
14	B	814	CLA	O2D-CGD-O1D	-4.48	115.09	123.84
14	B	812	CLA	CMB-C2B-C3B	4.48	133.05	124.68
14	b	836	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
14	a	832	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
14	a	835	CLA	CMB-C2B-C3B	4.46	133.02	124.68
14	b	818	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
14	b	804	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
13	a	801	CL0	CHD-C1D-ND	-4.42	120.39	124.45
14	A	823	CLA	CMB-C2B-C3B	4.42	132.95	124.68
14	b	810	CLA	CMB-C2B-C1B	-4.41	121.68	128.46
14	b	816	CLA	CMB-C2B-C3B	4.41	132.93	124.68
14	K	102	CLA	CMB-C2B-C1B	-4.41	121.68	128.46
14	b	820	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
14	A	808	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
14	B	822	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
14	B	809	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
13	A	801	CL0	CHD-C1D-ND	-4.39	120.42	124.45
14	a	809	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
14	a	839	CLA	CMB-C2B-C1B	-4.37	121.74	128.46
14	A	822	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
14	a	833	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
14	B	814	CLA	CMB-C2B-C3B	4.37	132.85	124.68
19	X	1702	SQD	O47-C7-C8	4.37	120.91	111.50
14	a	823	CLA	CMB-C2B-C3B	4.37	132.84	124.68
14	b	822	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
14	a	837	CLA	O2D-CGD-CBD	4.36	119.02	111.27
14	A	825	CLA	CMB-C2B-C3B	4.36	132.83	124.68
14	B	817	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
14	A	828	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
14	m	1201	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
14	b	830	CLA	CMB-C2B-C3B	4.35	132.82	124.68
18	i	103	LHG	O4-P-O5	4.34	133.72	112.24
14	a	837	CLA	O2D-CGD-O1D	-4.34	115.36	123.84
14	b	832	CLA	CMB-C2B-C3B	4.33	132.78	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	806	CLA	CMB-C2B-C3B	4.32	132.76	124.68
14	b	834	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
14	a	812	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
14	a	819	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
14	a	821	CLA	CMB-C2B-C3B	4.31	132.74	124.68
14	F	204	CLA	CMB-C2B-C1B	-4.30	121.85	128.46
18	a	850	LHG	O4-P-O5	4.29	133.47	112.24
14	b	843	CLA	CMC-C2C-C1C	-4.29	118.50	125.04
14	a	814	CLA	CMB-C2B-C3B	4.28	132.68	124.68
14	b	813	CLA	C4A-NA-C1A	4.28	108.63	106.71
14	A	829	CLA	CMB-C2B-C3B	4.27	132.66	124.68
14	a	805	CLA	CMB-C2B-C1B	-4.27	121.91	128.46
14	B	826	CLA	CMB-C2B-C3B	4.27	132.66	124.68
14	B	824	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
18	A	852	LHG	O4-P-O5	4.26	133.30	112.24
14	B	812	CLA	CAC-C3C-C4C	4.25	130.32	124.81
14	b	826	CLA	CMB-C2B-C3B	4.25	132.62	124.68
14	a	831	CLA	CMB-C2B-C3B	4.24	132.62	124.68
19	X	1702	SQD	O7-S-C6	4.24	111.98	106.94
14	b	815	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
14	A	836	CLA	CMB-C2B-C3B	4.23	132.59	124.68
14	B	820	CLA	O2D-CGD-O1D	-4.22	115.59	123.84
14	b	833	CLA	CMB-C2B-C1B	-4.21	122.00	128.46
14	A	827	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
14	a	803	CLA	CMB-C2B-C3B	4.20	132.53	124.68
14	B	840	CLA	CMB-C2B-C3B	4.20	132.53	124.68
14	B	811	CLA	O2D-CGD-CBD	4.19	118.72	111.27
19	l	202	SQD	O9-S-O7	-4.19	99.46	113.95
14	A	838	CLA	O2D-CGD-O1D	-4.18	115.66	123.84
14	a	837	CLA	CMB-C2B-C3B	4.18	132.50	124.68
14	l	205	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
14	a	804	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
14	b	814	CLA	O2D-CGD-O1D	-4.18	115.67	123.84
14	B	836	CLA	CMB-C2B-C3B	4.17	132.48	124.68
18	F	201	LHG	O4-P-O5	4.14	132.69	112.24
14	a	813	CLA	CMB-C2B-C3B	4.13	132.41	124.68
14	A	810	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
14	a	811	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
14	A	831	CLA	CHD-C1D-ND	-4.13	120.66	124.45
14	l	204	CLA	CHD-C1D-ND	-4.12	120.67	124.45
14	A	805	CLA	CMB-C2B-C3B	4.12	132.39	124.68
14	b	824	CLA	CMB-C2B-C1B	-4.12	122.13	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	808	CLA	O2D-CGD-O1D	-4.11	115.80	123.84
14	B	827	CLA	CMB-C2B-C3B	4.11	132.37	124.68
14	b	813	CLA	CAA-C2A-C3A	-4.10	101.54	112.78
17	b	848	BCR	C15-C16-C17	-4.09	115.09	123.47
14	X	1701	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
14	a	826	CLA	CMB-C2B-C3B	4.09	132.33	124.68
14	b	812	CLA	CMB-C2B-C3B	4.09	132.33	124.68
19	l	202	SQD	O9-S-C6	4.09	111.80	106.94
14	J	102	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
14	B	816	CLA	CMB-C2B-C3B	4.07	132.28	124.68
14	a	828	CLA	CMB-C2B-C3B	4.06	132.27	124.68
14	A	841	CLA	O2D-CGD-O1D	-4.06	115.91	123.84
14	B	833	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
14	f	203	CLA	CMB-C2B-C3B	4.05	132.26	124.68
14	B	832	CLA	C2D-C1D-ND	-4.05	107.12	110.10
14	a	824	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
19	b	801	SQD	O9-S-O7	-4.04	99.97	113.95
14	b	825	CLA	CMB-C2B-C3B	4.03	132.22	124.68
14	a	816	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
14	B	829	CLA	CMB-C2B-C3B	4.03	132.21	124.68
14	b	813	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
14	a	833	CLA	O2D-CGD-CBD	4.01	118.40	111.27
14	b	836	CLA	CAA-C2A-C3A	-4.01	101.80	112.78
14	a	841	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
14	b	809	CLA	CMB-C2B-C3B	4.00	132.16	124.68
14	A	818	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
14	B	842	CLA	CMB-C2B-C3B	3.99	132.15	124.68
14	A	834	CLA	CAC-C3C-C4C	3.99	129.98	124.81
14	b	840	CLA	CMB-C2B-C3B	3.99	132.13	124.68
14	B	808	CLA	CMB-C2B-C3B	3.99	132.13	124.68
14	b	843	CLA	CMC-C2C-C3C	3.98	136.92	126.12
17	B	846	BCR	C3-C4-C5	-3.98	106.97	114.08
14	L	1503	CLA	CMB-C2B-C3B	3.97	132.10	124.68
19	x	1702	SQD	O9-S-O7	-3.97	100.22	113.95
14	b	817	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
14	A	838	CLA	CMB-C2B-C3B	3.97	132.10	124.68
14	A	834	CLA	O2D-CGD-O1D	-3.96	116.09	123.84
14	B	810	CLA	CMB-C2B-C3B	3.94	132.05	124.68
14	l	204	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
14	b	829	CLA	CMB-C2B-C3B	3.93	132.02	124.68
14	A	813	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
14	l	204	CLA	O2D-CGD-CBD	3.92	118.24	111.27

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	813	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
14	b	806	CLA	O2D-CGD-O1D	-3.92	116.18	123.84
14	B	807	CLA	CMB-C2B-C1B	-3.92	122.45	128.46
14	b	808	CLA	CHB-C4A-NA	3.91	129.92	124.51
14	L	1503	CLA	CHD-C1D-ND	-3.90	120.87	124.45
19	x	1702	SQD	O47-C7-C8	3.90	119.91	111.50
14	a	839	CLA	CMB-C2B-C3B	3.90	131.97	124.68
14	A	807	CLA	CMB-C2B-C1B	-3.90	122.48	128.46
14	B	819	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
14	A	837	CLA	CAC-C3C-C4C	3.89	129.86	124.81
14	A	821	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
14	a	832	CLA	CMB-C2B-C3B	3.87	131.92	124.68
14	b	832	CLA	C2D-C1D-ND	-3.87	107.25	110.10
14	A	830	CLA	O2D-CGD-O1D	-3.87	116.28	123.84
14	a	817	CLA	O2D-CGD-O1D	-3.86	116.28	123.84
14	A	826	CLA	CMB-C2B-C3B	3.86	131.90	124.68
13	A	801	CL0	O2A-CGA-CBA	3.86	124.02	111.91
14	B	836	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
13	a	801	CL0	O2A-CGA-CBA	3.85	124.00	111.91
14	b	810	CLA	CMB-C2B-C3B	3.85	131.89	124.68
14	b	814	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
19	l	202	SQD	O7-S-C6	3.84	111.50	106.94
14	A	828	CLA	CMB-C2B-C3B	3.84	131.86	124.68
17	A	849	BCR	C7-C8-C9	-3.84	120.44	126.23
14	b	818	CLA	CMB-C2B-C3B	3.83	131.85	124.68
14	a	806	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
14	K	102	CLA	CMB-C2B-C3B	3.82	131.83	124.68
14	A	809	CLA	CMB-C2B-C3B	3.82	131.83	124.68
19	X	1702	SQD	O9-S-O7	-3.81	100.76	113.95
19	X	1702	SQD	O9-S-C6	3.81	111.46	106.94
14	a	810	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
17	J	103	BCR	C2-C1-C6	3.80	116.34	110.48
14	A	813	CLA	CAC-C3C-C4C	3.80	129.75	124.81
14	b	832	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
14	b	808	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
14	b	804	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
14	f	201	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
14	A	822	CLA	CMB-C2B-C3B	3.79	131.77	124.68
14	b	836	CLA	CMB-C2B-C3B	3.79	131.76	124.68
14	b	836	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
14	b	842	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
14	a	802	CLA	CMB-C2B-C3B	3.76	131.72	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	817	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
14	A	834	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
14	b	828	CLA	CMB-C2B-C3B	3.75	131.70	124.68
17	b	849	BCR	C15-C16-C17	-3.74	115.81	123.47
14	B	820	CLA	CMB-C2B-C3B	3.74	131.68	124.68
14	a	817	CLA	O2D-CGD-CBD	3.74	117.91	111.27
14	B	806	CLA	CHD-C1D-ND	-3.74	121.02	124.45
17	l	207	BCR	C24-C23-C22	-3.74	120.59	126.23
14	A	839	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
14	b	810	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
14	B	811	CLA	CHB-C4A-NA	3.71	129.64	124.51
14	L	1502	CLA	CHD-C1D-ND	-3.71	121.05	124.45
14	a	807	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
17	l	206	BCR	C2-C1-C6	3.70	116.18	110.48
14	B	805	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
14	a	833	CLA	C2D-C1D-ND	-3.70	107.38	110.10
14	F	202	CLA	CHD-C1D-ND	-3.70	121.06	124.45
14	b	838	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
14	j	102	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
18	A	853	LHG	O4-P-O5	3.68	130.45	112.24
14	B	802	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
14	a	808	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
14	B	813	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
14	B	840	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
19	x	1702	SQD	O9-S-C6	3.66	111.28	106.94
17	J	105	BCR	C11-C10-C9	-3.66	122.09	127.31
14	L	1502	CLA	CMB-C2B-C3B	3.65	131.50	124.68
14	A	835	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
14	a	824	CLA	CMB-C2B-C3B	3.65	131.50	124.68
14	A	837	CLA	O2D-CGD-O1D	-3.64	116.71	123.84
14	A	820	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
14	a	809	CLA	CMB-C2B-C3B	3.64	131.49	124.68
14	A	843	CLA	CAA-C2A-C3A	-3.64	102.82	112.78
14	k	102	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
14	L	1501	CLA	CHD-C1D-ND	-3.63	121.12	124.45
14	a	807	CLA	O2D-CGD-O1D	-3.62	116.75	123.84
14	B	805	CLA	O2D-CGD-O1D	-3.62	116.77	123.84
14	B	826	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
14	b	834	CLA	CMB-C2B-C3B	3.59	131.40	124.68
14	l	204	CLA	CMB-C2B-C3B	3.59	131.39	124.68
14	B	808	CLA	O2D-CGD-CBD	3.59	117.64	111.27
14	b	828	CLA	O2D-CGD-O1D	-3.58	116.84	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	805	CLA	CMB-C2B-C3B	3.57	131.36	124.68
14	A	802	CLA	CMB-C2B-C3B	3.57	131.36	124.68
14	B	828	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
14	b	820	CLA	CMB-C2B-C3B	3.57	131.35	124.68
14	a	841	CLA	CMB-C2B-C3B	3.56	131.34	124.68
17	b	849	BCR	C2-C1-C6	3.55	115.95	110.48
14	B	820	CLA	O2D-CGD-CBD	3.55	117.57	111.27
14	b	815	CLA	CMB-C2B-C3B	3.55	131.31	124.68
14	B	824	CLA	CMB-C2B-C3B	3.55	131.31	124.68
14	B	832	CLA	CMB-C2B-C3B	3.55	131.31	124.68
14	b	815	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
14	A	827	CLA	CMB-C2B-C3B	3.54	131.30	124.68
20	b	851	LMG	O6-C1-O1	-3.54	101.59	109.97
14	a	818	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
14	a	817	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
14	a	824	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
14	B	831	CLA	CMB-C2B-C3B	3.53	131.28	124.68
14	a	840	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
14	a	830	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
14	a	808	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
14	a	802	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
14	l	205	CLA	CMB-C2B-C3B	3.50	131.22	124.68
14	m	1201	CLA	CMB-C2B-C3B	3.50	131.22	124.68
14	B	836	CLA	CAA-C2A-C3A	-3.50	103.20	112.78
17	j	104	BCR	C2-C1-C6	3.50	115.86	110.48
14	B	827	CLA	CHB-C4A-NA	3.49	129.34	124.51
14	A	808	CLA	CMB-C2B-C3B	3.49	131.20	124.68
14	a	815	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
14	B	834	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
14	B	807	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
14	b	818	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
14	b	807	CLA	CHD-C1D-ND	-3.48	121.25	124.45
14	A	831	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
14	J	101	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
14	a	804	CLA	CMB-C2B-C3B	3.48	131.19	124.68
14	A	842	CLA	CMB-C2B-C3B	3.47	131.18	124.68
14	b	823	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
14	F	204	CLA	CMB-C2B-C3B	3.47	131.17	124.68
14	A	842	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
14	B	831	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
17	b	849	BCR	C15-C14-C13	-3.46	122.36	127.31
14	A	816	CLA	CMB-C2B-C1B	-3.46	123.14	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	k	101	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
17	j	106	BCR	C11-C10-C9	-3.46	122.37	127.31
14	a	828	CLA	O2D-CGD-O1D	-3.46	117.07	123.84
14	a	833	CLA	CHB-C4A-NA	3.46	129.30	124.51
14	A	818	CLA	CMB-C2B-C3B	3.46	131.15	124.68
14	B	842	CLA	O2D-CGD-O1D	-3.45	117.08	123.84
14	a	819	CLA	CMB-C2B-C3B	3.45	131.13	124.68
17	b	848	BCR	C20-C21-C22	-3.45	122.39	127.31
14	b	811	CLA	CBA-CAA-C2A	3.45	124.04	113.86
14	B	830	CLA	CMB-C2B-C3B	3.45	131.13	124.68
14	B	815	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
14	X	1701	CLA	CMB-C2B-C3B	3.45	131.13	124.68
14	b	824	CLA	CMB-C2B-C3B	3.45	131.13	124.68
14	A	810	CLA	CMB-C2B-C3B	3.44	131.12	124.68
14	a	836	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
14	b	841	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
14	A	843	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
14	A	832	CLA	CHB-C4A-NA	3.43	129.26	124.51
19	l	202	SQD	C1-C2-C3	-3.43	102.85	110.00
15	b	844	PQN	C14-C13-C15	3.43	121.04	115.27
17	A	847	BCR	C2-C1-C6	3.43	115.76	110.48
14	a	811	CLA	O2D-CGD-O1D	-3.42	117.14	123.84
14	b	828	CLA	CAA-C2A-C1A	-3.42	100.76	111.97
14	B	836	CLA	CHB-C4A-NA	3.42	129.24	124.51
14	B	817	CLA	CMB-C2B-C3B	3.42	131.08	124.68
14	b	834	CLA	O2D-CGD-O1D	-3.42	117.16	123.84
14	b	805	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
17	B	849	BCR	C2-C1-C6	3.40	115.71	110.48
14	A	828	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
14	l	204	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
14	b	828	CLA	CAA-C2A-C3A	-3.39	103.49	112.78
14	b	841	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
14	A	808	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
14	B	801	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
15	B	844	PQN	C11-C12-C13	-3.38	121.16	126.79
14	a	803	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
14	a	816	CLA	CMB-C2B-C3B	3.38	131.00	124.68
14	a	838	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
14	B	812	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
17	a	844	BCR	C15-C16-C17	-3.37	116.58	123.47
17	A	848	BCR	C2-C1-C6	3.37	115.66	110.48
14	B	809	CLA	CMB-C2B-C3B	3.37	130.98	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	811	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
17	l	207	BCR	C31-C1-C6	3.36	115.75	110.30
14	b	840	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
14	a	807	CLA	CMB-C2B-C3B	3.36	130.96	124.68
14	B	806	CLA	CAC-C3C-C4C	3.35	129.16	124.81
14	B	806	CLA	C3C-C4C-NC	-3.35	106.82	110.57
14	J	102	CLA	CMB-C2B-C3B	3.35	130.94	124.68
14	a	836	CLA	CMB-C2B-C1B	-3.34	123.32	128.46
14	J	102	CLA	CAA-C2A-C3A	-3.34	108.30	116.10
14	A	841	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
14	j	102	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
15	b	844	PQN	C11-C12-C13	-3.34	121.24	126.79
15	a	842	PQN	C14-C13-C15	3.34	120.88	115.27
17	j	106	BCR	C7-C8-C9	-3.33	121.20	126.23
14	b	812	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
14	F	202	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
14	B	819	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
14	A	805	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
17	b	848	BCR	C28-C27-C26	-3.32	108.15	114.08
14	B	805	CLA	CMB-C2B-C3B	3.31	130.88	124.68
14	a	836	CLA	CMB-C2B-C3B	3.31	130.88	124.68
14	B	816	CLA	CBC-CAC-C3C	3.31	121.56	112.43
14	A	826	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
14	A	803	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
14	b	803	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
17	i	102	BCR	C15-C14-C13	-3.31	122.59	127.31
14	A	833	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
14	B	839	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
14	j	103	CLA	CAA-C2A-C3A	-3.29	108.42	116.10
14	a	838	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
17	a	846	BCR	C2-C1-C6	3.29	115.54	110.48
14	A	804	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
14	b	836	CLA	CHB-C4A-NA	3.28	129.05	124.51
14	B	833	CLA	CMB-C2B-C3B	3.28	130.82	124.68
14	b	832	CLA	O2D-CGD-CBD	3.28	117.10	111.27
14	f	203	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
14	L	1503	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
14	A	837	CLA	CBC-CAC-C3C	3.28	121.47	112.43
14	B	823	CLA	CHB-C4A-NA	3.28	129.04	124.51
14	B	807	CLA	CMB-C2B-C3B	3.28	130.81	124.68
14	l	205	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
14	b	820	CLA	O2D-CGD-O1D	-3.27	117.45	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	843	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
17	l	206	BCR	C39-C30-C25	3.26	115.59	110.30
14	a	825	CLA	C2D-C1D-ND	-3.26	107.70	110.10
14	A	812	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
14	l	203	CLA	CAC-C3C-C4C	3.26	129.04	124.81
14	B	841	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
14	A	811	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
17	b	847	BCR	C2-C1-C6	3.26	115.49	110.48
14	B	802	CLA	CMB-C2B-C3B	3.25	130.76	124.68
14	b	807	CLA	CAC-C3C-C4C	3.25	129.03	124.81
17	j	106	BCR	C2-C1-C6	3.25	115.48	110.48
14	b	807	CLA	C1B-CHB-C4A	-3.25	123.69	130.12
14	B	838	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
14	b	817	CLA	CMB-C2B-C3B	3.24	130.73	124.68
14	B	829	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
14	b	817	CLA	CHB-C4A-NA	3.24	128.99	124.51
17	f	204	BCR	C11-C10-C9	-3.23	122.70	127.31
14	A	811	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
14	B	819	CLA	CMB-C2B-C3B	3.23	130.72	124.68
17	B	848	BCR	C28-C27-C26	-3.22	108.33	114.08
19	b	801	SQD	C4-C3-C2	3.22	116.44	110.82
14	a	824	CLA	C2A-C1A-CHA	3.22	129.48	123.86
14	b	811	CLA	CHB-C4A-NA	3.22	128.96	124.51
19	l	202	SQD	O5-C5-C4	3.22	115.53	109.69
14	a	812	CLA	CMB-C2B-C3B	3.21	130.69	124.68
14	A	805	CLA	CHB-C4A-NA	3.21	128.96	124.51
17	l	201	BCR	C31-C1-C6	3.21	115.50	110.30
14	K	101	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
14	J	101	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
19	x	1702	SQD	C4-C3-C2	3.20	116.41	110.82
14	b	803	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
14	a	820	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
17	l	207	BCR	C16-C15-C14	-3.20	116.92	123.47
14	j	101	CLA	CAA-C2A-C3A	-3.20	104.02	112.78
14	b	808	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
14	A	831	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
14	B	815	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
14	B	835	CLA	CAA-C2A-C3A	-3.19	104.05	112.78
14	b	821	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
14	b	814	CLA	CMB-C2B-C3B	3.18	130.63	124.68
14	j	101	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
14	b	807	CLA	CHB-C4A-NA	3.17	128.90	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	J	101	CLA	CHB-C4A-NA	3.17	128.90	124.51
14	a	840	CLA	CHB-C4A-NA	3.17	128.90	124.51
14	a	810	CLA	CHB-C4A-NA	3.17	128.89	124.51
14	b	811	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
14	A	825	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
14	B	816	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
14	a	835	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
17	B	846	BCR	C2-C1-C6	3.15	115.34	110.48
19	b	801	SQD	O5-C5-C4	3.15	115.42	109.69
14	a	829	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
14	A	806	CLA	CHB-C4A-NA	3.15	128.86	124.51
14	B	811	CLA	CBA-CAA-C2A	3.14	123.13	113.86
17	i	101	BCR	C31-C1-C6	3.14	115.39	110.30
14	A	813	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
14	A	824	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
17	m	1202	BCR	C15-C16-C17	-3.13	117.07	123.47
14	B	808	CLA	CHB-C4A-NA	3.13	128.83	124.51
17	L	1504	BCR	C2-C1-C6	3.12	115.29	110.48
14	B	843	CLA	CHB-C4A-NA	3.12	128.83	124.51
14	a	822	CLA	CHD-C1D-ND	-3.12	121.59	124.45
14	B	824	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
14	a	806	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
14	A	831	CLA	CMB-C2B-C3B	3.11	130.50	124.68
14	b	812	CLA	CAC-C3C-C4C	3.11	128.85	124.81
14	A	807	CLA	CMB-C2B-C3B	3.11	130.50	124.68
14	a	804	CLA	CHB-C4A-NA	3.11	128.81	124.51
17	b	846	BCR	C15-C16-C17	-3.11	117.10	123.47
14	b	833	CLA	CMB-C2B-C3B	3.11	130.49	124.68
14	a	825	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
17	B	849	BCR	C3-C4-C5	-3.10	108.53	114.08
14	a	841	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
14	A	814	CLA	CHB-C4A-NA	3.10	128.80	124.51
14	A	811	CLA	CHD-C1D-ND	-3.10	121.61	124.45
14	b	816	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
17	A	848	BCR	C3-C4-C5	-3.10	108.54	114.08
14	a	819	CLA	CHB-C4A-NA	3.10	128.80	124.51
14	a	814	CLA	CHB-C4A-NA	3.10	128.80	124.51
14	A	827	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
17	A	848	BCR	C40-C30-C25	3.10	115.32	110.30
14	j	103	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
14	b	838	CLA	CMB-C2B-C3B	3.09	130.47	124.68
14	j	102	CLA	CMB-C2B-C3B	3.09	130.46	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	840	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
14	a	806	CLA	CMB-C2B-C3B	3.09	130.46	124.68
20	b	851	LMG	O1-C7-C8	-3.09	103.44	110.90
14	a	834	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
20	b	851	LMG	O1-C1-C2	-3.09	103.48	108.30
14	b	807	CLA	O1D-CGD-CBD	3.09	130.80	124.48
14	A	812	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
14	a	818	CLA	O2D-CGD-CBD	3.09	116.75	111.27
14	b	841	CLA	CMB-C2B-C3B	3.09	130.45	124.68
14	b	813	CLA	C3B-C4B-NB	-3.09	105.22	109.21
14	b	815	CLA	CBC-CAC-C3C	3.08	120.93	112.43
14	A	815	CLA	CHB-C4A-NA	3.08	128.77	124.51
14	B	838	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
14	B	829	CLA	CHB-C4A-NA	3.08	128.77	124.51
14	b	818	CLA	CHB-C4A-NA	3.08	128.77	124.51
14	k	102	CLA	CHB-C4A-NA	3.08	128.76	124.51
14	a	821	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
14	b	811	CLA	O2A-CGA-O1A	-3.07	115.84	123.59
14	A	813	CLA	CMB-C2B-C3B	3.07	130.42	124.68
14	A	820	CLA	CHB-C4A-NA	3.07	128.75	124.51
17	l	206	BCR	C15-C14-C13	-3.06	122.94	127.31
14	B	808	CLA	O2A-C1-C2	-3.06	100.59	108.64
14	a	818	CLA	C1-C2-C3	-3.06	120.75	126.04
14	B	818	CLA	CHD-C1D-ND	-3.06	121.64	124.45
14	a	833	CLA	CHD-C1D-ND	-3.06	121.64	124.45
14	b	823	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
14	A	822	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
14	B	806	CLA	CHC-C1C-NC	3.05	128.83	124.20
14	B	837	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
14	A	829	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
14	a	824	CLA	O2D-CGD-CBD	3.05	116.68	111.27
14	B	830	CLA	O2A-CGA-O1A	-3.05	115.91	123.59
14	a	810	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
14	a	813	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
14	a	833	CLA	CMB-C2B-C3B	3.04	130.37	124.68
14	b	828	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
14	A	834	CLA	CMB-C2B-C3B	3.04	130.36	124.68
17	L	1504	BCR	C29-C30-C25	3.04	115.16	110.48
14	a	816	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
14	a	804	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
14	B	804	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
14	B	821	CLA	O2D-CGD-O1D	-3.03	117.91	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	817	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
14	B	823	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
14	a	815	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
14	b	813	CLA	CMB-C2B-C3B	3.03	130.34	124.68
14	a	810	CLA	CMB-C2B-C3B	3.03	130.34	124.68
14	a	819	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
20	B	851	LMG	O1-C7-C8	-3.02	103.60	110.90
14	f	201	CLA	CMB-C2B-C3B	3.02	130.33	124.68
14	a	814	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
14	B	808	CLA	C3C-C4C-NC	-3.01	107.19	110.57
14	B	828	CLA	C2D-C1D-ND	-3.01	107.88	110.10
14	a	830	CLA	CMB-C2B-C3B	3.01	130.31	124.68
14	b	824	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
14	a	808	CLA	CMB-C2B-C3B	3.01	130.31	124.68
14	B	818	CLA	O1D-CGD-CBD	3.01	130.63	124.48
14	b	835	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
14	K	102	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
14	F	202	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
14	l	203	CLA	CAA-C2A-C3A	-3.00	104.56	112.78
14	B	832	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
14	B	815	CLA	O2D-CGD-CBD	3.00	116.60	111.27
14	B	835	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
14	J	101	CLA	CMB-C2B-C3B	2.99	130.28	124.68
14	B	839	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
17	a	846	BCR	C3-C4-C5	-2.99	108.73	114.08
14	a	817	CLA	CMB-C2B-C3B	2.99	130.28	124.68
14	b	811	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
13	a	801	CL0	CMC-C2C-C1C	2.99	129.59	125.04
14	B	823	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
14	B	802	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
14	a	833	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
14	k	101	CLA	CHB-C4A-NA	2.98	128.64	124.51
14	B	818	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
14	A	808	CLA	CHB-C4A-NA	2.98	128.63	124.51
14	B	840	CLA	CHB-C4A-NA	2.98	128.63	124.51
14	a	803	CLA	CHB-C4A-NA	2.98	128.63	124.51
13	A	801	CL0	CMC-C2C-C1C	2.98	129.57	125.04
14	B	811	CLA	O2A-CGA-O1A	-2.98	116.08	123.59
14	A	820	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
14	F	202	CLA	CHB-C4A-NA	2.97	128.62	124.51
14	A	840	CLA	CMB-C2B-C1B	-2.97	123.91	128.46
13	A	801	CL0	CHB-C4A-NA	2.96	128.61	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	834	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
19	l	202	SQD	C4-C3-C2	2.96	115.99	110.82
17	l	206	BCR	C11-C10-C9	-2.96	123.09	127.31
14	A	808	CLA	O2D-CGD-CBD	2.96	116.53	111.27
14	A	832	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
14	A	823	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
14	B	825	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
19	x	1702	SQD	O5-C5-C4	2.95	115.06	109.69
17	j	105	BCR	C15-C16-C17	-2.95	117.42	123.47
14	a	834	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
14	B	812	CLA	CAC-C3C-C2C	-2.95	122.48	127.53
14	a	824	CLA	CHB-C4A-NA	2.95	128.60	124.51
14	B	810	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
14	B	830	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
20	B	851	LMG	O6-C1-O1	-2.95	102.98	109.97
14	B	808	CLA	CHD-C1D-ND	-2.95	121.74	124.45
14	b	808	CLA	O2D-CGD-CBD	2.95	116.50	111.27
14	l	205	CLA	O1D-CGD-CBD	2.95	130.51	124.48
14	A	824	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
17	A	848	BCR	C15-C14-C13	-2.94	123.11	127.31
14	b	824	CLA	CHB-C4A-NA	2.94	128.58	124.51
17	A	846	BCR	C15-C14-C13	-2.94	123.11	127.31
14	b	838	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
14	B	801	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
14	b	843	CLA	CHB-C4A-NA	2.94	128.58	124.51
14	L	1502	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
17	B	846	BCR	C28-C27-C26	-2.94	108.83	114.08
13	a	801	CL0	CHB-C4A-NA	2.94	128.57	124.51
14	L	1502	CLA	O2D-CGD-CBD	2.94	116.49	111.27
14	b	826	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
14	b	808	CLA	CMB-C2B-C3B	2.93	130.17	124.68
14	X	1701	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
14	A	830	CLA	C1D-ND-C4D	2.93	108.42	106.33
14	A	820	CLA	CMB-C2B-C3B	2.93	130.16	124.68
14	B	828	CLA	CAA-C2A-C3A	-2.93	104.77	112.78
14	A	828	CLA	CAA-CBA-CGA	-2.92	104.71	113.25
17	a	848	BCR	C15-C16-C17	-2.92	117.49	123.47
14	a	826	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
14	A	824	CLA	CMB-C2B-C3B	2.92	130.14	124.68
17	a	846	BCR	C40-C30-C25	2.92	115.03	110.30
14	x	1701	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
14	a	822	CLA	O2D-CGD-O1D	-2.92	118.13	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	829	CLA	CMC-C2C-C1C	-2.92	120.60	125.04
14	b	827	CLA	C2A-C1A-CHA	2.92	128.96	123.86
13	A	801	CL0	O2D-CGD-O1D	-2.91	118.14	123.84
17	F	205	BCR	C16-C15-C14	-2.91	117.51	123.47
14	b	842	CLA	CMB-C2B-C3B	2.91	130.12	124.68
14	a	825	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
13	a	801	CL0	O2D-CGD-O1D	-2.91	118.15	123.84
14	B	822	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
17	a	844	BCR	C15-C14-C13	-2.91	123.16	127.31
14	B	802	CLA	CHB-C4A-NA	2.91	128.53	124.51
14	B	843	CLA	CAA-C2A-C1A	-2.90	102.46	111.97
14	A	843	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
17	m	1202	BCR	C35-C13-C14	-2.90	118.86	122.92
14	b	802	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
14	b	828	CLA	O2D-CGD-CBD	2.90	116.41	111.27
14	b	819	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
14	b	805	CLA	CHD-C1D-ND	-2.89	121.80	124.45
17	B	850	BCR	C35-C13-C14	-2.89	118.88	122.92
17	B	849	BCR	C11-C10-C9	-2.89	123.19	127.31
14	A	833	CLA	CHD-C1D-ND	-2.89	121.80	124.45
14	A	811	CLA	C1-O2A-CGA	2.89	124.02	116.44
14	b	839	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
14	B	815	CLA	CHB-C4A-NA	2.88	128.50	124.51
14	B	834	CLA	CHB-C4A-NA	2.88	128.50	124.51
14	B	813	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
14	a	815	CLA	CHB-C4A-NA	2.88	128.50	124.51
14	A	809	CLA	CAA-CBA-CGA	-2.88	104.83	113.25
14	b	840	CLA	CHB-C4A-NA	2.88	128.50	124.51
14	b	833	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
14	b	814	CLA	CHB-C4A-NA	2.88	128.50	124.51
14	A	809	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
14	b	810	CLA	O2D-CGD-CBD	2.88	116.38	111.27
14	B	837	CLA	CHB-C4A-NA	2.88	128.49	124.51
14	b	829	CLA	CHB-C4A-NA	2.88	128.49	124.51
14	A	838	CLA	O2D-CGD-CBD	2.88	116.38	111.27
14	b	804	CLA	CHD-C1D-ND	-2.88	121.81	124.45
14	b	804	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
17	j	104	BCR	C3-C4-C5	-2.88	108.94	114.08
14	b	825	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
14	b	810	CLA	CHD-C1D-ND	-2.87	121.81	124.45
14	A	803	CLA	CHB-C4A-NA	2.87	128.49	124.51
14	a	839	CLA	CHB-C4A-NA	2.87	128.48	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	823	CLA	C2D-C1D-ND	-2.87	107.99	110.10
18	i	103	LHG	O8-C23-C24	2.87	120.91	111.91
14	B	841	CLA	CHB-C4A-NA	2.87	128.48	124.51
14	A	832	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
14	B	843	CLA	CAA-C2A-C3A	-2.87	104.93	112.78
14	L	1501	CLA	CAA-C2A-C3A	-2.87	104.93	112.78
19	x	1702	SQD	O8-S-C6	2.86	110.31	105.74
14	B	813	CLA	CMB-C2B-C3B	2.86	130.04	124.68
14	a	830	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
14	l	203	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
14	a	834	CLA	CHB-C4A-NA	2.86	128.47	124.51
14	a	809	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
14	A	834	CLA	C16-C15-C13	-2.86	106.68	115.92
14	b	814	CLA	CHD-C1D-ND	-2.86	121.83	124.45
14	B	804	CLA	CHB-C4A-NA	2.86	128.46	124.51
14	a	809	CLA	CHB-C4A-NA	2.86	128.46	124.51
14	B	828	CLA	C3C-C4C-NC	-2.86	107.37	110.57
17	J	104	BCR	C11-C10-C9	-2.86	123.23	127.31
14	A	831	CLA	CHB-C4A-NA	2.85	128.46	124.51
14	a	839	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
14	b	839	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
14	B	801	CLA	C1-C2-C3	-2.85	121.12	126.04
14	K	101	CLA	CHB-C4A-NA	2.85	128.45	124.51
17	a	849	BCR	C15-C16-C17	-2.84	117.65	123.47
14	k	101	CLA	CMB-C2B-C3B	2.84	130.00	124.68
14	A	826	CLA	CHB-C4A-NA	2.84	128.44	124.51
14	l	205	CLA	CHB-C4A-NA	2.84	128.44	124.51
14	A	814	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
14	B	811	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
14	b	843	CLA	C1B-CHB-C4A	-2.83	124.50	130.12
14	L	1501	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
14	B	806	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
17	B	849	BCR	C7-C8-C9	-2.83	121.95	126.23
14	X	1701	CLA	CHD-C1D-ND	-2.83	121.85	124.45
14	a	829	CLA	CMC-C2C-C1C	-2.83	120.73	125.04
14	X	1701	CLA	CHB-C4A-NA	2.83	128.43	124.51
14	a	839	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
14	b	842	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
14	b	822	CLA	CMC-C2C-C1C	-2.83	120.73	125.04
14	l	204	CLA	CHB-C4A-NA	2.83	128.42	124.51
14	k	102	CLA	CMB-C2B-C3B	2.83	129.97	124.68
17	a	845	BCR	C2-C1-C6	2.83	114.83	110.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	844	PQN	C2M-C2-C3	-2.82	119.79	124.40
18	a	850	LHG	O8-C23-C24	2.82	120.76	111.91
14	A	810	CLA	CHB-C4A-NA	2.82	128.41	124.51
17	b	847	BCR	C30-C25-C26	-2.82	118.64	122.61
14	B	823	CLA	CBC-CAC-C3C	-2.82	104.66	112.43
14	b	831	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
17	b	849	BCR	C3-C4-C5	-2.81	109.06	114.08
14	b	840	CLA	CHD-C1D-ND	-2.81	121.87	124.45
14	a	829	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
14	b	809	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
14	A	816	CLA	CMB-C2B-C3B	2.81	129.94	124.68
14	A	821	CLA	CMB-C2B-C3B	2.81	129.93	124.68
14	A	836	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
14	b	808	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
17	F	203	BCR	C24-C23-C22	-2.80	122.00	126.23
14	A	841	CLA	O2D-CGD-CBD	2.80	116.25	111.27
14	a	802	CLA	O2D-CGD-CBD	2.80	116.23	111.27
17	B	848	BCR	C15-C16-C17	-2.79	117.75	123.47
14	l	203	CLA	CBC-CAC-C3C	2.79	120.13	112.43
14	A	819	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
14	A	804	CLA	CHB-C4A-NA	2.79	128.37	124.51
14	A	835	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
14	b	809	CLA	C11-C12-C13	-2.79	106.91	115.92
14	k	102	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
14	A	809	CLA	CHB-C4A-NA	2.79	128.37	124.51
17	B	849	BCR	C27-C26-C25	2.79	126.78	122.73
14	K	102	CLA	CHB-C4A-NA	2.79	128.37	124.51
14	a	833	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
14	A	811	CLA	CHB-C4A-NA	2.78	128.36	124.51
14	a	828	CLA	CHB-C4A-NA	2.78	128.36	124.51
17	a	846	BCR	C27-C26-C25	2.78	126.77	122.73
14	B	804	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
17	a	846	BCR	C15-C16-C17	-2.78	117.77	123.47
14	L	1503	CLA	CHB-C4A-NA	2.78	128.36	124.51
14	a	832	CLA	C7-C6-C5	-2.78	105.81	113.36
14	B	840	CLA	C1-C2-C3	-2.78	121.23	126.04
14	j	102	CLA	CHB-C4A-NA	2.78	128.36	124.51
14	B	801	CLA	CHD-C1D-ND	-2.78	121.90	124.45
14	B	827	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
14	a	832	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
14	B	835	CLA	CMB-C2B-C3B	2.78	129.88	124.68
14	j	103	CLA	CHB-C4A-NA	2.78	128.36	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	817	CLA	C2D-C1D-ND	-2.78	108.06	110.10
14	B	832	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
17	b	849	BCR	C11-C10-C9	-2.78	123.34	127.31
14	A	802	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
14	a	811	CLA	CMB-C2B-C3B	2.78	129.87	124.68
14	A	817	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
14	A	817	CLA	CMB-C2B-C3B	2.78	129.87	124.68
19	X	1702	SQD	O8-S-C6	2.77	110.16	105.74
17	i	102	BCR	C35-C13-C14	-2.77	119.04	122.92
14	B	814	CLA	O2D-CGD-CBD	2.77	116.19	111.27
17	b	846	BCR	C28-C27-C26	-2.77	109.14	114.08
14	m	1201	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	B	808	CLA	CAC-C3C-C4C	2.77	128.40	124.81
17	F	205	BCR	C27-C26-C25	2.76	126.75	122.73
14	B	804	CLA	C2A-C1A-CHA	2.76	128.69	123.86
17	a	849	BCR	C28-C27-C26	-2.76	109.14	114.08
14	A	839	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	b	835	CLA	CHD-C1D-ND	-2.76	121.92	124.45
14	A	824	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	A	825	CLA	C2A-C1A-CHA	2.76	128.68	123.86
17	A	850	BCR	C35-C13-C14	-2.76	119.06	122.92
14	A	823	CLA	CHB-C4A-NA	2.76	128.33	124.51
14	A	842	CLA	O2D-CGD-CBD	2.76	116.17	111.27
17	I	101	BCR	C31-C1-C6	2.76	114.77	110.30
14	A	805	CLA	CHD-C1D-ND	-2.76	121.92	124.45
14	b	833	CLA	C2D-C1D-ND	-2.75	108.07	110.10
14	b	823	CLA	CHB-C4A-NA	2.75	128.32	124.51
17	A	848	BCR	C27-C26-C25	2.75	126.73	122.73
14	a	812	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
14	A	816	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	a	828	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
14	a	827	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
14	b	837	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	B	833	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
17	b	847	BCR	C27-C26-C25	2.75	126.72	122.73
14	A	841	CLA	CHB-C4A-NA	2.75	128.31	124.51
14	a	825	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
17	l	206	BCR	C27-C26-C25	2.75	126.72	122.73
17	a	848	BCR	C15-C14-C13	-2.75	123.39	127.31
14	a	826	CLA	CHB-C4A-NA	2.74	128.31	124.51
14	a	837	CLA	CHB-C4A-NA	2.74	128.31	124.51
14	b	826	CLA	C1B-CHB-C4A	-2.74	124.68	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	825	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
17	b	848	BCR	C15-C14-C13	-2.74	123.40	127.31
14	A	812	CLA	CHB-C4A-NA	2.74	128.30	124.51
14	a	831	CLA	CAA-C2A-C1A	2.74	120.95	111.97
14	b	810	CLA	CAC-C3C-C4C	2.74	128.36	124.81
14	b	827	CLA	CBA-CAA-C2A	2.74	121.95	113.86
14	b	828	CLA	CHB-C4A-NA	2.74	128.30	124.51
20	b	851	LMG	O3-C3-C2	-2.73	104.03	110.35
14	L	1502	CLA	CHB-C4A-NA	2.73	128.29	124.51
17	j	104	BCR	C15-C16-C17	-2.73	117.88	123.47
17	K	103	BCR	C15-C16-C17	-2.73	117.88	123.47
14	A	839	CLA	O2D-CGD-CBD	2.73	116.12	111.27
14	a	827	CLA	C11-C12-C13	-2.73	107.09	115.92
17	f	202	BCR	C16-C15-C14	-2.73	117.88	123.47
14	A	815	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
14	B	826	CLA	CHB-C4A-NA	2.73	128.29	124.51
14	b	828	CLA	C3A-C2A-C1A	2.73	105.43	101.34
14	A	828	CLA	CAC-C3C-C4C	2.73	128.35	124.81
20	B	803	LMG	O6-C1-O1	-2.73	103.52	109.97
14	A	811	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
14	A	836	CLA	CHB-C4A-NA	2.73	128.28	124.51
14	A	837	CLA	CHB-C4A-NA	2.72	128.28	124.51
17	M	101	BCR	C27-C26-C25	2.72	126.68	122.73
14	B	823	CLA	CMC-C2C-C3C	2.72	133.50	126.12
14	a	823	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
14	b	818	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
14	A	803	CLA	O2D-CGD-CBD	2.72	116.10	111.27
13	A	801	CL0	C3C-C4C-NC	2.72	113.62	110.57
14	A	837	CLA	O2A-CGA-O1A	-2.72	116.74	123.59
14	a	840	CLA	CMB-C2B-C3B	2.71	129.75	124.68
14	b	826	CLA	CHB-C4A-NA	2.71	128.26	124.51
17	A	847	BCR	C28-C27-C26	-2.71	109.23	114.08
15	a	842	PQN	C2M-C2-C3	-2.71	119.98	124.40
17	b	849	BCR	C27-C26-C25	2.71	126.67	122.73
14	a	832	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	a	807	CLA	CHB-C4A-NA	2.71	128.26	124.51
14	B	824	CLA	O2D-CGD-CBD	2.71	116.08	111.27
14	A	834	CLA	C2D-C1D-ND	-2.71	108.11	110.10
14	B	814	CLA	CHB-C4A-NA	2.71	128.25	124.51
14	b	819	CLA	CHB-C4A-NA	2.71	128.25	124.51
14	a	808	CLA	CHB-C4A-NA	2.70	128.25	124.51
14	A	818	CLA	O2D-CGD-O1D	-2.70	118.55	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	802	CLA	C2D-C1D-ND	-2.70	108.11	110.10
14	a	815	CLA	CMB-C2B-C3B	2.70	129.73	124.68
14	b	827	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
14	A	826	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
14	a	839	CLA	C1-C2-C3	-2.70	121.37	126.04
14	b	804	CLA	O2D-CGD-CBD	2.70	116.06	111.27
14	a	807	CLA	CAA-C2A-C1A	-2.69	103.14	111.97
14	L	1501	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
14	B	804	CLA	C7-C6-C5	-2.69	106.05	113.36
14	a	813	CLA	CHB-C4A-NA	2.69	128.23	124.51
13	a	801	CL0	C3C-C4C-NC	2.69	113.58	110.57
14	a	810	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
14	b	822	CLA	CHB-C4A-NA	2.69	128.23	124.51
14	m	1201	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
14	a	807	CLA	O2D-CGD-CBD	2.68	116.03	111.27
14	A	813	CLA	C1B-CHB-C4A	-2.68	124.82	130.12
17	A	846	BCR	C28-C27-C26	-2.68	109.30	114.08
17	I	102	BCR	C7-C8-C9	-2.68	122.19	126.23
14	b	817	CLA	C2D-C1D-ND	-2.68	108.13	110.10
18	a	850	LHG	C11-C10-C9	-2.68	100.84	114.42
14	a	833	CLA	C16-C15-C13	-2.67	107.28	115.92
14	b	823	CLA	CMB-C2B-C3B	2.67	129.68	124.68
14	A	823	CLA	O2D-CGD-CBD	2.67	116.01	111.27
14	B	806	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
14	B	815	CLA	CMB-C2B-C3B	2.66	129.66	124.68
14	a	802	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	A	828	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	x	1701	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	j	101	CLA	CHB-C4A-NA	2.66	128.19	124.51
14	a	827	CLA	CHB-C4A-NA	2.65	128.18	124.51
19	b	801	SQD	O48-C23-C24	2.65	120.24	111.91
18	a	850	LHG	C20-C19-C18	-2.65	100.95	114.42
17	I	101	BCR	C29-C30-C25	2.65	114.56	110.48
14	B	804	CLA	O2D-CGD-CBD	2.65	115.98	111.27
14	b	821	CLA	CHB-C4A-NA	2.65	128.18	124.51
14	b	817	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
17	J	104	BCR	C28-C27-C26	-2.65	109.34	114.08
14	A	807	CLA	CHB-C4A-NA	2.65	128.18	124.51
14	A	813	CLA	CHB-C4A-NA	2.65	128.18	124.51
17	A	851	BCR	C29-C30-C25	2.65	114.56	110.48
14	A	827	CLA	CHB-C4A-NA	2.65	128.18	124.51
14	b	820	CLA	C1B-CHB-C4A	-2.65	124.87	130.12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	848	BCR	C29-C30-C25	2.65	114.56	110.48
14	A	816	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
14	A	835	CLA	CMB-C2B-C3B	2.64	129.63	124.68
17	L	1504	BCR	C11-C10-C9	-2.64	123.54	127.31
14	b	825	CLA	CHB-C4A-NA	2.64	128.17	124.51
14	A	819	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
17	J	105	BCR	C7-C8-C9	-2.64	122.24	126.23
14	b	811	CLA	CMB-C2B-C3B	2.64	129.62	124.68
14	a	834	CLA	CMB-C2B-C3B	2.64	129.62	124.68
14	b	837	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
14	l	203	CLA	O2D-CGD-CBD	2.64	115.96	111.27
14	b	815	CLA	CHB-C4A-NA	2.64	128.16	124.51
14	B	827	CLA	C2A-C1A-CHA	2.64	128.47	123.86
17	A	846	BCR	C15-C16-C17	-2.64	118.07	123.47
14	K	101	CLA	CMB-C2B-C3B	2.63	129.61	124.68
14	A	828	CLA	O2D-CGD-CBD	2.63	115.95	111.27
14	B	832	CLA	O2D-CGD-CBD	2.63	115.95	111.27
14	A	833	CLA	CHB-C4A-NA	2.63	128.15	124.51
17	i	101	BCR	C37-C22-C21	-2.63	119.23	122.92
14	a	840	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
18	A	852	LHG	O8-C23-C24	2.63	120.17	111.91
14	B	826	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
14	A	810	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
14	B	842	CLA	CHB-C4A-NA	2.63	128.15	124.51
17	J	104	BCR	C24-C23-C22	-2.63	122.27	126.23
14	b	842	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
14	B	810	CLA	O2D-CGD-CBD	2.63	115.94	111.27
14	a	805	CLA	O1D-CGD-CBD	2.63	129.86	124.48
14	A	819	CLA	C7-C6-C5	-2.62	106.23	113.36
14	B	809	CLA	CHB-C4A-NA	2.62	128.14	124.51
14	a	812	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
14	a	836	CLA	O2D-CGD-CBD	2.62	115.92	111.27
14	A	833	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
14	a	838	CLA	CHB-C4A-NA	2.62	128.13	124.51
14	a	833	CLA	CHD-C1D-C2D	2.62	130.97	125.48
14	A	826	CLA	CBC-CAC-C3C	-2.62	105.22	112.43
14	A	815	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
17	J	105	BCR	C27-C26-C25	2.61	126.53	122.73
14	A	830	CLA	O2D-CGD-CBD	2.61	115.91	111.27
14	B	840	CLA	O2D-CGD-CBD	2.61	115.91	111.27
14	b	836	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
14	x	1701	CLA	O2D-CGD-O1D	-2.61	118.73	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	822	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	a	845	BCR	C28-C27-C26	-2.61	109.42	114.08
14	a	822	CLA	O2D-CGD-CBD	2.61	115.90	111.27
14	B	841	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
14	B	825	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
14	A	805	CLA	C3C-C4C-NC	-2.61	107.65	110.57
17	a	847	BCR	C7-C8-C9	-2.61	122.30	126.23
14	b	820	CLA	CHB-C4A-NA	2.61	128.12	124.51
14	b	830	CLA	C1-C2-C3	-2.61	121.54	126.04
14	B	809	CLA	O2A-CGA-O1A	-2.61	117.02	123.59
17	b	847	BCR	C15-C16-C17	-2.60	118.14	123.47
14	B	843	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
14	A	838	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
17	I	102	BCR	C15-C14-C13	-2.60	123.60	127.31
14	b	804	CLA	CMB-C2B-C3B	2.60	129.54	124.68
14	j	103	CLA	CMB-C2B-C3B	2.60	129.54	124.68
14	b	843	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
14	a	837	CLA	CGD-CBD-CAD	2.60	119.14	110.73
14	B	828	CLA	CHB-C4A-NA	2.60	128.10	124.51
14	A	824	CLA	CHD-C1D-ND	-2.60	122.07	124.45
14	B	835	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
14	a	804	CLA	O2A-CGA-O1A	-2.59	117.05	123.59
14	b	839	CLA	CBC-CAC-C3C	2.59	119.57	112.43
19	X	1702	SQD	O5-C5-C4	2.59	114.40	109.69
14	A	821	CLA	CHD-C1D-ND	-2.59	122.07	124.45
14	b	812	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
14	b	833	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
17	F	203	BCR	C20-C21-C22	-2.59	123.61	127.31
14	B	843	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
17	J	103	BCR	C11-C10-C9	-2.59	123.62	127.31
17	B	845	BCR	C24-C23-C22	-2.59	122.33	126.23
14	a	827	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
14	b	835	CLA	CHB-C4A-NA	2.58	128.09	124.51
14	B	808	CLA	CHD-C4C-C3C	2.58	128.63	124.84
14	A	843	CLA	CHB-C4A-NA	2.58	128.08	124.51
19	b	801	SQD	O47-C7-C8	2.58	117.06	111.50
14	A	826	CLA	CAA-C2A-C1A	-2.58	103.53	111.97
14	b	830	CLA	O2D-CGD-CBD	2.58	115.85	111.27
14	a	832	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
17	a	846	BCR	C15-C14-C13	-2.58	123.63	127.31
14	B	822	CLA	CMB-C2B-C3B	2.58	129.50	124.68
14	B	808	CLA	O2A-CGA-O1A	-2.57	117.09	123.59

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	l	202	SQD	C3-C4-C5	2.57	114.83	110.24
14	a	831	CLA	CHB-C4A-NA	2.57	128.07	124.51
14	A	805	CLA	O2D-CGD-CBD	2.57	115.84	111.27
14	A	828	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
14	A	843	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
17	F	205	BCR	C35-C13-C14	-2.57	119.32	122.92
17	j	105	BCR	C29-C30-C25	2.57	114.44	110.48
14	B	810	CLA	CHB-C4A-NA	2.57	128.07	124.51
17	l	206	BCR	C30-C25-C24	2.57	123.05	115.78
17	J	104	BCR	C15-C16-C17	-2.57	118.21	123.47
14	b	830	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
14	B	826	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
14	B	809	CLA	C1-O2A-CGA	2.57	123.18	116.44
14	B	826	CLA	CHD-C1D-ND	-2.57	122.09	124.45
14	b	807	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	b	834	CLA	CHB-C4A-NA	2.57	128.06	124.51
14	A	834	CLA	CAC-C3C-C2C	-2.57	123.14	127.53
14	B	802	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
14	B	821	CLA	CMB-C2B-C1B	-2.56	124.52	128.46
17	a	846	BCR	C11-C10-C9	-2.56	123.65	127.31
14	b	835	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
14	b	825	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
14	B	808	CLA	C3A-C2A-C1A	2.56	105.18	101.34
20	b	851	LMG	C40-C39-C38	-2.56	101.42	114.42
14	b	804	CLA	CHB-C4A-NA	2.56	128.05	124.51
14	B	830	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
14	b	802	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
14	b	822	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
17	A	850	BCR	C15-C14-C13	-2.56	123.66	127.31
14	B	823	CLA	CMB-C2B-C3B	2.56	129.46	124.68
17	k	103	BCR	C2-C1-C6	2.56	114.42	110.48
13	A	801	CL0	C4D-C3D-CAD	2.56	111.11	108.10
18	A	853	LHG	C18-C17-C16	-2.56	101.45	114.42
14	b	833	CLA	CHB-C4A-NA	2.56	128.05	124.51
14	A	843	CLA	O2D-CGD-CBD	2.56	115.81	111.27
17	B	847	BCR	C38-C26-C27	-2.55	108.71	113.62
13	a	801	CL0	C4D-C3D-CAD	2.55	111.11	108.10
19	l	202	SQD	O6-C44-C45	2.55	117.06	110.90
14	B	843	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
17	I	102	BCR	C27-C26-C25	2.55	126.44	122.73
14	a	818	CLA	C7-C6-C5	-2.55	106.43	113.36
14	B	806	CLA	CHB-C4A-NA	2.55	128.03	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	823	CLA	C1-C2-C3	-2.55	121.64	126.04
14	B	801	CLA	CHB-C4A-NA	2.54	128.03	124.51
14	B	821	CLA	C3C-C4C-NC	-2.54	107.72	110.57
18	a	851	LHG	O7-C7-C8	2.54	116.98	111.50
14	B	807	CLA	CHB-C4A-NA	2.54	128.03	124.51
14	B	829	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
14	A	814	CLA	CHD-C1D-ND	-2.54	122.12	124.45
17	b	849	BCR	C24-C23-C22	-2.54	122.40	126.23
14	B	836	CLA	O1D-CGD-CBD	2.54	129.68	124.48
14	B	840	CLA	CHD-C1D-ND	-2.54	122.12	124.45
14	B	811	CLA	C2D-C1D-ND	-2.54	108.23	110.10
14	b	827	CLA	CHA-C1A-NA	-2.54	120.59	126.40
14	b	803	CLA	C1D-ND-C4D	2.54	108.14	106.33
14	B	804	CLA	CMB-C2B-C3B	2.53	129.42	124.68
14	L	1501	CLA	CHB-C4A-NA	2.53	128.01	124.51
14	A	843	CLA	CMB-C2B-C3B	2.53	129.42	124.68
14	a	814	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
14	A	840	CLA	CMB-C2B-C3B	2.53	129.41	124.68
15	a	842	PQN	C12-C11-C3	-2.53	105.23	112.05
14	A	842	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
14	b	803	CLA	CHA-C1A-NA	-2.53	120.61	126.40
14	J	101	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
17	B	845	BCR	C15-C14-C13	-2.52	123.71	127.31
14	b	843	CLA	CHD-C1D-ND	-2.52	122.13	124.45
17	M	101	BCR	C16-C15-C14	-2.52	118.30	123.47
17	B	847	BCR	C27-C26-C25	2.52	126.39	122.73
14	A	817	CLA	CHB-C4A-NA	2.52	128.00	124.51
14	A	835	CLA	CHB-C4A-NA	2.52	128.00	124.51
14	b	827	CLA	CHB-C4A-NA	2.52	128.00	124.51
14	B	828	CLA	CMC-C2C-C1C	-2.52	121.20	125.04
14	A	828	CLA	C11-C12-C13	-2.52	107.77	115.92
14	b	826	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
14	A	821	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
17	B	845	BCR	C11-C10-C9	-2.52	123.72	127.31
14	L	1502	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
14	A	814	CLA	O2D-CGD-CBD	2.52	115.74	111.27
14	j	101	CLA	CMB-C2B-C1B	-2.52	124.60	128.46
14	B	808	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
14	b	806	CLA	O2D-CGD-CBD	2.51	115.74	111.27
14	A	829	CLA	CHB-C4A-NA	2.51	127.99	124.51
17	l	206	BCR	C23-C24-C25	2.51	134.26	127.20
14	a	807	CLA	C1B-CHB-C4A	-2.51	125.14	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	805	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
14	B	809	CLA	C11-C12-C13	-2.51	107.80	115.92
14	b	814	CLA	O2D-CGD-CBD	2.51	115.73	111.27
14	b	810	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	a	846	BCR	C38-C26-C27	-2.51	108.80	113.62
14	B	833	CLA	C2D-C1D-ND	-2.51	108.25	110.10
14	a	837	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
14	B	817	CLA	C3C-C4C-NC	-2.51	107.76	110.57
14	B	811	CLA	CMB-C2B-C1B	-2.51	124.61	128.46
17	J	104	BCR	C29-C30-C25	2.51	114.34	110.48
14	b	842	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	B	847	BCR	C15-C16-C17	-2.51	118.34	123.47
14	A	834	CLA	CHB-C4A-NA	2.51	127.98	124.51
14	b	810	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
14	a	829	CLA	C1-C2-C3	-2.51	121.71	126.04
14	a	811	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	k	103	BCR	C11-C10-C9	-2.50	123.74	127.31
14	B	821	CLA	CHB-C4A-NA	2.50	127.97	124.51
14	b	821	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
17	k	103	BCR	C15-C16-C17	-2.50	118.35	123.47
14	j	101	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
17	a	844	BCR	C24-C23-C22	-2.50	122.46	126.23
14	b	817	CLA	C1-C2-C3	-2.50	122.71	126.75
14	a	818	CLA	CHD-C1D-ND	-2.50	122.16	124.45
14	b	834	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
14	a	831	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
14	a	830	CLA	CHD-C1D-ND	-2.49	122.16	124.45
14	B	821	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
19	l	202	SQD	O47-C7-O49	-2.49	117.68	123.70
14	b	803	CLA	CHD-C1D-ND	-2.49	122.16	124.45
14	b	805	CLA	O2D-CGD-CBD	2.49	115.70	111.27
17	a	844	BCR	C7-C8-C9	-2.49	122.47	126.23
14	A	826	CLA	O2D-CGD-CBD	2.49	115.69	111.27
14	B	806	CLA	CMC-C2C-C1C	-2.49	121.25	125.04
14	B	839	CLA	CMB-C2B-C3B	2.49	129.34	124.68
14	B	827	CLA	CBA-CAA-C2A	2.49	121.21	113.86
14	A	806	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
17	J	105	BCR	C15-C14-C13	-2.49	123.76	127.31
14	a	825	CLA	CAA-C2A-C1A	-2.49	103.82	111.97
14	b	834	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
14	F	204	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
17	B	848	BCR	C20-C21-C22	-2.49	123.76	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	809	CLA	CHB-C4A-NA	2.49	127.95	124.51
14	a	833	CLA	CBC-CAC-C3C	2.49	119.28	112.43
13	A	801	CL0	C3D-C4D-ND	2.49	114.26	110.24
14	B	827	CLA	O1D-CGD-CBD	2.49	129.57	124.48
14	a	821	CLA	O2D-CGD-CBD	2.49	115.68	111.27
14	a	823	CLA	C2D-C1D-ND	-2.48	108.27	110.10
17	F	205	BCR	C40-C30-C25	2.48	114.33	110.30
14	A	825	CLA	CHB-C4A-NA	2.48	127.95	124.51
17	a	849	BCR	C29-C30-C25	2.48	114.31	110.48
17	i	101	BCR	C2-C1-C6	2.48	114.31	110.48
14	A	811	CLA	O2A-CGA-O1A	-2.48	117.32	123.59
17	A	848	BCR	C15-C16-C17	-2.48	118.39	123.47
17	i	101	BCR	C15-C16-C17	-2.48	118.39	123.47
14	a	840	CLA	O2A-CGA-O1A	-2.48	117.32	123.59
14	B	828	CLA	CMC-C2C-C3C	2.48	132.86	126.12
14	a	822	CLA	C1-C2-C3	-2.48	121.75	126.04
14	a	836	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
14	A	803	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
14	b	843	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
14	b	829	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
14	B	811	CLA	C3A-C2A-C1A	2.48	105.05	101.34
14	a	807	CLA	CHD-C1D-ND	-2.48	122.18	124.45
14	a	837	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
17	K	103	BCR	C7-C8-C9	-2.48	122.49	126.23
14	b	839	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
14	A	841	CLA	CMB-C2B-C3B	2.48	129.31	124.68
14	a	806	CLA	C4-C3-C5	2.48	119.44	115.27
17	i	101	BCR	C28-C27-C26	-2.48	109.65	114.08
17	a	847	BCR	C24-C23-C22	-2.48	122.49	126.23
14	J	102	CLA	CHB-C4A-NA	2.48	127.94	124.51
14	A	807	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
17	b	847	BCR	C38-C26-C27	-2.48	108.86	113.62
17	J	104	BCR	C15-C14-C13	-2.47	123.78	127.31
14	a	821	CLA	CHB-C4A-NA	2.47	127.93	124.51
13	a	801	CL0	C3D-C4D-ND	2.47	114.24	110.24
14	A	805	CLA	CAC-C3C-C4C	2.47	128.02	124.81
17	f	204	BCR	C27-C26-C25	2.47	126.32	122.73
17	A	849	BCR	C33-C5-C6	-2.47	121.75	124.53
14	b	822	CLA	CMB-C2B-C3B	2.47	129.29	124.68
14	B	823	CLA	CMC-C2C-C1C	-2.47	121.28	125.04
17	A	848	BCR	C30-C25-C26	-2.47	119.14	122.61
14	a	841	CLA	CHB-C4A-NA	2.47	127.92	124.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	820	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
14	A	809	CLA	C2A-C1A-CHA	2.46	128.17	123.86
17	m	1202	BCR	C27-C26-C25	2.46	126.31	122.73
19	X	1702	SQD	C1-C2-C3	-2.46	104.87	110.00
14	b	843	CLA	CBC-CAC-C3C	2.46	119.21	112.43
14	B	829	CLA	CHD-C1D-ND	-2.46	122.19	124.45
14	a	804	CLA	C1-O2A-CGA	2.46	122.89	116.44
17	K	103	BCR	C2-C1-C6	2.46	114.27	110.48
14	b	806	CLA	C4-C3-C5	2.46	119.40	115.27
17	a	846	BCR	C30-C25-C26	-2.46	119.15	122.61
14	b	806	CLA	O2A-C1-C2	-2.46	102.18	108.64
14	a	806	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
17	j	104	BCR	C15-C14-C13	-2.46	123.81	127.31
18	A	853	LHG	C20-C19-C18	-2.46	101.96	114.42
14	b	803	CLA	C2A-C1A-CHA	2.45	128.15	123.86
14	a	817	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
17	j	106	BCR	C27-C26-C25	2.45	126.29	122.73
14	b	811	CLA	O2D-CGD-CBD	2.45	115.63	111.27
19	l	202	SQD	O48-C23-O10	-2.45	117.40	123.59
17	F	205	BCR	C38-C26-C27	-2.45	108.91	113.62
14	a	805	CLA	CHB-C4A-NA	2.45	127.90	124.51
20	B	851	LMG	C40-C39-C38	-2.45	101.98	114.42
14	X	1701	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
14	b	808	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
14	X	1701	CLA	O1D-CGD-CBD	2.45	129.50	124.48
14	B	820	CLA	CBC-CAC-C3C	2.45	119.18	112.43
14	a	820	CLA	C2D-C1D-ND	-2.45	108.30	110.10
14	A	819	CLA	C1-C2-C3	-2.45	121.81	126.04
17	F	203	BCR	C15-C14-C13	-2.45	123.82	127.31
17	A	850	BCR	C27-C26-C25	2.45	126.28	122.73
14	b	841	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
14	b	838	CLA	CHB-C4A-NA	2.44	127.89	124.51
14	a	839	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
13	a	801	CL0	C1-O2A-CGA	2.44	122.86	116.44
14	b	816	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
17	m	1202	BCR	C33-C5-C6	-2.44	121.79	124.53
14	k	102	CLA	C2A-C1A-CHA	2.44	128.13	123.86
17	L	1504	BCR	C15-C16-C17	-2.44	118.47	123.47
13	A	801	CL0	C1-O2A-CGA	2.44	122.84	116.44
14	B	807	CLA	CHD-C1D-ND	-2.44	122.21	124.45
14	B	839	CLA	CHD-C1D-ND	-2.44	122.21	124.45
17	f	202	BCR	C27-C26-C25	2.44	126.27	122.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	l	204	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
14	A	808	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
17	J	105	BCR	C31-C1-C6	2.44	114.25	110.30
14	A	817	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
14	A	817	CLA	CHD-C1D-ND	-2.44	122.21	124.45
17	a	845	BCR	C15-C16-C17	-2.44	118.48	123.47
14	x	1701	CLA	CMB-C2B-C3B	2.44	129.24	124.68
14	J	102	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
18	a	850	LHG	C18-C17-C16	-2.44	102.06	114.42
14	B	839	CLA	CHB-C4A-NA	2.43	127.88	124.51
14	A	817	CLA	CAC-C3C-C4C	2.43	127.97	124.81
17	J	104	BCR	C7-C8-C9	-2.43	122.56	126.23
20	B	851	LMG	C1-C2-C3	-2.43	104.93	110.00
14	B	819	CLA	CHD-C1D-ND	-2.43	122.22	124.45
14	b	836	CLA	CAA-CBA-CGA	-2.43	106.15	113.25
14	A	808	CLA	C1-C2-C3	-2.43	121.84	126.04
14	A	833	CLA	C11-C10-C8	-2.43	108.07	115.92
14	B	812	CLA	CHD-C1D-ND	-2.43	122.22	124.45
14	F	204	CLA	CHD-C1D-ND	-2.43	122.22	124.45
17	F	203	BCR	C11-C10-C9	-2.43	123.84	127.31
14	b	839	CLA	CHA-C1A-NA	-2.42	120.84	126.40
14	B	804	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
14	B	824	CLA	CHB-C4A-NA	2.42	127.86	124.51
14	b	816	CLA	CAC-C3C-C4C	2.42	127.95	124.81
14	K	102	CLA	C2A-C1A-CHA	2.42	128.10	123.86
17	M	101	BCR	C40-C30-C25	2.42	114.23	110.30
14	A	812	CLA	CMB-C2B-C3B	2.42	129.21	124.68
18	F	201	LHG	C11-C10-C9	-2.42	102.15	114.42
14	B	808	CLA	C16-C15-C13	-2.42	108.10	115.92
14	b	839	CLA	CHB-C4A-NA	2.42	127.85	124.51
18	a	850	LHG	C27-C26-C25	-2.42	102.16	114.42
14	j	103	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
14	a	822	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
14	F	204	CLA	CHB-C4A-NA	2.41	127.85	124.51
14	a	820	CLA	CHB-C4A-NA	2.41	127.85	124.51
14	a	829	CLA	CHB-C4A-NA	2.41	127.84	124.51
14	b	841	CLA	O2D-CGD-CBD	2.41	115.55	111.27
14	B	835	CLA	CAA-CBA-CGA	-2.41	106.21	113.25
14	b	840	CLA	C1-C2-C3	-2.41	121.88	126.04
14	B	814	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
14	A	805	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
17	j	105	BCR	C24-C23-C22	-2.41	122.60	126.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	802	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
14	B	841	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
14	B	815	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
17	B	847	BCR	C30-C25-C26	-2.41	119.23	122.61
14	B	842	CLA	CHD-C1D-ND	-2.40	122.24	124.45
14	a	807	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
17	A	848	BCR	C38-C26-C27	-2.40	109.00	113.62
14	k	102	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
14	B	805	CLA	C1-C2-C3	-2.40	121.89	126.04
17	J	103	BCR	C3-C4-C5	-2.40	109.79	114.08
14	B	827	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
14	b	838	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
14	b	840	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
17	A	849	BCR	C15-C16-C17	-2.40	118.56	123.47
14	b	832	CLA	C1D-ND-C4D	2.40	108.04	106.33
14	b	835	CLA	CGD-CBD-CAD	-2.39	102.98	110.73
14	B	838	CLA	CHB-C4A-NA	2.39	127.82	124.51
14	A	835	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
14	b	812	CLA	CAC-C3C-C2C	-2.39	123.44	127.53
14	a	811	CLA	O2A-C1-C2	-2.39	102.34	108.64
14	A	826	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
14	A	811	CLA	CMB-C2B-C3B	2.39	129.15	124.68
17	F	205	BCR	C30-C25-C26	-2.39	119.25	122.61
14	a	816	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
14	a	824	CLA	CHA-C1A-NA	-2.39	120.92	126.40
14	A	829	CLA	CMC-C2C-C3C	2.39	132.60	126.12
17	M	101	BCR	C33-C5-C6	-2.39	121.84	124.53
14	b	813	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
14	b	815	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
14	B	837	CLA	C2A-C1A-CHA	2.39	128.04	123.86
14	B	810	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
17	b	845	BCR	C27-C26-C25	2.39	126.19	122.73
14	l	205	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
15	A	844	PQN	C11-C12-C13	-2.39	122.82	126.79
14	a	811	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
14	B	833	CLA	CHB-C4A-NA	2.38	127.81	124.51
14	B	807	CLA	O2A-CGA-O1A	-2.38	117.57	123.59
14	a	820	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
17	l	206	BCR	C31-C1-C6	2.38	114.17	110.30
14	b	842	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
14	a	833	CLA	CAC-C3C-C4C	2.38	127.90	124.81
14	B	837	CLA	C1B-CHB-C4A	-2.38	125.40	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	f	202	BCR	C10-C11-C12	-2.38	115.78	123.22
14	B	826	CLA	CAA-CBA-CGA	-2.38	106.29	113.25
14	B	842	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
19	X	1702	SQD	O48-C23-O10	-2.38	117.58	123.59
14	A	820	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
17	B	847	BCR	C20-C21-C22	-2.38	123.91	127.31
14	a	823	CLA	CHB-C4A-NA	2.38	127.80	124.51
14	A	837	CLA	O2D-CGD-CBD	2.38	115.50	111.27
14	b	839	CLA	C2A-C1A-CHA	2.38	128.02	123.86
17	B	846	BCR	C11-C10-C9	-2.38	123.92	127.31
17	k	103	BCR	C15-C14-C13	-2.38	123.92	127.31
14	a	806	CLA	CHB-C4A-NA	2.38	127.80	124.51
14	K	101	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
14	B	817	CLA	CHB-C4A-NA	2.38	127.80	124.51
14	A	842	CLA	CHB-C4A-NA	2.37	127.80	124.51
14	A	813	CLA	C2D-C1D-ND	-2.37	108.35	110.10
17	f	204	BCR	C24-C23-C22	-2.37	122.65	126.23
14	B	817	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
20	b	851	LMG	C42-C41-C40	-2.37	102.37	114.42
14	B	823	CLA	C3C-C4C-NC	-2.37	107.91	110.57
15	A	844	PQN	C2M-C2-C1	2.37	120.20	116.27
14	b	832	CLA	CHC-C1C-NC	2.37	127.80	124.20
14	B	825	CLA	CHB-C4A-NA	2.37	127.79	124.51
15	a	842	PQN	C2M-C2-C1	2.37	120.20	116.27
14	A	804	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
17	b	850	BCR	C15-C16-C17	-2.37	118.62	123.47
14	A	802	CLA	C1-C2-C3	-2.37	121.94	126.04
14	A	814	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
14	A	842	CLA	C4-C3-C5	2.37	119.26	115.27
17	b	849	BCR	C7-C8-C9	-2.37	122.66	126.23
17	m	1202	BCR	C30-C25-C26	-2.37	119.28	122.61
17	M	101	BCR	C38-C26-C27	-2.37	109.07	113.62
14	b	824	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
14	B	808	CLA	CHC-C1C-NC	2.37	127.79	124.20
17	I	102	BCR	C24-C23-C22	-2.36	122.66	126.23
14	A	805	CLA	CAA-CBA-CGA	-2.36	106.34	113.25
17	a	848	BCR	C24-C23-C22	-2.36	122.66	126.23
14	A	836	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
14	a	818	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
14	A	831	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
14	a	836	CLA	C2A-C1A-CHA	2.36	127.99	123.86
17	B	847	BCR	C40-C30-C25	2.36	114.13	110.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	831	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
14	A	842	CLA	CHD-C1D-ND	-2.36	122.29	124.45
14	B	823	CLA	CHD-C1D-ND	-2.36	122.29	124.45
17	A	846	BCR	C7-C8-C9	-2.36	122.67	126.23
14	a	822	CLA	C2D-C1D-ND	-2.36	108.37	110.10
19	l	202	SQD	O47-C7-C8	2.36	116.58	111.50
14	b	806	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
14	j	102	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
14	l	203	CLA	CHB-C4A-NA	2.35	127.77	124.51
14	A	834	CLA	O2D-CGD-CBD	2.35	115.45	111.27
14	B	843	CLA	O2D-CGD-CBD	2.35	115.45	111.27
14	F	204	CLA	O2A-CGA-O1A	-2.35	117.43	123.30
17	B	850	BCR	C27-C26-C25	2.35	126.15	122.73
14	b	830	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
14	a	826	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
14	A	835	CLA	CAA-CBA-CGA	-2.35	106.38	113.25
18	F	201	LHG	O8-C23-C24	2.35	119.29	111.91
20	B	851	LMG	O3-C3-C2	-2.35	104.91	110.35
14	B	829	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
14	b	813	CLA	CHD-C1D-ND	-2.35	122.29	124.45
14	A	829	CLA	C2D-C1D-ND	-2.35	108.37	110.10
14	b	828	CLA	CMC-C2C-C1C	-2.35	121.46	125.04
17	l	207	BCR	C28-C27-C26	-2.35	109.88	114.08
19	X	1702	SQD	C4-C3-C2	2.35	114.92	110.82
14	B	828	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
17	I	101	BCR	C15-C16-C17	-2.35	118.66	123.47
20	B	851	LMG	C42-C41-C40	-2.35	102.50	114.42
18	a	851	LHG	O4-P-O5	2.35	123.84	112.24
14	k	102	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
18	A	852	LHG	C27-C26-C25	-2.35	102.51	114.42
14	f	201	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
14	A	808	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
14	B	816	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
17	b	845	BCR	C15-C16-C17	-2.34	118.68	123.47
14	b	819	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
14	B	843	CLA	C1-C2-C3	-2.34	121.99	126.04
19	b	801	SQD	O47-C7-O49	-2.34	118.05	123.70
17	A	849	BCR	C16-C15-C14	-2.34	118.68	123.47
14	B	830	CLA	CHB-C4A-NA	2.34	127.75	124.51
18	A	852	LHG	C11-C10-C9	-2.34	102.55	114.42
14	A	839	CLA	CMB-C2B-C1B	-2.34	124.87	128.46
17	K	103	BCR	C24-C23-C22	-2.34	122.70	126.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	823	CLA	C2A-C1A-CHA	2.34	127.94	123.86
14	a	822	CLA	CHB-C4A-NA	2.34	127.74	124.51
14	m	1201	CLA	CHB-C4A-NA	2.34	127.74	124.51
14	A	817	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
14	A	806	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
17	B	849	BCR	C16-C15-C14	-2.33	118.70	123.47
14	a	818	CLA	C2D-C1D-ND	-2.33	108.39	110.10
14	A	838	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
14	B	828	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
14	b	841	CLA	CHB-C4A-NA	2.33	127.73	124.51
14	b	839	CLA	CAC-C3C-C2C	2.33	131.51	127.53
15	B	844	PQN	C14-C13-C15	2.33	119.19	115.27
17	A	850	BCR	C16-C17-C18	-2.33	123.99	127.31
13	a	801	CL0	CMD-C2D-C3D	-2.33	122.26	127.61
14	f	203	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
14	a	825	CLA	CHB-C4A-NA	2.33	127.73	124.51
17	l	206	BCR	C7-C8-C9	-2.33	122.72	126.23
14	b	837	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
14	a	825	CLA	CMB-C2B-C3B	2.33	129.03	124.68
18	i	103	LHG	O8-C23-O10	-2.33	117.72	123.59
13	A	801	CL0	CMA-C3A-C4A	-2.33	105.52	111.77
14	B	819	CLA	CHB-C4A-NA	2.32	127.73	124.51
17	b	847	BCR	C40-C30-C25	2.32	114.07	110.30
14	L	1502	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
13	A	801	CL0	CMD-C2D-C3D	-2.32	122.27	127.61
18	A	852	LHG	C20-C19-C18	-2.32	102.63	114.42
17	b	846	BCR	C7-C8-C9	-2.32	122.73	126.23
17	b	846	BCR	C2-C1-C6	2.32	114.05	110.48
14	a	827	CLA	C1-C2-C3	-2.32	122.03	126.04
14	L	1503	CLA	CHD-C1D-C2D	2.32	130.35	125.48
14	L	1503	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
14	B	805	CLA	O2D-CGD-CBD	2.32	115.39	111.27
14	A	822	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
17	A	849	BCR	C28-C27-C26	-2.32	109.94	114.08
17	J	103	BCR	C7-C8-C9	-2.32	122.73	126.23
14	b	821	CLA	C7-C6-C5	-2.32	107.07	113.36
14	a	816	CLA	CHB-C4A-NA	2.31	127.71	124.51
17	b	847	BCR	C3-C4-C5	-2.31	109.94	114.08
14	B	822	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
13	a	801	CL0	CMA-C3A-C4A	-2.31	105.56	111.77
17	B	846	BCR	C30-C25-C26	-2.31	119.36	122.61
14	A	841	CLA	CHD-C1D-ND	-2.31	122.33	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	807	CLA	C1-C2-C3	-2.31	122.04	126.04
17	I	101	BCR	C1-C6-C5	-2.31	119.36	122.61
14	b	813	CLA	O2D-CGD-CBD	2.31	115.38	111.27
14	a	835	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
14	b	803	CLA	C4D-C3D-CAD	-2.31	105.37	108.10
17	b	848	BCR	C29-C30-C25	2.31	114.04	110.48
14	a	803	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
17	A	849	BCR	C29-C30-C25	2.31	114.03	110.48
14	a	836	CLA	C2D-C1D-ND	-2.31	108.40	110.10
14	b	837	CLA	C2D-C1D-ND	-2.31	108.40	110.10
14	A	810	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
14	a	815	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
14	A	819	CLA	CHB-C4A-NA	2.30	127.70	124.51
14	L	1501	CLA	CAA-CBA-CGA	-2.30	106.52	113.25
14	b	805	CLA	C2A-C1A-CHA	2.30	127.89	123.86
14	A	810	CLA	O2A-CGA-O1A	-2.30	117.56	123.30
17	K	103	BCR	C11-C10-C9	-2.30	124.03	127.31
14	a	812	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
14	B	816	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
14	B	842	CLA	C2D-C1D-ND	-2.30	108.41	110.10
14	B	836	CLA	CHD-C1D-ND	-2.30	122.34	124.45
14	b	815	CLA	CHD-C1D-ND	-2.30	122.34	124.45
14	A	838	CLA	CHB-C4A-NA	2.30	127.69	124.51
14	a	830	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
14	a	832	CLA	O1D-CGD-CBD	2.29	129.18	124.48
14	A	830	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
17	a	848	BCR	C20-C21-C22	-2.29	124.04	127.31
14	A	821	CLA	CHB-C4A-NA	2.29	127.68	124.51
14	A	843	CLA	CHD-C1D-ND	-2.29	122.35	124.45
14	B	827	CLA	C6-C7-C8	-2.29	108.50	115.92
14	b	826	CLA	CAC-C3C-C4C	2.29	127.79	124.81
14	B	836	CLA	CAA-CBA-CGA	-2.29	106.55	113.25
14	X	1701	CLA	CAA-CBA-CGA	-2.29	106.56	113.25
14	A	833	CLA	C7-C6-C5	-2.29	107.14	113.36
14	a	833	CLA	C3C-C4C-NC	-2.29	108.00	110.57
14	B	807	CLA	O2D-CGD-CBD	2.29	115.34	111.27
18	A	853	LHG	O8-C23-C24	2.29	119.09	111.91
17	f	204	BCR	C16-C15-C14	-2.29	118.79	123.47
14	b	815	CLA	O2D-CGD-CBD	2.29	115.33	111.27
14	a	832	CLA	C1-C2-C3	-2.29	122.09	126.04
14	a	823	CLA	CMC-C2C-C3C	2.29	132.33	126.12
14	A	840	CLA	C1B-CHB-C4A	-2.29	125.59	130.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	827	CLA	C4-C3-C5	2.29	119.12	115.27
14	K	102	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
14	L	1501	CLA	C2A-C1A-CHA	2.29	127.86	123.86
17	j	104	BCR	C28-C27-C26	-2.28	110.00	114.08
14	A	802	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
14	a	818	CLA	CHB-C4A-NA	2.28	127.67	124.51
14	b	822	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
14	b	819	CLA	CHD-C1D-ND	-2.28	122.36	124.45
14	b	843	CLA	C4-C3-C5	2.28	119.11	115.27
14	b	822	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
14	A	821	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
17	J	103	BCR	C16-C15-C14	-2.28	118.80	123.47
17	B	847	BCR	C24-C23-C22	-2.28	122.79	126.23
18	A	853	LHG	C11-C10-C9	-2.28	102.86	114.42
14	A	834	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
14	b	809	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
14	B	822	CLA	CHB-C4A-NA	2.28	127.66	124.51
17	i	102	BCR	C27-C26-C25	2.28	126.04	122.73
14	A	819	CLA	O2D-CGD-CBD	2.28	115.31	111.27
17	A	851	BCR	C33-C5-C6	-2.28	121.97	124.53
14	B	834	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
14	A	842	CLA	C11-C12-C13	-2.28	108.56	115.92
17	B	848	BCR	C30-C25-C26	-2.28	119.41	122.61
17	m	1202	BCR	C24-C23-C22	-2.27	122.80	126.23
17	j	105	BCR	C11-C10-C9	-2.27	124.06	127.31
14	B	839	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
14	a	808	CLA	CAA-CBA-CGA	-2.27	106.61	113.25
14	a	814	CLA	C2A-C1A-CHA	2.27	127.83	123.86
14	b	840	CLA	O2D-CGD-CBD	2.27	115.31	111.27
14	k	101	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
14	A	814	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
15	B	844	PQN	O1-C1-C10	-2.27	117.88	121.56
14	b	828	CLA	CMC-C2C-C3C	2.27	132.28	126.12
14	B	837	CLA	CAA-CBA-CGA	-2.27	106.48	112.51
17	a	847	BCR	C15-C16-C17	-2.27	118.82	123.47
14	b	808	CLA	C2A-C1A-CHA	2.27	127.83	123.86
14	J	102	CLA	CMA-C3A-C2A	-2.27	110.80	116.10
14	b	835	CLA	CMB-C2B-C3B	2.27	128.92	124.68
14	b	805	CLA	C11-C10-C8	-2.27	108.58	115.92
14	A	820	CLA	C2D-C1D-ND	-2.27	108.43	110.10
14	B	830	CLA	C1-C2-C3	-2.27	122.12	126.04
14	b	843	CLA	C1C-C2C-C3C	-2.27	104.57	106.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	803	CLA	C2D-C1D-ND	-2.27	108.43	110.10
14	b	821	CLA	C3C-C4C-NC	-2.27	108.03	110.57
17	A	846	BCR	C29-C30-C25	2.27	113.97	110.48
14	f	201	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
14	b	814	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
14	A	807	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
14	a	810	CLA	O1D-CGD-CBD	2.26	129.12	124.48
17	a	847	BCR	C27-C26-C25	2.26	126.02	122.73
14	B	813	CLA	C3B-C4B-NB	-2.26	106.29	109.21
14	b	816	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
14	B	830	CLA	C2A-C1A-CHA	2.26	127.81	123.86
14	b	805	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
17	A	851	BCR	C28-C27-C26	-2.26	110.05	114.08
14	b	828	CLA	CHD-C1D-ND	-2.26	122.38	124.45
17	b	846	BCR	C1-C6-C5	-2.25	119.44	122.61
17	K	103	BCR	C15-C14-C13	-2.25	124.10	127.31
14	b	802	CLA	CHB-C4A-NA	2.25	127.63	124.51
14	A	819	CLA	CHD-C1D-ND	-2.25	122.39	124.45
14	B	832	CLA	C3A-C2A-C1A	2.25	104.71	101.34
17	j	106	BCR	C24-C23-C22	-2.25	122.84	126.23
17	I	102	BCR	C11-C10-C9	-2.25	124.10	127.31
14	B	840	CLA	C11-C12-C13	-2.25	108.65	115.92
15	b	844	PQN	C2M-C2-C3	-2.25	120.73	124.40
17	A	847	BCR	C29-C30-C25	2.25	113.94	110.48
14	A	811	CLA	O1D-CGD-CBD	2.25	129.08	124.48
20	B	803	LMG	O3-C3-C2	-2.25	105.16	110.35
14	A	822	CLA	O2D-CGD-CBD	2.25	115.26	111.27
14	A	825	CLA	CHA-C1A-NA	-2.24	121.26	126.40
14	b	821	CLA	C11-C12-C13	-2.24	108.67	115.92
17	f	204	BCR	C38-C26-C27	-2.24	109.31	113.62
14	b	821	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
17	l	201	BCR	C16-C15-C14	-2.24	118.89	123.47
14	A	827	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
14	B	801	CLA	O1D-CGD-CBD	2.24	129.07	124.48
20	b	851	LMG	C38-C37-C36	-2.24	103.06	114.42
14	b	817	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
17	a	848	BCR	C27-C26-C25	2.24	125.98	122.73
14	a	816	CLA	C2D-C1D-ND	-2.24	108.45	110.10
14	A	820	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
14	a	830	CLA	O2D-CGD-CBD	2.24	115.25	111.27
14	a	840	CLA	CHD-C1D-ND	-2.24	122.40	124.45
14	A	824	CLA	C2D-C1D-ND	-2.24	108.45	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	j	105	BCR	C28-C27-C26	-2.24	110.08	114.08
14	F	202	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
17	I	101	BCR	C28-C27-C26	-2.24	110.08	114.08
14	B	812	CLA	CAA-CBA-CGA	-2.24	106.72	113.25
14	B	827	CLA	CAC-C3C-C4C	2.23	127.71	124.81
14	B	812	CLA	O2D-CGD-CBD	2.23	115.24	111.27
14	A	834	CLA	CHC-C1C-NC	2.23	127.59	124.20
14	b	839	CLA	CAC-C3C-C4C	-2.23	121.91	124.81
14	b	818	CLA	CHD-C1D-ND	-2.23	122.40	124.45
14	A	804	CLA	O1D-CGD-CBD	2.23	129.05	124.48
14	f	203	CLA	CHB-C4A-NA	2.23	127.60	124.51
14	b	805	CLA	CHA-C1A-NA	-2.23	121.29	126.40
20	b	851	LMG	C1-C2-C3	-2.23	105.35	110.00
14	a	820	CLA	O2A-C1-C2	-2.23	102.78	108.64
14	b	835	CLA	C1-C2-C3	-2.23	122.19	126.04
14	F	202	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
14	B	814	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
14	B	814	CLA	CHD-C1D-ND	-2.23	122.41	124.45
14	b	816	CLA	CHB-C4A-NA	2.23	127.59	124.51
17	L	1504	BCR	C27-C26-C25	2.22	125.96	122.73
14	F	202	CLA	CBC-CAC-C3C	2.22	118.56	112.43
17	A	847	BCR	C3-C4-C5	-2.22	110.11	114.08
19	b	801	SQD	C3-C4-C5	2.22	114.20	110.24
14	A	802	CLA	C2A-C1A-CHA	2.22	127.75	123.86
14	A	839	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
14	B	822	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
17	M	101	BCR	C35-C13-C12	2.22	121.58	118.08
14	B	836	CLA	C1-O2A-CGA	2.22	122.27	116.44
14	a	831	CLA	C2A-C1A-CHA	2.22	127.74	123.86
17	m	1202	BCR	C15-C14-C13	-2.22	124.15	127.31
14	B	829	CLA	C2A-C1A-CHA	2.22	127.73	123.86
14	a	838	CLA	CMB-C2B-C3B	2.22	128.82	124.68
17	i	101	BCR	C29-C30-C25	2.22	113.89	110.48
14	b	822	CLA	CHC-C1C-NC	2.22	127.56	124.20
17	M	101	BCR	C30-C25-C26	-2.21	119.49	122.61
14	b	836	CLA	C2D-C1D-ND	-2.21	108.47	110.10
14	b	823	CLA	C2A-C1A-CHA	2.21	127.73	123.86
14	a	831	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
14	B	840	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
14	a	802	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
14	b	815	CLA	CAC-C3C-C2C	2.21	131.31	127.53
14	b	831	CLA	CHB-C4A-NA	2.21	127.57	124.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	809	CLA	O1D-CGD-CBD	2.21	129.01	124.48
14	a	832	CLA	C2D-C1D-ND	-2.21	108.47	110.10
14	a	808	CLA	O2D-CGD-CBD	2.21	115.20	111.27
14	b	841	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
14	b	841	CLA	CHD-C1D-ND	-2.21	122.42	124.45
14	B	830	CLA	O2D-CGD-CBD	2.21	115.19	111.27
14	b	832	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
14	A	822	CLA	CHD-C1D-ND	-2.21	122.43	124.45
20	B	803	LMG	O2-C2-C1	-2.21	104.69	110.05
15	a	842	PQN	C26-C25-C23	-2.21	108.79	115.92
14	A	816	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
17	f	204	BCR	C40-C30-C25	2.20	113.88	110.30
14	b	802	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
14	A	818	CLA	CHB-C4A-NA	2.20	127.56	124.51
14	B	813	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
14	B	812	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
14	B	811	CLA	CHC-C1C-NC	2.20	127.54	124.20
18	F	201	LHG	C27-C26-C25	-2.20	103.26	114.42
14	j	101	CLA	CAA-CBA-CGA	-2.20	106.83	113.25
14	b	826	CLA	CHD-C1D-ND	-2.20	122.43	124.45
14	B	806	CLA	O1D-CGD-CBD	2.20	128.98	124.48
14	B	838	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
17	m	1202	BCR	C40-C30-C25	2.20	113.86	110.30
14	b	829	CLA	CAA-C2A-C3A	-2.20	106.77	112.78
14	A	807	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
14	B	840	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
17	B	845	BCR	C27-C26-C25	2.20	125.92	122.73
14	B	802	CLA	O1D-CGD-CBD	2.19	128.97	124.48
14	b	820	CLA	O2D-CGD-CBD	2.19	115.17	111.27
17	I	101	BCR	C38-C26-C27	-2.19	109.40	113.62
14	a	804	CLA	O2D-CGD-CBD	2.19	115.16	111.27
14	A	834	CLA	CBC-CAC-C3C	2.19	118.47	112.43
14	B	822	CLA	C1-C2-C3	-2.19	122.25	126.04
14	B	828	CLA	C3A-C2A-C1A	2.19	104.62	101.34
14	F	204	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
17	A	849	BCR	C37-C22-C23	2.19	121.53	118.08
14	A	809	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
14	b	806	CLA	CBA-CAA-C2A	-2.19	107.41	113.86
17	a	848	BCR	C11-C10-C9	-2.19	124.19	127.31
14	b	834	CLA	CHD-C1D-ND	-2.19	122.44	124.45
14	J	101	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
14	b	837	CLA	O2A-CGA-O1A	-2.19	117.85	123.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	802	CLA	CHA-C1A-NA	-2.19	121.39	126.40
14	a	838	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
14	a	827	CLA	C16-C15-C13	-2.18	108.86	115.92
14	B	809	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
15	b	844	PQN	C12-C11-C3	-2.18	106.16	112.05
14	a	829	CLA	CMC-C2C-C3C	2.18	132.05	126.12
14	a	835	CLA	CHB-C4A-NA	2.18	127.53	124.51
14	a	833	CLA	C11-C12-C13	-2.18	108.86	115.92
14	a	821	CLA	O2A-CGA-O1A	-2.18	117.86	123.30
14	A	836	CLA	O2A-CGA-O1A	-2.18	117.86	123.30
18	i	103	LHG	C27-C26-C25	-2.18	103.35	114.42
14	a	833	CLA	O1D-CGD-CBD	2.18	128.95	124.48
14	b	816	CLA	CBC-CAC-C3C	2.18	118.44	112.43
14	b	836	CLA	C3C-C4C-NC	-2.18	108.12	110.57
14	B	839	CLA	CHA-C1A-NA	-2.18	121.40	126.40
17	j	105	BCR	C7-C8-C9	-2.18	122.94	126.23
17	f	202	BCR	C38-C26-C27	-2.18	109.43	113.62
14	b	842	CLA	C3A-C2A-C1A	2.18	104.61	101.34
17	k	103	BCR	C28-C27-C26	-2.18	110.19	114.08
14	a	829	CLA	C2A-C1A-CHA	2.18	127.67	123.86
14	a	831	CLA	CHD-C1D-ND	-2.18	122.45	124.45
14	a	821	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
14	b	821	CLA	C2A-C1A-CHA	2.18	127.67	123.86
17	i	101	BCR	C10-C11-C12	-2.18	116.42	123.22
17	B	847	BCR	C37-C22-C21	-2.18	119.87	122.92
14	A	838	CLA	C3A-C2A-C1A	2.18	104.60	101.34
14	B	819	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
14	a	827	CLA	C2A-C1A-CHA	2.17	127.66	123.86
14	B	827	CLA	CHA-C1A-NA	-2.17	121.42	126.40
14	B	828	CLA	CHD-C1D-ND	-2.17	122.46	124.45
14	B	818	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
14	B	804	CLA	C11-C12-C13	-2.17	108.89	115.92
14	A	806	CLA	C2A-C1A-CHA	2.17	127.66	123.86
14	a	816	CLA	CHD-C1D-ND	-2.17	122.46	124.45
14	B	811	CLA	C3C-C4C-NC	-2.17	108.13	110.57
14	A	826	CLA	C2D-C1D-ND	-2.17	108.50	110.10
14	B	839	CLA	C1-C2-C3	-2.17	122.29	126.04
14	B	813	CLA	C6-C7-C8	-2.17	108.90	115.92
18	A	853	LHG	C27-C26-C25	-2.17	103.40	114.42
14	B	839	CLA	O2D-CGD-CBD	2.17	115.13	111.27
14	A	826	CLA	CHD-C1D-ND	-2.17	122.46	124.45
14	A	809	CLA	O2A-CGA-O1A	-2.17	118.11	123.59

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	837	CLA	C3A-C2A-C1A	2.17	104.59	101.34
14	b	821	CLA	C2D-C1D-ND	-2.17	108.50	110.10
17	l	201	BCR	C11-C10-C9	-2.17	124.21	127.31
17	j	105	BCR	C33-C5-C6	-2.17	122.09	124.53
14	l	204	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
14	b	819	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
14	a	836	CLA	CHB-C4A-NA	2.17	127.51	124.51
14	B	812	CLA	C1-C2-C3	-2.17	122.30	126.04
20	B	803	LMG	O1-C7-C8	-2.17	105.67	110.90
14	B	828	CLA	CHC-C1C-NC	2.17	127.49	124.20
14	B	817	CLA	CHD-C1D-ND	-2.17	122.46	124.45
14	A	818	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
14	a	829	CLA	CHC-C1C-NC	2.17	127.49	124.20
14	B	802	CLA	CHD-C1D-ND	-2.17	122.46	124.45
17	F	203	BCR	C40-C30-C25	2.17	113.81	110.30
14	a	816	CLA	CAC-C3C-C4C	2.16	127.62	124.81
14	B	820	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
14	b	809	CLA	CBA-CAA-C2A	-2.16	107.48	113.86
14	b	807	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
14	f	201	CLA	CHB-C4A-NA	2.16	127.50	124.51
14	b	837	CLA	C2A-C1A-CHA	2.16	127.64	123.86
17	B	847	BCR	C7-C8-C9	-2.16	122.97	126.23
20	b	851	LMG	O7-C10-O9	-2.16	118.48	123.70
14	j	101	CLA	CMB-C2B-C3B	2.16	128.72	124.68
14	B	838	CLA	CMB-C2B-C3B	2.16	128.72	124.68
17	F	203	BCR	C16-C15-C14	-2.16	119.05	123.47
14	B	818	CLA	CHB-C4A-NA	2.16	127.50	124.51
14	A	831	CLA	CHD-C1D-C2D	2.16	130.01	125.48
17	l	207	BCR	C2-C1-C6	2.16	113.81	110.48
17	A	851	BCR	C7-C8-C9	-2.16	122.97	126.23
17	l	206	BCR	C35-C13-C14	-2.16	119.90	122.92
14	A	830	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
13	A	801	CL0	CMB-C2B-C3B	2.16	128.71	124.68
14	B	837	CLA	C2D-C1D-ND	-2.16	108.52	110.10
14	B	808	CLA	C2D-C1D-ND	-2.15	108.52	110.10
17	J	103	BCR	C27-C26-C25	2.15	125.86	122.73
14	A	818	CLA	C2A-C1A-CHA	2.15	127.62	123.86
14	B	809	CLA	CHA-C1A-NA	-2.15	121.47	126.40
14	K	102	CLA	CHA-C1A-NA	-2.15	121.47	126.40
17	l	201	BCR	C27-C26-C25	2.15	125.86	122.73
15	b	844	PQN	C2M-C2-C1	2.15	119.83	116.27
14	A	802	CLA	C4D-C3D-CAD	-2.15	105.56	108.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	828	CLA	C4-C3-C5	2.15	118.89	115.27
14	l	205	CLA	C2D-C1D-ND	-2.15	108.52	110.10
14	A	840	CLA	CHB-C4A-NA	2.15	127.48	124.51
14	A	813	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
17	j	104	BCR	C21-C20-C19	-2.15	116.52	123.22
17	I	101	BCR	C2-C1-C6	2.15	113.79	110.48
14	b	840	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
14	A	821	CLA	C3B-C4B-NB	-2.15	106.44	109.21
14	b	832	CLA	C7-C6-C5	-2.15	107.53	113.36
14	B	841	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
17	b	847	BCR	C16-C15-C14	-2.15	119.08	123.47
14	b	835	CLA	C3B-C4B-NB	-2.14	106.44	109.21
14	a	808	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
14	a	812	CLA	CHB-C4A-NA	2.14	127.48	124.51
14	B	809	CLA	C2A-C1A-CHA	2.14	127.61	123.86
20	B	851	LMG	O1-C1-C2	-2.14	104.96	108.30
14	B	828	CLA	O1D-CGD-CBD	2.14	128.87	124.48
14	A	835	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
13	a	801	CL0	CMB-C2B-C3B	2.14	128.69	124.68
14	a	808	CLA	C2D-C1D-ND	-2.14	108.53	110.10
14	A	834	CLA	C11-C12-C13	-2.14	109.00	115.92
14	B	824	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
14	b	812	CLA	C3C-C4C-NC	-2.14	108.17	110.57
14	B	829	CLA	O2D-CGD-CBD	2.14	115.07	111.27
14	b	812	CLA	O2D-CGD-CBD	2.14	115.07	111.27
14	B	819	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
14	a	822	CLA	CHD-C1D-C2D	2.14	129.97	125.48
17	j	104	BCR	C29-C30-C25	2.14	113.77	110.48
14	a	821	CLA	C2A-C1A-CHA	2.14	127.60	123.86
14	a	832	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
14	b	843	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
14	B	839	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
14	B	815	CLA	C2D-C1D-ND	-2.13	108.53	110.10
14	a	823	CLA	O2A-CGA-O1A	-2.13	117.98	123.30
17	K	103	BCR	C27-C26-C25	2.13	125.83	122.73
14	a	830	CLA	CHB-C4A-NA	2.13	127.46	124.51
14	j	102	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
14	k	102	CLA	CHA-C1A-NA	-2.13	121.52	126.40
14	A	809	CLA	C3A-C2A-C1A	2.13	104.53	101.34
17	M	101	BCR	C35-C13-C14	-2.13	119.94	122.92
14	A	823	CLA	CHD-C1D-ND	-2.13	122.50	124.45
14	b	803	CLA	O2D-CGD-CBD	2.13	115.05	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	811	CLA	C3A-C2A-C1A	2.13	104.53	101.34
17	A	847	BCR	C11-C10-C9	-2.13	124.27	127.31
14	a	826	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
14	a	841	CLA	CHD-C1D-ND	-2.13	122.50	124.45
17	B	846	BCR	C7-C8-C9	-2.13	123.02	126.23
17	k	103	BCR	C7-C8-C9	-2.13	123.02	126.23
17	i	102	BCR	C10-C11-C12	-2.13	116.58	123.22
14	a	835	CLA	O2D-CGD-CBD	2.13	115.05	111.27
15	b	844	PQN	C11-C3-C4	2.13	120.78	118.50
14	A	805	CLA	C1-C2-C3	-2.12	122.37	126.04
14	a	829	CLA	C2D-C1D-ND	-2.12	108.54	110.10
14	B	838	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
14	a	831	CLA	CHA-C1A-NA	-2.12	121.53	126.40
14	a	818	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
17	B	850	BCR	C10-C11-C12	-2.12	116.59	123.22
14	A	821	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
14	a	819	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
17	J	105	BCR	C34-C9-C10	-2.12	119.95	122.92
14	b	836	CLA	O2D-CGD-CBD	2.12	115.04	111.27
14	B	812	CLA	C3A-C2A-C1A	2.12	104.52	101.34
14	a	819	CLA	CHD-C1D-ND	-2.12	122.50	124.45
14	b	803	CLA	C4D-CHA-C1A	2.12	123.83	121.25
17	i	102	BCR	C1-C6-C5	-2.12	119.63	122.61
17	b	847	BCR	C10-C11-C12	-2.12	116.60	123.22
14	b	830	CLA	CHB-C4A-NA	2.12	127.44	124.51
14	a	810	CLA	C11-C12-C13	-2.12	109.07	115.92
14	a	810	CLA	C1-O2A-CGA	2.12	122.00	116.44
14	a	817	CLA	C2A-C1A-CHA	2.12	127.56	123.86
17	b	850	BCR	C27-C26-C25	2.12	125.81	122.73
14	b	827	CLA	C6-C7-C8	-2.12	109.07	115.92
14	a	837	CLA	C2A-C1A-CHA	2.12	127.56	123.86
14	b	813	CLA	CHB-C4A-NA	2.12	127.44	124.51
14	a	824	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
14	a	820	CLA	O2D-CGD-CBD	2.12	115.03	111.27
17	f	204	BCR	C35-C13-C14	-2.12	119.96	122.92
17	B	845	BCR	C39-C30-C25	2.12	113.73	110.30
14	b	829	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
14	b	832	CLA	CMC-C2C-C3C	2.12	131.86	126.12
17	l	201	BCR	C37-C22-C21	-2.12	119.96	122.92
14	l	203	CLA	O2A-CGA-O1A	-2.12	118.03	123.30
17	l	201	BCR	C35-C13-C14	-2.12	119.96	122.92
14	b	832	CLA	C3A-C2A-C1A	2.12	104.51	101.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	813	CLA	CAA-C2A-C3A	-2.12	106.99	112.78
17	l	207	BCR	C1-C6-C5	-2.11	119.64	122.61
14	B	812	CLA	C6-C7-C8	-2.11	109.08	115.92
14	A	829	CLA	O2D-CGD-CBD	2.11	115.03	111.27
14	B	832	CLA	C7-C6-C5	-2.11	107.62	113.36
17	J	104	BCR	C33-C5-C6	-2.11	122.15	124.53
14	A	833	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
18	A	852	LHG	C18-C17-C16	-2.11	103.71	114.42
15	b	844	PQN	C17-C16-C15	-2.11	107.63	113.36
14	a	805	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
14	B	843	CLA	C3A-C2A-C1A	2.11	104.50	101.34
14	a	827	CLA	CHD-C1D-ND	-2.11	122.52	124.45
14	j	101	CLA	C2A-C1A-CHA	2.11	127.54	123.86
14	j	103	CLA	CMA-C3A-C2A	-2.11	111.18	116.10
14	B	828	CLA	C6-C7-C8	-2.10	109.11	115.92
14	B	827	CLA	C1-C2-C3	-2.10	122.40	126.04
14	b	807	CLA	CHD-C1D-C2D	2.10	129.89	125.48
14	b	806	CLA	CMC-C2C-C1C	2.10	128.24	125.04
14	b	823	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
14	A	827	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
14	b	836	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
18	i	103	LHG	C20-C19-C18	-2.10	103.75	114.42
14	b	829	CLA	C2A-C1A-CHA	2.10	127.53	123.86
14	A	829	CLA	C1D-ND-C4D	2.10	107.83	106.33
17	a	847	BCR	C30-C25-C26	-2.10	119.65	122.61
14	A	841	CLA	C1-C2-C3	-2.10	122.41	126.04
14	b	813	CLA	C2A-C1A-CHA	2.10	127.53	123.86
14	B	824	CLA	CHD-C1D-ND	-2.10	122.52	124.45
14	b	812	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
14	B	826	CLA	O2D-CGD-CBD	2.10	115.00	111.27
14	a	813	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
14	B	818	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
14	A	837	CLA	CHD-C1D-ND	-2.10	122.53	124.45
17	A	850	BCR	C24-C23-C22	-2.10	123.06	126.23
14	A	831	CLA	O2D-CGD-CBD	2.10	114.99	111.27
14	b	832	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
14	A	838	CLA	C2D-C1D-ND	-2.10	108.56	110.10
14	a	828	CLA	C6-C7-C8	-2.09	109.15	115.92
17	M	101	BCR	C16-C17-C18	-2.09	124.32	127.31
17	A	849	BCR	C11-C10-C9	-2.09	124.32	127.31
14	b	832	CLA	CMC-C2C-C1C	-2.09	121.85	125.04
14	a	804	CLA	CHD-C1D-ND	-2.09	122.53	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	102	BCR	C30-C25-C26	-2.09	119.67	122.61
17	A	846	BCR	C11-C10-C9	-2.09	124.33	127.31
14	X	1701	CLA	C2A-C1A-CHA	2.09	127.52	123.86
14	B	823	CLA	CHC-C1C-NC	2.09	127.38	124.20
17	a	849	BCR	C3-C4-C5	-2.09	110.34	114.08
14	a	822	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
14	a	816	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
14	b	808	CLA	C16-C15-C13	-2.09	109.17	115.92
14	b	811	CLA	C3A-C2A-C1A	2.09	104.47	101.34
14	a	804	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
14	B	815	CLA	CBC-CAC-C3C	2.09	118.18	112.43
14	a	804	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
14	B	833	CLA	C1B-CHB-C4A	-2.09	125.99	130.12
14	B	836	CLA	CBA-CAA-C2A	2.09	120.02	113.86
14	a	824	CLA	CAA-C2A-C3A	-2.09	107.07	112.78
17	J	105	BCR	C35-C13-C14	-2.08	120.00	122.92
14	B	836	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
14	a	804	CLA	CMA-C3A-C2A	-2.08	105.42	113.83
14	A	830	CLA	CMC-C2C-C1C	-2.08	121.87	125.04
17	f	204	BCR	C2-C1-C6	2.08	113.69	110.48
14	A	832	CLA	CHA-C4D-ND	2.08	136.85	132.50
14	A	807	CLA	CHD-C1D-ND	-2.08	122.54	124.45
14	B	806	CLA	CHD-C4C-C3C	2.08	127.90	124.84
14	A	808	CLA	CAA-C2A-C1A	-2.08	105.16	111.97
14	B	832	CLA	CAA-CBA-CGA	-2.08	107.18	113.25
17	A	848	BCR	C35-C13-C14	-2.08	120.01	122.92
17	b	850	BCR	C35-C13-C14	-2.08	120.01	122.92
14	b	836	CLA	C2A-C1A-CHA	2.08	127.49	123.86
18	i	103	LHG	C11-C10-C9	-2.08	103.88	114.42
14	b	827	CLA	O2D-CGD-CBD	2.08	114.96	111.27
14	B	821	CLA	CBA-CAA-C2A	2.08	119.99	113.86
14	B	804	CLA	C16-C15-C13	-2.08	109.21	115.92
14	A	806	CLA	C16-C15-C13	-2.08	109.21	115.92
15	B	844	PQN	C2M-C2-C3	-2.08	121.01	124.40
14	a	821	CLA	C3A-C2A-C1A	2.08	104.45	101.34
14	L	1503	CLA	O1D-CGD-CBD	2.08	128.73	124.48
14	a	831	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
14	A	841	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
14	A	802	CLA	C1D-ND-C4D	2.07	107.81	106.33
14	b	820	CLA	C2D-C1D-ND	-2.07	108.58	110.10
14	B	814	CLA	O1D-CGD-CBD	2.07	128.73	124.48
14	B	816	CLA	O2D-CGD-CBD	2.07	114.95	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	821	CLA	CHD-C1D-ND	-2.07	122.55	124.45
14	A	829	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
14	A	820	CLA	CHD-C1D-ND	-2.07	122.55	124.45
14	B	843	CLA	CHD-C1D-ND	-2.07	122.55	124.45
17	A	847	BCR	C15-C16-C17	-2.07	119.23	123.47
17	A	846	BCR	C24-C23-C22	-2.07	123.11	126.23
14	A	829	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
14	A	840	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
19	b	801	SQD	O48-C23-O10	-2.07	118.37	123.59
14	A	833	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
14	B	813	CLA	CHB-C4A-NA	2.07	127.37	124.51
14	m	1201	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
14	B	835	CLA	C3A-C2A-C1A	2.07	104.44	101.34
17	l	207	BCR	C29-C30-C25	2.07	113.66	110.48
14	A	825	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
14	A	821	CLA	CHA-C1A-NA	-2.07	121.67	126.40
14	b	826	CLA	O2D-CGD-CBD	2.07	114.94	111.27
17	I	102	BCR	C38-C26-C27	-2.07	109.65	113.62
14	B	831	CLA	O2D-CGD-CBD	2.07	114.94	111.27
14	K	101	CLA	C2D-C1D-ND	-2.07	108.58	110.10
14	a	804	CLA	CAA-C2A-C3A	-2.06	107.12	112.78
17	k	103	BCR	C1-C6-C5	-2.06	119.71	122.61
14	b	824	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
17	I	101	BCR	C30-C25-C26	-2.06	119.71	122.61
19	X	1702	SQD	O48-C23-C24	2.06	118.38	111.91
17	i	101	BCR	C1-C6-C5	-2.06	119.71	122.61
14	B	808	CLA	C2A-C1A-CHA	2.06	127.47	123.86
14	B	841	CLA	CMB-C2B-C3B	2.06	128.54	124.68
14	l	205	CLA	C3A-C2A-C1A	2.06	104.43	101.34
17	A	850	BCR	C1-C6-C5	-2.06	119.71	122.61
14	a	829	CLA	CHA-C1A-NA	-2.06	121.68	126.40
14	B	832	CLA	CHB-C4A-NA	2.06	127.36	124.51
14	b	829	CLA	C16-C15-C13	-2.06	109.26	115.92
17	l	206	BCR	C15-C16-C17	-2.06	119.25	123.47
18	A	852	LHG	C29-C28-C27	-2.06	103.97	114.42
14	A	841	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
14	L	1501	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
14	a	830	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
14	F	202	CLA	CMB-C2B-C3B	2.06	128.53	124.68
14	a	836	CLA	C1D-ND-C4D	2.06	107.80	106.33
14	a	819	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
14	b	816	CLA	CHA-C1A-NA	-2.06	121.69	126.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	818	CLA	C3C-C4C-NC	-2.06	108.27	110.57
14	f	201	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
14	B	838	CLA	O1D-CGD-CBD	2.05	128.69	124.48
17	I	102	BCR	C37-C22-C21	-2.05	120.05	122.92
17	b	846	BCR	C38-C26-C27	-2.05	109.67	113.62
14	B	831	CLA	CHA-C4D-ND	2.05	136.79	132.50
20	B	851	LMG	O8-C28-O10	-2.05	118.41	123.59
14	A	805	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
17	J	105	BCR	C2-C1-C6	2.05	113.64	110.48
14	a	806	CLA	C2D-C1D-ND	-2.05	108.59	110.10
17	a	847	BCR	C38-C26-C27	-2.05	109.68	113.62
14	A	813	CLA	CAC-C3C-C2C	-2.05	124.02	127.53
17	f	202	BCR	C30-C25-C26	-2.05	119.73	122.61
17	i	102	BCR	C29-C30-C25	2.05	113.64	110.48
14	a	813	CLA	CHD-C1D-ND	-2.05	122.57	124.45
14	b	825	CLA	CHD-C1D-ND	-2.05	122.57	124.45
14	F	204	CLA	C2A-C1A-CHA	2.05	127.44	123.86
14	b	830	CLA	CHA-C1A-NA	-2.05	121.71	126.40
17	B	846	BCR	C29-C30-C25	2.05	113.63	110.48
14	a	838	CLA	O2D-CGD-CBD	2.05	114.90	111.27
17	l	206	BCR	C40-C30-C29	-2.05	100.72	108.91
14	a	822	CLA	CMB-C2B-C3B	2.05	128.51	124.68
17	m	1202	BCR	C12-C13-C14	-2.05	115.80	118.94
17	F	205	BCR	C2-C1-C6	2.04	113.62	110.48
14	B	811	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
17	b	846	BCR	C24-C23-C22	-2.04	123.15	126.23
17	i	101	BCR	C30-C25-C26	-2.04	119.74	122.61
14	B	828	CLA	C1D-ND-C4D	2.04	107.78	106.33
17	B	845	BCR	C15-C16-C17	-2.04	119.29	123.47
14	F	204	CLA	CHA-C1A-NA	-2.04	121.72	126.40
14	B	811	CLA	CAA-CBA-CGA	2.04	119.22	113.25
14	B	819	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
17	m	1202	BCR	C38-C26-C27	-2.04	109.70	113.62
14	a	804	CLA	O2A-C1-C2	-2.04	103.27	108.64
14	B	808	CLA	C11-C12-C13	-2.04	109.33	115.92
14	A	836	CLA	C2A-C1A-CHA	2.04	127.42	123.86
14	B	840	CLA	CBA-CAA-C2A	2.04	119.88	113.86
17	J	105	BCR	C30-C25-C26	-2.04	119.74	122.61
14	A	806	CLA	O1D-CGD-CBD	2.04	128.65	124.48
14	b	813	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
17	l	201	BCR	C21-C20-C19	-2.04	116.86	123.22
17	j	106	BCR	C3-C4-C5	-2.04	110.44	114.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	847	BCR	C7-C8-C9	-2.04	123.16	126.23
17	a	848	BCR	C38-C26-C27	-2.03	109.71	113.62
19	X	1702	SQD	O47-C45-C44	2.03	115.77	108.40
14	b	813	CLA	O1D-CGD-CBD	2.03	128.65	124.48
14	A	824	CLA	C2A-C1A-CHA	2.03	127.42	123.86
14	B	843	CLA	CMC-C2C-C3C	2.03	131.64	126.12
14	A	820	CLA	C2A-C1A-CHA	2.03	127.42	123.86
14	a	816	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
14	a	828	CLA	O2D-CGD-CBD	2.03	114.88	111.27
14	A	803	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
14	b	830	CLA	C2A-C1A-CHA	2.03	127.41	123.86
14	a	806	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
14	k	102	CLA	O2D-CGD-CBD	2.03	114.88	111.27
17	i	102	BCR	C16-C15-C14	-2.03	119.31	123.47
17	a	844	BCR	C38-C26-C27	-2.03	109.72	113.62
14	A	806	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
15	A	844	PQN	C14-C13-C15	2.03	118.69	115.27
14	B	842	CLA	O1D-CGD-CBD	2.03	128.64	124.48
14	a	802	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
14	j	101	CLA	O2D-CGD-CBD	2.03	114.87	111.27
14	B	841	CLA	CHD-C1D-ND	-2.03	122.59	124.45
14	B	843	CLA	CMB-C2B-C3B	2.03	128.47	124.68
19	x	1702	SQD	O48-C23-C24	2.03	118.27	111.91
14	b	839	CLA	CHA-C4D-ND	2.03	136.74	132.50
14	A	830	CLA	C2D-C1D-ND	-2.03	108.61	110.10
14	m	1201	CLA	C2D-C1D-ND	-2.03	108.61	110.10
14	b	828	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
17	B	846	BCR	C15-C16-C17	-2.03	119.32	123.47
17	L	1504	BCR	C40-C30-C29	-2.03	100.80	108.91
17	A	850	BCR	C30-C25-C26	-2.03	119.76	122.61
14	a	836	CLA	CHA-C1A-NA	-2.03	121.76	126.40
14	A	823	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
14	a	805	CLA	CAA-C2A-C3A	-2.02	107.23	112.78
14	a	805	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
14	A	839	CLA	C16-C15-C13	-2.02	109.38	115.92
17	L	1504	BCR	C30-C25-C26	-2.02	119.77	122.61
14	b	805	CLA	C3C-C4C-NC	-2.02	108.30	110.57
17	a	844	BCR	C28-C27-C26	-2.02	110.47	114.08
14	B	804	CLA	CGD-CBD-CAD	2.02	117.28	110.73
14	A	816	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
14	B	828	CLA	CAA-C2A-C1A	-2.02	105.35	111.97
17	F	203	BCR	C15-C16-C17	-2.02	119.34	123.47

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	801	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
14	a	826	CLA	CBC-CAC-C3C	2.02	117.99	112.43
14	B	825	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
14	A	839	CLA	CAC-C3C-C4C	2.02	127.43	124.81
14	B	823	CLA	CHD-C1D-C2D	2.02	129.71	125.48
17	F	203	BCR	C7-C8-C9	-2.02	123.19	126.23
14	L	1502	CLA	CAA-C2A-C1A	-2.02	105.37	111.97
14	A	812	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
14	A	805	CLA	CAA-C2A-C1A	-2.02	105.37	111.97
14	B	813	CLA	O2D-CGD-CBD	2.02	114.85	111.27
17	a	844	BCR	C11-C10-C9	-2.02	124.43	127.31
14	b	835	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
19	l	202	SQD	O48-C23-C24	2.01	118.23	111.91
14	B	837	CLA	O2D-CGD-CBD	2.01	114.85	111.27
14	b	821	CLA	CHA-C1A-NA	-2.01	121.79	126.40
14	a	823	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
17	l	201	BCR	C29-C30-C25	2.01	113.58	110.48
14	a	808	CLA	C2A-C1A-CHA	2.01	127.38	123.86
14	A	829	CLA	CHA-C1A-NA	-2.01	121.79	126.40
17	B	846	BCR	C29-C28-C27	-2.01	106.88	111.38
14	B	814	CLA	CMA-C3A-C2A	-2.01	105.71	113.83
14	B	830	CLA	CHD-C1D-ND	-2.01	122.61	124.45
14	b	804	CLA	C3C-C4C-NC	-2.01	108.31	110.57
14	A	816	CLA	C2A-C1A-CHA	2.01	127.38	123.86
14	b	827	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
14	B	801	CLA	C2A-C1A-CHA	2.01	127.38	123.86
17	b	845	BCR	C38-C26-C27	-2.01	109.75	113.62
14	b	837	CLA	CHA-C1A-NA	-2.01	121.79	126.40
14	a	811	CLA	O1D-CGD-CBD	2.01	128.60	124.48
14	J	101	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
14	b	835	CLA	C6-C7-C8	-2.01	109.42	115.92
14	A	825	CLA	C7-C6-C5	-2.01	107.90	113.36
14	B	837	CLA	C3C-C4C-NC	-2.01	108.32	110.57
14	b	814	CLA	O1D-CGD-CBD	2.01	128.60	124.48
14	A	839	CLA	C2A-C1A-CHA	2.01	127.37	123.86
20	b	851	LMG	O8-C28-O10	-2.01	118.52	123.59
14	b	804	CLA	C1-O2A-CGA	2.01	121.71	116.44
14	K	101	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
14	a	822	CLA	CMA-C3A-C2A	-2.01	105.73	113.83
17	J	104	BCR	C2-C1-C6	2.01	113.57	110.48
14	x	1701	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
17	a	844	BCR	C33-C5-C6	-2.01	122.27	124.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	811	CLA	C3C-C4C-NC	-2.01	108.32	110.57
14	b	818	CLA	O1D-CGD-CBD	2.01	128.59	124.48
14	A	823	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
14	B	838	CLA	CHD-C1D-ND	-2.01	122.61	124.45
14	l	203	CLA	C3A-C2A-C1A	2.00	104.34	101.34
14	A	839	CLA	C3A-C2A-C1A	2.00	104.34	101.34
14	b	808	CLA	C4D-C3D-CAD	2.00	110.46	108.10
14	A	840	CLA	C6-C7-C8	-2.00	109.44	115.92
14	a	817	CLA	CHA-C1A-NA	-2.00	121.81	126.40
14	L	1501	CLA	C3A-C2A-C1A	2.00	104.34	101.34
14	A	813	CLA	CHA-C1A-NA	-2.00	121.81	126.40
14	B	808	CLA	C4D-C3D-CAD	2.00	110.46	108.10
14	b	832	CLA	CHA-C4D-ND	2.00	136.69	132.50
14	a	817	CLA	CHB-C4A-NA	2.00	127.28	124.51
20	b	851	LMG	C6-C5-C4	-2.00	108.32	113.00
17	K	103	BCR	C1-C6-C5	-2.00	119.80	122.61
14	b	843	CLA	C2A-C1A-CHA	2.00	127.36	123.86
14	m	1201	CLA	O1D-CGD-CBD	2.00	128.58	124.48
14	a	817	CLA	C3B-C4B-NB	-2.00	106.62	109.21
14	A	812	CLA	C2D-C1D-ND	-2.00	108.63	110.10

All (187) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	NA
13	A	801	CL0	ND
13	A	801	CL0	NC
13	a	801	CL0	NA
13	a	801	CL0	ND
13	a	801	CL0	NC
14	A	802	CLA	ND
14	A	803	CLA	ND
14	A	804	CLA	ND
14	A	805	CLA	ND
14	A	806	CLA	ND
14	A	807	CLA	ND
14	A	808	CLA	ND
14	A	809	CLA	ND
14	A	810	CLA	ND
14	A	811	CLA	ND
14	A	812	CLA	ND
14	A	813	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
14	A	814	CLA	ND
14	A	815	CLA	ND
14	A	816	CLA	ND
14	A	817	CLA	ND
14	A	818	CLA	ND
14	A	819	CLA	ND
14	A	820	CLA	ND
14	A	821	CLA	ND
14	A	822	CLA	ND
14	A	823	CLA	ND
14	A	824	CLA	ND
14	A	825	CLA	ND
14	A	826	CLA	ND
14	A	827	CLA	ND
14	A	828	CLA	ND
14	A	829	CLA	ND
14	A	830	CLA	ND
14	A	831	CLA	ND
14	A	832	CLA	ND
14	A	833	CLA	ND
14	A	834	CLA	ND
14	A	835	CLA	ND
14	A	836	CLA	ND
14	A	837	CLA	ND
14	A	838	CLA	ND
14	A	840	CLA	ND
14	A	841	CLA	ND
14	A	842	CLA	ND
14	A	843	CLA	ND
14	X	1701	CLA	ND
14	B	801	CLA	ND
14	B	802	CLA	ND
14	B	804	CLA	ND
14	B	805	CLA	ND
14	B	806	CLA	ND
14	B	807	CLA	ND
14	B	808	CLA	ND
14	B	809	CLA	ND
14	B	810	CLA	ND
14	B	811	CLA	ND
14	B	812	CLA	ND
14	B	813	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
14	B	814	CLA	ND
14	B	815	CLA	ND
14	B	816	CLA	ND
14	B	817	CLA	ND
14	B	818	CLA	ND
14	B	819	CLA	ND
14	B	820	CLA	ND
14	B	821	CLA	ND
14	B	822	CLA	ND
14	B	823	CLA	ND
14	B	824	CLA	ND
14	B	825	CLA	ND
14	B	826	CLA	ND
14	B	827	CLA	ND
14	B	828	CLA	ND
14	B	829	CLA	ND
14	B	830	CLA	ND
14	B	831	CLA	ND
14	B	832	CLA	ND
14	B	833	CLA	ND
14	B	834	CLA	ND
14	B	835	CLA	ND
14	B	836	CLA	ND
14	B	837	CLA	ND
14	B	838	CLA	ND
14	B	839	CLA	ND
14	B	840	CLA	ND
14	B	841	CLA	ND
14	B	842	CLA	ND
14	B	843	CLA	ND
14	F	202	CLA	ND
14	F	204	CLA	ND
14	J	101	CLA	ND
14	J	102	CLA	ND
14	K	101	CLA	ND
14	K	102	CLA	ND
14	L	1501	CLA	ND
14	L	1503	CLA	ND
14	a	802	CLA	ND
14	a	803	CLA	ND
14	a	804	CLA	ND
14	a	805	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
14	a	806	CLA	ND
14	a	807	CLA	ND
14	a	808	CLA	ND
14	a	809	CLA	ND
14	a	810	CLA	ND
14	a	811	CLA	ND
14	a	812	CLA	ND
14	a	813	CLA	ND
14	a	814	CLA	ND
14	a	815	CLA	ND
14	a	816	CLA	ND
14	a	817	CLA	ND
14	a	818	CLA	ND
14	a	819	CLA	ND
14	a	820	CLA	ND
14	a	821	CLA	ND
14	a	822	CLA	ND
14	a	823	CLA	ND
14	a	824	CLA	ND
14	a	825	CLA	ND
14	a	827	CLA	ND
14	a	828	CLA	ND
14	a	829	CLA	ND
14	a	830	CLA	ND
14	a	831	CLA	ND
14	a	832	CLA	ND
14	a	833	CLA	ND
14	a	834	CLA	ND
14	a	835	CLA	ND
14	a	836	CLA	ND
14	a	837	CLA	ND
14	a	838	CLA	ND
14	a	839	CLA	ND
14	a	840	CLA	ND
14	a	841	CLA	ND
14	x	1701	CLA	ND
14	b	802	CLA	ND
14	b	803	CLA	ND
14	b	804	CLA	ND
14	b	805	CLA	ND
14	b	806	CLA	ND
14	b	807	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
14	b	808	CLA	ND
14	b	809	CLA	ND
14	b	810	CLA	ND
14	b	811	CLA	ND
14	b	812	CLA	ND
14	b	813	CLA	ND
14	b	814	CLA	ND
14	b	815	CLA	ND
14	b	817	CLA	ND
14	b	818	CLA	ND
14	b	819	CLA	ND
14	b	820	CLA	ND
14	b	821	CLA	ND
14	b	822	CLA	ND
14	b	823	CLA	ND
14	b	824	CLA	ND
14	b	825	CLA	ND
14	b	826	CLA	ND
14	b	828	CLA	ND
14	b	829	CLA	ND
14	b	830	CLA	ND
14	b	831	CLA	ND
14	b	832	CLA	ND
14	b	833	CLA	ND
14	b	834	CLA	ND
14	b	835	CLA	ND
14	b	836	CLA	ND
14	b	837	CLA	ND
14	b	838	CLA	ND
14	b	839	CLA	ND
14	b	840	CLA	ND
14	b	841	CLA	ND
14	b	842	CLA	ND
14	f	201	CLA	ND
14	f	203	CLA	ND
14	j	101	CLA	ND
14	j	102	CLA	ND
14	j	103	CLA	ND
14	k	101	CLA	ND
14	k	102	CLA	ND
14	l	203	CLA	ND
14	l	205	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
14	m	1201	CLA	ND

All (2625) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	805	CLA	CBA-CGA-O2A-C1
14	A	805	CLA	O1A-CGA-O2A-C1
14	A	805	CLA	CHA-CBD-CGD-O1D
14	A	805	CLA	CHA-CBD-CGD-O2D
14	A	806	CLA	C1A-C2A-CAA-CBA
14	A	807	CLA	CHA-CBD-CGD-O2D
14	A	807	CLA	C2-C3-C5-C6
14	A	807	CLA	C4-C3-C5-C6
14	A	808	CLA	C3A-C2A-CAA-CBA
14	A	808	CLA	CHA-CBD-CGD-O2D
14	A	808	CLA	C11-C12-C13-C15
14	A	810	CLA	C1A-C2A-CAA-CBA
14	A	811	CLA	CBA-CGA-O2A-C1
14	A	811	CLA	CBD-CGD-O2D-CED
14	A	819	CLA	C1A-C2A-CAA-CBA
14	A	819	CLA	C3A-C2A-CAA-CBA
14	A	820	CLA	C1A-C2A-CAA-CBA
14	A	820	CLA	C3A-C2A-CAA-CBA
14	A	821	CLA	CBD-CGD-O2D-CED
14	A	822	CLA	C1A-C2A-CAA-CBA
14	A	822	CLA	C3A-C2A-CAA-CBA
14	A	824	CLA	CHA-CBD-CGD-O1D
14	A	824	CLA	CHA-CBD-CGD-O2D
14	A	826	CLA	C1A-C2A-CAA-CBA
14	A	828	CLA	C4-C3-C5-C6
14	A	830	CLA	CHA-CBD-CGD-O1D
14	A	830	CLA	CHA-CBD-CGD-O2D
14	A	836	CLA	CHA-CBD-CGD-O1D
14	A	836	CLA	CHA-CBD-CGD-O2D
14	A	837	CLA	C1A-C2A-CAA-CBA
14	A	839	CLA	CHA-CBD-CGD-O1D
14	A	839	CLA	CHA-CBD-CGD-O2D
14	A	840	CLA	C1A-C2A-CAA-CBA
14	A	840	CLA	C3A-C2A-CAA-CBA
14	A	842	CLA	C4-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	A	843	CLA	C1A-C2A-CAA-CBA
14	A	843	CLA	CHA-CBD-CGD-O1D
14	A	843	CLA	CHA-CBD-CGD-O2D
14	X	1701	CLA	C3A-C2A-CAA-CBA
14	B	804	CLA	C1A-C2A-CAA-CBA
14	B	804	CLA	C3A-C2A-CAA-CBA
14	B	804	CLA	CHA-CBD-CGD-O1D
14	B	804	CLA	CHA-CBD-CGD-O2D
14	B	804	CLA	C2-C3-C5-C6
14	B	804	CLA	C4-C3-C5-C6
14	B	805	CLA	CBD-CGD-O2D-CED
14	B	808	CLA	C3A-C2A-CAA-CBA
14	B	809	CLA	CBA-CGA-O2A-C1
14	B	809	CLA	O1A-CGA-O2A-C1
14	B	812	CLA	C1A-C2A-CAA-CBA
14	B	812	CLA	C3A-C2A-CAA-CBA
14	B	815	CLA	C1A-C2A-CAA-CBA
14	B	815	CLA	C3A-C2A-CAA-CBA
14	B	820	CLA	C1A-C2A-CAA-CBA
14	B	820	CLA	C3A-C2A-CAA-CBA
14	B	821	CLA	C1A-C2A-CAA-CBA
14	B	821	CLA	C3A-C2A-CAA-CBA
14	B	822	CLA	CHA-CBD-CGD-O1D
14	B	822	CLA	CHA-CBD-CGD-O2D
14	B	823	CLA	C1A-C2A-CAA-CBA
14	B	823	CLA	C3A-C2A-CAA-CBA
14	B	830	CLA	C3A-C2A-CAA-CBA
14	B	831	CLA	C1A-C2A-CAA-CBA
14	B	831	CLA	C3A-C2A-CAA-CBA
14	B	834	CLA	C1A-C2A-CAA-CBA
14	B	836	CLA	CHA-CBD-CGD-O1D
14	B	836	CLA	CHA-CBD-CGD-O2D
14	B	837	CLA	CBD-CGD-O2D-CED
14	B	838	CLA	CHA-CBD-CGD-O1D
14	B	838	CLA	CHA-CBD-CGD-O2D
14	B	838	CLA	CAD-CBD-CGD-O1D
14	B	838	CLA	CAD-CBD-CGD-O2D
14	B	843	CLA	C1A-C2A-CAA-CBA
14	B	843	CLA	C3A-C2A-CAA-CBA
14	B	843	CLA	CBD-CGD-O2D-CED
14	J	101	CLA	CHA-CBD-CGD-O1D
14	J	101	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	J	101	CLA	CAD-CBD-CGD-O1D
14	K	101	CLA	C1A-C2A-CAA-CBA
14	K	101	CLA	C3A-C2A-CAA-CBA
14	L	1501	CLA	C1A-C2A-CAA-CBA
14	L	1501	CLA	C3A-C2A-CAA-CBA
14	L	1501	CLA	C2-C3-C5-C6
14	a	802	CLA	CHA-CBD-CGD-O1D
14	a	802	CLA	CHA-CBD-CGD-O2D
14	a	804	CLA	C1A-C2A-CAA-CBA
14	a	804	CLA	C3A-C2A-CAA-CBA
14	a	804	CLA	CBA-CGA-O2A-C1
14	a	804	CLA	CHA-CBD-CGD-O1D
14	a	804	CLA	CHA-CBD-CGD-O2D
14	a	805	CLA	C1A-C2A-CAA-CBA
14	a	806	CLA	C4-C3-C5-C6
14	a	807	CLA	C3A-C2A-CAA-CBA
14	a	809	CLA	C1A-C2A-CAA-CBA
14	a	809	CLA	C3A-C2A-CAA-CBA
14	a	809	CLA	CHA-CBD-CGD-O1D
14	a	809	CLA	CHA-CBD-CGD-O2D
14	a	816	CLA	C4-C3-C5-C6
14	a	818	CLA	C1A-C2A-CAA-CBA
14	a	818	CLA	C3A-C2A-CAA-CBA
14	a	819	CLA	C1A-C2A-CAA-CBA
14	a	819	CLA	C3A-C2A-CAA-CBA
14	a	819	CLA	C2A-CAA-CBA-CGA
14	a	820	CLA	C2-C3-C5-C6
14	a	820	CLA	C4-C3-C5-C6
14	a	821	CLA	C1A-C2A-CAA-CBA
14	a	821	CLA	C3A-C2A-CAA-CBA
14	a	822	CLA	C1A-C2A-CAA-CBA
14	a	822	CLA	C3A-C2A-CAA-CBA
14	a	826	CLA	CHA-CBD-CGD-O1D
14	a	826	CLA	CHA-CBD-CGD-O2D
14	a	831	CLA	C1A-C2A-CAA-CBA
14	a	831	CLA	C3A-C2A-CAA-CBA
14	a	831	CLA	C2-C3-C5-C6
14	a	831	CLA	C4-C3-C5-C6
14	a	835	CLA	CHA-CBD-CGD-O1D
14	a	835	CLA	CHA-CBD-CGD-O2D
14	a	836	CLA	C4-C3-C5-C6
14	a	837	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	a	837	CLA	CHA-CBD-CGD-O2D
14	a	839	CLA	CHA-CBD-CGD-O1D
14	a	841	CLA	C3A-C2A-CAA-CBA
14	x	1701	CLA	C1A-C2A-CAA-CBA
14	x	1701	CLA	C3A-C2A-CAA-CBA
14	b	804	CLA	CBD-CGD-O2D-CED
14	b	804	CLA	C2-C3-C5-C6
14	b	804	CLA	C4-C3-C5-C6
14	b	805	CLA	C3A-C2A-CAA-CBA
14	b	805	CLA	C2-C3-C5-C6
14	b	805	CLA	C4-C3-C5-C6
14	b	806	CLA	CHA-CBD-CGD-O1D
14	b	806	CLA	CHA-CBD-CGD-O2D
14	b	806	CLA	C2-C3-C5-C6
14	b	806	CLA	C4-C3-C5-C6
14	b	808	CLA	C3A-C2A-CAA-CBA
14	b	808	CLA	CBD-CGD-O2D-CED
14	b	811	CLA	CHA-CBD-CGD-O2D
14	b	813	CLA	C1A-C2A-CAA-CBA
14	b	814	CLA	CHA-CBD-CGD-O2D
14	b	815	CLA	C1A-C2A-CAA-CBA
14	b	815	CLA	C3A-C2A-CAA-CBA
14	b	816	CLA	C1A-C2A-CAA-CBA
14	b	821	CLA	C3A-C2A-CAA-CBA
14	b	823	CLA	C1A-C2A-CAA-CBA
14	b	823	CLA	C3A-C2A-CAA-CBA
14	b	826	CLA	C2-C3-C5-C6
14	b	826	CLA	C4-C3-C5-C6
14	b	827	CLA	C4-C3-C5-C6
14	b	829	CLA	C1A-C2A-CAA-CBA
14	b	829	CLA	C3A-C2A-CAA-CBA
14	b	830	CLA	C1A-C2A-CAA-CBA
14	b	830	CLA	C3A-C2A-CAA-CBA
14	b	831	CLA	C1A-C2A-CAA-CBA
14	b	831	CLA	C3A-C2A-CAA-CBA
14	b	836	CLA	CHA-CBD-CGD-O1D
14	b	836	CLA	CHA-CBD-CGD-O2D
14	b	837	CLA	CBD-CGD-O2D-CED
14	b	838	CLA	CHA-CBD-CGD-O1D
14	b	838	CLA	CHA-CBD-CGD-O2D
14	b	838	CLA	CAD-CBD-CGD-O1D
14	b	840	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	b	840	CLA	CHA-CBD-CGD-O2D
14	b	842	CLA	C2A-CAA-CBA-CGA
14	f	201	CLA	C1A-C2A-CAA-CBA
14	j	101	CLA	C1A-C2A-CAA-CBA
14	j	101	CLA	CBD-CGD-O2D-CED
14	j	102	CLA	C1A-C2A-CAA-CBA
14	j	102	CLA	C3A-C2A-CAA-CBA
14	j	102	CLA	CHA-CBD-CGD-O1D
14	j	102	CLA	CHA-CBD-CGD-O2D
14	j	102	CLA	CAD-CBD-CGD-O1D
14	j	102	CLA	CBD-CGD-O2D-CED
14	l	203	CLA	C1A-C2A-CAA-CBA
17	A	846	BCR	C7-C8-C9-C10
17	A	846	BCR	C7-C8-C9-C34
17	A	846	BCR	C21-C22-C23-C24
17	A	846	BCR	C37-C22-C23-C24
17	A	847	BCR	C20-C21-C22-C23
17	A	847	BCR	C20-C21-C22-C37
17	A	847	BCR	C21-C22-C23-C24
17	A	847	BCR	C37-C22-C23-C24
17	A	848	BCR	C7-C8-C9-C10
17	A	848	BCR	C11-C12-C13-C35
17	A	848	BCR	C21-C22-C23-C24
17	A	848	BCR	C37-C22-C23-C24
17	A	849	BCR	C16-C17-C18-C19
17	A	849	BCR	C20-C21-C22-C23
17	A	849	BCR	C37-C22-C23-C24
17	A	849	BCR	C22-C23-C24-C25
17	A	849	BCR	C23-C24-C25-C30
17	A	850	BCR	C1-C6-C7-C8
17	A	850	BCR	C11-C12-C13-C35
17	A	850	BCR	C35-C13-C14-C15
17	A	850	BCR	C37-C22-C23-C24
17	A	851	BCR	C6-C7-C8-C9
17	A	851	BCR	C16-C17-C18-C36
17	A	851	BCR	C18-C19-C20-C21
17	A	851	BCR	C21-C22-C23-C24
17	A	851	BCR	C37-C22-C23-C24
17	B	845	BCR	C10-C11-C12-C13
17	B	846	BCR	C1-C6-C7-C8
17	B	846	BCR	C35-C13-C14-C15
17	B	846	BCR	C37-C22-C23-C24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	B	847	BCR	C7-C8-C9-C10
17	B	847	BCR	C35-C13-C14-C15
17	B	847	BCR	C16-C17-C18-C36
17	B	847	BCR	C36-C18-C19-C20
17	B	847	BCR	C37-C22-C23-C24
17	B	848	BCR	C1-C6-C7-C8
17	B	848	BCR	C7-C8-C9-C10
17	B	848	BCR	C23-C24-C25-C30
17	B	849	BCR	C7-C8-C9-C10
17	B	849	BCR	C7-C8-C9-C34
17	B	849	BCR	C18-C19-C20-C21
17	B	849	BCR	C20-C21-C22-C23
17	B	849	BCR	C20-C21-C22-C37
17	B	849	BCR	C23-C24-C25-C26
17	B	850	BCR	C11-C12-C13-C35
17	F	203	BCR	C1-C6-C7-C8
17	F	203	BCR	C7-C8-C9-C10
17	F	203	BCR	C7-C8-C9-C34
17	F	203	BCR	C11-C12-C13-C35
17	F	203	BCR	C17-C18-C19-C20
17	F	203	BCR	C21-C22-C23-C24
17	F	205	BCR	C1-C6-C7-C8
17	F	205	BCR	C12-C13-C14-C15
17	F	205	BCR	C35-C13-C14-C15
17	F	205	BCR	C37-C22-C23-C24
17	J	103	BCR	C1-C6-C7-C8
17	J	103	BCR	C36-C18-C19-C20
17	J	103	BCR	C20-C21-C22-C37
17	J	103	BCR	C37-C22-C23-C24
17	J	104	BCR	C6-C7-C8-C9
17	J	104	BCR	C7-C8-C9-C34
17	J	104	BCR	C11-C12-C13-C35
17	J	104	BCR	C21-C22-C23-C24
17	J	105	BCR	C7-C8-C9-C10
17	J	105	BCR	C22-C23-C24-C25
17	K	103	BCR	C11-C12-C13-C14
17	K	103	BCR	C11-C12-C13-C35
17	K	103	BCR	C22-C23-C24-C25
17	I	101	BCR	C11-C12-C13-C14
17	I	101	BCR	C35-C13-C14-C15
17	I	102	BCR	C7-C8-C9-C34
17	I	102	BCR	C11-C12-C13-C35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	I	102	BCR	C18-C19-C20-C21
17	I	102	BCR	C20-C21-C22-C23
17	I	102	BCR	C20-C21-C22-C37
17	L	1504	BCR	C7-C8-C9-C10
17	L	1504	BCR	C7-C8-C9-C34
17	L	1504	BCR	C11-C12-C13-C35
17	L	1504	BCR	C21-C22-C23-C24
17	L	1504	BCR	C23-C24-C25-C26
17	L	1504	BCR	C23-C24-C25-C30
17	M	101	BCR	C7-C8-C9-C34
17	M	101	BCR	C16-C17-C18-C36
17	M	101	BCR	C20-C21-C22-C37
17	a	844	BCR	C1-C6-C7-C8
17	a	844	BCR	C7-C8-C9-C10
17	a	845	BCR	C21-C22-C23-C24
17	a	845	BCR	C23-C24-C25-C30
17	a	846	BCR	C7-C8-C9-C10
17	a	846	BCR	C7-C8-C9-C34
17	a	846	BCR	C36-C18-C19-C20
17	a	846	BCR	C21-C22-C23-C24
17	a	847	BCR	C1-C6-C7-C8
17	a	847	BCR	C17-C18-C19-C20
17	a	847	BCR	C18-C19-C20-C21
17	a	847	BCR	C20-C21-C22-C23
17	a	847	BCR	C20-C21-C22-C37
17	a	848	BCR	C1-C6-C7-C8
17	a	848	BCR	C11-C12-C13-C35
17	a	849	BCR	C6-C7-C8-C9
17	a	849	BCR	C11-C12-C13-C35
17	a	849	BCR	C21-C22-C23-C24
17	b	845	BCR	C1-C6-C7-C8
17	b	845	BCR	C7-C8-C9-C10
17	b	845	BCR	C7-C8-C9-C34
17	b	845	BCR	C22-C23-C24-C25
17	b	846	BCR	C21-C22-C23-C24
17	b	846	BCR	C37-C22-C23-C24
17	b	847	BCR	C1-C6-C7-C8
17	b	847	BCR	C11-C10-C9-C34
17	b	848	BCR	C1-C6-C7-C8
17	b	848	BCR	C7-C8-C9-C10
17	b	848	BCR	C16-C17-C18-C36
17	b	848	BCR	C20-C21-C22-C37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	b	848	BCR	C23-C24-C25-C30
17	b	849	BCR	C7-C8-C9-C10
17	b	849	BCR	C7-C8-C9-C34
17	b	850	BCR	C1-C6-C7-C8
17	b	850	BCR	C7-C8-C9-C34
17	b	850	BCR	C11-C12-C13-C14
17	b	850	BCR	C37-C22-C23-C24
17	b	850	BCR	C23-C24-C25-C30
17	f	202	BCR	C7-C8-C9-C10
17	f	202	BCR	C7-C8-C9-C34
17	f	202	BCR	C11-C12-C13-C35
17	f	202	BCR	C20-C21-C22-C23
17	f	202	BCR	C21-C22-C23-C24
17	f	202	BCR	C37-C22-C23-C24
17	f	204	BCR	C7-C8-C9-C10
17	f	204	BCR	C11-C10-C9-C8
17	f	204	BCR	C11-C12-C13-C35
17	f	204	BCR	C21-C22-C23-C24
17	j	104	BCR	C1-C6-C7-C8
17	j	104	BCR	C7-C8-C9-C34
17	j	104	BCR	C11-C12-C13-C35
17	j	104	BCR	C36-C18-C19-C20
17	j	104	BCR	C37-C22-C23-C24
17	j	105	BCR	C6-C7-C8-C9
17	j	105	BCR	C7-C8-C9-C34
17	j	105	BCR	C21-C22-C23-C24
17	j	105	BCR	C23-C24-C25-C30
17	j	106	BCR	C7-C8-C9-C10
17	j	106	BCR	C11-C10-C9-C34
17	j	106	BCR	C23-C24-C25-C30
17	k	103	BCR	C23-C24-C25-C30
17	i	101	BCR	C11-C12-C13-C35
17	i	101	BCR	C17-C18-C19-C20
17	i	101	BCR	C36-C18-C19-C20
17	i	101	BCR	C20-C21-C22-C23
17	i	101	BCR	C37-C22-C23-C24
17	i	102	BCR	C1-C6-C7-C8
17	i	102	BCR	C7-C8-C9-C10
17	i	102	BCR	C7-C8-C9-C34
17	i	102	BCR	C16-C17-C18-C36
17	i	102	BCR	C20-C21-C22-C23
17	l	201	BCR	C11-C12-C13-C35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	l	201	BCR	C17-C18-C19-C20
17	l	206	BCR	C7-C8-C9-C10
17	l	206	BCR	C11-C12-C13-C35
17	l	206	BCR	C37-C22-C23-C24
17	l	206	BCR	C22-C23-C24-C25
17	l	207	BCR	C11-C12-C13-C35
17	l	207	BCR	C23-C24-C25-C30
17	m	1202	BCR	C7-C8-C9-C34
17	m	1202	BCR	C11-C12-C13-C35
18	A	852	LHG	O7-C5-C6-O8
18	A	853	LHG	O2-C2-C3-O3
18	F	201	LHG	O2-C2-C3-O3
18	F	201	LHG	C3-O3-P-O4
18	a	850	LHG	O7-C5-C6-O8
18	a	851	LHG	C3-O3-P-O5
18	i	103	LHG	C1-C2-C3-O3
18	i	103	LHG	C3-O3-P-O5
18	i	103	LHG	C4-O6-P-O3
19	X	1702	SQD	C8-C7-O47-C45
19	x	1702	SQD	O5-C1-O6-C44
19	l	202	SQD	O5-C1-O6-C44
19	l	202	SQD	C5-C6-S-O8
19	l	202	SQD	C5-C6-S-O9
14	b	843	CLA	C4C-C3C-CAC-CBC
14	B	836	CLA	O1D-CGD-O2D-CED
14	b	836	CLA	O1D-CGD-O2D-CED
14	A	807	CLA	O1D-CGD-O2D-CED
14	A	811	CLA	O1D-CGD-O2D-CED
14	A	807	CLA	CBD-CGD-O2D-CED
14	A	809	CLA	CBD-CGD-O2D-CED
14	A	827	CLA	CBD-CGD-O2D-CED
14	X	1701	CLA	CBD-CGD-O2D-CED
14	B	807	CLA	CBD-CGD-O2D-CED
14	B	811	CLA	CBD-CGD-O2D-CED
14	B	836	CLA	CBD-CGD-O2D-CED
14	J	101	CLA	CBD-CGD-O2D-CED
14	a	808	CLA	CBD-CGD-O2D-CED
14	a	810	CLA	CBD-CGD-O2D-CED
14	a	820	CLA	CBD-CGD-O2D-CED
14	a	824	CLA	CBD-CGD-O2D-CED
14	b	836	CLA	CBD-CGD-O2D-CED
14	b	843	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	f	203	CLA	CBD-CGD-O2D-CED
14	l	205	CLA	CBD-CGD-O2D-CED
14	A	811	CLA	O1A-CGA-O2A-C1
14	B	815	CLA	O1A-CGA-O2A-C1
14	B	843	CLA	O1A-CGA-O2A-C1
14	a	804	CLA	O1A-CGA-O2A-C1
14	a	818	CLA	O1A-CGA-O2A-C1
14	a	836	CLA	O1A-CGA-O2A-C1
14	b	805	CLA	O1A-CGA-O2A-C1
14	b	834	CLA	O1A-CGA-O2A-C1
14	b	843	CLA	C2C-C3C-CAC-CBC
14	A	821	CLA	O1D-CGD-O2D-CED
14	B	805	CLA	O1D-CGD-O2D-CED
14	B	837	CLA	O1D-CGD-O2D-CED
14	b	804	CLA	O1D-CGD-O2D-CED
14	j	101	CLA	O1D-CGD-O2D-CED
14	j	102	CLA	O1D-CGD-O2D-CED
14	A	820	CLA	CBA-CGA-O2A-C1
14	a	836	CLA	CBA-CGA-O2A-C1
14	b	834	CLA	CBA-CGA-O2A-C1
14	A	833	CLA	CBD-CGD-O2D-CED
14	A	834	CLA	CBD-CGD-O2D-CED
14	A	837	CLA	CBD-CGD-O2D-CED
14	A	839	CLA	CBD-CGD-O2D-CED
14	A	841	CLA	CBD-CGD-O2D-CED
14	B	814	CLA	CBD-CGD-O2D-CED
14	B	834	CLA	CBD-CGD-O2D-CED
14	a	807	CLA	CBD-CGD-O2D-CED
14	a	811	CLA	CBD-CGD-O2D-CED
14	a	812	CLA	CBD-CGD-O2D-CED
14	a	814	CLA	CBD-CGD-O2D-CED
14	a	823	CLA	CBD-CGD-O2D-CED
14	b	806	CLA	CBD-CGD-O2D-CED
14	b	807	CLA	CBD-CGD-O2D-CED
14	b	813	CLA	CBD-CGD-O2D-CED
14	b	814	CLA	CBD-CGD-O2D-CED
14	b	825	CLA	CBD-CGD-O2D-CED
14	b	838	CLA	CBD-CGD-O2D-CED
14	A	820	CLA	O1A-CGA-O2A-C1
14	A	837	CLA	O1A-CGA-O2A-C1
14	B	804	CLA	O1A-CGA-O2A-C1
14	B	813	CLA	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	B	825	CLA	O1A-CGA-O2A-C1
14	a	819	CLA	O1A-CGA-O2A-C1
14	b	809	CLA	O1A-CGA-O2A-C1
14	b	815	CLA	O1A-CGA-O2A-C1
14	b	808	CLA	O1D-CGD-O2D-CED
14	a	827	CLA	C5-C6-C7-C8
14	B	843	CLA	O1D-CGD-O2D-CED
14	A	828	CLA	CBD-CGD-O2D-CED
14	B	838	CLA	CBD-CGD-O2D-CED
14	a	818	CLA	CBD-CGD-O2D-CED
14	a	833	CLA	CBD-CGD-O2D-CED
14	B	807	CLA	O1D-CGD-O2D-CED
14	b	837	CLA	O1D-CGD-O2D-CED
14	A	809	CLA	C3-C5-C6-C7
14	A	820	CLA	C3-C5-C6-C7
14	A	823	CLA	C3-C5-C6-C7
14	B	814	CLA	C3-C5-C6-C7
14	B	843	CLA	C3-C5-C6-C7
14	a	808	CLA	C3-C5-C6-C7
14	a	813	CLA	C3-C5-C6-C7
14	a	822	CLA	C3-C5-C6-C7
14	a	827	CLA	C3-C5-C6-C7
14	b	815	CLA	C3-C5-C6-C7
14	X	1701	CLA	CBA-CGA-O2A-C1
14	B	804	CLA	CBA-CGA-O2A-C1
14	B	815	CLA	CBA-CGA-O2A-C1
14	B	821	CLA	CBA-CGA-O2A-C1
14	B	843	CLA	CBA-CGA-O2A-C1
14	a	807	CLA	CBA-CGA-O2A-C1
14	a	818	CLA	CBA-CGA-O2A-C1
14	a	819	CLA	CBA-CGA-O2A-C1
14	a	828	CLA	CBA-CGA-O2A-C1
14	b	805	CLA	CBA-CGA-O2A-C1
14	b	809	CLA	CBA-CGA-O2A-C1
14	b	815	CLA	CBA-CGA-O2A-C1
14	b	818	CLA	CBA-CGA-O2A-C1
14	A	827	CLA	O1D-CGD-O2D-CED
14	A	802	CLA	CBD-CGD-O2D-CED
14	a	810	CLA	O1A-CGA-O2A-C1
14	A	817	CLA	C4-C3-C5-C6
14	A	823	CLA	C4-C3-C5-C6
14	B	812	CLA	C4-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	A	817	CLA	C2-C3-C5-C6
14	A	842	CLA	C2-C3-C5-C6
14	a	806	CLA	C2-C3-C5-C6
14	A	820	CLA	C2A-CAA-CBA-CGA
14	A	821	CLA	C2A-CAA-CBA-CGA
14	B	812	CLA	C2A-CAA-CBA-CGA
14	B	842	CLA	C2A-CAA-CBA-CGA
14	b	804	CLA	C2A-CAA-CBA-CGA
14	b	812	CLA	C2A-CAA-CBA-CGA
14	b	825	CLA	O1A-CGA-O2A-C1
14	a	810	CLA	O1D-CGD-O2D-CED
14	B	804	CLA	C3-C5-C6-C7
14	a	805	CLA	C3-C5-C6-C7
14	a	807	CLA	C3-C5-C6-C7
14	a	811	CLA	C3-C5-C6-C7
14	b	805	CLA	C3-C5-C6-C7
14	b	813	CLA	C3-C5-C6-C7
14	b	814	CLA	C3-C5-C6-C7
14	b	836	CLA	C3-C5-C6-C7
14	A	804	CLA	CBA-CGA-O2A-C1
14	A	819	CLA	CBA-CGA-O2A-C1
14	A	837	CLA	CBA-CGA-O2A-C1
14	B	813	CLA	CBA-CGA-O2A-C1
14	B	825	CLA	CBA-CGA-O2A-C1
14	B	834	CLA	CBA-CGA-O2A-C1
14	a	803	CLA	CBA-CGA-O2A-C1
14	b	825	CLA	CBA-CGA-O2A-C1
14	B	829	CLA	CBD-CGD-O2D-CED
14	B	839	CLA	CBD-CGD-O2D-CED
14	F	202	CLA	CBD-CGD-O2D-CED
14	a	834	CLA	CBD-CGD-O2D-CED
14	a	836	CLA	CBD-CGD-O2D-CED
14	b	803	CLA	CBD-CGD-O2D-CED
14	J	101	CLA	O1D-CGD-O2D-CED
14	a	808	CLA	O1D-CGD-O2D-CED
14	f	203	CLA	O1D-CGD-O2D-CED
14	A	808	CLA	O1A-CGA-O2A-C1
14	A	819	CLA	O1A-CGA-O2A-C1
14	B	821	CLA	O1A-CGA-O2A-C1
14	a	803	CLA	O1A-CGA-O2A-C1
14	a	807	CLA	O1A-CGA-O2A-C1
14	a	828	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	b	841	CLA	O1A-CGA-O2A-C1
14	l	205	CLA	O1D-CGD-O2D-CED
14	A	813	CLA	CBD-CGD-O2D-CED
14	L	1503	CLA	CBD-CGD-O2D-CED
14	a	817	CLA	CBD-CGD-O2D-CED
14	b	832	CLA	CBD-CGD-O2D-CED
14	b	841	CLA	CBD-CGD-O2D-CED
14	l	203	CLA	CBD-CGD-O2D-CED
14	m	1201	CLA	CBD-CGD-O2D-CED
14	a	820	CLA	O1D-CGD-O2D-CED
18	i	103	LHG	O2-C2-C3-O3
14	B	801	CLA	C3-C5-C6-C7
14	b	809	CLA	C3-C5-C6-C7
14	b	828	CLA	C3-C5-C6-C7
15	a	842	PQN	C13-C15-C16-C17
14	B	818	CLA	CBA-CGA-O2A-C1
14	a	831	CLA	CBA-CGA-O2A-C1
14	b	804	CLA	CBA-CGA-O2A-C1
14	b	821	CLA	CBA-CGA-O2A-C1
14	b	841	CLA	CBA-CGA-O2A-C1
14	b	843	CLA	CBA-CGA-O2A-C1
14	A	804	CLA	O1A-CGA-O2A-C1
14	X	1701	CLA	O1A-CGA-O2A-C1
14	B	818	CLA	O1A-CGA-O2A-C1
14	b	818	CLA	O1A-CGA-O2A-C1
14	b	843	CLA	O1A-CGA-O2A-C1
19	l	202	SQD	O10-C23-O48-C46
14	B	811	CLA	O1D-CGD-O2D-CED
14	b	843	CLA	O1D-CGD-O2D-CED
14	A	828	CLA	C5-C6-C7-C8
14	A	815	CLA	CBD-CGD-O2D-CED
14	A	842	CLA	CBD-CGD-O2D-CED
14	A	843	CLA	CBD-CGD-O2D-CED
14	B	823	CLA	CBD-CGD-O2D-CED
14	b	812	CLA	CBD-CGD-O2D-CED
14	b	833	CLA	CBD-CGD-O2D-CED
20	B	803	LMG	O6-C5-C6-O5
14	A	839	CLA	C3-C5-C6-C7
14	a	830	CLA	C3-C5-C6-C7
14	A	808	CLA	CBA-CGA-O2A-C1
14	a	810	CLA	CBA-CGA-O2A-C1
14	a	833	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	a	824	CLA	O1D-CGD-O2D-CED
20	B	851	LMG	C4-C5-C6-O5
20	b	851	LMG	C4-C5-C6-O5
14	B	834	CLA	O1A-CGA-O2A-C1
14	a	831	CLA	O1A-CGA-O2A-C1
18	A	853	LHG	C31-C32-C33-C34
20	b	851	LMG	O6-C5-C6-O5
14	A	841	CLA	C4-C3-C5-C6
14	b	843	CLA	C4-C3-C5-C6
14	A	828	CLA	C2-C3-C5-C6
14	A	841	CLA	C2-C3-C5-C6
14	B	812	CLA	C2-C3-C5-C6
14	a	816	CLA	C2-C3-C5-C6
14	b	827	CLA	C2-C3-C5-C6
14	b	843	CLA	C2-C3-C5-C6
14	A	829	CLA	C2A-CAA-CBA-CGA
14	L	1503	CLA	C2A-CAA-CBA-CGA
14	a	807	CLA	C2A-CAA-CBA-CGA
14	b	809	CLA	C2A-CAA-CBA-CGA
14	l	204	CLA	C2A-CAA-CBA-CGA
14	X	1701	CLA	O1D-CGD-O2D-CED
14	b	804	CLA	O1A-CGA-O2A-C1
18	a	851	LHG	C26-C27-C28-C29
14	A	839	CLA	CBA-CGA-O2A-C1
14	B	841	CLA	CBA-CGA-O2A-C1
14	a	805	CLA	CBA-CGA-O2A-C1
14	a	817	CLA	CBA-CGA-O2A-C1
18	F	201	LHG	C24-C23-O8-C6
19	l	202	SQD	C24-C23-O48-C46
20	B	851	LMG	O6-C5-C6-O5
14	A	809	CLA	O1D-CGD-O2D-CED
14	A	833	CLA	O1D-CGD-O2D-CED
14	A	834	CLA	O1D-CGD-O2D-CED
14	b	813	CLA	O1D-CGD-O2D-CED
14	b	821	CLA	O1A-CGA-O2A-C1
14	A	839	CLA	O1D-CGD-O2D-CED
14	B	814	CLA	O1D-CGD-O2D-CED
14	a	807	CLA	O1D-CGD-O2D-CED
14	a	814	CLA	O1D-CGD-O2D-CED
14	b	807	CLA	O1D-CGD-O2D-CED
14	b	838	CLA	O1D-CGD-O2D-CED
14	A	835	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	a	851	LHG	C1-C2-C3-O3
20	B	803	LMG	C4-C5-C6-O5
14	a	805	CLA	O1A-CGA-O2A-C1
14	a	833	CLA	O1A-CGA-O2A-C1
14	A	837	CLA	O1D-CGD-O2D-CED
14	A	830	CLA	CBA-CGA-O2A-C1
14	A	842	CLA	CBA-CGA-O2A-C1
14	B	817	CLA	CBA-CGA-O2A-C1
14	a	820	CLA	CBA-CGA-O2A-C1
14	a	829	CLA	CBA-CGA-O2A-C1
14	x	1701	CLA	CBA-CGA-O2A-C1
14	b	813	CLA	CBA-CGA-O2A-C1
19	X	1702	SQD	C24-C23-O48-C46
14	A	808	CLA	CBD-CGD-O2D-CED
14	B	802	CLA	CBD-CGD-O2D-CED
14	a	809	CLA	CBD-CGD-O2D-CED
14	B	834	CLA	O1D-CGD-O2D-CED
14	A	805	CLA	C13-C15-C16-C17
14	A	839	CLA	C13-C15-C16-C17
14	a	804	CLA	C8-C10-C11-C12
14	A	818	CLA	C8-C10-C11-C12
14	A	830	CLA	C5-C6-C7-C8
14	B	809	CLA	C15-C16-C17-C18
14	B	820	CLA	C8-C10-C11-C12
14	a	831	CLA	C8-C10-C11-C12
14	b	804	CLA	C13-C15-C16-C17
14	l	204	CLA	C8-C10-C11-C12
14	B	817	CLA	O1A-CGA-O2A-C1
14	B	841	CLA	O1A-CGA-O2A-C1
14	a	820	CLA	O1A-CGA-O2A-C1
14	b	831	CLA	C4-C3-C5-C6
14	A	823	CLA	C2-C3-C5-C6
14	b	831	CLA	C2-C3-C5-C6
14	A	806	CLA	C11-C10-C8-C9
14	A	818	CLA	C11-C10-C8-C9
14	A	825	CLA	C6-C7-C8-C9
14	A	827	CLA	C6-C7-C8-C9
14	A	832	CLA	C6-C7-C8-C9
14	B	809	CLA	C14-C13-C15-C16
14	F	202	CLA	C11-C12-C13-C14
14	b	804	CLA	C11-C10-C8-C9
14	b	813	CLA	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	b	832	CLA	C11-C12-C13-C14
14	b	835	CLA	C11-C12-C13-C14
14	A	841	CLA	O1D-CGD-O2D-CED
14	B	806	CLA	CBD-CGD-O2D-CED
14	A	811	CLA	C15-C16-C17-C18
14	A	810	CLA	C2A-CAA-CBA-CGA
14	B	830	CLA	C2A-CAA-CBA-CGA
14	B	843	CLA	C2A-CAA-CBA-CGA
17	A	848	BCR	C7-C8-C9-C34
17	A	849	BCR	C36-C18-C19-C20
17	A	851	BCR	C7-C8-C9-C34
17	B	845	BCR	C7-C8-C9-C34
17	B	845	BCR	C37-C22-C23-C24
17	B	846	BCR	C7-C8-C9-C34
17	F	203	BCR	C37-C22-C23-C24
17	J	104	BCR	C37-C22-C23-C24
17	K	103	BCR	C37-C22-C23-C24
17	a	844	BCR	C7-C8-C9-C34
17	a	844	BCR	C11-C12-C13-C35
17	a	844	BCR	C37-C22-C23-C24
17	a	845	BCR	C37-C22-C23-C24
17	a	846	BCR	C37-C22-C23-C24
17	a	847	BCR	C37-C22-C23-C24
17	a	849	BCR	C7-C8-C9-C34
17	b	845	BCR	C37-C22-C23-C24
17	b	847	BCR	C7-C8-C9-C34
17	b	848	BCR	C7-C8-C9-C34
17	f	204	BCR	C7-C8-C9-C34
17	k	103	BCR	C11-C12-C13-C35
17	l	206	BCR	C7-C8-C9-C34
17	A	850	BCR	C21-C22-C23-C24
17	A	851	BCR	C7-C8-C9-C10
17	B	845	BCR	C7-C8-C9-C10
17	a	849	BCR	C7-C8-C9-C10
17	b	845	BCR	C21-C22-C23-C24
17	b	848	BCR	C21-C22-C23-C24
17	k	103	BCR	C11-C12-C13-C14
14	A	837	CLA	C2C-C3C-CAC-CBC
18	a	851	LHG	C31-C32-C33-C34
14	A	842	CLA	O1A-CGA-O2A-C1
14	b	813	CLA	O1A-CGA-O2A-C1
14	A	821	CLA	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	B	809	CLA	C13-C15-C16-C17
14	B	811	CLA	C13-C15-C16-C17
14	B	826	CLA	C5-C6-C7-C8
14	a	804	CLA	C13-C15-C16-C17
14	a	808	CLA	C8-C10-C11-C12
14	a	831	CLA	C10-C11-C12-C13
14	b	827	CLA	C15-C16-C17-C18
14	b	806	CLA	O1D-CGD-O2D-CED
14	A	805	CLA	C8-C10-C11-C12
14	A	806	CLA	C15-C16-C17-C18
14	A	813	CLA	C8-C10-C11-C12
14	A	821	CLA	C8-C10-C11-C12
14	A	838	CLA	C8-C10-C11-C12
14	B	801	CLA	C15-C16-C17-C18
14	B	816	CLA	C10-C11-C12-C13
14	B	827	CLA	C15-C16-C17-C18
14	B	843	CLA	C13-C15-C16-C17
14	a	840	CLA	C15-C16-C17-C18
14	b	809	CLA	C13-C15-C16-C17
14	b	810	CLA	C15-C16-C17-C18
14	b	822	CLA	C8-C10-C11-C12
14	b	828	CLA	C15-C16-C17-C18
14	b	830	CLA	C8-C10-C11-C12
14	b	834	CLA	C8-C10-C11-C12
14	b	835	CLA	C10-C11-C12-C13
18	a	851	LHG	C7-C8-C9-C10
18	A	852	LHG	C29-C30-C31-C32
17	B	849	BCR	C14-C15-C16-C17
14	b	814	CLA	O1D-CGD-O2D-CED
14	A	803	CLA	C13-C15-C16-C17
14	A	821	CLA	C10-C11-C12-C13
14	A	829	CLA	C5-C6-C7-C8
14	A	829	CLA	C15-C16-C17-C18
14	A	834	CLA	C5-C6-C7-C8
14	A	841	CLA	C15-C16-C17-C18
14	A	842	CLA	C13-C15-C16-C17
14	B	801	CLA	C8-C10-C11-C12
14	B	809	CLA	C5-C6-C7-C8
14	B	810	CLA	C8-C10-C11-C12
14	B	826	CLA	C13-C15-C16-C17
14	B	831	CLA	C15-C16-C17-C18
14	B	834	CLA	C10-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	F	202	CLA	C10-C11-C12-C13
14	a	802	CLA	C10-C11-C12-C13
14	a	805	CLA	C15-C16-C17-C18
14	a	810	CLA	C15-C16-C17-C18
14	a	811	CLA	C5-C6-C7-C8
14	a	818	CLA	C15-C16-C17-C18
14	a	824	CLA	C8-C10-C11-C12
14	b	805	CLA	C10-C11-C12-C13
14	b	813	CLA	C5-C6-C7-C8
14	b	827	CLA	C5-C6-C7-C8
14	b	830	CLA	C15-C16-C17-C18
14	b	843	CLA	C5-C6-C7-C8
14	a	812	CLA	O1D-CGD-O2D-CED
18	a	851	LHG	C23-C24-C25-C26
19	X	1702	SQD	C7-C8-C9-C10
14	B	810	CLA	C15-C16-C17-C18
14	a	837	CLA	C13-C15-C16-C17
14	a	840	CLA	C13-C15-C16-C17
14	b	812	CLA	C5-C6-C7-C8
14	b	826	CLA	C8-C10-C11-C12
14	b	828	CLA	C8-C10-C11-C12
15	B	844	PQN	C25-C26-C27-C28
14	b	808	CLA	CBA-CGA-O2A-C1
14	b	825	CLA	O1D-CGD-O2D-CED
14	b	804	CLA	C2-C1-O2A-CGA
14	A	809	CLA	C8-C10-C11-C12
14	A	819	CLA	C8-C10-C11-C12
14	A	840	CLA	C8-C10-C11-C12
14	A	841	CLA	C10-C11-C12-C13
14	B	822	CLA	C8-C10-C11-C12
14	a	808	CLA	C13-C15-C16-C17
14	a	816	CLA	C8-C10-C11-C12
14	a	828	CLA	C15-C16-C17-C18
18	F	201	LHG	C23-C24-C25-C26
14	B	820	CLA	CBD-CGD-O2D-CED
14	B	832	CLA	CBD-CGD-O2D-CED
14	a	832	CLA	CBD-CGD-O2D-CED
14	a	804	CLA	C15-C16-C17-C18
14	a	811	CLA	O1D-CGD-O2D-CED
14	A	825	CLA	C6-C7-C8-C10
14	A	832	CLA	C12-C13-C15-C16
14	A	838	CLA	C11-C12-C13-C15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	B	804	CLA	C6-C7-C8-C10
14	B	806	CLA	C11-C10-C8-C7
14	B	829	CLA	C11-C10-C8-C7
14	F	202	CLA	C11-C12-C13-C15
14	a	837	CLA	C11-C10-C8-C7
14	b	810	CLA	C6-C7-C8-C10
14	b	820	CLA	C12-C13-C15-C16
14	A	830	CLA	O1A-CGA-O2A-C1
14	a	829	CLA	O1A-CGA-O2A-C1
14	x	1701	CLA	O1A-CGA-O2A-C1
17	a	847	BCR	C19-C20-C21-C22
17	i	101	BCR	C9-C10-C11-C12
14	A	829	CLA	CBA-CGA-O2A-C1
14	B	825	CLA	C2A-CAA-CBA-CGA
14	B	833	CLA	C2A-CAA-CBA-CGA
14	a	828	CLA	C2A-CAA-CBA-CGA
14	A	802	CLA	O1D-CGD-O2D-CED
14	B	838	CLA	O1D-CGD-O2D-CED
14	a	823	CLA	O1D-CGD-O2D-CED
14	a	833	CLA	O1D-CGD-O2D-CED
14	A	806	CLA	C5-C6-C7-C8
14	A	808	CLA	C5-C6-C7-C8
14	A	819	CLA	C15-C16-C17-C18
14	A	827	CLA	C10-C11-C12-C13
14	A	828	CLA	C15-C16-C17-C18
14	a	827	CLA	C8-C10-C11-C12
14	a	838	CLA	C5-C6-C7-C8
14	b	828	CLA	C5-C6-C7-C8
14	A	809	CLA	C5-C6-C7-C8
14	A	828	CLA	C8-C10-C11-C12
14	b	831	CLA	C15-C16-C17-C18
14	a	818	CLA	O1D-CGD-O2D-CED
17	A	847	BCR	C18-C19-C20-C21
17	A	851	BCR	C10-C11-C12-C13
17	B	846	BCR	C10-C11-C12-C13
17	J	103	BCR	C10-C11-C12-C13
17	I	102	BCR	C10-C11-C12-C13
17	a	846	BCR	C18-C19-C20-C21
17	b	846	BCR	C18-C19-C20-C21
17	b	848	BCR	C18-C19-C20-C21
17	f	202	BCR	C18-C19-C20-C21
17	m	1202	BCR	C18-C19-C20-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	a	851	LHG	O2-C2-C3-O3
18	A	852	LHG	O9-C7-O7-C5
14	A	814	CLA	C3-C5-C6-C7
14	a	804	CLA	C3-C5-C6-C7
15	A	844	PQN	C13-C15-C16-C17
14	A	832	CLA	C5-C6-C7-C8
14	A	841	CLA	C5-C6-C7-C8
14	A	841	CLA	C13-C15-C16-C17
14	B	812	CLA	C15-C16-C17-C18
14	a	826	CLA	C10-C11-C12-C13
14	a	837	CLA	C8-C10-C11-C12
14	b	808	CLA	C13-C15-C16-C17
14	A	839	CLA	O1A-CGA-O2A-C1
14	a	817	CLA	O1A-CGA-O2A-C1
14	A	805	CLA	C15-C16-C17-C18
14	A	811	CLA	C10-C11-C12-C13
14	A	838	CLA	C10-C11-C12-C13
14	A	838	CLA	C13-C15-C16-C17
14	B	834	CLA	C8-C10-C11-C12
14	B	843	CLA	C15-C16-C17-C18
14	a	804	CLA	C10-C11-C12-C13
14	a	820	CLA	C10-C11-C12-C13
14	a	837	CLA	C15-C16-C17-C18
14	b	810	CLA	C8-C10-C11-C12
14	b	816	CLA	C10-C11-C12-C13
14	A	805	CLA	C10-C11-C12-C13
14	A	808	CLA	C15-C16-C17-C18
14	A	832	CLA	C13-C15-C16-C17
14	B	828	CLA	C8-C10-C11-C12
14	L	1502	CLA	C8-C10-C11-C12
14	a	807	CLA	C15-C16-C17-C18
14	a	829	CLA	C5-C6-C7-C8
14	b	816	CLA	C5-C6-C7-C8
18	F	201	LHG	C3-O3-P-O6
18	a	851	LHG	C3-O3-P-O6
18	i	103	LHG	C3-O3-P-O6
14	B	822	CLA	CBA-CGA-O2A-C1
14	a	838	CLA	CBA-CGA-O2A-C1
14	B	829	CLA	O1D-CGD-O2D-CED
14	A	839	CLA	C5-C6-C7-C8
14	b	805	CLA	C13-C15-C16-C17
14	b	831	CLA	C13-C15-C16-C17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	b	844	PQN	C23-C25-C26-C27
14	b	808	CLA	O1A-CGA-O2A-C1
14	b	803	CLA	O1D-CGD-O2D-CED
18	A	853	LHG	C1-C2-C3-O3
18	F	201	LHG	C1-C2-C3-O3
18	A	853	LHG	O9-C7-O7-C5
19	X	1702	SQD	O49-C7-O47-C45
14	A	839	CLA	C4-C3-C5-C6
14	a	822	CLA	C4-C3-C5-C6
14	b	820	CLA	C13-C15-C16-C17
14	A	808	CLA	C2A-CAA-CBA-CGA
14	A	831	CLA	C2A-CAA-CBA-CGA
14	A	842	CLA	C2A-CAA-CBA-CGA
14	a	812	CLA	C2A-CAA-CBA-CGA
14	x	1701	CLA	C2A-CAA-CBA-CGA
14	b	825	CLA	C2A-CAA-CBA-CGA
14	b	826	CLA	C2A-CAA-CBA-CGA
14	b	830	CLA	C2A-CAA-CBA-CGA
14	b	805	CLA	C16-C17-C18-C20
14	A	828	CLA	C3-C5-C6-C7
14	b	833	CLA	CBA-CGA-O2A-C1
14	b	840	CLA	C15-C16-C17-C18
14	B	811	CLA	C10-C11-C12-C13
18	a	851	LHG	C9-C10-C11-C12
20	b	851	LMG	C16-C17-C18-C19
19	x	1702	SQD	C8-C7-O47-C45
17	A	849	BCR	C20-C21-C22-C37
17	A	850	BCR	C11-C10-C9-C34
17	A	850	BCR	C20-C21-C22-C37
17	B	846	BCR	C20-C21-C22-C37
17	B	847	BCR	C11-C10-C9-C34
17	B	847	BCR	C20-C21-C22-C37
17	B	848	BCR	C20-C21-C22-C37
17	B	850	BCR	C35-C13-C14-C15
17	F	203	BCR	C35-C13-C14-C15
17	J	105	BCR	C11-C10-C9-C34
17	K	103	BCR	C16-C17-C18-C36
17	K	103	BCR	C20-C21-C22-C37
17	I	101	BCR	C11-C10-C9-C34
17	I	101	BCR	C20-C21-C22-C37
17	L	1504	BCR	C16-C17-C18-C36
17	a	845	BCR	C20-C21-C22-C37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	a	849	BCR	C11-C10-C9-C34
17	a	849	BCR	C35-C13-C14-C15
17	b	846	BCR	C35-C13-C14-C15
17	b	846	BCR	C16-C17-C18-C36
17	b	846	BCR	C20-C21-C22-C37
17	b	847	BCR	C16-C17-C18-C36
17	b	850	BCR	C35-C13-C14-C15
17	f	204	BCR	C35-C13-C14-C15
17	f	204	BCR	C20-C21-C22-C37
17	j	105	BCR	C20-C21-C22-C37
17	i	101	BCR	C35-C13-C14-C15
17	i	101	BCR	C20-C21-C22-C37
17	i	102	BCR	C35-C13-C14-C15
17	l	201	BCR	C20-C21-C22-C37
17	l	206	BCR	C11-C10-C9-C34
17	l	206	BCR	C35-C13-C14-C15
17	l	206	BCR	C16-C17-C18-C36
17	l	207	BCR	C20-C21-C22-C37
17	m	1202	BCR	C35-C13-C14-C15
17	m	1202	BCR	C16-C17-C18-C36
17	m	1202	BCR	C20-C21-C22-C37
14	B	802	CLA	C3-C5-C6-C7
14	a	830	CLA	C5-C6-C7-C8
18	A	853	LHG	C27-C28-C29-C30
18	a	850	LHG	C24-C25-C26-C27
19	b	801	SQD	C33-C34-C35-C36
20	B	851	LMG	C20-C21-C22-C23
20	b	851	LMG	C35-C36-C37-C38
14	B	839	CLA	C11-C12-C13-C15
14	a	820	CLA	C16-C17-C18-C19
14	b	806	CLA	C16-C17-C18-C19
14	b	834	CLA	C11-C12-C13-C15
14	b	839	CLA	C11-C12-C13-C14
18	A	852	LHG	C34-C35-C36-C37
19	b	801	SQD	C11-C10-C9-C8
20	B	851	LMG	C17-C18-C19-C20
20	B	851	LMG	C19-C20-C21-C22
20	b	851	LMG	C13-C14-C15-C16
14	b	832	CLA	C8-C10-C11-C12
14	a	819	CLA	C5-C6-C7-C8
14	A	828	CLA	O1D-CGD-O2D-CED
14	a	834	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	a	836	CLA	O1D-CGD-O2D-CED
14	B	814	CLA	C5-C6-C7-C8
18	F	201	LHG	C32-C33-C34-C35
18	a	851	LHG	C13-C14-C15-C16
19	b	801	SQD	C26-C27-C28-C29
20	b	851	LMG	C36-C37-C38-C39
14	a	826	CLA	C8-C10-C11-C12
14	a	833	CLA	C10-C11-C12-C13
18	A	853	LHG	C34-C35-C36-C37
20	B	851	LMG	C22-C23-C24-C25
14	A	838	CLA	C3-C5-C6-C7
17	A	848	BCR	C11-C10-C9-C8
17	A	850	BCR	C12-C13-C14-C15
17	B	846	BCR	C12-C13-C14-C15
17	B	848	BCR	C11-C10-C9-C8
17	B	848	BCR	C20-C21-C22-C23
17	F	203	BCR	C20-C21-C22-C23
17	J	103	BCR	C12-C13-C14-C15
17	J	104	BCR	C11-C10-C9-C8
17	L	1504	BCR	C20-C21-C22-C23
17	M	101	BCR	C11-C10-C9-C8
17	a	844	BCR	C11-C10-C9-C8
17	a	847	BCR	C12-C13-C14-C15
17	b	846	BCR	C11-C10-C9-C8
17	b	846	BCR	C20-C21-C22-C23
17	b	847	BCR	C11-C10-C9-C8
17	b	848	BCR	C11-C10-C9-C8
17	b	848	BCR	C16-C17-C18-C19
17	f	202	BCR	C12-C13-C14-C15
17	f	202	BCR	C16-C17-C18-C19
17	j	104	BCR	C16-C17-C18-C19
17	j	105	BCR	C11-C10-C9-C8
17	j	106	BCR	C12-C13-C14-C15
17	i	102	BCR	C12-C13-C14-C15
14	L	1502	CLA	CBA-CGA-O2A-C1
14	a	825	CLA	CBA-CGA-O2A-C1
18	A	852	LHG	C32-C33-C34-C35
18	a	851	LHG	C28-C29-C30-C31
18	a	851	LHG	C30-C31-C32-C33
18	a	851	LHG	C33-C34-C35-C36
19	X	1702	SQD	C29-C30-C31-C32
20	B	851	LMG	C18-C19-C20-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	B	820	CLA	C13-C15-C16-C17
15	A	844	PQN	C15-C16-C17-C18
14	A	827	CLA	C16-C17-C18-C20
14	B	843	CLA	C16-C17-C18-C20
14	b	809	CLA	C16-C17-C18-C20
14	F	202	CLA	O1D-CGD-O2D-CED
14	L	1503	CLA	O1D-CGD-O2D-CED
14	b	832	CLA	O1D-CGD-O2D-CED
14	b	816	CLA	C4-C3-C5-C6
14	A	831	CLA	C5-C6-C7-C8
14	b	836	CLA	C5-C6-C7-C8
18	F	201	LHG	C25-C26-C27-C28
19	l	202	SQD	C24-C25-C26-C27
14	A	833	CLA	C2-C3-C5-C6
14	A	839	CLA	C2-C3-C5-C6
14	B	804	CLA	C6-C7-C8-C9
14	B	806	CLA	C11-C10-C8-C9
14	B	829	CLA	C11-C12-C13-C14
14	F	202	CLA	C6-C7-C8-C9
14	a	810	CLA	C11-C10-C8-C9
14	a	831	CLA	C14-C13-C15-C16
14	B	839	CLA	O1D-CGD-O2D-CED
14	A	835	CLA	C5-C6-C7-C8
14	a	834	CLA	C5-C6-C7-C8
18	F	201	LHG	C10-C11-C12-C13
18	F	201	LHG	C28-C29-C30-C31
20	B	851	LMG	C14-C15-C16-C17
14	A	807	CLA	C8-C10-C11-C12
14	B	808	CLA	C13-C15-C16-C17
14	B	832	CLA	C5-C6-C7-C8
14	A	809	CLA	C2A-CAA-CBA-CGA
14	A	836	CLA	C2A-CAA-CBA-CGA
14	B	827	CLA	C2A-CAA-CBA-CGA
14	a	808	CLA	C2A-CAA-CBA-CGA
14	a	809	CLA	C2A-CAA-CBA-CGA
14	a	841	CLA	C2A-CAA-CBA-CGA
14	b	831	CLA	C2A-CAA-CBA-CGA
14	A	829	CLA	O1A-CGA-O2A-C1
17	B	848	BCR	C7-C8-C9-C34
17	B	848	BCR	C37-C22-C23-C24
17	L	1504	BCR	C37-C22-C23-C24
17	a	847	BCR	C36-C18-C19-C20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	a	849	BCR	C37-C22-C23-C24
18	A	853	LHG	C30-C31-C32-C33
18	F	201	LHG	O1-C1-C2-C3
18	i	103	LHG	O1-C1-C2-C3
17	B	845	BCR	C21-C22-C23-C24
17	F	203	BCR	C11-C12-C13-C14
17	a	847	BCR	C21-C22-C23-C24
17	a	848	BCR	C11-C12-C13-C14
17	a	848	BCR	C21-C22-C23-C24
17	j	104	BCR	C21-C22-C23-C24
14	A	817	CLA	C8-C10-C11-C12
14	b	814	CLA	C5-C6-C7-C8
18	A	852	LHG	C24-C25-C26-C27
19	X	1702	SQD	C11-C12-C13-C14
14	b	815	CLA	C5-C6-C7-C8
19	b	801	SQD	C12-C13-C14-C15
19	l	202	SQD	C17-C18-C19-C20
20	b	851	LMG	C18-C19-C20-C21
13	A	801	CL0	C16-C17-C18-C19
13	a	801	CL0	C16-C17-C18-C19
14	A	806	CLA	C16-C17-C18-C20
14	A	842	CLA	C16-C17-C18-C19
14	B	807	CLA	C6-C7-C8-C9
14	B	807	CLA	C6-C7-C8-C10
14	a	837	CLA	C16-C17-C18-C20
14	b	805	CLA	C16-C17-C18-C19
14	b	839	CLA	C11-C12-C13-C15
14	B	805	CLA	C13-C15-C16-C17
14	b	809	CLA	C5-C6-C7-C8
14	b	809	CLA	C15-C16-C17-C18
18	F	201	LHG	C30-C31-C32-C33
19	l	202	SQD	C15-C16-C17-C18
14	A	813	CLA	O1D-CGD-O2D-CED
14	A	820	CLA	C5-C6-C7-C8
18	A	853	LHG	C10-C11-C12-C13
18	a	850	LHG	C32-C33-C34-C35
18	i	103	LHG	C18-C19-C20-C21
14	a	839	CLA	C8-C10-C11-C12
14	a	838	CLA	O1A-CGA-O2A-C1
18	a	850	LHG	O10-C23-O8-C6
20	B	851	LMG	C13-C14-C15-C16
20	b	851	LMG	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	m	1201	CLA	C3-C5-C6-C7
14	A	821	CLA	CBA-CGA-O2A-C1
14	a	830	CLA	CBA-CGA-O2A-C1
14	k	102	CLA	CBA-CGA-O2A-C1
18	A	853	LHG	C24-C23-O8-C6
20	B	851	LMG	C29-C28-O8-C9
18	F	201	LHG	C24-C25-C26-C27
14	a	817	CLA	O1D-CGD-O2D-CED
14	b	812	CLA	O1D-CGD-O2D-CED
14	A	805	CLA	C3A-C2A-CAA-CBA
14	A	806	CLA	C3A-C2A-CAA-CBA
14	A	837	CLA	C3A-C2A-CAA-CBA
14	B	806	CLA	C3A-C2A-CAA-CBA
14	B	813	CLA	C3A-C2A-CAA-CBA
14	B	816	CLA	C3A-C2A-CAA-CBA
14	B	835	CLA	C3A-C2A-CAA-CBA
14	a	805	CLA	C3A-C2A-CAA-CBA
14	b	807	CLA	C3A-C2A-CAA-CBA
14	b	812	CLA	C3A-C2A-CAA-CBA
14	b	816	CLA	C3A-C2A-CAA-CBA
14	f	201	CLA	C3A-C2A-CAA-CBA
14	l	203	CLA	C3A-C2A-CAA-CBA
14	b	828	CLA	C10-C11-C12-C13
18	a	851	LHG	C11-C12-C13-C14
19	b	801	SQD	C34-C35-C36-C37
20	B	851	LMG	C31-C32-C33-C34
14	l	203	CLA	O1D-CGD-O2D-CED
14	m	1201	CLA	O1D-CGD-O2D-CED
13	A	801	CL0	C16-C17-C18-C20
13	a	801	CL0	C16-C17-C18-C20
14	B	843	CLA	C16-C17-C18-C19
14	b	809	CLA	C16-C17-C18-C19
14	b	834	CLA	C11-C12-C13-C14
18	a	851	LHG	C24-C25-C26-C27
19	X	1702	SQD	C32-C33-C34-C35
20	b	851	LMG	C41-C42-C43-C44
14	b	834	CLA	CBD-CGD-O2D-CED
18	A	853	LHG	C25-C26-C27-C28
19	b	801	SQD	C25-C26-C27-C28
14	a	831	CLA	O2A-C1-C2-C3
17	A	850	BCR	C14-C15-C16-C17
17	I	101	BCR	C14-C15-C16-C17

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	a	847	BCR	C14-C15-C16-C17
17	f	202	BCR	C14-C15-C16-C17
17	i	101	BCR	C14-C15-C16-C17
14	A	807	CLA	C3-C5-C6-C7
14	A	841	CLA	C3-C5-C6-C7
14	A	825	CLA	C4-C3-C5-C6
14	A	833	CLA	C4-C3-C5-C6
14	a	837	CLA	C4-C3-C5-C6
14	A	838	CLA	CBA-CGA-O2A-C1
14	B	820	CLA	CBA-CGA-O2A-C1
14	B	830	CLA	CBA-CGA-O2A-C1
14	A	834	CLA	C2-C3-C5-C6
14	a	837	CLA	C2-C3-C5-C6
14	b	816	CLA	C2-C3-C5-C6
18	A	852	LHG	C31-C32-C33-C34
18	a	851	LHG	C15-C16-C17-C18
19	b	801	SQD	C29-C30-C31-C32
14	A	815	CLA	O1D-CGD-O2D-CED
14	B	822	CLA	O1A-CGA-O2A-C1
14	A	806	CLA	C16-C17-C18-C19
14	b	841	CLA	O1D-CGD-O2D-CED
14	a	802	CLA	C13-C15-C16-C17
14	b	814	CLA	CBA-CGA-O2A-C1
20	B	851	LMG	C33-C34-C35-C36
14	b	833	CLA	O1A-CGA-O2A-C1
14	a	822	CLA	C5-C6-C7-C8
14	l	203	CLA	C2C-C3C-CAC-CBC
19	l	202	SQD	C18-C19-C20-C21
14	B	836	CLA	C2-C1-O2A-CGA
19	l	202	SQD	C9-C10-C11-C12
20	b	851	LMG	C22-C23-C24-C25
14	B	816	CLA	C5-C6-C7-C8
14	a	831	CLA	C5-C6-C7-C8
14	b	832	CLA	C10-C11-C12-C13
14	a	825	CLA	O1A-CGA-O2A-C1
14	b	815	CLA	C4C-C3C-CAC-CBC
18	a	851	LHG	C10-C11-C12-C13
17	A	846	BCR	C5-C6-C7-C8
17	A	847	BCR	C23-C24-C25-C26
17	A	847	BCR	C23-C24-C25-C30
17	A	849	BCR	C1-C6-C7-C8
17	A	849	BCR	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	A	849	BCR	C23-C24-C25-C26
17	A	850	BCR	C5-C6-C7-C8
17	A	851	BCR	C1-C6-C7-C8
17	A	851	BCR	C5-C6-C7-C8
17	A	851	BCR	C23-C24-C25-C26
17	A	851	BCR	C23-C24-C25-C30
17	B	845	BCR	C1-C6-C7-C8
17	B	845	BCR	C5-C6-C7-C8
17	B	846	BCR	C5-C6-C7-C8
17	B	847	BCR	C5-C6-C7-C8
17	B	848	BCR	C5-C6-C7-C8
17	B	848	BCR	C23-C24-C25-C26
17	B	849	BCR	C23-C24-C25-C30
17	F	203	BCR	C5-C6-C7-C8
17	F	205	BCR	C5-C6-C7-C8
17	J	103	BCR	C5-C6-C7-C8
17	J	104	BCR	C1-C6-C7-C8
17	J	104	BCR	C5-C6-C7-C8
17	J	104	BCR	C23-C24-C25-C26
17	J	104	BCR	C23-C24-C25-C30
17	I	102	BCR	C5-C6-C7-C8
17	M	101	BCR	C1-C6-C7-C8
17	M	101	BCR	C5-C6-C7-C8
17	a	844	BCR	C5-C6-C7-C8
17	a	845	BCR	C23-C24-C25-C26
17	a	847	BCR	C5-C6-C7-C8
17	a	848	BCR	C5-C6-C7-C8
17	a	849	BCR	C1-C6-C7-C8
17	a	849	BCR	C5-C6-C7-C8
17	a	849	BCR	C23-C24-C25-C26
17	a	849	BCR	C23-C24-C25-C30
17	b	845	BCR	C5-C6-C7-C8
17	b	847	BCR	C5-C6-C7-C8
17	b	848	BCR	C5-C6-C7-C8
17	b	848	BCR	C23-C24-C25-C26
17	b	849	BCR	C23-C24-C25-C26
17	b	849	BCR	C23-C24-C25-C30
17	b	850	BCR	C5-C6-C7-C8
17	f	202	BCR	C5-C6-C7-C8
17	f	204	BCR	C1-C6-C7-C8
17	f	204	BCR	C5-C6-C7-C8
17	j	104	BCR	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	j	105	BCR	C1-C6-C7-C8
17	j	105	BCR	C5-C6-C7-C8
17	j	105	BCR	C23-C24-C25-C26
17	j	106	BCR	C23-C24-C25-C26
17	k	103	BCR	C23-C24-C25-C26
17	i	102	BCR	C5-C6-C7-C8
17	l	201	BCR	C23-C24-C25-C26
17	l	201	BCR	C23-C24-C25-C30
17	l	207	BCR	C23-C24-C25-C26
17	m	1202	BCR	C1-C6-C7-C8
17	m	1202	BCR	C5-C6-C7-C8
14	b	817	CLA	CBA-CGA-O2A-C1
14	b	822	CLA	CBA-CGA-O2A-C1
14	A	825	CLA	C8-C10-C11-C12
14	A	833	CLA	C15-C16-C17-C18
14	A	838	CLA	C15-C16-C17-C18
14	A	839	CLA	C15-C16-C17-C18
14	B	806	CLA	C13-C15-C16-C17
14	a	807	CLA	C5-C6-C7-C8
14	b	811	CLA	C13-C15-C16-C17
20	B	803	LMG	C11-C12-C13-C14
14	B	802	CLA	C5-C6-C7-C8
14	B	829	CLA	C15-C16-C17-C18
14	L	1502	CLA	C10-C11-C12-C13
14	A	843	CLA	O1D-CGD-O2D-CED
20	B	851	LMG	C29-C30-C31-C32
20	B	851	LMG	C36-C37-C38-C39
14	b	828	CLA	C4-C3-C5-C6
14	b	840	CLA	C4-C3-C5-C6
14	A	842	CLA	O1D-CGD-O2D-CED
14	A	825	CLA	C2-C3-C5-C6
14	A	828	CLA	C6-C7-C8-C10
14	A	832	CLA	C11-C10-C8-C7
14	B	810	CLA	C6-C7-C8-C10
14	B	812	CLA	C6-C7-C8-C10
14	B	820	CLA	C11-C10-C8-C7
14	B	820	CLA	C12-C13-C15-C16
14	B	839	CLA	C2-C3-C5-C6
14	F	202	CLA	C6-C7-C8-C10
14	a	804	CLA	C12-C13-C15-C16
14	a	810	CLA	C11-C10-C8-C7
14	b	804	CLA	C6-C7-C8-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	b	807	CLA	C11-C10-C8-C7
14	b	809	CLA	C11-C10-C8-C7
14	b	809	CLA	C12-C13-C15-C16
14	b	829	CLA	C11-C10-C8-C7
14	A	808	CLA	C3-C5-C6-C7
14	A	821	CLA	O1A-CGA-O2A-C1
14	L	1502	CLA	O1A-CGA-O2A-C1
14	a	830	CLA	O1A-CGA-O2A-C1
14	b	814	CLA	O1A-CGA-O2A-C1
14	k	102	CLA	O1A-CGA-O2A-C1
18	i	103	LHG	C10-C11-C12-C13
14	A	842	CLA	C8-C10-C11-C12
14	b	807	CLA	C10-C11-C12-C13
17	B	849	BCR	C15-C16-C17-C18
14	a	819	CLA	CBD-CGD-O2D-CED
14	b	830	CLA	CBD-CGD-O2D-CED
14	A	827	CLA	C16-C17-C18-C19
14	b	825	CLA	C6-C7-C8-C9
14	b	833	CLA	O1D-CGD-O2D-CED
18	F	201	LHG	O9-C7-O7-C5
19	l	202	SQD	O49-C7-O47-C45
18	A	853	LHG	C7-C8-C9-C10
14	j	101	CLA	CBA-CGA-O2A-C1
18	A	852	LHG	C30-C31-C32-C33
14	A	822	CLA	C2A-CAA-CBA-CGA
14	A	841	CLA	C2A-CAA-CBA-CGA
14	B	823	CLA	C2A-CAA-CBA-CGA
14	a	835	CLA	C2A-CAA-CBA-CGA
14	b	823	CLA	C2A-CAA-CBA-CGA
14	B	802	CLA	O1D-CGD-O2D-CED
14	B	825	CLA	C5-C6-C7-C8
14	a	802	CLA	C15-C16-C17-C18
19	x	1702	SQD	C7-C8-C9-C10
14	A	808	CLA	O1D-CGD-O2D-CED
14	b	825	CLA	C3-C5-C6-C7
19	X	1702	SQD	C34-C35-C36-C37
17	B	845	BCR	C22-C23-C24-C25
17	J	103	BCR	C6-C7-C8-C9
17	a	846	BCR	C22-C23-C24-C25
17	j	105	BCR	C22-C23-C24-C25
14	B	835	CLA	CBA-CGA-O2A-C1
14	B	822	CLA	C16-C17-C18-C20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	b	830	CLA	C16-C17-C18-C19
14	B	805	CLA	C5-C6-C7-C8
20	B	851	LMG	C21-C22-C23-C24
20	b	851	LMG	C28-C29-C30-C31
18	A	852	LHG	C8-C7-O7-C5
18	A	853	LHG	C8-C7-O7-C5
18	a	850	LHG	C8-C7-O7-C5
17	B	846	BCR	C14-C15-C16-C17
14	b	816	CLA	CBD-CGD-O2D-CED
14	f	201	CLA	C10-C11-C12-C13
19	x	1702	SQD	C32-C33-C34-C35
19	b	801	SQD	O49-C7-O47-C45
19	l	202	SQD	O47-C45-C46-O48
20	B	803	LMG	O7-C8-C9-O8
14	B	806	CLA	O1D-CGD-O2D-CED
14	B	804	CLA	C16-C17-C18-C19
14	B	839	CLA	C11-C12-C13-C14
18	a	851	LHG	C32-C33-C34-C35
19	l	202	SQD	C12-C13-C14-C15
14	a	817	CLA	C8-C10-C11-C12
14	b	827	CLA	C13-C15-C16-C17
14	A	834	CLA	C4-C3-C5-C6
18	i	103	LHG	C7-C8-C9-C10
14	A	819	CLA	C2-C3-C5-C6
14	a	822	CLA	C2-C3-C5-C6
14	b	828	CLA	C2-C3-C5-C6
14	b	840	CLA	C2-C3-C5-C6
14	b	833	CLA	C5-C6-C7-C8
14	A	805	CLA	C14-C13-C15-C16
14	A	809	CLA	C11-C12-C13-C14
14	A	828	CLA	C6-C7-C8-C9
14	A	828	CLA	C11-C12-C13-C14
14	A	832	CLA	C11-C12-C13-C14
14	A	832	CLA	C14-C13-C15-C16
14	A	838	CLA	C11-C12-C13-C14
14	B	802	CLA	C11-C10-C8-C9
14	B	810	CLA	C6-C7-C8-C9
14	B	812	CLA	C6-C7-C8-C9
14	B	820	CLA	C14-C13-C15-C16
14	a	804	CLA	C11-C10-C8-C9
14	a	804	CLA	C14-C13-C15-C16
14	a	805	CLA	C11-C12-C13-C14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	a	812	CLA	C11-C10-C8-C9
14	a	816	CLA	C11-C10-C8-C9
14	a	829	CLA	C11-C10-C8-C9
14	a	833	CLA	C6-C7-C8-C9
14	b	804	CLA	C6-C7-C8-C9
14	b	810	CLA	C6-C7-C8-C9
14	b	820	CLA	C14-C13-C15-C16
15	b	844	PQN	C21-C22-C23-C24
14	B	825	CLA	CBD-CGD-O2D-CED
20	B	851	LMG	C23-C24-C25-C26
14	B	828	CLA	C3-C5-C6-C7
14	b	826	CLA	C3-C5-C6-C7
14	b	840	CLA	C3-C5-C6-C7
18	A	853	LHG	C9-C10-C11-C12
20	b	851	LMG	C31-C32-C33-C34
17	b	848	BCR	C37-C22-C23-C24
14	A	835	CLA	O1D-CGD-O2D-CED
14	a	831	CLA	C15-C16-C17-C18
17	B	848	BCR	C21-C22-C23-C24
14	B	830	CLA	O1A-CGA-O2A-C1
14	b	822	CLA	O1A-CGA-O2A-C1
14	A	805	CLA	C1A-C2A-CAA-CBA
14	A	808	CLA	C1A-C2A-CAA-CBA
14	A	818	CLA	C1A-C2A-CAA-CBA
14	A	823	CLA	C1A-C2A-CAA-CBA
14	X	1701	CLA	C1A-C2A-CAA-CBA
14	B	806	CLA	C1A-C2A-CAA-CBA
14	B	808	CLA	C1A-C2A-CAA-CBA
14	B	813	CLA	C1A-C2A-CAA-CBA
14	B	816	CLA	C1A-C2A-CAA-CBA
14	B	818	CLA	C1A-C2A-CAA-CBA
14	B	819	CLA	C1A-C2A-CAA-CBA
14	B	830	CLA	C1A-C2A-CAA-CBA
14	B	832	CLA	C1A-C2A-CAA-CBA
14	B	833	CLA	C1A-C2A-CAA-CBA
14	B	835	CLA	C1A-C2A-CAA-CBA
14	K	102	CLA	C1A-C2A-CAA-CBA
14	a	807	CLA	C1A-C2A-CAA-CBA
14	a	817	CLA	C1A-C2A-CAA-CBA
14	a	828	CLA	C1A-C2A-CAA-CBA
14	a	841	CLA	C1A-C2A-CAA-CBA
14	b	805	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	b	808	CLA	C1A-C2A-CAA-CBA
14	b	812	CLA	C1A-C2A-CAA-CBA
14	b	814	CLA	C1A-C2A-CAA-CBA
14	b	821	CLA	C1A-C2A-CAA-CBA
14	b	833	CLA	C1A-C2A-CAA-CBA
14	b	836	CLA	C1A-C2A-CAA-CBA
14	k	102	CLA	C1A-C2A-CAA-CBA
14	A	842	CLA	C16-C17-C18-C20
14	a	820	CLA	C16-C17-C18-C20
18	A	853	LHG	C11-C10-C9-C8
18	a	851	LHG	C16-C17-C18-C19
17	J	105	BCR	C15-C16-C17-C18
14	A	825	CLA	C10-C11-C12-C13
14	a	833	CLA	C5-C6-C7-C8
14	a	837	CLA	C10-C11-C12-C13
14	a	838	CLA	C13-C15-C16-C17
14	b	815	CLA	C2C-C3C-CAC-CBC
14	A	803	CLA	C3-C5-C6-C7
14	B	823	CLA	O1D-CGD-O2D-CED
18	A	852	LHG	C28-C29-C30-C31
14	b	817	CLA	O1A-CGA-O2A-C1
14	B	821	CLA	C8-C10-C11-C12
14	b	843	CLA	C8-C10-C11-C12
14	l	204	CLA	C10-C11-C12-C13
19	x	1702	SQD	C24-C23-O48-C46
20	b	851	LMG	C17-C18-C19-C20
14	B	820	CLA	O1D-CGD-O2D-CED
19	b	801	SQD	C9-C10-C11-C12
14	B	808	CLA	C16-C17-C18-C20
14	b	830	CLA	C16-C17-C18-C20
18	i	103	LHG	C27-C28-C29-C30
14	A	826	CLA	C5-C6-C7-C8
19	x	1702	SQD	C23-C24-C25-C26
14	B	808	CLA	CBA-CGA-O2A-C1
14	B	828	CLA	C4-C3-C5-C6
14	B	839	CLA	C4-C3-C5-C6
14	A	841	CLA	C8-C10-C11-C12
14	A	838	CLA	O1A-CGA-O2A-C1
14	B	820	CLA	O1A-CGA-O2A-C1
14	B	835	CLA	O1A-CGA-O2A-C1
18	F	201	LHG	C29-C30-C31-C32
14	a	834	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	A	832	CLA	C16-C17-C18-C20
14	a	812	CLA	C11-C12-C13-C14
14	a	837	CLA	C16-C17-C18-C19
14	b	825	CLA	C6-C7-C8-C10
14	b	835	CLA	C3-C5-C6-C7
14	A	823	CLA	C6-C7-C8-C9
18	a	850	LHG	C4-C5-C6-O8
19	X	1702	SQD	C44-C45-C46-O48
20	B	803	LMG	C7-C8-C9-O8
14	b	816	CLA	C15-C16-C17-C18
18	A	852	LHG	O10-C23-O8-C6
14	a	809	CLA	O1D-CGD-O2D-CED
14	A	826	CLA	C6-C7-C8-C9
14	B	828	CLA	C10-C11-C12-C13
14	b	802	CLA	C5-C6-C7-C8
15	a	842	PQN	C20-C21-C22-C23
18	F	201	LHG	C33-C34-C35-C36
14	j	101	CLA	O1A-CGA-O2A-C1
14	a	822	CLA	C6-C7-C8-C9
14	A	837	CLA	C4C-C3C-CAC-CBC
18	F	201	LHG	C9-C10-C11-C12
20	B	803	LMG	C30-C31-C32-C33
20	B	851	LMG	C41-C42-C43-C44
14	B	835	CLA	CBD-CGD-O2D-CED
14	A	814	CLA	C6-C7-C8-C9
17	A	846	BCR	C16-C17-C18-C36
17	A	848	BCR	C35-C13-C14-C15
17	J	104	BCR	C35-C13-C14-C15
17	a	844	BCR	C16-C17-C18-C36
17	a	849	BCR	C16-C17-C18-C36
17	b	845	BCR	C20-C21-C22-C37
17	b	849	BCR	C20-C21-C22-C37
14	A	819	CLA	C4-C3-C5-C6
14	B	840	CLA	C4-C3-C5-C6
14	F	202	CLA	C4-C3-C5-C6
14	a	828	CLA	C4-C3-C5-C6
14	B	828	CLA	C2-C3-C5-C6
14	a	825	CLA	C2-C3-C5-C6
14	a	828	CLA	C2-C3-C5-C6
14	B	808	CLA	C16-C17-C18-C19
18	a	850	LHG	C24-C23-O8-C6
20	B	851	LMG	C16-C17-C18-C19

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	a	808	CLA	C5-C6-C7-C8
14	b	804	CLA	C8-C10-C11-C12
18	a	851	LHG	C35-C36-C37-C38
20	B	803	LMG	C16-C17-C18-C19
14	B	832	CLA	O1D-CGD-O2D-CED
14	B	807	CLA	C2A-CAA-CBA-CGA
14	A	807	CLA	C10-C11-C12-C13
14	A	831	CLA	C2-C1-O2A-CGA
14	A	835	CLA	C2-C1-O2A-CGA
14	A	841	CLA	C2-C1-O2A-CGA
14	b	809	CLA	C8-C10-C11-C12
14	b	813	CLA	C8-C10-C11-C12
20	B	803	LMG	C14-C15-C16-C17
18	i	103	LHG	O6-C4-C5-O7
14	A	819	CLA	C16-C17-C18-C20
14	B	809	CLA	C16-C17-C18-C19
14	B	822	CLA	C16-C17-C18-C19
14	b	804	CLA	C10-C11-C12-C13
14	a	832	CLA	O1D-CGD-O2D-CED
18	i	103	LHG	C13-C14-C15-C16
18	A	853	LHG	C23-C24-C25-C26
18	a	850	LHG	C7-C8-C9-C10
14	f	201	CLA	C5-C6-C7-C8
15	a	842	PQN	C15-C16-C17-C18
17	B	847	BCR	C12-C13-C14-C15
17	F	205	BCR	C20-C21-C22-C23
17	K	103	BCR	C20-C21-C22-C23
17	a	846	BCR	C11-C10-C9-C8
17	a	847	BCR	C11-C10-C9-C8
17	j	104	BCR	C12-C13-C14-C15
17	j	106	BCR	C11-C10-C9-C8
19	X	1702	SQD	C16-C17-C18-C19
20	B	851	LMG	C24-C25-C26-C27
20	B	851	LMG	O7-C8-C9-O8
14	B	813	CLA	C8-C10-C11-C12
14	b	811	CLA	C8-C10-C11-C12
14	b	829	CLA	C13-C15-C16-C17
14	B	808	CLA	O1A-CGA-O2A-C1
18	F	201	LHG	O10-C23-O8-C6
14	B	831	CLA	C4-C3-C5-C6
14	a	825	CLA	C4-C3-C5-C6
14	A	805	CLA	C12-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	A	807	CLA	C6-C7-C8-C10
14	A	808	CLA	C11-C10-C8-C7
14	A	809	CLA	C11-C12-C13-C15
14	A	811	CLA	C11-C12-C13-C15
14	A	828	CLA	C11-C12-C13-C15
14	A	829	CLA	C12-C13-C15-C16
14	A	832	CLA	C6-C7-C8-C10
14	A	832	CLA	C11-C12-C13-C15
14	A	833	CLA	C12-C13-C15-C16
14	A	842	CLA	C6-C7-C8-C10
14	B	802	CLA	C11-C10-C8-C7
14	B	809	CLA	C12-C13-C15-C16
14	B	811	CLA	C6-C7-C8-C10
14	B	829	CLA	C11-C12-C13-C15
14	B	840	CLA	C2-C3-C5-C6
14	B	840	CLA	C11-C10-C8-C7
14	F	202	CLA	C2-C3-C5-C6
14	L	1502	CLA	C11-C10-C8-C7
14	a	804	CLA	C11-C10-C8-C7
14	a	805	CLA	C11-C12-C13-C15
14	a	807	CLA	C11-C10-C8-C7
14	a	812	CLA	C11-C10-C8-C7
14	a	816	CLA	C6-C7-C8-C10
14	a	816	CLA	C11-C10-C8-C7
14	a	818	CLA	C11-C12-C13-C15
14	a	827	CLA	C6-C7-C8-C10
14	a	829	CLA	C11-C10-C8-C7
14	a	832	CLA	C12-C13-C15-C16
14	a	833	CLA	C11-C10-C8-C7
14	a	839	CLA	C11-C10-C8-C7
14	b	802	CLA	C11-C12-C13-C15
14	b	804	CLA	C11-C12-C13-C15
14	b	805	CLA	C12-C13-C15-C16
14	b	811	CLA	C6-C7-C8-C10
14	b	827	CLA	C12-C13-C15-C16
14	b	828	CLA	C11-C12-C13-C15
14	b	830	CLA	C6-C7-C8-C10
14	b	831	CLA	C12-C13-C15-C16
14	b	834	CLA	C6-C7-C8-C10
14	b	835	CLA	C11-C12-C13-C15
15	b	844	PQN	C21-C22-C23-C25
14	a	802	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	A	807	CLA	C6-C7-C8-C9
14	A	808	CLA	C11-C10-C8-C9
14	A	811	CLA	C11-C12-C13-C14
14	A	827	CLA	C11-C10-C8-C9
14	A	829	CLA	C14-C13-C15-C16
14	A	833	CLA	C14-C13-C15-C16
14	A	841	CLA	C11-C10-C8-C9
14	A	841	CLA	C14-C13-C15-C16
14	A	842	CLA	C6-C7-C8-C9
14	B	808	CLA	C14-C13-C15-C16
14	B	827	CLA	C14-C13-C15-C16
14	B	831	CLA	C14-C13-C15-C16
14	a	807	CLA	C11-C10-C8-C9
14	a	818	CLA	C11-C12-C13-C14
14	a	824	CLA	C14-C13-C15-C16
14	a	826	CLA	C11-C10-C8-C9
14	a	828	CLA	C14-C13-C15-C16
14	a	838	CLA	C11-C12-C13-C14
14	a	839	CLA	C11-C10-C8-C9
14	b	802	CLA	C6-C7-C8-C9
14	b	808	CLA	C14-C13-C15-C16
14	b	811	CLA	C6-C7-C8-C9
14	b	827	CLA	C14-C13-C15-C16
14	b	829	CLA	C6-C7-C8-C9
14	b	830	CLA	C6-C7-C8-C9
14	b	831	CLA	C14-C13-C15-C16
14	b	835	CLA	C6-C7-C8-C9
18	A	852	LHG	C27-C28-C29-C30
14	A	835	CLA	CBA-CGA-O2A-C1
14	B	834	CLA	C2A-CAA-CBA-CGA
14	B	808	CLA	O1D-CGD-O2D-CED
14	a	812	CLA	C11-C12-C13-C15
14	b	843	CLA	C16-C17-C18-C19
19	l	202	SQD	C19-C20-C21-C22
17	M	101	BCR	C7-C8-C9-C10
19	x	1702	SQD	O49-C7-O47-C45
14	A	814	CLA	CBA-CGA-O2A-C1
14	A	823	CLA	CBA-CGA-O2A-C1
14	A	831	CLA	CBA-CGA-O2A-C1
14	A	832	CLA	CBA-CGA-O2A-C1
14	a	812	CLA	CBA-CGA-O2A-C1
14	a	822	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	a	851	LHG	C29-C30-C31-C32
14	A	818	CLA	C10-C11-C12-C13
15	b	844	PQN	C20-C21-C22-C23
17	I	101	BCR	C6-C7-C8-C9
14	b	806	CLA	C16-C17-C18-C20
14	b	843	CLA	C16-C17-C18-C20
19	x	1702	SQD	C12-C13-C14-C15
18	A	852	LHG	C23-C24-C25-C26
14	b	826	CLA	CBA-CGA-O2A-C1
14	B	826	CLA	C4-C3-C5-C6
14	B	830	CLA	C4-C3-C5-C6
14	b	834	CLA	C4-C3-C5-C6
14	b	836	CLA	C6-C7-C8-C9
20	b	851	LMG	C40-C41-C42-C43
18	A	852	LHG	C11-C12-C13-C14
18	a	850	LHG	C31-C32-C33-C34
18	i	103	LHG	C11-C12-C13-C14
14	A	825	CLA	CBA-CGA-O2A-C1
14	B	832	CLA	CBA-CGA-O2A-C1
14	b	831	CLA	CBA-CGA-O2A-C1
14	A	810	CLA	C3A-C2A-CAA-CBA
14	A	823	CLA	C3A-C2A-CAA-CBA
14	A	826	CLA	C3A-C2A-CAA-CBA
14	A	843	CLA	C3A-C2A-CAA-CBA
14	B	834	CLA	C3A-C2A-CAA-CBA
14	j	101	CLA	C3A-C2A-CAA-CBA
19	b	801	SQD	C13-C14-C15-C16
19	b	801	SQD	C17-C18-C19-C20
17	b	848	BCR	C19-C20-C21-C22
18	i	103	LHG	C26-C27-C28-C29
14	B	806	CLA	C16-C17-C18-C20
14	B	830	CLA	C13-C15-C16-C17
14	a	820	CLA	C5-C6-C7-C8
15	B	844	PQN	C23-C25-C26-C27
18	A	852	LHG	C4-C5-C6-O8
18	i	103	LHG	C4-C5-C6-O8
20	B	803	LMG	O1-C7-C8-C9
19	l	202	SQD	C34-C35-C36-C37
18	i	103	LHG	C15-C16-C17-C18
14	B	809	CLA	C3-C5-C6-C7
18	A	853	LHG	C24-C25-C26-C27
14	b	839	CLA	C4C-C3C-CAC-CBC

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	A	834	CLA	C2C-C3C-CAC-CBC
14	B	835	CLA	C10-C11-C12-C13
19	l	202	SQD	C10-C11-C12-C13
14	A	805	CLA	C3-C5-C6-C7
18	F	201	LHG	O1-C1-C2-O2
14	A	825	CLA	C13-C15-C16-C17
14	B	804	CLA	C16-C17-C18-C20
14	B	812	CLA	C5-C6-C7-C8
14	b	802	CLA	C13-C15-C16-C17
14	b	830	CLA	CAA-CBA-CGA-O2A
18	i	103	LHG	O7-C5-C6-O8
14	B	808	CLA	CBD-CGD-O2D-CED
19	b	801	SQD	C19-C20-C21-C22
14	A	821	CLA	C16-C17-C18-C19
14	a	802	CLA	C16-C17-C18-C20
14	A	827	CLA	C8-C10-C11-C12
14	A	807	CLA	C2-C1-O2A-CGA
14	A	828	CLA	C2-C1-O2A-CGA
14	a	802	CLA	C2-C1-O2A-CGA
14	b	808	CLA	C2-C1-O2A-CGA
14	b	809	CLA	C2-C1-O2A-CGA
14	B	830	CLA	C2-C3-C5-C6
14	b	820	CLA	C8-C10-C11-C12
14	A	813	CLA	C11-C10-C8-C9
14	A	825	CLA	C14-C13-C15-C16
14	B	821	CLA	C11-C12-C13-C14
14	B	822	CLA	C11-C10-C8-C9
14	B	826	CLA	C6-C7-C8-C9
14	B	830	CLA	C11-C12-C13-C14
14	B	830	CLA	C14-C13-C15-C16
14	a	811	CLA	C6-C7-C8-C9
14	a	820	CLA	C11-C10-C8-C9
14	a	827	CLA	C6-C7-C8-C9
14	a	832	CLA	C14-C13-C15-C16
14	a	833	CLA	C11-C10-C8-C9
14	b	809	CLA	C14-C13-C15-C16
14	b	812	CLA	C11-C12-C13-C14
14	b	829	CLA	C14-C13-C15-C16
14	a	837	CLA	C5-C6-C7-C8
14	L	1501	CLA	C4-C3-C5-C6
14	a	812	CLA	O1A-CGA-O2A-C1
14	B	828	CLA	C2C-C3C-CAC-CBC

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	F	202	CLA	C2C-C3C-CAC-CBC
14	a	819	CLA	C6-C7-C8-C9
14	j	101	CLA	C10-C11-C12-C13
14	B	809	CLA	C2A-CAA-CBA-CGA
14	A	819	CLA	C16-C17-C18-C19
14	B	806	CLA	C16-C17-C18-C19
14	A	840	CLA	CBD-CGD-O2D-CED
17	A	846	BCR	C1-C6-C7-C8
17	A	846	BCR	C23-C24-C25-C26
17	A	846	BCR	C23-C24-C25-C30
17	A	847	BCR	C1-C6-C7-C8
17	A	847	BCR	C5-C6-C7-C8
17	A	848	BCR	C1-C6-C7-C8
17	A	848	BCR	C5-C6-C7-C8
17	A	848	BCR	C23-C24-C25-C26
17	A	850	BCR	C23-C24-C25-C30
17	B	845	BCR	C23-C24-C25-C26
17	B	847	BCR	C1-C6-C7-C8
17	B	849	BCR	C1-C6-C7-C8
17	B	849	BCR	C5-C6-C7-C8
17	B	850	BCR	C1-C6-C7-C8
17	B	850	BCR	C5-C6-C7-C8
17	B	850	BCR	C23-C24-C25-C26
17	F	203	BCR	C23-C24-C25-C30
17	J	103	BCR	C23-C24-C25-C26
17	J	105	BCR	C23-C24-C25-C26
17	J	105	BCR	C23-C24-C25-C30
17	K	103	BCR	C23-C24-C25-C26
17	K	103	BCR	C23-C24-C25-C30
17	I	102	BCR	C1-C6-C7-C8
17	I	102	BCR	C23-C24-C25-C26
17	I	102	BCR	C23-C24-C25-C30
17	M	101	BCR	C23-C24-C25-C26
17	a	845	BCR	C5-C6-C7-C8
17	a	846	BCR	C1-C6-C7-C8
17	a	846	BCR	C23-C24-C25-C26
17	a	847	BCR	C23-C24-C25-C26
17	a	848	BCR	C23-C24-C25-C26
17	a	848	BCR	C23-C24-C25-C30
17	b	846	BCR	C5-C6-C7-C8
17	b	849	BCR	C1-C6-C7-C8
17	b	849	BCR	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	b	850	BCR	C23-C24-C25-C26
17	f	202	BCR	C1-C6-C7-C8
17	f	204	BCR	C23-C24-C25-C26
17	j	104	BCR	C23-C24-C25-C26
17	j	104	BCR	C23-C24-C25-C30
17	j	106	BCR	C5-C6-C7-C8
17	i	101	BCR	C1-C6-C7-C8
17	i	101	BCR	C5-C6-C7-C8
17	i	102	BCR	C23-C24-C25-C26
17	i	102	BCR	C23-C24-C25-C30
17	l	201	BCR	C5-C6-C7-C8
17	l	206	BCR	C5-C6-C7-C8
17	l	207	BCR	C1-C6-C7-C8
17	l	207	BCR	C5-C6-C7-C8
17	m	1202	BCR	C23-C24-C25-C26
19	X	1702	SQD	C11-C10-C9-C8
17	A	849	BCR	C21-C22-C23-C24
17	J	103	BCR	C17-C18-C19-C20
17	f	204	BCR	C11-C12-C13-C14
14	b	834	CLA	O1D-CGD-O2D-CED
17	A	849	BCR	C14-C15-C16-C17
14	A	835	CLA	O1A-CGA-O2A-C1
14	A	832	CLA	C16-C17-C18-C19
14	B	843	CLA	C5-C6-C7-C8
14	a	822	CLA	O1A-CGA-O2A-C1
14	b	826	CLA	O1A-CGA-O2A-C1
14	B	825	CLA	O1D-CGD-O2D-CED
19	l	202	SQD	C14-C15-C16-C17
14	A	805	CLA	C11-C10-C8-C7
14	A	813	CLA	C11-C10-C8-C7
14	A	818	CLA	C11-C10-C8-C7
14	A	827	CLA	C11-C10-C8-C7
14	A	830	CLA	C11-C10-C8-C7
14	A	838	CLA	C12-C13-C15-C16
14	A	841	CLA	C11-C10-C8-C7
14	A	841	CLA	C12-C13-C15-C16
14	B	802	CLA	C12-C13-C15-C16
14	B	808	CLA	C12-C13-C15-C16
14	B	809	CLA	C6-C7-C8-C10
14	B	816	CLA	C11-C10-C8-C7
14	B	816	CLA	C12-C13-C15-C16
14	B	821	CLA	C6-C7-C8-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	B	821	CLA	C11-C10-C8-C7
14	B	821	CLA	C11-C12-C13-C15
14	B	822	CLA	C11-C10-C8-C7
14	B	827	CLA	C12-C13-C15-C16
14	B	828	CLA	C11-C12-C13-C15
14	B	830	CLA	C11-C12-C13-C15
14	B	831	CLA	C12-C13-C15-C16
14	F	202	CLA	C11-C10-C8-C7
14	a	805	CLA	C12-C13-C15-C16
14	a	818	CLA	C12-C13-C15-C16
14	a	820	CLA	C11-C10-C8-C7
14	a	824	CLA	C12-C13-C15-C16
14	a	826	CLA	C11-C10-C8-C7
14	a	828	CLA	C12-C13-C15-C16
14	b	802	CLA	C6-C7-C8-C10
14	b	804	CLA	C11-C10-C8-C7
14	b	807	CLA	C12-C13-C15-C16
14	b	808	CLA	C12-C13-C15-C16
14	b	812	CLA	C11-C12-C13-C15
14	b	829	CLA	C12-C13-C15-C16
14	b	832	CLA	C11-C12-C13-C15
14	b	835	CLA	C6-C7-C8-C10
14	a	819	CLA	O1D-CGD-O2D-CED
14	A	832	CLA	O1A-CGA-O2A-C1
17	A	849	BCR	C19-C20-C21-C22
17	I	102	BCR	C9-C10-C11-C12
17	i	101	BCR	C13-C14-C15-C16
14	K	101	CLA	C2A-CAA-CBA-CGA
14	B	839	CLA	C8-C10-C11-C12
17	A	849	BCR	C16-C17-C18-C36
17	B	845	BCR	C35-C13-C14-C15
17	a	846	BCR	C16-C17-C18-C36
17	a	846	BCR	C20-C21-C22-C37
17	b	845	BCR	C11-C10-C9-C34
17	b	850	BCR	C11-C10-C9-C34
17	j	106	BCR	C16-C17-C18-C36
17	l	201	BCR	C35-C13-C14-C15
19	l	202	SQD	C35-C36-C37-C38
14	A	802	CLA	C15-C16-C17-C18
14	F	202	CLA	CAA-CBA-CGA-O2A
14	b	835	CLA	CAA-CBA-CGA-O2A
19	X	1702	SQD	C18-C19-C20-C21

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	B	827	CLA	C10-C11-C12-C13
14	a	838	CLA	C10-C11-C12-C13
20	b	851	LMG	C37-C38-C39-C40
14	A	814	CLA	CAD-CBD-CGD-O2D
14	A	815	CLA	CAD-CBD-CGD-O2D
14	A	820	CLA	CAD-CBD-CGD-O2D
14	A	826	CLA	CAD-CBD-CGD-O2D
14	B	820	CLA	CAD-CBD-CGD-O2D
14	B	826	CLA	CAD-CBD-CGD-O2D
14	B	835	CLA	CAD-CBD-CGD-O2D
14	B	842	CLA	CAD-CBD-CGD-O2D
14	L	1501	CLA	CAD-CBD-CGD-O2D
14	a	811	CLA	CAD-CBD-CGD-O2D
14	a	813	CLA	CAD-CBD-CGD-O2D
14	a	816	CLA	CAD-CBD-CGD-O2D
14	a	820	CLA	CAD-CBD-CGD-O2D
14	a	830	CLA	CAD-CBD-CGD-O2D
14	a	832	CLA	CAD-CBD-CGD-O2D
14	a	840	CLA	CAD-CBD-CGD-O2D
14	b	803	CLA	CAD-CBD-CGD-O2D
14	b	813	CLA	CAD-CBD-CGD-O2D
14	b	817	CLA	CAD-CBD-CGD-O2D
14	b	818	CLA	CAD-CBD-CGD-O2D
14	b	823	CLA	CAD-CBD-CGD-O2D
14	b	825	CLA	CAD-CBD-CGD-O2D
14	b	829	CLA	CAD-CBD-CGD-O2D
14	b	842	CLA	CAD-CBD-CGD-O2D
14	f	203	CLA	CAD-CBD-CGD-O2D
14	j	102	CLA	CAD-CBD-CGD-O2D
14	l	205	CLA	CAD-CBD-CGD-O2D
14	m	1201	CLA	CAD-CBD-CGD-O2D
19	b	801	SQD	C11-C12-C13-C14
17	B	847	BCR	C6-C7-C8-C9
17	B	848	BCR	C22-C23-C24-C25
17	K	103	BCR	C6-C7-C8-C9
14	A	834	CLA	CBA-CGA-O2A-C1
14	a	837	CLA	CBA-CGA-O2A-C1
15	a	842	PQN	C14-C13-C15-C16
20	B	851	LMG	C30-C31-C32-C33
18	F	201	LHG	C2-C3-O3-P
18	F	201	LHG	C5-C4-O6-P
19	l	202	SQD	C44-C45-C46-O48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	A	814	CLA	O1A-CGA-O2A-C1
14	A	823	CLA	O1A-CGA-O2A-C1
14	A	831	CLA	O1A-CGA-O2A-C1
14	K	102	CLA	O2A-C1-C2-C3
18	i	103	LHG	C12-C13-C14-C15
14	A	802	CLA	C2A-CAA-CBA-CGA
14	B	833	CLA	CBD-CGD-O2D-CED
14	a	831	CLA	C16-C17-C18-C20
20	b	851	LMG	C20-C21-C22-C23
14	A	803	CLA	CHA-CBD-CGD-O1D
14	A	803	CLA	CHA-CBD-CGD-O2D
14	A	808	CLA	CHA-CBD-CGD-O1D
14	A	813	CLA	CHA-CBD-CGD-O1D
14	A	834	CLA	CHA-CBD-CGD-O1D
14	A	834	CLA	CHA-CBD-CGD-O2D
14	A	837	CLA	CHA-CBD-CGD-O1D
14	B	805	CLA	CHA-CBD-CGD-O1D
14	B	808	CLA	CHA-CBD-CGD-O1D
14	B	828	CLA	CHA-CBD-CGD-O1D
14	B	828	CLA	CHA-CBD-CGD-O2D
14	B	840	CLA	CHA-CBD-CGD-O1D
14	a	806	CLA	CHA-CBD-CGD-O1D
14	a	806	CLA	CHA-CBD-CGD-O2D
14	a	812	CLA	CHA-CBD-CGD-O1D
14	a	817	CLA	CHA-CBD-CGD-O1D
14	a	817	CLA	CHA-CBD-CGD-O2D
14	a	833	CLA	CHA-CBD-CGD-O1D
14	a	833	CLA	CHA-CBD-CGD-O2D
14	a	838	CLA	CHA-CBD-CGD-O1D
14	a	838	CLA	CHA-CBD-CGD-O2D
14	a	839	CLA	CHA-CBD-CGD-O2D
14	a	841	CLA	CHA-CBD-CGD-O1D
14	a	841	CLA	CHA-CBD-CGD-O2D
14	b	805	CLA	CHA-CBD-CGD-O1D
14	b	805	CLA	CHA-CBD-CGD-O2D
14	b	811	CLA	CHA-CBD-CGD-O1D
14	b	814	CLA	CHA-CBD-CGD-O1D
14	b	816	CLA	CHA-CBD-CGD-O1D
14	b	816	CLA	CHA-CBD-CGD-O2D
14	b	822	CLA	CHA-CBD-CGD-O1D
14	b	822	CLA	CHA-CBD-CGD-O2D
14	b	828	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	b	828	CLA	CHA-CBD-CGD-O2D
14	b	832	CLA	CHA-CBD-CGD-O1D
14	b	832	CLA	CHA-CBD-CGD-O2D
14	l	203	CLA	CHA-CBD-CGD-O1D
14	l	203	CLA	CHA-CBD-CGD-O2D
18	i	103	LHG	C16-C17-C18-C19
14	B	832	CLA	O1A-CGA-O2A-C1
14	b	831	CLA	O1A-CGA-O2A-C1
14	B	828	CLA	C4C-C3C-CAC-CBC
14	b	816	CLA	O1D-CGD-O2D-CED
17	J	104	BCR	C20-C21-C22-C23
17	I	101	BCR	C20-C21-C22-C23
17	j	106	BCR	C16-C17-C18-C19
14	B	808	CLA	C15-C16-C17-C18
14	a	824	CLA	C15-C16-C17-C18
14	A	825	CLA	O1A-CGA-O2A-C1
14	a	832	CLA	C16-C17-C18-C20
14	B	809	CLA	C8-C10-C11-C12
14	b	816	CLA	C8-C10-C11-C12
15	b	844	PQN	C25-C26-C27-C28
20	B	851	LMG	C37-C38-C39-C40
14	A	805	CLA	C11-C10-C8-C9
14	A	808	CLA	C11-C12-C13-C14
14	A	830	CLA	C11-C10-C8-C9
14	F	202	CLA	C11-C10-C8-C9
14	a	818	CLA	C14-C13-C15-C16
14	b	807	CLA	C11-C10-C8-C9
14	B	833	CLA	O1D-CGD-O2D-CED
14	B	806	CLA	C2C-C3C-CAC-CBC
14	b	812	CLA	C16-C17-C18-C20
17	M	101	BCR	C36-C18-C19-C20
17	b	847	BCR	C36-C18-C19-C20
14	A	823	CLA	C5-C6-C7-C8
19	X	1702	SQD	C31-C32-C33-C34
14	A	842	CLA	C5-C6-C7-C8
14	b	834	CLA	C5-C6-C7-C8
17	F	205	BCR	C17-C18-C19-C20
17	j	104	BCR	C11-C12-C13-C14
17	i	101	BCR	C7-C8-C9-C10
17	m	1202	BCR	C7-C8-C9-C10
14	A	807	CLA	C1A-C2A-CAA-CBA
14	A	811	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	A	830	CLA	C1A-C2A-CAA-CBA
14	A	831	CLA	C1A-C2A-CAA-CBA
14	A	835	CLA	C1A-C2A-CAA-CBA
14	A	841	CLA	C1A-C2A-CAA-CBA
14	b	807	CLA	C1A-C2A-CAA-CBA
14	b	832	CLA	C1A-C2A-CAA-CBA
14	a	831	CLA	C16-C17-C18-C19
19	l	202	SQD	C16-C17-C18-C19
14	B	825	CLA	C4-C3-C5-C6
18	i	103	LHG	C5-C4-O6-P
19	l	202	SQD	C11-C12-C13-C14
18	F	201	LHG	C3-O3-P-O5
18	a	851	LHG	C3-O3-P-O4
18	i	103	LHG	C3-O3-P-O4
18	i	103	LHG	C4-O6-P-O4
14	A	833	CLA	C16-C17-C18-C20
14	B	820	CLA	C16-C17-C18-C19
14	a	805	CLA	C16-C17-C18-C19
14	a	803	CLA	C6-C7-C8-C9
14	B	812	CLA	C8-C10-C11-C12
14	B	801	CLA	C2A-CAA-CBA-CGA
14	A	825	CLA	CBD-CGD-O2D-CED
14	B	842	CLA	C3-C5-C6-C7
14	B	809	CLA	C16-C17-C18-C20
14	B	813	CLA	C11-C12-C13-C15
14	A	805	CLA	CAD-CBD-CGD-O1D
14	A	813	CLA	CAD-CBD-CGD-O1D
14	A	837	CLA	CAD-CBD-CGD-O1D
14	A	843	CLA	CAD-CBD-CGD-O1D
14	B	804	CLA	CAD-CBD-CGD-O1D
14	a	804	CLA	CAD-CBD-CGD-O1D
14	a	812	CLA	CAD-CBD-CGD-O1D
14	a	817	CLA	CAD-CBD-CGD-O1D
14	a	836	CLA	C2-C3-C5-C6
14	a	837	CLA	CAD-CBD-CGD-O1D
14	a	841	CLA	CAD-CBD-CGD-O1D
14	b	805	CLA	CAD-CBD-CGD-O1D
14	b	816	CLA	CAD-CBD-CGD-O1D
14	b	832	CLA	CAD-CBD-CGD-O1D
14	l	203	CLA	CAD-CBD-CGD-O1D
19	l	202	SQD	C5-C6-S-O7
20	B	851	LMG	C40-C41-C42-C43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	a	838	CLA	C3-C5-C6-C7
14	A	830	CLA	C10-C11-C12-C13
19	l	202	SQD	C23-C24-C25-C26
18	i	103	LHG	C14-C15-C16-C17
14	B	810	CLA	CBA-CGA-O2A-C1
14	a	833	CLA	C2C-C3C-CAC-CBC
14	a	806	CLA	C11-C12-C13-C15
14	b	839	CLA	C4-C3-C5-C6
14	A	806	CLA	C6-C7-C8-C10
14	A	806	CLA	C12-C13-C15-C16
14	A	819	CLA	C12-C13-C15-C16
14	A	825	CLA	C12-C13-C15-C16
14	A	828	CLA	C11-C10-C8-C7
14	A	834	CLA	C12-C13-C15-C16
14	B	801	CLA	C11-C10-C8-C7
14	B	834	CLA	C11-C10-C8-C7
14	B	840	CLA	C12-C13-C15-C16
14	a	807	CLA	C12-C13-C15-C16
14	a	833	CLA	C11-C12-C13-C15
14	a	833	CLA	C12-C13-C15-C16
14	a	840	CLA	C11-C10-C8-C7
14	b	809	CLA	C6-C7-C8-C10
14	b	840	CLA	C11-C10-C8-C7
14	j	101	CLA	C11-C10-C8-C7
14	l	204	CLA	C3A-C2A-CAA-CBA
14	l	204	CLA	C11-C10-C8-C7
14	B	816	CLA	C8-C10-C11-C12
14	a	824	CLA	C13-C15-C16-C17
14	A	839	CLA	C10-C11-C12-C13
19	X	1702	SQD	C23-C24-C25-C26
14	A	808	CLA	C8-C10-C11-C12
14	a	820	CLA	C2A-CAA-CBA-CGA
14	A	807	CLA	C11-C12-C13-C15
14	b	804	CLA	C16-C17-C18-C19
14	b	816	CLA	C13-C15-C16-C17
19	x	1702	SQD	O6-C44-C45-C46
14	a	837	CLA	O1A-CGA-O2A-C1
20	B	803	LMG	O1-C7-C8-O7
20	b	851	LMG	C38-C39-C40-C41
14	A	818	CLA	O1A-CGA-O2A-C1
14	b	828	CLA	C4C-C3C-CAC-CBC
17	a	846	BCR	C14-C15-C16-C17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	l	202	SQD	C45-C44-O6-C1
14	B	820	CLA	C16-C17-C18-C20
14	A	807	CLA	C5-C6-C7-C8
14	A	832	CLA	C15-C16-C17-C18
14	a	812	CLA	C5-C6-C7-C8
14	A	839	CLA	C8-C10-C11-C12
14	m	1201	CLA	C5-C6-C7-C8
14	A	809	CLA	C4-C3-C5-C6
14	A	838	CLA	C4-C3-C5-C6
14	B	836	CLA	C5-C6-C7-C8
18	A	852	LHG	C11-C10-C9-C8
18	a	850	LHG	C28-C29-C30-C31
14	B	826	CLA	C2-C3-C5-C6
14	b	839	CLA	C2-C3-C5-C6
18	A	852	LHG	C25-C26-C27-C28
18	A	853	LHG	C32-C33-C34-C35
18	i	103	LHG	C24-C25-C26-C27
14	A	833	CLA	C13-C15-C16-C17
14	B	827	CLA	C13-C15-C16-C17
14	a	807	CLA	C13-C15-C16-C17
14	A	832	CLA	C11-C10-C8-C9
14	A	838	CLA	C14-C13-C15-C16
14	B	808	CLA	C11-C10-C8-C9
14	B	809	CLA	C6-C7-C8-C9
14	B	816	CLA	C11-C10-C8-C9
14	B	816	CLA	C14-C13-C15-C16
14	B	821	CLA	C6-C7-C8-C9
14	B	821	CLA	C11-C10-C8-C9
14	B	828	CLA	C11-C12-C13-C14
14	B	829	CLA	C11-C10-C8-C9
14	L	1502	CLA	C11-C10-C8-C9
14	a	805	CLA	C14-C13-C15-C16
14	b	802	CLA	C11-C12-C13-C14
14	b	805	CLA	C14-C13-C15-C16
15	A	844	PQN	C21-C22-C23-C24
17	a	848	BCR	C22-C23-C24-C25
17	j	106	BCR	C22-C23-C24-C25
14	A	834	CLA	O1A-CGA-O2A-C1
19	X	1702	SQD	O10-C23-O48-C46
19	b	801	SQD	C27-C28-C29-C30
19	b	801	SQD	C30-C31-C32-C33
19	l	202	SQD	C27-C28-C29-C30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	B	851	LMG	O10-C28-O8-C9
18	i	103	LHG	O1-C1-C2-O2
17	B	850	BCR	C36-C18-C19-C20
14	a	805	CLA	C10-C11-C12-C13
14	b	826	CLA	C5-C6-C7-C8
17	i	102	BCR	C20-C21-C22-C37
14	b	803	CLA	C4-C3-C5-C6
14	b	828	CLA	C2C-C3C-CAC-CBC
14	B	831	CLA	C2-C3-C5-C6
14	A	832	CLA	C8-C10-C11-C12
19	b	801	SQD	C16-C17-C18-C19
14	A	835	CLA	C6-C7-C8-C9
14	a	832	CLA	C13-C15-C16-C17
14	B	818	CLA	C1-C2-C3-C4
14	b	818	CLA	C1-C2-C3-C4
14	B	835	CLA	O1D-CGD-O2D-CED
18	a	851	LHG	C34-C35-C36-C37
18	i	103	LHG	O6-C4-C5-C6
14	X	1701	CLA	C2A-CAA-CBA-CGA
14	B	831	CLA	C2A-CAA-CBA-CGA
14	b	803	CLA	C2A-CAA-CBA-CGA
18	a	850	LHG	O9-C7-O7-C5
14	A	818	CLA	CBA-CGA-O2A-C1
14	B	814	CLA	CBA-CGA-O2A-C1
14	A	803	CLA	C2-C1-O2A-CGA
14	A	818	CLA	C2-C1-O2A-CGA
14	A	842	CLA	C2-C1-O2A-CGA
14	a	817	CLA	C2-C1-O2A-CGA
14	b	812	CLA	C2-C1-O2A-CGA
14	b	839	CLA	C2C-C3C-CAC-CBC
14	B	833	CLA	O1A-CGA-O2A-C1
14	B	836	CLA	O1A-CGA-O2A-C1
14	A	827	CLA	C3-C5-C6-C7
14	B	833	CLA	CBA-CGA-O2A-C1
14	b	804	CLA	C16-C17-C18-C20
14	A	808	CLA	C4-C3-C5-C6
14	B	816	CLA	C4-C3-C5-C6
14	a	827	CLA	C4-C3-C5-C6
14	b	825	CLA	C4-C3-C5-C6
19	X	1702	SQD	C28-C29-C30-C31
17	A	848	BCR	C23-C24-C25-C30
17	A	850	BCR	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	B	845	BCR	C23-C24-C25-C30
17	F	203	BCR	C23-C24-C25-C26
17	F	205	BCR	C23-C24-C25-C26
17	J	103	BCR	C23-C24-C25-C30
17	J	105	BCR	C5-C6-C7-C8
17	K	103	BCR	C5-C6-C7-C8
17	M	101	BCR	C23-C24-C25-C30
17	a	846	BCR	C5-C6-C7-C8
17	a	846	BCR	C23-C24-C25-C30
17	b	845	BCR	C23-C24-C25-C26
17	k	103	BCR	C5-C6-C7-C8
17	l	201	BCR	C1-C6-C7-C8
14	b	834	CLA	C10-C11-C12-C13
14	B	831	CLA	CBA-CGA-O2A-C1
14	B	832	CLA	C16-C17-C18-C20
14	B	842	CLA	O1D-CGD-O2D-CED
14	B	806	CLA	C8-C10-C11-C12
14	B	826	CLA	C2A-CAA-CBA-CGA
17	A	851	BCR	C11-C10-C9-C8
17	A	851	BCR	C16-C17-C18-C19
17	a	848	BCR	C16-C17-C18-C19
17	b	848	BCR	C20-C21-C22-C23
19	x	1702	SQD	O6-C44-C45-O47
14	a	820	CLA	C15-C16-C17-C18
18	A	852	LHG	C3-O3-P-O6
18	A	853	LHG	C3-O3-P-O6
18	a	850	LHG	C3-O3-P-O6
18	A	853	LHG	C33-C34-C35-C36
14	A	840	CLA	O1D-CGD-O2D-CED
14	A	802	CLA	C4-C3-C5-C6
14	b	830	CLA	C4-C3-C5-C6
14	f	201	CLA	C4-C3-C5-C6
15	A	844	PQN	C14-C13-C15-C16
14	A	813	CLA	C6-C7-C8-C10
14	A	839	CLA	C11-C10-C8-C7
14	B	809	CLA	C11-C10-C8-C7
14	B	843	CLA	C6-C7-C8-C10
14	a	805	CLA	C11-C10-C8-C7
14	a	808	CLA	C11-C10-C8-C7
14	b	834	CLA	C2-C3-C5-C6
20	B	851	LMG	C34-C35-C36-C37
14	B	801	CLA	C11-C10-C8-C9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	B	811	CLA	C6-C7-C8-C9
14	B	834	CLA	C11-C10-C8-C9
14	B	840	CLA	C11-C10-C8-C9
14	a	807	CLA	C14-C13-C15-C16
14	a	816	CLA	C6-C7-C8-C9
14	a	837	CLA	C11-C10-C8-C9
14	a	840	CLA	C11-C10-C8-C9
14	b	804	CLA	C11-C12-C13-C14
14	b	807	CLA	C14-C13-C15-C16
14	b	828	CLA	C11-C12-C13-C14
14	b	829	CLA	C11-C10-C8-C9
14	b	834	CLA	C6-C7-C8-C9
17	J	104	BCR	C19-C20-C21-C22
17	I	101	BCR	C13-C14-C15-C16
14	B	805	CLA	C16-C17-C18-C19
14	A	813	CLA	C2A-CAA-CBA-CGA
14	A	807	CLA	C11-C12-C13-C14
14	a	802	CLA	C16-C17-C18-C19
14	a	805	CLA	C16-C17-C18-C20
14	a	832	CLA	C16-C17-C18-C19
14	b	812	CLA	C16-C17-C18-C19
18	a	850	LHG	C10-C11-C12-C13
17	l	201	BCR	C21-C22-C23-C24
14	x	1701	CLA	O2A-C1-C2-C3
14	A	821	CLA	C16-C17-C18-C20
14	B	813	CLA	C11-C12-C13-C14
14	B	832	CLA	C16-C17-C18-C19
14	a	806	CLA	C11-C12-C13-C14
14	A	828	CLA	CBA-CGA-O2A-C1
14	B	836	CLA	CBA-CGA-O2A-C1
20	b	851	LMG	C29-C30-C31-C32
14	A	825	CLA	C15-C16-C17-C18
14	B	814	CLA	O1A-CGA-O2A-C1
14	m	1201	CLA	CBA-CGA-O2A-C1
14	A	828	CLA	C2A-CAA-CBA-CGA
14	B	805	CLA	C16-C17-C18-C20
14	B	842	CLA	C15-C16-C17-C18
17	F	203	BCR	C9-C10-C11-C12
17	j	104	BCR	C13-C14-C15-C16
13	A	801	CL0	O1A-CGA-O2A-C1
13	a	801	CL0	O1A-CGA-O2A-C1
18	F	201	LHG	O6-C4-C5-O7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
18	A	853	LHG	O10-C23-O8-C6
14	B	834	CLA	C4-C3-C5-C6
15	a	842	PQN	C12-C13-C15-C16
14	a	825	CLA	C6-C7-C8-C9
14	A	839	CLA	C2-C1-O2A-CGA
14	B	804	CLA	C2-C1-O2A-CGA
14	B	832	CLA	C2-C1-O2A-CGA
14	a	812	CLA	C2-C1-O2A-CGA
14	b	828	CLA	C16-C17-C18-C20
19	b	801	SQD	C24-C25-C26-C27
14	a	816	CLA	C2A-CAA-CBA-CGA
19	x	1702	SQD	C11-C10-C9-C8
14	A	841	CLA	C3A-C2A-CAA-CBA
14	b	813	CLA	C3A-C2A-CAA-CBA
14	a	828	CLA	C16-C17-C18-C19
17	A	846	BCR	C9-C10-C11-C12
17	M	101	BCR	C13-C14-C15-C16
17	f	204	BCR	C19-C20-C21-C22
17	j	106	BCR	C9-C10-C11-C12
14	B	830	CLA	C10-C11-C12-C13
14	B	814	CLA	C6-C7-C8-C9
14	B	836	CLA	C4-C3-C5-C6
14	b	802	CLA	C4-C3-C5-C6
14	b	835	CLA	C4-C3-C5-C6
14	a	829	CLA	O1D-CGD-O2D-CED
14	A	803	CLA	C11-C12-C13-C14
14	A	819	CLA	C14-C13-C15-C16
14	A	821	CLA	C6-C7-C8-C9
14	A	827	CLA	C14-C13-C15-C16
14	B	813	CLA	C11-C10-C8-C9
14	L	1502	CLA	C6-C7-C8-C9
14	a	833	CLA	C11-C12-C13-C14
14	a	833	CLA	C14-C13-C15-C16
14	b	803	CLA	C14-C13-C15-C16
14	b	809	CLA	C6-C7-C8-C9
14	b	810	CLA	C11-C10-C8-C9
14	b	813	CLA	C11-C10-C8-C9
19	b	801	SQD	C15-C16-C17-C18
17	A	851	BCR	C11-C10-C9-C34
17	B	850	BCR	C20-C21-C22-C37
17	J	103	BCR	C35-C13-C14-C15
17	J	105	BCR	C20-C21-C22-C37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	b	847	BCR	C20-C21-C22-C37
17	f	202	BCR	C20-C21-C22-C37
14	A	812	CLA	C3-C5-C6-C7
14	A	841	CLA	CAA-CBA-CGA-O2A
14	b	823	CLA	CAA-CBA-CGA-O1A
14	a	828	CLA	C16-C17-C18-C20
14	b	828	CLA	C16-C17-C18-C19
18	i	103	LHG	C17-C18-C19-C20
14	A	806	CLA	C3-C5-C6-C7
14	a	841	CLA	CAA-CBA-CGA-O1A
14	A	813	CLA	C1A-C2A-CAA-CBA
14	B	825	CLA	C1A-C2A-CAA-CBA
14	a	803	CLA	C1A-C2A-CAA-CBA
14	a	808	CLA	C1A-C2A-CAA-CBA
14	a	838	CLA	C1A-C2A-CAA-CBA
14	b	803	CLA	C1A-C2A-CAA-CBA
14	b	819	CLA	C1A-C2A-CAA-CBA
14	l	204	CLA	C1A-C2A-CAA-CBA
14	m	1201	CLA	C1A-C2A-CAA-CBA
14	A	809	CLA	C2-C3-C5-C6
14	B	808	CLA	C11-C10-C8-C7
14	a	806	CLA	C6-C7-C8-C10
14	a	811	CLA	C6-C7-C8-C10
14	b	816	CLA	C11-C10-C8-C7
14	b	822	CLA	C11-C10-C8-C7
14	b	827	CLA	C6-C7-C8-C10
14	b	829	CLA	C6-C7-C8-C10
14	b	835	CLA	C2-C3-C5-C6
14	A	841	CLA	O1A-CGA-O2A-C1
14	b	823	CLA	CAA-CBA-CGA-O2A
14	b	814	CLA	C6-C7-C8-C9
17	b	845	BCR	C13-C14-C15-C16
18	A	852	LHG	C24-C23-O8-C6
14	a	841	CLA	CAA-CBA-CGA-O2A
14	A	825	CLA	C16-C17-C18-C20
14	b	813	CLA	C11-C12-C13-C14
14	A	812	CLA	C2A-CAA-CBA-CGA
14	a	805	CLA	C2A-CAA-CBA-CGA
14	B	802	CLA	C13-C15-C16-C17
14	b	808	CLA	C15-C16-C17-C18
18	F	201	LHG	C11-C10-C9-C8
18	a	850	LHG	C35-C36-C37-C38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	x	1702	SQD	C17-C18-C19-C20
20	b	851	LMG	C15-C16-C17-C18
14	B	805	CLA	C15-C16-C17-C18
14	A	822	CLA	CAA-CBA-CGA-O2A
14	b	803	CLA	C2-C3-C5-C6
14	A	817	CLA	C11-C12-C13-C14
19	x	1702	SQD	C19-C20-C21-C22
17	B	847	BCR	C20-C21-C22-C23
17	M	101	BCR	C16-C17-C18-C19
17	a	849	BCR	C11-C10-C9-C8
17	a	849	BCR	C16-C17-C18-C19
17	b	847	BCR	C20-C21-C22-C23
14	b	842	CLA	CBA-CGA-O2A-C1
17	B	849	BCR	C13-C14-C15-C16
17	b	850	BCR	C13-C14-C15-C16
17	i	101	BCR	C15-C16-C17-C18
19	x	1702	SQD	C14-C15-C16-C17
14	A	803	CLA	O1D-CGD-O2D-CED
14	A	833	CLA	C16-C17-C18-C19
14	b	811	CLA	C15-C16-C17-C18
14	B	801	CLA	C4-C3-C5-C6
14	A	809	CLA	C2-C1-O2A-CGA
14	A	832	CLA	C2-C1-O2A-CGA
14	b	806	CLA	C2-C1-O2A-CGA
14	A	838	CLA	C2-C3-C5-C6
14	b	802	CLA	C2-C3-C5-C6
14	b	830	CLA	C2-C3-C5-C6
14	f	201	CLA	C2-C3-C5-C6
14	b	835	CLA	C13-C15-C16-C17
17	f	202	BCR	C10-C11-C12-C13
17	j	106	BCR	C18-C19-C20-C21
14	A	822	CLA	CAA-CBA-CGA-O1A
14	B	810	CLA	C11-C10-C8-C9
14	B	829	CLA	C6-C7-C8-C9
14	a	838	CLA	C11-C10-C8-C9
14	B	806	CLA	C10-C11-C12-C13
14	B	831	CLA	O1A-CGA-O2A-C1
14	a	827	CLA	C2A-CAA-CBA-CGA
14	a	830	CLA	C2A-CAA-CBA-CGA
14	b	808	CLA	C16-C17-C18-C19
14	B	810	CLA	O1A-CGA-O2A-C1
17	B	850	BCR	C23-C24-C25-C30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	F	205	BCR	C23-C24-C25-C30
17	J	105	BCR	C1-C6-C7-C8
17	K	103	BCR	C1-C6-C7-C8
17	I	101	BCR	C1-C6-C7-C8
17	I	101	BCR	C5-C6-C7-C8
17	L	1504	BCR	C1-C6-C7-C8
17	a	844	BCR	C23-C24-C25-C26
17	a	844	BCR	C23-C24-C25-C30
17	a	845	BCR	C1-C6-C7-C8
17	a	847	BCR	C23-C24-C25-C30
17	b	845	BCR	C23-C24-C25-C30
17	b	846	BCR	C1-C6-C7-C8
17	f	202	BCR	C23-C24-C25-C26
17	f	202	BCR	C23-C24-C25-C30
17	f	204	BCR	C23-C24-C25-C30
17	j	106	BCR	C1-C6-C7-C8
17	k	103	BCR	C1-C6-C7-C8
17	l	206	BCR	C1-C6-C7-C8
17	m	1202	BCR	C23-C24-C25-C30
14	A	809	CLA	C10-C11-C12-C13
14	a	817	CLA	C10-C11-C12-C13
14	L	1503	CLA	CAA-CBA-CGA-O2A
14	B	809	CLA	C10-C11-C12-C13
14	m	1201	CLA	O1A-CGA-O2A-C1
17	j	106	BCR	C15-C16-C17-C18
18	a	851	LHG	C11-C10-C9-C8
14	B	835	CLA	C4-C3-C5-C6
17	b	846	BCR	C7-C8-C9-C10
14	A	802	CLA	C2-C3-C5-C6
14	A	808	CLA	C2-C3-C5-C6
14	B	816	CLA	C2-C3-C5-C6
15	A	844	PQN	C12-C13-C15-C16
14	L	1502	CLA	C3-C5-C6-C7
14	b	819	CLA	CBD-CGD-O2D-CED
14	k	101	CLA	CAA-CBA-CGA-O2A
14	b	842	CLA	O1A-CGA-O2A-C1
14	b	807	CLA	C8-C10-C11-C12
14	L	1503	CLA	CAA-CBA-CGA-O1A
14	k	101	CLA	CAA-CBA-CGA-O1A
14	B	823	CLA	CAA-CBA-CGA-O2A
14	A	829	CLA	C4-C3-C5-C6
14	a	807	CLA	C4-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	a	808	CLA	C4-C3-C5-C6
14	A	803	CLA	C11-C12-C13-C15
14	A	821	CLA	C12-C13-C15-C16
14	B	805	CLA	C6-C7-C8-C10
14	a	807	CLA	C2-C3-C5-C6
14	b	805	CLA	C6-C7-C8-C10
14	b	821	CLA	C6-C7-C8-C10
14	K	101	CLA	CAA-CBA-CGA-O2A
13	A	801	CL0	CBA-CGA-O2A-C1
14	A	826	CLA	C3-C5-C6-C7
14	b	830	CLA	CAA-CBA-CGA-O1A
14	A	829	CLA	C16-C17-C18-C19
14	A	812	CLA	C5-C6-C7-C8
14	X	1701	CLA	O2A-C1-C2-C3
20	B	851	LMG	O7-C10-C11-C12
14	m	1201	CLA	C2A-CAA-CBA-CGA
14	f	203	CLA	CAA-CBA-CGA-O2A
13	a	801	CL0	CBA-CGA-O2A-C1
14	A	841	CLA	CBA-CGA-O2A-C1
14	b	827	CLA	CBA-CGA-O2A-C1
17	A	848	BCR	C16-C17-C18-C36
17	A	849	BCR	C35-C13-C14-C15
17	A	851	BCR	C20-C21-C22-C37
17	b	846	BCR	C11-C10-C9-C34
17	b	849	BCR	C35-C13-C14-C15
17	k	103	BCR	C20-C21-C22-C37
14	B	813	CLA	C4-C3-C5-C6
14	a	805	CLA	C4-C3-C5-C6
14	a	811	CLA	C4-C3-C5-C6
14	j	101	CLA	C4-C3-C5-C6
18	A	852	LHG	C10-C11-C12-C13
14	B	825	CLA	C2-C3-C5-C6
14	a	808	CLA	C2-C3-C5-C6
14	a	827	CLA	C2-C3-C5-C6
14	A	829	CLA	C16-C17-C18-C20
14	b	832	CLA	C13-C15-C16-C17
14	A	842	CLA	CAA-CBA-CGA-O2A
14	B	820	CLA	C4C-C3C-CAC-CBC
14	A	806	CLA	C14-C13-C15-C16
14	A	834	CLA	C14-C13-C15-C16
14	A	842	CLA	C14-C13-C15-C16
14	B	840	CLA	C14-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	B	843	CLA	C6-C7-C8-C9
14	F	202	CLA	C14-C13-C15-C16
14	a	824	CLA	C6-C7-C8-C9
14	b	802	CLA	C11-C10-C8-C9
14	b	807	CLA	C11-C12-C13-C14
14	b	809	CLA	C11-C10-C8-C9
14	b	816	CLA	C11-C10-C8-C9
14	b	822	CLA	C11-C10-C8-C9
14	b	827	CLA	C6-C7-C8-C9
14	b	831	CLA	C11-C12-C13-C14
14	b	840	CLA	C11-C10-C8-C9
14	j	101	CLA	C11-C10-C8-C9
14	l	204	CLA	C6-C7-C8-C9
14	B	815	CLA	C4C-C3C-CAC-CBC
14	A	813	CLA	C3A-C2A-CAA-CBA
14	a	803	CLA	C3A-C2A-CAA-CBA
14	a	835	CLA	C3A-C2A-CAA-CBA
14	b	803	CLA	C3A-C2A-CAA-CBA
19	b	801	SQD	O47-C7-C8-C9
14	K	101	CLA	CAA-CBA-CGA-O1A
14	A	817	CLA	CAD-CBD-CGD-O2D
14	A	825	CLA	CAD-CBD-CGD-O2D
14	X	1701	CLA	CAD-CBD-CGD-O2D
14	B	807	CLA	CAD-CBD-CGD-O2D
14	B	811	CLA	CAD-CBD-CGD-O2D
14	B	816	CLA	CAD-CBD-CGD-O2D
14	B	818	CLA	CAD-CBD-CGD-O2D
14	B	824	CLA	CAD-CBD-CGD-O2D
14	B	829	CLA	CAD-CBD-CGD-O2D
14	F	202	CLA	CAD-CBD-CGD-O2D
14	F	204	CLA	CAD-CBD-CGD-O2D
14	J	101	CLA	CAD-CBD-CGD-O2D
14	a	825	CLA	CAD-CBD-CGD-O2D
14	a	836	CLA	CAD-CBD-CGD-O2D
14	x	1701	CLA	CAD-CBD-CGD-O2D
14	b	833	CLA	CAD-CBD-CGD-O2D
14	b	835	CLA	CAD-CBD-CGD-O2D
14	b	839	CLA	CAD-CBD-CGD-O2D
14	b	808	CLA	C16-C17-C18-C20
14	b	813	CLA	C11-C12-C13-C15
14	b	821	CLA	C16-C17-C18-C20
14	B	825	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	b	834	CLA	C3-C5-C6-C7
19	b	801	SQD	C32-C33-C34-C35
18	a	850	LHG	C11-C12-C13-C14
14	A	827	CLA	CAA-CBA-CGA-O2A
14	a	828	CLA	CAA-CBA-CGA-O2A
20	B	803	LMG	O7-C10-C11-C12
14	A	825	CLA	O1D-CGD-O2D-CED
17	a	847	BCR	C6-C7-C8-C9
17	i	102	BCR	C22-C23-C24-C25
14	B	812	CLA	CAA-CBA-CGA-O2A
14	B	835	CLA	CAA-CBA-CGA-O2A
17	F	205	BCR	C21-C22-C23-C24
14	b	842	CLA	O1D-CGD-O2D-CED
20	B	851	LMG	C7-C8-C9-O8
14	B	823	CLA	CAA-CBA-CGA-O1A
14	a	829	CLA	CBD-CGD-O2D-CED
14	B	813	CLA	CAA-CBA-CGA-O2A
20	b	851	LMG	O7-C10-C11-C12
14	a	818	CLA	C16-C17-C18-C20
14	b	842	CLA	CBD-CGD-O2D-CED
14	A	820	CLA	O2A-C1-C2-C3
14	A	832	CLA	O2A-C1-C2-C3
14	a	817	CLA	O2A-C1-C2-C3
14	b	827	CLA	O1A-CGA-O2A-C1
14	a	820	CLA	C8-C10-C11-C12
14	A	840	CLA	C11-C12-C13-C14
14	B	805	CLA	CAA-CBA-CGA-O2A
14	a	807	CLA	CAA-CBA-CGA-O2A
14	A	806	CLA	CBD-CGD-O2D-CED
14	b	822	CLA	CBD-CGD-O2D-CED
14	A	807	CLA	CHA-CBD-CGD-O1D
14	A	813	CLA	CHA-CBD-CGD-O2D
14	A	822	CLA	CHA-CBD-CGD-O1D
14	A	837	CLA	CHA-CBD-CGD-O2D
14	B	801	CLA	CHA-CBD-CGD-O1D
14	B	801	CLA	CHA-CBD-CGD-O2D
14	B	802	CLA	CHA-CBD-CGD-O1D
14	B	802	CLA	CHA-CBD-CGD-O2D
14	B	805	CLA	CHA-CBD-CGD-O2D
14	B	808	CLA	CHA-CBD-CGD-O2D
14	B	810	CLA	CHA-CBD-CGD-O1D
14	B	810	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	B	814	CLA	CHA-CBD-CGD-O2D
14	B	824	CLA	CHA-CBD-CGD-O2D
14	B	831	CLA	CHA-CBD-CGD-O2D
14	B	834	CLA	CHA-CBD-CGD-O1D
14	B	834	CLA	CHA-CBD-CGD-O2D
14	B	840	CLA	CHA-CBD-CGD-O2D
14	L	1503	CLA	CHA-CBD-CGD-O2D
14	a	807	CLA	CHA-CBD-CGD-O2D
14	a	812	CLA	CHA-CBD-CGD-O2D
14	a	814	CLA	CHA-CBD-CGD-O1D
14	a	821	CLA	CHA-CBD-CGD-O1D
14	a	821	CLA	CHA-CBD-CGD-O2D
14	a	824	CLA	CHA-CBD-CGD-O1D
14	a	824	CLA	CHA-CBD-CGD-O2D
14	a	829	CLA	CHA-CBD-CGD-O2D
14	b	812	CLA	CHA-CBD-CGD-O1D
14	b	812	CLA	CHA-CBD-CGD-O2D
14	b	824	CLA	CHA-CBD-CGD-O1D
14	b	824	CLA	CHA-CBD-CGD-O2D
14	b	827	CLA	CHA-CBD-CGD-O1D
14	b	827	CLA	CHA-CBD-CGD-O2D
14	b	812	CLA	C15-C16-C17-C18
14	a	823	CLA	C4C-C3C-CAC-CBC
17	A	850	BCR	C20-C21-C22-C23
17	B	847	BCR	C11-C10-C9-C8
17	f	204	BCR	C12-C13-C14-C15
17	j	104	BCR	C11-C10-C9-C8
14	a	808	CLA	C16-C17-C18-C20
14	b	807	CLA	C16-C17-C18-C20
14	A	813	CLA	CAA-CBA-CGA-O2A
14	a	824	CLA	CAA-CBA-CGA-O2A
14	B	828	CLA	C5-C6-C7-C8
14	J	101	CLA	CAA-CBA-CGA-O2A
20	b	851	LMG	O9-C10-O7-C8
14	A	812	CLA	C4C-C3C-CAC-CBC
14	a	824	CLA	C10-C11-C12-C13
14	A	808	CLA	CAA-CBA-CGA-O2A
14	A	812	CLA	CAA-CBA-CGA-O2A
14	a	840	CLA	C2A-CAA-CBA-CGA
14	b	813	CLA	C10-C11-C12-C13
14	a	804	CLA	C4-C3-C5-C6
14	B	841	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	B	813	CLA	C2-C3-C5-C6
14	B	827	CLA	C11-C10-C8-C7
14	F	202	CLA	C12-C13-C15-C16
14	a	828	CLA	C11-C12-C13-C15
14	b	825	CLA	C2-C3-C5-C6
14	b	834	CLA	C11-C10-C8-C7
14	b	809	CLA	CAA-CBA-CGA-O2A
14	b	825	CLA	CAA-CBA-CGA-O2A
14	A	806	CLA	C6-C7-C8-C9
14	A	842	CLA	C11-C12-C13-C14
14	B	802	CLA	C14-C13-C15-C16
14	a	806	CLA	C6-C7-C8-C9
14	a	828	CLA	C6-C7-C8-C9
14	b	809	CLA	C11-C12-C13-C14
14	b	812	CLA	C11-C10-C8-C9
14	b	821	CLA	C6-C7-C8-C9
14	b	821	CLA	C11-C12-C13-C14
14	l	204	CLA	C11-C10-C8-C9
17	a	847	BCR	C15-C16-C17-C18
14	b	818	CLA	O2A-C1-C2-C3
17	f	204	BCR	C14-C15-C16-C17
14	a	835	CLA	CAA-CBA-CGA-O2A
14	b	804	CLA	CAA-CBA-CGA-O2A
14	b	821	CLA	C16-C17-C18-C19
14	f	203	CLA	CAA-CBA-CGA-O1A
14	b	805	CLA	C2A-CAA-CBA-CGA
14	b	812	CLA	CAA-CBA-CGA-O2A
14	B	836	CLA	C6-C7-C8-C9
14	a	827	CLA	C16-C17-C18-C20
14	a	829	CLA	C16-C17-C18-C19
14	b	814	CLA	C4-C3-C5-C6
15	B	844	PQN	C14-C13-C15-C16
14	A	842	CLA	CAA-CBA-CGA-O1A
17	j	105	BCR	C7-C8-C9-C10
14	l	204	CLA	CBA-CGA-O2A-C1
14	A	802	CLA	C1A-C2A-CAA-CBA
14	A	827	CLA	C1A-C2A-CAA-CBA
14	B	829	CLA	C1A-C2A-CAA-CBA
14	a	812	CLA	C1A-C2A-CAA-CBA
14	a	835	CLA	C1A-C2A-CAA-CBA
14	a	836	CLA	C1A-C2A-CAA-CBA
14	b	820	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	b	822	CLA	C1A-C2A-CAA-CBA
14	b	835	CLA	C1A-C2A-CAA-CBA
14	B	812	CLA	CAA-CBA-CGA-O1A
14	a	830	CLA	C2-C1-O2A-CGA
14	f	201	CLA	C2-C1-O2A-CGA
19	b	801	SQD	C18-C19-C20-C21
14	B	813	CLA	CAA-CBA-CGA-O1A
20	b	851	LMG	C19-C20-C21-C22
17	L	1504	BCR	C15-C16-C17-C18
14	A	817	CLA	C2A-CAA-CBA-CGA
14	a	811	CLA	C2A-CAA-CBA-CGA
14	b	813	CLA	C2A-CAA-CBA-CGA
14	b	809	CLA	CAA-CBA-CGA-O1A
18	a	850	LHG	O10-C23-C24-C25
14	j	102	CLA	CAA-CBA-CGA-O2A
19	X	1702	SQD	C14-C15-C16-C17
14	b	830	CLA	O1D-CGD-O2D-CED
18	i	103	LHG	C2-C3-O3-P
14	b	804	CLA	CAA-CBA-CGA-O1A
14	B	834	CLA	C2-C3-C5-C6
14	a	835	CLA	CAA-CBA-CGA-O1A
18	A	853	LHG	C3-O3-P-O5
18	a	850	LHG	C3-O3-P-O4
14	A	827	CLA	CAA-CBA-CGA-O1A
14	a	828	CLA	CAA-CBA-CGA-O1A
14	b	812	CLA	CAA-CBA-CGA-O1A
18	A	852	LHG	O10-C23-C24-C25
18	F	201	LHG	O10-C23-C24-C25
20	B	803	LMG	O9-C10-C11-C12
14	k	102	CLA	O2A-C1-C2-C3
14	a	826	CLA	CAA-CBA-CGA-O2A
18	F	201	LHG	O8-C23-C24-C25
17	L	1504	BCR	C35-C13-C14-C15
14	J	101	CLA	CAA-CBA-CGA-O1A
17	L	1504	BCR	C5-C6-C7-C8
17	b	847	BCR	C23-C24-C25-C26
14	B	812	CLA	C10-C11-C12-C13
14	A	808	CLA	CAA-CBA-CGA-O1A
14	A	813	CLA	CAA-CBA-CGA-O1A
14	a	807	CLA	CAA-CBA-CGA-O1A
14	b	835	CLA	C5-C6-C7-C8
14	b	840	CLA	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
15	B	844	PQN	C15-C16-C17-C18
14	a	814	CLA	CAA-CBA-CGA-O2A
14	a	817	CLA	C2A-CAA-CBA-CGA
14	B	825	CLA	CAA-CBA-CGA-O2A
14	b	830	CLA	C10-C11-C12-C13
14	b	839	CLA	C8-C10-C11-C12
14	B	835	CLA	CAA-CBA-CGA-O1A
14	F	202	CLA	CAA-CBA-CGA-O1A
14	a	824	CLA	CAA-CBA-CGA-O1A
14	A	807	CLA	CAD-CBD-CGD-O1D
14	B	805	CLA	CAD-CBD-CGD-O1D
14	B	808	CLA	CAD-CBD-CGD-O1D
14	B	816	CLA	CAD-CBD-CGD-O1D
14	B	834	CLA	CAD-CBD-CGD-O1D
14	a	814	CLA	CAD-CBD-CGD-O1D
14	a	823	CLA	CAD-CBD-CGD-O1D
14	b	812	CLA	CAD-CBD-CGD-O1D
19	b	801	SQD	C5-C6-S-O7
14	A	803	CLA	CBD-CGD-O2D-CED
14	a	808	CLA	CAA-CBA-CGA-O2A
14	a	831	CLA	C11-C10-C8-C9
14	b	834	CLA	C11-C10-C8-C9
14	A	812	CLA	CAA-CBA-CGA-O1A
14	a	811	CLA	CAA-CBA-CGA-O2A
14	b	841	CLA	CAA-CBA-CGA-O2A
18	F	201	LHG	O7-C7-C8-C9
14	A	812	CLA	C10-C11-C12-C13
14	b	815	CLA	C2A-CAA-CBA-CGA
14	l	205	CLA	C2A-CAA-CBA-CGA
14	B	826	CLA	CAA-CBA-CGA-O2A
14	a	829	CLA	C16-C17-C18-C20
14	B	814	CLA	C4-C3-C5-C6
14	B	801	CLA	C13-C15-C16-C17
14	B	840	CLA	C15-C16-C17-C18
14	b	835	CLA	C8-C10-C11-C12
17	j	106	BCR	C11-C12-C13-C35
14	A	802	CLA	C3A-C2A-CAA-CBA
14	A	834	CLA	C11-C12-C13-C15
14	A	842	CLA	C12-C13-C15-C16
14	B	813	CLA	C11-C10-C8-C7
14	B	835	CLA	C2-C3-C5-C6
14	B	836	CLA	C2-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

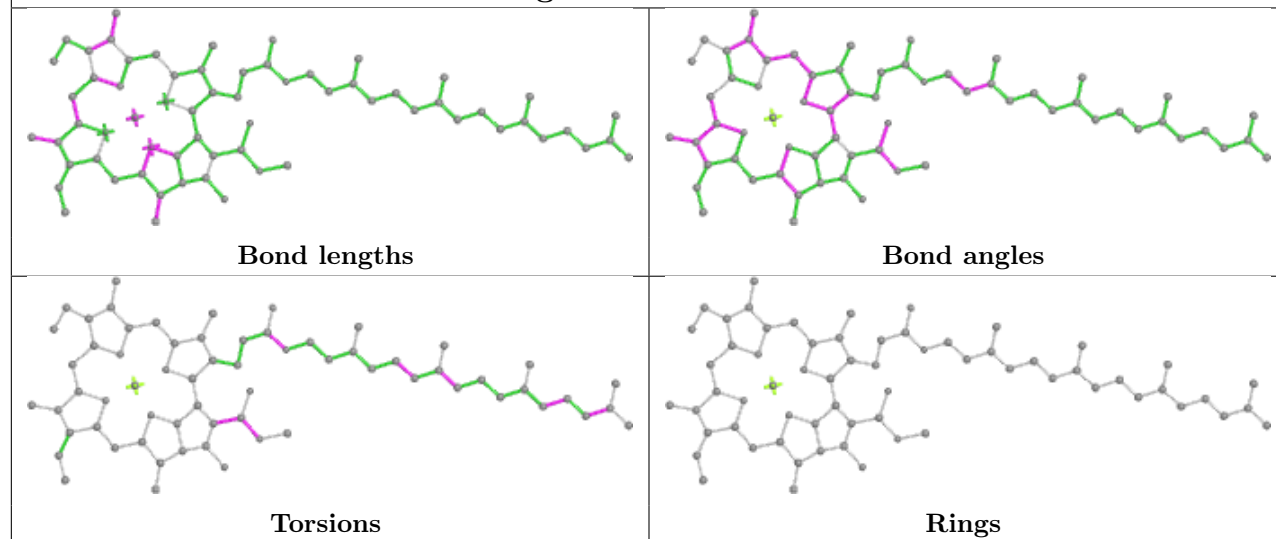
Mol	Chain	Res	Type	Atoms
14	b	812	CLA	C11-C10-C8-C7
14	a	811	CLA	CAA-CBA-CGA-O1A
14	b	825	CLA	CAA-CBA-CGA-O1A
14	A	811	CLA	C13-C15-C16-C17
20	b	851	LMG	C33-C34-C35-C36
17	A	847	BCR	C17-C18-C19-C20
17	B	850	BCR	C21-C22-C23-C24
17	a	844	BCR	C11-C12-C13-C14
17	B	845	BCR	C15-C16-C17-C18
17	I	101	BCR	C15-C16-C17-C18
14	a	802	CLA	CAA-CBA-CGA-O2A
14	B	822	CLA	C5-C6-C7-C8
20	B	851	LMG	C35-C36-C37-C38
14	B	826	CLA	CAA-CBA-CGA-O1A
14	b	841	CLA	CAA-CBA-CGA-O1A
14	b	802	CLA	C8-C10-C11-C12
14	A	840	CLA	C5-C6-C7-C8
14	b	810	CLA	C2A-CAA-CBA-CGA
14	b	841	CLA	C2A-CAA-CBA-CGA
14	B	802	CLA	C16-C17-C18-C20
14	A	806	CLA	O1D-CGD-O2D-CED
14	a	818	CLA	C8-C10-C11-C12
14	a	829	CLA	C13-C15-C16-C17
14	b	810	CLA	C10-C11-C12-C13
14	b	835	CLA	CAA-CBA-CGA-O1A
14	a	814	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

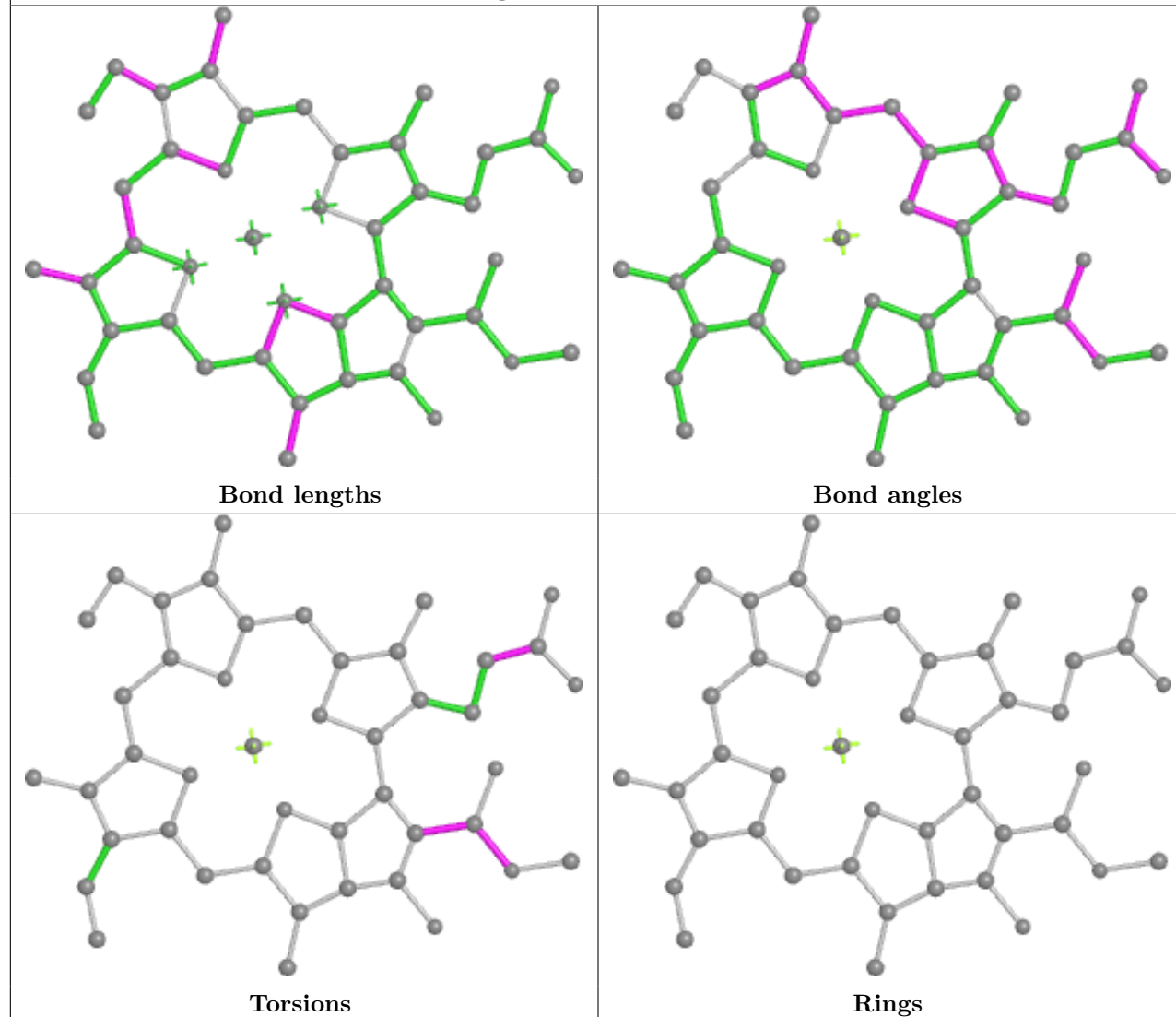
No monomer is involved in short contacts.

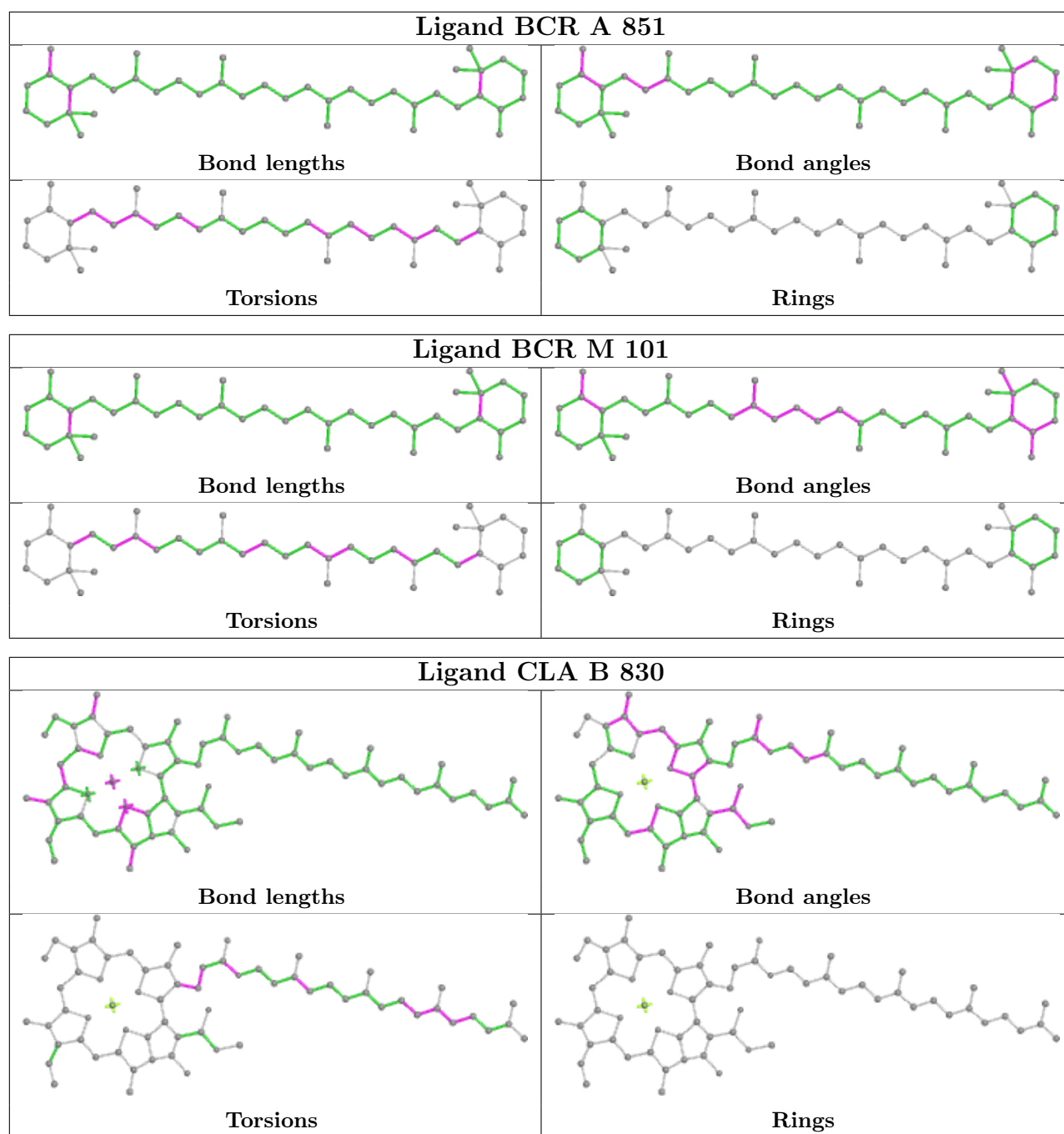
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

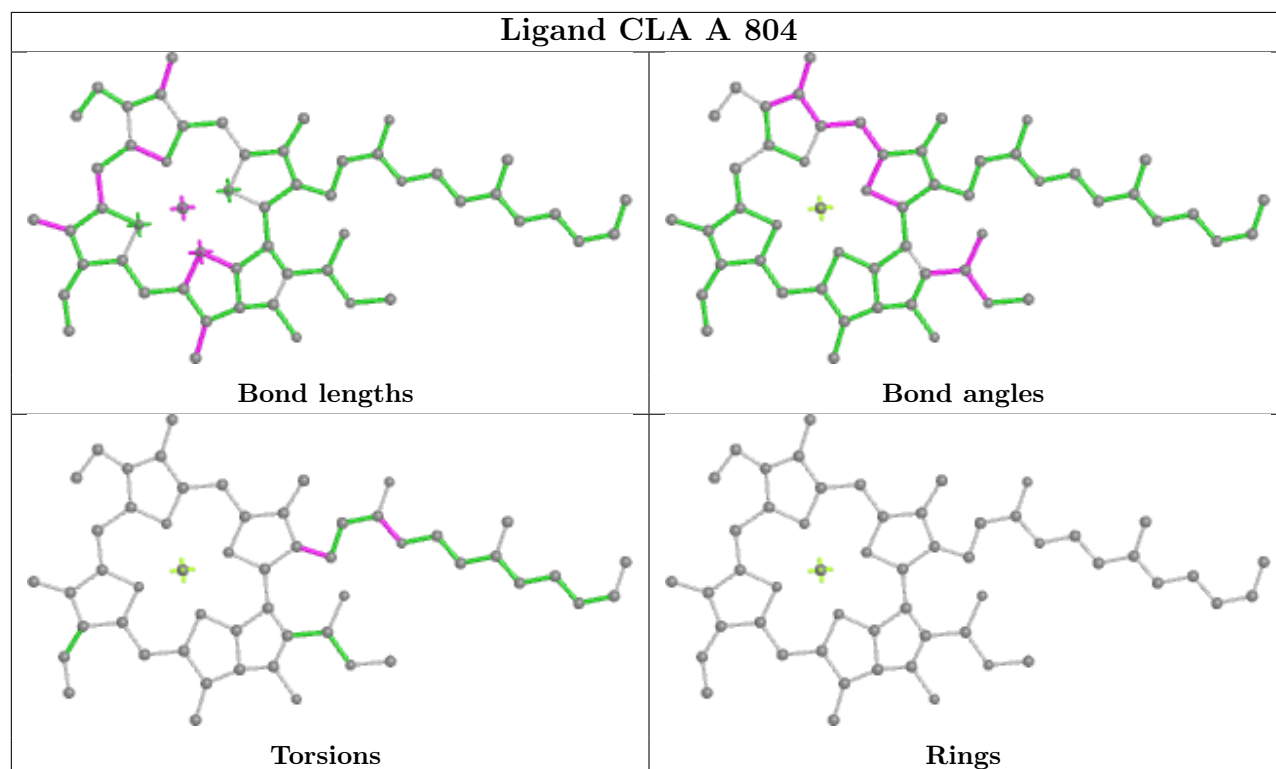
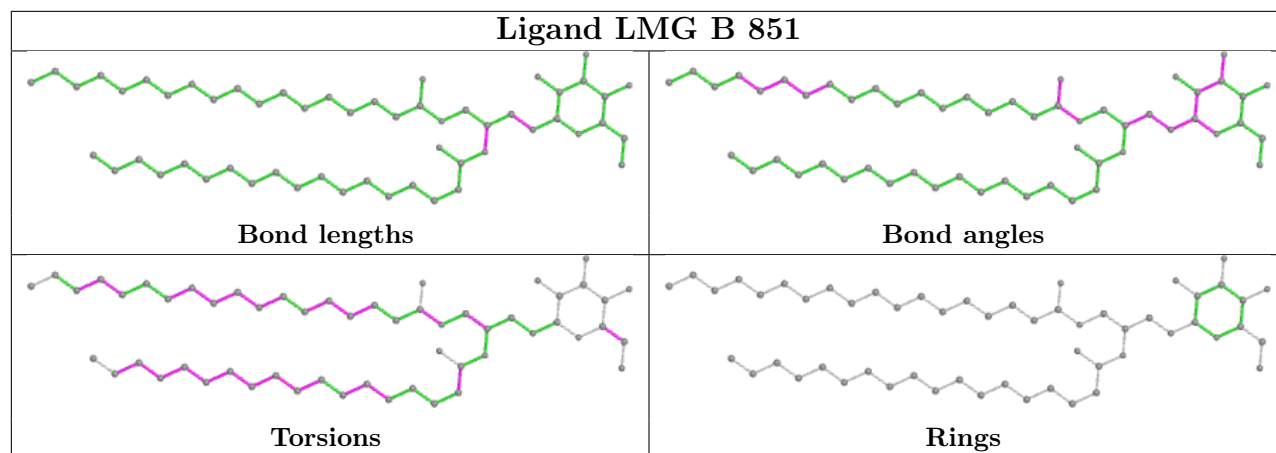
## Ligand CLA a 829



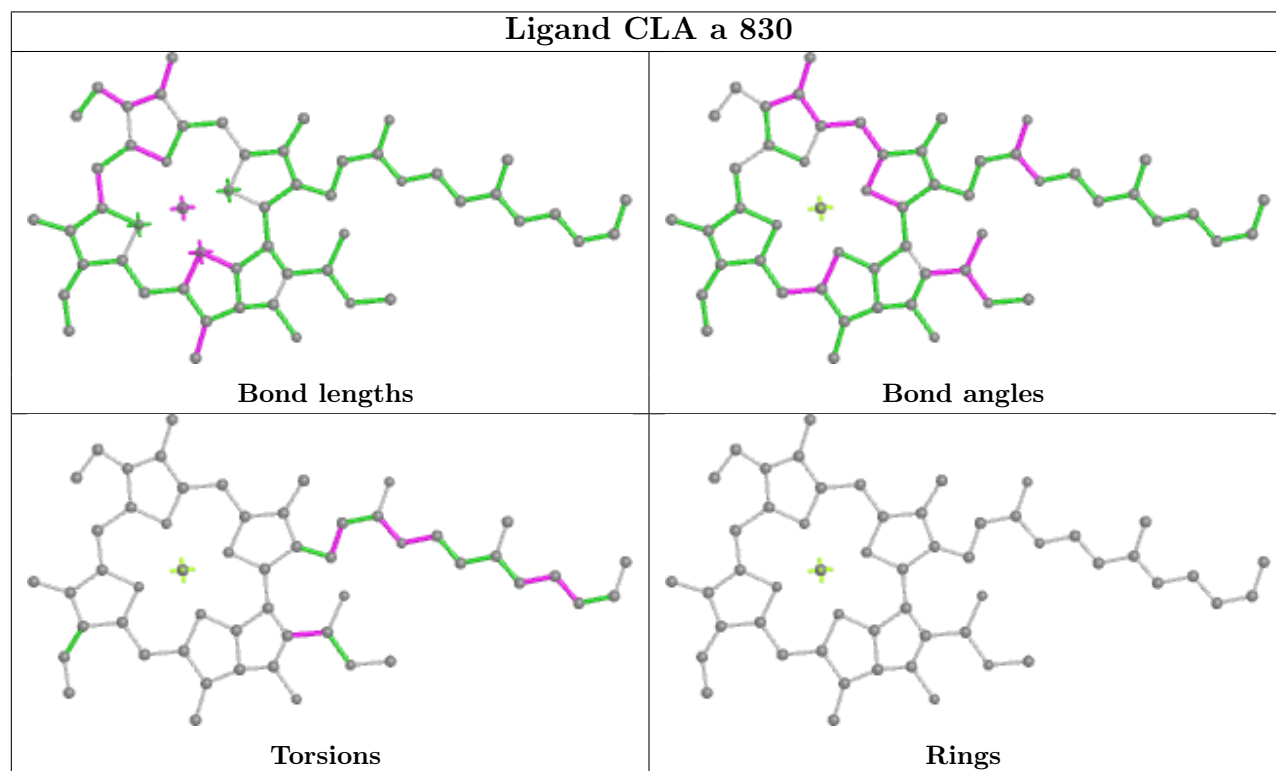
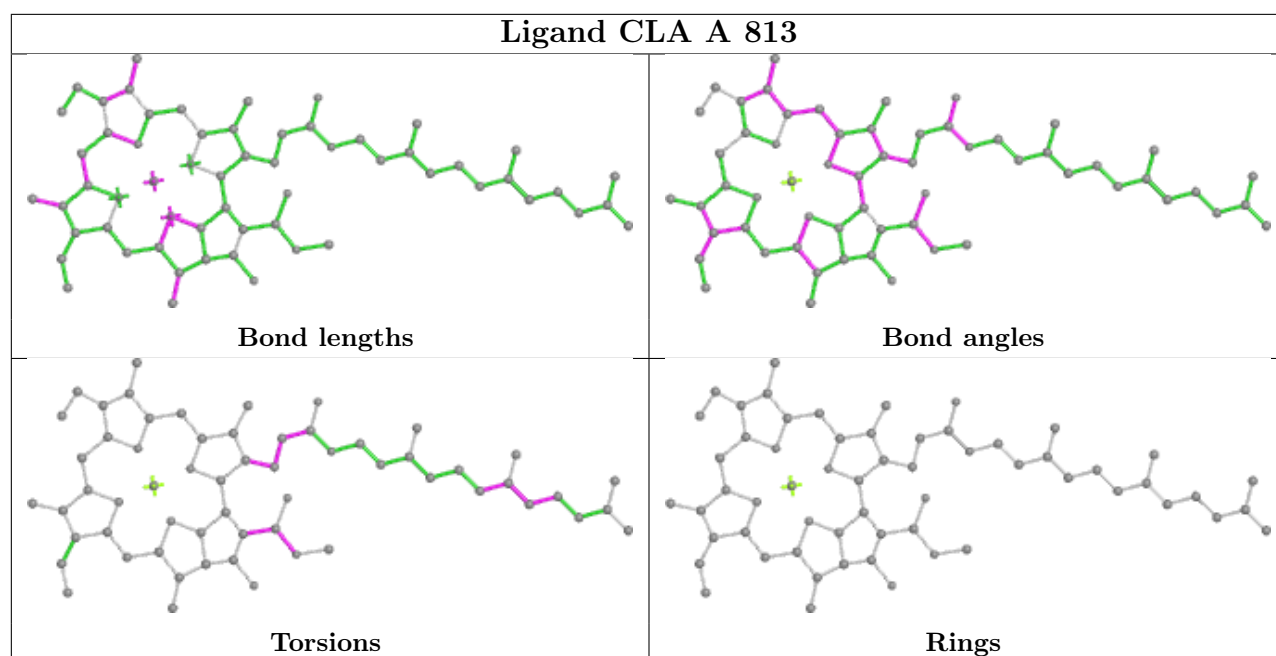
## Ligand CLA J 101



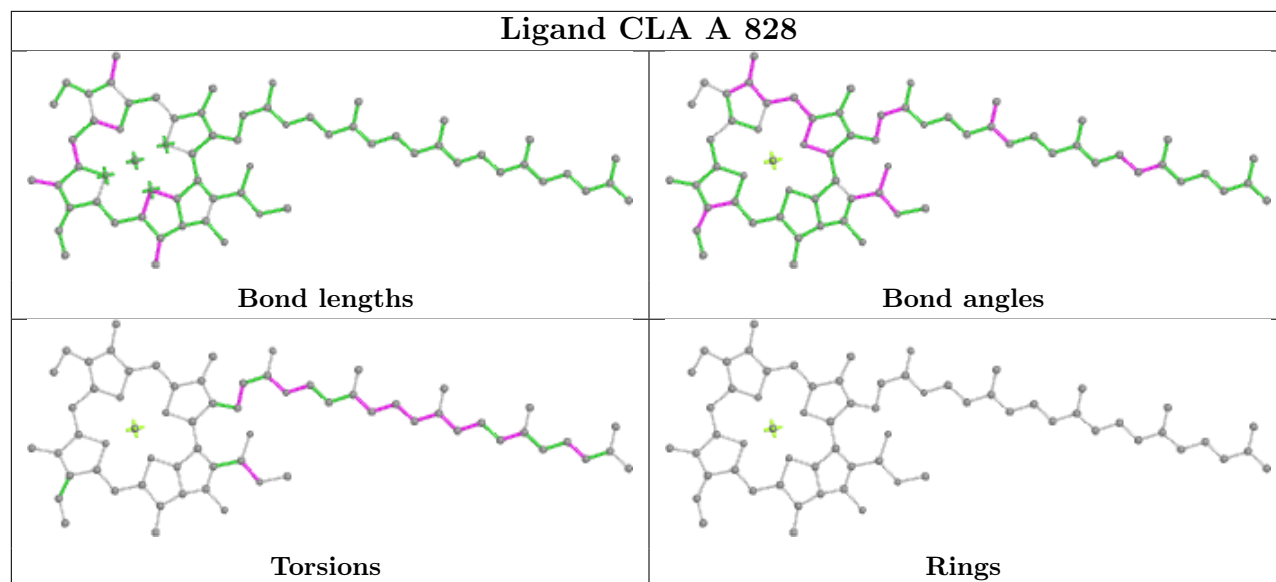




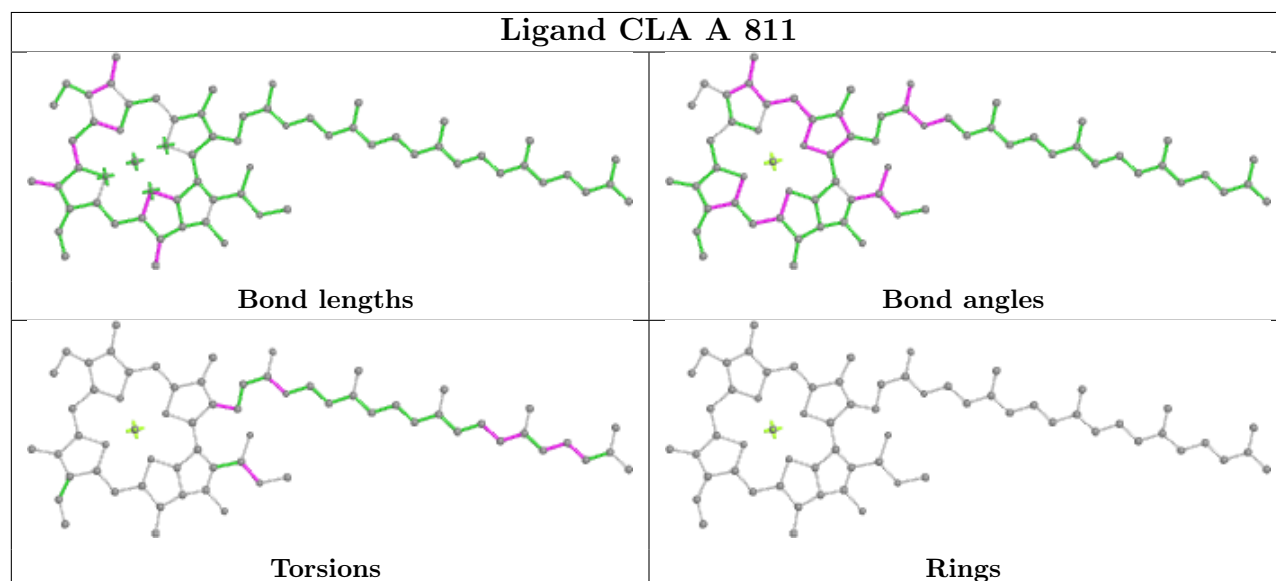




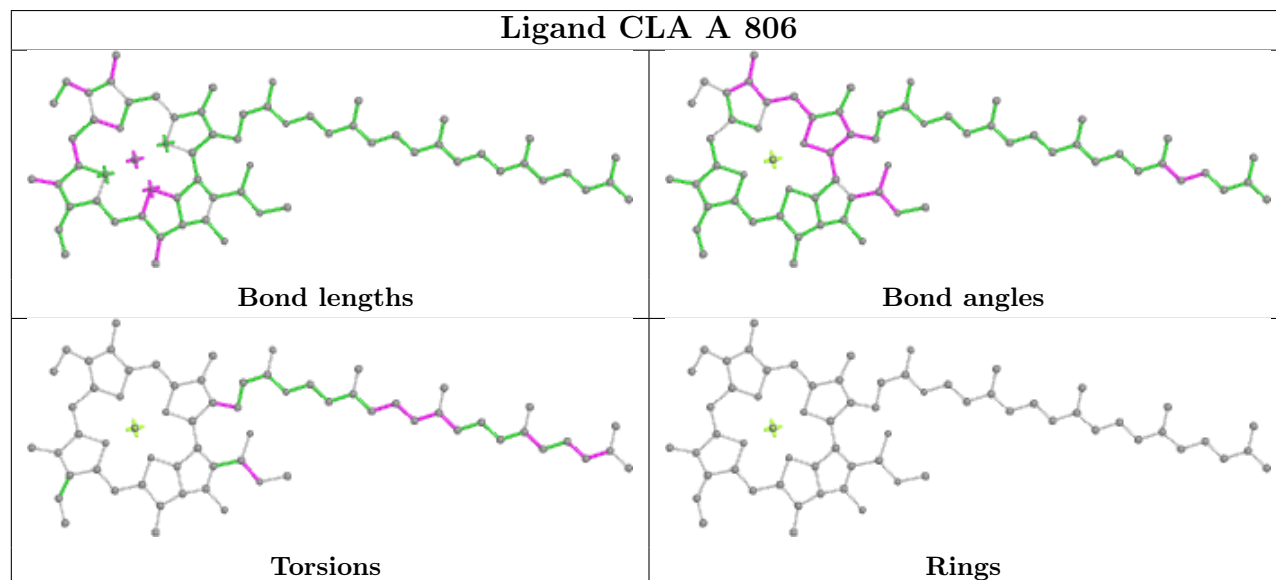
## Ligand CLA A 828



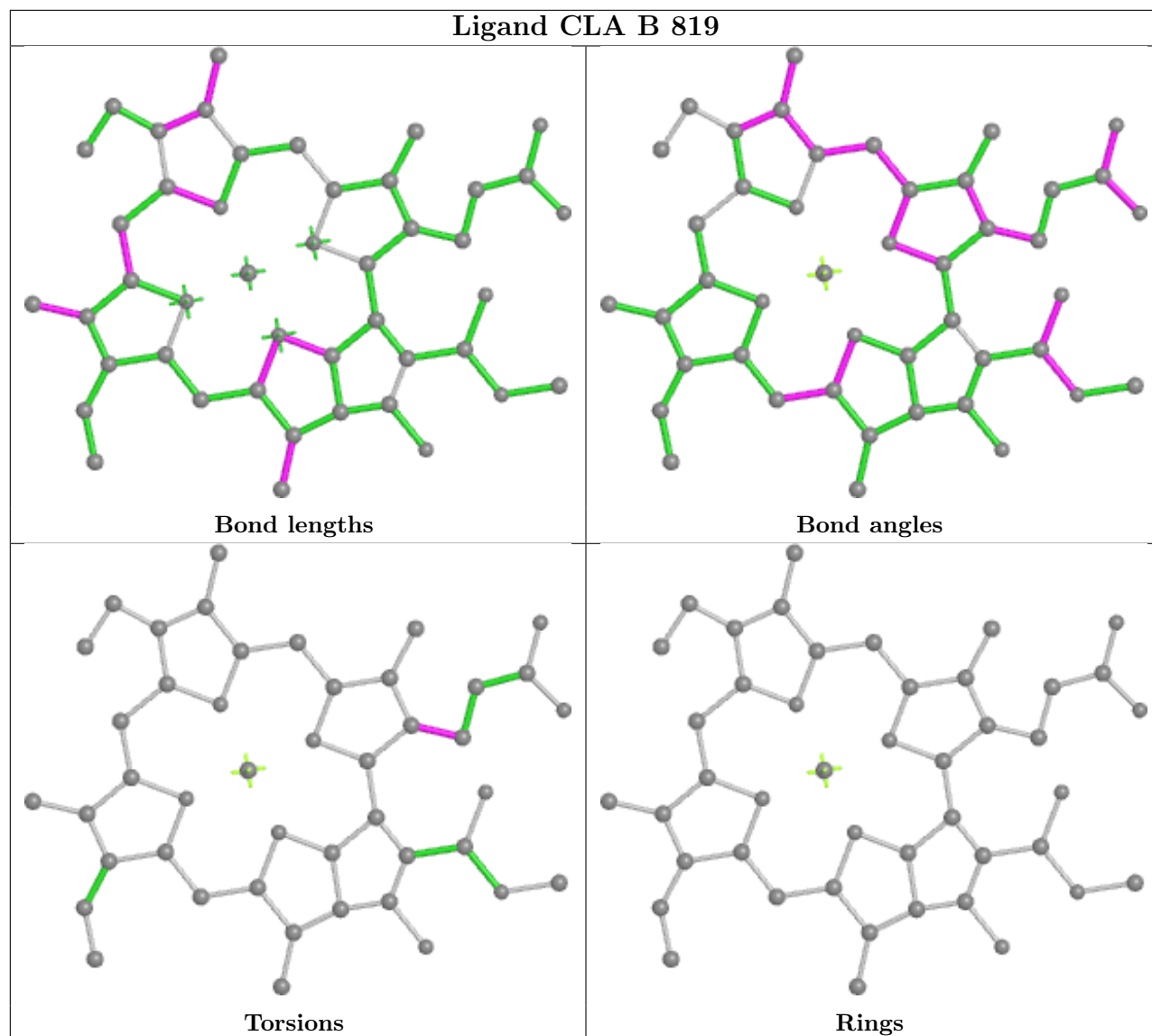
## Ligand CLA A 811



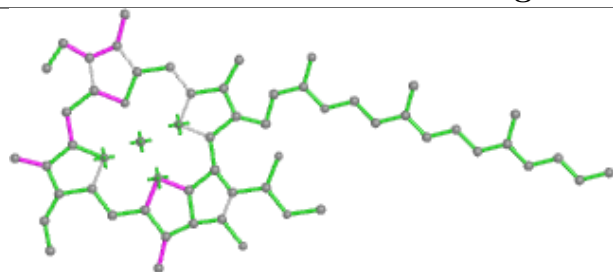
## Ligand CLA A 806



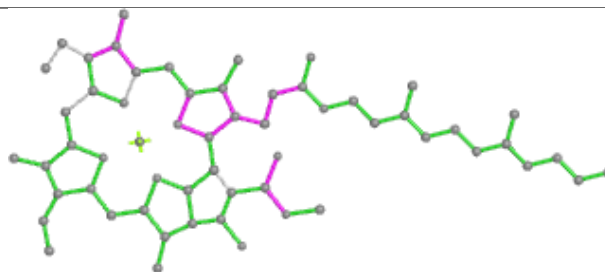
## Ligand CLA B 819



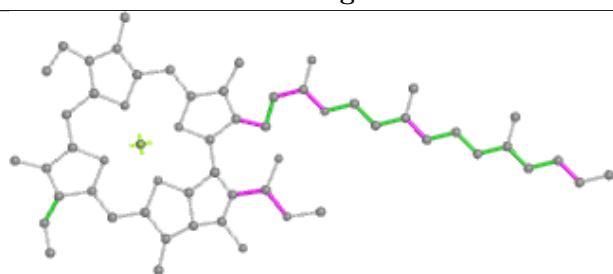
## Ligand CLA B 835



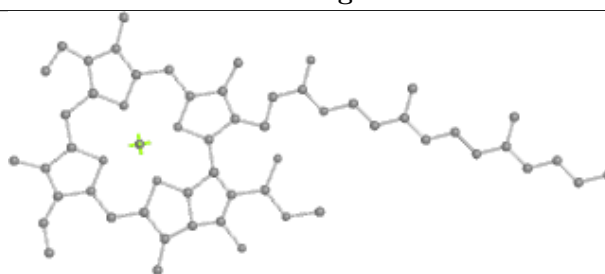
Bond lengths



Bond angles

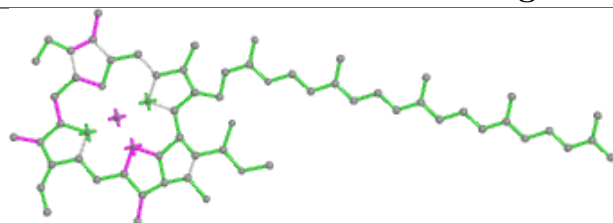


Torsions

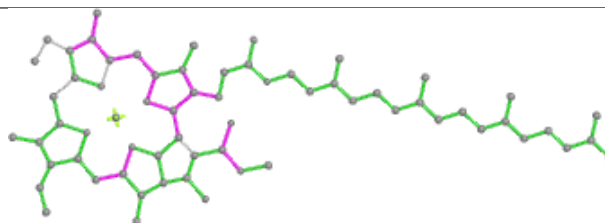


Rings

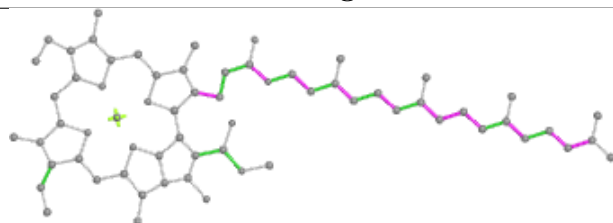
## Ligand CLA a 831



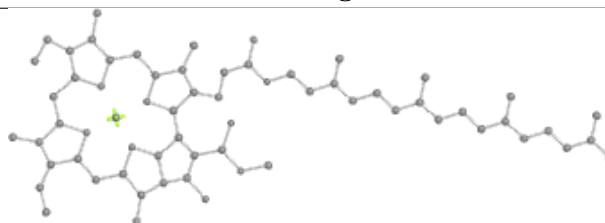
Bond lengths



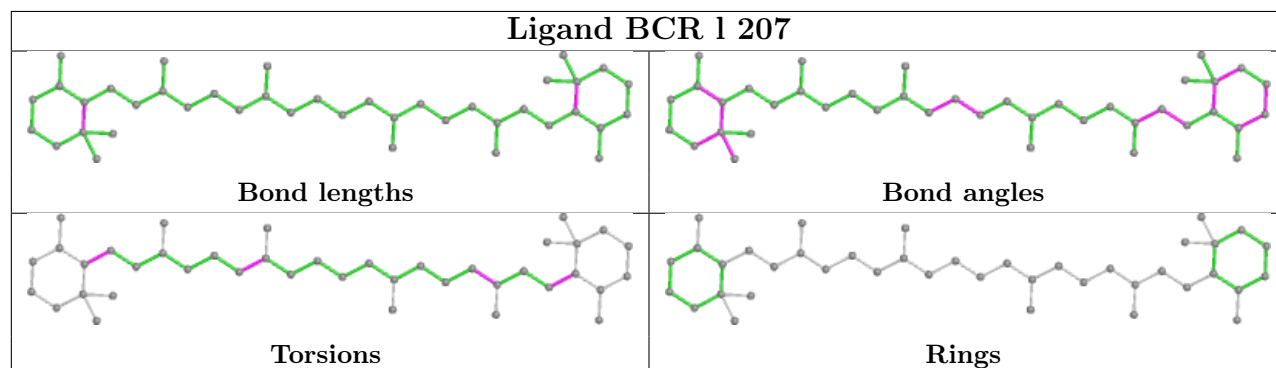
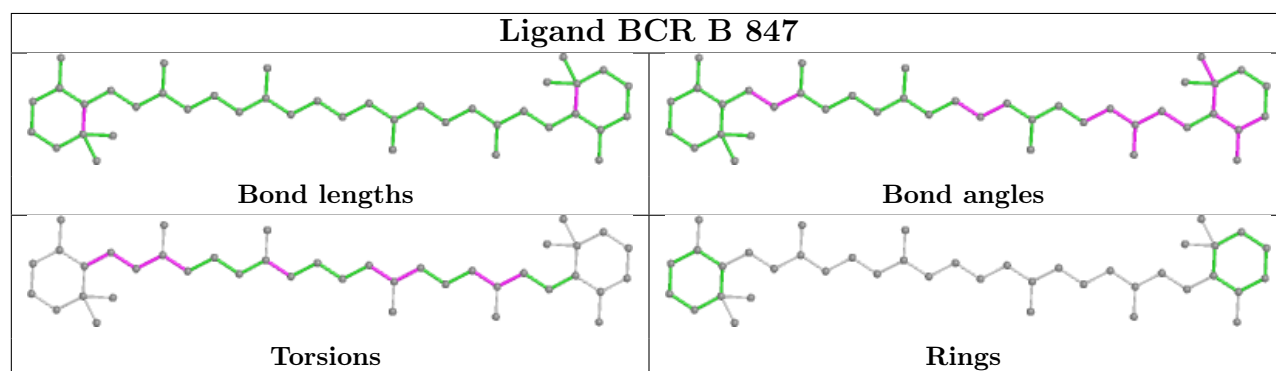
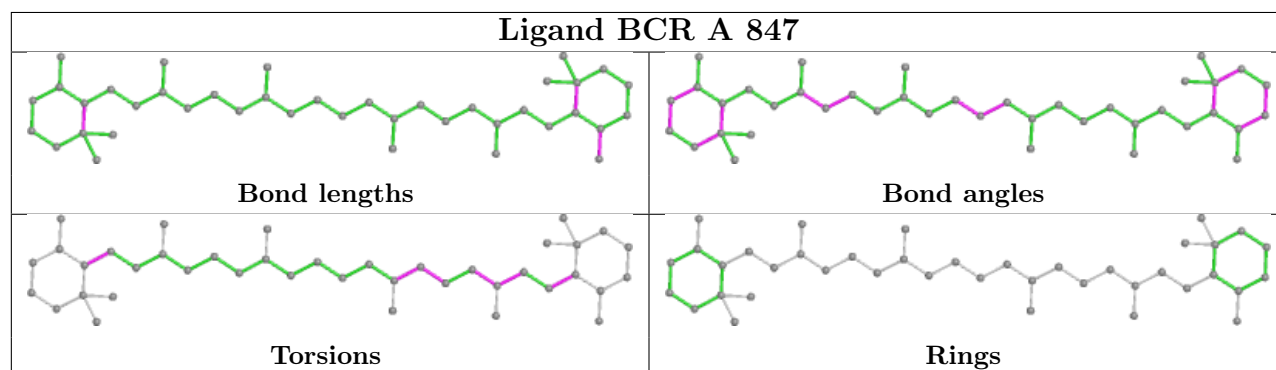
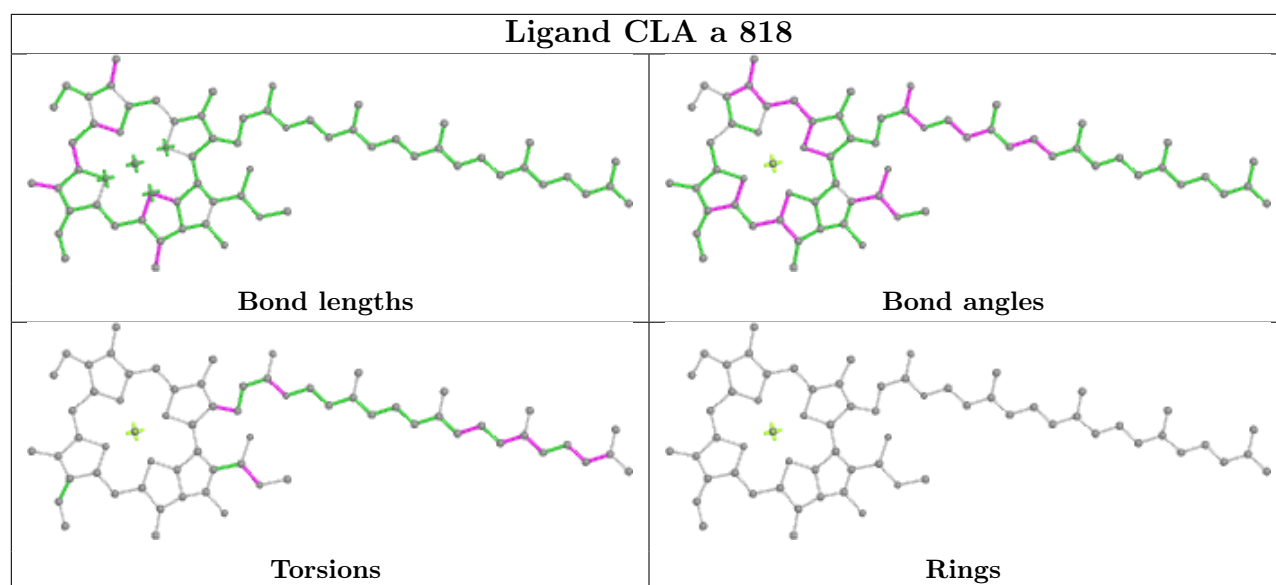
Bond angles

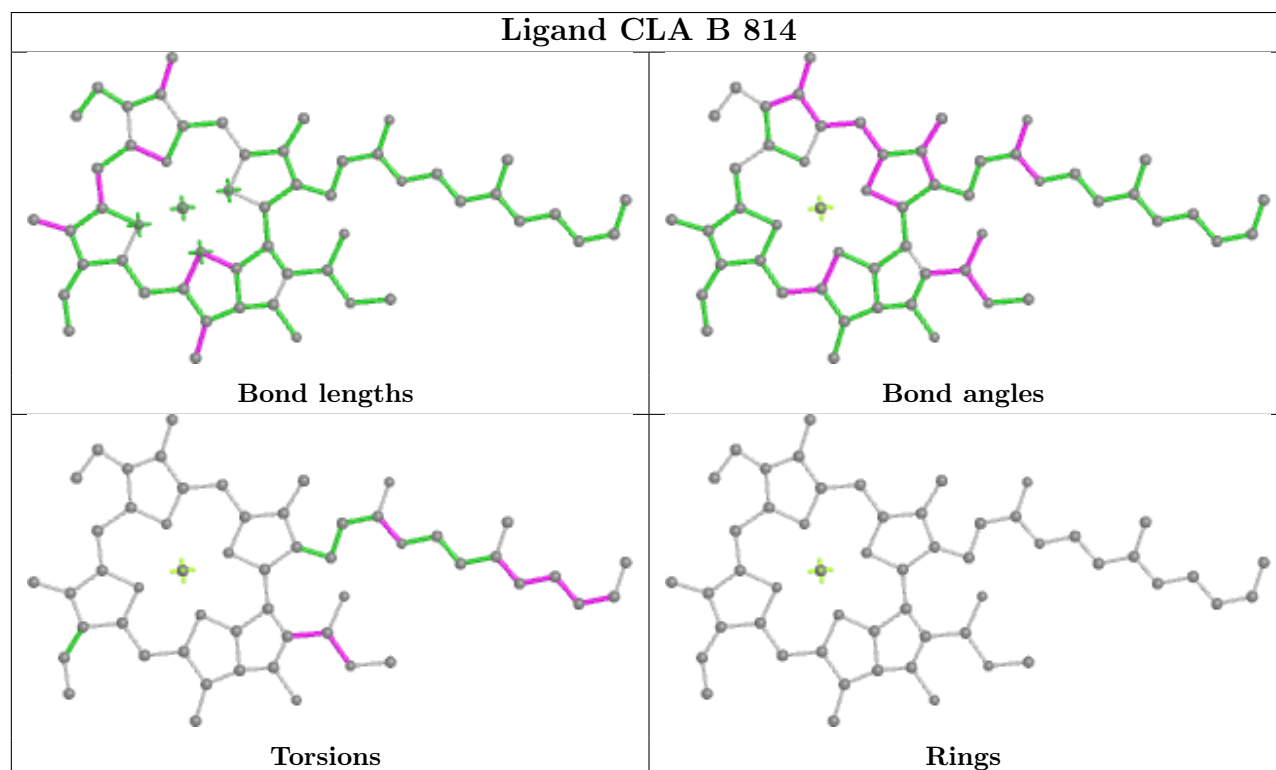
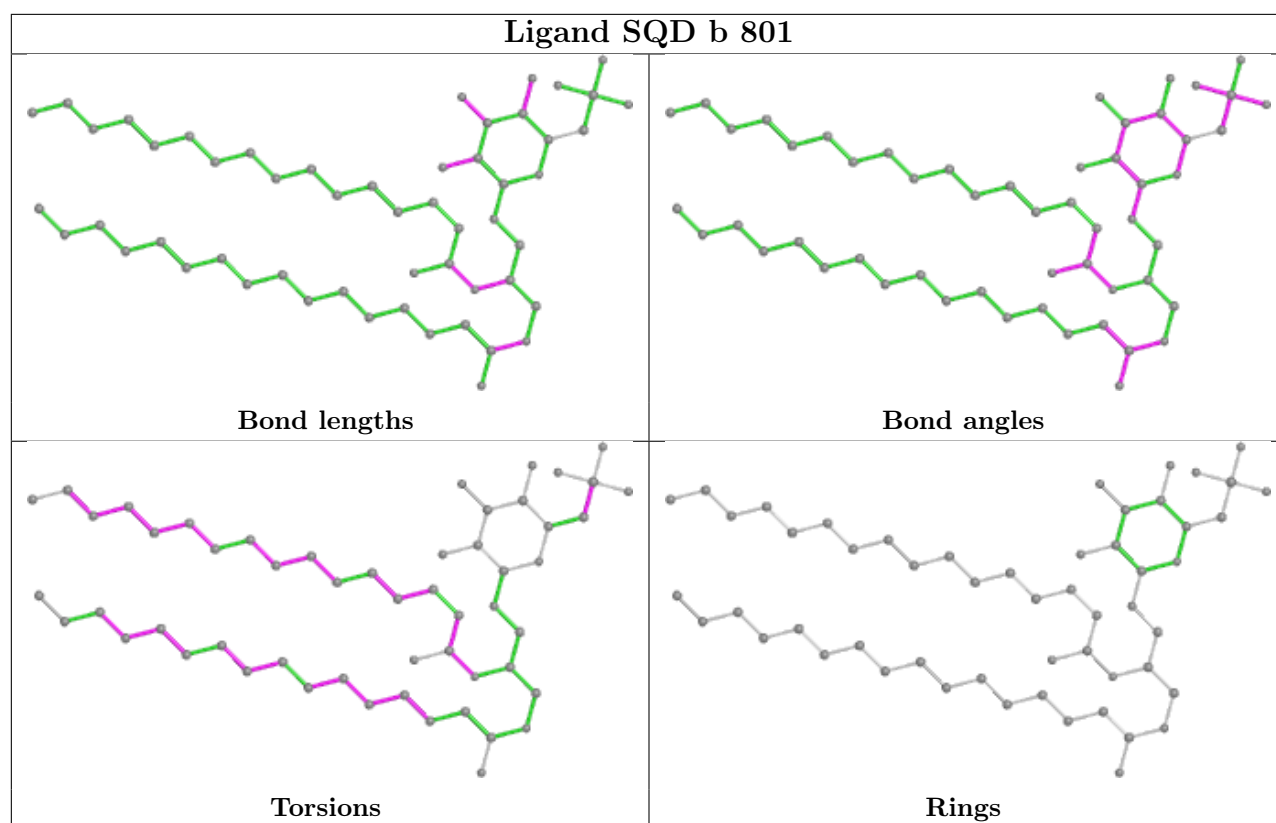


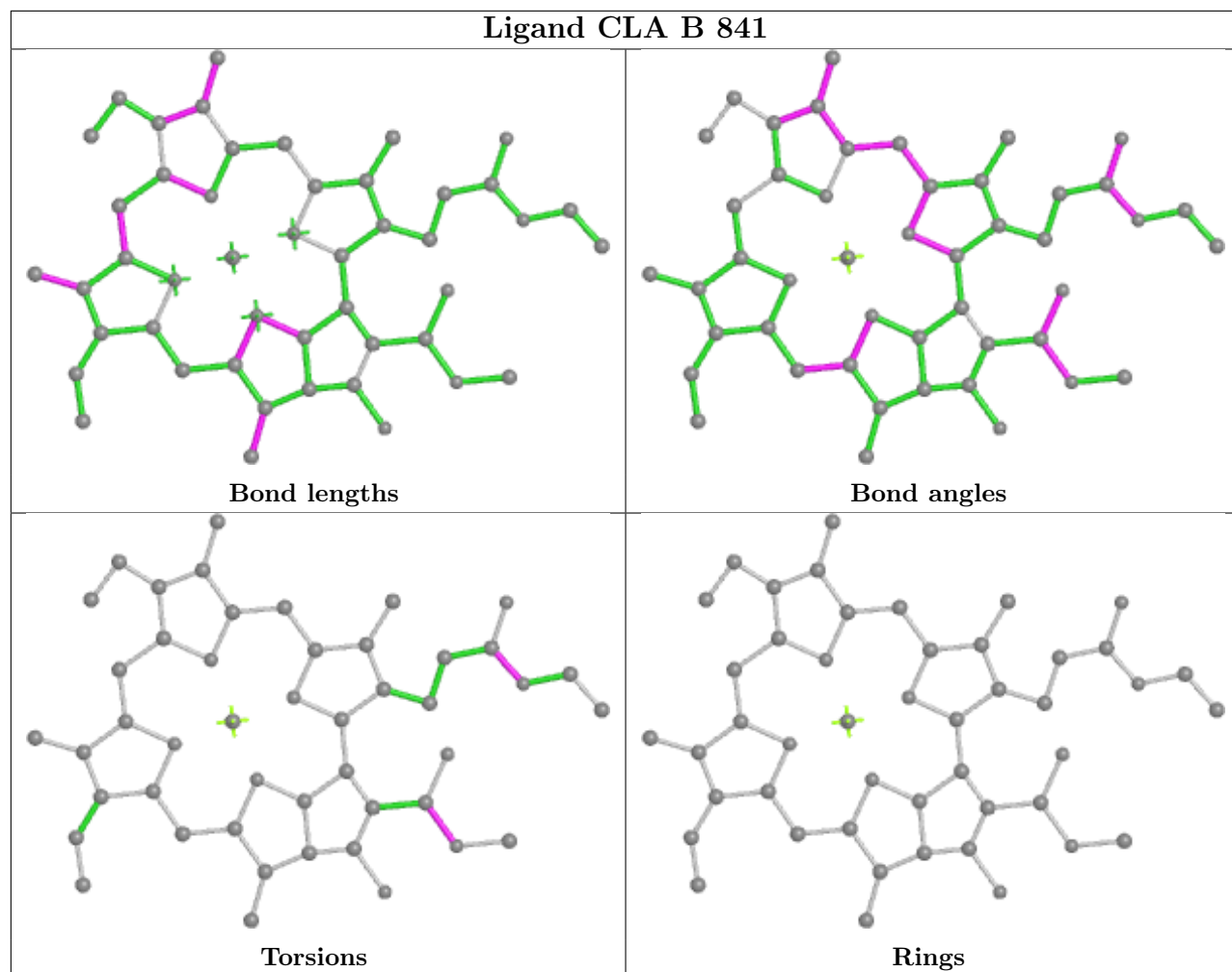
Torsions



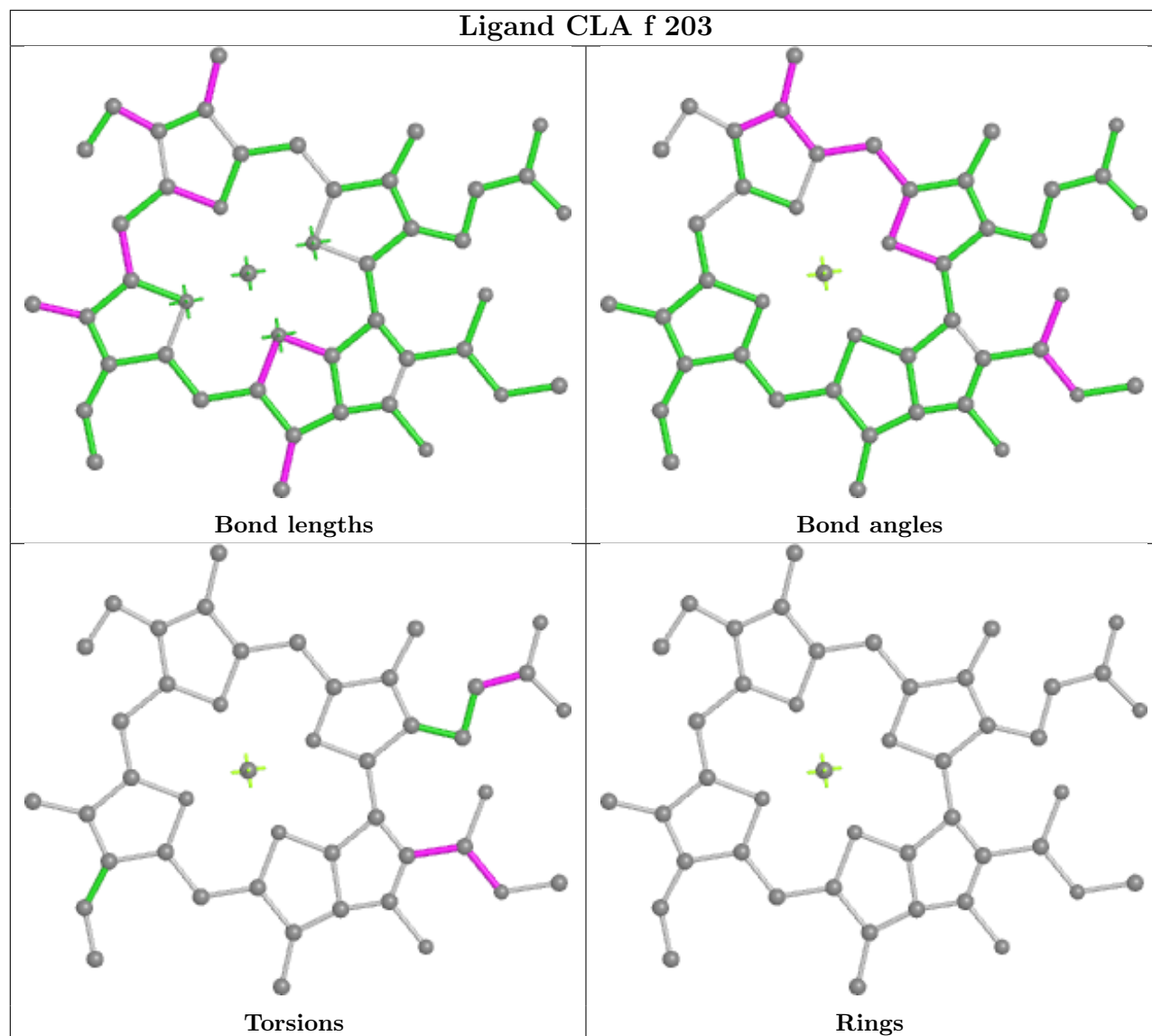
Rings



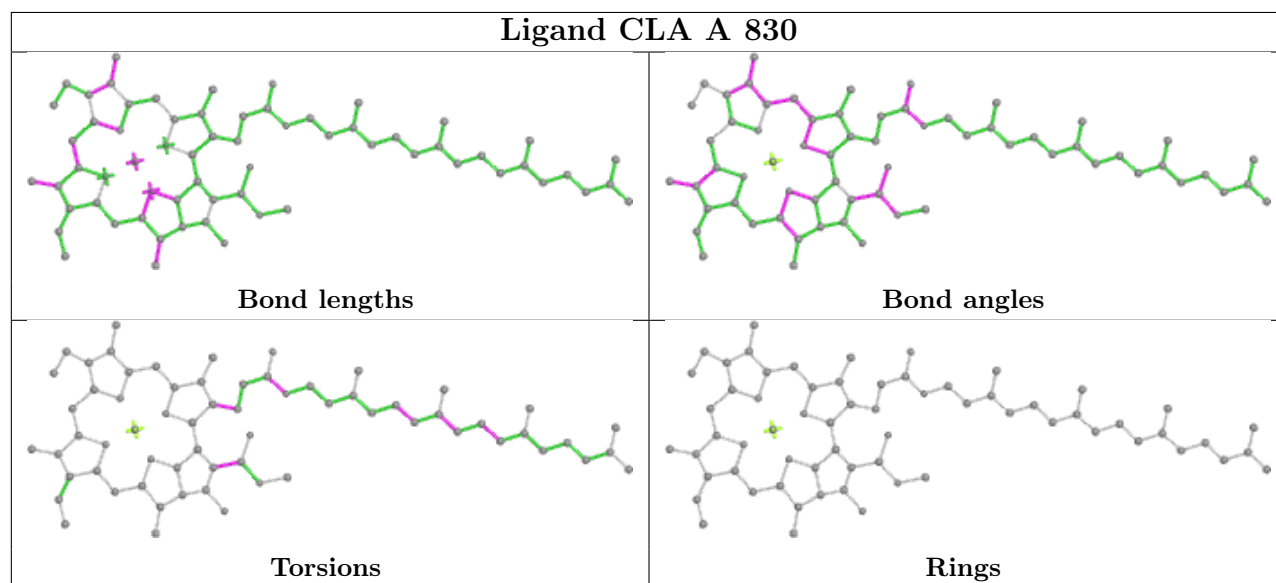
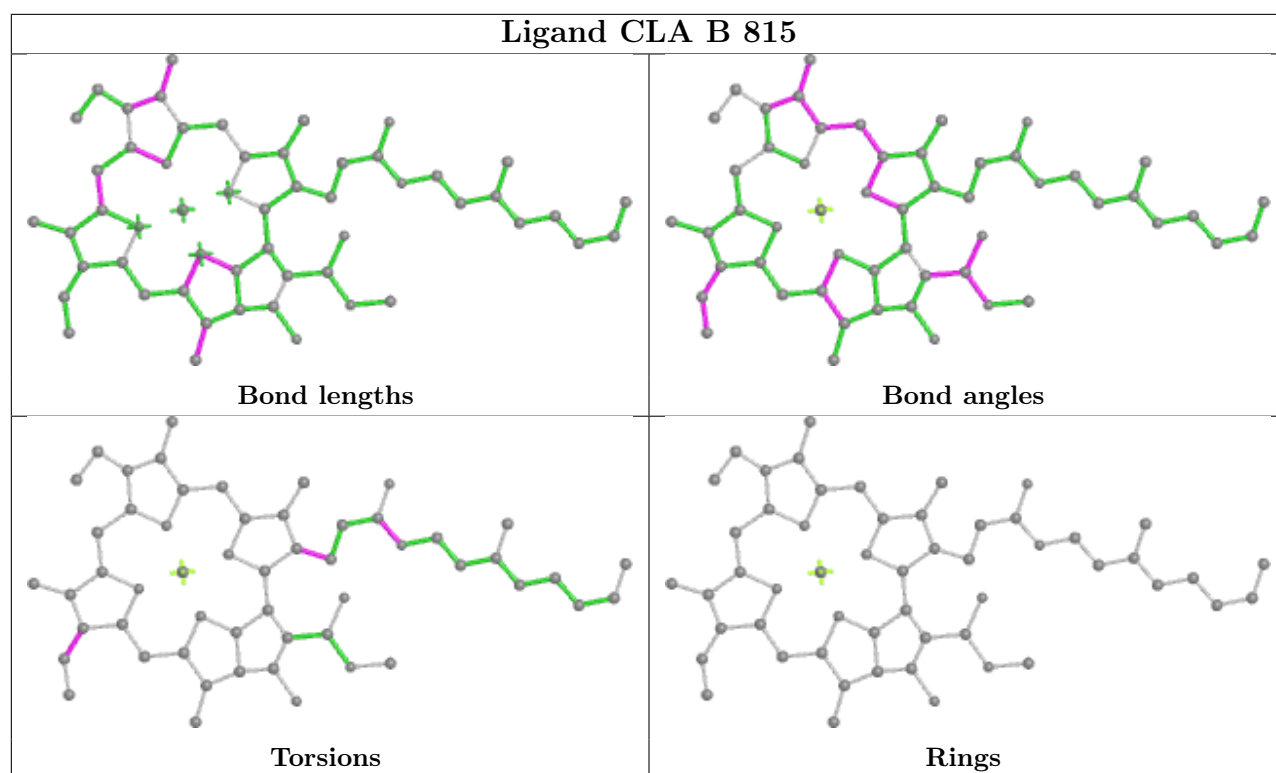


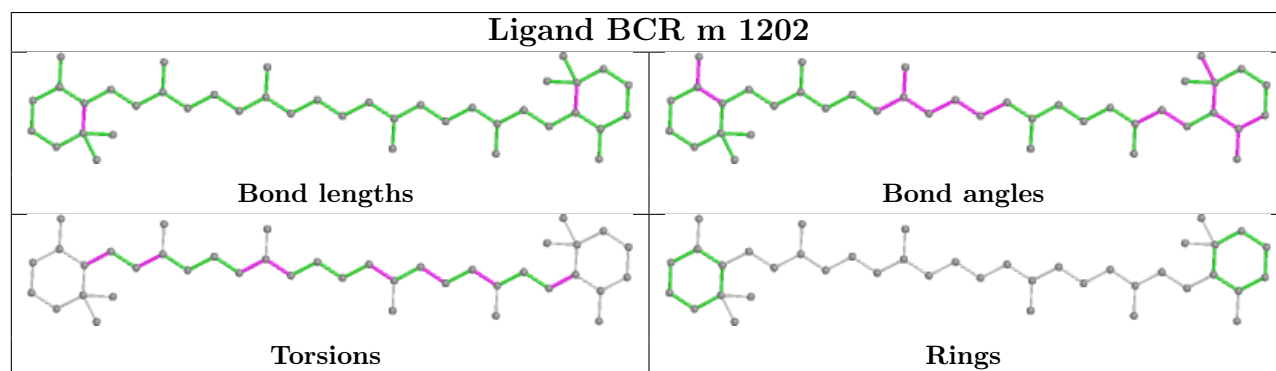
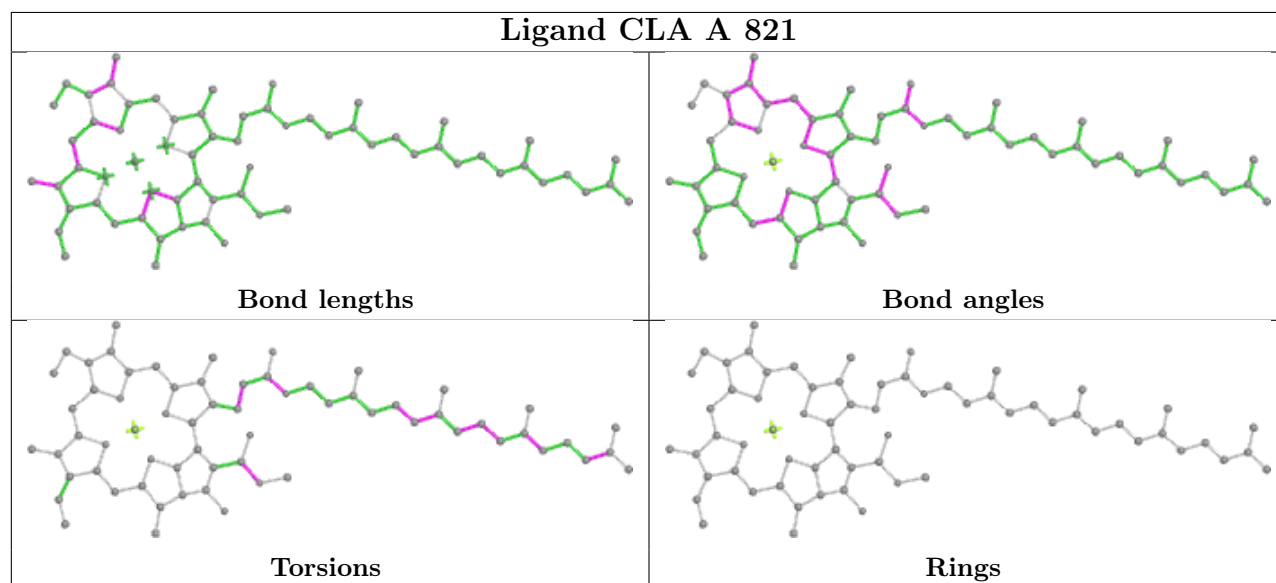
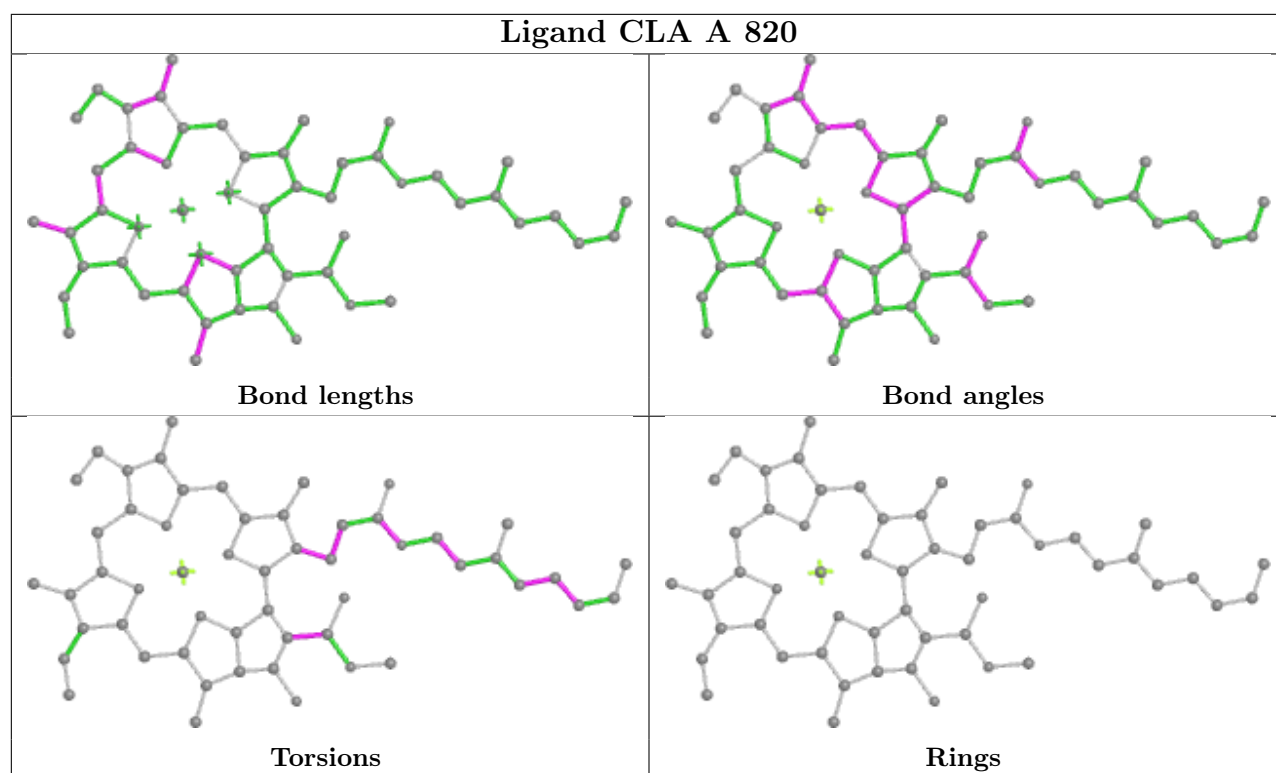


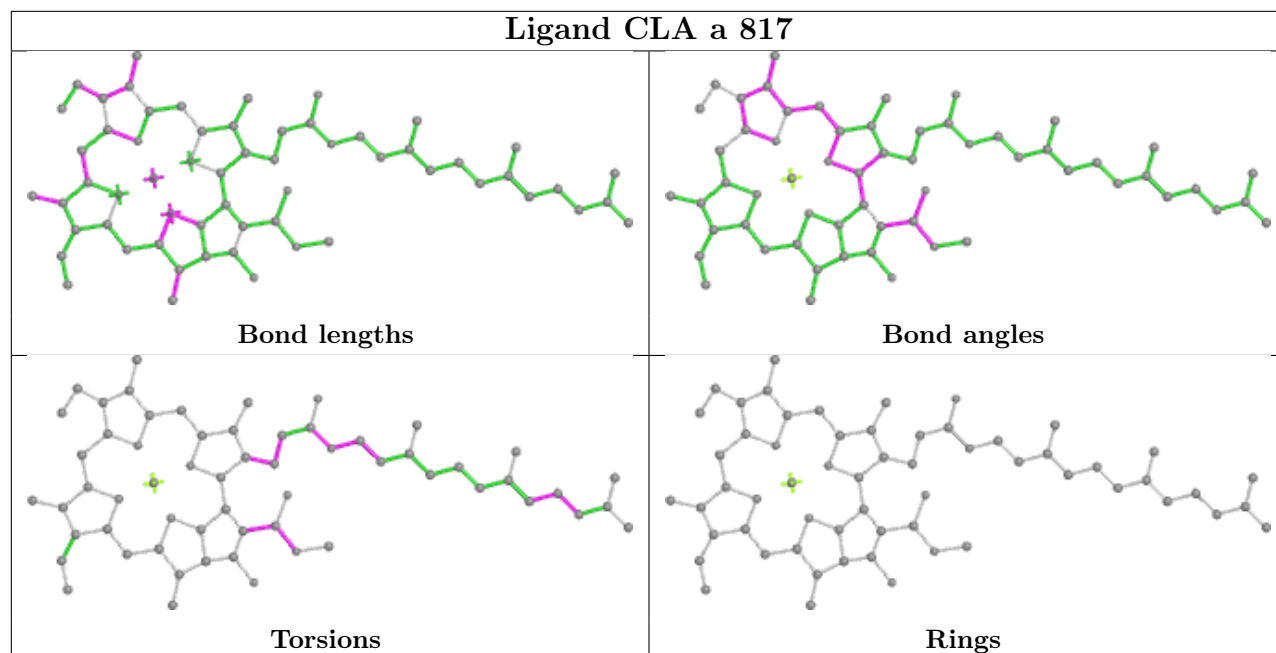
## Ligand CLA f 203

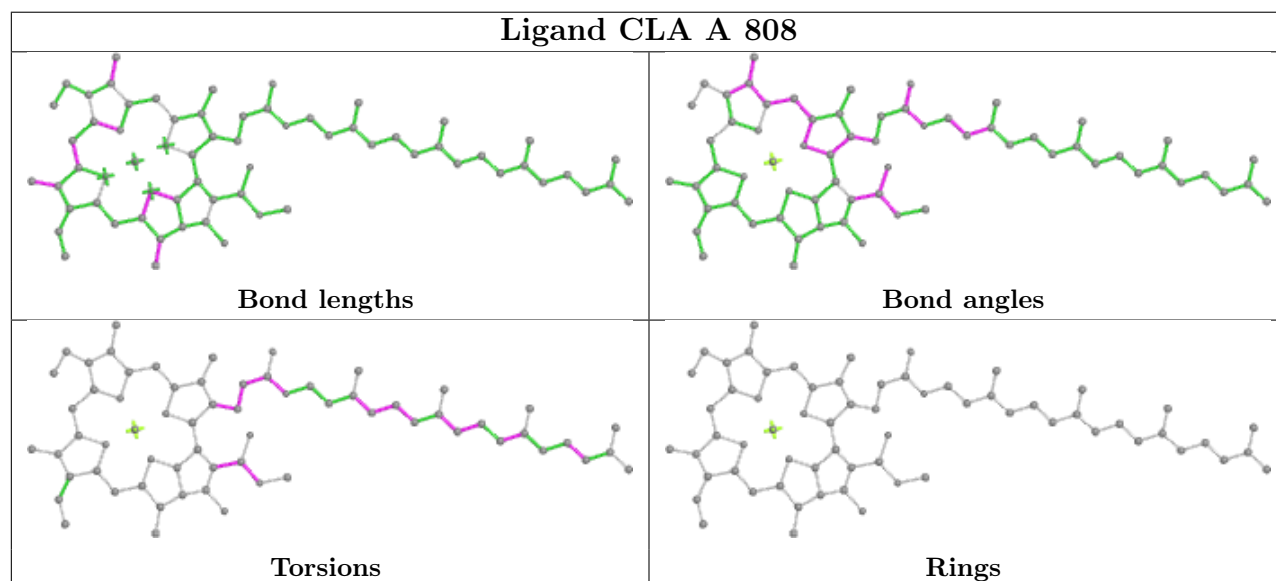
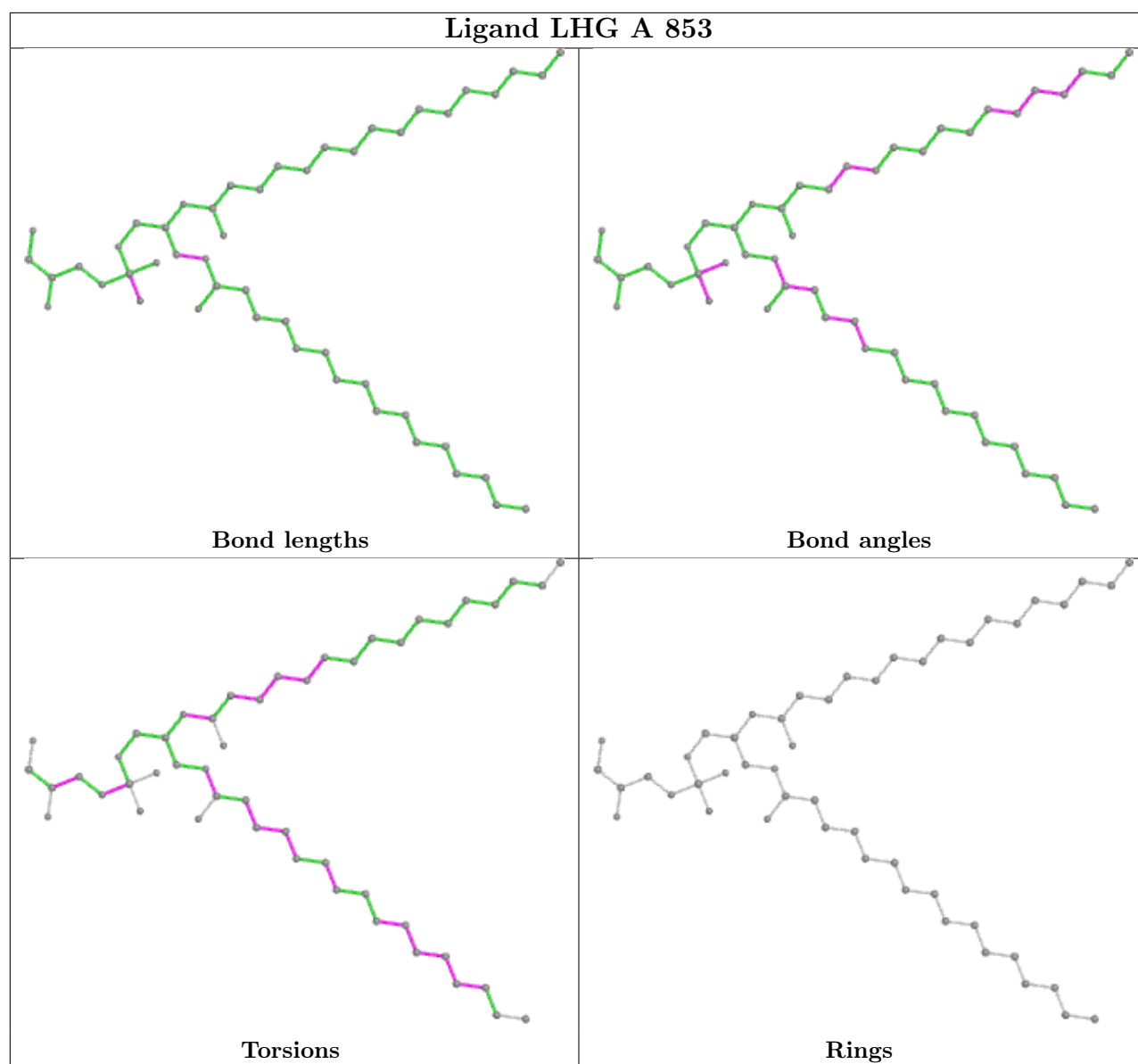


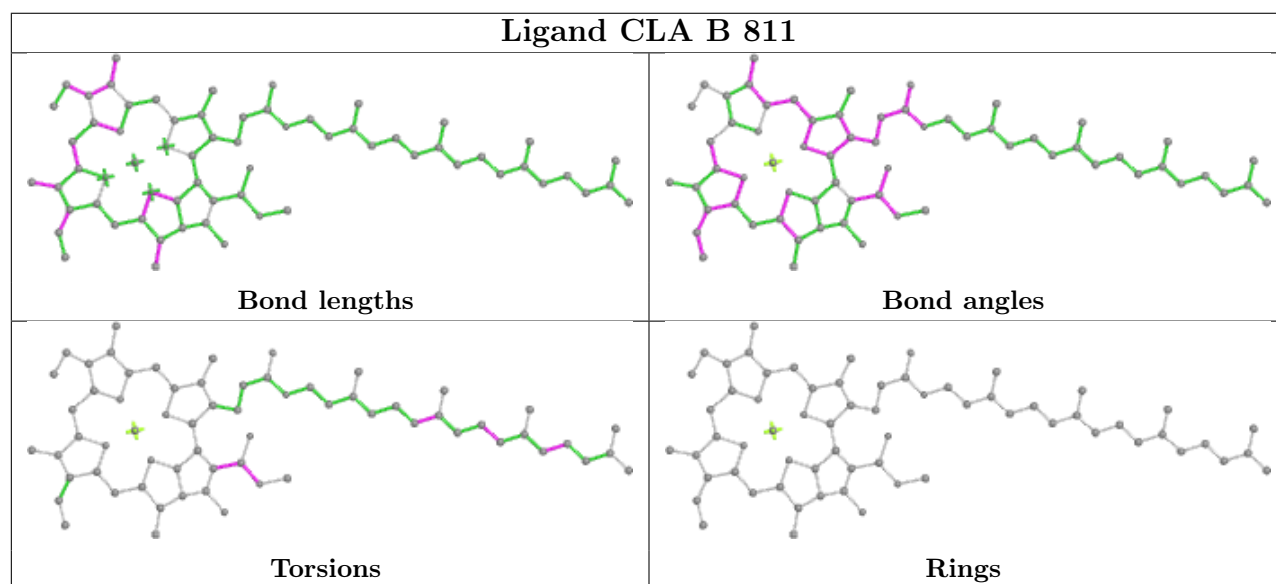
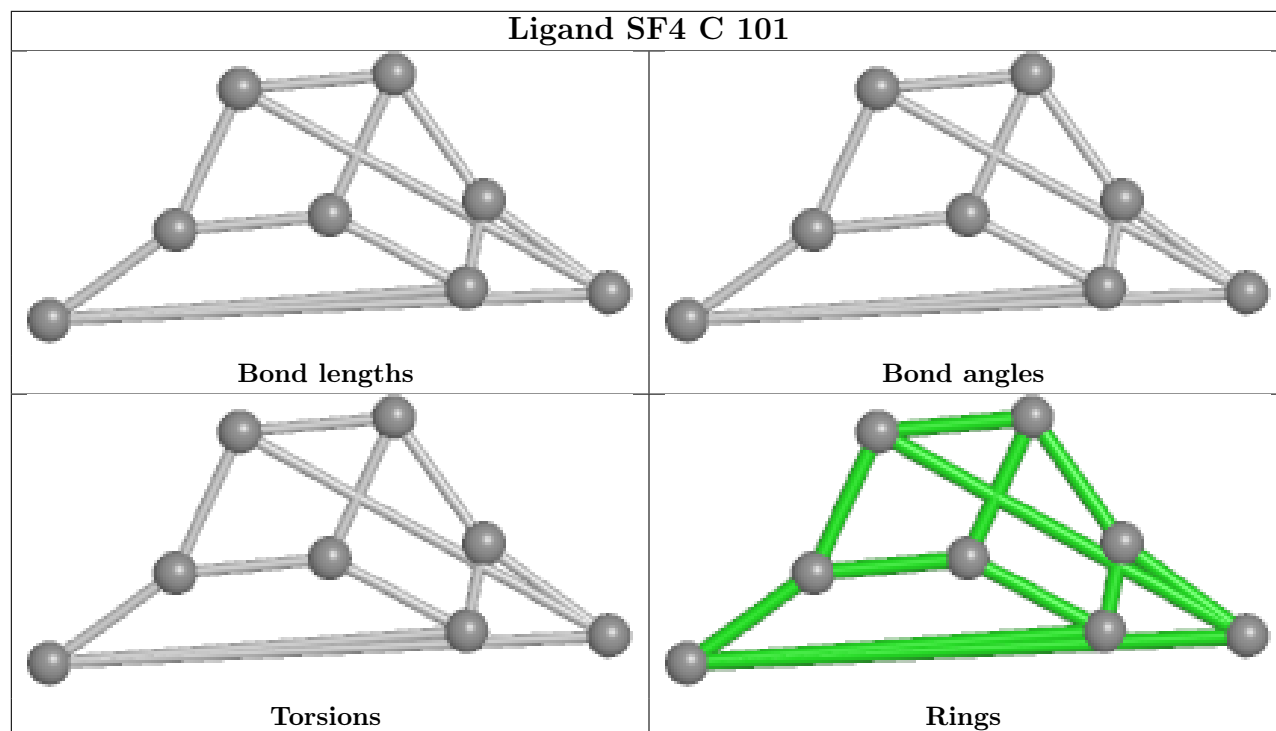
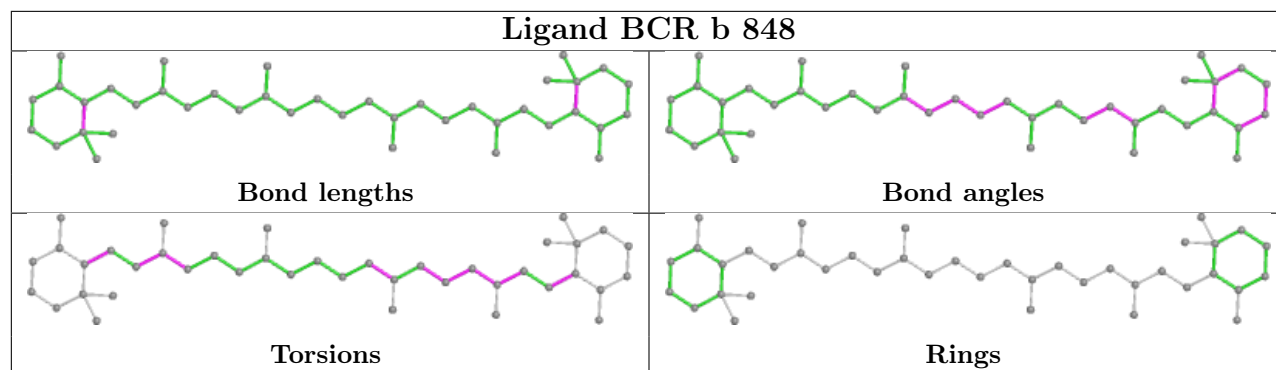


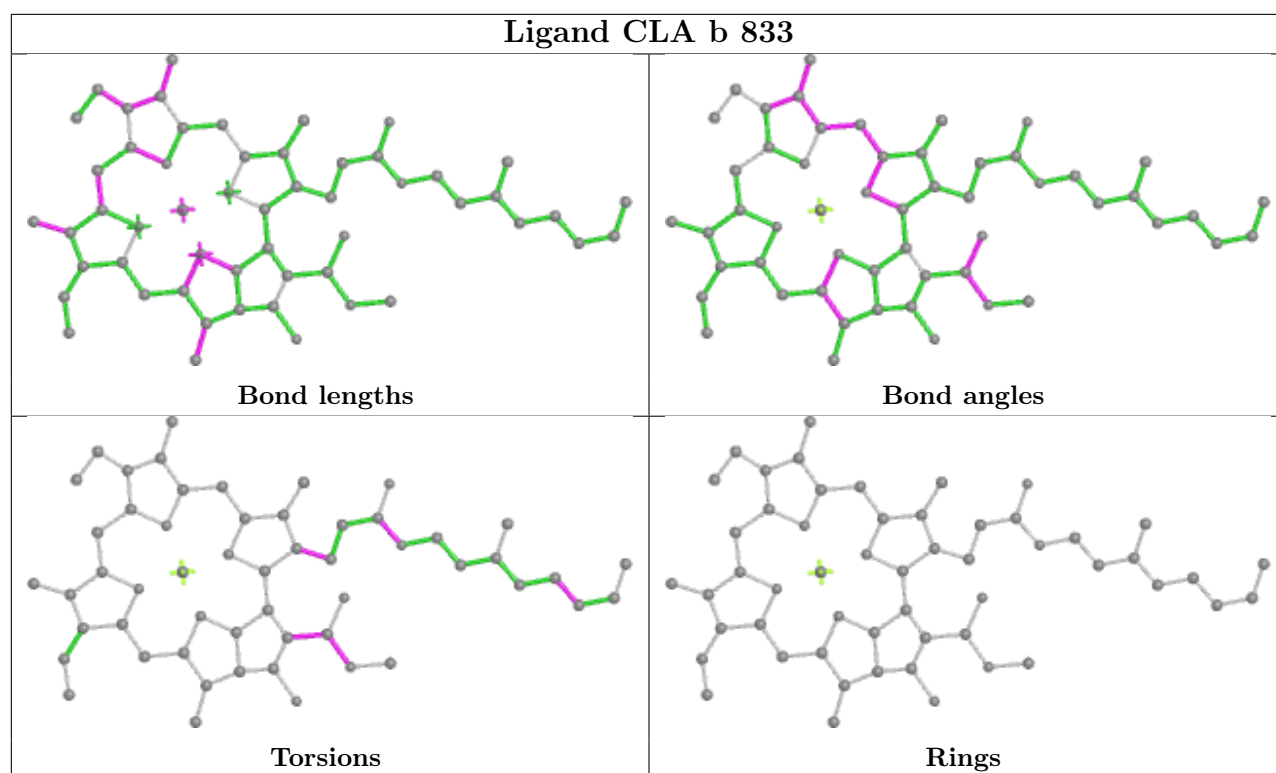




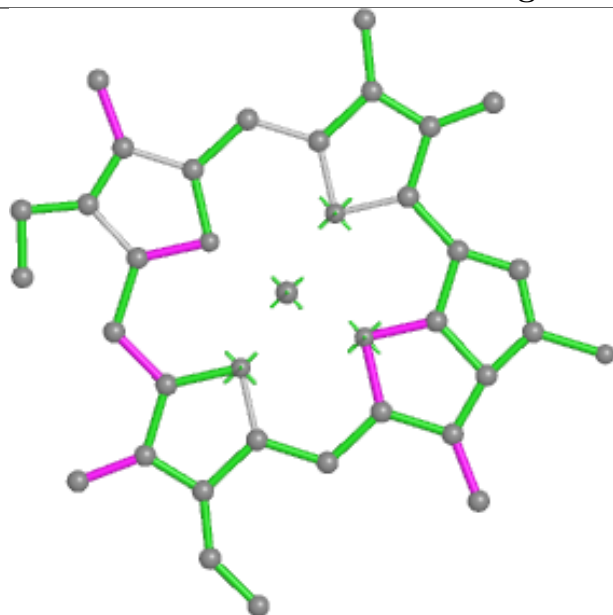




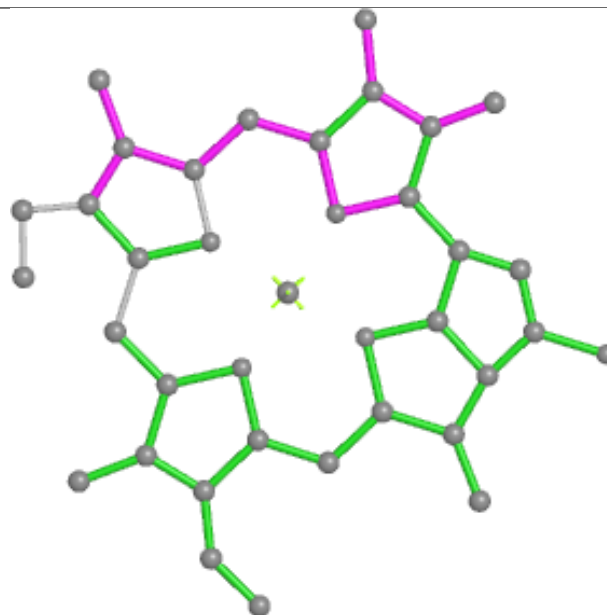




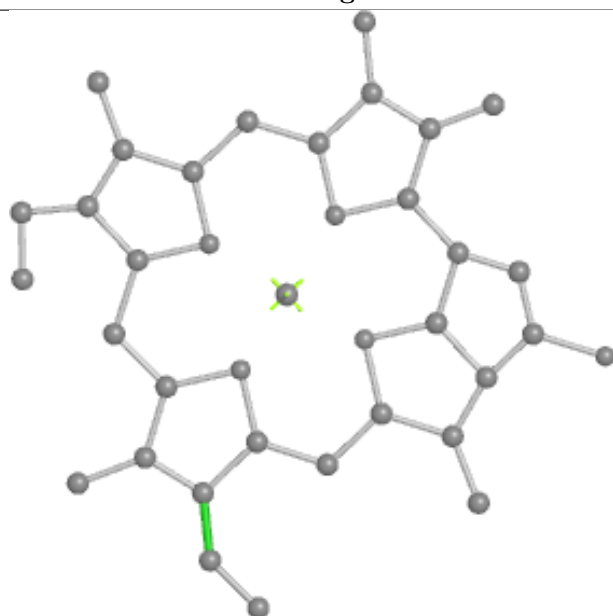
## Ligand CLA J 102



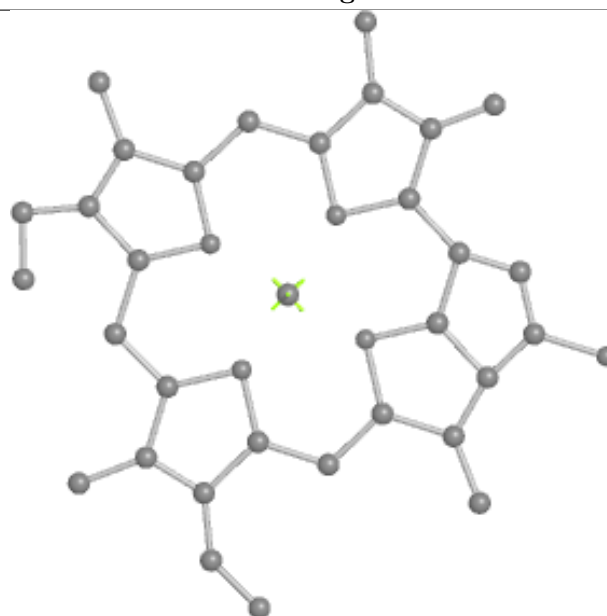
Bond lengths



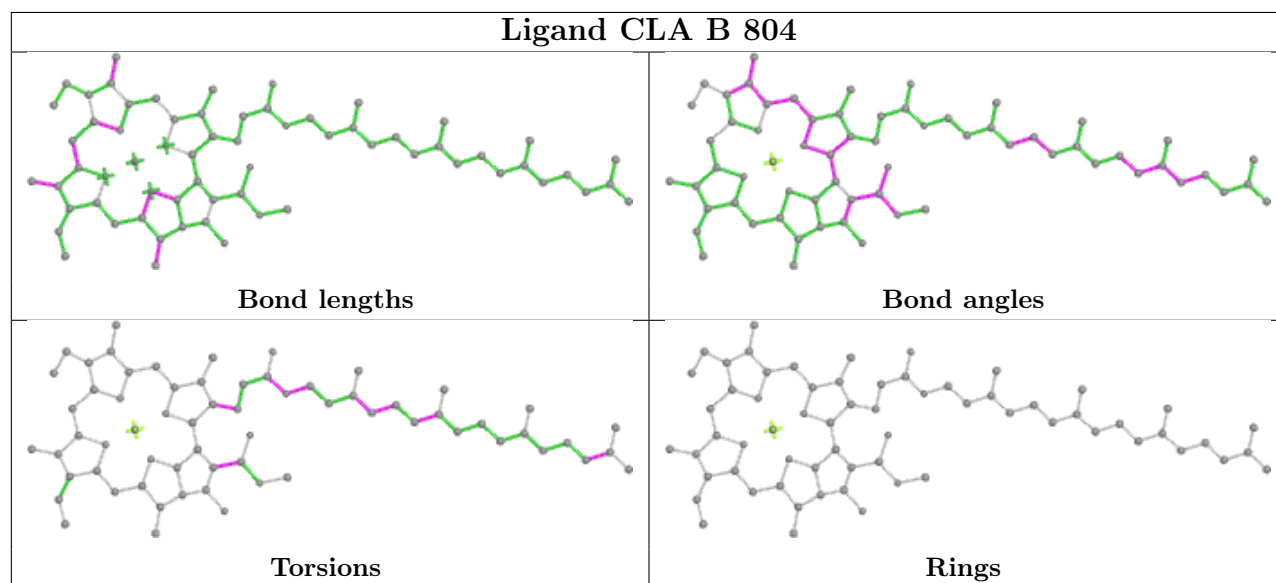
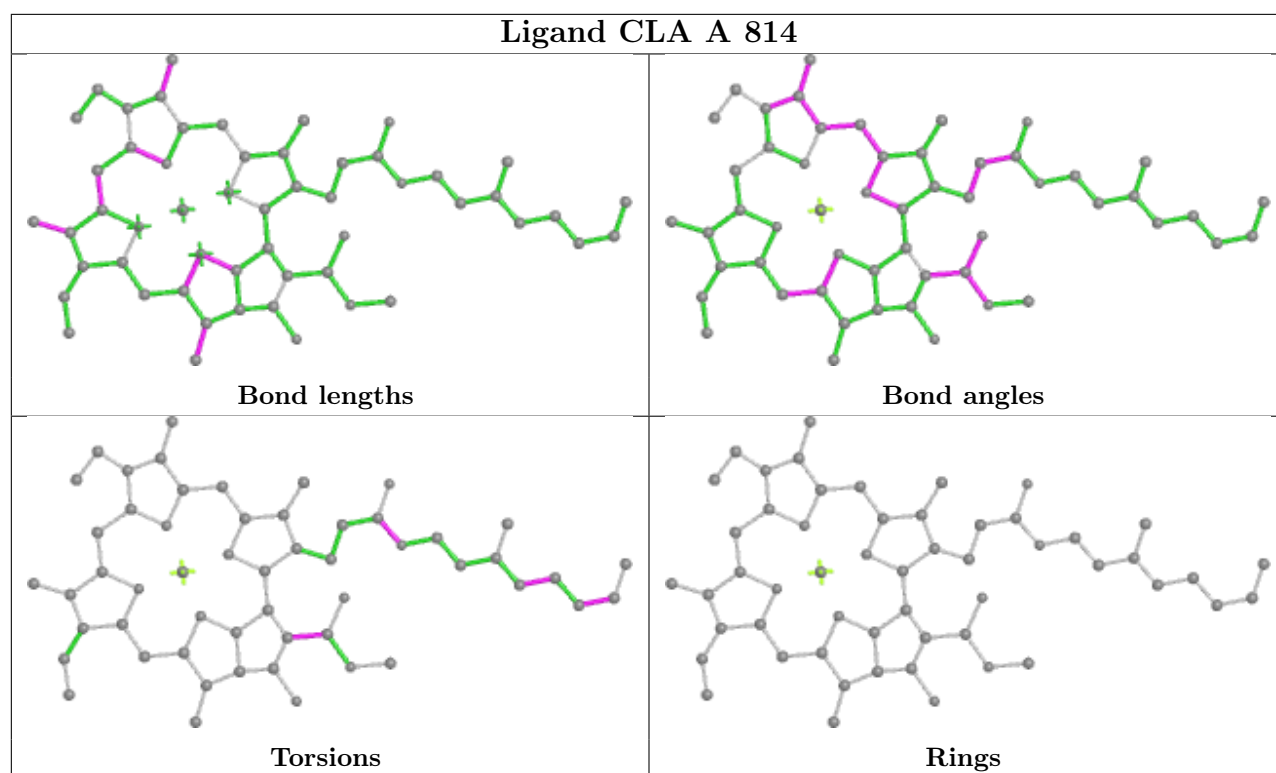
Bond angles



Torsions

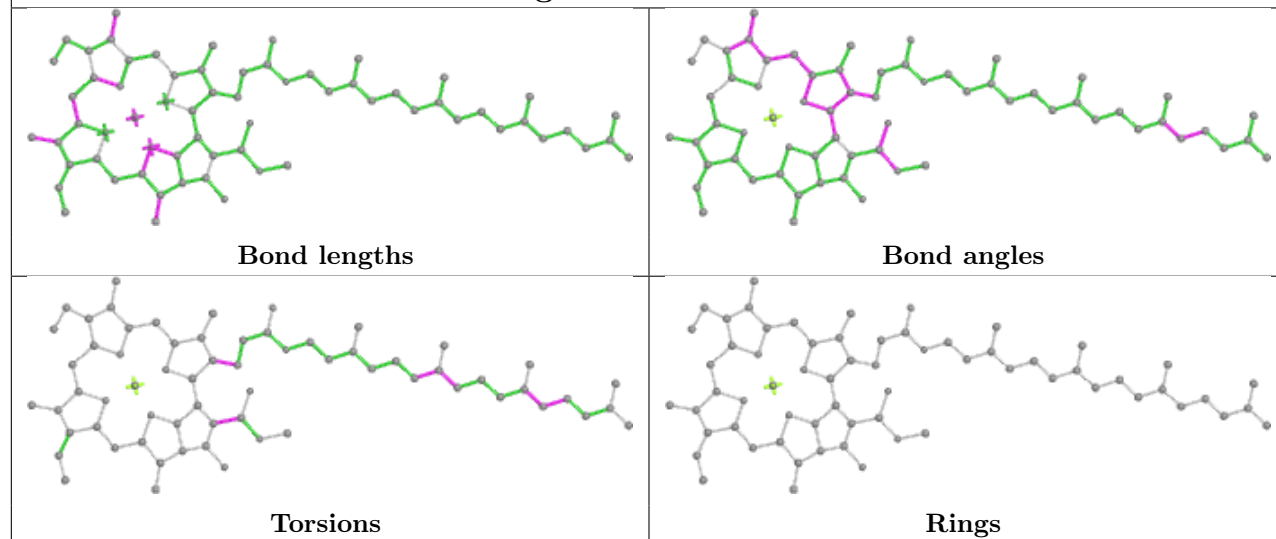


Rings

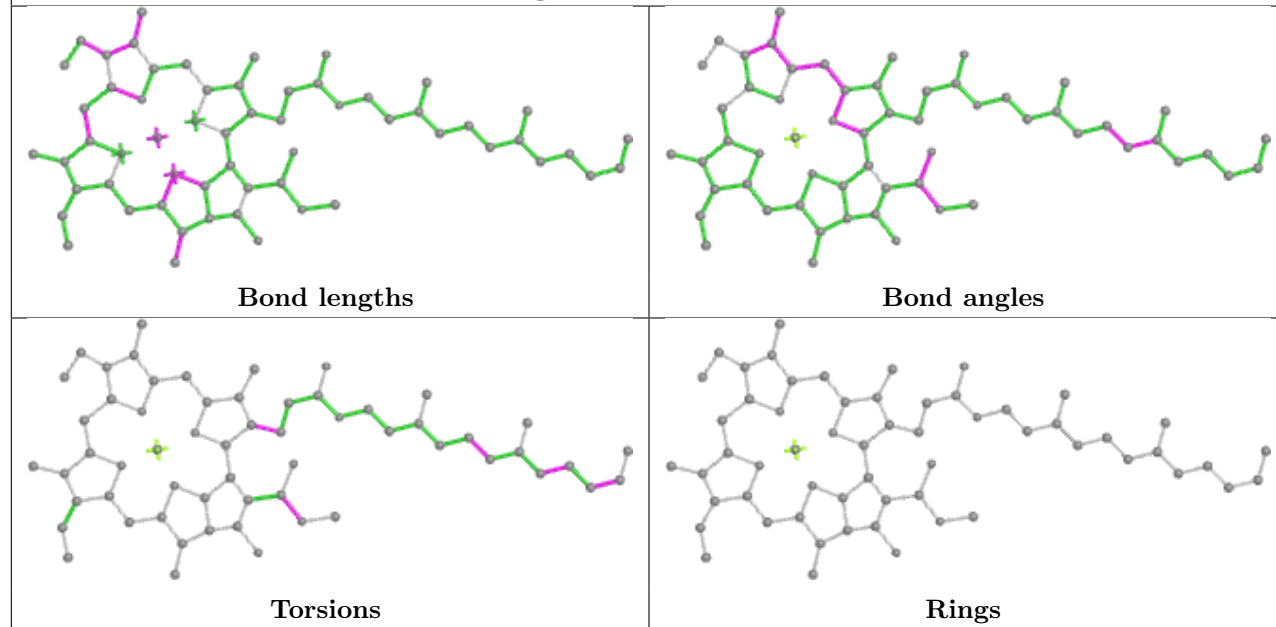


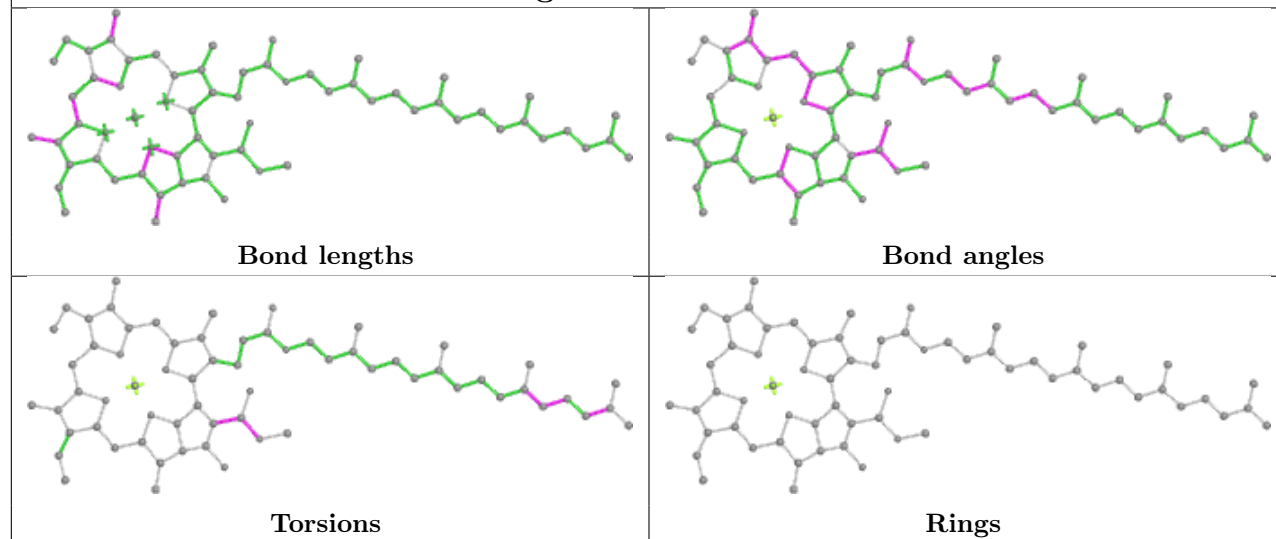
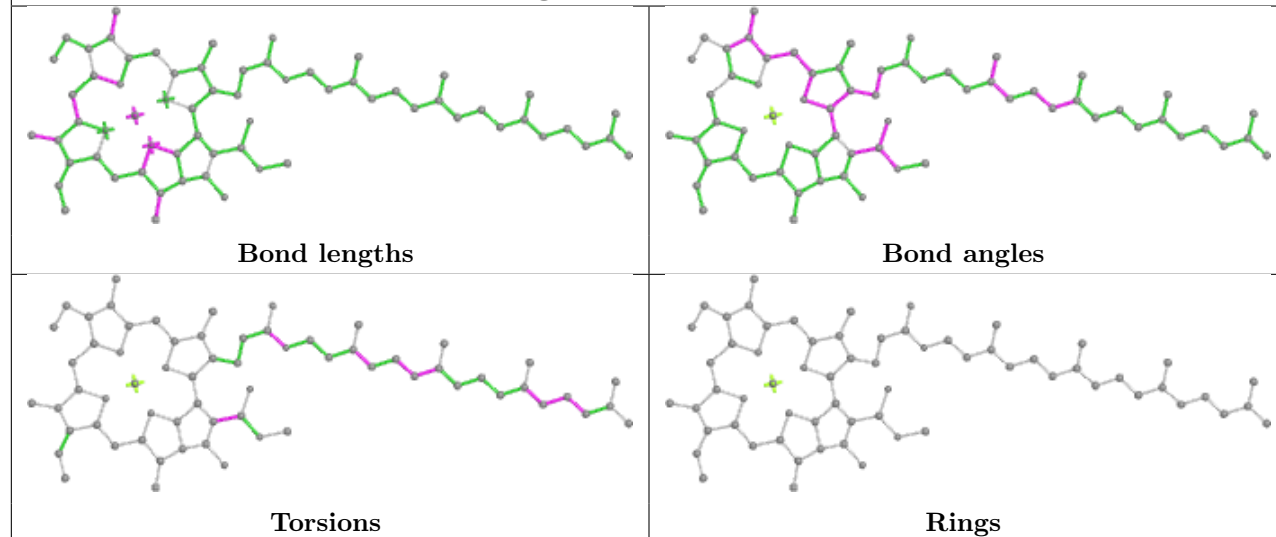
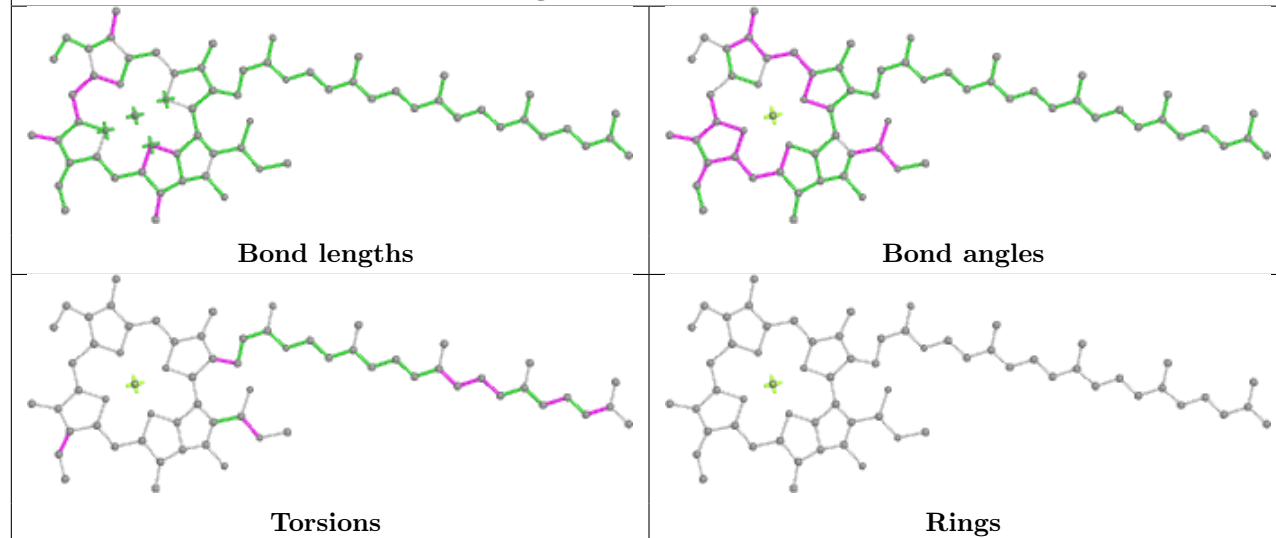


## Ligand CLA b 829

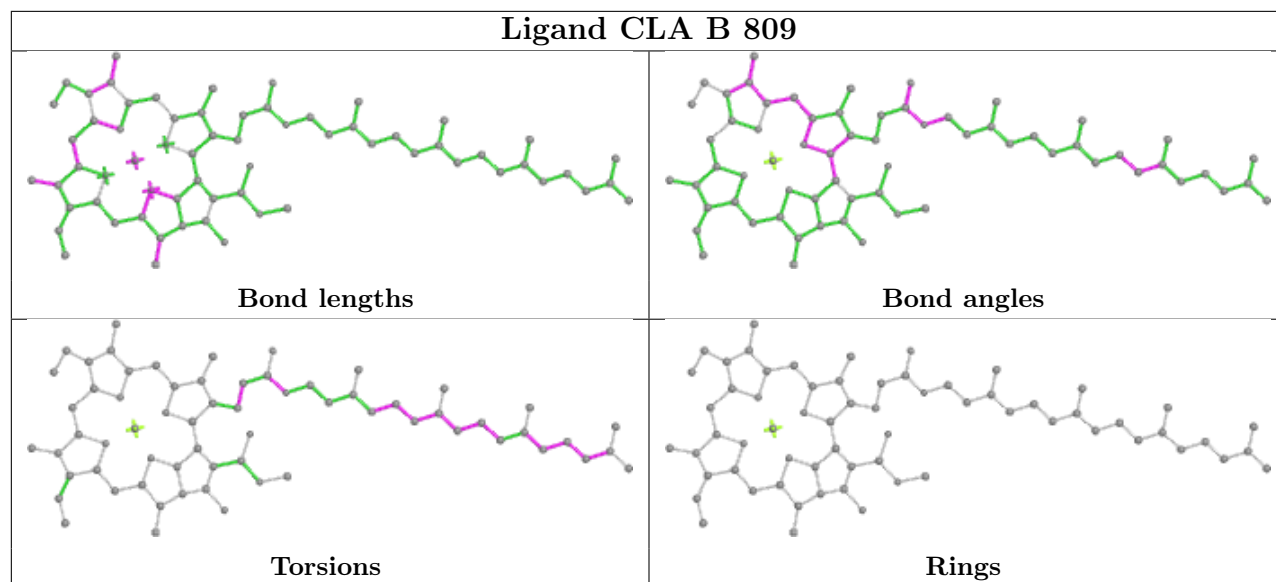


## Ligand CLA A 840

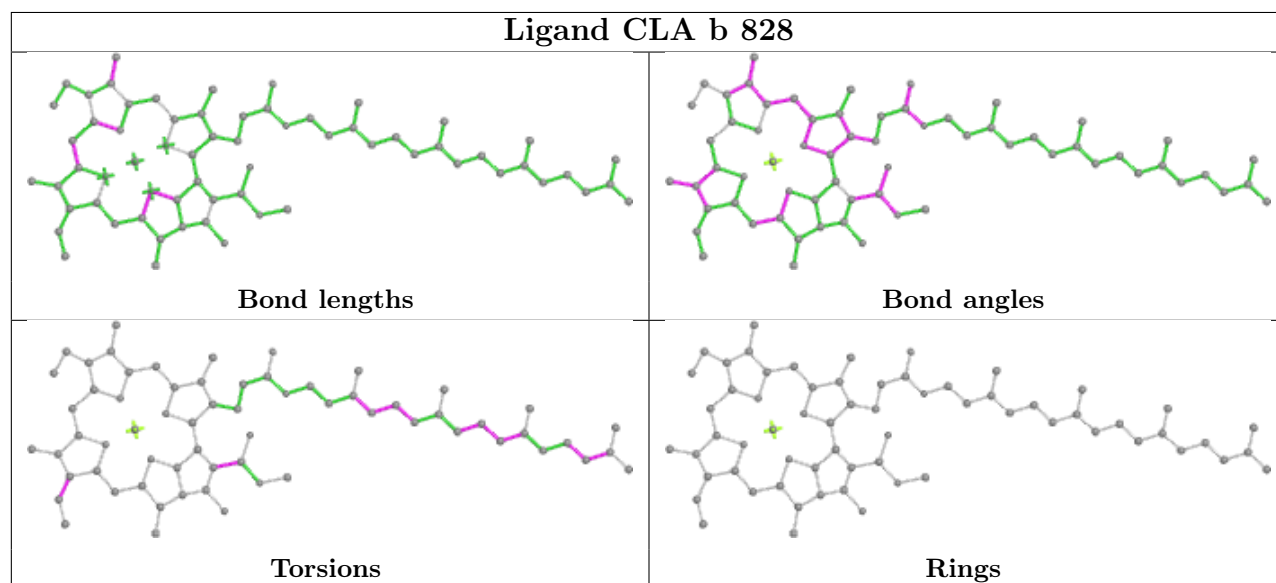


**Ligand CLA a 832****Ligand CLA b 827****Ligand CLA B 806**

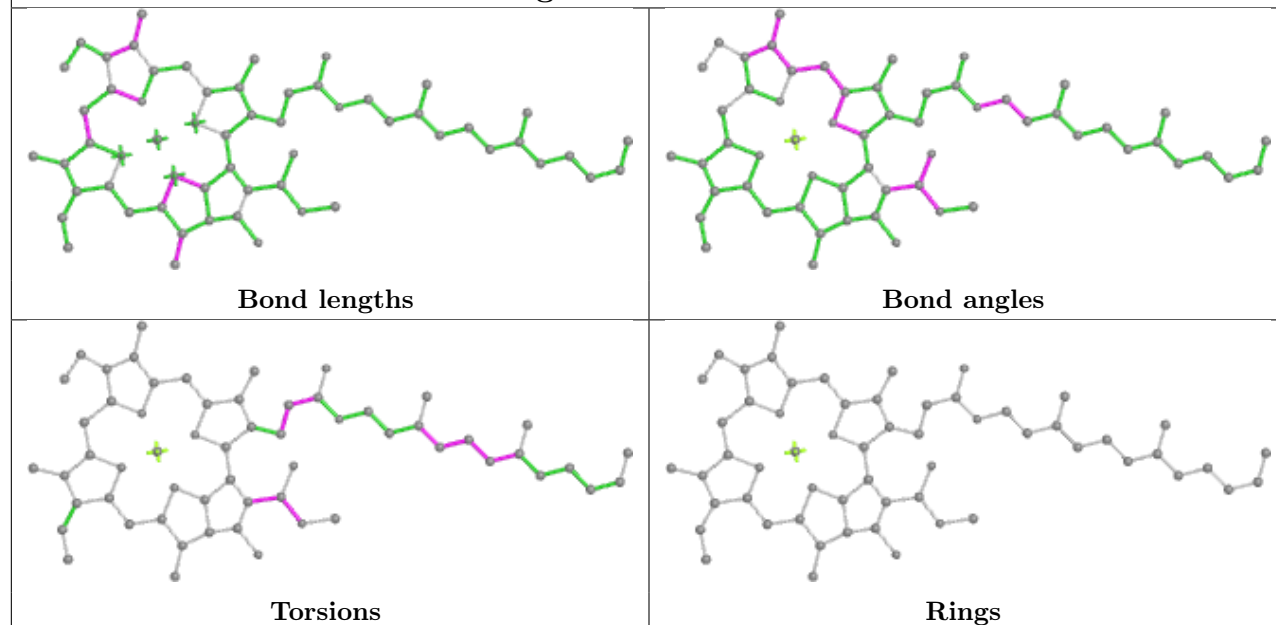
## Ligand CLA B 809



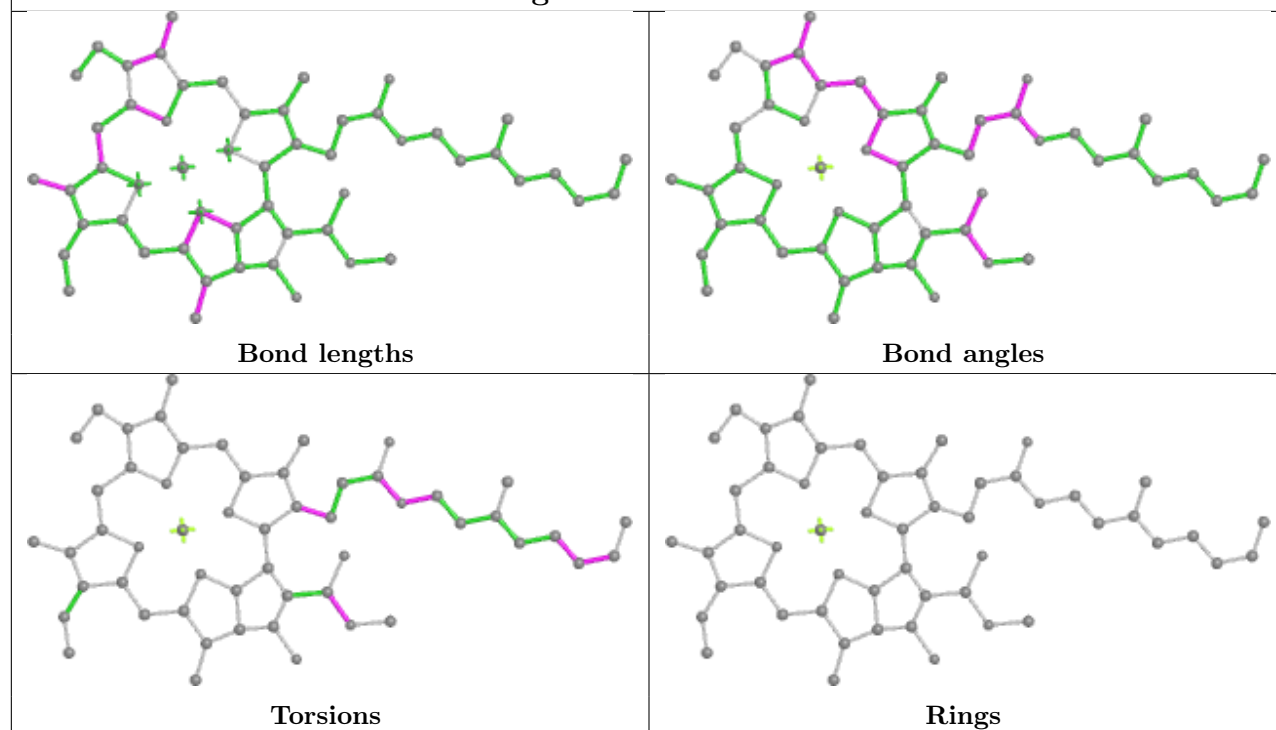
## Ligand CLA b 828



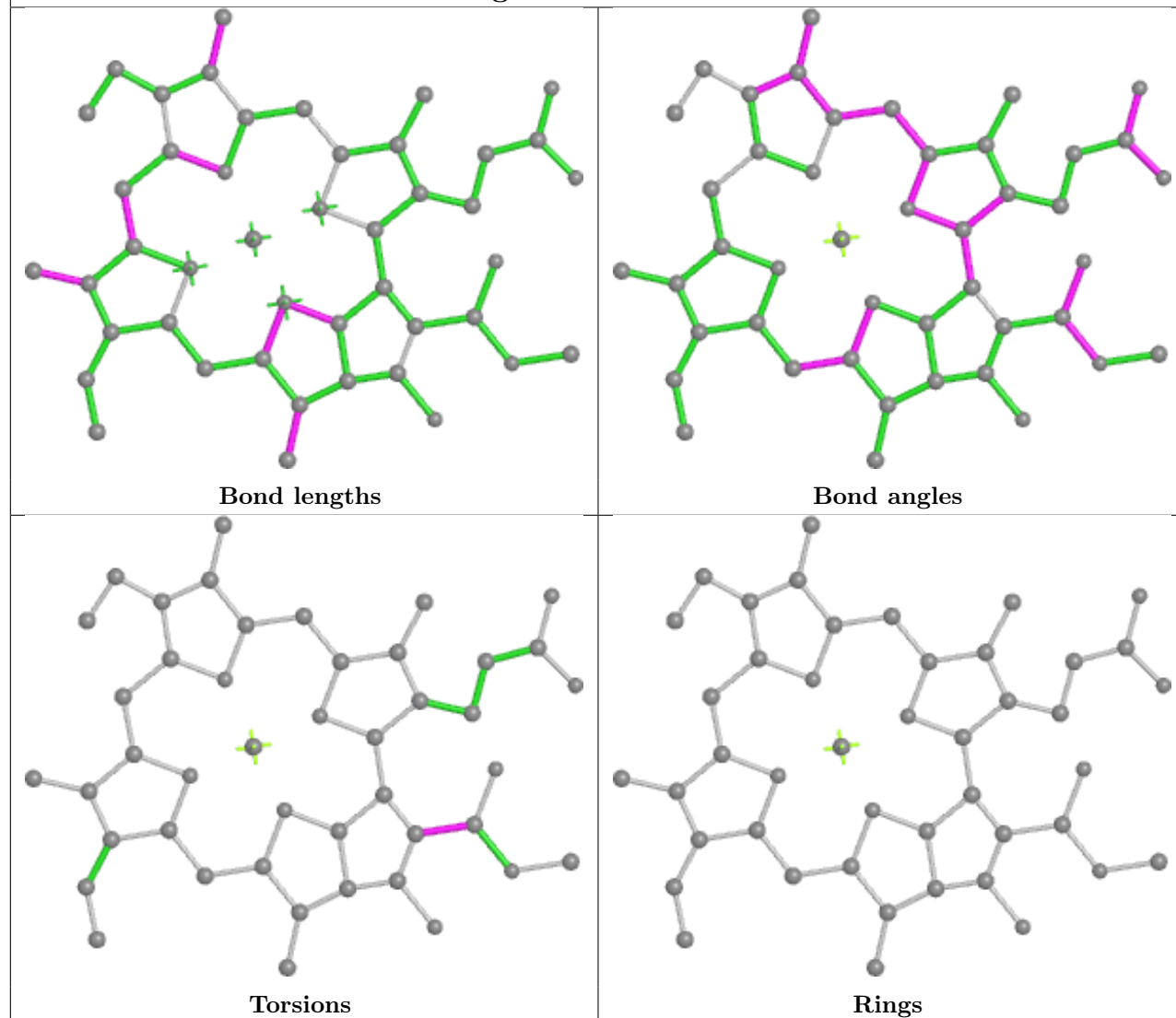
## Ligand CLA a 811



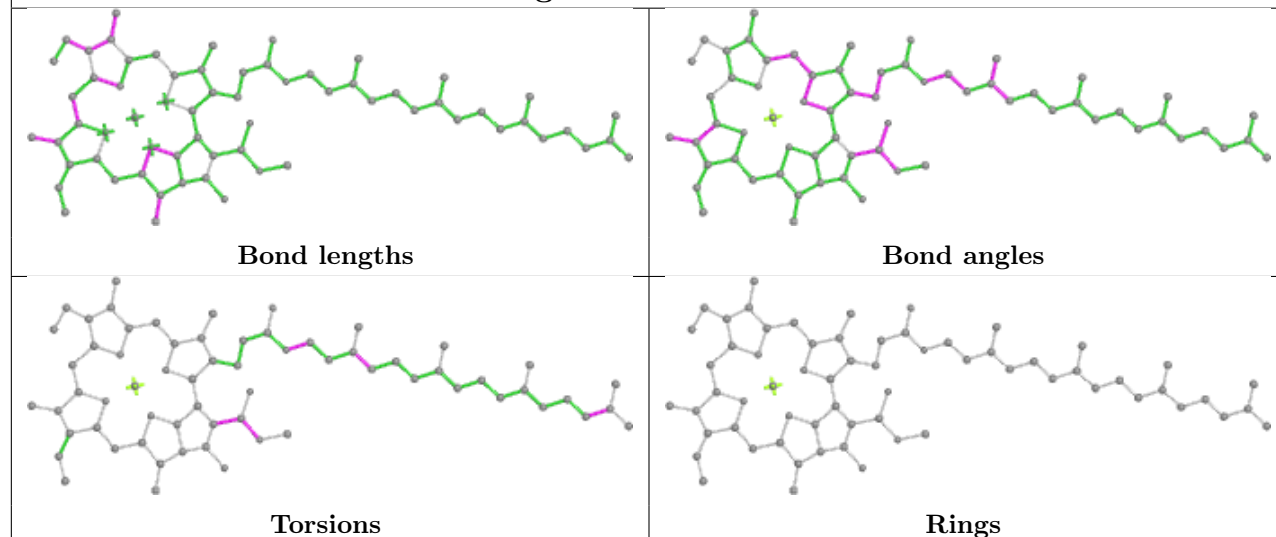
## Ligand CLA A 835



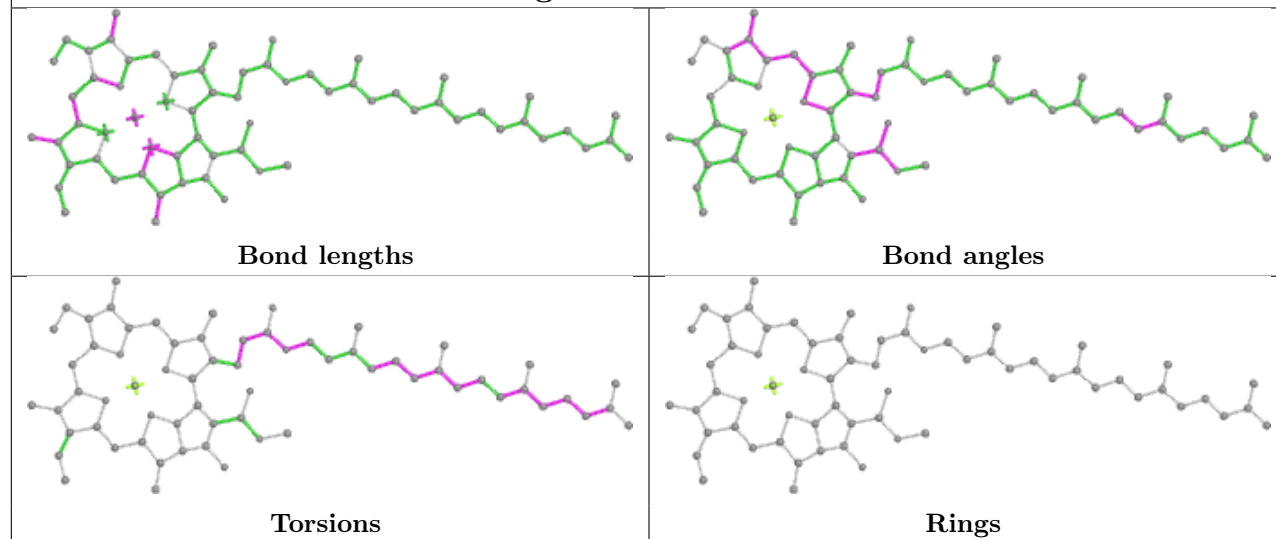
## Ligand CLA F 204



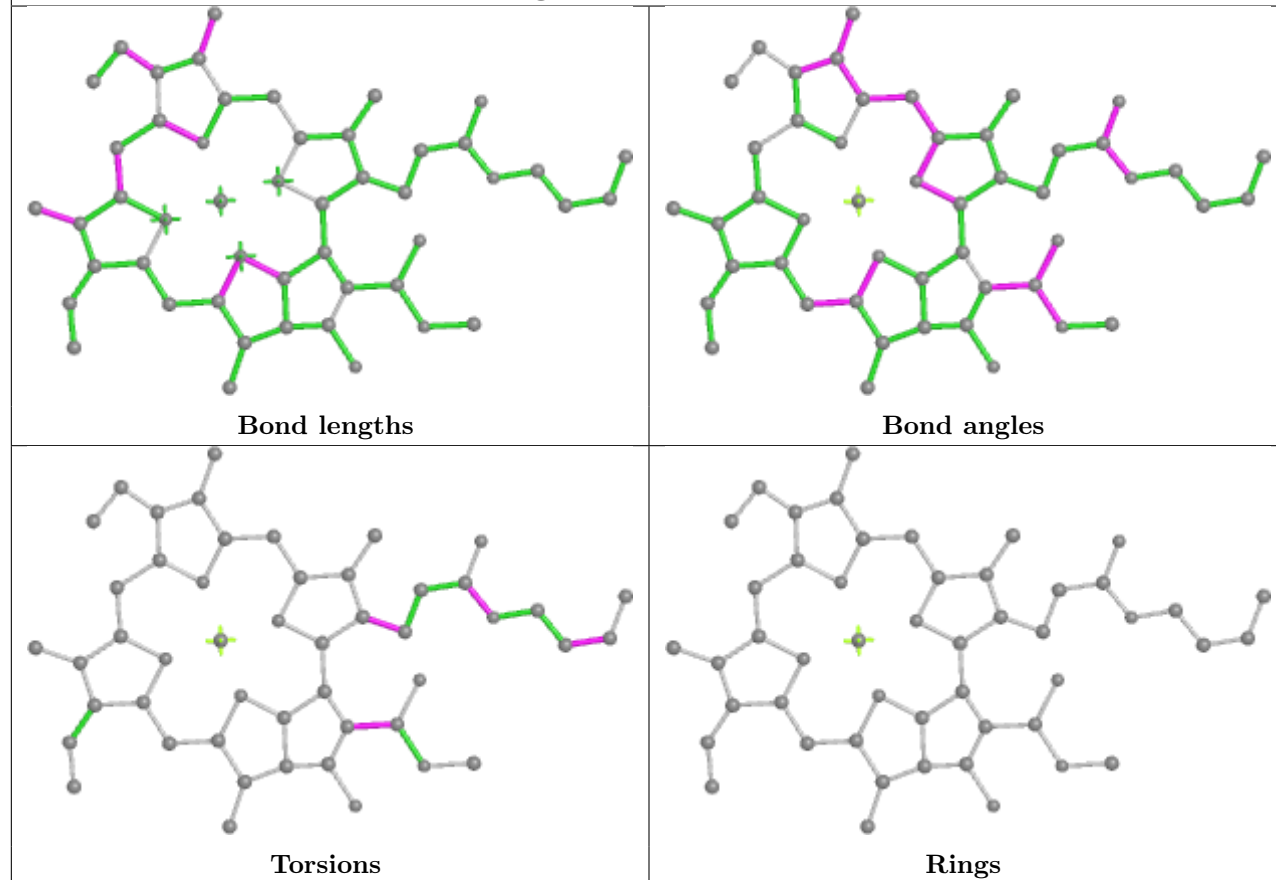
## Ligand CLA b 806

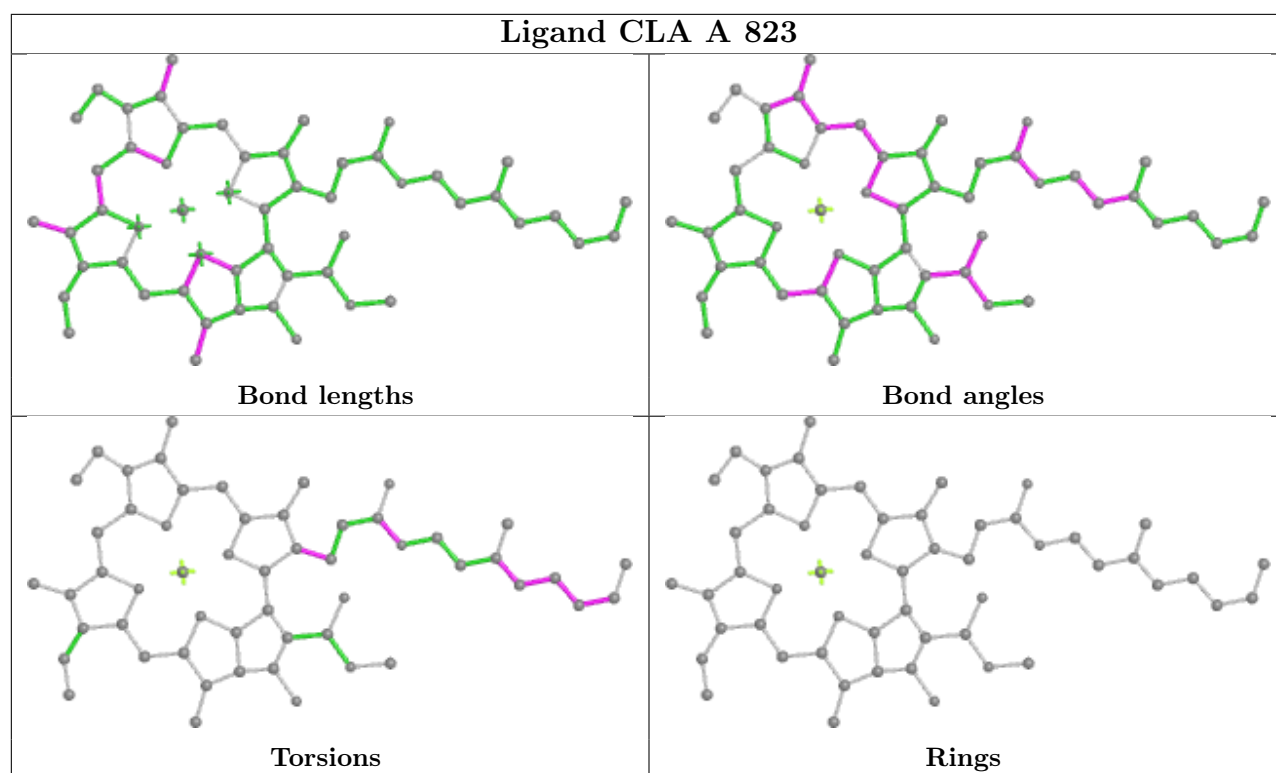


## Ligand CLA b 809

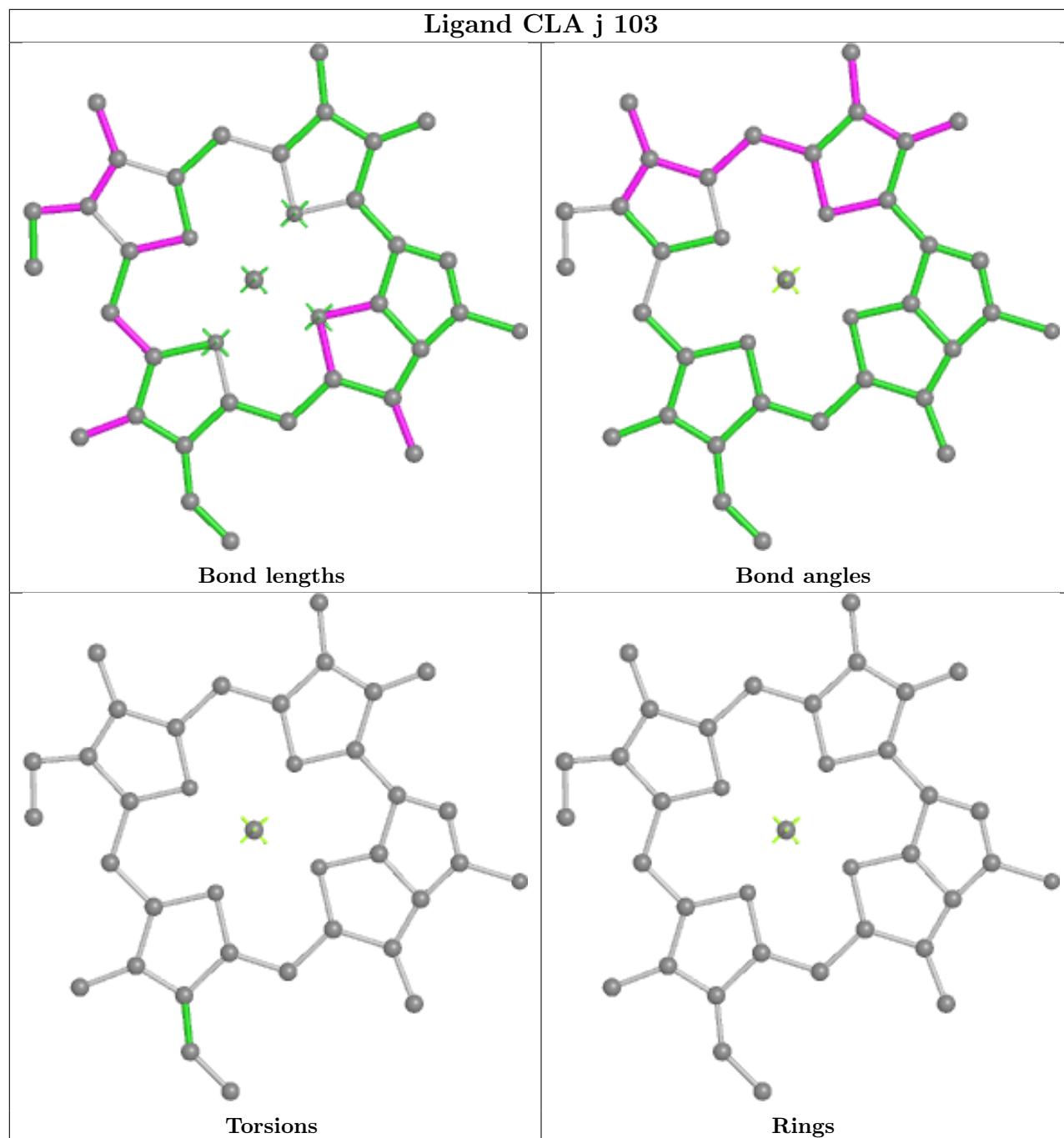


## Ligand CLA B 818

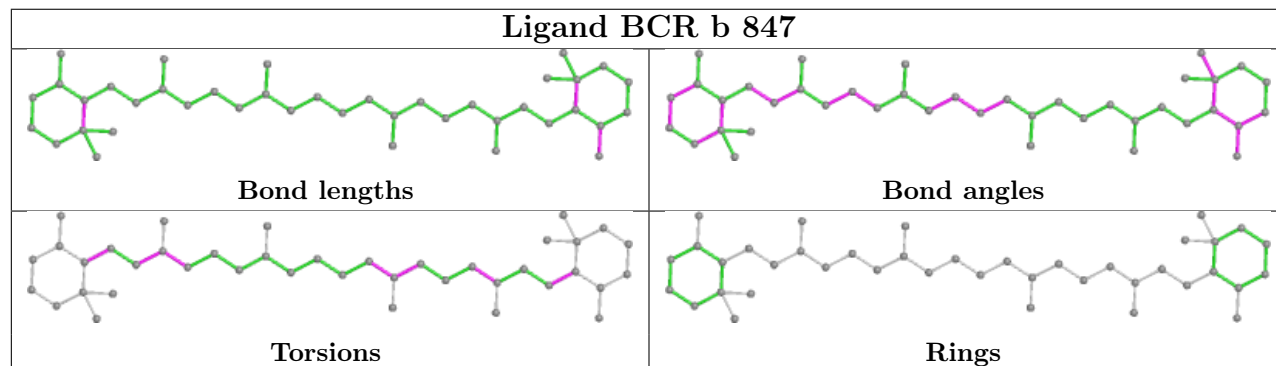




## Ligand CLA j 103

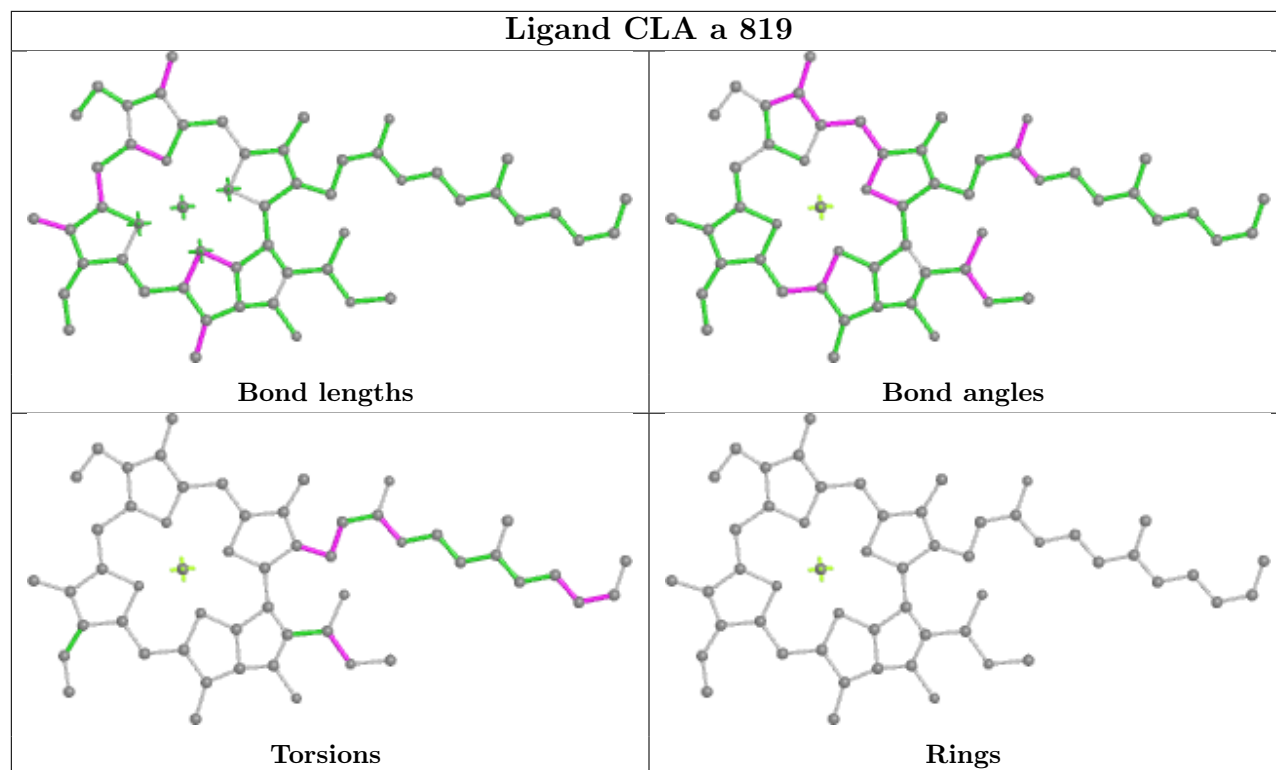


## Ligand BCR b 847

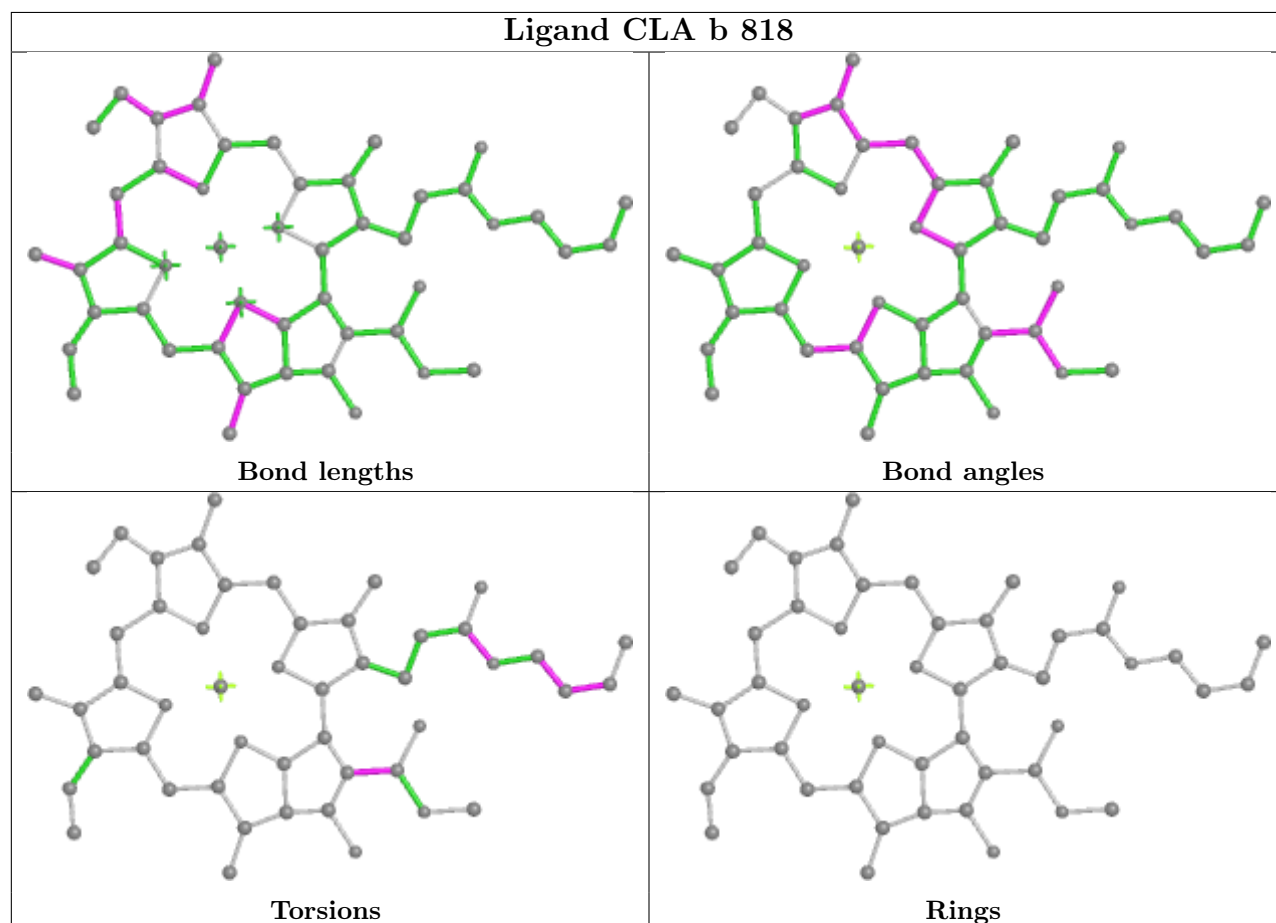


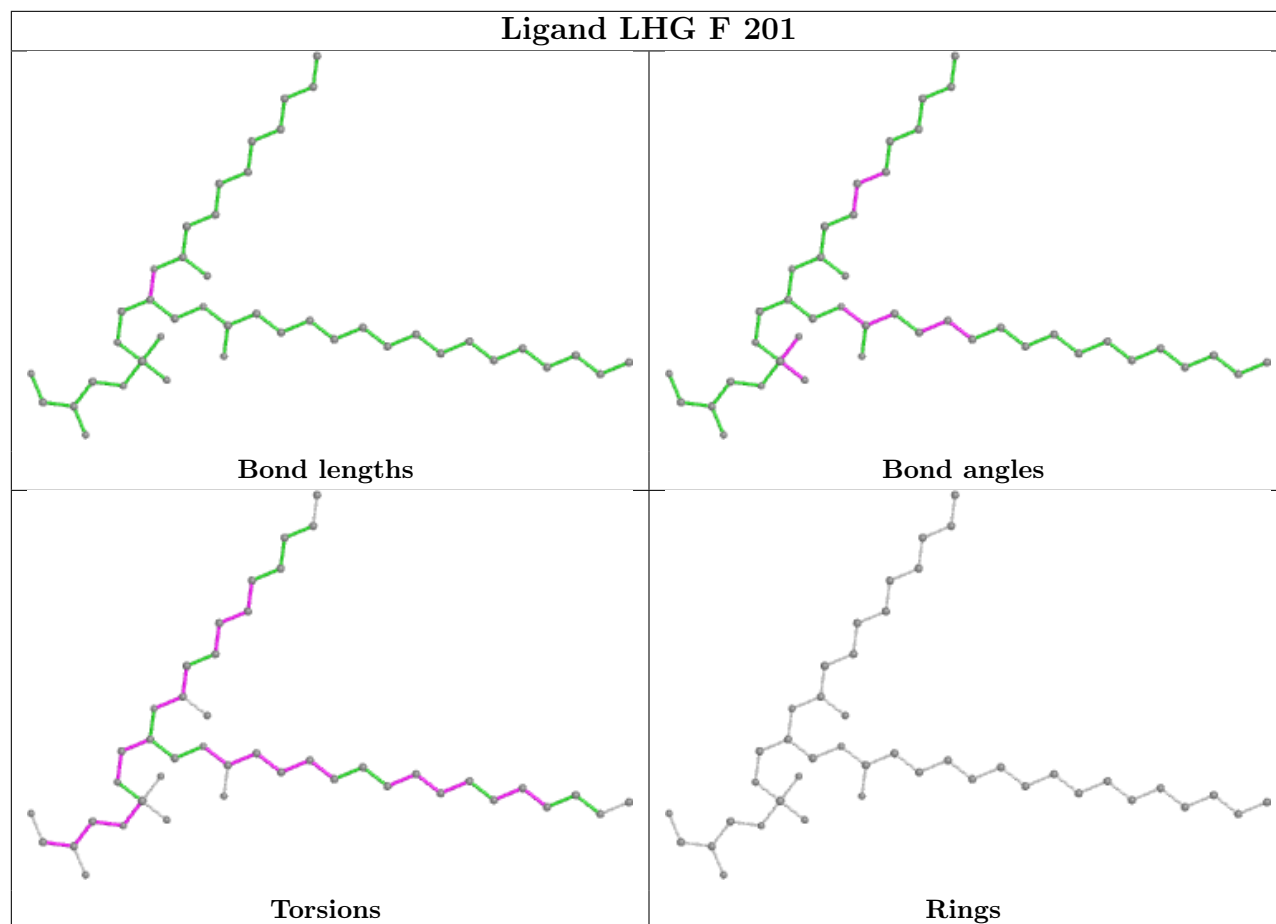
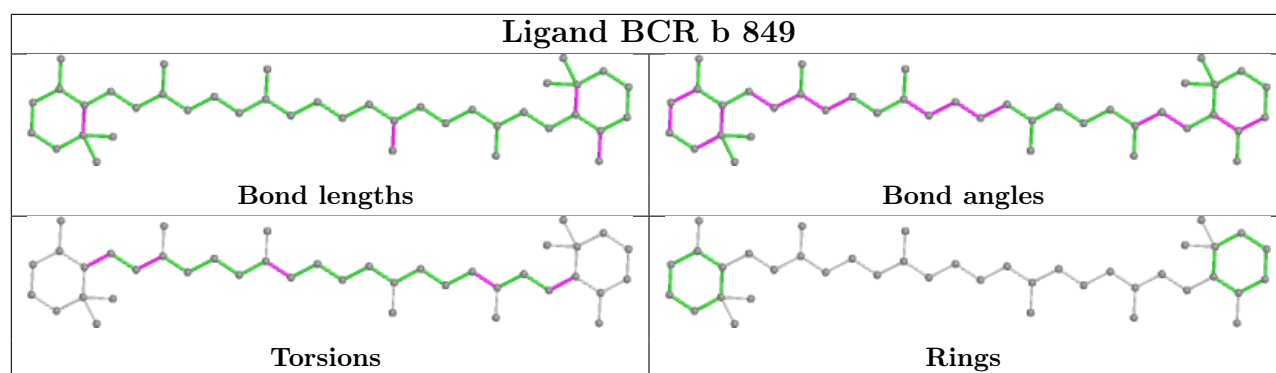


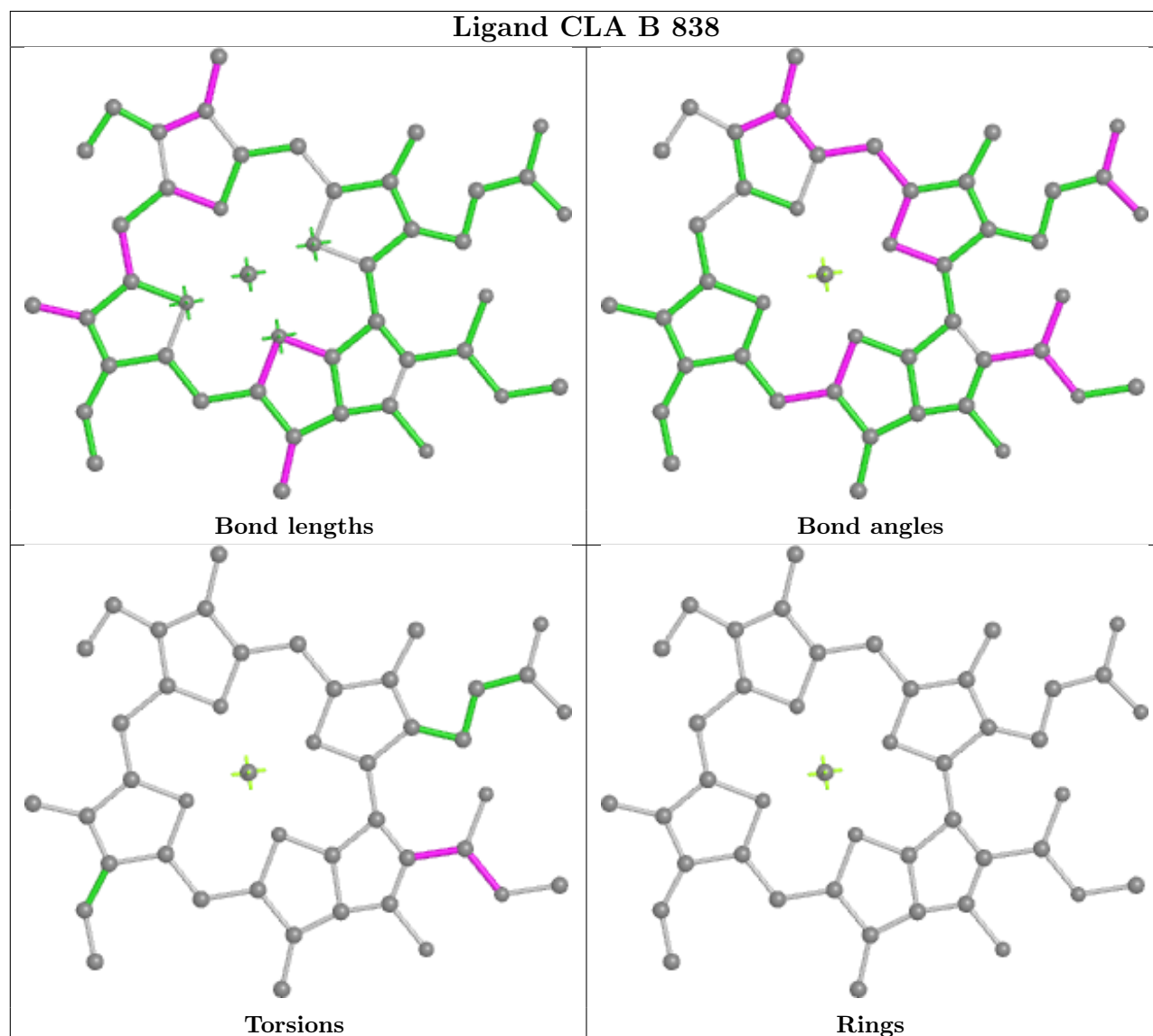
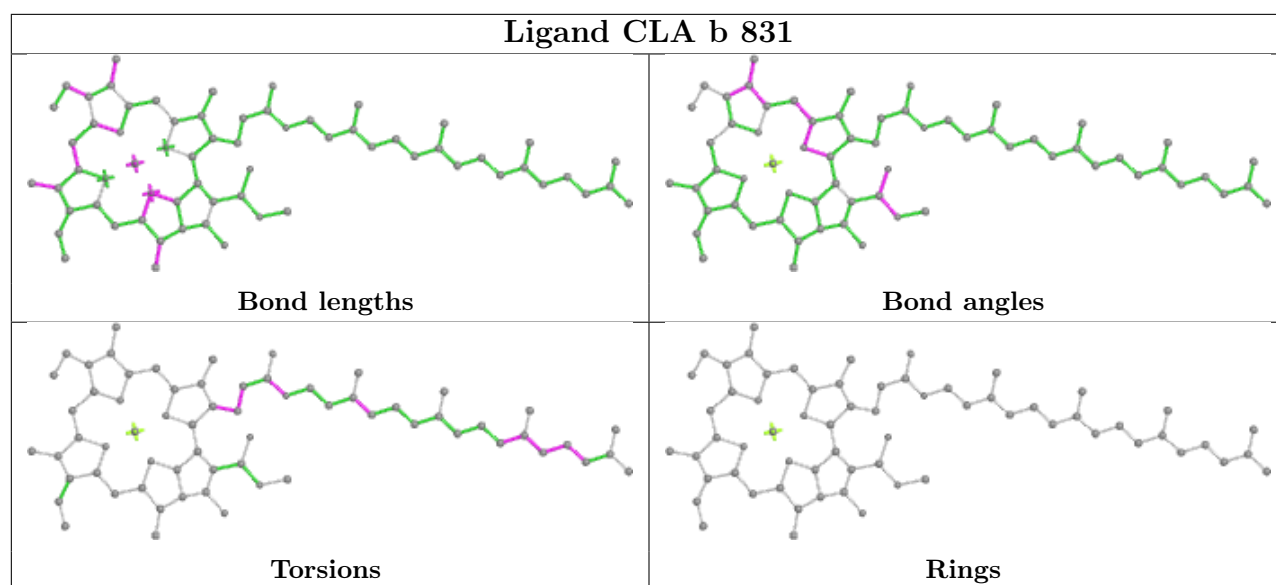
## Ligand CLA a 819

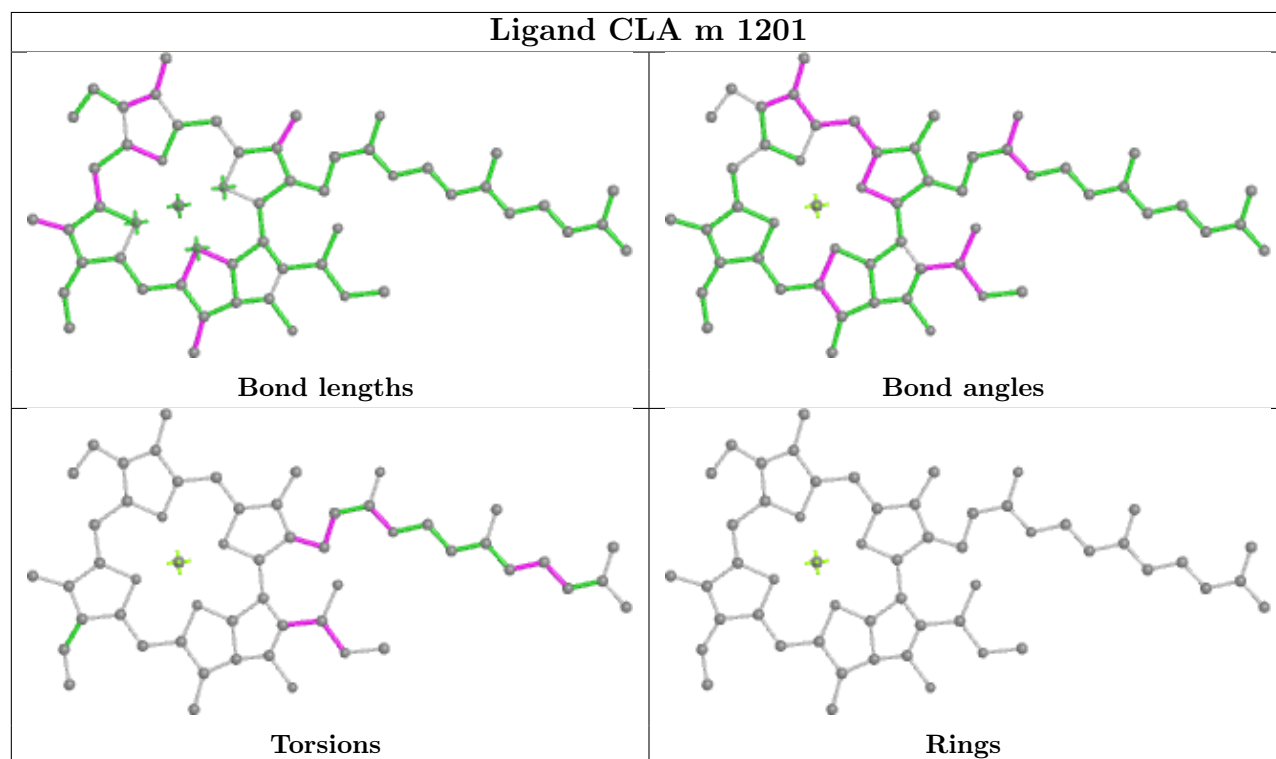
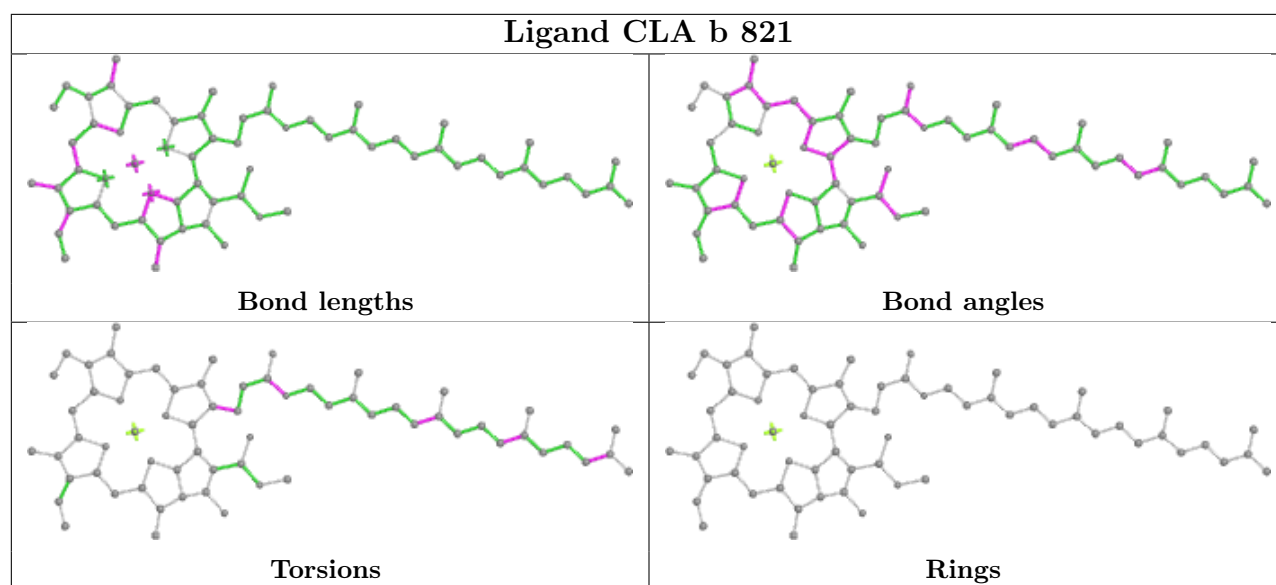


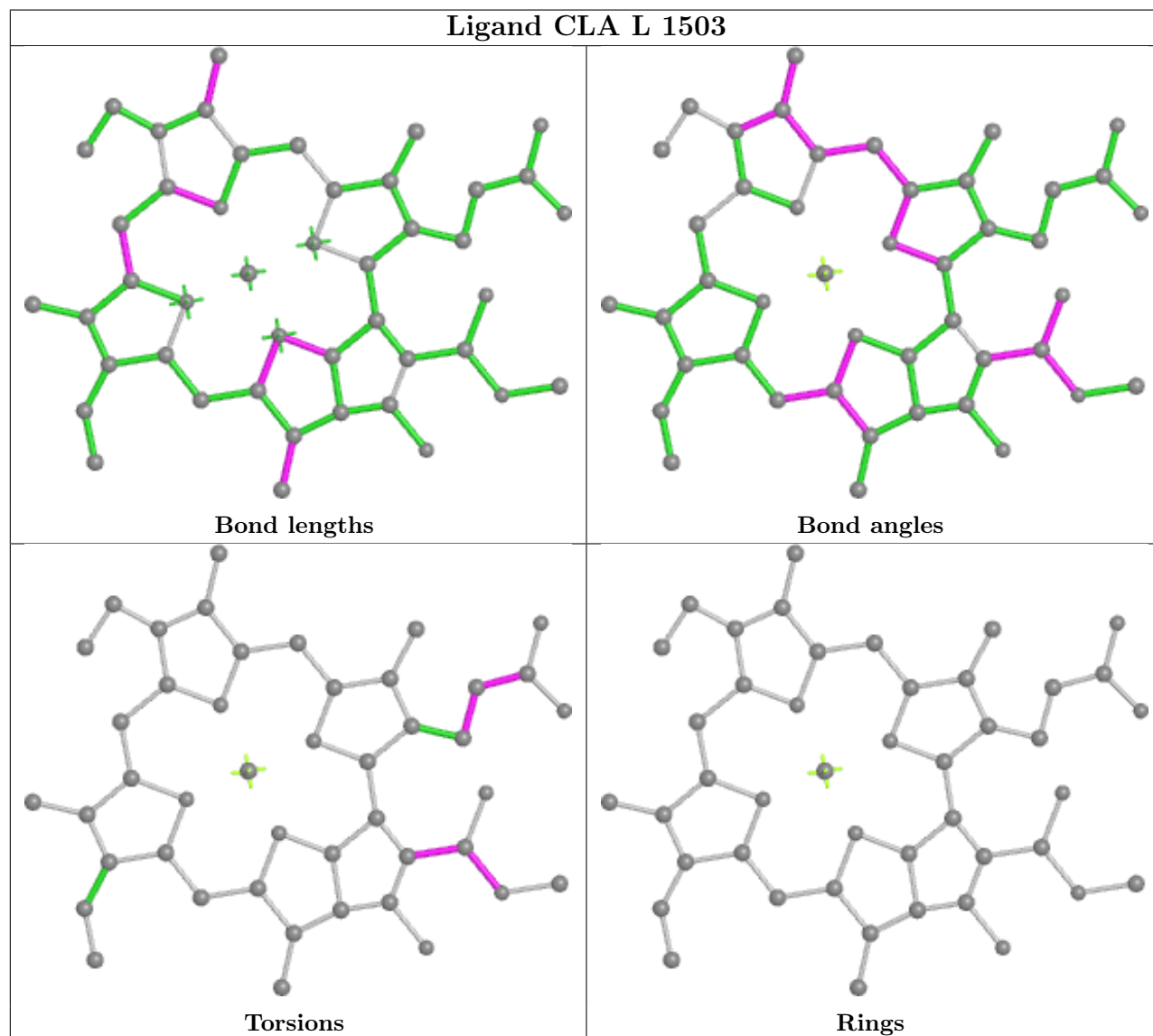
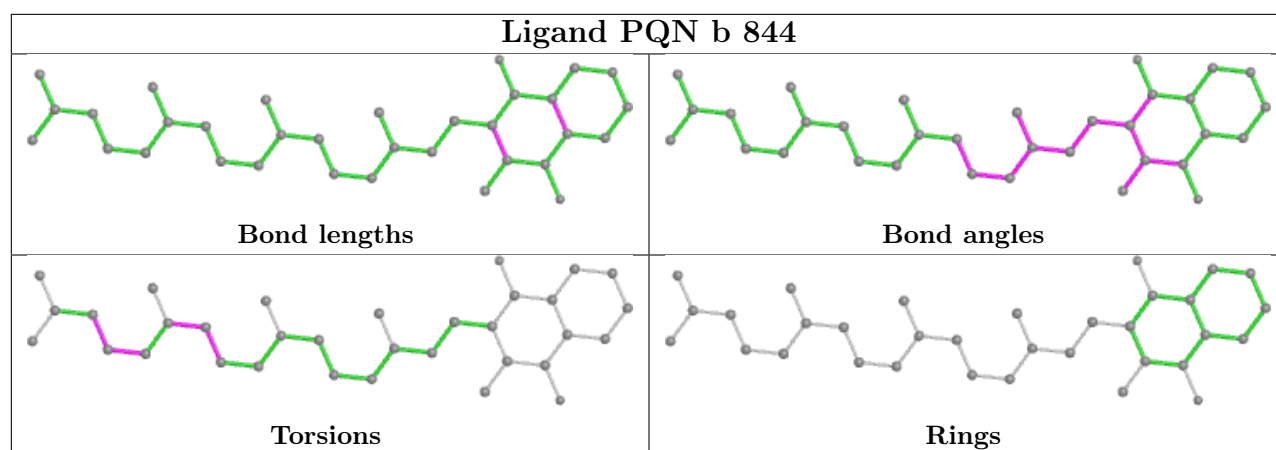
## Ligand CLA b 818



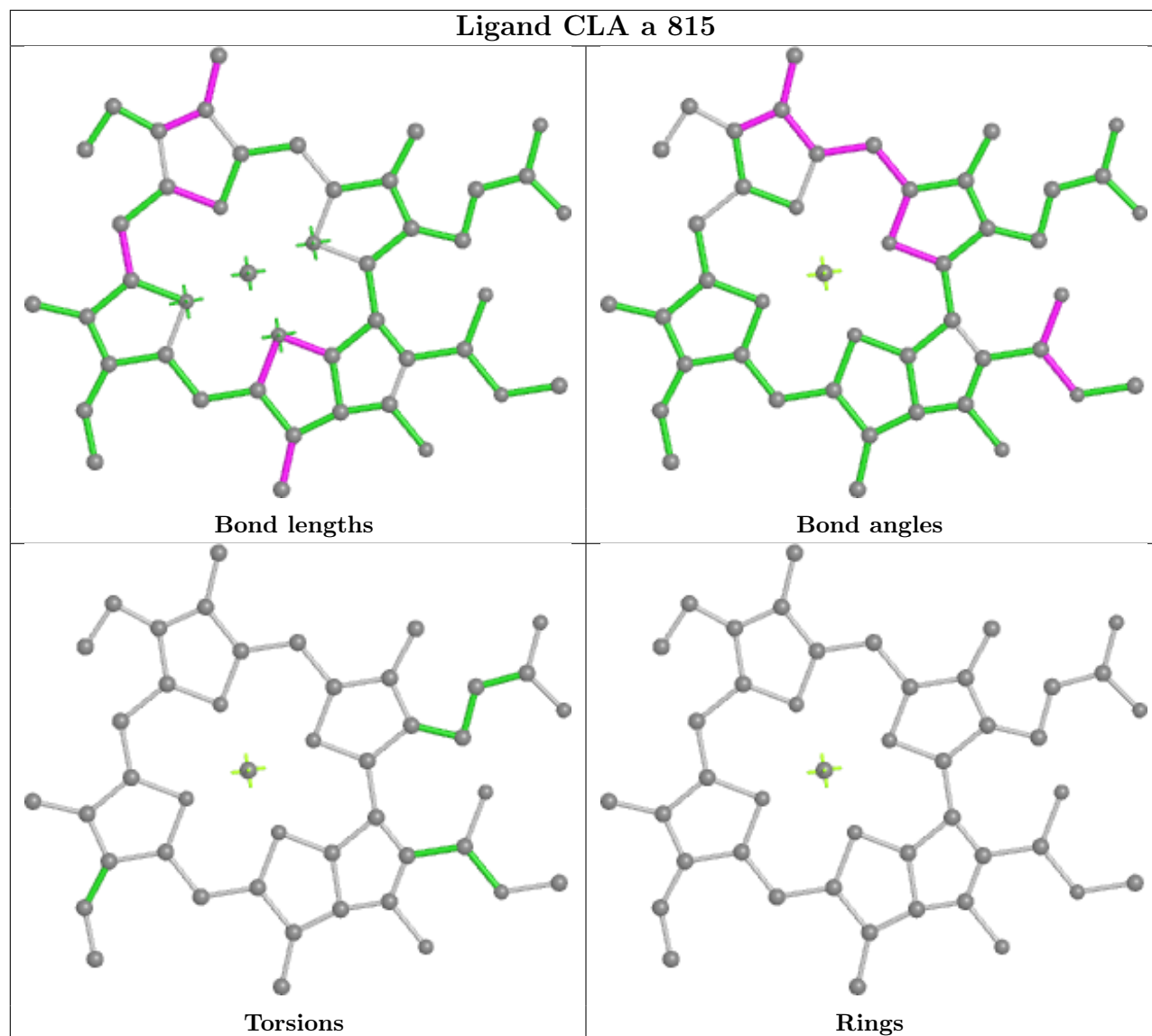




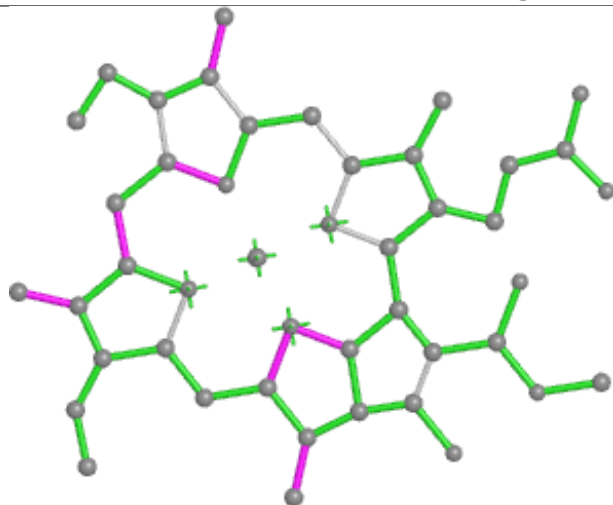




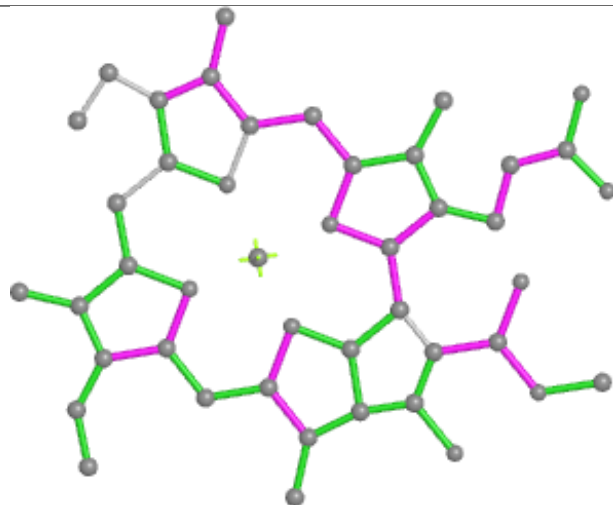
## Ligand CLA a 815



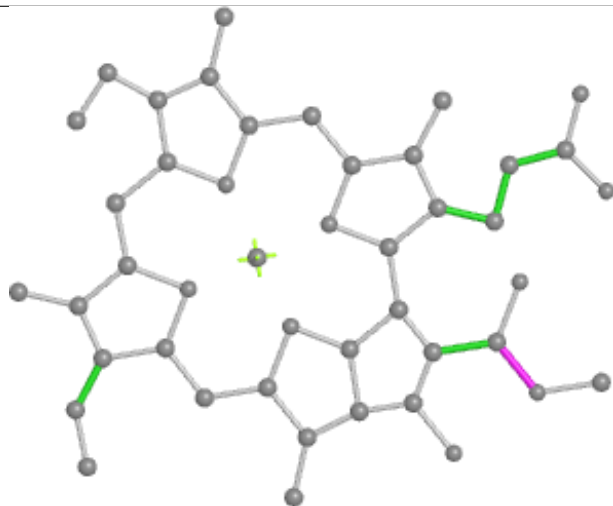
## Ligand CLA B 837



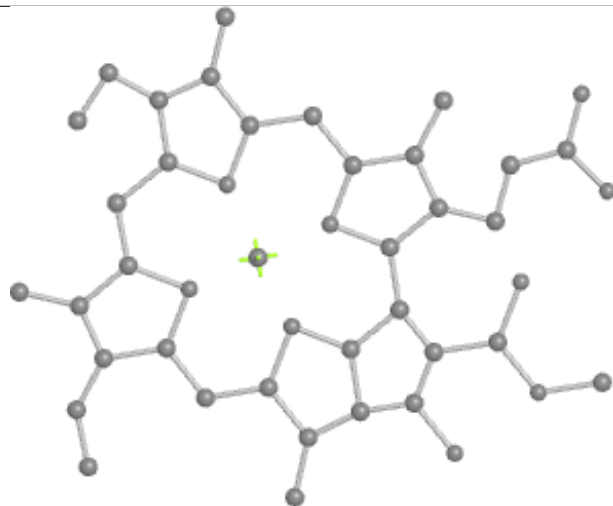
Bond lengths



Bond angles

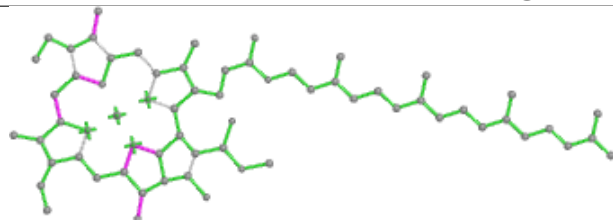


Torsions

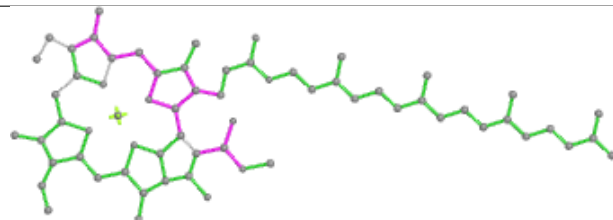


Rings

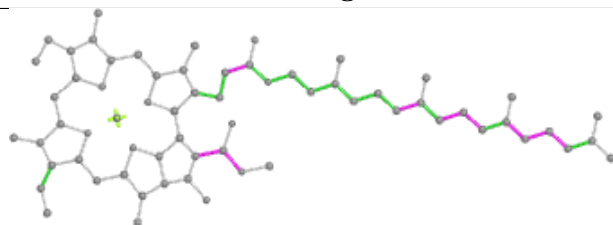
## Ligand CLA a 824



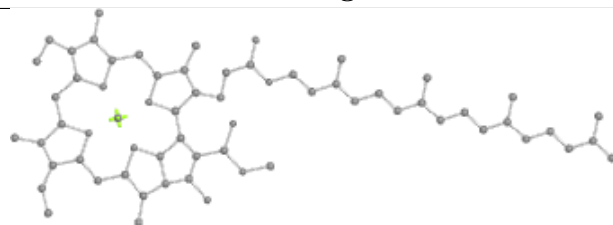
Bond lengths



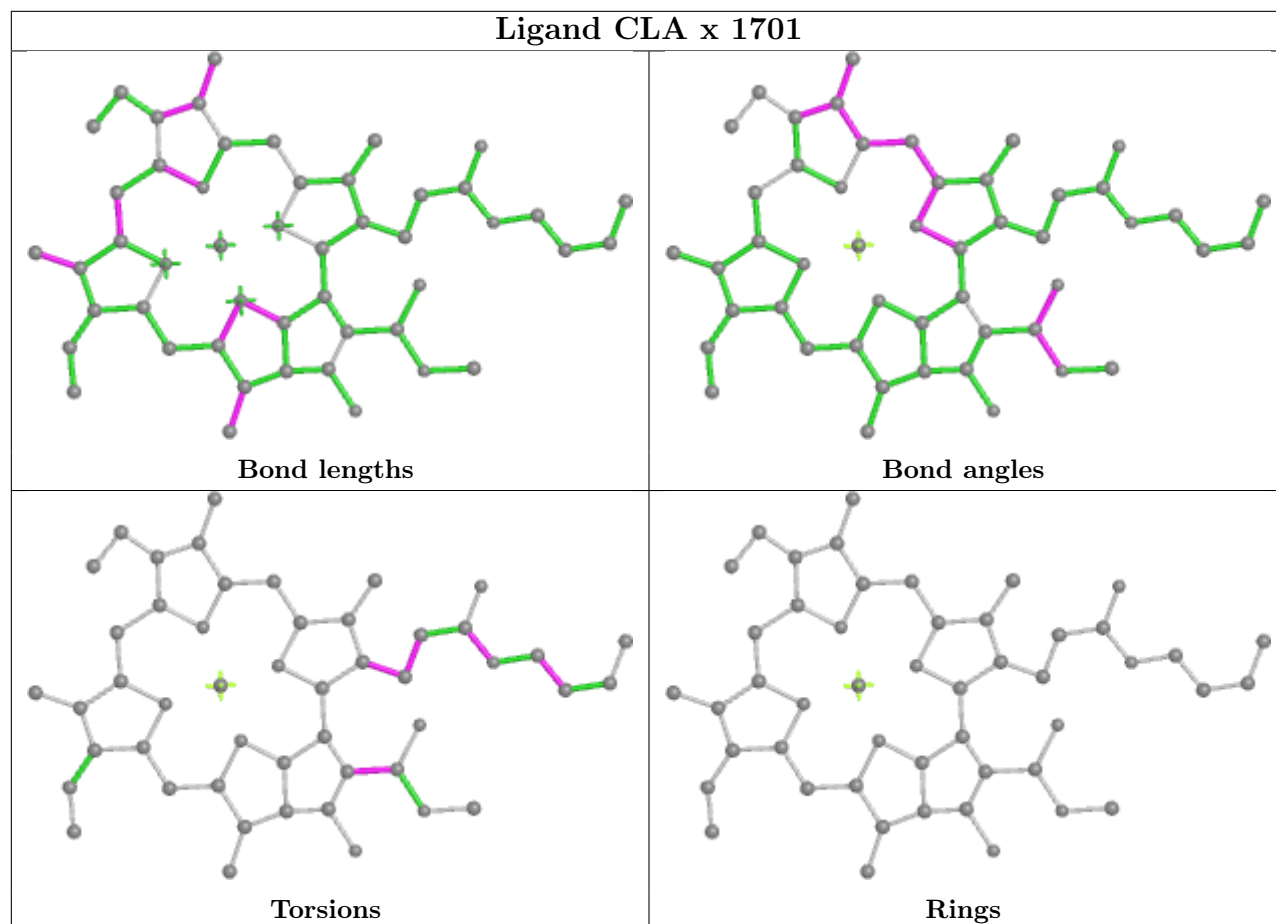
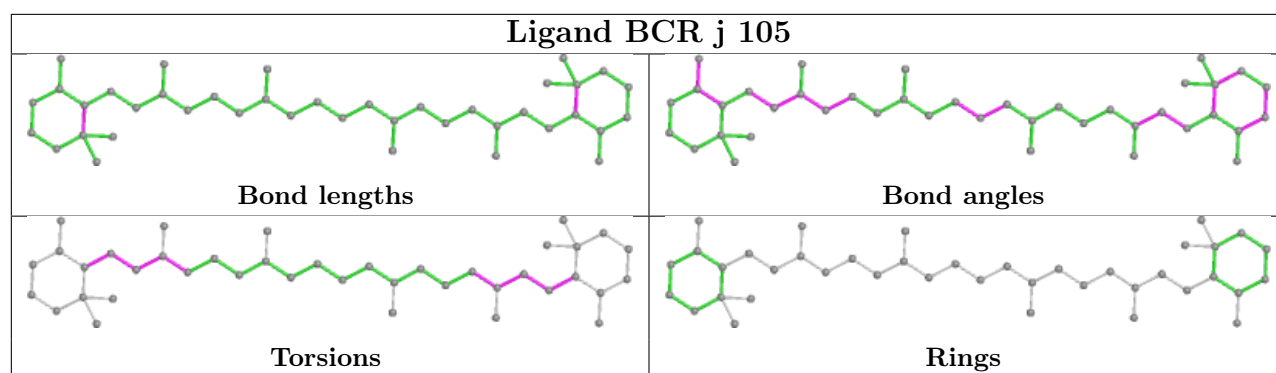
Bond angles



Torsions

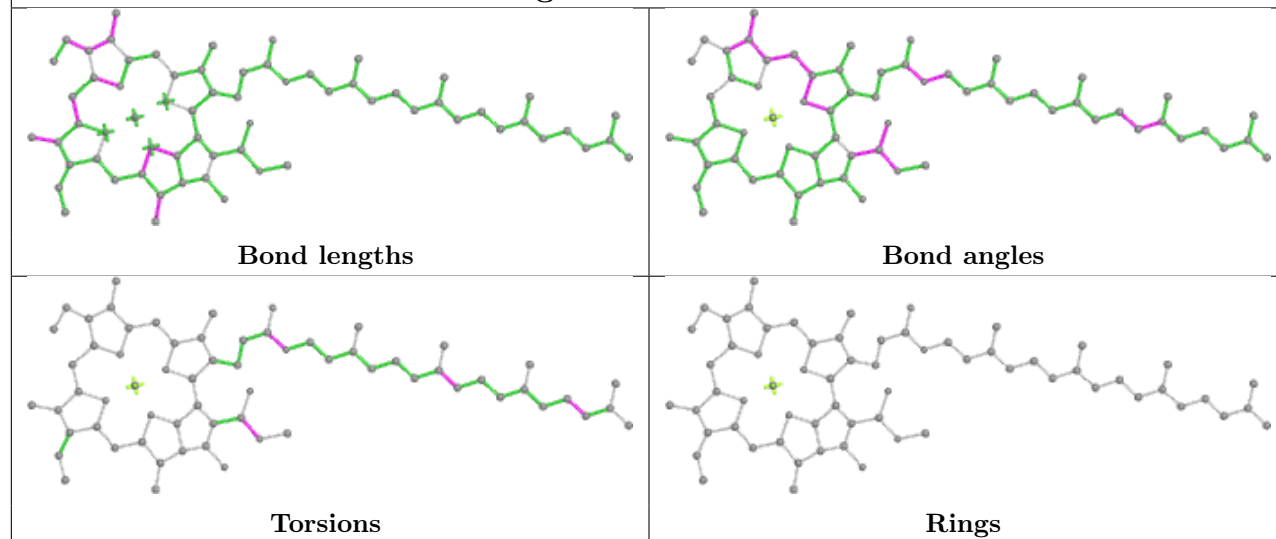


Rings

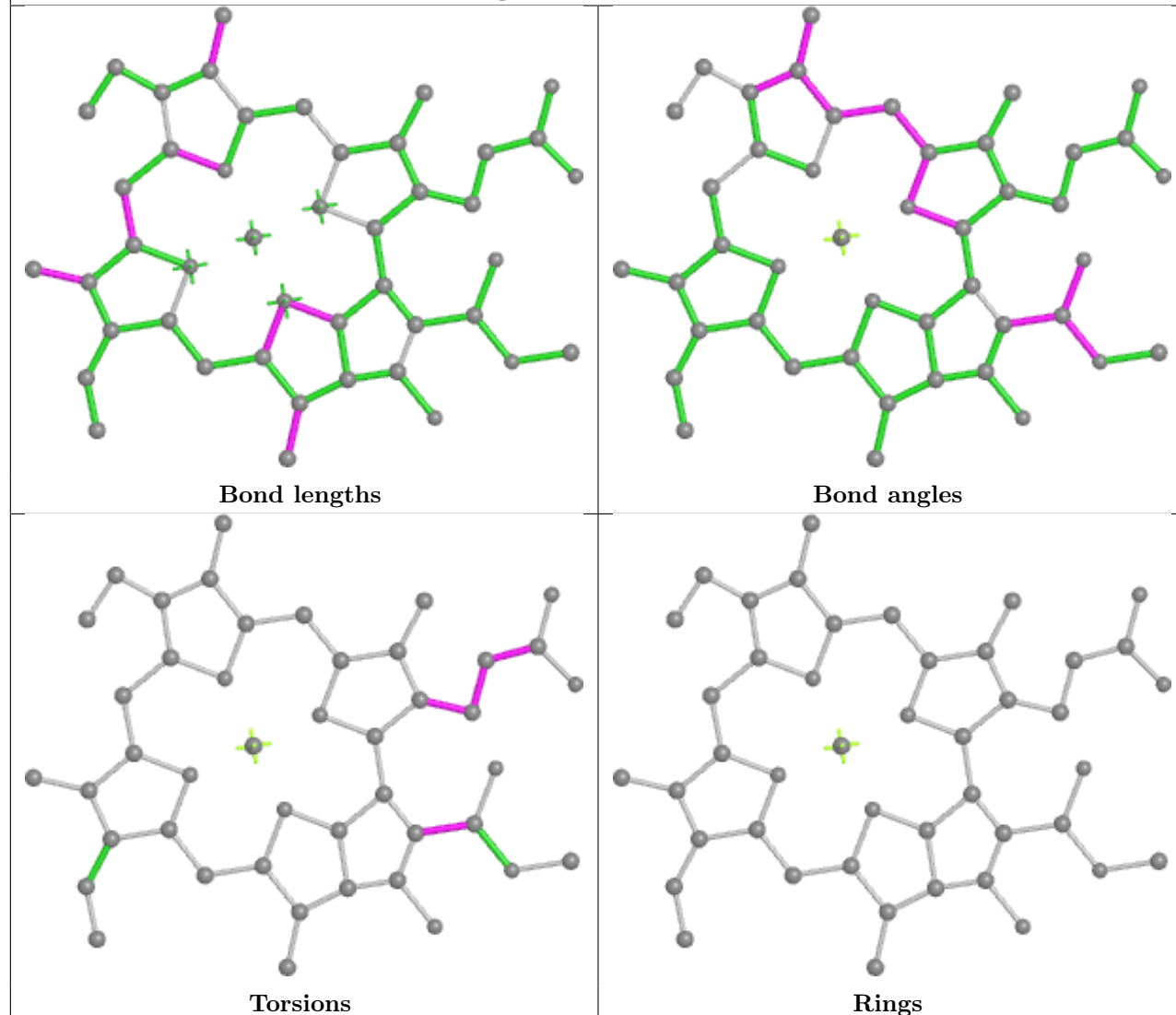




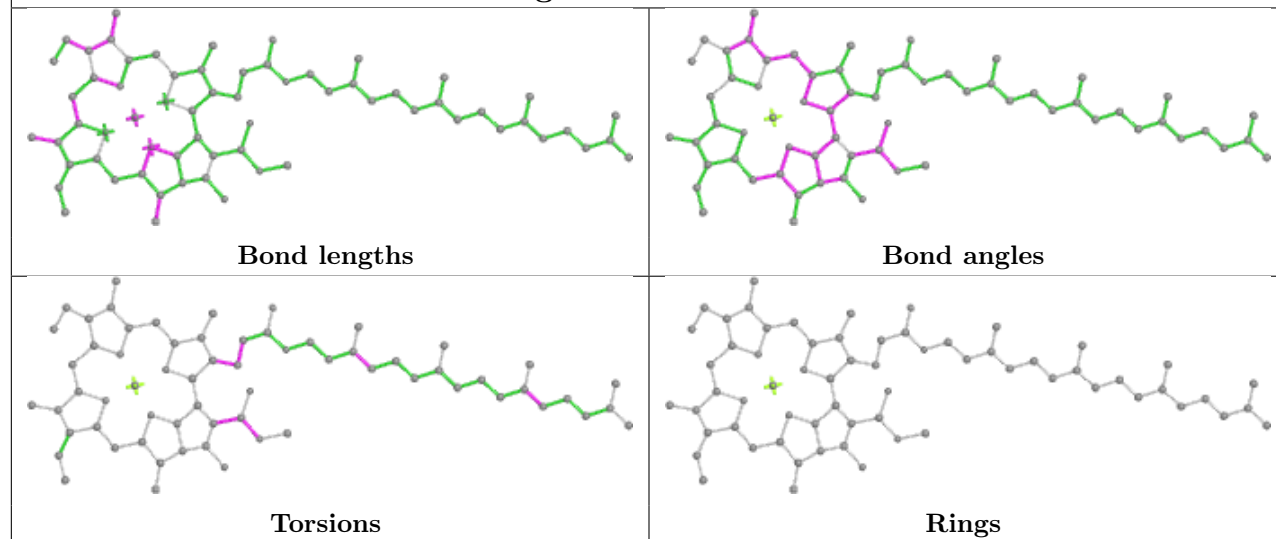
## Ligand CLA a 810



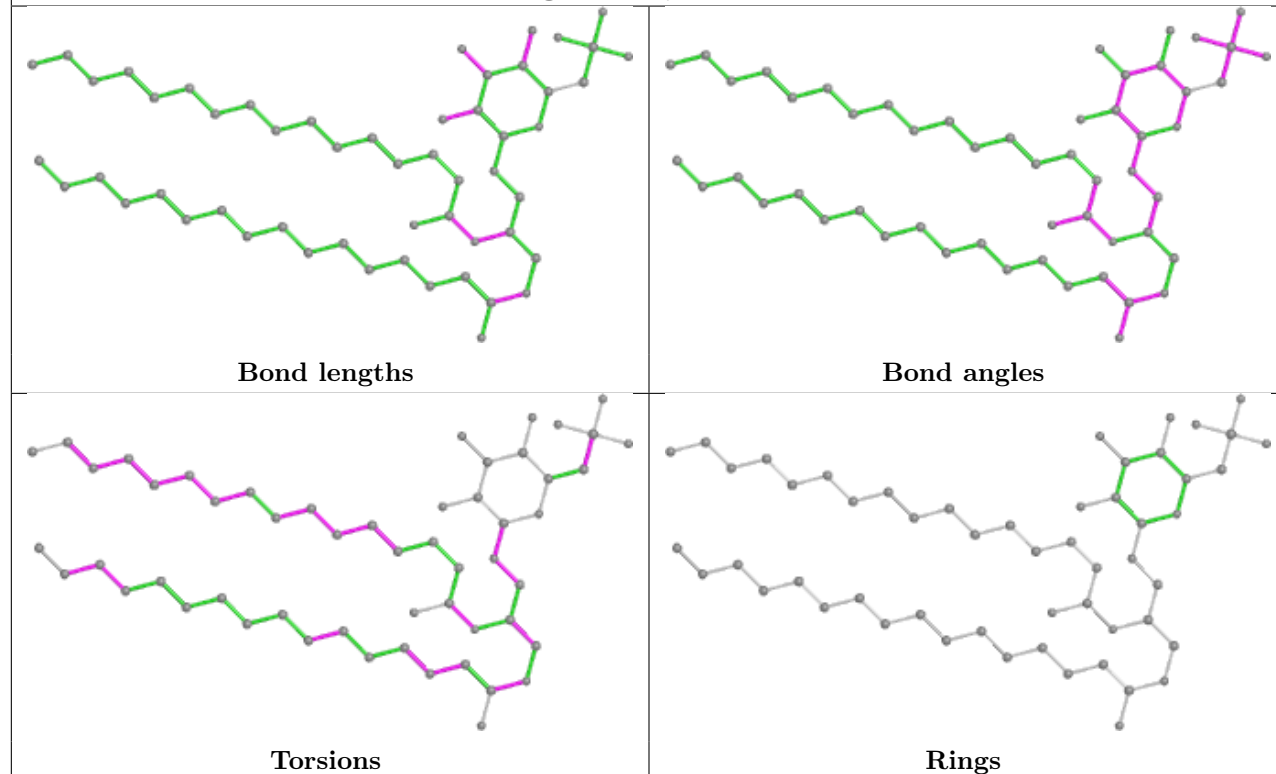
## Ligand CLA a 835

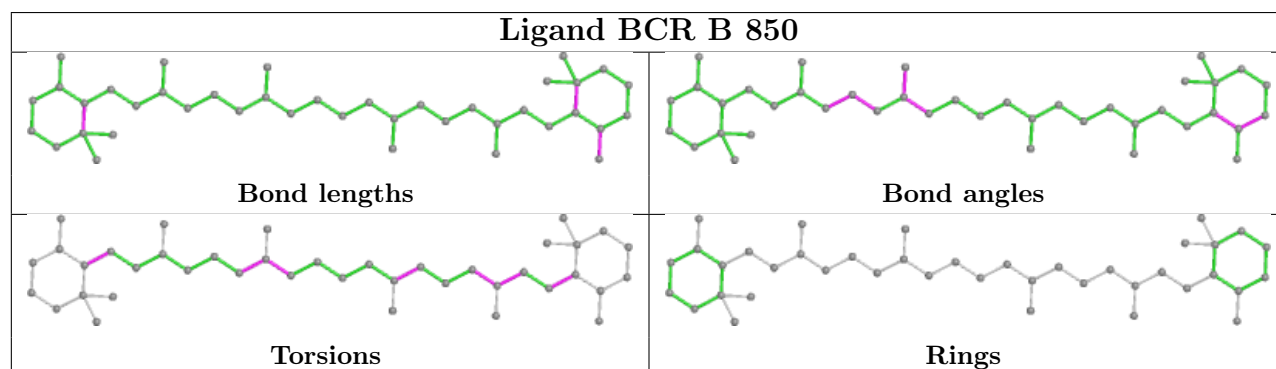
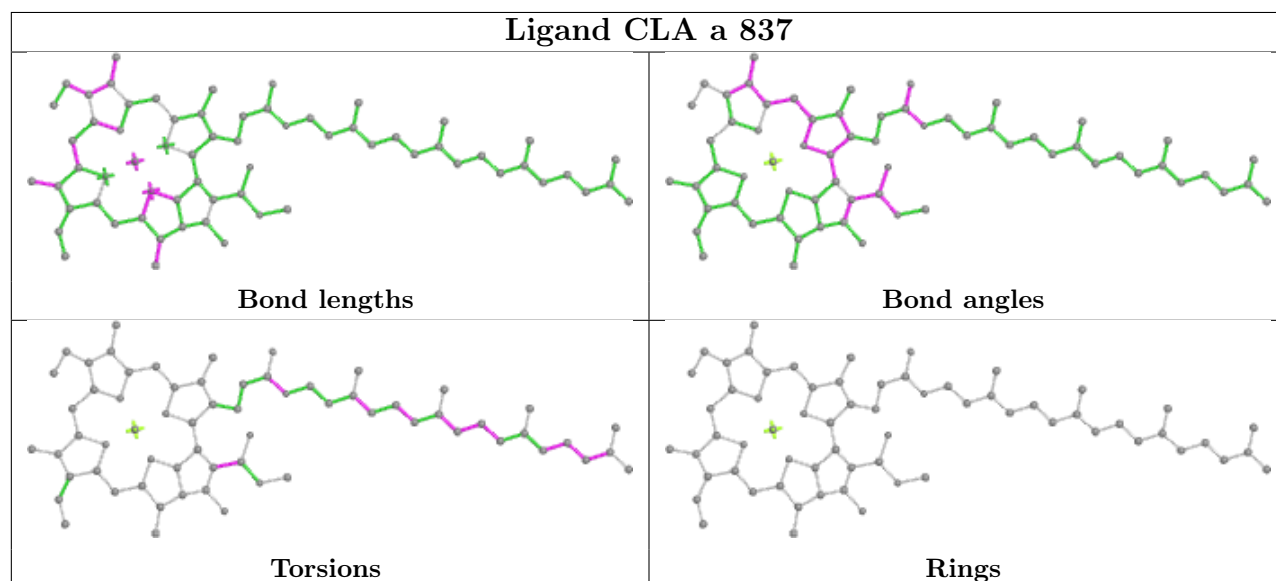
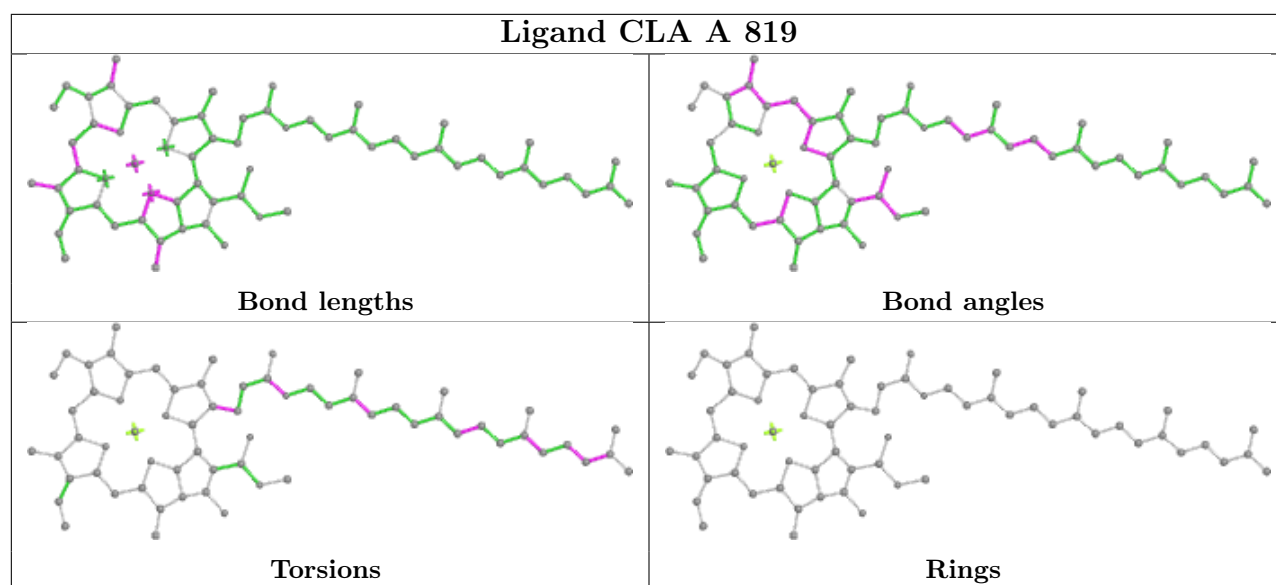


## Ligand CLA b 803

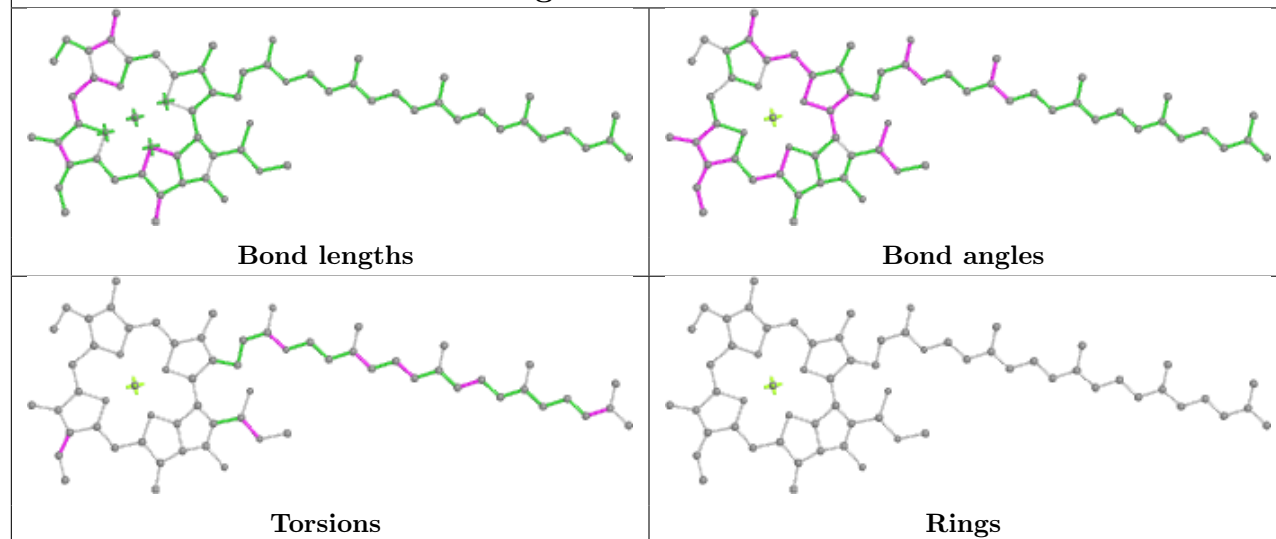


## Ligand SQD 1 202

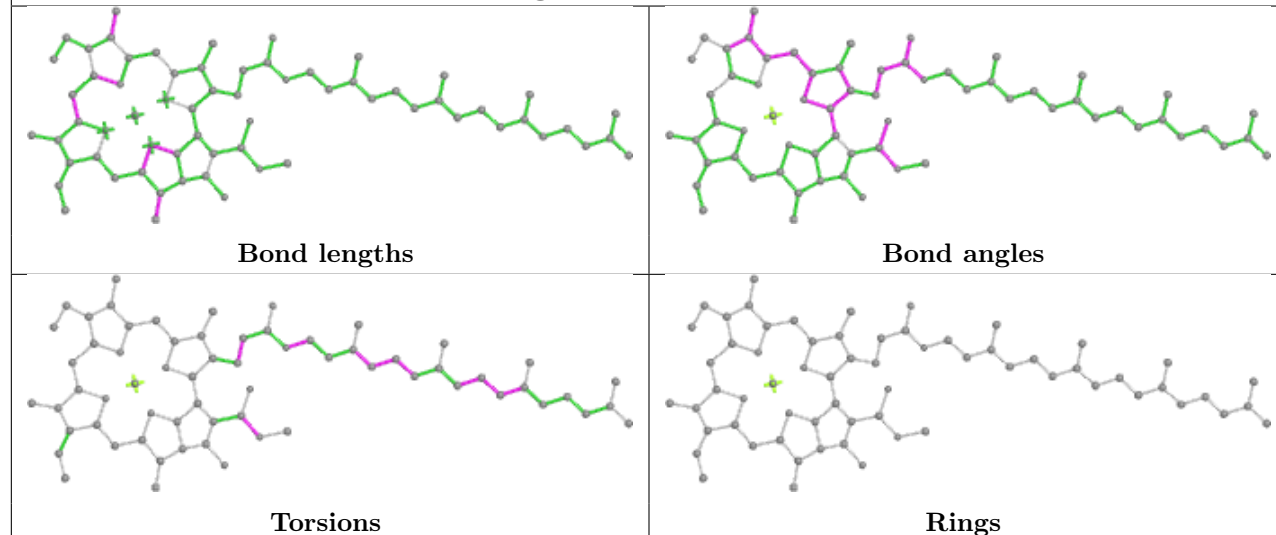




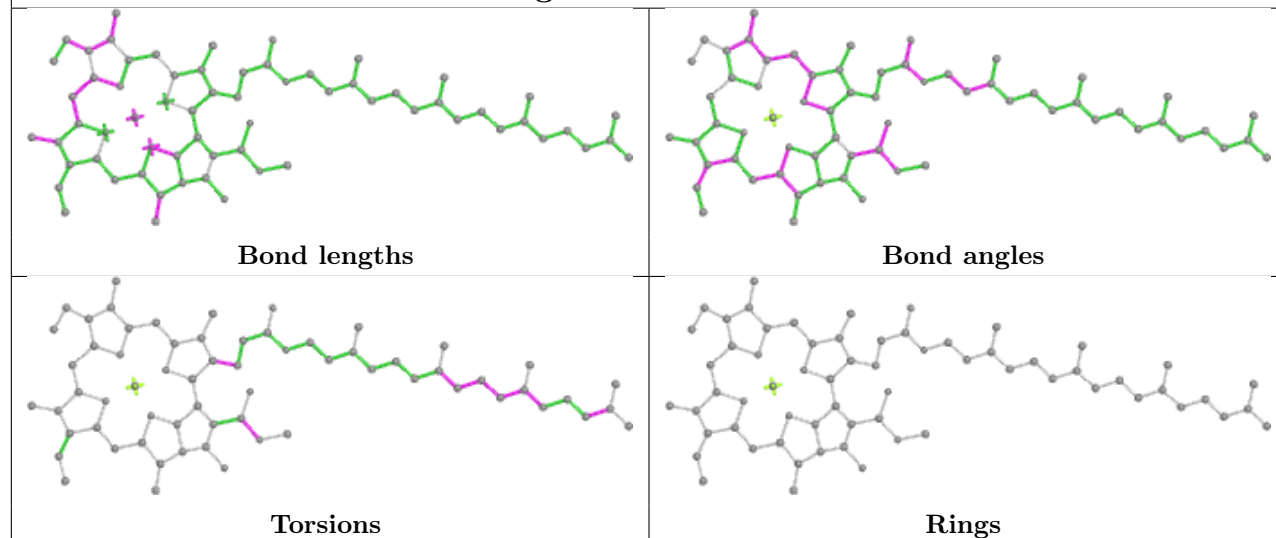
## Ligand CLA b 843

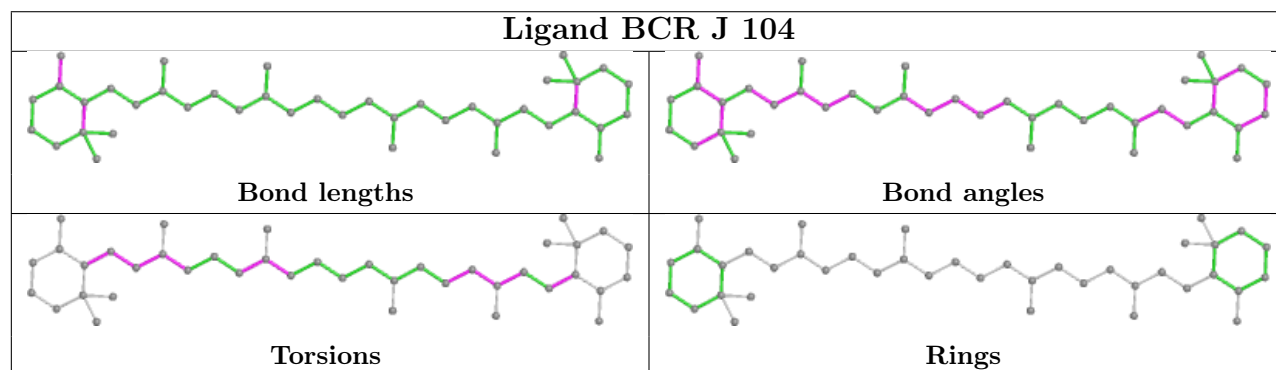
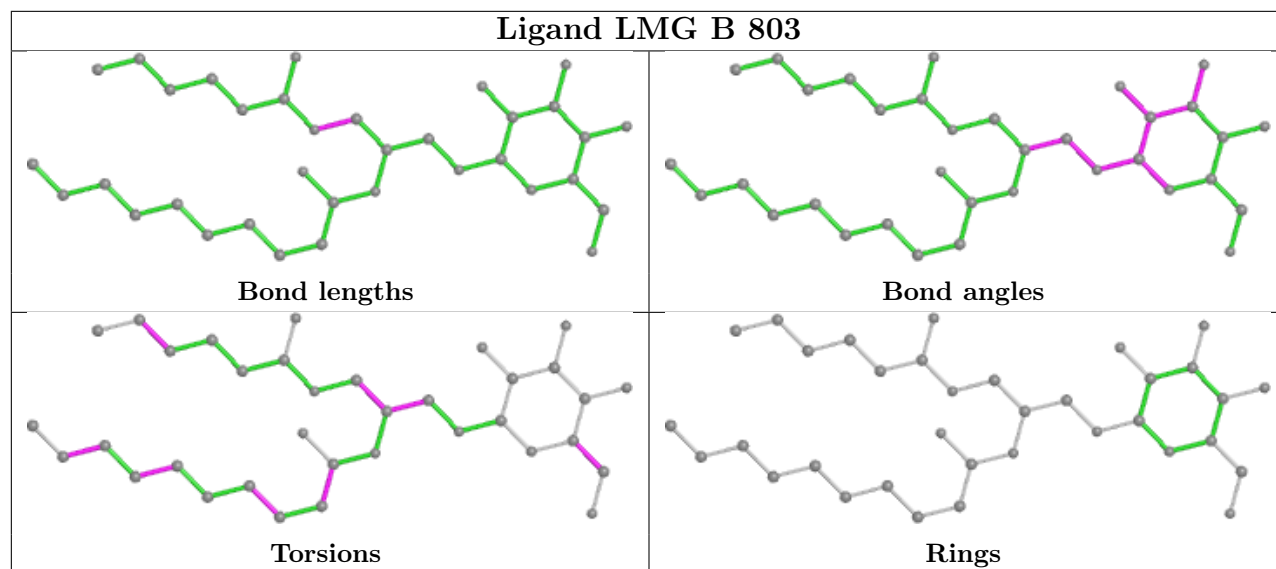
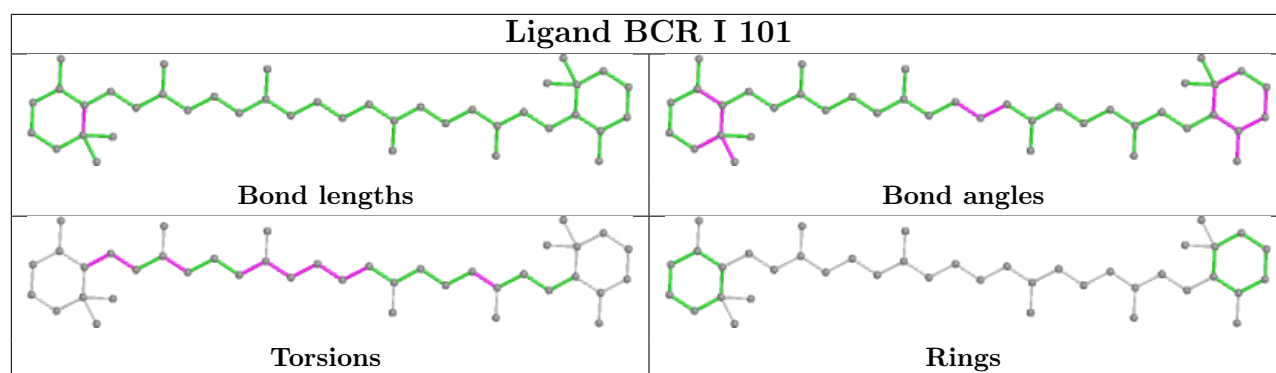


## Ligand CLA A 809

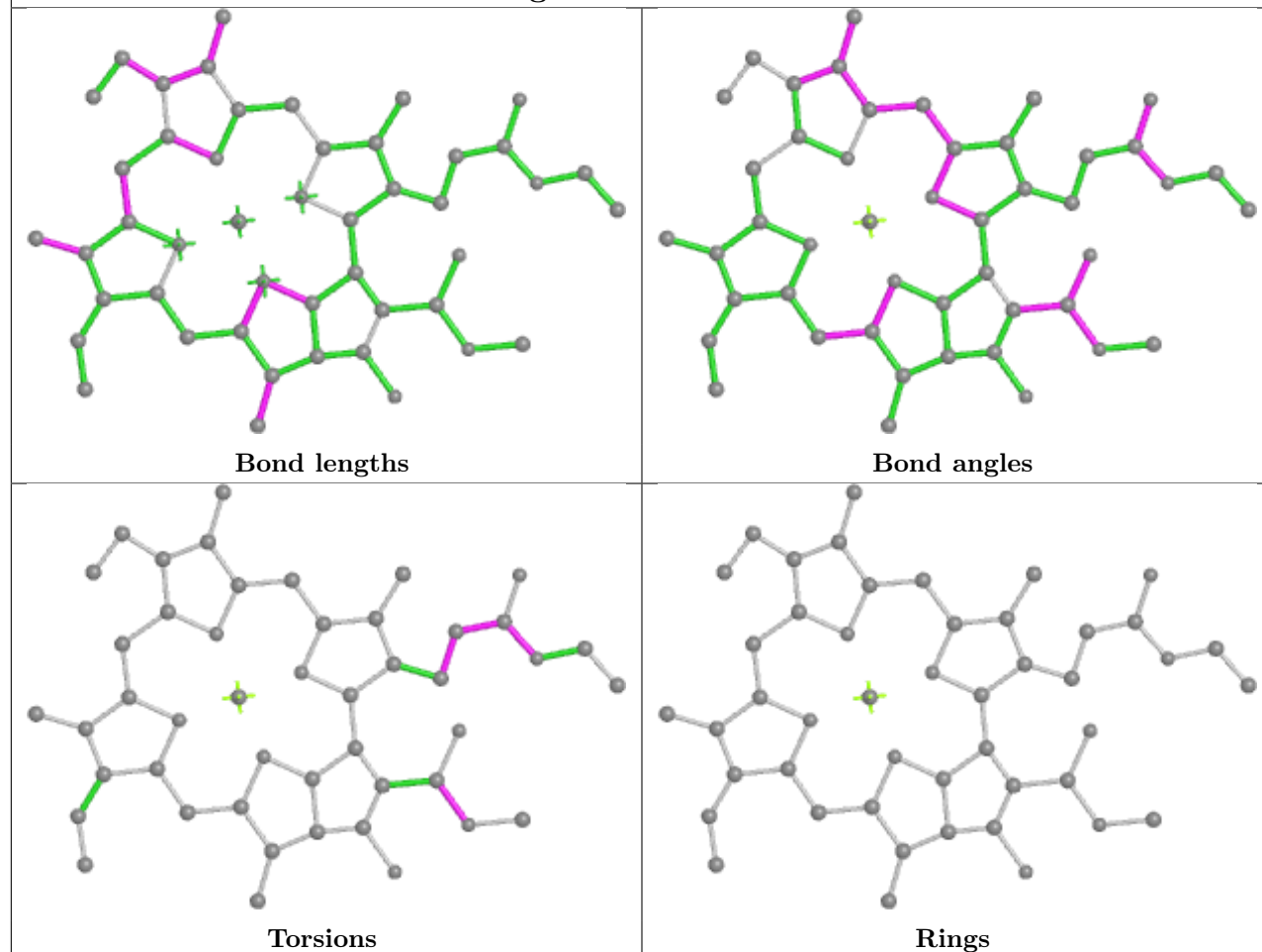


## Ligand CLA b 807

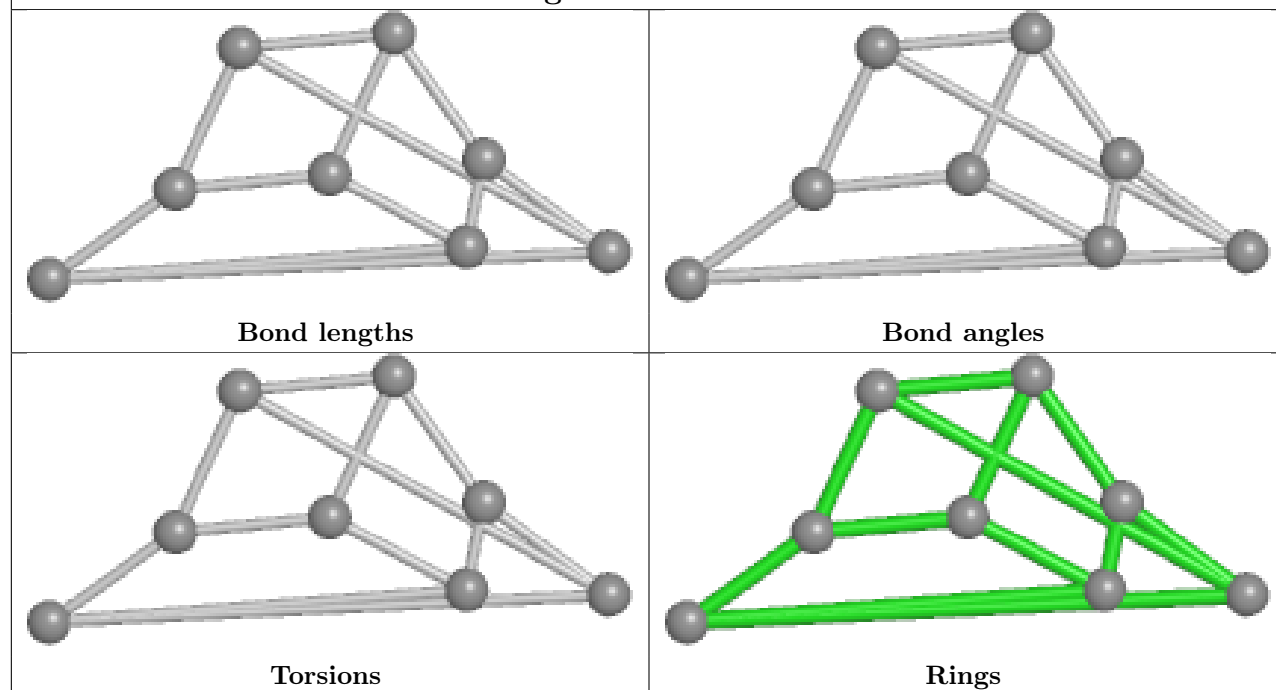


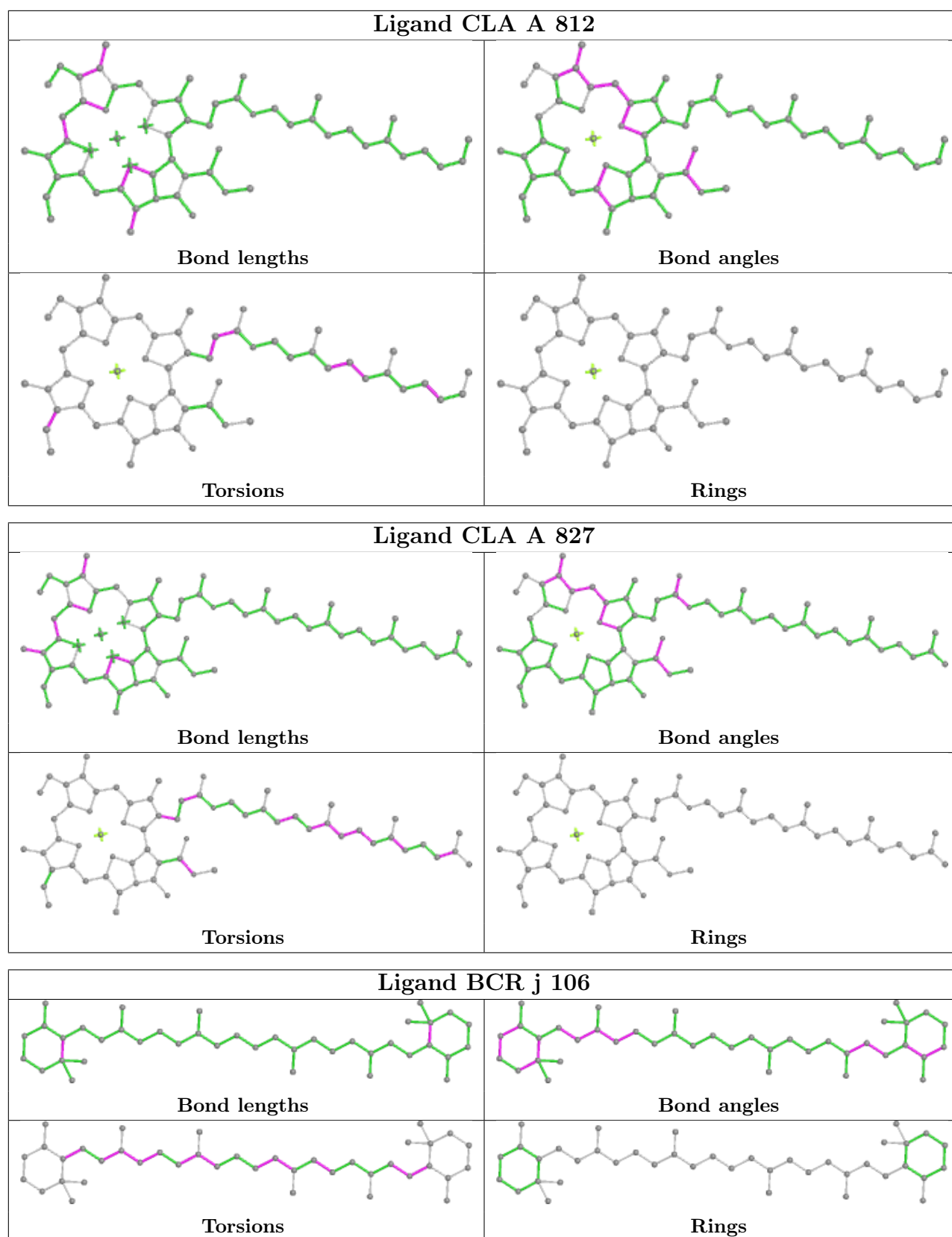


## Ligand CLA b 841

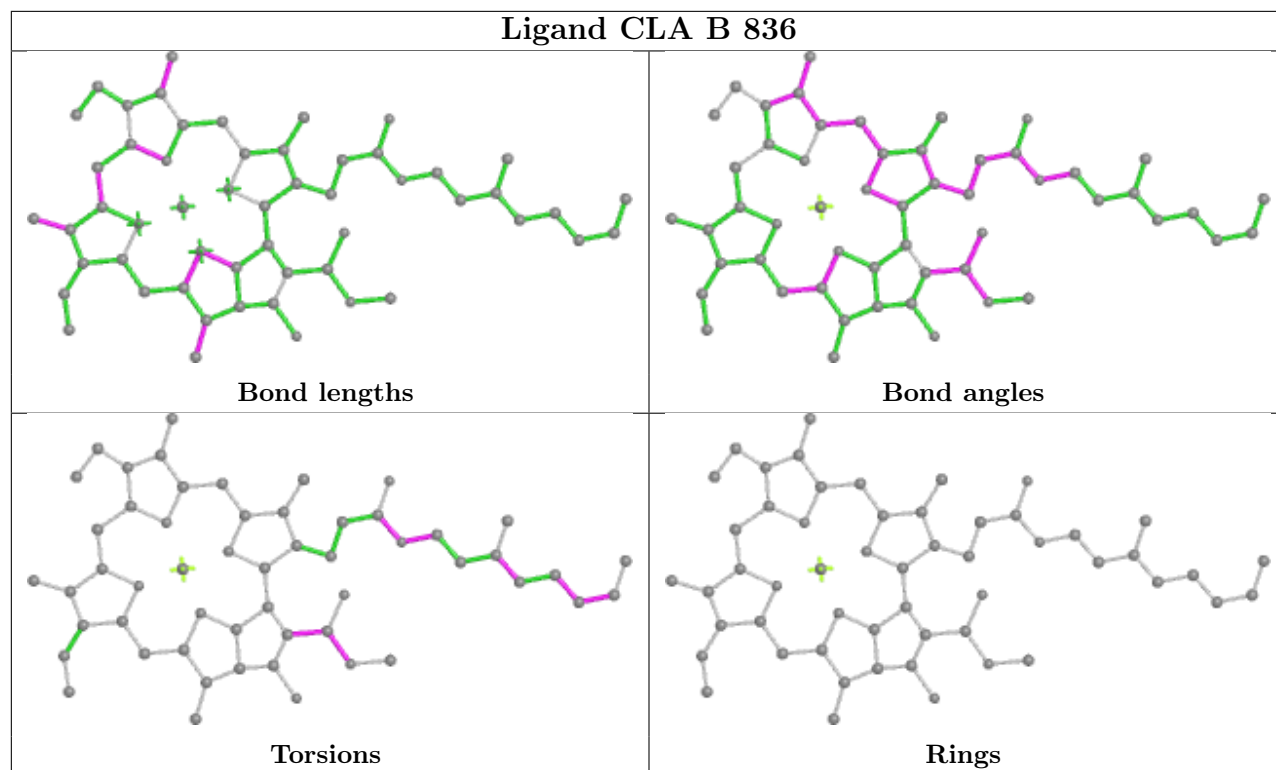


## Ligand SF4 c 101

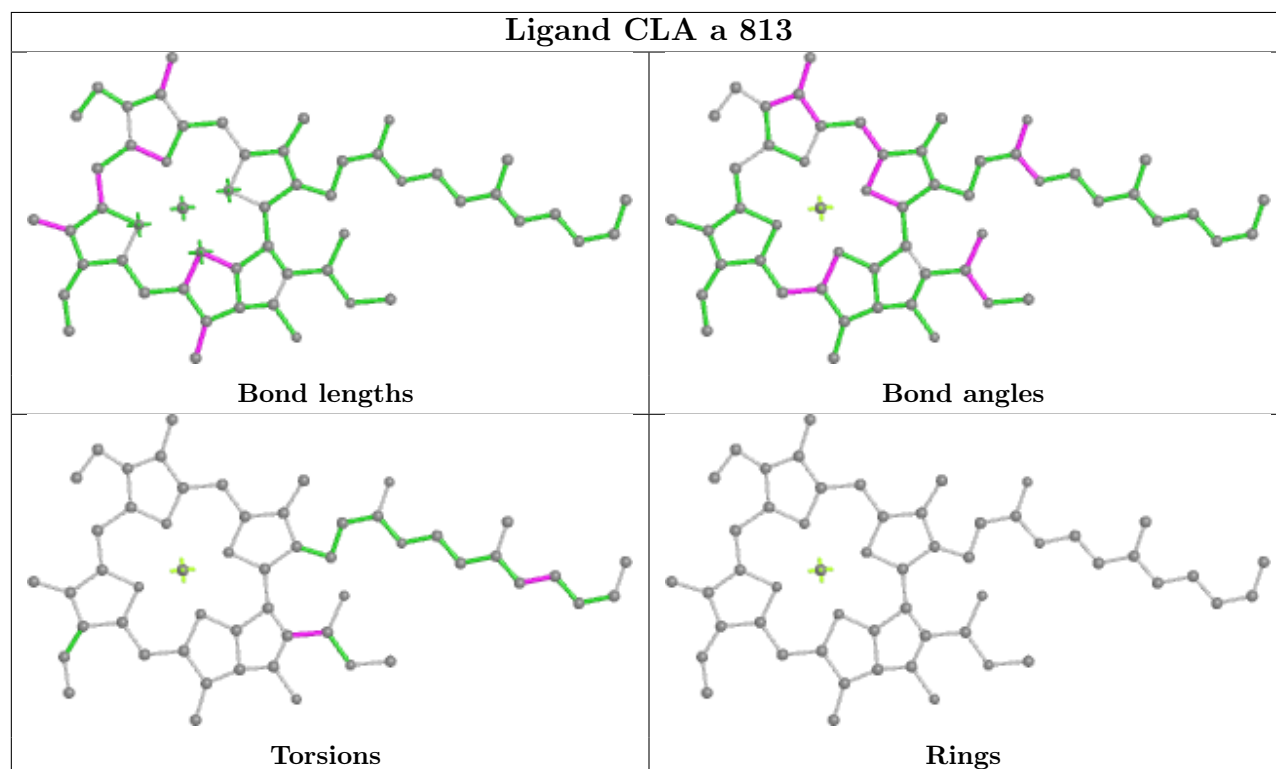




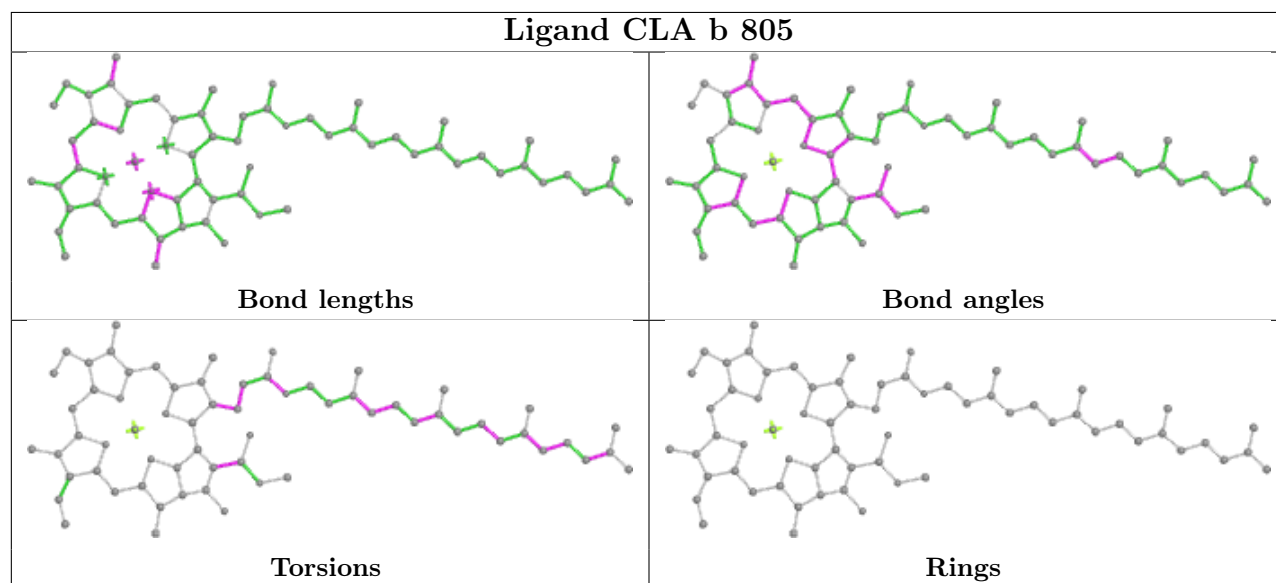
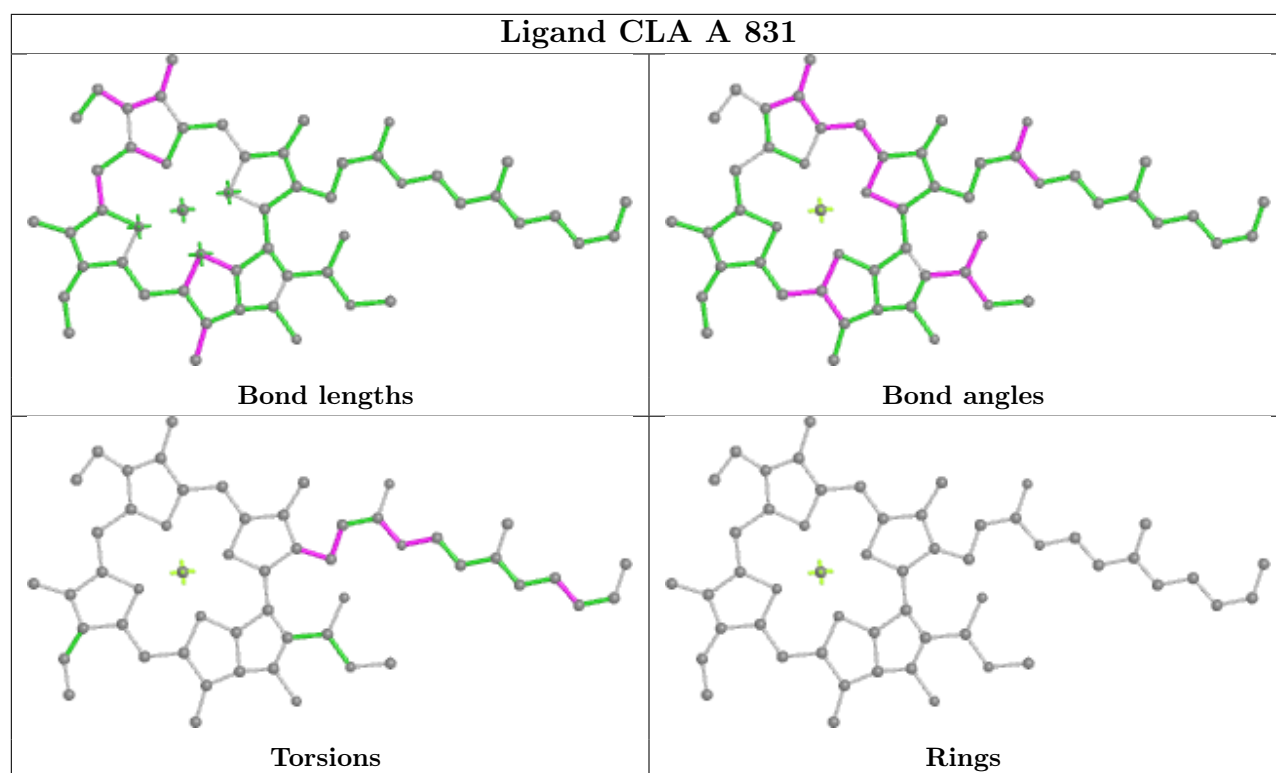
## Ligand CLA B 836



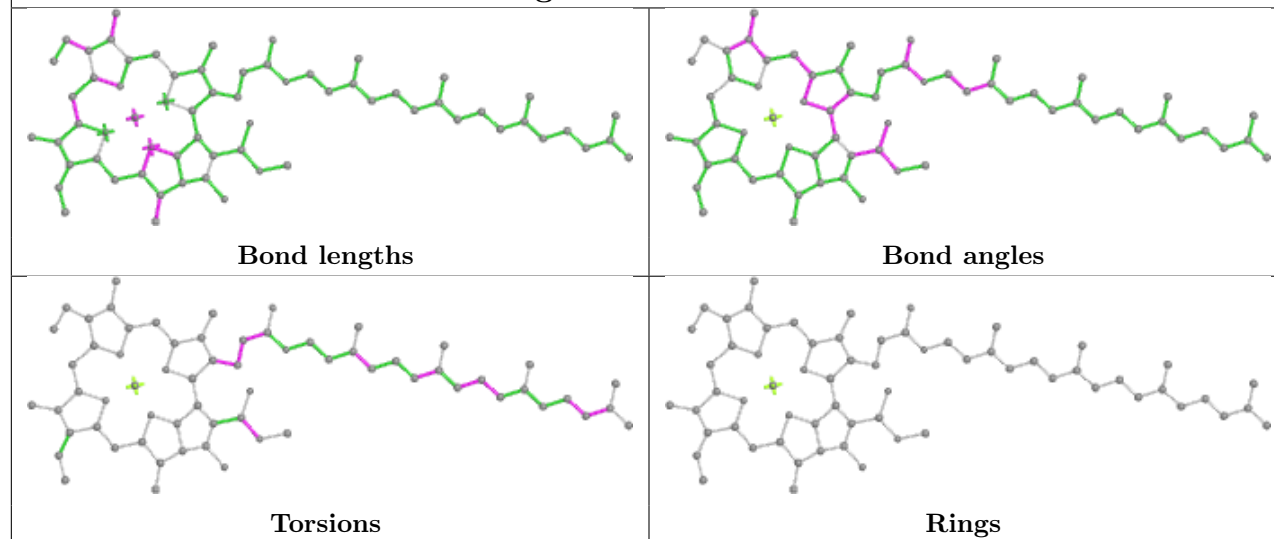
## Ligand CLA a 813



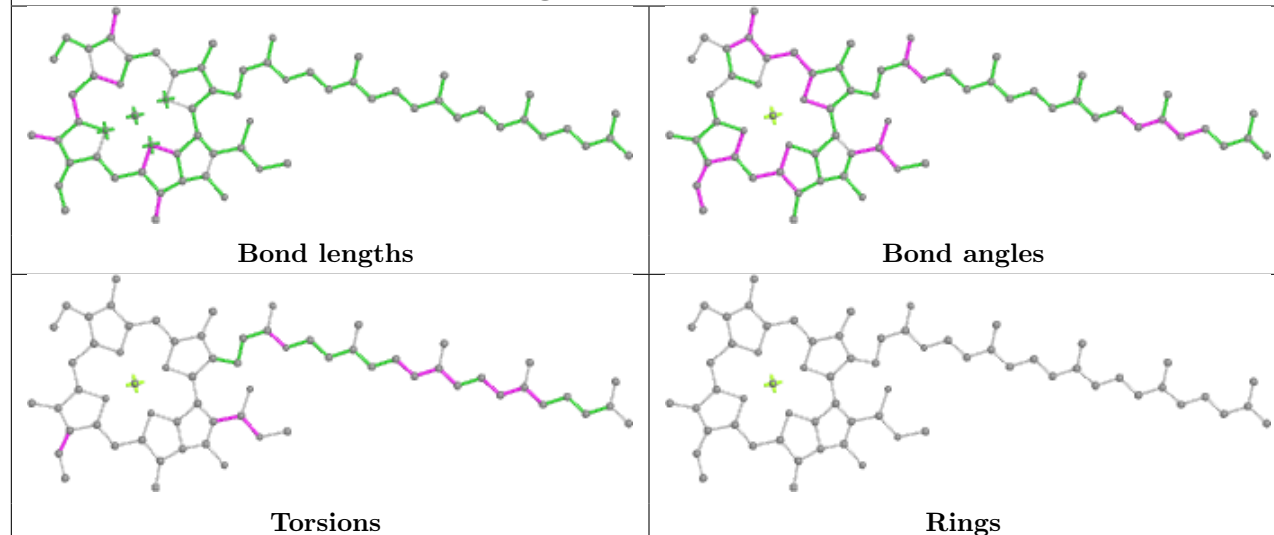




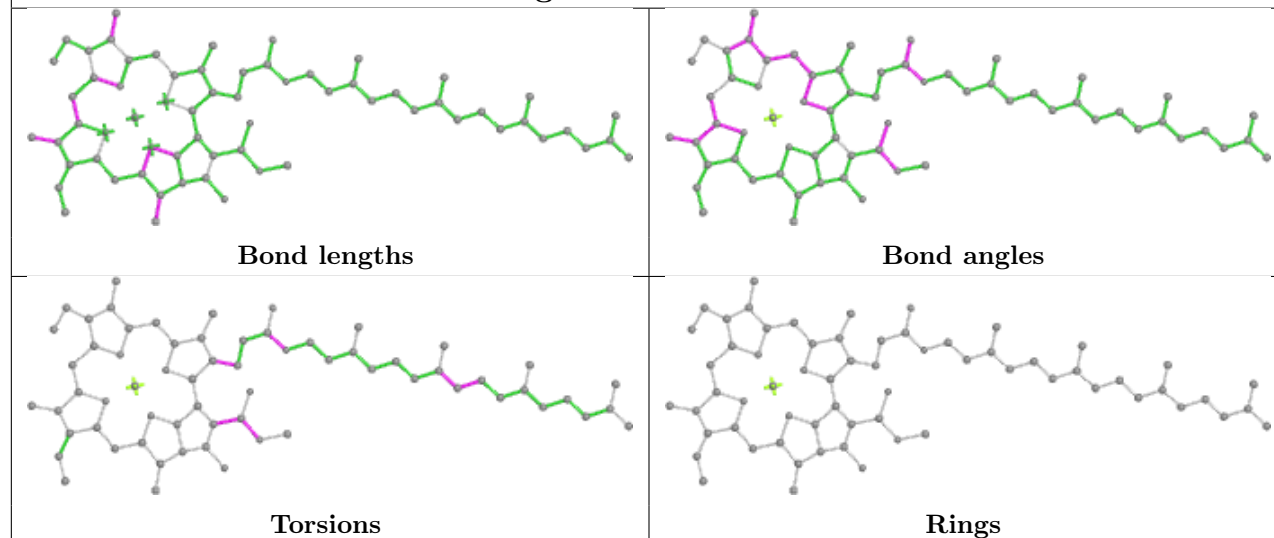
## Ligand CLA b 830

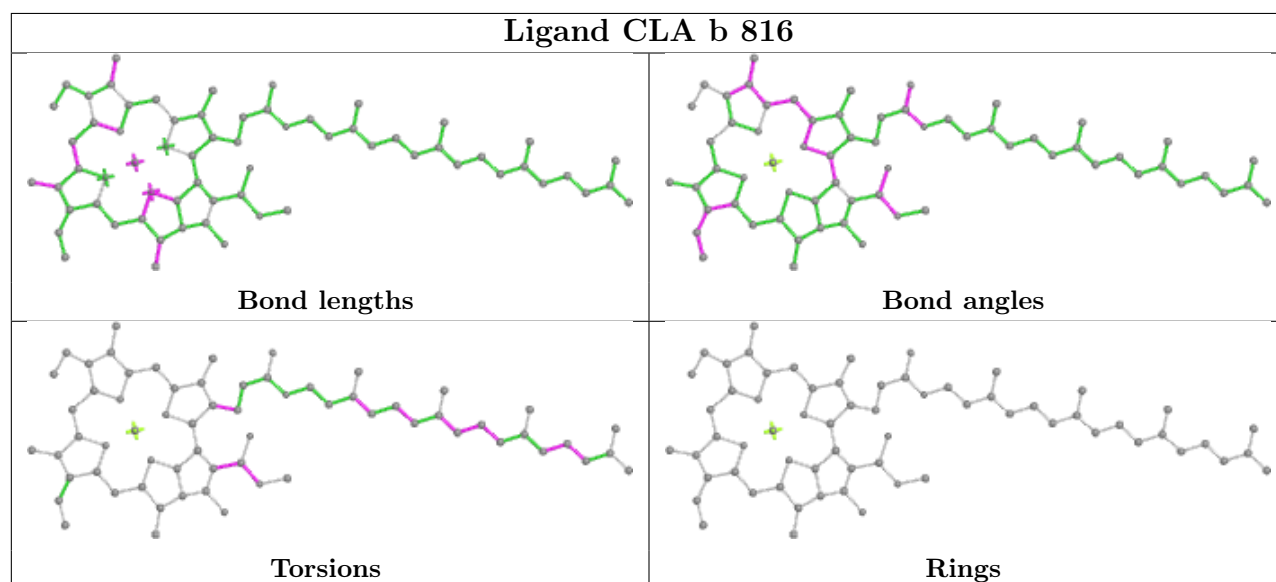
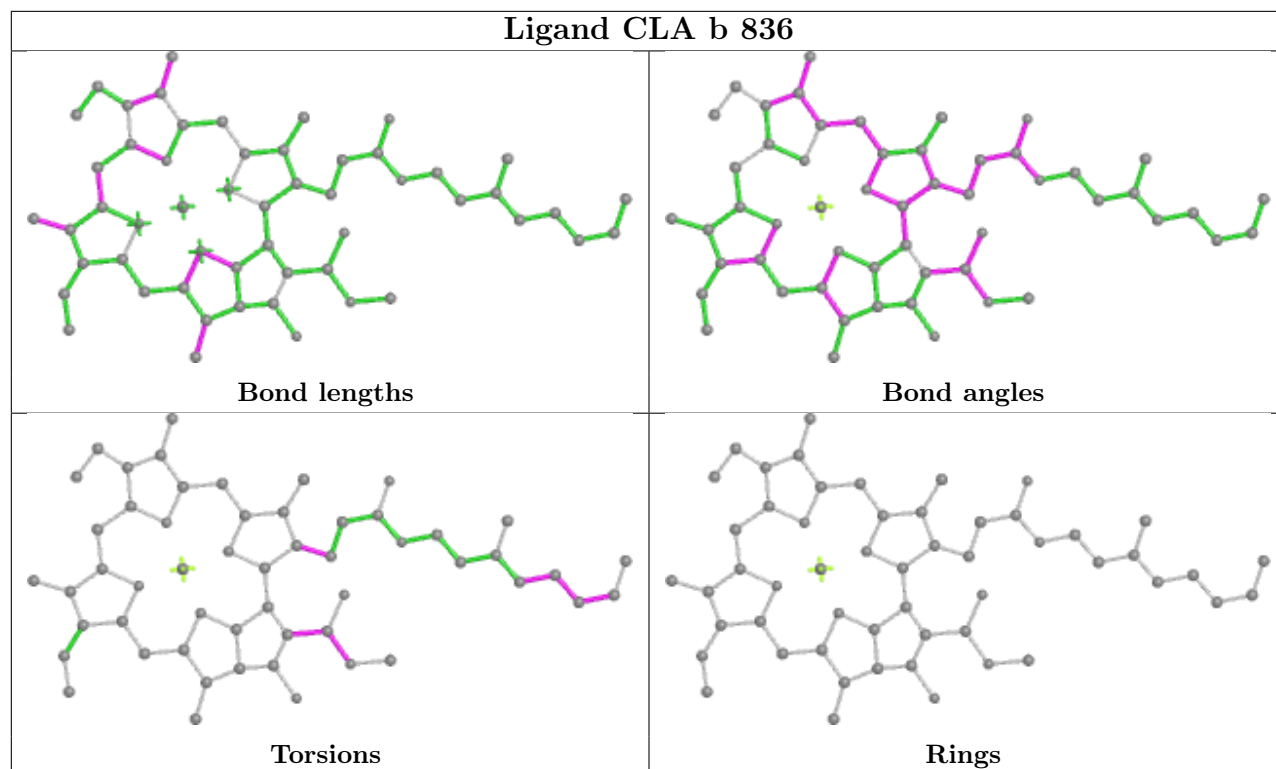
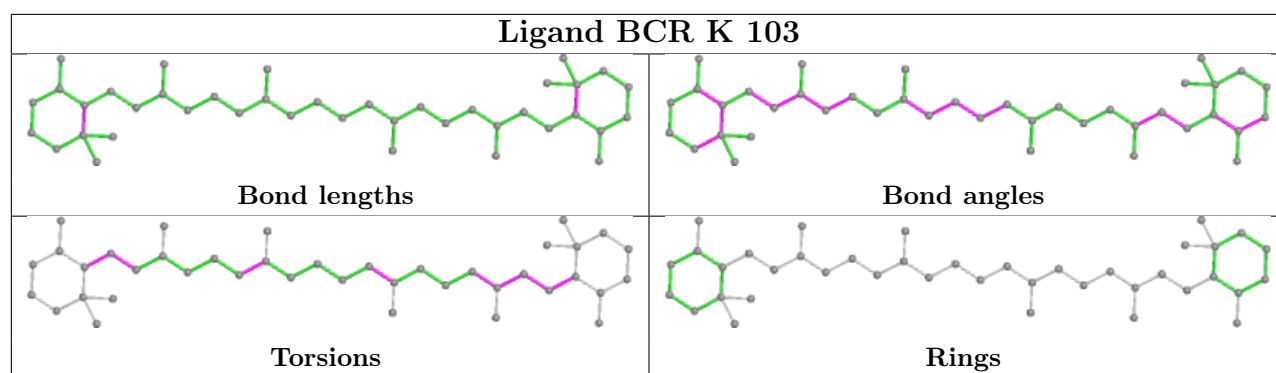


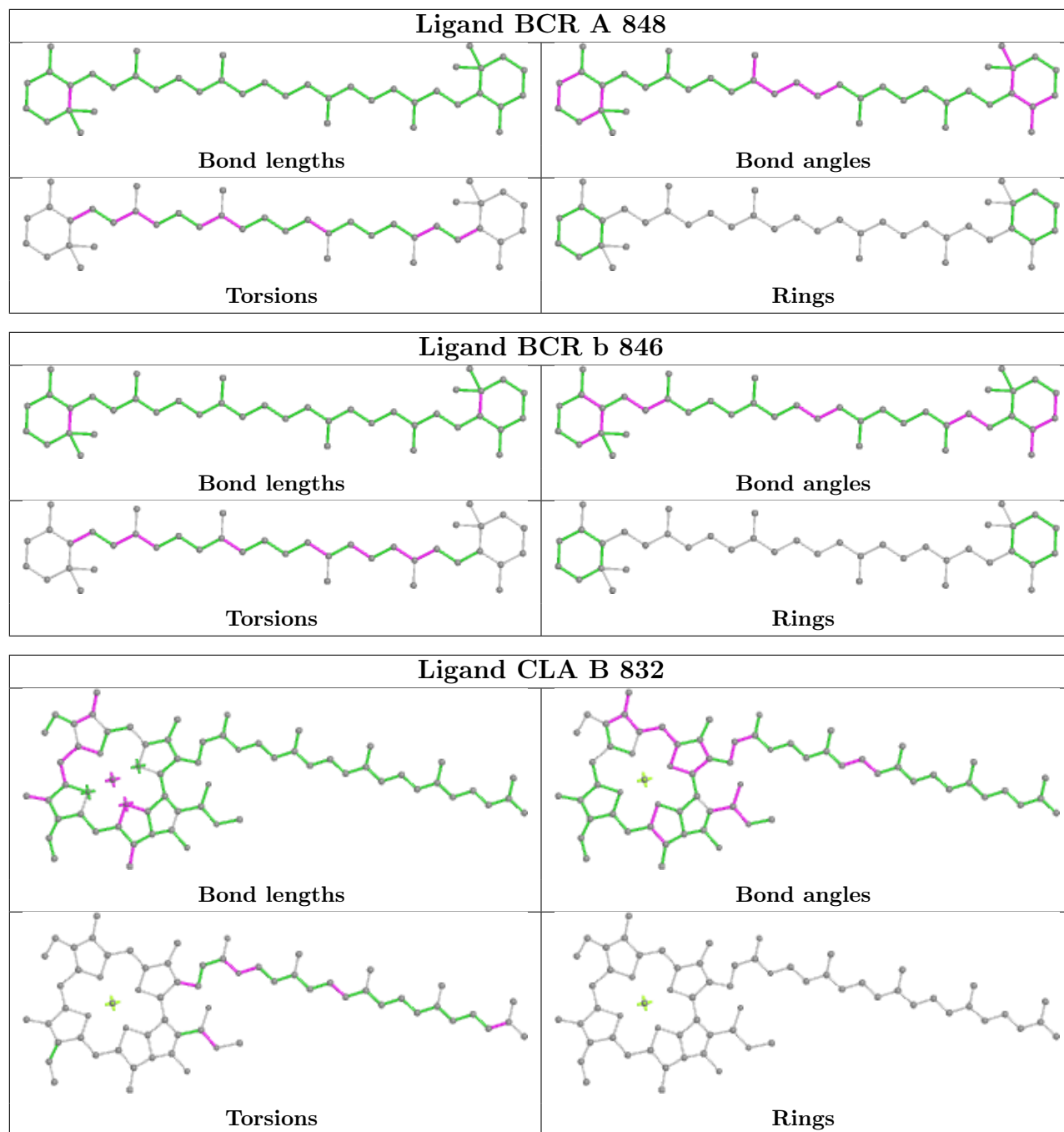
## Ligand CLA a 833



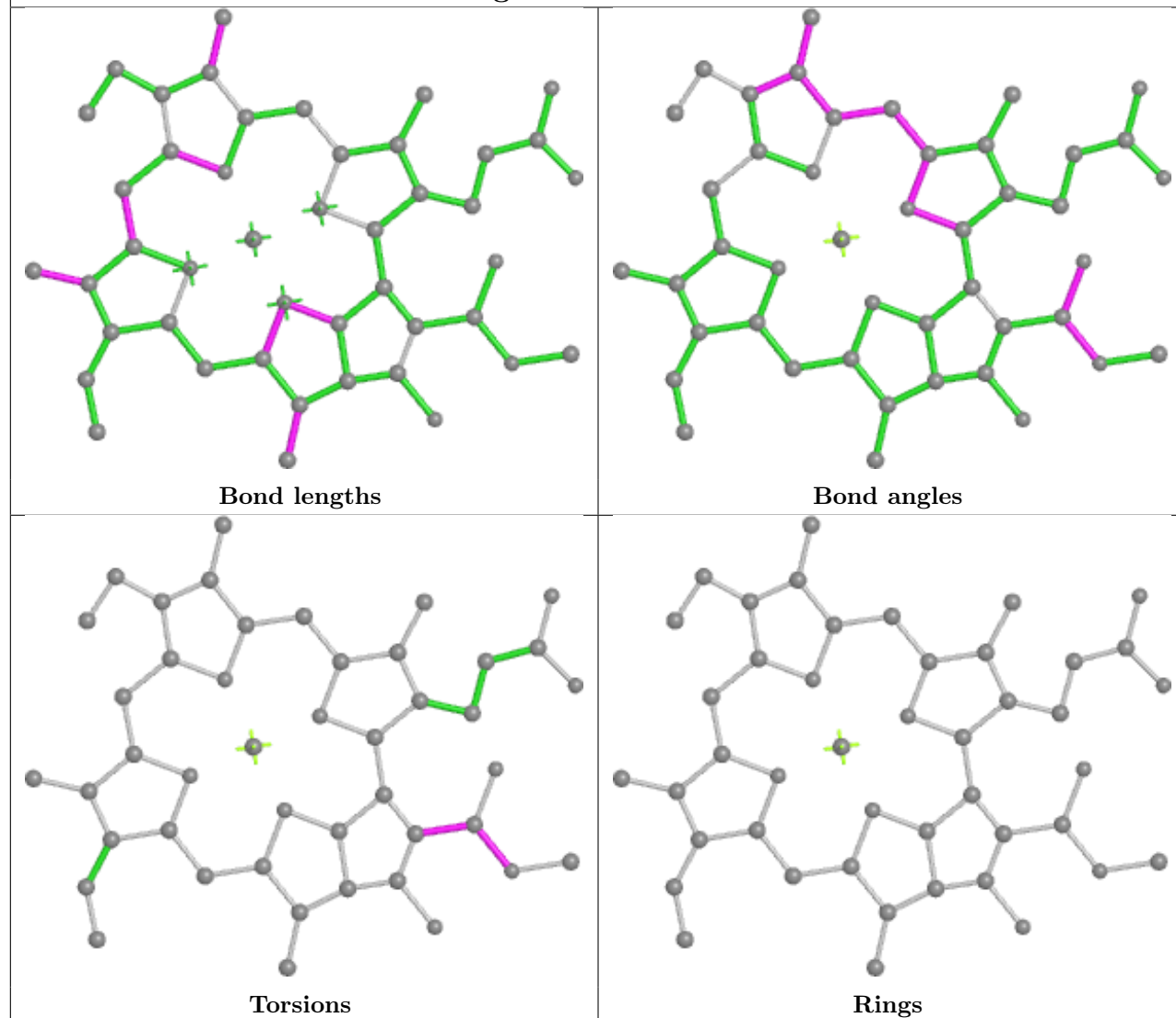
## Ligand CLA b 822



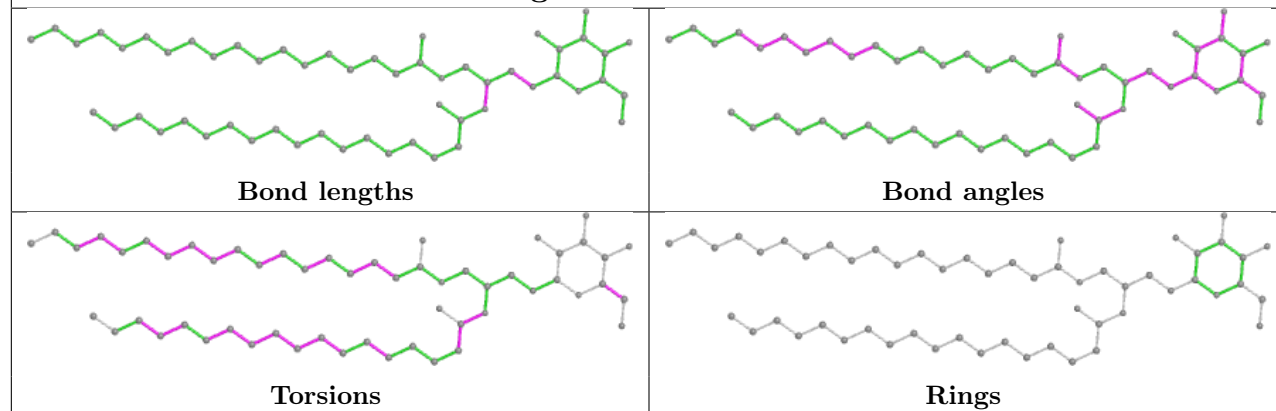


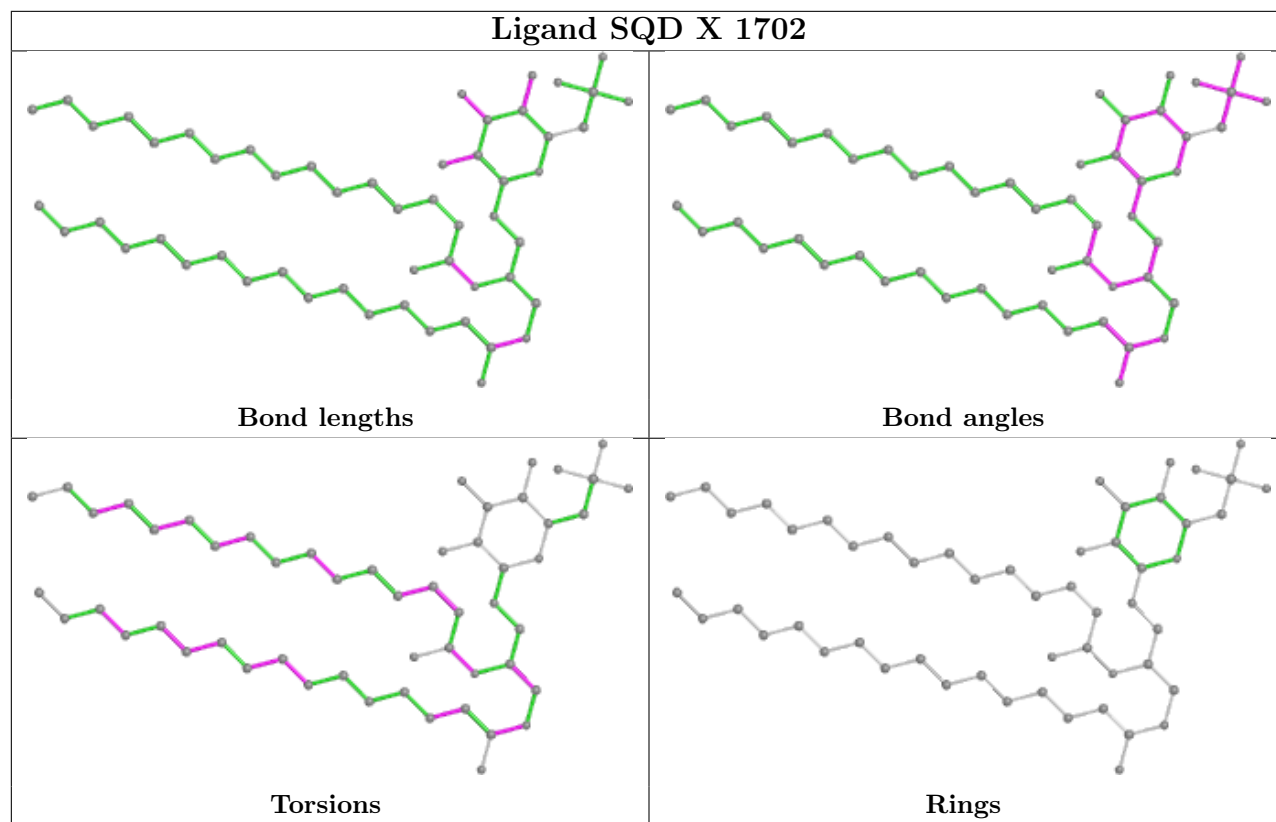
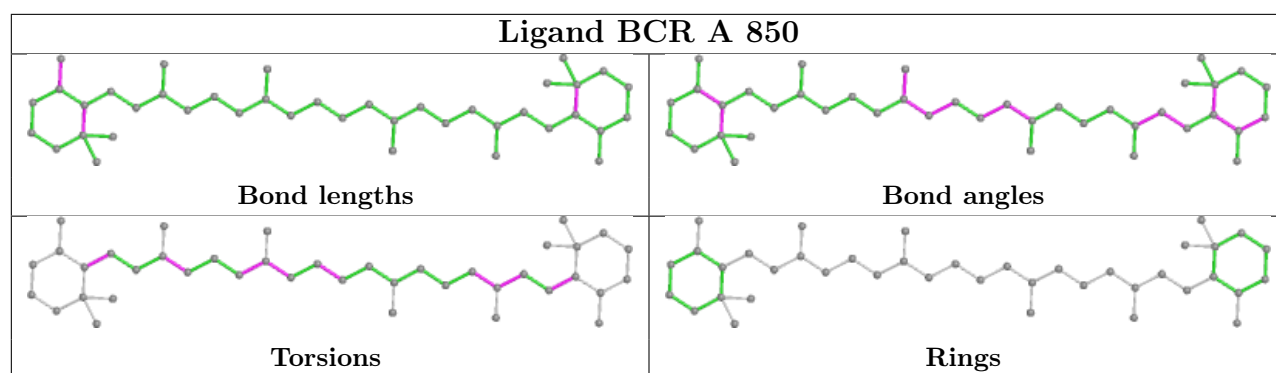


## Ligand CLA b 838

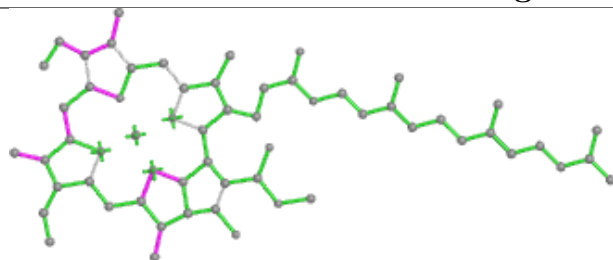


## Ligand LMG b 851

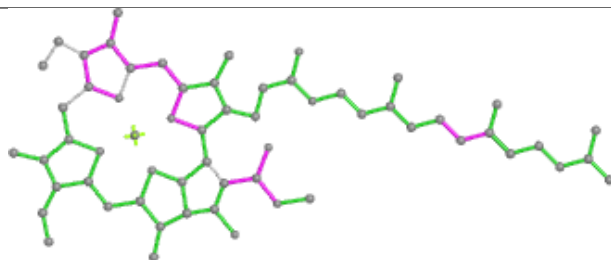




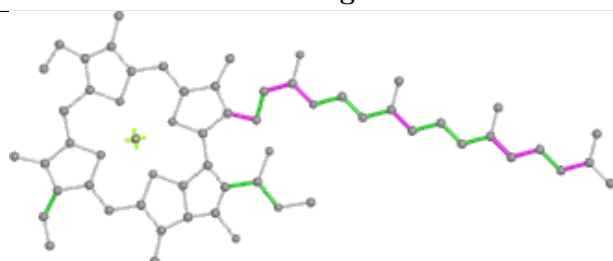
## Ligand CLA B 813



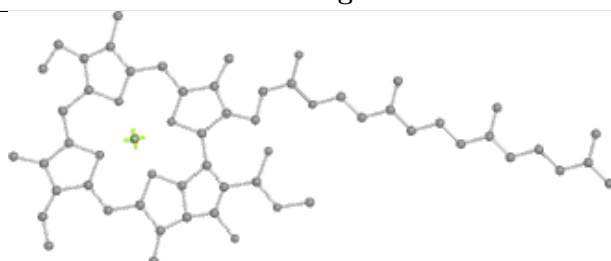
Bond lengths



Bond angles

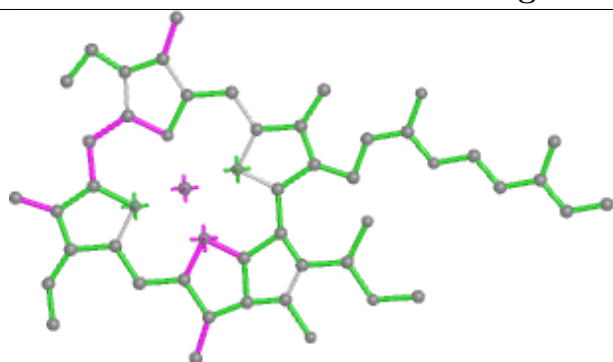


Torsions

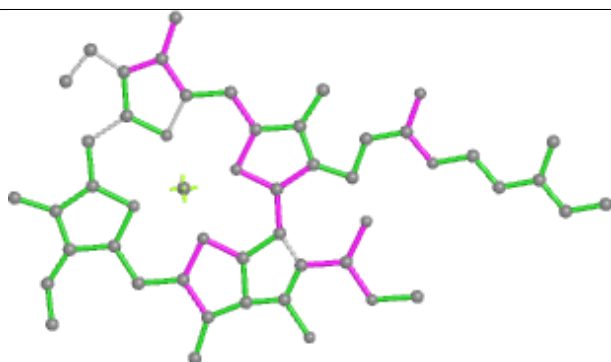


Rings

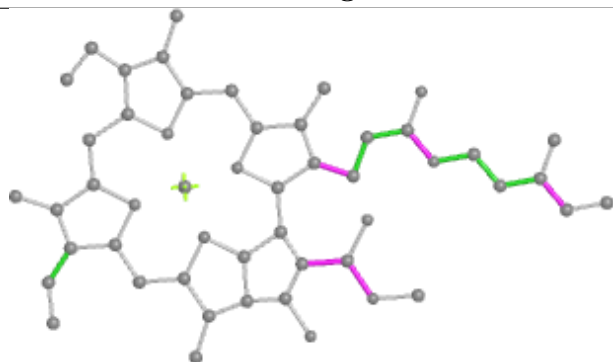
## Ligand CLA a 836



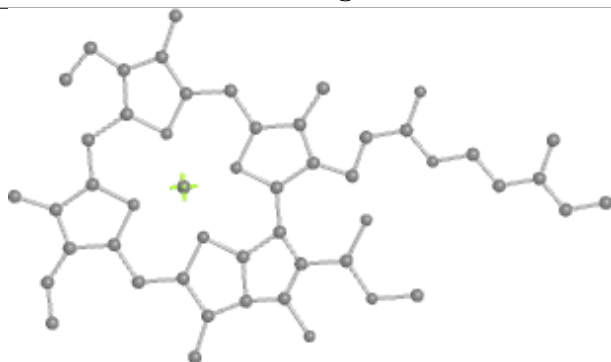
Bond lengths



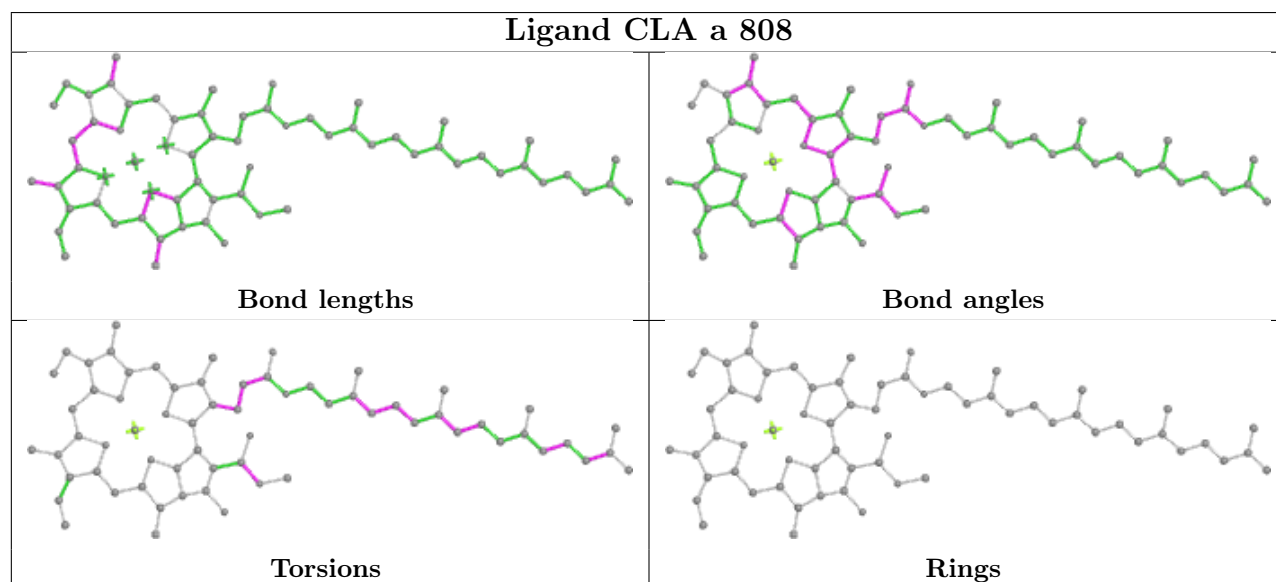
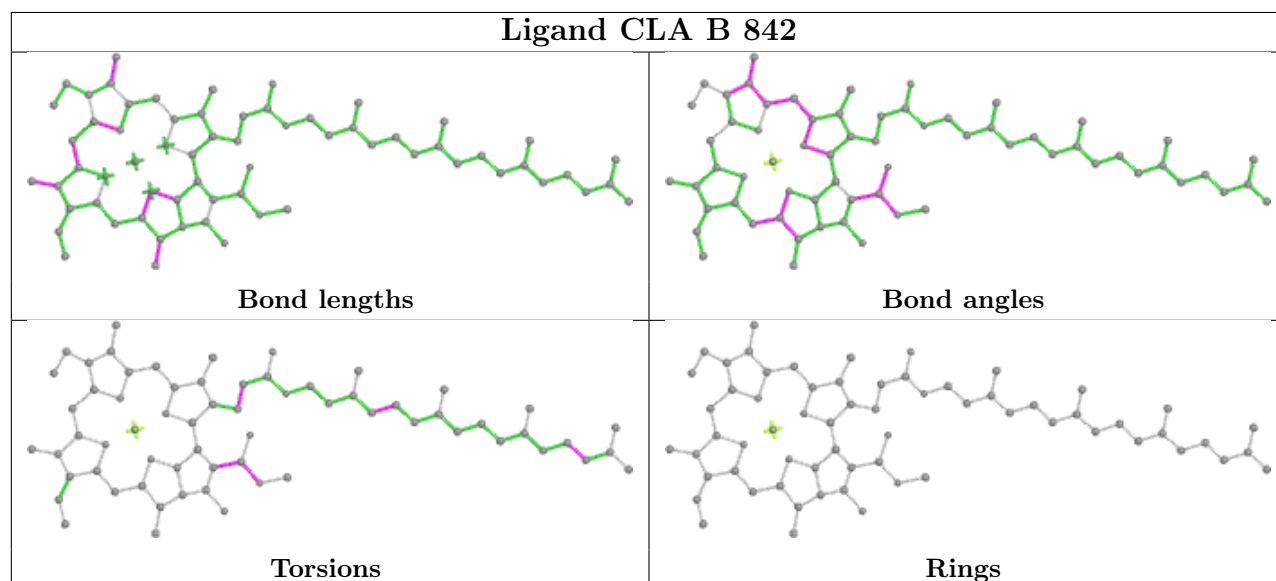
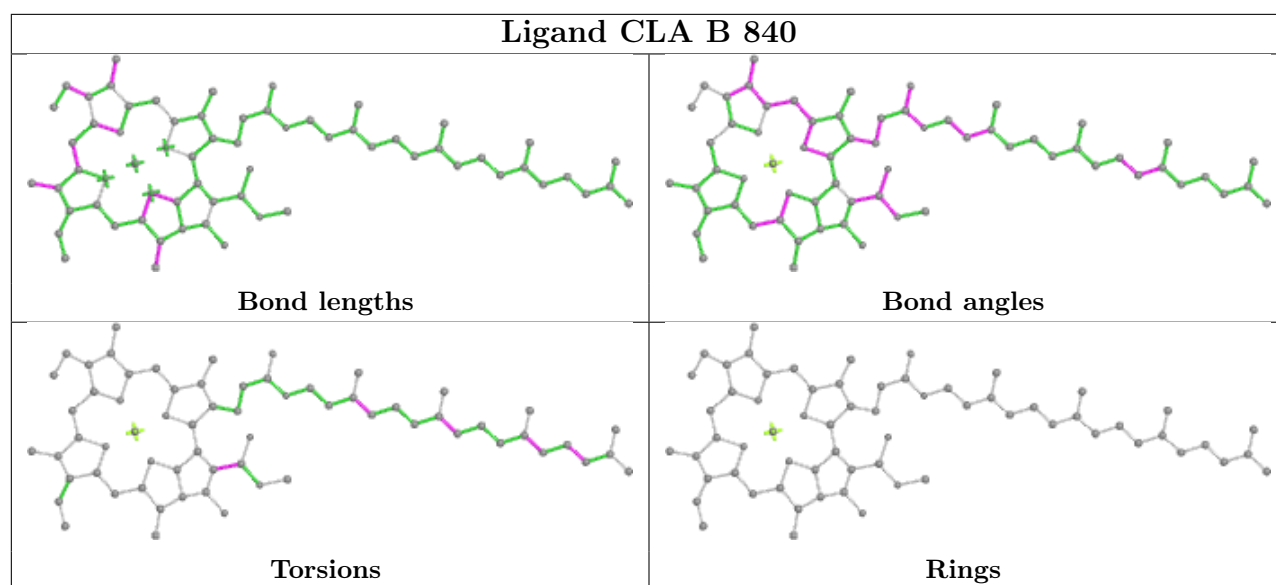
Bond angles



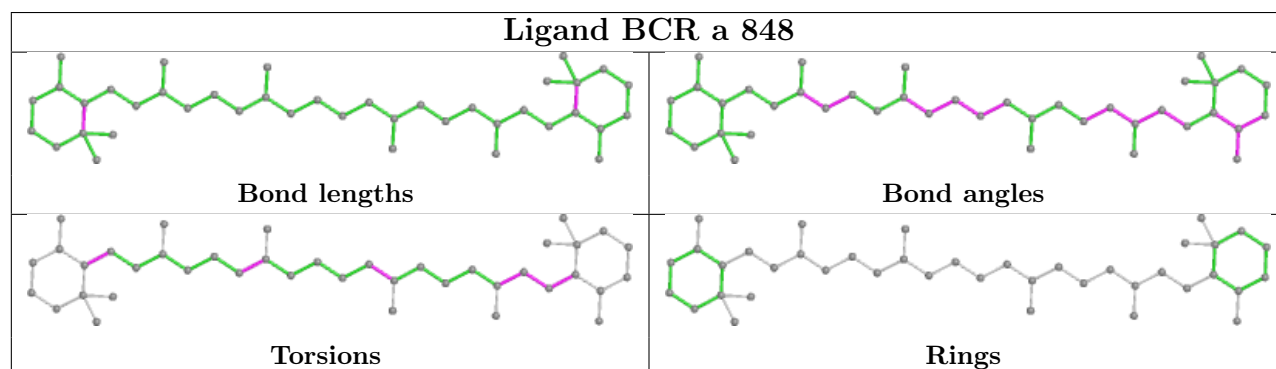
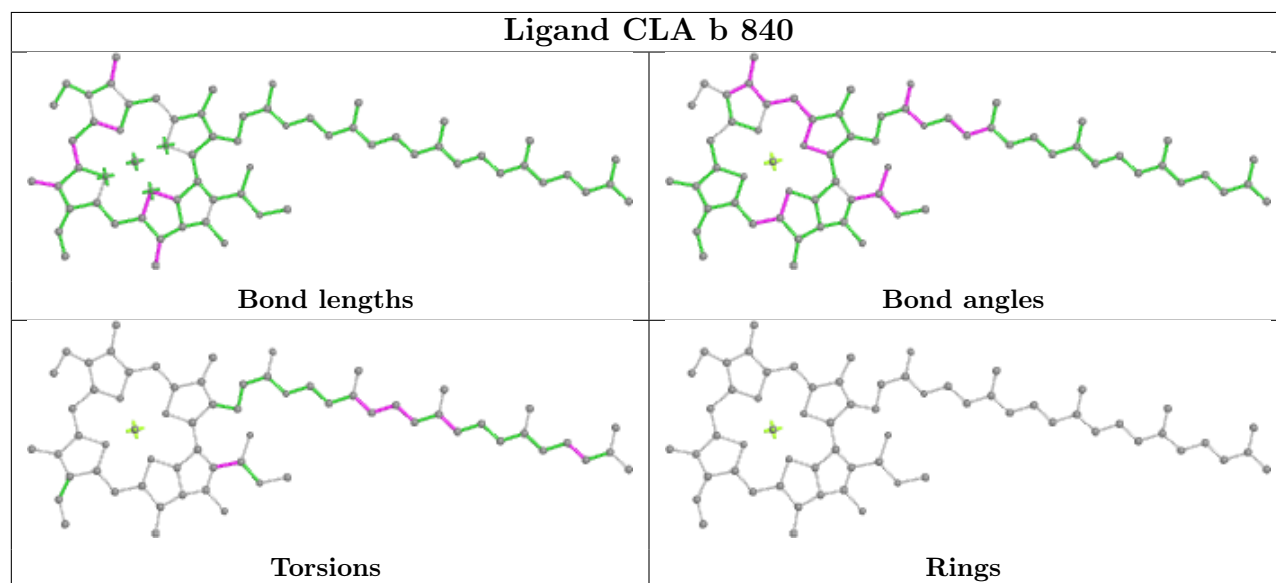
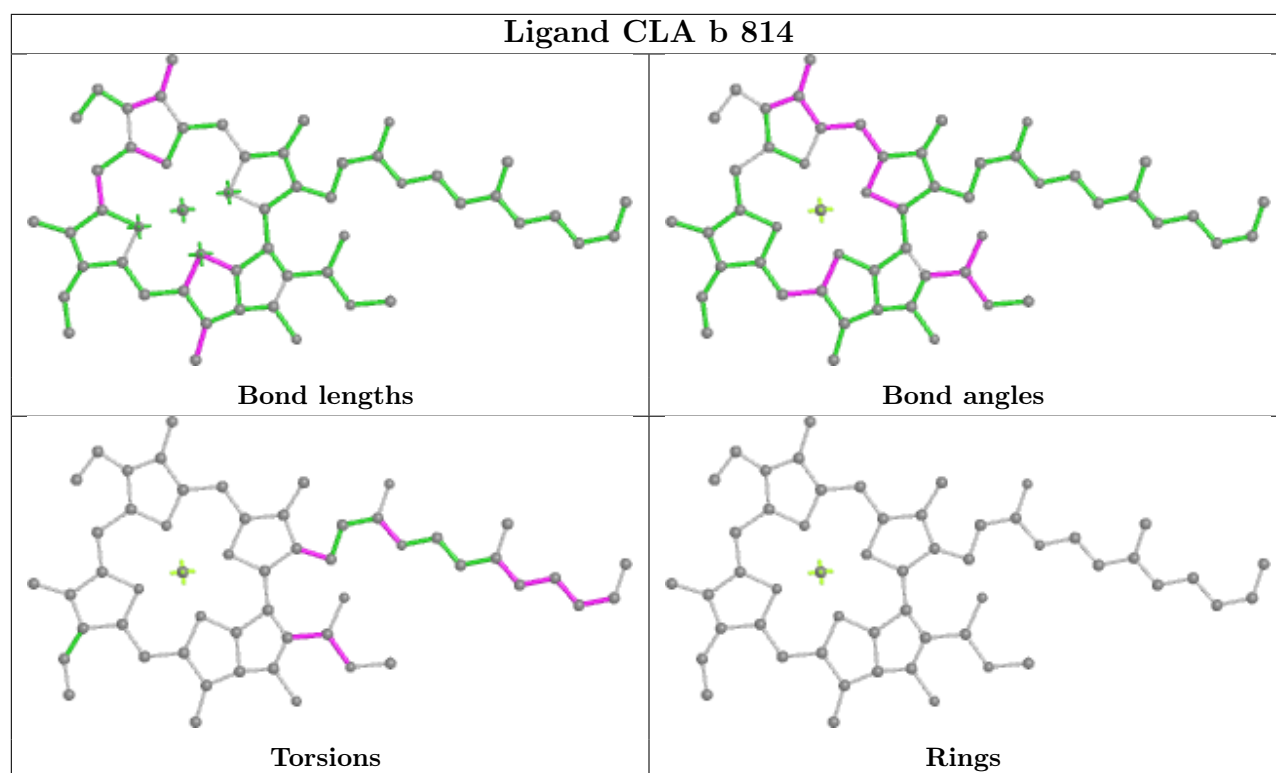
Torsions



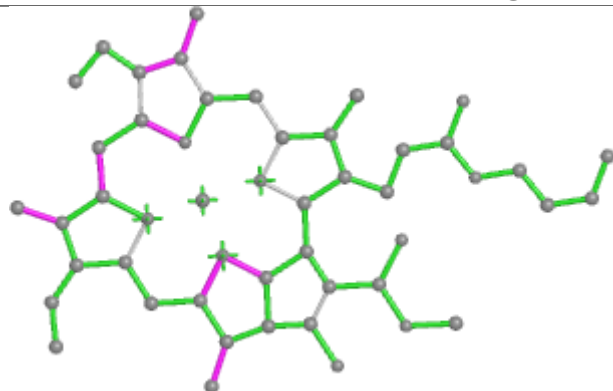
Rings



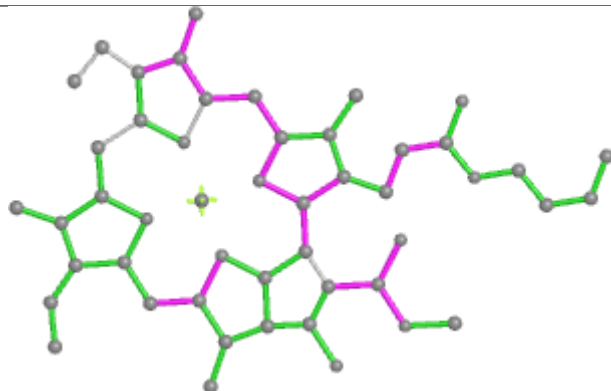




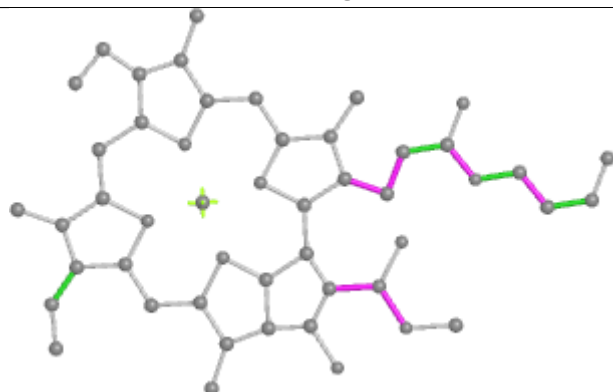
## Ligand CLA X 1701



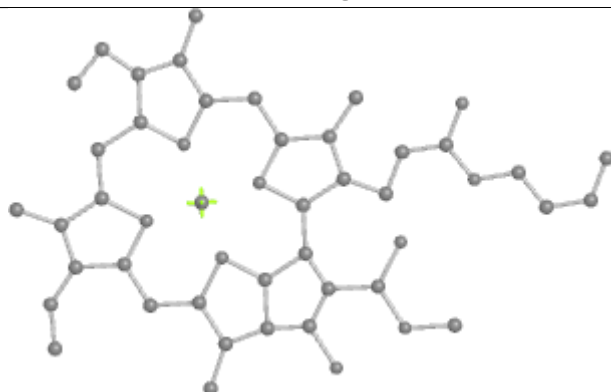
Bond lengths



Bond angles

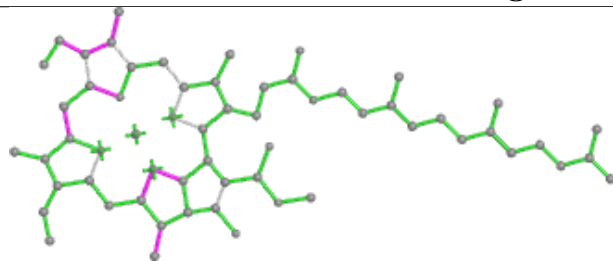


Torsions

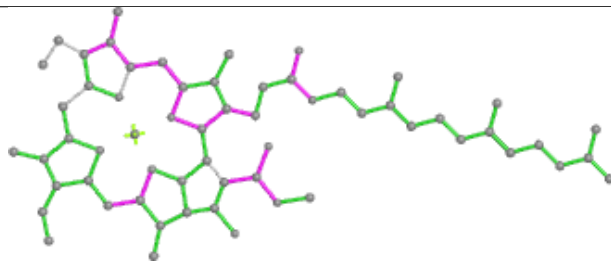


Rings

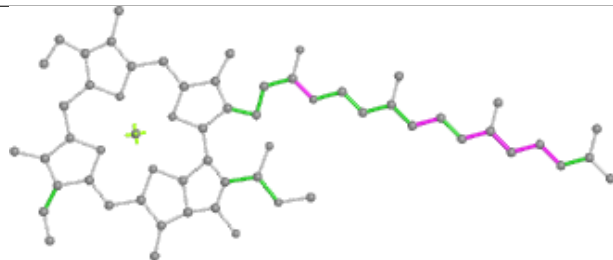
## Ligand CLA L 1502



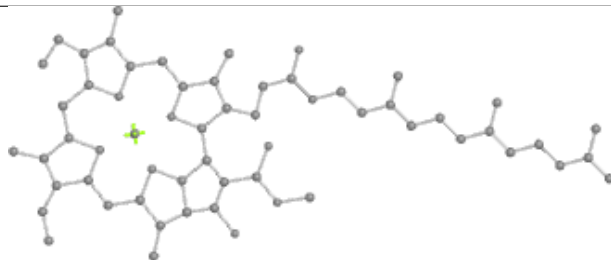
Bond lengths



Bond angles

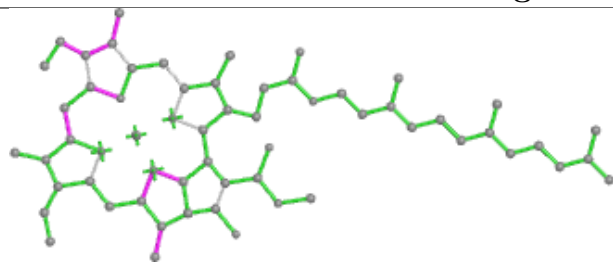


Torsions

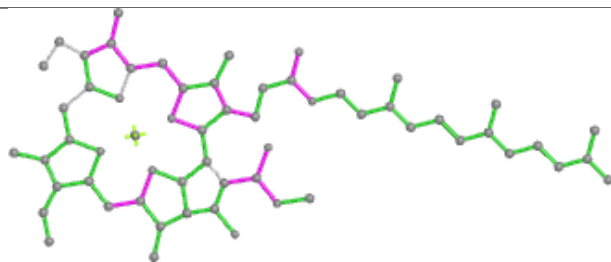


Rings

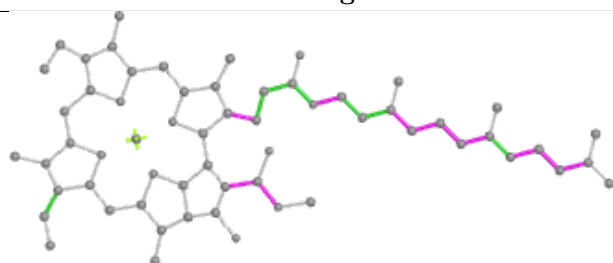
## Ligand CLA A 807



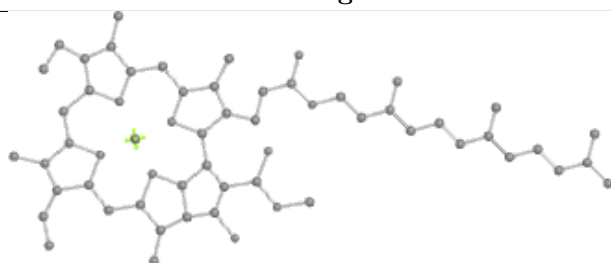
Bond lengths



Bond angles

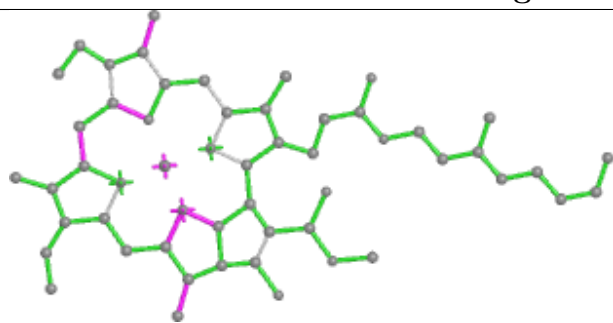


Torsions

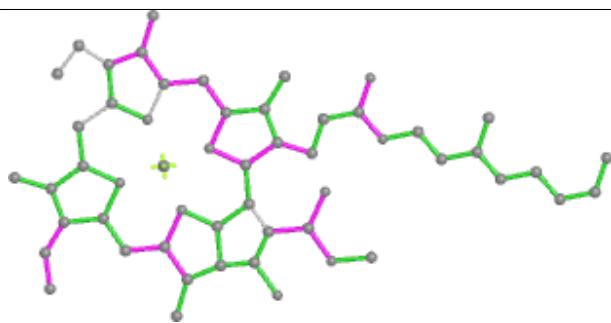


Rings

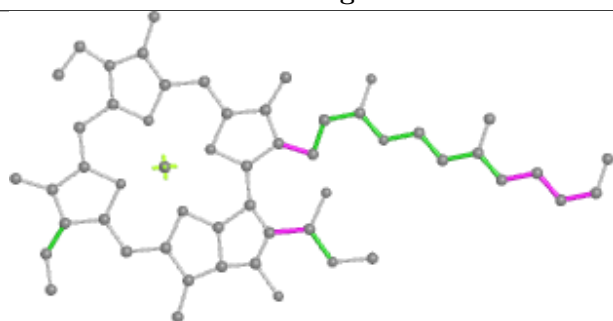
## Ligand CLA A 826



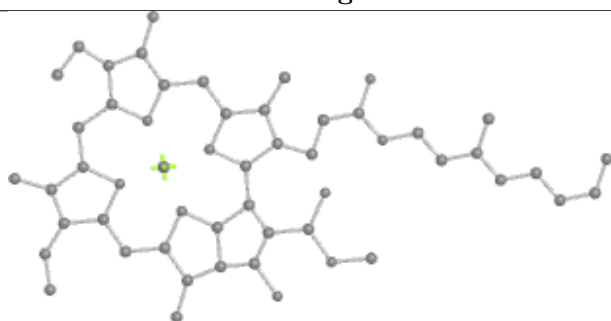
Bond lengths



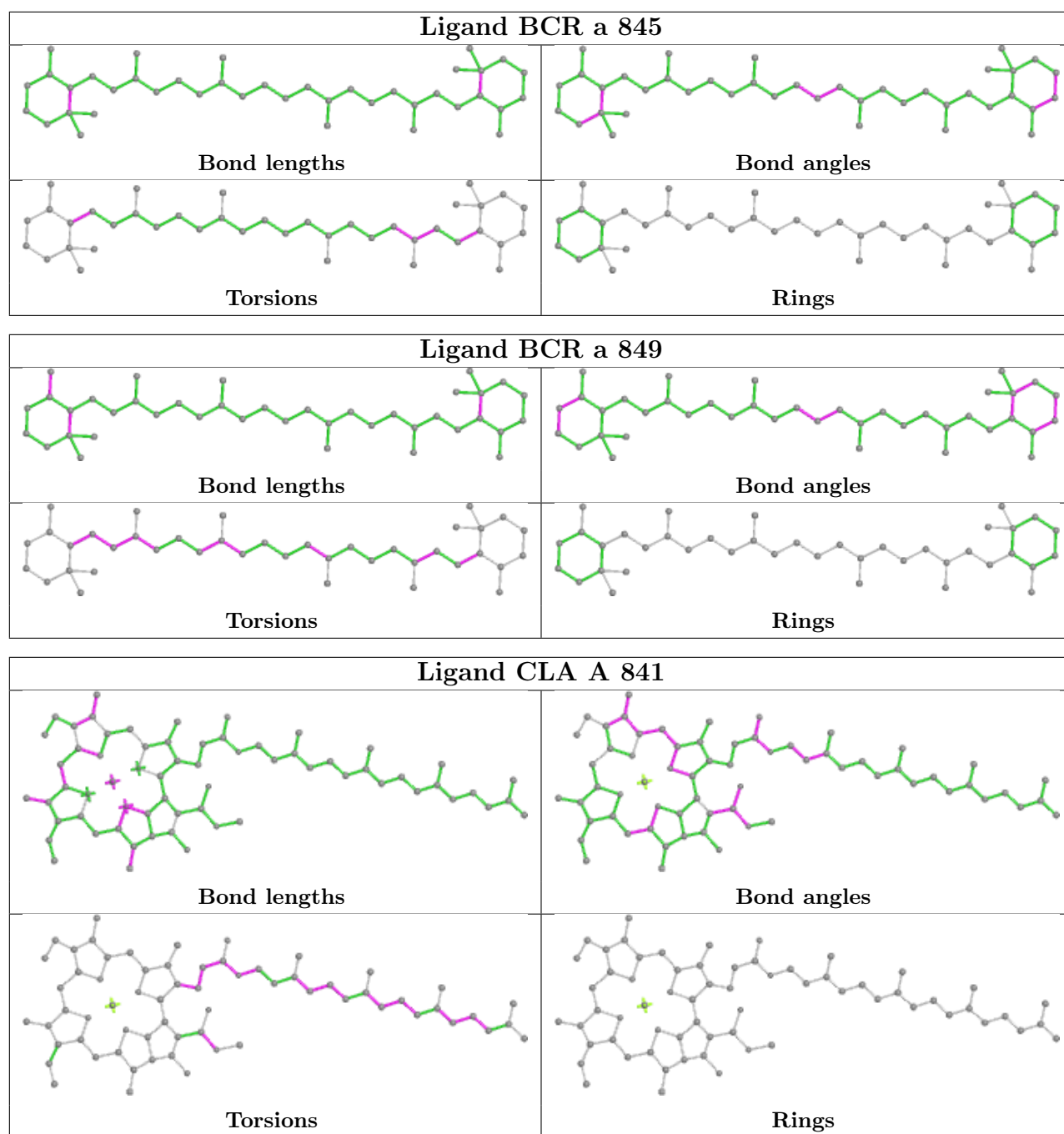
Bond angles



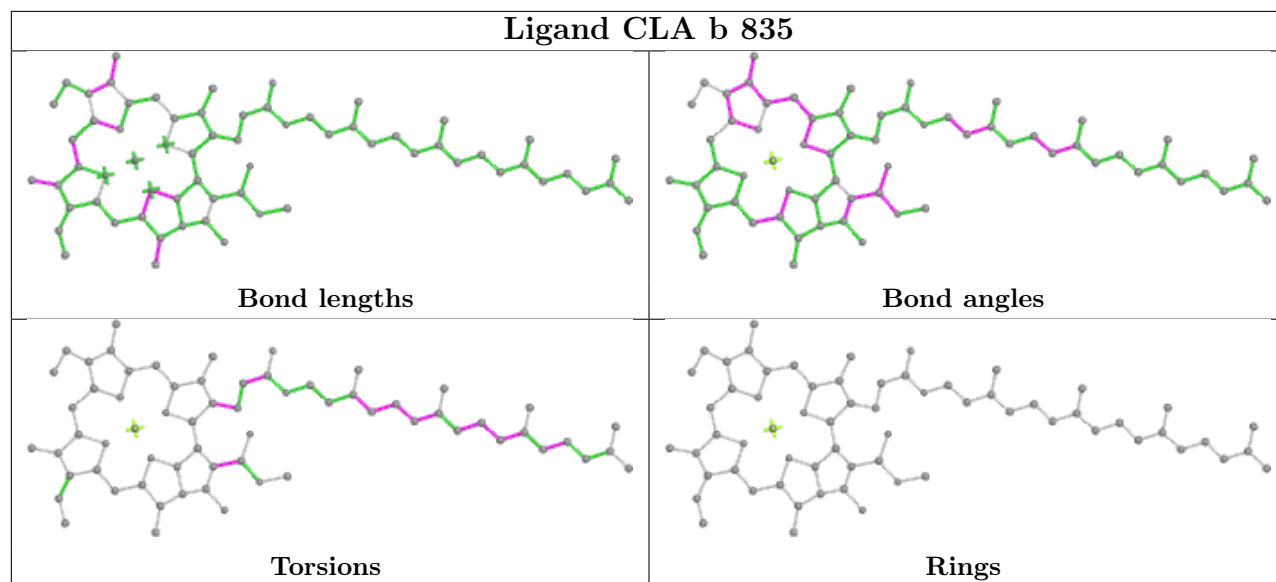
Torsions



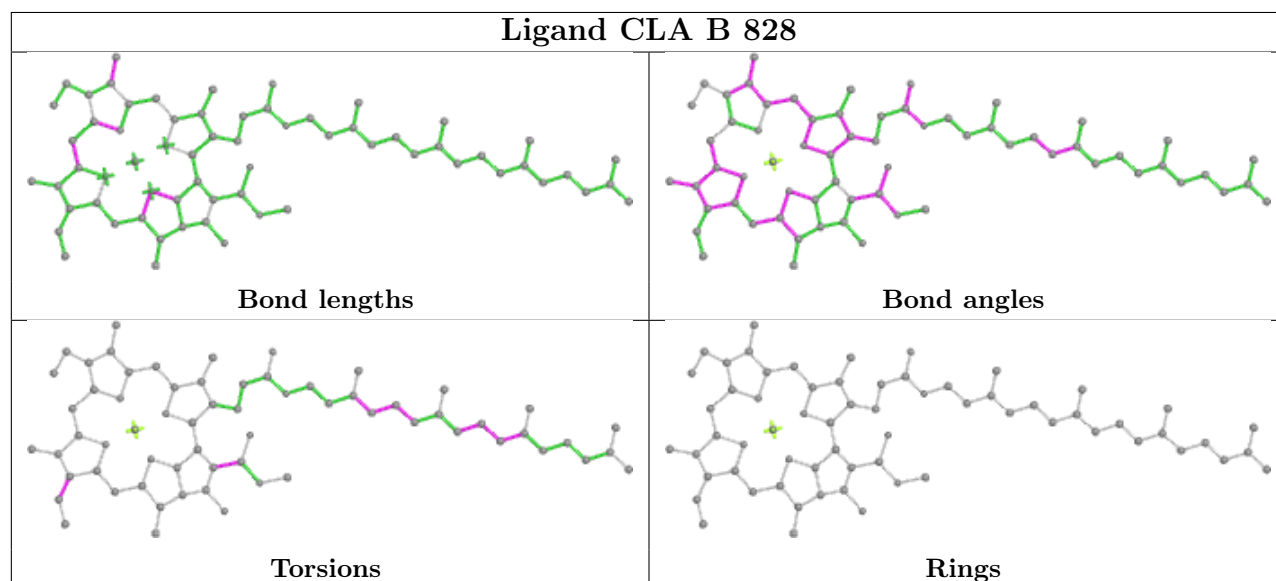
Rings



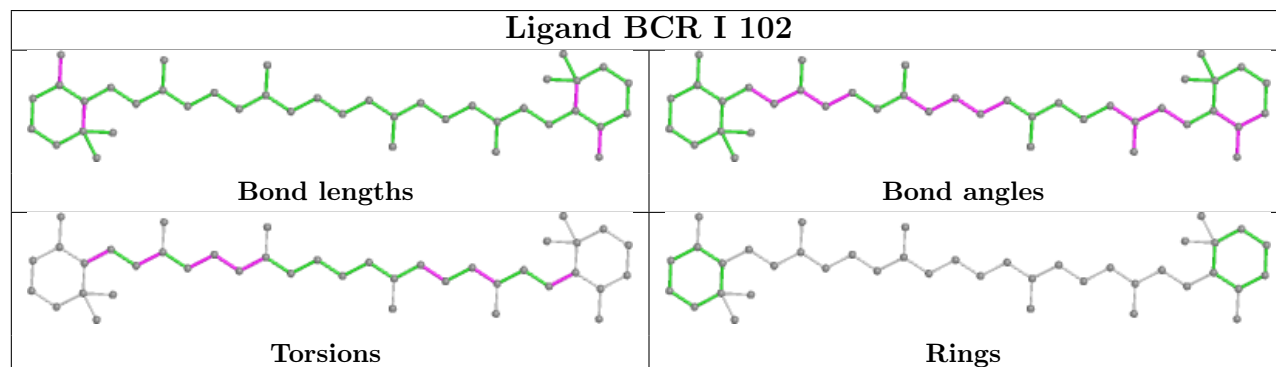
## Ligand CLA b 835



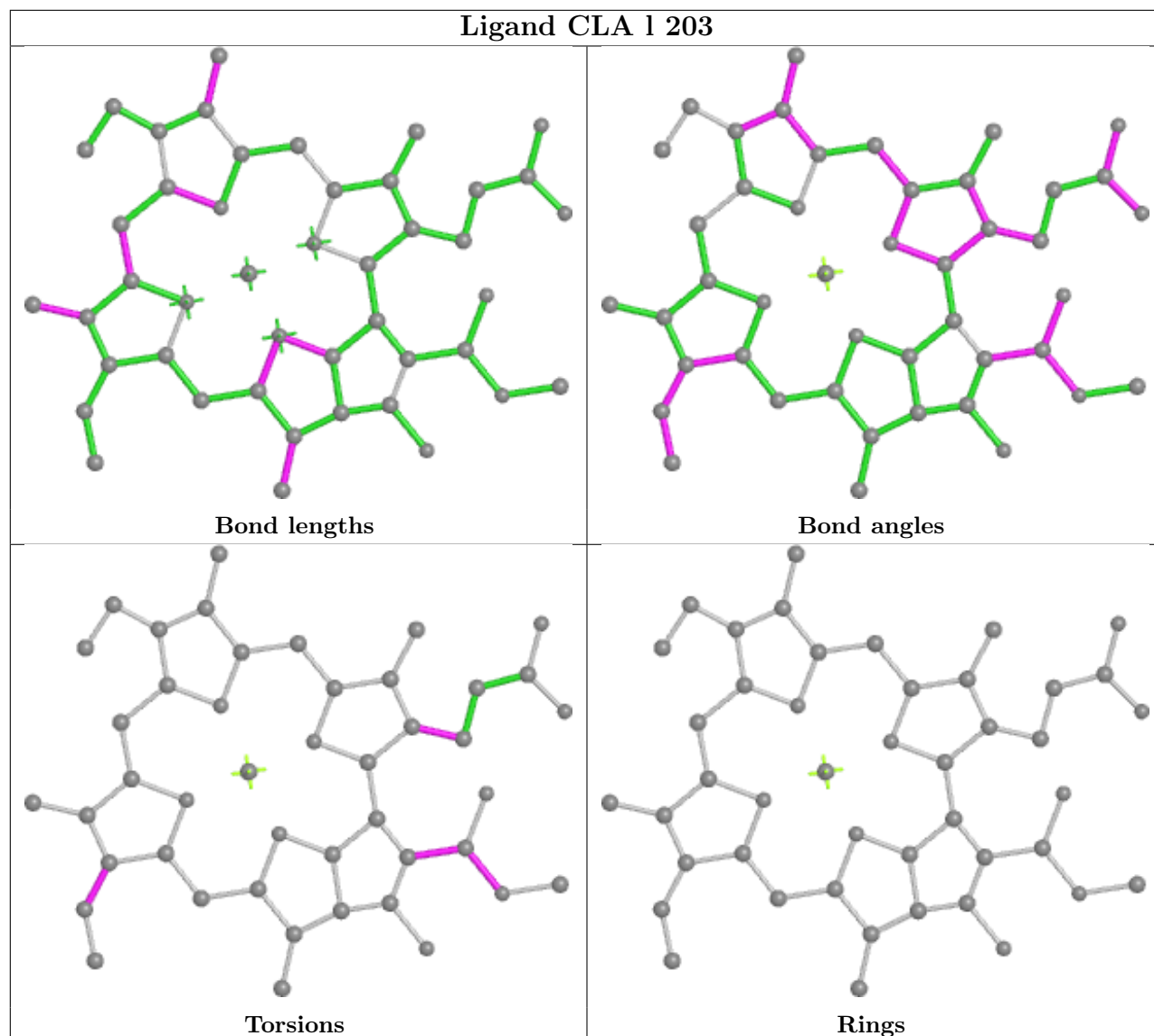
## Ligand CLA B 828



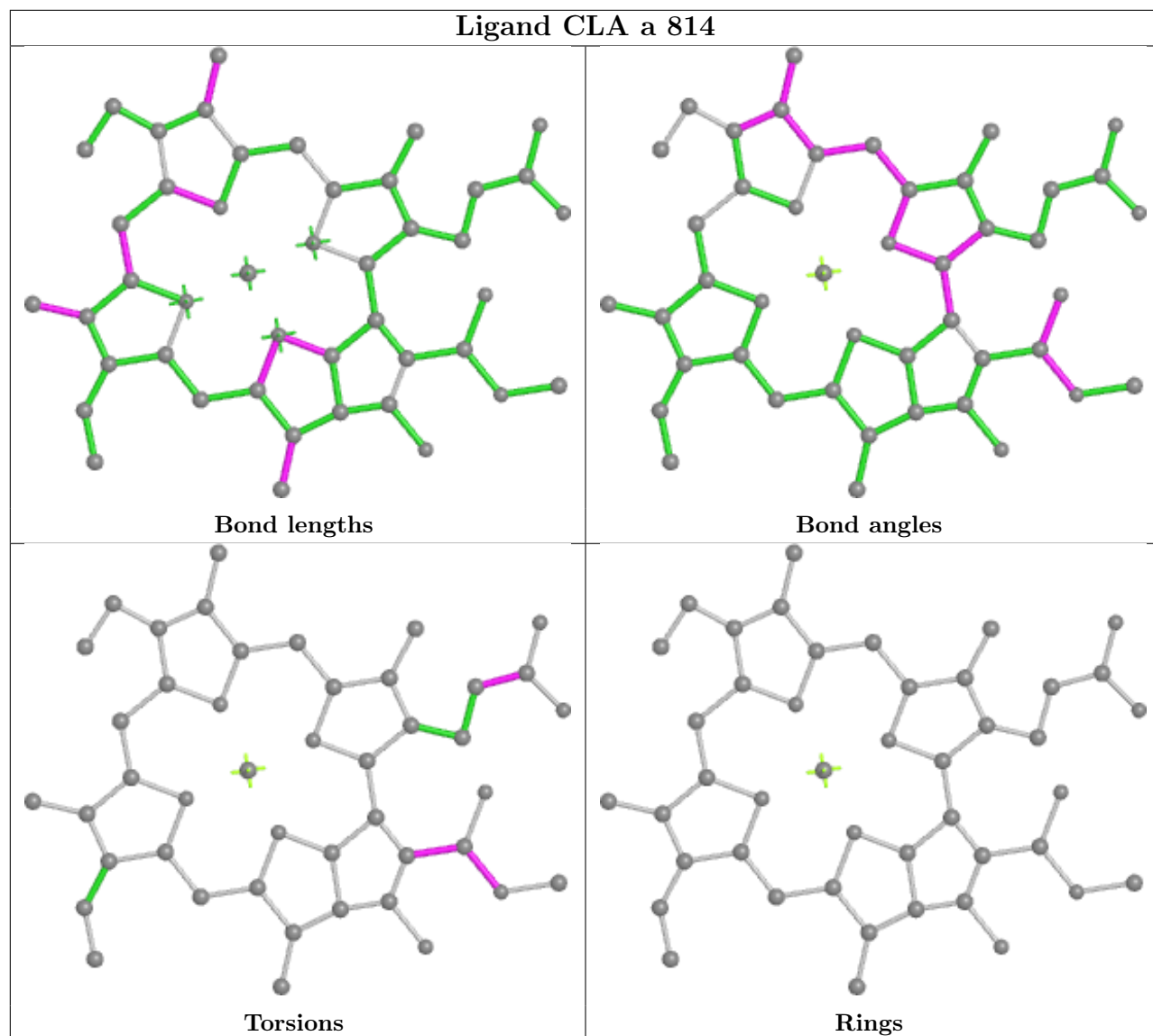
## Ligand BCR I 102



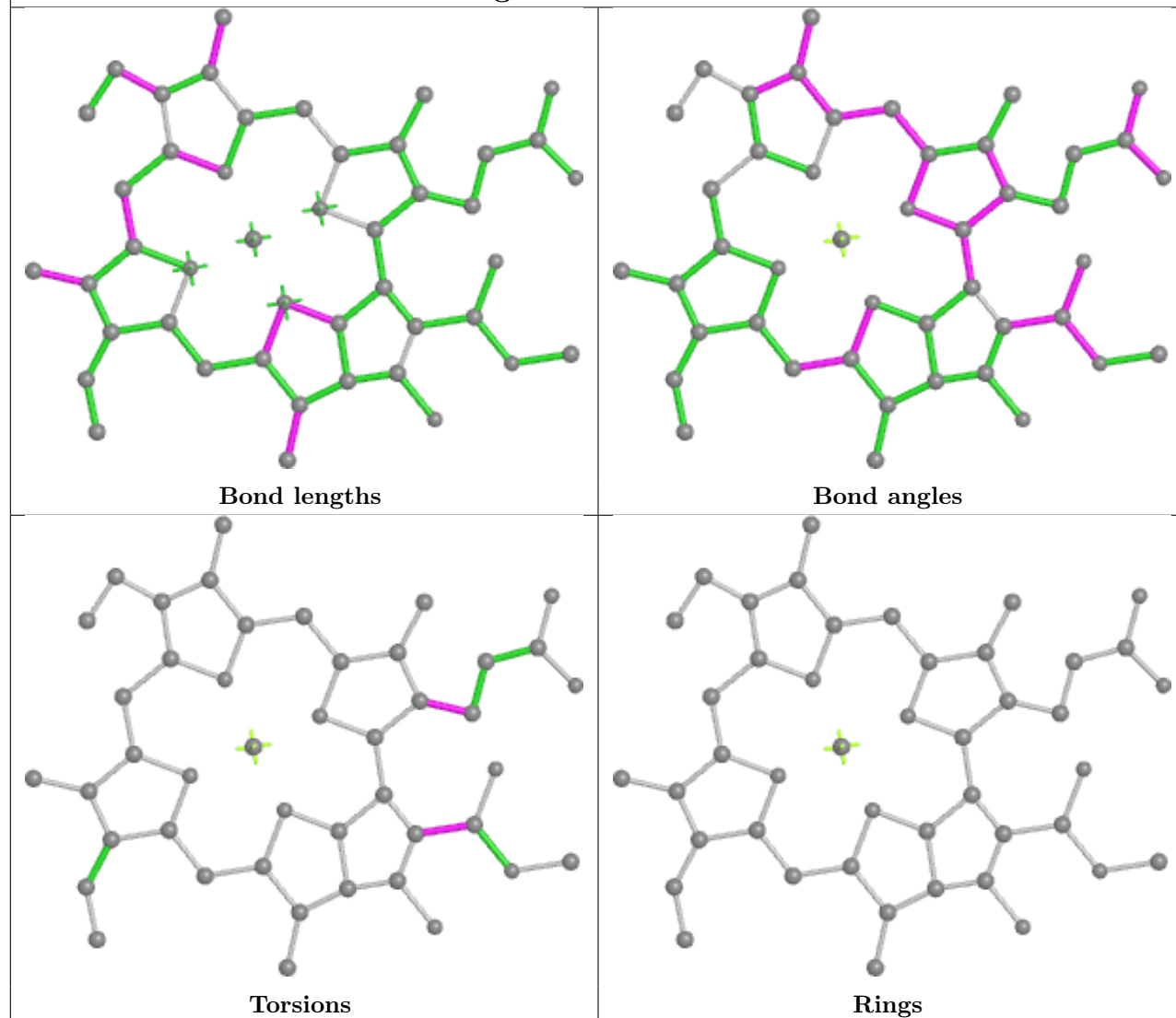
## Ligand CLA 1 203



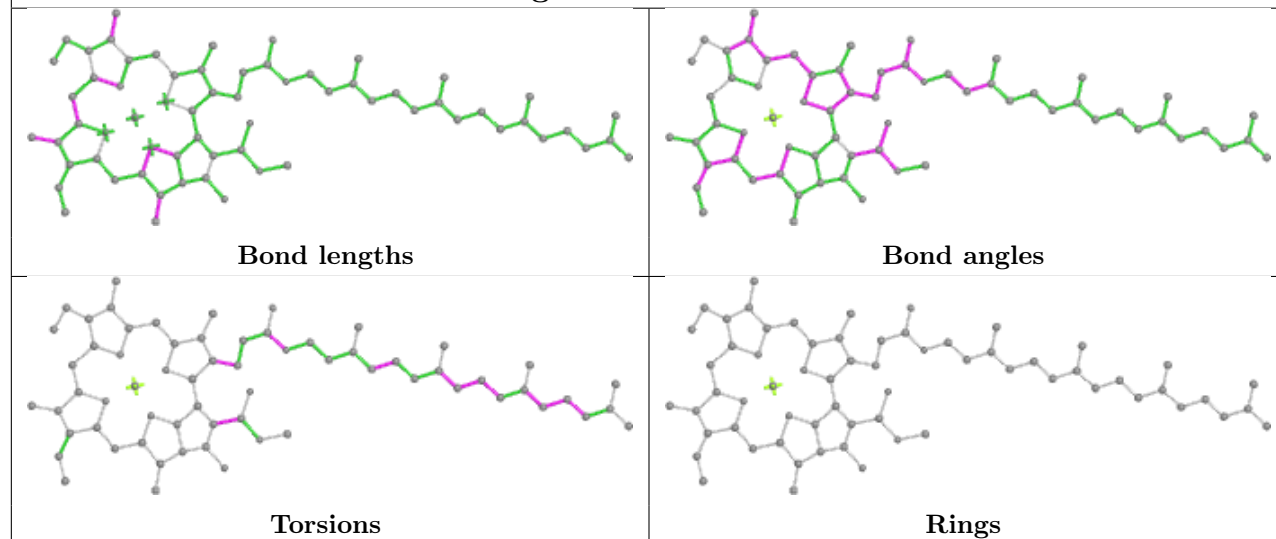
## Ligand CLA a 814



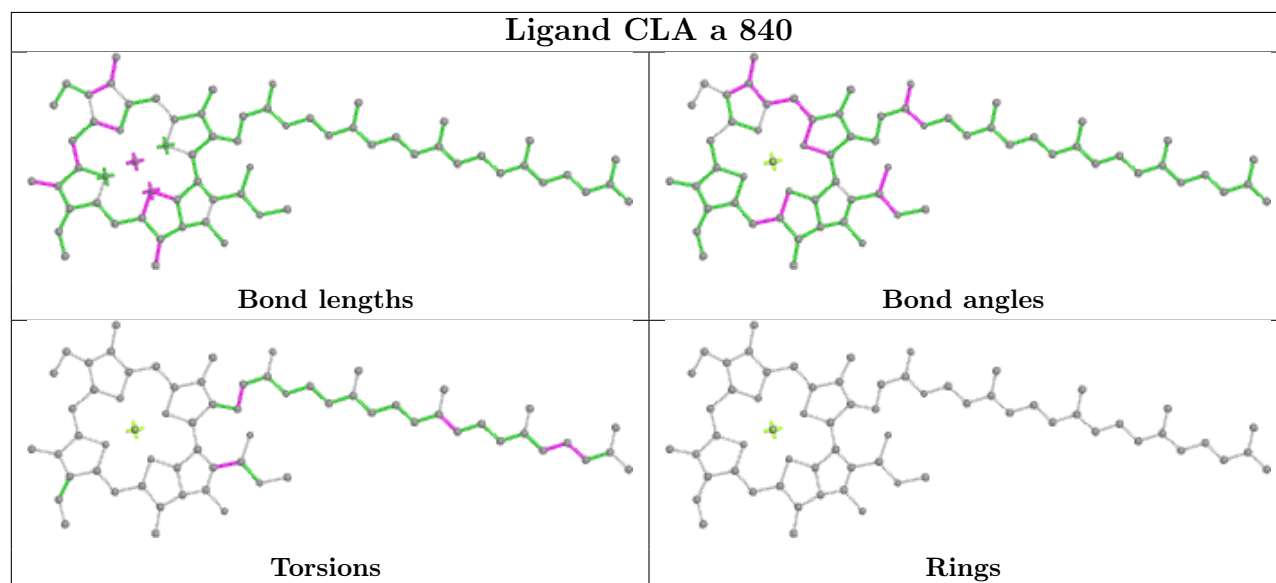
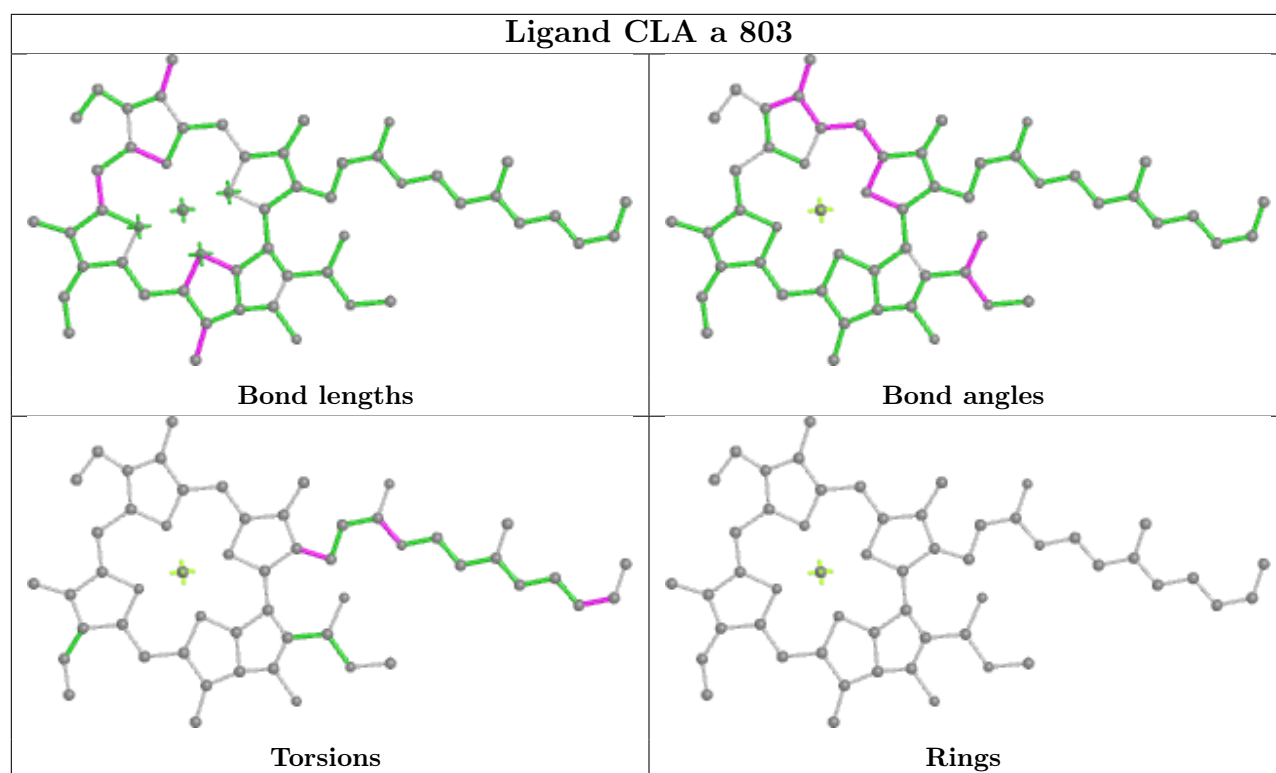
## Ligand CLA a 821



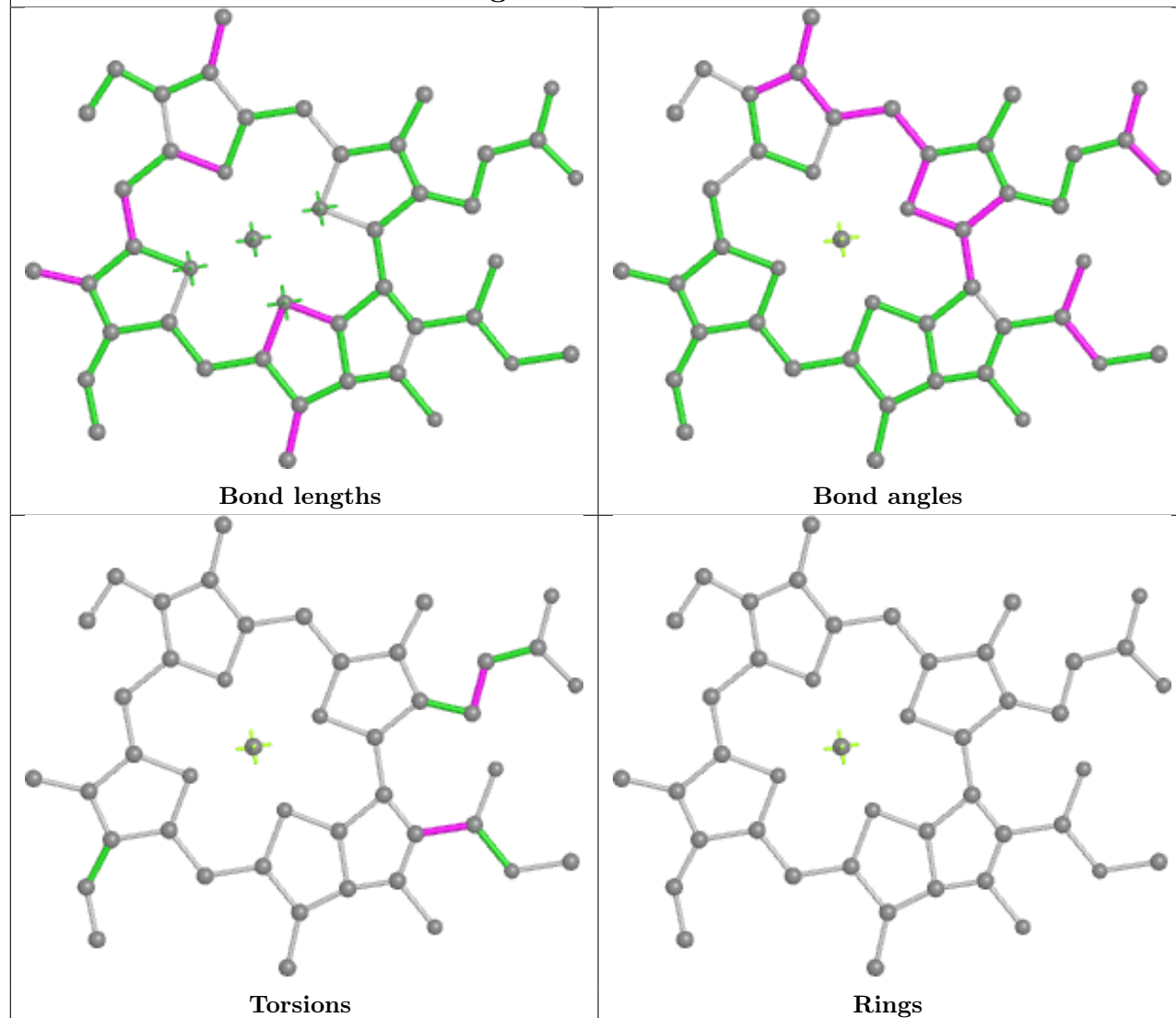
## Ligand CLA A 805



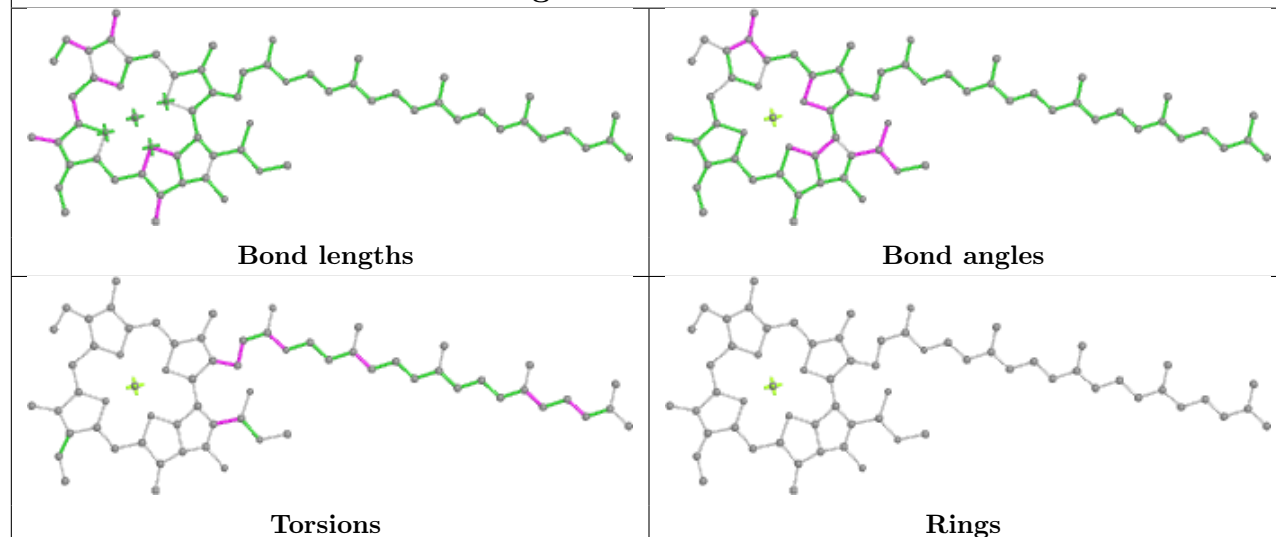


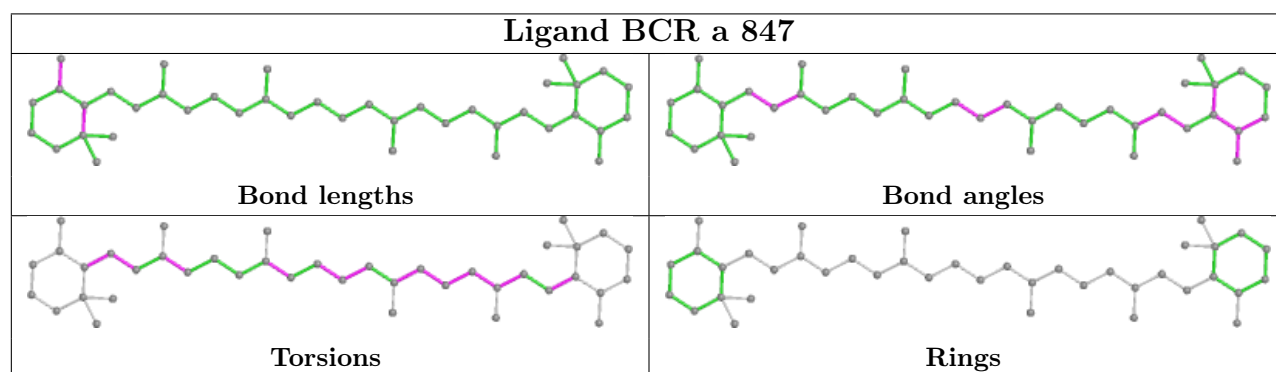
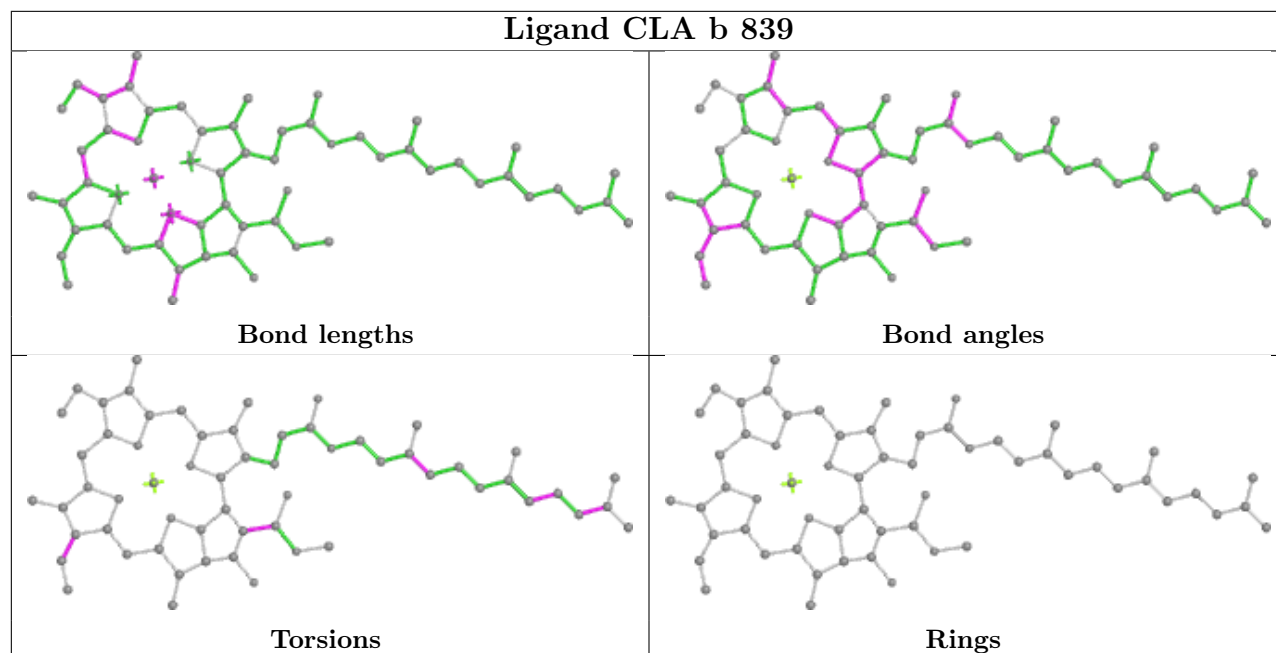
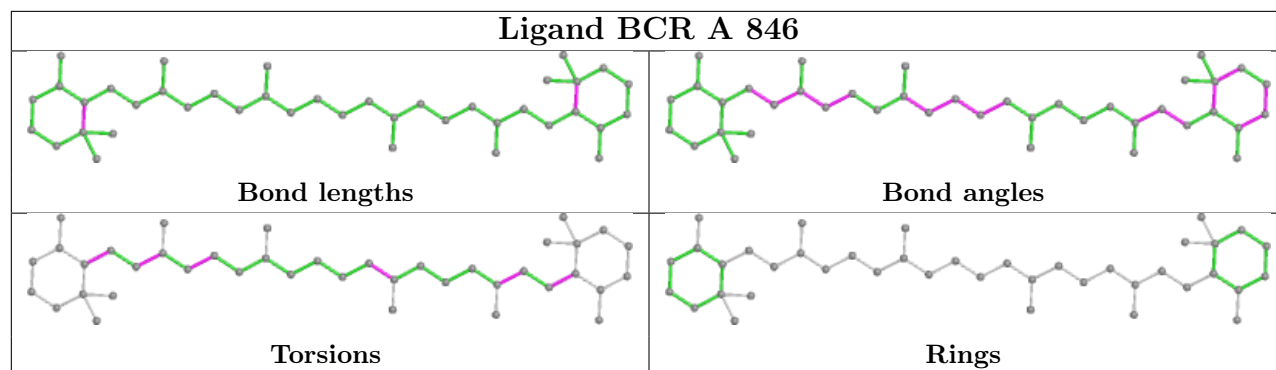


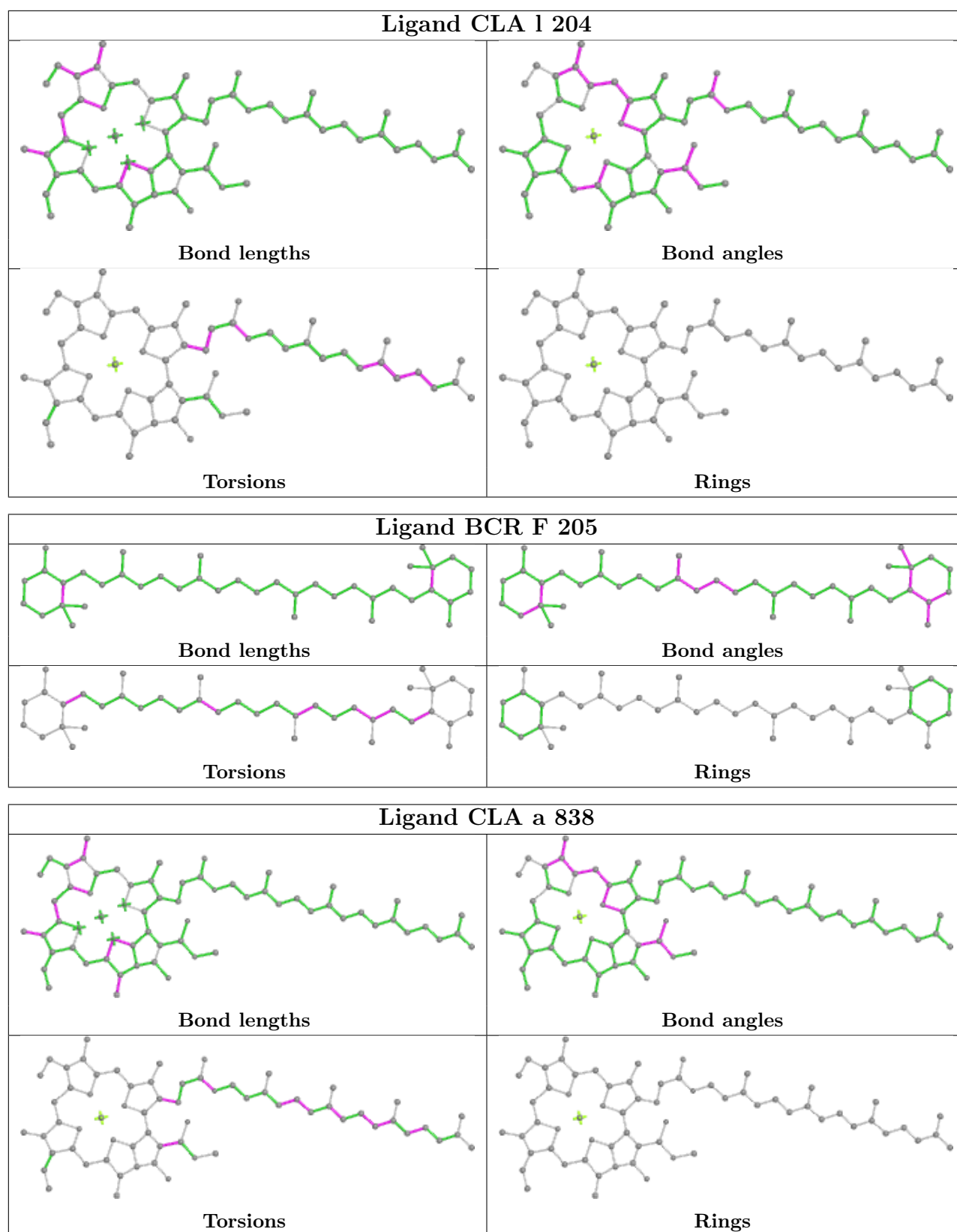
## Ligand CLA A 836

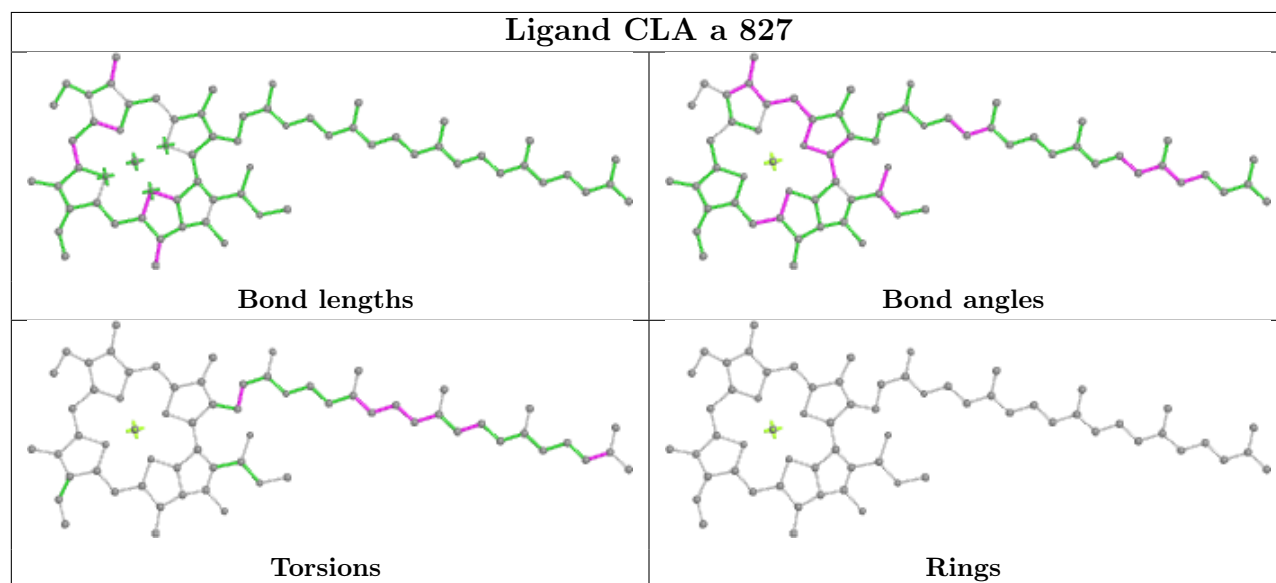
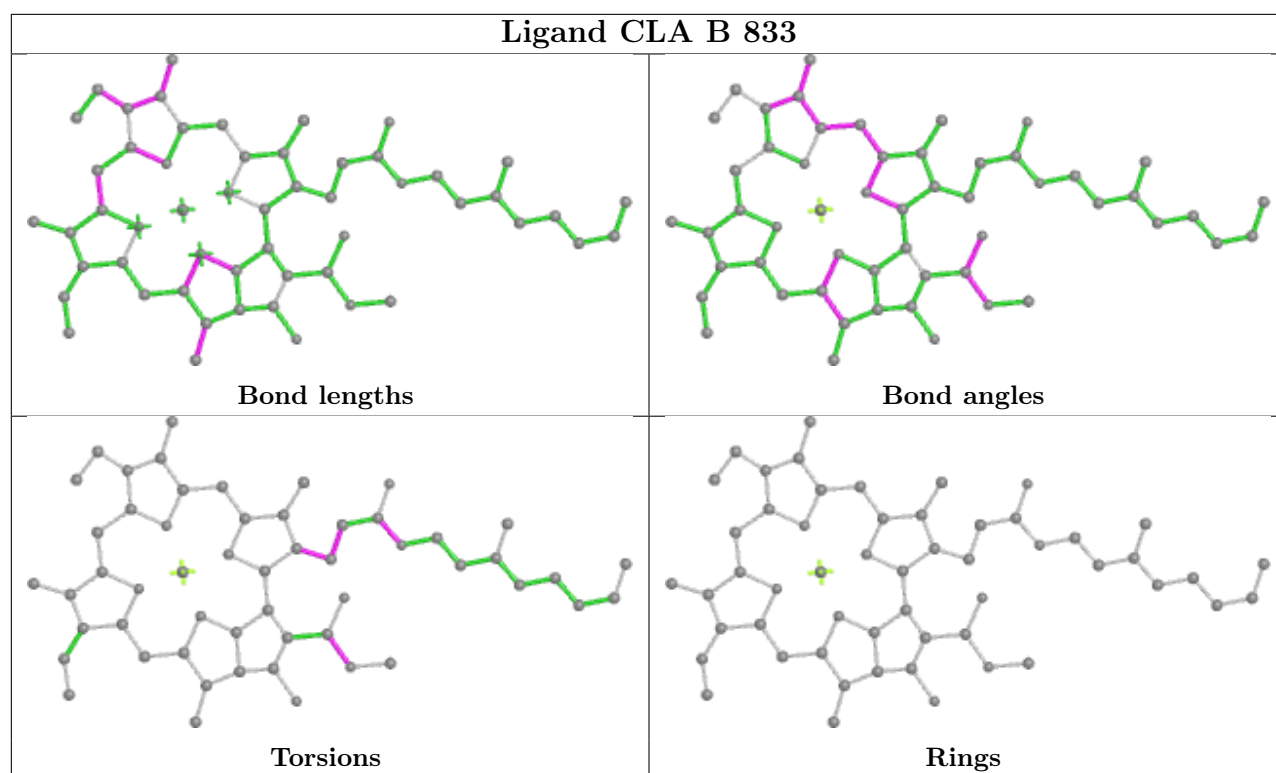


## Ligand CLA B 831

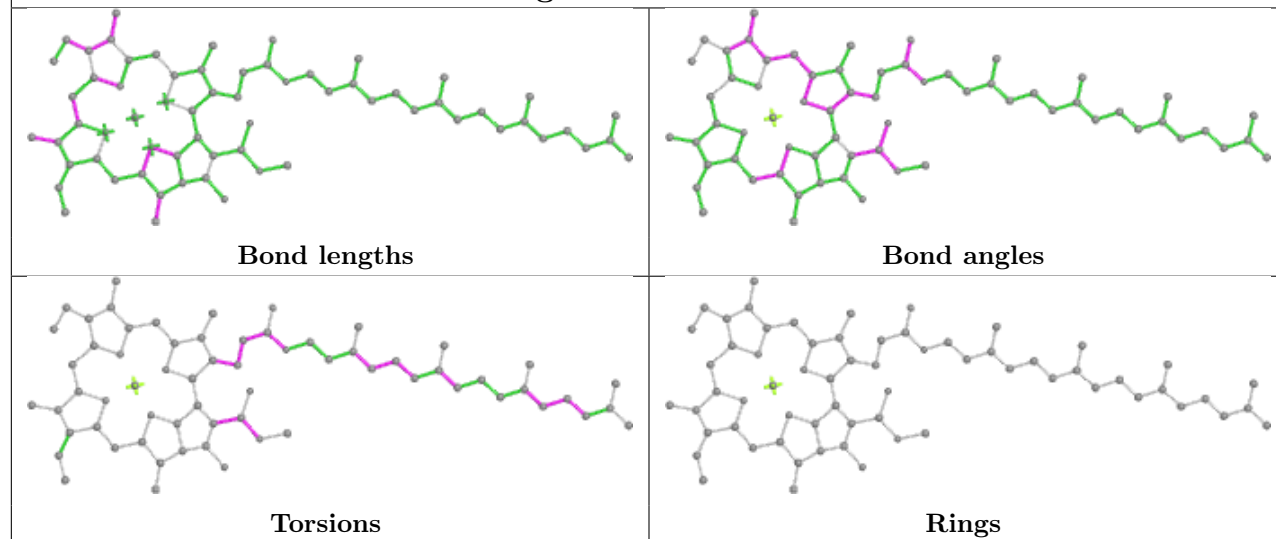




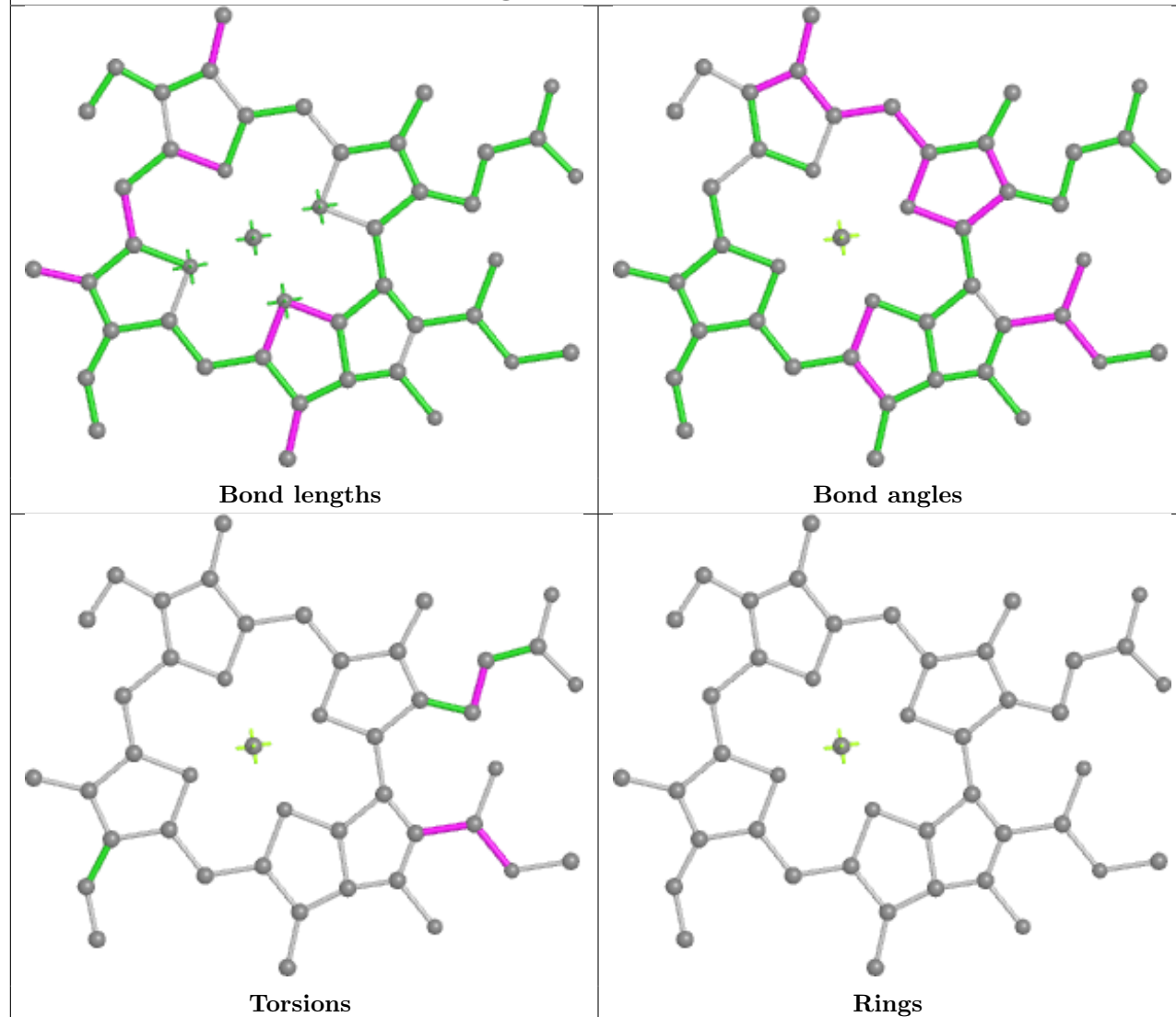




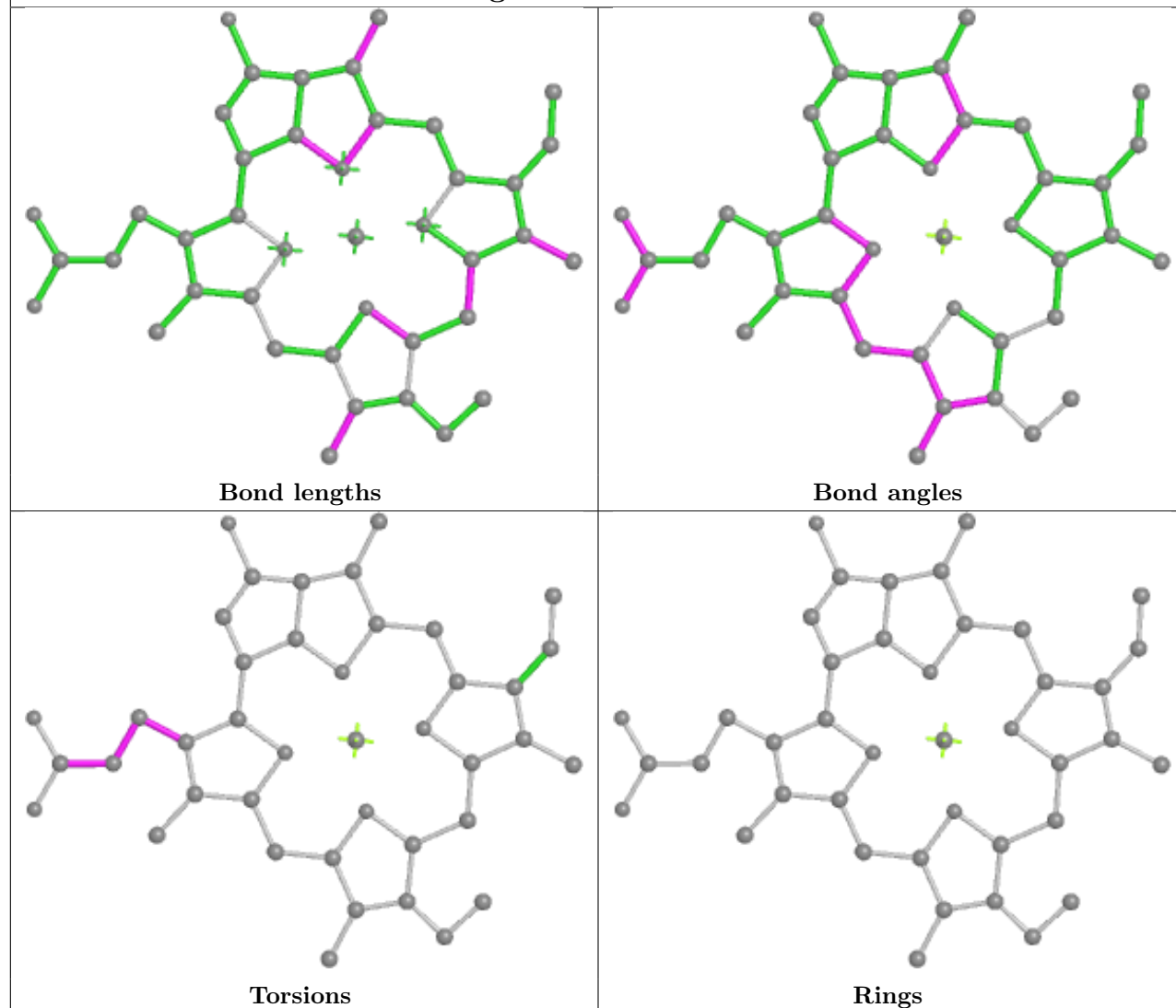
## Ligand CLA a 807



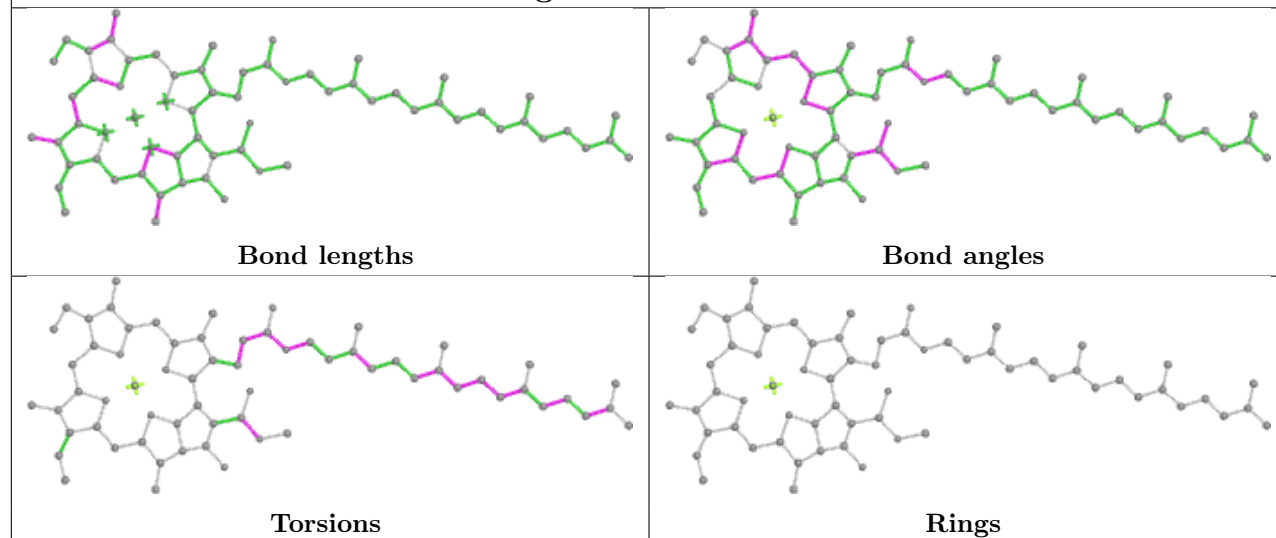
## Ligand CLA l 205

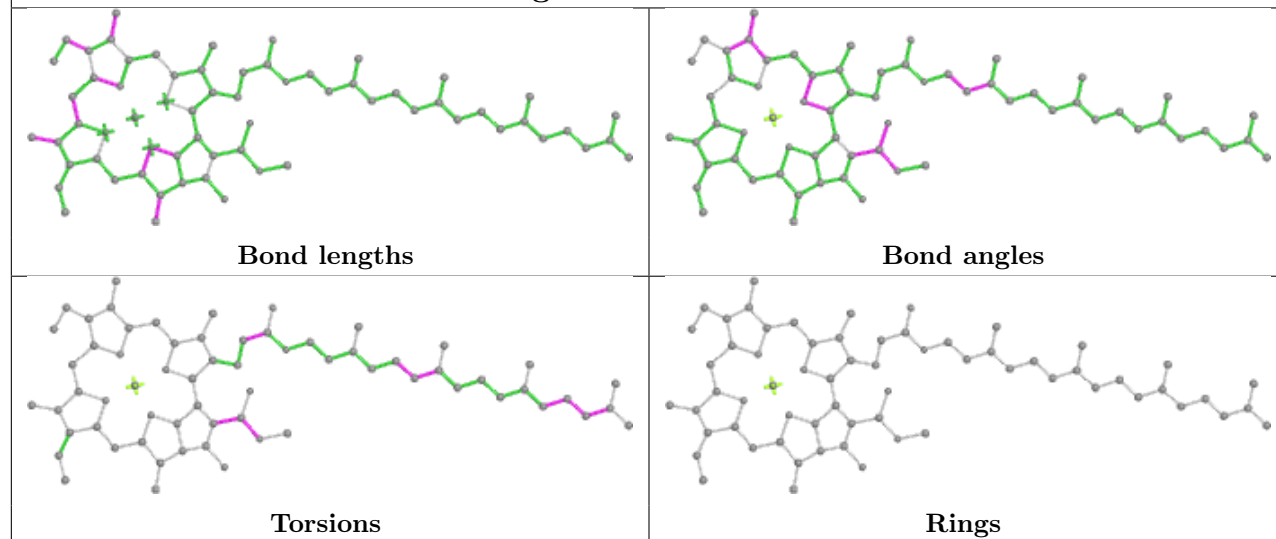
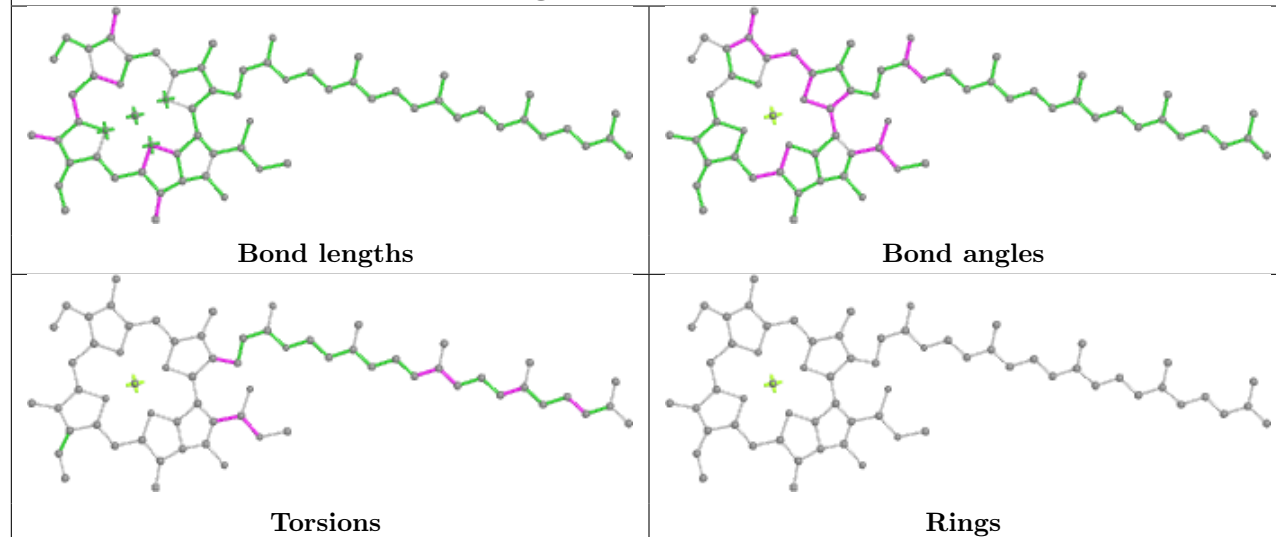


## Ligand CLA K 101



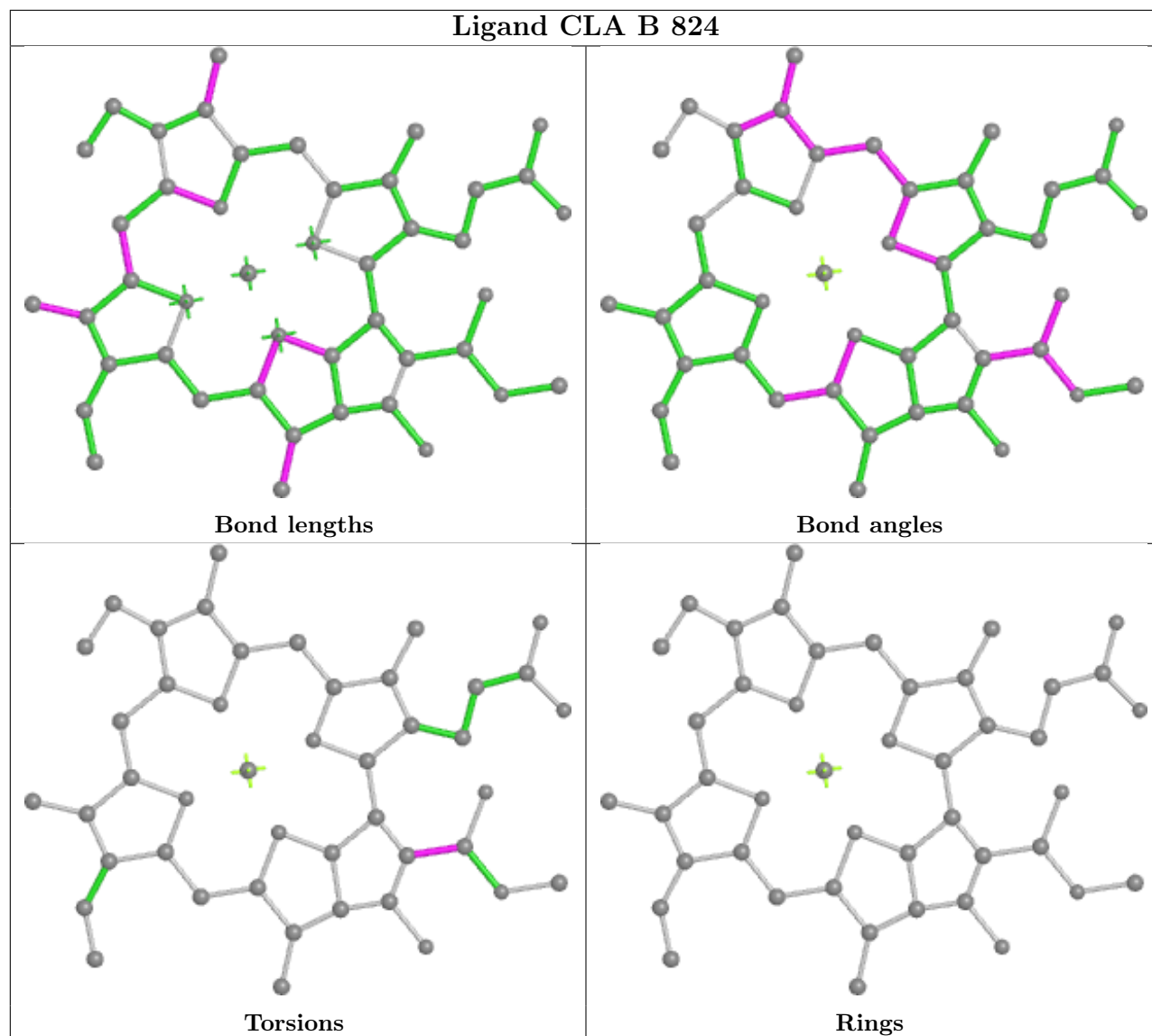
## Ligand CLA b 804



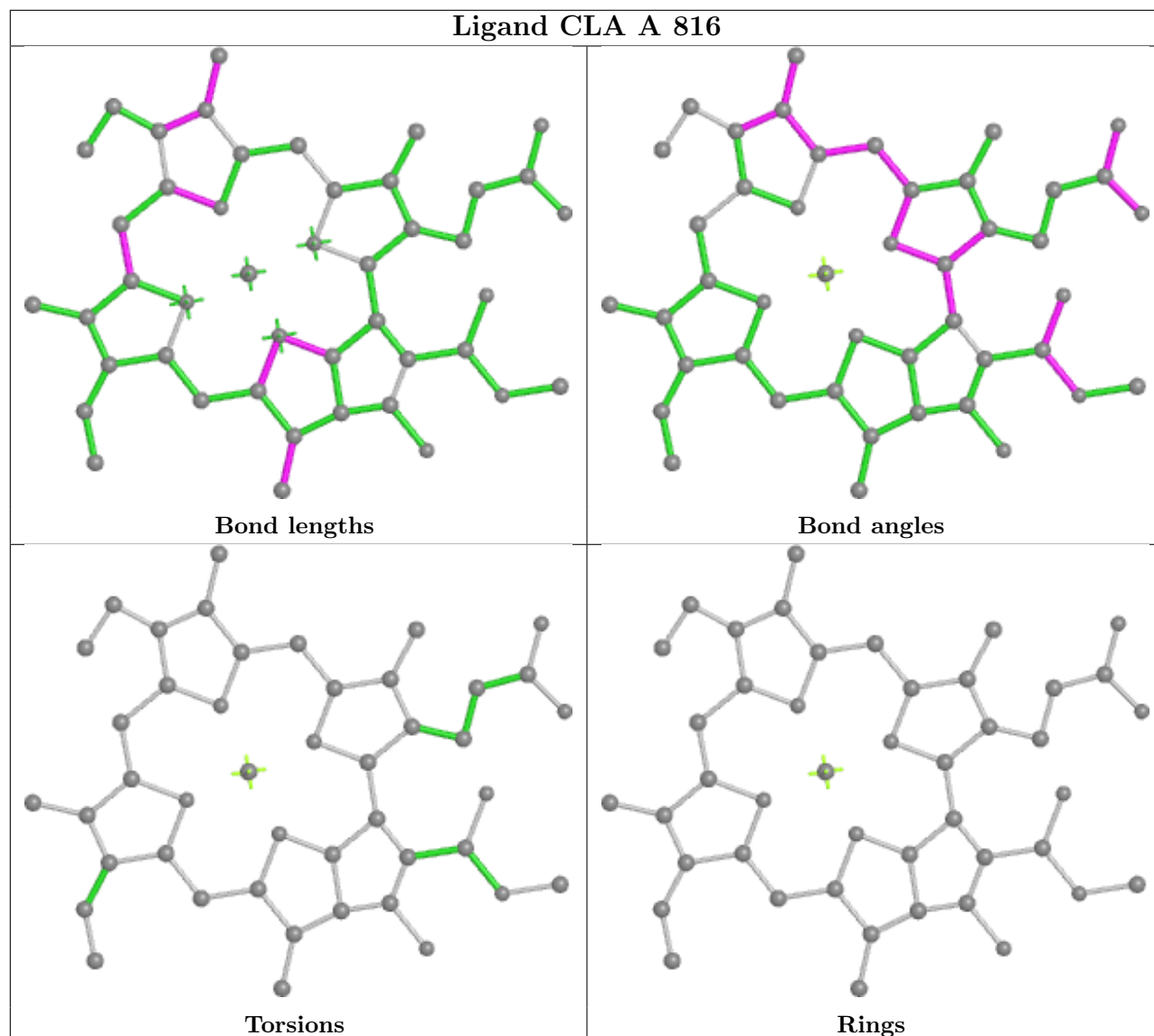
**Ligand CLA B 805****Ligand CLA B 829**



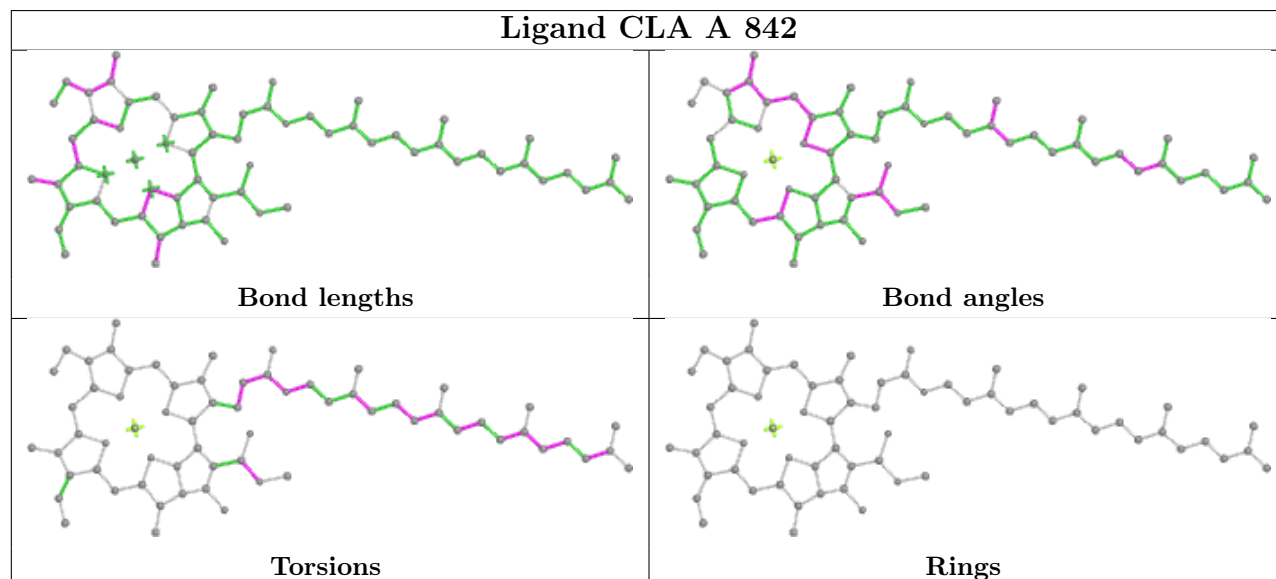
## Ligand CLA B 824



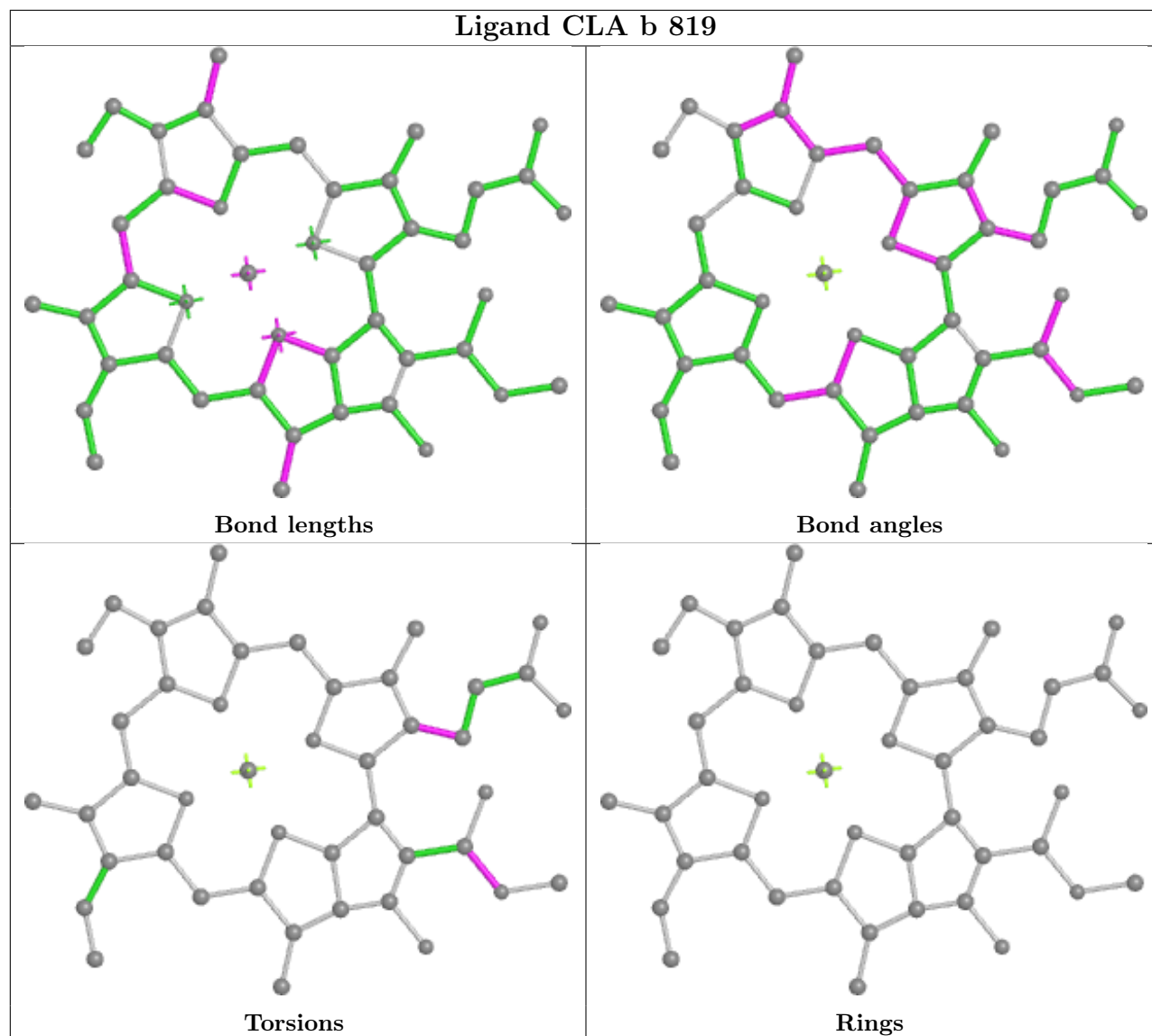
## Ligand CLA A 816



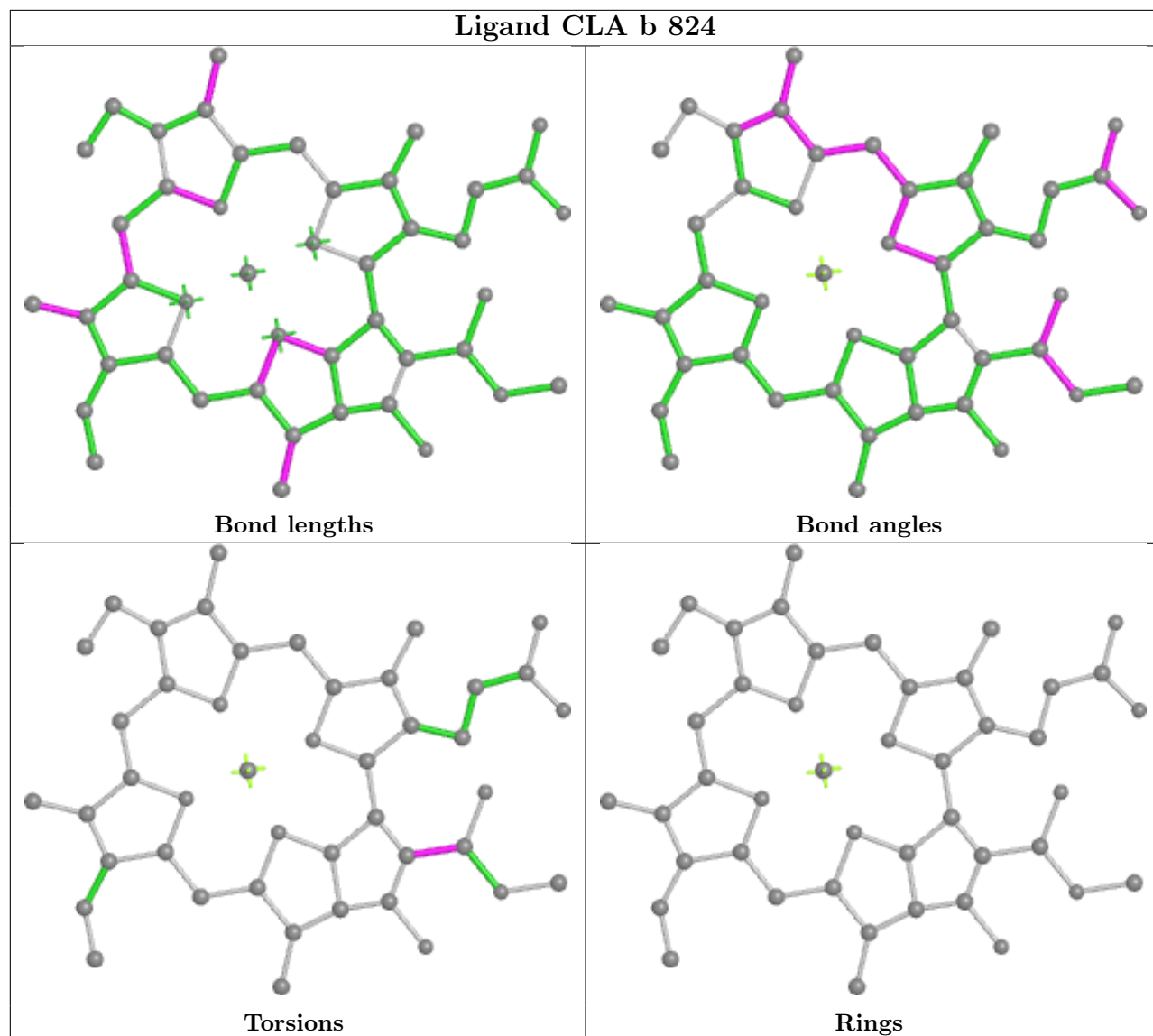
## Ligand CLA A 842



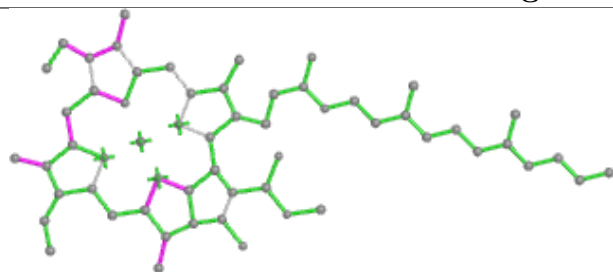
## Ligand CLA b 819



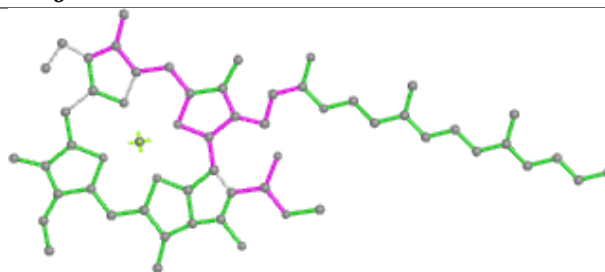
## Ligand CLA b 824



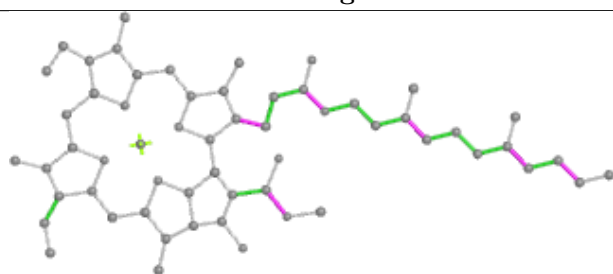
## Ligand CLA j 101



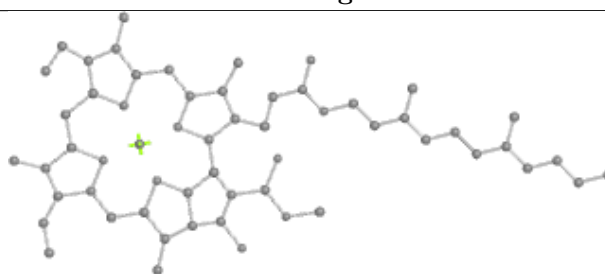
Bond lengths



Bond angles

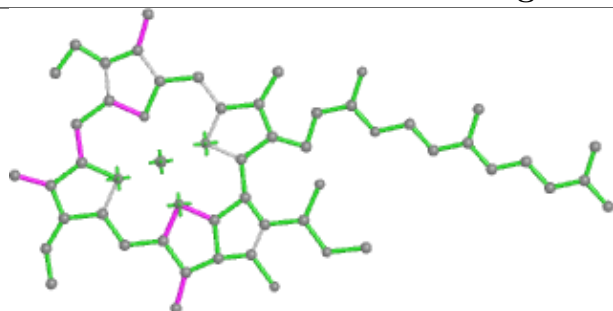


Torsions

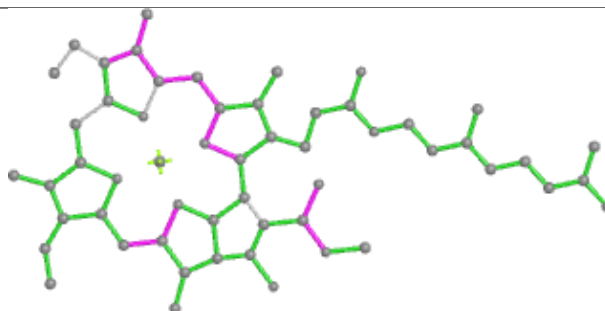


Rings

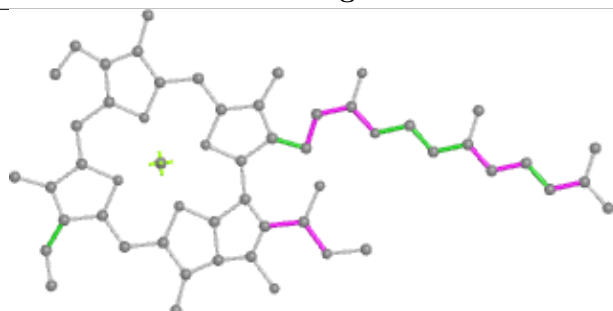
## Ligand CLA b 825



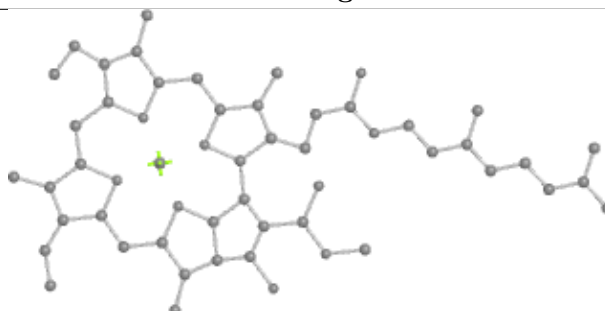
Bond lengths



Bond angles

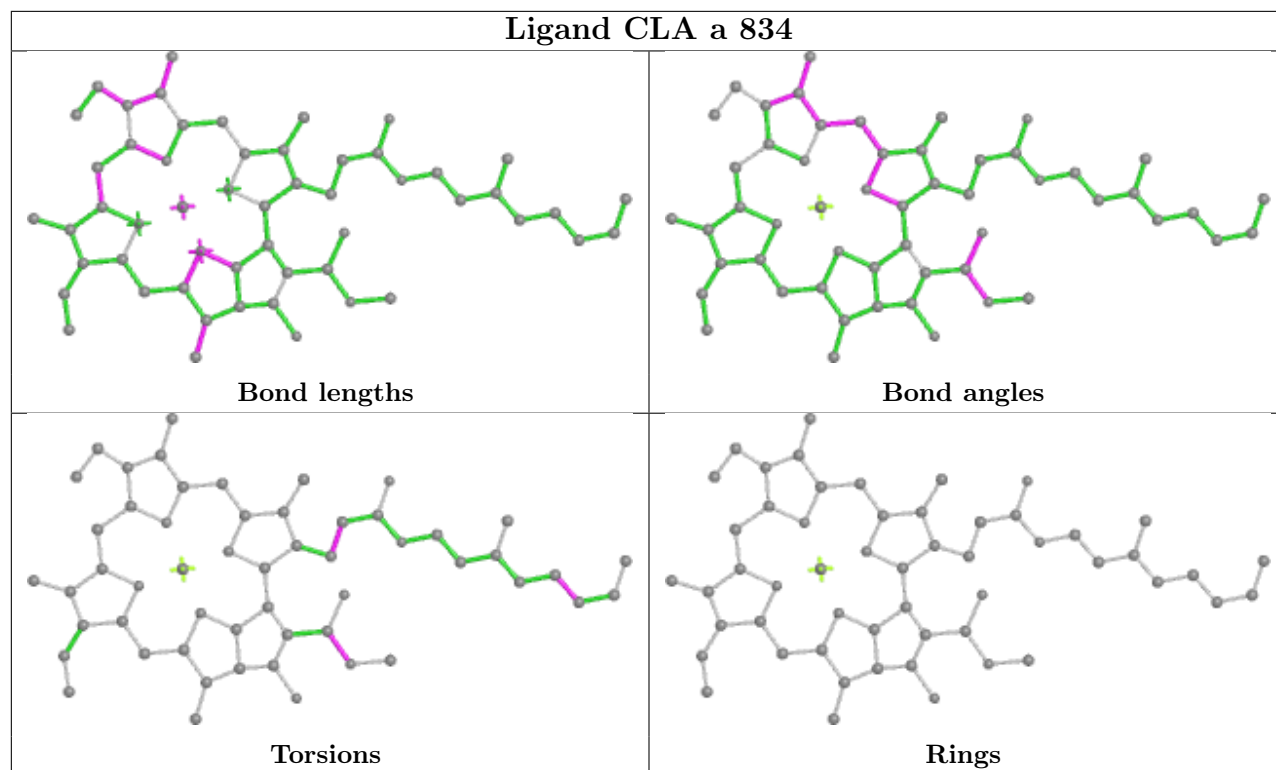


Torsions

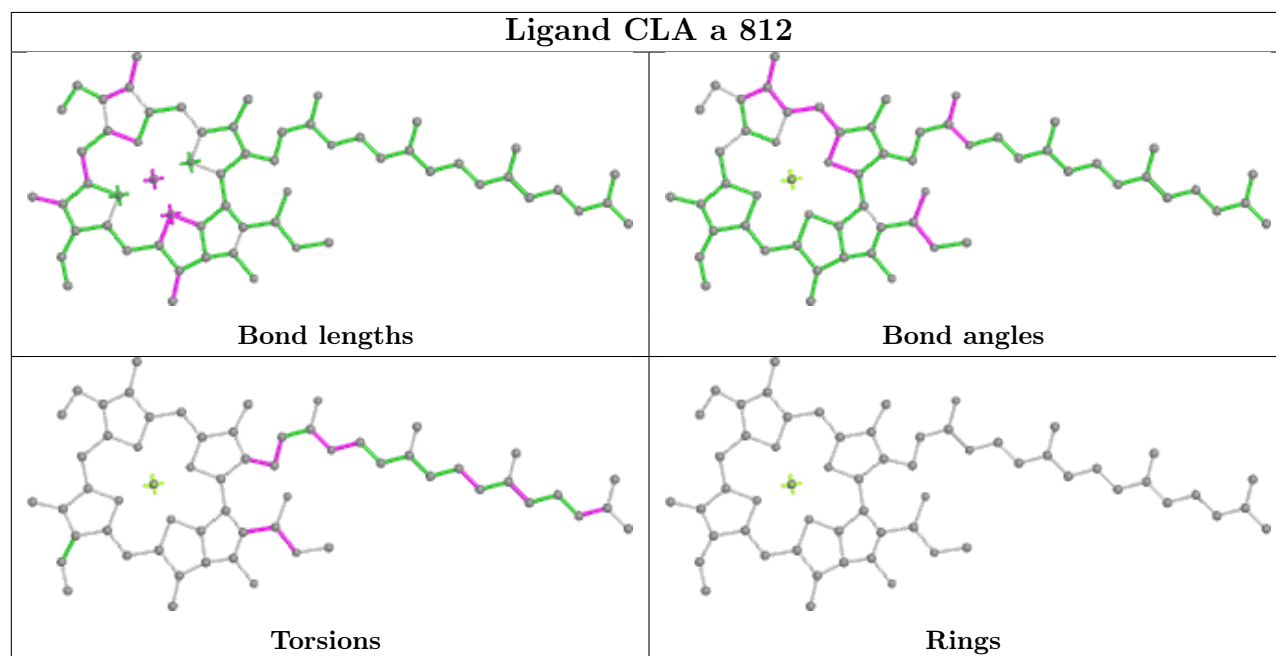


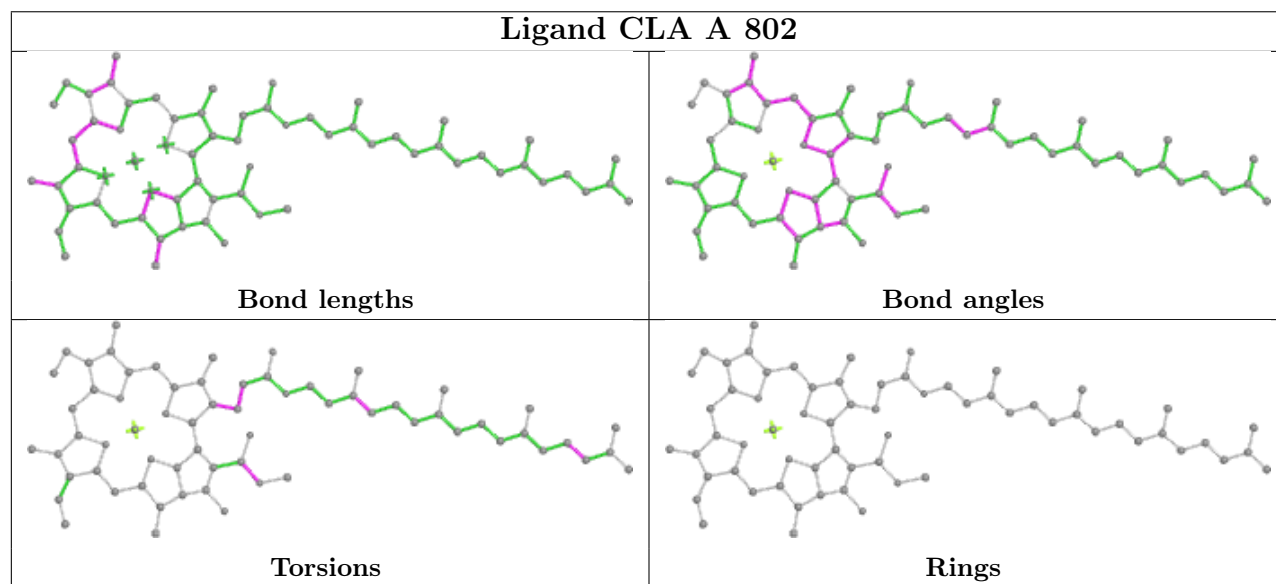
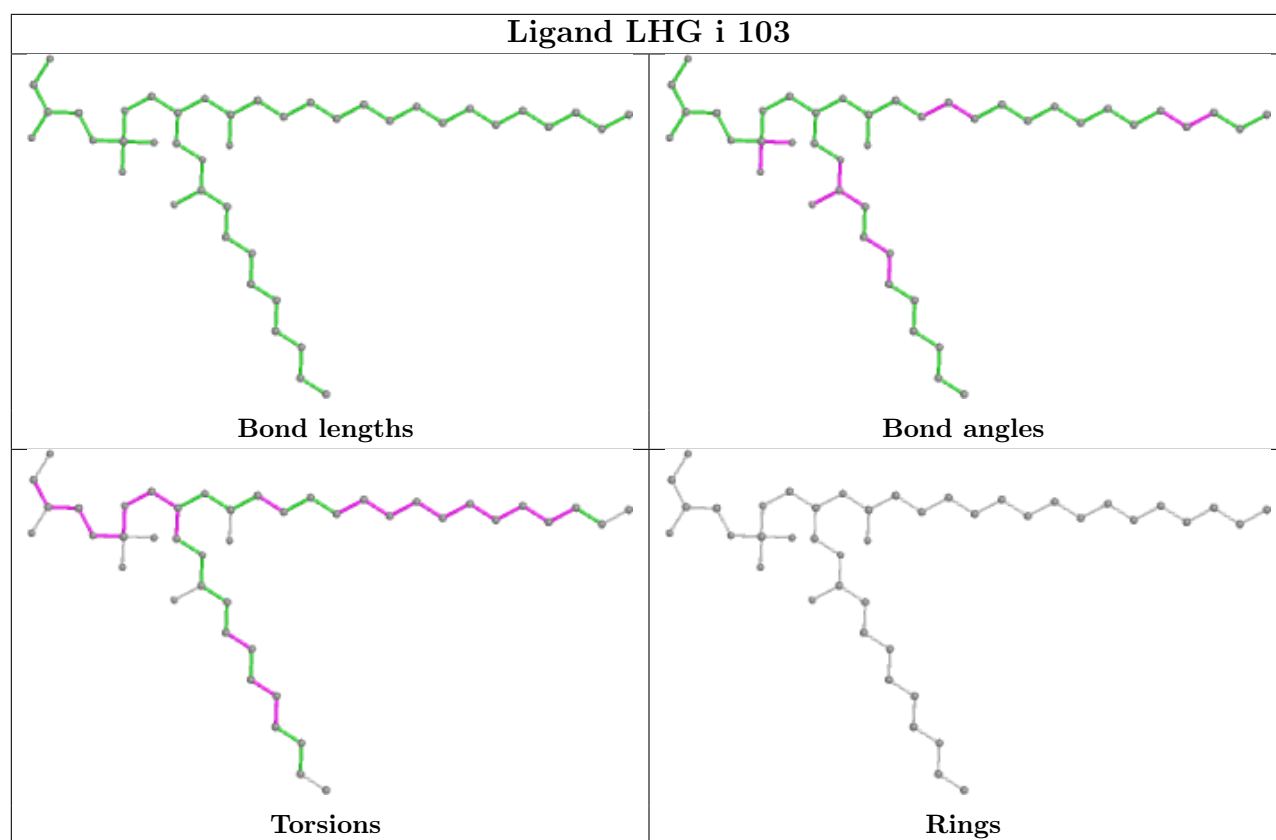
Rings

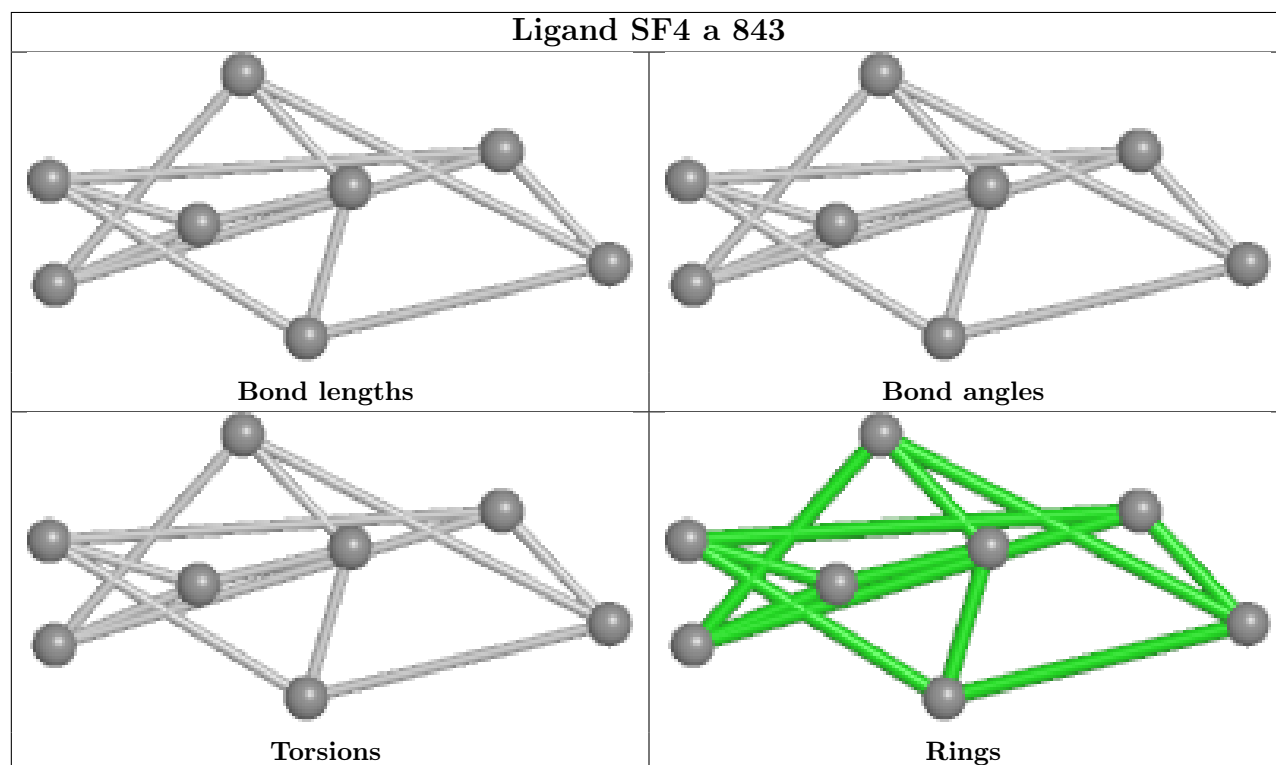
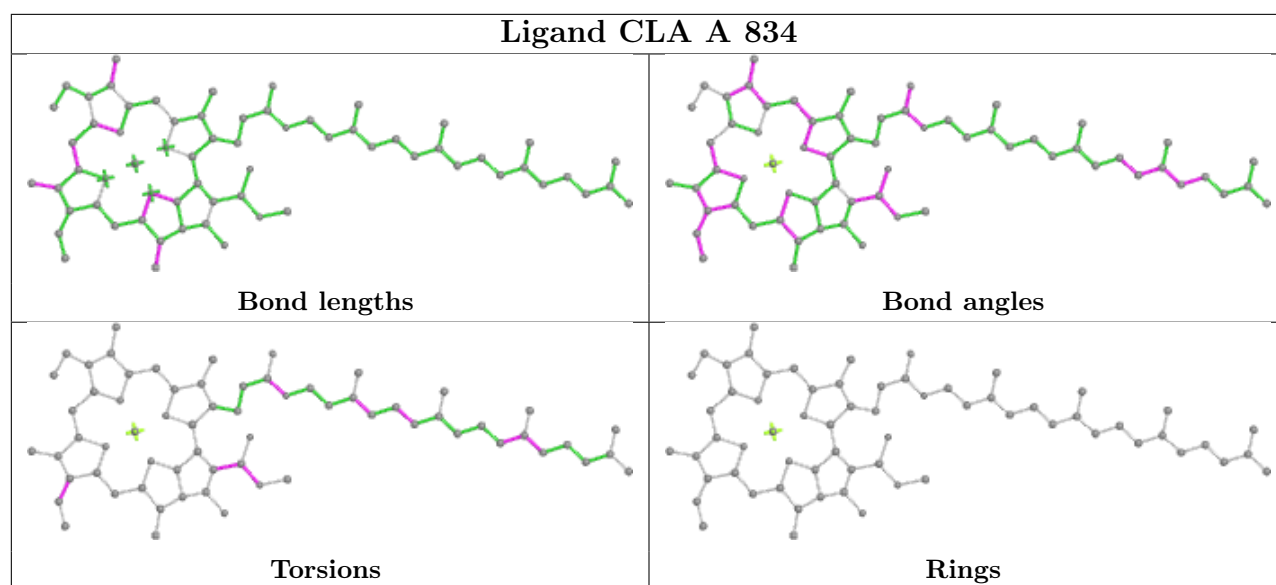
## Ligand CLA a 834



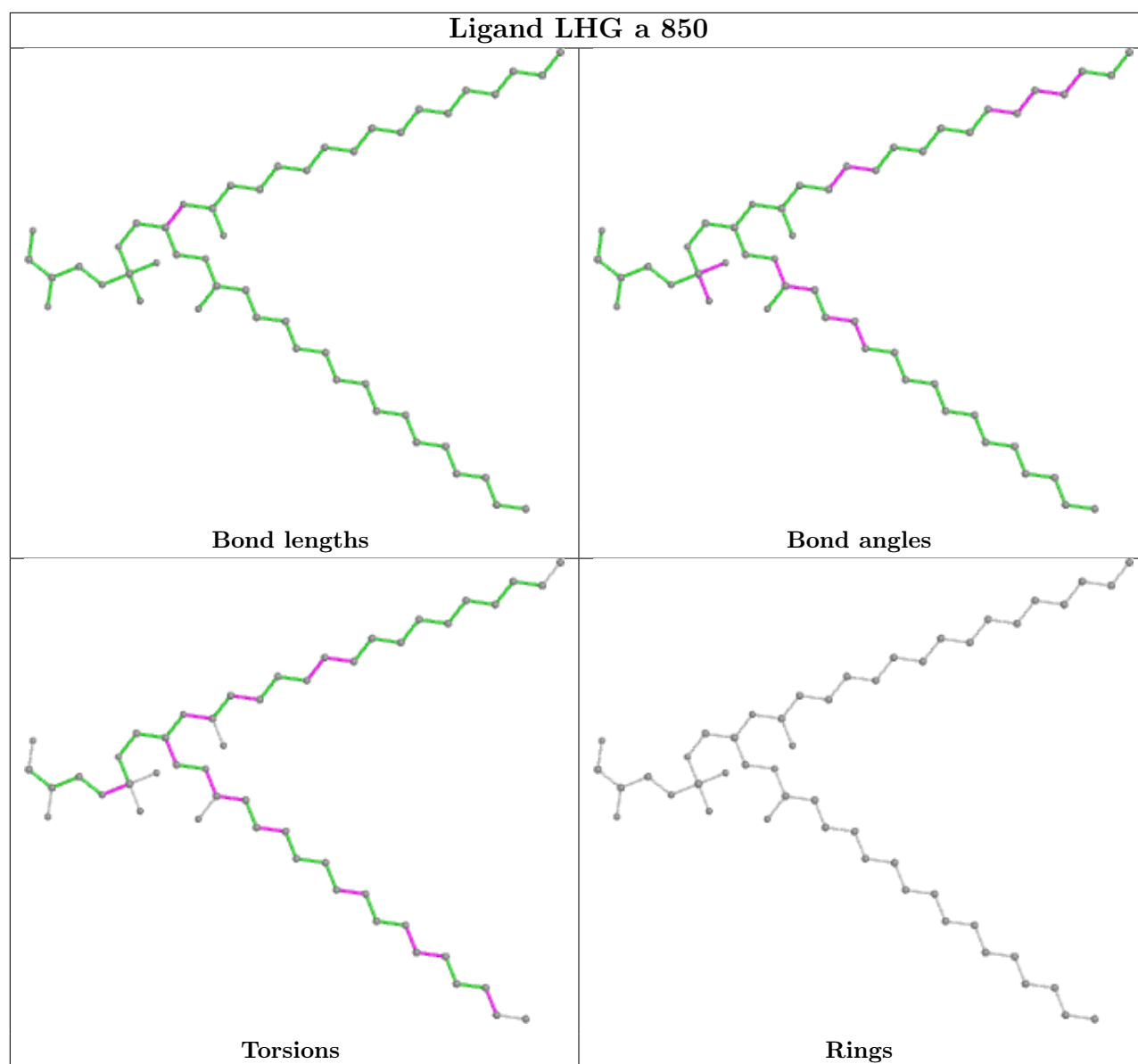
## Ligand CLA a 812

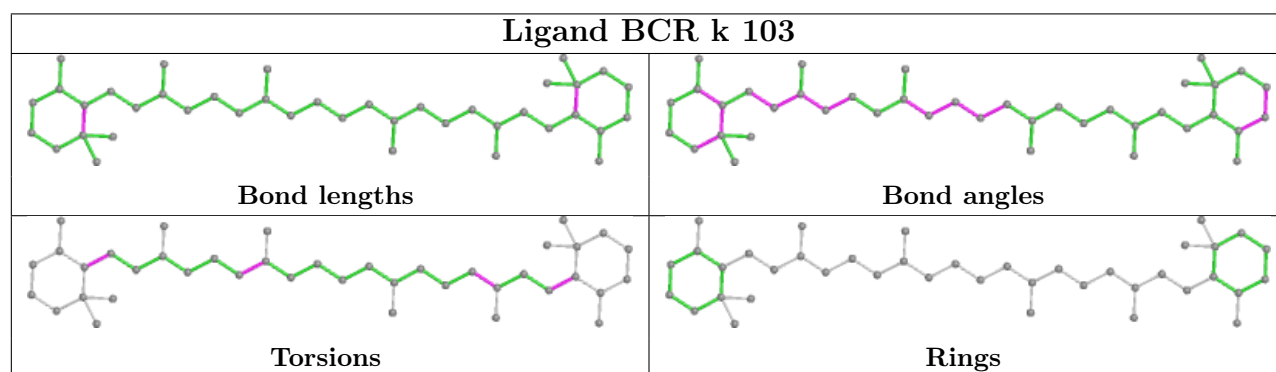
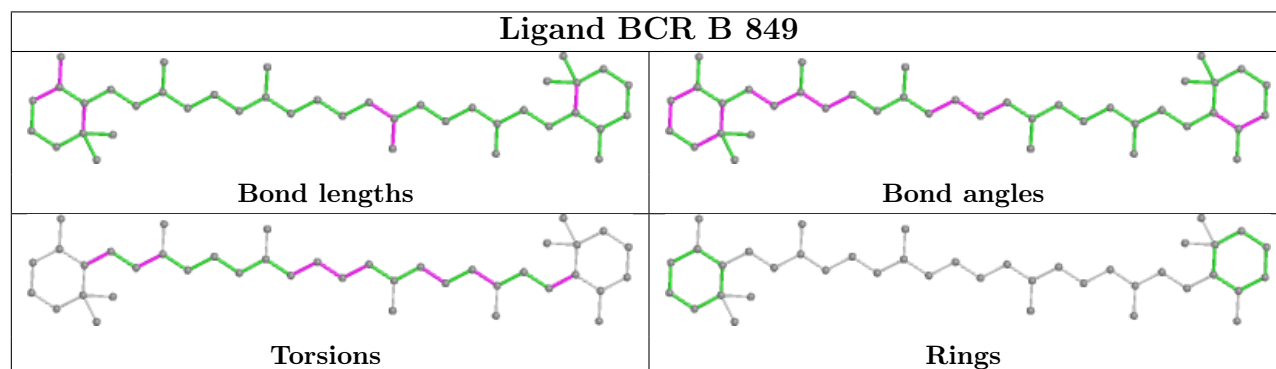
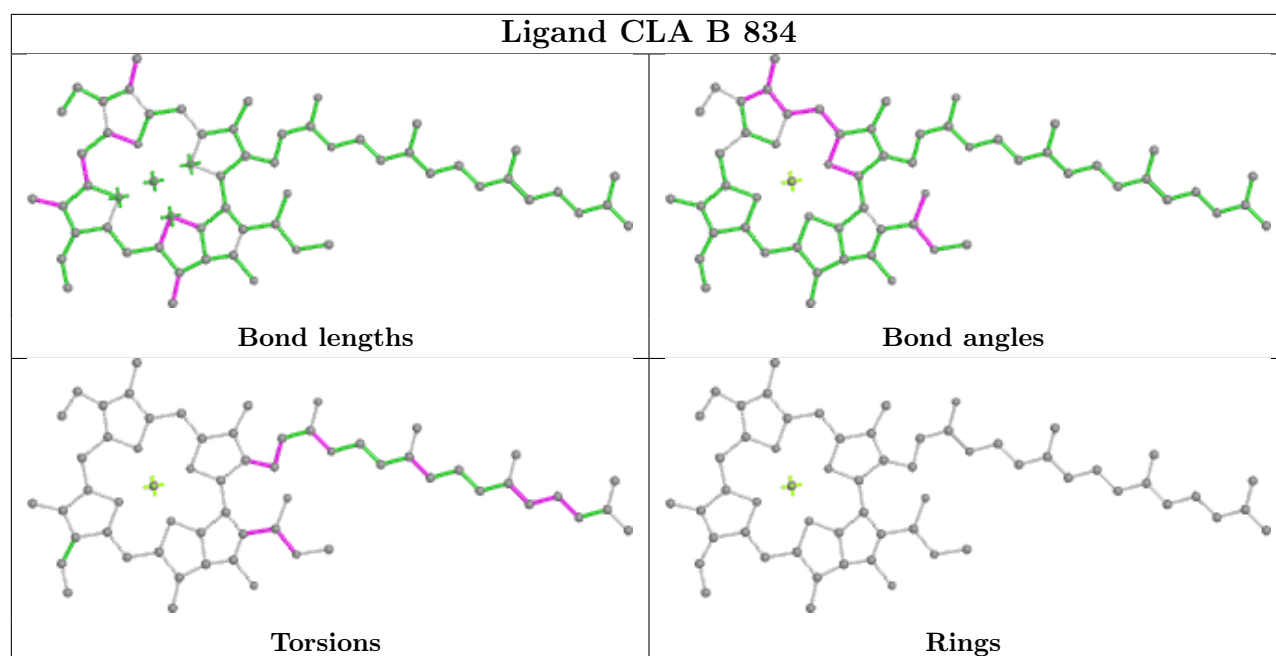


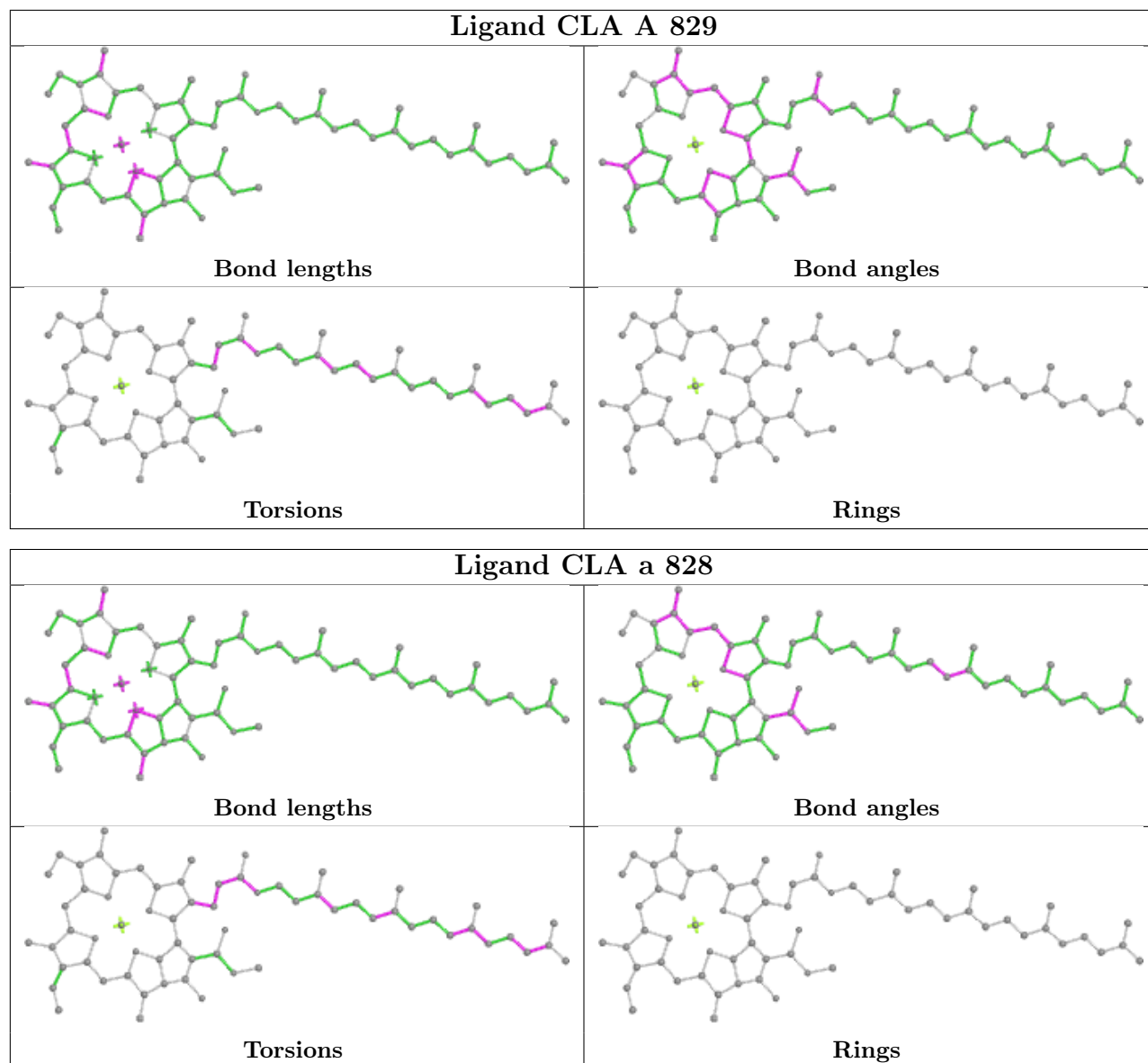


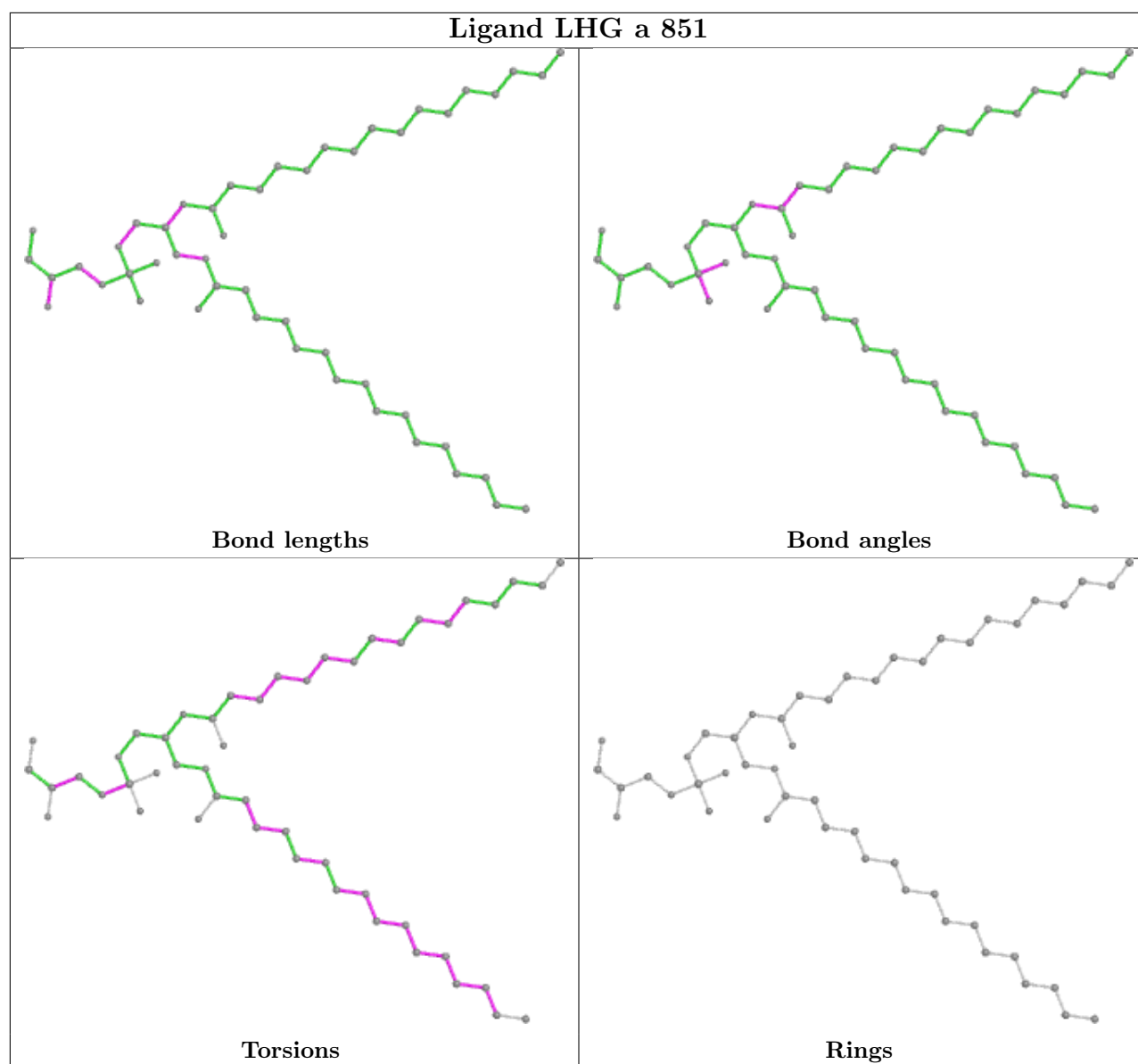




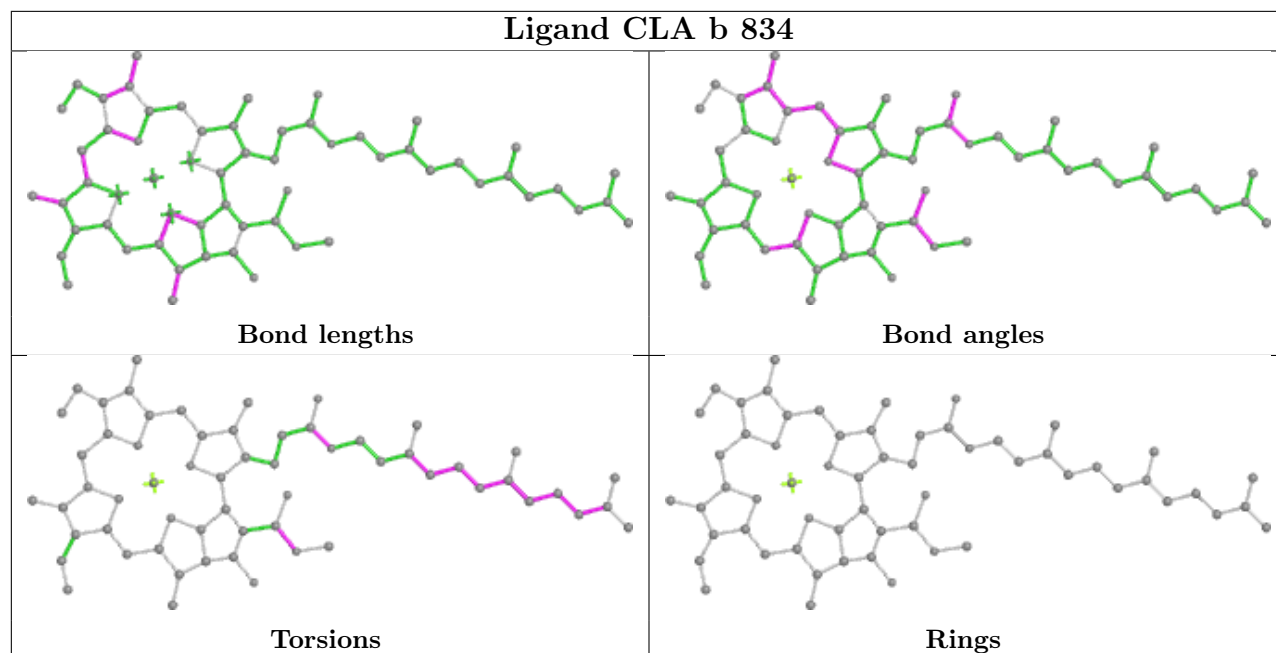




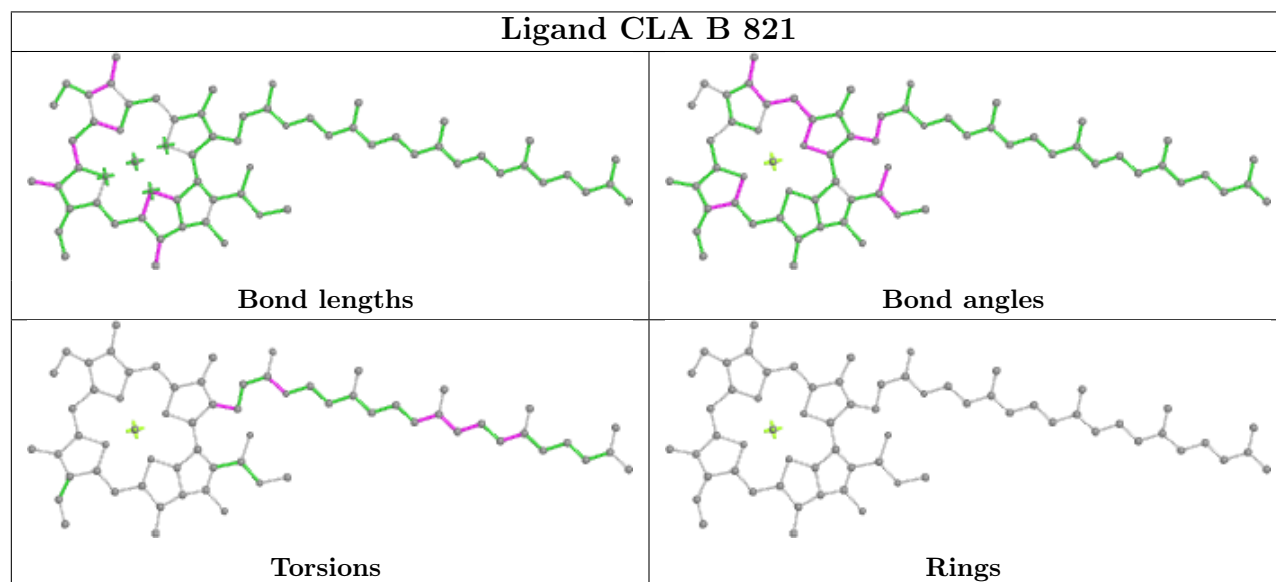




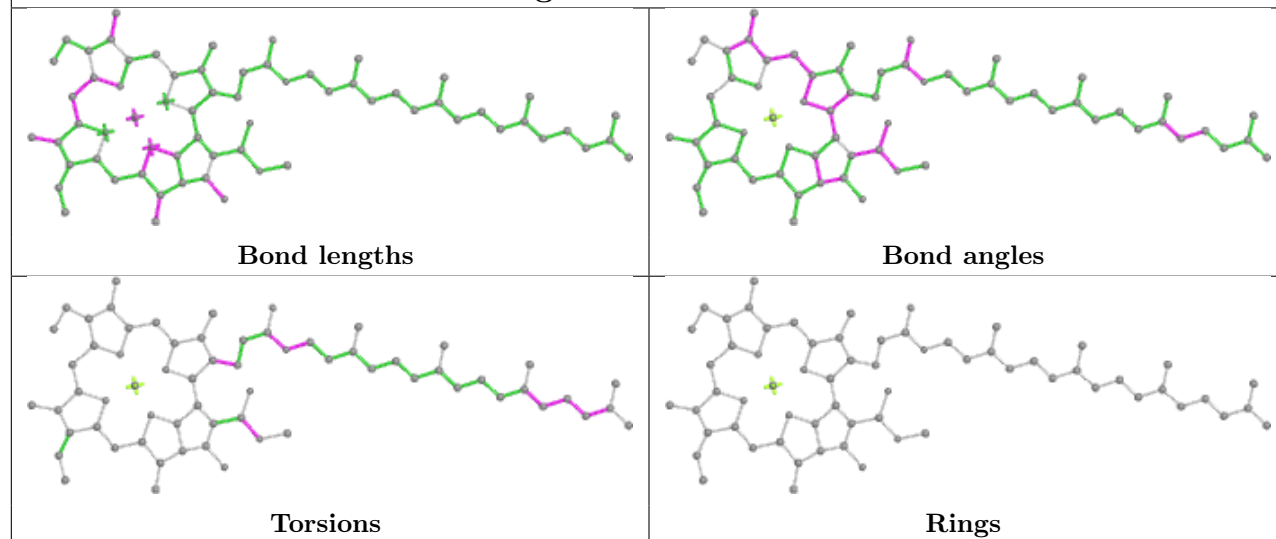
## Ligand CLA b 834



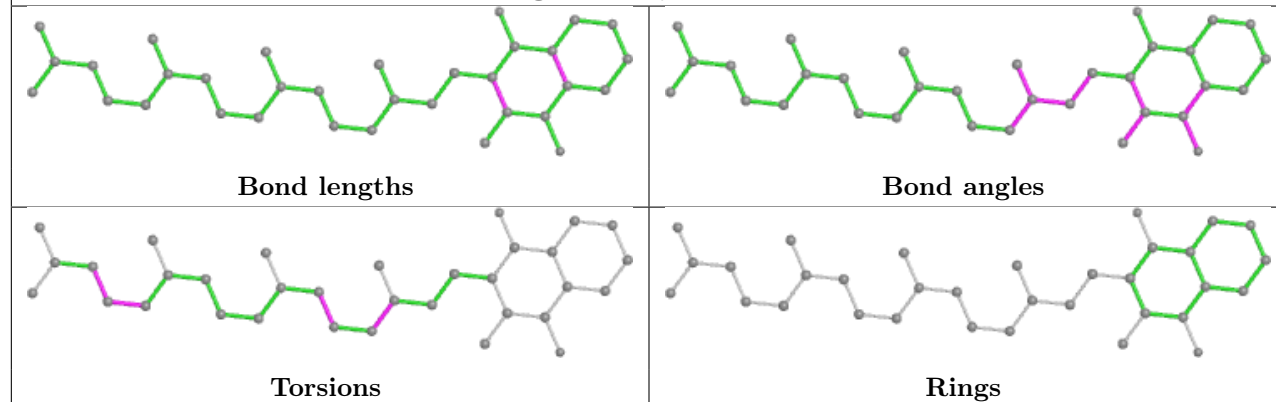
## Ligand CLA B 821



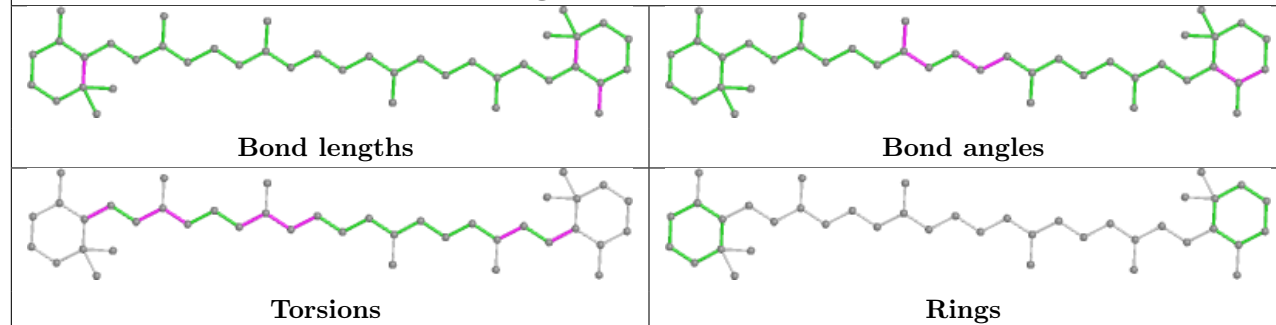
## Ligand CLA b 808



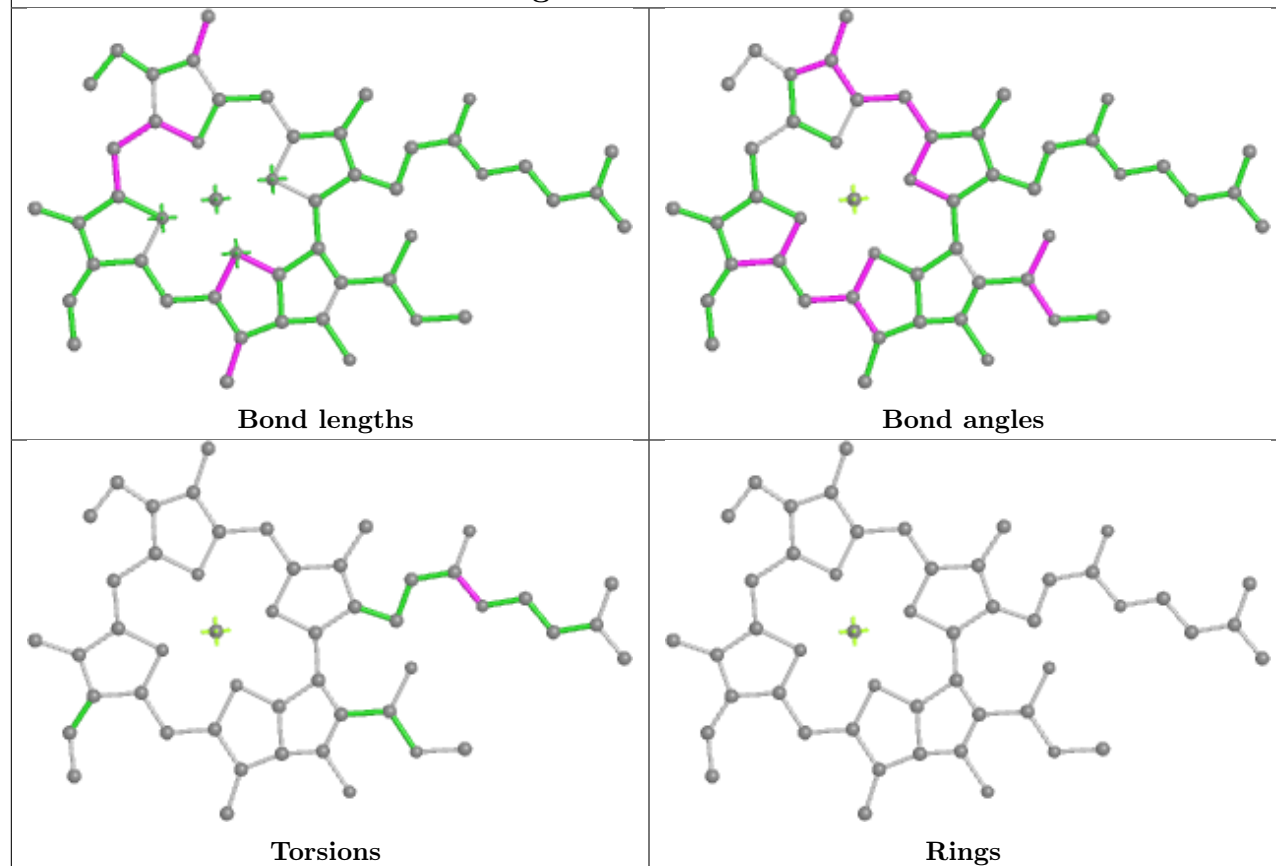
## Ligand PQN B 844



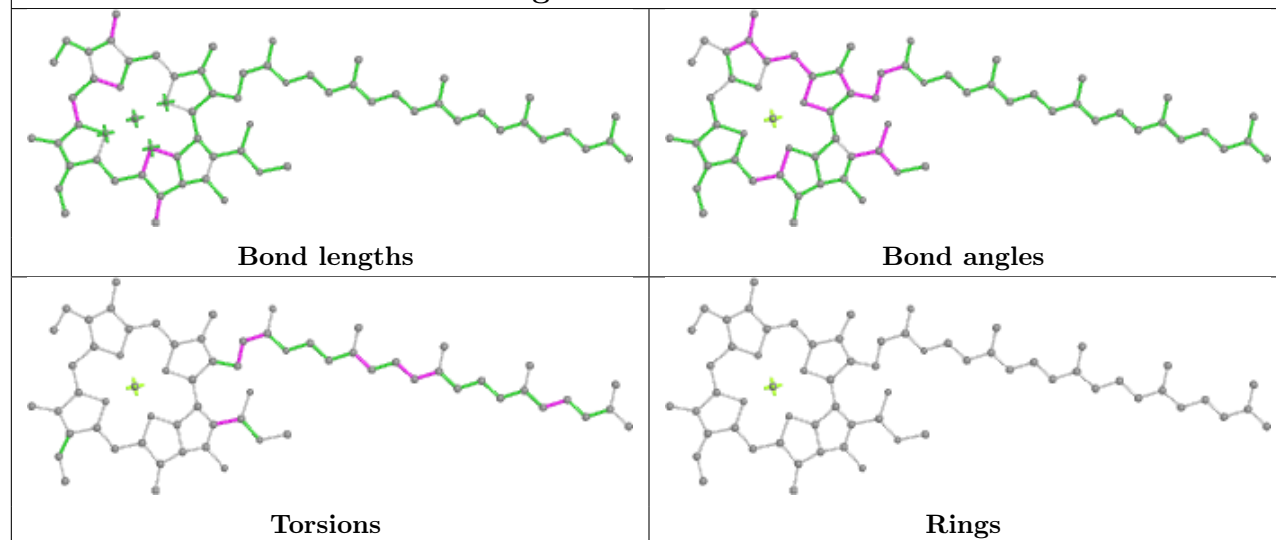
## Ligand BCR b 850

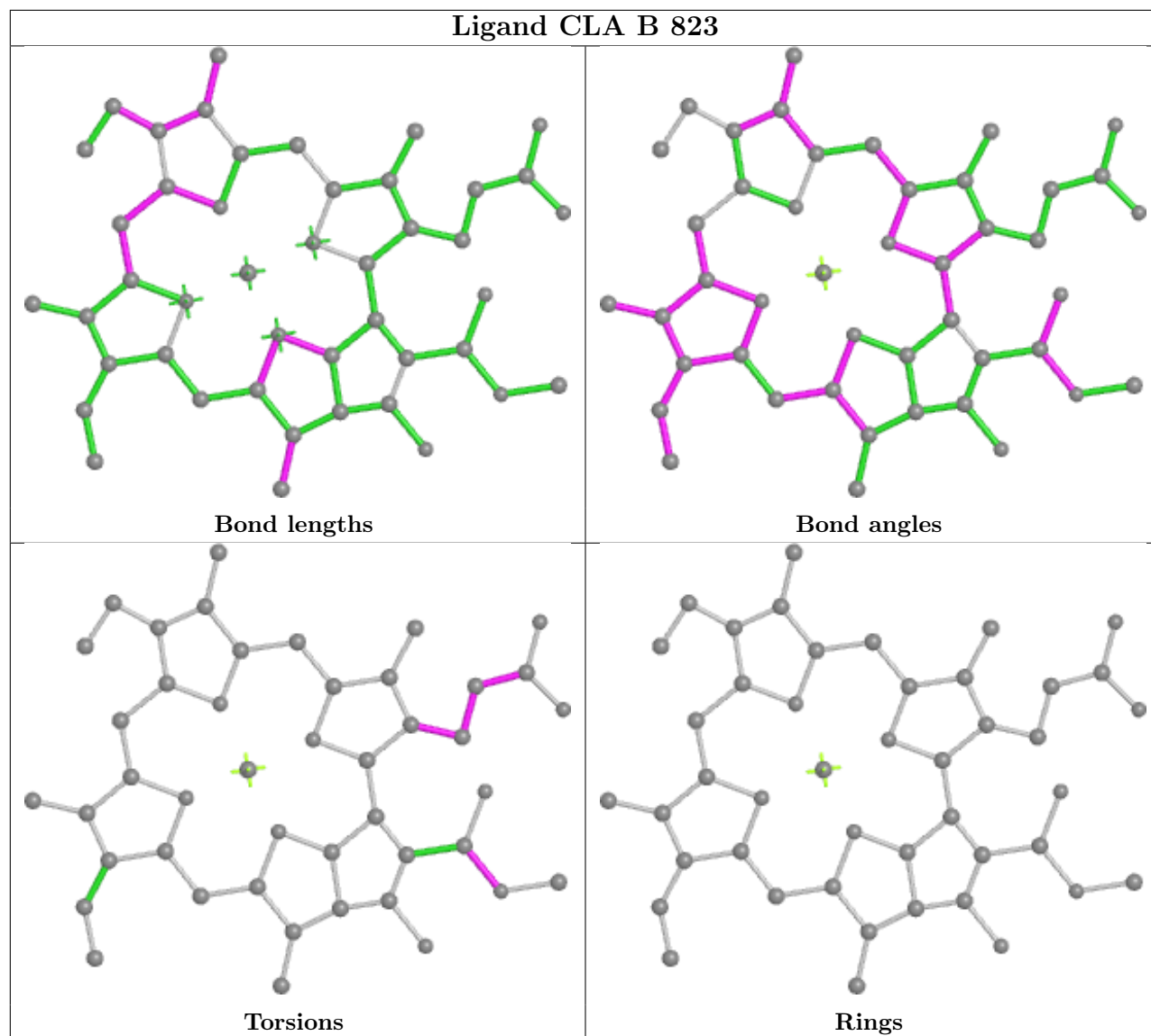
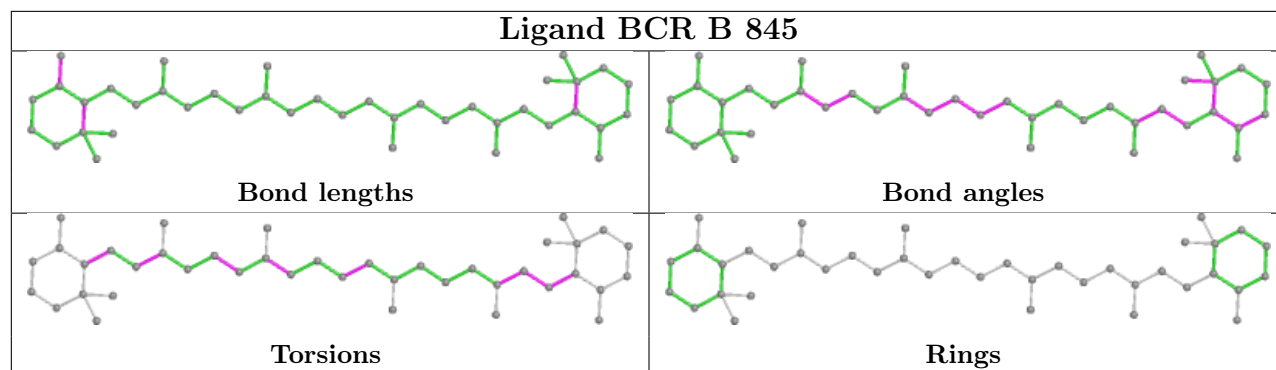


## Ligand CLA B 817



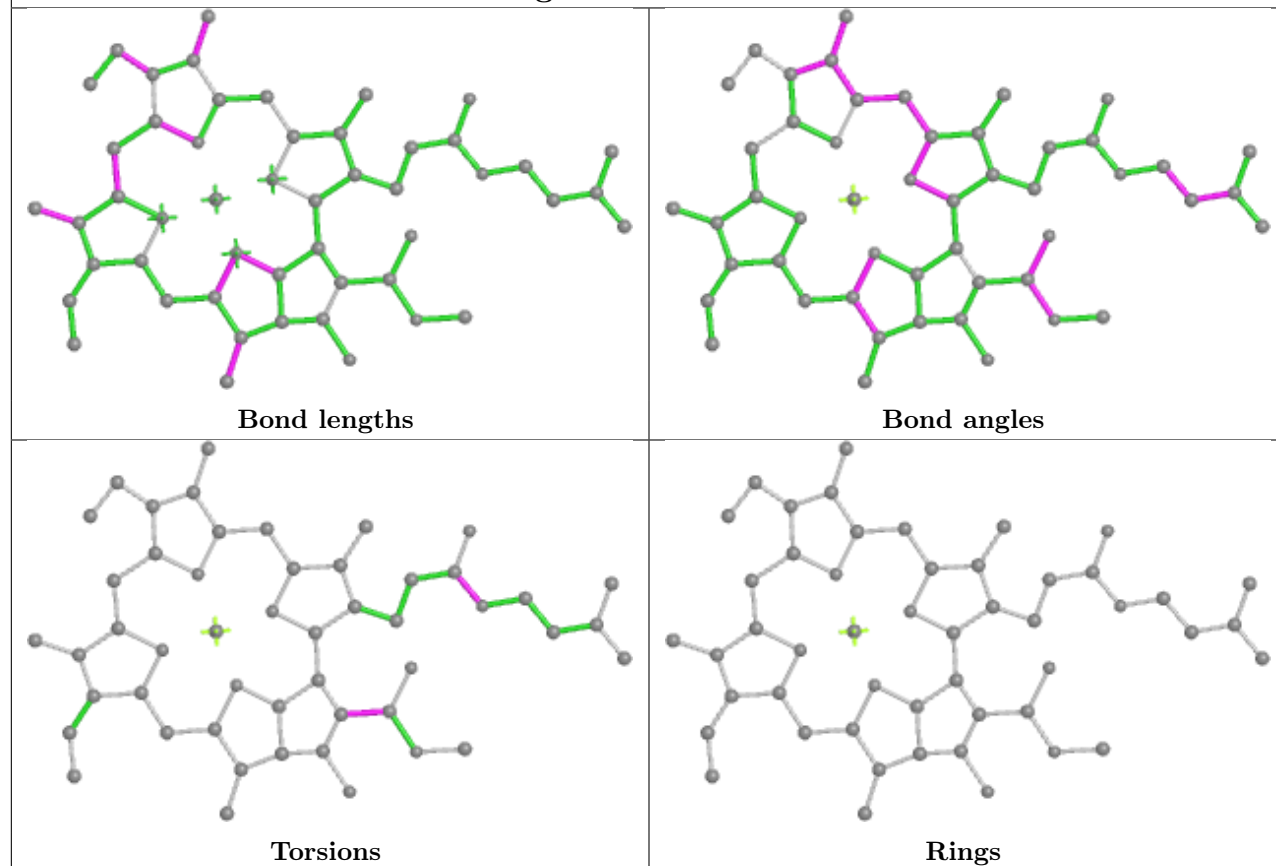
## Ligand CLA B 826



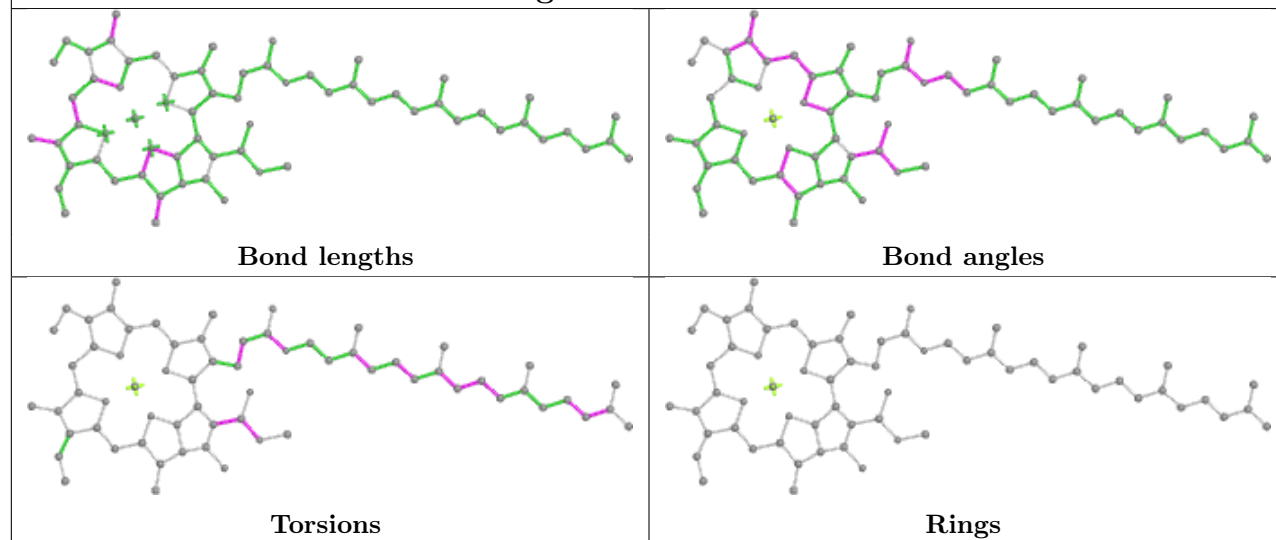


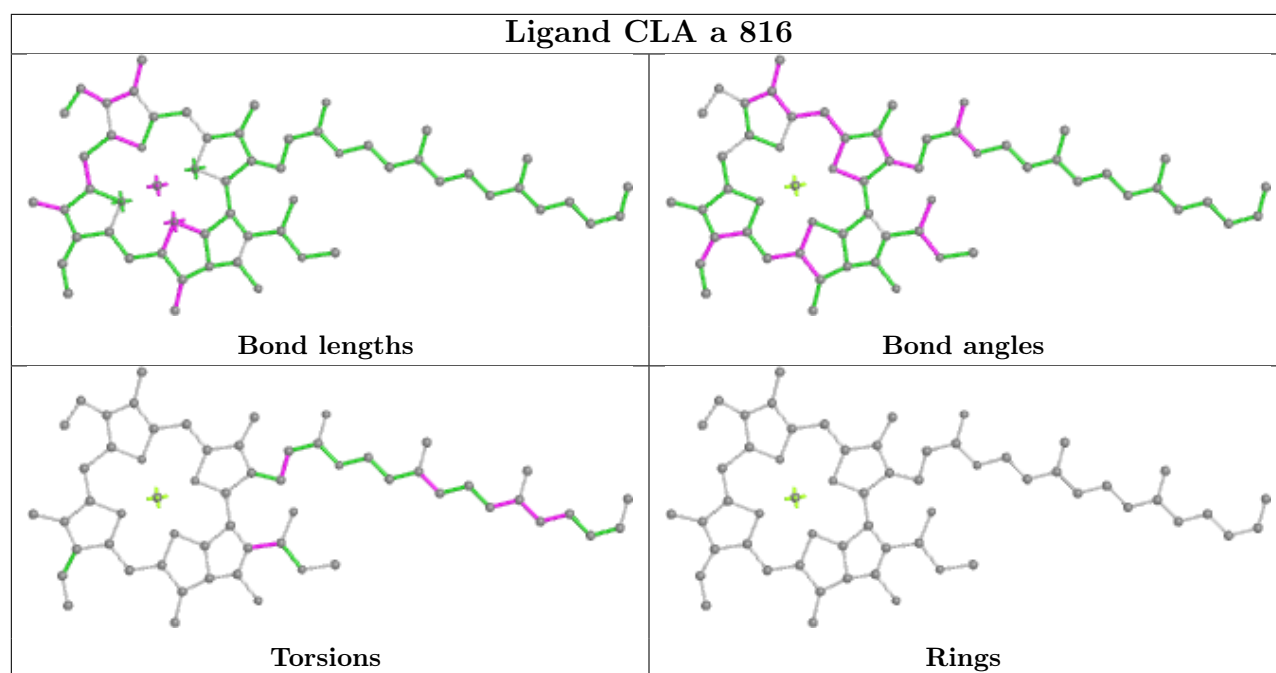


## Ligand CLA b 817

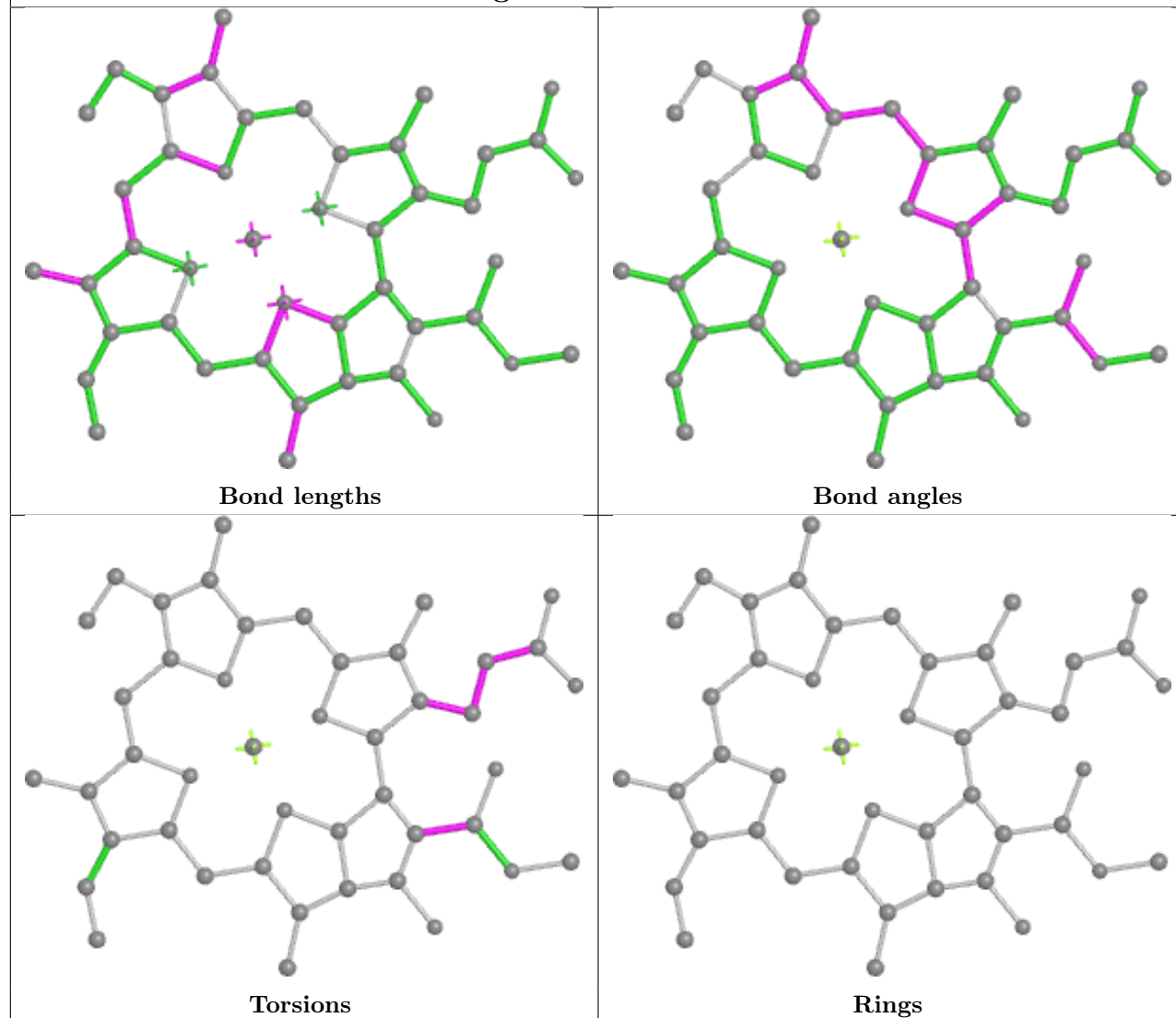


## Ligand CLA a 820

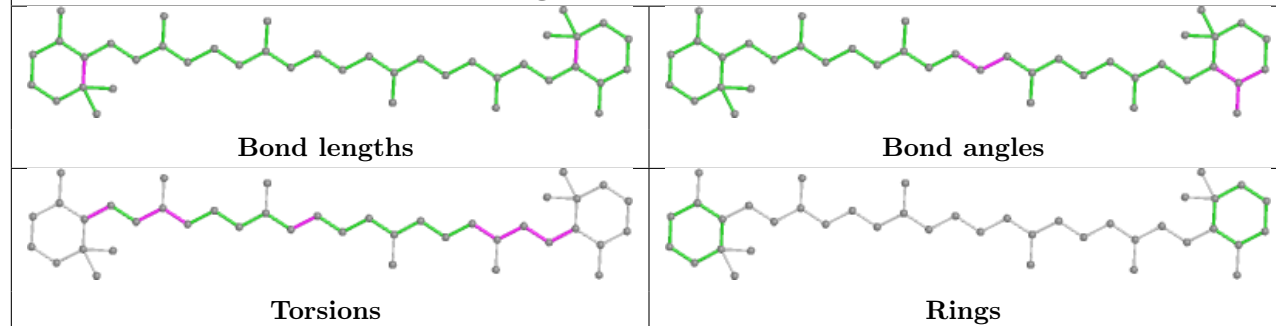




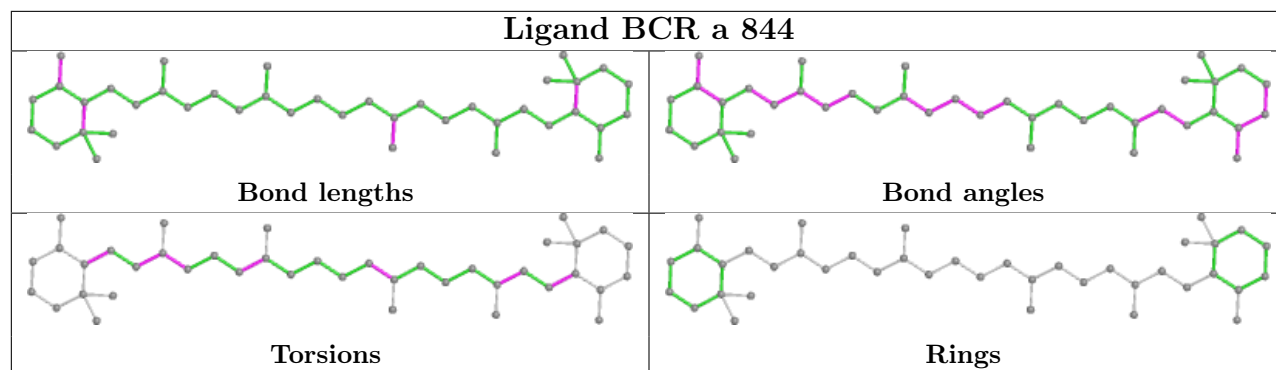
## Ligand CLA b 823



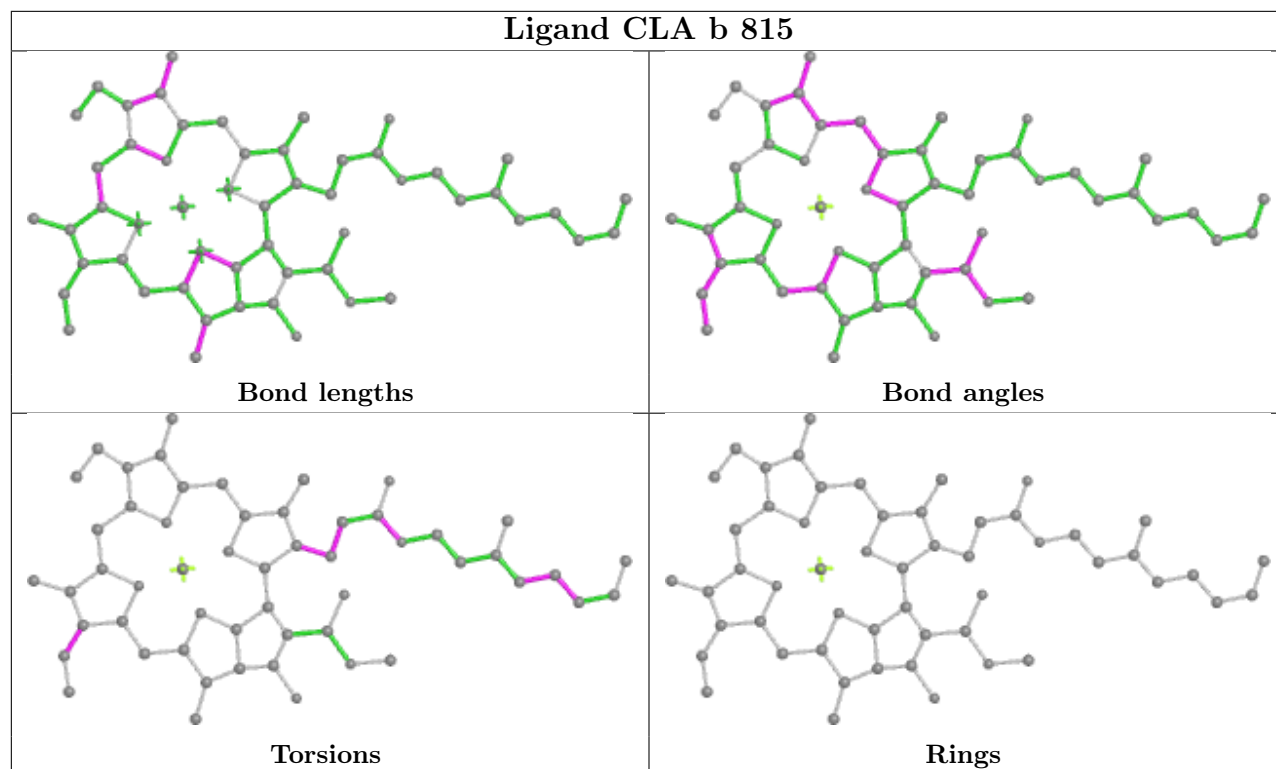
## Ligand BCR b 845



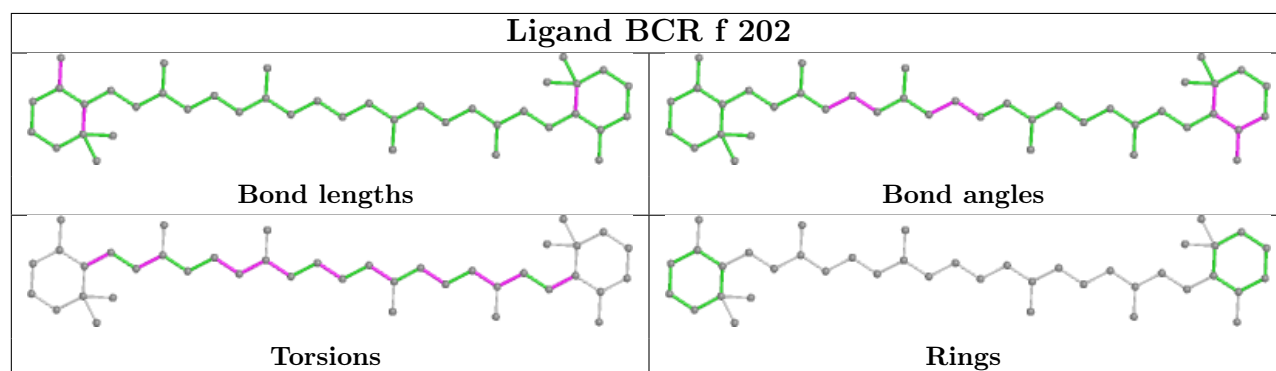
## Ligand BCR a 844



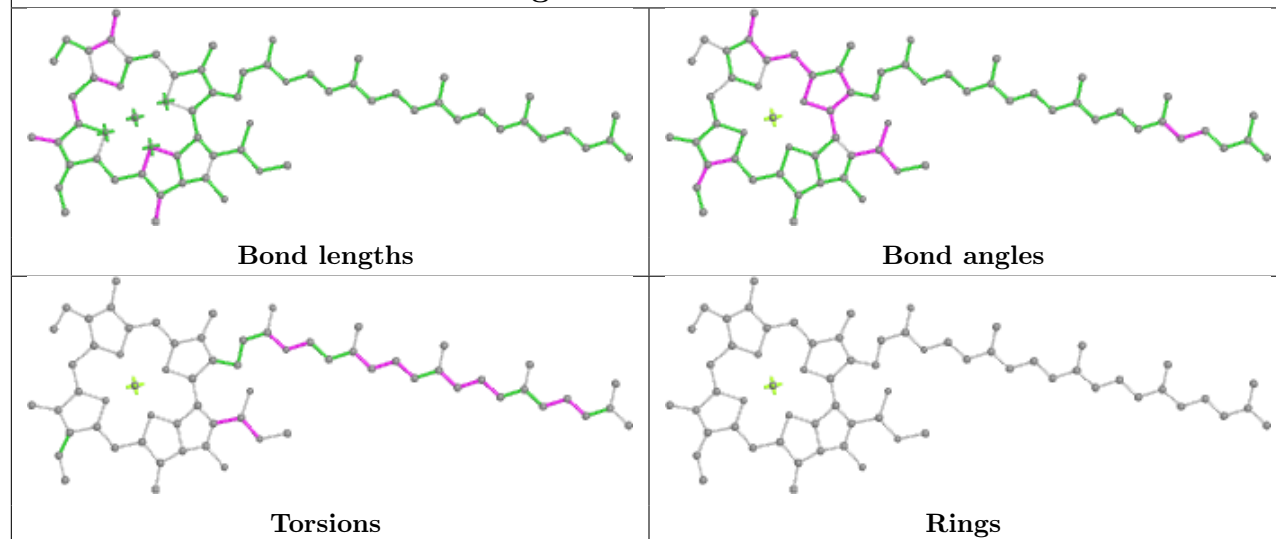
## Ligand CLA b 815



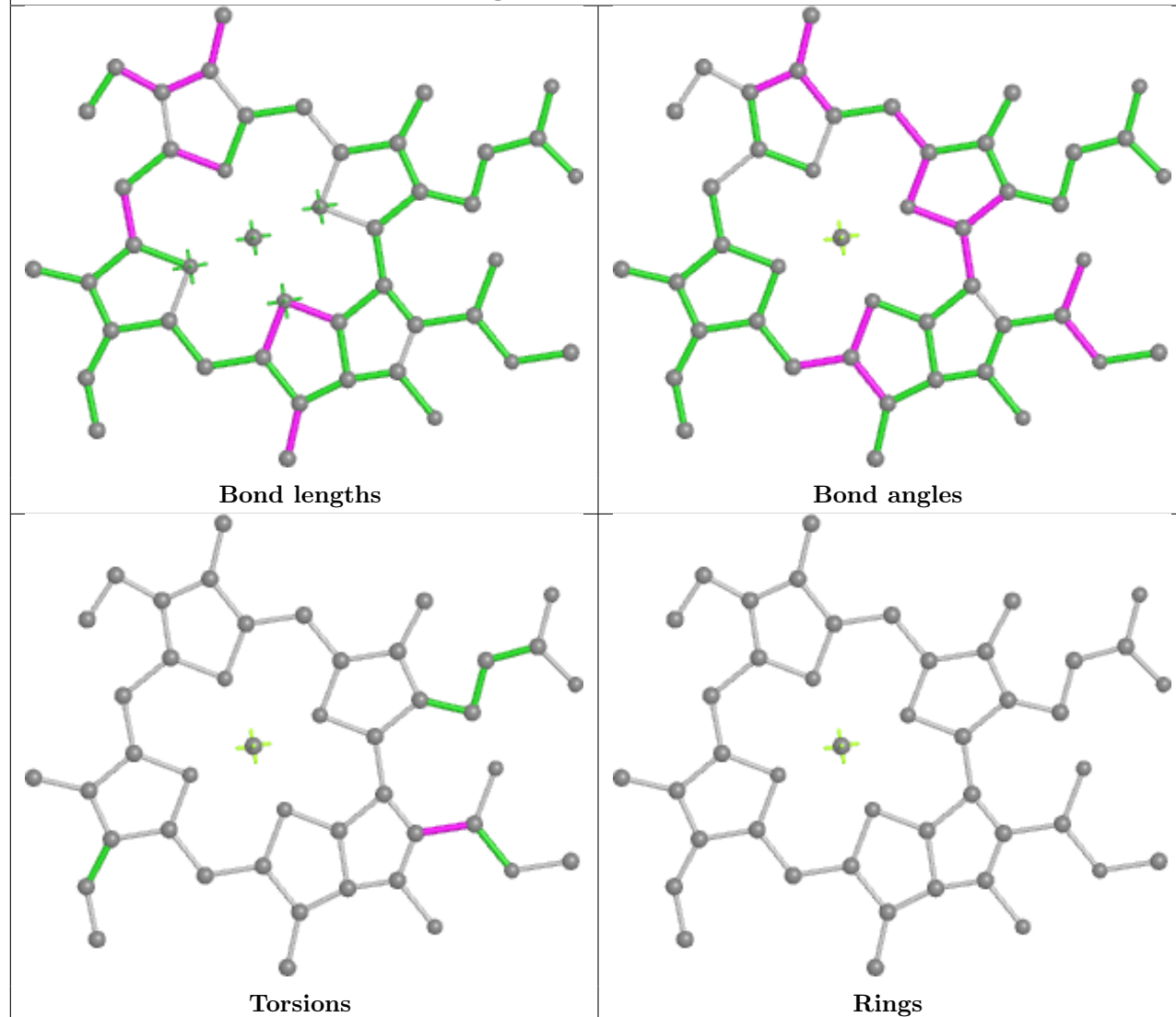
## Ligand BCR f 202

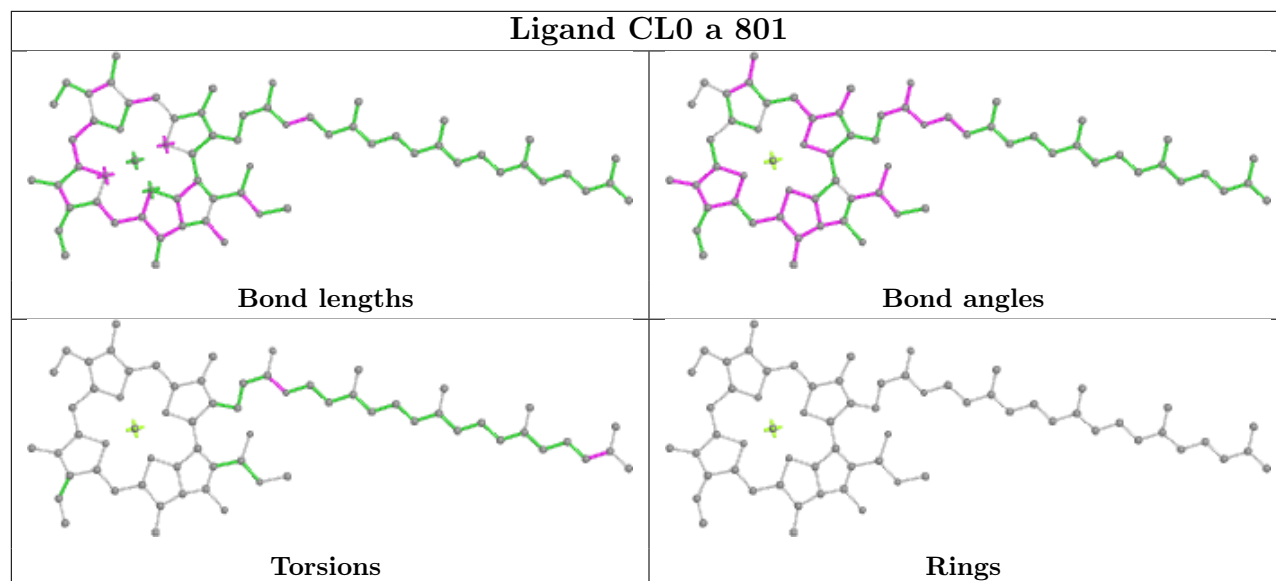
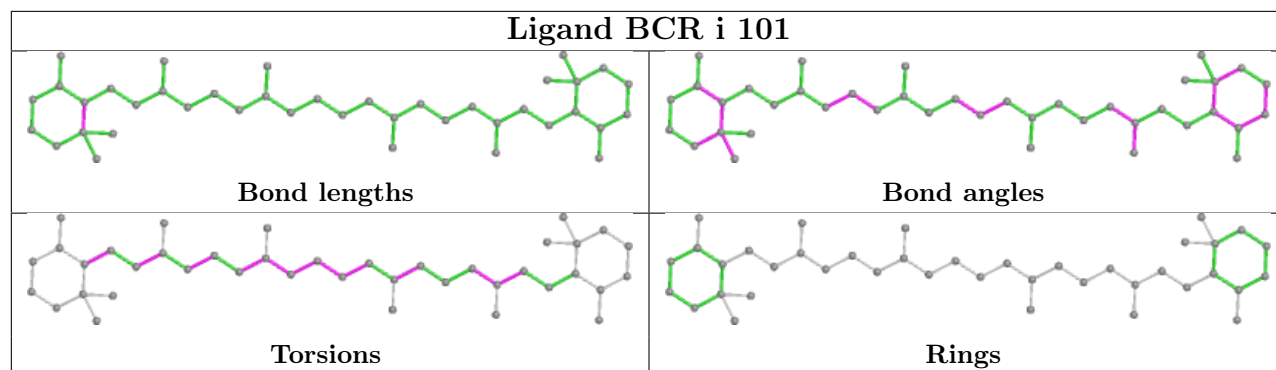


## Ligand CLA A 839

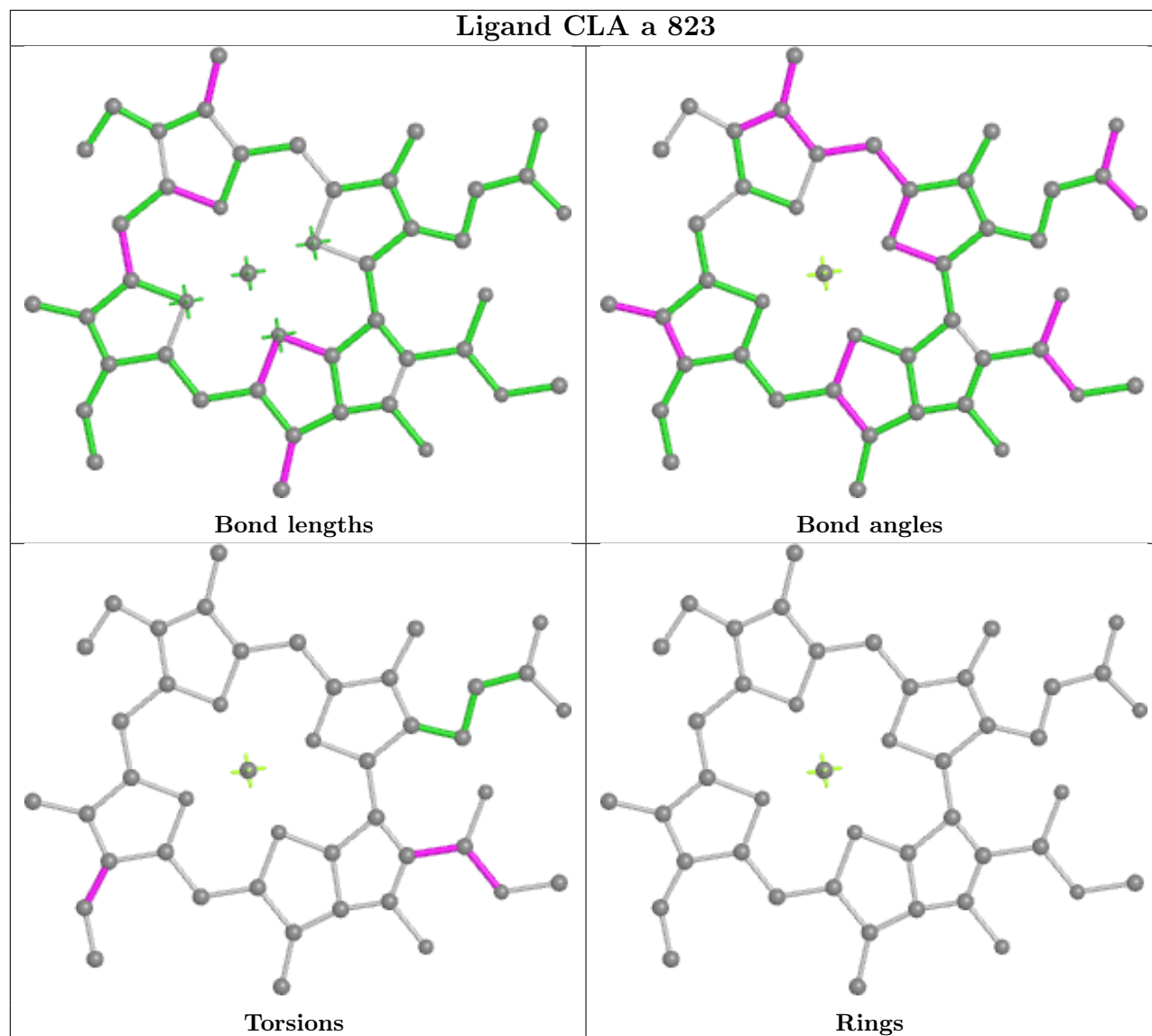


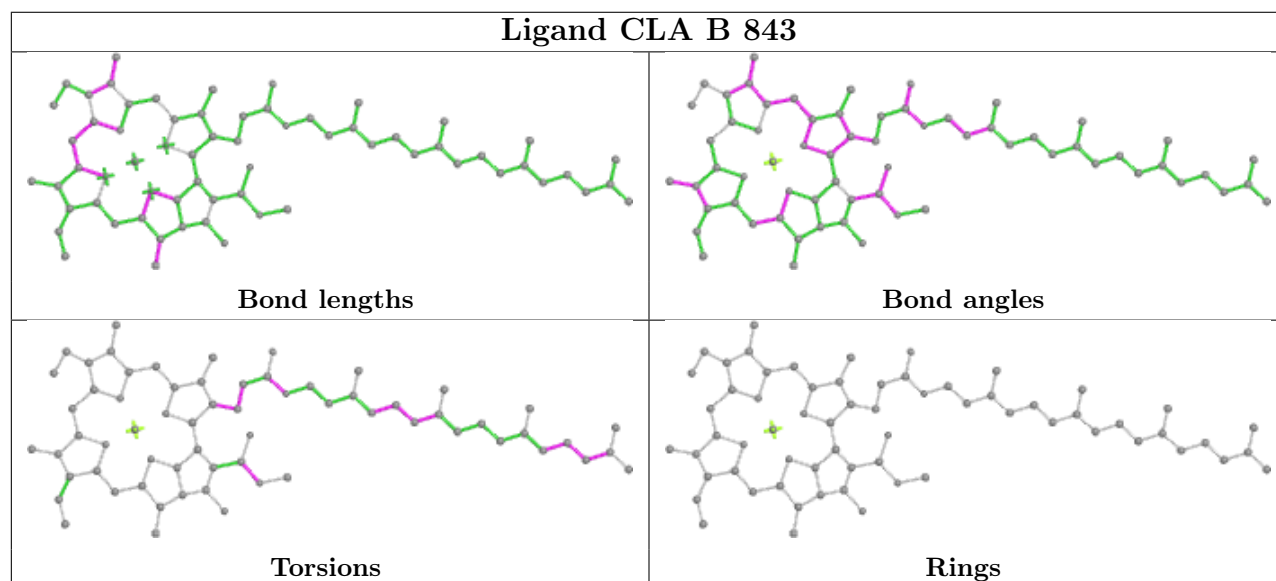
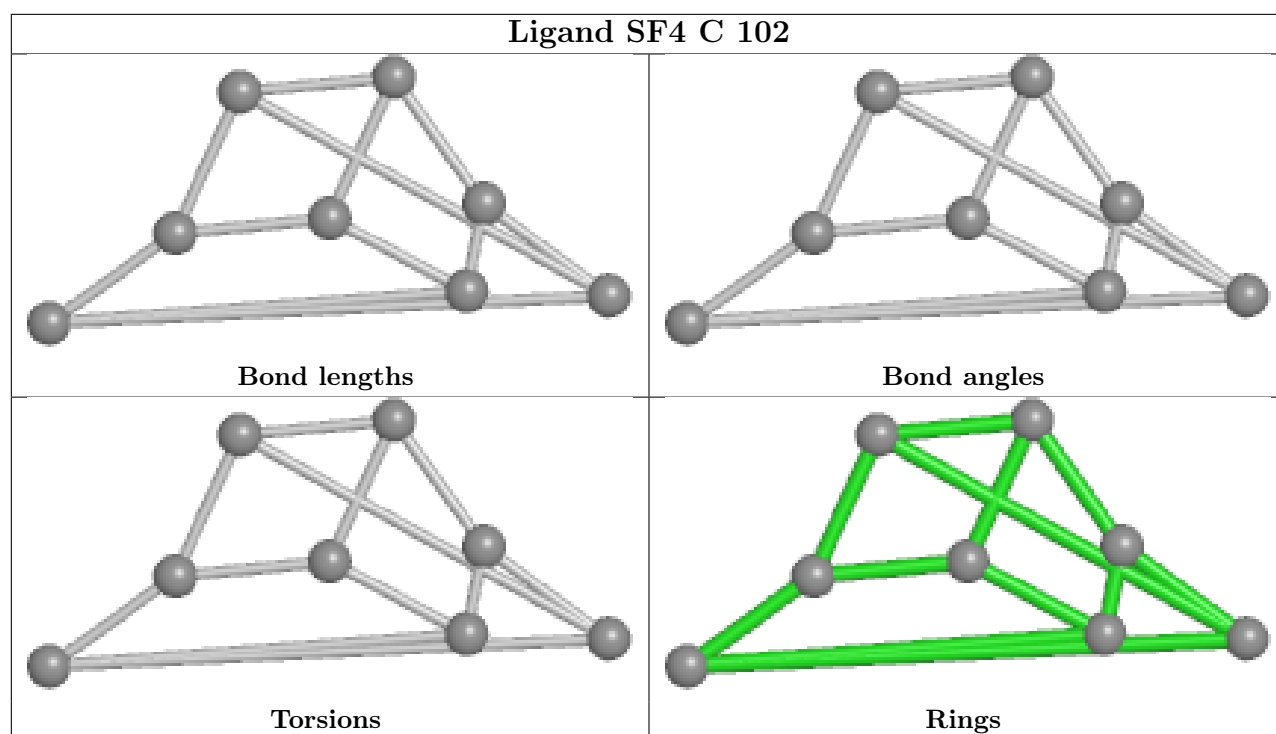
## Ligand CLA A 824





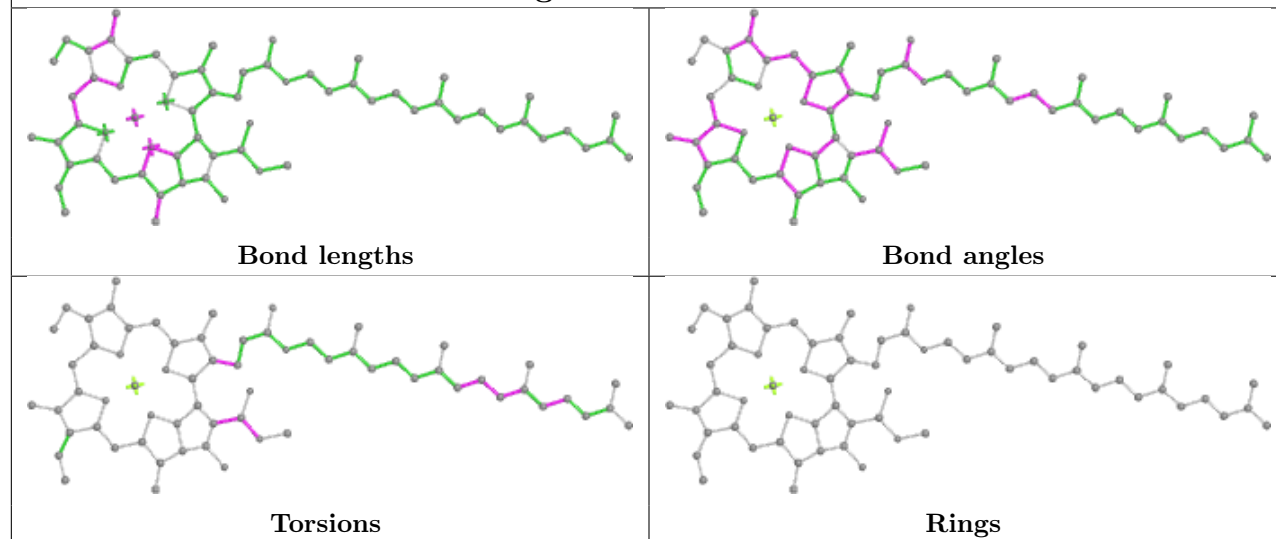
## Ligand CLA a 823



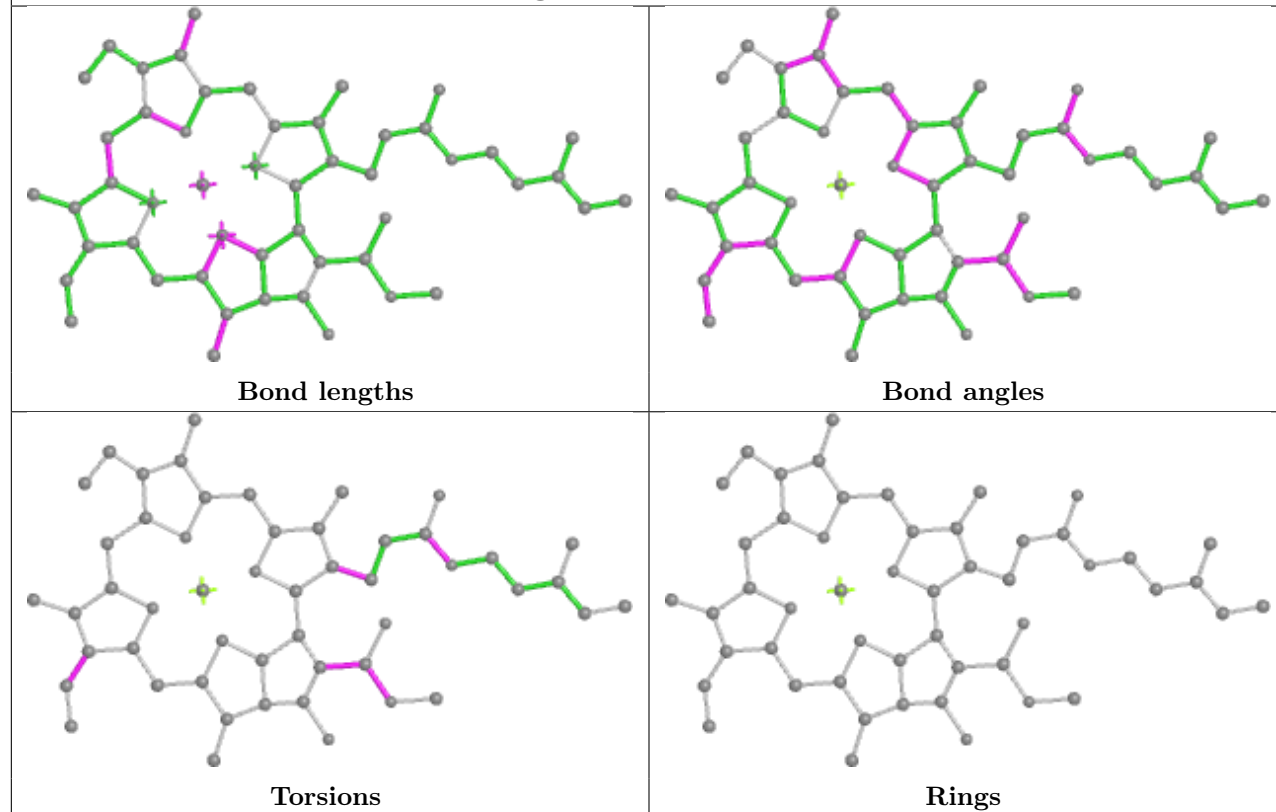


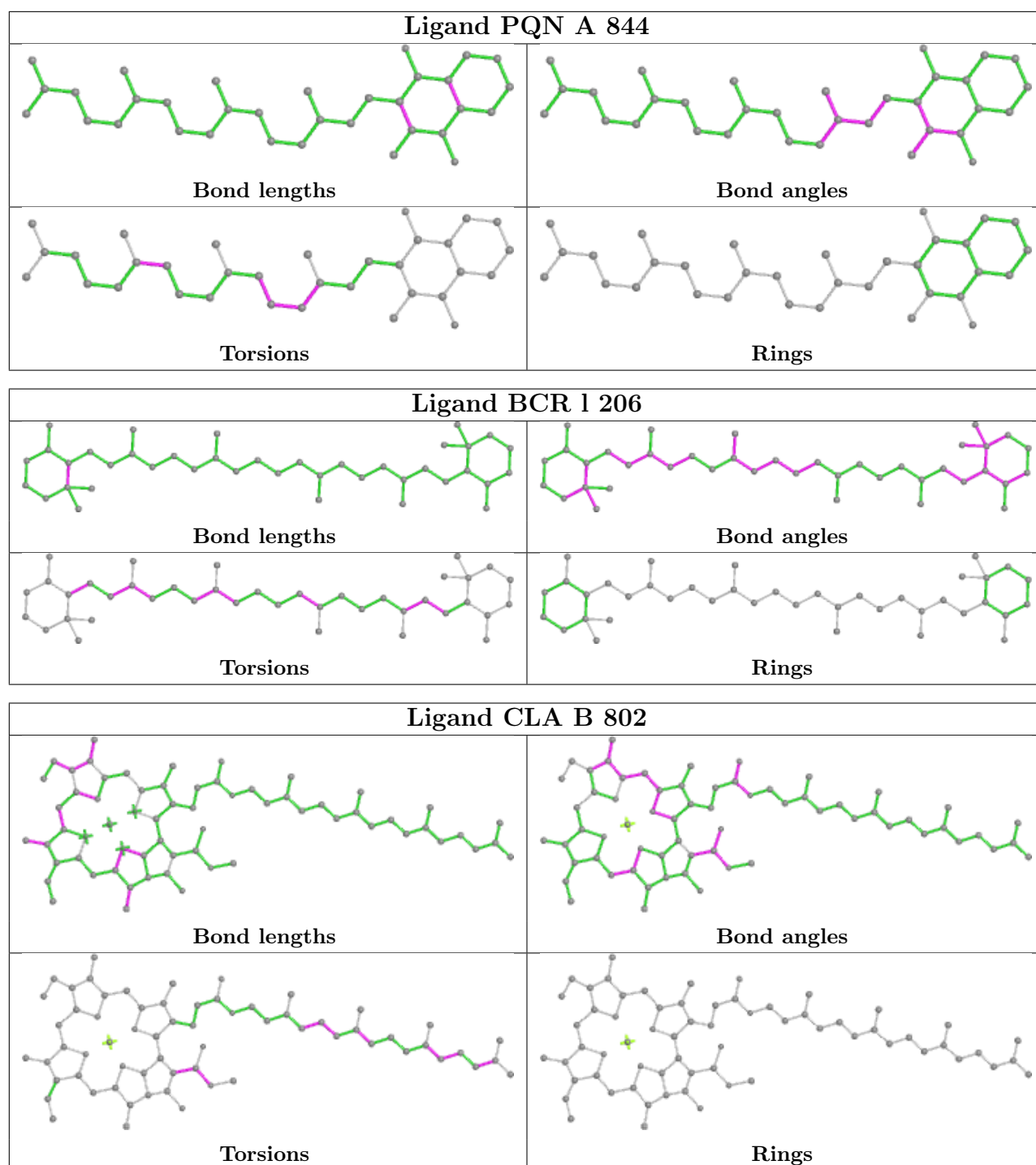


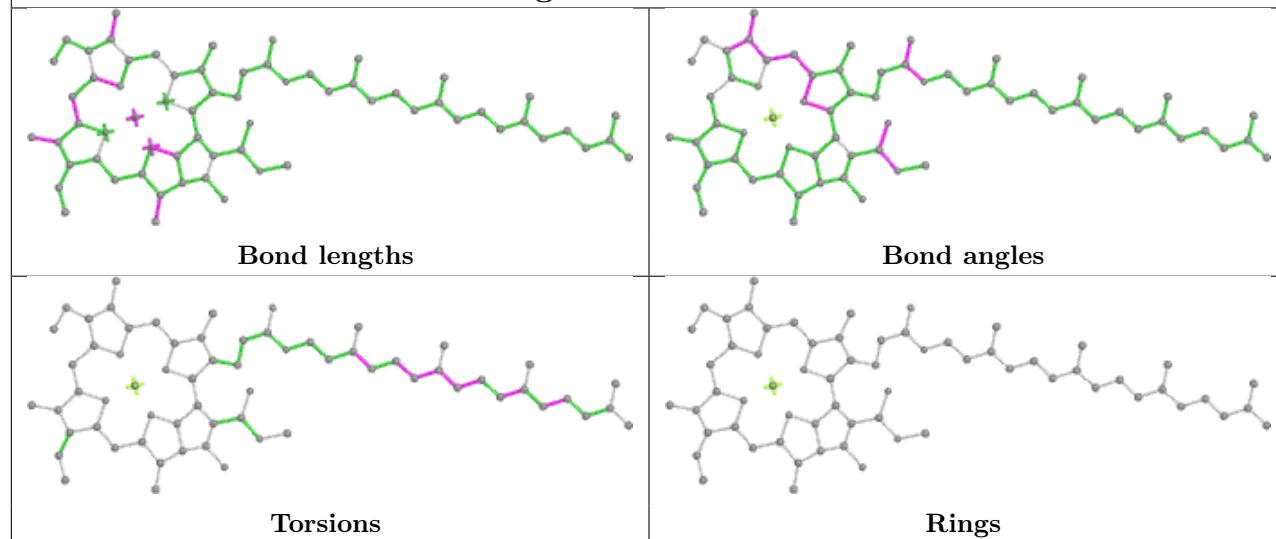
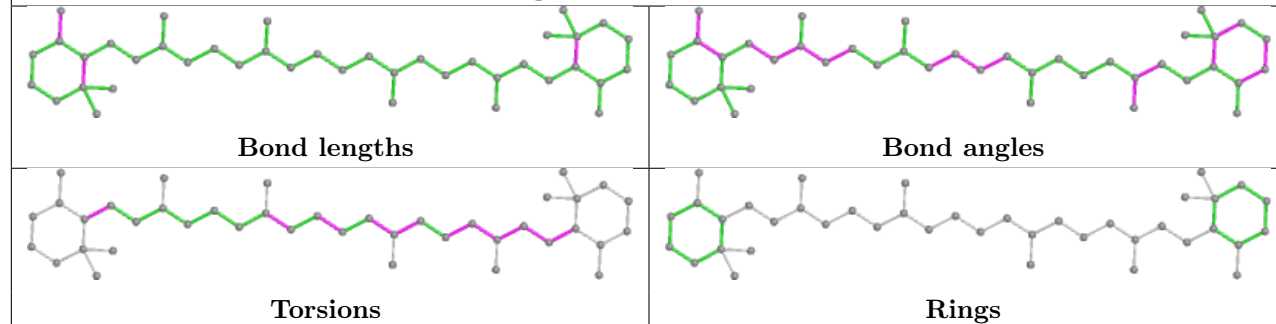
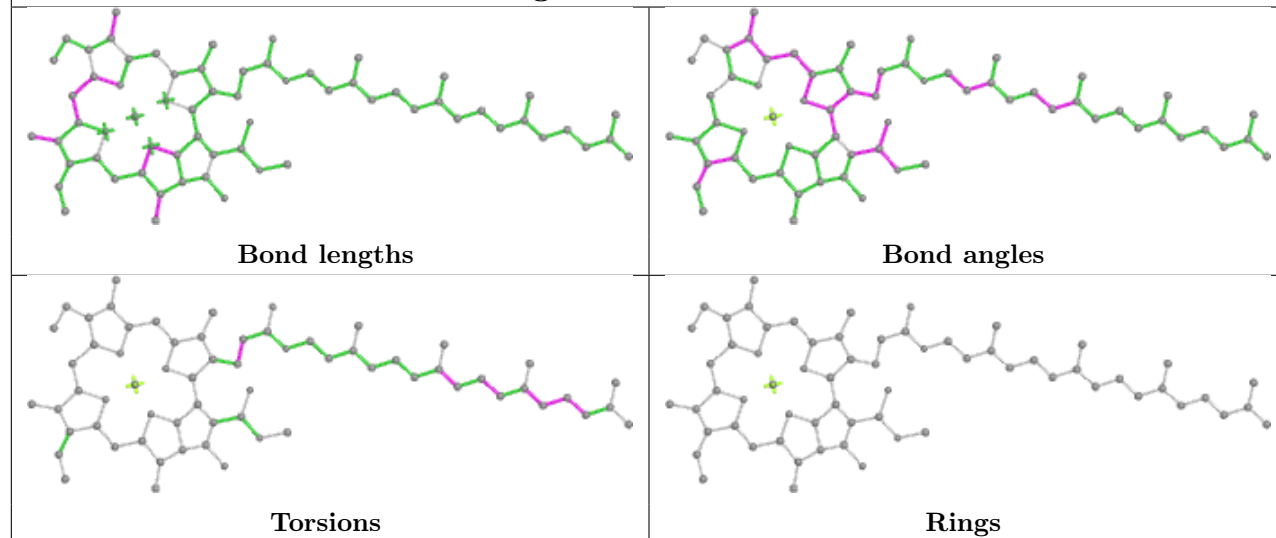
## Ligand CLA b 832

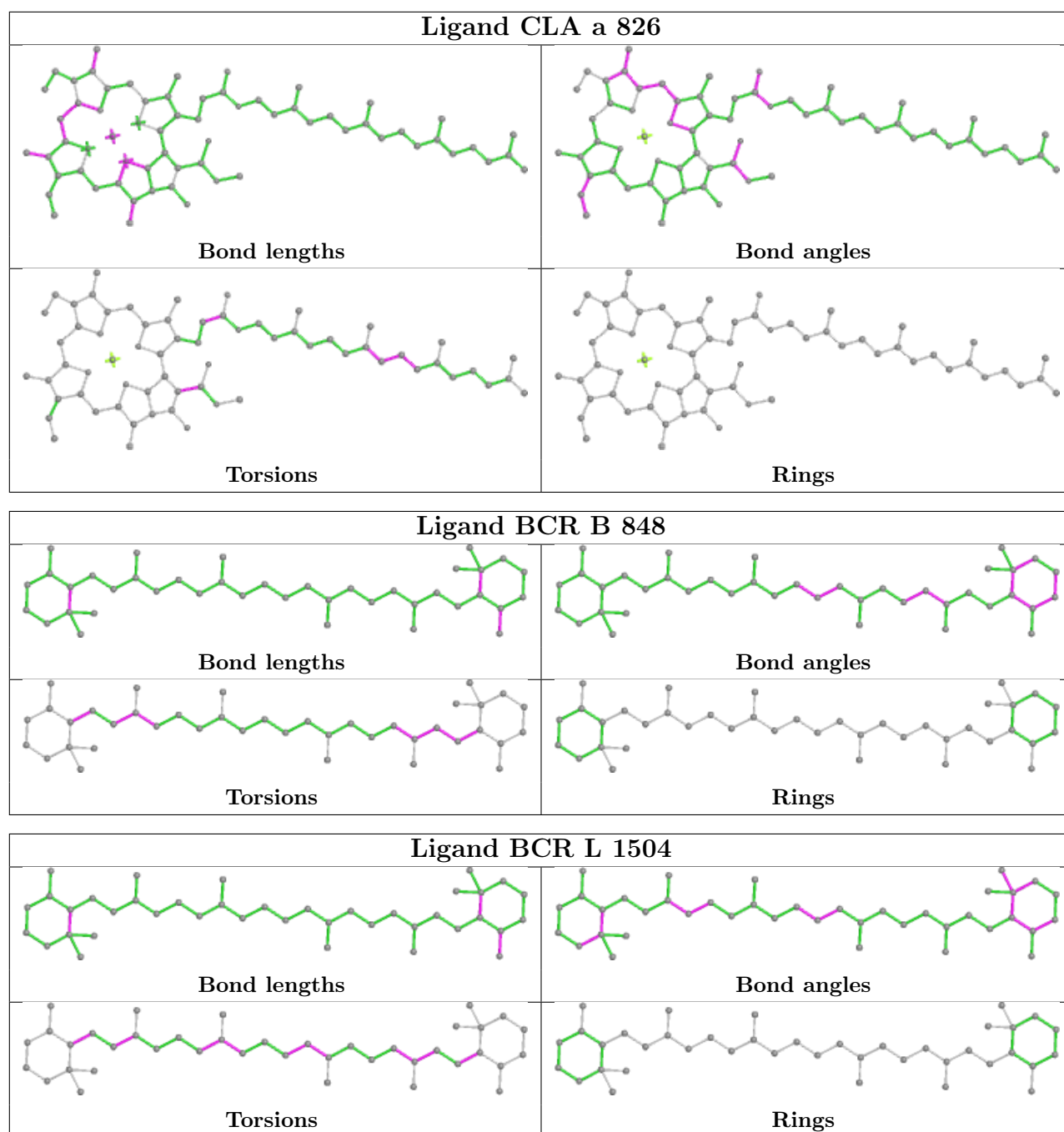


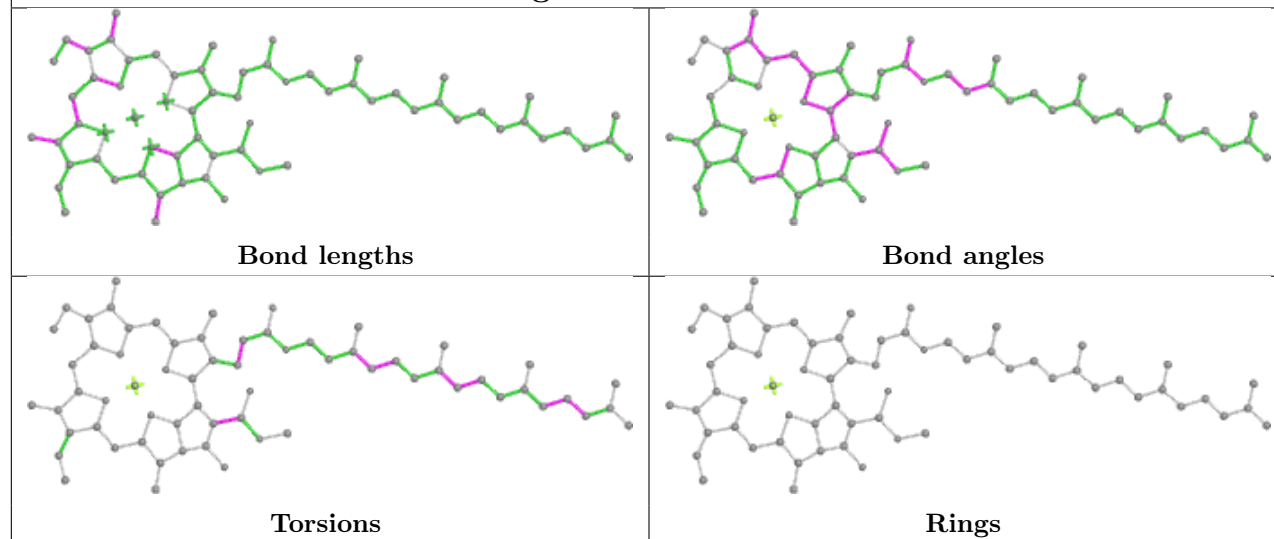
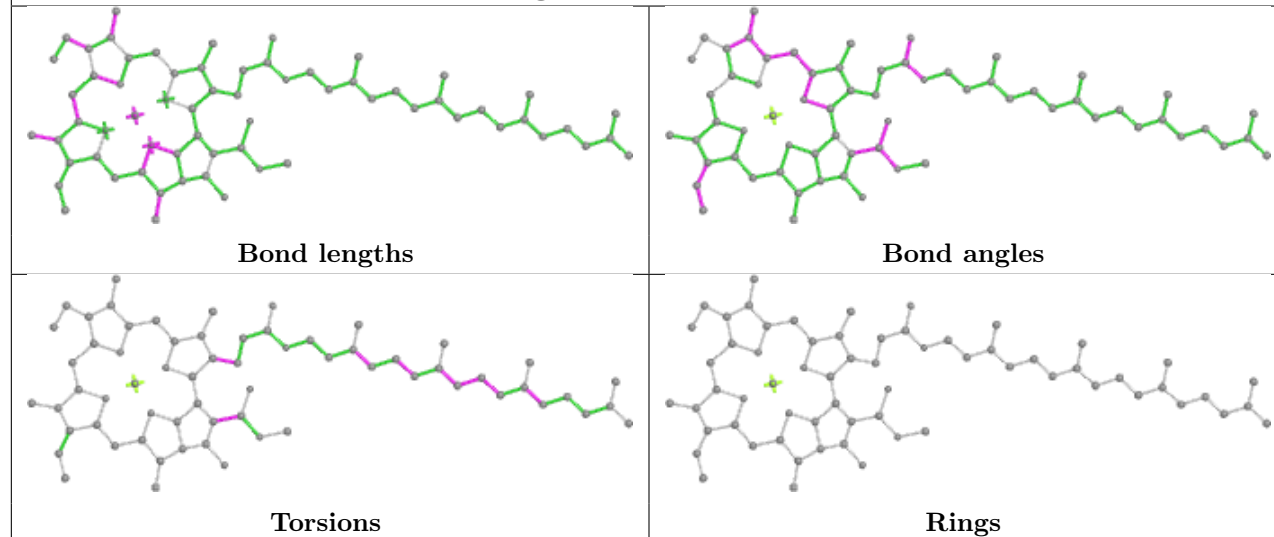
## Ligand CLA A 837



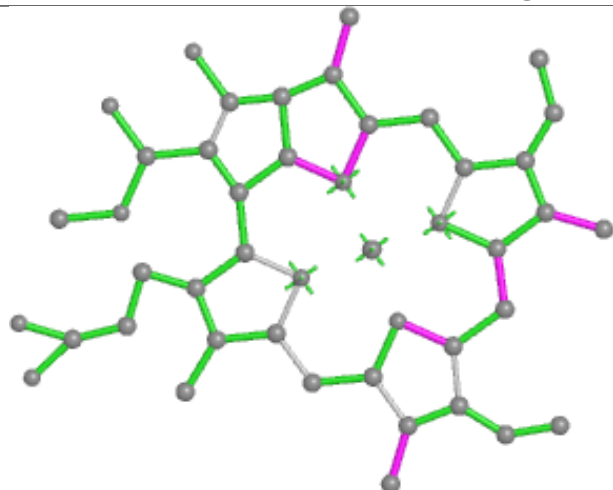


**Ligand CLA b 802****Ligand BCR A 849****Ligand CLA B 827**

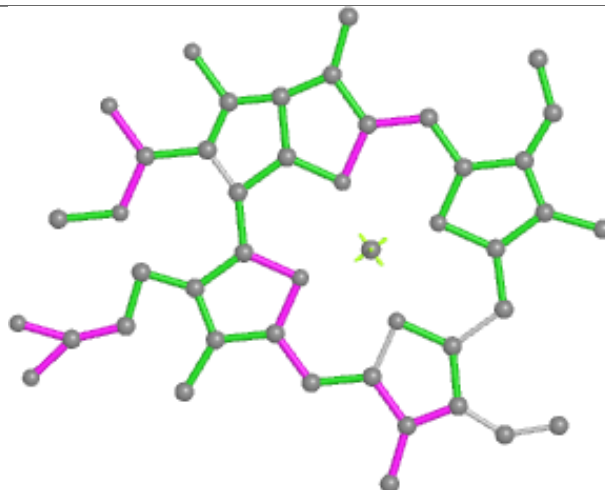


**Ligand CLA B 801****Ligand CLA B 816**

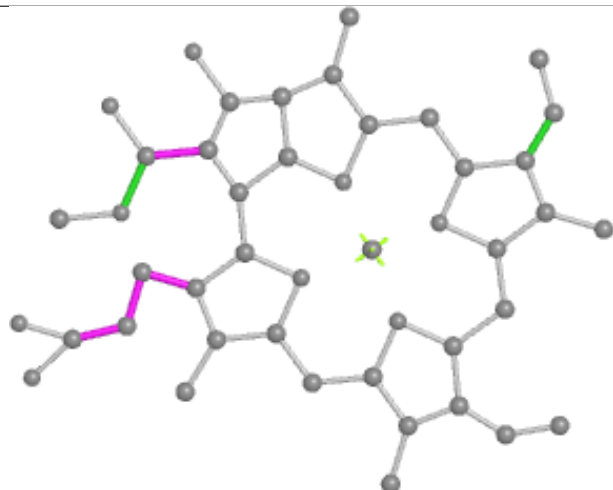
## Ligand CLA a 841



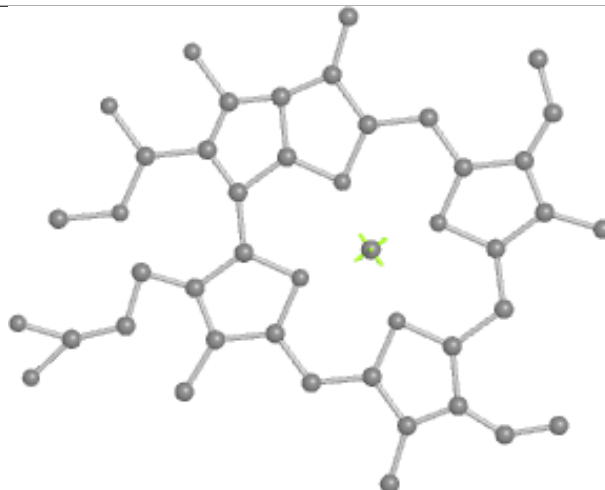
Bond lengths



Bond angles

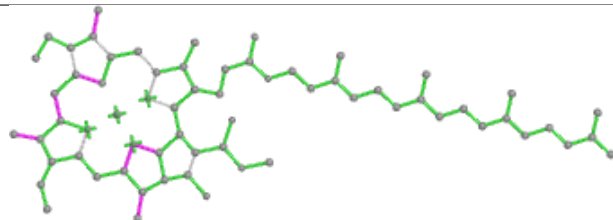


Torsions

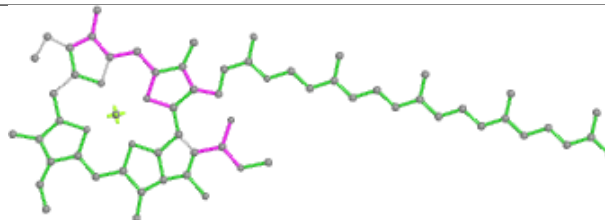


Rings

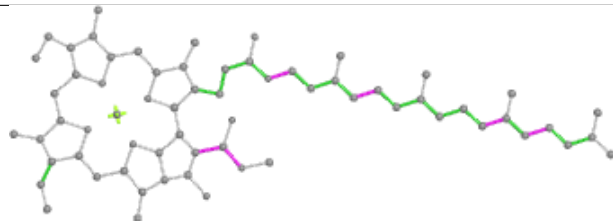
## Ligand CLA A 803



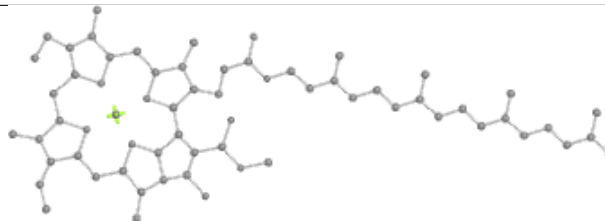
Bond lengths



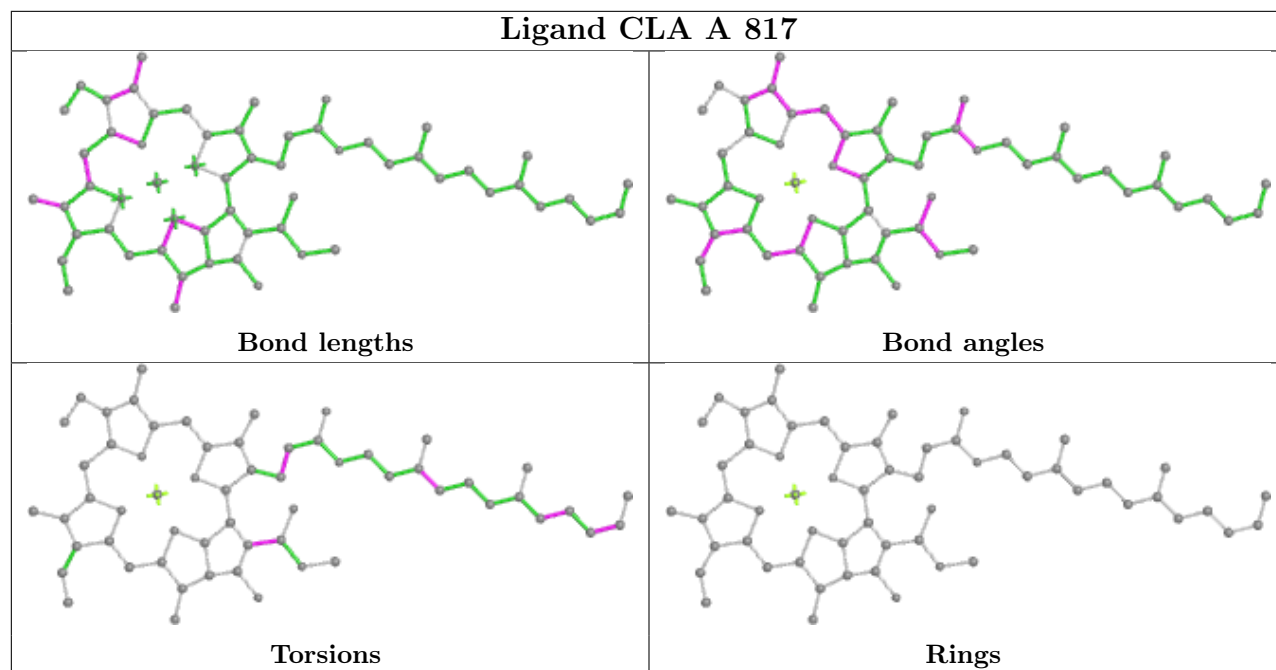
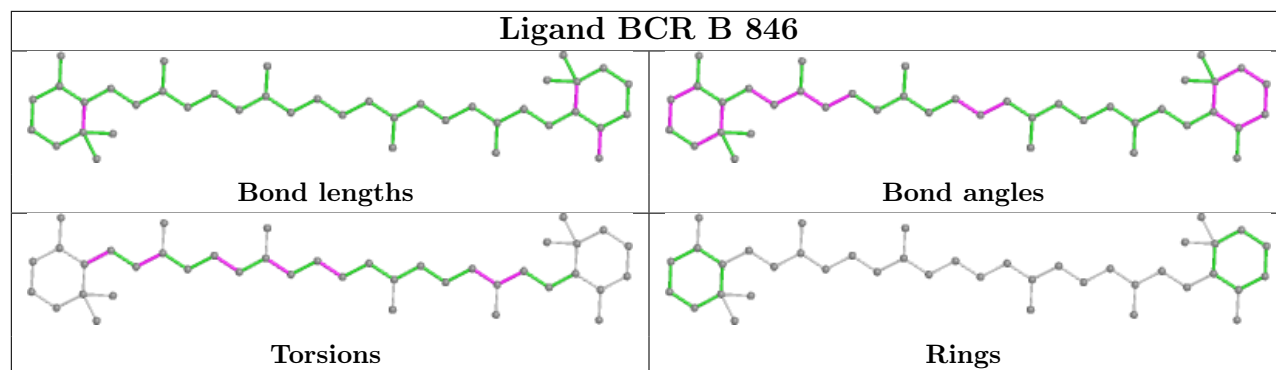
Bond angles

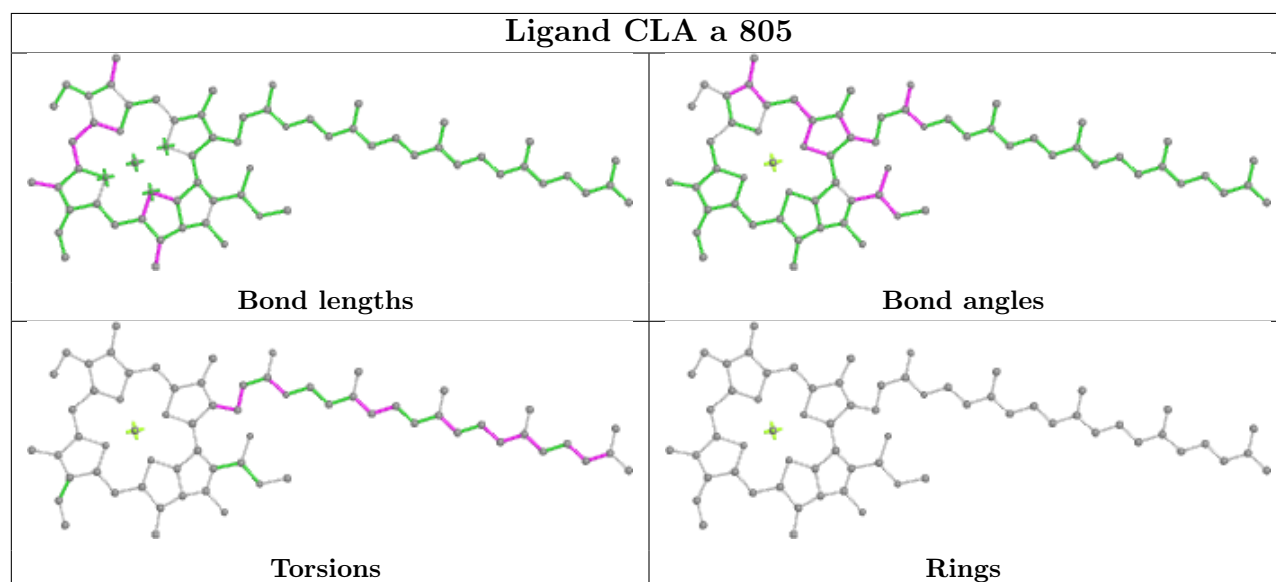
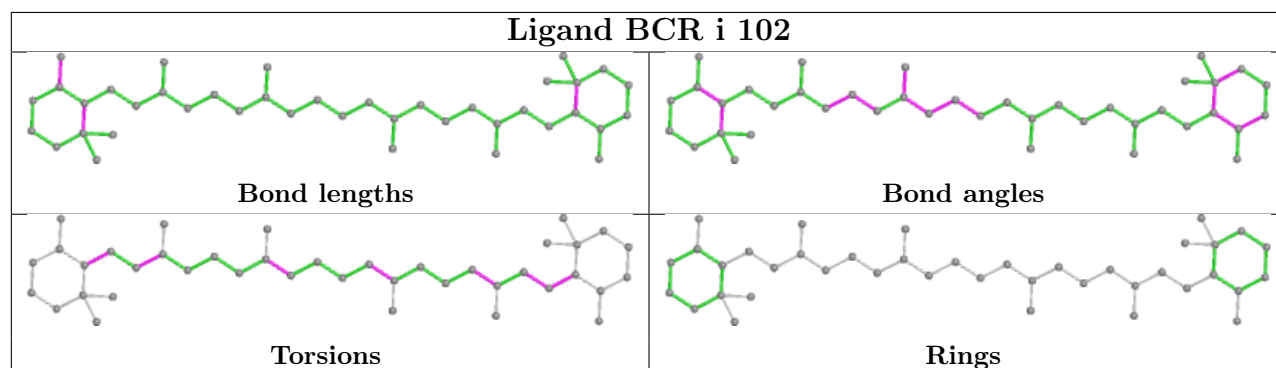
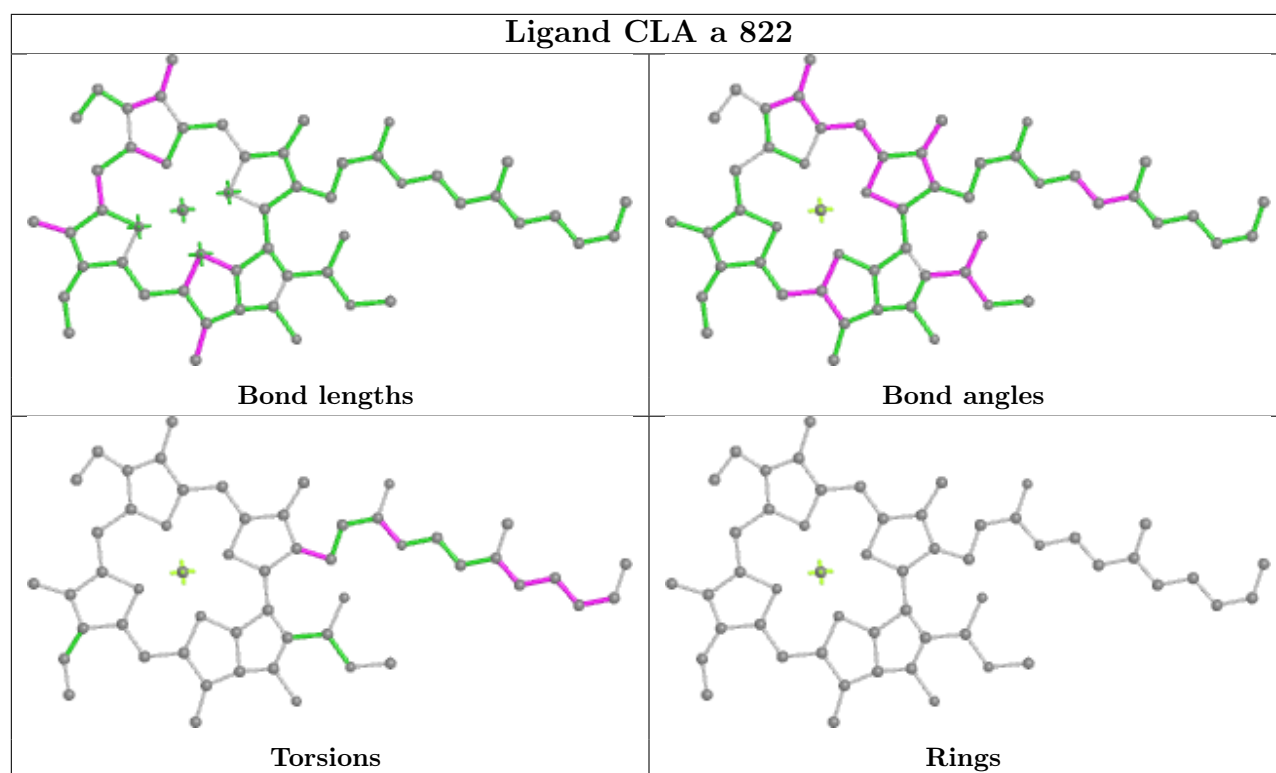


Torsions

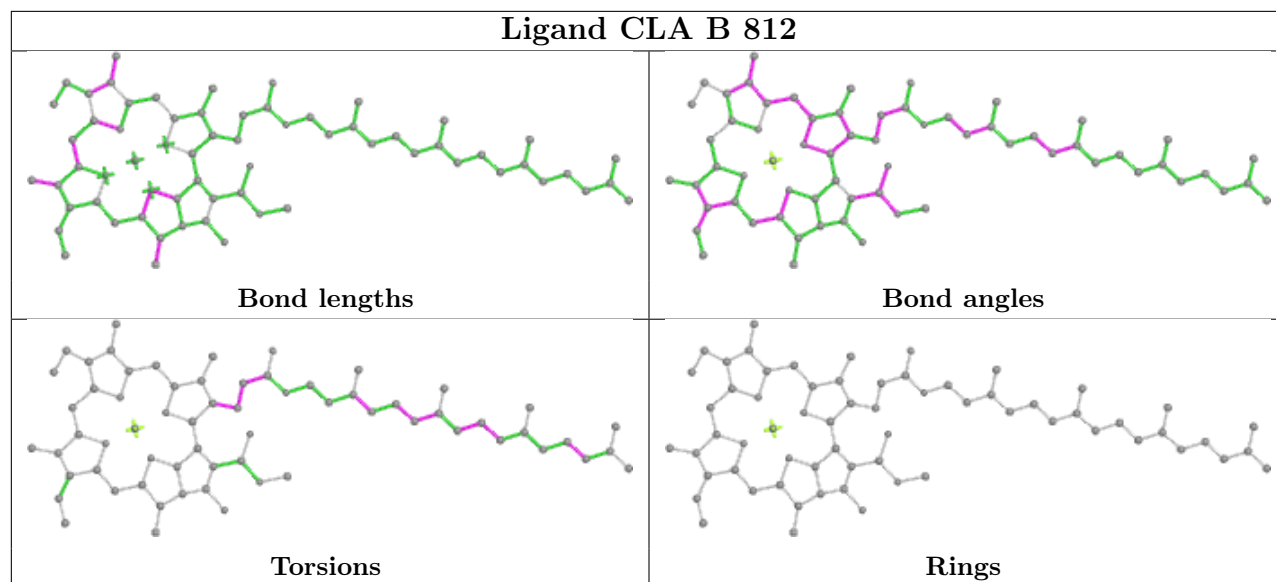
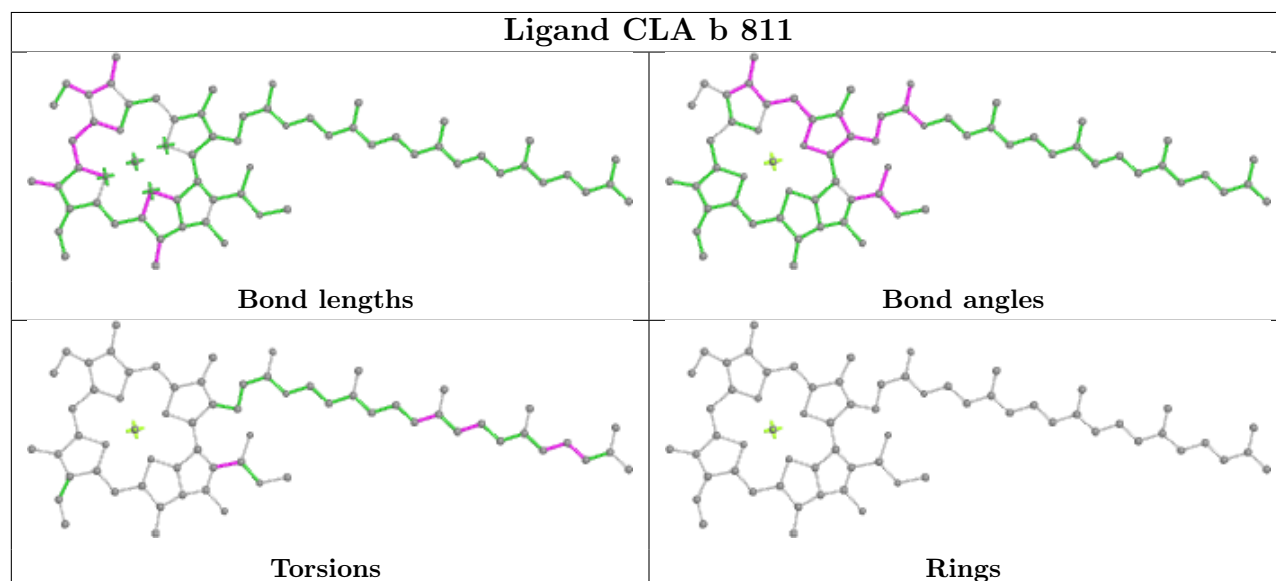
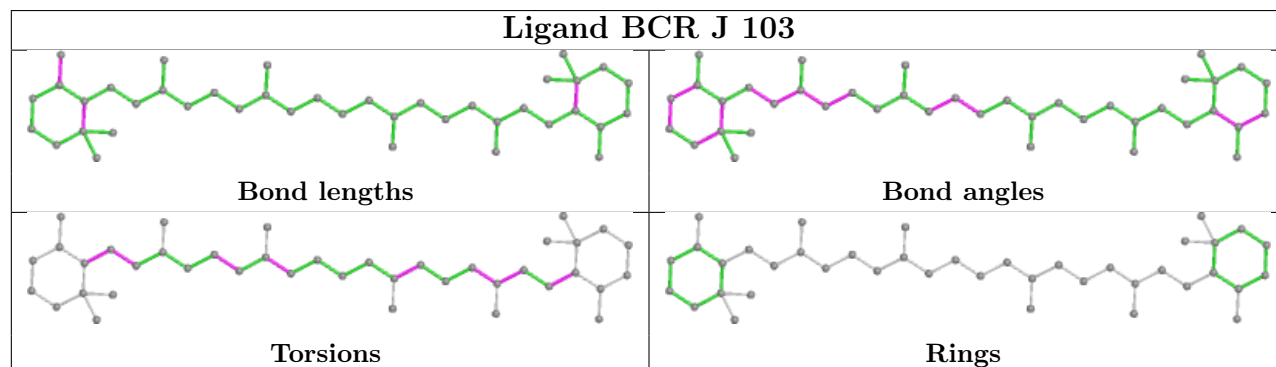


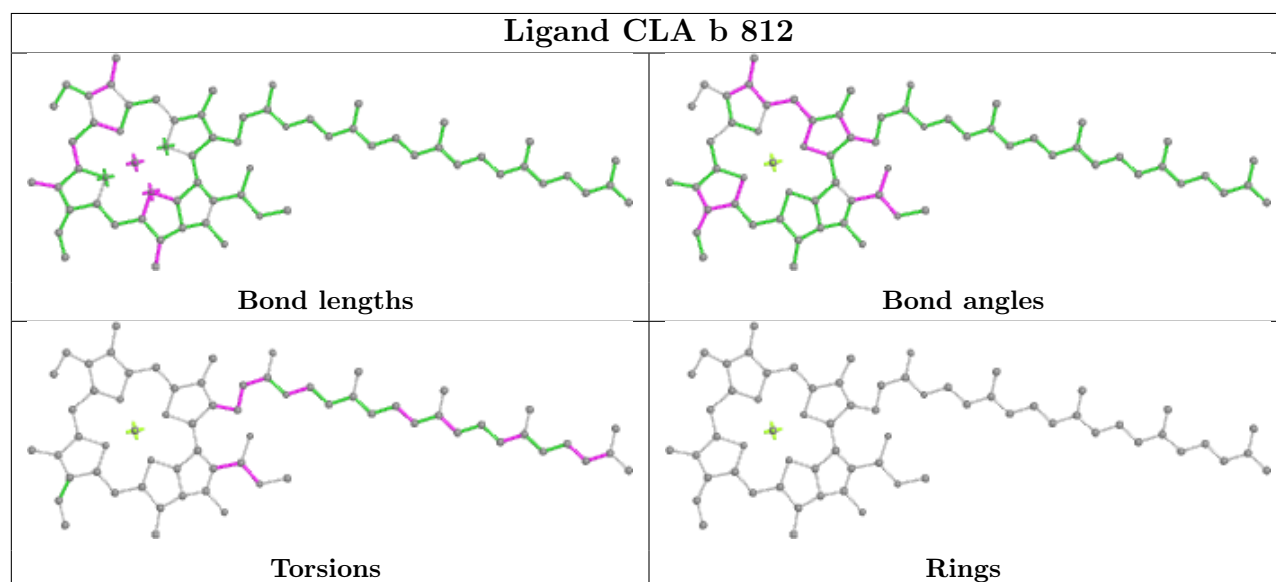
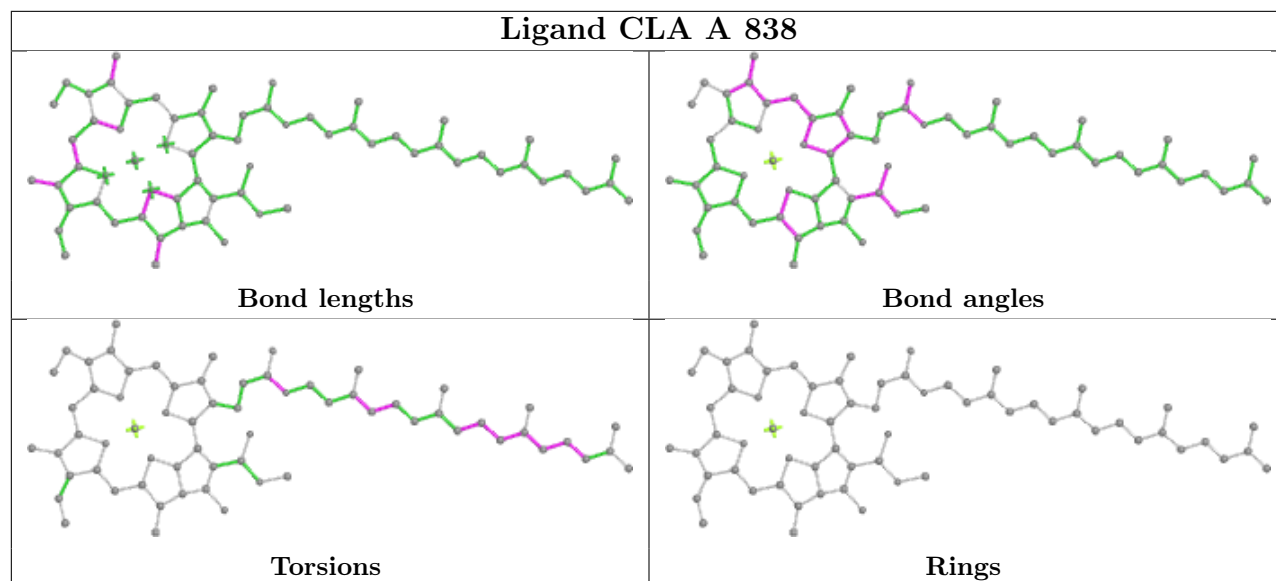
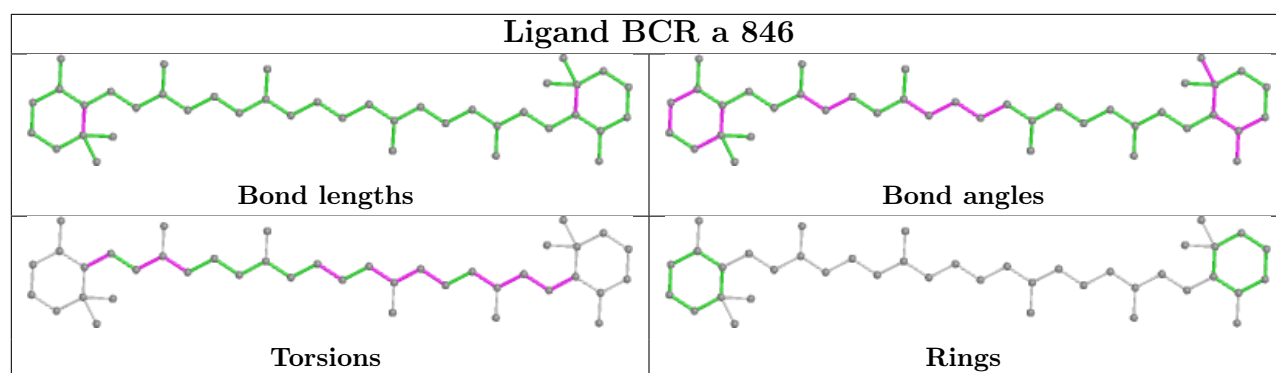
Rings



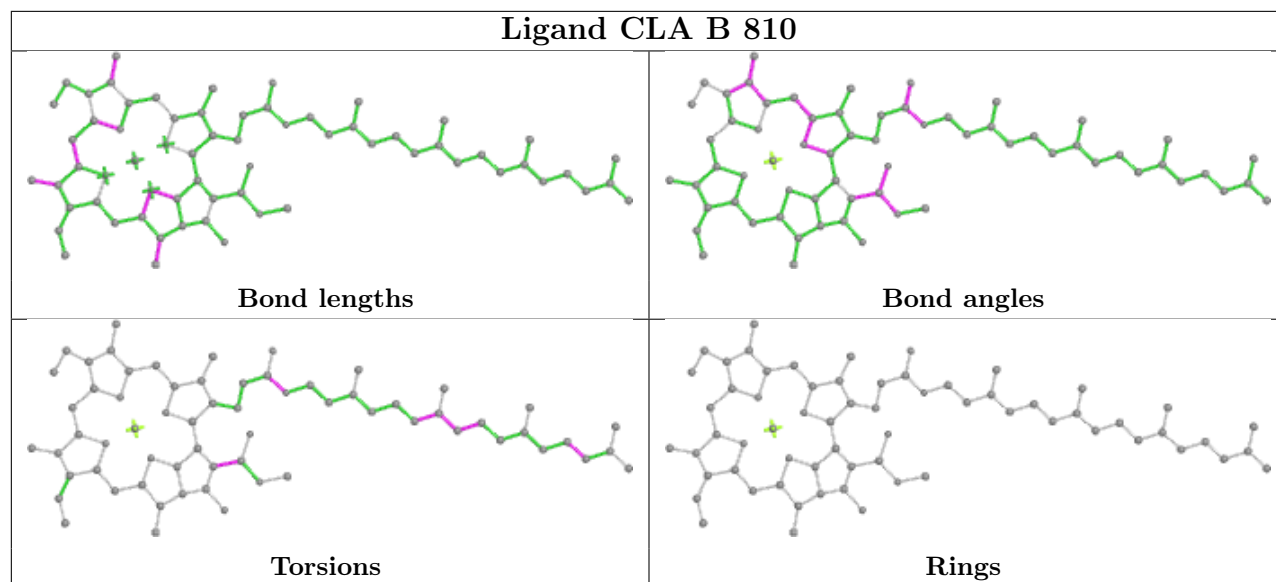




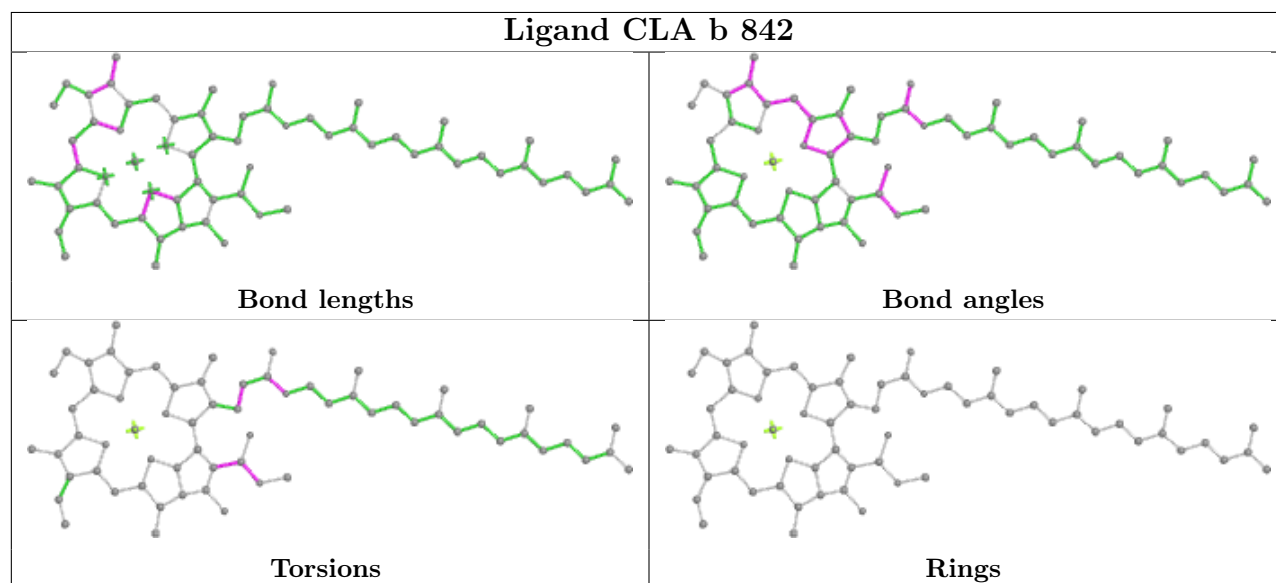
**Ligand CLA B 812****Ligand CLA b 811****Ligand BCR J 103**

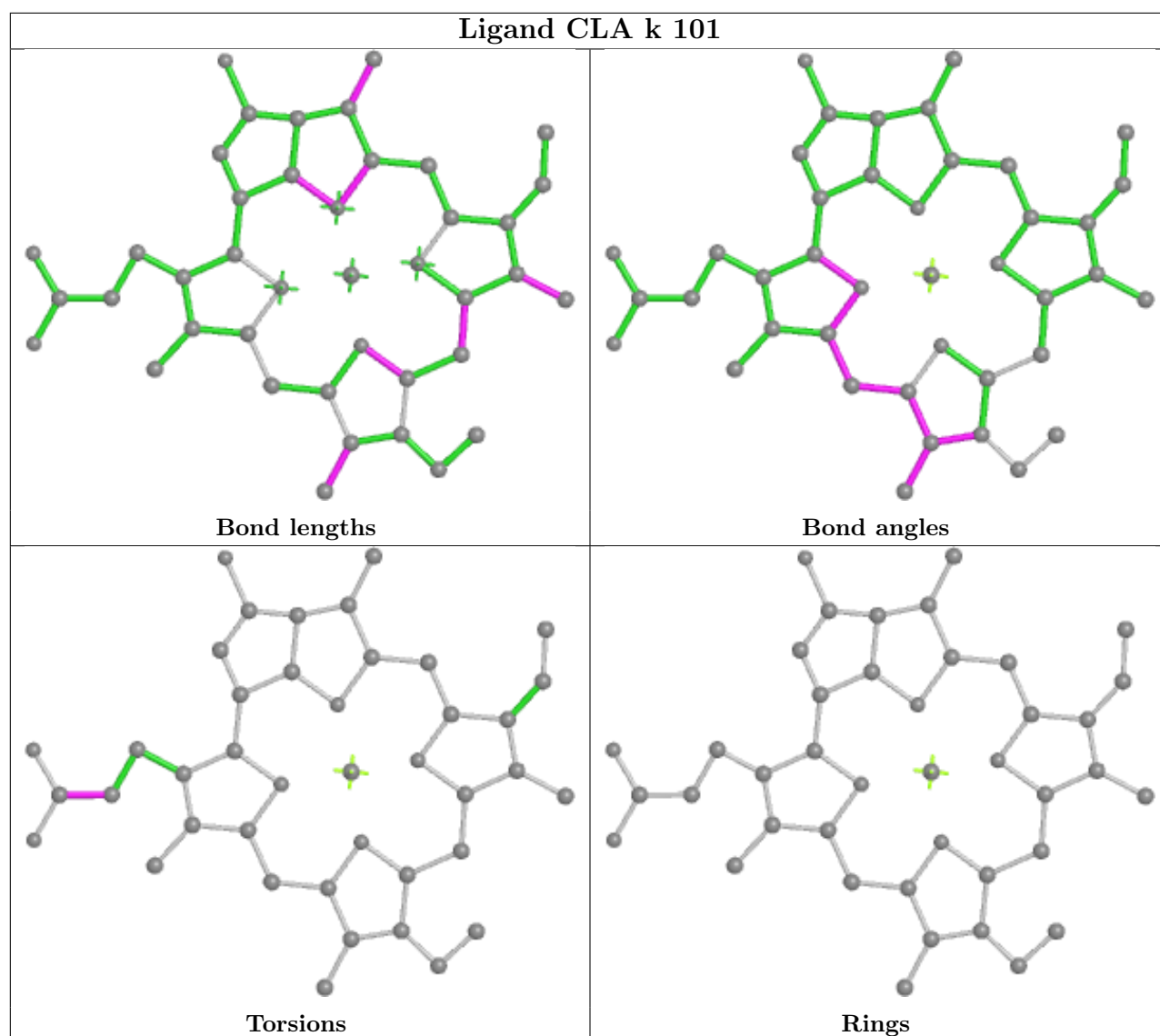


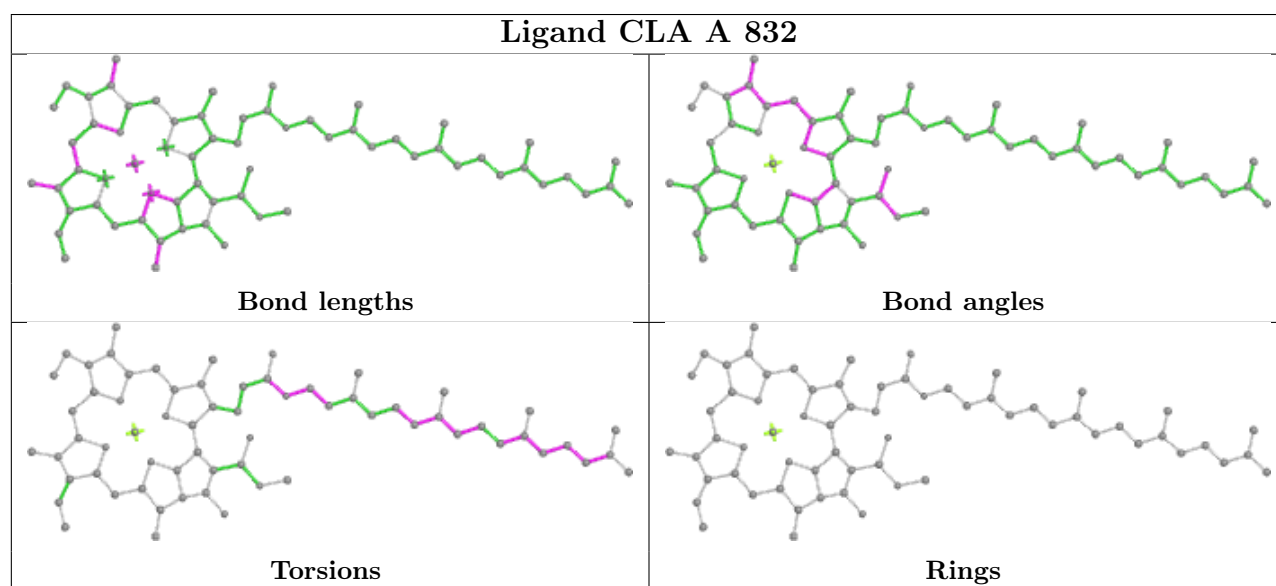
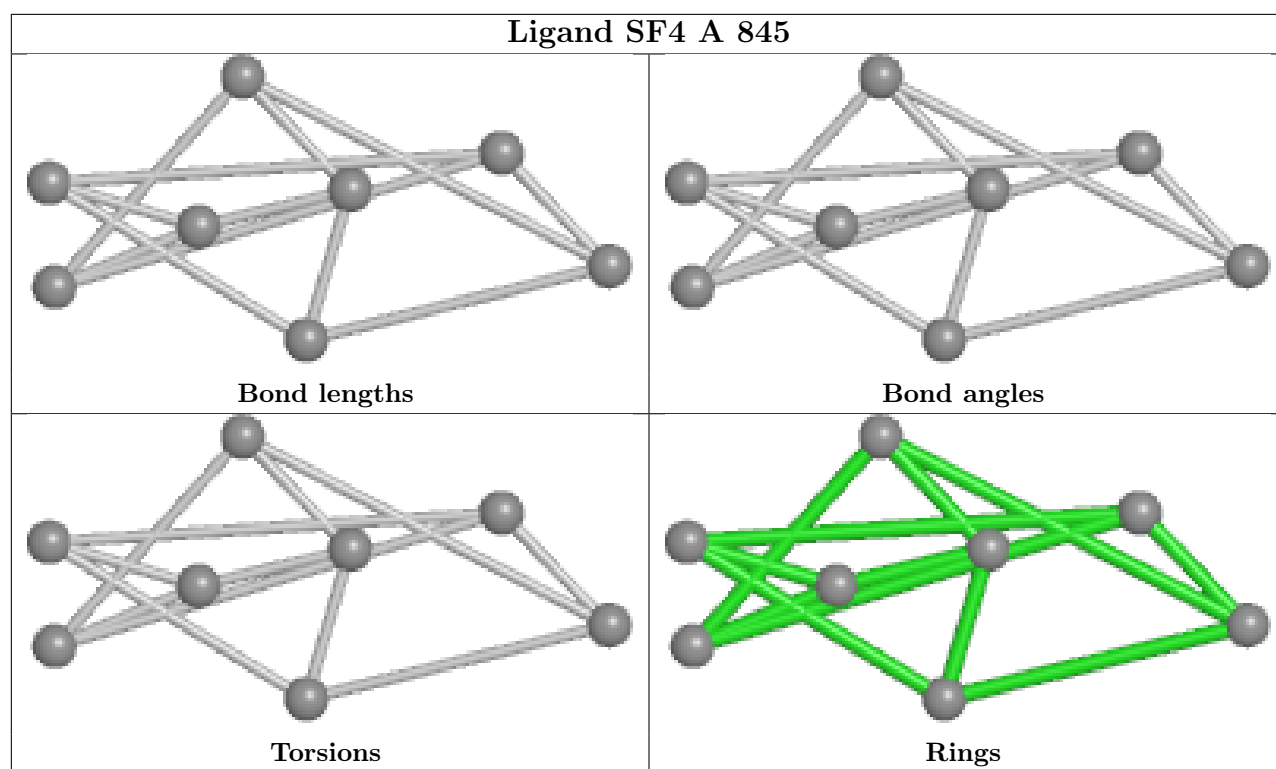
## Ligand CLA B 810



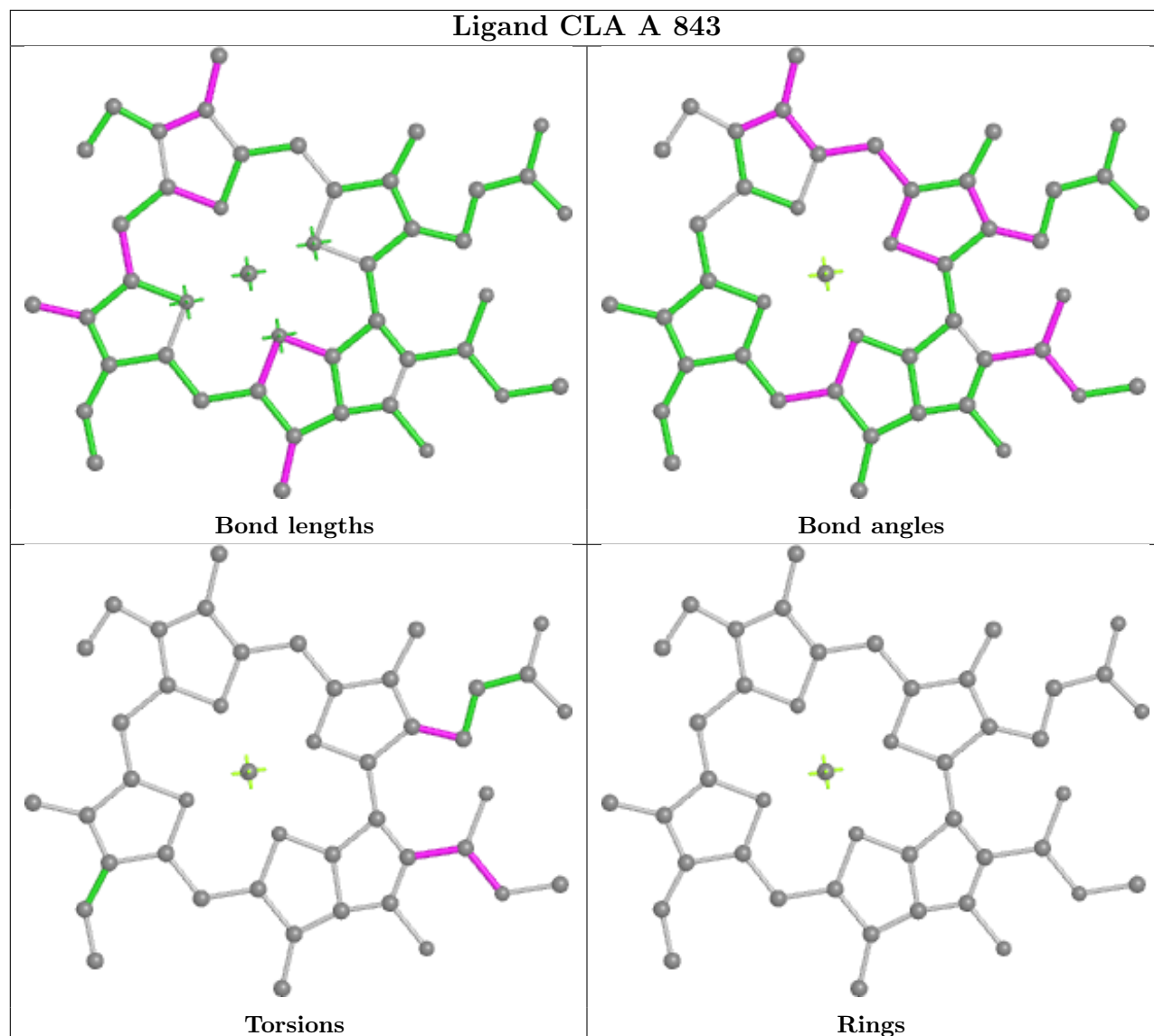
## Ligand CLA b 842



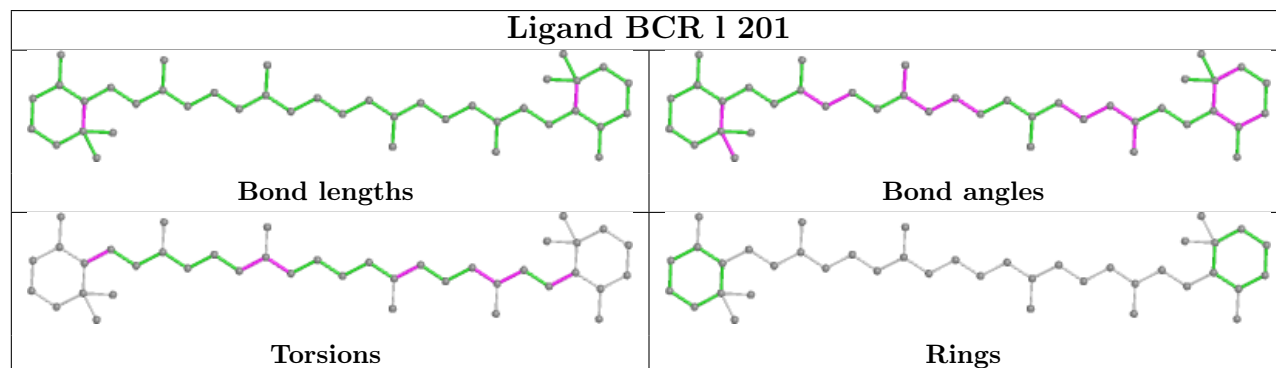


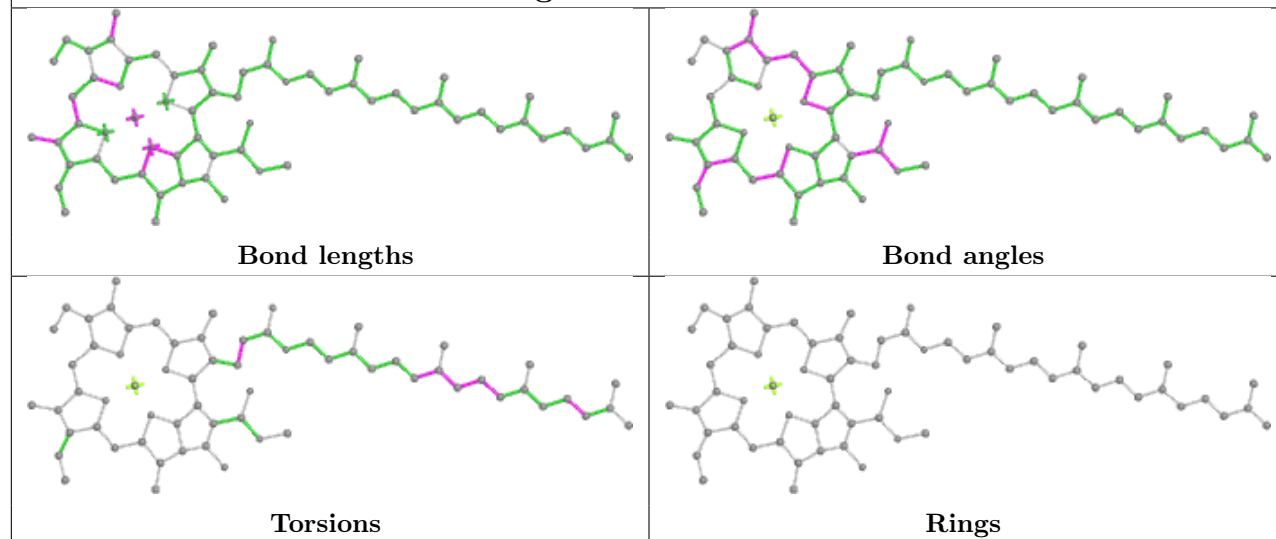
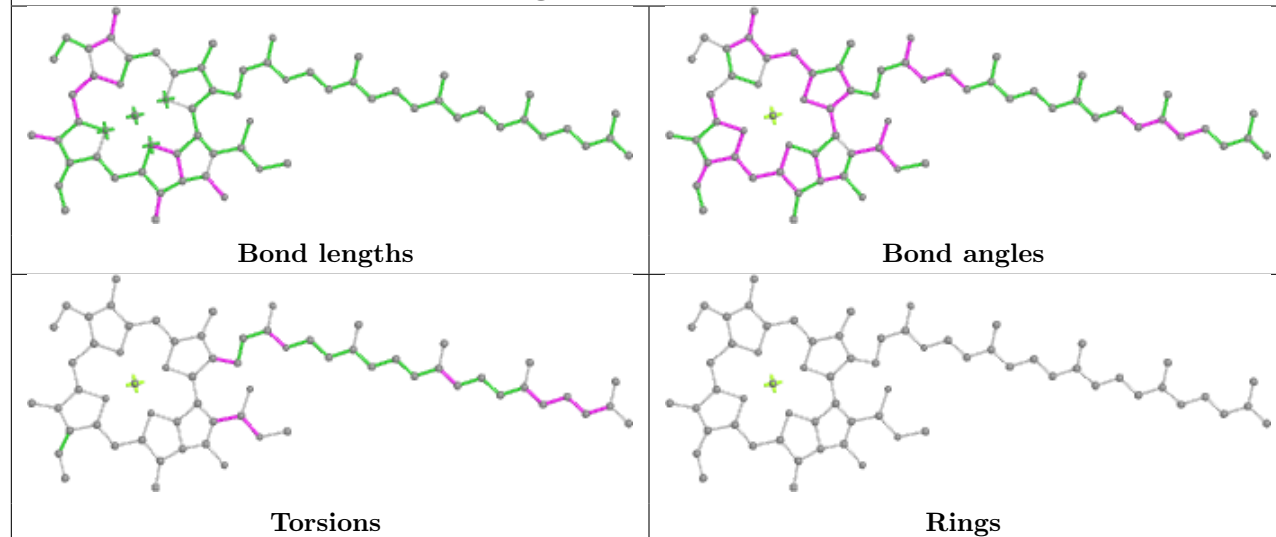


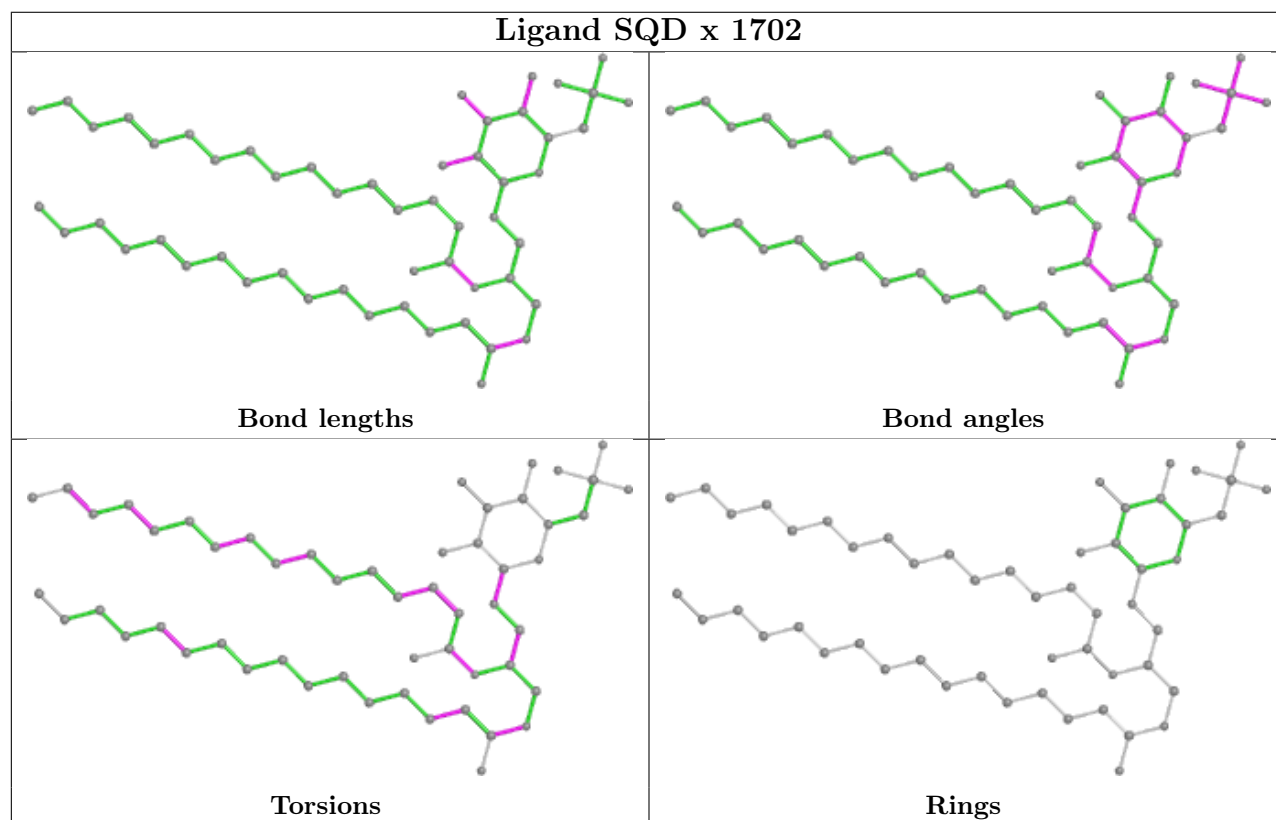
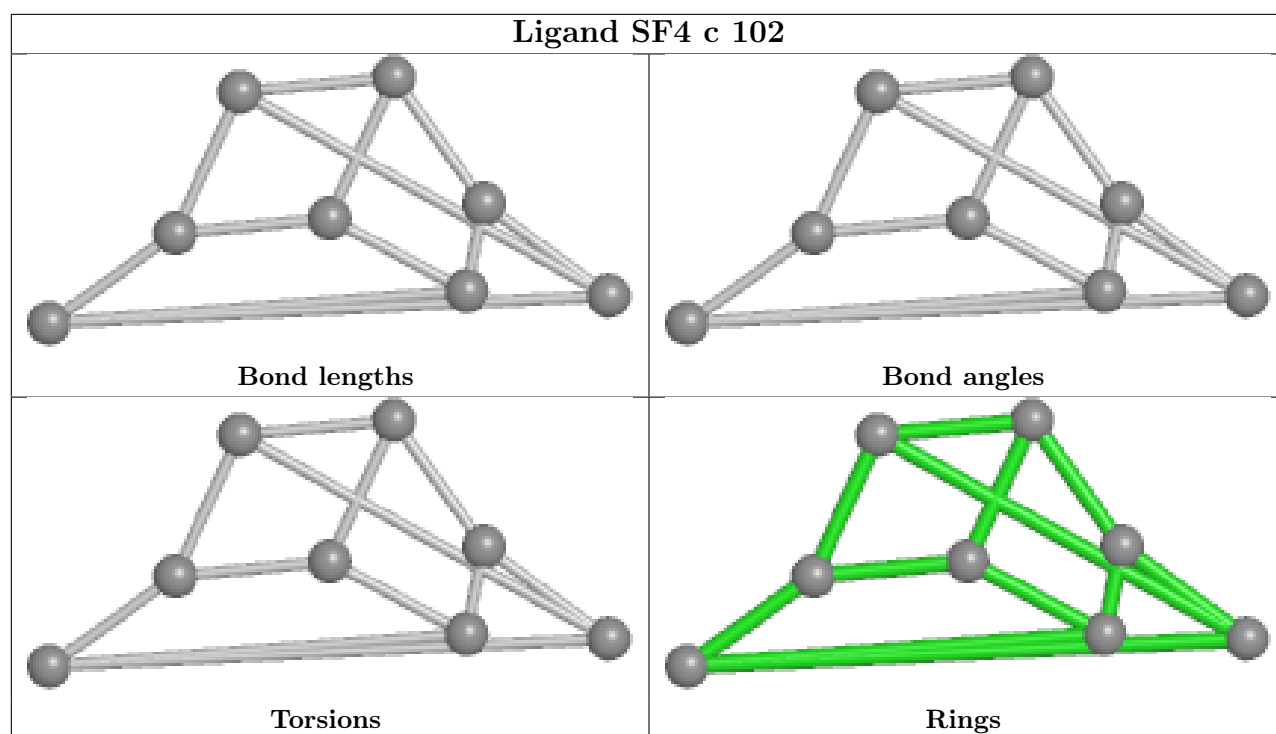
## Ligand CLA A 843



## Ligand BCR 1 201

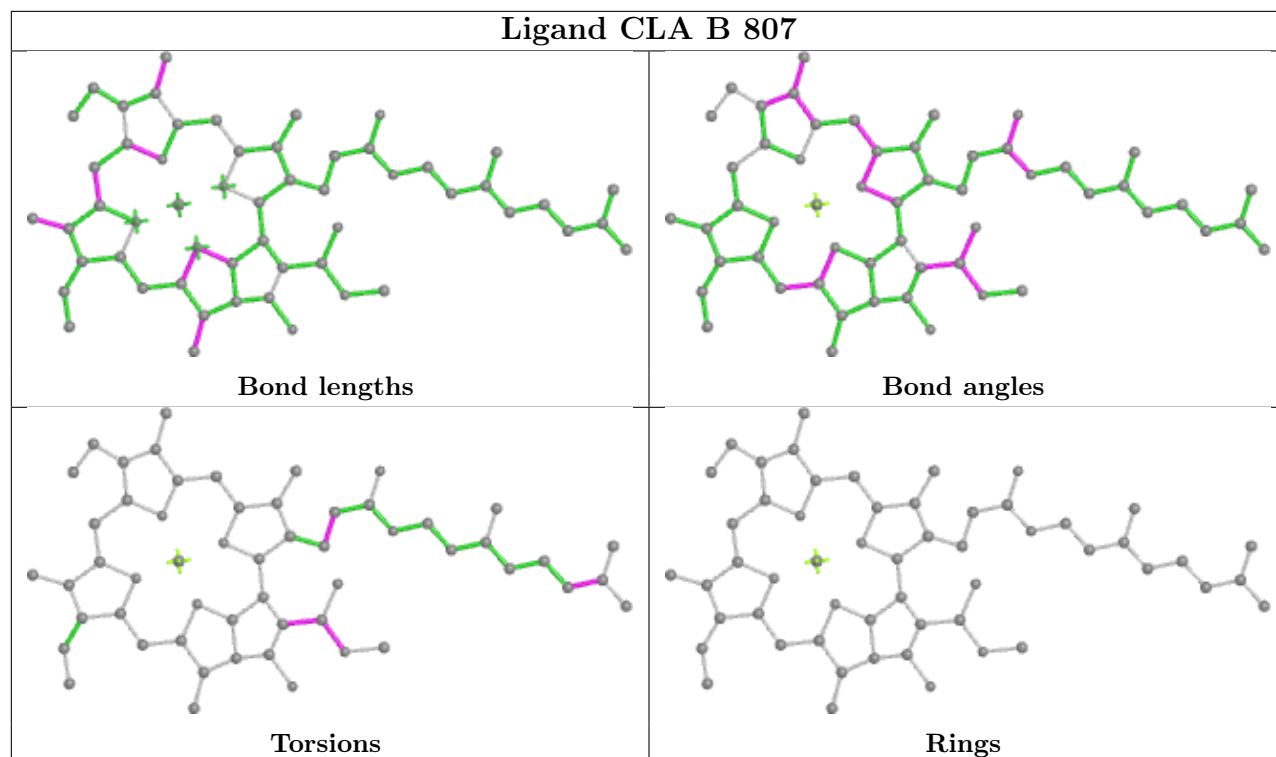


**Ligand CLA b 810****Ligand CLA B 808**

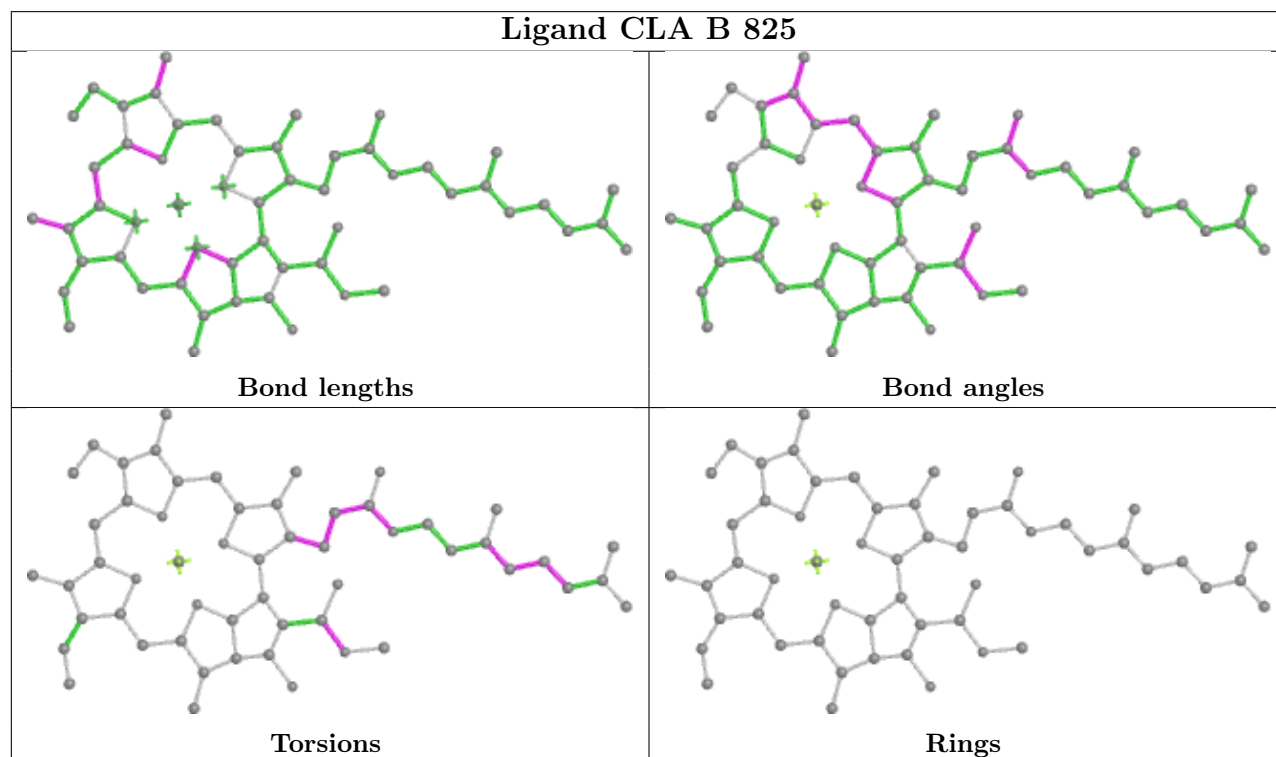


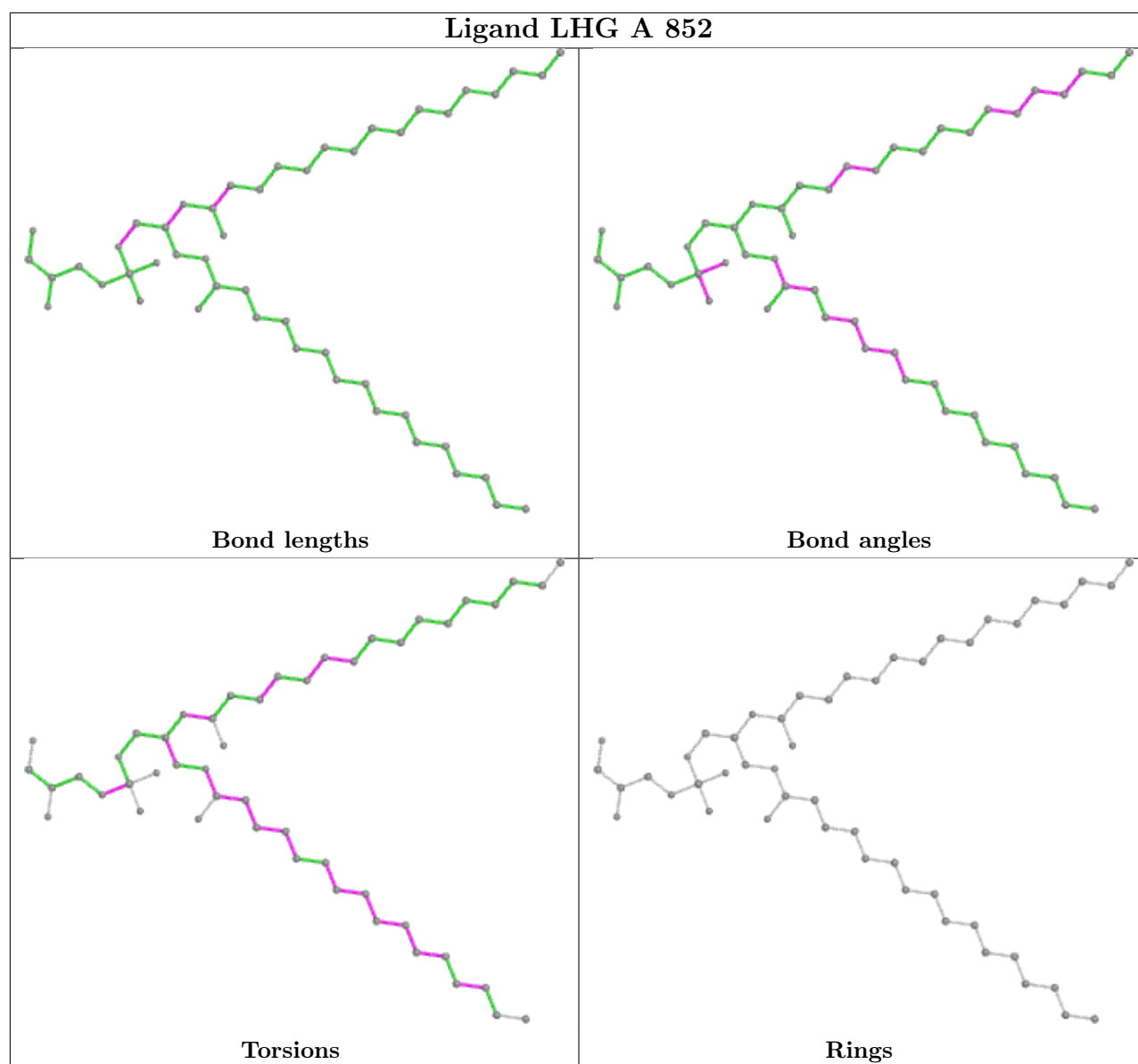


## Ligand CLA B 807

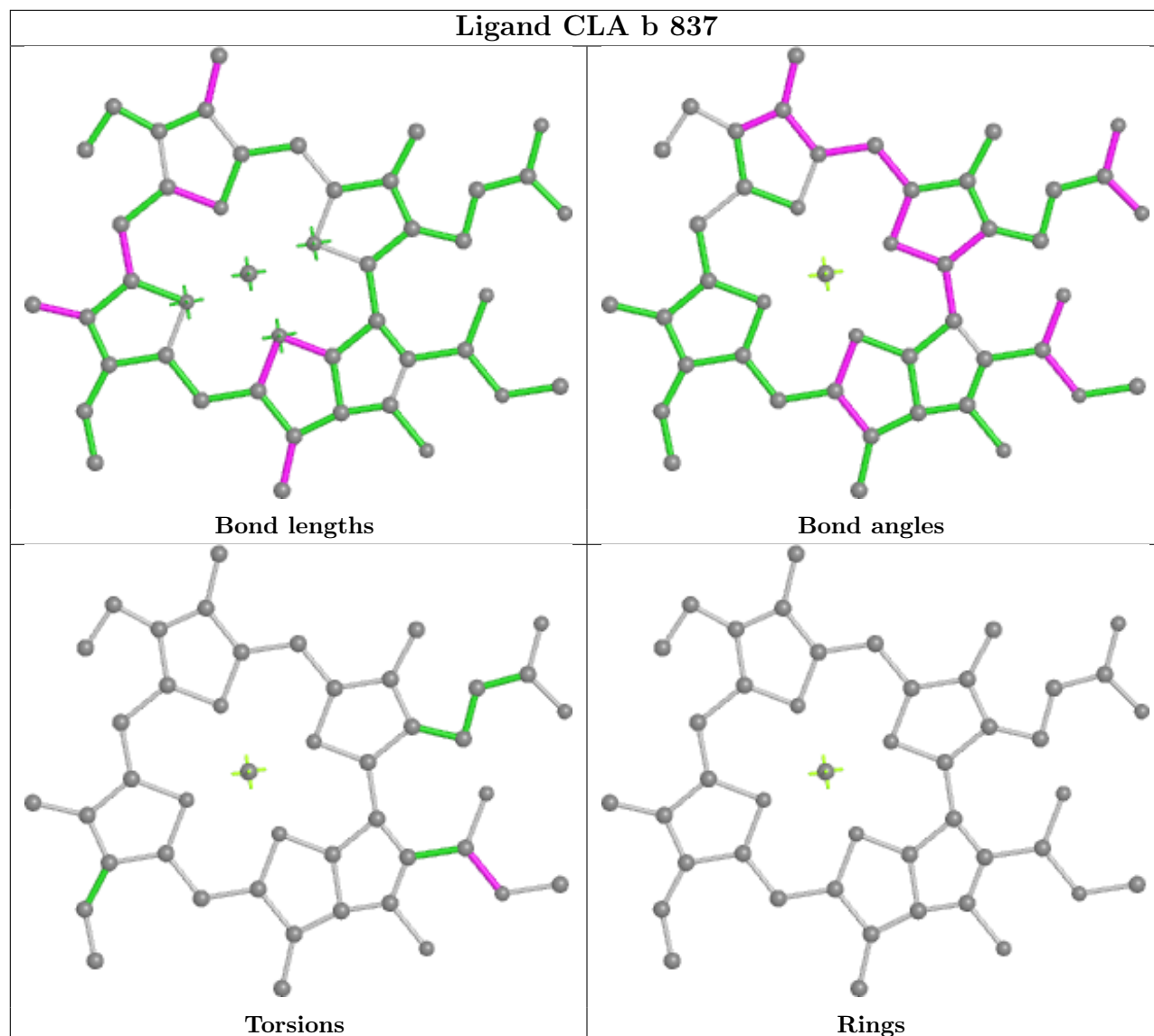


## Ligand CLA B 825

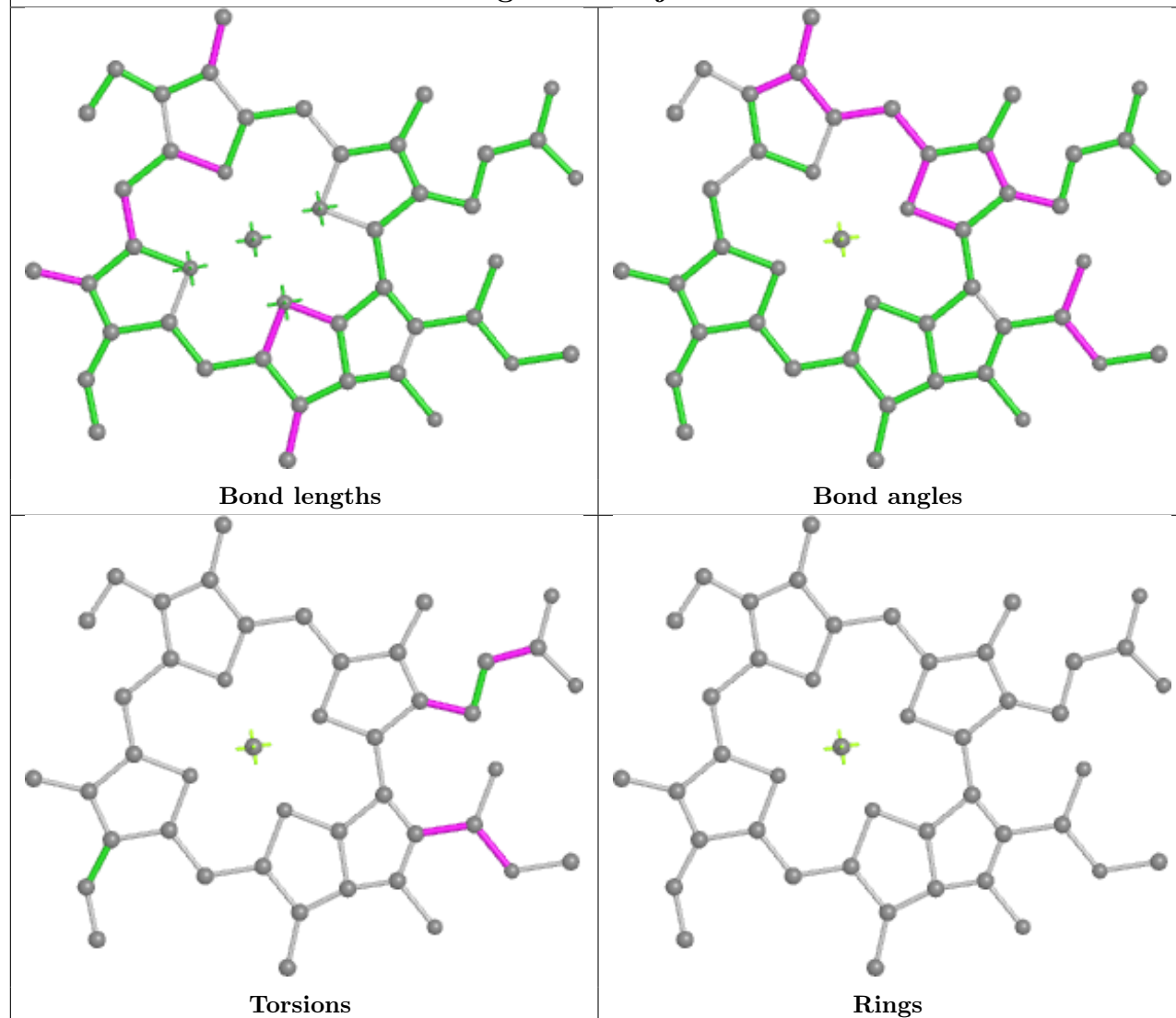




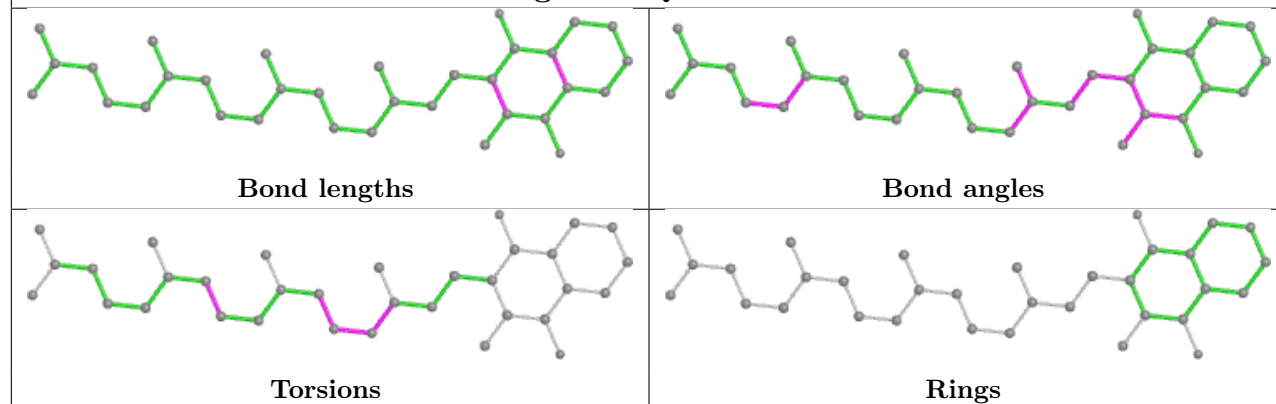
## Ligand CLA b 837



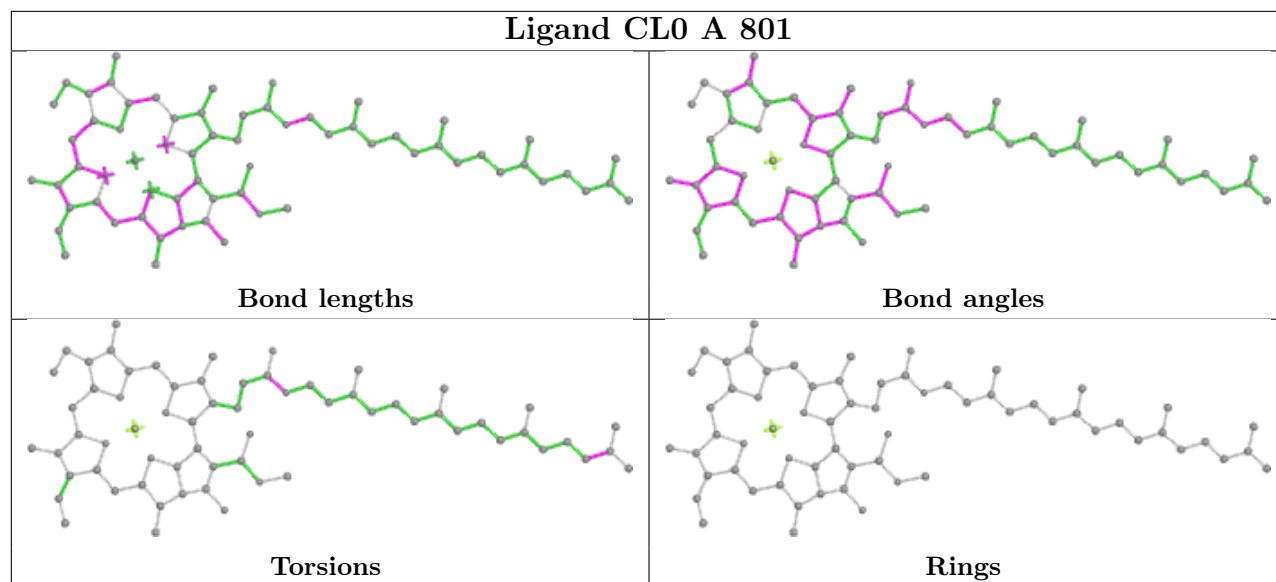
## Ligand CLA j 102



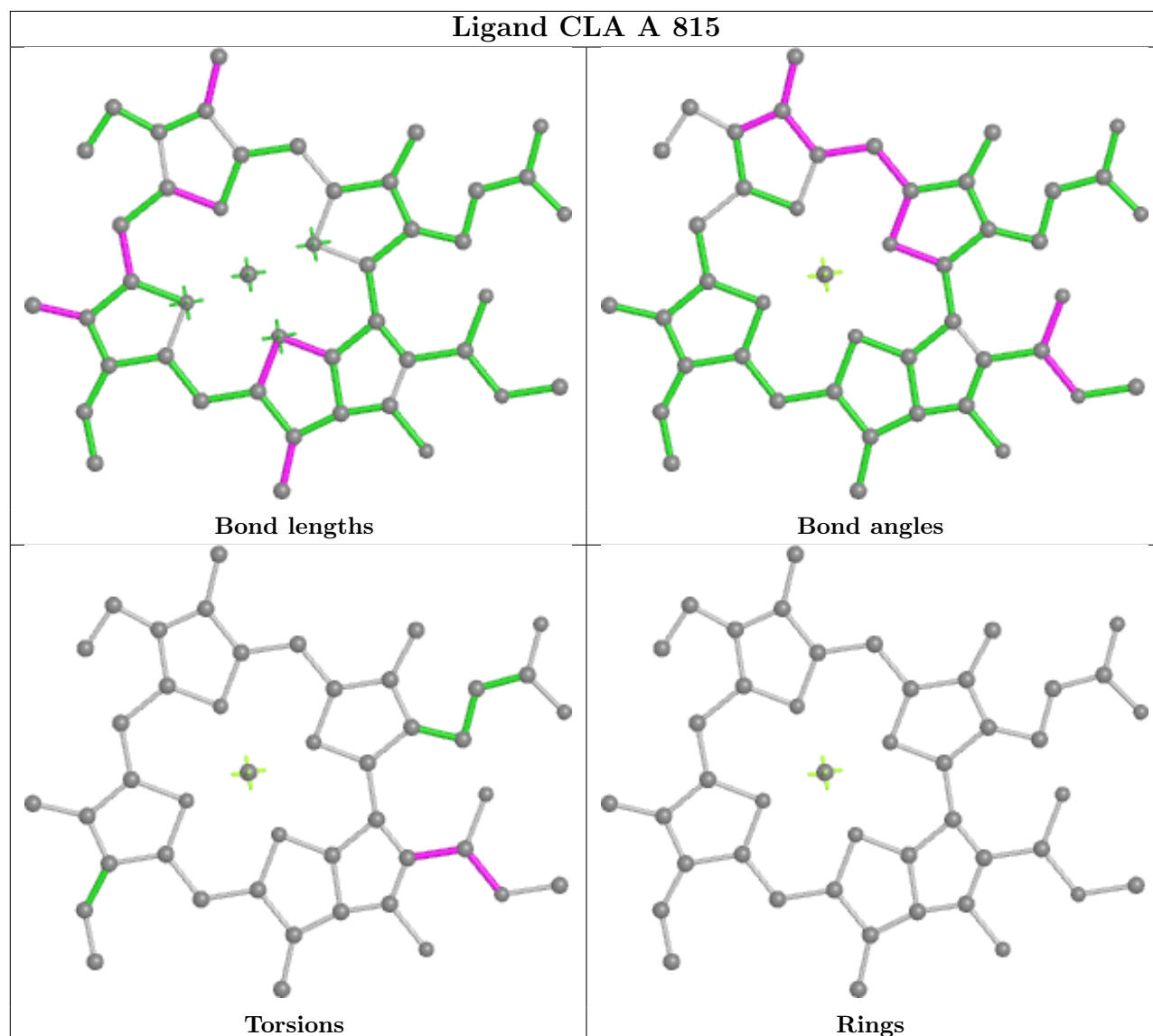
## Ligand PQN a 842

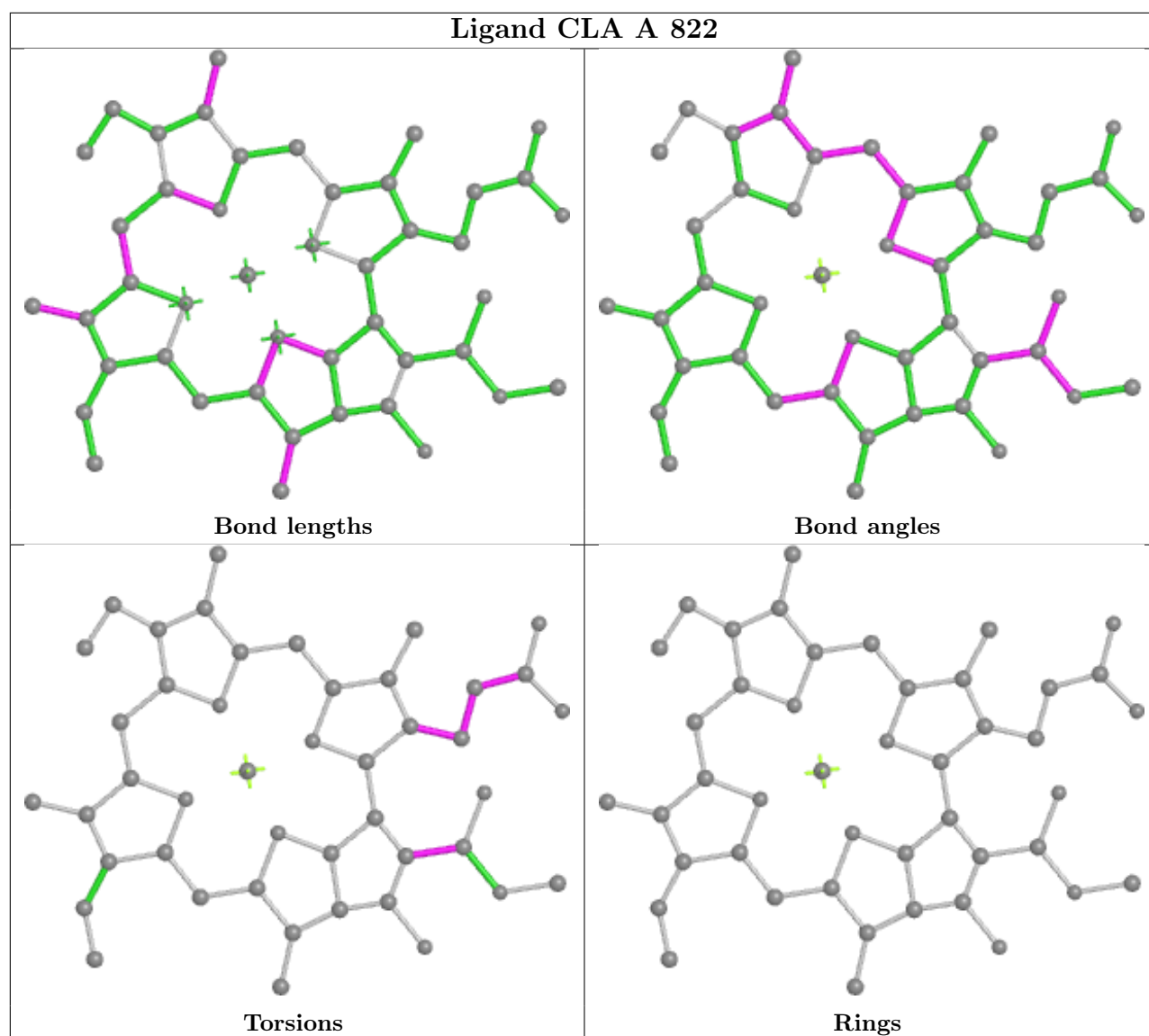


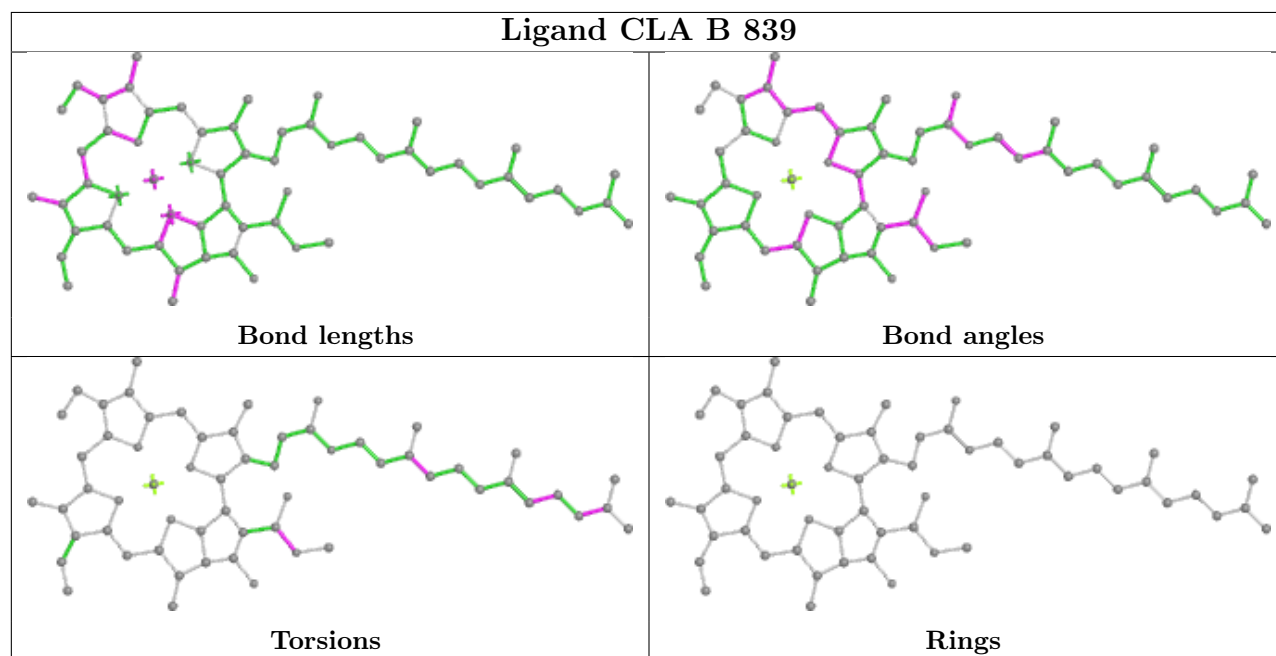
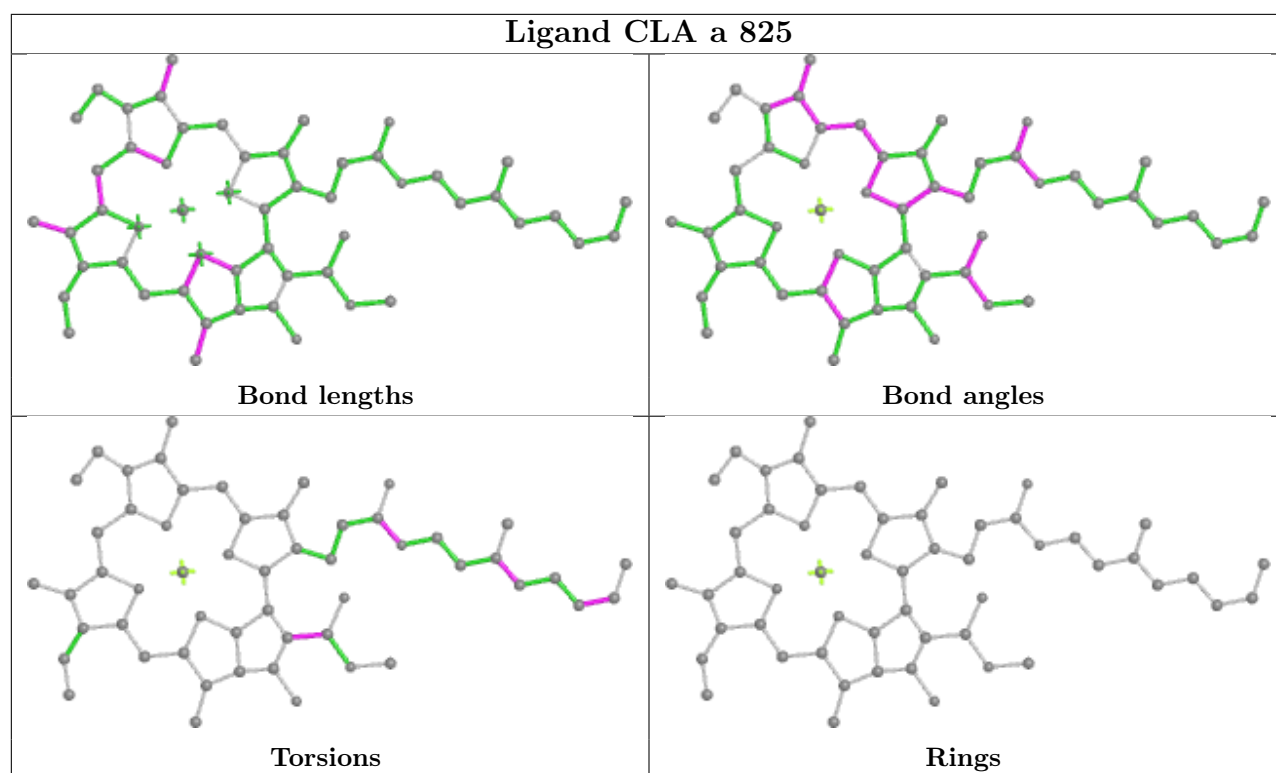
## Ligand CL0 A 801

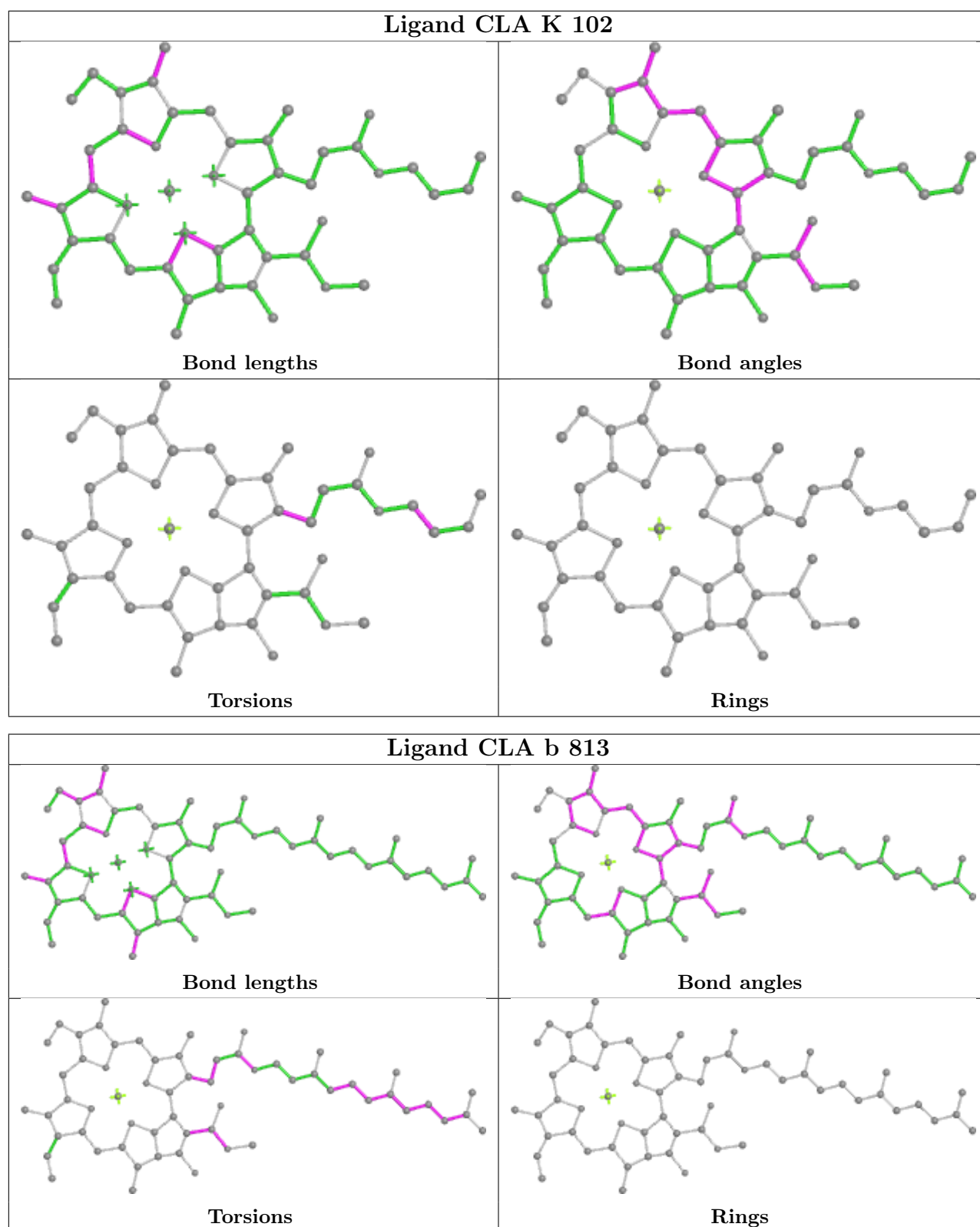


## Ligand CLA A 815

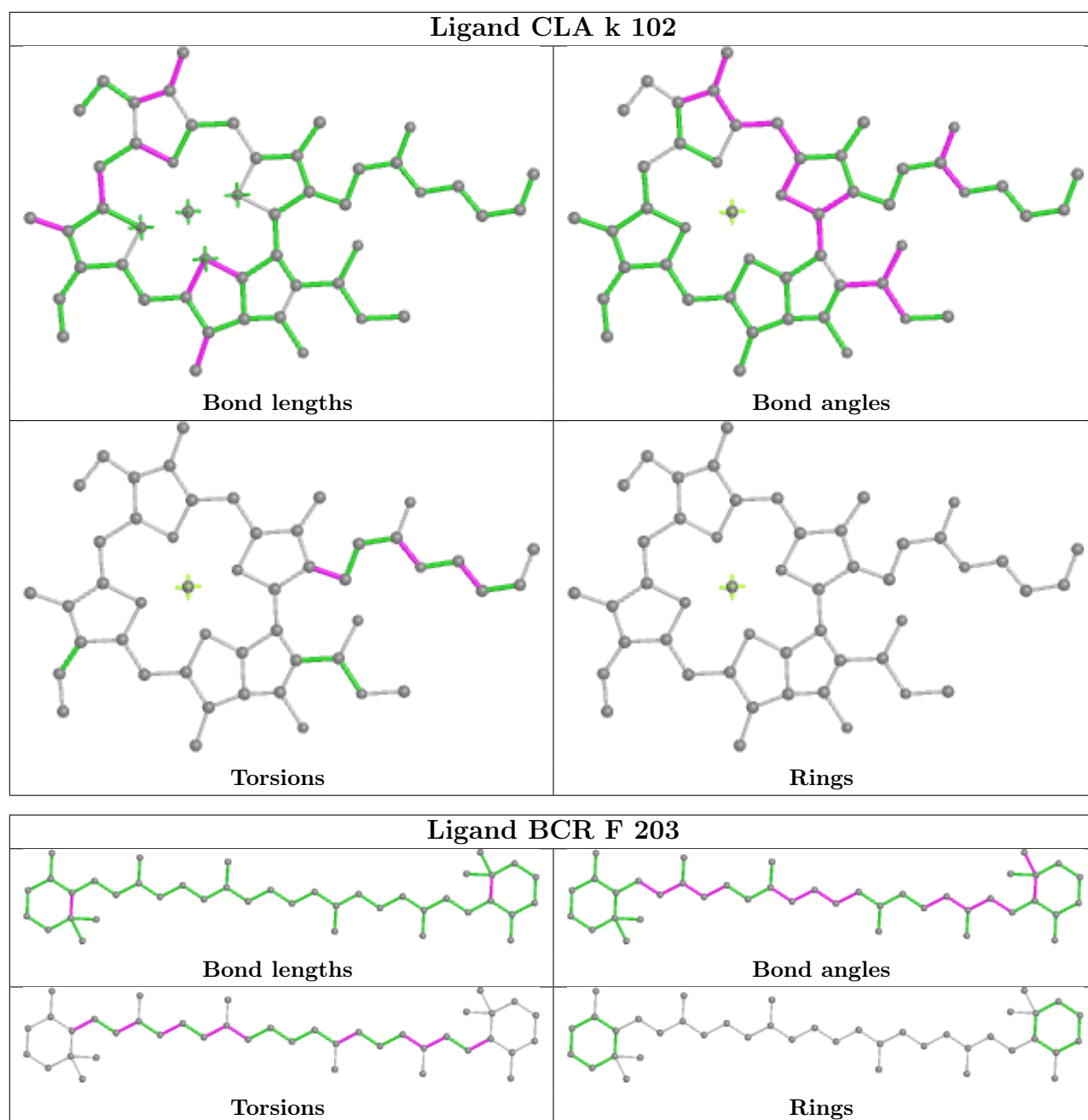


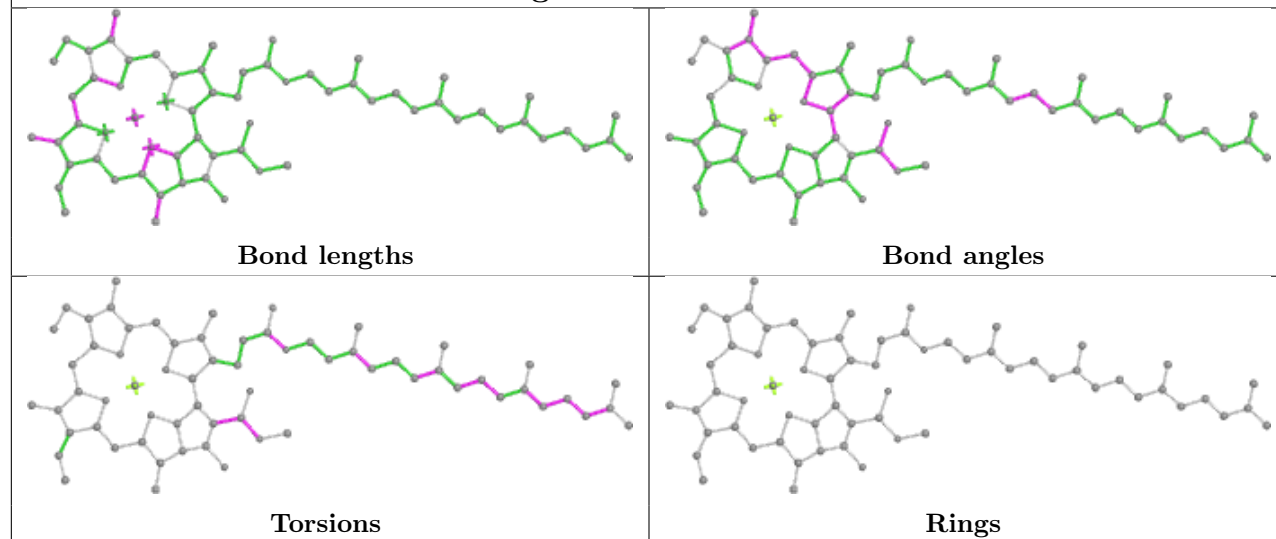
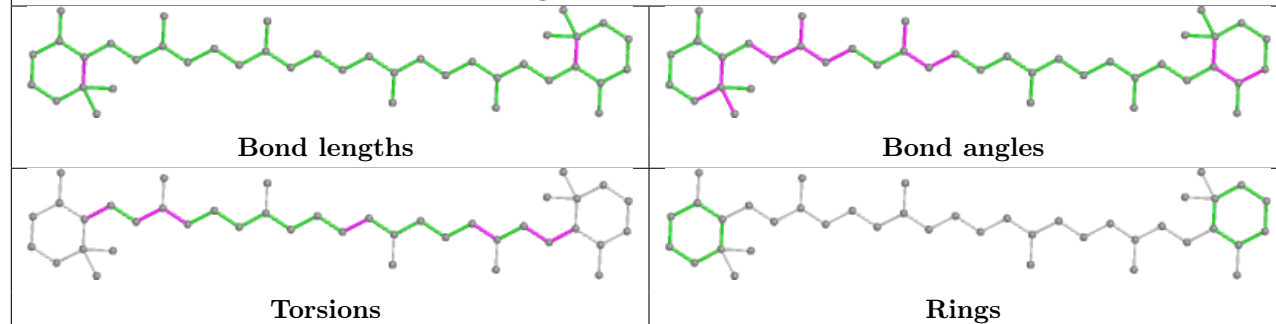
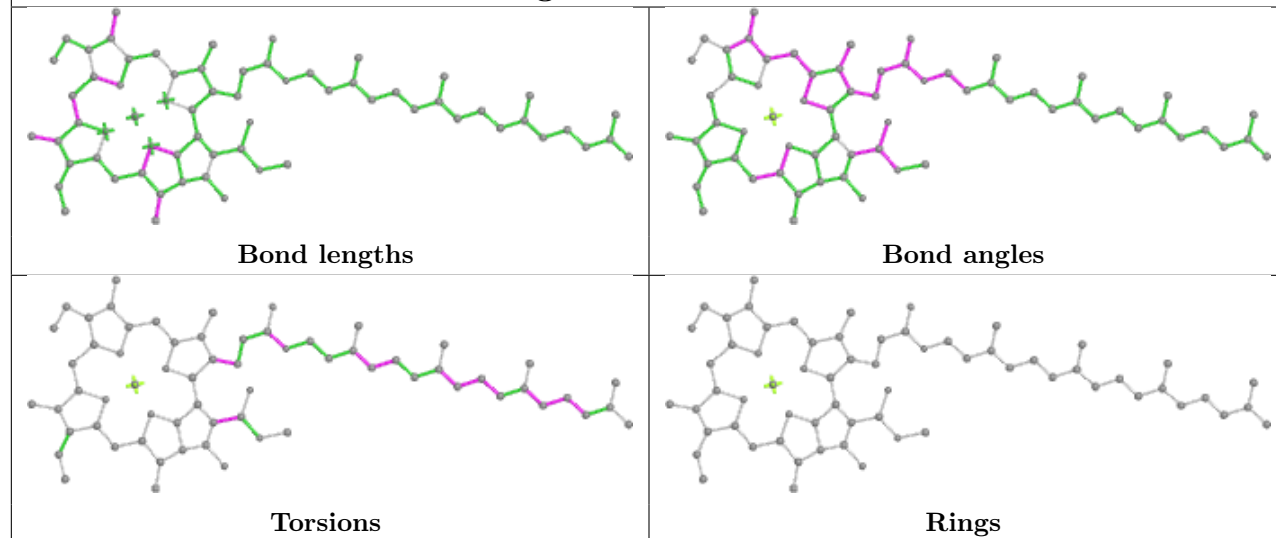


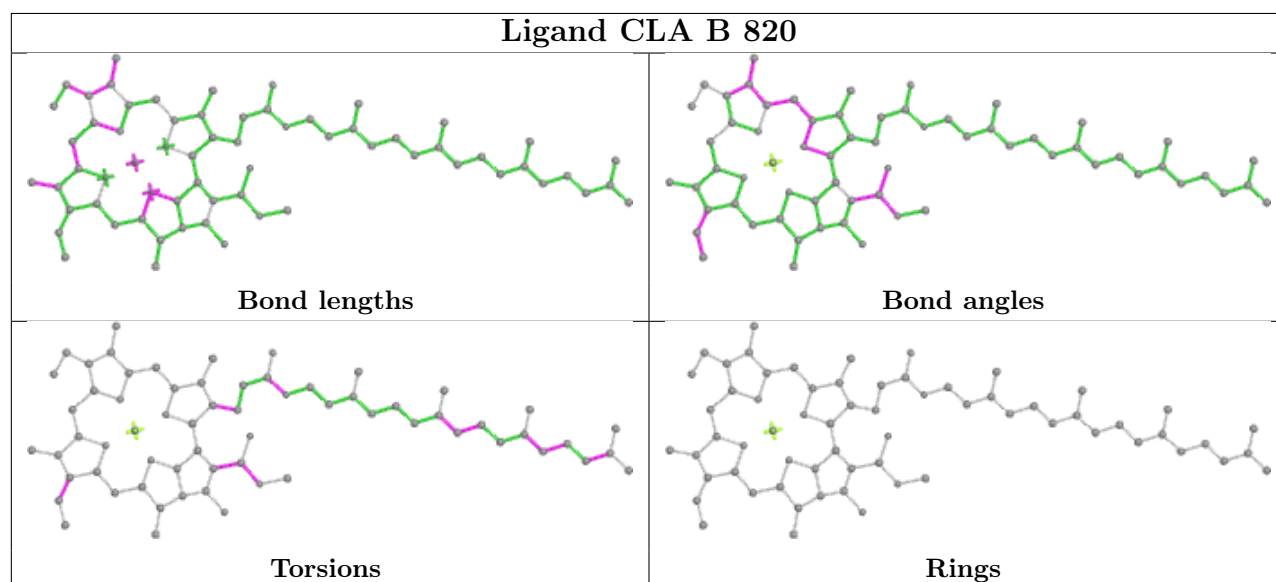
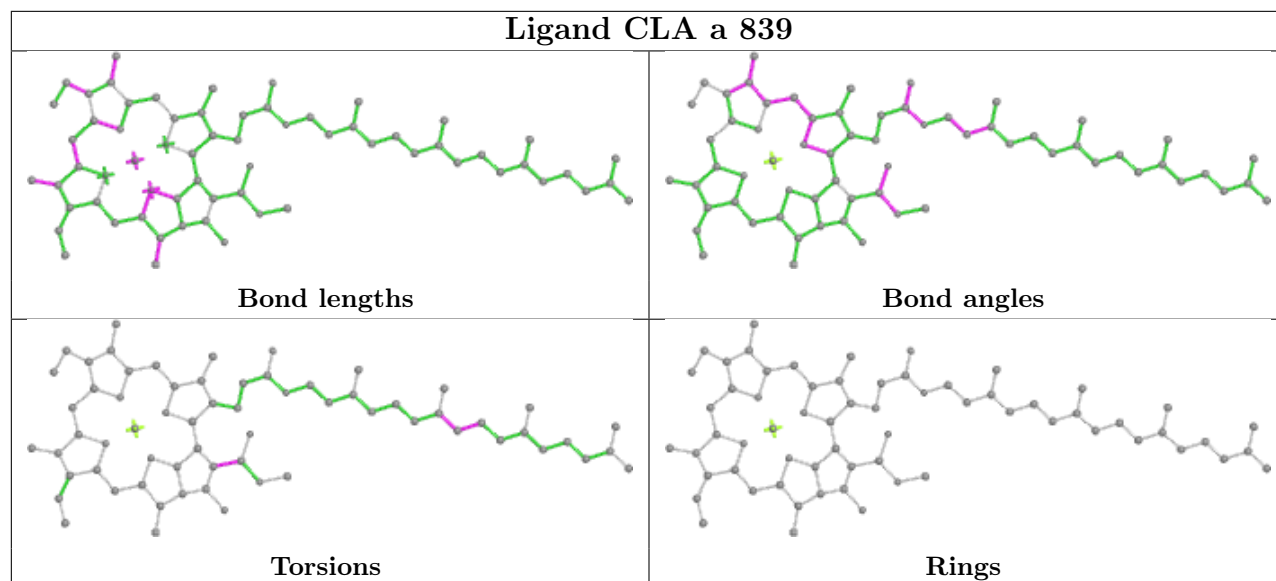
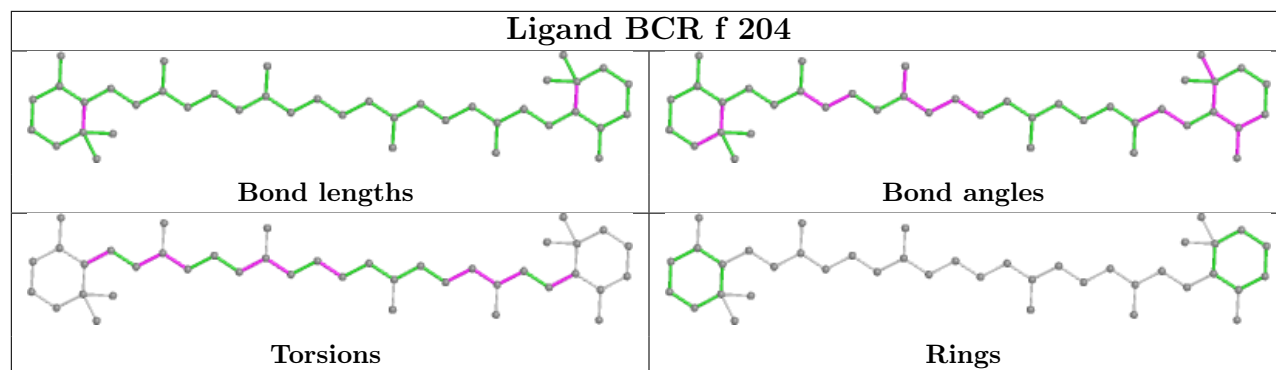


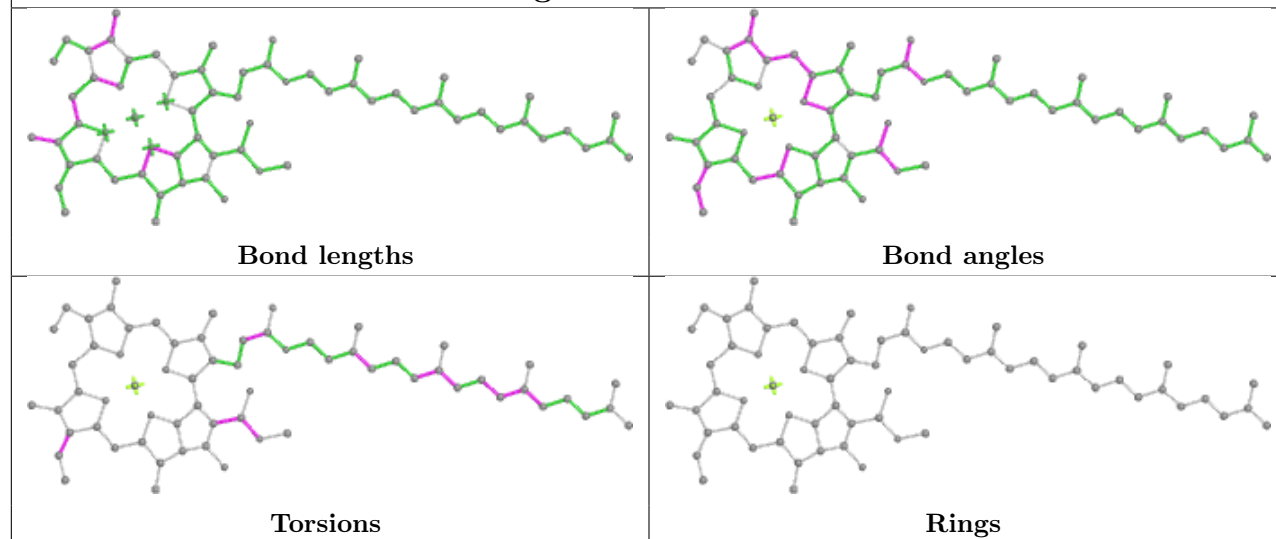
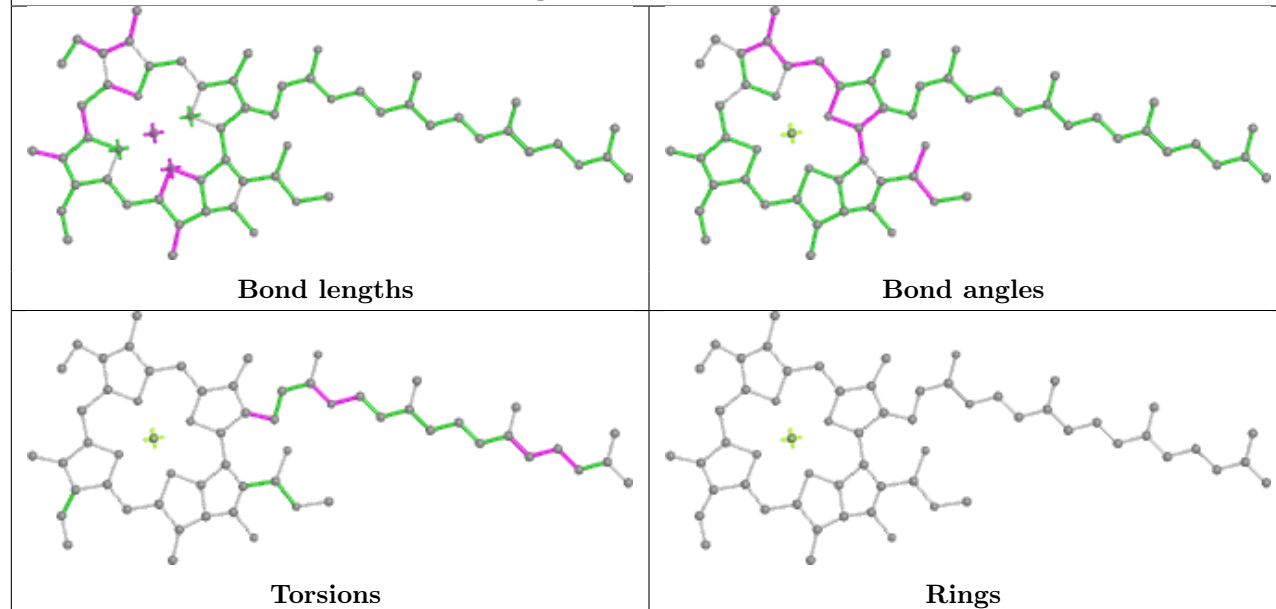




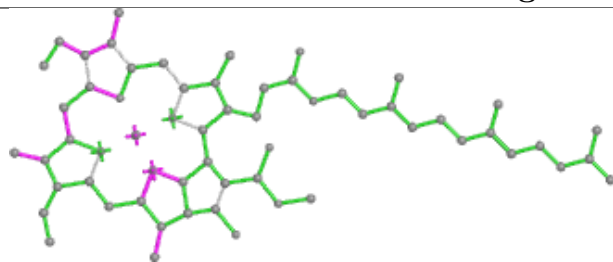


**Ligand CLA A 825****Ligand BCR J 105****Ligand CLA a 804**

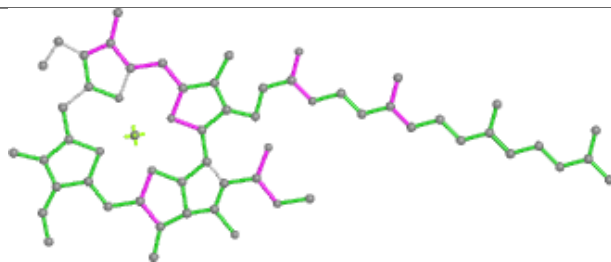


**Ligand CLA F 202****Ligand CLA A 818**

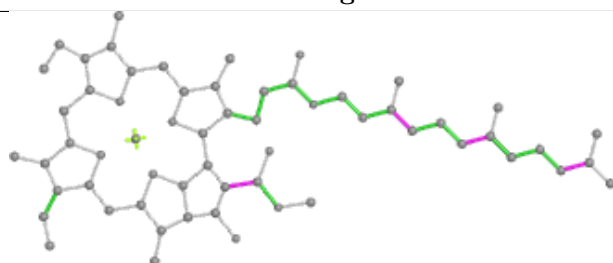
## Ligand CLA a 806



Bond lengths



Bond angles

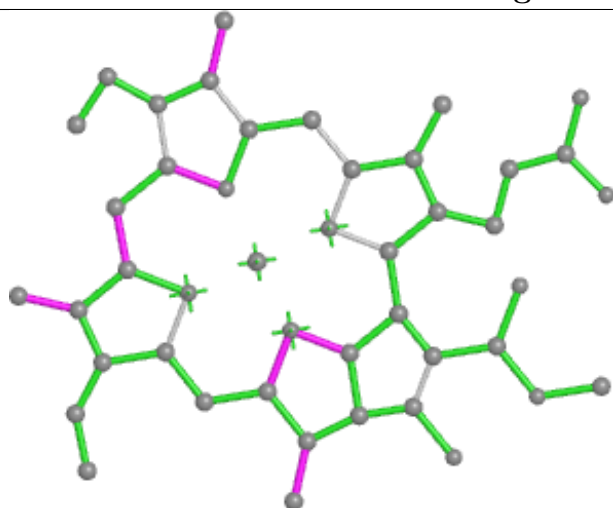


Torsions

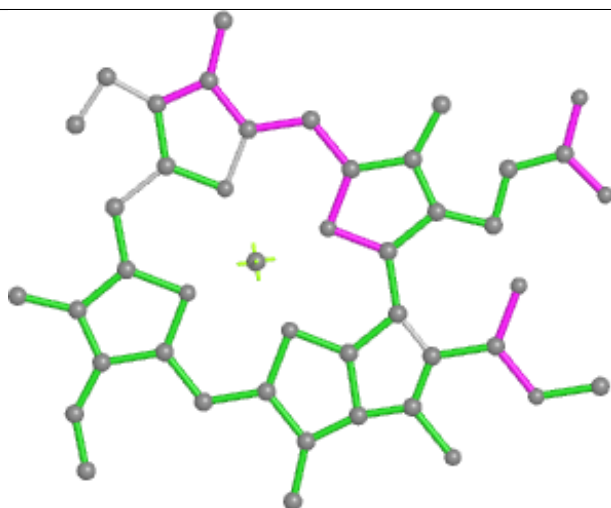


Rings

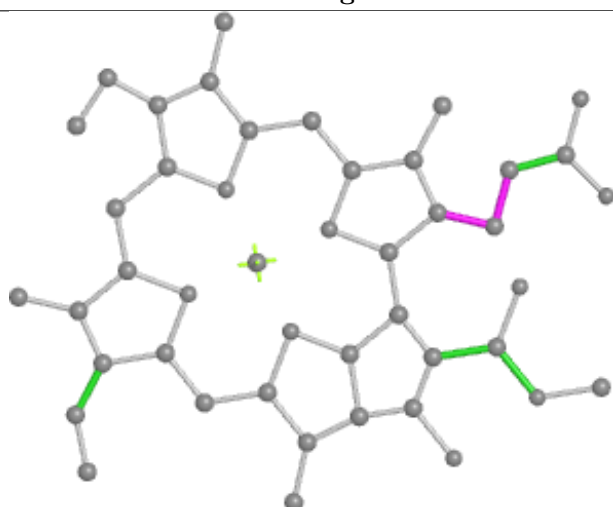
## Ligand CLA A 810



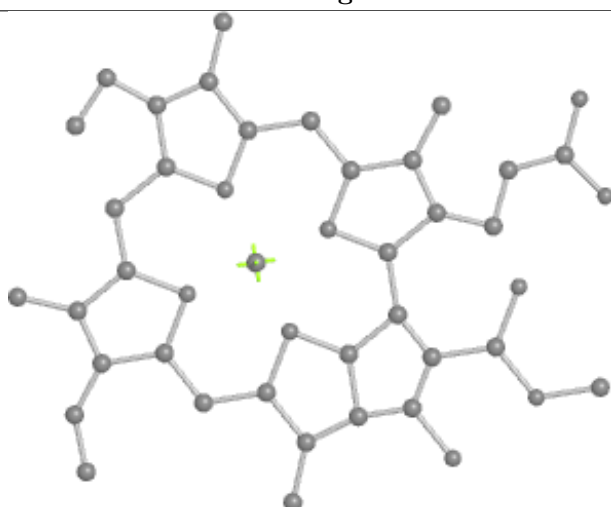
Bond lengths



Bond angles

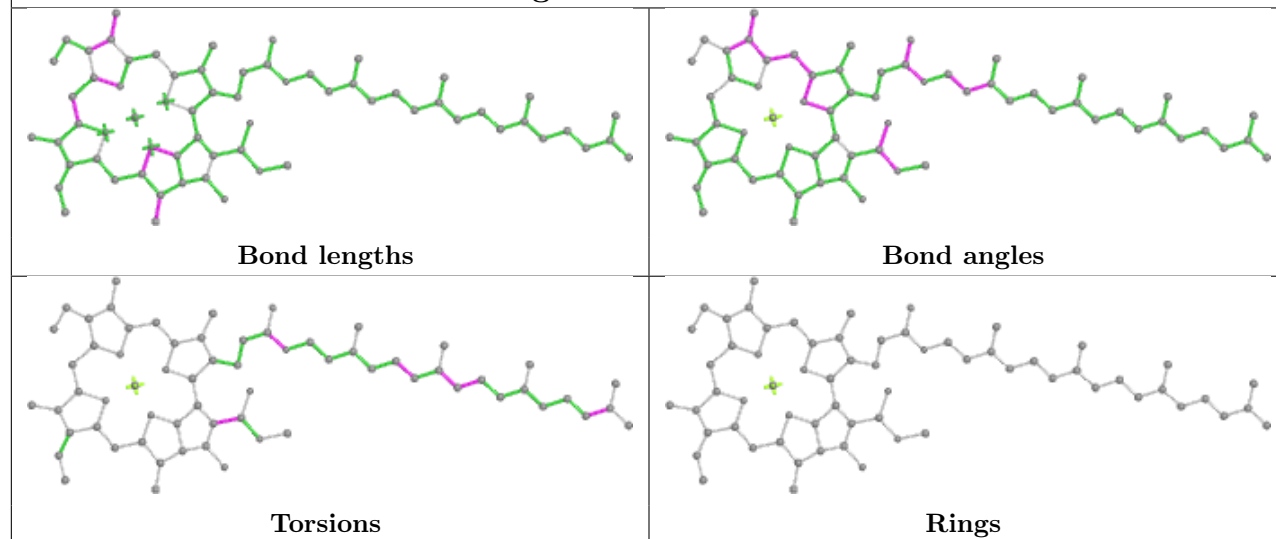


Torsions

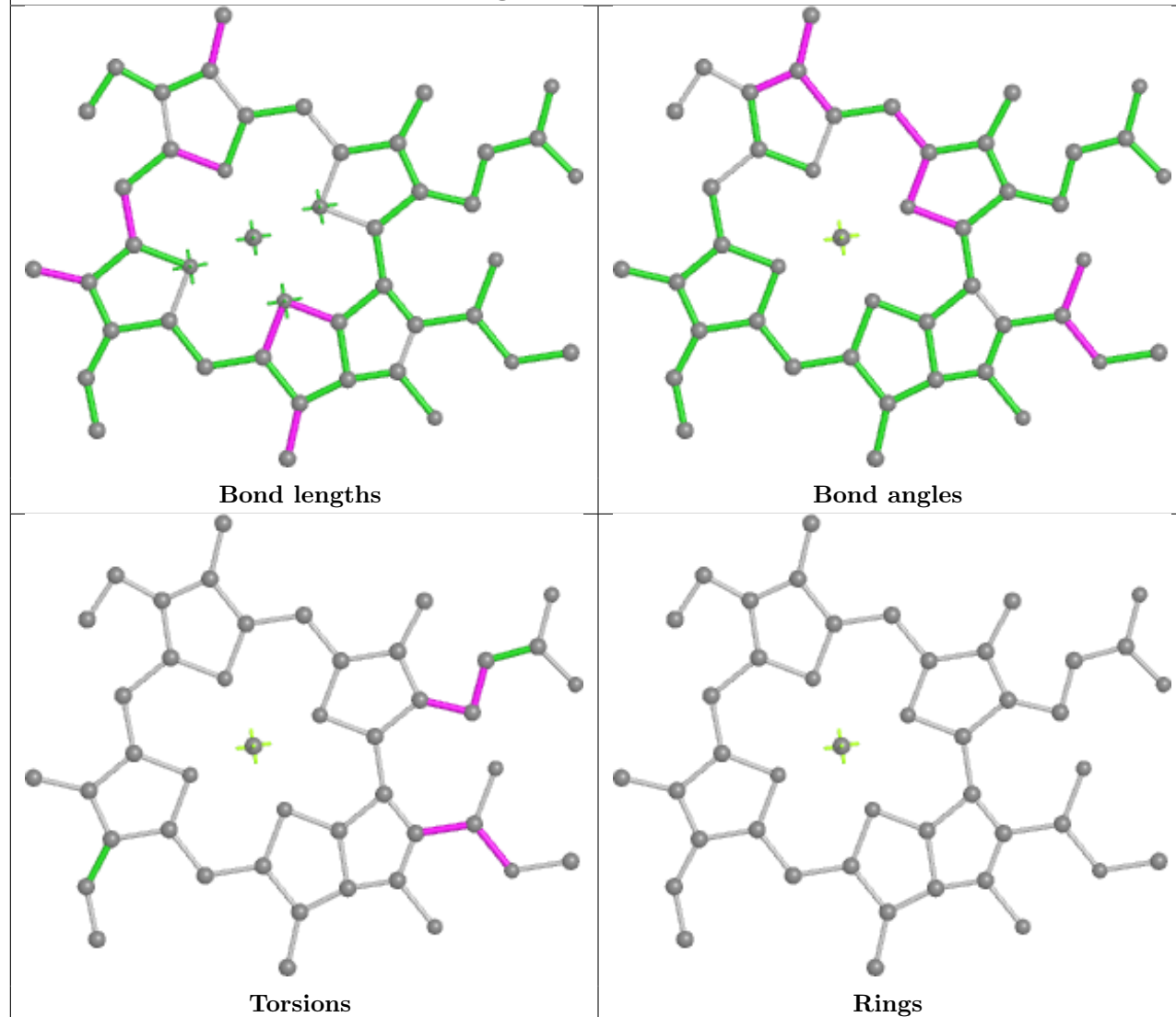


Rings

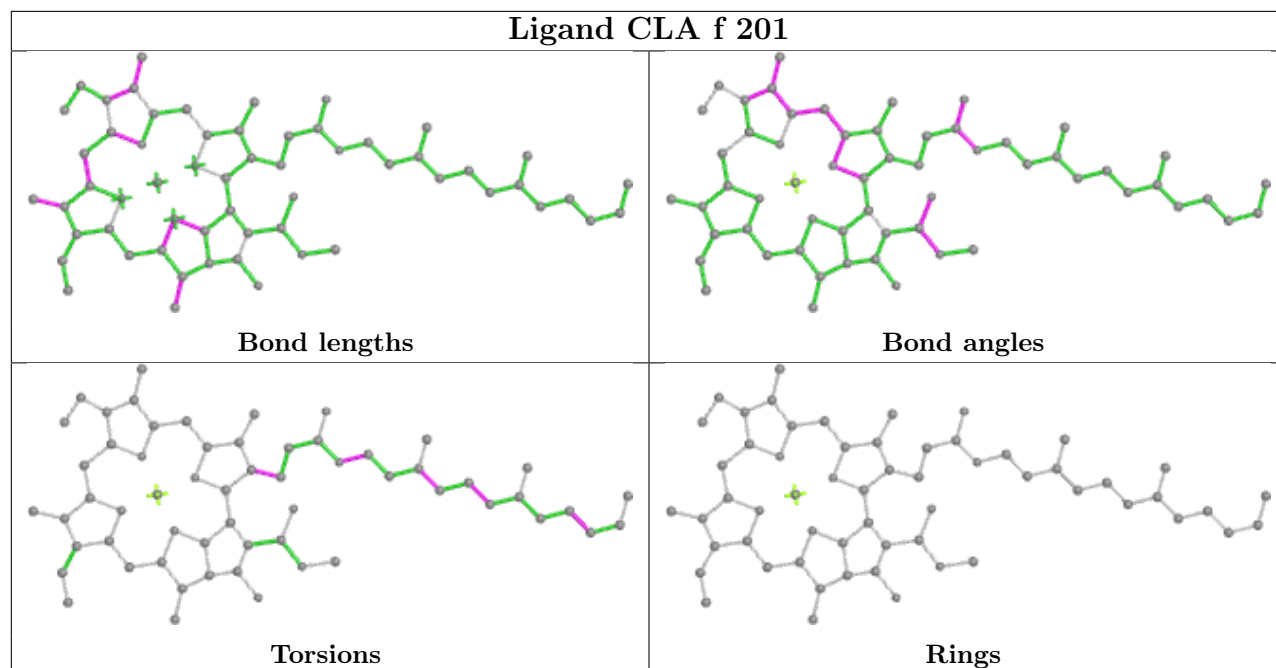
## Ligand CLA B 822



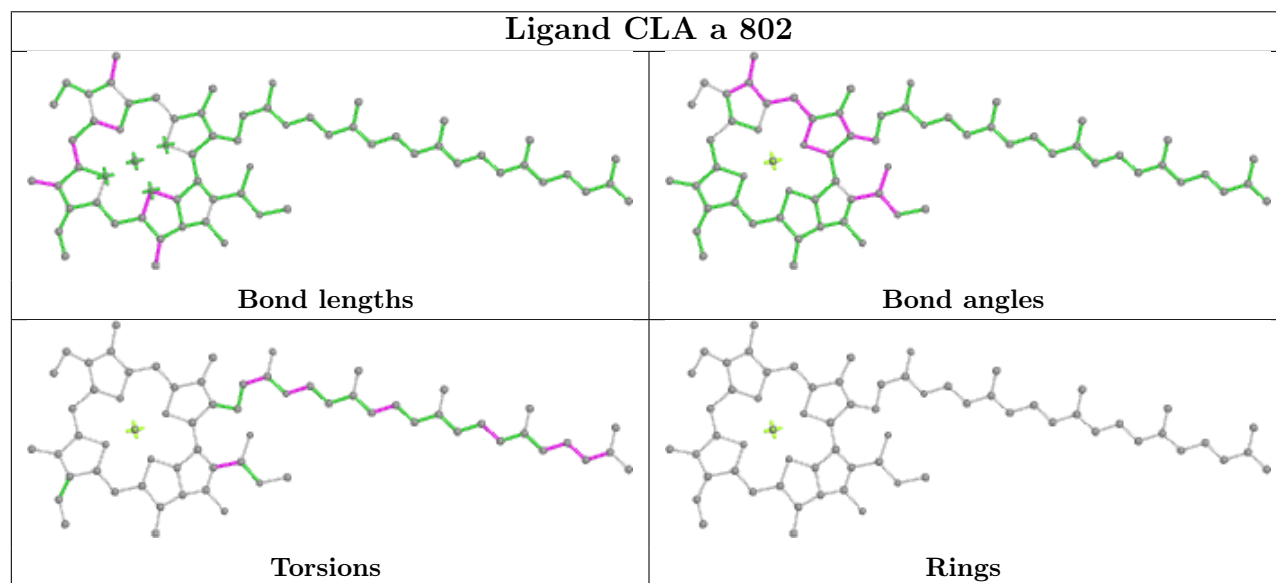
## Ligand CLA a 809

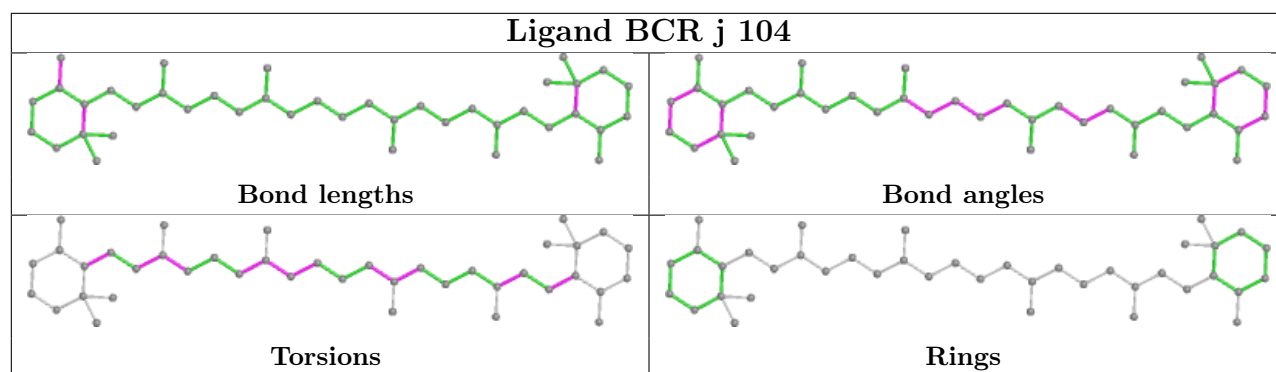
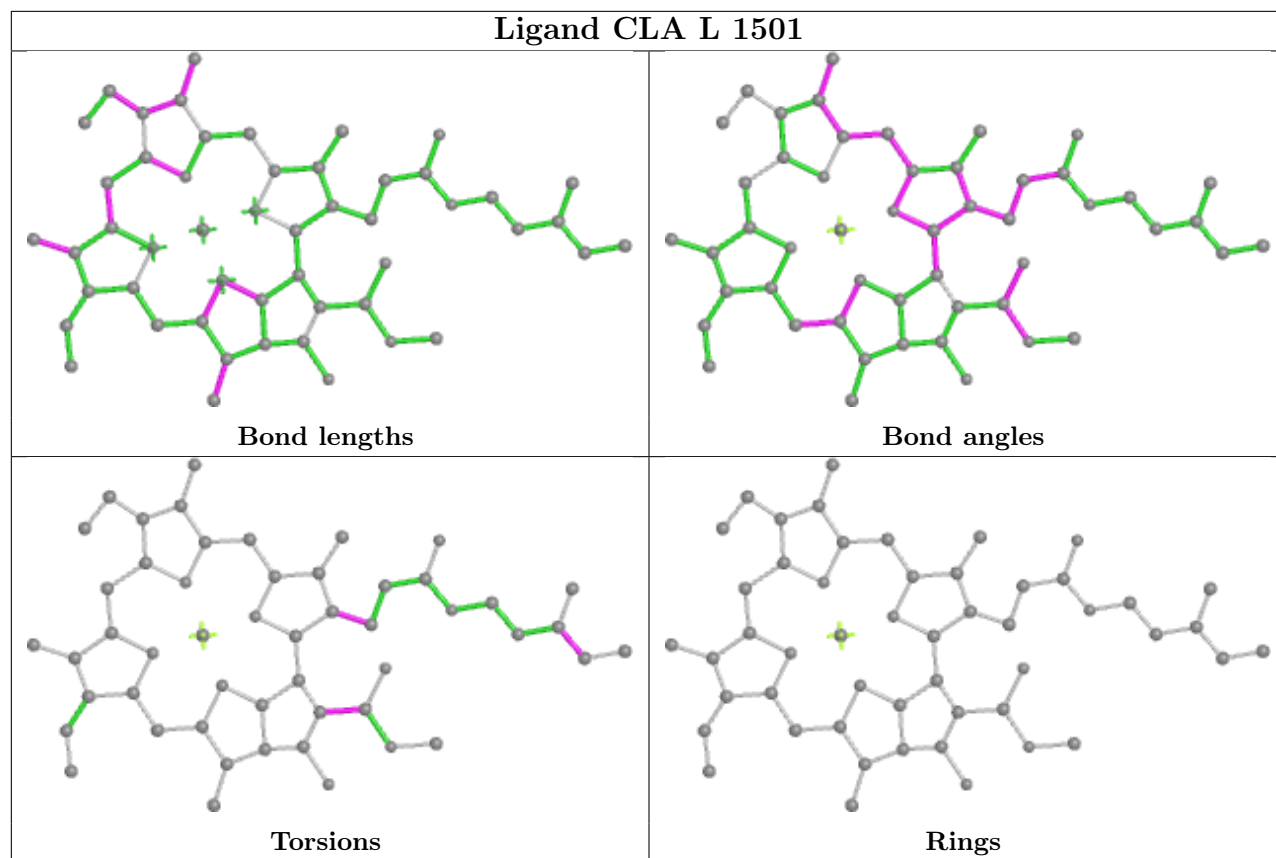


## Ligand CLA f 201



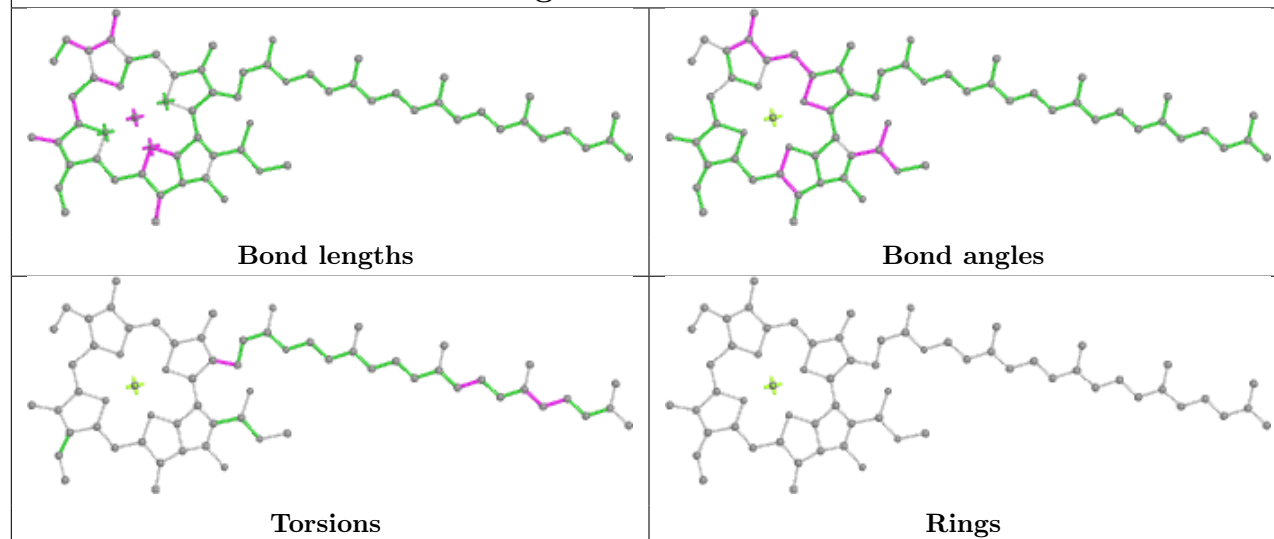
## Ligand CLA a 802



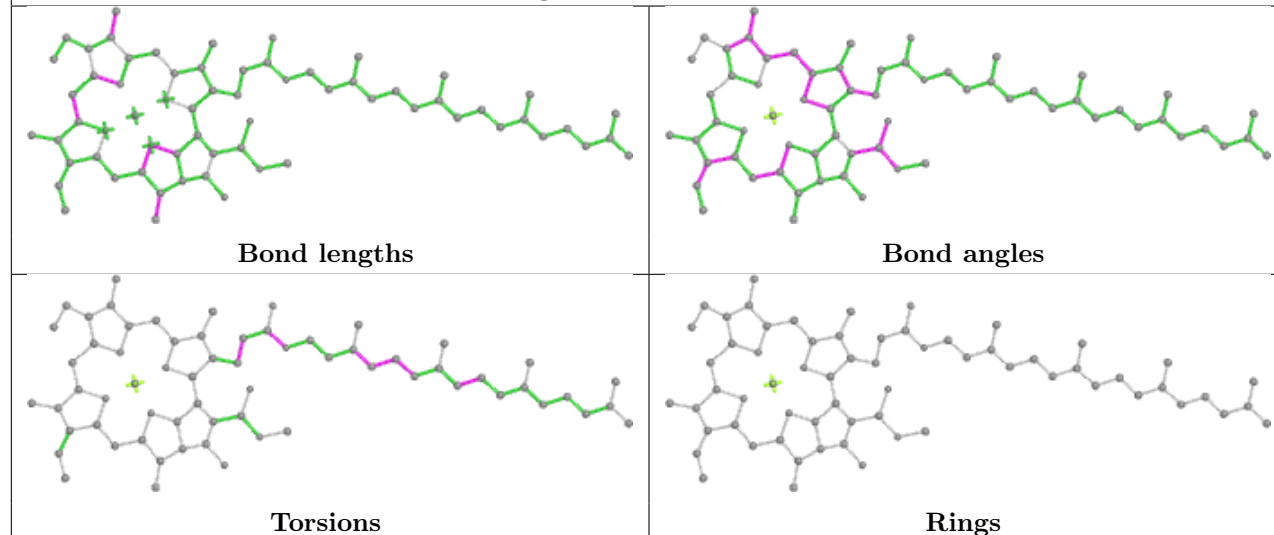




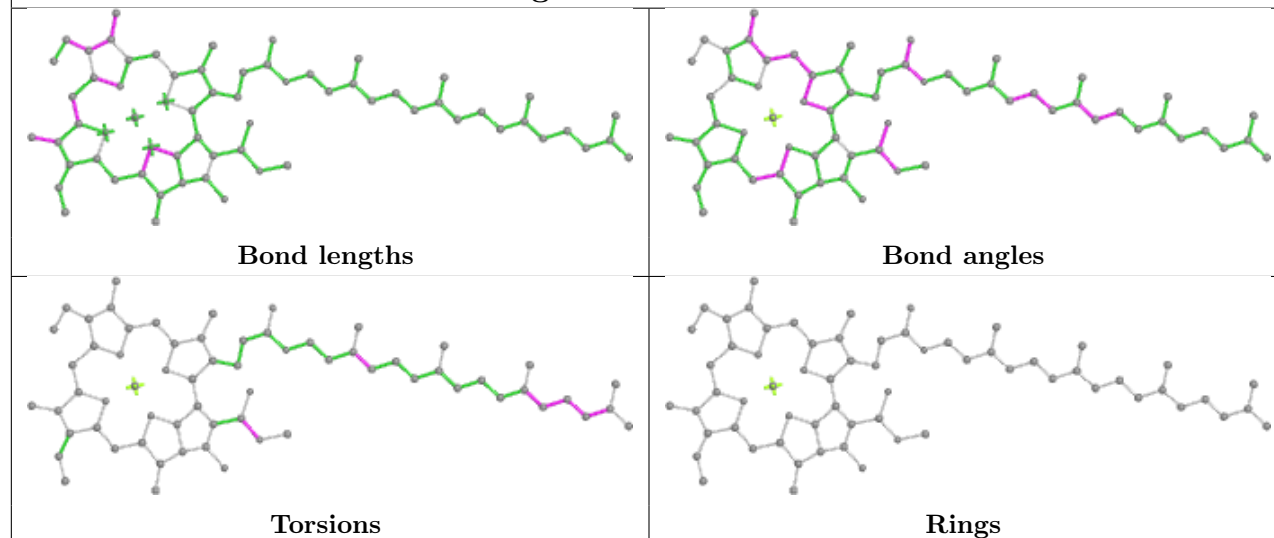
## Ligand CLA b 820



## Ligand CLA b 826



## Ligand CLA A 833



## 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.

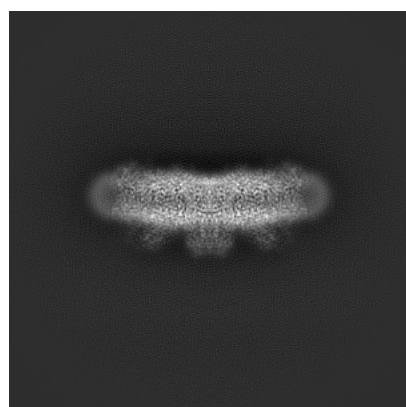
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9918. These allow visual inspection of the internal detail of the map and identification of artifacts.

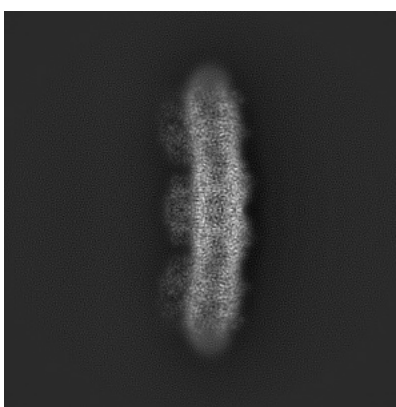
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

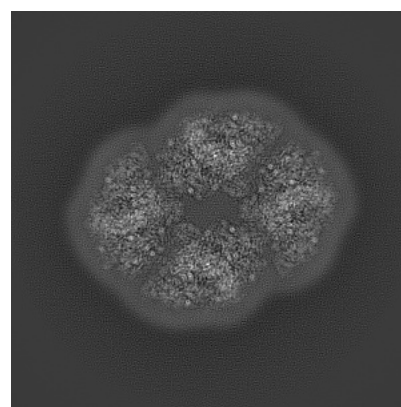
#### 6.1.1 Primary map



X



Y

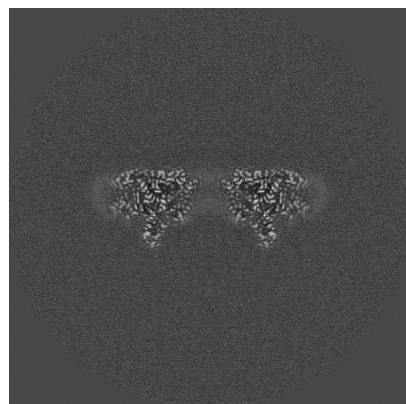


Z

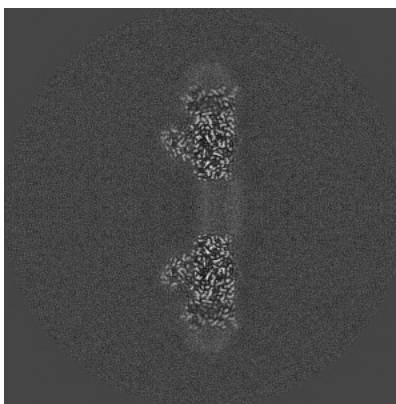
The images above show the map projected in three orthogonal directions.

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

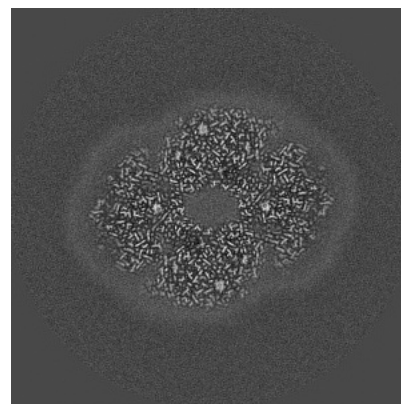
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

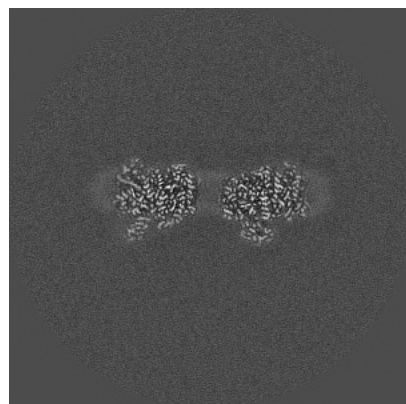


Z Index: 200

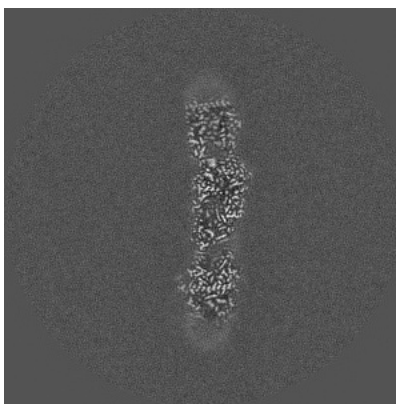
The images above show central slices of the map in three orthogonal directions.

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

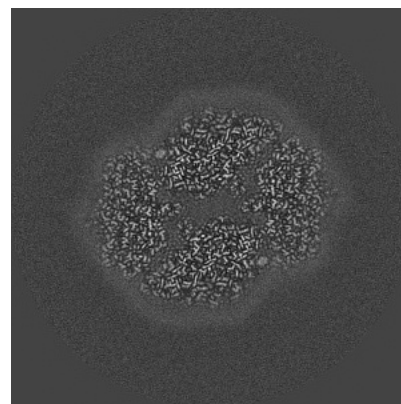
### 6.3.1 Primary map



X Index: 219



Y Index: 171

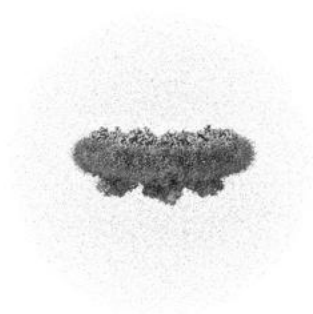


Z Index: 223

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

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

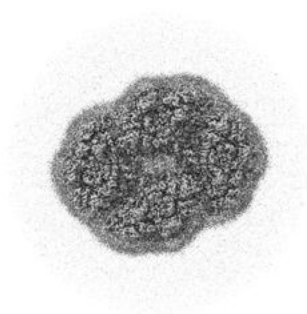
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

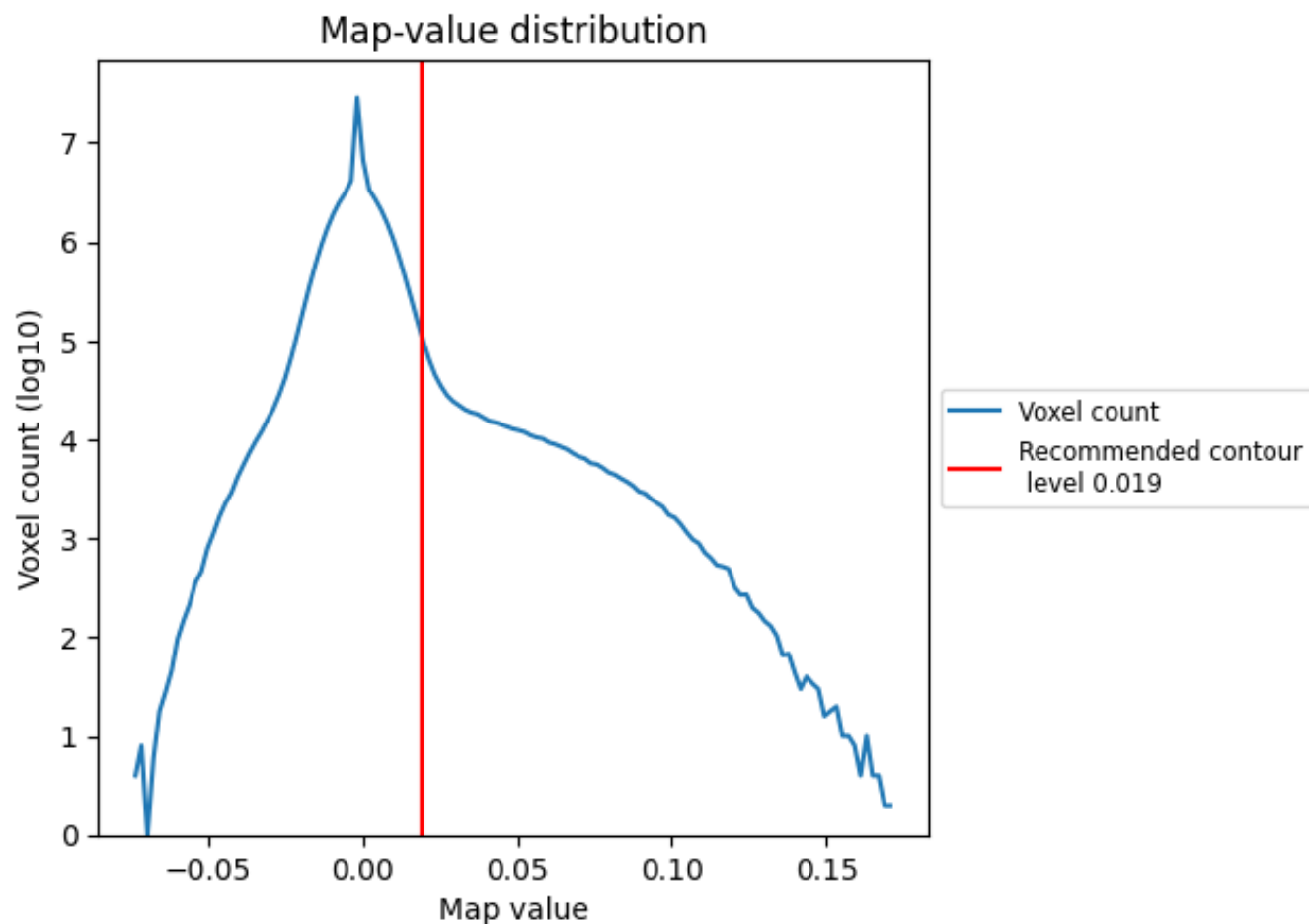
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

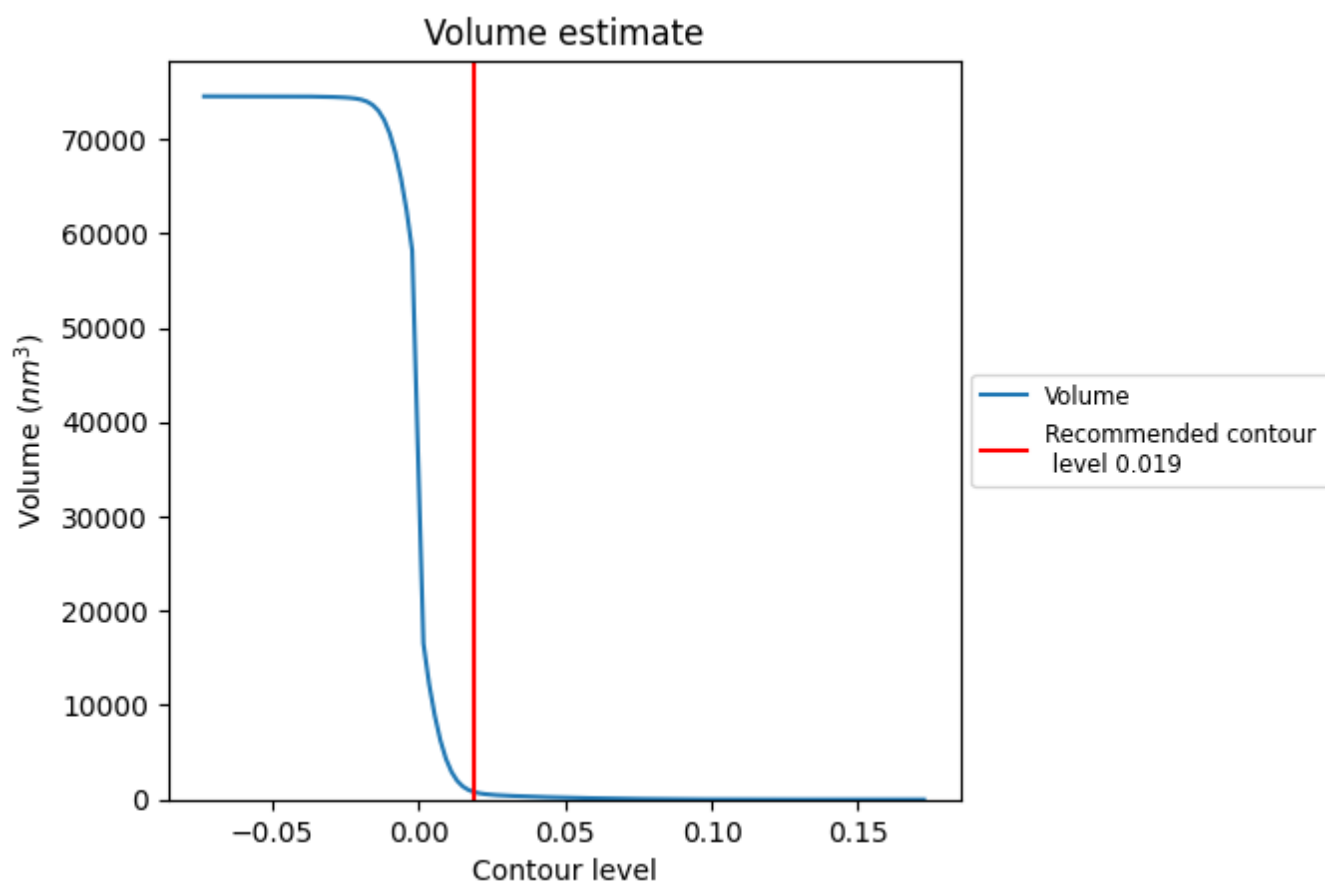
This section contains the results of statistical analysis of the map.

### 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.

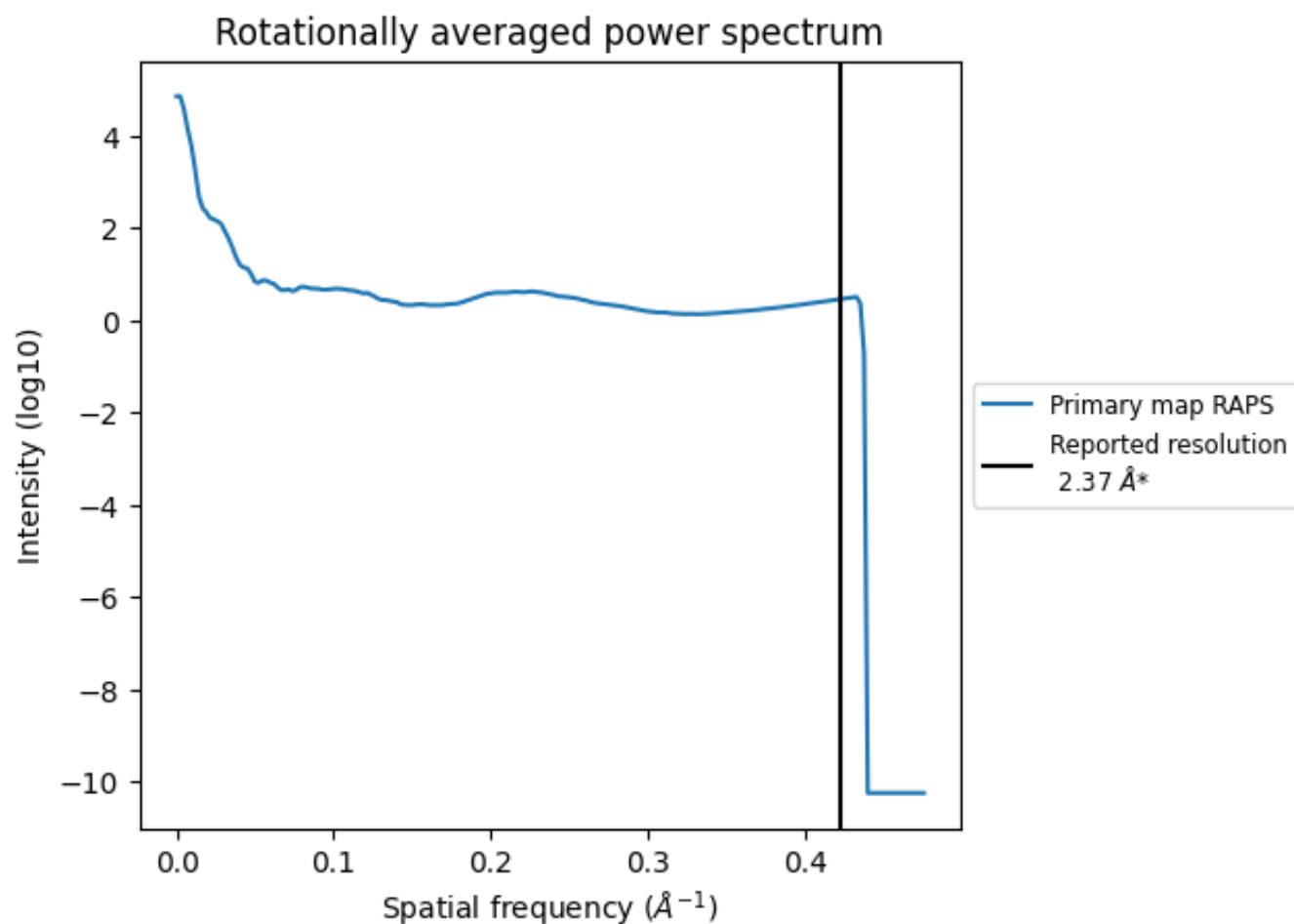
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 790  $\text{nm}^3$ ; this corresponds to an approximate mass of 714 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.422 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](#)

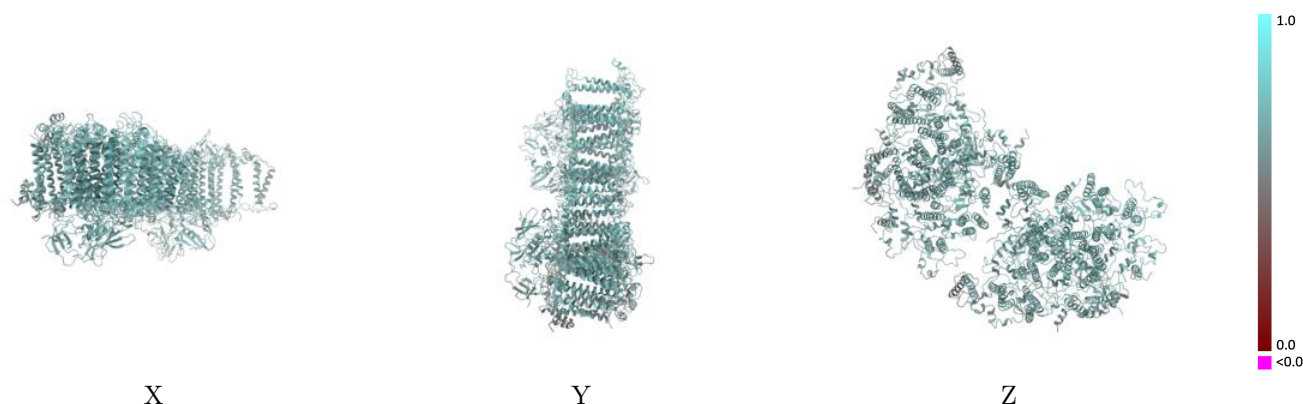
This section contains information regarding the fit between EMDB map EMD-9918 and PDB model 6K61. Per-residue inclusion information can be found in section [3](#) on page [28](#).

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



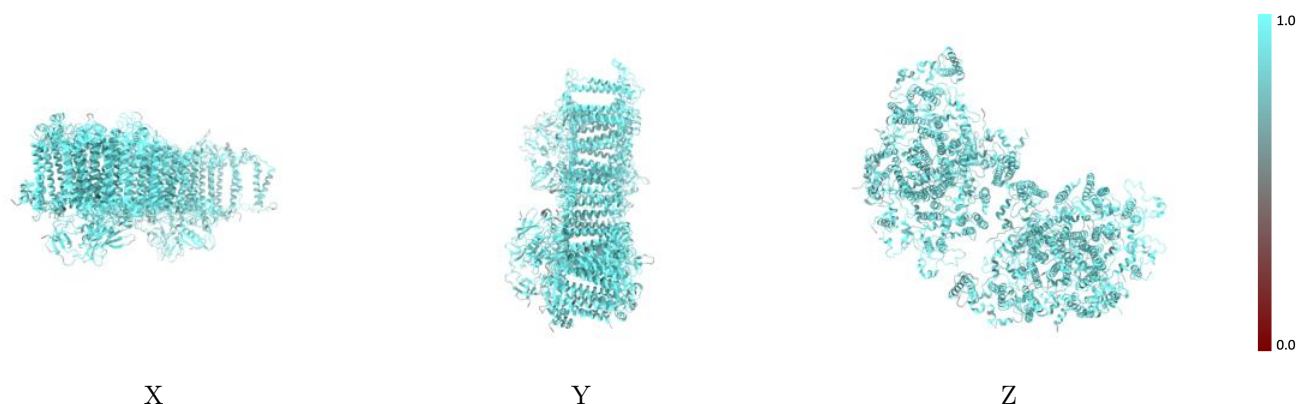
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



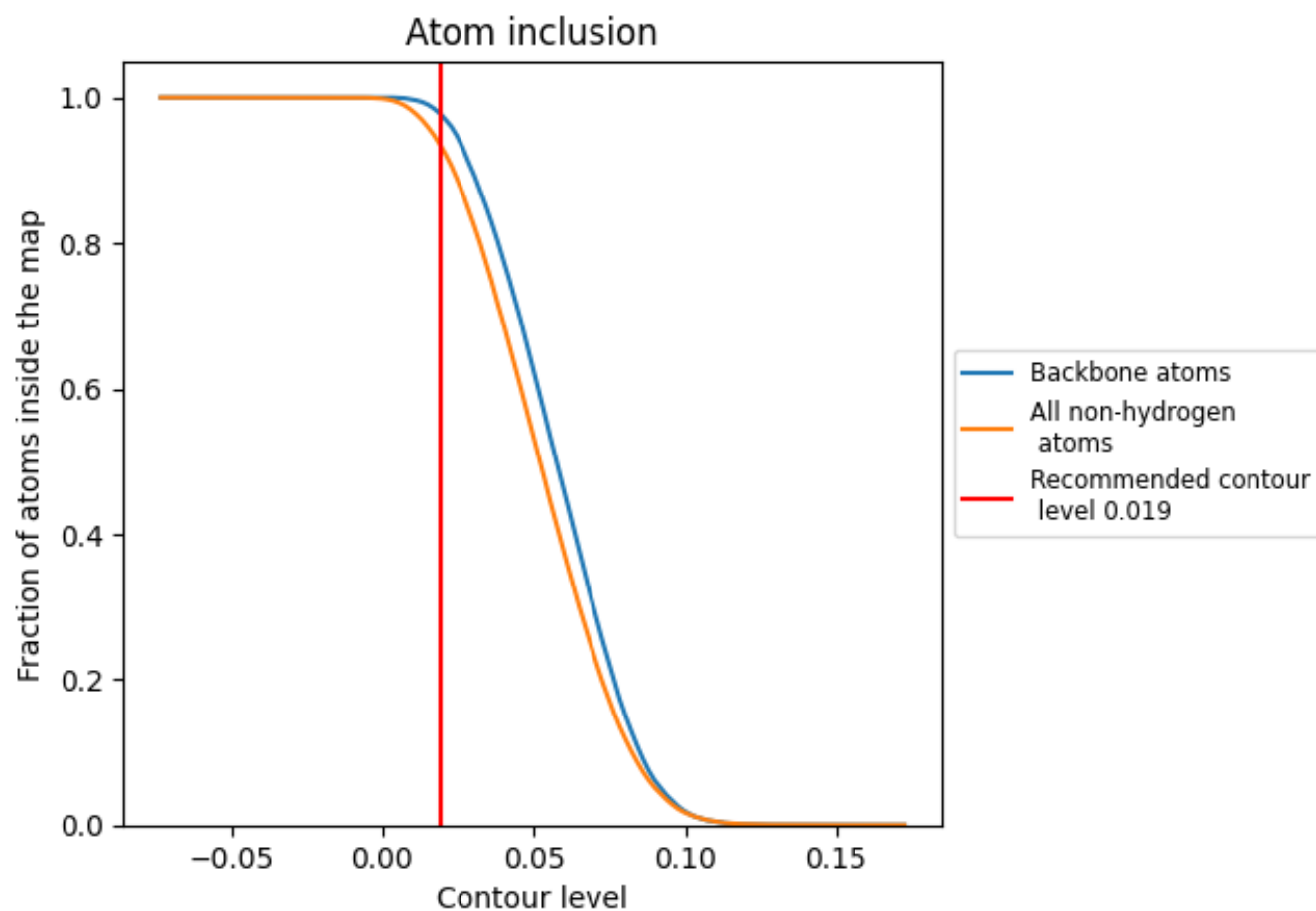
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9353	 0.6500
A	 0.9498	 0.6610
B	 0.9671	 0.6840
C	 0.9600	 0.6560
D	 0.9187	 0.6340
E	 0.8787	 0.5980
F	 0.8910	 0.6090
I	 0.9601	 0.6630
J	 0.9217	 0.6240
K	 0.7810	 0.5180
L	 0.9473	 0.6660
M	 0.9384	 0.6720
X	 0.8743	 0.6140
a	 0.9412	 0.6510
b	 0.9495	 0.6590
c	 0.9633	 0.6480
d	 0.9066	 0.6180
e	 0.8473	 0.5610
f	 0.8470	 0.5680
i	 0.9137	 0.6670
j	 0.8706	 0.5820
k	 0.7880	 0.5380
l	 0.9299	 0.6700
m	 0.9480	 0.6580
x	 0.7686	 0.5330

