



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 07:09 AM JST

PDB ID : 6KMW
EMDB ID : EMD-0726
Title : Structure of PSI from *H. hongdechloris* grown under white light condition
Authors : Kato, K.; Nagao, R.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on : 2019-08-01
Resolution : 2.35 Å (reported)
Based on initial model : 1JB0

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.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

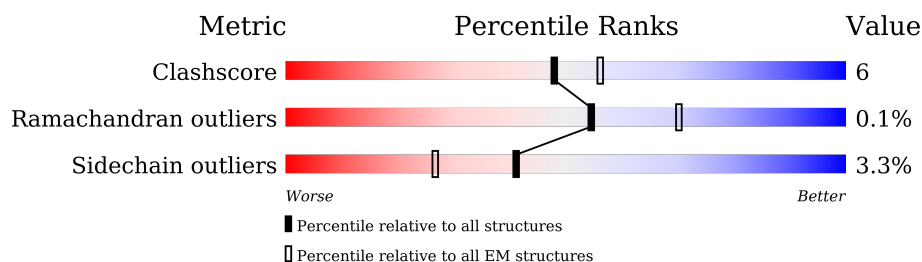
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.35 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	aA	764	
1	bA	764	
1	cA	764	
2	aB	742	
2	bB	742	
2	cB	742	
3	aC	81	
3	bC	81	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	cC	81	
4	aD	142	
4	bD	142	
4	cD	142	
5	aE	68	
5	bE	68	
5	cE	68	
6	aI	38	
6	bI	38	
6	cI	38	
7	aL	159	
7	bL	159	
7	cL	159	
8	aM	31	
8	bM	31	
8	cM	31	

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
10	CLA	aA	802	X	-	-	-
10	CLA	aA	803	X	-	-	-
10	CLA	aA	804	X	-	-	-
10	CLA	aA	805	X	-	-	-
10	CLA	aA	806	X	-	-	-
10	CLA	aA	807	X	-	-	-
10	CLA	aA	808	X	-	-	-
10	CLA	aA	809	X	-	-	-
10	CLA	aA	810	X	-	-	-
10	CLA	aA	811	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	aA	812	X	-	-	-
10	CLA	aA	813	X	-	-	-
10	CLA	aA	814	X	-	-	-
10	CLA	aA	815	X	-	-	-
10	CLA	aA	818	X	-	-	-
10	CLA	aA	819	X	-	-	-
10	CLA	aA	820	X	-	-	-
10	CLA	aA	821	X	-	-	-
10	CLA	aA	822	X	-	-	-
10	CLA	aA	823	X	-	-	-
10	CLA	aA	824	X	-	-	-
10	CLA	aA	825	X	-	-	-
10	CLA	aA	826	X	-	-	-
10	CLA	aA	827	X	-	-	-
10	CLA	aA	828	X	-	-	-
10	CLA	aA	829	X	-	-	-
10	CLA	aA	830	X	-	-	-
10	CLA	aA	831	X	-	-	-
10	CLA	aA	832	X	-	-	-
10	CLA	aA	833	X	-	-	-
10	CLA	aA	834	X	-	-	-
10	CLA	aA	835	X	-	-	-
10	CLA	aA	836	X	-	-	-
10	CLA	aA	837	X	-	-	-
10	CLA	aA	838	X	-	-	-
10	CLA	aA	839	X	-	-	-
10	CLA	aA	840	X	-	-	-
10	CLA	aA	841	X	-	-	-
10	CLA	aA	842	X	-	-	-
10	CLA	aA	843	X	-	-	-
10	CLA	aA	856	X	-	-	-
10	CLA	aB	801	X	-	-	-
10	CLA	aB	802	X	-	-	-
10	CLA	aB	803	X	-	-	-
10	CLA	aB	804	X	-	-	-
10	CLA	aB	805	X	-	-	-
10	CLA	aB	806	X	-	-	-
10	CLA	aB	807	X	-	-	-
10	CLA	aB	808	X	-	-	-
10	CLA	aB	809	X	-	-	-
10	CLA	aB	810	X	-	-	-
10	CLA	aB	811	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	aB	812	X	-	-	-
10	CLA	aB	814	X	-	-	-
10	CLA	aB	815	X	-	-	-
10	CLA	aB	816	X	-	-	-
10	CLA	aB	817	X	-	-	-
10	CLA	aB	818	X	-	-	-
10	CLA	aB	819	X	-	-	-
10	CLA	aB	820	X	-	-	-
10	CLA	aB	821	X	-	-	-
10	CLA	aB	823	X	-	-	-
10	CLA	aB	824	X	-	-	-
10	CLA	aB	825	X	-	-	-
10	CLA	aB	826	X	-	-	-
10	CLA	aB	827	X	-	-	-
10	CLA	aB	828	X	-	-	-
10	CLA	aB	829	X	-	-	-
10	CLA	aB	830	X	-	-	-
10	CLA	aB	831	X	-	-	-
10	CLA	aB	832	X	-	-	-
10	CLA	aB	833	X	-	-	-
10	CLA	aB	834	X	-	-	-
10	CLA	aB	835	X	-	-	-
10	CLA	aB	836	X	-	-	-
10	CLA	aB	837	X	-	-	-
10	CLA	aB	838	X	-	-	-
10	CLA	aB	839	X	-	-	-
10	CLA	aB	840	X	-	-	-
10	CLA	aB	841	X	-	-	-
10	CLA	aL	202	X	-	-	-
10	CLA	aL	204	X	-	-	-
10	CLA	bA	802	X	-	-	-
10	CLA	bA	803	X	-	-	-
10	CLA	bA	804	X	-	-	-
10	CLA	bA	805	X	-	-	-
10	CLA	bA	806	X	-	-	-
10	CLA	bA	807	X	-	-	-
10	CLA	bA	808	X	-	-	-
10	CLA	bA	809	X	-	-	-
10	CLA	bA	810	X	-	-	-
10	CLA	bA	811	X	-	-	-
10	CLA	bA	812	X	-	-	-
10	CLA	bA	813	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	bA	814	X	-	-	-
10	CLA	bA	815	X	-	-	-
10	CLA	bA	818	X	-	-	-
10	CLA	bA	819	X	-	-	-
10	CLA	bA	820	X	-	-	-
10	CLA	bA	821	X	-	-	-
10	CLA	bA	822	X	-	-	-
10	CLA	bA	823	X	-	-	-
10	CLA	bA	824	X	-	-	-
10	CLA	bA	825	X	-	-	-
10	CLA	bA	826	X	-	-	-
10	CLA	bA	827	X	-	-	-
10	CLA	bA	828	X	-	-	-
10	CLA	bA	829	X	-	-	-
10	CLA	bA	830	X	-	-	-
10	CLA	bA	831	X	-	-	-
10	CLA	bA	832	X	-	-	-
10	CLA	bA	833	X	-	-	-
10	CLA	bA	834	X	-	-	-
10	CLA	bA	835	X	-	-	-
10	CLA	bA	836	X	-	-	-
10	CLA	bA	837	X	-	-	-
10	CLA	bA	838	X	-	-	-
10	CLA	bA	839	X	-	-	-
10	CLA	bA	840	X	-	-	-
10	CLA	bA	841	X	-	-	-
10	CLA	bA	842	X	-	-	-
10	CLA	bA	843	X	-	-	-
10	CLA	bA	856	X	-	-	-
10	CLA	bB	801	X	-	-	-
10	CLA	bB	802	X	-	-	-
10	CLA	bB	803	X	-	-	-
10	CLA	bB	804	X	-	-	-
10	CLA	bB	805	X	-	-	-
10	CLA	bB	806	X	-	-	-
10	CLA	bB	807	X	-	-	-
10	CLA	bB	808	X	-	-	-
10	CLA	bB	809	X	-	-	-
10	CLA	bB	810	X	-	-	-
10	CLA	bB	811	X	-	-	-
10	CLA	bB	812	X	-	-	-
10	CLA	bB	814	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	bB	815	X	-	-	-
10	CLA	bB	816	X	-	-	-
10	CLA	bB	817	X	-	-	-
10	CLA	bB	818	X	-	-	-
10	CLA	bB	819	X	-	-	-
10	CLA	bB	820	X	-	-	-
10	CLA	bB	821	X	-	-	-
10	CLA	bB	823	X	-	-	-
10	CLA	bB	824	X	-	-	-
10	CLA	bB	825	X	-	-	-
10	CLA	bB	826	X	-	-	-
10	CLA	bB	827	X	-	-	-
10	CLA	bB	828	X	-	-	-
10	CLA	bB	829	X	-	-	-
10	CLA	bB	830	X	-	-	-
10	CLA	bB	831	X	-	-	-
10	CLA	bB	832	X	-	-	-
10	CLA	bB	833	X	-	-	-
10	CLA	bB	834	X	-	-	-
10	CLA	bB	835	X	-	-	-
10	CLA	bB	836	X	-	-	-
10	CLA	bB	837	X	-	-	-
10	CLA	bB	838	X	-	-	-
10	CLA	bB	839	X	-	-	-
10	CLA	bB	840	X	-	-	-
10	CLA	bB	841	X	-	-	-
10	CLA	bL	202	X	-	-	-
10	CLA	bL	204	X	-	-	-
10	CLA	cA	802	X	-	-	-
10	CLA	cA	803	X	-	-	-
10	CLA	cA	804	X	-	-	-
10	CLA	cA	805	X	-	-	-
10	CLA	cA	806	X	-	-	-
10	CLA	cA	807	X	-	-	-
10	CLA	cA	808	X	-	-	-
10	CLA	cA	809	X	-	-	-
10	CLA	cA	810	X	-	-	-
10	CLA	cA	811	X	-	-	-
10	CLA	cA	812	X	-	-	-
10	CLA	cA	813	X	-	-	-
10	CLA	cA	814	X	-	-	-
10	CLA	cA	815	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	cA	818	X	-	-	-
10	CLA	cA	819	X	-	-	-
10	CLA	cA	820	X	-	-	-
10	CLA	cA	821	X	-	-	-
10	CLA	cA	822	X	-	-	-
10	CLA	cA	823	X	-	-	-
10	CLA	cA	824	X	-	-	-
10	CLA	cA	825	X	-	-	-
10	CLA	cA	826	X	-	-	-
10	CLA	cA	827	X	-	-	-
10	CLA	cA	828	X	-	-	-
10	CLA	cA	829	X	-	-	-
10	CLA	cA	830	X	-	-	-
10	CLA	cA	831	X	-	-	-
10	CLA	cA	832	X	-	-	-
10	CLA	cA	833	X	-	-	-
10	CLA	cA	834	X	-	-	-
10	CLA	cA	835	X	-	-	-
10	CLA	cA	836	X	-	-	-
10	CLA	cA	837	X	-	-	-
10	CLA	cA	838	X	-	-	-
10	CLA	cA	839	X	-	-	-
10	CLA	cA	840	X	-	-	-
10	CLA	cA	841	X	-	-	-
10	CLA	cA	842	X	-	-	-
10	CLA	cA	843	X	-	-	-
10	CLA	cA	856	X	-	-	-
10	CLA	cB	801	X	-	-	-
10	CLA	cB	802	X	-	-	-
10	CLA	cB	803	X	-	-	-
10	CLA	cB	804	X	-	-	-
10	CLA	cB	805	X	-	-	-
10	CLA	cB	806	X	-	-	-
10	CLA	cB	807	X	-	-	-
10	CLA	cB	808	X	-	-	-
10	CLA	cB	809	X	-	-	-
10	CLA	cB	810	X	-	-	-
10	CLA	cB	811	X	-	-	-
10	CLA	cB	812	X	-	-	-
10	CLA	cB	814	X	-	-	-
10	CLA	cB	815	X	-	-	-
10	CLA	cB	816	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	cB	817	X	-	-	-
10	CLA	cB	818	X	-	-	-
10	CLA	cB	819	X	-	-	-
10	CLA	cB	820	X	-	-	-
10	CLA	cB	821	X	-	-	-
10	CLA	cB	823	X	-	-	-
10	CLA	cB	824	X	-	-	-
10	CLA	cB	825	X	-	-	-
10	CLA	cB	826	X	-	-	-
10	CLA	cB	827	X	-	-	-
10	CLA	cB	828	X	-	-	-
10	CLA	cB	829	X	-	-	-
10	CLA	cB	830	X	-	-	-
10	CLA	cB	831	X	-	-	-
10	CLA	cB	832	X	-	-	-
10	CLA	cB	833	X	-	-	-
10	CLA	cB	834	X	-	-	-
10	CLA	cB	835	X	-	-	-
10	CLA	cB	836	X	-	-	-
10	CLA	cB	837	X	-	-	-
10	CLA	cB	838	X	-	-	-
10	CLA	cB	839	X	-	-	-
10	CLA	cB	840	X	-	-	-
10	CLA	cB	841	X	-	-	-
10	CLA	cL	202	X	-	-	-
10	CLA	cL	204	X	-	-	-
9	CL0	aA	801	X	-	-	-
9	CL0	bA	801	X	-	-	-
9	CL0	cA	801	X	-	-	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 64083 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	aA	721	Total	C	N	O	S	0	0
			5629	3692	953	958	26		
1	bA	721	Total	C	N	O	S	0	0
			5629	3692	953	958	26		
1	cA	721	Total	C	N	O	S	0	0
			5629	3692	953	958	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	740	Total	C	N	O	S	0	0
			5884	3866	990	1005	23		
2	bB	740	Total	C	N	O	S	0	0
			5884	3866	990	1005	23		
2	cB	740	Total	C	N	O	S	0	0
			5884	3866	990	1005	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			596	366	102	117	11		
3	bC	80	Total	C	N	O	S	0	0
			596	366	102	117	11		
3	cC	80	Total	C	N	O	S	0	0
			596	366	102	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	98	Total	C	N	O	S	0	0
			768	492	130	143	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	98	Total	C	N	O	S	0	0
			768	492	130	143	3		
4	cD	98	Total	C	N	O	S	0	0
			768	492	130	143	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	aE	61	Total	C	N	O		0	0
			499	317	87	95			
5	bE	61	Total	C	N	O		0	0
			499	317	87	95			
5	cE	61	Total	C	N	O		0	0
			499	317	87	95			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aI	38	Total	C	N	O	S	0	0
			305	210	41	51	3		
6	bI	38	Total	C	N	O	S	0	0
			305	210	41	51	3		
6	cI	38	Total	C	N	O	S	0	0
			305	210	41	51	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aL	144	Total	C	N	O	S	0	0
			1065	694	173	192	6		
7	bL	144	Total	C	N	O	S	0	0
			1065	694	173	192	6		
7	cL	144	Total	C	N	O	S	0	0
			1065	694	173	192	6		

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

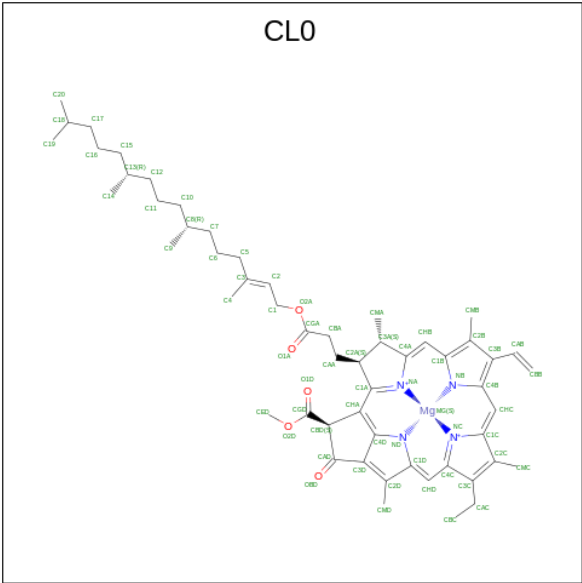
Mol	Chain	Residues	Atoms					AltConf	Trace
8	aM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		
8	bM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	cM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		

- Molecule 9 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
9	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 10 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Continued on next page...

[illegible]

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	aL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	aL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	aL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	

Continued on next page...

[illegible]

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	

Continued on next page...

[illegible]

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bL	1	Total 250	C 210	Mg 4	N 16	O 20	0
10	bL	1	Total 250	C 210	Mg 4	N 16	O 20	0
10	bL	1	Total 250	C 210	Mg 4	N 16	O 20	0
10	bL	1	Total 250	C 210	Mg 4	N 16	O 20	0
10	cA	1	Total 2491	C 2053	Mg 44	N 176	O 218	0
10	cA	1	Total 2491	C 2053	Mg 44	N 176	O 218	0
10	cA	1	Total 2491	C 2053	Mg 44	N 176	O 218	0
10	cA	1	Total 2491	C 2053	Mg 44	N 176	O 218	0

Continued on next page...

[illegible]

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

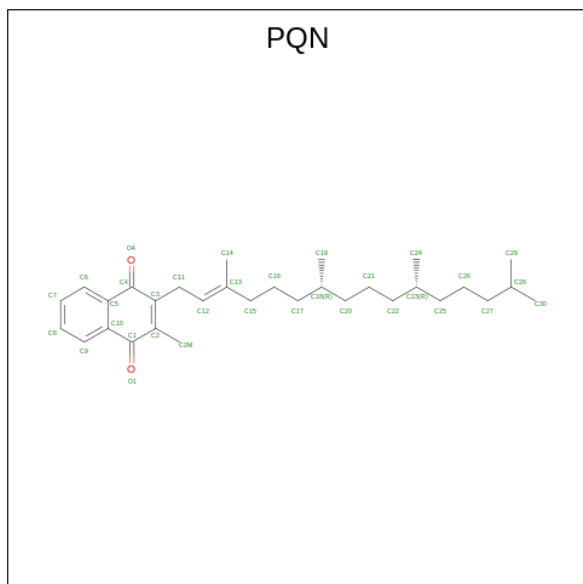
Mol	Chain	Residues	Atoms					AltConf
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cL	1	Total 250	C 210	Mg 4	N 16	O 20	0
10	cL	1	Total 250	C 210	Mg 4	N 16	O 20	0
10	cL	1	Total 250	C 210	Mg 4	N 16	O 20	0

Continued on next page...

Continued from previous page...

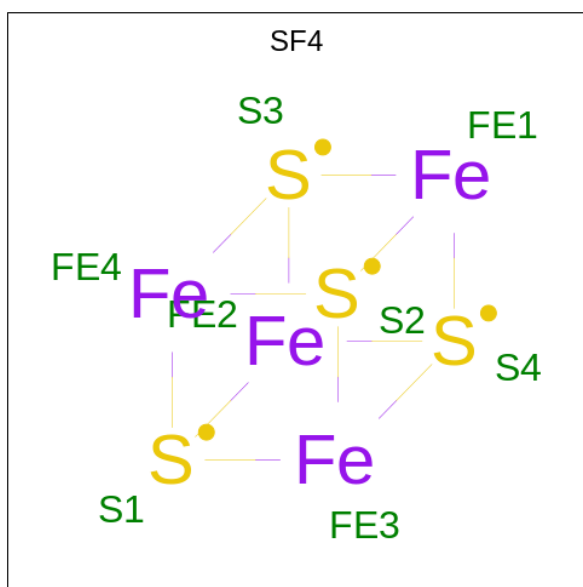
Mol	Chain	Residues	Atoms					AltConf
10	cL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	

- Molecule 11 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



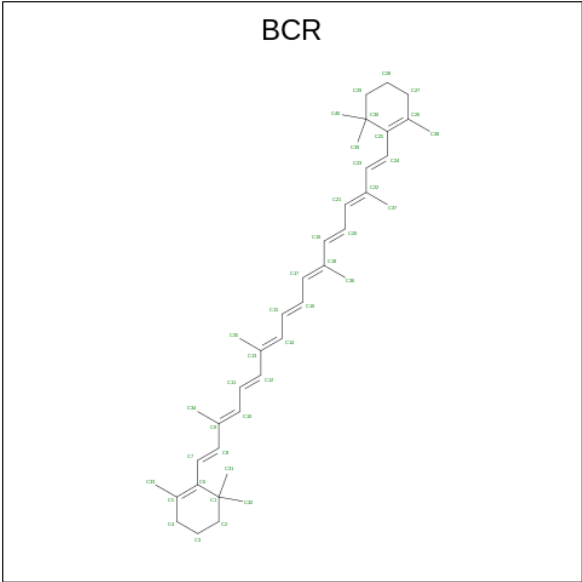
Mol	Chain	Residues	Atoms			AltConf
11	aA	1	Total	C	O	0
			33	31	2	
11	aB	1	Total	C	O	0
			33	31	2	
11	bA	1	Total	C	O	0
			33	31	2	
11	bB	1	Total	C	O	0
			33	31	2	
11	cA	1	Total	C	O	0
			33	31	2	
11	cB	1	Total	C	O	0
			33	31	2	

- Molecule 12 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
12	aA	1	Total	Fe	S	0
			8	4	4	
12	aC	1	Total	Fe	S	0
			16	8	8	
12	aC	1	Total	Fe	S	0
			16	8	8	
12	bA	1	Total	Fe	S	0
			8	4	4	
12	bC	1	Total	Fe	S	0
			16	8	8	
12	bC	1	Total	Fe	S	0
			16	8	8	
12	cA	1	Total	Fe	S	0
			8	4	4	
12	cC	1	Total	Fe	S	0
			16	8	8	
12	cC	1	Total	Fe	S	0
			16	8	8	

- Molecule 13 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
13	aA	1	Total	C	0
			240	240	
13	aA	1	Total	C	0
			240	240	
13	aA	1	Total	C	0
			240	240	
13	aA	1	Total	C	0
			240	240	
13	aA	1	Total	C	0
			240	240	
13	aA	1	Total	C	0
			240	240	
13	aB	1	Total	C	0
			240	240	
13	aB	1	Total	C	0
			240	240	
13	aB	1	Total	C	0
			240	240	
13	aB	1	Total	C	0
			240	240	
13	aB	1	Total	C	0
			240	240	
13	aI	1	Total	C	0
			80	80	
13	aI	1	Total	C	0
			80	80	

Continued on next page...

Continued from previous page...

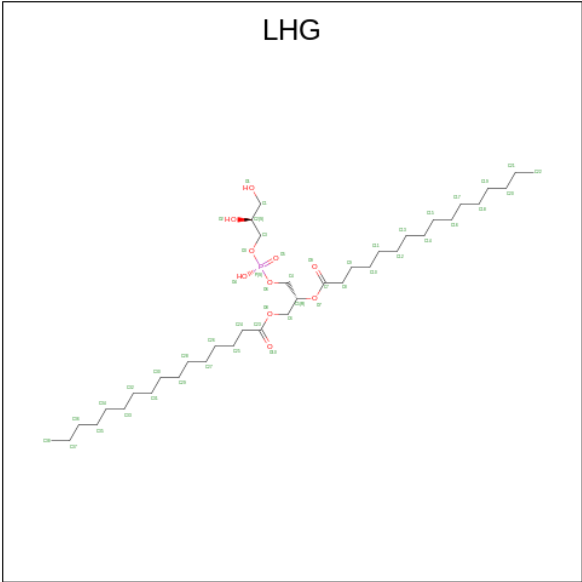
Mol	Chain	Residues	Atoms	AltConf
13	aL	1	Total C 80 80	0
13	aL	1	Total C 80 80	0
13	aM	1	Total C 40 40	0
13	bA	1	Total C 240 240	0
13	bA	1	Total C 240 240	0
13	bA	1	Total C 240 240	0
13	bA	1	Total C 240 240	0
13	bA	1	Total C 240 240	0
13	bA	1	Total C 240 240	0
13	bB	1	Total C 240 240	0
13	bB	1	Total C 240 240	0
13	bB	1	Total C 240 240	0
13	bB	1	Total C 240 240	0
13	bB	1	Total C 240 240	0
13	bB	1	Total C 240 240	0
13	bB	1	Total C 240 240	0
13	bI	1	Total C 80 80	0
13	bI	1	Total C 80 80	0
13	bL	1	Total C 80 80	0
13	bL	1	Total C 80 80	0
13	bM	1	Total C 40 40	0
13	cA	1	Total C 240 240	0

Continued on next page...

Continued from previous page...

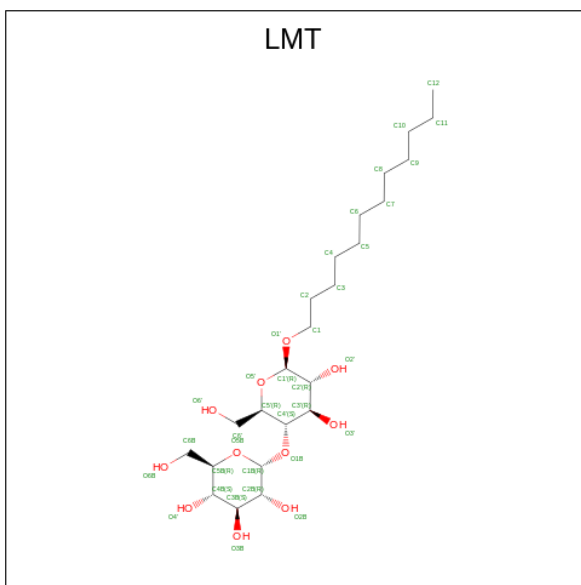
Mol	Chain	Residues	Atoms		AltConf
13	cA	1	Total	C	0
			240	240	
13	cA	1	Total	C	0
			240	240	
13	cA	1	Total	C	0
			240	240	
13	cA	1	Total	C	0
			240	240	
13	cA	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cI	1	Total	C	0
			80	80	
13	cI	1	Total	C	0
			80	80	
13	cL	1	Total	C	0
			80	80	
13	cL	1	Total	C	0
			80	80	
13	cM	1	Total	C	0
			40	40	

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



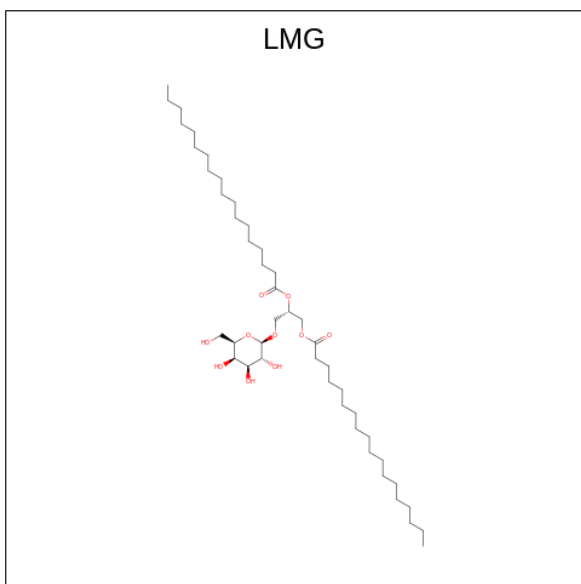
Mol	Chain	Residues	Atoms				AltConf
14	aA	1	Total	C	O	P	0
			76	54	20	2	
14	aA	1	Total	C	O	P	0
			76	54	20	2	
14	bA	1	Total	C	O	P	0
			76	54	20	2	
14	bA	1	Total	C	O	P	0
			76	54	20	2	
14	cA	1	Total	C	O	P	0
			76	54	20	2	
14	cA	1	Total	C	O	P	0
			76	54	20	2	

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
15	aA	1	Total 35	C 24	O 11	0
15	bA	1	Total 35	C 24	O 11	0
15	cA	1	Total 35	C 24	O 11	0

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
16	aB	1	Total	C	O	0
			55	45	10	
16	bB	1	Total	C	O	0
			55	45	10	
16	cB	1	Total	C	O	0
			55	45	10	

- Molecule 17 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			AltConf
17	aI	1	Total	C		0
			9	9		
17	aL	4	Total	C	O	0
			56	52	4	
17	bI	1	Total	C		0
			9	9		
17	bL	4	Total	C	O	0
			56	52	4	
17	cI	1	Total	C		0
			9	9		
17	cL	4	Total	C	O	0
			56	52	4	

- Molecule 18 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
18	aL	1	Total	Ca	0
			1	1	
18	bL	1	Total	Ca	0
			1	1	
18	cL	1	Total	Ca	0
			1	1	

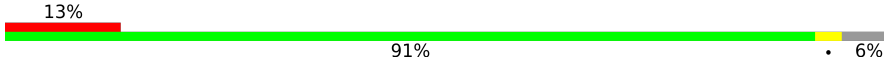
- Molecule 19 is water.

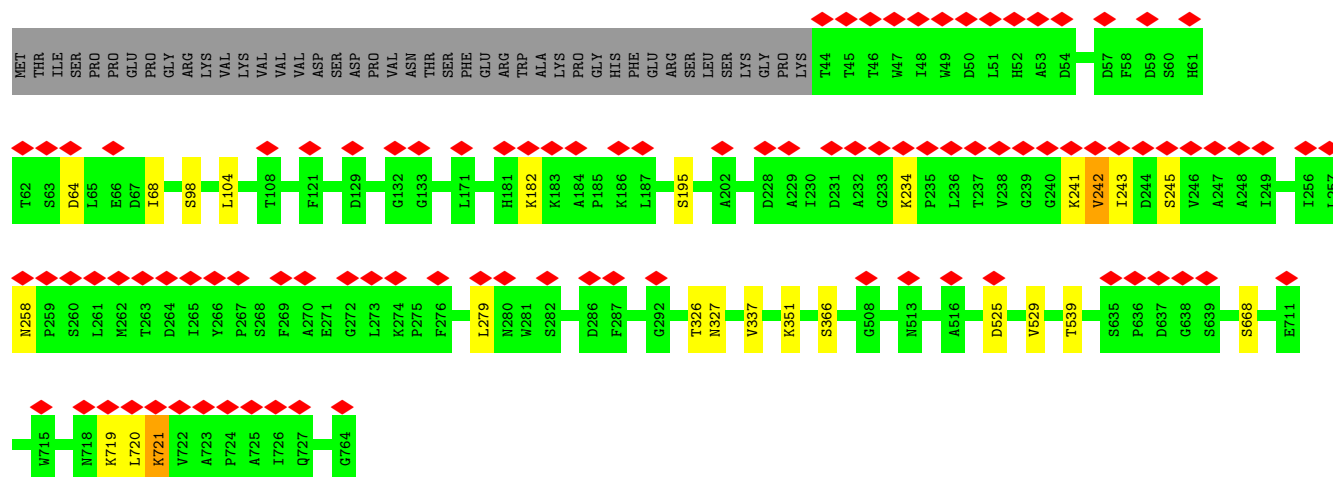
Mol	Chain	Residues	Atoms		AltConf
19	aA	64	Total	O	0
			64	64	
19	aB	85	Total	O	0
			85	85	
19	aC	16	Total	O	0
			16	16	

Continued on next page...

Continued from previous page...

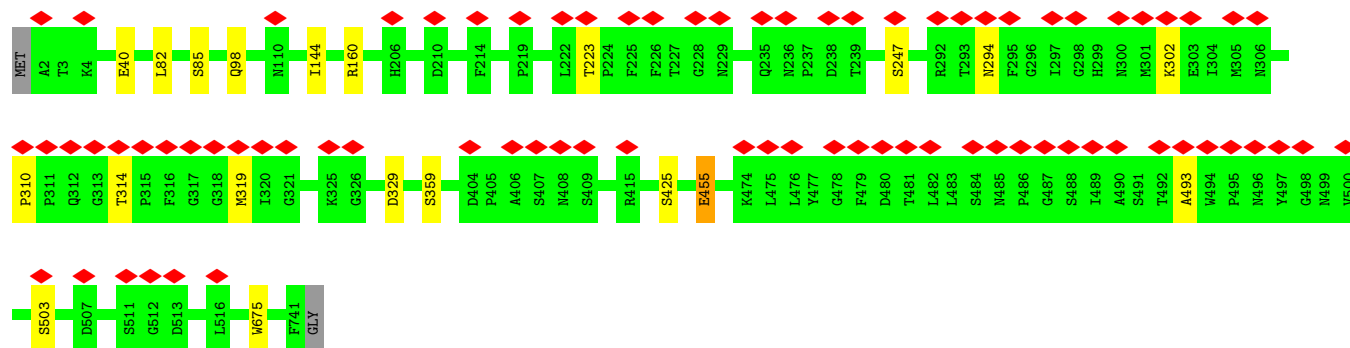
Mol	Chain	Residues	Atoms		AltConf
19	aD	12	Total 12	O 12	0
19	aI	1	Total 1	O 1	0
19	aL	30	Total 30	O 30	0
19	aM	1	Total 1	O 1	0
19	bA	63	Total 63	O 63	0
19	bB	85	Total 85	O 85	0
19	bC	17	Total 17	O 17	0
19	bD	12	Total 12	O 12	0
19	bI	1	Total 1	O 1	0
19	bL	30	Total 30	O 30	0
19	bM	1	Total 1	O 1	0
19	cA	63	Total 63	O 63	0
19	cB	86	Total 86	O 86	0
19	cC	15	Total 15	O 15	0
19	cD	13	Total 13	O 13	0
19	cI	1	Total 1	O 1	0
19	cL	30	Total 30	O 30	0
19	cM	1	Total 1	O 1	0

Chain cA: 



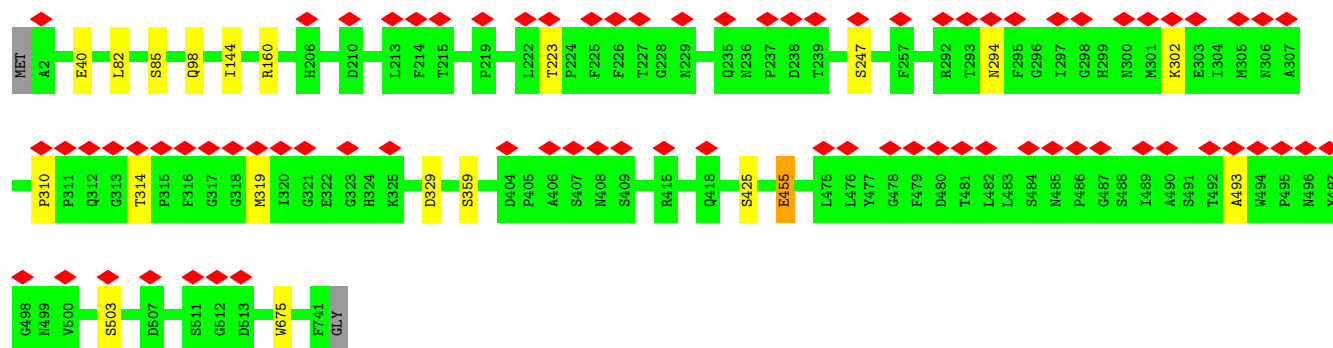
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain aB: 



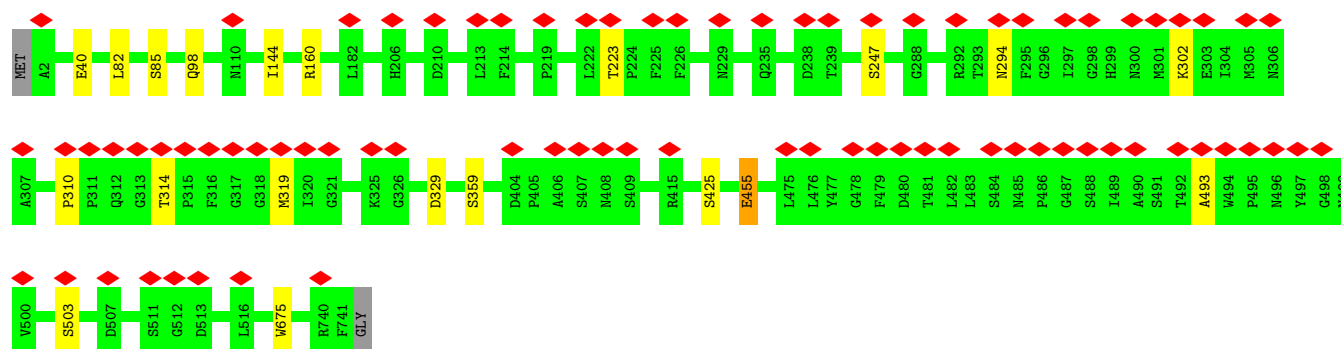
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain bB: 

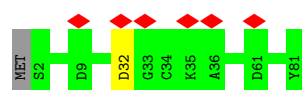


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

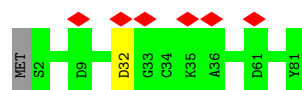
Chain cB: 



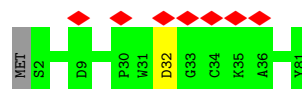
- Molecule 3: Photosystem I iron-sulfur center



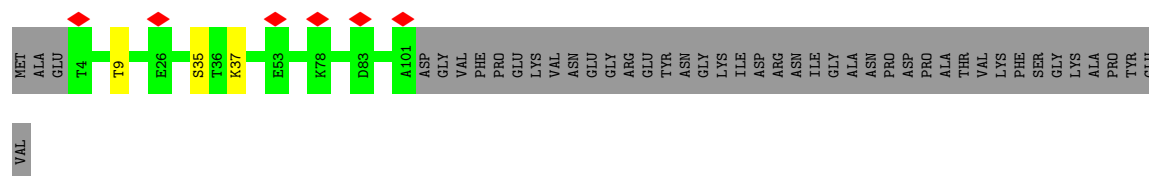
- Molecule 3: Photosystem I iron-sulfur center



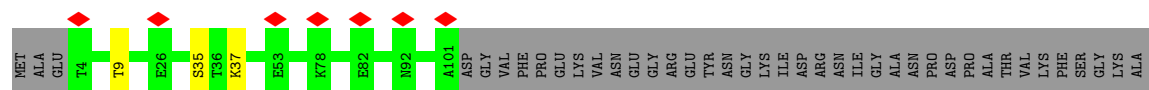
- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II

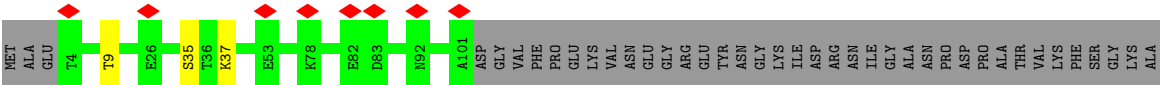


- Molecule 4: Photosystem I reaction center subunit II



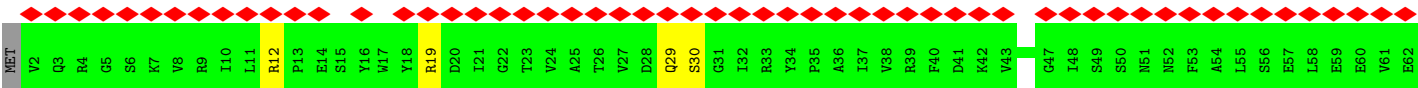
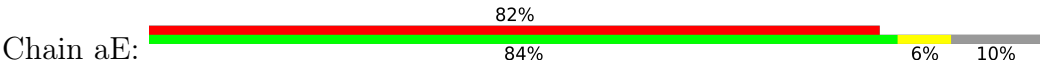
TYR
GLU
VAL

• Molecule 4: Photosystem I reaction center subunit II



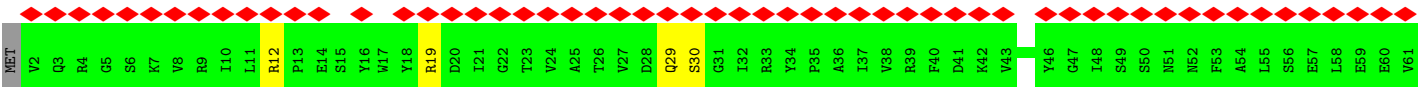
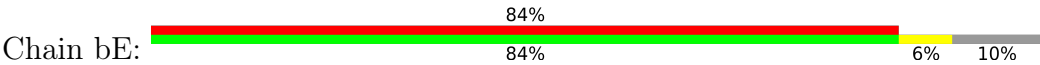
PRO
TYR
GLU
VAL

• Molecule 5: Photosystem I reaction center subunit IV



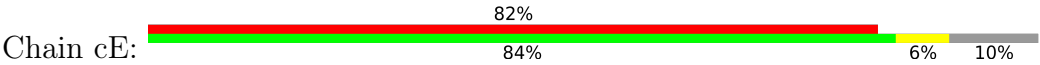
PRO
PRO
LYS
LYS
LYS

• Molecule 5: Photosystem I reaction center subunit IV



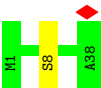
E62
PRO
PRO
LYS
LYS
LYS

• Molecule 5: Photosystem I reaction center subunit IV



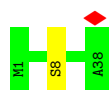
PRO
PRO
LYS
LYS
LYS

• Molecule 6: Photosystem I reaction center subunit VIII



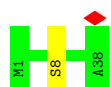
- Molecule 6: Photosystem I reaction center subunit VIII

Chain bI:  97%




- Molecule 6: Photosystem I reaction center subunit VIII

Chain cI:  97%




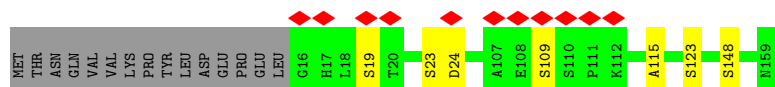
- Molecule 7: Photosystem I reaction center subunit XI

Chain aL:  86%




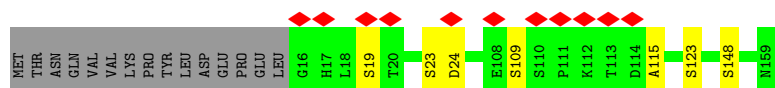
- Molecule 7: Photosystem I reaction center subunit XI

Chain bL:  86%



- Molecule 7: Photosystem I reaction center subunit XI

Chain cL:  86%



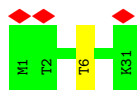
- Molecule 8: Photosystem I reaction center subunit XII

Chain aM:  97%

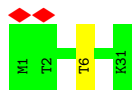


- Molecule 8: Photosystem I reaction center subunit XII

Chain bM:  97%



- Molecule 8: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	546366	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 ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.453	Depositor
Minimum map value	-0.267	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	313.2, 313.2, 313.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, BCR, LMT, UNL, LHG, SF4, CA, CLA, LMG, CL0

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	aA	0.34	0/5825	0.52	1/7944 (0.0%)
1	bA	0.34	0/5825	0.52	1/7944 (0.0%)
1	cA	0.34	0/5825	0.52	1/7944 (0.0%)
2	aB	0.35	0/6105	0.53	2/8343 (0.0%)
2	bB	0.35	0/6105	0.53	2/8343 (0.0%)
2	cB	0.35	0/6105	0.53	2/8343 (0.0%)
3	aC	0.32	0/606	0.59	1/820 (0.1%)
3	bC	0.33	0/606	0.59	1/820 (0.1%)
3	cC	0.33	0/606	0.59	1/820 (0.1%)
4	aD	0.31	0/785	0.52	0/1061
4	bD	0.31	0/785	0.51	0/1061
4	cD	0.31	0/785	0.51	0/1061
5	aE	0.31	0/509	0.59	1/689 (0.1%)
5	bE	0.31	0/509	0.59	1/689 (0.1%)
5	cE	0.31	0/509	0.59	1/689 (0.1%)
6	aI	0.36	0/317	0.60	0/436
6	bI	0.36	0/317	0.60	0/436
6	cI	0.36	0/317	0.60	0/436
7	aL	0.34	0/1093	0.52	0/1481
7	bL	0.34	0/1093	0.52	0/1481
7	cL	0.34	0/1093	0.52	0/1481
8	aM	0.30	0/244	0.56	0/332
8	bM	0.30	0/244	0.56	0/332
8	cM	0.30	0/244	0.56	0/332
All	All	0.34	0/46452	0.53	15/63318 (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	aA	0	4
1	bA	0	4
1	cA	0	4
2	aB	0	3
2	bB	0	3
2	cB	0	3
All	All	0	21

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	cC	32	ASP	CB-CG-OD1	7.78	125.30	118.30
3	aC	32	ASP	CB-CG-OD1	7.78	125.30	118.30
3	bC	32	ASP	CB-CG-OD1	7.75	125.27	118.30
2	bB	310	PRO	C-N-CD	-6.41	106.49	120.60
2	aB	310	PRO	C-N-CD	-6.41	106.51	120.60
2	cB	310	PRO	C-N-CD	-6.39	106.55	120.60
2	aB	455	GLU	CA-CB-CG	5.90	126.37	113.40
2	bB	455	GLU	CA-CB-CG	5.87	126.32	113.40
2	cB	455	GLU	CA-CB-CG	5.87	126.32	113.40
5	cE	19	ARG	CA-CB-CG	5.52	125.54	113.40
5	bE	19	ARG	CA-CB-CG	5.52	125.54	113.40
5	aE	19	ARG	CA-CB-CG	5.49	125.48	113.40
1	bA	721	LYS	C-N-CA	5.09	134.43	121.70
1	cA	721	LYS	C-N-CA	5.08	134.41	121.70
1	aA	721	LYS	C-N-CA	5.08	134.40	121.70

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	aA	242	VAL	Peptide
1	aA	529	VAL	Peptide
1	aA	720	LEU	Peptide
1	aA	721	LYS	Peptide
2	aB	314	THR	Peptide
2	aB	493	ALA	Peptide
2	aB	675	TRP	Peptide
1	bA	242	VAL	Peptide
1	bA	529	VAL	Peptide
1	bA	720	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	bA	721	LYS	Peptide
2	bB	314	THR	Peptide
2	bB	493	ALA	Peptide
2	bB	675	TRP	Peptide
1	cA	242	VAL	Peptide
1	cA	529	VAL	Peptide
1	cA	720	LEU	Peptide
1	cA	721	LYS	Peptide
2	cB	314	THR	Peptide
2	cB	493	ALA	Peptide
2	cB	675	TRP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	5629	0	5454	0	0
1	bA	5629	0	5454	0	0
1	cA	5629	0	5454	0	0
2	aB	5884	0	5623	0	0
2	bB	5884	0	5623	0	0
2	cB	5884	0	5623	0	0
3	aC	596	0	576	0	0
3	bC	596	0	576	0	0
3	cC	596	0	576	0	0
4	aD	768	0	774	0	0
4	bD	768	0	774	0	0
4	cD	768	0	774	0	0
5	aE	499	0	488	0	0
5	bE	499	0	488	0	0
5	cE	499	0	488	0	0
6	aI	305	0	304	0	0
6	bI	305	0	304	0	0
6	cI	305	0	304	0	0
7	aL	1065	0	1064	0	0
7	bL	1065	0	1064	0	0
7	cL	1065	0	1064	0	0
8	aM	241	0	266	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	bM	241	0	266	0	0
8	cM	241	0	266	0	0
9	aA	65	0	72	0	0
9	bA	65	0	72	0	0
9	cA	65	0	72	0	0
10	aA	2491	0	2400	0	0
10	aB	2357	0	2305	0	0
10	aL	250	0	265	0	0
10	bA	2491	0	2400	0	0
10	bB	2357	0	2305	0	0
10	bL	250	0	265	0	0
10	cA	2491	0	2400	0	0
10	cB	2357	0	2305	0	0
10	cL	250	0	265	0	0
11	aA	33	0	46	0	0
11	aB	33	0	46	0	0
11	bA	33	0	46	0	0
11	bB	33	0	46	0	0
11	cA	33	0	46	0	0
11	cB	33	0	46	0	0
12	aA	8	0	0	0	0
12	aC	16	0	0	0	0
12	bA	8	0	0	0	0
12	bC	16	0	0	0	0
12	cA	8	0	0	0	0
12	cC	16	0	0	0	0
13	aA	240	0	336	0	0
13	aB	240	0	333	0	0
13	aI	80	0	112	0	0
13	aL	80	0	112	0	0
13	aM	40	0	56	0	0
13	bA	240	0	336	0	0
13	bB	240	0	333	0	0
13	bI	80	0	112	0	0
13	bL	80	0	112	0	0
13	bM	40	0	56	0	0
13	cA	240	0	336	0	0
13	cB	240	0	333	0	0
13	cI	80	0	112	0	0
13	cL	80	0	112	0	0
13	cM	40	0	56	0	0
14	aA	76	0	98	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	bA	76	0	98	0	0
14	cA	76	0	98	0	0
15	aA	35	0	46	0	0
15	bA	35	0	46	0	0
15	cA	35	0	46	0	0
16	aB	55	0	84	0	0
16	bB	55	0	84	0	0
16	cB	55	0	84	0	0
17	aI	9	0	0	0	0
17	aL	56	0	0	0	0
17	bI	9	0	0	0	0
17	bL	56	0	0	0	0
17	cI	9	0	0	0	0
17	cL	56	0	0	0	0
18	aL	1	0	0	0	0
18	bL	1	0	0	0	0
18	cL	1	0	0	0	0
19	aA	64	0	0	0	0
19	aB	85	0	0	0	0
19	aC	16	0	0	0	0
19	aD	12	0	0	0	0
19	aI	1	0	0	0	0
19	aL	30	0	0	0	0
19	aM	1	0	0	0	0
19	bA	63	0	0	0	0
19	bB	85	0	0	0	0
19	bC	17	0	0	0	0
19	bD	12	0	0	0	0
19	bI	1	0	0	0	0
19	bL	30	0	0	0	0
19	bM	1	0	0	0	0
19	cA	63	0	0	0	0
19	cB	86	0	0	0	0
19	cC	15	0	0	0	0
19	cD	13	0	0	0	0
19	cI	1	0	0	0	0
19	cL	30	0	0	0	0
19	cM	1	0	0	0	0
All	All	64083	0	62580	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	719/764 (94%)	691 (96%)	27 (4%)	1 (0%)	51	63
1	bA	719/764 (94%)	691 (96%)	27 (4%)	1 (0%)	51	63
1	cA	719/764 (94%)	691 (96%)	27 (4%)	1 (0%)	51	63
2	aB	738/742 (100%)	705 (96%)	33 (4%)	0	100	100
2	bB	738/742 (100%)	705 (96%)	33 (4%)	0	100	100
2	cB	738/742 (100%)	705 (96%)	33 (4%)	0	100	100
3	aC	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
3	bC	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
3	cC	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	aD	96/142 (68%)	93 (97%)	3 (3%)	0	100	100
4	bD	96/142 (68%)	93 (97%)	3 (3%)	0	100	100
4	cD	96/142 (68%)	93 (97%)	3 (3%)	0	100	100
5	aE	59/68 (87%)	51 (86%)	8 (14%)	0	100	100
5	bE	59/68 (87%)	51 (86%)	8 (14%)	0	100	100
5	cE	59/68 (87%)	51 (86%)	8 (14%)	0	100	100
6	aI	36/38 (95%)	36 (100%)	0	0	100	100
6	bI	36/38 (95%)	36 (100%)	0	0	100	100
6	cI	36/38 (95%)	36 (100%)	0	0	100	100
7	aL	142/159 (89%)	138 (97%)	3 (2%)	1 (1%)	22	23
7	bL	142/159 (89%)	138 (97%)	3 (2%)	1 (1%)	22	23
7	cL	142/159 (89%)	138 (97%)	3 (2%)	1 (1%)	22	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	aM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
8	bM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
8	cM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
All	All	5691/6075 (94%)	5442 (96%)	243 (4%)	6 (0%)	54	63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	aL	115	ALA
7	bL	115	ALA
7	cL	115	ALA
1	aA	242	VAL
1	bA	242	VAL
1	cA	242	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	574/614 (94%)	553 (96%)	21 (4%)	34	42
1	bA	574/614 (94%)	553 (96%)	21 (4%)	34	42
1	cA	574/614 (94%)	553 (96%)	21 (4%)	34	42
2	aB	597/598 (100%)	581 (97%)	16 (3%)	44	55
2	bB	597/598 (100%)	581 (97%)	16 (3%)	44	55
2	cB	597/598 (100%)	581 (97%)	16 (3%)	44	55
3	aC	68/69 (99%)	68 (100%)	0	100	100
3	bC	68/69 (99%)	68 (100%)	0	100	100
3	cC	68/69 (99%)	68 (100%)	0	100	100
4	aD	80/115 (70%)	77 (96%)	3 (4%)	33	41
4	bD	80/115 (70%)	77 (96%)	3 (4%)	33	41
4	cD	80/115 (70%)	77 (96%)	3 (4%)	33	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	aE	54/61 (88%)	51 (94%)	3 (6%)	21	23
5	bE	54/61 (88%)	51 (94%)	3 (6%)	21	23
5	cE	54/61 (88%)	51 (94%)	3 (6%)	21	23
6	aI	32/32 (100%)	31 (97%)	1 (3%)	40	48
6	bI	32/32 (100%)	31 (97%)	1 (3%)	40	48
6	cI	32/32 (100%)	31 (97%)	1 (3%)	40	48
7	aL	108/123 (88%)	102 (94%)	6 (6%)	21	23
7	bL	108/123 (88%)	102 (94%)	6 (6%)	21	23
7	cL	108/123 (88%)	102 (94%)	6 (6%)	21	23
8	aM	27/27 (100%)	26 (96%)	1 (4%)	34	42
8	bM	27/27 (100%)	26 (96%)	1 (4%)	34	42
8	cM	27/27 (100%)	26 (96%)	1 (4%)	34	42
All	All	4620/4917 (94%)	4467 (97%)	153 (3%)	41	46

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	aA	64	ASP
1	aA	68	ILE
1	aA	98	SER
1	aA	104	LEU
1	aA	182	LYS
1	aA	195	SER
1	aA	234	LYS
1	aA	241	LYS
1	aA	243	ILE
1	aA	245	SER
1	aA	258	ASN
1	aA	279	LEU
1	aA	326	THR
1	aA	327	ASN
1	aA	337	VAL
1	aA	351	LYS
1	aA	366	SER
1	aA	525	ASP
1	aA	539	THR
1	aA	668	SER
1	aA	719	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	aB	40	GLU
2	aB	82	LEU
2	aB	85	SER
2	aB	98	GLN
2	aB	144	ILE
2	aB	160	ARG
2	aB	223	THR
2	aB	247	SER
2	aB	294	ASN
2	aB	302	LYS
2	aB	319	MET
2	aB	329	ASP
2	aB	359	SER
2	aB	425	SER
2	aB	455	GLU
2	aB	503	SER
4	aD	9	THR
4	aD	35	SER
4	aD	37	LYS
5	aE	12	ARG
5	aE	29	GLN
5	aE	30	SER
6	aI	8	SER
7	aL	19	SER
7	aL	23	SER
7	aL	24	ASP
7	aL	109	SER
7	aL	123	SER
7	aL	148	SER
8	aM	6	THR
1	bA	64	ASP
1	bA	68	ILE
1	bA	98	SER
1	bA	104	LEU
1	bA	182	LYS
1	bA	195	SER
1	bA	234	LYS
1	bA	241	LYS
1	bA	243	ILE
1	bA	245	SER
1	bA	258	ASN
1	bA	279	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	bA	326	THR
1	bA	327	ASN
1	bA	337	VAL
1	bA	351	LYS
1	bA	366	SER
1	bA	525	ASP
1	bA	539	THR
1	bA	668	SER
1	bA	719	LYS
2	bB	40	GLU
2	bB	82	LEU
2	bB	85	SER
2	bB	98	GLN
2	bB	144	ILE
2	bB	160	ARG
2	bB	223	THR
2	bB	247	SER
2	bB	294	ASN
2	bB	302	LYS
2	bB	319	MET
2	bB	329	ASP
2	bB	359	SER
2	bB	425	SER
2	bB	455	GLU
2	bB	503	SER
4	bD	9	THR
4	bD	35	SER
4	bD	37	LYS
5	bE	12	ARG
5	bE	29	GLN
5	bE	30	SER
6	bI	8	SER
7	bL	19	SER
7	bL	23	SER
7	bL	24	ASP
7	bL	109	SER
7	bL	123	SER
7	bL	148	SER
8	bM	6	THR
1	cA	64	ASP
1	cA	68	ILE
1	cA	98	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	cA	104	LEU
1	cA	182	LYS
1	cA	195	SER
1	cA	234	LYS
1	cA	241	LYS
1	cA	243	ILE
1	cA	245	SER
1	cA	258	ASN
1	cA	279	LEU
1	cA	326	THR
1	cA	327	ASN
1	cA	337	VAL
1	cA	351	LYS
1	cA	366	SER
1	cA	525	ASP
1	cA	539	THR
1	cA	668	SER
1	cA	719	LYS
2	cB	40	GLU
2	cB	82	LEU
2	cB	85	SER
2	cB	98	GLN
2	cB	144	ILE
2	cB	160	ARG
2	cB	223	THR
2	cB	247	SER
2	cB	294	ASN
2	cB	302	LYS
2	cB	319	MET
2	cB	329	ASP
2	cB	359	SER
2	cB	425	SER
2	cB	455	GLU
2	cB	503	SER
4	cD	9	THR
4	cD	35	SER
4	cD	37	LYS
5	cE	12	ARG
5	cE	29	GLN
5	cE	30	SER
6	cI	8	SER
7	cL	19	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	cL	23	SER
7	cL	24	ASP
7	cL	109	SER
7	cL	123	SER
7	cL	148	SER
8	cM	6	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	aA	135	HIS
1	aA	150	ASN
1	aA	362	HIS
1	aA	368	ASN
1	aA	381	HIS
1	aA	454	ASN
1	aA	513	ASN
1	aA	571	ASN
1	aA	727	GLN
2	aB	262	HIS
2	aB	306	ASN
2	aB	332	ASN
2	aB	333	ASN
2	aB	342	HIS
2	aB	373	GLN
2	aB	496	ASN
2	aB	618	ASN
2	aB	641	ASN
2	aB	680	GLN
4	aD	56	ASN
4	aD	99	HIS
5	aE	51	ASN
7	aL	98	HIS
1	bA	135	HIS
1	bA	150	ASN
1	bA	362	HIS
1	bA	368	ASN
1	bA	381	HIS
1	bA	454	ASN
1	bA	513	ASN
1	bA	571	ASN
1	bA	727	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	bB	262	HIS
2	bB	306	ASN
2	bB	332	ASN
2	bB	333	ASN
2	bB	342	HIS
2	bB	373	GLN
2	bB	496	ASN
2	bB	618	ASN
2	bB	641	ASN
2	bB	680	GLN
4	bD	56	ASN
4	bD	99	HIS
5	bE	51	ASN
7	bL	98	HIS
1	cA	135	HIS
1	cA	150	ASN
1	cA	362	HIS
1	cA	368	ASN
1	cA	381	HIS
1	cA	454	ASN
1	cA	571	ASN
1	cA	727	GLN
2	cB	262	HIS
2	cB	306	ASN
2	cB	332	ASN
2	cB	333	ASN
2	cB	342	HIS
2	cB	373	GLN
2	cB	496	ASN
2	cB	618	ASN
2	cB	641	ASN
2	cB	680	GLN
4	cD	56	ASN
4	cD	99	HIS
5	cE	51	ASN
7	cL	98	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 366 ligands modelled in this entry, 15 are unknown and 3 are monoatomic - leaving 348 for Mogul analysis.

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
10	CLA	cB	819	2	60,68,73	2.08	15 (25%)	70,107,113	2.89	30 (42%)
10	CLA	bA	816	1	54,62,73	2.20	16 (29%)	62,99,113	3.05	28 (45%)
9	CL0	aA	801	1	65,73,73	1.93	17 (26%)	76,113,113	2.69	31 (40%)
10	CLA	cA	837	1	65,73,73	1.94	18 (27%)	76,113,113	2.72	27 (35%)
10	CLA	cA	811	1	54,62,73	2.22	17 (31%)	62,99,113	2.90	27 (43%)
10	CLA	bA	808	1	45,53,73	2.38	17 (37%)	52,89,113	3.14	23 (44%)
10	CLA	aA	838	1	50,58,73	2.24	17 (34%)	58,95,113	3.35	30 (51%)
10	CLA	aB	831	2	45,53,73	2.46	16 (35%)	52,89,113	3.12	25 (48%)
13	BCR	bA	848	-	41,41,41	1.03	2 (4%)	56,56,56	1.29	8 (14%)
10	CLA	bA	835	1	65,73,73	2.02	17 (26%)	76,113,113	2.64	28 (36%)
13	BCR	bL	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	3 (5%)
10	CLA	bB	805	-	65,73,73	1.94	18 (27%)	76,113,113	2.59	23 (30%)
10	CLA	cB	808	2	65,73,73	1.98	18 (27%)	76,113,113	2.68	27 (35%)
10	CLA	cB	829	2	65,73,73	2.01	19 (29%)	76,113,113	2.51	26 (34%)
10	CLA	aB	836	-	45,53,73	2.49	17 (37%)	52,89,113	3.12	25 (48%)
13	BCR	cA	850	-	41,41,41	1.12	2 (4%)	56,56,56	1.18	5 (8%)
10	CLA	aA	827	1	65,73,73	2.04	19 (29%)	76,113,113	2.78	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCR	cA	849	-	41,41,41	1.11	3 (7%)	56,56,56	1.27	7 (12%)
10	CLA	bB	841	2	65,73,73	1.95	16 (24%)	76,113,113	2.70	27 (35%)
10	CLA	aA	821	1	49,57,73	2.34	16 (32%)	55,93,113	3.17	26 (47%)
10	CLA	aB	805	-	65,73,73	1.94	18 (27%)	76,113,113	2.59	23 (30%)
10	CLA	cB	830	2	65,73,73	2.04	16 (24%)	76,113,113	2.67	29 (38%)
10	CLA	aA	814	1	45,53,73	2.45	17 (37%)	52,89,113	3.12	24 (46%)
10	CLA	bA	856	2	49,57,73	2.38	17 (34%)	55,93,113	3.00	24 (43%)
10	CLA	aA	843	-	42,49,73	2.42	14 (33%)	48,83,113	3.19	21 (43%)
10	CLA	cB	802	-	65,73,73	1.99	17 (26%)	76,113,113	2.64	27 (35%)
10	CLA	cA	843	-	42,49,73	2.42	14 (33%)	48,83,113	3.18	21 (43%)
10	CLA	bA	807	1	45,53,73	2.42	19 (42%)	52,89,113	3.25	26 (50%)
13	BCR	bA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.30	5 (8%)
10	CLA	cA	821	1	49,57,73	2.34	16 (32%)	55,93,113	3.18	26 (47%)
10	CLA	cA	804	1	65,73,73	1.97	17 (26%)	76,113,113	2.74	26 (34%)
10	CLA	aA	839	1	65,73,73	2.04	16 (24%)	76,113,113	2.66	26 (34%)
9	CL0	bA	801	1	65,73,73	1.93	17 (26%)	76,113,113	2.69	30 (39%)
10	CLA	aB	824	2	45,53,73	2.48	16 (35%)	52,89,113	3.14	24 (46%)
13	BCR	aB	849	-	41,41,41	1.02	2 (4%)	56,56,56	1.16	4 (7%)
10	CLA	bB	822	2	45,53,73	2.45	17 (37%)	52,89,113	3.31	22 (42%)
10	CLA	cA	813	1	45,53,73	2.50	18 (40%)	52,89,113	3.11	25 (48%)
10	CLA	aB	840	-	65,73,73	1.97	17 (26%)	76,113,113	2.65	28 (36%)
13	BCR	bB	844	-	41,41,41	1.04	2 (4%)	56,56,56	1.32	5 (8%)
10	CLA	bB	816	2	45,53,73	2.41	16 (35%)	52,89,113	3.15	25 (48%)
10	CLA	cL	205	-	65,73,73	1.99	19 (29%)	76,113,113	2.72	26 (34%)
10	CLA	aA	802	1	45,53,73	2.48	16 (35%)	52,89,113	3.21	24 (46%)
13	BCR	aA	846	-	41,41,41	1.11	3 (7%)	56,56,56	1.23	6 (10%)
13	BCR	cI	102	-	41,41,41	1.08	3 (7%)	56,56,56	1.27	6 (10%)
10	CLA	aA	806	1	51,59,73	2.29	16 (31%)	59,96,113	3.05	28 (47%)
10	CLA	aA	833	1	65,73,73	1.97	16 (24%)	76,113,113	2.77	27 (35%)
10	CLA	cB	838	2	65,73,73	2.01	15 (23%)	76,113,113	2.73	28 (36%)
10	CLA	cA	823	1	65,73,73	2.02	16 (24%)	76,113,113	2.62	25 (32%)
10	CLA	aB	830	2	65,73,73	2.04	17 (26%)	76,113,113	2.67	29 (38%)
10	CLA	bL	205	-	65,73,73	1.99	19 (29%)	76,113,113	2.73	26 (34%)
10	CLA	bB	835	-	45,53,73	2.46	18 (40%)	52,89,113	3.10	24 (46%)
10	CLA	cA	854	14	52,60,73	2.26	17 (32%)	60,97,113	3.11	26 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	bB	814	2	65,73,73	2.03	18 (27%)	76,113,113	2.67	28 (36%)
10	CLA	cB	837	2	60,68,73	2.05	18 (30%)	70,107,113	2.84	27 (38%)
10	CLA	aB	839	2	47,55,73	2.33	17 (36%)	54,91,113	3.17	25 (46%)
13	BCR	bB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	4 (7%)
10	CLA	bA	809	1	45,53,73	2.43	16 (35%)	52,89,113	3.20	23 (44%)
10	CLA	cB	836	-	45,53,73	2.49	17 (37%)	52,89,113	3.11	24 (46%)
10	CLA	aA	840	-	51,59,73	2.34	17 (33%)	59,96,113	3.05	27 (45%)
10	CLA	bB	837	2	60,68,73	2.05	18 (30%)	70,107,113	2.84	27 (38%)
15	LMT	bA	853	-	36,36,36	0.45	0	47,47,47	0.91	3 (6%)
10	CLA	aB	814	2	65,73,73	2.04	19 (29%)	76,113,113	2.68	28 (36%)
14	LHG	aA	852	-	48,48,48	0.67	2 (4%)	51,54,54	1.23	7 (13%)
10	CLA	aA	837	1	65,73,73	1.94	18 (27%)	76,113,113	2.72	27 (35%)
10	CLA	bA	830	1	50,58,73	2.26	17 (34%)	58,95,113	3.00	27 (46%)
10	CLA	bA	817	1	54,62,73	2.22	16 (29%)	62,99,113	2.94	28 (45%)
10	CLA	aA	826	1	65,73,73	1.99	16 (24%)	76,113,113	2.70	27 (35%)
10	CLA	aB	811	2	65,73,73	1.94	17 (26%)	76,113,113	2.65	25 (32%)
10	CLA	cA	827	1	65,73,73	2.04	19 (29%)	76,113,113	2.77	28 (36%)
10	CLA	cB	831	2	45,53,73	2.45	15 (33%)	52,89,113	3.11	26 (50%)
16	LMG	bB	848	-	55,55,55	0.77	1 (1%)	63,63,63	1.36	9 (14%)
10	CLA	cB	827	2	65,73,73	2.01	17 (26%)	76,113,113	2.79	28 (36%)
10	CLA	cB	823	2	55,63,73	2.27	17 (30%)	64,101,113	2.86	27 (42%)
10	CLA	cA	807	1	45,53,73	2.42	18 (40%)	52,89,113	3.24	26 (50%)
13	BCR	cL	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	3 (5%)
10	CLA	cB	821	2	47,55,73	2.39	16 (34%)	54,91,113	3.00	26 (48%)
10	CLA	cB	812	2	45,53,73	2.41	16 (35%)	52,89,113	3.19	23 (44%)
10	CLA	bA	829	1	65,73,73	2.01	17 (26%)	76,113,113	2.77	27 (35%)
10	CLA	aA	841	-	65,73,73	2.02	17 (26%)	76,113,113	2.69	27 (35%)
10	CLA	bB	806	2	54,62,73	2.20	17 (31%)	62,99,113	3.06	31 (50%)
12	SF4	bA	845	2,1	0,12,12	-	-	-	-	-
10	CLA	bB	813	2	45,53,73	2.46	17 (37%)	52,89,113	3.09	22 (42%)
10	CLA	bB	809	2	65,73,73	1.97	19 (29%)	76,113,113	2.75	26 (34%)
10	CLA	aB	804	-	57,65,73	2.10	15 (26%)	66,103,113	3.08	29 (43%)
10	CLA	aA	832	1	65,73,73	1.96	16 (24%)	76,113,113	2.73	29 (38%)
13	BCR	aB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	4 (7%)
10	CLA	bB	810	2	55,63,73	2.11	14 (25%)	64,101,113	2.90	30 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCR	cB	847	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	6 (10%)
10	CLA	bA	802	1	45,53,73	2.47	16 (35%)	52,89,113	3.20	24 (46%)
10	CLA	cL	202	2	55,63,73	2.13	18 (32%)	64,101,113	2.94	27 (42%)
10	CLA	bA	826	1	65,73,73	1.99	16 (24%)	76,113,113	2.69	27 (35%)
10	CLA	bA	843	-	42,49,73	2.42	14 (33%)	48,83,113	3.19	21 (43%)
12	SF4	aC	101	3	0,12,12	-	-	-	-	-
10	CLA	cA	830	1	50,58,73	2.26	16 (32%)	58,95,113	3.00	27 (46%)
10	CLA	cA	825	-	55,63,73	2.16	18 (32%)	64,101,113	2.98	26 (40%)
10	CLA	cA	815	-	49,57,73	2.35	16 (32%)	55,93,113	3.11	24 (43%)
10	CLA	cB	809	2	65,73,73	1.96	19 (29%)	76,113,113	2.74	26 (34%)
10	CLA	cB	826	-	65,73,73	2.08	16 (24%)	76,113,113	2.79	30 (39%)
10	CLA	bA	813	1	45,53,73	2.49	18 (40%)	52,89,113	3.12	24 (46%)
10	CLA	cB	811	2	65,73,73	1.94	17 (26%)	76,113,113	2.66	25 (32%)
10	CLA	bA	810	1	65,73,73	2.07	15 (23%)	76,113,113	2.73	27 (35%)
10	CLA	aA	824	-	65,73,73	1.96	17 (26%)	76,113,113	2.77	24 (31%)
10	CLA	bA	838	1	50,58,73	2.23	15 (30%)	58,95,113	3.35	30 (51%)
10	CLA	bA	834	1	54,62,73	2.17	16 (29%)	62,99,113	2.88	29 (46%)
10	CLA	cA	856	2	49,57,73	2.38	16 (32%)	55,93,113	2.99	24 (43%)
10	CLA	aB	826	-	65,73,73	2.08	16 (24%)	76,113,113	2.79	30 (39%)
10	CLA	cB	824	2	45,53,73	2.48	16 (35%)	52,89,113	3.14	24 (46%)
10	CLA	bA	823	1	65,73,73	2.02	16 (24%)	76,113,113	2.62	25 (32%)
13	BCR	cA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.29	5 (8%)
10	CLA	aA	825	-	55,63,73	2.15	16 (29%)	64,101,113	2.98	26 (40%)
10	CLA	aA	817	1	54,62,73	2.22	16 (29%)	62,99,113	2.94	29 (46%)
10	CLA	aB	835	-	45,53,73	2.46	17 (37%)	52,89,113	3.10	24 (46%)
10	CLA	aL	202	2	55,63,73	2.13	19 (34%)	64,101,113	2.94	26 (40%)
10	CLA	aB	813	2	45,53,73	2.46	17 (37%)	52,89,113	3.10	22 (42%)
10	CLA	bA	854	-	52,60,73	2.27	16 (30%)	60,97,113	3.10	26 (43%)
10	CLA	bA	812	1	65,73,73	2.04	16 (24%)	76,113,113	2.75	28 (36%)
10	CLA	aA	811	1	54,62,73	2.22	17 (31%)	62,99,113	2.91	27 (43%)
10	CLA	cB	814	2	65,73,73	2.03	19 (29%)	76,113,113	2.68	27 (35%)
10	CLA	bA	836	1	51,59,73	2.26	17 (33%)	59,96,113	5.96	30 (50%)
13	BCR	cB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	4 (7%)
10	CLA	bA	820	-	65,73,73	2.03	16 (24%)	76,113,113	2.62	27 (35%)
10	CLA	aB	822	2	45,53,73	2.46	17 (37%)	52,89,113	3.32	22 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCR	cA	848	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	8 (14%)
10	CLA	aA	822	1	51,59,73	2.31	16 (31%)	59,96,113	3.05	27 (45%)
10	CLA	aB	816	2	45,53,73	2.41	16 (35%)	52,89,113	3.16	25 (48%)
12	SF4	cC	102	3	0,12,12	-	-	-	-	-
10	CLA	bB	807	2	65,73,73	1.99	19 (29%)	76,113,113	2.78	29 (38%)
10	CLA	aA	819	1	61,69,73	2.12	17 (27%)	71,108,113	2.71	26 (36%)
13	BCR	bA	850	-	41,41,41	1.12	2 (4%)	56,56,56	1.18	5 (8%)
10	CLA	aB	807	2	65,73,73	1.99	19 (29%)	76,113,113	2.78	30 (39%)
14	LHG	bA	855	-	26,26,48	0.83	0	29,32,54	1.33	3 (10%)
10	CLA	aB	818	2	59,67,73	2.16	17 (28%)	68,105,113	2.84	27 (39%)
10	CLA	cB	806	2	54,62,73	2.19	17 (31%)	62,99,113	3.06	31 (50%)
10	CLA	bA	827	1	65,73,73	2.04	19 (29%)	76,113,113	2.77	28 (36%)
10	CLA	cA	842	-	65,73,73	1.93	17 (26%)	76,113,113	2.64	29 (38%)
10	CLA	cA	809	1	45,53,73	2.44	17 (37%)	52,89,113	3.21	23 (44%)
13	BCR	aA	849	-	41,41,41	1.11	3 (7%)	56,56,56	1.26	7 (12%)
10	CLA	bL	203	7	65,73,73	2.00	18 (27%)	76,113,113	2.69	27 (35%)
10	CLA	cB	828	2	65,73,73	1.94	19 (29%)	76,113,113	2.76	27 (35%)
10	CLA	bA	818	1	65,73,73	2.07	16 (24%)	76,113,113	2.91	29 (38%)
10	CLA	bA	821	1	49,57,73	2.34	16 (32%)	55,93,113	3.18	26 (47%)
10	CLA	aA	805	1	65,73,73	2.03	18 (27%)	76,113,113	2.81	30 (39%)
10	CLA	cB	804	-	57,65,73	2.09	15 (26%)	66,103,113	3.08	29 (43%)
13	BCR	cA	851	-	41,41,41	1.04	2 (4%)	56,56,56	1.21	3 (5%)
10	CLA	bB	823	2	55,63,73	2.27	17 (30%)	64,101,113	2.86	27 (42%)
11	PQN	cA	844	-	34,34,34	1.53	2 (5%)	42,45,45	1.21	4 (9%)
12	SF4	cA	845	2,1	0,12,12	-	-	-	-	-
13	BCR	bB	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	3 (5%)
10	CLA	bA	839	1	65,73,73	2.04	16 (24%)	76,113,113	2.66	26 (34%)
10	CLA	aB	815	2	56,64,73	2.18	16 (28%)	65,102,113	2.80	27 (41%)
10	CLA	cA	834	1	54,62,73	2.17	16 (29%)	62,99,113	2.90	29 (46%)
10	CLA	aA	830	1	50,58,73	2.26	17 (34%)	58,95,113	2.99	27 (46%)
10	CLA	bB	808	2	65,73,73	1.98	18 (27%)	76,113,113	2.69	27 (35%)
10	CLA	cB	816	2	45,53,73	2.41	16 (35%)	52,89,113	3.15	25 (48%)
10	CLA	aA	815	-	49,57,73	2.35	17 (34%)	55,93,113	3.11	24 (43%)
10	CLA	cA	802	1	45,53,73	2.47	16 (35%)	52,89,113	3.20	24 (46%)
10	CLA	bA	824	-	65,73,73	1.96	17 (26%)	76,113,113	2.77	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCR	aB	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	3 (5%)
14	LHG	cA	855	10	26,26,48	0.83	0	29,32,54	1.33	3 (10%)
16	LMG	aB	848	-	55,55,55	0.76	1 (1%)	63,63,63	1.36	9 (14%)
11	PQN	bB	842	-	34,34,34	1.51	2 (5%)	42,45,45	1.05	3 (7%)
10	CLA	bL	202	2	55,63,73	2.12	19 (34%)	64,101,113	2.94	26 (40%)
10	CLA	cB	841	2	65,73,73	1.95	16 (24%)	76,113,113	2.70	27 (35%)
10	CLA	cA	810	1	65,73,73	2.06	15 (23%)	76,113,113	2.73	27 (35%)
10	CLA	cB	822	2	45,53,73	2.46	17 (37%)	52,89,113	3.32	22 (42%)
10	CLA	cA	820	-	65,73,73	2.03	15 (23%)	76,113,113	2.62	27 (35%)
13	BCR	cB	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	3 (5%)
13	BCR	aB	844	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	5 (8%)
14	LHG	bA	852	-	48,48,48	0.66	2 (4%)	51,54,54	1.23	7 (13%)
13	BCR	bL	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	7 (12%)
13	BCR	aA	850	-	41,41,41	1.12	2 (4%)	56,56,56	1.18	5 (8%)
10	CLA	cA	831	1	65,73,73	2.01	17 (26%)	76,113,113	2.68	25 (32%)
10	CLA	cB	801	-	65,73,73	1.98	16 (24%)	76,113,113	2.78	28 (36%)
13	BCR	bB	847	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	6 (10%)
10	CLA	bA	825	-	55,63,73	2.15	17 (30%)	64,101,113	2.99	26 (40%)
13	BCR	bM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	10 (17%)
10	CLA	bA	815	-	49,57,73	2.35	17 (34%)	55,93,113	3.11	24 (43%)
10	CLA	aB	828	2	65,73,73	1.95	19 (29%)	76,113,113	2.76	27 (35%)
10	CLA	bB	821	2	47,55,73	2.39	16 (34%)	54,91,113	2.99	26 (48%)
10	CLA	aA	808	1	45,53,73	2.38	17 (37%)	52,89,113	3.14	23 (44%)
10	CLA	cA	808	1	45,53,73	2.39	17 (37%)	52,89,113	3.13	23 (44%)
10	CLA	bA	822	1	51,59,73	2.31	16 (31%)	59,96,113	3.05	28 (47%)
10	CLA	cB	805	-	65,73,73	1.94	18 (27%)	76,113,113	2.59	23 (30%)
10	CLA	bA	814	1	45,53,73	2.45	17 (37%)	52,89,113	3.12	24 (46%)
10	CLA	bA	833	1	65,73,73	1.98	16 (24%)	76,113,113	2.78	28 (36%)
10	CLA	bB	803	2	65,73,73	1.94	17 (26%)	76,113,113	2.78	29 (38%)
13	BCR	bB	849	-	41,41,41	1.02	2 (4%)	56,56,56	1.15	4 (7%)
10	CLA	bB	839	2	47,55,73	2.33	17 (36%)	54,91,113	3.16	25 (46%)
10	CLA	aA	818	1	65,73,73	2.08	16 (24%)	76,113,113	2.91	29 (38%)
12	SF4	bC	102	3	0,12,12	-	-	-	-	-
16	LMG	cB	848	-	55,55,55	0.76	1 (1%)	63,63,63	1.36	9 (14%)
10	CLA	bA	804	1	65,73,73	1.97	16 (24%)	76,113,113	2.74	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	aB	817	2	55,63,73	2.19	17 (30%)	64,101,113	2.89	27 (42%)
10	CLA	bA	842	-	65,73,73	1.94	16 (24%)	76,113,113	2.64	29 (38%)
10	CLA	cA	840	-	51,59,73	2.34	17 (33%)	59,96,113	3.06	27 (45%)
10	CLA	aA	842	-	65,73,73	1.93	17 (26%)	76,113,113	2.64	29 (38%)
13	BCR	bI	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	6 (10%)
10	CLA	cL	204	7	65,73,73	1.93	16 (24%)	76,113,113	2.80	26 (34%)
10	CLA	bB	829	2	65,73,73	2.01	18 (27%)	76,113,113	2.51	26 (34%)
13	BCR	cB	849	-	41,41,41	1.02	2 (4%)	56,56,56	1.15	4 (7%)
10	CLA	bB	820	-	65,73,73	2.05	16 (24%)	76,113,113	2.65	27 (35%)
10	CLA	bB	815	2	56,64,73	2.17	16 (28%)	65,102,113	2.80	27 (41%)
10	CLA	aB	809	2	65,73,73	1.96	19 (29%)	76,113,113	2.74	26 (34%)
10	CLA	bA	819	1	61,69,73	2.11	17 (27%)	71,108,113	2.70	26 (36%)
10	CLA	bA	806	1	51,59,73	2.30	16 (31%)	59,96,113	3.07	29 (49%)
10	CLA	cB	834	2	45,53,73	2.45	17 (37%)	52,89,113	3.22	27 (51%)
10	CLA	aA	813	1	45,53,73	2.49	17 (37%)	52,89,113	3.11	24 (46%)
10	CLA	bA	841	1	65,73,73	2.03	17 (26%)	76,113,113	2.69	27 (35%)
11	PQN	bA	844	-	34,34,34	1.53	2 (5%)	42,45,45	1.22	4 (9%)
13	BCR	cA	846	-	41,41,41	1.10	3 (7%)	56,56,56	1.23	7 (12%)
10	CLA	bB	830	2	65,73,73	2.04	17 (26%)	76,113,113	2.67	29 (38%)
12	SF4	aC	102	3	0,12,12	-	-	-	-	-
10	CLA	bB	834	2	45,53,73	2.45	17 (37%)	52,89,113	3.23	27 (51%)
10	CLA	cL	203	7	65,73,73	2.00	18 (27%)	76,113,113	2.69	27 (35%)
10	CLA	cB	820	-	65,73,73	2.05	16 (24%)	76,113,113	2.65	27 (35%)
10	CLA	cB	815	2	56,64,73	2.18	16 (28%)	65,102,113	2.80	27 (41%)
10	CLA	aB	834	2	45,53,73	2.44	17 (37%)	52,89,113	3.23	27 (51%)
13	BCR	bB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
10	CLA	cA	838	1	50,58,73	2.23	17 (34%)	58,95,113	3.35	30 (51%)
13	BCR	cI	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	5 (8%)
10	CLA	aA	834	1	54,62,73	2.17	16 (29%)	62,99,113	2.89	29 (46%)
10	CLA	bB	812	2	45,53,73	2.41	16 (35%)	52,89,113	3.20	23 (44%)
10	CLA	aB	808	2	65,73,73	1.98	18 (27%)	76,113,113	2.68	28 (36%)
14	LHG	cA	852	-	48,48,48	0.67	1 (2%)	51,54,54	1.23	7 (13%)
14	LHG	aA	855	-	26,26,48	0.83	0	29,32,54	1.33	3 (10%)
10	CLA	aB	810	2	55,63,73	2.11	15 (27%)	64,101,113	2.90	30 (46%)
10	CLA	bL	204	7	65,73,73	1.93	16 (24%)	76,113,113	2.79	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	aB	820	-	65,73,73	2.05	16 (24%)	76,113,113	2.65	28 (36%)
10	CLA	cA	817	1	54,62,73	2.23	17 (31%)	62,99,113	2.95	29 (46%)
10	CLA	aA	828	1	65,73,73	2.02	17 (26%)	76,113,113	2.64	28 (36%)
13	BCR	bI	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
10	CLA	bA	837	1	65,73,73	1.94	16 (24%)	76,113,113	2.72	27 (35%)
13	BCR	cL	206	-	41,41,41	1.03	2 (4%)	56,56,56	1.29	6 (10%)
13	BCR	cB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
10	CLA	bB	818	2	59,67,73	2.16	16 (27%)	68,105,113	2.83	27 (39%)
13	BCR	cM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	10 (17%)
10	CLA	cA	818	1	65,73,73	2.08	17 (26%)	76,113,113	2.91	29 (38%)
10	CLA	aB	838	2	65,73,73	2.01	15 (23%)	76,113,113	2.74	28 (36%)
10	CLA	aA	816	1	54,62,73	2.20	16 (29%)	62,99,113	3.06	28 (45%)
10	CLA	aL	203	7	65,73,73	2.01	18 (27%)	76,113,113	2.69	27 (35%)
10	CLA	cB	803	2	65,73,73	1.93	17 (26%)	76,113,113	2.77	29 (38%)
10	CLA	cA	803	1	45,53,73	2.50	17 (37%)	52,89,113	3.21	25 (48%)
10	CLA	bA	831	1	65,73,73	2.01	17 (26%)	76,113,113	2.67	25 (32%)
13	BCR	aB	847	-	41,41,41	1.09	3 (7%)	56,56,56	1.30	6 (10%)
10	CLA	aB	837	2	60,68,73	2.05	18 (30%)	70,107,113	2.84	27 (38%)
15	LMT	aA	853	-	36,36,36	0.45	0	47,47,47	0.91	3 (6%)
10	CLA	cB	817	2	55,63,73	2.18	17 (30%)	64,101,113	2.88	27 (42%)
10	CLA	aB	827	2	65,73,73	2.01	17 (26%)	76,113,113	2.79	27 (35%)
10	CLA	aA	807	1	45,53,73	2.42	19 (42%)	52,89,113	3.24	26 (50%)
13	BCR	aA	847	-	41,41,41	1.04	2 (4%)	56,56,56	1.29	5 (8%)
13	BCR	aA	848	-	41,41,41	1.03	2 (4%)	56,56,56	1.29	8 (14%)
10	CLA	aA	835	1	65,73,73	2.02	17 (26%)	76,113,113	2.64	28 (36%)
10	CLA	aA	854	-	52,60,73	2.27	17 (32%)	60,97,113	3.11	26 (43%)
10	CLA	aB	823	2	55,63,73	2.27	17 (30%)	64,101,113	2.86	27 (42%)
10	CLA	aB	801	-	65,73,73	1.98	16 (24%)	76,113,113	2.77	28 (36%)
13	BCR	aM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	10 (17%)
10	CLA	aB	821	2	47,55,73	2.39	16 (34%)	54,91,113	3.00	26 (48%)
10	CLA	cA	814	1	45,53,73	2.46	17 (37%)	52,89,113	3.12	24 (46%)
13	BCR	aL	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	6 (10%)
10	CLA	bA	805	1	65,73,73	2.03	18 (27%)	76,113,113	2.81	30 (39%)
10	CLA	cA	829	1	65,73,73	2.01	17 (26%)	76,113,113	2.76	27 (35%)
10	CLA	cA	833	1	65,73,73	1.98	16 (24%)	76,113,113	2.77	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	bB	838	2	65,73,73	2.01	15 (23%)	76,113,113	2.73	28 (36%)
10	CLA	bA	828	1	65,73,73	2.02	17 (26%)	76,113,113	2.64	28 (36%)
12	SF4	bC	101	3	0,12,12	-	-	-		
11	PQN	aA	844	-	34,34,34	1.53	2 (5%)	42,45,45	1.22	4 (9%)
12	SF4	aA	845	2,1	0,12,12	-	-	-		
10	CLA	cA	832	1	65,73,73	1.96	16 (24%)	76,113,113	2.73	29 (38%)
10	CLA	cB	810	2	55,63,73	2.11	14 (25%)	64,101,113	2.90	30 (46%)
10	CLA	cA	839	1	65,73,73	2.04	16 (24%)	76,113,113	2.67	26 (34%)
10	CLA	cB	813	2	45,53,73	2.46	18 (40%)	52,89,113	3.08	22 (42%)
13	BCR	bA	849	-	41,41,41	1.11	3 (7%)	56,56,56	1.26	7 (12%)
10	CLA	bA	832	1	65,73,73	1.96	16 (24%)	76,113,113	2.74	29 (38%)
10	CLA	cA	806	1	51,59,73	2.29	16 (31%)	59,96,113	3.07	28 (47%)
10	CLA	cA	841	1	65,73,73	2.03	18 (27%)	76,113,113	2.68	27 (35%)
10	CLA	aB	833	2	58,66,73	2.16	17 (29%)	67,104,113	2.85	29 (43%)
10	CLA	cA	812	1	65,73,73	2.04	16 (24%)	76,113,113	2.75	28 (36%)
10	CLA	bA	840	-	51,59,73	2.34	17 (33%)	59,96,113	3.06	27 (45%)
10	CLA	aA	810	1	65,73,73	2.06	15 (23%)	76,113,113	2.73	27 (35%)
10	CLA	bB	831	2	45,53,73	2.45	15 (33%)	52,89,113	3.11	25 (48%)
10	CLA	cA	826	1	65,73,73	1.99	16 (24%)	76,113,113	2.69	27 (35%)
10	CLA	aB	825	2	54,62,73	2.22	17 (31%)	62,99,113	2.93	28 (45%)
10	CLA	aA	809	1	45,53,73	2.43	16 (35%)	52,89,113	3.21	23 (44%)
10	CLA	cA	835	1	65,73,73	2.03	17 (26%)	76,113,113	2.64	28 (36%)
10	CLA	bB	825	2	54,62,73	2.22	15 (27%)	62,99,113	2.94	28 (45%)
10	CLA	bB	817	2	55,63,73	2.18	17 (30%)	64,101,113	2.88	27 (42%)
10	CLA	bB	827	2	65,73,73	2.02	18 (27%)	76,113,113	2.79	28 (36%)
10	CLA	bA	803	1	45,53,73	2.50	18 (40%)	52,89,113	3.21	25 (48%)
10	CLA	bA	811	1	54,62,73	2.22	17 (31%)	62,99,113	2.90	27 (43%)
11	PQN	cB	842	-	34,34,34	1.50	2 (5%)	42,45,45	1.05	3 (7%)
10	CLA	cB	835	-	45,53,73	2.46	17 (37%)	52,89,113	3.10	24 (46%)
10	CLA	bB	819	2	60,68,73	2.08	15 (25%)	70,107,113	2.88	30 (42%)
10	CLA	cA	816	1	54,62,73	2.20	15 (27%)	62,99,113	3.06	28 (45%)
10	CLA	cA	819	1	61,69,73	2.11	17 (27%)	71,108,113	2.70	26 (36%)
10	CLA	bB	811	2	65,73,73	1.94	17 (26%)	76,113,113	2.66	25 (32%)
10	CLA	aA	836	1	51,59,73	2.26	17 (33%)	59,96,113	5.96	30 (50%)
10	CLA	cB	825	2	54,62,73	2.22	16 (29%)	62,99,113	2.93	28 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	aA	820	-	65,73,73	2.03	15 (23%)	76,113,113	2.62	27 (35%)
10	CLA	cA	836	1	51,59,73	2.27	17 (33%)	59,96,113	5.96	30 (50%)
10	CLA	bB	802	-	65,73,73	1.99	17 (26%)	76,113,113	2.63	27 (35%)
13	BCR	cB	844	-	41,41,41	1.04	2 (4%)	56,56,56	1.32	5 (8%)
10	CLA	aB	803	2	65,73,73	1.93	17 (26%)	76,113,113	2.77	29 (38%)
10	CLA	bB	824	2	45,53,73	2.47	16 (35%)	52,89,113	3.13	24 (46%)
10	CLA	cB	833	2	58,66,73	2.16	17 (29%)	67,104,113	2.85	28 (41%)
10	CLA	cB	818	2	59,67,73	2.16	17 (28%)	68,105,113	2.83	27 (39%)
10	CLA	aA	803	1	45,53,73	2.50	18 (40%)	52,89,113	3.21	25 (48%)
10	CLA	bB	840	-	65,73,73	1.97	17 (26%)	76,113,113	2.66	28 (36%)
10	CLA	aA	831	1	65,73,73	2.01	17 (26%)	76,113,113	2.68	25 (32%)
10	CLA	aB	802	-	65,73,73	1.98	17 (26%)	76,113,113	2.64	27 (35%)
13	BCR	aB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
10	CLA	bB	833	2	58,66,73	2.16	17 (29%)	67,104,113	2.84	28 (41%)
10	CLA	cB	839	2	47,55,73	2.33	18 (38%)	54,91,113	3.17	25 (46%)
10	CLA	cB	832	2	65,73,73	2.03	18 (27%)	76,113,113	2.72	28 (36%)
10	CLA	aB	819	2	60,68,73	2.09	15 (25%)	70,107,113	2.89	30 (42%)
10	CLA	aB	841	2	65,73,73	1.95	16 (24%)	76,113,113	2.70	27 (35%)
10	CLA	cA	828	1	65,73,73	2.02	17 (26%)	76,113,113	2.64	28 (36%)
10	CLA	aA	804	1	65,73,73	1.97	16 (24%)	76,113,113	2.75	26 (34%)
10	CLA	cA	824	-	65,73,73	1.96	17 (26%)	76,113,113	2.77	24 (31%)
10	CLA	aB	829	2	65,73,73	2.01	18 (27%)	76,113,113	2.51	26 (34%)
10	CLA	bB	826	-	65,73,73	2.08	16 (24%)	76,113,113	2.79	30 (39%)
13	BCR	bA	851	-	41,41,41	1.06	2 (4%)	56,56,56	1.20	3 (5%)
10	CLA	bB	836	-	45,53,73	2.49	17 (37%)	52,89,113	3.11	25 (48%)
10	CLA	bB	832	2	65,73,73	2.03	17 (26%)	76,113,113	2.72	28 (36%)
10	CLA	aL	205	-	65,73,73	1.99	19 (29%)	76,113,113	2.73	26 (34%)
10	CLA	aA	829	1	65,73,73	2.01	17 (26%)	76,113,113	2.77	27 (35%)
10	CLA	cB	840	-	65,73,73	1.97	17 (26%)	76,113,113	2.66	28 (36%)
10	CLA	cA	805	1	65,73,73	2.03	18 (27%)	76,113,113	2.80	30 (39%)
10	CLA	aL	204	7	65,73,73	1.93	16 (24%)	76,113,113	2.80	26 (34%)
10	CLA	aA	856	2	49,57,73	2.38	17 (34%)	55,93,113	3.00	24 (43%)
9	CL0	cA	801	1	65,73,73	1.93	17 (26%)	76,113,113	2.69	30 (39%)
10	CLA	aB	832	2	65,73,73	2.03	17 (26%)	76,113,113	2.72	28 (36%)
13	BCR	aA	851	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	cB	807	2	65,73,73	1.99	19 (29%)	76,113,113	2.77	30 (39%)
13	BCR	bA	846	-	41,41,41	1.10	3 (7%)	56,56,56	1.23	7 (12%)
15	LMT	cA	853	-	36,36,36	0.45	0	47,47,47	0.91	3 (6%)
13	BCR	aI	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.27	6 (10%)
13	BCR	aL	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	3 (5%)
10	CLA	aB	806	2	54,62,73	2.20	17 (31%)	62,99,113	3.06	31 (50%)
10	CLA	cA	822	1	51,59,73	2.31	16 (31%)	59,96,113	3.05	28 (47%)
10	CLA	bB	828	2	65,73,73	1.95	19 (29%)	76,113,113	2.76	27 (35%)
10	CLA	aB	812	2	45,53,73	2.40	16 (35%)	52,89,113	3.19	23 (44%)
10	CLA	aA	823	1	65,73,73	2.02	17 (26%)	76,113,113	2.62	25 (32%)
10	CLA	bB	804	-	57,65,73	2.10	15 (26%)	66,103,113	3.08	29 (43%)
13	BCR	aI	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	5 (8%)
11	PQN	aB	842	-	34,34,34	1.51	2 (5%)	42,45,45	1.05	3 (7%)
10	CLA	aA	812	1	65,73,73	2.04	17 (26%)	76,113,113	2.75	28 (36%)
12	SF4	cC	101	3	0,12,12	-	-	-	-	-
10	CLA	bB	801	-	65,73,73	1.97	16 (24%)	76,113,113	2.77	29 (38%)

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
10	CLA	cB	819	2	1/1/14/20	10/31/109/115	-
10	CLA	bA	816	1	-	10/24/102/115	-
9	CL0	aA	801	1	3/3/20/25	6/37/135/135	-
10	CLA	cA	837	1	1/1/15/20	7/37/115/115	-
10	CLA	cA	811	1	1/1/12/20	8/24/102/115	-
10	CLA	bA	808	1	1/1/11/20	4/13/91/115	-
10	CLA	aA	838	1	1/1/12/20	9/19/97/115	-
10	CLA	aB	831	2	1/1/11/20	6/13/91/115	-
13	BCR	bA	848	-	-	16/29/63/63	0/2/2/2
10	CLA	bA	835	1	1/1/15/20	12/37/115/115	-
13	BCR	bL	207	-	-	7/29/63/63	0/2/2/2
10	CLA	bB	805	-	1/1/15/20	10/37/115/115	-
10	CLA	cB	808	2	1/1/15/20	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cB	829	2	1/1/15/20	12/37/115/115	-
10	CLA	aB	836	-	1/1/11/20	2/13/91/115	-
13	BCR	cA	850	-	-	9/29/63/63	0/2/2/2
10	CLA	aA	827	1	1/1/15/20	17/37/115/115	-
13	BCR	cA	849	-	-	13/29/63/63	0/2/2/2
10	CLA	bB	841	2	1/1/15/20	10/37/115/115	-
10	CLA	aA	821	1	1/1/11/20	4/18/96/115	-
10	CLA	aB	805	-	1/1/15/20	10/37/115/115	-
10	CLA	cB	830	2	1/1/15/20	9/37/115/115	-
10	CLA	aA	814	1	1/1/11/20	2/13/91/115	-
10	CLA	bA	856	2	1/1/11/20	7/18/96/115	-
10	CLA	aA	843	-	1/1/9/20	2/7/81/115	-
10	CLA	cB	802	-	1/1/15/20	13/37/115/115	-
10	CLA	cA	843	-	1/1/9/20	2/7/81/115	-
10	CLA	bA	807	1	1/1/11/20	7/13/91/115	-
13	BCR	bA	847	-	-	9/29/63/63	0/2/2/2
10	CLA	cA	821	1	1/1/11/20	4/18/96/115	-
10	CLA	cA	804	1	1/1/15/20	10/37/115/115	-
10	CLA	aA	839	1	1/1/15/20	6/37/115/115	-
9	CL0	bA	801	1	3/3/20/25	6/37/135/135	-
10	CLA	aB	824	2	1/1/11/20	5/13/91/115	-
13	BCR	aB	849	-	-	18/29/63/63	0/2/2/2
10	CLA	bB	822	2	-	7/13/91/115	-
10	CLA	cA	813	1	1/1/11/20	1/13/91/115	-
10	CLA	aB	840	-	1/1/15/20	2/37/115/115	-
13	BCR	bB	844	-	-	10/29/63/63	0/2/2/2
10	CLA	bB	816	2	1/1/11/20	2/13/91/115	-
10	CLA	cL	205	-	-	11/37/115/115	-
10	CLA	aA	802	1	1/1/11/20	7/13/91/115	-
13	BCR	aA	846	-	-	14/29/63/63	0/2/2/2
13	BCR	cI	102	-	-	8/29/63/63	0/2/2/2
10	CLA	aA	806	1	1/1/12/20	3/21/99/115	-
10	CLA	aA	833	1	1/1/15/20	10/37/115/115	-
10	CLA	cB	838	2	1/1/15/20	9/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cA	823	1	1/1/15/20	12/37/115/115	-
10	CLA	aB	830	2	1/1/15/20	9/37/115/115	-
10	CLA	bL	205	-	-	11/37/115/115	-
10	CLA	bB	835	-	1/1/11/20	5/13/91/115	-
10	CLA	cA	854	14	-	8/22/100/115	-
10	CLA	bB	814	2	1/1/15/20	14/37/115/115	-
10	CLA	cB	837	2	1/1/14/20	10/31/109/115	-
10	CLA	aB	839	2	1/1/11/20	5/16/94/115	-
13	BCR	bB	843	-	-	11/29/63/63	0/2/2/2
10	CLA	bA	809	1	1/1/11/20	2/13/91/115	-
10	CLA	cB	836	-	1/1/11/20	2/13/91/115	-
10	CLA	aA	840	-	1/1/12/20	6/21/99/115	-
10	CLA	bB	837	2	1/1/14/20	10/31/109/115	-
15	LMT	bA	853	-	-	9/21/61/61	0/2/2/2
10	CLA	aB	814	2	1/1/15/20	14/37/115/115	-
14	LHG	aA	852	-	-	31/53/53/53	-
10	CLA	aA	837	1	1/1/15/20	7/37/115/115	-
10	CLA	bA	830	1	1/1/12/20	5/19/97/115	-
10	CLA	bA	817	1	-	10/24/102/115	-
10	CLA	aA	826	1	1/1/15/20	8/37/115/115	-
10	CLA	aB	811	2	1/1/15/20	17/37/115/115	-
10	CLA	cA	827	1	1/1/15/20	17/37/115/115	-
10	CLA	cB	831	2	1/1/11/20	6/13/91/115	-
16	LMG	bB	848	-	-	19/50/70/70	0/1/1/1
10	CLA	cB	827	2	1/1/15/20	9/37/115/115	-
10	CLA	cB	823	2	1/1/13/20	13/25/103/115	-
10	CLA	cA	807	1	1/1/11/20	7/13/91/115	-
13	BCR	cL	207	-	-	7/29/63/63	0/2/2/2
10	CLA	cB	821	2	1/1/11/20	4/16/94/115	-
10	CLA	cB	812	2	1/1/11/20	1/13/91/115	-
10	CLA	bA	829	1	1/1/15/20	12/37/115/115	-
10	CLA	aA	841	-	1/1/15/20	11/37/115/115	-
10	CLA	bB	806	2	1/1/12/20	12/24/102/115	-
12	SF4	bA	845	2,1	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bB	813	2	-	4/13/91/115	-
10	CLA	bB	809	2	1/1/15/20	6/37/115/115	-
10	CLA	aB	804	-	1/1/13/20	14/28/106/115	-
10	CLA	aA	832	1	1/1/15/20	6/37/115/115	-
13	BCR	aB	843	-	-	11/29/63/63	0/2/2/2
10	CLA	bB	810	2	1/1/13/20	9/25/103/115	-
13	BCR	cB	847	-	-	10/29/63/63	0/2/2/2
10	CLA	bA	802	1	1/1/11/20	7/13/91/115	-
10	CLA	cL	202	2	1/1/13/20	7/25/103/115	-
10	CLA	bA	826	1	1/1/15/20	8/37/115/115	-
10	CLA	bA	843	-	1/1/9/20	2/7/81/115	-
12	SF4	aC	101	3	-	-	0/6/5/5
10	CLA	cA	830	1	1/1/12/20	5/19/97/115	-
10	CLA	cA	825	-	1/1/13/20	9/25/103/115	-
10	CLA	cA	815	-	1/1/11/20	3/18/96/115	-
10	CLA	cB	809	2	1/1/15/20	6/37/115/115	-
10	CLA	cB	826	-	1/1/15/20	12/37/115/115	-
10	CLA	bA	813	1	1/1/11/20	1/13/91/115	-
10	CLA	cB	811	2	1/1/15/20	17/37/115/115	-
10	CLA	bA	810	1	1/1/15/20	10/37/115/115	-
10	CLA	aA	824	-	1/1/15/20	11/37/115/115	-
10	CLA	bA	838	1	1/1/12/20	9/19/97/115	-
10	CLA	bA	834	1	1/1/12/20	8/24/102/115	-
10	CLA	cA	856	2	1/1/11/20	7/18/96/115	-
10	CLA	aB	826	-	1/1/15/20	12/37/115/115	-
10	CLA	cB	824	2	1/1/11/20	5/13/91/115	-
10	CLA	bA	823	1	1/1/15/20	12/37/115/115	-
13	BCR	cA	847	-	-	9/29/63/63	0/2/2/2
10	CLA	aA	825	-	1/1/13/20	9/25/103/115	-
10	CLA	aB	835	-	1/1/11/20	5/13/91/115	-
10	CLA	aL	202	2	1/1/13/20	7/25/103/115	-
10	CLA	aA	817	1	-	10/24/102/115	-
10	CLA	aB	813	2	-	4/13/91/115	-
10	CLA	bA	854	-	-	8/22/100/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bA	812	1	1/1/15/20	15/37/115/115	-
10	CLA	aA	811	1	1/1/12/20	8/24/102/115	-
10	CLA	cB	814	2	1/1/15/20	14/37/115/115	-
10	CLA	bA	836	1	1/1/12/20	7/21/99/115	-
13	BCR	cB	843	-	-	11/29/63/63	0/2/2/2
10	CLA	bA	820	-	1/1/15/20	13/37/115/115	-
10	CLA	aB	822	2	-	7/13/91/115	-
13	BCR	cA	848	-	-	16/29/63/63	0/2/2/2
10	CLA	aA	822	1	1/1/12/20	10/21/99/115	-
10	CLA	aB	816	2	1/1/11/20	2/13/91/115	-
12	SF4	cC	102	3	-	-	0/6/5/5
10	CLA	bB	807	2	1/1/15/20	12/37/115/115	-
10	CLA	aA	819	1	1/1/14/20	11/33/111/115	-
13	BCR	bA	850	-	-	9/29/63/63	0/2/2/2
10	CLA	aB	807	2	1/1/15/20	12/37/115/115	-
14	LHG	bA	855	-	-	15/31/31/53	-
10	CLA	aB	818	2	1/1/13/20	11/30/108/115	-
10	CLA	cB	806	2	1/1/12/20	11/24/102/115	-
10	CLA	bA	827	1	1/1/15/20	17/37/115/115	-
10	CLA	cA	842	-	1/1/15/20	13/37/115/115	-
10	CLA	cA	809	1	1/1/11/20	2/13/91/115	-
13	BCR	aA	849	-	-	13/29/63/63	0/2/2/2
10	CLA	bL	203	7	-	11/37/115/115	-
10	CLA	cB	828	2	1/1/15/20	11/37/115/115	-
10	CLA	bA	818	1	1/1/15/20	13/37/115/115	-
10	CLA	bA	821	1	1/1/11/20	4/18/96/115	-
10	CLA	aA	805	1	1/1/15/20	10/37/115/115	-
10	CLA	cB	804	-	1/1/13/20	14/28/106/115	-
13	BCR	cA	851	-	-	13/29/63/63	0/2/2/2
10	CLA	bB	823	2	1/1/13/20	13/25/103/115	-
11	PQN	cA	844	-	-	8/23/43/43	0/2/2/2
12	SF4	cA	845	2,1	-	-	0/6/5/5
13	BCR	bB	846	-	-	8/29/63/63	0/2/2/2
10	CLA	bA	839	1	1/1/15/20	6/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	aB	815	2	1/1/13/20	7/27/105/115	-
10	CLA	cA	834	1	1/1/12/20	8/24/102/115	-
10	CLA	aA	830	1	1/1/12/20	5/19/97/115	-
10	CLA	bB	808	2	1/1/15/20	12/37/115/115	-
10	CLA	cB	816	2	1/1/11/20	2/13/91/115	-
10	CLA	aA	815	-	1/1/11/20	3/18/96/115	-
10	CLA	cA	802	1	1/1/11/20	7/13/91/115	-
10	CLA	bA	824	-	1/1/15/20	11/37/115/115	-
13	BCR	aB	846	-	-	8/29/63/63	0/2/2/2
14	LHG	cA	855	10	-	15/31/31/53	-
16	LMG	aB	848	-	-	19/50/70/70	0/1/1/1
11	PQN	bB	842	-	-	2/23/43/43	0/2/2/2
10	CLA	bL	202	2	1/1/13/20	7/25/103/115	-
10	CLA	cB	841	2	1/1/15/20	10/37/115/115	-
10	CLA	cA	810	1	1/1/15/20	10/37/115/115	-
10	CLA	cB	822	2	-	7/13/91/115	-
10	CLA	cA	820	-	1/1/15/20	13/37/115/115	-
13	BCR	cB	846	-	-	8/29/63/63	0/2/2/2
13	BCR	aB	844	-	-	10/29/63/63	0/2/2/2
14	LHG	bA	852	-	-	31/53/53/53	-
13	BCR	bL	206	-	-	8/29/63/63	0/2/2/2
13	BCR	aA	850	-	-	9/29/63/63	0/2/2/2
10	CLA	cA	831	1	1/1/15/20	13/37/115/115	-
10	CLA	cB	801	-	1/1/15/20	7/37/115/115	-
13	BCR	bB	847	-	-	10/29/63/63	0/2/2/2
10	CLA	bA	825	-	1/1/13/20	9/25/103/115	-
13	BCR	bM	101	-	-	13/29/63/63	0/2/2/2
10	CLA	bA	815	-	1/1/11/20	3/18/96/115	-
10	CLA	aB	828	2	1/1/15/20	11/37/115/115	-
10	CLA	bB	821	2	1/1/11/20	4/16/94/115	-
10	CLA	aA	808	1	1/1/11/20	4/13/91/115	-
10	CLA	cA	808	1	1/1/11/20	4/13/91/115	-
10	CLA	bA	822	1	1/1/12/20	10/21/99/115	-
10	CLA	cB	805	-	1/1/15/20	10/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bA	814	1	1/1/11/20	2/13/91/115	-
10	CLA	bA	833	1	1/1/15/20	10/37/115/115	-
10	CLA	bB	803	2	1/1/15/20	4/37/115/115	-
13	BCR	bB	849	-	-	18/29/63/63	0/2/2/2
10	CLA	bB	839	2	1/1/11/20	5/16/94/115	-
10	CLA	aA	818	1	1/1/15/20	13/37/115/115	-
12	SF4	bC	102	3	-	-	0/6/5/5
16	LMG	cB	848	-	-	19/50/70/70	0/1/1/1
10	CLA	bA	804	1	1/1/15/20	10/37/115/115	-
10	CLA	aB	817	2	1/1/13/20	10/25/103/115	-
10	CLA	bA	842	-	1/1/15/20	13/37/115/115	-
10	CLA	cA	840	-	1/1/12/20	6/21/99/115	-
10	CLA	aA	842	-	1/1/15/20	13/37/115/115	-
13	BCR	bI	102	-	-	8/29/63/63	0/2/2/2
10	CLA	cL	204	7	1/1/15/20	8/37/115/115	-
10	CLA	bB	829	2	1/1/15/20	12/37/115/115	-
13	BCR	cB	849	-	-	18/29/63/63	0/2/2/2
10	CLA	bB	820	-	1/1/15/20	11/37/115/115	-
10	CLA	bB	815	2	1/1/13/20	7/27/105/115	-
10	CLA	aB	809	2	1/1/15/20	6/37/115/115	-
10	CLA	bA	819	1	1/1/14/20	11/33/111/115	-
10	CLA	bA	806	1	1/1/12/20	3/21/99/115	-
10	CLA	cB	834	2	1/1/11/20	0/13/91/115	-
10	CLA	aA	813	1	1/1/11/20	1/13/91/115	-
10	CLA	bA	841	1	1/1/15/20	11/37/115/115	-
11	PQN	bA	844	-	-	8/23/43/43	0/2/2/2
13	BCR	cA	846	-	-	14/29/63/63	0/2/2/2
10	CLA	bB	830	2	1/1/15/20	9/37/115/115	-
12	SF4	aC	102	3	-	-	0/6/5/5
10	CLA	bB	834	2	1/1/11/20	0/13/91/115	-
10	CLA	cL	203	7	-	11/37/115/115	-
10	CLA	cB	820	-	1/1/15/20	11/37/115/115	-
10	CLA	cB	815	2	1/1/13/20	7/27/105/115	-
10	CLA	aB	834	2	1/1/11/20	0/13/91/115	-
13	BCR	bB	845	-	-	12/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cA	838	1	1/1/12/20	9/19/97/115	-
13	BCR	cI	103	-	-	8/29/63/63	0/2/2/2
10	CLA	aA	834	1	1/1/12/20	8/24/102/115	-
10	CLA	bB	812	2	1/1/11/20	1/13/91/115	-
10	CLA	aB	808	2	1/1/15/20	12/37/115/115	-
14	LHG	cA	852	-	-	31/53/53/53	-
14	LHG	aA	855	-	-	15/31/31/53	-
10	CLA	aB	810	2	1/1/13/20	9/25/103/115	-
10	CLA	bL	204	7	1/1/15/20	8/37/115/115	-
10	CLA	aB	820	-	1/1/15/20	11/37/115/115	-
10	CLA	cA	817	1	-	10/24/102/115	-
10	CLA	aA	828	1	1/1/15/20	6/37/115/115	-
13	BCR	bI	101	-	-	8/29/63/63	0/2/2/2
10	CLA	bA	837	1	1/1/15/20	7/37/115/115	-
13	BCR	cL	206	-	-	8/29/63/63	0/2/2/2
13	BCR	cB	845	-	-	12/29/63/63	0/2/2/2
10	CLA	bB	818	2	1/1/13/20	11/30/108/115	-
13	BCR	cM	101	-	-	13/29/63/63	0/2/2/2
10	CLA	cA	818	1	1/1/15/20	13/37/115/115	-
10	CLA	aB	838	2	1/1/15/20	9/37/115/115	-
10	CLA	aA	816	1	-	10/24/102/115	-
10	CLA	aL	203	7	-	11/37/115/115	-
10	CLA	cB	803	2	1/1/15/20	4/37/115/115	-
10	CLA	cA	803	1	1/1/11/20	3/13/91/115	-
10	CLA	bA	831	1	1/1/15/20	13/37/115/115	-
13	BCR	aB	847	-	-	10/29/63/63	0/2/2/2
10	CLA	aB	837	2	1/1/14/20	10/31/109/115	-
15	LMT	aA	853	-	-	9/21/61/61	0/2/2/2
10	CLA	cB	817	2	1/1/13/20	10/25/103/115	-
10	CLA	aB	827	2	1/1/15/20	9/37/115/115	-
10	CLA	aA	807	1	1/1/11/20	7/13/91/115	-
13	BCR	aA	847	-	-	9/29/63/63	0/2/2/2
13	BCR	aA	848	-	-	16/29/63/63	0/2/2/2
10	CLA	aA	835	1	1/1/15/20	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	aA	854	-	-	8/22/100/115	-
10	CLA	aB	823	2	1/1/13/20	13/25/103/115	-
10	CLA	aB	801	-	1/1/15/20	7/37/115/115	-
13	BCR	aM	101	-	-	13/29/63/63	0/2/2/2
10	CLA	aB	821	2	1/1/11/20	4/16/94/115	-
10	CLA	cA	814	1	1/1/11/20	2/13/91/115	-
13	BCR	aL	206	-	-	8/29/63/63	0/2/2/2
10	CLA	bA	805	1	1/1/15/20	10/37/115/115	-
10	CLA	cA	829	1	1/1/15/20	12/37/115/115	-
10	CLA	cA	833	1	1/1/15/20	10/37/115/115	-
10	CLA	bB	838	2	1/1/15/20	9/37/115/115	-
10	CLA	bA	828	1	1/1/15/20	6/37/115/115	-
12	SF4	bC	101	3	-	-	0/6/5/5
11	PQN	aA	844	-	-	8/23/43/43	0/2/2/2
12	SF4	aA	845	2,1	-	-	0/6/5/5
10	CLA	cA	832	1	1/1/15/20	6/37/115/115	-
10	CLA	cB	810	2	1/1/13/20	9/25/103/115	-
10	CLA	cA	839	1	1/1/15/20	6/37/115/115	-
10	CLA	cB	813	2	-	4/13/91/115	-
13	BCR	bA	849	-	-	13/29/63/63	0/2/2/2
10	CLA	bA	832	1	1/1/15/20	6/37/115/115	-
10	CLA	cA	806	1	1/1/12/20	3/21/99/115	-
10	CLA	cA	841	1	1/1/15/20	11/37/115/115	-
10	CLA	aB	833	2	1/1/13/20	14/29/107/115	-
10	CLA	cA	812	1	1/1/15/20	15/37/115/115	-
10	CLA	bA	840	-	1/1/12/20	6/21/99/115	-
10	CLA	aA	810	1	1/1/15/20	10/37/115/115	-
10	CLA	bB	831	2	1/1/11/20	6/13/91/115	-
10	CLA	cA	826	1	1/1/15/20	8/37/115/115	-
10	CLA	aB	825	2	1/1/12/20	7/24/102/115	-
10	CLA	aA	809	1	1/1/11/20	2/13/91/115	-
10	CLA	cA	835	1	1/1/15/20	12/37/115/115	-
10	CLA	bB	825	2	1/1/12/20	7/24/102/115	-
10	CLA	bB	817	2	1/1/13/20	10/25/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bB	827	2	1/1/15/20	9/37/115/115	-
10	CLA	bA	803	1	1/1/11/20	3/13/91/115	-
10	CLA	bA	811	1	1/1/12/20	8/24/102/115	-
11	PQN	cB	842	-	-	2/23/43/43	0/2/2/2
10	CLA	cB	835	-	1/1/11/20	5/13/91/115	-
10	CLA	bB	819	2	1/1/14/20	10/31/109/115	-
10	CLA	cA	816	1	-	10/24/102/115	-
10	CLA	cA	819	1	1/1/14/20	11/33/111/115	-
10	CLA	bB	811	2	1/1/15/20	17/37/115/115	-
10	CLA	aA	836	1	1/1/12/20	7/21/99/115	-
10	CLA	cB	825	2	1/1/12/20	7/24/102/115	-
10	CLA	aA	820	-	1/1/15/20	13/37/115/115	-
10	CLA	cA	836	1	1/1/12/20	7/21/99/115	-
10	CLA	bB	802	-	1/1/15/20	13/37/115/115	-
13	BCR	cB	844	-	-	10/29/63/63	0/2/2/2
10	CLA	aB	803	2	1/1/15/20	4/37/115/115	-
10	CLA	bB	824	2	1/1/11/20	5/13/91/115	-
10	CLA	cB	833	2	1/1/13/20	14/29/107/115	-
10	CLA	cB	818	2	1/1/13/20	11/30/108/115	-
10	CLA	aA	803	1	1/1/11/20	3/13/91/115	-
10	CLA	bB	840	-	1/1/15/20	2/37/115/115	-
10	CLA	aA	831	1	1/1/15/20	13/37/115/115	-
10	CLA	aB	802	-	1/1/15/20	13/37/115/115	-
13	BCR	aB	845	-	-	12/29/63/63	0/2/2/2
10	CLA	bB	833	2	1/1/13/20	14/29/107/115	-
10	CLA	cB	839	2	1/1/11/20	5/16/94/115	-
10	CLA	cB	832	2	1/1/15/20	14/37/115/115	-
10	CLA	aB	819	2	1/1/14/20	10/31/109/115	-
10	CLA	aB	841	2	1/1/15/20	10/37/115/115	-
10	CLA	cA	828	1	1/1/15/20	6/37/115/115	-
10	CLA	aA	804	1	1/1/15/20	10/37/115/115	-
10	CLA	cA	824	-	1/1/15/20	11/37/115/115	-
10	CLA	aB	829	2	1/1/15/20	12/37/115/115	-
10	CLA	bB	826	-	1/1/15/20	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCR	bA	851	-	-	13/29/63/63	0/2/2/2
10	CLA	bB	836	-	1/1/11/20	2/13/91/115	-
10	CLA	bB	832	2	1/1/15/20	14/37/115/115	-
10	CLA	aL	205	-	-	11/37/115/115	-
10	CLA	aA	829	1	1/1/15/20	12/37/115/115	-
10	CLA	cB	840	-	1/1/15/20	2/37/115/115	-
10	CLA	cA	805	1	1/1/15/20	10/37/115/115	-
10	CLA	aL	204	7	1/1/15/20	8/37/115/115	-
10	CLA	aA	856	2	1/1/11/20	7/18/96/115	-
9	CL0	cA	801	1	3/3/20/25	6/37/135/135	-
10	CLA	aB	832	2	1/1/15/20	14/37/115/115	-
13	BCR	aA	851	-	-	13/29/63/63	0/2/2/2
10	CLA	cB	807	2	1/1/15/20	12/37/115/115	-
13	BCR	bA	846	-	-	14/29/63/63	0/2/2/2
15	LMT	cA	853	-	-	9/21/61/61	0/2/2/2
13	BCR	aI	101	-	-	8/29/63/63	0/2/2/2
13	BCR	aL	207	-	-	7/29/63/63	0/2/2/2
10	CLA	aB	806	2	1/1/12/20	11/24/102/115	-
10	CLA	cA	822	1	1/1/12/20	10/21/99/115	-
10	CLA	bB	828	2	1/1/15/20	11/37/115/115	-
10	CLA	aB	812	2	1/1/11/20	1/13/91/115	-
10	CLA	aA	823	1	1/1/15/20	12/37/115/115	-
10	CLA	bB	804	-	1/1/13/20	14/28/106/115	-
13	BCR	aI	102	-	-	8/29/63/63	0/2/2/2
11	PQN	aB	842	-	-	2/23/43/43	0/2/2/2
10	CLA	aA	812	1	1/1/15/20	15/37/115/115	-
12	SF4	cC	101	3	-	-	0/6/5/5
10	CLA	bB	801	-	1/1/15/20	7/37/115/115	-

All (4662) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	844	PQN	C3-C2	7.31	1.48	1.35
11	bA	844	PQN	C3-C2	7.31	1.48	1.35
11	aA	844	PQN	C3-C2	7.31	1.48	1.35
11	aB	842	PQN	C3-C2	7.23	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cB	842	PQN	C3-C2	7.22	1.48	1.35
11	bB	842	PQN	C3-C2	7.22	1.48	1.35
10	aA	828	CLA	C3B-C2B	6.55	1.49	1.40
10	bA	828	CLA	C3B-C2B	6.53	1.49	1.40
10	cA	828	CLA	C3B-C2B	6.53	1.49	1.40
10	cA	836	CLA	C3B-C2B	6.40	1.49	1.40
10	bA	836	CLA	C3B-C2B	6.33	1.49	1.40
10	aA	836	CLA	C3B-C2B	6.33	1.49	1.40
10	aB	827	CLA	C3B-C2B	6.30	1.49	1.40
10	bA	813	CLA	C3B-C2B	6.30	1.49	1.40
10	aA	813	CLA	C3B-C2B	6.28	1.49	1.40
10	cB	827	CLA	C3B-C2B	6.26	1.49	1.40
10	cA	813	CLA	C3B-C2B	6.26	1.49	1.40
10	bB	827	CLA	C3B-C2B	6.26	1.49	1.40
10	aA	831	CLA	C3B-C2B	6.24	1.49	1.40
10	cA	831	CLA	C3B-C2B	6.23	1.49	1.40
10	aA	827	CLA	C3B-C2B	6.21	1.49	1.40
10	aA	822	CLA	C3B-C2B	6.20	1.49	1.40
10	cA	827	CLA	C3B-C2B	6.20	1.49	1.40
10	bA	831	CLA	C3B-C2B	6.19	1.49	1.40
10	cA	822	CLA	C3B-C2B	6.19	1.49	1.40
10	bA	827	CLA	C3B-C2B	6.19	1.49	1.40
10	bA	822	CLA	C3B-C2B	6.15	1.48	1.40
10	bB	825	CLA	C3B-C2B	6.14	1.48	1.40
10	aB	825	CLA	C3B-C2B	6.10	1.48	1.40
10	cB	825	CLA	C3B-C2B	6.09	1.48	1.40
10	bA	805	CLA	C3B-C2B	6.09	1.48	1.40
10	cA	803	CLA	C3B-C2B	6.09	1.48	1.40
10	cA	802	CLA	C3B-C2B	6.07	1.48	1.40
10	bA	803	CLA	C3B-C2B	6.04	1.48	1.40
10	aA	805	CLA	C3B-C2B	6.04	1.48	1.40
10	aB	826	CLA	C3B-C2B	6.03	1.48	1.40
10	cA	805	CLA	C3B-C2B	6.02	1.48	1.40
10	bB	826	CLA	C3B-C2B	6.02	1.48	1.40
10	aB	806	CLA	C3B-C2B	6.02	1.48	1.40
10	aA	802	CLA	C3B-C2B	6.01	1.48	1.40
10	bB	806	CLA	C3B-C2B	6.01	1.48	1.40
10	bA	802	CLA	C3B-C2B	6.01	1.48	1.40
10	cB	826	CLA	C3B-C2B	6.01	1.48	1.40
10	aA	803	CLA	C3B-C2B	6.01	1.48	1.40
10	cB	806	CLA	C3B-C2B	6.00	1.48	1.40
10	bB	804	CLA	C3B-C2B	5.98	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	821	CLA	C3B-C2B	5.96	1.48	1.40
10	aB	830	CLA	C3B-C2B	5.96	1.48	1.40
10	bA	821	CLA	C3B-C2B	5.96	1.48	1.40
10	cA	821	CLA	C3B-C2B	5.96	1.48	1.40
10	bB	830	CLA	C3B-C2B	5.93	1.48	1.40
10	aB	804	CLA	C3B-C2B	5.93	1.48	1.40
10	aA	819	CLA	C3B-C2B	5.92	1.48	1.40
10	cB	830	CLA	C3B-C2B	5.92	1.48	1.40
10	bB	821	CLA	C3B-C2B	5.91	1.48	1.40
10	bB	829	CLA	C3B-C2B	5.91	1.48	1.40
10	aB	815	CLA	C3B-C2B	5.91	1.48	1.40
10	aB	829	CLA	C3B-C2B	5.91	1.48	1.40
10	cB	829	CLA	C3B-C2B	5.91	1.48	1.40
10	cB	804	CLA	C3B-C2B	5.91	1.48	1.40
10	bA	819	CLA	C3B-C2B	5.90	1.48	1.40
10	cB	821	CLA	C3B-C2B	5.89	1.48	1.40
10	aB	821	CLA	C3B-C2B	5.89	1.48	1.40
10	bB	815	CLA	C3B-C2B	5.89	1.48	1.40
10	cB	815	CLA	C3B-C2B	5.89	1.48	1.40
10	cA	819	CLA	C3B-C2B	5.88	1.48	1.40
10	cB	813	CLA	C3B-C2B	5.83	1.48	1.40
10	bB	813	CLA	C3B-C2B	5.83	1.48	1.40
10	cB	823	CLA	C3B-C2B	5.82	1.48	1.40
10	bA	829	CLA	C3B-C2B	5.81	1.48	1.40
10	cB	840	CLA	C3B-C2B	5.81	1.48	1.40
10	aB	813	CLA	C3B-C2B	5.81	1.48	1.40
10	cB	802	CLA	C3B-C2B	5.81	1.48	1.40
10	aA	840	CLA	C3B-C2B	5.80	1.48	1.40
10	aB	828	CLA	C3B-C2B	5.79	1.48	1.40
10	bA	840	CLA	C3B-C2B	5.79	1.48	1.40
10	bB	823	CLA	C3B-C2B	5.79	1.48	1.40
10	bB	802	CLA	C3B-C2B	5.78	1.48	1.40
10	aB	802	CLA	C3B-C2B	5.78	1.48	1.40
10	aA	843	CLA	C3B-C2B	5.78	1.48	1.40
10	cA	829	CLA	C3B-C2B	5.78	1.48	1.40
10	aB	823	CLA	C3B-C2B	5.77	1.48	1.40
10	aB	824	CLA	C3B-C2B	5.77	1.48	1.40
10	bB	822	CLA	C3B-C2B	5.77	1.48	1.40
10	aB	822	CLA	C3B-C2B	5.76	1.48	1.40
10	aA	807	CLA	C3B-C2B	5.76	1.48	1.40
10	aA	829	CLA	C3B-C2B	5.76	1.48	1.40
10	cA	814	CLA	C3B-C2B	5.76	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	840	CLA	C3B-C2B	5.75	1.48	1.40
10	cB	824	CLA	C3B-C2B	5.75	1.48	1.40
10	aB	840	CLA	C3B-C2B	5.75	1.48	1.40
10	bB	828	CLA	C3B-C2B	5.75	1.48	1.40
10	cB	828	CLA	C3B-C2B	5.74	1.48	1.40
10	cA	843	CLA	C3B-C2B	5.74	1.48	1.40
10	aA	808	CLA	C3B-C2B	5.74	1.48	1.40
10	aA	814	CLA	C3B-C2B	5.73	1.48	1.40
10	bB	840	CLA	C3B-C2B	5.73	1.48	1.40
10	bA	814	CLA	C3B-C2B	5.72	1.48	1.40
10	bA	856	CLA	C3B-C2B	5.72	1.48	1.40
10	bA	807	CLA	C3B-C2B	5.72	1.48	1.40
10	bA	843	CLA	C3B-C2B	5.71	1.48	1.40
10	cA	808	CLA	C3B-C2B	5.71	1.48	1.40
10	cB	822	CLA	C3B-C2B	5.71	1.48	1.40
10	bB	824	CLA	C3B-C2B	5.70	1.48	1.40
10	aA	856	CLA	C3B-C2B	5.70	1.48	1.40
10	cA	807	CLA	C3B-C2B	5.69	1.48	1.40
10	cA	856	CLA	C3B-C2B	5.69	1.48	1.40
10	aB	801	CLA	C3B-C2B	5.69	1.48	1.40
10	bB	814	CLA	C3B-C2B	5.69	1.48	1.40
10	aB	833	CLA	C3B-C2B	5.68	1.48	1.40
10	bA	841	CLA	C3B-C2B	5.68	1.48	1.40
10	bA	817	CLA	C3B-C2B	5.68	1.48	1.40
10	aA	841	CLA	C3B-C2B	5.68	1.48	1.40
10	cA	817	CLA	C3B-C2B	5.68	1.48	1.40
10	aB	814	CLA	C3B-C2B	5.67	1.48	1.40
10	cB	801	CLA	C3B-C2B	5.67	1.48	1.40
10	cB	807	CLA	C3B-C2B	5.67	1.48	1.40
10	aB	807	CLA	C3B-C2B	5.67	1.48	1.40
10	bA	808	CLA	C3B-C2B	5.67	1.48	1.40
10	cA	825	CLA	C3B-C2B	5.66	1.48	1.40
10	aB	838	CLA	C3B-C2B	5.66	1.48	1.40
10	cA	841	CLA	C3B-C2B	5.66	1.48	1.40
10	cB	832	CLA	C3B-C2B	5.66	1.48	1.40
10	bB	833	CLA	C3B-C2B	5.65	1.48	1.40
10	bB	838	CLA	C3B-C2B	5.65	1.48	1.40
10	bB	807	CLA	C3B-C2B	5.64	1.48	1.40
10	cB	833	CLA	C3B-C2B	5.64	1.48	1.40
10	bA	810	CLA	C3B-C2B	5.64	1.48	1.40
10	aA	817	CLA	C3B-C2B	5.64	1.48	1.40
10	cB	814	CLA	C3B-C2B	5.63	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	805	CLA	C3B-C2B	5.63	1.48	1.40
10	aA	818	CLA	C3B-C2B	5.63	1.48	1.40
10	cB	838	CLA	C3B-C2B	5.63	1.48	1.40
10	aB	832	CLA	C3B-C2B	5.62	1.48	1.40
10	cB	836	CLA	C3B-C2B	5.61	1.48	1.40
10	bA	818	CLA	C3B-C2B	5.61	1.48	1.40
10	bB	832	CLA	C3B-C2B	5.61	1.48	1.40
10	bB	801	CLA	C3B-C2B	5.60	1.48	1.40
10	aB	805	CLA	C3B-C2B	5.60	1.48	1.40
10	bB	836	CLA	C3B-C2B	5.60	1.48	1.40
10	cA	818	CLA	C3B-C2B	5.60	1.48	1.40
10	bB	805	CLA	C3B-C2B	5.59	1.48	1.40
10	cB	834	CLA	C3B-C2B	5.59	1.48	1.40
10	cA	810	CLA	C3B-C2B	5.59	1.48	1.40
10	aA	811	CLA	C3B-C2B	5.58	1.48	1.40
10	bA	825	CLA	C3B-C2B	5.58	1.48	1.40
10	bB	818	CLA	C3B-C2B	5.58	1.48	1.40
10	cB	818	CLA	C3B-C2B	5.57	1.48	1.40
10	cA	818	CLA	C3C-C2C	5.57	1.48	1.36
10	aA	810	CLA	C3B-C2B	5.57	1.48	1.40
10	bA	815	CLA	C3B-C2B	5.56	1.48	1.40
10	cA	811	CLA	C3B-C2B	5.55	1.48	1.40
10	aA	825	CLA	C3B-C2B	5.55	1.48	1.40
10	aA	812	CLA	C3B-C2B	5.55	1.48	1.40
10	aB	834	CLA	C3B-C2B	5.55	1.48	1.40
10	cB	839	CLA	C3B-C2B	5.55	1.48	1.40
10	bB	839	CLA	C3B-C2B	5.55	1.48	1.40
10	aA	818	CLA	C3C-C2C	5.55	1.48	1.36
10	aB	836	CLA	C3B-C2B	5.54	1.48	1.40
10	aL	203	CLA	C3B-C2B	5.54	1.48	1.40
10	bA	811	CLA	C3B-C2B	5.54	1.48	1.40
10	bA	812	CLA	C3B-C2B	5.54	1.48	1.40
10	bB	834	CLA	C3B-C2B	5.54	1.48	1.40
10	aB	818	CLA	C3B-C2B	5.54	1.48	1.40
10	bA	818	CLA	C3C-C2C	5.54	1.48	1.36
10	aA	839	CLA	C3B-C2B	5.53	1.48	1.40
10	bB	808	CLA	C3B-C2B	5.53	1.48	1.40
10	bA	816	CLA	C3B-C2B	5.52	1.48	1.40
10	cA	812	CLA	C3B-C2B	5.52	1.48	1.40
10	cA	816	CLA	C3B-C2B	5.52	1.48	1.40
10	aA	816	CLA	C3B-C2B	5.52	1.48	1.40
10	cL	203	CLA	C3B-C2B	5.52	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bL	203	CLA	C3B-C2B	5.51	1.48	1.40
10	aA	815	CLA	C3B-C2B	5.50	1.48	1.40
10	aB	808	CLA	C3B-C2B	5.50	1.48	1.40
10	cA	815	CLA	C3B-C2B	5.50	1.48	1.40
10	cA	839	CLA	C3B-C2B	5.50	1.48	1.40
10	bA	839	CLA	C3B-C2B	5.50	1.48	1.40
10	aL	205	CLA	C3B-C2B	5.49	1.48	1.40
10	cB	808	CLA	C3B-C2B	5.49	1.48	1.40
10	aA	815	CLA	C3C-C2C	5.49	1.48	1.36
10	bA	815	CLA	C3C-C2C	5.49	1.48	1.36
10	aB	839	CLA	C3B-C2B	5.47	1.48	1.40
10	cA	809	CLA	C3B-C2B	5.45	1.47	1.40
10	cA	815	CLA	C3C-C2C	5.45	1.48	1.36
10	cA	856	CLA	O2D-CGD	5.45	1.46	1.33
10	cA	835	CLA	C3B-C2B	5.44	1.47	1.40
10	aL	202	CLA	C3B-C2B	5.44	1.47	1.40
10	bL	205	CLA	C3B-C2B	5.43	1.47	1.40
10	bA	840	CLA	C3C-C2C	5.43	1.48	1.36
10	bA	854	CLA	C3B-C2B	5.43	1.47	1.40
10	aA	840	CLA	C3C-C2C	5.43	1.48	1.36
10	cL	205	CLA	C3B-C2B	5.43	1.47	1.40
10	aA	835	CLA	C3B-C2B	5.43	1.47	1.40
10	aB	817	CLA	C3B-C2B	5.43	1.47	1.40
10	bA	854	CLA	C3C-C2C	5.42	1.48	1.36
10	cA	854	CLA	C3C-C2C	5.42	1.48	1.36
10	bA	835	CLA	C3B-C2B	5.42	1.47	1.40
10	cB	817	CLA	C3B-C2B	5.42	1.47	1.40
10	aB	813	CLA	C3C-C2C	5.42	1.48	1.36
10	cL	202	CLA	C3B-C2B	5.41	1.47	1.40
10	aA	854	CLA	C3C-C2C	5.41	1.48	1.36
10	bA	856	CLA	O2D-CGD	5.41	1.46	1.33
10	bA	820	CLA	C3B-C2B	5.41	1.47	1.40
10	bB	813	CLA	C3C-C2C	5.40	1.48	1.36
10	bA	809	CLA	C3B-C2B	5.40	1.47	1.40
10	cA	840	CLA	C3C-C2C	5.40	1.48	1.36
10	cB	813	CLA	C3C-C2C	5.40	1.48	1.36
10	cA	854	CLA	C3B-C2B	5.39	1.47	1.40
10	aA	820	CLA	C3B-C2B	5.39	1.47	1.40
10	aA	854	CLA	C3B-C2B	5.39	1.47	1.40
10	cA	823	CLA	C3B-C2B	5.38	1.47	1.40
10	cA	820	CLA	C3B-C2B	5.38	1.47	1.40
10	bA	810	CLA	C3C-C2C	5.37	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	856	CLA	O2D-CGD	5.37	1.46	1.33
10	aA	809	CLA	C3B-C2B	5.37	1.47	1.40
10	aB	835	CLA	C3C-C2C	5.37	1.48	1.36
10	bA	823	CLA	C3B-C2B	5.37	1.47	1.40
10	cB	826	CLA	C3C-C2C	5.36	1.48	1.36
10	cA	806	CLA	C3B-C2B	5.36	1.47	1.40
10	aA	826	CLA	C3C-C2C	5.36	1.48	1.36
10	cB	835	CLA	C3C-C2C	5.35	1.48	1.36
10	aB	823	CLA	C1D-ND	5.35	1.44	1.37
10	bL	202	CLA	C3B-C2B	5.35	1.47	1.40
10	bB	817	CLA	C3B-C2B	5.35	1.47	1.40
10	cA	826	CLA	C3C-C2C	5.35	1.48	1.36
10	bA	812	CLA	C3C-C2C	5.35	1.48	1.36
10	aA	819	CLA	C3C-C2C	5.35	1.48	1.36
10	bB	826	CLA	C3C-C2C	5.35	1.48	1.36
10	cA	810	CLA	C3C-C2C	5.35	1.48	1.36
10	cA	804	CLA	C3B-C2B	5.34	1.47	1.40
10	aA	843	CLA	C3C-C2C	5.34	1.48	1.36
10	bA	820	CLA	C3C-C2C	5.34	1.48	1.36
10	aA	823	CLA	C3B-C2B	5.34	1.47	1.40
10	aA	810	CLA	C3C-C2C	5.34	1.48	1.36
10	aA	804	CLA	C3B-C2B	5.34	1.47	1.40
10	cL	204	CLA	C3B-C2B	5.34	1.47	1.40
10	cA	820	CLA	C3C-C2C	5.33	1.48	1.36
10	bB	823	CLA	C1D-ND	5.33	1.44	1.37
10	cB	816	CLA	C3B-C2B	5.33	1.47	1.40
10	bA	843	CLA	C3C-C2C	5.33	1.48	1.36
10	bA	826	CLA	C3C-C2C	5.33	1.48	1.36
10	cA	843	CLA	C3C-C2C	5.33	1.48	1.36
10	bA	802	CLA	C1D-ND	5.32	1.44	1.37
10	bA	810	CLA	C1D-ND	5.32	1.44	1.37
10	bA	806	CLA	C3B-C2B	5.32	1.47	1.40
10	bB	836	CLA	C3C-C2C	5.32	1.48	1.36
10	cA	819	CLA	C3C-C2C	5.32	1.48	1.36
10	cB	836	CLA	C3C-C2C	5.32	1.48	1.36
10	bA	803	CLA	C3C-C2C	5.32	1.48	1.36
10	bB	834	CLA	C3C-C2C	5.32	1.48	1.36
10	bB	823	CLA	C3C-C2C	5.32	1.48	1.36
9	cA	801	CL0	C3B-C2B	5.32	1.47	1.40
10	aB	818	CLA	C3C-C2C	5.32	1.48	1.36
10	aB	819	CLA	C3B-C2B	5.31	1.47	1.40
10	cA	812	CLA	C3C-C2C	5.31	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	806	CLA	C3B-C2B	5.31	1.47	1.40
10	bA	827	CLA	C3C-C2C	5.31	1.48	1.36
10	bB	835	CLA	C3C-C2C	5.31	1.48	1.36
10	aA	820	CLA	C3C-C2C	5.31	1.48	1.36
10	aB	836	CLA	C3C-C2C	5.31	1.48	1.36
10	aB	835	CLA	C3B-C2B	5.31	1.47	1.40
10	cB	823	CLA	C3C-C2C	5.30	1.48	1.36
9	bA	801	CL0	C3B-C2B	5.30	1.47	1.40
10	bA	856	CLA	C3C-C2C	5.30	1.48	1.36
10	bB	816	CLA	C3B-C2B	5.30	1.47	1.40
10	aB	820	CLA	C3C-C2C	5.30	1.48	1.36
10	aA	812	CLA	C3C-C2C	5.30	1.48	1.36
10	bA	819	CLA	C3C-C2C	5.30	1.48	1.36
10	aB	816	CLA	C3B-C2B	5.30	1.47	1.40
10	aB	823	CLA	C3C-C2C	5.30	1.48	1.36
10	aB	834	CLA	C3C-C2C	5.30	1.48	1.36
10	bB	818	CLA	C3C-C2C	5.30	1.48	1.36
10	cB	818	CLA	C3C-C2C	5.30	1.48	1.36
9	aA	801	CL0	C3B-C2B	5.30	1.47	1.40
10	cB	834	CLA	C3C-C2C	5.29	1.48	1.36
10	aB	826	CLA	C3C-C2C	5.29	1.48	1.36
10	bA	822	CLA	C3C-C2C	5.29	1.48	1.36
10	bA	804	CLA	C3B-C2B	5.29	1.47	1.40
10	bB	835	CLA	C3B-C2B	5.29	1.47	1.40
10	cB	823	CLA	C1D-ND	5.29	1.44	1.37
10	aA	827	CLA	C3C-C2C	5.29	1.48	1.36
10	aA	802	CLA	C1D-ND	5.28	1.44	1.37
10	aA	822	CLA	C3C-C2C	5.28	1.48	1.36
10	aA	810	CLA	C1D-ND	5.28	1.44	1.37
10	aA	803	CLA	C3C-C2C	5.28	1.48	1.36
10	bB	809	CLA	C3B-C2B	5.28	1.47	1.40
10	bB	820	CLA	C3C-C2C	5.28	1.47	1.36
10	cA	856	CLA	C3C-C2C	5.27	1.47	1.36
10	cA	802	CLA	C1D-ND	5.27	1.44	1.37
10	aA	829	CLA	C3C-C2C	5.27	1.47	1.36
10	aA	814	CLA	C3C-C2C	5.27	1.47	1.36
10	aA	809	CLA	C3C-C2C	5.26	1.47	1.36
10	cB	820	CLA	C3C-C2C	5.26	1.47	1.36
10	aL	204	CLA	C3B-C2B	5.26	1.47	1.40
10	bB	803	CLA	C3B-C2B	5.26	1.47	1.40
10	cA	803	CLA	C3C-C2C	5.26	1.47	1.36
10	cB	819	CLA	C3B-C2B	5.26	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	806	CLA	C3C-C2C	5.26	1.47	1.36
10	aA	813	CLA	C3C-C2C	5.26	1.47	1.36
10	bA	813	CLA	C3C-C2C	5.26	1.47	1.36
10	bA	823	CLA	C3C-C2C	5.26	1.47	1.36
10	bA	832	CLA	C3B-C2B	5.26	1.47	1.40
10	cA	823	CLA	C3C-C2C	5.26	1.47	1.36
10	aA	823	CLA	C3C-C2C	5.26	1.47	1.36
10	bB	819	CLA	C3B-C2B	5.26	1.47	1.40
10	aB	841	CLA	C3B-C2B	5.26	1.47	1.40
10	bA	809	CLA	C3C-C2C	5.26	1.47	1.36
10	cB	835	CLA	C3B-C2B	5.26	1.47	1.40
10	cA	843	CLA	C1D-ND	5.26	1.44	1.37
10	aB	832	CLA	C3C-C2C	5.25	1.47	1.36
10	bA	806	CLA	C3C-C2C	5.25	1.47	1.36
10	cA	811	CLA	C3C-C2C	5.25	1.47	1.36
10	cA	827	CLA	C3C-C2C	5.25	1.47	1.36
10	bB	812	CLA	C3C-C2C	5.25	1.47	1.36
10	bA	811	CLA	C3C-C2C	5.25	1.47	1.36
10	aB	809	CLA	C3B-C2B	5.25	1.47	1.40
10	cB	831	CLA	C3B-C2B	5.25	1.47	1.40
10	cA	835	CLA	C3C-C2C	5.25	1.47	1.36
10	cA	829	CLA	C3C-C2C	5.24	1.47	1.36
10	bL	204	CLA	C3B-C2B	5.24	1.47	1.40
10	aA	811	CLA	C3C-C2C	5.24	1.47	1.36
10	cA	809	CLA	C3C-C2C	5.24	1.47	1.36
10	aA	832	CLA	C3B-C2B	5.24	1.47	1.40
10	bB	841	CLA	C3B-C2B	5.24	1.47	1.40
10	cB	824	CLA	C1D-ND	5.24	1.44	1.37
10	aA	856	CLA	C3C-C2C	5.24	1.47	1.36
10	cB	822	CLA	O2D-CGD	5.24	1.46	1.33
10	cB	812	CLA	C3C-C2C	5.24	1.47	1.36
10	cA	822	CLA	C3C-C2C	5.23	1.47	1.36
10	aB	838	CLA	C3C-C2C	5.23	1.47	1.36
10	cA	813	CLA	C3C-C2C	5.23	1.47	1.36
10	bA	843	CLA	C1D-ND	5.23	1.44	1.37
10	bA	814	CLA	C3C-C2C	5.23	1.47	1.36
10	cA	810	CLA	C1D-ND	5.23	1.44	1.37
10	aA	806	CLA	C3C-C2C	5.23	1.47	1.36
10	aB	816	CLA	C3C-C2C	5.23	1.47	1.36
10	cA	832	CLA	C3B-C2B	5.23	1.47	1.40
10	bB	832	CLA	C3C-C2C	5.23	1.47	1.36
10	bA	835	CLA	C3C-C2C	5.23	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	831	CLA	C3B-C2B	5.23	1.47	1.40
10	cA	814	CLA	C3C-C2C	5.23	1.47	1.36
10	bA	829	CLA	C3C-C2C	5.23	1.47	1.36
10	cA	826	CLA	CHC-C1C	5.23	1.48	1.35
10	bB	815	CLA	C3C-C2C	5.23	1.47	1.36
10	aB	812	CLA	C3C-C2C	5.23	1.47	1.36
10	cB	832	CLA	C3C-C2C	5.22	1.47	1.36
10	bB	816	CLA	C3C-C2C	5.22	1.47	1.36
10	cB	816	CLA	C3C-C2C	5.22	1.47	1.36
10	aB	815	CLA	C3C-C2C	5.22	1.47	1.36
10	cA	840	CLA	O2D-CGD	5.22	1.45	1.33
10	bB	827	CLA	C3C-C2C	5.22	1.47	1.36
10	bB	821	CLA	C3C-C2C	5.22	1.47	1.36
10	aA	835	CLA	C3C-C2C	5.22	1.47	1.36
10	cB	815	CLA	C3C-C2C	5.22	1.47	1.36
10	bA	824	CLA	C3B-C2B	5.22	1.47	1.40
10	bB	838	CLA	C3C-C2C	5.22	1.47	1.36
10	cA	824	CLA	C3B-C2B	5.22	1.47	1.40
10	bB	831	CLA	C3C-C2C	5.21	1.47	1.36
10	aA	843	CLA	C1D-ND	5.21	1.44	1.37
10	bA	834	CLA	C3C-C2C	5.21	1.47	1.36
10	aB	824	CLA	C1D-ND	5.21	1.44	1.37
10	aA	824	CLA	C3B-C2B	5.21	1.47	1.40
10	cA	834	CLA	C3C-C2C	5.21	1.47	1.36
10	cB	836	CLA	O2D-CGD	5.21	1.45	1.33
10	bA	803	CLA	C1D-ND	5.21	1.44	1.37
10	cB	809	CLA	C3B-C2B	5.21	1.47	1.40
10	bB	824	CLA	C3C-C2C	5.21	1.47	1.36
10	aA	817	CLA	C3C-C2C	5.21	1.47	1.36
10	aB	824	CLA	C3C-C2C	5.21	1.47	1.36
10	aB	803	CLA	C3B-C2B	5.21	1.47	1.40
10	aA	826	CLA	CHC-C1C	5.21	1.48	1.35
10	aB	822	CLA	O2D-CGD	5.21	1.45	1.33
10	aA	856	CLA	C1D-ND	5.20	1.44	1.37
10	aA	837	CLA	C3B-C2B	5.20	1.47	1.40
10	aB	827	CLA	C3C-C2C	5.20	1.47	1.36
10	cB	831	CLA	C3C-C2C	5.20	1.47	1.36
10	aB	831	CLA	C3B-C2B	5.20	1.47	1.40
10	bA	826	CLA	CHC-C1C	5.20	1.48	1.35
10	cB	824	CLA	C3C-C2C	5.20	1.47	1.36
10	cB	841	CLA	C3B-C2B	5.20	1.47	1.40
10	aB	821	CLA	C3C-C2C	5.20	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	821	CLA	C3C-C2C	5.20	1.47	1.36
10	aA	839	CLA	C3C-C2C	5.20	1.47	1.36
10	aA	834	CLA	C3C-C2C	5.20	1.47	1.36
10	bA	840	CLA	O2D-CGD	5.20	1.45	1.33
10	bA	833	CLA	C3B-C2B	5.19	1.47	1.40
10	cL	203	CLA	C3C-C2C	5.19	1.47	1.36
10	cA	803	CLA	C1D-ND	5.19	1.44	1.37
10	cA	839	CLA	C3C-C2C	5.19	1.47	1.36
10	aB	836	CLA	O2D-CGD	5.19	1.45	1.33
10	aB	831	CLA	C3C-C2C	5.19	1.47	1.36
10	cB	822	CLA	C3C-C2C	5.19	1.47	1.36
10	bL	203	CLA	C3C-C2C	5.19	1.47	1.36
10	bA	839	CLA	C3C-C2C	5.19	1.47	1.36
10	cB	803	CLA	C3B-C2B	5.19	1.47	1.40
10	bA	803	CLA	CHC-C1C	5.18	1.48	1.35
10	aB	826	CLA	CHC-C1C	5.18	1.48	1.35
10	cB	822	CLA	C1D-ND	5.18	1.44	1.37
10	cB	835	CLA	C1D-ND	5.18	1.44	1.37
10	cA	817	CLA	C3C-C2C	5.18	1.47	1.36
10	aA	803	CLA	C1D-ND	5.18	1.44	1.37
10	cA	803	CLA	CHC-C1C	5.18	1.48	1.35
10	cB	833	CLA	C3C-C2C	5.18	1.47	1.36
10	cB	838	CLA	C3C-C2C	5.18	1.47	1.36
10	bB	822	CLA	O2D-CGD	5.18	1.45	1.33
10	bB	826	CLA	CHC-C1C	5.18	1.48	1.35
10	aA	839	CLA	O2D-CGD	5.18	1.45	1.33
10	cB	823	CLA	O2D-CGD	5.18	1.45	1.33
10	aA	840	CLA	O2D-CGD	5.18	1.45	1.33
10	bA	821	CLA	O2D-CGD	5.18	1.45	1.33
10	cB	826	CLA	CHC-C1C	5.18	1.48	1.35
10	aB	822	CLA	C3C-C2C	5.18	1.47	1.36
10	cA	821	CLA	O2D-CGD	5.17	1.45	1.33
10	bB	836	CLA	O2D-CGD	5.17	1.45	1.33
10	cB	827	CLA	C3C-C2C	5.17	1.47	1.36
10	aB	839	CLA	C3C-C2C	5.17	1.47	1.36
10	aA	821	CLA	O2D-CGD	5.17	1.45	1.33
10	aB	823	CLA	O2D-CGD	5.17	1.45	1.33
10	aA	802	CLA	O2D-CGD	5.17	1.45	1.33
10	aA	803	CLA	CHC-C1C	5.17	1.48	1.35
10	cA	833	CLA	C3B-C2B	5.16	1.47	1.40
10	bB	839	CLA	C3C-C2C	5.16	1.47	1.36
10	cA	832	CLA	C3C-C2C	5.16	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	824	CLA	C1D-ND	5.16	1.44	1.37
10	bA	802	CLA	O2D-CGD	5.16	1.45	1.33
10	bB	822	CLA	C3C-C2C	5.16	1.47	1.36
10	bB	835	CLA	C1D-ND	5.16	1.44	1.37
10	aL	205	CLA	C3C-C2C	5.16	1.47	1.36
10	cB	807	CLA	C3C-C2C	5.16	1.47	1.36
10	cA	839	CLA	O2D-CGD	5.16	1.45	1.33
10	bA	809	CLA	O2D-CGD	5.16	1.45	1.33
10	bA	807	CLA	C3C-C2C	5.16	1.47	1.36
10	cL	205	CLA	C3C-C2C	5.16	1.47	1.36
10	cA	856	CLA	C1D-ND	5.16	1.44	1.37
10	aL	203	CLA	C3C-C2C	5.15	1.47	1.36
10	bA	824	CLA	C3C-C2C	5.15	1.47	1.36
10	bA	817	CLA	C3C-C2C	5.15	1.47	1.36
10	bB	822	CLA	C1D-ND	5.15	1.44	1.37
10	cA	823	CLA	C1D-ND	5.15	1.44	1.37
10	bA	823	CLA	C1D-ND	5.15	1.44	1.37
10	bA	837	CLA	C3B-C2B	5.15	1.47	1.40
10	bB	823	CLA	O2D-CGD	5.15	1.45	1.33
10	bB	833	CLA	C3C-C2C	5.15	1.47	1.36
10	cA	807	CLA	C3C-C2C	5.15	1.47	1.36
10	cA	802	CLA	O2D-CGD	5.15	1.45	1.33
10	aA	824	CLA	C3C-C2C	5.15	1.47	1.36
10	aA	809	CLA	O2D-CGD	5.15	1.45	1.33
10	bA	832	CLA	C3C-C2C	5.15	1.47	1.36
10	aA	813	CLA	C1D-ND	5.15	1.44	1.37
10	cA	837	CLA	C3B-C2B	5.15	1.47	1.40
10	bB	829	CLA	C3C-C2C	5.15	1.47	1.36
10	aA	830	CLA	C3C-C2C	5.14	1.47	1.36
10	aB	833	CLA	C3C-C2C	5.14	1.47	1.36
10	aB	822	CLA	C1D-ND	5.14	1.44	1.37
10	bA	839	CLA	O2D-CGD	5.14	1.45	1.33
10	aA	802	CLA	C3C-C2C	5.14	1.47	1.36
10	bA	821	CLA	C3C-C2C	5.14	1.47	1.36
10	bL	205	CLA	C3C-C2C	5.14	1.47	1.36
10	aB	829	CLA	C3C-C2C	5.14	1.47	1.36
10	cA	825	CLA	CHC-C1C	5.14	1.48	1.35
10	cA	802	CLA	C3C-C2C	5.14	1.47	1.36
10	bA	856	CLA	C1D-ND	5.14	1.44	1.37
10	bB	807	CLA	C3C-C2C	5.14	1.47	1.36
10	aA	821	CLA	C3C-C2C	5.14	1.47	1.36
10	cA	824	CLA	C3C-C2C	5.14	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	831	CLA	O2D-CGD	5.13	1.45	1.33
10	cA	830	CLA	C3C-C2C	5.13	1.47	1.36
10	aB	807	CLA	C3C-C2C	5.13	1.47	1.36
10	bA	802	CLA	C3C-C2C	5.13	1.47	1.36
10	bB	835	CLA	CHC-C1C	5.13	1.48	1.35
10	bA	805	CLA	C3C-C2C	5.13	1.47	1.36
10	bA	830	CLA	C3C-C2C	5.13	1.47	1.36
10	cA	806	CLA	CHC-C1C	5.13	1.48	1.35
10	aA	808	CLA	C3C-C2C	5.13	1.47	1.36
10	aA	832	CLA	C3C-C2C	5.13	1.47	1.36
10	cA	825	CLA	C3C-C2C	5.13	1.47	1.36
10	cA	821	CLA	C3C-C2C	5.13	1.47	1.36
10	bB	836	CLA	C1D-ND	5.13	1.44	1.37
10	bA	806	CLA	CHC-C1C	5.13	1.48	1.35
10	cB	839	CLA	C3C-C2C	5.13	1.47	1.36
10	aB	835	CLA	C1D-ND	5.13	1.44	1.37
10	cB	829	CLA	C3C-C2C	5.12	1.47	1.36
10	bA	825	CLA	CHC-C1C	5.12	1.48	1.35
10	cA	813	CLA	C1D-ND	5.12	1.44	1.37
10	aB	831	CLA	O2D-CGD	5.12	1.45	1.33
10	bA	804	CLA	C3C-C2C	5.12	1.47	1.36
10	cA	826	CLA	C3B-C2B	5.12	1.47	1.40
10	cB	827	CLA	C1D-ND	5.12	1.44	1.37
10	cA	820	CLA	CHC-C1C	5.11	1.48	1.35
10	aB	836	CLA	C1D-ND	5.11	1.44	1.37
10	cB	802	CLA	C3C-C2C	5.11	1.47	1.36
10	aA	839	CLA	C1D-ND	5.11	1.44	1.37
10	aA	854	CLA	O2D-CGD	5.11	1.45	1.33
10	aA	825	CLA	CHC-C1C	5.11	1.48	1.35
10	aA	805	CLA	C3C-C2C	5.11	1.47	1.36
10	aA	806	CLA	CHC-C1C	5.11	1.48	1.35
10	aB	835	CLA	CHC-C1C	5.11	1.48	1.35
10	cB	835	CLA	CHC-C1C	5.11	1.48	1.35
10	bA	825	CLA	C3C-C2C	5.11	1.47	1.36
10	cA	809	CLA	O2D-CGD	5.11	1.45	1.33
10	cA	805	CLA	C3C-C2C	5.11	1.47	1.36
10	cB	836	CLA	C1D-ND	5.11	1.44	1.37
10	bA	854	CLA	O2D-CGD	5.11	1.45	1.33
10	aA	833	CLA	C3B-C2B	5.10	1.47	1.40
10	bB	802	CLA	C3C-C2C	5.10	1.47	1.36
10	bA	810	CLA	O2D-CGD	5.10	1.45	1.33
10	bA	839	CLA	C1D-ND	5.10	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	831	CLA	O2D-CGD	5.10	1.45	1.33
10	aA	807	CLA	C3C-C2C	5.10	1.47	1.36
10	cA	854	CLA	CHC-C1C	5.10	1.48	1.35
10	aB	835	CLA	O2D-CGD	5.10	1.45	1.33
10	bB	808	CLA	O2D-CGD	5.10	1.45	1.33
10	bB	837	CLA	C3B-C2B	5.10	1.47	1.40
10	cA	854	CLA	O2D-CGD	5.10	1.45	1.33
10	cA	824	CLA	CHC-C1C	5.10	1.48	1.35
10	aA	806	CLA	O2D-CGD	5.10	1.45	1.33
10	aB	832	CLA	C1D-ND	5.10	1.44	1.37
10	aA	825	CLA	C3C-C2C	5.10	1.47	1.36
10	bB	827	CLA	C1D-ND	5.10	1.44	1.37
10	aA	814	CLA	O2D-CGD	5.10	1.45	1.33
10	cA	831	CLA	C3C-C2C	5.10	1.47	1.36
10	bA	814	CLA	O2D-CGD	5.10	1.45	1.33
10	bA	833	CLA	C3C-C2C	5.10	1.47	1.36
10	bB	812	CLA	C3B-C2B	5.10	1.47	1.40
10	cB	820	CLA	O2D-CGD	5.09	1.45	1.33
10	bA	831	CLA	C3C-C2C	5.09	1.47	1.36
10	aB	810	CLA	C3B-C2B	5.09	1.47	1.40
10	cA	808	CLA	C3C-C2C	5.09	1.47	1.36
10	aB	817	CLA	C1D-ND	5.09	1.44	1.37
10	cB	812	CLA	C3B-C2B	5.09	1.47	1.40
10	aB	818	CLA	O2D-CGD	5.09	1.45	1.33
10	cA	833	CLA	C3C-C2C	5.09	1.47	1.36
10	bA	806	CLA	O2D-CGD	5.09	1.45	1.33
10	aL	202	CLA	C3C-C2C	5.09	1.47	1.36
10	aB	806	CLA	CHC-C1C	5.09	1.48	1.35
10	cL	202	CLA	C3C-C2C	5.09	1.47	1.36
10	aA	837	CLA	C3C-C2C	5.09	1.47	1.36
10	cA	830	CLA	C3B-C2B	5.09	1.47	1.40
10	cA	816	CLA	CHC-C1C	5.09	1.48	1.35
10	bA	813	CLA	C1D-ND	5.09	1.44	1.37
10	aB	837	CLA	C3B-C2B	5.09	1.47	1.40
10	bA	824	CLA	CHC-C1C	5.09	1.48	1.35
10	bA	854	CLA	CHC-C1C	5.09	1.48	1.35
10	bA	814	CLA	C1D-ND	5.09	1.44	1.37
10	cA	814	CLA	C1D-ND	5.09	1.44	1.37
10	cA	834	CLA	O2D-CGD	5.08	1.45	1.33
10	bB	833	CLA	C1D-ND	5.08	1.44	1.37
10	bB	806	CLA	CHC-C1C	5.08	1.48	1.35
10	bA	837	CLA	C3C-C2C	5.08	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	810	CLA	O2D-CGD	5.08	1.45	1.33
10	aA	854	CLA	CHC-C1C	5.08	1.48	1.35
10	bL	202	CLA	C3C-C2C	5.08	1.47	1.36
10	cB	818	CLA	O2D-CGD	5.08	1.45	1.33
10	cB	835	CLA	O2D-CGD	5.08	1.45	1.33
10	aB	808	CLA	O2D-CGD	5.08	1.45	1.33
10	bB	818	CLA	O2D-CGD	5.08	1.45	1.33
10	cB	833	CLA	C1D-ND	5.08	1.44	1.37
10	bA	828	CLA	C3C-C2C	5.08	1.47	1.36
10	cA	809	CLA	CHC-C1C	5.08	1.48	1.35
10	bA	820	CLA	CHC-C1C	5.08	1.48	1.35
10	cB	806	CLA	CHC-C1C	5.08	1.48	1.35
10	bA	834	CLA	O2D-CGD	5.08	1.45	1.33
10	cA	810	CLA	O2D-CGD	5.08	1.45	1.33
10	cA	814	CLA	O2D-CGD	5.08	1.45	1.33
10	aA	824	CLA	CHC-C1C	5.08	1.48	1.35
10	aA	804	CLA	C3C-C2C	5.08	1.47	1.36
10	cA	804	CLA	C3C-C2C	5.08	1.47	1.36
10	cA	837	CLA	C3C-C2C	5.08	1.47	1.36
10	aB	827	CLA	C1D-ND	5.08	1.44	1.37
10	bB	810	CLA	C3B-C2B	5.08	1.47	1.40
10	aB	802	CLA	C3C-C2C	5.08	1.47	1.36
10	cA	806	CLA	O2D-CGD	5.08	1.45	1.33
10	aA	833	CLA	C3C-C2C	5.07	1.47	1.36
10	aA	834	CLA	O2D-CGD	5.07	1.45	1.33
10	aA	816	CLA	CHC-C1C	5.07	1.48	1.35
10	cA	812	CLA	CHC-C1C	5.07	1.48	1.35
10	aA	826	CLA	C3B-C2B	5.07	1.47	1.40
10	cB	810	CLA	C3B-C2B	5.07	1.47	1.40
10	cB	804	CLA	C3C-C2C	5.07	1.47	1.36
10	bA	808	CLA	C3C-C2C	5.07	1.47	1.36
10	cA	841	CLA	C3C-C2C	5.07	1.47	1.36
10	cB	834	CLA	CHC-C1C	5.07	1.48	1.35
10	cB	808	CLA	O2D-CGD	5.07	1.45	1.33
10	bB	804	CLA	CHC-C1C	5.07	1.48	1.35
10	bB	809	CLA	C3C-C2C	5.07	1.47	1.36
10	cB	811	CLA	C3C-C2C	5.07	1.47	1.36
10	bA	830	CLA	C3B-C2B	5.06	1.47	1.40
10	aL	204	CLA	C3C-C2C	5.06	1.47	1.36
10	aB	838	CLA	CHC-C1C	5.06	1.47	1.35
10	bA	816	CLA	CHC-C1C	5.06	1.47	1.35
10	aB	818	CLA	CHC-C1C	5.06	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	809	CLA	C3C-C2C	5.06	1.47	1.36
10	bB	830	CLA	C3C-C2C	5.06	1.47	1.36
10	aA	823	CLA	C1D-ND	5.06	1.44	1.37
10	aB	812	CLA	C3B-C2B	5.06	1.47	1.40
10	aB	817	CLA	C3C-C2C	5.06	1.47	1.36
10	bB	834	CLA	CHC-C1C	5.06	1.47	1.35
10	cB	837	CLA	C3B-C2B	5.06	1.47	1.40
10	aA	841	CLA	C3C-C2C	5.06	1.47	1.36
10	cA	839	CLA	C1D-ND	5.06	1.44	1.37
10	cB	832	CLA	C1D-ND	5.06	1.44	1.37
10	aA	804	CLA	O2D-CGD	5.06	1.45	1.33
10	bA	804	CLA	O2D-CGD	5.06	1.45	1.33
10	aA	812	CLA	CHC-C1C	5.06	1.47	1.35
10	bB	818	CLA	CHC-C1C	5.06	1.47	1.35
10	bA	826	CLA	C3B-C2B	5.06	1.47	1.40
10	aA	831	CLA	C3C-C2C	5.05	1.47	1.36
10	cA	804	CLA	O2D-CGD	5.05	1.45	1.33
10	bB	811	CLA	C3C-C2C	5.05	1.47	1.36
10	aB	834	CLA	CHC-C1C	5.05	1.47	1.35
10	bB	835	CLA	O2D-CGD	5.05	1.45	1.33
10	cA	836	CLA	C3C-C2C	5.05	1.47	1.36
10	aB	831	CLA	C1D-ND	5.05	1.44	1.37
10	aB	804	CLA	CHC-C1C	5.05	1.47	1.35
10	bA	809	CLA	CHC-C1C	5.05	1.47	1.35
10	aB	804	CLA	C3C-C2C	5.05	1.47	1.36
10	cB	817	CLA	O2D-CGD	5.05	1.45	1.33
10	bL	204	CLA	C3C-C2C	5.05	1.47	1.36
10	aA	817	CLA	CHC-C1C	5.05	1.47	1.35
10	aA	820	CLA	CHC-C1C	5.05	1.47	1.35
10	cA	815	CLA	O2D-CGD	5.05	1.45	1.33
10	bA	812	CLA	CHC-C1C	5.05	1.47	1.35
10	cA	828	CLA	C3C-C2C	5.05	1.47	1.36
10	aB	817	CLA	O2D-CGD	5.05	1.45	1.33
10	bB	838	CLA	CHC-C1C	5.05	1.47	1.35
10	aA	809	CLA	CHC-C1C	5.05	1.47	1.35
10	aA	828	CLA	C3C-C2C	5.04	1.47	1.36
10	aA	803	CLA	O2D-CGD	5.04	1.45	1.33
10	aB	820	CLA	CHC-C1C	5.04	1.47	1.35
10	aA	822	CLA	CHC-C1C	5.04	1.47	1.35
10	bB	832	CLA	C1D-ND	5.04	1.44	1.37
10	bB	817	CLA	C3C-C2C	5.04	1.47	1.36
10	bB	831	CLA	CHC-C1C	5.04	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	838	CLA	CHC-C1C	5.04	1.47	1.35
10	bB	804	CLA	C3C-C2C	5.04	1.47	1.36
10	bA	822	CLA	CHC-C1C	5.04	1.47	1.35
10	bA	840	CLA	CHC-C1C	5.04	1.47	1.35
10	aA	814	CLA	C1D-ND	5.04	1.44	1.37
10	cB	837	CLA	C3C-C2C	5.04	1.47	1.36
10	aA	841	CLA	CHC-C1C	5.04	1.47	1.35
10	aA	816	CLA	O2D-CGD	5.04	1.45	1.33
10	bA	836	CLA	C3C-C2C	5.04	1.47	1.36
10	cL	204	CLA	C3C-C2C	5.04	1.47	1.36
10	aA	816	CLA	C3C-C2C	5.04	1.47	1.36
10	aB	831	CLA	CHC-C1C	5.04	1.47	1.35
10	aB	811	CLA	C3C-C2C	5.04	1.47	1.36
10	bA	838	CLA	C3C-C2C	5.04	1.47	1.36
10	cA	822	CLA	CHC-C1C	5.04	1.47	1.35
10	cB	831	CLA	CHC-C1C	5.04	1.47	1.35
10	cA	838	CLA	C3B-C2B	5.04	1.47	1.40
10	aA	836	CLA	C3C-C2C	5.04	1.47	1.36
10	bA	816	CLA	C3C-C2C	5.04	1.47	1.36
10	aB	833	CLA	O2D-CGD	5.03	1.45	1.33
10	bA	816	CLA	O2D-CGD	5.03	1.45	1.33
10	cB	820	CLA	CHC-C1C	5.03	1.47	1.35
10	cB	809	CLA	C3C-C2C	5.03	1.47	1.36
10	aB	833	CLA	C1D-ND	5.03	1.44	1.37
10	aA	838	CLA	C3B-C2B	5.03	1.47	1.40
10	cB	838	CLA	O2D-CGD	5.03	1.45	1.33
10	bA	820	CLA	O2D-CGD	5.03	1.45	1.33
10	aA	820	CLA	O2D-CGD	5.03	1.45	1.33
10	aB	837	CLA	C3C-C2C	5.03	1.47	1.36
10	bB	817	CLA	O2D-CGD	5.03	1.45	1.33
10	cB	804	CLA	CHC-C1C	5.03	1.47	1.35
10	cA	816	CLA	O2D-CGD	5.03	1.45	1.33
10	cA	820	CLA	O2D-CGD	5.03	1.45	1.33
10	bB	837	CLA	C3C-C2C	5.03	1.47	1.36
10	bA	816	CLA	C1D-ND	5.03	1.44	1.37
10	cA	840	CLA	CHC-C1C	5.03	1.47	1.35
10	cB	808	CLA	C3C-C2C	5.03	1.47	1.36
10	aA	815	CLA	O2D-CGD	5.03	1.45	1.33
10	cB	831	CLA	C1D-ND	5.03	1.44	1.37
10	aB	820	CLA	O2D-CGD	5.03	1.45	1.33
10	cA	841	CLA	CHC-C1C	5.03	1.47	1.35
10	aA	840	CLA	CHC-C1C	5.02	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	816	CLA	C3C-C2C	5.02	1.47	1.36
10	bB	817	CLA	C1D-ND	5.02	1.44	1.37
10	bA	815	CLA	O2D-CGD	5.02	1.45	1.33
10	cA	841	CLA	O2D-CGD	5.02	1.45	1.33
10	bB	814	CLA	C3C-C2C	5.02	1.47	1.36
10	bA	803	CLA	O2D-CGD	5.02	1.45	1.33
10	aA	819	CLA	CHC-C1C	5.02	1.47	1.35
10	cA	815	CLA	C1D-ND	5.02	1.44	1.37
10	bB	833	CLA	O2D-CGD	5.02	1.45	1.33
10	aA	818	CLA	CHC-C1C	5.02	1.47	1.35
10	cB	814	CLA	C3C-C2C	5.02	1.47	1.36
10	cB	818	CLA	CHC-C1C	5.02	1.47	1.35
10	cA	803	CLA	O2D-CGD	5.02	1.45	1.33
10	bA	819	CLA	CHC-C1C	5.02	1.47	1.35
10	bA	841	CLA	C3C-C2C	5.02	1.47	1.36
10	bA	817	CLA	CHC-C1C	5.02	1.47	1.35
10	bA	841	CLA	CHC-C1C	5.02	1.47	1.35
10	bA	815	CLA	C1D-ND	5.02	1.44	1.37
10	bB	816	CLA	CHC-C1C	5.02	1.47	1.35
10	bB	808	CLA	C3C-C2C	5.02	1.47	1.36
10	cB	803	CLA	C3C-C2C	5.02	1.47	1.36
10	bB	841	CLA	C3C-C2C	5.02	1.47	1.36
10	cB	817	CLA	C3C-C2C	5.01	1.47	1.36
10	aA	830	CLA	C3B-C2B	5.01	1.47	1.40
10	bA	817	CLA	O2D-CGD	5.01	1.45	1.33
10	bA	841	CLA	O2D-CGD	5.01	1.45	1.33
10	cB	833	CLA	O2D-CGD	5.01	1.45	1.33
10	bA	818	CLA	CHC-C1C	5.01	1.47	1.35
10	bB	803	CLA	C3C-C2C	5.01	1.47	1.36
10	aA	823	CLA	O2D-CGD	5.01	1.45	1.33
10	cA	816	CLA	C1D-ND	5.01	1.43	1.37
10	cA	811	CLA	CHC-C1C	5.01	1.47	1.35
10	aB	830	CLA	C3C-C2C	5.01	1.47	1.36
10	aB	808	CLA	C3C-C2C	5.01	1.47	1.36
10	bB	838	CLA	O2D-CGD	5.01	1.45	1.33
10	bB	820	CLA	O2D-CGD	5.01	1.45	1.33
10	aB	821	CLA	O2D-CGD	5.01	1.45	1.33
10	cA	817	CLA	O2D-CGD	5.01	1.45	1.33
10	bA	811	CLA	CHC-C1C	5.01	1.47	1.35
10	bB	840	CLA	O2D-CGD	5.00	1.45	1.33
10	bA	806	CLA	C1D-ND	5.00	1.43	1.37
10	aA	811	CLA	CHC-C1C	5.00	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	833	CLA	CHC-C1C	5.00	1.47	1.35
10	bB	820	CLA	CHC-C1C	5.00	1.47	1.35
10	aB	828	CLA	C3C-C2C	5.00	1.47	1.36
10	aA	815	CLA	C1D-ND	5.00	1.43	1.37
10	cA	823	CLA	O2D-CGD	5.00	1.45	1.33
10	cA	819	CLA	CHC-C1C	5.00	1.47	1.35
10	aB	814	CLA	C3C-C2C	5.00	1.47	1.36
10	aL	204	CLA	CHC-C1C	4.99	1.47	1.35
10	cA	821	CLA	CHC-C1C	4.99	1.47	1.35
10	bA	838	CLA	C3B-C2B	4.99	1.47	1.40
10	cB	813	CLA	CHC-C1C	4.99	1.47	1.35
10	bB	833	CLA	CHC-C1C	4.99	1.47	1.35
10	aB	824	CLA	O2D-CGD	4.99	1.45	1.33
10	aA	821	CLA	CHC-C1C	4.99	1.47	1.35
10	aB	803	CLA	C3C-C2C	4.99	1.47	1.36
10	bB	824	CLA	O2D-CGD	4.99	1.45	1.33
10	aA	817	CLA	O2D-CGD	4.99	1.45	1.33
10	bB	821	CLA	O2D-CGD	4.99	1.45	1.33
10	bA	821	CLA	CHC-C1C	4.99	1.47	1.35
10	cA	817	CLA	CHC-C1C	4.99	1.47	1.35
10	cB	830	CLA	C3C-C2C	4.99	1.47	1.36
10	cA	818	CLA	CHC-C1C	4.99	1.47	1.35
10	bB	828	CLA	C3C-C2C	4.99	1.47	1.36
10	cB	816	CLA	CHC-C1C	4.99	1.47	1.35
10	cB	841	CLA	C3C-C2C	4.98	1.47	1.36
10	bA	842	CLA	O2D-CGD	4.98	1.45	1.33
10	aB	841	CLA	C3C-C2C	4.98	1.47	1.36
10	aL	203	CLA	CHC-C1C	4.98	1.47	1.35
10	aA	838	CLA	C3C-C2C	4.98	1.47	1.36
10	cA	813	CLA	CHC-C1C	4.98	1.47	1.35
10	aA	822	CLA	O2D-CGD	4.98	1.45	1.33
9	cA	801	CL0	C3C-C2C	4.98	1.47	1.36
10	bA	822	CLA	O2D-CGD	4.98	1.45	1.33
10	bL	203	CLA	CHC-C1C	4.98	1.47	1.35
10	bL	204	CLA	CHC-C1C	4.98	1.47	1.35
10	bA	823	CLA	O2D-CGD	4.98	1.45	1.33
10	cL	204	CLA	CHC-C1C	4.98	1.47	1.35
10	cA	854	CLA	C1D-ND	4.98	1.43	1.37
10	aB	840	CLA	O2D-CGD	4.98	1.45	1.33
10	cB	817	CLA	C1D-ND	4.98	1.43	1.37
10	aA	841	CLA	O2D-CGD	4.98	1.45	1.33
10	cA	828	CLA	O2D-CGD	4.98	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	821	CLA	O2D-CGD	4.97	1.45	1.33
10	aB	816	CLA	C1D-ND	4.97	1.43	1.37
10	bB	813	CLA	CHC-C1C	4.97	1.47	1.35
10	aA	819	CLA	O2D-CGD	4.97	1.45	1.33
9	bA	801	CL0	C3C-C2C	4.97	1.47	1.36
10	bA	815	CLA	CHC-C1C	4.97	1.47	1.35
10	bB	831	CLA	C1D-ND	4.97	1.43	1.37
10	aB	808	CLA	CHC-C1C	4.97	1.47	1.35
10	aB	812	CLA	O2D-CGD	4.97	1.45	1.33
10	cB	825	CLA	CHC-C1C	4.97	1.47	1.35
10	bA	811	CLA	O2D-CGD	4.97	1.45	1.33
10	aB	816	CLA	CHC-C1C	4.97	1.47	1.35
10	cB	820	CLA	C3B-C2B	4.97	1.47	1.40
10	bB	816	CLA	C1D-ND	4.97	1.43	1.37
10	cB	836	CLA	CHC-C1C	4.97	1.47	1.35
10	aA	816	CLA	C1D-ND	4.97	1.43	1.37
10	cB	840	CLA	O2D-CGD	4.97	1.45	1.33
10	aA	842	CLA	O2D-CGD	4.97	1.45	1.33
10	aB	813	CLA	O2D-CGD	4.97	1.45	1.33
10	cB	829	CLA	O2D-CGD	4.97	1.45	1.33
10	bB	825	CLA	CHC-C1C	4.97	1.47	1.35
10	bA	828	CLA	CHC-C1C	4.96	1.47	1.35
10	aB	838	CLA	O2D-CGD	4.96	1.45	1.33
10	bB	836	CLA	CHC-C1C	4.96	1.47	1.35
10	cA	838	CLA	C3C-C2C	4.96	1.47	1.36
10	aA	811	CLA	O2D-CGD	4.96	1.45	1.33
10	cA	827	CLA	O2D-CGD	4.96	1.45	1.33
10	aA	827	CLA	O2D-CGD	4.96	1.45	1.33
10	bA	804	CLA	CHC-C1C	4.96	1.47	1.35
10	cB	828	CLA	C3C-C2C	4.96	1.47	1.36
10	bA	828	CLA	O2D-CGD	4.96	1.45	1.33
10	aB	836	CLA	CHC-C1C	4.96	1.47	1.35
10	aB	806	CLA	C3C-C2C	4.96	1.47	1.36
10	cB	815	CLA	CHC-C1C	4.96	1.47	1.35
10	bB	820	CLA	C3B-C2B	4.96	1.47	1.40
10	cA	819	CLA	O2D-CGD	4.96	1.45	1.33
10	aB	813	CLA	CHC-C1C	4.96	1.47	1.35
10	aA	813	CLA	CHC-C1C	4.96	1.47	1.35
10	bA	809	CLA	C1D-ND	4.96	1.43	1.37
10	bA	826	CLA	O2D-CGD	4.96	1.45	1.33
10	cA	842	CLA	O2D-CGD	4.96	1.45	1.33
10	cB	833	CLA	CHC-C1C	4.96	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	812	CLA	O2D-CGD	4.96	1.45	1.33
10	bB	823	CLA	CHC-C1C	4.95	1.47	1.35
10	cL	203	CLA	CHC-C1C	4.95	1.47	1.35
10	aA	827	CLA	CHC-C1C	4.95	1.47	1.35
10	aA	828	CLA	O2D-CGD	4.95	1.45	1.33
10	bA	810	CLA	CHC-C1C	4.95	1.47	1.35
10	cB	828	CLA	O2D-CGD	4.95	1.45	1.33
10	cA	811	CLA	O2D-CGD	4.95	1.45	1.33
10	cA	828	CLA	CHC-C1C	4.95	1.47	1.35
10	bA	827	CLA	O2D-CGD	4.95	1.45	1.33
10	cB	824	CLA	O2D-CGD	4.95	1.45	1.33
9	aA	801	CL0	C3C-C2C	4.95	1.47	1.36
10	aA	856	CLA	CHC-C1C	4.95	1.47	1.35
10	aA	804	CLA	CHC-C1C	4.95	1.47	1.35
10	cA	856	CLA	CHC-C1C	4.95	1.47	1.35
10	aA	828	CLA	CHC-C1C	4.95	1.47	1.35
10	aB	815	CLA	CHC-C1C	4.95	1.47	1.35
10	bA	819	CLA	O2D-CGD	4.95	1.45	1.33
10	aA	854	CLA	C1D-ND	4.95	1.43	1.37
10	bB	806	CLA	C3C-C2C	4.94	1.47	1.36
10	bB	840	CLA	C3C-C2C	4.94	1.47	1.36
10	bB	811	CLA	O2D-CGD	4.94	1.45	1.33
10	bB	808	CLA	CHC-C1C	4.94	1.47	1.35
10	cA	809	CLA	C1D-ND	4.94	1.43	1.37
10	cA	810	CLA	CHC-C1C	4.94	1.47	1.35
10	aA	815	CLA	CHC-C1C	4.94	1.47	1.35
10	bA	854	CLA	C1D-ND	4.94	1.43	1.37
10	aB	829	CLA	O2D-CGD	4.94	1.45	1.33
10	cA	840	CLA	C1D-ND	4.94	1.43	1.37
10	bB	815	CLA	CHC-C1C	4.94	1.47	1.35
10	bB	832	CLA	CHC-C1C	4.94	1.47	1.35
10	aA	817	CLA	C1D-ND	4.94	1.43	1.37
10	aA	840	CLA	C1D-ND	4.94	1.43	1.37
10	cB	811	CLA	C3B-C2B	4.94	1.47	1.40
10	cA	827	CLA	CHC-C1C	4.94	1.47	1.35
10	aB	825	CLA	CHC-C1C	4.94	1.47	1.35
10	aA	810	CLA	CHC-C1C	4.94	1.47	1.35
10	aB	820	CLA	C3B-C2B	4.94	1.47	1.40
10	bB	819	CLA	O2D-CGD	4.93	1.45	1.33
10	cB	827	CLA	O2D-CGD	4.93	1.45	1.33
10	aB	827	CLA	O2D-CGD	4.93	1.45	1.33
10	bA	839	CLA	CHC-C1C	4.93	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	827	CLA	CHC-C1C	4.93	1.47	1.35
10	cA	815	CLA	CHC-C1C	4.93	1.47	1.35
10	aB	823	CLA	CHC-C1C	4.93	1.47	1.35
10	cA	839	CLA	CHC-C1C	4.93	1.47	1.35
10	bB	828	CLA	O2D-CGD	4.93	1.45	1.33
10	bA	856	CLA	CHC-C1C	4.93	1.47	1.35
10	cB	811	CLA	O2D-CGD	4.93	1.45	1.33
10	cB	812	CLA	O2D-CGD	4.93	1.45	1.33
10	bB	829	CLA	O2D-CGD	4.93	1.45	1.33
10	cB	813	CLA	O2D-CGD	4.93	1.45	1.33
10	aA	805	CLA	C1D-ND	4.93	1.43	1.37
10	aA	802	CLA	CHC-C1C	4.93	1.47	1.35
10	cB	808	CLA	CHC-C1C	4.93	1.47	1.35
10	bL	205	CLA	CHC-C1C	4.93	1.47	1.35
10	aA	839	CLA	CHC-C1C	4.92	1.47	1.35
10	cB	819	CLA	O2D-CGD	4.92	1.45	1.33
10	cB	823	CLA	CHC-C1C	4.92	1.47	1.35
10	bA	813	CLA	CHC-C1C	4.92	1.47	1.35
10	aB	801	CLA	C3C-C2C	4.92	1.47	1.36
10	cB	840	CLA	C3C-C2C	4.92	1.47	1.36
10	aA	809	CLA	C1D-ND	4.92	1.43	1.37
10	aA	812	CLA	C1D-ND	4.92	1.43	1.37
10	bB	811	CLA	C3B-C2B	4.92	1.47	1.40
10	cB	806	CLA	C3C-C2C	4.92	1.47	1.36
10	cB	803	CLA	CHC-C1C	4.92	1.47	1.35
10	aA	807	CLA	CHC-C1C	4.92	1.47	1.35
10	cA	817	CLA	C1D-ND	4.92	1.43	1.37
10	bA	840	CLA	C1D-ND	4.92	1.43	1.37
10	aB	811	CLA	O2D-CGD	4.92	1.45	1.33
10	aB	819	CLA	O2D-CGD	4.92	1.45	1.33
10	aA	835	CLA	CHC-C1C	4.92	1.47	1.35
10	cA	822	CLA	O2D-CGD	4.92	1.45	1.33
10	bB	809	CLA	CHC-C1C	4.92	1.47	1.35
10	aB	840	CLA	C3C-C2C	4.92	1.47	1.36
10	cA	826	CLA	O2D-CGD	4.92	1.45	1.33
10	bA	835	CLA	CHC-C1C	4.92	1.47	1.35
10	cA	804	CLA	CHC-C1C	4.92	1.47	1.35
10	aB	828	CLA	O2D-CGD	4.92	1.45	1.33
10	aA	818	CLA	O2D-CGD	4.92	1.45	1.33
10	cB	832	CLA	CHC-C1C	4.92	1.47	1.35
10	bA	802	CLA	CHC-C1C	4.92	1.47	1.35
10	bB	803	CLA	CHC-C1C	4.92	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aL	205	CLA	CHC-C1C	4.91	1.47	1.35
10	aA	806	CLA	C1D-ND	4.91	1.43	1.37
10	bA	807	CLA	CHC-C1C	4.91	1.47	1.35
10	bB	827	CLA	O2D-CGD	4.91	1.45	1.33
10	cA	835	CLA	CHC-C1C	4.91	1.47	1.35
10	bB	813	CLA	O2D-CGD	4.91	1.45	1.33
10	bA	807	CLA	O2D-CGD	4.91	1.45	1.33
10	cA	813	CLA	O2D-CGD	4.91	1.45	1.33
10	cB	809	CLA	CHC-C1C	4.91	1.47	1.35
10	cA	807	CLA	O2D-CGD	4.91	1.45	1.33
10	cA	834	CLA	C3B-C2B	4.91	1.47	1.40
10	cA	814	CLA	CHC-C1C	4.91	1.47	1.35
10	cB	816	CLA	C1D-ND	4.91	1.43	1.37
10	cL	205	CLA	CHC-C1C	4.91	1.47	1.35
10	bB	801	CLA	C3C-C2C	4.91	1.47	1.36
10	bB	824	CLA	CHC-C1C	4.91	1.47	1.35
10	aB	809	CLA	CHC-C1C	4.90	1.47	1.35
10	bB	840	CLA	CHC-C1C	4.90	1.47	1.35
10	cB	801	CLA	C3C-C2C	4.90	1.47	1.36
10	aB	832	CLA	CHC-C1C	4.90	1.47	1.35
10	bA	817	CLA	C1D-ND	4.90	1.43	1.37
10	aA	826	CLA	O2D-CGD	4.90	1.45	1.33
10	bB	821	CLA	CHC-C1C	4.90	1.47	1.35
10	cA	802	CLA	CHC-C1C	4.90	1.47	1.35
10	aB	803	CLA	CHC-C1C	4.90	1.47	1.35
10	bA	842	CLA	C3C-C2C	4.90	1.47	1.36
10	cA	826	CLA	C1D-ND	4.90	1.43	1.37
10	cA	830	CLA	CHC-C1C	4.90	1.47	1.35
10	bA	818	CLA	O2D-CGD	4.90	1.45	1.33
10	cB	834	CLA	C1D-ND	4.89	1.43	1.37
10	cB	827	CLA	CHC-C1C	4.89	1.47	1.35
10	aA	808	CLA	CHC-C1C	4.89	1.47	1.35
10	bA	813	CLA	O2D-CGD	4.89	1.45	1.33
10	cB	821	CLA	CHC-C1C	4.89	1.47	1.35
10	cA	807	CLA	CHC-C1C	4.89	1.47	1.35
10	bA	808	CLA	CHC-C1C	4.89	1.47	1.35
10	cA	824	CLA	O2D-CGD	4.89	1.45	1.33
10	cA	808	CLA	CHC-C1C	4.89	1.47	1.35
10	aB	802	CLA	O2D-CGD	4.89	1.45	1.33
10	aB	834	CLA	C1D-ND	4.89	1.43	1.37
10	cA	818	CLA	O2D-CGD	4.89	1.45	1.33
10	aA	813	CLA	O2D-CGD	4.89	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	825	CLA	C3C-C2C	4.89	1.47	1.36
10	bB	837	CLA	O2D-CGD	4.89	1.45	1.33
10	bB	834	CLA	C1D-ND	4.89	1.43	1.37
10	aB	824	CLA	CHC-C1C	4.89	1.47	1.35
10	cB	802	CLA	O2D-CGD	4.89	1.45	1.33
10	cB	837	CLA	O2D-CGD	4.89	1.45	1.33
10	cB	824	CLA	CHC-C1C	4.89	1.47	1.35
10	bA	814	CLA	CHC-C1C	4.88	1.47	1.35
10	aA	842	CLA	C3C-C2C	4.88	1.47	1.36
10	bB	818	CLA	C1D-ND	4.88	1.43	1.37
10	cB	807	CLA	O2D-CGD	4.88	1.45	1.33
10	aB	811	CLA	C3B-C2B	4.88	1.47	1.40
10	aA	831	CLA	CHC-C1C	4.88	1.47	1.35
10	cB	840	CLA	CHC-C1C	4.88	1.47	1.35
10	aA	807	CLA	O2D-CGD	4.88	1.45	1.33
10	bB	814	CLA	C1D-ND	4.88	1.43	1.37
10	aB	827	CLA	CHC-C1C	4.88	1.47	1.35
10	bB	802	CLA	O2D-CGD	4.88	1.45	1.33
10	aA	824	CLA	O2D-CGD	4.88	1.45	1.33
10	cA	805	CLA	C1D-ND	4.88	1.43	1.37
10	aB	802	CLA	CHC-C1C	4.87	1.47	1.35
10	cA	808	CLA	O2D-CGD	4.87	1.45	1.33
10	aA	826	CLA	C1D-ND	4.87	1.43	1.37
10	cA	812	CLA	C1D-ND	4.87	1.43	1.37
10	aA	843	CLA	CHC-C1C	4.87	1.47	1.35
10	aB	825	CLA	C3C-C2C	4.87	1.47	1.36
10	cB	812	CLA	CHC-C1C	4.87	1.47	1.35
10	bA	824	CLA	O2D-CGD	4.87	1.45	1.33
10	cB	820	CLA	C1D-ND	4.87	1.43	1.37
10	aL	203	CLA	O2D-CGD	4.87	1.45	1.33
10	bB	825	CLA	C3C-C2C	4.87	1.47	1.36
10	bA	841	CLA	C1D-ND	4.87	1.43	1.37
10	cA	842	CLA	C3C-C2C	4.87	1.47	1.36
10	bB	802	CLA	CHC-C1C	4.87	1.47	1.35
10	aB	821	CLA	CHC-C1C	4.87	1.47	1.35
10	aA	805	CLA	CHC-C1C	4.86	1.47	1.35
10	cA	806	CLA	C1D-ND	4.86	1.43	1.37
10	aB	839	CLA	CHC-C1C	4.86	1.47	1.35
10	aB	840	CLA	CHC-C1C	4.86	1.47	1.35
10	cB	802	CLA	CHC-C1C	4.86	1.47	1.35
10	bA	805	CLA	C1D-ND	4.86	1.43	1.37
10	bA	843	CLA	CHC-C1C	4.86	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	812	CLA	C1D-ND	4.86	1.43	1.37
10	cB	825	CLA	O2D-CGD	4.86	1.45	1.33
10	cA	805	CLA	O2D-CGD	4.86	1.45	1.33
10	cA	835	CLA	O2D-CGD	4.86	1.45	1.33
10	cB	839	CLA	O2D-CGD	4.86	1.45	1.33
10	bB	813	CLA	C1D-ND	4.86	1.43	1.37
10	bA	832	CLA	CHC-C1C	4.86	1.47	1.35
10	bA	835	CLA	O2D-CGD	4.86	1.45	1.33
10	cA	843	CLA	CHC-C1C	4.86	1.47	1.35
10	aA	835	CLA	O2D-CGD	4.86	1.45	1.33
10	bB	807	CLA	O2D-CGD	4.85	1.45	1.33
10	bB	839	CLA	CHC-C1C	4.85	1.47	1.35
10	aA	830	CLA	CHC-C1C	4.85	1.47	1.35
10	bB	827	CLA	CHC-C1C	4.85	1.47	1.35
10	aB	818	CLA	C1D-ND	4.85	1.43	1.37
10	bA	812	CLA	C1D-ND	4.85	1.43	1.37
10	cB	816	CLA	O2D-CGD	4.85	1.45	1.33
10	cB	839	CLA	CHC-C1C	4.85	1.47	1.35
10	aA	814	CLA	CHC-C1C	4.85	1.47	1.35
10	bA	805	CLA	CHC-C1C	4.85	1.47	1.35
10	bB	825	CLA	O2D-CGD	4.85	1.45	1.33
10	bB	812	CLA	C1D-ND	4.85	1.43	1.37
10	aB	825	CLA	O2D-CGD	4.85	1.45	1.33
10	cA	831	CLA	CHC-C1C	4.85	1.47	1.35
10	aB	807	CLA	O2D-CGD	4.85	1.45	1.33
10	bB	812	CLA	CHC-C1C	4.85	1.47	1.35
10	aA	805	CLA	O2D-CGD	4.85	1.45	1.33
10	cA	831	CLA	O2D-CGD	4.84	1.45	1.33
10	bA	808	CLA	O2D-CGD	4.84	1.45	1.33
10	cB	817	CLA	CHC-C1C	4.84	1.47	1.35
10	aB	810	CLA	C3C-C2C	4.84	1.47	1.36
10	aB	837	CLA	O2D-CGD	4.84	1.45	1.33
10	bA	831	CLA	O2D-CGD	4.84	1.45	1.33
10	aB	812	CLA	C1D-ND	4.84	1.43	1.37
10	aB	839	CLA	O2D-CGD	4.84	1.45	1.33
10	bA	830	CLA	CHC-C1C	4.84	1.47	1.35
10	aA	808	CLA	O2D-CGD	4.84	1.45	1.33
10	aB	812	CLA	CHC-C1C	4.84	1.47	1.35
10	cB	810	CLA	C3C-C2C	4.84	1.47	1.36
10	bB	820	CLA	C1D-ND	4.84	1.43	1.37
10	aA	831	CLA	O2D-CGD	4.83	1.45	1.33
10	aA	832	CLA	CHC-C1C	4.83	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	814	CLA	CHC-C1C	4.83	1.47	1.35
10	bB	817	CLA	CHC-C1C	4.83	1.47	1.35
10	aB	817	CLA	CHC-C1C	4.83	1.47	1.35
10	cA	805	CLA	CHC-C1C	4.83	1.47	1.35
10	bB	841	CLA	O2D-CGD	4.83	1.45	1.33
10	bA	826	CLA	C1D-ND	4.83	1.43	1.37
10	bB	816	CLA	O2D-CGD	4.83	1.45	1.33
10	aB	816	CLA	O2D-CGD	4.83	1.45	1.33
10	cA	841	CLA	C1D-ND	4.83	1.43	1.37
10	bA	838	CLA	CHC-C1C	4.83	1.47	1.35
10	cL	203	CLA	O2D-CGD	4.83	1.45	1.33
10	cA	832	CLA	CHC-C1C	4.83	1.47	1.35
10	bB	839	CLA	O2D-CGD	4.83	1.45	1.33
10	aB	810	CLA	O2D-CGD	4.82	1.45	1.33
10	aB	841	CLA	O2D-CGD	4.82	1.45	1.33
10	bL	203	CLA	O2D-CGD	4.82	1.45	1.33
10	bA	822	CLA	C1D-ND	4.82	1.43	1.37
10	bA	837	CLA	CHC-C1C	4.82	1.47	1.35
10	cA	838	CLA	CHC-C1C	4.82	1.47	1.35
10	cB	818	CLA	C1D-ND	4.82	1.43	1.37
11	cA	844	PQN	C10-C5	4.82	1.48	1.40
10	bA	833	CLA	CHC-C1C	4.82	1.47	1.35
10	aA	834	CLA	C3B-C2B	4.82	1.47	1.40
10	aB	826	CLA	C1D-ND	4.82	1.43	1.37
10	bA	831	CLA	CHC-C1C	4.81	1.47	1.35
10	aB	838	CLA	C1D-ND	4.81	1.43	1.37
10	aA	833	CLA	CHC-C1C	4.81	1.47	1.35
11	bA	844	PQN	C10-C5	4.81	1.48	1.40
10	bB	810	CLA	O2D-CGD	4.81	1.44	1.33
10	bB	810	CLA	C3C-C2C	4.81	1.46	1.36
10	aA	818	CLA	C1D-ND	4.81	1.43	1.37
10	cB	837	CLA	CHC-C1C	4.81	1.47	1.35
9	bA	801	CL0	O2D-CGD	4.80	1.44	1.33
10	bA	805	CLA	O2D-CGD	4.80	1.44	1.33
10	cB	819	CLA	C3C-C2C	4.80	1.46	1.36
10	aA	838	CLA	CHC-C1C	4.80	1.47	1.35
10	bL	204	CLA	O2D-CGD	4.80	1.44	1.33
10	bB	828	CLA	CHC-C1C	4.80	1.47	1.35
10	bA	834	CLA	C3B-C2B	4.80	1.47	1.40
10	cA	822	CLA	C1D-ND	4.80	1.43	1.37
10	aB	813	CLA	C1D-ND	4.80	1.43	1.37
10	cA	811	CLA	C1D-ND	4.80	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	841	CLA	O2D-CGD	4.80	1.44	1.33
10	cB	826	CLA	C1D-ND	4.80	1.43	1.37
10	aB	807	CLA	CHC-C1C	4.80	1.47	1.35
10	cB	829	CLA	CHC-C1C	4.80	1.47	1.35
10	aB	828	CLA	CHC-C1C	4.80	1.47	1.35
10	aA	837	CLA	CHC-C1C	4.80	1.47	1.35
9	cA	801	CL0	O2D-CGD	4.80	1.44	1.33
10	bB	807	CLA	CHC-C1C	4.80	1.47	1.35
10	bB	830	CLA	O2D-CGD	4.80	1.44	1.33
10	aB	820	CLA	C1D-ND	4.79	1.43	1.37
10	bA	829	CLA	CHC-C1C	4.79	1.47	1.35
9	aA	801	CL0	O2D-CGD	4.79	1.44	1.33
10	aL	204	CLA	O2D-CGD	4.79	1.44	1.33
10	cB	830	CLA	O2D-CGD	4.79	1.44	1.33
10	aA	811	CLA	C1D-ND	4.79	1.43	1.37
10	aB	814	CLA	C1D-ND	4.79	1.43	1.37
10	cB	810	CLA	O2D-CGD	4.79	1.44	1.33
10	cB	814	CLA	CHC-C1C	4.79	1.47	1.35
10	aB	815	CLA	O2D-CGD	4.79	1.44	1.33
10	aB	819	CLA	C3C-C2C	4.79	1.46	1.36
10	aA	822	CLA	C1D-ND	4.79	1.43	1.37
10	aB	806	CLA	C1D-ND	4.79	1.43	1.37
10	bA	811	CLA	C1D-ND	4.79	1.43	1.37
10	bB	806	CLA	C1D-ND	4.79	1.43	1.37
10	bB	808	CLA	C1D-ND	4.79	1.43	1.37
10	aB	837	CLA	CHC-C1C	4.79	1.47	1.35
10	bA	821	CLA	C1D-ND	4.78	1.43	1.37
10	cA	837	CLA	O2D-CGD	4.78	1.44	1.33
10	cB	815	CLA	O2D-CGD	4.78	1.44	1.33
10	cA	833	CLA	CHC-C1C	4.78	1.47	1.35
10	aA	841	CLA	C1D-ND	4.78	1.43	1.37
10	aB	805	CLA	CHC-C1C	4.78	1.47	1.35
10	cB	807	CLA	CHC-C1C	4.78	1.47	1.35
11	aA	844	PQN	C10-C5	4.78	1.48	1.40
10	cB	828	CLA	CHC-C1C	4.78	1.47	1.35
10	bB	814	CLA	CHC-C1C	4.78	1.47	1.35
10	aB	829	CLA	CHC-C1C	4.78	1.47	1.35
10	cA	818	CLA	C1D-ND	4.78	1.43	1.37
10	cB	814	CLA	C1D-ND	4.78	1.43	1.37
10	cB	821	CLA	C1D-ND	4.78	1.43	1.37
10	cB	838	CLA	C1D-ND	4.78	1.43	1.37
10	bB	829	CLA	CHC-C1C	4.78	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	809	CLA	O2D-CGD	4.78	1.44	1.33
10	cL	204	CLA	O2D-CGD	4.78	1.44	1.33
10	bB	819	CLA	C3C-C2C	4.78	1.46	1.36
10	cA	837	CLA	CHC-C1C	4.78	1.47	1.35
10	cB	813	CLA	C1D-ND	4.77	1.43	1.37
10	bB	826	CLA	C1D-ND	4.77	1.43	1.37
10	bB	837	CLA	CHC-C1C	4.77	1.47	1.35
10	cA	819	CLA	C1D-ND	4.77	1.43	1.37
10	cB	825	CLA	C1D-ND	4.77	1.43	1.37
10	cA	829	CLA	CHC-C1C	4.77	1.47	1.35
10	bA	837	CLA	O2D-CGD	4.77	1.44	1.33
10	bB	805	CLA	CHC-C1C	4.77	1.47	1.35
10	cL	205	CLA	O2D-CGD	4.77	1.44	1.33
10	aA	819	CLA	C1D-ND	4.77	1.43	1.37
10	aB	830	CLA	O2D-CGD	4.76	1.44	1.33
10	bB	815	CLA	O2D-CGD	4.76	1.44	1.33
10	aA	829	CLA	CHC-C1C	4.76	1.47	1.35
10	bA	825	CLA	O2D-CGD	4.76	1.44	1.33
10	cB	801	CLA	CHC-C1C	4.76	1.47	1.35
10	cB	809	CLA	O2D-CGD	4.76	1.44	1.33
10	bB	838	CLA	C1D-ND	4.76	1.43	1.37
10	cA	838	CLA	O2D-CGD	4.76	1.44	1.33
10	bA	834	CLA	CHC-C1C	4.76	1.47	1.35
10	cB	805	CLA	CHC-C1C	4.76	1.47	1.35
10	aA	837	CLA	O2D-CGD	4.76	1.44	1.33
10	bB	809	CLA	O2D-CGD	4.76	1.44	1.33
10	cA	829	CLA	O2D-CGD	4.75	1.44	1.33
10	aL	205	CLA	O2D-CGD	4.75	1.44	1.33
10	cB	806	CLA	C1D-ND	4.75	1.43	1.37
10	bB	825	CLA	C1D-ND	4.75	1.43	1.37
10	aB	801	CLA	CHC-C1C	4.75	1.47	1.35
10	bA	829	CLA	O2D-CGD	4.75	1.44	1.33
10	aA	825	CLA	O2D-CGD	4.74	1.44	1.33
10	bB	830	CLA	CHC-C1C	4.74	1.47	1.35
10	aB	830	CLA	CHC-C1C	4.74	1.47	1.35
10	bA	819	CLA	C1D-ND	4.74	1.43	1.37
10	cA	832	CLA	O2D-CGD	4.74	1.44	1.33
10	cA	834	CLA	CHC-C1C	4.74	1.47	1.35
10	bB	826	CLA	O2D-CGD	4.74	1.44	1.33
10	cB	814	CLA	O2D-CGD	4.74	1.44	1.33
10	cB	830	CLA	CHC-C1C	4.73	1.47	1.35
10	bL	205	CLA	O2D-CGD	4.73	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	826	CLA	O2D-CGD	4.73	1.44	1.33
10	bB	801	CLA	CHC-C1C	4.73	1.47	1.35
10	aB	821	CLA	C1D-ND	4.73	1.43	1.37
10	aA	812	CLA	O2D-CGD	4.73	1.44	1.33
10	aB	832	CLA	O2D-CGD	4.73	1.44	1.33
10	cB	832	CLA	O2D-CGD	4.73	1.44	1.33
10	bA	807	CLA	C1D-ND	4.73	1.43	1.37
10	aB	814	CLA	O2D-CGD	4.73	1.44	1.33
10	aB	839	CLA	C1D-ND	4.73	1.43	1.37
10	bL	203	CLA	C1D-ND	4.73	1.43	1.37
10	aB	826	CLA	O2D-CGD	4.72	1.44	1.33
10	aA	838	CLA	O2D-CGD	4.72	1.44	1.33
10	aA	834	CLA	CHC-C1C	4.72	1.47	1.35
10	bA	827	CLA	C1D-ND	4.72	1.43	1.37
10	aA	829	CLA	O2D-CGD	4.72	1.44	1.33
10	cL	203	CLA	C1D-ND	4.72	1.43	1.37
10	bA	823	CLA	CHC-C1C	4.72	1.47	1.35
10	bA	812	CLA	O2D-CGD	4.72	1.44	1.33
10	cA	825	CLA	O2D-CGD	4.72	1.44	1.33
10	aA	832	CLA	O2D-CGD	4.72	1.44	1.33
10	aA	821	CLA	C1D-ND	4.71	1.43	1.37
10	bA	838	CLA	O2D-CGD	4.71	1.44	1.33
10	bB	832	CLA	O2D-CGD	4.71	1.44	1.33
10	bB	834	CLA	O2D-CGD	4.71	1.44	1.33
10	cB	808	CLA	C1D-ND	4.71	1.43	1.37
10	aB	808	CLA	C1D-ND	4.70	1.43	1.37
10	cA	833	CLA	C1D-ND	4.70	1.43	1.37
10	aB	825	CLA	C1D-ND	4.70	1.43	1.37
10	aA	807	CLA	C1D-ND	4.70	1.43	1.37
10	cA	812	CLA	O2D-CGD	4.70	1.44	1.33
10	bB	814	CLA	O2D-CGD	4.70	1.44	1.33
10	cA	823	CLA	CHC-C1C	4.70	1.47	1.35
10	bB	806	CLA	O2D-CGD	4.70	1.44	1.33
10	aB	806	CLA	O2D-CGD	4.70	1.44	1.33
10	bA	818	CLA	C1D-ND	4.70	1.43	1.37
10	aB	805	CLA	C3C-C2C	4.70	1.46	1.36
10	aA	827	CLA	C1D-ND	4.69	1.43	1.37
10	cA	807	CLA	C1D-ND	4.69	1.43	1.37
10	aA	823	CLA	CHC-C1C	4.69	1.47	1.35
10	cA	821	CLA	C1D-ND	4.69	1.43	1.37
10	cB	806	CLA	O2D-CGD	4.69	1.44	1.33
10	cB	839	CLA	C1D-ND	4.69	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aL	203	CLA	C1D-ND	4.68	1.43	1.37
10	cA	827	CLA	C1D-ND	4.68	1.43	1.37
10	bB	839	CLA	C1D-ND	4.68	1.43	1.37
10	aB	834	CLA	O2D-CGD	4.68	1.44	1.33
10	cB	805	CLA	C3C-C2C	4.68	1.46	1.36
10	aA	833	CLA	C1D-ND	4.68	1.43	1.37
10	bA	832	CLA	O2D-CGD	4.68	1.44	1.33
10	bB	821	CLA	C1D-ND	4.67	1.43	1.37
10	bA	833	CLA	C1D-ND	4.67	1.43	1.37
10	aA	838	CLA	C1D-ND	4.67	1.43	1.37
10	aA	836	CLA	CHC-C1C	4.66	1.46	1.35
10	aA	830	CLA	O2D-CGD	4.66	1.44	1.33
10	bB	805	CLA	C3C-C2C	4.66	1.46	1.36
10	cA	836	CLA	CHC-C1C	4.66	1.46	1.35
10	cB	834	CLA	O2D-CGD	4.65	1.44	1.33
10	bA	830	CLA	O2D-CGD	4.65	1.44	1.33
10	bA	820	CLA	C1D-ND	4.65	1.43	1.37
10	bB	841	CLA	C1D-ND	4.65	1.43	1.37
10	cA	830	CLA	O2D-CGD	4.64	1.44	1.33
10	aA	820	CLA	C1D-ND	4.64	1.43	1.37
10	aA	836	CLA	O2D-CGD	4.64	1.44	1.33
10	cA	835	CLA	C1D-ND	4.64	1.43	1.37
10	bA	838	CLA	C1D-ND	4.64	1.43	1.37
10	bA	836	CLA	CHC-C1C	4.64	1.46	1.35
10	aA	835	CLA	C1D-ND	4.63	1.43	1.37
10	cA	833	CLA	O2D-CGD	4.62	1.44	1.33
10	bA	833	CLA	O2D-CGD	4.62	1.44	1.33
10	aB	822	CLA	OBD-CAD	4.62	1.30	1.22
10	cB	837	CLA	C1D-ND	4.62	1.43	1.37
10	aA	842	CLA	CHC-C1C	4.62	1.46	1.35
10	aB	837	CLA	C1D-ND	4.62	1.43	1.37
10	aB	807	CLA	C1D-ND	4.62	1.43	1.37
10	cA	836	CLA	O2D-CGD	4.62	1.44	1.33
10	cA	842	CLA	C3B-C2B	4.62	1.46	1.40
10	cB	822	CLA	CHC-C1C	4.62	1.46	1.35
10	bA	835	CLA	C1D-ND	4.62	1.43	1.37
10	bB	822	CLA	OBD-CAD	4.62	1.30	1.22
10	bA	836	CLA	O2D-CGD	4.61	1.44	1.33
10	bA	842	CLA	CHC-C1C	4.61	1.46	1.35
10	cB	822	CLA	OBD-CAD	4.61	1.30	1.22
10	cA	842	CLA	CHC-C1C	4.61	1.46	1.35
10	aB	822	CLA	CHC-C1C	4.60	1.46	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bL	205	CLA	C1D-ND	4.60	1.43	1.37
10	aA	833	CLA	O2D-CGD	4.60	1.44	1.33
10	bA	842	CLA	C3B-C2B	4.60	1.46	1.40
10	aA	842	CLA	C3B-C2B	4.60	1.46	1.40
10	cL	202	CLA	C1D-ND	4.60	1.43	1.37
10	cL	202	CLA	CHC-C1C	4.60	1.46	1.35
10	aA	808	CLA	C1D-ND	4.59	1.43	1.37
10	aB	841	CLA	C1D-ND	4.59	1.43	1.37
10	cL	205	CLA	C1D-ND	4.59	1.43	1.37
10	aL	202	CLA	CHC-C1C	4.59	1.46	1.35
10	aL	205	CLA	C1D-ND	4.58	1.43	1.37
10	bB	822	CLA	CHC-C1C	4.58	1.46	1.35
10	cA	820	CLA	C1D-ND	4.58	1.43	1.37
10	cB	803	CLA	O2D-CGD	4.58	1.44	1.33
9	bA	801	CL0	CHC-C1C	4.58	1.46	1.35
10	aB	820	CLA	CHD-C1D	4.58	1.47	1.38
10	cA	808	CLA	C1D-ND	4.58	1.43	1.37
10	aB	831	CLA	O2A-CGA	4.57	1.46	1.30
10	bB	805	CLA	O2D-CGD	4.57	1.44	1.33
9	cA	801	CL0	CHC-C1C	4.57	1.46	1.35
10	bB	819	CLA	C1D-ND	4.57	1.43	1.37
10	cA	838	CLA	C1D-ND	4.57	1.43	1.37
10	cB	805	CLA	O2D-CGD	4.57	1.44	1.33
10	bB	837	CLA	C1D-ND	4.57	1.43	1.37
10	aB	801	CLA	O2D-CGD	4.57	1.44	1.33
10	bL	202	CLA	CHC-C1C	4.57	1.46	1.35
10	aB	819	CLA	C1D-ND	4.57	1.43	1.37
10	bB	810	CLA	CHC-C1C	4.57	1.46	1.35
10	bB	803	CLA	O2D-CGD	4.57	1.44	1.33
10	aB	810	CLA	CHC-C1C	4.56	1.46	1.35
10	bA	808	CLA	C1D-ND	4.56	1.43	1.37
10	bB	831	CLA	O2A-CGA	4.56	1.46	1.30
10	bL	202	CLA	C1D-ND	4.56	1.43	1.37
10	cB	801	CLA	O2D-CGD	4.56	1.44	1.33
10	cB	841	CLA	C1D-ND	4.56	1.43	1.37
10	cB	807	CLA	C1D-ND	4.56	1.43	1.37
10	aB	803	CLA	O2D-CGD	4.56	1.44	1.33
9	aA	801	CL0	CHC-C1C	4.55	1.46	1.35
10	aA	809	CLA	O2A-CGA	4.55	1.46	1.30
10	bB	801	CLA	O2D-CGD	4.55	1.44	1.33
10	cB	820	CLA	CHD-C1D	4.55	1.47	1.38
10	cB	822	CLA	O2A-CGA	4.55	1.46	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	809	CLA	O2A-CGA	4.55	1.46	1.30
10	cB	810	CLA	CHC-C1C	4.55	1.46	1.35
10	cB	819	CLA	C1D-ND	4.55	1.43	1.37
10	cB	831	CLA	O2A-CGA	4.55	1.46	1.30
10	cB	814	CLA	CHD-C1D	4.54	1.47	1.38
10	aB	816	CLA	O2A-CGA	4.54	1.46	1.30
10	aB	822	CLA	O2A-CGA	4.54	1.46	1.30
10	bB	822	CLA	O2A-CGA	4.54	1.46	1.30
10	bA	809	CLA	O2A-CGA	4.54	1.46	1.30
10	aL	202	CLA	C1D-ND	4.54	1.43	1.37
10	bL	202	CLA	O2D-CGD	4.54	1.44	1.33
10	cL	202	CLA	O2D-CGD	4.54	1.44	1.33
10	bA	831	CLA	C1D-ND	4.53	1.43	1.37
10	aL	202	CLA	O2D-CGD	4.53	1.44	1.33
10	bB	820	CLA	CHD-C1D	4.53	1.47	1.38
10	aB	815	CLA	C1D-ND	4.53	1.43	1.37
10	aB	814	CLA	CHD-C1D	4.53	1.47	1.38
10	aA	825	CLA	C1D-ND	4.53	1.43	1.37
10	cA	843	CLA	O2A-CGA	4.53	1.46	1.30
10	aB	805	CLA	O2D-CGD	4.53	1.44	1.33
10	bB	816	CLA	O2A-CGA	4.53	1.46	1.30
10	cB	816	CLA	O2A-CGA	4.53	1.46	1.30
10	aA	831	CLA	C1D-ND	4.52	1.43	1.37
10	aB	824	CLA	O2A-CGA	4.52	1.46	1.30
10	cB	825	CLA	O2A-CGA	4.52	1.46	1.33
10	cA	836	CLA	C1D-ND	4.52	1.43	1.37
10	bA	802	CLA	O2A-CGA	4.52	1.45	1.30
10	aA	843	CLA	O2A-CGA	4.52	1.45	1.30
10	cB	813	CLA	O2A-CGA	4.52	1.45	1.30
10	bA	803	CLA	O2A-CGA	4.52	1.45	1.30
10	cB	824	CLA	O2A-CGA	4.52	1.45	1.30
10	bB	824	CLA	O2A-CGA	4.51	1.45	1.30
10	bB	813	CLA	O2A-CGA	4.51	1.45	1.30
10	aA	803	CLA	O2A-CGA	4.51	1.45	1.30
10	bA	843	CLA	O2A-CGA	4.51	1.45	1.30
10	bB	814	CLA	CHD-C1D	4.51	1.47	1.38
10	bB	807	CLA	C1D-ND	4.51	1.43	1.37
10	aA	802	CLA	O2A-CGA	4.51	1.45	1.30
11	bB	842	PQN	C10-C5	4.51	1.48	1.40
10	bA	807	CLA	O2A-CGA	4.50	1.45	1.30
10	aB	813	CLA	O2A-CGA	4.50	1.45	1.30
10	bB	804	CLA	O2D-CGD	4.50	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	803	CLA	O2A-CGA	4.50	1.45	1.30
10	bB	825	CLA	O2A-CGA	4.50	1.46	1.33
10	aA	836	CLA	C1D-ND	4.50	1.43	1.37
10	aB	836	CLA	CHD-C1D	4.50	1.47	1.38
10	aB	825	CLA	O2A-CGA	4.50	1.46	1.33
10	aB	836	CLA	O2A-CGA	4.50	1.45	1.30
10	cB	804	CLA	O2D-CGD	4.50	1.44	1.33
10	aA	807	CLA	O2A-CGA	4.49	1.45	1.30
10	cB	836	CLA	O2A-CGA	4.49	1.45	1.30
10	aB	804	CLA	O2D-CGD	4.49	1.44	1.33
10	cA	825	CLA	C1D-ND	4.49	1.43	1.37
10	cA	802	CLA	O2A-CGA	4.49	1.45	1.30
11	aB	842	PQN	C10-C5	4.49	1.48	1.40
10	bA	836	CLA	C1D-ND	4.49	1.43	1.37
10	bB	836	CLA	O2A-CGA	4.48	1.45	1.30
10	cA	807	CLA	O2A-CGA	4.48	1.45	1.30
10	cA	831	CLA	C1D-ND	4.48	1.43	1.37
10	cB	819	CLA	CHC-C1C	4.48	1.46	1.35
10	bA	837	CLA	C1D-ND	4.48	1.43	1.37
10	cB	836	CLA	CHD-C1D	4.48	1.47	1.38
10	bB	815	CLA	C1D-ND	4.48	1.43	1.37
10	bB	819	CLA	CHC-C1C	4.48	1.46	1.35
10	bA	804	CLA	C1D-ND	4.47	1.43	1.37
10	cB	834	CLA	O2A-CGA	4.47	1.45	1.30
10	bB	836	CLA	CHD-C1D	4.47	1.47	1.38
10	cB	815	CLA	C1D-ND	4.47	1.43	1.37
10	bB	834	CLA	O2A-CGA	4.47	1.45	1.30
10	cA	804	CLA	C1D-ND	4.47	1.43	1.37
10	aB	819	CLA	CHC-C1C	4.47	1.46	1.35
11	cB	842	PQN	C10-C5	4.46	1.48	1.40
10	aA	828	CLA	C1D-ND	4.46	1.43	1.37
10	bA	843	CLA	CHD-C1D	4.46	1.47	1.38
10	bA	825	CLA	C1D-ND	4.46	1.43	1.37
10	bB	835	CLA	O2A-CGA	4.46	1.45	1.30
10	cB	835	CLA	O2A-CGA	4.46	1.45	1.30
10	aA	808	CLA	O2A-CGA	4.46	1.45	1.30
10	cA	837	CLA	C1D-ND	4.45	1.43	1.37
10	bA	808	CLA	O2A-CGA	4.45	1.45	1.30
10	cB	840	CLA	C1D-ND	4.45	1.43	1.37
10	aB	840	CLA	C1D-ND	4.45	1.43	1.37
10	aB	835	CLA	O2A-CGA	4.45	1.45	1.30
10	cA	808	CLA	O2A-CGA	4.45	1.45	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	830	CLA	CHD-C1D	4.45	1.47	1.38
10	bB	812	CLA	O2A-CGA	4.45	1.45	1.30
10	cB	812	CLA	O2A-CGA	4.44	1.45	1.30
10	aA	830	CLA	O2A-CGA	4.44	1.46	1.33
10	cA	843	CLA	CHD-C1D	4.44	1.47	1.38
10	aB	831	CLA	CHD-C1D	4.44	1.47	1.38
10	bB	840	CLA	C1D-ND	4.44	1.43	1.37
10	aA	814	CLA	O2A-CGA	4.44	1.45	1.30
10	cL	202	CLA	O2A-CGA	4.44	1.46	1.33
10	cA	814	CLA	O2A-CGA	4.44	1.45	1.30
10	aA	843	CLA	CHD-C1D	4.44	1.47	1.38
10	aB	812	CLA	O2A-CGA	4.43	1.45	1.30
10	bB	824	CLA	CHD-C1D	4.43	1.47	1.38
10	aA	837	CLA	C1D-ND	4.43	1.43	1.37
10	aB	834	CLA	O2A-CGA	4.43	1.45	1.30
10	cA	830	CLA	O2A-CGA	4.43	1.46	1.33
10	bA	814	CLA	O2A-CGA	4.43	1.45	1.30
10	cB	824	CLA	CHD-C1D	4.42	1.47	1.38
10	aL	202	CLA	O2A-CGA	4.42	1.46	1.33
10	aA	818	CLA	O2A-CGA	4.42	1.46	1.33
10	aB	824	CLA	CHD-C1D	4.42	1.47	1.38
10	aA	804	CLA	C1D-ND	4.42	1.43	1.37
10	cA	818	CLA	O2A-CGA	4.42	1.46	1.33
10	cA	813	CLA	O2A-CGA	4.41	1.45	1.30
10	bA	828	CLA	C1D-ND	4.41	1.43	1.37
10	aB	811	CLA	CHC-C1C	4.41	1.46	1.35
10	bA	830	CLA	O2A-CGA	4.41	1.46	1.33
10	bB	809	CLA	C1D-ND	4.41	1.43	1.37
10	aB	823	CLA	CHD-C1D	4.41	1.46	1.38
10	cA	828	CLA	C1D-ND	4.40	1.43	1.37
10	bB	831	CLA	CHD-C1D	4.40	1.46	1.38
10	bA	818	CLA	O2A-CGA	4.40	1.46	1.33
10	aA	823	CLA	CHD-C1D	4.40	1.46	1.38
10	bB	837	CLA	O2A-CGA	4.40	1.46	1.33
10	cB	837	CLA	O2A-CGA	4.40	1.46	1.33
10	bL	202	CLA	O2A-CGA	4.40	1.46	1.33
10	bB	823	CLA	CHD-C1D	4.40	1.46	1.38
10	cB	831	CLA	CHD-C1D	4.40	1.46	1.38
10	cA	810	CLA	O2A-CGA	4.40	1.46	1.33
10	aB	826	CLA	CHD-C1D	4.40	1.46	1.38
10	cB	830	CLA	CHD-C1D	4.39	1.46	1.38
10	cA	830	CLA	C1D-ND	4.39	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	823	CLA	CHD-C1D	4.39	1.46	1.38
10	aB	809	CLA	C1D-ND	4.39	1.43	1.37
10	aA	813	CLA	O2A-CGA	4.39	1.45	1.30
10	cA	840	CLA	O2A-CGA	4.39	1.46	1.33
10	bA	840	CLA	O2A-CGA	4.39	1.46	1.33
10	bA	813	CLA	O2A-CGA	4.39	1.45	1.30
10	bB	826	CLA	CHD-C1D	4.38	1.46	1.38
10	bB	834	CLA	CHD-C1D	4.38	1.46	1.38
10	cB	811	CLA	CHC-C1C	4.38	1.46	1.35
10	bB	811	CLA	CHC-C1C	4.38	1.46	1.35
10	aA	830	CLA	C1D-ND	4.38	1.43	1.37
10	bA	830	CLA	C1D-ND	4.38	1.43	1.37
10	bB	830	CLA	CHD-C1D	4.38	1.46	1.38
10	bA	810	CLA	O2A-CGA	4.38	1.46	1.33
10	aA	840	CLA	O2A-CGA	4.38	1.46	1.33
10	aA	810	CLA	O2A-CGA	4.38	1.46	1.33
10	aB	837	CLA	O2A-CGA	4.37	1.46	1.33
10	bB	828	CLA	O2A-CGA	4.37	1.46	1.33
10	cB	828	CLA	O2A-CGA	4.37	1.46	1.33
10	cB	820	CLA	O2A-CGA	4.36	1.46	1.33
10	bA	823	CLA	CHD-C1D	4.36	1.46	1.38
10	aB	829	CLA	O2A-CGA	4.36	1.46	1.33
10	aB	828	CLA	O2A-CGA	4.36	1.46	1.33
10	aA	854	CLA	O2A-CGA	4.35	1.46	1.33
10	aB	834	CLA	CHD-C1D	4.35	1.46	1.38
10	bA	854	CLA	O2A-CGA	4.35	1.46	1.33
10	cB	809	CLA	C1D-ND	4.35	1.43	1.37
10	aB	820	CLA	O2A-CGA	4.35	1.46	1.33
10	bA	814	CLA	CHD-C1D	4.35	1.46	1.38
10	cA	823	CLA	CHD-C1D	4.35	1.46	1.38
10	aA	839	CLA	CHD-C1D	4.34	1.46	1.38
10	cA	839	CLA	CHD-C1D	4.34	1.46	1.38
10	aA	824	CLA	C1D-ND	4.34	1.43	1.37
10	cA	824	CLA	C1D-ND	4.34	1.43	1.37
10	cB	841	CLA	CHC-C1C	4.34	1.46	1.35
10	cB	834	CLA	CHD-C1D	4.34	1.46	1.38
10	cB	826	CLA	CHD-C1D	4.34	1.46	1.38
10	cA	821	CLA	O2A-CGA	4.34	1.46	1.33
10	bB	820	CLA	O2A-CGA	4.33	1.46	1.33
10	cL	204	CLA	O2A-CGA	4.33	1.46	1.33
10	cB	829	CLA	O2A-CGA	4.33	1.46	1.33
10	bB	829	CLA	O2A-CGA	4.33	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	832	CLA	C1D-ND	4.33	1.43	1.37
10	cA	832	CLA	C1D-ND	4.33	1.43	1.37
10	aB	841	CLA	CHC-C1C	4.32	1.46	1.35
10	aA	812	CLA	CHD-C1D	4.32	1.46	1.38
10	aA	803	CLA	CHD-C1D	4.32	1.46	1.38
10	bB	833	CLA	O2A-CGA	4.32	1.46	1.33
10	aA	821	CLA	O2A-CGA	4.32	1.46	1.33
10	bA	813	CLA	CHD-C1D	4.32	1.46	1.38
10	bA	822	CLA	O2A-CGA	4.32	1.46	1.33
10	cA	835	CLA	CHD-C1D	4.32	1.46	1.38
10	aB	835	CLA	CHD-C1D	4.32	1.46	1.38
10	cB	833	CLA	CHD-C1D	4.32	1.46	1.38
10	aL	204	CLA	O2A-CGA	4.32	1.46	1.33
10	bA	834	CLA	C1D-ND	4.32	1.43	1.37
10	cA	854	CLA	O2A-CGA	4.32	1.46	1.33
10	cA	822	CLA	O2A-CGA	4.32	1.46	1.33
10	bA	832	CLA	C1D-ND	4.32	1.43	1.37
10	bA	819	CLA	O2A-CGA	4.32	1.46	1.33
10	bA	821	CLA	O2A-CGA	4.31	1.45	1.33
10	cA	810	CLA	CHD-C1D	4.31	1.46	1.38
10	bA	812	CLA	CHD-C1D	4.31	1.46	1.38
10	bA	856	CLA	CHD-C1D	4.31	1.46	1.38
10	aA	819	CLA	O2A-CGA	4.31	1.45	1.33
10	cB	821	CLA	O2A-CGA	4.31	1.45	1.33
10	aA	822	CLA	O2A-CGA	4.31	1.45	1.33
10	cA	834	CLA	C1D-ND	4.31	1.43	1.37
10	bB	817	CLA	O2A-CGA	4.31	1.45	1.33
10	aA	815	CLA	CHD-C1D	4.31	1.46	1.38
10	bB	835	CLA	CHD-C1D	4.31	1.46	1.38
10	bA	815	CLA	CHD-C1D	4.31	1.46	1.38
10	aA	835	CLA	CHD-C1D	4.31	1.46	1.38
10	cA	806	CLA	CHD-C1D	4.31	1.46	1.38
10	bB	839	CLA	O2A-CGA	4.31	1.45	1.33
10	bA	810	CLA	CHD-C1D	4.31	1.46	1.38
10	bA	839	CLA	CHD-C1D	4.30	1.46	1.38
10	cA	812	CLA	CHD-C1D	4.30	1.46	1.38
10	cA	819	CLA	O2A-CGA	4.30	1.45	1.33
10	cB	817	CLA	O2A-CGA	4.30	1.45	1.33
10	cA	813	CLA	CHD-C1D	4.30	1.46	1.38
10	aA	856	CLA	CHD-C1D	4.30	1.46	1.38
10	bL	204	CLA	O2A-CGA	4.30	1.45	1.33
10	aA	814	CLA	CHD-C1D	4.30	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	840	CLA	O2A-CGA	4.30	1.45	1.33
10	cB	833	CLA	O2A-CGA	4.30	1.45	1.33
10	cB	839	CLA	O2A-CGA	4.30	1.45	1.33
10	bB	841	CLA	CHC-C1C	4.30	1.46	1.35
10	aB	817	CLA	O2A-CGA	4.29	1.45	1.33
10	aB	833	CLA	O2A-CGA	4.29	1.45	1.33
10	aA	810	CLA	CHD-C1D	4.29	1.46	1.38
10	cA	815	CLA	CHD-C1D	4.29	1.46	1.38
10	aB	821	CLA	O2A-CGA	4.29	1.45	1.33
10	aA	834	CLA	C1D-ND	4.29	1.43	1.37
10	bA	835	CLA	CHD-C1D	4.29	1.46	1.38
10	bB	812	CLA	CHD-C1D	4.29	1.46	1.38
10	cA	814	CLA	CHD-C1D	4.29	1.46	1.38
10	bA	806	CLA	CHD-C1D	4.29	1.46	1.38
10	bB	821	CLA	O2A-CGA	4.29	1.45	1.33
10	aB	832	CLA	CHD-C1D	4.29	1.46	1.38
10	bB	840	CLA	O2A-CGA	4.29	1.45	1.33
10	bB	832	CLA	CHD-C1D	4.28	1.46	1.38
10	aB	839	CLA	O2A-CGA	4.28	1.45	1.33
10	bA	833	CLA	O2A-CGA	4.28	1.45	1.33
10	cA	856	CLA	CHD-C1D	4.28	1.46	1.38
10	aA	820	CLA	O2A-CGA	4.28	1.45	1.33
10	aB	818	CLA	CHD-C1D	4.28	1.46	1.38
10	bB	833	CLA	CHD-C1D	4.28	1.46	1.38
10	cA	803	CLA	CHD-C1D	4.28	1.46	1.38
10	cB	818	CLA	CHD-C1D	4.28	1.46	1.38
10	bA	824	CLA	C1D-ND	4.28	1.43	1.37
10	cB	804	CLA	O2A-CGA	4.28	1.45	1.33
10	cB	840	CLA	O2A-CGA	4.28	1.45	1.33
10	cB	835	CLA	CHD-C1D	4.27	1.46	1.38
10	aA	815	CLA	O2A-CGA	4.27	1.45	1.33
10	bA	820	CLA	O2A-CGA	4.27	1.45	1.33
10	bA	803	CLA	CHD-C1D	4.27	1.46	1.38
10	cB	832	CLA	CHD-C1D	4.27	1.46	1.38
10	aA	856	CLA	O2A-CGA	4.27	1.45	1.33
10	bA	856	CLA	O2A-CGA	4.27	1.45	1.33
10	aA	813	CLA	CHD-C1D	4.27	1.46	1.38
10	bA	827	CLA	O2A-CGA	4.27	1.45	1.33
10	aB	812	CLA	CHD-C1D	4.27	1.46	1.38
10	aA	823	CLA	O2A-CGA	4.27	1.45	1.33
10	aB	833	CLA	CHD-C1D	4.26	1.46	1.38
10	aA	833	CLA	O2A-CGA	4.26	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	812	CLA	CHD-C1D	4.26	1.46	1.38
10	cA	820	CLA	O2A-CGA	4.26	1.45	1.33
10	aA	827	CLA	O2A-CGA	4.26	1.45	1.33
10	bB	810	CLA	C1D-ND	4.26	1.43	1.37
10	cA	833	CLA	O2A-CGA	4.26	1.45	1.33
10	bB	804	CLA	O2A-CGA	4.26	1.45	1.33
10	bA	815	CLA	O2A-CGA	4.26	1.45	1.33
10	cA	827	CLA	O2A-CGA	4.26	1.45	1.33
10	aB	804	CLA	O2A-CGA	4.25	1.45	1.33
10	cA	815	CLA	O2A-CGA	4.25	1.45	1.33
10	cB	810	CLA	C1D-ND	4.25	1.43	1.37
10	bB	832	CLA	O2A-CGA	4.25	1.45	1.33
10	aB	810	CLA	C1D-ND	4.25	1.43	1.37
10	cA	856	CLA	O2A-CGA	4.24	1.45	1.33
10	aA	806	CLA	CHD-C1D	4.24	1.46	1.38
10	bA	823	CLA	O2A-CGA	4.24	1.45	1.33
10	cA	823	CLA	O2A-CGA	4.24	1.45	1.33
10	bA	842	CLA	C1D-ND	4.23	1.43	1.37
10	bA	826	CLA	O2A-CGA	4.23	1.45	1.33
10	aA	819	CLA	CHD-C1D	4.23	1.46	1.38
10	bA	829	CLA	C1D-ND	4.23	1.43	1.37
10	aA	842	CLA	C1D-ND	4.23	1.43	1.37
10	cB	821	CLA	CHD-C1D	4.23	1.46	1.38
10	cA	835	CLA	O2A-CGA	4.22	1.45	1.33
10	cA	839	CLA	O2A-CGA	4.22	1.45	1.33
10	aB	821	CLA	CHD-C1D	4.22	1.46	1.38
10	cB	841	CLA	O2A-CGA	4.22	1.45	1.33
10	bB	811	CLA	O2A-CGA	4.22	1.45	1.33
10	cB	815	CLA	O2A-CGA	4.22	1.45	1.33
10	cB	832	CLA	O2A-CGA	4.22	1.45	1.33
10	aB	832	CLA	O2A-CGA	4.22	1.45	1.33
10	aB	811	CLA	O2A-CGA	4.22	1.45	1.33
10	bB	818	CLA	CHD-C1D	4.22	1.46	1.38
10	cB	811	CLA	O2A-CGA	4.22	1.45	1.33
10	cA	829	CLA	C1D-ND	4.22	1.43	1.37
10	aA	826	CLA	O2A-CGA	4.22	1.45	1.33
10	aA	835	CLA	O2A-CGA	4.22	1.45	1.33
10	cA	838	CLA	O2A-CGA	4.22	1.45	1.33
10	aA	839	CLA	O2A-CGA	4.21	1.45	1.33
10	cB	826	CLA	CHD-C4C	4.21	1.48	1.39
10	bA	835	CLA	O2A-CGA	4.21	1.45	1.33
10	aB	815	CLA	O2A-CGA	4.21	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	827	CLA	O2A-CGA	4.21	1.45	1.33
10	cA	816	CLA	O2A-CGA	4.21	1.45	1.33
10	bA	817	CLA	CHD-C1D	4.21	1.46	1.38
10	bB	803	CLA	C1D-ND	4.21	1.43	1.37
10	cB	830	CLA	C1D-ND	4.21	1.43	1.37
10	aB	826	CLA	CHD-C4C	4.20	1.48	1.39
10	cA	826	CLA	O2A-CGA	4.20	1.45	1.33
10	bB	826	CLA	CHD-C4C	4.20	1.48	1.39
10	aB	841	CLA	O2A-CGA	4.20	1.45	1.33
10	cB	827	CLA	O2A-CGA	4.20	1.45	1.33
10	aA	829	CLA	C1D-ND	4.20	1.42	1.37
10	bB	841	CLA	O2A-CGA	4.20	1.45	1.33
10	aA	841	CLA	O2A-CGA	4.20	1.45	1.33
10	bB	826	CLA	O2A-CGA	4.20	1.45	1.33
10	bB	821	CLA	CHD-C1D	4.20	1.46	1.38
10	bA	839	CLA	O2A-CGA	4.20	1.45	1.33
10	cA	842	CLA	C1D-ND	4.19	1.42	1.37
10	aA	816	CLA	O2A-CGA	4.19	1.45	1.33
10	aB	826	CLA	O2A-CGA	4.19	1.45	1.33
10	cB	819	CLA	CHD-C1D	4.19	1.46	1.38
10	bB	815	CLA	O2A-CGA	4.19	1.45	1.33
10	cA	802	CLA	CHD-C1D	4.19	1.46	1.38
10	cA	841	CLA	O2A-CGA	4.19	1.45	1.33
10	cA	840	CLA	CHD-C1D	4.19	1.46	1.38
10	aA	802	CLA	CHD-C1D	4.19	1.46	1.38
10	cA	834	CLA	O2A-CGA	4.19	1.45	1.33
10	bA	819	CLA	CHD-C1D	4.19	1.46	1.38
10	aA	838	CLA	O2A-CGA	4.19	1.45	1.33
10	bA	816	CLA	O2A-CGA	4.19	1.45	1.33
10	bB	830	CLA	C1D-ND	4.18	1.42	1.37
10	aA	830	CLA	CHD-C1D	4.18	1.46	1.38
10	aB	827	CLA	O2A-CGA	4.18	1.45	1.33
10	bA	830	CLA	CHD-C1D	4.18	1.46	1.38
10	cB	816	CLA	CHD-C1D	4.18	1.46	1.38
10	aB	813	CLA	CHD-C1D	4.18	1.46	1.38
10	aB	819	CLA	CHD-C1D	4.18	1.46	1.38
10	cA	817	CLA	CHD-C1D	4.18	1.46	1.38
10	bA	838	CLA	O2A-CGA	4.18	1.45	1.33
10	bA	802	CLA	CHD-C1D	4.18	1.46	1.38
10	aB	823	CLA	O2A-CGA	4.18	1.45	1.33
10	bA	824	CLA	O2A-CGA	4.18	1.45	1.33
10	bA	841	CLA	O2A-CGA	4.18	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	840	CLA	CHD-C1D	4.18	1.46	1.38
10	aB	830	CLA	C1D-ND	4.18	1.42	1.37
10	cA	836	CLA	O2A-CGA	4.17	1.45	1.33
10	aA	809	CLA	CHD-C1D	4.17	1.46	1.38
10	cB	826	CLA	O2A-CGA	4.17	1.45	1.33
10	aB	815	CLA	CHD-C1D	4.17	1.46	1.38
10	cA	820	CLA	CHD-C1D	4.17	1.46	1.38
10	cB	802	CLA	O2A-CGA	4.17	1.45	1.33
10	cA	811	CLA	O2A-CGA	4.17	1.45	1.33
10	aA	834	CLA	O2A-CGA	4.17	1.45	1.33
10	aA	820	CLA	CHD-C1D	4.17	1.46	1.38
10	aA	806	CLA	O2A-CGA	4.17	1.45	1.33
10	cA	819	CLA	CHD-C1D	4.17	1.46	1.38
10	bB	816	CLA	CHD-C1D	4.17	1.46	1.38
10	bB	823	CLA	O2A-CGA	4.17	1.45	1.33
10	cB	803	CLA	C1D-ND	4.17	1.42	1.37
10	bA	820	CLA	CHD-C1D	4.17	1.46	1.38
10	aA	804	CLA	CHD-C1D	4.17	1.46	1.38
10	aB	816	CLA	CHD-C1D	4.17	1.46	1.38
10	cB	815	CLA	CHD-C1D	4.17	1.46	1.38
10	bB	813	CLA	CHD-C1D	4.17	1.46	1.38
10	cA	818	CLA	CHD-C1D	4.17	1.46	1.38
10	aA	836	CLA	O2A-CGA	4.17	1.45	1.33
10	cA	806	CLA	O2A-CGA	4.16	1.45	1.33
10	cB	823	CLA	O2A-CGA	4.16	1.45	1.33
10	cL	203	CLA	CHD-C1D	4.16	1.46	1.38
10	bA	806	CLA	O2A-CGA	4.16	1.45	1.33
10	bA	834	CLA	O2A-CGA	4.16	1.45	1.33
10	cA	809	CLA	CHD-C1D	4.16	1.46	1.38
10	bB	806	CLA	O2A-CGA	4.16	1.45	1.33
10	bB	838	CLA	O2A-CGA	4.16	1.45	1.33
10	bB	819	CLA	CHD-C1D	4.16	1.46	1.38
10	aA	811	CLA	O2A-CGA	4.16	1.45	1.33
10	cA	824	CLA	O2A-CGA	4.16	1.45	1.33
10	aA	824	CLA	O2A-CGA	4.16	1.45	1.33
10	bA	836	CLA	O2A-CGA	4.16	1.45	1.33
10	cA	830	CLA	CHD-C1D	4.16	1.46	1.38
10	bB	807	CLA	CHD-C1D	4.15	1.46	1.38
10	cB	813	CLA	CHD-C1D	4.15	1.46	1.38
10	bB	802	CLA	O2A-CGA	4.15	1.45	1.33
10	aA	840	CLA	CHD-C1D	4.15	1.46	1.38
10	aA	817	CLA	CHD-C1D	4.15	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	806	CLA	O2A-CGA	4.15	1.45	1.33
10	cB	838	CLA	O2A-CGA	4.15	1.45	1.33
10	bL	203	CLA	CHD-C1D	4.15	1.46	1.38
10	bB	817	CLA	CHD-C1D	4.14	1.46	1.38
10	aB	807	CLA	CHD-C1D	4.14	1.46	1.38
10	aL	203	CLA	CHD-C1D	4.14	1.46	1.38
10	aA	831	CLA	O2A-CGA	4.14	1.45	1.33
10	aB	817	CLA	CHD-C1D	4.14	1.46	1.38
10	aB	838	CLA	O2A-CGA	4.14	1.45	1.33
10	aB	802	CLA	O2A-CGA	4.14	1.45	1.33
10	bA	809	CLA	CHD-C1D	4.14	1.46	1.38
10	bB	809	CLA	O2A-CGA	4.14	1.45	1.33
10	aB	814	CLA	O2A-CGA	4.14	1.45	1.33
10	aB	803	CLA	C1D-ND	4.14	1.42	1.37
10	bB	834	CLA	CHD-C4C	4.14	1.48	1.39
10	aB	806	CLA	O2A-CGA	4.14	1.45	1.33
10	bA	811	CLA	O2A-CGA	4.14	1.45	1.33
10	aA	817	CLA	O2A-CGA	4.13	1.45	1.33
10	aB	834	CLA	CHD-C4C	4.13	1.48	1.39
10	aB	809	CLA	O2A-CGA	4.13	1.45	1.33
10	bA	818	CLA	CHD-C1D	4.13	1.46	1.38
10	cB	807	CLA	CHD-C1D	4.13	1.46	1.38
10	cA	812	CLA	O2A-CGA	4.13	1.45	1.33
10	bA	804	CLA	CHD-C1D	4.13	1.46	1.38
10	aB	801	CLA	CHD-C1D	4.13	1.46	1.38
10	bA	817	CLA	O2A-CGA	4.13	1.45	1.33
10	bB	814	CLA	O2A-CGA	4.13	1.45	1.33
10	cB	818	CLA	O2A-CGA	4.13	1.45	1.33
10	bB	818	CLA	O2A-CGA	4.12	1.45	1.33
10	cB	817	CLA	CHD-C1D	4.12	1.46	1.38
10	bB	801	CLA	CHD-C1D	4.12	1.46	1.38
10	cL	203	CLA	O2A-CGA	4.12	1.45	1.33
10	aB	818	CLA	O2A-CGA	4.12	1.45	1.33
10	cB	801	CLA	CHD-C1D	4.12	1.46	1.38
10	aA	818	CLA	CHD-C1D	4.12	1.46	1.38
10	cB	834	CLA	CHD-C4C	4.12	1.48	1.39
10	aA	842	CLA	CHD-C1D	4.11	1.46	1.38
10	aA	811	CLA	CHD-C1D	4.11	1.46	1.38
10	cA	804	CLA	CHD-C1D	4.11	1.46	1.38
10	bA	831	CLA	O2A-CGA	4.11	1.45	1.33
10	cA	831	CLA	O2A-CGA	4.11	1.45	1.33
10	cB	814	CLA	O2A-CGA	4.11	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	833	CLA	CHD-C1D	4.11	1.46	1.38
10	aA	812	CLA	O2A-CGA	4.11	1.45	1.33
10	bB	815	CLA	CHD-C1D	4.11	1.46	1.38
10	aL	205	CLA	CHD-C1D	4.11	1.46	1.38
10	bA	842	CLA	CHD-C1D	4.11	1.46	1.38
10	bA	812	CLA	O2A-CGA	4.10	1.45	1.33
10	cA	817	CLA	O2A-CGA	4.10	1.45	1.33
10	aL	203	CLA	O2A-CGA	4.10	1.45	1.33
10	cB	809	CLA	O2A-CGA	4.10	1.45	1.33
10	cA	834	CLA	CHD-C1D	4.10	1.46	1.38
10	cB	807	CLA	O2A-CGA	4.10	1.45	1.33
10	bB	820	CLA	CHD-C4C	4.10	1.48	1.39
10	aB	820	CLA	CHD-C4C	4.09	1.48	1.39
10	cA	811	CLA	CHD-C1D	4.09	1.46	1.38
10	aB	808	CLA	O2A-CGA	4.09	1.45	1.33
10	bB	836	CLA	CHD-C4C	4.09	1.48	1.39
10	bB	837	CLA	CHD-C1D	4.09	1.46	1.38
10	aB	836	CLA	CHD-C4C	4.09	1.48	1.39
10	bA	833	CLA	CHD-C1D	4.09	1.46	1.38
10	cA	822	CLA	CHD-C1D	4.09	1.46	1.38
10	cA	833	CLA	CHD-C1D	4.09	1.46	1.38
10	bB	831	CLA	CHD-C4C	4.08	1.48	1.39
10	bA	837	CLA	O2A-CGA	4.08	1.45	1.33
10	bB	803	CLA	O2A-CGA	4.08	1.45	1.33
10	cB	808	CLA	O2A-CGA	4.08	1.45	1.33
10	bB	823	CLA	CHD-C4C	4.08	1.48	1.39
10	bL	203	CLA	O2A-CGA	4.08	1.45	1.33
10	bA	811	CLA	CHD-C1D	4.08	1.46	1.38
10	bL	205	CLA	CHD-C1D	4.08	1.46	1.38
10	cB	823	CLA	CHD-C4C	4.08	1.48	1.39
10	aA	841	CLA	CHD-C1D	4.08	1.46	1.38
10	aB	837	CLA	CHD-C1D	4.08	1.46	1.38
10	aA	837	CLA	O2A-CGA	4.08	1.45	1.33
10	cA	837	CLA	O2A-CGA	4.08	1.45	1.33
10	aA	805	CLA	O2A-CGA	4.08	1.45	1.33
10	aB	828	CLA	C1D-ND	4.08	1.42	1.37
10	cA	842	CLA	CHD-C1D	4.08	1.46	1.38
10	cB	822	CLA	CHD-C1D	4.07	1.46	1.38
10	cB	820	CLA	CHD-C4C	4.07	1.48	1.39
10	cB	836	CLA	CHD-C4C	4.07	1.48	1.39
10	aB	805	CLA	O2A-CGA	4.07	1.45	1.33
10	cB	835	CLA	CHD-C4C	4.07	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	828	CLA	C1D-ND	4.07	1.42	1.37
10	aB	807	CLA	O2A-CGA	4.07	1.45	1.33
10	cB	803	CLA	O2A-CGA	4.07	1.45	1.33
10	aB	835	CLA	CHD-C4C	4.06	1.48	1.39
10	bB	808	CLA	O2A-CGA	4.06	1.45	1.33
10	bB	805	CLA	O2A-CGA	4.06	1.45	1.33
10	cA	842	CLA	O2A-CGA	4.06	1.45	1.33
10	cB	801	CLA	C1D-ND	4.06	1.42	1.37
10	cB	837	CLA	CHD-C1D	4.06	1.46	1.38
10	aA	834	CLA	CHD-C1D	4.06	1.46	1.38
10	aA	842	CLA	O2A-CGA	4.06	1.45	1.33
10	bA	822	CLA	CHD-C1D	4.06	1.46	1.38
10	aB	823	CLA	CHD-C4C	4.06	1.48	1.39
10	cL	205	CLA	CHD-C1D	4.06	1.46	1.38
10	cA	821	CLA	CHD-C1D	4.06	1.46	1.38
10	aA	822	CLA	CHD-C1D	4.06	1.46	1.38
10	cA	805	CLA	O2A-CGA	4.06	1.45	1.33
10	aB	838	CLA	CHD-C1D	4.05	1.46	1.38
10	bA	829	CLA	O2A-CGA	4.05	1.45	1.33
10	aA	843	CLA	CHD-C4C	4.05	1.48	1.39
10	aA	816	CLA	CHD-C1D	4.05	1.46	1.38
10	aB	803	CLA	O2A-CGA	4.05	1.45	1.33
10	bA	805	CLA	O2A-CGA	4.05	1.45	1.33
10	bA	842	CLA	O2A-CGA	4.05	1.45	1.33
10	cB	828	CLA	C1D-ND	4.05	1.42	1.37
10	aA	829	CLA	O2A-CGA	4.05	1.45	1.33
10	bB	807	CLA	O2A-CGA	4.05	1.45	1.33
10	cA	829	CLA	O2A-CGA	4.04	1.45	1.33
10	aA	854	CLA	CHD-C1D	4.04	1.46	1.38
10	aB	831	CLA	CHD-C4C	4.04	1.48	1.39
10	bB	835	CLA	CHD-C4C	4.04	1.48	1.39
10	cB	805	CLA	O2A-CGA	4.04	1.45	1.33
10	bB	801	CLA	C1D-ND	4.04	1.42	1.37
10	bA	841	CLA	CHD-C1D	4.04	1.46	1.38
10	cA	827	CLA	CHD-C1D	4.04	1.46	1.38
10	cB	831	CLA	CHD-C4C	4.04	1.48	1.39
10	aB	822	CLA	CHD-C1D	4.03	1.46	1.38
10	bA	854	CLA	CHD-C1D	4.03	1.46	1.38
10	aA	827	CLA	CHD-C1D	4.03	1.46	1.38
10	bA	827	CLA	CHD-C1D	4.03	1.46	1.38
10	bB	822	CLA	CHD-C1D	4.03	1.46	1.38
10	bA	821	CLA	CHD-C1D	4.03	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	841	CLA	CHD-C1D	4.03	1.46	1.38
10	aA	821	CLA	CHD-C1D	4.02	1.46	1.38
10	bB	824	CLA	CHD-C4C	4.02	1.48	1.39
10	aA	805	CLA	CHD-C1D	4.02	1.46	1.38
10	cB	830	CLA	O2A-CGA	4.02	1.45	1.33
10	bB	810	CLA	CHD-C1D	4.02	1.46	1.38
10	bA	805	CLA	CHD-C1D	4.02	1.46	1.38
10	bA	834	CLA	CHD-C1D	4.02	1.46	1.38
10	cB	838	CLA	CHD-C1D	4.02	1.46	1.38
10	aA	838	CLA	CHD-C1D	4.02	1.46	1.38
10	bB	830	CLA	O2A-CGA	4.02	1.45	1.33
10	aB	801	CLA	C1D-ND	4.02	1.42	1.37
10	aB	810	CLA	CHD-C1D	4.02	1.46	1.38
10	cA	839	CLA	CHD-C4C	4.02	1.48	1.39
10	aB	824	CLA	CHD-C4C	4.01	1.48	1.39
10	cA	838	CLA	CHD-C1D	4.01	1.46	1.38
10	bA	843	CLA	CHD-C4C	4.01	1.48	1.39
10	bA	807	CLA	CHD-C1D	4.01	1.46	1.38
9	cA	801	CL0	O2A-CGA	4.01	1.45	1.33
10	cA	810	CLA	CHD-C4C	4.01	1.48	1.39
10	aB	830	CLA	O2A-CGA	4.01	1.45	1.33
10	bB	838	CLA	CHD-C1D	4.01	1.46	1.38
10	cA	805	CLA	CHD-C1D	4.01	1.46	1.38
10	bA	839	CLA	CHD-C4C	4.01	1.48	1.39
10	cA	843	CLA	CHD-C4C	4.01	1.48	1.39
10	bA	810	CLA	CHD-C4C	4.01	1.48	1.39
10	cA	812	CLA	CHD-C4C	4.00	1.48	1.39
10	cB	824	CLA	CHD-C4C	4.00	1.48	1.39
10	bA	812	CLA	CHD-C4C	4.00	1.48	1.39
9	bA	801	CL0	O2A-CGA	4.00	1.45	1.33
10	cA	807	CLA	CHD-C1D	4.00	1.46	1.38
10	aA	818	CLA	CHD-C4C	4.00	1.48	1.39
10	bA	818	CLA	CHD-C4C	4.00	1.48	1.39
10	cA	854	CLA	CHD-C1D	4.00	1.46	1.38
9	aA	801	CL0	O2A-CGA	4.00	1.45	1.33
10	cB	810	CLA	CHD-C1D	4.00	1.46	1.38
10	cA	818	CLA	CHD-C4C	4.00	1.48	1.39
10	aB	804	CLA	C1D-ND	4.00	1.42	1.37
10	bA	806	CLA	CHD-C4C	3.99	1.48	1.39
10	cB	841	CLA	CHD-C1D	3.99	1.46	1.38
10	aA	807	CLA	CHD-C1D	3.99	1.46	1.38
10	cB	819	CLA	O2A-CGA	3.99	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	839	CLA	CHD-C1D	3.99	1.46	1.38
10	aA	810	CLA	CHD-C4C	3.98	1.48	1.39
10	cA	816	CLA	CHD-C1D	3.98	1.46	1.38
10	aB	841	CLA	CHD-C1D	3.98	1.46	1.38
10	aA	839	CLA	CHD-C4C	3.98	1.48	1.39
10	bA	828	CLA	O2A-CGA	3.98	1.45	1.33
10	bB	839	CLA	CHD-C1D	3.98	1.46	1.38
10	aA	828	CLA	O2A-CGA	3.98	1.45	1.33
10	aA	806	CLA	CHD-C4C	3.98	1.48	1.39
10	bA	832	CLA	O2A-CGA	3.97	1.44	1.33
10	aA	812	CLA	CHD-C4C	3.97	1.48	1.39
10	cA	803	CLA	CHD-C4C	3.97	1.48	1.39
10	aB	818	CLA	CHD-C4C	3.97	1.48	1.39
10	cA	828	CLA	CHD-C1D	3.97	1.46	1.38
10	bL	205	CLA	O2A-CGA	3.97	1.44	1.33
10	cB	839	CLA	CHD-C1D	3.97	1.46	1.38
10	bA	816	CLA	CHD-C1D	3.97	1.46	1.38
10	bB	841	CLA	CHD-C1D	3.97	1.46	1.38
10	bB	810	CLA	O2A-CGA	3.97	1.44	1.33
10	cA	802	CLA	CHD-C4C	3.96	1.48	1.39
10	cL	205	CLA	O2A-CGA	3.96	1.44	1.33
10	aB	819	CLA	O2A-CGA	3.96	1.44	1.33
10	cB	810	CLA	O2A-CGA	3.96	1.44	1.33
10	bB	819	CLA	O2A-CGA	3.96	1.44	1.33
10	aA	813	CLA	CHD-C4C	3.96	1.48	1.39
10	aB	810	CLA	O2A-CGA	3.96	1.44	1.33
10	bA	838	CLA	CHD-C1D	3.96	1.46	1.38
10	cB	818	CLA	CHD-C4C	3.96	1.48	1.39
10	bA	803	CLA	CHD-C4C	3.95	1.48	1.39
10	cA	832	CLA	O2A-CGA	3.95	1.44	1.33
10	bB	812	CLA	CHD-C4C	3.95	1.48	1.39
10	cA	819	CLA	CHD-C4C	3.95	1.48	1.39
10	aL	205	CLA	O2A-CGA	3.95	1.44	1.33
10	bA	802	CLA	CHD-C4C	3.95	1.48	1.39
10	aA	803	CLA	CHD-C4C	3.95	1.48	1.39
10	bA	828	CLA	CHD-C1D	3.95	1.46	1.38
10	bB	829	CLA	CHD-C1D	3.95	1.46	1.38
10	cA	806	CLA	CHD-C4C	3.95	1.48	1.39
10	aB	833	CLA	CHD-C4C	3.95	1.48	1.39
10	aA	828	CLA	CHD-C1D	3.95	1.46	1.38
10	cB	829	CLA	CHD-C1D	3.95	1.46	1.38
10	aA	832	CLA	CHD-C1D	3.94	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	802	CLA	CHD-C4C	3.94	1.48	1.39
10	bB	830	CLA	CHD-C4C	3.94	1.48	1.39
10	bA	837	CLA	CHD-C1D	3.94	1.46	1.38
10	cA	828	CLA	O2A-CGA	3.94	1.44	1.33
10	aB	825	CLA	CHD-C1D	3.94	1.46	1.38
10	bB	804	CLA	C1D-ND	3.94	1.42	1.37
10	bB	829	CLA	C1D-ND	3.94	1.42	1.37
10	aB	814	CLA	CHD-C4C	3.94	1.48	1.39
10	cB	814	CLA	CHD-C4C	3.94	1.48	1.39
10	cB	833	CLA	CHD-C4C	3.94	1.48	1.39
10	aB	829	CLA	CHD-C1D	3.94	1.46	1.38
10	aA	832	CLA	O2A-CGA	3.94	1.44	1.33
10	bB	818	CLA	CHD-C4C	3.93	1.48	1.39
10	bA	813	CLA	CHD-C4C	3.93	1.48	1.39
10	aB	832	CLA	CHD-C4C	3.93	1.48	1.39
10	bB	833	CLA	CHD-C4C	3.93	1.48	1.39
10	bA	832	CLA	CHD-C1D	3.93	1.46	1.38
10	cB	838	CLA	CHD-C4C	3.93	1.48	1.39
10	bB	801	CLA	O2A-CGA	3.93	1.44	1.33
10	aB	812	CLA	CHD-C4C	3.92	1.48	1.39
10	cB	812	CLA	CHD-C4C	3.92	1.48	1.39
10	bB	832	CLA	CHD-C4C	3.92	1.48	1.39
10	aA	814	CLA	CHD-C4C	3.92	1.48	1.39
10	bA	814	CLA	CHD-C4C	3.92	1.48	1.39
10	bA	815	CLA	CHD-C4C	3.92	1.48	1.39
10	cB	804	CLA	C3D-C2D	3.92	1.49	1.39
10	cB	804	CLA	C1D-ND	3.91	1.42	1.37
9	aA	801	CL0	C1D-ND	3.91	1.42	1.37
10	cA	831	CLA	CHD-C1D	3.91	1.46	1.38
10	bB	825	CLA	CHD-C1D	3.91	1.46	1.38
10	cA	837	CLA	CHD-C1D	3.91	1.46	1.38
10	cB	830	CLA	CHD-C4C	3.91	1.48	1.39
10	aB	838	CLA	CHD-C4C	3.91	1.48	1.39
10	cA	856	CLA	CHD-C4C	3.91	1.48	1.39
10	cB	816	CLA	CHD-C4C	3.91	1.48	1.39
10	cA	832	CLA	CHD-C1D	3.91	1.46	1.38
10	cB	832	CLA	CHD-C4C	3.91	1.48	1.39
10	cA	813	CLA	CHD-C4C	3.91	1.48	1.39
10	cA	814	CLA	CHD-C4C	3.91	1.48	1.39
10	aA	836	CLA	CHD-C1D	3.91	1.46	1.38
10	aB	804	CLA	C3D-C2D	3.91	1.49	1.39
10	aB	839	CLA	CHD-C4C	3.91	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	819	CLA	CHD-C4C	3.91	1.48	1.39
10	aA	837	CLA	CHD-C1D	3.91	1.46	1.38
10	bA	835	CLA	CHD-C4C	3.90	1.48	1.39
10	bB	816	CLA	CHD-C4C	3.90	1.48	1.39
10	aB	830	CLA	CHD-C4C	3.90	1.48	1.39
10	bA	804	CLA	O2A-CGA	3.90	1.44	1.33
10	aA	815	CLA	CHD-C4C	3.90	1.48	1.39
10	cA	836	CLA	CHD-C1D	3.90	1.46	1.38
10	bB	838	CLA	CHD-C4C	3.90	1.48	1.39
10	cA	804	CLA	O2A-CGA	3.90	1.44	1.33
10	aB	816	CLA	CHD-C4C	3.90	1.48	1.39
10	cB	839	CLA	CHD-C4C	3.90	1.48	1.39
10	bA	817	CLA	CHD-C4C	3.90	1.48	1.39
10	bB	814	CLA	CHD-C4C	3.90	1.48	1.39
10	cA	815	CLA	CHD-C4C	3.90	1.48	1.39
10	bA	836	CLA	CHD-C1D	3.89	1.46	1.38
10	cB	829	CLA	C1D-ND	3.89	1.42	1.37
10	cA	817	CLA	CHD-C4C	3.89	1.48	1.39
10	aA	831	CLA	CHD-C1D	3.89	1.45	1.38
10	cA	835	CLA	CHD-C4C	3.89	1.48	1.39
10	bB	822	CLA	CHD-C4C	3.89	1.48	1.39
10	aA	856	CLA	CHD-C4C	3.89	1.48	1.39
10	aA	804	CLA	O2A-CGA	3.89	1.44	1.33
10	aB	829	CLA	C1D-ND	3.89	1.42	1.37
10	aB	801	CLA	O2A-CGA	3.89	1.44	1.33
10	aA	821	CLA	C3D-C2D	3.89	1.49	1.39
10	aA	817	CLA	CHD-C4C	3.89	1.48	1.39
10	aA	835	CLA	CHD-C4C	3.89	1.48	1.39
10	aA	843	CLA	C3D-C2D	3.88	1.49	1.39
10	bB	804	CLA	C3D-C2D	3.88	1.49	1.39
10	bA	843	CLA	C3D-C2D	3.88	1.49	1.39
10	cB	801	CLA	O2A-CGA	3.88	1.44	1.33
10	bA	821	CLA	C3D-C2D	3.88	1.49	1.39
10	bA	856	CLA	CHD-C4C	3.88	1.48	1.39
10	cL	204	CLA	C1D-ND	3.88	1.42	1.37
10	bA	825	CLA	CHD-C1D	3.88	1.45	1.38
10	aA	819	CLA	CHD-C4C	3.88	1.48	1.39
10	cA	825	CLA	CHD-C1D	3.88	1.45	1.38
10	cB	822	CLA	CHD-C4C	3.88	1.48	1.39
10	aL	203	CLA	CHD-C4C	3.87	1.48	1.39
10	cA	809	CLA	CHD-C4C	3.87	1.48	1.39
10	aA	826	CLA	CHD-C1D	3.87	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	823	CLA	CHD-C4C	3.87	1.48	1.39
10	aB	808	CLA	CHD-C1D	3.87	1.45	1.38
9	cA	801	CL0	C1D-ND	3.87	1.42	1.37
10	aA	825	CLA	CHD-C1D	3.87	1.45	1.38
10	aB	819	CLA	CHD-C4C	3.87	1.48	1.39
10	cA	829	CLA	CHD-C1D	3.87	1.45	1.38
10	cB	825	CLA	CHD-C1D	3.87	1.45	1.38
10	cB	819	CLA	CHD-C4C	3.87	1.48	1.39
10	aA	829	CLA	CHD-C1D	3.87	1.45	1.38
10	bA	833	CLA	CHD-C4C	3.86	1.48	1.39
10	aA	807	CLA	CHD-C4C	3.86	1.48	1.39
10	aB	822	CLA	CHD-C4C	3.86	1.48	1.39
10	bB	839	CLA	CHD-C4C	3.86	1.48	1.39
10	cB	811	CLA	CHD-C1D	3.86	1.45	1.38
10	cA	843	CLA	C3D-C2D	3.86	1.49	1.39
10	bA	823	CLA	CHD-C4C	3.86	1.48	1.39
10	bA	808	CLA	CHD-C1D	3.86	1.45	1.38
10	bA	829	CLA	CHD-C1D	3.85	1.45	1.38
10	cA	821	CLA	C3D-C2D	3.85	1.49	1.39
10	bA	807	CLA	CHD-C4C	3.85	1.48	1.39
10	aB	807	CLA	CHD-C4C	3.85	1.48	1.39
10	cA	811	CLA	CHD-C4C	3.85	1.48	1.39
10	aB	811	CLA	CHD-C1D	3.85	1.45	1.38
10	bB	819	CLA	CHD-C4C	3.85	1.48	1.39
10	cL	202	CLA	CHD-C1D	3.85	1.45	1.38
10	bB	811	CLA	CHD-C1D	3.85	1.45	1.38
10	bA	841	CLA	CHD-C4C	3.85	1.48	1.39
10	aB	802	CLA	C3D-C2D	3.85	1.49	1.39
10	cB	808	CLA	CHD-C1D	3.85	1.45	1.38
10	cA	807	CLA	CHD-C4C	3.85	1.48	1.39
10	bB	802	CLA	C3D-C2D	3.85	1.49	1.39
10	bA	811	CLA	CHD-C4C	3.84	1.48	1.39
10	bA	821	CLA	CHD-C4C	3.84	1.48	1.39
10	aA	811	CLA	CHD-C4C	3.84	1.48	1.39
10	aL	204	CLA	C1D-ND	3.84	1.42	1.37
10	bA	840	CLA	CHD-C4C	3.84	1.48	1.39
10	cA	833	CLA	CHD-C4C	3.84	1.48	1.39
10	cA	856	CLA	C3D-C2D	3.84	1.49	1.39
10	aL	202	CLA	CHD-C1D	3.84	1.45	1.38
10	bA	826	CLA	CHD-C1D	3.84	1.45	1.38
10	aA	820	CLA	CHD-C4C	3.84	1.48	1.39
10	aA	833	CLA	CHD-C4C	3.84	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bL	203	CLA	CHD-C4C	3.84	1.48	1.39
10	cA	825	CLA	O2A-CGA	3.84	1.44	1.33
10	bA	809	CLA	CHD-C4C	3.84	1.48	1.39
10	aA	825	CLA	O2A-CGA	3.84	1.44	1.33
10	bL	202	CLA	CHD-C1D	3.84	1.45	1.38
10	aA	856	CLA	C3D-C2D	3.83	1.49	1.39
10	bA	831	CLA	CHD-C1D	3.83	1.45	1.38
9	bA	801	CL0	C1D-ND	3.83	1.42	1.37
10	cA	808	CLA	CHD-C1D	3.83	1.45	1.38
10	aA	809	CLA	CHD-C4C	3.83	1.48	1.39
10	bB	808	CLA	CHD-C1D	3.83	1.45	1.38
10	cB	807	CLA	CHD-C4C	3.83	1.48	1.39
10	bA	856	CLA	C3D-C2D	3.83	1.49	1.39
10	cB	802	CLA	C3D-C2D	3.83	1.49	1.39
10	bB	840	CLA	CHD-C1D	3.82	1.45	1.38
10	aA	823	CLA	CHD-C4C	3.82	1.48	1.39
10	bB	807	CLA	CHD-C4C	3.82	1.48	1.39
10	bA	825	CLA	O2A-CGA	3.82	1.44	1.33
10	bB	836	CLA	C3D-C2D	3.82	1.49	1.39
10	aB	824	CLA	C3D-C2D	3.82	1.49	1.39
10	aA	840	CLA	CHD-C4C	3.82	1.48	1.39
10	cA	840	CLA	CHD-C4C	3.82	1.48	1.39
10	aB	818	CLA	C3D-C2D	3.82	1.49	1.39
10	bA	820	CLA	CHD-C4C	3.82	1.48	1.39
10	cL	203	CLA	CHD-C4C	3.82	1.48	1.39
10	cB	806	CLA	CHD-C1D	3.82	1.45	1.38
10	bB	801	CLA	C3D-C2D	3.82	1.49	1.39
10	bB	806	CLA	CHD-C1D	3.82	1.45	1.38
10	aA	841	CLA	CHD-C4C	3.81	1.47	1.39
10	cA	820	CLA	CHD-C4C	3.81	1.47	1.39
10	cB	814	CLA	C3D-C2D	3.81	1.49	1.39
10	cA	804	CLA	CHD-C4C	3.81	1.47	1.39
10	cB	836	CLA	C3D-C2D	3.81	1.49	1.39
10	aB	811	CLA	C1B-NB	-3.81	1.31	1.35
10	bB	824	CLA	C3D-C2D	3.81	1.49	1.39
10	cA	826	CLA	CHD-C1D	3.81	1.45	1.38
10	cA	841	CLA	CHD-C4C	3.81	1.47	1.39
10	aA	808	CLA	CHD-C1D	3.80	1.45	1.38
10	aB	806	CLA	CHD-C1D	3.80	1.45	1.38
10	cA	816	CLA	CHD-C4C	3.80	1.47	1.39
10	cA	821	CLA	CHD-C4C	3.80	1.47	1.39
10	aB	814	CLA	C3D-C2D	3.80	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	818	CLA	C3D-C2D	3.80	1.49	1.39
10	aB	840	CLA	CHD-C1D	3.80	1.45	1.38
10	cB	816	CLA	C3D-C2D	3.80	1.49	1.39
10	bA	804	CLA	CHD-C4C	3.80	1.47	1.39
10	bA	826	CLA	CHD-C4C	3.79	1.47	1.39
10	cB	818	CLA	C3D-C2D	3.79	1.49	1.39
10	aB	801	CLA	C3D-C2D	3.79	1.49	1.39
10	bL	204	CLA	C1D-ND	3.79	1.42	1.37
10	aA	821	CLA	CHD-C4C	3.79	1.47	1.39
10	bB	813	CLA	CHD-C4C	3.79	1.47	1.39
10	aB	821	CLA	CHD-C4C	3.79	1.47	1.39
10	cA	826	CLA	CHD-C4C	3.79	1.47	1.39
10	aB	836	CLA	C3D-C2D	3.79	1.49	1.39
10	aB	816	CLA	C3D-C2D	3.79	1.49	1.39
10	bB	814	CLA	C3D-C2D	3.79	1.49	1.39
10	aA	804	CLA	CHD-C4C	3.79	1.47	1.39
10	bL	205	CLA	CHD-C4C	3.79	1.47	1.39
10	aB	811	CLA	C1D-ND	3.79	1.42	1.37
10	cB	811	CLA	C1D-ND	3.79	1.42	1.37
10	bB	811	CLA	C1B-NB	-3.79	1.31	1.35
10	cB	801	CLA	C3D-C2D	3.79	1.49	1.39
10	cB	813	CLA	CHD-C4C	3.79	1.47	1.39
10	cL	205	CLA	CHD-C4C	3.78	1.47	1.39
10	cB	824	CLA	C3D-C2D	3.78	1.49	1.39
10	cB	840	CLA	CHD-C1D	3.78	1.45	1.38
10	bB	817	CLA	CHD-C4C	3.78	1.47	1.39
10	cB	817	CLA	CHD-C4C	3.78	1.47	1.39
10	aB	831	CLA	C3D-C2D	3.78	1.49	1.39
10	bB	816	CLA	C3D-C2D	3.78	1.49	1.39
10	cA	829	CLA	C1B-NB	-3.78	1.31	1.35
10	aA	829	CLA	C3D-C2D	3.78	1.49	1.39
10	cB	802	CLA	CHD-C4C	3.78	1.47	1.39
10	cA	839	CLA	C3D-C2D	3.77	1.49	1.39
10	bB	811	CLA	C1D-ND	3.77	1.42	1.37
10	aB	813	CLA	CHD-C4C	3.77	1.47	1.39
10	bB	815	CLA	CHD-C4C	3.77	1.47	1.39
10	bA	824	CLA	CHD-C4C	3.77	1.47	1.39
10	bB	802	CLA	CHD-C4C	3.77	1.47	1.39
10	cA	854	CLA	CHD-C4C	3.77	1.47	1.39
10	aA	816	CLA	CHD-C4C	3.77	1.47	1.39
10	aB	833	CLA	C3D-C2D	3.77	1.49	1.39
10	aB	820	CLA	C3D-C2D	3.76	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	826	CLA	CHD-C4C	3.76	1.47	1.39
10	aB	821	CLA	C3D-C2D	3.76	1.49	1.39
10	cB	831	CLA	C3D-C2D	3.76	1.49	1.39
10	cB	815	CLA	CHD-C4C	3.76	1.47	1.39
10	bB	831	CLA	C3D-C2D	3.76	1.49	1.39
10	bB	821	CLA	CHD-C4C	3.76	1.47	1.39
10	bA	816	CLA	CHD-C4C	3.76	1.47	1.39
10	aA	854	CLA	CHD-C4C	3.76	1.47	1.39
10	bB	820	CLA	C3D-C2D	3.76	1.49	1.39
10	aA	839	CLA	C3D-C2D	3.76	1.49	1.39
10	aL	205	CLA	CHD-C4C	3.76	1.47	1.39
10	cB	823	CLA	C3D-C2D	3.75	1.49	1.39
10	bB	833	CLA	C3D-C2D	3.75	1.49	1.39
10	cB	821	CLA	CHD-C4C	3.75	1.47	1.39
10	aB	817	CLA	CHD-C4C	3.75	1.47	1.39
10	bB	809	CLA	CHD-C4C	3.75	1.47	1.39
10	aB	811	CLA	C3D-C2D	3.75	1.49	1.39
10	cA	829	CLA	C3D-C2D	3.75	1.49	1.39
10	bA	829	CLA	C1B-NB	-3.75	1.31	1.35
10	cA	834	CLA	C3D-C2D	3.75	1.49	1.39
10	bA	834	CLA	C3D-C2D	3.75	1.49	1.39
10	aA	831	CLA	C3D-C2D	3.75	1.49	1.39
10	cB	827	CLA	CHD-C1D	3.75	1.45	1.38
10	bA	834	CLA	CHD-C4C	3.75	1.47	1.39
10	cA	824	CLA	CHD-C4C	3.75	1.47	1.39
10	bA	818	CLA	C3D-C2D	3.75	1.49	1.39
10	aA	824	CLA	CHD-C4C	3.75	1.47	1.39
10	bA	829	CLA	C3D-C2D	3.75	1.49	1.39
10	bA	839	CLA	C3D-C2D	3.74	1.49	1.39
10	cA	831	CLA	C3D-C2D	3.74	1.49	1.39
10	aA	830	CLA	CHD-C4C	3.74	1.47	1.39
10	cB	820	CLA	C3D-C2D	3.74	1.49	1.39
10	bB	823	CLA	C3D-C2D	3.74	1.49	1.39
10	bA	854	CLA	CHD-C4C	3.74	1.47	1.39
10	aA	810	CLA	C3D-C2D	3.74	1.49	1.39
10	bA	838	CLA	CHD-C4C	3.74	1.47	1.39
10	cA	838	CLA	CHD-C4C	3.74	1.47	1.39
10	aB	809	CLA	CHD-C4C	3.74	1.47	1.39
10	bB	811	CLA	C3D-C2D	3.74	1.49	1.39
10	cL	204	CLA	CHD-C4C	3.74	1.47	1.39
10	cB	833	CLA	C3D-C2D	3.74	1.49	1.39
9	cA	801	CL0	CHD-C1D	3.74	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	830	CLA	CHD-C4C	3.74	1.47	1.39
10	bA	830	CLA	CHD-C4C	3.73	1.47	1.39
10	cB	811	CLA	C3D-C2D	3.73	1.49	1.39
10	cB	801	CLA	CHD-C4C	3.73	1.47	1.39
10	aA	834	CLA	CHD-C4C	3.73	1.47	1.39
10	aA	838	CLA	CHD-C4C	3.73	1.47	1.39
10	aA	834	CLA	C3D-C2D	3.73	1.49	1.39
10	bA	831	CLA	C3D-C2D	3.73	1.49	1.39
9	bA	801	CL0	CHD-C1D	3.73	1.45	1.38
10	aB	823	CLA	C3D-C2D	3.73	1.49	1.39
10	aB	802	CLA	CHD-C4C	3.73	1.47	1.39
10	cA	810	CLA	C3D-C2D	3.73	1.49	1.39
10	cA	834	CLA	CHD-C4C	3.73	1.47	1.39
10	cA	803	CLA	C3D-C2D	3.73	1.49	1.39
10	aA	832	CLA	CHD-C4C	3.73	1.47	1.39
10	cA	818	CLA	C3D-C2D	3.73	1.49	1.39
10	cA	822	CLA	CHD-C4C	3.73	1.47	1.39
10	aA	803	CLA	C3D-C2D	3.73	1.49	1.39
10	aB	808	CLA	CHD-C4C	3.73	1.47	1.39
10	aB	815	CLA	CHD-C4C	3.73	1.47	1.39
10	aB	827	CLA	CHD-C1D	3.73	1.45	1.38
10	cB	809	CLA	CHD-C4C	3.72	1.47	1.39
10	bL	204	CLA	CHD-C4C	3.72	1.47	1.39
10	cB	836	CLA	OBD-CAD	3.72	1.28	1.22
10	aB	813	CLA	C3D-C2D	3.72	1.49	1.39
10	cB	821	CLA	C3D-C2D	3.72	1.49	1.39
10	bA	810	CLA	C3D-C2D	3.72	1.49	1.39
10	bA	822	CLA	CHD-C4C	3.72	1.47	1.39
10	bB	813	CLA	C3D-C2D	3.72	1.49	1.39
10	aB	801	CLA	CHD-C4C	3.72	1.47	1.39
10	aL	204	CLA	CHD-C4C	3.72	1.47	1.39
10	aA	818	CLA	C3D-C2D	3.72	1.49	1.39
10	bB	808	CLA	CHD-C4C	3.72	1.47	1.39
10	bA	803	CLA	C3D-C2D	3.71	1.49	1.39
10	bA	825	CLA	CHD-C4C	3.71	1.47	1.39
10	bA	832	CLA	CHD-C4C	3.71	1.47	1.39
10	cB	811	CLA	C1B-NB	-3.71	1.31	1.35
10	aA	827	CLA	CHD-C4C	3.71	1.47	1.39
10	aA	822	CLA	CHD-C4C	3.71	1.47	1.39
10	bB	809	CLA	CHD-C1D	3.71	1.45	1.38
10	aA	829	CLA	C1B-NB	-3.71	1.31	1.35
9	aA	801	CL0	CHD-C1D	3.71	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	827	CLA	CHD-C1D	3.71	1.45	1.38
10	cB	808	CLA	CHD-C4C	3.71	1.47	1.39
10	bB	821	CLA	OBD-CAD	3.71	1.28	1.22
10	cA	842	CLA	C3D-C2D	3.71	1.49	1.39
10	bA	834	CLA	OBD-CAD	3.71	1.28	1.22
10	cA	827	CLA	CHD-C4C	3.71	1.47	1.39
10	aB	826	CLA	C3D-C2D	3.71	1.49	1.39
10	cA	832	CLA	CHD-C4C	3.70	1.47	1.39
10	cB	837	CLA	CHD-C4C	3.70	1.47	1.39
10	bB	826	CLA	C3D-C2D	3.70	1.49	1.39
10	bB	817	CLA	OBD-CAD	3.70	1.28	1.22
10	bB	821	CLA	C3D-C2D	3.70	1.49	1.39
10	bB	820	CLA	OBD-CAD	3.70	1.28	1.22
10	cB	809	CLA	CHD-C1D	3.70	1.45	1.38
10	aB	809	CLA	C3D-C2D	3.70	1.49	1.39
10	aB	809	CLA	CHD-C1D	3.70	1.45	1.38
10	bA	842	CLA	C3D-C2D	3.70	1.49	1.39
10	cB	821	CLA	OBD-CAD	3.70	1.28	1.22
10	cB	804	CLA	CHD-C1D	3.69	1.45	1.38
10	bB	837	CLA	CHD-C4C	3.69	1.47	1.39
10	cB	826	CLA	C3D-C2D	3.69	1.49	1.39
10	bA	833	CLA	C3D-C2D	3.69	1.49	1.39
10	aB	804	CLA	CHD-C1D	3.69	1.45	1.38
10	bB	804	CLA	CHD-C1D	3.69	1.45	1.38
10	aA	805	CLA	CHD-C4C	3.69	1.47	1.39
10	bB	805	CLA	C3D-C2D	3.69	1.49	1.39
10	aA	828	CLA	C3D-C2D	3.69	1.49	1.39
10	cB	809	CLA	C3D-C2D	3.69	1.49	1.39
10	aA	834	CLA	OBD-CAD	3.68	1.28	1.22
10	bB	836	CLA	OBD-CAD	3.68	1.28	1.22
10	cB	817	CLA	C3D-C2D	3.68	1.49	1.39
10	cB	825	CLA	CHD-C4C	3.68	1.47	1.39
10	aB	821	CLA	OBD-CAD	3.68	1.28	1.22
10	cA	805	CLA	CHD-C4C	3.68	1.47	1.39
10	bA	805	CLA	CHD-C4C	3.68	1.47	1.39
10	cB	817	CLA	OBD-CAD	3.68	1.28	1.22
10	cA	825	CLA	CHD-C4C	3.68	1.47	1.39
10	aB	838	CLA	C3D-C2D	3.68	1.49	1.39
10	bB	838	CLA	C3D-C2D	3.68	1.49	1.39
10	cA	814	CLA	C3D-C2D	3.68	1.49	1.39
10	aA	833	CLA	C3D-C2D	3.68	1.49	1.39
10	bB	809	CLA	C3D-C2D	3.68	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	803	CLA	OBD-CAD	3.68	1.28	1.22
10	bB	823	CLA	OBD-CAD	3.68	1.28	1.22
10	bA	812	CLA	C3D-C2D	3.68	1.49	1.39
10	cA	805	CLA	C3D-C2D	3.68	1.49	1.39
10	bB	825	CLA	CHD-C4C	3.67	1.47	1.39
10	aB	817	CLA	OBD-CAD	3.67	1.28	1.22
10	bA	827	CLA	CHD-C4C	3.67	1.47	1.39
10	aA	842	CLA	C3D-C2D	3.67	1.49	1.39
10	cB	838	CLA	C3D-C2D	3.67	1.49	1.39
10	bA	803	CLA	OBD-CAD	3.67	1.28	1.22
10	aB	837	CLA	CHD-C4C	3.67	1.47	1.39
10	bB	801	CLA	CHD-C4C	3.67	1.47	1.39
10	aA	825	CLA	CHD-C4C	3.67	1.47	1.39
10	bB	841	CLA	CHD-C4C	3.67	1.47	1.39
10	aB	836	CLA	OBD-CAD	3.67	1.28	1.22
10	bA	828	CLA	C3D-C2D	3.67	1.49	1.39
10	cB	823	CLA	OBD-CAD	3.67	1.28	1.22
10	cB	805	CLA	C3D-C2D	3.66	1.49	1.39
10	aB	837	CLA	C3D-C2D	3.66	1.49	1.39
10	aA	828	CLA	CHD-C4C	3.66	1.47	1.39
10	aB	820	CLA	OBD-CAD	3.66	1.28	1.22
10	cB	813	CLA	C3D-C2D	3.66	1.49	1.39
10	aA	811	CLA	C3D-C2D	3.66	1.49	1.39
10	aA	820	CLA	C3D-C2D	3.66	1.49	1.39
10	cA	812	CLA	C3D-C2D	3.66	1.49	1.39
10	cB	825	CLA	C3D-C2D	3.66	1.49	1.39
10	cA	834	CLA	OBD-CAD	3.66	1.28	1.22
10	cB	820	CLA	OBD-CAD	3.66	1.28	1.22
10	bA	819	CLA	C3D-C2D	3.66	1.49	1.39
10	aB	805	CLA	C3D-C2D	3.66	1.49	1.39
10	bB	825	CLA	C3D-C2D	3.66	1.49	1.39
10	aB	817	CLA	C3D-C2D	3.66	1.49	1.39
10	bA	811	CLA	C3D-C2D	3.66	1.49	1.39
10	bL	205	CLA	C3D-C2D	3.66	1.49	1.39
10	aA	805	CLA	C3D-C2D	3.66	1.49	1.39
10	aB	823	CLA	OBD-CAD	3.65	1.28	1.22
10	bA	820	CLA	C3D-C2D	3.65	1.49	1.39
10	cB	819	CLA	C3D-C2D	3.65	1.49	1.39
10	aA	819	CLA	C3D-C2D	3.65	1.49	1.39
10	bA	805	CLA	C3D-C2D	3.65	1.49	1.39
10	cA	828	CLA	CHD-C4C	3.65	1.47	1.39
10	cA	811	CLA	C3D-C2D	3.65	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	819	CLA	C3D-C2D	3.65	1.49	1.39
10	cA	803	CLA	OBD-CAD	3.65	1.28	1.22
10	cA	815	CLA	OBD-CAD	3.65	1.28	1.22
10	aB	825	CLA	C3D-C2D	3.65	1.49	1.39
10	bA	828	CLA	CHD-C4C	3.65	1.47	1.39
10	bA	813	CLA	C3D-C2D	3.65	1.49	1.39
10	aA	814	CLA	C3D-C2D	3.65	1.49	1.39
10	aB	819	CLA	C3D-C2D	3.65	1.49	1.39
10	bB	803	CLA	CHD-C1D	3.65	1.45	1.38
10	cB	832	CLA	C3D-C2D	3.65	1.49	1.39
10	aB	803	CLA	CHD-C1D	3.65	1.45	1.38
10	bB	817	CLA	C3D-C2D	3.65	1.49	1.39
10	cA	806	CLA	C3D-C2D	3.65	1.49	1.39
10	aB	832	CLA	C3D-C2D	3.65	1.49	1.39
10	cA	828	CLA	C3D-C2D	3.65	1.49	1.39
10	cB	830	CLA	C1B-NB	-3.64	1.32	1.35
10	cA	820	CLA	C3D-C2D	3.64	1.49	1.39
10	cB	837	CLA	C3D-C2D	3.64	1.49	1.39
10	bA	837	CLA	CHD-C4C	3.64	1.47	1.39
10	bB	837	CLA	C3D-C2D	3.64	1.49	1.39
10	cA	833	CLA	C3D-C2D	3.64	1.49	1.39
10	aA	837	CLA	CHD-C4C	3.64	1.47	1.39
10	bB	806	CLA	CHD-C4C	3.64	1.47	1.39
10	aA	802	CLA	C3D-C2D	3.64	1.49	1.39
10	cB	803	CLA	CHD-C1D	3.64	1.45	1.38
10	cA	840	CLA	C3D-C2D	3.64	1.49	1.39
10	bB	830	CLA	C1B-NB	-3.64	1.32	1.35
10	cA	824	CLA	CHD-C1D	3.64	1.45	1.38
10	aA	812	CLA	C3D-C2D	3.64	1.49	1.39
10	cA	802	CLA	C3D-C2D	3.64	1.49	1.39
10	cA	815	CLA	C3D-C2D	3.64	1.49	1.39
10	bA	840	CLA	OBD-CAD	3.64	1.28	1.22
10	bA	836	CLA	CHD-C4C	3.64	1.47	1.39
10	aB	825	CLA	CHD-C4C	3.64	1.47	1.39
10	aA	840	CLA	OBD-CAD	3.64	1.28	1.22
10	bB	819	CLA	C3D-C2D	3.64	1.49	1.39
10	cL	205	CLA	C3D-C2D	3.64	1.49	1.39
10	bA	824	CLA	CHD-C1D	3.63	1.45	1.38
10	bA	840	CLA	C3D-C2D	3.63	1.49	1.39
10	aA	836	CLA	CHD-C4C	3.63	1.47	1.39
10	aA	816	CLA	OBD-CAD	3.63	1.28	1.22
10	bB	802	CLA	C1B-NB	-3.63	1.32	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	832	CLA	C3D-C2D	3.63	1.49	1.39
10	aB	841	CLA	CHD-C4C	3.63	1.47	1.39
10	cB	801	CLA	C1B-NB	-3.63	1.32	1.35
10	bA	830	CLA	C3D-C2D	3.63	1.49	1.39
10	cB	804	CLA	CHD-C4C	3.63	1.47	1.39
10	cA	809	CLA	OBD-CAD	3.63	1.28	1.22
10	cA	813	CLA	OBD-CAD	3.63	1.28	1.22
10	aB	830	CLA	C1B-NB	-3.62	1.32	1.35
10	aA	815	CLA	OBD-CAD	3.62	1.28	1.22
10	cB	802	CLA	C1B-NB	-3.62	1.32	1.35
10	bA	814	CLA	C3D-C2D	3.62	1.49	1.39
10	cA	837	CLA	CHD-C4C	3.62	1.47	1.39
10	bA	806	CLA	C3D-C2D	3.62	1.49	1.39
10	bA	815	CLA	C3D-C2D	3.62	1.49	1.39
10	aA	809	CLA	OBD-CAD	3.62	1.28	1.22
10	aL	205	CLA	C3D-C2D	3.62	1.49	1.39
10	aB	829	CLA	CHD-C4C	3.62	1.47	1.39
10	cA	831	CLA	CHD-C4C	3.62	1.47	1.39
10	cB	813	CLA	OBD-CAD	3.62	1.28	1.22
10	aB	812	CLA	C3D-C2D	3.62	1.49	1.39
10	aA	806	CLA	C3D-C2D	3.62	1.49	1.39
10	bB	813	CLA	OBD-CAD	3.62	1.28	1.22
10	bB	827	CLA	CHD-C4C	3.62	1.47	1.39
10	cA	836	CLA	CHD-C4C	3.62	1.47	1.39
10	aA	813	CLA	C3D-C2D	3.62	1.49	1.39
10	bA	841	CLA	C3D-C2D	3.62	1.49	1.39
10	bA	831	CLA	CHD-C4C	3.62	1.47	1.39
10	bA	842	CLA	CHD-C4C	3.62	1.47	1.39
10	cB	827	CLA	CHD-C4C	3.62	1.47	1.39
10	bA	802	CLA	C3D-C2D	3.61	1.49	1.39
10	aA	840	CLA	C3D-C2D	3.61	1.49	1.39
10	cA	813	CLA	C3D-C2D	3.61	1.49	1.39
10	bA	809	CLA	OBD-CAD	3.61	1.28	1.22
10	aA	815	CLA	C3D-C2D	3.61	1.49	1.39
10	aB	802	CLA	C1B-NB	-3.61	1.32	1.35
10	cA	840	CLA	OBD-CAD	3.61	1.28	1.22
10	aB	804	CLA	CHD-C4C	3.61	1.47	1.39
10	cL	204	CLA	C3D-C2D	3.61	1.49	1.39
10	aA	824	CLA	CHD-C1D	3.61	1.45	1.38
10	aB	801	CLA	C1B-NB	-3.61	1.32	1.35
10	cA	830	CLA	C3D-C2D	3.61	1.49	1.39
10	aA	813	CLA	OBD-CAD	3.61	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	813	CLA	OBD-CAD	3.61	1.28	1.22
10	cB	841	CLA	CHD-C4C	3.61	1.47	1.39
10	cA	841	CLA	C3D-C2D	3.61	1.49	1.39
10	bA	816	CLA	OBD-CAD	3.61	1.28	1.22
10	aB	841	CLA	C3D-C2D	3.60	1.49	1.39
10	cA	809	CLA	C3D-C2D	3.60	1.49	1.39
10	aA	818	CLA	OBD-CAD	3.60	1.28	1.22
10	bB	812	CLA	C3D-C2D	3.60	1.49	1.39
10	bA	829	CLA	CHD-C4C	3.60	1.47	1.39
10	aB	806	CLA	CHD-C4C	3.60	1.47	1.39
10	aA	841	CLA	C3D-C2D	3.60	1.49	1.39
10	bL	204	CLA	C3D-C2D	3.60	1.49	1.39
10	cA	816	CLA	OBD-CAD	3.60	1.28	1.22
10	aB	827	CLA	CHD-C4C	3.60	1.47	1.39
10	aA	830	CLA	C3D-C2D	3.60	1.48	1.39
10	bB	829	CLA	CHD-C4C	3.60	1.47	1.39
10	cB	806	CLA	CHD-C4C	3.60	1.47	1.39
10	cL	202	CLA	CHD-C4C	3.60	1.47	1.39
10	aA	842	CLA	CHD-C4C	3.60	1.47	1.39
10	aA	831	CLA	CHD-C4C	3.60	1.47	1.39
10	bB	835	CLA	C3D-C2D	3.60	1.48	1.39
10	aB	825	CLA	OBD-CAD	3.60	1.28	1.22
10	bB	801	CLA	C1B-NB	-3.60	1.32	1.35
10	bB	841	CLA	C3D-C2D	3.59	1.48	1.39
10	aL	202	CLA	CHD-C4C	3.59	1.47	1.39
10	bB	832	CLA	OBD-CAD	3.59	1.28	1.22
10	cB	825	CLA	OBD-CAD	3.59	1.28	1.22
10	aL	203	CLA	C3D-C2D	3.59	1.48	1.39
10	cB	835	CLA	C3D-C2D	3.59	1.48	1.39
10	aB	805	CLA	CHD-C4C	3.59	1.47	1.39
10	bL	203	CLA	C3D-C2D	3.59	1.48	1.39
10	bB	804	CLA	CHD-C4C	3.59	1.47	1.39
10	bA	809	CLA	C3D-C2D	3.59	1.48	1.39
10	cA	854	CLA	C3D-C2D	3.59	1.48	1.39
10	cB	832	CLA	OBD-CAD	3.59	1.28	1.22
10	bL	202	CLA	CHD-C4C	3.58	1.47	1.39
10	aB	822	CLA	C3D-C2D	3.58	1.48	1.39
10	aA	812	CLA	OBD-CAD	3.58	1.28	1.22
10	aB	835	CLA	C3D-C2D	3.58	1.48	1.39
10	bA	807	CLA	C3D-C2D	3.58	1.48	1.39
10	aA	854	CLA	C3D-C2D	3.58	1.48	1.39
10	cA	812	CLA	OBD-CAD	3.58	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	809	CLA	C3D-C2D	3.58	1.48	1.39
10	bB	805	CLA	CHD-C4C	3.58	1.47	1.39
10	cB	829	CLA	CHD-C4C	3.58	1.47	1.39
10	bB	825	CLA	OBD-CAD	3.58	1.28	1.22
10	bA	823	CLA	C3D-C2D	3.58	1.48	1.39
10	cA	823	CLA	C3D-C2D	3.57	1.48	1.39
10	cA	816	CLA	C3D-C2D	3.57	1.48	1.39
10	bB	822	CLA	C3D-C2D	3.57	1.48	1.39
10	cB	822	CLA	C3D-C2D	3.57	1.48	1.39
10	aA	856	CLA	OBD-CAD	3.57	1.28	1.22
10	cB	812	CLA	C3D-C2D	3.57	1.48	1.39
10	cB	841	CLA	C3D-C2D	3.57	1.48	1.39
10	aB	832	CLA	OBD-CAD	3.57	1.28	1.22
10	cA	856	CLA	OBD-CAD	3.57	1.28	1.22
10	cA	808	CLA	OBD-CAD	3.57	1.28	1.22
10	bA	812	CLA	OBD-CAD	3.57	1.28	1.22
10	aA	823	CLA	C3D-C2D	3.57	1.48	1.39
10	cB	805	CLA	CHD-C1D	3.57	1.45	1.38
10	cA	806	CLA	OBD-CAD	3.57	1.28	1.22
10	cA	842	CLA	CHD-C4C	3.57	1.47	1.39
10	cA	818	CLA	OBD-CAD	3.57	1.28	1.22
10	bA	854	CLA	C3D-C2D	3.56	1.48	1.39
10	cA	835	CLA	C3D-C2D	3.56	1.48	1.39
10	aL	204	CLA	C3D-C2D	3.56	1.48	1.39
10	bA	822	CLA	OBD-CAD	3.56	1.28	1.22
10	cA	829	CLA	CHD-C4C	3.56	1.47	1.39
10	cL	203	CLA	C3D-C2D	3.56	1.48	1.39
10	cB	815	CLA	C3D-C2D	3.56	1.48	1.39
10	bA	813	CLA	OBD-CAD	3.56	1.28	1.22
10	aB	824	CLA	OBD-CAD	3.56	1.28	1.22
10	bA	815	CLA	OBD-CAD	3.56	1.28	1.22
10	bB	839	CLA	C3D-C2D	3.56	1.48	1.39
10	aA	829	CLA	CHD-C4C	3.56	1.47	1.39
10	cA	819	CLA	OBD-CAD	3.56	1.28	1.22
10	cB	840	CLA	CHD-C4C	3.56	1.47	1.39
10	aA	835	CLA	C3D-C2D	3.55	1.48	1.39
10	cB	831	CLA	OBD-CAD	3.55	1.28	1.22
10	bA	819	CLA	OBD-CAD	3.55	1.28	1.22
10	cB	806	CLA	C3D-C2D	3.55	1.48	1.39
10	bB	835	CLA	OBD-CAD	3.55	1.28	1.22
10	cA	807	CLA	C3D-C2D	3.55	1.48	1.39
10	cA	822	CLA	OBD-CAD	3.55	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	818	CLA	OBD-CAD	3.55	1.28	1.22
10	cA	817	CLA	C3D-C2D	3.55	1.48	1.39
10	bA	806	CLA	OBD-CAD	3.55	1.28	1.22
10	cA	820	CLA	OBD-CAD	3.55	1.28	1.22
10	bA	854	CLA	OBD-CAD	3.55	1.28	1.22
10	cB	805	CLA	CHD-C4C	3.55	1.47	1.39
10	aA	822	CLA	OBD-CAD	3.55	1.28	1.22
10	aB	802	CLA	CHD-C1D	3.54	1.45	1.38
10	aA	807	CLA	C3D-C2D	3.54	1.48	1.39
10	bA	816	CLA	C3D-C2D	3.54	1.48	1.39
10	bA	835	CLA	C3D-C2D	3.54	1.48	1.39
10	bB	831	CLA	OBD-CAD	3.54	1.28	1.22
10	aB	806	CLA	C3D-C2D	3.54	1.48	1.39
10	aB	840	CLA	CHD-C4C	3.54	1.47	1.39
10	bA	856	CLA	OBD-CAD	3.54	1.28	1.22
10	bB	806	CLA	C3D-C2D	3.54	1.48	1.39
10	bB	805	CLA	CHD-C1D	3.54	1.45	1.38
10	aB	835	CLA	OBD-CAD	3.54	1.28	1.22
10	bB	815	CLA	C3D-C2D	3.54	1.48	1.39
10	bA	817	CLA	C3D-C2D	3.54	1.48	1.39
10	aA	814	CLA	OBD-CAD	3.54	1.28	1.22
10	aB	831	CLA	OBD-CAD	3.54	1.28	1.22
10	aB	805	CLA	CHD-C1D	3.53	1.45	1.38
10	aA	808	CLA	CHD-C4C	3.53	1.47	1.39
10	cA	835	CLA	OBD-CAD	3.53	1.28	1.22
10	aB	815	CLA	OBD-CAD	3.53	1.28	1.22
10	aA	808	CLA	OBD-CAD	3.53	1.28	1.22
10	aB	815	CLA	C3D-C2D	3.53	1.48	1.39
10	bB	840	CLA	CHD-C4C	3.53	1.47	1.39
10	cA	811	CLA	OBD-CAD	3.53	1.28	1.22
10	aA	817	CLA	C3D-C2D	3.53	1.48	1.39
10	bA	839	CLA	OBD-CAD	3.53	1.28	1.22
10	aA	806	CLA	OBD-CAD	3.53	1.28	1.22
10	cB	824	CLA	OBD-CAD	3.53	1.28	1.22
10	cA	814	CLA	OBD-CAD	3.52	1.28	1.22
10	aA	854	CLA	OBD-CAD	3.52	1.28	1.22
10	cA	808	CLA	CHD-C4C	3.52	1.47	1.39
10	cB	815	CLA	OBD-CAD	3.52	1.28	1.22
10	aB	839	CLA	C3D-C2D	3.52	1.48	1.39
10	aA	819	CLA	OBD-CAD	3.52	1.28	1.22
10	bA	837	CLA	C3D-C2D	3.52	1.48	1.39
10	bA	814	CLA	OBD-CAD	3.52	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	816	CLA	C3D-C2D	3.52	1.48	1.39
10	aA	832	CLA	C3D-C2D	3.52	1.48	1.39
10	bB	807	CLA	C3D-C2D	3.52	1.48	1.39
10	bA	835	CLA	OBD-CAD	3.52	1.28	1.22
10	bB	815	CLA	OBD-CAD	3.51	1.28	1.22
10	aA	807	CLA	OBD-CAD	3.51	1.28	1.22
10	bA	808	CLA	OBD-CAD	3.51	1.28	1.22
10	cA	832	CLA	C3D-C2D	3.51	1.48	1.39
10	bB	834	CLA	OBD-CAD	3.51	1.28	1.22
10	cB	839	CLA	C3D-C2D	3.51	1.48	1.39
10	cB	834	CLA	OBD-CAD	3.51	1.28	1.22
10	cB	807	CLA	C3D-C2D	3.51	1.48	1.39
10	cA	841	CLA	OBD-CAD	3.51	1.28	1.22
10	bA	808	CLA	CHD-C4C	3.51	1.47	1.39
10	aA	810	CLA	OBD-CAD	3.50	1.28	1.22
10	cA	839	CLA	OBD-CAD	3.50	1.28	1.22
10	aA	839	CLA	OBD-CAD	3.50	1.28	1.22
10	bB	824	CLA	OBD-CAD	3.50	1.28	1.22
10	bA	841	CLA	OBD-CAD	3.50	1.28	1.22
10	bA	807	CLA	OBD-CAD	3.50	1.28	1.22
10	cA	810	CLA	OBD-CAD	3.50	1.28	1.22
10	aA	811	CLA	OBD-CAD	3.50	1.28	1.22
10	cA	837	CLA	C3D-C2D	3.50	1.48	1.39
10	cB	802	CLA	CHD-C1D	3.50	1.45	1.38
10	bA	832	CLA	C3D-C2D	3.50	1.48	1.39
10	aA	837	CLA	C3D-C2D	3.50	1.48	1.39
10	bB	802	CLA	CHD-C1D	3.50	1.45	1.38
10	aA	820	CLA	OBD-CAD	3.50	1.28	1.22
10	bA	811	CLA	OBD-CAD	3.49	1.28	1.22
10	cA	854	CLA	OBD-CAD	3.49	1.28	1.22
10	aB	829	CLA	OBD-CAD	3.49	1.28	1.22
10	aA	841	CLA	OBD-CAD	3.49	1.28	1.22
10	cB	810	CLA	CHD-C4C	3.49	1.47	1.39
9	bA	801	CL0	C3D-C2D	3.49	1.48	1.39
10	aB	807	CLA	C3D-C2D	3.48	1.48	1.39
10	aA	829	CLA	OBD-CAD	3.48	1.28	1.22
10	cB	835	CLA	OBD-CAD	3.48	1.28	1.22
10	bB	833	CLA	OBD-CAD	3.48	1.28	1.22
10	cA	807	CLA	OBD-CAD	3.48	1.28	1.22
10	bA	826	CLA	C3D-C2D	3.48	1.48	1.39
10	aB	806	CLA	OBD-CAD	3.48	1.28	1.22
10	aA	835	CLA	OBD-CAD	3.48	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	820	CLA	OBD-CAD	3.48	1.28	1.22
10	cB	829	CLA	OBD-CAD	3.47	1.28	1.22
10	aB	805	CLA	C1D-ND	3.47	1.42	1.37
10	bA	817	CLA	OBD-CAD	3.47	1.28	1.22
10	cB	806	CLA	OBD-CAD	3.47	1.28	1.22
10	bA	810	CLA	OBD-CAD	3.47	1.28	1.22
10	bB	811	CLA	CHD-C4C	3.47	1.47	1.39
10	aB	811	CLA	CHD-C4C	3.47	1.47	1.39
10	cB	818	CLA	OBD-CAD	3.46	1.28	1.22
9	cA	801	CL0	C3D-C2D	3.46	1.48	1.39
10	cA	826	CLA	C3D-C2D	3.46	1.48	1.39
10	aB	818	CLA	OBD-CAD	3.46	1.28	1.22
10	cB	833	CLA	OBD-CAD	3.46	1.28	1.22
10	bB	829	CLA	OBD-CAD	3.46	1.28	1.22
10	aB	834	CLA	OBD-CAD	3.46	1.28	1.22
10	bB	806	CLA	OBD-CAD	3.45	1.28	1.22
10	aB	833	CLA	OBD-CAD	3.45	1.28	1.22
10	cA	829	CLA	OBD-CAD	3.45	1.28	1.22
10	bB	805	CLA	C1D-ND	3.45	1.42	1.37
10	cA	823	CLA	OBD-CAD	3.45	1.28	1.22
9	aA	801	CL0	C3D-C2D	3.45	1.48	1.39
10	aB	810	CLA	CHD-C4C	3.45	1.47	1.39
10	cB	827	CLA	C3D-C2D	3.45	1.48	1.39
10	cA	825	CLA	C3D-C2D	3.45	1.48	1.39
10	aA	817	CLA	OBD-CAD	3.45	1.28	1.22
10	bB	810	CLA	CHD-C4C	3.45	1.47	1.39
10	aA	824	CLA	C3D-C2D	3.45	1.48	1.39
10	bB	808	CLA	C3D-C2D	3.45	1.48	1.39
10	bA	824	CLA	C3D-C2D	3.45	1.48	1.39
10	aB	808	CLA	C3D-C2D	3.44	1.48	1.39
10	cA	838	CLA	C3D-C2D	3.44	1.48	1.39
10	bB	827	CLA	C3D-C2D	3.44	1.48	1.39
10	aA	822	CLA	C3D-C2D	3.44	1.48	1.39
10	aB	827	CLA	C3D-C2D	3.44	1.48	1.39
10	aA	825	CLA	C3D-C2D	3.44	1.48	1.39
10	cB	812	CLA	OBD-CAD	3.44	1.28	1.22
10	bB	818	CLA	OBD-CAD	3.44	1.28	1.22
10	bA	825	CLA	C3D-C2D	3.44	1.48	1.39
10	bB	812	CLA	OBD-CAD	3.44	1.28	1.22
10	bB	803	CLA	CHD-C4C	3.44	1.47	1.39
10	cB	808	CLA	C3D-C2D	3.43	1.48	1.39
10	aA	826	CLA	C3D-C2D	3.43	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	823	CLA	OBD-CAD	3.43	1.28	1.22
10	cB	811	CLA	CHD-C4C	3.43	1.47	1.39
10	aB	812	CLA	OBD-CAD	3.43	1.28	1.22
10	aA	823	CLA	OBD-CAD	3.43	1.28	1.22
10	cB	802	CLA	OBD-CAD	3.43	1.28	1.22
10	cA	818	CLA	C1B-NB	-3.43	1.32	1.35
10	aA	838	CLA	C3D-C2D	3.43	1.48	1.39
10	bA	822	CLA	C3D-C2D	3.43	1.48	1.39
10	cB	805	CLA	C1D-ND	3.43	1.42	1.37
10	bA	805	CLA	OBD-CAD	3.42	1.28	1.22
10	cA	817	CLA	OBD-CAD	3.42	1.28	1.22
10	bA	829	CLA	OBD-CAD	3.42	1.28	1.22
10	cA	822	CLA	C3D-C2D	3.42	1.48	1.39
10	bA	838	CLA	C3D-C2D	3.41	1.48	1.39
10	cA	805	CLA	OBD-CAD	3.41	1.28	1.22
10	aA	802	CLA	OBD-CAD	3.41	1.28	1.22
10	aB	819	CLA	OBD-CAD	3.41	1.28	1.22
10	cA	824	CLA	C3D-C2D	3.41	1.48	1.39
10	aB	810	CLA	C3D-C2D	3.41	1.48	1.39
10	aB	803	CLA	CHD-C4C	3.41	1.47	1.39
10	cA	804	CLA	C3D-C2D	3.41	1.48	1.39
10	cB	837	CLA	OBD-CAD	3.41	1.28	1.22
10	cB	810	CLA	C3D-C2D	3.40	1.48	1.39
10	bB	830	CLA	C3D-C2D	3.40	1.48	1.39
10	cA	827	CLA	C3D-C2D	3.40	1.48	1.39
10	bL	202	CLA	C3D-C2D	3.40	1.48	1.39
10	cL	202	CLA	C3D-C2D	3.40	1.48	1.39
10	bB	830	CLA	OBD-CAD	3.40	1.28	1.22
10	aL	202	CLA	C3D-C2D	3.40	1.48	1.39
10	bA	802	CLA	OBD-CAD	3.40	1.28	1.22
10	aA	804	CLA	C3D-C2D	3.40	1.48	1.39
10	cB	830	CLA	OBD-CAD	3.40	1.28	1.22
10	bA	821	CLA	OBD-CAD	3.40	1.28	1.22
10	cB	830	CLA	C3D-C2D	3.40	1.48	1.39
10	cB	803	CLA	CHD-C4C	3.39	1.47	1.39
10	bB	810	CLA	C3D-C2D	3.39	1.48	1.39
10	bB	819	CLA	OBD-CAD	3.39	1.28	1.22
13	aA	846	BCR	C1-C6	-3.39	1.49	1.53
10	aB	837	CLA	OBD-CAD	3.39	1.28	1.22
10	aB	819	CLA	C1B-NB	-3.39	1.32	1.35
10	aB	830	CLA	C3D-C2D	3.39	1.48	1.39
10	cB	834	CLA	C3D-C2D	3.39	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	837	CLA	OBD-CAD	3.39	1.28	1.22
10	cA	802	CLA	OBD-CAD	3.39	1.28	1.22
10	cA	821	CLA	OBD-CAD	3.39	1.28	1.22
10	aA	821	CLA	OBD-CAD	3.38	1.28	1.22
10	bA	804	CLA	C3D-C2D	3.38	1.48	1.39
10	aB	803	CLA	OBD-CAD	3.38	1.28	1.22
10	aA	824	CLA	OBD-CAD	3.38	1.28	1.22
10	bB	802	CLA	OBD-CAD	3.38	1.28	1.22
10	cB	819	CLA	OBD-CAD	3.38	1.28	1.22
10	aB	834	CLA	C3D-C2D	3.38	1.48	1.39
10	bA	836	CLA	C3D-C2D	3.38	1.48	1.39
9	aA	801	CL0	CHD-C4C	3.38	1.46	1.39
10	aA	818	CLA	C1B-NB	-3.37	1.32	1.35
10	aA	805	CLA	OBD-CAD	3.37	1.28	1.22
10	aB	830	CLA	OBD-CAD	3.37	1.28	1.22
9	cA	801	CL0	CHD-C4C	3.37	1.46	1.39
10	aA	836	CLA	C3D-C2D	3.37	1.48	1.39
10	bA	832	CLA	OBD-CAD	3.37	1.28	1.22
10	aA	833	CLA	OBD-CAD	3.36	1.28	1.22
10	bB	828	CLA	CHD-C1D	3.36	1.44	1.38
10	aA	827	CLA	C3D-C2D	3.36	1.48	1.39
10	bB	802	CLA	C1D-ND	3.36	1.41	1.37
10	bB	834	CLA	C3D-C2D	3.36	1.48	1.39
10	cA	830	CLA	OBD-CAD	3.36	1.28	1.22
10	aL	204	CLA	OBD-CAD	3.36	1.28	1.22
10	cB	819	CLA	C1B-NB	-3.36	1.32	1.35
10	cA	836	CLA	C3D-C2D	3.36	1.48	1.39
10	bB	803	CLA	OBD-CAD	3.36	1.28	1.22
10	cA	824	CLA	OBD-CAD	3.35	1.28	1.22
10	aB	829	CLA	C3D-C2D	3.35	1.48	1.39
10	bB	819	CLA	C1B-NB	-3.35	1.32	1.35
10	aB	802	CLA	C1D-ND	3.35	1.41	1.37
10	cL	203	CLA	OBD-CAD	3.35	1.28	1.22
10	cL	204	CLA	OBD-CAD	3.35	1.28	1.22
10	aB	828	CLA	CHD-C1D	3.35	1.44	1.38
10	cB	841	CLA	OBD-CAD	3.35	1.28	1.22
9	bA	801	CL0	CHD-C4C	3.35	1.46	1.39
10	cB	803	CLA	OBD-CAD	3.35	1.28	1.22
10	aL	203	CLA	OBD-CAD	3.35	1.28	1.22
10	bL	205	CLA	OBD-CAD	3.35	1.28	1.22
10	cB	802	CLA	C1D-ND	3.35	1.41	1.37
10	cB	829	CLA	C3D-C2D	3.34	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	803	CLA	C3D-C2D	3.34	1.48	1.39
10	bA	824	CLA	OBD-CAD	3.34	1.28	1.22
10	bB	829	CLA	C3D-C2D	3.34	1.48	1.39
10	bA	827	CLA	C3D-C2D	3.34	1.48	1.39
10	cA	833	CLA	OBD-CAD	3.34	1.28	1.22
13	cA	846	BCR	C1-C6	-3.34	1.49	1.53
10	bB	803	CLA	C3D-C2D	3.34	1.48	1.39
10	aB	803	CLA	C3D-C2D	3.33	1.48	1.39
10	bL	204	CLA	OBD-CAD	3.33	1.28	1.22
10	bB	810	CLA	C1B-NB	-3.33	1.32	1.35
10	cL	205	CLA	OBD-CAD	3.33	1.28	1.22
10	cA	832	CLA	OBD-CAD	3.33	1.28	1.22
10	cB	828	CLA	C3D-C2D	3.33	1.48	1.39
10	bL	203	CLA	OBD-CAD	3.33	1.28	1.22
10	aB	802	CLA	OBD-CAD	3.33	1.28	1.22
10	bA	830	CLA	OBD-CAD	3.33	1.28	1.22
10	bA	833	CLA	OBD-CAD	3.33	1.28	1.22
13	bA	846	BCR	C1-C6	-3.32	1.49	1.53
10	cB	828	CLA	CHD-C1D	3.32	1.44	1.38
10	aB	810	CLA	C1B-NB	-3.31	1.32	1.35
10	cB	810	CLA	C1B-NB	-3.31	1.32	1.35
10	aA	830	CLA	OBD-CAD	3.31	1.28	1.22
10	bB	828	CLA	C3D-C2D	3.31	1.48	1.39
10	aB	841	CLA	OBD-CAD	3.31	1.28	1.22
10	aL	205	CLA	OBD-CAD	3.31	1.28	1.22
10	aB	828	CLA	C3D-C2D	3.31	1.48	1.39
10	cB	828	CLA	CHD-C4C	3.31	1.46	1.39
10	bB	841	CLA	OBD-CAD	3.30	1.28	1.22
10	aA	832	CLA	OBD-CAD	3.30	1.28	1.22
10	aA	838	CLA	OBD-CAD	3.30	1.28	1.22
10	bA	827	CLA	OBD-CAD	3.30	1.28	1.22
10	bA	842	CLA	OBD-CAD	3.30	1.28	1.22
10	bA	818	CLA	C1B-NB	-3.30	1.32	1.35
10	aB	828	CLA	CHD-C4C	3.30	1.46	1.39
10	cA	827	CLA	OBD-CAD	3.30	1.28	1.22
10	bB	828	CLA	CHD-C4C	3.30	1.46	1.39
10	aB	805	CLA	C1B-NB	-3.28	1.32	1.35
10	aA	827	CLA	OBD-CAD	3.28	1.28	1.22
10	cB	809	CLA	OBD-CAD	3.28	1.28	1.22
10	aB	814	CLA	OBD-CAD	3.27	1.28	1.22
10	bB	809	CLA	OBD-CAD	3.27	1.28	1.22
10	aB	809	CLA	OBD-CAD	3.27	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	816	CLA	OBD-CAD	3.27	1.28	1.22
10	bB	805	CLA	C1B-NB	-3.27	1.32	1.35
10	bA	838	CLA	OBD-CAD	3.27	1.28	1.22
10	bB	814	CLA	OBD-CAD	3.27	1.28	1.22
10	cA	838	CLA	OBD-CAD	3.27	1.28	1.22
10	bB	826	CLA	OBD-CAD	3.26	1.28	1.22
10	aA	804	CLA	OBD-CAD	3.26	1.28	1.22
10	aB	816	CLA	OBD-CAD	3.26	1.28	1.22
9	bA	801	CL0	OBD-CAD	3.26	1.28	1.22
10	bL	204	CLA	CHD-C1D	3.25	1.44	1.38
9	aA	801	CL0	OBD-CAD	3.25	1.28	1.22
10	cB	816	CLA	OBD-CAD	3.25	1.28	1.22
9	cA	801	CL0	OBD-CAD	3.25	1.28	1.22
10	cB	814	CLA	OBD-CAD	3.24	1.28	1.22
10	cL	204	CLA	CHD-C1D	3.24	1.44	1.38
10	aA	842	CLA	OBD-CAD	3.24	1.28	1.22
10	bA	808	CLA	C3D-C2D	3.24	1.48	1.39
10	aA	808	CLA	C3D-C2D	3.24	1.48	1.39
10	aL	204	CLA	CHD-C1D	3.23	1.44	1.38
10	cA	808	CLA	C3D-C2D	3.23	1.47	1.39
10	cB	826	CLA	OBD-CAD	3.23	1.28	1.22
10	cA	842	CLA	OBD-CAD	3.22	1.28	1.22
10	bA	804	CLA	OBD-CAD	3.22	1.28	1.22
10	cA	836	CLA	C1B-NB	-3.21	1.32	1.35
10	aB	826	CLA	OBD-CAD	3.20	1.28	1.22
10	cB	805	CLA	C1B-NB	-3.20	1.32	1.35
10	aB	805	CLA	OBD-CAD	3.19	1.28	1.22
10	cA	804	CLA	OBD-CAD	3.19	1.28	1.22
10	cB	810	CLA	OBD-CAD	3.18	1.28	1.22
10	bA	831	CLA	OBD-CAD	3.18	1.28	1.22
10	bB	810	CLA	OBD-CAD	3.17	1.27	1.22
10	aB	828	CLA	OBD-CAD	3.16	1.27	1.22
10	cB	805	CLA	OBD-CAD	3.16	1.27	1.22
10	aB	810	CLA	OBD-CAD	3.16	1.27	1.22
10	bB	828	CLA	OBD-CAD	3.16	1.27	1.22
10	cB	828	CLA	OBD-CAD	3.14	1.27	1.22
13	cB	845	BCR	C1-C6	-3.13	1.49	1.53
13	bB	843	BCR	C1-C6	-3.12	1.49	1.53
10	bB	805	CLA	OBD-CAD	3.12	1.27	1.22
10	aB	839	CLA	OBD-CAD	3.11	1.27	1.22
10	cA	831	CLA	OBD-CAD	3.11	1.27	1.22
13	bB	846	BCR	C30-C25	-3.11	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	836	CLA	C1B-NB	-3.10	1.32	1.35
13	cB	846	BCR	C30-C25	-3.09	1.49	1.53
10	aA	831	CLA	OBD-CAD	3.09	1.27	1.22
10	bB	839	CLA	OBD-CAD	3.09	1.27	1.22
10	cB	839	CLA	OBD-CAD	3.08	1.27	1.22
10	aA	836	CLA	C1B-NB	-3.07	1.32	1.35
13	cB	843	BCR	C1-C6	-3.07	1.49	1.53
10	aB	840	CLA	C3D-C2D	3.07	1.47	1.39
10	cB	840	CLA	C3D-C2D	3.07	1.47	1.39
10	bB	840	CLA	C3D-C2D	3.06	1.47	1.39
13	aB	843	BCR	C1-C6	-3.06	1.49	1.53
13	bB	845	BCR	C1-C6	-3.06	1.49	1.53
13	aB	846	BCR	C30-C25	-3.05	1.49	1.53
10	bB	829	CLA	C1B-NB	-3.04	1.32	1.35
10	aB	840	CLA	C3D-C4D	-3.04	1.37	1.44
13	cA	849	BCR	C1-C6	-3.03	1.49	1.53
10	bB	840	CLA	C3D-C4D	-3.03	1.37	1.44
13	aB	845	BCR	C1-C6	-3.03	1.49	1.53
10	cB	829	CLA	C1B-NB	-3.02	1.32	1.35
13	aA	849	BCR	C1-C6	-3.02	1.49	1.53
13	bA	849	BCR	C1-C6	-3.02	1.49	1.53
10	cB	840	CLA	C3D-C4D	-3.01	1.37	1.44
10	bA	826	CLA	OBD-CAD	2.99	1.27	1.22
13	cM	101	BCR	C30-C25	-2.99	1.49	1.53
13	bM	101	BCR	C30-C25	-2.99	1.49	1.53
13	aM	101	BCR	C30-C25	-2.98	1.49	1.53
10	cA	826	CLA	OBD-CAD	2.98	1.27	1.22
10	aA	826	CLA	OBD-CAD	2.96	1.27	1.22
10	cA	835	CLA	C1B-NB	-2.96	1.32	1.35
13	cA	850	BCR	C30-C25	-2.95	1.49	1.53
13	bA	850	BCR	C30-C25	-2.94	1.49	1.53
13	aA	850	BCR	C30-C25	-2.93	1.49	1.53
10	aB	829	CLA	C1B-NB	-2.93	1.32	1.35
10	cL	204	CLA	C1B-NB	-2.91	1.32	1.35
10	cB	804	CLA	OBD-CAD	2.91	1.27	1.22
13	bL	207	BCR	C30-C25	-2.90	1.49	1.53
10	bB	804	CLA	C1B-NB	-2.89	1.32	1.35
10	aB	804	CLA	OBD-CAD	2.89	1.27	1.22
10	bA	843	CLA	OBD-CAD	2.88	1.28	1.23
13	aL	207	BCR	C30-C25	-2.88	1.49	1.53
10	cA	843	CLA	OBD-CAD	2.88	1.28	1.23
10	aB	804	CLA	C1B-NB	-2.87	1.32	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	804	CLA	C1B-NB	-2.87	1.32	1.35
10	bA	835	CLA	C1B-NB	-2.87	1.32	1.35
10	aA	830	CLA	C1B-NB	-2.86	1.32	1.35
10	bB	827	CLA	OBD-CAD	2.86	1.27	1.22
10	bB	804	CLA	OBD-CAD	2.86	1.27	1.22
10	cA	825	CLA	OBD-CAD	2.86	1.27	1.22
10	aA	843	CLA	OBD-CAD	2.86	1.28	1.23
10	aL	204	CLA	C1B-NB	-2.86	1.32	1.35
10	bA	834	CLA	C1B-NB	-2.85	1.32	1.35
10	aA	835	CLA	C1B-NB	-2.85	1.32	1.35
10	aB	805	CLA	C1C-NC	-2.85	1.33	1.37
10	bB	805	CLA	C1C-NC	-2.85	1.33	1.37
10	cB	826	CLA	C1B-NB	-2.85	1.32	1.35
13	aM	101	BCR	C1-C6	-2.84	1.49	1.53
13	bM	101	BCR	C1-C6	-2.84	1.49	1.53
13	cL	207	BCR	C30-C25	-2.84	1.49	1.53
10	cB	807	CLA	C1B-NB	-2.83	1.32	1.35
10	bL	204	CLA	C1B-NB	-2.83	1.32	1.35
10	aA	825	CLA	OBD-CAD	2.83	1.27	1.22
10	cB	827	CLA	OBD-CAD	2.82	1.27	1.22
10	bB	808	CLA	OBD-CAD	2.81	1.27	1.22
10	bA	831	CLA	C1B-NB	-2.81	1.32	1.35
13	cM	101	BCR	C1-C6	-2.81	1.49	1.53
13	cI	102	BCR	C1-C6	-2.81	1.49	1.53
10	aB	827	CLA	OBD-CAD	2.80	1.27	1.22
10	bB	826	CLA	C1B-NB	-2.80	1.32	1.35
10	aB	807	CLA	C1B-NB	-2.80	1.32	1.35
10	cB	838	CLA	OBD-CAD	2.79	1.27	1.22
10	bA	825	CLA	OBD-CAD	2.79	1.27	1.22
10	aA	831	CLA	C1B-NB	-2.79	1.32	1.35
10	cB	811	CLA	OBD-CAD	2.79	1.27	1.22
10	aB	808	CLA	OBD-CAD	2.78	1.27	1.22
13	bI	101	BCR	C1-C6	-2.78	1.49	1.53
10	cA	832	CLA	C1B-NB	-2.78	1.32	1.35
10	bA	830	CLA	C1B-NB	-2.78	1.32	1.35
10	aB	826	CLA	C1B-NB	-2.78	1.32	1.35
10	cB	805	CLA	C1C-NC	-2.77	1.33	1.37
10	bB	838	CLA	OBD-CAD	2.77	1.27	1.22
10	cB	812	CLA	C1B-NB	-2.77	1.32	1.35
10	aA	805	CLA	C1B-NB	-2.77	1.32	1.35
10	aA	836	CLA	C4B-NB	-2.77	1.32	1.35
10	cL	202	CLA	OBD-CAD	2.76	1.27	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	834	CLA	C1B-NB	-2.76	1.32	1.35
10	cB	808	CLA	OBD-CAD	2.76	1.27	1.22
10	cA	830	CLA	C1B-NB	-2.76	1.32	1.35
10	cA	856	CLA	C4D-CHA	2.75	1.48	1.38
10	bB	807	CLA	C1B-NB	-2.75	1.32	1.35
10	cA	831	CLA	C1B-NB	-2.75	1.32	1.35
10	aB	838	CLA	OBD-CAD	2.75	1.27	1.22
10	bB	830	CLA	C3D-C4D	-2.74	1.38	1.44
10	aB	830	CLA	C3D-C4D	-2.74	1.38	1.44
10	bA	803	CLA	C4D-CHA	2.74	1.48	1.38
10	bB	835	CLA	C4D-CHA	2.74	1.48	1.38
10	aL	202	CLA	OBD-CAD	2.74	1.27	1.22
10	aB	840	CLA	C1B-NB	-2.74	1.32	1.35
10	bA	856	CLA	C4D-CHA	2.74	1.48	1.38
10	aA	832	CLA	C1B-NB	-2.74	1.32	1.35
10	aA	856	CLA	C4D-CHA	2.73	1.48	1.38
13	aI	101	BCR	C1-C6	-2.73	1.50	1.53
10	cA	825	CLA	C3D-C4D	-2.73	1.38	1.44
10	bB	811	CLA	OBD-CAD	2.73	1.27	1.22
9	bA	801	CL0	C1B-NB	-2.73	1.32	1.35
10	aB	825	CLA	C1B-NB	-2.73	1.32	1.35
10	bA	836	CLA	C4B-NB	-2.73	1.32	1.35
10	aB	835	CLA	C4D-CHA	2.72	1.48	1.38
10	aA	838	CLA	C1B-NB	-2.72	1.32	1.35
10	cB	816	CLA	C4D-CHA	2.72	1.48	1.38
10	aB	818	CLA	C1B-NB	-2.72	1.32	1.35
10	aA	834	CLA	C1B-NB	-2.72	1.32	1.35
10	bB	812	CLA	C1B-NB	-2.72	1.32	1.35
10	bA	825	CLA	C3D-C4D	-2.72	1.38	1.44
10	cB	823	CLA	C4D-CHA	2.72	1.48	1.38
10	aB	831	CLA	C4D-CHA	2.72	1.48	1.38
10	bB	840	CLA	C1B-NB	-2.72	1.32	1.35
10	aA	825	CLA	C3D-C4D	-2.71	1.38	1.44
10	aA	810	CLA	C4D-CHA	2.71	1.48	1.38
10	cB	835	CLA	C4D-CHA	2.71	1.48	1.38
10	bB	816	CLA	C4D-CHA	2.71	1.48	1.38
10	bB	823	CLA	C4D-CHA	2.71	1.48	1.38
10	cB	831	CLA	C4D-CHA	2.71	1.48	1.38
10	bL	202	CLA	OBD-CAD	2.71	1.27	1.22
10	cA	803	CLA	C4D-CHA	2.71	1.48	1.38
10	aA	803	CLA	C4D-CHA	2.71	1.48	1.38
10	aB	816	CLA	C4D-CHA	2.71	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	832	CLA	C1B-NB	-2.71	1.32	1.35
10	bB	818	CLA	C1B-NB	-2.71	1.32	1.35
13	bB	849	BCR	C30-C25	-2.70	1.50	1.53
10	aB	836	CLA	C4D-CHA	2.70	1.48	1.38
10	cB	830	CLA	C3D-C4D	-2.70	1.38	1.44
10	cA	836	CLA	C4B-NB	-2.70	1.32	1.35
10	aA	836	CLA	C3D-C4D	-2.70	1.38	1.44
10	bB	831	CLA	C4D-CHA	2.70	1.48	1.38
10	cB	840	CLA	C1B-NB	-2.69	1.32	1.35
10	bA	839	CLA	C4D-CHA	2.69	1.48	1.38
10	aA	839	CLA	C4D-CHA	2.69	1.48	1.38
10	aB	827	CLA	C4D-CHA	2.69	1.48	1.38
10	aB	823	CLA	C4D-CHA	2.69	1.48	1.38
10	aB	812	CLA	C1B-NB	-2.69	1.32	1.35
10	bA	842	CLA	C1B-NB	-2.69	1.32	1.35
10	bA	810	CLA	C4D-CHA	2.69	1.48	1.38
10	bA	836	CLA	C3D-C4D	-2.69	1.38	1.44
10	cA	810	CLA	C4D-CHA	2.69	1.47	1.38
13	aB	845	BCR	C30-C25	-2.69	1.50	1.53
10	bB	817	CLA	C4D-CHA	2.68	1.47	1.38
10	aB	828	CLA	C1B-NB	-2.68	1.32	1.35
10	cB	818	CLA	C1B-NB	-2.68	1.32	1.35
10	cB	801	CLA	OBD-CAD	2.67	1.27	1.22
10	aA	805	CLA	C4D-CHA	2.67	1.47	1.38
10	aB	817	CLA	C4D-CHA	2.67	1.47	1.38
10	bA	838	CLA	C1B-NB	-2.67	1.32	1.35
10	bB	836	CLA	C4D-CHA	2.67	1.47	1.38
10	cB	827	CLA	C4D-CHA	2.67	1.47	1.38
13	aB	849	BCR	C30-C25	-2.67	1.50	1.53
10	cB	836	CLA	C4D-CHA	2.67	1.47	1.38
13	cB	847	BCR	C30-C25	-2.67	1.50	1.53
10	aB	811	CLA	OBD-CAD	2.67	1.27	1.22
13	bB	845	BCR	C30-C25	-2.67	1.50	1.53
10	bB	828	CLA	C1B-NB	-2.67	1.32	1.35
10	bB	827	CLA	C4D-CHA	2.67	1.47	1.38
10	cB	817	CLA	C4D-CHA	2.67	1.47	1.38
10	cA	843	CLA	C4C-C3C	2.67	1.49	1.45
13	aB	847	BCR	C30-C25	-2.67	1.50	1.53
10	cA	836	CLA	OBD-CAD	2.67	1.27	1.22
10	aA	838	CLA	C3D-C4D	-2.67	1.38	1.44
10	aB	826	CLA	C3D-C4D	-2.67	1.38	1.44
10	cA	836	CLA	C3D-C4D	-2.67	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	826	CLA	C3D-C4D	-2.66	1.38	1.44
10	bB	801	CLA	OBD-CAD	2.66	1.27	1.22
10	cA	839	CLA	C4D-CHA	2.66	1.47	1.38
10	bA	826	CLA	C3D-C4D	-2.66	1.38	1.44
10	cB	830	CLA	C4C-C3C	2.66	1.49	1.45
10	aA	826	CLA	C3D-C4D	-2.66	1.38	1.44
10	aA	836	CLA	OBD-CAD	2.66	1.27	1.22
10	cA	827	CLA	C1B-NB	-2.66	1.32	1.35
10	cA	805	CLA	C4D-CHA	2.65	1.47	1.38
10	aB	824	CLA	C4D-CHA	2.65	1.47	1.38
13	aA	850	BCR	C1-C6	-2.65	1.50	1.53
10	aA	807	CLA	C4D-CHA	2.65	1.47	1.38
10	cA	804	CLA	C3D-C4D	-2.65	1.38	1.44
10	bA	836	CLA	OBD-CAD	2.65	1.27	1.22
10	cA	807	CLA	C4D-CHA	2.65	1.47	1.38
13	cA	850	BCR	C1-C6	-2.65	1.50	1.53
10	bA	805	CLA	C4D-CHA	2.65	1.47	1.38
10	cB	820	CLA	C4C-C3C	2.65	1.49	1.45
10	aL	203	CLA	C1B-NB	-2.65	1.32	1.35
10	bA	828	CLA	C1B-NB	-2.65	1.32	1.35
10	aA	802	CLA	C4D-CHA	2.65	1.47	1.38
10	bB	824	CLA	C4D-CHA	2.65	1.47	1.38
10	cA	816	CLA	C4D-CHA	2.65	1.47	1.38
10	cB	826	CLA	C3D-C4D	-2.65	1.38	1.44
10	bA	854	CLA	C1B-NB	-2.65	1.32	1.35
10	bA	838	CLA	C3D-C4D	-2.64	1.38	1.44
10	aA	813	CLA	C4D-CHA	2.64	1.47	1.38
10	bA	802	CLA	C4D-CHA	2.64	1.47	1.38
10	cA	805	CLA	C1B-NB	-2.64	1.32	1.35
10	cA	824	CLA	C1B-NB	-2.64	1.32	1.35
10	aA	819	CLA	C4D-CHA	2.64	1.47	1.38
10	aA	824	CLA	C1B-NB	-2.64	1.32	1.35
10	aB	820	CLA	C1B-NB	-2.64	1.32	1.35
10	bA	807	CLA	C4D-CHA	2.64	1.47	1.38
10	bB	830	CLA	C4C-C3C	2.64	1.49	1.45
10	bB	826	CLA	C3D-C4D	-2.64	1.38	1.44
10	cA	813	CLA	C4D-CHA	2.64	1.47	1.38
10	aL	202	CLA	C3D-C4D	-2.64	1.38	1.44
10	cA	838	CLA	C3D-C4D	-2.64	1.38	1.44
13	aA	851	BCR	C30-C25	-2.64	1.50	1.53
10	bA	819	CLA	C4D-CHA	2.64	1.47	1.38
10	cB	821	CLA	C4D-CHA	2.63	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	828	CLA	C1B-NB	-2.63	1.32	1.35
13	bA	850	BCR	C1-C6	-2.63	1.50	1.53
10	aB	821	CLA	C4D-CHA	2.63	1.47	1.38
10	bL	202	CLA	C4D-CHA	2.63	1.47	1.38
10	cA	837	CLA	C3D-C4D	-2.63	1.38	1.44
10	aB	801	CLA	OBD-CAD	2.63	1.27	1.22
10	bB	841	CLA	C4D-CHA	2.63	1.47	1.38
10	bA	827	CLA	C1B-NB	-2.63	1.32	1.35
10	bA	813	CLA	C4D-CHA	2.63	1.47	1.38
10	cA	819	CLA	C4D-CHA	2.63	1.47	1.38
10	aB	833	CLA	C4D-CHA	2.63	1.47	1.38
10	bA	814	CLA	C4D-CHA	2.63	1.47	1.38
10	bA	837	CLA	C3D-C4D	-2.63	1.38	1.44
10	bA	843	CLA	C4C-C3C	2.63	1.49	1.45
10	cB	824	CLA	C4D-CHA	2.63	1.47	1.38
13	cB	849	BCR	C30-C25	-2.63	1.50	1.53
10	aA	809	CLA	C4D-CHA	2.63	1.47	1.38
10	aA	837	CLA	C3D-C4D	-2.63	1.38	1.44
10	aA	827	CLA	C1B-NB	-2.63	1.32	1.35
13	bA	851	BCR	C30-C25	-2.63	1.50	1.53
10	aB	830	CLA	C4C-C3C	2.63	1.49	1.45
10	bB	833	CLA	C4D-CHA	2.63	1.47	1.38
10	bA	816	CLA	C4D-CHA	2.63	1.47	1.38
10	bB	820	CLA	C4C-C3C	2.63	1.49	1.45
10	aA	816	CLA	C4D-CHA	2.63	1.47	1.38
10	cA	802	CLA	C4D-CHA	2.63	1.47	1.38
10	cB	828	CLA	C1B-NB	-2.63	1.32	1.35
10	aA	843	CLA	C4C-C3C	2.63	1.49	1.45
10	cA	823	CLA	C4D-CHA	2.63	1.47	1.38
10	cA	822	CLA	C4D-CHA	2.63	1.47	1.38
10	cB	841	CLA	C4D-CHA	2.63	1.47	1.38
10	aA	854	CLA	C1B-NB	-2.62	1.32	1.35
10	bL	202	CLA	C3D-C4D	-2.62	1.38	1.44
10	bA	809	CLA	C4D-CHA	2.62	1.47	1.38
10	cB	803	CLA	C1B-NB	-2.62	1.32	1.35
10	cA	837	CLA	OBD-CAD	2.62	1.27	1.22
10	bA	841	CLA	C4D-CHA	2.62	1.47	1.38
10	aA	814	CLA	C4D-CHA	2.62	1.47	1.38
10	aA	842	CLA	C1B-NB	-2.62	1.32	1.35
10	aL	202	CLA	C4D-CHA	2.62	1.47	1.38
10	cA	809	CLA	C4D-CHA	2.62	1.47	1.38
10	aA	804	CLA	C3D-C4D	-2.62	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	840	CLA	C4B-CHC	2.62	1.48	1.41
10	aB	811	CLA	C3D-C4D	-2.62	1.38	1.44
10	aA	822	CLA	C4D-CHA	2.62	1.47	1.38
10	cB	833	CLA	C4D-CHA	2.61	1.47	1.38
10	aA	823	CLA	C4D-CHA	2.61	1.47	1.38
10	aA	817	CLA	C4D-CHA	2.61	1.47	1.38
10	aA	841	CLA	C4D-CHA	2.61	1.47	1.38
10	cL	202	CLA	C4D-CHA	2.61	1.47	1.38
10	cA	842	CLA	C1B-NB	-2.61	1.32	1.35
10	bB	841	CLA	C1C-NC	-2.61	1.33	1.37
10	bB	815	CLA	C4D-CHA	2.61	1.47	1.38
10	bB	810	CLA	C3D-C4D	-2.61	1.38	1.44
10	bB	821	CLA	C4D-CHA	2.61	1.47	1.38
10	cA	814	CLA	C4D-CHA	2.61	1.47	1.38
10	bB	813	CLA	C4D-CHA	2.61	1.47	1.38
10	bB	839	CLA	C3D-C4D	-2.61	1.38	1.44
10	aB	815	CLA	C4D-CHA	2.61	1.47	1.38
10	cB	813	CLA	C4D-CHA	2.61	1.47	1.38
10	cB	815	CLA	C4D-CHA	2.61	1.47	1.38
10	aB	803	CLA	C1B-NB	-2.61	1.32	1.35
10	bA	804	CLA	C3D-C4D	-2.61	1.38	1.44
10	cA	821	CLA	C4D-CHA	2.61	1.47	1.38
10	cA	840	CLA	C4B-CHC	2.61	1.48	1.41
10	aB	835	CLA	C1B-NB	-2.61	1.32	1.35
13	bB	847	BCR	C30-C25	-2.60	1.50	1.53
10	cB	820	CLA	C4D-CHA	2.60	1.47	1.38
10	cA	841	CLA	C4D-CHA	2.60	1.47	1.38
10	cA	817	CLA	C4D-CHA	2.60	1.47	1.38
10	aB	810	CLA	C3D-C4D	-2.60	1.38	1.44
10	aB	841	CLA	C4D-CHA	2.60	1.47	1.38
10	aA	820	CLA	C1B-NB	-2.60	1.32	1.35
10	bA	817	CLA	C4D-CHA	2.60	1.47	1.38
13	cI	103	BCR	C30-C25	-2.60	1.50	1.53
10	bA	822	CLA	C4D-CHA	2.60	1.47	1.38
10	bB	809	CLA	C3D-C4D	-2.60	1.38	1.44
10	cB	841	CLA	C3D-C4D	-2.60	1.38	1.44
10	cA	815	CLA	C4D-CHA	2.60	1.47	1.38
10	cB	825	CLA	C1B-NB	-2.60	1.32	1.35
10	bA	837	CLA	OBD-CAD	2.60	1.27	1.22
10	bA	823	CLA	C4D-CHA	2.60	1.47	1.38
10	bA	832	CLA	C3D-C4D	-2.60	1.38	1.44
10	aA	837	CLA	OBD-CAD	2.60	1.27	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	820	CLA	C1B-NB	-2.60	1.32	1.35
10	aB	813	CLA	C4D-CHA	2.60	1.47	1.38
10	aA	815	CLA	C4D-CHA	2.60	1.47	1.38
10	cB	825	CLA	C4D-CHA	2.60	1.47	1.38
10	bB	825	CLA	C4D-CHA	2.60	1.47	1.38
10	aA	833	CLA	C4D-CHA	2.60	1.47	1.38
10	aB	820	CLA	C4D-CHA	2.60	1.47	1.38
10	cA	854	CLA	C4D-CHA	2.60	1.47	1.38
10	cB	810	CLA	C3D-C4D	-2.60	1.38	1.44
10	bB	820	CLA	C4D-CHA	2.60	1.47	1.38
10	bA	840	CLA	C4B-CHC	2.60	1.48	1.41
10	aA	854	CLA	C4D-CHA	2.60	1.47	1.38
10	aB	841	CLA	C3D-C4D	-2.59	1.38	1.44
10	aB	808	CLA	C4D-CHA	2.59	1.47	1.38
10	aB	841	CLA	C1C-NC	-2.59	1.33	1.37
10	cB	841	CLA	C1C-NC	-2.59	1.33	1.37
10	bB	811	CLA	C3D-C4D	-2.59	1.38	1.44
10	aB	827	CLA	C3D-C4D	-2.59	1.38	1.44
10	bA	815	CLA	C4D-CHA	2.59	1.47	1.38
10	bA	833	CLA	C4D-CHA	2.59	1.47	1.38
10	aA	826	CLA	C4D-CHA	2.59	1.47	1.38
10	aB	825	CLA	C4D-CHA	2.59	1.47	1.38
10	bA	824	CLA	C1B-NB	-2.59	1.32	1.35
9	cA	801	CL0	C1B-NB	-2.59	1.32	1.35
10	cL	203	CLA	C1B-NB	-2.59	1.32	1.35
10	cA	831	CLA	C4D-CHA	2.59	1.47	1.38
10	cA	854	CLA	C1B-NB	-2.59	1.32	1.35
10	bA	821	CLA	C4D-CHA	2.59	1.47	1.38
10	bA	818	CLA	C4D-CHA	2.59	1.47	1.38
13	cA	851	BCR	C30-C25	-2.59	1.50	1.53
10	cA	828	CLA	C4D-CHA	2.59	1.47	1.38
13	cB	845	BCR	C30-C25	-2.59	1.50	1.53
10	cB	827	CLA	C3D-C4D	-2.59	1.38	1.44
10	cB	826	CLA	C4D-CHA	2.59	1.47	1.38
10	bB	827	CLA	C3D-C4D	-2.59	1.38	1.44
10	bB	803	CLA	C1B-NB	-2.59	1.32	1.35
13	aI	102	BCR	C1-C6	-2.59	1.50	1.53
10	aB	839	CLA	C3D-C4D	-2.59	1.38	1.44
10	cA	836	CLA	C4D-CHA	2.59	1.47	1.38
10	cA	833	CLA	C4D-CHA	2.58	1.47	1.38
10	aA	821	CLA	C4D-CHA	2.58	1.47	1.38
10	cA	820	CLA	C4D-CHA	2.58	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	808	CLA	C4D-CHA	2.58	1.47	1.38
10	cB	808	CLA	C3D-C4D	-2.58	1.38	1.44
10	cL	202	CLA	C3D-C4D	-2.58	1.38	1.44
9	aA	801	CL0	C1B-NB	-2.58	1.32	1.35
10	aA	828	CLA	C1B-NB	-2.58	1.32	1.35
10	cA	840	CLA	C4D-CHA	2.58	1.47	1.38
10	aA	832	CLA	C3D-C4D	-2.58	1.38	1.44
10	aB	829	CLA	C3D-C4D	-2.58	1.38	1.44
10	bB	807	CLA	OBD-CAD	2.58	1.26	1.22
10	aB	820	CLA	C4C-C3C	2.58	1.49	1.45
10	aB	806	CLA	C4D-CHA	2.58	1.47	1.38
13	aB	843	BCR	C30-C25	-2.58	1.50	1.53
13	bB	843	BCR	C30-C25	-2.58	1.50	1.53
10	bA	830	CLA	C3D-C4D	-2.58	1.38	1.44
10	cB	818	CLA	C4D-CHA	2.58	1.47	1.38
10	bB	808	CLA	C4D-CHA	2.58	1.47	1.38
10	cA	806	CLA	C4D-CHA	2.58	1.47	1.38
10	cA	838	CLA	C1B-NB	-2.58	1.32	1.35
10	cB	815	CLA	C1B-NB	-2.58	1.32	1.35
10	cA	825	CLA	C1C-C2C	2.58	1.49	1.44
10	aB	808	CLA	C3D-C4D	-2.58	1.38	1.44
10	cB	811	CLA	C3D-C4D	-2.58	1.38	1.44
10	cB	832	CLA	C4D-CHA	2.58	1.47	1.38
10	cA	818	CLA	C4D-CHA	2.58	1.47	1.38
10	aA	828	CLA	C4D-CHA	2.58	1.47	1.38
10	bA	831	CLA	C4D-CHA	2.58	1.47	1.38
10	cA	830	CLA	C4D-CHA	2.58	1.47	1.38
10	aB	828	CLA	C3D-C4D	-2.57	1.38	1.44
10	bA	828	CLA	C4D-CHA	2.57	1.47	1.38
10	bB	826	CLA	C4D-CHA	2.57	1.47	1.38
10	bB	818	CLA	C4D-CHA	2.57	1.47	1.38
10	aA	830	CLA	C4D-CHA	2.57	1.47	1.38
10	aA	831	CLA	C4D-CHA	2.57	1.47	1.38
10	aA	840	CLA	C4D-CHA	2.57	1.47	1.38
10	cB	838	CLA	C3D-C4D	-2.57	1.38	1.44
10	aB	818	CLA	C4D-CHA	2.57	1.47	1.38
10	bA	826	CLA	C4D-CHA	2.57	1.47	1.38
10	bB	828	CLA	C3D-C4D	-2.57	1.38	1.44
10	bL	203	CLA	C1B-NB	-2.57	1.32	1.35
10	aB	807	CLA	OBD-CAD	2.57	1.26	1.22
10	bA	806	CLA	C4D-CHA	2.57	1.47	1.38
10	aA	836	CLA	C4D-CHA	2.57	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	819	CLA	C4D-CHA	2.57	1.47	1.38
10	cB	807	CLA	OBD-CAD	2.57	1.26	1.22
10	bA	825	CLA	C1C-C2C	2.57	1.49	1.44
10	aB	822	CLA	C4D-CHA	2.57	1.47	1.38
10	bA	836	CLA	C4D-CHA	2.57	1.47	1.38
10	bB	829	CLA	C3D-C4D	-2.57	1.38	1.44
10	aB	809	CLA	C3D-C4D	-2.57	1.38	1.44
10	cB	820	CLA	C1B-NB	-2.57	1.32	1.35
10	bA	824	CLA	C4D-CHA	2.56	1.47	1.38
10	bB	822	CLA	C4D-CHA	2.56	1.47	1.38
10	aA	825	CLA	C1C-C2C	2.56	1.49	1.44
10	bB	825	CLA	C1B-NB	-2.56	1.32	1.35
10	bA	811	CLA	C4D-CHA	2.56	1.47	1.38
10	bB	841	CLA	C3D-C4D	-2.56	1.38	1.44
10	cB	822	CLA	C4D-CHA	2.56	1.47	1.38
10	cA	828	CLA	OBD-CAD	2.56	1.26	1.22
10	bA	830	CLA	C4D-CHA	2.56	1.47	1.38
10	bA	854	CLA	C4D-CHA	2.56	1.47	1.38
10	cB	808	CLA	C1B-NB	-2.56	1.32	1.35
10	aB	826	CLA	C4D-CHA	2.56	1.47	1.38
10	aA	806	CLA	C4D-CHA	2.56	1.47	1.38
10	bA	840	CLA	C4D-CHA	2.56	1.47	1.38
10	aA	835	CLA	C4D-CHA	2.56	1.47	1.38
10	cA	826	CLA	C4D-CHA	2.56	1.47	1.38
10	cB	829	CLA	C3D-C4D	-2.56	1.38	1.44
10	bA	805	CLA	C1B-NB	-2.56	1.32	1.35
10	aA	818	CLA	C4D-CHA	2.56	1.47	1.38
10	cB	806	CLA	C4D-CHA	2.56	1.47	1.38
10	cB	809	CLA	C3D-C4D	-2.56	1.38	1.44
10	cA	811	CLA	C4D-CHA	2.56	1.47	1.38
10	cB	839	CLA	C3D-C4D	-2.56	1.38	1.44
10	cA	832	CLA	C3D-C4D	-2.55	1.38	1.44
13	cI	103	BCR	C1-C6	-2.55	1.50	1.53
10	aA	826	CLA	C4B-CHC	2.55	1.48	1.41
10	aB	824	CLA	C4C-C3C	2.55	1.49	1.45
10	bB	801	CLA	C3D-C4D	-2.55	1.38	1.44
10	bA	829	CLA	C4D-CHA	2.55	1.47	1.38
10	aA	811	CLA	C4D-CHA	2.55	1.47	1.38
10	bB	808	CLA	C1B-NB	-2.55	1.32	1.35
10	cB	835	CLA	C1B-NB	-2.55	1.32	1.35
10	cA	830	CLA	C3D-C4D	-2.55	1.38	1.44
10	cB	819	CLA	C4D-CHA	2.55	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aL	203	CLA	C4D-CHA	2.55	1.47	1.38
10	cB	828	CLA	C3D-C4D	-2.55	1.38	1.44
10	aA	829	CLA	C4D-CHA	2.55	1.47	1.38
10	aL	202	CLA	C1C-NC	-2.55	1.34	1.37
10	bB	834	CLA	C4C-C3C	2.55	1.49	1.45
9	cA	801	CL0	C3D-C4D	-2.55	1.38	1.44
13	aB	846	BCR	C1-C6	-2.55	1.50	1.53
10	aB	838	CLA	C3D-C4D	-2.55	1.38	1.44
10	aA	820	CLA	C4D-CHA	2.55	1.47	1.38
10	bB	806	CLA	C4D-CHA	2.55	1.47	1.38
10	bB	835	CLA	C1B-NB	-2.55	1.32	1.35
10	cB	830	CLA	C4D-CHA	2.55	1.47	1.38
10	bB	832	CLA	C4D-CHA	2.54	1.47	1.38
13	bI	102	BCR	C1-C6	-2.54	1.50	1.53
10	bB	808	CLA	C3D-C4D	-2.54	1.38	1.44
10	bA	820	CLA	C4D-CHA	2.54	1.47	1.38
10	cA	835	CLA	C4D-CHA	2.54	1.47	1.38
10	cA	824	CLA	C4D-CHA	2.54	1.47	1.38
10	cB	809	CLA	C1B-NB	-2.54	1.32	1.35
10	aB	801	CLA	C3D-C4D	-2.54	1.38	1.44
10	aB	832	CLA	C4D-CHA	2.54	1.47	1.38
10	cA	829	CLA	C4D-CHA	2.54	1.47	1.38
10	aA	830	CLA	C3D-C4D	-2.54	1.38	1.44
10	cB	801	CLA	C3D-C4D	-2.54	1.38	1.44
10	cL	205	CLA	C3D-C4D	-2.54	1.38	1.44
10	aA	824	CLA	C4D-CHA	2.54	1.47	1.38
10	bL	205	CLA	C3D-C4D	-2.54	1.38	1.44
10	bL	205	CLA	C4D-CHA	2.54	1.47	1.38
10	cL	203	CLA	C4D-CHA	2.54	1.47	1.38
13	cA	846	BCR	C30-C25	-2.54	1.50	1.53
10	bA	811	CLA	C1B-NB	-2.54	1.32	1.35
10	bB	819	CLA	C4D-CHA	2.54	1.47	1.38
10	aA	834	CLA	C4D-CHA	2.54	1.47	1.38
10	bL	203	CLA	C4D-CHA	2.54	1.47	1.38
13	bB	846	BCR	C1-C6	-2.54	1.50	1.53
10	bA	828	CLA	OBD-CAD	2.54	1.26	1.22
10	cB	834	CLA	C4C-C3C	2.54	1.49	1.45
10	cB	802	CLA	C4D-CHA	2.54	1.47	1.38
10	cB	838	CLA	C4D-CHA	2.54	1.47	1.38
10	aB	810	CLA	C4D-CHA	2.54	1.47	1.38
9	bA	801	CL0	C3D-C4D	-2.54	1.38	1.44
10	aB	812	CLA	C4D-CHA	2.53	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bL	202	CLA	C1C-NC	-2.53	1.34	1.37
10	cL	202	CLA	C1C-NC	-2.53	1.34	1.37
10	aB	805	CLA	C4B-NB	-2.53	1.32	1.35
10	bA	820	CLA	C1B-NB	-2.53	1.32	1.35
10	aB	838	CLA	C4D-CHA	2.53	1.47	1.38
10	aB	814	CLA	C4C-C3C	2.53	1.49	1.45
10	aB	837	CLA	C4D-CHA	2.53	1.47	1.38
10	bB	810	CLA	C4D-CHA	2.53	1.47	1.38
10	cA	834	CLA	C4D-CHA	2.53	1.47	1.38
10	cB	807	CLA	C4D-CHA	2.53	1.47	1.38
10	cA	820	CLA	C1B-NB	-2.53	1.32	1.35
10	cB	814	CLA	C4D-CHA	2.53	1.47	1.38
10	bB	838	CLA	C3D-C4D	-2.53	1.38	1.44
10	aB	814	CLA	C4D-CHA	2.53	1.47	1.38
10	bA	834	CLA	C4D-CHA	2.53	1.47	1.38
13	cB	843	BCR	C30-C25	-2.53	1.50	1.53
10	aL	205	CLA	C3D-C4D	-2.53	1.38	1.44
10	cA	822	CLA	C1B-NB	-2.53	1.33	1.35
10	bA	835	CLA	C4D-CHA	2.53	1.47	1.38
10	cB	812	CLA	C4D-CHA	2.53	1.47	1.38
10	aL	205	CLA	C4D-CHA	2.53	1.47	1.38
13	bA	846	BCR	C30-C25	-2.52	1.50	1.53
10	bB	837	CLA	C4D-CHA	2.52	1.47	1.38
9	aA	801	CL0	C3D-C4D	-2.52	1.38	1.44
10	aL	203	CLA	C3D-C4D	-2.52	1.38	1.44
10	bB	814	CLA	C4C-C3C	2.52	1.49	1.45
10	aB	807	CLA	C4D-CHA	2.52	1.47	1.38
10	aB	834	CLA	C3D-C4D	-2.52	1.38	1.44
10	aA	825	CLA	C4D-CHA	2.52	1.47	1.38
9	bA	801	CL0	C1B-CHB	2.52	1.48	1.41
10	bB	830	CLA	C4D-CHA	2.52	1.47	1.38
10	aB	840	CLA	OBD-CAD	2.52	1.26	1.22
10	cA	826	CLA	C4B-CHC	2.52	1.48	1.41
10	aA	810	CLA	C4C-C3C	2.52	1.49	1.45
10	bL	203	CLA	C3D-C4D	-2.52	1.38	1.44
10	cL	203	CLA	C3D-C4D	-2.52	1.38	1.44
9	cA	801	CL0	C1B-CHB	2.52	1.48	1.41
13	aA	846	BCR	C30-C25	-2.52	1.50	1.53
10	bB	805	CLA	C4B-NB	-2.52	1.33	1.35
10	bB	809	CLA	C4D-CHA	2.52	1.47	1.38
10	cB	814	CLA	C4C-C3C	2.52	1.49	1.45
10	cA	827	CLA	C3D-C4D	-2.52	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	810	CLA	C4C-C3C	2.51	1.49	1.45
10	cB	805	CLA	C4B-NB	-2.51	1.33	1.35
10	aB	834	CLA	C4C-C3C	2.51	1.49	1.45
10	bA	842	CLA	C4D-CHA	2.51	1.47	1.38
10	cL	205	CLA	C4D-CHA	2.51	1.47	1.38
10	bB	802	CLA	C4D-CHA	2.51	1.47	1.38
10	bB	812	CLA	C4D-CHA	2.51	1.47	1.38
10	cA	835	CLA	C3D-C4D	-2.51	1.38	1.44
10	aA	838	CLA	C4D-CHA	2.51	1.47	1.38
10	aA	828	CLA	OBD-CAD	2.51	1.26	1.22
10	aB	815	CLA	C1B-NB	-2.51	1.33	1.35
13	bI	102	BCR	C30-C25	-2.51	1.50	1.53
10	bA	808	CLA	C4B-CHC	2.51	1.48	1.41
10	aB	840	CLA	C4D-CHA	2.51	1.47	1.38
10	cA	825	CLA	C4D-CHA	2.51	1.47	1.38
10	bB	804	CLA	C4D-CHA	2.51	1.47	1.38
10	aB	809	CLA	C4D-CHA	2.51	1.47	1.38
10	aA	827	CLA	C3D-C4D	-2.51	1.38	1.44
10	bB	809	CLA	C1B-NB	-2.51	1.33	1.35
10	bB	814	CLA	C4D-CHA	2.51	1.47	1.38
10	cB	837	CLA	C4D-CHA	2.51	1.47	1.38
10	bB	838	CLA	C4D-CHA	2.51	1.47	1.38
10	bB	824	CLA	C4C-C3C	2.51	1.49	1.45
10	cB	804	CLA	C4D-CHA	2.51	1.47	1.38
10	aB	802	CLA	C4D-CHA	2.51	1.47	1.38
10	aB	830	CLA	C4D-CHA	2.51	1.47	1.38
10	bA	825	CLA	C4D-CHA	2.51	1.47	1.38
10	cB	824	CLA	C4C-C3C	2.51	1.49	1.45
10	cB	840	CLA	C4D-CHA	2.50	1.47	1.38
9	aA	801	CL0	C1B-CHB	2.50	1.48	1.41
13	cB	846	BCR	C1-C6	-2.50	1.50	1.53
10	bB	807	CLA	C4D-CHA	2.50	1.47	1.38
10	bB	815	CLA	C1B-NB	-2.50	1.33	1.35
10	bA	808	CLA	C4D-CHA	2.50	1.47	1.38
10	cB	809	CLA	C4D-CHA	2.50	1.47	1.38
10	cA	832	CLA	C4D-CHA	2.50	1.47	1.38
10	cA	838	CLA	C4D-CHA	2.50	1.47	1.38
10	aB	819	CLA	C3D-C4D	-2.50	1.38	1.44
10	cB	810	CLA	C4D-CHA	2.50	1.47	1.38
10	aA	842	CLA	C4D-CHA	2.50	1.47	1.38
10	bA	838	CLA	C4D-CHA	2.50	1.47	1.38
10	bA	826	CLA	C4B-CHC	2.50	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	842	CLA	C3D-C4D	-2.50	1.38	1.44
10	cA	817	CLA	C1B-NB	-2.50	1.33	1.35
10	aB	804	CLA	C4D-CHA	2.50	1.47	1.38
10	bA	827	CLA	C3D-C4D	-2.50	1.38	1.44
10	aB	839	CLA	C4D-CHA	2.50	1.47	1.38
10	bB	811	CLA	C4D-CHA	2.49	1.47	1.38
10	bB	838	CLA	C1B-NB	-2.49	1.33	1.35
10	bA	842	CLA	C3D-C4D	-2.49	1.38	1.44
10	aA	808	CLA	C4D-CHA	2.49	1.47	1.38
10	bB	840	CLA	C4D-CHA	2.49	1.47	1.38
10	aB	808	CLA	C1B-NB	-2.49	1.33	1.35
10	bB	839	CLA	C4D-CHA	2.49	1.47	1.38
10	aB	823	CLA	C4C-C3C	2.49	1.49	1.45
13	aI	102	BCR	C30-C25	-2.49	1.50	1.53
10	cA	842	CLA	C3D-C4D	-2.49	1.38	1.44
13	bA	848	BCR	C30-C25	-2.49	1.50	1.53
10	bB	834	CLA	C3D-C4D	-2.49	1.38	1.44
10	aA	832	CLA	C4D-CHA	2.49	1.47	1.38
10	cA	842	CLA	C4D-CHA	2.49	1.47	1.38
10	cB	803	CLA	C3D-C4D	-2.49	1.38	1.44
10	cB	814	CLA	C3D-C4D	-2.49	1.38	1.44
13	bB	844	BCR	C30-C25	-2.49	1.50	1.53
10	cB	828	CLA	C4D-CHA	2.49	1.47	1.38
10	cL	204	CLA	C3D-C4D	-2.49	1.38	1.44
10	aA	817	CLA	C3D-C4D	-2.49	1.38	1.44
10	cA	808	CLA	C4B-CHC	2.49	1.47	1.41
10	bA	835	CLA	C3D-C4D	-2.49	1.38	1.44
10	aL	204	CLA	C3D-C4D	-2.49	1.38	1.44
10	bA	832	CLA	C4D-CHA	2.49	1.47	1.38
10	cB	834	CLA	C3D-C4D	-2.49	1.38	1.44
10	cB	840	CLA	OBD-CAD	2.49	1.26	1.22
10	aA	811	CLA	C1B-NB	-2.49	1.33	1.35
10	bB	840	CLA	OBD-CAD	2.48	1.26	1.22
10	cA	837	CLA	C1B-NB	-2.48	1.33	1.35
10	aA	835	CLA	C3D-C4D	-2.48	1.38	1.44
10	aA	808	CLA	C3D-C4D	-2.48	1.38	1.44
10	cA	808	CLA	C4D-CHA	2.48	1.47	1.38
10	bB	828	CLA	C4D-CHA	2.48	1.47	1.38
10	bL	204	CLA	C3D-C4D	-2.48	1.38	1.44
10	bB	836	CLA	C4C-C3C	2.48	1.49	1.45
10	bB	819	CLA	C3D-C4D	-2.48	1.38	1.44
10	bA	810	CLA	C4C-C3C	2.48	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	839	CLA	C4D-CHA	2.48	1.47	1.38
10	cB	819	CLA	C3D-C4D	-2.48	1.38	1.44
10	aB	836	CLA	C4C-C3C	2.48	1.49	1.45
10	aA	837	CLA	C4D-CHA	2.47	1.47	1.38
10	bA	808	CLA	C3D-C4D	-2.47	1.38	1.44
10	aB	834	CLA	C4B-CHC	2.47	1.47	1.41
10	bB	807	CLA	C3D-C4D	-2.47	1.38	1.44
13	aA	848	BCR	C30-C25	-2.47	1.50	1.53
10	aA	808	CLA	C4B-CHC	2.47	1.47	1.41
10	aB	811	CLA	C4D-CHA	2.47	1.47	1.38
10	bA	831	CLA	C3D-C4D	-2.47	1.38	1.44
10	bB	823	CLA	C4C-C3C	2.47	1.49	1.45
10	cA	817	CLA	C3D-C4D	-2.47	1.38	1.44
10	bB	806	CLA	C1B-NB	-2.47	1.33	1.35
10	cB	823	CLA	C4C-C3C	2.47	1.49	1.45
10	bB	814	CLA	C3D-C4D	-2.47	1.38	1.44
10	aB	807	CLA	C3D-C4D	-2.46	1.38	1.44
10	cA	841	CLA	C3D-C4D	-2.46	1.38	1.44
10	aB	814	CLA	C3D-C4D	-2.46	1.38	1.44
10	cA	837	CLA	C4D-CHA	2.46	1.47	1.38
10	aB	829	CLA	C4D-CHA	2.46	1.47	1.38
10	aB	809	CLA	C1B-NB	-2.46	1.33	1.35
10	aA	812	CLA	C4D-CHA	2.46	1.47	1.38
10	cB	811	CLA	C4D-CHA	2.46	1.47	1.38
10	bA	817	CLA	C3D-C4D	-2.46	1.38	1.44
10	bA	812	CLA	C4D-CHA	2.46	1.47	1.38
10	aB	828	CLA	C4D-CHA	2.46	1.47	1.38
10	bA	827	CLA	C4D-CHA	2.46	1.47	1.38
10	aB	803	CLA	C3D-C4D	-2.46	1.38	1.44
10	cB	836	CLA	C4C-C3C	2.46	1.49	1.45
10	bB	811	CLA	C1C-NC	-2.46	1.34	1.37
10	cA	812	CLA	C4D-CHA	2.45	1.47	1.38
10	cB	810	CLA	C1C-NC	-2.45	1.34	1.37
10	cA	833	CLA	C3D-C4D	-2.45	1.38	1.44
10	cB	807	CLA	C3D-C4D	-2.45	1.38	1.44
10	cA	840	CLA	C1C-C2C	2.45	1.49	1.44
10	bA	837	CLA	C4D-CHA	2.45	1.47	1.38
10	cA	827	CLA	C4D-CHA	2.45	1.47	1.38
10	cB	829	CLA	C4D-CHA	2.45	1.47	1.38
10	cB	831	CLA	C4C-C3C	2.45	1.49	1.45
10	bB	829	CLA	C4D-CHA	2.45	1.47	1.38
10	bA	840	CLA	C1C-C2C	2.45	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	819	CLA	C4C-C3C	2.44	1.49	1.45
10	bB	801	CLA	C4D-CHA	2.44	1.47	1.38
10	cB	801	CLA	C4D-CHA	2.44	1.47	1.38
10	bA	819	CLA	C4C-C3C	2.44	1.49	1.45
10	aA	827	CLA	C4D-CHA	2.44	1.47	1.38
13	aB	844	BCR	C30-C25	-2.44	1.50	1.53
10	aB	840	CLA	C4B-CHC	2.44	1.47	1.41
10	bA	833	CLA	C3D-C4D	-2.44	1.38	1.44
10	bA	837	CLA	C1B-NB	-2.44	1.33	1.35
13	bA	851	BCR	C1-C6	-2.44	1.50	1.53
10	bB	810	CLA	C1C-NC	-2.44	1.34	1.37
10	cA	808	CLA	C3D-C4D	-2.44	1.38	1.44
10	cA	819	CLA	C4C-C3C	2.44	1.49	1.45
10	cA	816	CLA	C4B-CHC	2.44	1.47	1.41
10	cA	811	CLA	C1B-NB	-2.44	1.33	1.35
13	cB	844	BCR	C30-C25	-2.44	1.50	1.53
10	aB	812	CLA	C3D-C4D	-2.44	1.38	1.44
10	cB	811	CLA	C1C-NC	-2.44	1.34	1.37
10	aB	801	CLA	C4B-NB	-2.44	1.33	1.35
10	bB	834	CLA	C4B-CHC	2.44	1.47	1.41
10	bB	803	CLA	C3D-C4D	-2.43	1.38	1.44
10	bA	816	CLA	C4B-CHC	2.43	1.47	1.41
9	aA	801	CL0	C4D-CHA	2.43	1.47	1.38
10	aB	810	CLA	C1C-NC	-2.43	1.34	1.37
10	aA	816	CLA	C4B-CHC	2.43	1.47	1.41
10	aA	831	CLA	C3D-C4D	-2.43	1.38	1.44
10	cB	834	CLA	C4B-CHC	2.43	1.47	1.41
10	aB	801	CLA	C4D-CHA	2.43	1.47	1.38
10	aB	806	CLA	C1B-NB	-2.43	1.33	1.35
9	cA	801	CL0	C4D-CHA	2.43	1.47	1.38
10	cA	822	CLA	C1C-C2C	2.43	1.49	1.44
10	aA	837	CLA	C1B-NB	-2.43	1.33	1.35
10	cA	831	CLA	C3D-C4D	-2.43	1.38	1.44
10	aA	822	CLA	C1B-NB	-2.43	1.33	1.35
10	cL	205	CLA	C1B-NB	-2.43	1.33	1.35
10	bA	841	CLA	C3D-C4D	-2.43	1.38	1.44
10	cA	841	CLA	C4B-CHC	2.43	1.47	1.41
10	aB	837	CLA	C3D-C4D	-2.42	1.38	1.44
10	bA	826	CLA	C1C-C2C	2.42	1.49	1.44
10	aA	812	CLA	C3D-C4D	-2.42	1.38	1.44
13	aA	849	BCR	C30-C25	-2.42	1.50	1.53
13	cB	847	BCR	C1-C6	-2.42	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	820	CLA	C4B-CHC	2.42	1.47	1.41
10	bA	828	CLA	C3D-C4D	-2.42	1.38	1.44
10	bA	820	CLA	C4B-CHC	2.42	1.47	1.41
10	aL	204	CLA	C4D-CHA	2.42	1.47	1.38
10	aA	841	CLA	C3D-C4D	-2.42	1.38	1.44
13	cB	849	BCR	C1-C6	-2.42	1.50	1.53
10	aB	826	CLA	C4B-CHC	2.42	1.47	1.41
10	aA	820	CLA	C4B-CHC	2.42	1.47	1.41
10	aA	840	CLA	C1C-C2C	2.42	1.49	1.44
9	bA	801	CL0	C4D-CHA	2.42	1.47	1.38
10	aA	817	CLA	C4B-CHC	2.42	1.47	1.41
10	bB	840	CLA	C4B-CHC	2.42	1.47	1.41
10	bL	204	CLA	C4D-CHA	2.42	1.47	1.38
13	bA	847	BCR	C1-C6	-2.41	1.50	1.53
13	cA	851	BCR	C1-C6	-2.41	1.50	1.53
10	aL	202	CLA	C1B-NB	-2.41	1.33	1.35
10	bA	833	CLA	C4B-NB	-2.41	1.33	1.35
10	aB	811	CLA	C1C-NC	-2.41	1.34	1.37
13	aA	851	BCR	C1-C6	-2.41	1.50	1.53
10	cA	802	CLA	C4C-C3C	2.41	1.49	1.45
10	bA	812	CLA	C3D-C4D	-2.41	1.38	1.44
10	cB	812	CLA	C3D-C4D	-2.41	1.38	1.44
10	cB	818	CLA	C3D-C4D	-2.41	1.38	1.44
10	cB	838	CLA	C1B-NB	-2.41	1.33	1.35
10	bA	841	CLA	C4B-CHC	2.41	1.47	1.41
10	cB	837	CLA	C3D-C4D	-2.41	1.38	1.44
10	cA	831	CLA	C4B-NB	-2.41	1.33	1.35
10	aA	833	CLA	C3D-C4D	-2.41	1.38	1.44
10	cB	834	CLA	C4D-CHA	2.41	1.47	1.38
10	aL	205	CLA	C1B-NB	-2.41	1.33	1.35
10	bA	825	CLA	C4B-CHC	2.41	1.47	1.41
10	cA	817	CLA	C4B-CHC	2.41	1.47	1.41
10	bA	803	CLA	C4B-CHC	2.41	1.47	1.41
10	cA	825	CLA	C4B-CHC	2.41	1.47	1.41
10	bB	840	CLA	C1C-NC	-2.41	1.34	1.37
10	bA	831	CLA	C4B-NB	-2.41	1.33	1.35
10	cA	803	CLA	C4B-CHC	2.41	1.47	1.41
10	aA	822	CLA	C3D-C4D	-2.41	1.38	1.44
10	cA	828	CLA	C3D-C4D	-2.41	1.38	1.44
10	bA	817	CLA	C4B-CHC	2.41	1.47	1.41
10	bB	812	CLA	C3D-C4D	-2.41	1.38	1.44
13	aB	849	BCR	C1-C6	-2.41	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cL	204	CLA	C4D-CHA	2.41	1.47	1.38
10	cB	818	CLA	C4B-CHC	2.41	1.47	1.41
10	cA	813	CLA	C1B-NB	-2.41	1.33	1.35
10	bB	834	CLA	C4D-CHA	2.41	1.47	1.38
10	cA	804	CLA	C4D-CHA	2.41	1.47	1.38
10	cB	840	CLA	C4B-CHC	2.41	1.47	1.41
13	cA	847	BCR	C1-C6	-2.41	1.50	1.53
10	cB	832	CLA	C4B-CHC	2.41	1.47	1.41
10	bA	822	CLA	C1B-NB	-2.41	1.33	1.35
10	bB	805	CLA	C4D-CHA	2.41	1.47	1.38
10	bB	803	CLA	C1C-C2C	2.41	1.49	1.44
10	aB	840	CLA	C1C-NC	-2.40	1.34	1.37
10	bL	202	CLA	C1B-NB	-2.40	1.33	1.35
13	aA	847	BCR	C1-C6	-2.40	1.50	1.53
10	bA	822	CLA	C1C-C2C	2.40	1.49	1.44
10	cA	822	CLA	C3D-C4D	-2.40	1.38	1.44
10	aA	802	CLA	C4C-C3C	2.40	1.49	1.45
10	aB	818	CLA	C3D-C4D	-2.40	1.38	1.44
10	aA	841	CLA	C4B-CHC	2.40	1.47	1.41
13	bA	849	BCR	C30-C25	-2.40	1.50	1.53
10	bB	818	CLA	C3D-C4D	-2.40	1.38	1.44
10	aA	825	CLA	C4B-CHC	2.40	1.47	1.41
10	cA	833	CLA	C1B-NB	-2.40	1.33	1.35
10	cB	814	CLA	C4B-NB	-2.40	1.33	1.35
10	aB	834	CLA	C4D-CHA	2.40	1.46	1.38
10	bB	831	CLA	C4C-C3C	2.40	1.49	1.45
10	cB	826	CLA	C4B-CHC	2.40	1.47	1.41
10	aB	831	CLA	C4C-C3C	2.40	1.49	1.45
10	aA	828	CLA	C3D-C4D	-2.40	1.38	1.44
10	aB	832	CLA	C4B-CHC	2.40	1.47	1.41
10	bB	804	CLA	C1C-C2C	2.39	1.49	1.44
10	aA	819	CLA	C4B-CHC	2.39	1.47	1.41
10	aB	806	CLA	C4B-CHC	2.39	1.47	1.41
10	cB	805	CLA	C4D-CHA	2.39	1.46	1.38
10	aB	805	CLA	C4D-CHA	2.39	1.46	1.38
10	aB	818	CLA	C4B-CHC	2.39	1.47	1.41
10	cB	801	CLA	C4B-NB	-2.39	1.33	1.35
10	aA	803	CLA	C4B-CHC	2.39	1.47	1.41
10	aB	803	CLA	C1C-C2C	2.39	1.49	1.44
10	bB	806	CLA	C4B-CHC	2.39	1.47	1.41
10	bB	837	CLA	C3D-C4D	-2.39	1.38	1.44
10	aB	816	CLA	C4C-C3C	2.39	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	842	CLA	C1C-NC	-2.39	1.34	1.37
10	cB	806	CLA	C4B-CHC	2.39	1.47	1.41
10	aA	826	CLA	C1C-C2C	2.39	1.49	1.44
10	cB	840	CLA	C1C-NC	-2.39	1.34	1.37
10	bA	813	CLA	C1B-NB	-2.39	1.33	1.35
10	aA	804	CLA	C4D-CHA	2.39	1.46	1.38
13	cA	848	BCR	C30-C25	-2.39	1.50	1.53
10	aB	813	CLA	C4B-CHC	2.39	1.47	1.41
10	cB	803	CLA	C1C-C2C	2.38	1.49	1.44
10	bA	837	CLA	C1C-NC	-2.38	1.34	1.37
13	cA	849	BCR	C30-C25	-2.38	1.50	1.53
10	aB	838	CLA	C4B-CHC	2.38	1.47	1.41
10	cA	824	CLA	C4C-C3C	2.38	1.49	1.45
10	bA	804	CLA	C4D-CHA	2.38	1.46	1.38
10	bA	839	CLA	C4C-C3C	2.38	1.49	1.45
10	aA	818	CLA	C3D-C4D	-2.38	1.38	1.44
13	aB	847	BCR	C1-C6	-2.38	1.50	1.53
10	aA	822	CLA	C1C-C2C	2.38	1.49	1.44
10	cB	803	CLA	C4D-CHA	2.38	1.46	1.38
10	bA	843	CLA	C4B-CHC	2.38	1.47	1.41
10	aA	843	CLA	C4B-CHC	2.38	1.47	1.41
10	cA	811	CLA	C4B-CHC	2.38	1.47	1.41
10	cB	825	CLA	C3D-C4D	-2.38	1.38	1.44
10	aB	838	CLA	C1B-NB	-2.38	1.33	1.35
10	cA	808	CLA	C1C-C2C	2.38	1.49	1.44
10	bB	818	CLA	C4B-CHC	2.38	1.47	1.41
10	aB	815	CLA	C3D-C4D	-2.38	1.38	1.44
10	cB	813	CLA	C4B-CHC	2.37	1.47	1.41
10	bA	806	CLA	C4B-CHC	2.37	1.47	1.41
10	aB	804	CLA	C1C-C2C	2.37	1.49	1.44
10	bB	832	CLA	C4B-CHC	2.37	1.47	1.41
10	aA	811	CLA	C4B-CHC	2.37	1.47	1.41
10	cA	812	CLA	C3D-C4D	-2.37	1.38	1.44
10	aB	806	CLA	C1C-C2C	2.37	1.49	1.44
10	bA	806	CLA	C1C-C2C	2.37	1.49	1.44
10	bA	822	CLA	C3D-C4D	-2.37	1.38	1.44
10	aA	831	CLA	C4B-NB	-2.37	1.33	1.35
10	bA	811	CLA	C4B-CHC	2.37	1.47	1.41
10	cA	843	CLA	C4B-CHC	2.37	1.47	1.41
10	bB	806	CLA	C3D-C4D	-2.37	1.38	1.44
10	bB	837	CLA	C4B-CHC	2.37	1.47	1.41
10	aA	806	CLA	C3D-C4D	-2.37	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	803	CLA	C4D-CHA	2.37	1.46	1.38
10	aA	825	CLA	C1B-NB	-2.37	1.33	1.35
10	cA	819	CLA	C4B-CHC	2.37	1.47	1.41
13	bB	849	BCR	C1-C6	-2.37	1.50	1.53
10	cB	806	CLA	C1C-C2C	2.37	1.49	1.44
10	bB	838	CLA	C4B-CHC	2.37	1.47	1.41
10	cA	826	CLA	C1C-C2C	2.37	1.49	1.44
10	aA	838	CLA	C4B-CHC	2.37	1.47	1.41
10	cA	806	CLA	C3D-C4D	-2.37	1.38	1.44
10	aB	837	CLA	C4B-CHC	2.37	1.47	1.41
10	cA	838	CLA	C4B-CHC	2.37	1.47	1.41
10	bA	841	CLA	C1B-NB	-2.37	1.33	1.35
10	bB	825	CLA	C3D-C4D	-2.37	1.38	1.44
10	bB	833	CLA	C3D-C4D	-2.37	1.38	1.44
10	bB	813	CLA	C4B-CHC	2.37	1.47	1.41
10	cB	838	CLA	C4B-CHC	2.37	1.47	1.41
10	bB	826	CLA	C4B-CHC	2.37	1.47	1.41
10	aA	823	CLA	C1B-NB	-2.36	1.33	1.35
10	aA	833	CLA	C4B-NB	-2.36	1.33	1.35
10	bB	819	CLA	C4B-NB	-2.36	1.33	1.35
10	bA	838	CLA	C4B-CHC	2.36	1.47	1.41
10	bB	815	CLA	C3D-C4D	-2.36	1.38	1.44
10	cB	804	CLA	C1C-C2C	2.36	1.49	1.44
10	aA	813	CLA	C1B-NB	-2.36	1.33	1.35
10	bA	819	CLA	C4B-CHC	2.36	1.47	1.41
10	cA	837	CLA	C1C-NC	-2.36	1.34	1.37
10	cA	840	CLA	C3D-C4D	-2.36	1.38	1.44
10	aB	803	CLA	C4D-CHA	2.36	1.46	1.38
10	cA	854	CLA	C4B-CHC	2.36	1.47	1.41
10	cA	823	CLA	C1B-NB	-2.36	1.33	1.35
10	bA	818	CLA	C3D-C4D	-2.36	1.38	1.44
10	cA	839	CLA	C4C-C3C	2.36	1.49	1.45
10	aA	804	CLA	C4B-CHC	2.36	1.47	1.41
10	cA	825	CLA	C1B-NB	-2.36	1.33	1.35
10	cB	837	CLA	C4B-CHC	2.36	1.47	1.41
10	bA	808	CLA	C1C-C2C	2.36	1.49	1.44
10	bA	842	CLA	C1B-CHB	2.36	1.47	1.41
10	bA	806	CLA	C3D-C4D	-2.36	1.38	1.44
10	aA	833	CLA	C1B-NB	-2.36	1.33	1.35
10	aB	839	CLA	C1B-NB	-2.36	1.33	1.35
10	bB	801	CLA	C4B-NB	-2.36	1.33	1.35
10	cB	839	CLA	C1B-NB	-2.36	1.33	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	818	CLA	C3D-C4D	-2.36	1.38	1.44
10	bA	802	CLA	C4C-C3C	2.35	1.49	1.45
10	aB	806	CLA	C3D-C4D	-2.35	1.38	1.44
10	aA	828	CLA	C4B-NB	-2.35	1.33	1.35
10	cB	806	CLA	C1B-NB	-2.35	1.33	1.35
10	bB	835	CLA	C4C-C3C	2.35	1.49	1.45
10	aA	842	CLA	C1B-CHB	2.35	1.47	1.41
10	bB	821	CLA	C4B-CHC	2.35	1.47	1.41
10	cB	806	CLA	C3D-C4D	-2.35	1.38	1.44
10	cB	841	CLA	C1B-NB	-2.35	1.33	1.35
10	bB	816	CLA	C4C-C3C	2.35	1.49	1.45
10	aA	854	CLA	C3D-C4D	-2.35	1.38	1.44
10	cB	831	CLA	C4B-CHC	2.35	1.47	1.41
10	aA	839	CLA	C4C-C3C	2.35	1.49	1.45
10	bL	205	CLA	C1B-NB	-2.35	1.33	1.35
10	aA	806	CLA	C4B-CHC	2.35	1.47	1.41
10	cB	833	CLA	C4B-CHC	2.35	1.47	1.41
10	aB	814	CLA	C4B-NB	-2.35	1.33	1.35
10	aA	854	CLA	C4B-CHC	2.34	1.47	1.41
10	bA	824	CLA	C4C-C3C	2.34	1.49	1.45
10	cA	842	CLA	C1B-CHB	2.34	1.47	1.41
10	bA	825	CLA	C1B-NB	-2.34	1.33	1.35
10	aB	825	CLA	C3D-C4D	-2.34	1.38	1.44
10	cB	832	CLA	C3D-C4D	-2.34	1.38	1.44
10	aA	803	CLA	C4C-C3C	2.34	1.49	1.45
10	aA	814	CLA	C4B-CHC	2.34	1.47	1.41
10	cA	806	CLA	C4B-CHC	2.34	1.47	1.41
10	aA	837	CLA	C1C-NC	-2.34	1.34	1.37
10	cB	839	CLA	C4B-CHC	2.34	1.47	1.41
10	aA	806	CLA	C1C-C2C	2.34	1.49	1.44
10	bA	804	CLA	C4B-CHC	2.34	1.47	1.41
10	cA	804	CLA	C1B-NB	-2.34	1.33	1.35
10	bA	829	CLA	C3D-C4D	-2.34	1.38	1.44
10	bA	854	CLA	C3D-C4D	-2.34	1.38	1.44
10	cA	806	CLA	C1C-C2C	2.34	1.49	1.44
10	aB	831	CLA	C4B-CHC	2.34	1.47	1.41
10	cB	815	CLA	C3D-C4D	-2.34	1.38	1.44
10	cA	805	CLA	C3D-C4D	-2.34	1.38	1.44
10	cB	808	CLA	C4B-CHC	2.34	1.47	1.41
10	bA	854	CLA	C4B-CHC	2.34	1.47	1.41
10	cA	854	CLA	C3D-C4D	-2.34	1.38	1.44
10	cB	816	CLA	C4C-C3C	2.34	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	823	CLA	C1B-NB	-2.34	1.33	1.35
10	bB	806	CLA	C1C-C2C	2.33	1.49	1.44
10	aA	824	CLA	C4C-C3C	2.33	1.49	1.45
10	cB	821	CLA	C4B-CHC	2.33	1.47	1.41
10	aB	835	CLA	C4B-CHC	2.33	1.47	1.41
10	cA	804	CLA	C4B-CHC	2.33	1.47	1.41
10	cA	803	CLA	C4C-C3C	2.33	1.49	1.45
10	aA	822	CLA	C4B-CHC	2.33	1.47	1.41
10	bB	831	CLA	C4B-CHC	2.33	1.47	1.41
10	cA	814	CLA	C4B-CHC	2.33	1.47	1.41
13	aB	844	BCR	C1-C6	-2.33	1.50	1.53
10	aB	821	CLA	C4B-CHC	2.33	1.47	1.41
10	aB	832	CLA	C3D-C4D	-2.33	1.38	1.44
13	cA	848	BCR	C1-C6	-2.33	1.50	1.53
10	aA	808	CLA	C1C-C2C	2.33	1.49	1.44
10	aB	833	CLA	C3D-C4D	-2.33	1.38	1.44
10	cA	818	CLA	C4C-C3C	2.33	1.49	1.45
10	aA	835	CLA	C4B-CHC	2.33	1.47	1.41
10	bA	820	CLA	C3D-C4D	-2.33	1.38	1.44
10	bB	839	CLA	C4B-CHC	2.33	1.47	1.41
10	bA	840	CLA	C3D-C4D	-2.33	1.38	1.44
10	cA	824	CLA	C3D-C4D	-2.33	1.38	1.44
10	bA	817	CLA	C1B-NB	-2.33	1.33	1.35
10	bA	824	CLA	C3D-C4D	-2.33	1.38	1.44
10	bA	856	CLA	C4C-C3C	2.33	1.49	1.45
10	cB	835	CLA	C4C-C3C	2.33	1.49	1.45
10	cB	804	CLA	C4B-CHC	2.33	1.47	1.41
10	bA	815	CLA	C3D-C4D	-2.32	1.38	1.44
10	bA	822	CLA	C4B-CHC	2.32	1.47	1.41
10	cA	822	CLA	C4B-CHC	2.32	1.47	1.41
10	aA	842	CLA	C1C-NC	-2.32	1.34	1.37
10	aB	841	CLA	C1B-NB	-2.32	1.33	1.35
10	cA	820	CLA	C3D-C4D	-2.32	1.38	1.44
10	aB	813	CLA	C4C-C3C	2.32	1.49	1.45
10	cA	829	CLA	C3D-C4D	-2.32	1.38	1.44
10	bB	802	CLA	C4B-NB	-2.32	1.33	1.35
10	cA	828	CLA	C4B-NB	-2.32	1.33	1.35
10	aA	815	CLA	C3D-C4D	-2.32	1.38	1.44
10	aA	803	CLA	C1C-C2C	2.32	1.49	1.44
13	cB	844	BCR	C1-C6	-2.32	1.50	1.53
10	cB	813	CLA	C4C-C3C	2.32	1.49	1.45
10	aA	805	CLA	C3D-C4D	-2.32	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	841	CLA	C1C-C2C	2.32	1.49	1.44
10	cB	831	CLA	C1C-C2C	2.32	1.49	1.44
10	cB	833	CLA	C3D-C4D	-2.32	1.38	1.44
10	aA	818	CLA	C4C-C3C	2.32	1.49	1.45
10	cA	841	CLA	C1B-NB	-2.32	1.33	1.35
10	aA	829	CLA	C3D-C4D	-2.32	1.38	1.44
10	bL	204	CLA	C4B-CHC	2.32	1.47	1.41
10	bA	816	CLA	C1C-C2C	2.32	1.49	1.44
10	aA	817	CLA	C1B-NB	-2.32	1.33	1.35
10	cA	833	CLA	C4B-NB	-2.32	1.33	1.35
10	bA	842	CLA	C1C-NC	-2.32	1.34	1.37
10	aA	840	CLA	C3D-C4D	-2.32	1.38	1.44
10	cA	819	CLA	C3D-C4D	-2.32	1.38	1.44
10	cA	803	CLA	C1C-C2C	2.32	1.49	1.44
10	aB	804	CLA	C4B-CHC	2.32	1.47	1.41
10	bA	807	CLA	C3D-C4D	-2.31	1.38	1.44
10	bB	833	CLA	C4B-CHC	2.31	1.47	1.41
10	aA	824	CLA	C3D-C4D	-2.31	1.39	1.44
10	cB	835	CLA	C4B-CHC	2.31	1.47	1.41
13	aA	848	BCR	C1-C6	-2.31	1.50	1.53
10	bB	814	CLA	C4B-NB	-2.31	1.33	1.35
10	cL	202	CLA	C1B-NB	-2.31	1.33	1.35
13	bB	847	BCR	C1-C6	-2.31	1.50	1.53
10	bA	835	CLA	C4B-CHC	2.31	1.47	1.41
10	bB	804	CLA	C4B-CHC	2.31	1.47	1.41
10	cA	807	CLA	C3D-C4D	-2.31	1.39	1.44
10	aB	833	CLA	C4B-CHC	2.31	1.47	1.41
10	aB	839	CLA	C4B-CHC	2.31	1.47	1.41
10	aB	813	CLA	C3D-C4D	-2.31	1.39	1.44
10	bB	832	CLA	C3D-C4D	-2.31	1.39	1.44
10	cA	815	CLA	C3D-C4D	-2.31	1.39	1.44
10	aA	812	CLA	C4B-CHC	2.31	1.47	1.41
10	bA	815	CLA	C4B-CHC	2.31	1.47	1.41
10	cB	819	CLA	C4B-NB	-2.31	1.33	1.35
10	cA	816	CLA	C1C-C2C	2.31	1.49	1.44
10	bA	826	CLA	C1B-NB	-2.31	1.33	1.35
13	bB	844	BCR	C1-C6	-2.30	1.50	1.53
10	bA	802	CLA	C4B-CHC	2.30	1.47	1.41
10	cA	824	CLA	C4B-CHC	2.30	1.47	1.41
10	aB	807	CLA	C4C-C3C	2.30	1.49	1.45
10	bA	803	CLA	C4C-C3C	2.30	1.49	1.45
10	bB	821	CLA	C3D-C4D	-2.30	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	802	CLA	C4B-CHC	2.30	1.47	1.41
10	cA	809	CLA	C4B-CHC	2.30	1.47	1.41
10	cA	815	CLA	C4B-CHC	2.30	1.47	1.41
10	aA	806	CLA	C4C-C3C	2.30	1.49	1.45
10	cA	828	CLA	C1C-C2C	2.30	1.49	1.44
10	aA	856	CLA	C4C-C3C	2.30	1.49	1.45
10	bA	806	CLA	C4C-C3C	2.30	1.49	1.45
10	bA	833	CLA	C1B-NB	-2.30	1.33	1.35
10	cA	835	CLA	C4B-CHC	2.30	1.47	1.41
10	aB	821	CLA	C3D-C4D	-2.30	1.39	1.44
10	cA	821	CLA	C3D-C4D	-2.30	1.39	1.44
10	bA	814	CLA	C4B-CHC	2.30	1.47	1.41
10	cL	204	CLA	C4B-CHC	2.30	1.47	1.41
10	bB	808	CLA	C4B-CHC	2.30	1.47	1.41
10	cA	856	CLA	C4C-C3C	2.30	1.49	1.45
10	aA	820	CLA	C3D-C4D	-2.30	1.39	1.44
10	bB	823	CLA	C4B-CHC	2.30	1.47	1.41
10	bA	841	CLA	C1C-C2C	2.30	1.49	1.44
10	aA	813	CLA	C3D-C4D	-2.30	1.39	1.44
10	aA	837	CLA	C4B-CHC	2.30	1.47	1.41
10	aB	819	CLA	C4B-NB	-2.30	1.33	1.35
10	aB	831	CLA	C3D-C4D	-2.30	1.39	1.44
10	cB	824	CLA	C4B-CHC	2.30	1.47	1.41
10	aA	809	CLA	C4B-CHC	2.29	1.47	1.41
10	aA	815	CLA	C4B-CHC	2.29	1.47	1.41
10	bB	813	CLA	C3D-C4D	-2.29	1.39	1.44
10	aA	802	CLA	C4B-CHC	2.29	1.47	1.41
10	bA	809	CLA	C4B-CHC	2.29	1.47	1.41
10	aA	807	CLA	C3D-C4D	-2.29	1.39	1.44
10	cA	823	CLA	C3D-C4D	-2.29	1.39	1.44
10	aA	808	CLA	C1B-CHB	2.29	1.47	1.41
10	bB	839	CLA	C1B-NB	-2.29	1.33	1.35
10	aB	808	CLA	C4B-CHC	2.29	1.47	1.41
10	cA	806	CLA	C4C-C3C	2.29	1.49	1.45
10	aB	823	CLA	C4B-CHC	2.29	1.47	1.41
10	bA	808	CLA	C1B-CHB	2.29	1.47	1.41
10	cA	837	CLA	C4B-CHC	2.29	1.47	1.41
10	aA	824	CLA	C4B-CHC	2.29	1.47	1.41
10	bB	841	CLA	C1B-NB	-2.29	1.33	1.35
10	bA	824	CLA	C4B-CHC	2.29	1.47	1.41
10	bA	837	CLA	C4B-CHC	2.29	1.47	1.41
10	bA	812	CLA	C4B-CHC	2.29	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	838	CLA	C1C-NC	-2.29	1.34	1.37
13	bL	206	BCR	C30-C25	-2.29	1.50	1.53
10	bA	813	CLA	C3D-C4D	-2.29	1.39	1.44
10	cB	823	CLA	C4B-CHC	2.29	1.47	1.41
10	aA	840	CLA	C4C-C3C	2.29	1.49	1.45
10	aA	834	CLA	C3D-C4D	-2.29	1.39	1.44
10	aA	828	CLA	C1C-C2C	2.29	1.49	1.44
10	bA	803	CLA	C1C-C2C	2.29	1.49	1.44
10	bA	819	CLA	C3D-C4D	-2.29	1.39	1.44
10	bA	823	CLA	C3D-C4D	-2.29	1.39	1.44
10	cA	808	CLA	C1B-NB	-2.29	1.33	1.35
10	aA	823	CLA	C3D-C4D	-2.28	1.39	1.44
10	bA	828	CLA	C4B-NB	-2.28	1.33	1.35
10	aL	204	CLA	C4B-CHC	2.28	1.47	1.41
10	bB	824	CLA	C4B-CHC	2.28	1.47	1.41
10	aB	831	CLA	C1C-C2C	2.28	1.49	1.44
10	bA	805	CLA	C3D-C4D	-2.28	1.39	1.44
10	bB	807	CLA	C4C-C3C	2.28	1.49	1.45
10	cB	839	CLA	C4C-C3C	2.28	1.49	1.45
10	aB	832	CLA	C1C-C2C	2.28	1.49	1.44
10	bB	835	CLA	C4B-CHC	2.28	1.47	1.41
13	cL	206	BCR	C30-C25	-2.28	1.50	1.53
10	bB	828	CLA	C1B-CHB	2.28	1.47	1.41
10	cA	812	CLA	C4B-CHC	2.28	1.47	1.41
13	aL	206	BCR	C30-C25	-2.28	1.50	1.53
13	bA	848	BCR	C1-C6	-2.28	1.50	1.53
10	cB	813	CLA	C3D-C4D	-2.28	1.39	1.44
10	cA	856	CLA	C4B-CHC	2.28	1.47	1.41
10	bA	810	CLA	C1C-C2C	2.28	1.49	1.44
10	cA	810	CLA	C1C-C2C	2.28	1.49	1.44
10	cB	816	CLA	C4B-CHC	2.28	1.47	1.41
10	cA	838	CLA	C1C-NC	-2.28	1.34	1.37
10	cA	808	CLA	C1B-CHB	2.28	1.47	1.41
10	bA	835	CLA	C4C-C3C	2.28	1.49	1.45
10	cA	812	CLA	C4C-C3C	2.28	1.49	1.45
10	aB	802	CLA	C4B-NB	-2.28	1.33	1.35
10	cA	814	CLA	C3D-C4D	-2.28	1.39	1.44
10	cA	834	CLA	C3D-C4D	-2.28	1.39	1.44
10	bB	835	CLA	C3D-C4D	-2.28	1.39	1.44
10	aB	828	CLA	C1B-CHB	2.28	1.47	1.41
10	cB	821	CLA	C3D-C4D	-2.28	1.39	1.44
13	cI	102	BCR	C30-C25	-2.27	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	821	CLA	C1C-C2C	2.27	1.49	1.44
10	aB	824	CLA	C4B-CHC	2.27	1.47	1.41
10	aB	816	CLA	C4B-CHC	2.27	1.47	1.41
10	cB	840	CLA	C1C-C2C	2.27	1.49	1.44
10	bB	823	CLA	C3D-C4D	-2.27	1.39	1.44
10	cB	802	CLA	C4B-NB	-2.27	1.33	1.35
10	aA	802	CLA	C3D-C4D	-2.27	1.39	1.44
10	bB	827	CLA	C4B-CHC	2.27	1.47	1.41
10	bA	818	CLA	C4C-C3C	2.27	1.49	1.45
10	aA	804	CLA	C1B-NB	-2.27	1.33	1.35
10	aA	819	CLA	C3D-C4D	-2.27	1.39	1.44
10	bA	802	CLA	C3D-C4D	-2.27	1.39	1.44
10	bA	829	CLA	C1C-NC	-2.27	1.34	1.37
10	cA	812	CLA	C1C-C2C	2.27	1.49	1.44
10	aA	856	CLA	C4B-CHC	2.27	1.47	1.41
10	aA	835	CLA	C4C-C3C	2.27	1.48	1.45
10	bA	856	CLA	C4B-CHC	2.27	1.47	1.41
10	aA	816	CLA	C1C-C2C	2.27	1.49	1.44
10	bB	840	CLA	C1C-C2C	2.27	1.49	1.44
10	aA	812	CLA	C4C-C3C	2.27	1.48	1.45
9	cA	801	CL0	C4B-NB	-2.27	1.33	1.35
10	aA	841	CLA	C1B-NB	-2.27	1.33	1.35
10	aB	835	CLA	C4C-C3C	2.27	1.48	1.45
10	aA	829	CLA	C1C-NC	-2.27	1.34	1.37
10	cB	832	CLA	C1C-C2C	2.27	1.49	1.44
10	aB	827	CLA	C1B-CHB	2.27	1.47	1.41
10	aA	841	CLA	C1C-C2C	2.26	1.48	1.44
10	cA	843	CLA	C1C-C2C	2.26	1.48	1.44
10	aB	820	CLA	C3D-C4D	-2.26	1.39	1.44
10	aA	843	CLA	C1C-C2C	2.26	1.48	1.44
10	bA	828	CLA	C1C-C2C	2.26	1.48	1.44
10	bA	838	CLA	C1C-NC	-2.26	1.34	1.37
10	bB	803	CLA	C1B-CHB	2.26	1.47	1.41
10	bA	827	CLA	C1C-C2C	2.26	1.48	1.44
10	cA	813	CLA	C3D-C4D	-2.26	1.39	1.44
10	cA	807	CLA	C1C-C2C	2.26	1.48	1.44
10	cA	802	CLA	C3D-C4D	-2.26	1.39	1.44
10	aA	856	CLA	C1B-NB	-2.26	1.33	1.35
10	aA	810	CLA	C1C-C2C	2.26	1.48	1.44
10	aB	824	CLA	C3D-C4D	-2.26	1.39	1.44
10	bB	828	CLA	C1C-C2C	2.26	1.48	1.44
10	bA	814	CLA	C1B-NB	-2.26	1.33	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	827	CLA	C4B-CHC	2.26	1.47	1.41
10	aA	815	CLA	C4C-C3C	2.26	1.48	1.45
10	bB	820	CLA	C3D-C4D	-2.26	1.39	1.44
10	bA	819	CLA	C1C-C2C	2.26	1.48	1.44
10	aA	802	CLA	C1B-CHB	2.26	1.47	1.41
10	cB	820	CLA	C3D-C4D	-2.26	1.39	1.44
10	cB	827	CLA	C4B-CHC	2.26	1.47	1.41
10	aA	814	CLA	C3D-C4D	-2.26	1.39	1.44
10	bA	821	CLA	C3D-C4D	-2.26	1.39	1.44
10	aB	840	CLA	C1C-C2C	2.25	1.48	1.44
10	bA	814	CLA	C4C-C3C	2.25	1.48	1.45
10	cA	809	CLA	C1B-NB	-2.25	1.33	1.35
10	bB	826	CLA	C4C-C3C	2.25	1.48	1.45
10	cB	807	CLA	C4C-C3C	2.25	1.48	1.45
10	cB	828	CLA	C1B-CHB	2.25	1.47	1.41
10	bB	827	CLA	C1B-CHB	2.25	1.47	1.41
10	aA	821	CLA	C3D-C4D	-2.25	1.39	1.44
10	bA	807	CLA	C1B-NB	-2.25	1.33	1.35
10	bB	832	CLA	C1B-NB	-2.25	1.33	1.35
10	aB	803	CLA	C1B-CHB	2.25	1.47	1.41
10	aA	812	CLA	C1C-C2C	2.25	1.48	1.44
10	aB	828	CLA	C1C-C2C	2.25	1.48	1.44
10	cA	814	CLA	C4C-C3C	2.25	1.48	1.45
10	bB	816	CLA	C4B-CHC	2.25	1.47	1.41
10	cB	820	CLA	C4B-CHC	2.25	1.47	1.41
10	cA	840	CLA	C4C-C3C	2.25	1.48	1.45
10	aB	836	CLA	C3D-C4D	-2.25	1.39	1.44
10	cB	824	CLA	C3D-C4D	-2.25	1.39	1.44
10	cA	829	CLA	C1C-NC	-2.25	1.34	1.37
10	bB	820	CLA	C4B-CHC	2.25	1.47	1.41
10	cB	823	CLA	C3D-C4D	-2.25	1.39	1.44
10	bB	829	CLA	C4B-NB	-2.25	1.33	1.35
10	aB	818	CLA	C4C-C3C	2.25	1.48	1.45
13	bI	101	BCR	C30-C25	-2.25	1.50	1.53
9	aA	801	CL0	C4B-NB	-2.25	1.33	1.35
10	bA	807	CLA	C1C-C2C	2.25	1.48	1.44
10	bA	843	CLA	C1C-C2C	2.25	1.48	1.44
10	bA	811	CLA	C4C-C3C	2.25	1.48	1.45
10	bA	834	CLA	C3D-C4D	-2.25	1.39	1.44
10	cB	818	CLA	C4C-C3C	2.25	1.48	1.45
10	cB	827	CLA	C1B-CHB	2.25	1.47	1.41
10	bB	831	CLA	C1C-C2C	2.25	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	821	CLA	C1C-C2C	2.25	1.48	1.44
10	bA	828	CLA	C4B-CHC	2.24	1.47	1.41
10	aA	811	CLA	C3D-C4D	-2.24	1.39	1.44
10	bB	839	CLA	C4C-C3C	2.24	1.48	1.45
10	bA	840	CLA	C4C-C3C	2.24	1.48	1.45
10	cA	811	CLA	C3D-C4D	-2.24	1.39	1.44
10	aB	809	CLA	C4B-CHC	2.24	1.47	1.41
10	cB	835	CLA	C3D-C4D	-2.24	1.39	1.44
10	bB	813	CLA	C4C-C3C	2.24	1.48	1.45
10	cB	802	CLA	C3D-C4D	-2.24	1.39	1.44
10	cB	836	CLA	C3D-C4D	-2.24	1.39	1.44
10	cB	809	CLA	C4B-CHC	2.24	1.47	1.41
10	cA	828	CLA	C4B-CHC	2.24	1.47	1.41
10	cA	807	CLA	C4B-CHC	2.24	1.47	1.41
10	cB	825	CLA	C4B-CHC	2.24	1.47	1.41
10	bA	814	CLA	C3D-C4D	-2.24	1.39	1.44
10	bB	824	CLA	C3D-C4D	-2.24	1.39	1.44
10	bB	821	CLA	C1C-C2C	2.24	1.48	1.44
10	bB	832	CLA	C1C-C2C	2.24	1.48	1.44
10	cA	815	CLA	C4C-C3C	2.24	1.48	1.45
10	bA	807	CLA	C4B-CHC	2.24	1.47	1.41
10	cA	802	CLA	C1B-CHB	2.24	1.47	1.41
10	aB	816	CLA	C1C-C2C	2.24	1.48	1.44
10	bA	815	CLA	C4C-C3C	2.24	1.48	1.45
10	bB	822	CLA	C1B-NB	-2.24	1.33	1.35
10	bB	805	CLA	C3D-C4D	-2.24	1.39	1.44
10	cB	841	CLA	C1B-CHB	2.24	1.47	1.41
10	aB	836	CLA	C4B-CHC	2.24	1.47	1.41
10	bA	809	CLA	C3D-C4D	-2.24	1.39	1.44
10	bB	816	CLA	C1C-C2C	2.24	1.48	1.44
10	bA	810	CLA	C4B-CHC	2.24	1.47	1.41
10	aA	827	CLA	C4B-NB	-2.24	1.33	1.35
10	bB	802	CLA	C3D-C4D	-2.24	1.39	1.44
10	bA	802	CLA	C1B-CHB	2.24	1.47	1.41
10	aA	832	CLA	C4B-CHC	2.23	1.47	1.41
10	aB	820	CLA	C4B-CHC	2.23	1.47	1.41
10	aB	832	CLA	C1B-NB	-2.23	1.33	1.35
10	bB	817	CLA	C1B-NB	-2.23	1.33	1.35
10	aB	837	CLA	C1C-NC	-2.23	1.34	1.37
10	aA	807	CLA	C4B-CHC	2.23	1.47	1.41
10	aA	809	CLA	C3D-C4D	-2.23	1.39	1.44
10	cB	803	CLA	C1B-CHB	2.23	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	822	CLA	C1B-NB	-2.23	1.33	1.35
10	cB	831	CLA	C3D-C4D	-2.23	1.39	1.44
10	aA	827	CLA	C1C-C2C	2.23	1.48	1.44
10	bA	812	CLA	C1C-C2C	2.23	1.48	1.44
10	cA	827	CLA	C1C-C2C	2.23	1.48	1.44
10	bB	809	CLA	C4B-CHC	2.23	1.47	1.41
10	aB	835	CLA	C3D-C4D	-2.23	1.39	1.44
10	cA	810	CLA	C4B-CHC	2.23	1.47	1.41
10	bA	827	CLA	C4B-NB	-2.23	1.33	1.35
10	aB	813	CLA	C1C-C2C	2.23	1.48	1.44
13	aI	101	BCR	C30-C25	-2.23	1.50	1.53
10	aB	825	CLA	C4B-CHC	2.23	1.47	1.41
10	aA	807	CLA	C1C-C2C	2.23	1.48	1.44
10	cA	827	CLA	C4B-NB	-2.23	1.33	1.35
10	bB	808	CLA	C1C-C2C	2.23	1.48	1.44
10	aB	808	CLA	C1C-C2C	2.23	1.48	1.44
10	bB	831	CLA	C3D-C4D	-2.23	1.39	1.44
10	bB	836	CLA	C3D-C4D	-2.23	1.39	1.44
10	bA	827	CLA	C4B-CHC	2.23	1.47	1.41
10	aA	810	CLA	C4B-CHC	2.23	1.47	1.41
10	cA	839	CLA	C4B-CHC	2.23	1.47	1.41
10	bB	825	CLA	C4B-CHC	2.23	1.47	1.41
10	bB	818	CLA	C4C-C3C	2.23	1.48	1.45
10	bB	805	CLA	C4C-C3C	2.22	1.48	1.45
10	cB	813	CLA	C1C-C2C	2.22	1.48	1.44
10	cA	835	CLA	C4C-C3C	2.22	1.48	1.45
10	bA	811	CLA	C3D-C4D	-2.22	1.39	1.44
10	aA	811	CLA	C4C-C3C	2.22	1.48	1.45
10	aA	826	CLA	C1B-NB	-2.22	1.33	1.35
10	cB	826	CLA	C4C-C3C	2.22	1.48	1.45
10	aA	828	CLA	C4B-CHC	2.22	1.47	1.41
10	bL	204	CLA	C1C-C2C	2.22	1.48	1.44
10	bA	841	CLA	C1B-CHB	2.22	1.47	1.41
10	cA	821	CLA	C1B-CHB	2.22	1.47	1.41
10	aB	839	CLA	C4C-C3C	2.22	1.48	1.45
10	bB	838	CLA	C1C-C2C	2.22	1.48	1.44
10	bA	821	CLA	C4B-CHC	2.22	1.47	1.41
10	bA	839	CLA	C4B-CHC	2.22	1.47	1.41
13	aA	847	BCR	C30-C25	-2.22	1.50	1.53
10	cB	808	CLA	C1C-C2C	2.22	1.48	1.44
10	bA	812	CLA	C4C-C3C	2.22	1.48	1.45
10	cB	809	CLA	C4C-C3C	2.22	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	819	CLA	C1C-C2C	2.22	1.48	1.44
10	cA	824	CLA	C1C-C2C	2.22	1.48	1.44
10	cB	828	CLA	C1C-C2C	2.22	1.48	1.44
10	aB	814	CLA	C1C-NC	-2.22	1.34	1.37
10	bA	816	CLA	C3D-C4D	-2.22	1.39	1.44
10	aA	819	CLA	C1C-C2C	2.22	1.48	1.44
10	cB	822	CLA	C1B-NB	-2.22	1.33	1.35
10	cA	816	CLA	C3D-C4D	-2.21	1.39	1.44
10	cB	829	CLA	C4B-NB	-2.21	1.33	1.35
10	cB	832	CLA	C1B-NB	-2.21	1.33	1.35
10	cA	832	CLA	C4B-CHC	2.21	1.47	1.41
10	cA	811	CLA	C4C-C3C	2.21	1.48	1.45
10	aB	823	CLA	C1C-C2C	2.21	1.48	1.44
10	cB	829	CLA	C1B-CHB	2.21	1.47	1.41
10	aA	824	CLA	C1C-C2C	2.21	1.48	1.44
10	cB	812	CLA	C4C-C3C	2.21	1.48	1.45
10	cB	837	CLA	C1C-NC	-2.21	1.34	1.37
10	aB	812	CLA	C4C-C3C	2.21	1.48	1.45
10	bB	812	CLA	C4C-C3C	2.21	1.48	1.45
10	cA	821	CLA	C4B-CHC	2.21	1.47	1.41
10	aB	802	CLA	C3D-C4D	-2.21	1.39	1.44
10	cA	809	CLA	C3D-C4D	-2.21	1.39	1.44
10	bA	821	CLA	C1B-CHB	2.21	1.47	1.41
10	cB	821	CLA	C1B-CHB	2.21	1.47	1.41
10	bB	802	CLA	C1C-NC	-2.21	1.34	1.37
10	cA	804	CLA	C1C-NC	-2.21	1.34	1.37
10	aA	843	CLA	C1B-CHB	2.21	1.47	1.41
10	bA	808	CLA	C1B-NB	-2.21	1.33	1.35
10	aB	829	CLA	C1B-CHB	2.21	1.47	1.41
10	bA	834	CLA	C1B-CHB	2.21	1.47	1.41
10	cA	813	CLA	C4C-C3C	2.21	1.48	1.45
10	aA	816	CLA	C3D-C4D	-2.21	1.39	1.44
10	aA	808	CLA	C1B-NB	-2.21	1.33	1.35
10	cB	816	CLA	C1C-C2C	2.21	1.48	1.44
10	cA	811	CLA	C1C-C2C	2.21	1.48	1.44
10	aA	821	CLA	C4B-CHC	2.21	1.47	1.41
10	bA	805	CLA	C1B-CHB	2.21	1.47	1.41
10	cB	823	CLA	C1C-C2C	2.21	1.48	1.44
10	aA	805	CLA	C1B-CHB	2.21	1.47	1.41
10	bA	832	CLA	C4B-CHC	2.20	1.47	1.41
10	cA	841	CLA	C1B-CHB	2.20	1.47	1.41
10	bL	205	CLA	C4C-C3C	2.20	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	803	CLA	C4B-CHC	2.20	1.47	1.41
10	cA	805	CLA	C4B-CHC	2.20	1.47	1.41
10	cA	827	CLA	C4B-CHC	2.20	1.47	1.41
10	cB	838	CLA	C1C-C2C	2.20	1.48	1.44
10	cB	827	CLA	C1C-NC	-2.20	1.34	1.37
10	aA	821	CLA	C1B-CHB	2.20	1.47	1.41
10	aA	814	CLA	C4C-C3C	2.20	1.48	1.45
10	bB	823	CLA	C1C-C2C	2.20	1.48	1.44
10	aA	827	CLA	C4B-CHC	2.20	1.47	1.41
10	aA	830	CLA	C4B-CHC	2.20	1.47	1.41
10	bL	202	CLA	C4B-CHC	2.20	1.47	1.41
10	aB	828	CLA	C1C-NC	-2.20	1.34	1.37
10	bB	835	CLA	C1C-C2C	2.20	1.48	1.44
10	bA	804	CLA	C1C-NC	-2.20	1.34	1.37
10	bB	829	CLA	C1B-CHB	2.20	1.47	1.41
10	bB	841	CLA	C1B-CHB	2.20	1.47	1.41
10	cB	826	CLA	C1C-C2C	2.20	1.48	1.44
10	cB	802	CLA	C1C-NC	-2.20	1.34	1.37
10	aB	809	CLA	C4C-C3C	2.20	1.48	1.45
10	cA	805	CLA	C1C-C2C	2.20	1.48	1.44
13	aA	846	BCR	C33-C5	-2.20	1.47	1.50
10	aA	805	CLA	C4B-CHC	2.20	1.47	1.41
10	aL	203	CLA	C4B-CHC	2.20	1.47	1.41
10	aB	835	CLA	C1C-C2C	2.20	1.48	1.44
10	bB	813	CLA	C1C-C2C	2.20	1.48	1.44
10	aB	817	CLA	C4B-CHC	2.20	1.47	1.41
10	aA	839	CLA	C4B-CHC	2.20	1.47	1.41
10	bA	805	CLA	C4B-CHC	2.20	1.47	1.41
10	aA	809	CLA	C1B-NB	-2.20	1.33	1.35
10	aB	823	CLA	C3D-C4D	-2.20	1.39	1.44
10	aB	802	CLA	C1C-NC	-2.20	1.34	1.37
10	aB	841	CLA	C1B-CHB	2.20	1.47	1.41
10	cB	803	CLA	C4B-CHC	2.20	1.47	1.41
10	cA	834	CLA	C1B-CHB	2.20	1.47	1.41
10	aB	826	CLA	C4C-C3C	2.20	1.48	1.45
10	bA	821	CLA	C1C-C2C	2.20	1.48	1.44
10	bB	836	CLA	C4B-CHC	2.20	1.47	1.41
10	cL	203	CLA	C4B-CHC	2.20	1.47	1.41
10	cB	836	CLA	C4B-CHC	2.20	1.47	1.41
10	aB	808	CLA	C4B-NB	-2.19	1.33	1.35
10	bB	828	CLA	C1C-NC	-2.19	1.34	1.37
10	bL	203	CLA	C4B-CHC	2.19	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cL	205	CLA	C1B-CHB	2.19	1.47	1.41
10	cB	835	CLA	C1C-C2C	2.19	1.48	1.44
10	aA	841	CLA	C1B-CHB	2.19	1.47	1.41
14	aA	852	LHG	P-O6	2.19	1.68	1.59
10	cA	821	CLA	C1C-C2C	2.19	1.48	1.44
9	bA	801	CL0	C4B-NB	-2.19	1.33	1.35
10	cA	817	CLA	C1C-C2C	2.19	1.48	1.44
10	aA	834	CLA	C1B-CHB	2.19	1.47	1.41
14	bA	852	LHG	P-O6	2.19	1.68	1.59
10	cA	810	CLA	C3D-C4D	-2.19	1.39	1.44
10	aL	205	CLA	C1B-CHB	2.19	1.47	1.41
10	bB	837	CLA	C1C-NC	-2.19	1.34	1.37
10	aB	805	CLA	C3D-C4D	-2.19	1.39	1.44
14	cA	852	LHG	P-O6	2.19	1.68	1.59
10	aA	815	CLA	C1B-NB	-2.19	1.33	1.35
9	aA	801	CL0	C1C-NC	-2.19	1.34	1.37
10	bB	826	CLA	C1C-C2C	2.19	1.48	1.44
13	cA	847	BCR	C30-C25	-2.19	1.50	1.53
10	cA	805	CLA	C1B-CHB	2.19	1.47	1.41
10	cA	819	CLA	C1B-NB	-2.19	1.33	1.35
10	bB	803	CLA	C4B-CHC	2.19	1.47	1.41
10	bB	821	CLA	C4C-C3C	2.19	1.48	1.45
10	aB	821	CLA	C1B-CHB	2.19	1.47	1.41
10	bA	805	CLA	C1C-C2C	2.19	1.48	1.44
10	bB	821	CLA	C1B-CHB	2.19	1.47	1.41
10	aB	822	CLA	C3D-C4D	-2.19	1.39	1.44
10	bA	811	CLA	C1C-C2C	2.19	1.48	1.44
10	aB	829	CLA	C4B-NB	-2.18	1.33	1.35
10	aL	202	CLA	C4B-CHC	2.18	1.47	1.41
10	cB	805	CLA	C3D-C4D	-2.18	1.39	1.44
10	bA	804	CLA	C1B-NB	-2.18	1.33	1.35
10	cB	813	CLA	C1B-NB	-2.18	1.33	1.35
10	cB	805	CLA	C4C-C3C	2.18	1.48	1.45
10	cA	843	CLA	C1B-CHB	2.18	1.47	1.41
10	bA	824	CLA	C1C-C2C	2.18	1.48	1.44
10	bB	813	CLA	C1B-NB	-2.18	1.33	1.35
10	aB	815	CLA	C4B-CHC	2.18	1.47	1.41
10	bB	814	CLA	C1C-NC	-2.18	1.34	1.37
10	aA	804	CLA	C1C-NC	-2.18	1.34	1.37
10	bB	827	CLA	C1C-NC	-2.18	1.34	1.37
10	aB	805	CLA	C4C-C3C	2.18	1.48	1.45
10	cL	202	CLA	C4B-CHC	2.18	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	807	CLA	C1B-NB	-2.18	1.33	1.35
10	cA	814	CLA	C1B-NB	-2.18	1.33	1.35
10	cB	823	CLA	C1B-CHB	2.18	1.47	1.41
10	aB	827	CLA	C1C-NC	-2.18	1.34	1.37
10	cB	821	CLA	C4C-C3C	2.18	1.48	1.45
10	aB	838	CLA	C1C-C2C	2.18	1.48	1.44
10	cB	808	CLA	C4B-NB	-2.18	1.33	1.35
10	cA	815	CLA	C1B-CHB	2.18	1.47	1.41
10	cB	840	CLA	C1B-CHB	2.18	1.47	1.41
10	aB	823	CLA	C1B-CHB	2.18	1.47	1.41
10	aA	813	CLA	C4C-C3C	2.18	1.48	1.45
10	bB	813	CLA	C1B-CHB	2.18	1.47	1.41
10	aB	817	CLA	C4C-C3C	2.17	1.48	1.45
10	aA	814	CLA	C1B-NB	-2.17	1.33	1.35
10	cA	840	CLA	C1B-NB	-2.17	1.33	1.35
10	aA	811	CLA	C1C-C2C	2.17	1.48	1.44
10	bA	813	CLA	C4B-CHC	2.17	1.47	1.41
10	bB	809	CLA	C4C-C3C	2.17	1.48	1.45
10	cA	824	CLA	C1B-CHB	2.17	1.47	1.41
10	cL	204	CLA	C1C-C2C	2.17	1.48	1.44
10	aB	811	CLA	C1B-CHB	2.17	1.47	1.41
10	aL	205	CLA	C4C-C3C	2.17	1.48	1.45
10	bA	813	CLA	C4C-C3C	2.17	1.48	1.45
10	bA	815	CLA	C1B-NB	-2.17	1.33	1.35
10	bA	843	CLA	C1B-CHB	2.17	1.47	1.41
13	bA	847	BCR	C30-C25	-2.17	1.50	1.53
10	aB	834	CLA	C1B-NB	-2.17	1.33	1.35
10	cA	856	CLA	C1B-NB	-2.17	1.33	1.35
10	bA	830	CLA	C4B-CHC	2.17	1.47	1.41
10	cA	840	CLA	C1B-CHB	2.17	1.47	1.41
10	cB	817	CLA	C3D-C4D	-2.17	1.39	1.44
10	bB	802	CLA	C4B-CHC	2.17	1.47	1.41
10	aA	830	CLA	C4C-C3C	2.17	1.48	1.45
10	cB	813	CLA	C1B-CHB	2.17	1.47	1.41
10	aB	840	CLA	C1B-CHB	2.17	1.47	1.41
10	cB	817	CLA	C4B-CHC	2.17	1.47	1.41
10	aB	837	CLA	C1B-CHB	2.17	1.47	1.41
10	bB	840	CLA	C1B-CHB	2.16	1.47	1.41
10	cA	813	CLA	C4B-CHC	2.16	1.47	1.41
10	bB	801	CLA	C1C-NC	-2.16	1.34	1.37
10	cA	830	CLA	C4C-C3C	2.16	1.48	1.45
10	bL	205	CLA	C4B-CHC	2.16	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	817	CLA	C1C-C2C	2.16	1.48	1.44
10	cA	831	CLA	C4B-CHC	2.16	1.47	1.41
10	bB	834	CLA	C1B-NB	-2.16	1.33	1.35
10	bB	809	CLA	C1C-C2C	2.16	1.48	1.44
10	aB	829	CLA	C1C-C2C	2.16	1.48	1.44
10	aA	840	CLA	C1B-CHB	2.16	1.47	1.41
10	aB	824	CLA	C1B-CHB	2.16	1.47	1.41
10	bA	856	CLA	C1B-NB	-2.16	1.33	1.35
10	cB	824	CLA	C1C-C2C	2.16	1.48	1.44
10	bB	801	CLA	C4C-C3C	2.16	1.48	1.45
10	cB	822	CLA	C3D-C4D	-2.16	1.39	1.44
10	cA	832	CLA	C1C-C2C	2.16	1.48	1.44
10	bA	824	CLA	C1B-CHB	2.16	1.47	1.41
10	bL	205	CLA	C1B-CHB	2.16	1.47	1.41
10	aB	836	CLA	C1B-CHB	2.16	1.47	1.41
10	aA	821	CLA	C1C-C2C	2.16	1.48	1.44
10	cB	809	CLA	C1C-C2C	2.16	1.48	1.44
10	aB	801	CLA	C1C-NC	-2.16	1.34	1.37
10	aB	817	CLA	C1B-NB	-2.16	1.33	1.35
10	aL	205	CLA	C4B-CHC	2.16	1.47	1.41
10	aB	817	CLA	C3D-C4D	-2.16	1.39	1.44
10	aB	833	CLA	C4C-C3C	2.16	1.48	1.45
10	cL	205	CLA	C4C-C3C	2.16	1.48	1.45
10	bA	832	CLA	C1C-NC	-2.16	1.34	1.37
10	cB	828	CLA	C1C-NC	-2.16	1.34	1.37
10	cB	811	CLA	C4B-NB	-2.16	1.33	1.35
10	cB	815	CLA	C4B-CHC	2.16	1.47	1.41
10	aA	819	CLA	C1B-NB	-2.16	1.33	1.35
10	aA	813	CLA	C4B-CHC	2.16	1.47	1.41
10	bB	817	CLA	C4B-CHC	2.16	1.47	1.41
10	cL	205	CLA	C4B-CHC	2.16	1.47	1.41
9	cA	801	CL0	C1C-NC	-2.16	1.34	1.37
10	bB	818	CLA	C1C-C2C	2.16	1.48	1.44
10	aA	815	CLA	C1B-CHB	2.16	1.47	1.41
10	cB	822	CLA	C1B-CHB	2.16	1.47	1.41
10	cB	836	CLA	C1B-CHB	2.16	1.47	1.41
13	aB	847	BCR	C33-C5	-2.16	1.47	1.50
10	cA	807	CLA	C1B-NB	-2.15	1.33	1.35
10	bB	817	CLA	C4C-C3C	2.15	1.48	1.45
10	aL	204	CLA	C1C-C2C	2.15	1.48	1.44
10	bA	840	CLA	C1B-CHB	2.15	1.47	1.41
10	bB	815	CLA	C4B-CHC	2.15	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	829	CLA	C4C-C3C	2.15	1.48	1.45
10	aB	822	CLA	C1B-CHB	2.15	1.47	1.41
10	aB	826	CLA	C1C-C2C	2.15	1.48	1.44
10	bB	823	CLA	C1B-CHB	2.15	1.47	1.41
10	bA	840	CLA	C1B-NB	-2.15	1.33	1.35
10	bA	830	CLA	C4C-C3C	2.15	1.48	1.45
10	cA	841	CLA	C4C-C3C	2.15	1.48	1.45
10	cA	830	CLA	C4B-CHC	2.15	1.47	1.41
10	aB	802	CLA	C4B-CHC	2.15	1.47	1.41
9	bA	801	CL0	C1C-NC	-2.15	1.34	1.37
10	aB	824	CLA	C1C-C2C	2.15	1.48	1.44
10	aA	820	CLA	C1C-C2C	2.15	1.48	1.44
10	cA	820	CLA	C1C-C2C	2.15	1.48	1.44
10	cB	822	CLA	C1A-CHA	2.15	1.52	1.43
10	cA	815	CLA	C1B-NB	-2.15	1.33	1.35
10	cL	202	CLA	C4B-NB	-2.15	1.33	1.35
10	bB	822	CLA	C3D-C4D	-2.15	1.39	1.44
10	cA	823	CLA	C1C-NC	-2.15	1.34	1.37
10	bB	811	CLA	C1B-CHB	2.15	1.47	1.41
10	bB	836	CLA	C1B-CHB	2.15	1.47	1.41
10	cB	801	CLA	C1C-NC	-2.15	1.34	1.37
13	bB	847	BCR	C33-C5	-2.15	1.47	1.50
10	aA	834	CLA	C1C-NC	-2.14	1.34	1.37
10	cB	815	CLA	C4C-C3C	2.14	1.48	1.45
10	aB	822	CLA	C1A-CHA	2.14	1.52	1.43
16	cB	848	LMG	O7-C8	-2.14	1.41	1.46
10	cB	814	CLA	C1C-NC	-2.14	1.34	1.37
10	aA	831	CLA	C4B-CHC	2.14	1.46	1.41
10	bB	833	CLA	C4C-C3C	2.14	1.48	1.45
10	aA	805	CLA	C1C-C2C	2.14	1.48	1.44
10	aB	804	CLA	C3D-C4D	-2.14	1.39	1.44
10	cA	839	CLA	C3D-C4D	-2.14	1.39	1.44
10	aA	832	CLA	C1C-C2C	2.14	1.48	1.44
10	bB	822	CLA	C1B-CHB	2.14	1.46	1.41
10	aA	807	CLA	C4C-C3C	2.14	1.48	1.45
10	bA	829	CLA	C4C-C3C	2.14	1.48	1.45
10	bA	843	CLA	C3D-C4D	-2.14	1.39	1.44
10	bA	815	CLA	C1B-CHB	2.14	1.46	1.41
10	bB	807	CLA	C4B-NB	-2.14	1.33	1.35
10	bB	829	CLA	C1C-C2C	2.14	1.48	1.44
10	aB	813	CLA	C1B-CHB	2.14	1.46	1.41
10	aB	821	CLA	C4C-C3C	2.14	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	810	CLA	C3D-C4D	-2.14	1.39	1.44
10	bB	817	CLA	C3D-C4D	-2.14	1.39	1.44
10	bA	823	CLA	C1C-NC	-2.14	1.34	1.37
10	cB	814	CLA	C1B-NB	-2.14	1.33	1.35
10	bB	822	CLA	C1A-CHA	2.14	1.52	1.43
10	cB	802	CLA	C4B-CHC	2.14	1.46	1.41
10	bB	824	CLA	C1C-C2C	2.14	1.48	1.44
10	cB	829	CLA	C1C-C2C	2.14	1.48	1.44
10	aB	814	CLA	C1B-NB	-2.14	1.33	1.35
10	bA	809	CLA	C1B-NB	-2.14	1.33	1.35
10	cB	837	CLA	C1B-CHB	2.14	1.46	1.41
10	aA	843	CLA	C3D-C4D	-2.14	1.39	1.44
13	bL	207	BCR	C1-C6	-2.14	1.50	1.53
10	cB	818	CLA	C1C-C2C	2.14	1.48	1.44
10	bA	831	CLA	C4B-CHC	2.14	1.46	1.41
10	aA	839	CLA	C3D-C4D	-2.14	1.39	1.44
10	aA	824	CLA	C1B-CHB	2.14	1.46	1.41
10	cB	811	CLA	C1B-CHB	2.13	1.46	1.41
13	cL	207	BCR	C1-C6	-2.13	1.50	1.53
16	bB	848	LMG	O7-C8	-2.13	1.41	1.46
13	bA	846	BCR	C33-C5	-2.13	1.47	1.50
10	aB	813	CLA	C1B-NB	-2.13	1.33	1.35
10	bA	806	CLA	C1B-NB	-2.13	1.33	1.35
10	cA	834	CLA	C1C-NC	-2.13	1.34	1.37
10	aA	829	CLA	C4C-C3C	2.13	1.48	1.45
10	bA	820	CLA	C1C-C2C	2.13	1.48	1.44
10	bA	803	CLA	C3D-C4D	-2.13	1.39	1.44
10	bA	809	CLA	C1C-C2C	2.13	1.48	1.44
10	cB	833	CLA	C4C-C3C	2.13	1.48	1.45
10	aB	814	CLA	C1B-CHB	2.13	1.46	1.41
10	aA	829	CLA	C1B-CHB	2.13	1.46	1.41
10	bA	819	CLA	C1B-NB	-2.13	1.33	1.35
10	bB	808	CLA	C4B-NB	-2.13	1.33	1.35
10	bA	810	CLA	C3D-C4D	-2.13	1.39	1.44
10	aA	806	CLA	C1B-NB	-2.13	1.33	1.35
10	aB	825	CLA	C4C-C3C	2.13	1.48	1.45
10	aB	833	CLA	C1C-NC	-2.13	1.34	1.37
10	bB	824	CLA	C1B-CHB	2.13	1.46	1.41
10	aB	836	CLA	C1C-C2C	2.13	1.48	1.44
10	bA	839	CLA	C3D-C4D	-2.13	1.39	1.44
10	aB	805	CLA	C4B-CHC	2.13	1.46	1.41
10	cA	829	CLA	C1B-CHB	2.13	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	832	CLA	C1C-NC	-2.13	1.34	1.37
10	bB	837	CLA	C1B-CHB	2.13	1.46	1.41
10	aB	801	CLA	C4C-C3C	2.13	1.48	1.45
10	bA	841	CLA	C4C-C3C	2.13	1.48	1.45
10	bA	832	CLA	C1C-C2C	2.13	1.48	1.44
10	aB	808	CLA	C1C-NC	-2.13	1.34	1.37
10	bA	808	CLA	C1C-NC	-2.13	1.34	1.37
10	bA	833	CLA	C4B-CHC	2.13	1.46	1.41
10	cA	803	CLA	C3D-C4D	-2.12	1.39	1.44
10	aA	833	CLA	C1C-NC	-2.12	1.34	1.37
10	cB	834	CLA	C1B-NB	-2.12	1.33	1.35
10	aB	807	CLA	C4B-CHC	2.12	1.46	1.41
10	cA	836	CLA	C1B-CHB	2.12	1.46	1.41
10	cB	807	CLA	C4B-CHC	2.12	1.46	1.41
10	aA	837	CLA	C1B-CHB	2.12	1.46	1.41
10	aA	817	CLA	C1C-C2C	2.12	1.48	1.44
10	bB	806	CLA	C1B-CHB	2.12	1.46	1.41
10	cA	826	CLA	C1B-NB	-2.12	1.33	1.35
10	cB	824	CLA	C1B-CHB	2.12	1.46	1.41
10	cL	205	CLA	C1C-NC	-2.12	1.34	1.37
10	cB	817	CLA	C4C-C3C	2.12	1.48	1.45
10	cB	836	CLA	C1C-C2C	2.12	1.48	1.44
10	bA	836	CLA	C1C-NC	-2.12	1.34	1.37
10	aA	821	CLA	C4B-NB	-2.12	1.33	1.35
10	cB	825	CLA	C4C-C3C	2.12	1.48	1.45
10	aB	839	CLA	C1C-C2C	2.12	1.48	1.44
10	cB	820	CLA	C1C-C2C	2.12	1.48	1.44
16	aB	848	LMG	O7-C8	-2.12	1.41	1.46
10	cB	814	CLA	C1B-CHB	2.12	1.46	1.41
10	bB	839	CLA	C1C-C2C	2.12	1.48	1.44
10	cB	814	CLA	C4B-CHC	2.12	1.46	1.41
10	bA	834	CLA	C1C-NC	-2.12	1.34	1.37
10	cA	805	CLA	C1C-NC	-2.12	1.34	1.37
10	cB	828	CLA	C4B-CHC	2.12	1.46	1.41
10	cA	836	CLA	C1C-NC	-2.12	1.34	1.37
10	aL	205	CLA	C1C-NC	-2.12	1.34	1.37
10	cA	813	CLA	C1B-CHB	2.12	1.46	1.41
10	bB	825	CLA	C4C-C3C	2.12	1.48	1.45
10	cB	839	CLA	C1C-C2C	2.12	1.48	1.44
10	aB	807	CLA	C1C-NC	-2.12	1.34	1.37
10	bB	839	CLA	C1B-CHB	2.12	1.46	1.41
10	aA	836	CLA	C1C-NC	-2.12	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	833	CLA	C1C-NC	-2.12	1.34	1.37
10	aA	841	CLA	C4C-C3C	2.12	1.48	1.45
10	bA	831	CLA	C1B-CHB	2.11	1.46	1.41
10	bB	814	CLA	C1B-CHB	2.11	1.46	1.41
10	cB	839	CLA	C1B-CHB	2.11	1.46	1.41
10	cB	822	CLA	C1C-C2C	2.11	1.48	1.44
10	cA	843	CLA	C3D-C4D	-2.11	1.39	1.44
10	bA	818	CLA	C4B-NB	-2.11	1.33	1.35
10	cA	833	CLA	C4B-CHC	2.11	1.46	1.41
13	cA	846	BCR	C33-C5	-2.11	1.47	1.50
10	aB	806	CLA	C1B-CHB	2.11	1.46	1.41
10	bA	813	CLA	C1B-CHB	2.11	1.46	1.41
10	cA	837	CLA	C1B-CHB	2.11	1.46	1.41
10	aA	823	CLA	C1C-NC	-2.11	1.34	1.37
10	aA	809	CLA	C1C-C2C	2.11	1.48	1.44
10	bL	205	CLA	C4B-NB	-2.11	1.33	1.35
13	aL	207	BCR	C1-C6	-2.11	1.50	1.53
10	bB	834	CLA	C1C-C2C	2.11	1.48	1.44
10	aB	809	CLA	C1C-C2C	2.11	1.48	1.44
10	bA	814	CLA	C1C-NC	-2.11	1.34	1.37
10	aA	856	CLA	C1B-CHB	2.11	1.46	1.41
10	cB	804	CLA	C3D-C4D	-2.11	1.39	1.44
10	bA	829	CLA	C1B-CHB	2.11	1.46	1.41
10	aA	835	CLA	C1C-C2C	2.11	1.48	1.44
10	aA	805	CLA	C1C-NC	-2.11	1.34	1.37
10	aA	834	CLA	C4B-CHC	2.11	1.46	1.41
10	cB	834	CLA	C1C-C2C	2.11	1.48	1.44
10	cB	805	CLA	C4B-CHC	2.11	1.46	1.41
10	bB	809	CLA	C1C-NC	-2.11	1.34	1.37
10	cA	809	CLA	C1C-C2C	2.11	1.48	1.44
10	aA	831	CLA	C1B-CHB	2.11	1.46	1.41
10	aA	837	CLA	C4B-NB	-2.11	1.33	1.35
10	bB	820	CLA	C1C-C2C	2.11	1.48	1.44
10	bB	804	CLA	C3D-C4D	-2.11	1.39	1.44
10	bA	834	CLA	C4B-CHC	2.11	1.46	1.41
10	bB	807	CLA	C4B-CHC	2.11	1.46	1.41
10	bA	827	CLA	C1C-NC	-2.11	1.34	1.37
10	bB	819	CLA	C1C-NC	-2.11	1.34	1.37
10	cA	819	CLA	C1B-CHB	2.10	1.46	1.41
10	bB	808	CLA	C1C-NC	-2.10	1.34	1.37
10	aA	836	CLA	C1B-CHB	2.10	1.46	1.41
10	cA	832	CLA	C1C-NC	-2.10	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	814	CLA	C1C-NC	-2.10	1.34	1.37
10	aL	205	CLA	C1C-C2C	2.10	1.48	1.44
10	aA	813	CLA	C1B-CHB	2.10	1.46	1.41
10	bB	833	CLA	C1C-NC	-2.10	1.34	1.37
10	aB	834	CLA	C1C-C2C	2.10	1.48	1.44
10	aA	833	CLA	C4B-CHC	2.10	1.46	1.41
10	cB	809	CLA	C1B-CHB	2.10	1.46	1.41
10	bB	814	CLA	C4B-CHC	2.10	1.46	1.41
10	bL	205	CLA	C1C-NC	-2.10	1.34	1.37
10	cB	803	CLA	C1C-NC	-2.10	1.34	1.37
10	cB	837	CLA	C1C-C2C	2.10	1.48	1.44
10	aA	803	CLA	C3D-C4D	-2.10	1.39	1.44
10	cA	806	CLA	C1B-NB	-2.10	1.33	1.35
10	bB	837	CLA	C4C-C3C	2.10	1.48	1.45
10	aB	815	CLA	C4C-C3C	2.10	1.48	1.45
10	bA	807	CLA	C4C-C3C	2.10	1.48	1.45
10	bA	805	CLA	C1C-NC	-2.10	1.34	1.37
10	cA	834	CLA	C4B-CHC	2.10	1.46	1.41
10	aB	822	CLA	C1C-C2C	2.09	1.48	1.44
10	bB	805	CLA	C4B-CHC	2.09	1.46	1.41
10	bB	832	CLA	C4C-C3C	2.09	1.48	1.45
10	aB	814	CLA	C4B-CHC	2.09	1.46	1.41
10	aB	820	CLA	C1C-C2C	2.09	1.48	1.44
10	bA	837	CLA	C1B-CHB	2.09	1.46	1.41
10	bB	816	CLA	C3D-C4D	-2.09	1.39	1.44
10	cB	828	CLA	C4B-NB	-2.09	1.33	1.35
10	bA	826	CLA	C1B-CHB	2.09	1.46	1.41
10	cA	825	CLA	C4B-NB	-2.09	1.33	1.35
10	bA	811	CLA	C1B-CHB	2.09	1.46	1.41
10	bB	815	CLA	C4C-C3C	2.09	1.48	1.45
10	cA	807	CLA	C4B-NB	-2.09	1.33	1.35
10	bA	833	CLA	C1C-NC	-2.09	1.34	1.37
10	aA	804	CLA	C4C-C3C	2.09	1.48	1.45
10	bA	836	CLA	C1B-CHB	2.09	1.46	1.41
10	aA	826	CLA	C1B-CHB	2.09	1.46	1.41
10	cA	831	CLA	C1B-CHB	2.09	1.46	1.41
10	bB	828	CLA	C4B-CHC	2.09	1.46	1.41
10	bB	809	CLA	C1B-CHB	2.09	1.46	1.41
10	cB	830	CLA	C1B-CHB	2.09	1.46	1.41
10	bA	828	CLA	C1B-CHB	2.09	1.46	1.41
10	aB	811	CLA	C4B-NB	-2.09	1.33	1.35
10	cB	819	CLA	C1C-NC	-2.09	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	818	CLA	C1C-C2C	2.09	1.48	1.44
10	cA	856	CLA	C1B-CHB	2.09	1.46	1.41
10	aB	823	CLA	C1B-NB	-2.09	1.33	1.35
10	cB	801	CLA	C4C-C3C	2.09	1.48	1.45
10	aB	815	CLA	C1C-C2C	2.09	1.48	1.44
10	aA	828	CLA	C1B-CHB	2.09	1.46	1.41
10	bA	802	CLA	C1C-C2C	2.09	1.48	1.44
10	cL	205	CLA	C1C-C2C	2.09	1.48	1.44
13	cB	847	BCR	C33-C5	-2.09	1.47	1.50
10	cB	812	CLA	C1B-CHB	2.09	1.46	1.41
10	bB	814	CLA	C1B-NB	-2.09	1.33	1.35
10	cB	823	CLA	C1B-NB	-2.09	1.33	1.35
10	aA	819	CLA	C1B-CHB	2.08	1.46	1.41
10	aB	828	CLA	C4B-CHC	2.08	1.46	1.41
10	bB	827	CLA	C4C-C3C	2.08	1.48	1.45
10	cB	806	CLA	C1B-CHB	2.08	1.46	1.41
10	cB	827	CLA	C4C-C3C	2.08	1.48	1.45
10	bA	803	CLA	C1B-CHB	2.08	1.46	1.41
10	bA	818	CLA	C4B-CHC	2.08	1.46	1.41
10	cA	835	CLA	C1C-C2C	2.08	1.48	1.44
10	aA	818	CLA	C4B-CHC	2.08	1.46	1.41
10	cB	808	CLA	C1C-NC	-2.08	1.34	1.37
10	aB	839	CLA	C1B-CHB	2.08	1.46	1.41
10	cA	807	CLA	C4C-C3C	2.08	1.48	1.45
10	cB	816	CLA	C3D-C4D	-2.08	1.39	1.44
10	bB	837	CLA	C1C-C2C	2.08	1.48	1.44
10	bA	819	CLA	C1B-CHB	2.08	1.46	1.41
10	cA	828	CLA	C1B-CHB	2.08	1.46	1.41
10	cB	817	CLA	C1B-NB	-2.08	1.33	1.35
10	cL	204	CLA	C1B-CHB	2.08	1.46	1.41
10	cB	815	CLA	C1C-C2C	2.08	1.48	1.44
10	cB	841	CLA	C4C-C3C	2.08	1.48	1.45
10	aA	807	CLA	C4B-NB	-2.08	1.33	1.35
10	bA	836	CLA	C1C-C2C	2.08	1.48	1.44
10	cA	842	CLA	C4C-C3C	2.08	1.48	1.45
10	bA	805	CLA	C4B-NB	-2.08	1.33	1.35
10	aB	809	CLA	C1B-CHB	2.08	1.46	1.41
10	aA	823	CLA	C4B-CHC	2.08	1.46	1.41
10	cA	813	CLA	C1A-CHA	2.08	1.51	1.43
10	cB	829	CLA	C4B-CHC	2.08	1.46	1.41
10	cL	203	CLA	C1B-CHB	2.08	1.46	1.41
10	bA	839	CLA	C1B-NB	-2.08	1.33	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	856	CLA	C1B-CHB	2.08	1.46	1.41
10	aA	802	CLA	C1C-C2C	2.08	1.48	1.44
10	bL	204	CLA	C1B-CHB	2.08	1.46	1.41
10	bB	827	CLA	C4B-NB	-2.08	1.33	1.35
10	cA	826	CLA	C1B-CHB	2.07	1.46	1.41
10	cA	854	CLA	C1B-CHB	2.07	1.46	1.41
10	aB	819	CLA	C1C-NC	-2.07	1.34	1.37
10	bL	205	CLA	C1C-C2C	2.07	1.48	1.44
10	aB	816	CLA	C3D-C4D	-2.07	1.39	1.44
10	bB	833	CLA	C1B-CHB	2.07	1.46	1.41
10	bB	817	CLA	C1C-C2C	2.07	1.48	1.44
10	aB	837	CLA	C1B-NB	-2.07	1.33	1.35
10	cB	836	CLA	C1B-NB	-2.07	1.33	1.35
10	cL	203	CLA	C1C-C2C	2.07	1.48	1.44
10	aA	835	CLA	C1B-CHB	2.07	1.46	1.41
10	cA	803	CLA	C1B-CHB	2.07	1.46	1.41
10	cA	808	CLA	C1C-NC	-2.07	1.34	1.37
10	cA	823	CLA	C4C-C3C	2.07	1.48	1.45
10	aA	803	CLA	C1A-CHA	2.07	1.51	1.43
10	aA	842	CLA	C4C-C3C	2.07	1.48	1.45
10	cB	837	CLA	C4C-C3C	2.07	1.48	1.45
10	aA	839	CLA	C1B-NB	-2.07	1.33	1.35
10	aB	807	CLA	C4B-NB	-2.07	1.33	1.35
10	bA	804	CLA	C4C-C3C	2.07	1.48	1.45
10	aA	839	CLA	C1C-C2C	2.07	1.48	1.44
10	bL	203	CLA	C1B-CHB	2.07	1.46	1.41
10	aB	832	CLA	C1C-NC	-2.07	1.34	1.37
10	aL	202	CLA	C4B-NB	-2.07	1.33	1.35
10	aA	816	CLA	C1B-CHB	2.07	1.46	1.41
10	cB	817	CLA	C1C-C2C	2.07	1.48	1.44
10	aA	836	CLA	C1C-C2C	2.07	1.48	1.44
10	aA	822	CLA	C1B-CHB	2.07	1.46	1.41
10	cA	811	CLA	C1B-CHB	2.07	1.46	1.41
10	cA	827	CLA	C1C-NC	-2.07	1.34	1.37
10	bA	854	CLA	C1B-CHB	2.07	1.46	1.41
10	aA	840	CLA	C1B-NB	-2.07	1.33	1.35
10	cL	203	CLA	C4B-NB	-2.07	1.33	1.35
10	cB	809	CLA	C1C-NC	-2.07	1.34	1.37
10	aL	203	CLA	C1C-C2C	2.07	1.48	1.44
10	aA	823	CLA	C4C-C3C	2.07	1.48	1.45
10	cA	818	CLA	C4B-NB	-2.06	1.33	1.35
10	cB	832	CLA	C4C-C3C	2.06	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	827	CLA	C1A-CHA	2.06	1.51	1.43
10	bB	817	CLA	C1A-CHA	2.06	1.51	1.43
10	aA	827	CLA	C1C-NC	-2.06	1.34	1.37
10	cA	804	CLA	C4C-C3C	2.06	1.48	1.45
10	bB	811	CLA	C4B-NB	-2.06	1.33	1.35
10	bB	803	CLA	C1C-NC	-2.06	1.34	1.37
10	cA	833	CLA	C1C-NC	-2.06	1.34	1.37
10	aB	829	CLA	C4B-CHC	2.06	1.46	1.41
10	cB	829	CLA	C4C-C3C	2.06	1.48	1.45
10	cA	839	CLA	C1C-C2C	2.06	1.48	1.44
10	bB	828	CLA	C1A-CHA	2.06	1.51	1.43
10	bA	822	CLA	C1B-CHB	2.06	1.46	1.41
10	bB	830	CLA	C1B-CHB	2.06	1.46	1.41
10	bB	807	CLA	C1C-C2C	2.06	1.48	1.44
10	bB	836	CLA	C1C-C2C	2.06	1.48	1.44
10	cA	818	CLA	C4B-CHC	2.06	1.46	1.41
10	cB	835	CLA	C1B-CHB	2.06	1.46	1.41
10	bA	831	CLA	C1C-C2C	2.06	1.48	1.44
10	aA	814	CLA	C1C-NC	-2.06	1.34	1.37
10	cB	807	CLA	C1C-NC	-2.06	1.34	1.37
10	aB	812	CLA	C1B-CHB	2.06	1.46	1.41
10	bA	823	CLA	C4B-CHC	2.06	1.46	1.41
10	cA	807	CLA	C1A-CHA	2.06	1.51	1.43
9	aA	801	CL0	C1C-C2C	2.06	1.48	1.44
10	aA	808	CLA	C1C-NC	-2.06	1.34	1.37
10	aB	830	CLA	C1C-NC	-2.06	1.34	1.37
10	aB	830	CLA	C1B-CHB	2.06	1.46	1.41
10	bB	815	CLA	C1C-C2C	2.06	1.48	1.44
10	aB	837	CLA	C4C-C3C	2.06	1.48	1.45
10	aB	837	CLA	C1C-C2C	2.06	1.48	1.44
10	bA	803	CLA	C1B-NB	-2.06	1.33	1.35
10	bL	202	CLA	C4B-NB	-2.06	1.33	1.35
10	cB	812	CLA	C4B-CHC	2.06	1.46	1.41
10	aB	809	CLA	C4B-NB	-2.06	1.33	1.35
10	aB	809	CLA	C1C-NC	-2.06	1.34	1.37
10	aA	813	CLA	C1A-CHA	2.06	1.51	1.43
10	cA	803	CLA	C1A-CHA	2.06	1.51	1.43
10	cA	830	CLA	C1B-CHB	2.06	1.46	1.41
13	bA	849	BCR	C33-C5	-2.06	1.47	1.50
10	aA	811	CLA	C1B-CHB	2.06	1.46	1.41
10	cB	817	CLA	C1A-CHA	2.06	1.51	1.43
13	aL	206	BCR	C1-C6	-2.06	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aL	204	CLA	C1B-CHB	2.06	1.46	1.41
10	cB	828	CLA	C1A-CHA	2.06	1.51	1.43
10	aB	828	CLA	C4B-NB	-2.05	1.33	1.35
10	aL	205	CLA	C4B-NB	-2.05	1.33	1.35
10	bB	829	CLA	C4C-C3C	2.05	1.48	1.45
10	cA	809	CLA	C4C-C3C	2.05	1.48	1.45
10	aB	830	CLA	C4B-NB	-2.05	1.33	1.35
10	cA	837	CLA	C4B-NB	-2.05	1.33	1.35
10	cL	202	CLA	C4C-C3C	2.05	1.48	1.45
10	cA	836	CLA	C1C-C2C	2.05	1.48	1.44
10	cB	822	CLA	C4B-CHC	2.05	1.46	1.41
10	bA	807	CLA	C1A-CHA	2.05	1.51	1.43
10	bA	835	CLA	C1C-C2C	2.05	1.48	1.44
10	bB	812	CLA	C1B-CHB	2.05	1.46	1.41
10	aB	803	CLA	C1C-NC	-2.05	1.34	1.37
10	cA	827	CLA	C1B-CHB	2.05	1.46	1.41
10	bA	813	CLA	C1A-CHA	2.05	1.51	1.43
10	cA	835	CLA	C1B-CHB	2.05	1.46	1.41
10	cB	808	CLA	C1B-CHB	2.05	1.46	1.41
10	bB	806	CLA	C1A-CHA	2.05	1.51	1.43
10	bA	825	CLA	C4B-NB	-2.05	1.33	1.35
10	bA	835	CLA	C1B-CHB	2.05	1.46	1.41
10	bA	827	CLA	C1A-CHA	2.05	1.51	1.43
10	aB	812	CLA	C4B-CHC	2.05	1.46	1.41
10	aB	835	CLA	C1B-CHB	2.05	1.46	1.41
10	aB	822	CLA	C4B-CHC	2.05	1.46	1.41
10	aA	803	CLA	C1B-CHB	2.05	1.46	1.41
10	aB	817	CLA	C1A-CHA	2.05	1.51	1.43
10	cA	825	CLA	C1C-NC	-2.05	1.34	1.37
10	aB	836	CLA	C1B-NB	-2.05	1.33	1.35
10	cA	816	CLA	C1B-CHB	2.05	1.46	1.41
10	aB	807	CLA	C1C-C2C	2.05	1.48	1.44
10	cB	834	CLA	C1B-CHB	2.05	1.46	1.41
10	cB	837	CLA	C1B-NB	-2.05	1.33	1.35
10	aA	854	CLA	C1C-C2C	2.05	1.48	1.44
10	aA	807	CLA	C1A-CHA	2.05	1.51	1.43
10	cA	809	CLA	C1B-CHB	2.05	1.46	1.41
13	cL	206	BCR	C1-C6	-2.05	1.51	1.53
10	bB	829	CLA	C4B-CHC	2.05	1.46	1.41
10	cA	823	CLA	C4B-CHC	2.05	1.46	1.41
10	cA	821	CLA	C4B-NB	-2.05	1.33	1.35
10	aA	827	CLA	C1A-CHA	2.05	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	822	CLA	C1C-C2C	2.05	1.48	1.44
10	cA	802	CLA	C1C-C2C	2.05	1.48	1.44
10	cA	831	CLA	C1C-C2C	2.05	1.48	1.44
10	cA	822	CLA	C1B-CHB	2.04	1.46	1.41
10	cA	842	CLA	C4B-NB	-2.04	1.33	1.35
10	aA	830	CLA	C1B-CHB	2.04	1.46	1.41
10	aA	814	CLA	C1B-CHB	2.04	1.46	1.41
10	aB	833	CLA	C1B-CHB	2.04	1.46	1.41
10	aA	831	CLA	C1C-C2C	2.04	1.48	1.44
10	aB	829	CLA	C4C-C3C	2.04	1.48	1.45
10	bB	830	CLA	C1C-NC	-2.04	1.34	1.37
10	bA	803	CLA	C1A-CHA	2.04	1.51	1.43
10	bB	808	CLA	C1B-CHB	2.04	1.46	1.41
9	bA	801	CL0	C1C-C2C	2.04	1.48	1.44
10	aB	808	CLA	C1B-CHB	2.04	1.46	1.41
10	aL	203	CLA	C1B-CHB	2.04	1.46	1.41
10	bA	821	CLA	C4B-NB	-2.04	1.33	1.35
10	bA	816	CLA	C1B-CHB	2.04	1.46	1.41
10	aB	828	CLA	C1A-CHA	2.04	1.51	1.43
10	aB	827	CLA	C4C-C3C	2.04	1.48	1.45
10	bA	820	CLA	C4C-C3C	2.04	1.48	1.45
10	bA	809	CLA	C4C-C3C	2.04	1.48	1.45
10	cB	827	CLA	C4B-NB	-2.04	1.33	1.35
10	cB	829	CLA	C1C-NC	-2.04	1.34	1.37
10	bL	202	CLA	C1B-CHB	2.04	1.46	1.41
10	cB	833	CLA	C1B-CHB	2.04	1.46	1.41
10	bA	856	CLA	C1A-CHA	2.04	1.51	1.43
10	cA	839	CLA	C1B-NB	-2.04	1.33	1.35
10	bB	807	CLA	C1C-NC	-2.04	1.34	1.37
10	aA	856	CLA	C1A-CHA	2.04	1.51	1.43
10	bB	828	CLA	C4B-NB	-2.04	1.33	1.35
10	cB	830	CLA	C4B-NB	-2.04	1.33	1.35
10	bB	809	CLA	C4B-NB	-2.04	1.33	1.35
10	bB	830	CLA	C4B-NB	-2.04	1.33	1.35
10	aA	854	CLA	C1C-NC	-2.04	1.34	1.37
10	aB	817	CLA	C1C-C2C	2.04	1.48	1.44
10	cA	817	CLA	C1B-CHB	2.04	1.46	1.41
10	aA	809	CLA	C1B-CHB	2.04	1.46	1.41
10	aB	841	CLA	C4C-C3C	2.04	1.48	1.45
10	cA	837	CLA	C1C-C2C	2.04	1.48	1.44
10	bB	822	CLA	C4B-CHC	2.03	1.46	1.41
10	bB	833	CLA	C1B-NB	-2.03	1.33	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	832	CLA	C4C-C3C	2.03	1.48	1.45
10	cB	832	CLA	C1C-NC	-2.03	1.34	1.37
10	aB	806	CLA	C1A-CHA	2.03	1.51	1.43
10	cA	856	CLA	C1A-CHA	2.03	1.51	1.43
10	bA	854	CLA	C1C-C2C	2.03	1.48	1.44
10	aA	827	CLA	C1B-CHB	2.03	1.46	1.41
10	cA	841	CLA	C1C-NC	-2.03	1.34	1.37
10	aA	854	CLA	C1B-CHB	2.03	1.46	1.41
10	bB	812	CLA	C4B-CHC	2.03	1.46	1.41
10	bL	203	CLA	C4B-NB	-2.03	1.33	1.35
10	aB	825	CLA	C1C-C2C	2.03	1.48	1.44
10	aA	829	CLA	C4B-CHC	2.03	1.46	1.41
10	aA	817	CLA	C1B-CHB	2.03	1.46	1.41
10	aA	812	CLA	C1B-CHB	2.03	1.46	1.41
13	aI	101	BCR	C33-C5	-2.03	1.47	1.50
10	bA	813	CLA	C4B-NB	-2.03	1.33	1.35
10	bB	816	CLA	C1B-CHB	2.03	1.46	1.41
10	aL	202	CLA	C4C-C3C	2.03	1.48	1.45
10	bA	807	CLA	C4B-NB	-2.03	1.33	1.35
10	bB	836	CLA	C1B-NB	-2.03	1.33	1.35
10	aB	818	CLA	C1C-NC	-2.03	1.34	1.37
10	aB	814	CLA	C1C-C2C	2.03	1.48	1.44
10	bA	830	CLA	C1C-C2C	2.03	1.48	1.44
10	bL	203	CLA	C4C-C3C	2.03	1.48	1.45
10	aL	202	CLA	C1B-CHB	2.03	1.46	1.41
10	bB	837	CLA	C1B-NB	-2.03	1.33	1.35
10	cB	833	CLA	C1B-NB	-2.03	1.33	1.35
10	cL	205	CLA	C4B-NB	-2.03	1.33	1.35
10	cB	805	CLA	C1A-CHA	2.03	1.51	1.43
10	aB	834	CLA	C1B-CHB	2.03	1.46	1.41
10	aA	818	CLA	C4B-NB	-2.03	1.33	1.35
10	aB	802	CLA	C4C-C3C	2.03	1.48	1.45
10	cA	812	CLA	C1B-CHB	2.03	1.46	1.41
10	aL	203	CLA	C4C-C3C	2.03	1.48	1.45
10	cA	854	CLA	C1C-C2C	2.03	1.48	1.44
10	aA	803	CLA	C1B-NB	-2.03	1.33	1.35
10	cA	825	CLA	C4C-C3C	2.03	1.48	1.45
10	cA	805	CLA	C4B-NB	-2.02	1.33	1.35
10	cB	814	CLA	C1C-C2C	2.02	1.48	1.44
10	bA	823	CLA	C4C-C3C	2.02	1.48	1.45
10	bA	842	CLA	C4C-C3C	2.02	1.48	1.45
10	bL	202	CLA	C1C-C2C	2.02	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aL	203	CLA	C4B-NB	-2.02	1.33	1.35
10	bA	817	CLA	C1B-CHB	2.02	1.46	1.41
13	bL	206	BCR	C1-C6	-2.02	1.51	1.53
10	aL	202	CLA	C1C-C2C	2.02	1.48	1.44
10	cB	807	CLA	C4B-NB	-2.02	1.33	1.35
10	aB	811	CLA	C4C-C3C	2.02	1.48	1.45
10	aA	837	CLA	C1C-C2C	2.02	1.48	1.44
10	bA	812	CLA	C1B-CHB	2.02	1.46	1.41
10	bL	202	CLA	C4C-C3C	2.02	1.48	1.45
10	aB	833	CLA	C1B-NB	-2.02	1.33	1.35
10	bL	203	CLA	C1C-C2C	2.02	1.48	1.44
13	cI	102	BCR	C33-C5	-2.02	1.47	1.50
10	cA	829	CLA	C4B-CHC	2.02	1.46	1.41
10	cB	806	CLA	C1A-CHA	2.02	1.51	1.43
10	aA	825	CLA	C4B-NB	-2.02	1.33	1.35
10	bB	823	CLA	C1B-NB	-2.02	1.33	1.35
10	bA	814	CLA	C1B-CHB	2.02	1.46	1.41
10	bB	807	CLA	C1B-CHB	2.02	1.46	1.41
10	bB	835	CLA	C1B-CHB	2.02	1.46	1.41
10	bA	825	CLA	C1C-NC	-2.02	1.34	1.37
10	bB	805	CLA	C1A-CHA	2.02	1.51	1.43
10	cB	839	CLA	C1C-NC	-2.02	1.34	1.37
9	cA	801	CL0	C1C-C2C	2.02	1.48	1.44
10	aB	805	CLA	C1A-CHA	2.02	1.51	1.43
10	aB	807	CLA	C1B-CHB	2.01	1.46	1.41
10	bA	827	CLA	C1B-CHB	2.01	1.46	1.41
10	cB	816	CLA	C1B-NB	-2.01	1.33	1.35
10	bA	830	CLA	C1B-CHB	2.01	1.46	1.41
10	cA	814	CLA	C1B-CHB	2.01	1.46	1.41
10	bA	839	CLA	C1C-C2C	2.01	1.48	1.44
10	cB	813	CLA	C1C-NC	-2.01	1.34	1.37
10	aA	838	CLA	C1C-C2C	2.01	1.48	1.44
10	cA	813	CLA	C4B-NB	-2.01	1.33	1.35
10	cA	817	CLA	C4C-C3C	2.01	1.48	1.45
10	aB	825	CLA	C1B-CHB	2.01	1.46	1.41
10	bB	832	CLA	C1C-NC	-2.01	1.34	1.37
10	cB	807	CLA	C1C-C2C	2.01	1.48	1.44
10	cB	825	CLA	C1C-C2C	2.01	1.48	1.44
10	cB	832	CLA	C1B-CHB	2.01	1.46	1.41
10	aA	830	CLA	C1C-C2C	2.01	1.48	1.44
10	cA	838	CLA	C4C-C3C	2.01	1.48	1.45
13	cA	849	BCR	C33-C5	-2.01	1.47	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	838	CLA	C1C-C2C	2.01	1.48	1.44
10	bA	816	CLA	C1A-CHA	2.01	1.51	1.43
13	aA	849	BCR	C33-C5	-2.01	1.47	1.50
10	bA	856	CLA	C3D-C4D	-2.01	1.39	1.44
10	aA	812	CLA	C1B-NB	-2.01	1.33	1.35
10	aB	827	CLA	C4B-NB	-2.01	1.33	1.35
10	bA	815	CLA	C1C-C2C	2.01	1.48	1.44
10	cA	804	CLA	C1C-C2C	2.01	1.48	1.44
10	bB	802	CLA	C4C-C3C	2.01	1.48	1.45
10	cB	811	CLA	C4C-C3C	2.01	1.48	1.45
10	aA	816	CLA	C1A-CHA	2.01	1.51	1.43
10	cB	818	CLA	C1C-NC	-2.01	1.34	1.37
10	aB	831	CLA	C1B-NB	-2.01	1.33	1.35
10	bB	835	CLA	C1A-CHA	2.01	1.51	1.43
10	aA	856	CLA	C3D-C4D	-2.01	1.39	1.44
10	aA	805	CLA	C4B-NB	-2.01	1.33	1.35
10	cB	809	CLA	C4B-NB	-2.01	1.33	1.35
10	cL	203	CLA	C4C-C3C	2.01	1.48	1.45
10	bA	829	CLA	C4B-CHC	2.01	1.46	1.41
14	bA	852	LHG	O7-C5	-2.01	1.41	1.46
10	cB	802	CLA	C4C-C3C	2.00	1.48	1.45
14	aA	852	LHG	O7-C5	-2.00	1.41	1.46
10	bB	827	CLA	C1B-NB	-2.00	1.33	1.35
10	bB	841	CLA	C4C-C3C	2.00	1.48	1.45
10	cA	818	CLA	C1C-NC	-2.00	1.34	1.37
10	aB	816	CLA	C1B-CHB	2.00	1.46	1.41
10	bB	811	CLA	C4C-C3C	2.00	1.48	1.45
10	aA	842	CLA	C4B-NB	-2.00	1.33	1.35
10	aB	810	CLA	C4B-CHC	2.00	1.46	1.41
10	aA	815	CLA	C1C-C2C	2.00	1.48	1.44
10	aA	823	CLA	C1A-CHA	2.00	1.51	1.43
10	cB	807	CLA	C1B-CHB	2.00	1.46	1.41
10	bA	807	CLA	C1B-CHB	2.00	1.46	1.41
10	cL	202	CLA	C1C-C2C	2.00	1.48	1.44
10	aA	807	CLA	C1B-CHB	2.00	1.46	1.41
10	bB	834	CLA	C1B-CHB	2.00	1.46	1.41
10	aA	838	CLA	C4C-C3C	2.00	1.48	1.45
10	cA	854	CLA	C1C-NC	-2.00	1.34	1.37

All (7586) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	836	CLA	C4-C3-C5	-31.70	79.75	115.98
10	bA	836	CLA	C4-C3-C5	-31.68	79.77	115.98
10	aA	836	CLA	C4-C3-C5	-31.64	79.81	115.98
10	cA	836	CLA	C4-C3-C2	-17.16	79.65	123.68
10	aA	836	CLA	C4-C3-C2	-17.15	79.68	123.68
10	bA	836	CLA	C4-C3-C2	-17.15	79.69	123.68
10	aA	836	CLA	C5-C3-C2	15.76	159.48	120.50
10	bA	836	CLA	C5-C3-C2	15.75	159.45	120.50
10	cA	836	CLA	C5-C3-C2	15.72	159.38	120.50
10	cL	204	CLA	C1D-ND-C4D	-10.34	98.99	106.33
10	aL	204	CLA	C1D-ND-C4D	-10.33	99.00	106.33
10	bL	204	CLA	C1D-ND-C4D	-10.25	99.05	106.33
10	cL	204	CLA	C2D-C1D-ND	10.00	117.47	110.10
10	bL	204	CLA	C2D-C1D-ND	9.99	117.47	110.10
10	aL	204	CLA	C2D-C1D-ND	9.97	117.45	110.10
10	aB	822	CLA	C1D-ND-C4D	-9.70	99.45	106.33
10	cB	822	CLA	C1D-ND-C4D	-9.69	99.45	106.33
10	bB	822	CLA	C1D-ND-C4D	-9.67	99.47	106.33
10	cA	854	CLA	C1D-ND-C4D	-9.58	99.53	106.33
10	aA	854	CLA	C1D-ND-C4D	-9.55	99.55	106.33
10	aA	816	CLA	C1D-ND-C4D	-9.52	99.57	106.33
10	bA	816	CLA	C1D-ND-C4D	-9.51	99.58	106.33
10	cA	816	CLA	C1D-ND-C4D	-9.51	99.58	106.33
10	bA	808	CLA	C1D-ND-C4D	-9.50	99.59	106.33
10	bA	854	CLA	C1D-ND-C4D	-9.47	99.61	106.33
10	aA	808	CLA	C1D-ND-C4D	-9.46	99.61	106.33
10	cA	808	CLA	C1D-ND-C4D	-9.44	99.63	106.33
10	bB	834	CLA	C1D-ND-C4D	-9.32	99.71	106.33
10	aB	834	CLA	C1D-ND-C4D	-9.30	99.72	106.33
10	bL	205	CLA	C1D-ND-C4D	-9.30	99.73	106.33
10	aL	205	CLA	C1D-ND-C4D	-9.30	99.73	106.33
10	aB	813	CLA	C1D-ND-C4D	-9.30	99.73	106.33
10	cA	815	CLA	C1D-ND-C4D	-9.29	99.74	106.33
10	bA	815	CLA	C1D-ND-C4D	-9.28	99.75	106.33
10	cB	834	CLA	C1D-ND-C4D	-9.28	99.75	106.33
10	aA	815	CLA	C1D-ND-C4D	-9.27	99.75	106.33
10	bB	813	CLA	C1D-ND-C4D	-9.25	99.76	106.33
10	cL	205	CLA	C1D-ND-C4D	-9.24	99.77	106.33
10	aA	809	CLA	C1D-ND-C4D	-9.23	99.78	106.33
10	cA	824	CLA	C1D-ND-C4D	-9.23	99.78	106.33
10	aA	824	CLA	C1D-ND-C4D	-9.22	99.79	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	824	CLA	C1D-ND-C4D	-9.21	99.79	106.33
10	cB	838	CLA	C1D-ND-C4D	-9.21	99.79	106.33
10	cA	809	CLA	C1D-ND-C4D	-9.20	99.80	106.33
10	aL	203	CLA	C1D-ND-C4D	-9.20	99.80	106.33
10	cA	804	CLA	C1D-ND-C4D	-9.19	99.81	106.33
10	cL	203	CLA	C1D-ND-C4D	-9.19	99.81	106.33
10	aA	804	CLA	C1D-ND-C4D	-9.18	99.81	106.33
10	bB	803	CLA	C1D-ND-C4D	-9.18	99.81	106.33
10	cB	813	CLA	C1D-ND-C4D	-9.18	99.82	106.33
10	aA	812	CLA	C1D-ND-C4D	-9.17	99.82	106.33
10	bL	203	CLA	C1D-ND-C4D	-9.17	99.82	106.33
10	aB	838	CLA	C1D-ND-C4D	-9.17	99.82	106.33
10	bA	809	CLA	C1D-ND-C4D	-9.16	99.83	106.33
10	bB	809	CLA	C1D-ND-C4D	-9.15	99.84	106.33
10	cB	803	CLA	C1D-ND-C4D	-9.14	99.84	106.33
10	cB	805	CLA	C2D-C1D-ND	9.14	116.84	110.10
10	bA	804	CLA	C1D-ND-C4D	-9.13	99.85	106.33
10	bA	812	CLA	C1D-ND-C4D	-9.13	99.85	106.33
10	aA	838	CLA	C1D-ND-C4D	-9.13	99.85	106.33
10	bA	838	CLA	C1D-ND-C4D	-9.13	99.85	106.33
10	aB	841	CLA	C1D-ND-C4D	-9.12	99.86	106.33
10	aB	803	CLA	C1D-ND-C4D	-9.11	99.86	106.33
10	cB	841	CLA	C1D-ND-C4D	-9.11	99.86	106.33
10	cA	840	CLA	C1D-ND-C4D	-9.10	99.87	106.33
10	cA	812	CLA	C1D-ND-C4D	-9.10	99.87	106.33
10	aB	809	CLA	C1D-ND-C4D	-9.10	99.87	106.33
10	bB	805	CLA	C2D-C1D-ND	9.10	116.81	110.10
10	aB	839	CLA	C1D-ND-C4D	-9.10	99.87	106.33
10	cA	838	CLA	C1D-ND-C4D	-9.09	99.87	106.33
10	bB	838	CLA	C1D-ND-C4D	-9.09	99.88	106.33
10	bB	841	CLA	C1D-ND-C4D	-9.08	99.88	106.33
10	cB	839	CLA	C1D-ND-C4D	-9.07	99.89	106.33
10	cA	834	CLA	C1D-ND-C4D	-9.07	99.89	106.33
10	aB	805	CLA	C2D-C1D-ND	9.07	116.78	110.10
10	cA	837	CLA	C1D-ND-C4D	-9.06	99.90	106.33
10	aB	832	CLA	C1D-ND-C4D	-9.06	99.90	106.33
10	aA	834	CLA	C1D-ND-C4D	-9.06	99.90	106.33
10	aA	811	CLA	C1D-ND-C4D	-9.06	99.90	106.33
10	aB	807	CLA	C1D-ND-C4D	-9.06	99.90	106.33
10	cB	809	CLA	C1D-ND-C4D	-9.06	99.90	106.33
10	cB	804	CLA	C2D-C1D-ND	9.05	116.77	110.10
10	cB	832	CLA	C1D-ND-C4D	-9.04	99.91	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	837	CLA	C1D-ND-C4D	-9.04	99.91	106.33
10	bB	806	CLA	C1D-ND-C4D	-9.04	99.91	106.33
10	bA	811	CLA	C1D-ND-C4D	-9.04	99.92	106.33
10	cB	827	CLA	C1D-ND-C4D	-9.03	99.92	106.33
10	bB	839	CLA	C1D-ND-C4D	-9.03	99.92	106.33
10	bA	840	CLA	C1D-ND-C4D	-9.03	99.92	106.33
10	bA	837	CLA	C1D-ND-C4D	-9.03	99.92	106.33
10	bB	832	CLA	C1D-ND-C4D	-9.02	99.92	106.33
10	cA	817	CLA	C1D-ND-C4D	-9.02	99.93	106.33
10	cA	820	CLA	C1D-ND-C4D	-9.02	99.93	106.33
10	bA	832	CLA	C1D-ND-C4D	-9.01	99.93	106.33
10	aA	840	CLA	C1D-ND-C4D	-9.01	99.93	106.33
10	cA	811	CLA	C1D-ND-C4D	-9.01	99.94	106.33
10	aB	806	CLA	C1D-ND-C4D	-9.00	99.94	106.33
10	bA	806	CLA	C1D-ND-C4D	-8.99	99.95	106.33
10	bA	843	CLA	C1D-ND-C4D	-8.99	99.95	106.33
10	aA	820	CLA	C1D-ND-C4D	-8.99	99.95	106.33
10	bB	827	CLA	C1D-ND-C4D	-8.99	99.95	106.33
10	aA	802	CLA	C1D-ND-C4D	-8.99	99.95	106.33
10	aB	804	CLA	C2D-C1D-ND	8.99	116.73	110.10
10	bB	804	CLA	C2D-C1D-ND	8.98	116.72	110.10
10	bA	820	CLA	C1D-ND-C4D	-8.98	99.95	106.33
10	cB	806	CLA	C1D-ND-C4D	-8.98	99.96	106.33
10	bA	834	CLA	C1D-ND-C4D	-8.98	99.96	106.33
10	aA	843	CLA	C1D-ND-C4D	-8.98	99.96	106.33
10	bB	807	CLA	C1D-ND-C4D	-8.97	99.96	106.33
10	aB	802	CLA	C2D-C1D-ND	8.97	116.72	110.10
10	bB	802	CLA	C2D-C1D-ND	8.97	116.71	110.10
10	aB	827	CLA	C1D-ND-C4D	-8.97	99.97	106.33
10	aA	832	CLA	C1D-ND-C4D	-8.96	99.97	106.33
10	bA	817	CLA	C1D-ND-C4D	-8.95	99.98	106.33
10	cB	807	CLA	C1D-ND-C4D	-8.94	99.98	106.33
10	cA	832	CLA	C1D-ND-C4D	-8.94	99.99	106.33
10	aB	817	CLA	C1D-ND-C4D	-8.94	99.99	106.33
10	bA	810	CLA	C1D-ND-C4D	-8.94	99.99	106.33
10	cB	833	CLA	C1D-ND-C4D	-8.93	99.99	106.33
10	aA	817	CLA	C1D-ND-C4D	-8.93	99.99	106.33
10	cB	802	CLA	C2D-C1D-ND	8.93	116.69	110.10
10	bA	802	CLA	C1D-ND-C4D	-8.93	99.99	106.33
10	cA	843	CLA	C1D-ND-C4D	-8.93	99.99	106.33
10	cA	806	CLA	C1D-ND-C4D	-8.93	99.99	106.33
10	cA	810	CLA	C1D-ND-C4D	-8.92	100.00	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	802	CLA	C1D-ND-C4D	-8.92	100.00	106.33
10	cB	812	CLA	C1D-ND-C4D	-8.92	100.00	106.33
10	bB	812	CLA	C1D-ND-C4D	-8.91	100.00	106.33
10	bA	841	CLA	C1D-ND-C4D	-8.91	100.00	106.33
10	aA	839	CLA	C1D-ND-C4D	-8.90	100.01	106.33
10	cB	827	CLA	C2D-C1D-ND	8.90	116.66	110.10
10	aA	805	CLA	C1D-ND-C4D	-8.90	100.02	106.33
10	aA	810	CLA	C1D-ND-C4D	-8.89	100.02	106.33
10	bA	807	CLA	C1D-ND-C4D	-8.89	100.02	106.33
10	cA	818	CLA	C1D-ND-C4D	-8.89	100.02	106.33
10	aA	841	CLA	C1D-ND-C4D	-8.88	100.03	106.33
10	bA	831	CLA	C1D-ND-C4D	-8.88	100.03	106.33
10	aB	827	CLA	C2D-C1D-ND	8.87	116.64	110.10
10	aA	818	CLA	C1D-ND-C4D	-8.87	100.03	106.33
10	aB	812	CLA	C1D-ND-C4D	-8.87	100.03	106.33
10	bB	827	CLA	C2D-C1D-ND	8.87	116.64	110.10
10	aA	803	CLA	C1D-ND-C4D	-8.87	100.03	106.33
10	aB	837	CLA	C1D-ND-C4D	-8.87	100.03	106.33
10	aB	828	CLA	C1D-ND-C4D	-8.87	100.03	106.33
10	aA	827	CLA	C1D-ND-C4D	-8.87	100.04	106.33
10	aA	831	CLA	C1D-ND-C4D	-8.86	100.04	106.33
10	bB	833	CLA	C1D-ND-C4D	-8.86	100.04	106.33
10	bA	839	CLA	C1D-ND-C4D	-8.86	100.04	106.33
10	aB	833	CLA	C1D-ND-C4D	-8.86	100.04	106.33
10	bA	827	CLA	C1D-ND-C4D	-8.85	100.05	106.33
10	bA	805	CLA	C1D-ND-C4D	-8.85	100.05	106.33
10	bB	817	CLA	C1D-ND-C4D	-8.85	100.05	106.33
10	cA	841	CLA	C1D-ND-C4D	-8.85	100.05	106.33
10	aA	806	CLA	C1D-ND-C4D	-8.85	100.05	106.33
10	aA	807	CLA	C1D-ND-C4D	-8.85	100.05	106.33
10	aB	818	CLA	C1D-ND-C4D	-8.84	100.05	106.33
10	cB	837	CLA	C1D-ND-C4D	-8.84	100.05	106.33
10	cA	807	CLA	C1D-ND-C4D	-8.84	100.06	106.33
10	cA	831	CLA	C1D-ND-C4D	-8.84	100.06	106.33
10	bB	828	CLA	C1D-ND-C4D	-8.84	100.06	106.33
10	cA	839	CLA	C1D-ND-C4D	-8.84	100.06	106.33
10	cB	828	CLA	C1D-ND-C4D	-8.83	100.06	106.33
10	bB	837	CLA	C1D-ND-C4D	-8.83	100.06	106.33
10	aA	825	CLA	C1D-ND-C4D	-8.83	100.06	106.33
10	cA	827	CLA	C1D-ND-C4D	-8.83	100.06	106.33
10	bA	818	CLA	C1D-ND-C4D	-8.83	100.06	106.33
10	aB	804	CLA	C1D-ND-C4D	-8.82	100.07	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	820	CLA	C1D-ND-C4D	-8.82	100.07	106.33
10	bA	803	CLA	C1D-ND-C4D	-8.82	100.07	106.33
10	cA	803	CLA	C1D-ND-C4D	-8.81	100.07	106.33
10	cB	820	CLA	C1D-ND-C4D	-8.81	100.08	106.33
10	cB	818	CLA	C1D-ND-C4D	-8.81	100.08	106.33
10	bB	818	CLA	C1D-ND-C4D	-8.81	100.08	106.33
10	cB	817	CLA	C1D-ND-C4D	-8.81	100.08	106.33
10	cA	825	CLA	C1D-ND-C4D	-8.80	100.08	106.33
10	cB	804	CLA	C1D-ND-C4D	-8.80	100.08	106.33
10	cA	805	CLA	C1D-ND-C4D	-8.80	100.08	106.33
10	cA	829	CLA	C1D-ND-C4D	-8.80	100.09	106.33
10	cA	821	CLA	C1D-ND-C4D	-8.79	100.09	106.33
10	bB	805	CLA	C1D-ND-C4D	-8.79	100.09	106.33
10	bB	820	CLA	C1D-ND-C4D	-8.79	100.09	106.33
10	bA	829	CLA	C1D-ND-C4D	-8.79	100.09	106.33
10	cB	802	CLA	C1D-ND-C4D	-8.79	100.09	106.33
10	bA	825	CLA	C1D-ND-C4D	-8.79	100.09	106.33
10	aA	826	CLA	C1D-ND-C4D	-8.78	100.10	106.33
10	bB	804	CLA	C1D-ND-C4D	-8.78	100.10	106.33
10	cB	805	CLA	C1D-ND-C4D	-8.78	100.10	106.33
10	bB	802	CLA	C1D-ND-C4D	-8.78	100.10	106.33
10	aA	829	CLA	C1D-ND-C4D	-8.77	100.11	106.33
10	cA	814	CLA	C1D-ND-C4D	-8.76	100.11	106.33
10	aB	805	CLA	C1D-ND-C4D	-8.76	100.11	106.33
10	bA	814	CLA	C1D-ND-C4D	-8.76	100.11	106.33
10	aB	802	CLA	C1D-ND-C4D	-8.76	100.11	106.33
10	bB	835	CLA	C1D-ND-C4D	-8.75	100.12	106.33
10	bA	821	CLA	C1D-ND-C4D	-8.75	100.12	106.33
10	bA	826	CLA	C1D-ND-C4D	-8.75	100.12	106.33
10	cB	828	CLA	C2D-C1D-ND	8.73	116.54	110.10
10	cA	826	CLA	C1D-ND-C4D	-8.73	100.13	106.33
10	cB	835	CLA	C1D-ND-C4D	-8.73	100.13	106.33
10	aB	828	CLA	C2D-C1D-ND	8.73	116.53	110.10
10	aA	814	CLA	C1D-ND-C4D	-8.72	100.14	106.33
10	cB	824	CLA	C1D-ND-C4D	-8.72	100.14	106.33
10	bA	833	CLA	C1D-ND-C4D	-8.72	100.14	106.33
10	cA	833	CLA	C1D-ND-C4D	-8.71	100.15	106.33
10	bB	828	CLA	C2D-C1D-ND	8.71	116.52	110.10
10	aB	824	CLA	C1D-ND-C4D	-8.70	100.15	106.33
10	aA	821	CLA	C1D-ND-C4D	-8.70	100.15	106.33
10	aB	835	CLA	C1D-ND-C4D	-8.70	100.16	106.33
10	aA	835	CLA	C1D-ND-C4D	-8.70	100.16	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	833	CLA	C1D-ND-C4D	-8.69	100.16	106.33
10	aA	842	CLA	C1D-ND-C4D	-8.68	100.17	106.33
10	bA	842	CLA	C1D-ND-C4D	-8.67	100.18	106.33
10	aB	840	CLA	C1D-ND-C4D	-8.66	100.19	106.33
10	bA	835	CLA	C1D-ND-C4D	-8.65	100.19	106.33
10	cA	835	CLA	C1D-ND-C4D	-8.65	100.19	106.33
10	bB	824	CLA	C1D-ND-C4D	-8.64	100.19	106.33
10	aA	856	CLA	C1D-ND-C4D	-8.63	100.21	106.33
10	cB	840	CLA	C1D-ND-C4D	-8.63	100.21	106.33
10	aA	819	CLA	C1D-ND-C4D	-8.63	100.21	106.33
10	bB	840	CLA	C1D-ND-C4D	-8.62	100.21	106.33
10	aA	824	CLA	C2D-C1D-ND	8.62	116.46	110.10
10	cA	842	CLA	C1D-ND-C4D	-8.62	100.21	106.33
10	bB	823	CLA	C1D-ND-C4D	-8.61	100.22	106.33
9	aA	801	CL0	C1D-ND-C4D	-8.59	100.23	106.33
10	cA	819	CLA	C1D-ND-C4D	-8.59	100.23	106.33
10	cB	823	CLA	C1D-ND-C4D	-8.59	100.23	106.33
10	aB	822	CLA	C2D-C1D-ND	8.59	116.43	110.10
10	bA	824	CLA	C2D-C1D-ND	8.58	116.43	110.10
10	bA	819	CLA	C1D-ND-C4D	-8.58	100.24	106.33
10	cA	822	CLA	C1D-ND-C4D	-8.58	100.24	106.33
9	cA	801	CL0	C1D-ND-C4D	-8.58	100.24	106.33
10	aB	836	CLA	C1D-ND-C4D	-8.58	100.24	106.33
10	cA	824	CLA	C2D-C1D-ND	8.57	116.42	110.10
10	bB	822	CLA	C2D-C1D-ND	8.57	116.42	110.10
10	bA	856	CLA	C1D-ND-C4D	-8.56	100.25	106.33
10	cB	836	CLA	C1D-ND-C4D	-8.56	100.25	106.33
10	cB	822	CLA	C2D-C1D-ND	8.56	116.41	110.10
10	bB	816	CLA	C1D-ND-C4D	-8.56	100.26	106.33
10	aB	823	CLA	C1D-ND-C4D	-8.55	100.26	106.33
10	aA	822	CLA	C1D-ND-C4D	-8.55	100.26	106.33
10	cB	821	CLA	C1D-ND-C4D	-8.55	100.26	106.33
10	bA	813	CLA	C1D-ND-C4D	-8.54	100.27	106.33
10	bB	836	CLA	C1D-ND-C4D	-8.54	100.27	106.33
10	aB	816	CLA	C1D-ND-C4D	-8.54	100.27	106.33
10	bA	822	CLA	C1D-ND-C4D	-8.53	100.27	106.33
10	cB	816	CLA	C1D-ND-C4D	-8.53	100.27	106.33
10	aB	808	CLA	C1D-ND-C4D	-8.53	100.28	106.33
10	bB	808	CLA	C1D-ND-C4D	-8.53	100.28	106.33
10	cA	823	CLA	C1D-ND-C4D	-8.53	100.28	106.33
10	cB	808	CLA	C1D-ND-C4D	-8.53	100.28	106.33
10	cA	856	CLA	C1D-ND-C4D	-8.52	100.28	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	830	CLA	C1D-ND-C4D	-8.52	100.28	106.33
10	cA	813	CLA	C1D-ND-C4D	-8.52	100.28	106.33
9	bA	801	CL0	C1D-ND-C4D	-8.52	100.28	106.33
10	aA	813	CLA	C1D-ND-C4D	-8.51	100.29	106.33
10	aB	821	CLA	C1D-ND-C4D	-8.51	100.29	106.33
10	aA	830	CLA	C1D-ND-C4D	-8.51	100.29	106.33
10	bA	823	CLA	C1D-ND-C4D	-8.51	100.29	106.33
10	aA	816	CLA	C2D-C1D-ND	8.50	116.37	110.10
10	cA	830	CLA	C1D-ND-C4D	-8.49	100.30	106.33
10	cA	816	CLA	C2D-C1D-ND	8.49	116.36	110.10
10	aL	202	CLA	C1D-ND-C4D	-8.48	100.31	106.33
10	aB	831	CLA	C1D-ND-C4D	-8.48	100.31	106.33
10	bB	829	CLA	C1D-ND-C4D	-8.47	100.32	106.33
10	bL	202	CLA	C1D-ND-C4D	-8.47	100.32	106.33
10	bA	816	CLA	C2D-C1D-ND	8.47	116.34	110.10
10	aA	823	CLA	C1D-ND-C4D	-8.47	100.32	106.33
10	bB	821	CLA	C1D-ND-C4D	-8.46	100.32	106.33
10	aB	815	CLA	C1D-ND-C4D	-8.45	100.33	106.33
10	cB	815	CLA	C1D-ND-C4D	-8.45	100.33	106.33
10	cL	202	CLA	C1D-ND-C4D	-8.45	100.33	106.33
10	bB	815	CLA	C1D-ND-C4D	-8.45	100.33	106.33
10	aB	826	CLA	C1D-ND-C4D	-8.43	100.34	106.33
10	bB	809	CLA	C2D-C1D-ND	8.43	116.32	110.10
10	aB	809	CLA	C2D-C1D-ND	8.41	116.30	110.10
10	cB	829	CLA	C1D-ND-C4D	-8.41	100.36	106.33
10	aB	829	CLA	C1D-ND-C4D	-8.40	100.36	106.33
10	aA	831	CLA	C2D-C1D-ND	8.40	116.29	110.10
10	cA	828	CLA	C1D-ND-C4D	-8.39	100.38	106.33
10	cB	809	CLA	C2D-C1D-ND	8.39	116.29	110.10
10	cA	854	CLA	C2D-C1D-ND	8.39	116.28	110.10
10	aA	854	CLA	C2D-C1D-ND	8.39	116.28	110.10
10	aA	829	CLA	C2D-C1D-ND	8.38	116.28	110.10
10	bB	826	CLA	C1D-ND-C4D	-8.38	100.38	106.33
10	cA	829	CLA	C2D-C1D-ND	8.36	116.27	110.10
10	cB	826	CLA	C1D-ND-C4D	-8.36	100.40	106.33
10	cA	821	CLA	C2D-C1D-ND	8.35	116.26	110.10
10	cB	831	CLA	C1D-ND-C4D	-8.35	100.40	106.33
10	cA	831	CLA	C2D-C1D-ND	8.35	116.26	110.10
10	cA	836	CLA	C1D-ND-C4D	-8.34	100.41	106.33
10	bB	831	CLA	C1D-ND-C4D	-8.34	100.41	106.33
10	aA	828	CLA	C1D-ND-C4D	-8.34	100.41	106.33
10	aA	836	CLA	C1D-ND-C4D	-8.34	100.41	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	854	CLA	C2D-C1D-ND	8.33	116.25	110.10
10	bA	828	CLA	C1D-ND-C4D	-8.32	100.42	106.33
10	bB	806	CLA	C2D-C1D-ND	8.32	116.24	110.10
10	cB	806	CLA	C2D-C1D-ND	8.32	116.24	110.10
10	aA	821	CLA	C2D-C1D-ND	8.32	116.23	110.10
10	bA	836	CLA	C1D-ND-C4D	-8.32	100.43	106.33
10	bA	831	CLA	C2D-C1D-ND	8.31	116.23	110.10
10	bA	821	CLA	C2D-C1D-ND	8.31	116.22	110.10
10	bA	829	CLA	C2D-C1D-ND	8.30	116.22	110.10
10	bB	803	CLA	C2D-C1D-ND	8.29	116.22	110.10
10	bA	807	CLA	C2D-C1D-ND	8.29	116.21	110.10
10	aL	202	CLA	C2D-C1D-ND	8.27	116.20	110.10
10	cA	807	CLA	C2D-C1D-ND	8.26	116.19	110.10
10	bA	826	CLA	C2D-C1D-ND	8.26	116.19	110.10
10	aB	806	CLA	C2D-C1D-ND	8.25	116.19	110.10
10	bB	825	CLA	C1D-ND-C4D	-8.25	100.47	106.33
10	aB	841	CLA	C2D-C1D-ND	8.25	116.19	110.10
10	bL	202	CLA	C2D-C1D-ND	8.24	116.18	110.10
10	aA	826	CLA	C2D-C1D-ND	8.24	116.17	110.10
10	cL	202	CLA	C2D-C1D-ND	8.23	116.17	110.10
10	cB	803	CLA	C2D-C1D-ND	8.23	116.17	110.10
10	cB	841	CLA	C2D-C1D-ND	8.23	116.17	110.10
10	aA	807	CLA	C2D-C1D-ND	8.22	116.16	110.10
10	aB	803	CLA	C2D-C1D-ND	8.22	116.16	110.10
10	cB	825	CLA	C1D-ND-C4D	-8.22	100.50	106.33
10	aB	825	CLA	C1D-ND-C4D	-8.21	100.50	106.33
10	bB	841	CLA	C2D-C1D-ND	8.20	116.15	110.10
10	cA	826	CLA	C2D-C1D-ND	8.20	116.15	110.10
10	aB	810	CLA	C1D-ND-C4D	-8.20	100.51	106.33
10	bB	810	CLA	C1D-ND-C4D	-8.19	100.52	106.33
10	cA	838	CLA	C2D-C1D-ND	8.15	116.11	110.10
10	aA	809	CLA	C2D-C1D-ND	8.14	116.10	110.10
10	cA	809	CLA	C2D-C1D-ND	8.13	116.10	110.10
10	aA	838	CLA	C2D-C1D-ND	8.13	116.09	110.10
10	bA	838	CLA	C2D-C1D-ND	8.13	116.09	110.10
10	cA	837	CLA	C2D-C1D-ND	8.13	116.09	110.10
10	bL	205	CLA	C2D-C1D-ND	8.11	116.08	110.10
10	bA	837	CLA	C2D-C1D-ND	8.11	116.08	110.10
10	cB	810	CLA	C1D-ND-C4D	-8.11	100.58	106.33
10	cB	814	CLA	C1D-ND-C4D	-8.10	100.58	106.33
10	aA	837	CLA	C2D-C1D-ND	8.09	116.06	110.10
10	cA	834	CLA	C2D-C1D-ND	8.08	116.06	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	814	CLA	C1D-ND-C4D	-8.08	100.60	106.33
10	aL	205	CLA	C2D-C1D-ND	8.07	116.05	110.10
10	bA	825	CLA	C2D-C1D-ND	8.07	116.05	110.10
10	bA	832	CLA	C2D-C1D-ND	8.07	116.05	110.10
10	aA	832	CLA	C2D-C1D-ND	8.07	116.05	110.10
10	aA	834	CLA	C2D-C1D-ND	8.05	116.03	110.10
10	aA	825	CLA	C2D-C1D-ND	8.05	116.03	110.10
10	bA	833	CLA	C2D-C1D-ND	8.04	116.03	110.10
10	cA	825	CLA	C2D-C1D-ND	8.04	116.03	110.10
10	cA	832	CLA	C2D-C1D-ND	8.03	116.03	110.10
10	bA	809	CLA	C2D-C1D-ND	8.03	116.02	110.10
10	bA	838	CLA	CAA-C2A-C3A	-8.02	90.83	112.78
10	aB	814	CLA	C1D-ND-C4D	-8.02	100.64	106.33
10	cL	205	CLA	C2D-C1D-ND	8.01	116.01	110.10
10	aA	833	CLA	C2D-C1D-ND	8.01	116.00	110.10
10	cA	838	CLA	CAA-C2A-C3A	-8.00	90.86	112.78
10	aB	808	CLA	C2D-C1D-ND	7.99	116.00	110.10
10	aB	817	CLA	C2D-C1D-ND	7.99	115.99	110.10
10	aA	838	CLA	CAA-C2A-C3A	-7.99	90.90	112.78
10	bA	834	CLA	C2D-C1D-ND	7.99	115.99	110.10
10	bB	830	CLA	C1D-ND-C4D	-7.98	100.66	106.33
10	aA	841	CLA	C2D-C1D-ND	7.98	115.98	110.10
10	aB	830	CLA	C1D-ND-C4D	-7.98	100.67	106.33
10	cB	830	CLA	C1D-ND-C4D	-7.97	100.67	106.33
10	bB	808	CLA	C2D-C1D-ND	7.97	115.98	110.10
10	cA	810	CLA	C2D-C1D-ND	7.97	115.98	110.10
10	bB	817	CLA	C2D-C1D-ND	7.97	115.97	110.10
10	cB	808	CLA	C2D-C1D-ND	7.97	115.97	110.10
10	bA	810	CLA	C2D-C1D-ND	7.96	115.97	110.10
10	cB	817	CLA	C2D-C1D-ND	7.96	115.97	110.10
10	cA	833	CLA	C2D-C1D-ND	7.96	115.97	110.10
10	aB	819	CLA	C1D-ND-C4D	-7.96	100.68	106.33
10	cB	838	CLA	C2D-C1D-ND	7.95	115.97	110.10
10	bA	841	CLA	C2D-C1D-ND	7.94	115.96	110.10
10	bA	808	CLA	C2D-C1D-ND	7.94	115.95	110.10
10	aA	803	CLA	C2D-C1D-ND	7.94	115.95	110.10
10	aA	810	CLA	C2D-C1D-ND	7.93	115.95	110.10
10	aB	838	CLA	C2D-C1D-ND	7.93	115.95	110.10
10	cB	819	CLA	C1D-ND-C4D	-7.93	100.70	106.33
10	bA	805	CLA	C2D-C1D-ND	7.92	115.94	110.10
10	aL	203	CLA	C2D-C1D-ND	7.91	115.93	110.10
10	cA	803	CLA	C2D-C1D-ND	7.91	115.93	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	841	CLA	C2D-C1D-ND	7.91	115.93	110.10
10	aA	805	CLA	C2D-C1D-ND	7.90	115.93	110.10
10	aA	811	CLA	C2D-C1D-ND	7.90	115.93	110.10
10	cL	203	CLA	C2D-C1D-ND	7.90	115.92	110.10
10	bB	838	CLA	C2D-C1D-ND	7.89	115.92	110.10
10	cB	839	CLA	C2D-C1D-ND	7.89	115.92	110.10
10	bL	203	CLA	C2D-C1D-ND	7.89	115.92	110.10
10	aA	808	CLA	C2D-C1D-ND	7.88	115.91	110.10
10	aB	839	CLA	C2D-C1D-ND	7.88	115.91	110.10
10	cA	808	CLA	C2D-C1D-ND	7.88	115.91	110.10
10	aB	813	CLA	C2D-C1D-ND	7.87	115.90	110.10
10	cA	817	CLA	C2D-C1D-ND	7.86	115.90	110.10
10	bB	819	CLA	C1D-ND-C4D	-7.86	100.75	106.33
10	bA	818	CLA	C2D-C1D-ND	7.86	115.89	110.10
10	bA	803	CLA	C2D-C1D-ND	7.86	115.89	110.10
10	bA	811	CLA	C2D-C1D-ND	7.86	115.89	110.10
10	aB	816	CLA	C2D-C1D-ND	7.85	115.89	110.10
10	aB	832	CLA	C2D-C1D-ND	7.85	115.89	110.10
10	cA	818	CLA	C2D-C1D-ND	7.85	115.89	110.10
10	cA	805	CLA	C2D-C1D-ND	7.85	115.89	110.10
10	bB	832	CLA	C2D-C1D-ND	7.84	115.88	110.10
10	cB	816	CLA	C2D-C1D-ND	7.84	115.88	110.10
10	bA	843	CLA	C2D-C1D-ND	7.84	115.88	110.10
10	bB	812	CLA	C2D-C1D-ND	7.83	115.88	110.10
10	bB	816	CLA	C2D-C1D-ND	7.83	115.87	110.10
10	bB	839	CLA	C2D-C1D-ND	7.83	115.87	110.10
10	cA	811	CLA	C2D-C1D-ND	7.82	115.87	110.10
10	cB	832	CLA	C2D-C1D-ND	7.82	115.87	110.10
10	aA	843	CLA	C2D-C1D-ND	7.81	115.86	110.10
10	aA	802	CLA	C2D-C1D-ND	7.81	115.86	110.10
10	aB	812	CLA	C2D-C1D-ND	7.80	115.86	110.10
10	bA	817	CLA	C2D-C1D-ND	7.80	115.85	110.10
10	cB	812	CLA	C2D-C1D-ND	7.80	115.85	110.10
10	aA	818	CLA	C2D-C1D-ND	7.80	115.85	110.10
10	bB	813	CLA	C2D-C1D-ND	7.79	115.85	110.10
10	cA	820	CLA	C2D-C1D-ND	7.78	115.84	110.10
10	bB	807	CLA	C2D-C1D-ND	7.77	115.83	110.10
10	bB	837	CLA	C2D-C1D-ND	7.77	115.83	110.10
10	bA	856	CLA	C2D-C1D-ND	7.77	115.83	110.10
10	cA	802	CLA	C2D-C1D-ND	7.77	115.83	110.10
10	cB	813	CLA	C2D-C1D-ND	7.76	115.82	110.10
10	cA	843	CLA	C2D-C1D-ND	7.76	115.82	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	820	CLA	C2D-C1D-ND	7.76	115.82	110.10
10	cB	837	CLA	C2D-C1D-ND	7.75	115.82	110.10
10	bA	820	CLA	C2D-C1D-ND	7.75	115.81	110.10
10	aB	837	CLA	C2D-C1D-ND	7.74	115.81	110.10
10	bA	815	CLA	C2D-C1D-ND	7.74	115.81	110.10
10	cA	815	CLA	C2D-C1D-ND	7.74	115.81	110.10
10	aB	807	CLA	C2D-C1D-ND	7.74	115.81	110.10
10	aA	856	CLA	C2D-C1D-ND	7.73	115.80	110.10
10	aA	817	CLA	C2D-C1D-ND	7.73	115.80	110.10
10	aA	815	CLA	C2D-C1D-ND	7.72	115.80	110.10
10	aA	827	CLA	C2D-C1D-ND	7.72	115.80	110.10
10	cB	801	CLA	C1D-ND-C4D	-7.72	100.85	106.33
10	cB	807	CLA	C2D-C1D-ND	7.72	115.79	110.10
10	cA	856	CLA	C2D-C1D-ND	7.71	115.79	110.10
10	cA	827	CLA	C2D-C1D-ND	7.71	115.79	110.10
10	cA	839	CLA	C2D-C1D-ND	7.71	115.78	110.10
10	aA	836	CLA	C2D-C1D-ND	7.71	115.78	110.10
10	bA	802	CLA	C2D-C1D-ND	7.70	115.78	110.10
10	aA	828	CLA	C2D-C1D-ND	7.70	115.78	110.10
10	cA	828	CLA	C2D-C1D-ND	7.70	115.78	110.10
10	bA	836	CLA	C2D-C1D-ND	7.68	115.76	110.10
10	aA	839	CLA	C2D-C1D-ND	7.67	115.76	110.10
10	bB	811	CLA	C1D-ND-C4D	-7.67	100.88	106.33
10	cB	833	CLA	C2D-C1D-ND	7.67	115.76	110.10
10	bB	801	CLA	C1D-ND-C4D	-7.67	100.89	106.33
10	aB	811	CLA	C1D-ND-C4D	-7.67	100.89	106.33
10	cA	842	CLA	C2D-C1D-ND	7.67	115.75	110.10
10	aA	842	CLA	C2D-C1D-ND	7.66	115.75	110.10
10	bA	842	CLA	C2D-C1D-ND	7.66	115.75	110.10
10	cB	811	CLA	C1D-ND-C4D	-7.66	100.90	106.33
10	aB	833	CLA	C2D-C1D-ND	7.65	115.75	110.10
10	aB	801	CLA	C1D-ND-C4D	-7.65	100.90	106.33
10	cA	814	CLA	C2D-C1D-ND	7.65	115.74	110.10
10	bA	828	CLA	C2D-C1D-ND	7.65	115.74	110.10
10	bA	839	CLA	C2D-C1D-ND	7.64	115.73	110.10
10	bA	827	CLA	C2D-C1D-ND	7.64	115.73	110.10
10	cA	836	CLA	C2D-C1D-ND	7.63	115.73	110.10
10	bB	804	CLA	O2D-CGD-CBD	7.62	124.81	111.27
10	aB	824	CLA	C2D-C1D-ND	7.62	115.72	110.10
10	aB	818	CLA	C2D-C1D-ND	7.61	115.72	110.10
10	bB	833	CLA	C2D-C1D-ND	7.61	115.72	110.10
10	aA	814	CLA	C2D-C1D-ND	7.61	115.71	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	814	CLA	C2D-C1D-ND	7.61	115.71	110.10
10	bB	835	CLA	C2D-C1D-ND	7.60	115.71	110.10
10	bB	811	CLA	C2D-C1D-ND	7.60	115.70	110.10
10	cB	824	CLA	C2D-C1D-ND	7.60	115.70	110.10
10	aB	835	CLA	C2D-C1D-ND	7.59	115.70	110.10
10	bB	824	CLA	C2D-C1D-ND	7.58	115.69	110.10
10	cB	811	CLA	C2D-C1D-ND	7.58	115.69	110.10
10	aB	834	CLA	CMD-C2D-C1D	7.58	138.07	124.71
10	aB	804	CLA	O2D-CGD-CBD	7.58	124.74	111.27
10	cB	804	CLA	O2D-CGD-CBD	7.58	124.74	111.27
10	bB	834	CLA	CMD-C2D-C1D	7.57	138.06	124.71
10	aB	811	CLA	C2D-C1D-ND	7.57	115.68	110.10
10	cB	834	CLA	CMD-C2D-C1D	7.57	138.05	124.71
10	cB	818	CLA	C2D-C1D-ND	7.57	115.68	110.10
10	cB	835	CLA	C2D-C1D-ND	7.57	115.68	110.10
10	bB	840	CLA	CMD-C2D-C1D	7.54	138.00	124.71
10	bB	818	CLA	C2D-C1D-ND	7.54	115.66	110.10
10	cB	840	CLA	CMD-C2D-C1D	7.53	137.99	124.71
10	cA	840	CLA	C2D-C1D-ND	7.53	115.65	110.10
10	bA	840	CLA	C2D-C1D-ND	7.52	115.65	110.10
10	aB	840	CLA	CMD-C2D-C1D	7.52	137.96	124.71
9	aA	801	CL0	C2D-C1D-ND	7.52	115.64	110.10
10	cA	822	CLA	C2D-C1D-ND	7.51	115.64	110.10
10	cA	806	CLA	C2D-C1D-ND	7.51	115.64	110.10
10	aA	822	CLA	C2D-C1D-ND	7.50	115.63	110.10
10	bA	822	CLA	C2D-C1D-ND	7.50	115.63	110.10
9	bA	801	CL0	C2D-C1D-ND	7.50	115.63	110.10
9	cA	801	CL0	C2D-C1D-ND	7.50	115.63	110.10
10	bA	806	CLA	C2D-C1D-ND	7.48	115.62	110.10
10	aB	825	CLA	C2D-C1D-ND	7.45	115.59	110.10
10	aB	831	CLA	C2D-C1D-ND	7.44	115.59	110.10
10	aA	840	CLA	C2D-C1D-ND	7.44	115.58	110.10
10	bB	825	CLA	C2D-C1D-ND	7.44	115.58	110.10
10	bA	812	CLA	C2D-C1D-ND	7.43	115.58	110.10
10	bB	834	CLA	C2D-C1D-ND	7.42	115.57	110.10
10	cA	812	CLA	C2D-C1D-ND	7.42	115.57	110.10
10	aB	834	CLA	C2D-C1D-ND	7.41	115.57	110.10
10	bB	831	CLA	C2D-C1D-ND	7.41	115.57	110.10
10	aA	812	CLA	C2D-C1D-ND	7.41	115.56	110.10
10	aA	804	CLA	C2D-C1D-ND	7.40	115.56	110.10
10	aB	840	CLA	C2D-C1D-ND	7.39	115.55	110.10
10	cB	834	CLA	C2D-C1D-ND	7.38	115.55	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	813	CLA	C2D-C1D-ND	7.38	115.54	110.10
10	cB	840	CLA	C2D-C1D-ND	7.38	115.54	110.10
10	aA	806	CLA	C2D-C1D-ND	7.37	115.54	110.10
10	cB	825	CLA	C2D-C1D-ND	7.37	115.54	110.10
10	bB	840	CLA	C2D-C1D-ND	7.36	115.53	110.10
10	aA	819	CLA	C2D-C1D-ND	7.36	115.53	110.10
10	aB	821	CLA	C2D-C1D-ND	7.35	115.52	110.10
10	bA	819	CLA	C2D-C1D-ND	7.35	115.52	110.10
10	cB	831	CLA	C2D-C1D-ND	7.35	115.52	110.10
10	cB	821	CLA	C2D-C1D-ND	7.35	115.52	110.10
10	cA	804	CLA	C2D-C1D-ND	7.34	115.51	110.10
10	cA	813	CLA	C2D-C1D-ND	7.33	115.50	110.10
10	cB	823	CLA	C2D-C1D-ND	7.32	115.50	110.10
10	cA	819	CLA	C2D-C1D-ND	7.30	115.48	110.10
10	bB	821	CLA	C2D-C1D-ND	7.29	115.48	110.10
10	bA	804	CLA	C2D-C1D-ND	7.29	115.48	110.10
10	bB	823	CLA	C2D-C1D-ND	7.29	115.48	110.10
10	aB	823	CLA	C2D-C1D-ND	7.29	115.47	110.10
10	aB	820	CLA	C2D-C1D-ND	7.28	115.47	110.10
10	cB	819	CLA	C2D-C1D-ND	7.27	115.47	110.10
10	aA	813	CLA	C2D-C1D-ND	7.26	115.45	110.10
10	aB	819	CLA	C2D-C1D-ND	7.24	115.44	110.10
10	bA	830	CLA	C2D-C1D-ND	7.24	115.44	110.10
10	bB	820	CLA	C2D-C1D-ND	7.23	115.44	110.10
10	cB	820	CLA	C2D-C1D-ND	7.23	115.44	110.10
10	bB	819	CLA	C2D-C1D-ND	7.21	115.42	110.10
10	aA	830	CLA	C2D-C1D-ND	7.18	115.40	110.10
10	cB	815	CLA	C2D-C1D-ND	7.18	115.40	110.10
10	cB	836	CLA	C2D-C1D-ND	7.18	115.40	110.10
10	aA	827	CLA	CMD-C2D-C1D	7.18	137.37	124.71
10	aB	836	CLA	C2D-C1D-ND	7.18	115.40	110.10
10	cA	830	CLA	C2D-C1D-ND	7.17	115.39	110.10
10	cA	827	CLA	CMD-C2D-C1D	7.17	137.35	124.71
10	bA	806	CLA	CMD-C2D-C1D	7.16	137.34	124.71
10	bB	836	CLA	C2D-C1D-ND	7.16	115.38	110.10
10	aB	815	CLA	C2D-C1D-ND	7.16	115.38	110.10
10	cA	806	CLA	CMD-C2D-C1D	7.15	137.32	124.71
10	bB	815	CLA	C2D-C1D-ND	7.14	115.36	110.10
10	aA	806	CLA	CMD-C2D-C1D	7.13	137.29	124.71
10	bA	827	CLA	CMD-C2D-C1D	7.13	137.28	124.71
10	aB	826	CLA	C2D-C1D-ND	7.09	115.33	110.10
10	bB	835	CLA	CMD-C2D-C1D	7.08	137.20	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	835	CLA	CMD-C2D-C1D	7.08	137.18	124.71
10	aA	823	CLA	C2D-C1D-ND	7.08	115.32	110.10
10	bB	826	CLA	C2D-C1D-ND	7.07	115.31	110.10
10	cA	823	CLA	C2D-C1D-ND	7.06	115.31	110.10
10	cB	835	CLA	CMD-C2D-C1D	7.06	137.16	124.71
10	bA	823	CLA	C2D-C1D-ND	7.06	115.31	110.10
10	bA	826	CLA	CMD-C2D-C1D	7.04	137.13	124.71
10	cA	826	CLA	CMD-C2D-C1D	7.02	137.09	124.71
10	cB	801	CLA	C2D-C1D-ND	7.02	115.27	110.10
10	cB	826	CLA	C2D-C1D-ND	7.02	115.27	110.10
10	aA	826	CLA	CMD-C2D-C1D	7.01	137.06	124.71
10	bB	801	CLA	C2D-C1D-ND	6.99	115.25	110.10
10	bA	833	CLA	O2D-CGD-CBD	6.99	123.69	111.27
10	aA	833	CLA	O2D-CGD-CBD	6.98	123.67	111.27
10	bA	825	CLA	CMD-C2D-C1D	6.97	137.00	124.71
10	cA	833	CLA	O2D-CGD-CBD	6.97	123.66	111.27
10	cA	825	CLA	CMD-C2D-C1D	6.97	137.00	124.71
10	aB	801	CLA	C2D-C1D-ND	6.97	115.24	110.10
10	cA	817	CLA	CMD-C2D-C1D	6.97	137.00	124.71
10	aA	802	CLA	CMD-C2D-C1D	6.96	136.98	124.71
10	bA	817	CLA	CMD-C2D-C1D	6.95	136.97	124.71
10	aA	825	CLA	CMD-C2D-C1D	6.95	136.96	124.71
10	aA	817	CLA	CMD-C2D-C1D	6.95	136.96	124.71
10	cA	835	CLA	C2D-C1D-ND	6.95	115.22	110.10
10	aA	835	CLA	C2D-C1D-ND	6.94	115.22	110.10
10	bA	835	CLA	C2D-C1D-ND	6.94	115.22	110.10
10	cA	802	CLA	CMD-C2D-C1D	6.94	136.94	124.71
10	aB	826	CLA	CMD-C2D-C1D	6.93	136.93	124.71
10	aB	830	CLA	CMD-C2D-C1D	6.93	136.93	124.71
10	bA	802	CLA	CMD-C2D-C1D	6.93	136.92	124.71
10	bB	830	CLA	CMD-C2D-C1D	6.92	136.90	124.71
10	cB	830	CLA	CMD-C2D-C1D	6.91	136.90	124.71
10	cB	814	CLA	C2D-C1D-ND	6.91	115.20	110.10
10	cB	826	CLA	CMD-C2D-C1D	6.91	136.89	124.71
10	bB	826	CLA	CMD-C2D-C1D	6.90	136.88	124.71
10	cB	806	CLA	CMD-C2D-C1D	6.90	136.87	124.71
10	bA	815	CLA	CMD-C2D-C1D	6.89	136.85	124.71
10	aA	854	CLA	CMD-C2D-C1D	6.89	136.85	124.71
10	aB	806	CLA	CMD-C2D-C1D	6.89	136.85	124.71
10	bA	813	CLA	CMD-C2D-C1D	6.89	136.85	124.71
10	bB	806	CLA	CMD-C2D-C1D	6.88	136.85	124.71
10	cA	854	CLA	CMD-C2D-C1D	6.88	136.84	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	815	CLA	CMD-C2D-C1D	6.87	136.83	124.71
10	bA	807	CLA	CMD-C2D-C1D	6.87	136.83	124.71
10	bA	812	CLA	CMD-C2D-C1D	6.87	136.82	124.71
10	cA	812	CLA	CMD-C2D-C1D	6.87	136.82	124.71
10	aA	815	CLA	CMD-C2D-C1D	6.87	136.82	124.71
10	cA	813	CLA	CMD-C2D-C1D	6.86	136.81	124.71
10	cA	807	CLA	CMD-C2D-C1D	6.86	136.81	124.71
10	aB	810	CLA	C2D-C1D-ND	6.85	115.16	110.10
10	cA	804	CLA	CMD-C2D-C1D	6.85	136.79	124.71
10	aB	808	CLA	CMD-C2D-C1D	6.85	136.78	124.71
10	aB	814	CLA	C2D-C1D-ND	6.85	115.15	110.10
10	aA	807	CLA	CMD-C2D-C1D	6.85	136.78	124.71
10	bB	814	CLA	C2D-C1D-ND	6.84	115.15	110.10
10	aA	813	CLA	CMD-C2D-C1D	6.84	136.77	124.71
10	bB	808	CLA	CMD-C2D-C1D	6.84	136.77	124.71
10	cB	808	CLA	CMD-C2D-C1D	6.84	136.77	124.71
10	aA	804	CLA	CMD-C2D-C1D	6.84	136.77	124.71
10	bA	854	CLA	CMD-C2D-C1D	6.84	136.77	124.71
10	bA	824	CLA	O2D-CGD-CBD	6.84	123.42	111.27
10	aA	812	CLA	CMD-C2D-C1D	6.84	136.76	124.71
10	bA	804	CLA	CMD-C2D-C1D	6.83	136.75	124.71
10	bB	832	CLA	CMD-C2D-C1D	6.82	136.74	124.71
10	aB	832	CLA	CMD-C2D-C1D	6.82	136.73	124.71
10	cB	832	CLA	CMD-C2D-C1D	6.82	136.73	124.71
10	cA	824	CLA	O2D-CGD-CBD	6.82	123.38	111.27
10	bB	810	CLA	C2D-C1D-ND	6.81	115.12	110.10
10	aA	823	CLA	CMD-C2D-C1D	6.81	136.71	124.71
10	aA	824	CLA	O2D-CGD-CBD	6.81	123.36	111.27
10	cA	838	CLA	CMD-C2D-C1D	6.81	136.71	124.71
10	cA	818	CLA	CHD-C1D-ND	-6.80	118.21	124.45
10	cB	810	CLA	C2D-C1D-ND	6.79	115.11	110.10
10	aA	838	CLA	CMD-C2D-C1D	6.79	136.68	124.71
10	bA	838	CLA	CMD-C2D-C1D	6.79	136.68	124.71
10	cA	823	CLA	CMD-C2D-C1D	6.79	136.68	124.71
10	bA	823	CLA	CMD-C2D-C1D	6.78	136.67	124.71
10	cA	832	CLA	CMD-C2D-C1D	6.76	136.63	124.71
10	aA	818	CLA	CHD-C1D-ND	-6.76	118.24	124.45
10	cB	827	CLA	CMD-C2D-C1D	6.75	136.62	124.71
10	aA	832	CLA	CMD-C2D-C1D	6.75	136.61	124.71
10	aL	203	CLA	CMD-C2D-C1D	6.75	136.61	124.71
10	cB	823	CLA	CMD-C2D-C1D	6.75	136.61	124.71
10	aB	827	CLA	CMD-C2D-C1D	6.75	136.61	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	810	CLA	CMD-C2D-C1D	6.75	136.60	124.71
10	cL	203	CLA	CMD-C2D-C1D	6.74	136.60	124.71
10	bL	203	CLA	CMD-C2D-C1D	6.74	136.59	124.71
10	bA	818	CLA	CHD-C1D-ND	-6.74	118.26	124.45
10	bB	829	CLA	C2D-C1D-ND	6.73	115.06	110.10
10	bA	832	CLA	CMD-C2D-C1D	6.73	136.57	124.71
10	cA	803	CLA	CMD-C2D-C1D	6.73	136.57	124.71
10	bB	827	CLA	CMD-C2D-C1D	6.73	136.57	124.71
10	bA	810	CLA	CMD-C2D-C1D	6.73	136.57	124.71
10	cA	822	CLA	CMD-C2D-C1D	6.72	136.56	124.71
10	aB	823	CLA	CMD-C2D-C1D	6.72	136.56	124.71
10	aA	822	CLA	CMD-C2D-C1D	6.72	136.56	124.71
10	cA	810	CLA	CMD-C2D-C1D	6.72	136.56	124.71
10	bB	823	CLA	CMD-C2D-C1D	6.72	136.55	124.71
10	bA	803	CLA	CMD-C2D-C1D	6.71	136.54	124.71
10	bA	822	CLA	CMD-C2D-C1D	6.71	136.53	124.71
10	aA	803	CLA	CMD-C2D-C1D	6.70	136.53	124.71
10	aB	812	CLA	CMD-C2D-C1D	6.69	136.51	124.71
10	cA	809	CLA	CMD-C2D-C1D	6.68	136.49	124.71
10	bB	812	CLA	CMD-C2D-C1D	6.68	136.49	124.71
10	cB	812	CLA	CMD-C2D-C1D	6.67	136.47	124.71
10	aB	829	CLA	C2D-C1D-ND	6.67	115.02	110.10
10	cB	829	CLA	C2D-C1D-ND	6.67	115.02	110.10
10	aB	838	CLA	CMD-C2D-C1D	6.67	136.46	124.71
10	aA	836	CLA	CMD-C2D-C1D	6.66	136.45	124.71
10	bB	838	CLA	CMD-C2D-C1D	6.66	136.44	124.71
10	bA	836	CLA	CMD-C2D-C1D	6.66	136.44	124.71
10	aA	809	CLA	CMD-C2D-C1D	6.65	136.44	124.71
10	cA	816	CLA	CMD-C2D-C1D	6.65	136.43	124.71
10	bA	805	CLA	CMD-C2D-C1D	6.65	136.43	124.71
10	aA	805	CLA	CMD-C2D-C1D	6.65	136.43	124.71
10	bA	818	CLA	CMD-C2D-C1D	6.64	136.42	124.71
10	bB	807	CLA	CMD-C2D-C1D	6.64	136.42	124.71
10	cB	807	CLA	CMD-C2D-C1D	6.64	136.42	124.71
10	bB	820	CLA	CMD-C2D-C1D	6.64	136.41	124.71
10	aA	816	CLA	CMD-C2D-C1D	6.64	136.41	124.71
10	cB	838	CLA	CMD-C2D-C1D	6.64	136.41	124.71
10	aB	820	CLA	CMD-C2D-C1D	6.63	136.40	124.71
10	bA	809	CLA	CMD-C2D-C1D	6.63	136.40	124.71
10	bA	816	CLA	CMD-C2D-C1D	6.63	136.40	124.71
10	aB	824	CLA	CMD-C2D-C1D	6.63	136.40	124.71
10	cA	805	CLA	CMD-C2D-C1D	6.63	136.40	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	836	CLA	CMD-C2D-C1D	6.63	136.39	124.71
10	bB	824	CLA	CMD-C2D-C1D	6.63	136.39	124.71
10	cB	839	CLA	CMD-C2D-C1D	6.63	136.39	124.71
10	aB	841	CLA	C2C-C1C-NC	6.63	116.18	109.97
10	bB	839	CLA	CMD-C2D-C1D	6.63	136.39	124.71
10	cB	820	CLA	CMD-C2D-C1D	6.62	136.39	124.71
10	aB	839	CLA	CMD-C2D-C1D	6.62	136.38	124.71
10	cA	818	CLA	CMD-C2D-C1D	6.62	136.37	124.71
10	aB	807	CLA	CMD-C2D-C1D	6.61	136.36	124.71
10	bL	205	CLA	CMD-C2D-C1D	6.61	136.36	124.71
10	aL	202	CLA	CMD-C2D-C1D	6.60	136.35	124.71
10	bL	202	CLA	CMD-C2D-C1D	6.60	136.35	124.71
10	cB	841	CLA	C2C-C1C-NC	6.60	116.16	109.97
10	aL	205	CLA	CMD-C2D-C1D	6.60	136.34	124.71
10	cA	837	CLA	CMD-C2D-C1D	6.60	136.34	124.71
10	aA	818	CLA	CMD-C2D-C1D	6.60	136.34	124.71
10	bB	836	CLA	CMD-C2D-C1D	6.59	136.33	124.71
10	bB	841	CLA	C2C-C1C-NC	6.59	116.15	109.97
10	aB	836	CLA	CMD-C2D-C1D	6.59	136.33	124.71
10	aA	835	CLA	CMD-C2D-C1D	6.59	136.33	124.71
10	cB	824	CLA	CMD-C2D-C1D	6.59	136.33	124.71
10	cB	817	CLA	CMD-C2D-C1D	6.59	136.32	124.71
10	bA	837	CLA	CMD-C2D-C1D	6.59	136.32	124.71
10	cA	835	CLA	CMD-C2D-C1D	6.59	136.32	124.71
10	cB	819	CLA	CMD-C2D-C1D	6.58	136.32	124.71
10	cB	836	CLA	CMD-C2D-C1D	6.58	136.31	124.71
10	cL	202	CLA	CMD-C2D-C1D	6.58	136.31	124.71
10	bB	819	CLA	CMD-C2D-C1D	6.58	136.31	124.71
10	bB	817	CLA	CMD-C2D-C1D	6.58	136.31	124.71
10	aA	837	CLA	CMD-C2D-C1D	6.58	136.30	124.71
10	aB	819	CLA	CMD-C2D-C1D	6.57	136.30	124.71
10	bB	822	CLA	CMD-C2D-C1D	6.57	136.30	124.71
10	aB	822	CLA	CMD-C2D-C1D	6.57	136.30	124.71
10	aB	817	CLA	CMD-C2D-C1D	6.57	136.29	124.71
10	cL	205	CLA	CMD-C2D-C1D	6.57	136.29	124.71
10	bA	835	CLA	CMD-C2D-C1D	6.57	136.29	124.71
10	cB	822	CLA	CHD-C1D-ND	-6.57	118.42	124.45
10	bB	831	CLA	CMD-C2D-C1D	6.56	136.28	124.71
10	bB	825	CLA	O2D-CGD-CBD	6.56	122.92	111.27
10	aB	831	CLA	CMD-C2D-C1D	6.55	136.26	124.71
10	aB	822	CLA	CHD-C1D-ND	-6.55	118.43	124.45
10	cB	831	CLA	CMD-C2D-C1D	6.55	136.25	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	822	CLA	CMD-C2D-C1D	6.55	136.25	124.71
10	bA	843	CLA	CMD-C2D-C1D	6.54	136.24	124.71
10	bB	822	CLA	CHD-C1D-ND	-6.54	118.44	124.45
10	aB	825	CLA	O2D-CGD-CBD	6.54	122.89	111.27
10	bB	811	CLA	C2C-C1C-NC	6.54	116.10	109.97
10	cB	825	CLA	O2D-CGD-CBD	6.53	122.88	111.27
10	cA	818	CLA	O2D-CGD-CBD	6.52	122.86	111.27
10	cA	843	CLA	CMD-C2D-C1D	6.52	136.20	124.71
10	aA	843	CLA	CMD-C2D-C1D	6.52	136.20	124.71
10	bA	806	CLA	CHD-C1D-ND	-6.52	118.46	124.45
10	cA	806	CLA	CHD-C1D-ND	-6.52	118.47	124.45
10	bA	818	CLA	O2D-CGD-CBD	6.51	122.84	111.27
10	aA	824	CLA	CMD-C2D-C1D	6.51	136.18	124.71
10	aA	818	CLA	O2D-CGD-CBD	6.51	122.83	111.27
10	cB	811	CLA	C2C-C1C-NC	6.50	116.06	109.97
10	bA	824	CLA	CMD-C2D-C1D	6.50	136.17	124.71
10	aB	811	CLA	C2C-C1C-NC	6.49	116.06	109.97
10	aA	839	CLA	CMD-C2D-C1D	6.49	136.15	124.71
10	cA	814	CLA	CMD-C2D-C1D	6.49	136.15	124.71
10	cA	839	CLA	CMD-C2D-C1D	6.49	136.15	124.71
10	cA	824	CLA	CMD-C2D-C1D	6.49	136.15	124.71
10	cA	856	CLA	CMD-C2D-C1D	6.48	136.13	124.71
10	bA	856	CLA	CMD-C2D-C1D	6.48	136.13	124.71
10	aB	818	CLA	CMD-C2D-C1D	6.48	136.13	124.71
10	bB	818	CLA	CMD-C2D-C1D	6.47	136.12	124.71
10	bA	833	CLA	CMD-C2D-C1D	6.47	136.12	124.71
10	bA	839	CLA	CMD-C2D-C1D	6.47	136.11	124.71
10	bA	814	CLA	CMD-C2D-C1D	6.47	136.11	124.71
10	aA	814	CLA	CMD-C2D-C1D	6.47	136.11	124.71
10	cB	818	CLA	CMD-C2D-C1D	6.47	136.11	124.71
10	aA	856	CLA	CMD-C2D-C1D	6.46	136.10	124.71
10	aA	833	CLA	CMD-C2D-C1D	6.46	136.10	124.71
10	bB	833	CLA	CMD-C2D-C1D	6.46	136.09	124.71
10	aB	833	CLA	CMD-C2D-C1D	6.45	136.08	124.71
10	cB	805	CLA	CHD-C1D-ND	-6.45	118.53	124.45
10	cB	833	CLA	CMD-C2D-C1D	6.44	136.06	124.71
10	cB	816	CLA	O2D-CGD-CBD	6.43	122.69	111.27
10	aA	806	CLA	CHD-C1D-ND	-6.43	118.55	124.45
10	cA	833	CLA	CMD-C2D-C1D	6.43	136.04	124.71
10	bA	808	CLA	CMD-C2D-C1D	6.43	136.04	124.71
10	aA	808	CLA	CMD-C2D-C1D	6.42	136.03	124.71
10	cB	814	CLA	C4A-NA-C1A	-6.42	103.82	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	803	CLA	O2D-CGD-CBD	6.42	122.67	111.27
10	aB	814	CLA	CMD-C2D-C1D	6.42	136.03	124.71
10	aB	816	CLA	O2D-CGD-CBD	6.42	122.67	111.27
10	bB	814	CLA	CMD-C2D-C1D	6.42	136.02	124.71
10	cA	803	CLA	O2D-CGD-CBD	6.42	122.67	111.27
10	aB	805	CLA	CHD-C1D-ND	-6.42	118.56	124.45
10	aB	826	CLA	CHD-C1D-ND	-6.42	118.56	124.45
10	cB	814	CLA	CMD-C2D-C1D	6.42	136.02	124.71
10	aA	854	CLA	CHD-C4C-C3C	-6.41	115.41	124.84
10	cB	826	CLA	CHD-C1D-ND	-6.41	118.56	124.45
10	aB	828	CLA	CHD-C4C-C3C	-6.41	115.42	124.84
10	cA	808	CLA	CMD-C2D-C1D	6.41	136.00	124.71
10	bB	826	CLA	CHD-C1D-ND	-6.40	118.57	124.45
10	bB	828	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
10	bA	840	CLA	CMD-C2D-C1D	6.40	136.00	124.71
10	bB	805	CLA	CHD-C1D-ND	-6.40	118.57	124.45
10	cB	828	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
10	bB	816	CLA	O2D-CGD-CBD	6.40	122.64	111.27
10	bA	841	CLA	CMD-C2D-C1D	6.40	135.98	124.71
10	bA	854	CLA	CHD-C4C-C3C	-6.39	115.44	124.84
10	aA	803	CLA	O2D-CGD-CBD	6.39	122.62	111.27
10	cA	840	CLA	CMD-C2D-C1D	6.39	135.98	124.71
10	cA	854	CLA	CHD-C4C-C3C	-6.39	115.45	124.84
10	aA	833	CLA	CHD-C1D-ND	-6.39	118.58	124.45
10	bA	830	CLA	CMD-C2D-C1D	6.39	135.97	124.71
10	bB	803	CLA	CMD-C2D-C1D	6.38	135.97	124.71
10	aA	841	CLA	CMD-C2D-C1D	6.38	135.96	124.71
10	bA	833	CLA	CHD-C1D-ND	-6.38	118.59	124.45
10	cB	803	CLA	CMD-C2D-C1D	6.37	135.94	124.71
10	aB	803	CLA	CMD-C2D-C1D	6.37	135.93	124.71
10	aB	814	CLA	C4A-NA-C1A	-6.36	103.85	106.71
10	cA	833	CLA	CHD-C1D-ND	-6.36	118.61	124.45
10	aA	840	CLA	CMD-C2D-C1D	6.36	135.92	124.71
10	cA	841	CLA	CMD-C2D-C1D	6.36	135.92	124.71
10	aA	830	CLA	CMD-C2D-C1D	6.35	135.91	124.71
10	cA	830	CLA	CMD-C2D-C1D	6.35	135.90	124.71
10	aA	812	CLA	CHD-C1D-ND	-6.35	118.62	124.45
10	cL	203	CLA	CHD-C1D-ND	-6.34	118.62	124.45
10	bA	829	CLA	O2D-CGD-CBD	6.33	122.52	111.27
10	cB	837	CLA	C4A-NA-C1A	-6.33	103.86	106.71
10	bB	808	CLA	CHD-C4C-C3C	-6.32	115.54	124.84
10	cB	808	CLA	CHD-C4C-C3C	-6.32	115.55	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bL	203	CLA	CHD-C1D-ND	-6.32	118.64	124.45
10	aB	808	CLA	CHD-C4C-C3C	-6.32	115.55	124.84
10	aA	829	CLA	O2D-CGD-CBD	6.32	122.49	111.27
10	cA	829	CLA	O2D-CGD-CBD	6.32	122.49	111.27
10	bA	812	CLA	CHD-C1D-ND	-6.31	118.66	124.45
10	aA	826	CLA	CHD-C4C-C3C	-6.31	115.57	124.84
10	bA	826	CLA	CHD-C4C-C3C	-6.30	115.57	124.84
10	cB	827	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
10	cB	820	CLA	CHD-C1D-ND	-6.30	118.66	124.45
10	bB	806	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
10	aB	820	CLA	CHD-C1D-ND	-6.29	118.67	124.45
10	bB	814	CLA	C4A-NA-C1A	-6.29	103.88	106.71
10	cA	812	CLA	CHD-C1D-ND	-6.29	118.67	124.45
10	aL	203	CLA	CHD-C1D-ND	-6.29	118.67	124.45
10	bA	819	CLA	CMD-C2D-C1D	6.29	135.80	124.71
10	bB	803	CLA	CHD-C4C-C3C	-6.29	115.60	124.84
10	bB	827	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
10	aA	819	CLA	CMD-C2D-C1D	6.28	135.78	124.71
10	aB	806	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
10	cA	826	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
10	cB	806	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
10	bB	841	CLA	CMD-C2D-C1D	6.27	135.76	124.71
10	aA	816	CLA	O2D-CGD-CBD	6.27	122.41	111.27
10	aB	803	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
10	cA	819	CLA	CMD-C2D-C1D	6.27	135.76	124.71
10	aB	827	CLA	CHD-C4C-C3C	-6.27	115.63	124.84
10	aB	841	CLA	CMD-C2D-C1D	6.27	135.76	124.71
10	cA	816	CLA	O2D-CGD-CBD	6.26	122.39	111.27
10	cB	803	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
10	bB	820	CLA	CHD-C1D-ND	-6.25	118.71	124.45
10	aB	805	CLA	CAC-C3C-C4C	6.25	132.92	124.81
10	cB	805	CLA	CAC-C3C-C4C	6.25	132.92	124.81
10	bB	805	CLA	CAC-C3C-C4C	6.25	132.92	124.81
10	cB	841	CLA	CMD-C2D-C1D	6.25	135.72	124.71
10	bB	837	CLA	C4A-NA-C1A	-6.24	103.90	106.71
10	cA	820	CLA	CMD-C2D-C1D	6.24	135.71	124.71
10	bA	820	CLA	CMD-C2D-C1D	6.23	135.68	124.71
9	bA	801	CL0	C2C-C1C-NC	6.22	115.80	109.97
10	bA	816	CLA	O2D-CGD-CBD	6.22	122.32	111.27
10	bA	822	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
10	aB	837	CLA	C4A-NA-C1A	-6.21	103.91	106.71
10	aA	820	CLA	CMD-C2D-C1D	6.21	135.66	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	822	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
10	cA	822	CLA	CHD-C4C-C3C	-6.21	115.72	124.84
10	cB	819	CLA	C2C-C1C-NC	6.21	115.79	109.97
9	cA	801	CL0	C2C-C1C-NC	6.20	115.78	109.97
10	cB	815	CLA	CMD-C2D-C1D	6.20	135.63	124.71
10	cB	834	CLA	CHD-C1D-ND	-6.19	118.77	124.45
10	cB	838	CLA	CHD-C1D-ND	-6.19	118.77	124.45
10	aB	815	CLA	CMD-C2D-C1D	6.18	135.61	124.71
10	bB	834	CLA	CHD-C1D-ND	-6.18	118.78	124.45
10	aB	838	CLA	CHD-C1D-ND	-6.18	118.78	124.45
10	aB	830	CLA	C2D-C1D-ND	6.18	114.66	110.10
10	aB	801	CLA	C2C-C1C-NC	6.17	115.76	109.97
10	aB	834	CLA	CHD-C1D-ND	-6.17	118.78	124.45
9	aA	801	CL0	C2C-C1C-NC	6.17	115.75	109.97
10	aA	825	CLA	CHD-C1D-ND	-6.16	118.79	124.45
10	cB	801	CLA	CHD-C1D-ND	-6.16	118.79	124.45
10	aB	819	CLA	C2C-C1C-NC	6.16	115.75	109.97
10	aA	811	CLA	CMD-C2D-C1D	6.16	135.57	124.71
10	bB	838	CLA	CHD-C1D-ND	-6.16	118.79	124.45
10	bA	811	CLA	CMD-C2D-C1D	6.16	135.57	124.71
10	bB	815	CLA	CMD-C2D-C1D	6.16	135.57	124.71
10	cB	801	CLA	C2C-C1C-NC	6.16	115.74	109.97
10	bB	819	CLA	C2C-C1C-NC	6.16	115.74	109.97
10	cB	810	CLA	O2D-CGD-CBD	6.15	122.20	111.27
10	bB	830	CLA	C2D-C1D-ND	6.15	114.64	110.10
10	bB	801	CLA	CHD-C1D-ND	-6.15	118.81	124.45
10	cB	830	CLA	C2D-C1D-ND	6.14	114.63	110.10
10	aB	831	CLA	CHD-C1D-ND	-6.14	118.81	124.45
10	cB	812	CLA	CHD-C1D-ND	-6.14	118.81	124.45
10	cA	815	CLA	CHD-C1D-ND	-6.14	118.81	124.45
10	bB	812	CLA	CHD-C1D-ND	-6.13	118.82	124.45
10	aA	816	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
10	cA	811	CLA	CMD-C2D-C1D	6.13	135.52	124.71
10	cA	816	CLA	CHD-C4C-C3C	-6.12	115.85	124.84
10	bA	832	CLA	CHD-C1D-ND	-6.12	118.83	124.45
10	bL	205	CLA	CHD-C1D-ND	-6.12	118.83	124.45
10	aL	205	CLA	CHD-C1D-ND	-6.11	118.84	124.45
10	bB	810	CLA	O2D-CGD-CBD	6.11	122.13	111.27
10	aB	810	CLA	O2D-CGD-CBD	6.11	122.12	111.27
10	bA	842	CLA	C2C-C1C-NC	6.11	115.69	109.97
10	cL	205	CLA	CHD-C1D-ND	-6.11	118.84	124.45
10	cA	802	CLA	CHD-C1D-ND	-6.10	118.84	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	801	CLA	C2C-C1C-NC	6.10	115.68	109.97
10	aA	802	CLA	CHD-C1D-ND	-6.10	118.85	124.45
10	bA	802	CLA	CHD-C1D-ND	-6.10	118.85	124.45
10	bA	807	CLA	CHD-C1D-ND	-6.10	118.85	124.45
10	aB	801	CLA	CHD-C1D-ND	-6.09	118.85	124.45
10	aB	812	CLA	CHD-C1D-ND	-6.09	118.85	124.45
10	cA	825	CLA	CHD-C1D-ND	-6.09	118.86	124.45
10	bA	825	CLA	CHD-C1D-ND	-6.09	118.86	124.45
10	cL	204	CLA	O2D-CGD-CBD	6.09	122.09	111.27
10	bA	816	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
10	aA	832	CLA	CHD-C1D-ND	-6.08	118.87	124.45
10	cA	807	CLA	CHD-C1D-ND	-6.08	118.87	124.45
10	aA	843	CLA	CHD-C1D-ND	-6.08	118.87	124.45
10	bA	815	CLA	CHD-C1D-ND	-6.08	118.87	124.45
10	aB	816	CLA	CMD-C2D-C1D	6.07	135.41	124.71
10	bL	204	CLA	O2D-CGD-CBD	6.07	122.06	111.27
10	aL	204	CLA	O2D-CGD-CBD	6.07	122.05	111.27
10	bL	202	CLA	C2C-C1C-NC	6.07	115.66	109.97
10	cA	842	CLA	C2C-C1C-NC	6.07	115.66	109.97
10	aB	826	CLA	O2D-CGD-CBD	6.07	122.05	111.27
10	cA	807	CLA	O2D-CGD-CBD	6.07	122.05	111.27
10	aA	815	CLA	CHD-C1D-ND	-6.06	118.88	124.45
10	bA	843	CLA	CHD-C1D-ND	-6.06	118.88	124.45
10	cB	819	CLA	CHD-C1D-ND	-6.06	118.88	124.45
10	aA	807	CLA	O2D-CGD-CBD	6.06	122.04	111.27
10	aA	842	CLA	C2C-C1C-NC	6.06	115.65	109.97
10	aA	807	CLA	CHD-C1D-ND	-6.05	118.89	124.45
10	bA	807	CLA	O2D-CGD-CBD	6.05	122.02	111.27
10	cB	828	CLA	CMD-C2D-C1D	6.05	135.38	124.71
10	bB	826	CLA	O2D-CGD-CBD	6.05	122.02	111.27
10	cA	832	CLA	CHD-C1D-ND	-6.05	118.89	124.45
10	bA	828	CLA	CHD-C4C-C3C	-6.05	115.95	124.84
10	cB	816	CLA	CMD-C2D-C1D	6.05	135.37	124.71
10	cB	826	CLA	O2D-CGD-CBD	6.05	122.01	111.27
10	cA	843	CLA	CHD-C1D-ND	-6.05	118.90	124.45
10	bB	816	CLA	CMD-C2D-C1D	6.05	135.37	124.71
10	aL	202	CLA	C2C-C1C-NC	6.04	115.63	109.97
10	cL	202	CLA	C2C-C1C-NC	6.04	115.63	109.97
10	cB	840	CLA	CHD-C4C-C3C	-6.04	115.97	124.84
10	bB	840	CLA	CHD-C4C-C3C	-6.03	115.97	124.84
10	aB	840	CLA	CHD-C4C-C3C	-6.03	115.97	124.84
10	bB	819	CLA	CHD-C1D-ND	-6.03	118.92	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	805	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
10	bB	835	CLA	CHD-C1D-ND	-6.02	118.92	124.45
10	cA	854	CLA	CHD-C1D-ND	-6.02	118.92	124.45
10	bB	828	CLA	CMD-C2D-C1D	6.02	135.32	124.71
10	cB	831	CLA	CHD-C1D-ND	-6.02	118.92	124.45
10	aB	828	CLA	CMD-C2D-C1D	6.02	135.32	124.71
10	cA	831	CLA	CHD-C4C-C3C	-6.02	116.00	124.84
10	cA	828	CLA	CHD-C4C-C3C	-6.02	116.00	124.84
10	aB	819	CLA	CHD-C1D-ND	-6.02	118.93	124.45
10	bA	854	CLA	CHD-C1D-ND	-6.02	118.93	124.45
10	aA	854	CLA	CHD-C1D-ND	-6.01	118.93	124.45
10	bB	831	CLA	CHD-C1D-ND	-6.01	118.93	124.45
10	cB	835	CLA	CHD-C1D-ND	-6.01	118.93	124.45
10	aA	808	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
10	cA	805	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
10	cA	808	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
10	bA	831	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
10	cA	821	CLA	CHD-C1D-ND	-6.00	118.94	124.45
10	aA	828	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
10	bA	830	CLA	CHD-C1D-ND	-6.00	118.94	124.45
10	bA	805	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
10	aA	821	CLA	CHD-C1D-ND	-6.00	118.94	124.45
10	aB	837	CLA	CMD-C2D-C1D	5.98	135.26	124.71
10	bA	821	CLA	CHD-C1D-ND	-5.98	118.96	124.45
10	bB	837	CLA	CMD-C2D-C1D	5.98	135.25	124.71
10	aB	838	CLA	CHD-C4C-C3C	-5.98	116.06	124.84
10	aB	835	CLA	CHD-C1D-ND	-5.98	118.96	124.45
10	aA	839	CLA	CHD-C1D-ND	-5.98	118.96	124.45
10	bA	808	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
10	cB	822	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
10	cB	824	CLA	CHD-C1D-ND	-5.97	118.96	124.45
10	cA	830	CLA	CHD-C1D-ND	-5.97	118.97	124.45
10	aA	831	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
10	cB	826	CLA	C4A-NA-C1A	-5.97	104.02	106.71
10	cB	837	CLA	CMD-C2D-C1D	5.97	135.23	124.71
10	cA	839	CLA	CHD-C1D-ND	-5.97	118.97	124.45
10	aB	814	CLA	O2D-CGD-CBD	5.96	121.87	111.27
10	aB	818	CLA	CHD-C1D-ND	-5.96	118.97	124.45
10	aA	821	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
10	bB	838	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
10	bA	821	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
10	aA	838	CLA	CHD-C1D-ND	-5.96	118.98	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	807	CLA	CHD-C1D-ND	-5.96	118.98	124.45
10	aA	809	CLA	CHD-C1D-ND	-5.96	118.98	124.45
10	aB	822	CLA	C2C-C1C-NC	5.96	115.55	109.97
10	aB	836	CLA	CHD-C1D-ND	-5.95	118.98	124.45
10	bA	804	CLA	O2D-CGD-CBD	5.95	121.85	111.27
10	cB	836	CLA	CHD-C1D-ND	-5.95	118.98	124.45
10	cB	822	CLA	C2C-C1C-NC	5.95	115.55	109.97
10	aB	807	CLA	CHD-C1D-ND	-5.95	118.99	124.45
10	bB	814	CLA	O2D-CGD-CBD	5.95	121.84	111.27
10	aB	839	CLA	CHD-C1D-ND	-5.95	118.99	124.45
10	bB	822	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
10	cA	804	CLA	O2D-CGD-CBD	5.94	121.83	111.27
10	cB	814	CLA	O2D-CGD-CBD	5.94	121.83	111.27
10	cB	839	CLA	CHD-C1D-ND	-5.94	118.99	124.45
10	aB	822	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
10	cB	818	CLA	CHD-C1D-ND	-5.94	119.00	124.45
10	aA	830	CLA	CHD-C1D-ND	-5.93	119.00	124.45
10	cA	809	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
10	bA	838	CLA	CHD-C1D-ND	-5.93	119.00	124.45
10	bB	818	CLA	CHD-C1D-ND	-5.93	119.00	124.45
10	bA	809	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
10	bB	822	CLA	C2C-C1C-NC	5.93	115.53	109.97
10	aA	804	CLA	CHD-C1D-ND	-5.93	119.01	124.45
10	bA	805	CLA	O2D-CGD-CBD	5.92	121.80	111.27
10	bB	806	CLA	CHD-C1D-ND	-5.92	119.01	124.45
10	cB	807	CLA	CHD-C1D-ND	-5.92	119.01	124.45
10	bB	832	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
10	bB	836	CLA	CHD-C1D-ND	-5.92	119.01	124.45
10	cB	806	CLA	CHD-C1D-ND	-5.92	119.01	124.45
10	cB	838	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
10	aB	810	CLA	CMD-C2D-C1D	5.92	135.15	124.71
10	cB	810	CLA	CMD-C2D-C1D	5.92	135.15	124.71
10	cA	821	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
10	aB	832	CLA	CHD-C1D-ND	-5.92	119.02	124.45
10	cB	825	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
10	bA	839	CLA	CHD-C1D-ND	-5.92	119.02	124.45
10	cA	838	CLA	CHD-C1D-ND	-5.92	119.02	124.45
10	bA	827	CLA	CHD-C1D-ND	-5.92	119.02	124.45
10	aA	827	CLA	CHD-C1D-ND	-5.92	119.02	124.45
10	aA	843	CLA	C2C-C1C-NC	5.91	115.51	109.97
10	bB	830	CLA	C2C-C1C-NC	5.91	115.51	109.97
10	bB	810	CLA	CMD-C2D-C1D	5.91	135.14	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	804	CLA	O2D-CGD-CBD	5.91	121.78	111.27
10	aB	804	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
10	cB	830	CLA	C2C-C1C-NC	5.91	115.51	109.97
10	aB	824	CLA	CHD-C1D-ND	-5.91	119.02	124.45
10	aB	826	CLA	C4A-NA-C1A	-5.91	104.05	106.71
10	aA	809	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
10	aB	830	CLA	C2C-C1C-NC	5.91	115.51	109.97
10	bA	841	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
9	cA	801	CL0	CHD-C4C-C3C	-5.91	116.16	124.84
10	cA	805	CLA	O2D-CGD-CBD	5.90	121.76	111.27
10	bA	821	CLA	CMD-C2D-C1D	5.90	135.12	124.71
10	cA	817	CLA	CHD-C1D-ND	-5.90	119.03	124.45
10	cB	804	CLA	CHD-C4C-C3C	-5.90	116.16	124.84
10	cA	821	CLA	CMD-C2D-C1D	5.90	135.12	124.71
10	aA	805	CLA	O2D-CGD-CBD	5.90	121.75	111.27
10	aB	806	CLA	CHD-C1D-ND	-5.90	119.03	124.45
9	aA	801	CL0	CHD-C4C-C3C	-5.90	116.17	124.84
10	aA	832	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
10	aA	821	CLA	CMD-C2D-C1D	5.89	135.10	124.71
10	bB	825	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
10	aA	841	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
10	aB	825	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
10	bA	832	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
10	aB	809	CLA	CMD-C2D-C1D	5.89	135.09	124.71
10	aB	832	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
10	aB	821	CLA	CMD-C2D-C1D	5.89	135.09	124.71
9	bA	801	CL0	CHD-C4C-C3C	-5.89	116.19	124.84
10	bB	824	CLA	CHD-C1D-ND	-5.89	119.04	124.45
10	bB	839	CLA	CHD-C1D-ND	-5.89	119.04	124.45
10	bB	804	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
10	bA	843	CLA	C2C-C1C-NC	5.88	115.48	109.97
10	bA	802	CLA	C2C-C1C-NC	5.88	115.48	109.97
10	cA	804	CLA	CHD-C1D-ND	-5.88	119.05	124.45
10	aA	831	CLA	CMD-C2D-C1D	5.88	135.08	124.71
10	cA	841	CLA	CHD-C4C-C3C	-5.88	116.19	124.84
10	bB	809	CLA	CHD-C1D-ND	-5.88	119.05	124.45
10	cA	827	CLA	CHD-C1D-ND	-5.88	119.05	124.45
10	bA	825	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
10	bA	823	CLA	CHD-C1D-ND	-5.88	119.05	124.45
10	bA	837	CLA	CHD-C1D-ND	-5.88	119.05	124.45
10	bB	826	CLA	C4A-NA-C1A	-5.87	104.06	106.71
10	aA	829	CLA	C2C-C1C-NC	5.87	115.47	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	832	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
10	cA	823	CLA	CHD-C1D-ND	-5.87	119.06	124.45
10	cB	809	CLA	CMD-C2D-C1D	5.87	135.06	124.71
10	cB	821	CLA	CMD-C2D-C1D	5.87	135.06	124.71
10	cB	832	CLA	CHD-C1D-ND	-5.87	119.06	124.45
10	bB	809	CLA	CMD-C2D-C1D	5.87	135.06	124.71
10	aA	803	CLA	CHD-C1D-ND	-5.87	119.06	124.45
10	cA	825	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
10	cA	832	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
10	cA	843	CLA	C2C-C1C-NC	5.86	115.47	109.97
10	bA	817	CLA	CHD-C1D-ND	-5.86	119.06	124.45
10	bA	804	CLA	CHD-C1D-ND	-5.86	119.07	124.45
10	cA	809	CLA	CHD-C1D-ND	-5.86	119.07	124.45
10	bB	821	CLA	CMD-C2D-C1D	5.86	135.04	124.71
10	aA	817	CLA	CHD-C1D-ND	-5.86	119.07	124.45
10	bA	831	CLA	CMD-C2D-C1D	5.86	135.04	124.71
10	bA	809	CLA	CHD-C1D-ND	-5.86	119.07	124.45
10	aA	802	CLA	C2C-C1C-NC	5.86	115.46	109.97
10	aA	825	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
10	bB	832	CLA	CHD-C1D-ND	-5.86	119.07	124.45
10	aA	823	CLA	CHD-C1D-ND	-5.86	119.07	124.45
10	bA	837	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
10	cB	837	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
10	cA	838	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
10	aA	838	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
10	cA	837	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
10	aB	823	CLA	CHD-C1D-ND	-5.85	119.08	124.45
10	cA	831	CLA	CMD-C2D-C1D	5.85	135.02	124.71
10	aA	837	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
10	cA	803	CLA	CHD-C1D-ND	-5.85	119.08	124.45
10	bA	829	CLA	C2C-C1C-NC	5.85	115.45	109.97
10	cA	837	CLA	CHD-C1D-ND	-5.84	119.08	124.45
10	aA	837	CLA	CHD-C1D-ND	-5.84	119.08	124.45
10	bA	827	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
10	bB	837	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
10	bA	821	CLA	O2D-CGD-CBD	5.84	121.64	111.27
10	bA	803	CLA	CHD-C1D-ND	-5.83	119.09	124.45
10	aB	809	CLA	CHD-C1D-ND	-5.83	119.09	124.45
10	cB	809	CLA	CHD-C1D-ND	-5.82	119.11	124.45
10	bB	823	CLA	CHD-C1D-ND	-5.82	119.11	124.45
10	cA	827	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
10	aA	827	CLA	CHD-C4C-C3C	-5.82	116.29	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	838	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
10	cA	802	CLA	C2C-C1C-NC	5.81	115.42	109.97
10	cB	809	CLA	O2D-CGD-CBD	5.81	121.59	111.27
10	cA	829	CLA	C2C-C1C-NC	5.81	115.41	109.97
10	aB	809	CLA	O2D-CGD-CBD	5.81	121.59	111.27
10	aB	837	CLA	CHD-C4C-C3C	-5.81	116.31	124.84
10	bA	805	CLA	CHD-C1D-ND	-5.81	119.12	124.45
10	aA	816	CLA	CHD-C1D-ND	-5.80	119.12	124.45
10	bA	816	CLA	CHD-C1D-ND	-5.80	119.12	124.45
10	cB	823	CLA	CHD-C1D-ND	-5.80	119.12	124.45
10	cA	821	CLA	O2D-CGD-CBD	5.80	121.58	111.27
10	cA	816	CLA	CHD-C1D-ND	-5.80	119.12	124.45
10	cB	824	CLA	C2C-C1C-NC	5.80	115.40	109.97
10	bA	819	CLA	O2D-CGD-CBD	5.80	121.57	111.27
10	bB	801	CLA	CMD-C2D-C1D	5.79	134.93	124.71
10	bB	809	CLA	O2D-CGD-CBD	5.79	121.56	111.27
10	aA	819	CLA	O2D-CGD-CBD	5.79	121.56	111.27
10	aA	821	CLA	O2D-CGD-CBD	5.79	121.56	111.27
10	cA	813	CLA	CHD-C1D-ND	-5.79	119.13	124.45
10	bA	823	CLA	C2C-C1C-NC	5.79	115.40	109.97
10	aB	836	CLA	C2C-C1C-NC	5.79	115.40	109.97
10	aA	823	CLA	C2C-C1C-NC	5.79	115.39	109.97
10	bB	836	CLA	C2C-C1C-NC	5.79	115.39	109.97
10	aB	813	CLA	CMD-C2D-C1D	5.79	134.91	124.71
10	aB	824	CLA	C2C-C1C-NC	5.79	115.39	109.97
10	cB	836	CLA	C2C-C1C-NC	5.79	115.39	109.97
10	bB	824	CLA	C2C-C1C-NC	5.78	115.39	109.97
10	aB	801	CLA	CMD-C2D-C1D	5.78	134.91	124.71
10	bA	803	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
10	aA	840	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
10	cB	822	CLA	O2D-CGD-CBD	5.77	121.53	111.27
10	bA	810	CLA	CHD-C1D-ND	-5.77	119.15	124.45
10	bA	840	CLA	CHD-C4C-C3C	-5.77	116.35	124.84
10	cA	803	CLA	CHD-C4C-C3C	-5.77	116.35	124.84
10	bB	821	CLA	O2D-CGD-CBD	5.77	121.53	111.27
10	aA	803	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
10	cB	801	CLA	CMD-C2D-C1D	5.77	134.88	124.71
10	aB	822	CLA	O2D-CGD-CBD	5.77	121.52	111.27
10	aB	804	CLA	CHD-C1D-ND	-5.77	119.15	124.45
10	cA	840	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
10	aB	806	CLA	O2D-CGD-CBD	5.77	121.52	111.27
10	bB	817	CLA	CHD-C4C-C3C	-5.77	116.36	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	819	CLA	O2D-CGD-CBD	5.77	121.52	111.27
10	bA	836	CLA	C2C-C1C-NC	5.77	115.37	109.97
10	aB	821	CLA	CHD-C4C-C3C	-5.77	116.37	124.84
10	aA	805	CLA	CHD-C1D-ND	-5.76	119.16	124.45
10	aA	826	CLA	CHD-C1D-ND	-5.76	119.16	124.45
10	bA	813	CLA	CHD-C1D-ND	-5.76	119.16	124.45
10	cA	810	CLA	CHD-C1D-ND	-5.76	119.16	124.45
10	bB	822	CLA	O2D-CGD-CBD	5.76	121.51	111.27
10	cA	817	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
10	bB	821	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
10	cA	823	CLA	C2C-C1C-NC	5.76	115.37	109.97
10	bB	813	CLA	CMD-C2D-C1D	5.76	134.86	124.71
10	bB	833	CLA	CHD-C1D-ND	-5.76	119.16	124.45
10	bA	834	CLA	C2C-C1C-NC	5.76	115.36	109.97
10	bB	801	CLA	C4A-NA-C1A	-5.75	104.12	106.71
10	aA	817	CLA	CHD-C4C-C3C	-5.75	116.38	124.84
10	aA	836	CLA	CHD-C4C-C3C	-5.75	116.38	124.84
10	bB	806	CLA	O2D-CGD-CBD	5.75	121.49	111.27
10	cB	806	CLA	O2D-CGD-CBD	5.75	121.49	111.27
10	cA	812	CLA	O2D-CGD-CBD	5.75	121.49	111.27
10	cB	813	CLA	CMD-C2D-C1D	5.75	134.85	124.71
10	bA	820	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
10	cB	810	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
10	aB	817	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
10	aA	834	CLA	C2C-C1C-NC	5.75	115.36	109.97
10	cB	821	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
10	aB	833	CLA	CHD-C1D-ND	-5.75	119.17	124.45
10	cA	836	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
10	cB	821	CLA	O2D-CGD-CBD	5.74	121.47	111.27
10	cL	202	CLA	O2D-CGD-CBD	5.74	121.47	111.27
10	bB	810	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
10	cB	817	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
10	cA	836	CLA	C2C-C1C-NC	5.74	115.35	109.97
10	bA	817	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
10	aB	810	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
10	aB	821	CLA	O2D-CGD-CBD	5.74	121.46	111.27
10	aA	813	CLA	CHD-C1D-ND	-5.73	119.19	124.45
10	cB	833	CLA	CHD-C1D-ND	-5.73	119.19	124.45
10	cA	820	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
10	bA	812	CLA	O2D-CGD-CBD	5.73	121.45	111.27
10	bA	836	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
10	bL	202	CLA	O2D-CGD-CBD	5.73	121.45	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aL	202	CLA	O2D-CGD-CBD	5.73	121.45	111.27
10	cB	804	CLA	CHD-C1D-ND	-5.73	119.19	124.45
10	cB	815	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
10	aB	801	CLA	C4A-NA-C1A	-5.73	104.13	106.71
10	aA	820	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
10	aA	818	CLA	C2C-C1C-NC	5.72	115.33	109.97
10	aA	812	CLA	O2D-CGD-CBD	5.72	121.44	111.27
10	bA	818	CLA	C4A-NA-C1A	-5.72	104.13	106.71
10	bB	804	CLA	CHD-C1D-ND	-5.72	119.19	124.45
10	cA	805	CLA	CHD-C1D-ND	-5.72	119.19	124.45
10	aA	836	CLA	C2C-C1C-NC	5.72	115.33	109.97
10	cA	834	CLA	C2C-C1C-NC	5.72	115.33	109.97
10	aA	810	CLA	CHD-C1D-ND	-5.71	119.20	124.45
10	aB	837	CLA	O2D-CGD-CBD	5.71	121.42	111.27
10	aL	204	CLA	CHD-C1D-ND	-5.71	119.21	124.45
10	cB	813	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
10	bB	813	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
10	aB	813	CLA	CHD-C4C-C3C	-5.70	116.45	124.84
10	cA	833	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
10	aB	817	CLA	CHD-C1D-ND	-5.70	119.21	124.45
10	cL	204	CLA	CHD-C1D-ND	-5.70	119.21	124.45
10	cB	837	CLA	O2D-CGD-CBD	5.70	121.40	111.27
10	bB	815	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
10	bB	837	CLA	O2D-CGD-CBD	5.70	121.39	111.27
10	aA	833	CLA	CHD-C4C-C3C	-5.70	116.47	124.84
10	aB	815	CLA	CHD-C4C-C3C	-5.70	116.47	124.84
10	bA	820	CLA	CHD-C1D-ND	-5.70	119.22	124.45
10	cA	818	CLA	C4A-NA-C1A	-5.70	104.14	106.71
10	aA	818	CLA	C4A-NA-C1A	-5.69	104.15	106.71
10	bA	821	CLA	C2C-C1C-NC	5.69	115.30	109.97
10	bA	833	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
10	cA	820	CLA	CHD-C1D-ND	-5.69	119.23	124.45
10	aA	820	CLA	CHD-C1D-ND	-5.69	119.23	124.45
10	bA	818	CLA	C2C-C1C-NC	5.69	115.30	109.97
10	bB	823	CLA	C2C-C1C-NC	5.69	115.30	109.97
10	bA	826	CLA	CHD-C1D-ND	-5.68	119.23	124.45
10	cA	842	CLA	CMD-C2D-C1D	5.68	134.73	124.71
10	bL	204	CLA	CHD-C1D-ND	-5.68	119.23	124.45
10	cA	826	CLA	CHD-C1D-ND	-5.68	119.23	124.45
10	cB	830	CLA	CHD-C1D-ND	-5.68	119.23	124.45
10	aB	830	CLA	CHD-C1D-ND	-5.68	119.23	124.45
10	bA	842	CLA	CMD-C2D-C1D	5.68	134.72	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	842	CLA	CMD-C2D-C1D	5.67	134.71	124.71
10	cL	202	CLA	CHD-C1D-ND	-5.67	119.24	124.45
10	aB	829	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
10	cA	821	CLA	C2C-C1C-NC	5.67	115.28	109.97
10	bB	814	CLA	CHD-C1D-ND	-5.67	119.25	124.45
10	aB	835	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
10	cB	829	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
10	aL	202	CLA	CHD-C1D-ND	-5.65	119.26	124.45
10	cA	834	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
10	cB	814	CLA	CHD-C1D-ND	-5.65	119.26	124.45
10	cA	818	CLA	C2C-C1C-NC	5.65	115.26	109.97
10	bA	837	CLA	O2D-CGD-CBD	5.64	121.30	111.27
10	bB	829	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
10	bL	202	CLA	CHD-C1D-ND	-5.64	119.27	124.45
10	cB	835	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
10	cB	801	CLA	C4A-NA-C1A	-5.64	104.17	106.71
10	cB	821	CLA	C2C-C1C-NC	5.64	115.25	109.97
10	bB	817	CLA	CHD-C1D-ND	-5.63	119.28	124.45
10	aA	821	CLA	C2C-C1C-NC	5.63	115.25	109.97
10	cB	823	CLA	C2C-C1C-NC	5.63	115.25	109.97
10	cA	837	CLA	O2D-CGD-CBD	5.63	121.27	111.27
10	aA	815	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
10	bA	814	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
10	cA	813	CLA	C2C-C1C-NC	5.63	115.24	109.97
10	cB	816	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
10	aB	816	CLA	CHD-C4C-C3C	-5.62	116.57	124.84
10	aA	837	CLA	O2D-CGD-CBD	5.62	121.26	111.27
10	aA	819	CLA	C2C-C1C-NC	5.62	115.24	109.97
10	aB	823	CLA	C2C-C1C-NC	5.62	115.24	109.97
10	bB	835	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
10	aA	834	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
10	bA	819	CLA	C2C-C1C-NC	5.62	115.23	109.97
10	bB	821	CLA	C2C-C1C-NC	5.62	115.23	109.97
10	bA	834	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
10	cA	815	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
10	bB	828	CLA	C2C-C1C-NC	5.61	115.23	109.97
10	cA	810	CLA	C4A-NA-C1A	-5.61	104.18	106.71
10	aB	841	CLA	CHD-C1D-ND	-5.61	119.30	124.45
10	bB	830	CLA	CHD-C1D-ND	-5.61	119.30	124.45
10	aA	836	CLA	CHD-C1D-ND	-5.61	119.30	124.45
10	bA	836	CLA	CHD-C1D-ND	-5.61	119.30	124.45
10	bA	810	CLA	C2C-C1C-NC	5.61	115.22	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	809	CLA	C2C-C1C-NC	5.61	115.22	109.97
10	bB	812	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
10	cB	817	CLA	CHD-C1D-ND	-5.60	119.31	124.45
10	bB	808	CLA	CHD-C1D-ND	-5.60	119.31	124.45
10	aA	814	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
10	cB	841	CLA	CHD-C1D-ND	-5.60	119.31	124.45
10	bA	815	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
10	aA	824	CLA	CHD-C1D-ND	-5.60	119.31	124.45
10	aB	816	CLA	CHD-C1D-ND	-5.60	119.31	124.45
10	cB	839	CLA	O2D-CGD-CBD	5.60	121.21	111.27
10	aB	821	CLA	C2C-C1C-NC	5.60	115.22	109.97
10	cA	835	CLA	C2C-C1C-NC	5.60	115.22	109.97
10	cA	810	CLA	C2C-C1C-NC	5.60	115.21	109.97
10	cB	828	CLA	C2C-C1C-NC	5.60	115.21	109.97
10	aB	828	CLA	C2C-C1C-NC	5.59	115.21	109.97
10	cA	814	CLA	CHD-C1D-ND	-5.59	119.31	124.45
10	aA	810	CLA	C2C-C1C-NC	5.59	115.21	109.97
10	cA	838	CLA	O2D-CGD-CBD	5.59	121.20	111.27
10	aB	814	CLA	CHD-C1D-ND	-5.59	119.31	124.45
10	bA	810	CLA	C4A-NA-C1A	-5.59	104.19	106.71
10	aA	807	CLA	CHD-C4C-C3C	-5.59	116.63	124.84
10	cA	813	CLA	CHD-C4C-C3C	-5.59	116.63	124.84
10	cA	830	CLA	C2C-C1C-NC	5.59	115.20	109.97
10	bB	816	CLA	CHD-C4C-C3C	-5.59	116.63	124.84
10	aA	813	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
10	cA	839	CLA	C2C-C1C-NC	5.58	115.20	109.97
10	cA	836	CLA	CHD-C1D-ND	-5.58	119.33	124.45
10	aA	831	CLA	CHD-C1D-ND	-5.58	119.33	124.45
10	cA	814	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
10	aA	813	CLA	C2C-C1C-NC	5.58	115.20	109.97
10	bA	835	CLA	C2C-C1C-NC	5.58	115.20	109.97
10	bB	841	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
10	aB	827	CLA	C3D-C2D-C1D	-5.58	98.22	105.83
10	bB	829	CLA	C2C-C1C-NC	5.58	115.20	109.97
10	cA	819	CLA	C2C-C1C-NC	5.58	115.19	109.97
10	bA	813	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
10	bB	827	CLA	C3D-C2D-C1D	-5.57	98.22	105.83
10	aB	809	CLA	C2C-C1C-NC	5.57	115.19	109.97
10	cB	829	CLA	C2C-C1C-NC	5.57	115.19	109.97
10	aA	835	CLA	CHD-C1D-ND	-5.57	119.33	124.45
10	aA	802	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
10	aB	808	CLA	CHD-C1D-ND	-5.57	119.33	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	802	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
10	bA	838	CLA	O2D-CGD-CBD	5.57	121.17	111.27
10	bB	816	CLA	CHD-C1D-ND	-5.57	119.33	124.45
10	aA	835	CLA	C2C-C1C-NC	5.57	115.19	109.97
10	aB	839	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
10	bB	809	CLA	C2C-C1C-NC	5.57	115.19	109.97
10	bA	807	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
10	cB	841	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
10	bA	839	CLA	C2C-C1C-NC	5.57	115.19	109.97
10	cB	839	CLA	C2C-C1C-NC	5.57	115.19	109.97
10	bB	839	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
10	aA	814	CLA	CHD-C1D-ND	-5.56	119.34	124.45
10	bA	814	CLA	CHD-C1D-ND	-5.56	119.34	124.45
10	bB	839	CLA	O2D-CGD-CBD	5.56	121.16	111.27
10	cB	812	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
10	cB	839	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
10	bB	841	CLA	CHD-C1D-ND	-5.56	119.34	124.45
10	cB	813	CLA	C2C-C1C-NC	5.56	115.18	109.97
10	aB	812	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
10	cA	824	CLA	CHD-C1D-ND	-5.56	119.34	124.45
10	aA	839	CLA	C2C-C1C-NC	5.56	115.18	109.97
10	aA	811	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
10	bA	813	CLA	C2C-C1C-NC	5.56	115.18	109.97
10	bA	830	CLA	C2C-C1C-NC	5.56	115.18	109.97
10	bA	831	CLA	CHD-C1D-ND	-5.56	119.35	124.45
10	aB	839	CLA	O2D-CGD-CBD	5.56	121.14	111.27
10	bA	811	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
10	cA	807	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
10	aA	830	CLA	C2C-C1C-NC	5.55	115.17	109.97
10	bB	801	CLA	O2D-CGD-CBD	5.55	121.14	111.27
10	aB	801	CLA	O2D-CGD-CBD	5.55	121.14	111.27
10	cA	835	CLA	CHD-C1D-ND	-5.55	119.35	124.45
10	aB	841	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
10	cB	808	CLA	CHD-C1D-ND	-5.55	119.35	124.45
10	cB	825	CLA	CMD-C2D-C1D	5.55	134.50	124.71
10	cA	811	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
10	aB	829	CLA	C2C-C1C-NC	5.55	115.17	109.97
10	bA	815	CLA	C2C-C1C-NC	5.55	115.17	109.97
10	aA	810	CLA	C4A-NA-C1A	-5.55	104.21	106.71
10	bA	802	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
10	bB	803	CLA	CHD-C1D-ND	-5.55	119.36	124.45
10	aB	825	CLA	CMD-C2D-C1D	5.55	134.49	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	827	CLA	C3D-C2D-C1D	-5.55	98.26	105.83
10	cA	831	CLA	CHD-C1D-ND	-5.55	119.36	124.45
10	bB	828	CLA	O2D-CGD-CBD	5.54	121.12	111.27
10	aA	831	CLA	C2C-C1C-NC	5.54	115.16	109.97
10	cB	816	CLA	CHD-C1D-ND	-5.54	119.36	124.45
10	cB	833	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
10	aB	839	CLA	C2C-C1C-NC	5.54	115.16	109.97
10	bB	813	CLA	C2C-C1C-NC	5.54	115.16	109.97
10	aA	838	CLA	O2D-CGD-CBD	5.54	121.11	111.27
10	bA	829	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
10	cA	831	CLA	C2C-C1C-NC	5.53	115.16	109.97
10	cB	801	CLA	O2D-CGD-CBD	5.53	121.10	111.27
10	aA	829	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
10	bA	856	CLA	C2C-C1C-NC	5.53	115.15	109.97
10	bB	825	CLA	CMD-C2D-C1D	5.53	134.46	124.71
10	aB	837	CLA	C2C-C1C-NC	5.53	115.15	109.97
10	cB	837	CLA	C2C-C1C-NC	5.53	115.15	109.97
10	aB	833	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
10	bB	833	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
10	bA	835	CLA	CHD-C1D-ND	-5.52	119.38	124.45
10	aB	828	CLA	O2D-CGD-CBD	5.52	121.08	111.27
10	aB	803	CLA	CHD-C1D-ND	-5.52	119.38	124.45
10	cB	803	CLA	CHD-C1D-ND	-5.51	119.39	124.45
10	bA	824	CLA	CHD-C1D-ND	-5.51	119.39	124.45
10	aB	814	CLA	C2C-C1C-NC	5.51	115.13	109.97
10	aA	815	CLA	C2C-C1C-NC	5.51	115.13	109.97
10	bB	839	CLA	C2C-C1C-NC	5.51	115.13	109.97
10	cA	815	CLA	C2C-C1C-NC	5.51	115.13	109.97
10	aB	813	CLA	C2C-C1C-NC	5.51	115.13	109.97
10	aA	856	CLA	CHD-C1D-ND	-5.50	119.40	124.45
10	cA	829	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
10	cA	856	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
10	bA	856	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
10	cB	828	CLA	O2D-CGD-CBD	5.50	121.03	111.27
10	bB	837	CLA	C2C-C1C-NC	5.50	115.12	109.97
10	aB	817	CLA	C2C-C1C-NC	5.49	115.11	109.97
10	cB	810	CLA	C2C-C1C-NC	5.49	115.11	109.97
10	bA	856	CLA	CHD-C1D-ND	-5.49	119.41	124.45
10	aA	856	CLA	CHD-C4C-C3C	-5.49	116.78	124.84
10	cA	856	CLA	C2C-C1C-NC	5.49	115.11	109.97
10	aA	808	CLA	C2C-C1C-NC	5.48	115.11	109.97
10	cA	810	CLA	CHD-C4C-C3C	-5.48	116.78	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	810	CLA	C2C-C1C-NC	5.48	115.11	109.97
10	bB	814	CLA	C2C-C1C-NC	5.48	115.10	109.97
10	bA	810	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
10	bA	808	CLA	C2C-C1C-NC	5.47	115.10	109.97
10	bA	806	CLA	CHD-C4C-C3C	-5.47	116.79	124.84
10	bL	205	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
10	cL	202	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
10	cL	205	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
10	aL	205	CLA	CHD-C4C-C3C	-5.47	116.81	124.84
10	cA	823	CLA	CHD-C4C-C3C	-5.47	116.81	124.84
10	cA	808	CLA	C2C-C1C-NC	5.46	115.09	109.97
10	aA	829	CLA	CHD-C1D-ND	-5.46	119.43	124.45
10	cA	840	CLA	O2D-CGD-CBD	5.46	120.98	111.27
10	aB	810	CLA	C2C-C1C-NC	5.46	115.09	109.97
10	aA	840	CLA	O2D-CGD-CBD	5.46	120.97	111.27
10	aA	811	CLA	CHD-C1D-ND	-5.46	119.44	124.45
10	cB	811	CLA	CHD-C1D-ND	-5.46	119.44	124.45
10	aA	806	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
10	cA	806	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
10	bA	835	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
10	cA	840	CLA	CHD-C1D-ND	-5.45	119.44	124.45
10	aA	856	CLA	C2C-C1C-NC	5.45	115.08	109.97
10	cB	814	CLA	C2C-C1C-NC	5.45	115.08	109.97
10	bA	824	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
10	bA	840	CLA	O2D-CGD-CBD	5.45	120.96	111.27
10	aA	810	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
10	aA	835	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
10	bA	831	CLA	C2C-C1C-NC	5.45	115.08	109.97
10	aA	823	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
10	bL	204	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
10	aB	840	CLA	CHD-C1D-ND	-5.44	119.45	124.45
10	bA	823	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
10	cA	841	CLA	CHD-C1D-ND	-5.44	119.45	124.45
10	bB	809	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
10	cA	835	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
10	cA	824	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
10	cB	817	CLA	C2C-C1C-NC	5.44	115.07	109.97
10	aB	809	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
10	aA	841	CLA	CHD-C1D-ND	-5.44	119.46	124.45
10	aL	204	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
10	bA	838	CLA	C2C-C1C-NC	5.44	115.06	109.97
10	cA	811	CLA	CHD-C1D-ND	-5.44	119.46	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cL	204	CLA	CHD-C4C-C3C	-5.43	116.85	124.84
10	aL	202	CLA	CHD-C4C-C3C	-5.43	116.85	124.84
10	bA	814	CLA	O2D-CGD-CBD	5.43	120.92	111.27
10	cA	856	CLA	CHD-C1D-ND	-5.43	119.46	124.45
10	cA	829	CLA	CHD-C1D-ND	-5.43	119.47	124.45
10	aB	833	CLA	O2D-CGD-CBD	5.43	120.91	111.27
10	cB	807	CLA	C2C-C1C-NC	5.43	115.06	109.97
10	bB	811	CLA	CHD-C1D-ND	-5.43	119.47	124.45
10	bL	202	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
10	aA	842	CLA	CHD-C1D-ND	-5.42	119.47	124.45
10	aB	807	CLA	C2C-C1C-NC	5.42	115.05	109.97
10	cA	819	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
10	bA	840	CLA	CHD-C1D-ND	-5.42	119.47	124.45
10	cA	822	CLA	O2D-CGD-CBD	5.42	120.90	111.27
10	cA	812	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
10	bB	833	CLA	O2D-CGD-CBD	5.42	120.89	111.27
10	aA	814	CLA	O2D-CGD-CBD	5.41	120.89	111.27
10	cB	809	CLA	CHD-C4C-C3C	-5.41	116.88	124.84
10	aB	815	CLA	O2D-CGD-CBD	5.41	120.89	111.27
10	cB	815	CLA	O2D-CGD-CBD	5.41	120.88	111.27
10	bA	811	CLA	CHD-C1D-ND	-5.41	119.48	124.45
10	aL	203	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
10	bB	817	CLA	C2C-C1C-NC	5.41	115.04	109.97
10	aA	824	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
10	cB	833	CLA	O2D-CGD-CBD	5.41	120.88	111.27
10	cB	807	CLA	O2D-CGD-CBD	5.41	120.88	111.27
10	bA	829	CLA	CHD-C1D-ND	-5.41	119.49	124.45
10	cA	842	CLA	CHD-C1D-ND	-5.41	119.49	124.45
10	aA	819	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
10	bB	819	CLA	C4A-NA-C1A	-5.40	104.28	106.71
10	aB	823	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
10	aA	822	CLA	O2D-CGD-CBD	5.40	120.86	111.27
10	bA	812	CLA	CHD-C4C-C3C	-5.40	116.91	124.84
10	bA	841	CLA	CHD-C1D-ND	-5.39	119.50	124.45
10	aA	812	CLA	CHD-C4C-C3C	-5.39	116.91	124.84
10	aB	811	CLA	CHD-C1D-ND	-5.39	119.50	124.45
10	bB	807	CLA	O2D-CGD-CBD	5.39	120.85	111.27
10	bB	815	CLA	O2D-CGD-CBD	5.39	120.85	111.27
10	bL	203	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
10	bA	822	CLA	O2D-CGD-CBD	5.39	120.85	111.27
10	bA	832	CLA	C2C-C1C-NC	5.39	115.02	109.97
10	cL	203	CLA	CHD-C4C-C3C	-5.39	116.92	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	814	CLA	O2D-CGD-CBD	5.39	120.84	111.27
10	aB	836	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
10	bB	836	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
10	bA	819	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
10	bA	842	CLA	CHD-C1D-ND	-5.39	119.50	124.45
10	bB	823	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
10	cB	823	CLA	CHD-C4C-C3C	-5.38	116.92	124.84
10	aA	838	CLA	C2C-C1C-NC	5.38	115.02	109.97
10	bB	807	CLA	C2C-C1C-NC	5.38	115.02	109.97
10	aB	807	CLA	O2D-CGD-CBD	5.38	120.83	111.27
10	aB	819	CLA	CHD-C4C-C3C	-5.38	116.94	124.84
10	cB	840	CLA	CHD-C1D-ND	-5.38	119.51	124.45
10	bA	833	CLA	C2C-C1C-NC	5.37	115.01	109.97
10	cA	838	CLA	C2C-C1C-NC	5.37	115.00	109.97
10	bA	825	CLA	O2D-CGD-CBD	5.37	120.81	111.27
10	cB	815	CLA	C2C-C1C-NC	5.37	115.00	109.97
10	bB	840	CLA	CHD-C1D-ND	-5.37	119.52	124.45
10	aA	840	CLA	CHD-C1D-ND	-5.37	119.52	124.45
10	aB	815	CLA	C2C-C1C-NC	5.36	115.00	109.97
10	aA	825	CLA	O2D-CGD-CBD	5.36	120.79	111.27
10	cA	825	CLA	O2D-CGD-CBD	5.36	120.79	111.27
10	aA	829	CLA	CMD-C2D-C1D	5.36	134.16	124.71
10	cA	829	CLA	CMD-C2D-C1D	5.36	134.15	124.71
10	cA	832	CLA	C2C-C1C-NC	5.36	114.99	109.97
10	bB	819	CLA	CHD-C4C-C3C	-5.36	116.97	124.84
10	aB	837	CLA	CHD-C1D-ND	-5.35	119.54	124.45
10	cB	819	CLA	C4A-NA-C1A	-5.35	104.30	106.71
10	cB	819	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
10	bB	815	CLA	C2C-C1C-NC	5.35	114.98	109.97
10	cB	836	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
10	cL	204	CLA	CMD-C2D-C1D	5.35	134.13	124.71
10	aB	818	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
10	bL	204	CLA	CMD-C2D-C1D	5.34	134.13	124.71
10	aB	807	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
10	aB	819	CLA	C4A-NA-C1A	-5.34	104.31	106.71
10	bA	829	CLA	CMD-C2D-C1D	5.34	134.12	124.71
10	cB	818	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
10	aL	204	CLA	CMD-C2D-C1D	5.33	134.11	124.71
10	aA	833	CLA	C2C-C1C-NC	5.33	114.97	109.97
10	cA	828	CLA	CMD-C2D-C1D	5.33	134.11	124.71
10	aA	828	CLA	CMD-C2D-C1D	5.33	134.11	124.71
10	aA	832	CLA	C2C-C1C-NC	5.33	114.97	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	831	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
10	cA	833	CLA	C2C-C1C-NC	5.33	114.97	109.97
10	aB	827	CLA	O2D-CGD-CBD	5.33	120.73	111.27
10	aA	827	CLA	C2C-C1C-NC	5.32	114.96	109.97
10	cA	814	CLA	C2C-C1C-NC	5.32	114.96	109.97
10	cB	832	CLA	C2C-C1C-NC	5.32	114.96	109.97
10	cA	812	CLA	C4A-NA-C1A	-5.32	104.31	106.71
10	aB	834	CLA	C2C-C1C-NC	5.32	114.96	109.97
10	cB	837	CLA	CHD-C1D-ND	-5.32	119.56	124.45
10	bB	824	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
10	aA	812	CLA	C4A-NA-C1A	-5.32	104.31	106.71
10	cA	811	CLA	C2C-C1C-NC	5.32	114.96	109.97
10	bB	837	CLA	CHD-C1D-ND	-5.32	119.56	124.45
10	bB	807	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
10	bA	828	CLA	CMD-C2D-C1D	5.32	134.09	124.71
10	cB	831	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
10	cB	820	CLA	C2C-C1C-NC	5.32	114.95	109.97
10	bA	840	CLA	C4A-NA-C1A	-5.31	104.32	106.71
10	cA	811	CLA	O2D-CGD-CBD	5.31	120.71	111.27
10	aA	804	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
10	bA	804	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
10	cA	804	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
10	aB	835	CLA	C2C-C1C-NC	5.31	114.95	109.97
10	aB	831	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
10	bB	832	CLA	C2C-C1C-NC	5.31	114.94	109.97
10	cA	843	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
10	cA	840	CLA	C4A-NA-C1A	-5.31	104.32	106.71
10	bB	834	CLA	C2C-C1C-NC	5.31	114.94	109.97
10	aB	824	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
10	aA	840	CLA	C2C-C1C-NC	5.31	114.94	109.97
10	cB	827	CLA	O2D-CGD-CBD	5.30	120.69	111.27
10	cB	824	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
10	aA	841	CLA	O2D-CGD-CBD	5.30	120.69	111.27
10	aA	837	CLA	C2C-C1C-NC	5.30	114.94	109.97
10	aA	819	CLA	CHD-C1D-ND	-5.30	119.58	124.45
10	cA	841	CLA	O2D-CGD-CBD	5.30	120.68	111.27
10	bA	814	CLA	C2C-C1C-NC	5.30	114.94	109.97
10	bA	811	CLA	O2D-CGD-CBD	5.30	120.68	111.27
10	cB	807	CLA	CHD-C4C-C3C	-5.30	117.06	124.84
10	bA	827	CLA	C2C-C1C-NC	5.29	114.93	109.97
10	aA	811	CLA	O2D-CGD-CBD	5.29	120.68	111.27
10	aA	830	CLA	CHD-C4C-C3C	-5.29	117.06	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	843	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
10	bA	811	CLA	C2C-C1C-NC	5.29	114.93	109.97
10	bB	820	CLA	C2C-C1C-NC	5.29	114.93	109.97
10	bA	841	CLA	O2D-CGD-CBD	5.29	120.67	111.27
10	cA	854	CLA	O2D-CGD-CBD	5.29	120.67	111.27
10	cA	830	CLA	CHD-C4C-C3C	-5.29	117.07	124.84
10	aA	840	CLA	C4A-NA-C1A	-5.29	104.33	106.71
10	bB	835	CLA	C2C-C1C-NC	5.29	114.92	109.97
10	bB	827	CLA	O2D-CGD-CBD	5.29	120.66	111.27
10	bA	843	CLA	CHD-C4C-C3C	-5.29	117.07	124.84
10	aA	854	CLA	O2D-CGD-CBD	5.29	120.66	111.27
10	cA	840	CLA	C2C-C1C-NC	5.28	114.92	109.97
10	aA	811	CLA	C2C-C1C-NC	5.28	114.92	109.97
10	aB	804	CLA	CAA-C2A-C3A	-5.28	98.31	112.78
10	aB	820	CLA	C2C-C1C-NC	5.28	114.92	109.97
10	aB	832	CLA	C2C-C1C-NC	5.28	114.92	109.97
10	bA	840	CLA	C2C-C1C-NC	5.28	114.92	109.97
10	cB	804	CLA	CAA-C2A-C3A	-5.28	98.32	112.78
10	bA	812	CLA	C4A-NA-C1A	-5.28	104.33	106.71
10	bB	816	CLA	C2C-C1C-NC	5.27	114.91	109.97
10	cB	812	CLA	C2C-C1C-NC	5.27	114.91	109.97
10	bB	804	CLA	CAA-C2A-C3A	-5.27	98.34	112.78
10	aL	202	CLA	C3D-C2D-C1D	-5.27	98.63	105.83
10	bA	831	CLA	O2D-CGD-CBD	5.27	120.64	111.27
10	cA	831	CLA	O2D-CGD-CBD	5.27	120.64	111.27
10	aA	814	CLA	C2C-C1C-NC	5.27	114.91	109.97
10	bA	837	CLA	C2C-C1C-NC	5.27	114.91	109.97
10	bA	854	CLA	O2D-CGD-CBD	5.27	120.63	111.27
10	bA	830	CLA	CHD-C4C-C3C	-5.27	117.10	124.84
10	bA	826	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
10	bB	818	CLA	CHD-C4C-C3C	-5.27	117.10	124.84
10	cB	834	CLA	C2C-C1C-NC	5.27	114.91	109.97
10	bA	807	CLA	C2C-C1C-NC	5.26	114.90	109.97
10	cA	837	CLA	C2C-C1C-NC	5.26	114.90	109.97
10	bA	819	CLA	CHD-C1D-ND	-5.26	119.62	124.45
10	bL	202	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
10	aA	831	CLA	O2D-CGD-CBD	5.26	120.62	111.27
10	aB	812	CLA	C2C-C1C-NC	5.26	114.90	109.97
10	cA	826	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
10	bB	805	CLA	CMD-C2D-C1D	5.26	133.98	124.71
10	cB	805	CLA	CMD-C2D-C1D	5.26	133.98	124.71
10	bL	205	CLA	C2C-C1C-NC	5.26	114.90	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	805	CLA	CMD-C2D-C1D	5.26	133.98	124.71
10	cA	827	CLA	C2C-C1C-NC	5.25	114.89	109.97
10	aB	831	CLA	C4A-NA-C1A	-5.25	104.34	106.71
10	aB	803	CLA	C2C-C1C-NC	5.25	114.89	109.97
10	aB	831	CLA	C2C-C1C-NC	5.25	114.89	109.97
10	cB	831	CLA	C2C-C1C-NC	5.25	114.89	109.97
10	bB	803	CLA	C2C-C1C-NC	5.25	114.89	109.97
10	aA	826	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
10	cB	816	CLA	C2C-C1C-NC	5.25	114.89	109.97
10	cB	803	CLA	C2C-C1C-NC	5.25	114.89	109.97
10	cL	205	CLA	C2C-C1C-NC	5.24	114.88	109.97
10	aB	813	CLA	CHD-C1D-ND	-5.24	119.64	124.45
10	bB	812	CLA	C2C-C1C-NC	5.24	114.88	109.97
10	cB	835	CLA	C2C-C1C-NC	5.24	114.88	109.97
10	aB	811	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
10	bB	811	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
10	aB	816	CLA	C2C-C1C-NC	5.24	114.88	109.97
10	bB	813	CLA	CHD-C1D-ND	-5.24	119.64	124.45
10	cL	202	CLA	C3D-C2D-C1D	-5.24	98.69	105.83
10	bB	831	CLA	C2C-C1C-NC	5.24	114.88	109.97
10	aB	802	CLA	CHD-C1D-ND	-5.23	119.65	124.45
10	cB	811	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
10	aA	822	CLA	CHD-C1D-ND	-5.23	119.65	124.45
10	bA	822	CLA	CHD-C1D-ND	-5.22	119.65	124.45
10	cB	838	CLA	O2D-CGD-CBD	5.22	120.55	111.27
10	aL	205	CLA	C2C-C1C-NC	5.22	114.86	109.97
10	aA	807	CLA	C2C-C1C-NC	5.22	114.86	109.97
10	bB	818	CLA	C4A-NA-C1A	-5.22	104.36	106.71
10	aA	842	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
10	bB	838	CLA	O2D-CGD-CBD	5.22	120.54	111.27
10	aB	818	CLA	C4A-NA-C1A	-5.22	104.36	106.71
10	cA	822	CLA	CHD-C1D-ND	-5.22	119.66	124.45
10	bB	840	CLA	C2C-C1C-NC	5.22	114.86	109.97
10	bB	831	CLA	C4A-NA-C1A	-5.22	104.36	106.71
10	bA	842	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
10	aB	838	CLA	O2D-CGD-CBD	5.21	120.52	111.27
10	cA	819	CLA	CHD-C1D-ND	-5.21	119.67	124.45
10	cA	807	CLA	C2C-C1C-NC	5.21	114.85	109.97
10	aB	801	CLA	CHD-C4C-C3C	-5.20	117.19	124.84
10	aA	805	CLA	C2C-C1C-NC	5.20	114.84	109.97
10	cA	842	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
10	cB	831	CLA	C4A-NA-C1A	-5.20	104.37	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	830	CLA	O2D-CGD-CBD	5.19	120.50	111.27
10	cA	835	CLA	O2D-CGD-CBD	5.19	120.50	111.27
10	aB	815	CLA	CHD-C1D-ND	-5.19	119.68	124.45
10	bA	835	CLA	O2D-CGD-CBD	5.19	120.49	111.27
10	bA	830	CLA	O2D-CGD-CBD	5.19	120.48	111.27
10	cB	813	CLA	CHD-C1D-ND	-5.19	119.69	124.45
10	bB	801	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
10	cB	802	CLA	CHD-C1D-ND	-5.18	119.69	124.45
10	cB	801	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
10	cL	204	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
10	aA	835	CLA	O2D-CGD-CBD	5.18	120.47	111.27
10	bL	204	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
10	aA	830	CLA	O2D-CGD-CBD	5.17	120.46	111.27
10	aL	205	CLA	O2D-CGD-CBD	5.17	120.46	111.27
10	bB	802	CLA	CHD-C1D-ND	-5.17	119.70	124.45
10	cA	836	CLA	O2D-CGD-CBD	5.17	120.45	111.27
10	cL	205	CLA	O2D-CGD-CBD	5.17	120.45	111.27
10	bB	811	CLA	CMD-C2D-C1D	5.17	133.82	124.71
10	bA	805	CLA	C2C-C1C-NC	5.16	114.81	109.97
10	aB	811	CLA	CMD-C2D-C1D	5.16	133.81	124.71
10	bB	808	CLA	C4A-NA-C1A	-5.16	104.39	106.71
10	aL	204	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
10	cA	839	CLA	C4A-NA-C1A	-5.16	104.39	106.71
10	cB	808	CLA	C4A-NA-C1A	-5.16	104.39	106.71
10	cA	839	CLA	CHD-C4C-C3C	-5.16	117.26	124.84
10	bL	205	CLA	O2D-CGD-CBD	5.16	120.43	111.27
10	cB	811	CLA	CMD-C2D-C1D	5.16	133.80	124.71
10	bA	836	CLA	O2D-CGD-CBD	5.15	120.43	111.27
10	bA	839	CLA	CHD-C4C-C3C	-5.15	117.27	124.84
10	aA	836	CLA	O2D-CGD-CBD	5.15	120.42	111.27
10	cB	827	CLA	CHD-C1D-ND	-5.15	119.72	124.45
10	aA	822	CLA	C2C-C1C-NC	5.15	114.79	109.97
10	bB	815	CLA	CHD-C1D-ND	-5.15	119.72	124.45
10	aB	808	CLA	C4A-NA-C1A	-5.14	104.39	106.71
10	cB	840	CLA	C2C-C1C-NC	5.14	114.79	109.97
10	aB	825	CLA	C4A-NA-C1A	-5.14	104.39	106.71
10	bB	804	CLA	C4A-NA-C1A	-5.14	104.40	106.71
10	cB	826	CLA	CAA-C2A-C3A	-5.14	98.71	112.78
10	bB	825	CLA	C2C-C1C-NC	5.14	114.78	109.97
10	aA	839	CLA	C4A-NA-C1A	-5.14	104.40	106.71
10	aB	827	CLA	CHD-C1D-ND	-5.13	119.74	124.45
10	aB	804	CLA	C4A-NA-C1A	-5.13	104.40	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	825	CLA	C4A-NA-C1A	-5.13	104.40	106.71
10	cB	825	CLA	C2C-C1C-NC	5.13	114.78	109.97
10	aA	839	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
10	bB	826	CLA	CAA-C2A-C3A	-5.13	98.74	112.78
10	bA	822	CLA	C2C-C1C-NC	5.13	114.78	109.97
10	aB	826	CLA	CAA-C2A-C3A	-5.13	98.74	112.78
10	bB	807	CLA	C4A-NA-C1A	-5.12	104.40	106.71
10	aB	840	CLA	C2C-C1C-NC	5.12	114.77	109.97
10	bB	827	CLA	CHD-C1D-ND	-5.12	119.75	124.45
10	aB	807	CLA	C4A-NA-C1A	-5.12	104.41	106.71
10	cB	815	CLA	CHD-C1D-ND	-5.12	119.75	124.45
10	cB	830	CLA	C4A-NA-C1A	-5.12	104.41	106.71
10	cA	818	CLA	CHD-C4C-C3C	-5.11	117.32	124.84
10	aA	828	CLA	C2C-C1C-NC	5.11	114.76	109.97
10	bA	828	CLA	C2C-C1C-NC	5.11	114.76	109.97
10	cA	803	CLA	C2C-C1C-NC	5.11	114.76	109.97
10	cA	805	CLA	C2C-C1C-NC	5.11	114.76	109.97
10	cB	826	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
10	cB	818	CLA	C4A-NA-C1A	-5.10	104.41	106.71
10	cB	825	CLA	C4A-NA-C1A	-5.10	104.41	106.71
10	bA	806	CLA	C2C-C1C-NC	5.10	114.75	109.97
10	bA	839	CLA	C4A-NA-C1A	-5.10	104.42	106.71
10	bA	804	CLA	C2C-C1C-NC	5.09	114.75	109.97
10	cB	804	CLA	C4A-NA-C1A	-5.09	104.42	106.71
10	bA	803	CLA	C2C-C1C-NC	5.09	114.74	109.97
10	bB	826	CLA	CHD-C4C-C3C	-5.09	117.36	124.84
10	aA	803	CLA	C2C-C1C-NC	5.09	114.74	109.97
10	aB	827	CLA	C2C-C1C-NC	5.09	114.74	109.97
10	cB	827	CLA	C2C-C1C-NC	5.09	114.74	109.97
10	bB	827	CLA	C2C-C1C-NC	5.08	114.73	109.97
10	aB	825	CLA	C2C-C1C-NC	5.08	114.73	109.97
10	cA	824	CLA	C2C-C1C-NC	5.08	114.73	109.97
10	cB	802	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
10	cA	822	CLA	C2C-C1C-NC	5.08	114.73	109.97
10	cB	812	CLA	O2D-CGD-CBD	5.08	120.29	111.27
10	cA	828	CLA	C2C-C1C-NC	5.07	114.72	109.97
10	cB	807	CLA	C4A-NA-C1A	-5.07	104.43	106.71
10	bB	828	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
10	bB	834	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
10	aB	802	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
10	bB	829	CLA	CMD-C2D-C1D	5.07	133.64	124.71
10	aB	829	CLA	CMD-C2D-C1D	5.07	133.64	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	aA	801	CL0	O2D-CGD-CBD	5.07	120.27	111.27
9	cA	801	CL0	O2D-CGD-CBD	5.07	120.27	111.27
10	aB	826	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
10	cA	804	CLA	C2C-C1C-NC	5.07	114.72	109.97
9	bA	801	CL0	O2D-CGD-CBD	5.06	120.27	111.27
10	aB	812	CLA	O2D-CGD-CBD	5.06	120.27	111.27
10	cA	816	CLA	C2C-C1C-NC	5.06	114.71	109.97
10	cB	828	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
10	bB	812	CLA	O2D-CGD-CBD	5.06	120.26	111.27
10	aB	830	CLA	C4A-NA-C1A	-5.06	104.43	106.71
10	aA	804	CLA	C2C-C1C-NC	5.06	114.71	109.97
10	bA	825	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
10	aA	818	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
10	bL	203	CLA	C2C-C1C-NC	5.05	114.70	109.97
10	aA	802	CLA	O2D-CGD-CBD	5.05	120.24	111.27
10	bA	818	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
10	cB	829	CLA	CMD-C2D-C1D	5.04	133.60	124.71
10	aB	819	CLA	O2D-CGD-CBD	5.04	120.23	111.27
10	aA	806	CLA	C2C-C1C-NC	5.04	114.70	109.97
10	bB	802	CLA	CHD-C4C-C3C	-5.04	117.43	124.84
10	cB	819	CLA	O2D-CGD-CBD	5.04	120.23	111.27
10	cB	805	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
10	bA	812	CLA	C2C-C1C-NC	5.04	114.69	109.97
10	cA	806	CLA	O2D-CGD-CBD	5.04	120.22	111.27
10	aB	830	CLA	O2D-CGD-CBD	5.03	120.22	111.27
10	bB	805	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
10	bA	824	CLA	C2C-C1C-NC	5.03	114.69	109.97
10	aB	828	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
10	cA	806	CLA	C2C-C1C-NC	5.03	114.68	109.97
10	cB	834	CLA	CHD-C4C-C3C	-5.02	117.46	124.84
10	bA	806	CLA	O2D-CGD-CBD	5.02	120.19	111.27
10	aB	832	CLA	O2D-CGD-CBD	5.02	120.19	111.27
10	aB	834	CLA	CHD-C4C-C3C	-5.02	117.46	124.84
10	bA	802	CLA	O2D-CGD-CBD	5.02	120.19	111.27
10	bB	819	CLA	O2D-CGD-CBD	5.02	120.19	111.27
10	bB	832	CLA	O2D-CGD-CBD	5.02	120.19	111.27
10	aB	808	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
10	aA	806	CLA	O2D-CGD-CBD	5.02	120.18	111.27
10	cB	832	CLA	O2D-CGD-CBD	5.02	120.18	111.27
10	aB	814	CLA	CHD-C4C-C3C	-5.02	117.47	124.84
10	cA	812	CLA	C2C-C1C-NC	5.02	114.67	109.97
10	aA	828	CLA	C4A-NA-C1A	-5.02	104.45	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	802	CLA	O2D-CGD-CBD	5.02	120.18	111.27
10	bA	828	CLA	C4A-NA-C1A	-5.01	104.45	106.71
10	bB	830	CLA	O2D-CGD-CBD	5.01	120.17	111.27
10	cB	814	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
10	bB	808	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
10	aA	825	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
10	cB	808	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
10	cB	830	CLA	O2D-CGD-CBD	5.01	120.17	111.27
10	aA	812	CLA	C2C-C1C-NC	5.01	114.67	109.97
10	cB	821	CLA	CHD-C1D-ND	-5.01	119.85	124.45
10	bA	815	CLA	O2D-CGD-CBD	5.00	120.16	111.27
10	aA	824	CLA	C2C-C1C-NC	5.00	114.66	109.97
10	cL	203	CLA	C2C-C1C-NC	5.00	114.66	109.97
10	aB	828	CLA	CHD-C1D-ND	-5.00	119.86	124.45
10	aA	838	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
10	cA	825	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
10	bB	830	CLA	C4A-NA-C1A	-5.00	104.46	106.71
10	aA	816	CLA	C2C-C1C-NC	5.00	114.66	109.97
10	bB	814	CLA	CHD-C4C-C3C	-4.99	117.50	124.84
10	cA	838	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
10	aL	203	CLA	C2C-C1C-NC	4.99	114.65	109.97
10	aB	805	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
10	bA	838	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
10	aA	815	CLA	O2D-CGD-CBD	4.98	120.12	111.27
10	bL	203	CLA	O2D-CGD-CBD	4.98	120.12	111.27
10	cA	815	CLA	O2D-CGD-CBD	4.98	120.11	111.27
10	cA	821	CLA	C3D-C2D-C1D	-4.97	99.04	105.83
10	bA	808	CLA	CHD-C1D-ND	-4.97	119.88	124.45
10	bB	802	CLA	C2C-C1C-NC	4.97	114.63	109.97
10	aA	821	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
10	aA	838	CLA	C4A-NA-C1A	-4.97	104.47	106.71
10	aA	810	CLA	O2D-CGD-CBD	4.97	120.09	111.27
10	bA	816	CLA	C2C-C1C-NC	4.96	114.62	109.97
10	bB	806	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
10	aB	808	CLA	C2C-C1C-NC	4.96	114.62	109.97
10	aB	802	CLA	C2C-C1C-NC	4.96	114.62	109.97
10	cB	828	CLA	CHD-C1D-ND	-4.96	119.90	124.45
10	aB	821	CLA	CHD-C1D-ND	-4.95	119.90	124.45
10	aB	804	CLA	C2C-C1C-NC	4.95	114.61	109.97
10	cB	802	CLA	C2C-C1C-NC	4.95	114.61	109.97
10	cB	806	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
10	cA	807	CLA	C3D-C2D-C1D	-4.95	99.08	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	808	CLA	CHD-C1D-ND	-4.95	119.91	124.45
10	bB	808	CLA	C2C-C1C-NC	4.95	114.61	109.97
10	aL	203	CLA	O2D-CGD-CBD	4.95	120.06	111.27
10	cA	828	CLA	C4A-NA-C1A	-4.95	104.48	106.71
10	bB	828	CLA	CHD-C1D-ND	-4.95	119.91	124.45
10	bB	801	CLA	CAA-C2A-C3A	-4.95	99.23	112.78
10	bA	810	CLA	O2D-CGD-CBD	4.95	120.06	111.27
10	cL	203	CLA	O2D-CGD-CBD	4.94	120.05	111.27
10	cB	828	CLA	C3C-C4C-NC	4.94	116.11	110.57
10	bB	809	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
10	cB	809	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
10	bB	820	CLA	O2D-CGD-CBD	4.94	120.04	111.27
10	cA	810	CLA	O2D-CGD-CBD	4.94	120.04	111.27
10	bB	804	CLA	C2C-C1C-NC	4.94	114.60	109.97
10	bA	821	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
10	cB	833	CLA	C2C-C1C-NC	4.94	114.60	109.97
10	aA	831	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
10	cB	801	CLA	CAA-C2A-C3A	-4.94	99.26	112.78
10	aB	806	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
10	cB	808	CLA	C2C-C1C-NC	4.93	114.59	109.97
10	aB	801	CLA	CAA-C2A-C3A	-4.93	99.28	112.78
10	cB	804	CLA	C2C-C1C-NC	4.93	114.59	109.97
10	aA	809	CLA	C4A-NA-C1A	-4.93	104.49	106.71
10	bB	828	CLA	C3C-C4C-NC	4.93	116.10	110.57
10	aB	833	CLA	C2C-C1C-NC	4.93	114.59	109.97
10	cA	838	CLA	C4A-NA-C1A	-4.93	104.49	106.71
10	bA	807	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
10	aA	828	CLA	CHD-C1D-ND	-4.92	119.93	124.45
10	aB	820	CLA	O2D-CGD-CBD	4.92	120.02	111.27
10	bB	821	CLA	CHD-C1D-ND	-4.92	119.93	124.45
10	bB	833	CLA	C2C-C1C-NC	4.92	114.58	109.97
10	cB	823	CLA	O2D-CGD-CBD	4.92	120.01	111.27
10	aB	820	CLA	CHD-C4C-C3C	-4.92	117.61	124.84
10	aA	836	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
10	aB	809	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
10	cA	808	CLA	CHD-C1D-ND	-4.91	119.94	124.45
10	bB	823	CLA	O2D-CGD-CBD	4.91	119.99	111.27
10	aA	817	CLA	C2C-C1C-NC	4.91	114.57	109.97
10	bA	836	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
10	aB	823	CLA	O2D-CGD-CBD	4.91	119.99	111.27
10	bB	820	CLA	CHD-C4C-C3C	-4.91	117.63	124.84
10	aB	818	CLA	C2C-C1C-NC	4.91	114.57	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	822	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
10	aA	807	CLA	C3D-C2D-C1D	-4.91	99.14	105.83
10	bA	827	CLA	O2D-CGD-CBD	4.90	119.98	111.27
10	bB	804	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
10	cA	828	CLA	CHD-C1D-ND	-4.90	119.95	124.45
10	cB	804	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
10	cA	831	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
10	cB	820	CLA	O2D-CGD-CBD	4.89	119.97	111.27
10	bA	828	CLA	CHD-C1D-ND	-4.89	119.96	124.45
10	bA	833	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
10	cA	827	CLA	O2D-CGD-CBD	4.89	119.96	111.27
10	cB	820	CLA	CHD-C4C-C3C	-4.89	117.65	124.84
10	cB	804	CLA	CMD-C2D-C1D	4.89	133.33	124.71
10	bA	804	CLA	C4A-NA-C1A	-4.89	104.51	106.71
10	cB	822	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
10	aB	804	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
10	cA	834	CLA	CHD-C1D-ND	-4.88	119.97	124.45
10	aA	841	CLA	C2C-C1C-NC	4.88	114.55	109.97
10	aA	827	CLA	O2D-CGD-CBD	4.88	119.94	111.27
10	cB	841	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
10	bA	831	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
10	aA	833	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
10	aA	834	CLA	CHD-C1D-ND	-4.88	119.97	124.45
10	aB	834	CLA	C4A-NA-C1A	-4.88	104.51	106.71
10	aB	841	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
10	cA	834	CLA	CMD-C2D-C1D	4.87	133.30	124.71
10	bA	837	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
10	bB	818	CLA	C2C-C1C-NC	4.87	114.54	109.97
10	cA	837	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
10	aB	828	CLA	C3C-C4C-NC	4.87	116.03	110.57
10	cA	817	CLA	C2C-C1C-NC	4.87	114.53	109.97
10	bA	809	CLA	C4A-NA-C1A	-4.86	104.52	106.71
10	bA	809	CLA	C2C-C1C-NC	4.86	114.53	109.97
10	bB	822	CLA	C3D-C2D-C1D	-4.86	99.19	105.83
10	aA	837	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
10	bB	804	CLA	CMD-C2D-C1D	4.86	133.28	124.71
10	cB	818	CLA	C2C-C1C-NC	4.86	114.53	109.97
10	cA	809	CLA	C2C-C1C-NC	4.86	114.52	109.97
10	aB	832	CLA	C4A-NA-C1A	-4.86	104.52	106.71
10	cA	809	CLA	C4A-NA-C1A	-4.86	104.52	106.71
10	cB	811	CLA	CAA-C2A-C3A	-4.85	99.49	112.78
10	cA	833	CLA	C3D-C2D-C1D	-4.85	99.21	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	841	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
10	cA	836	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
10	aB	804	CLA	CMD-C2D-C1D	4.85	133.26	124.71
10	bA	841	CLA	C2C-C1C-NC	4.85	114.51	109.97
10	cA	841	CLA	C2C-C1C-NC	4.85	114.51	109.97
10	bA	834	CLA	CMD-C2D-C1D	4.84	133.25	124.71
10	aA	834	CLA	CMD-C2D-C1D	4.84	133.25	124.71
10	aA	809	CLA	C2C-C1C-NC	4.84	114.51	109.97
10	bA	817	CLA	C2C-C1C-NC	4.84	114.50	109.97
10	cB	804	CLA	C3C-C4C-NC	4.84	116.00	110.57
10	aA	832	CLA	C3D-C2D-C1D	-4.83	99.23	105.83
10	bB	816	CLA	C4A-NA-C1A	-4.83	104.53	106.71
10	cB	832	CLA	C4A-NA-C1A	-4.83	104.53	106.71
10	bA	838	CLA	C4A-NA-C1A	-4.83	104.54	106.71
10	bB	804	CLA	C3C-C4C-NC	4.83	115.98	110.57
10	aA	824	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
10	bB	811	CLA	CAA-C2A-C3A	-4.83	99.56	112.78
10	cA	854	CLA	C2C-C1C-NC	4.83	114.49	109.97
10	aB	811	CLA	CAA-C2A-C3A	-4.83	99.57	112.78
9	aA	801	CL0	CAA-C2A-C3A	-4.83	99.57	112.78
10	bB	840	CLA	C4A-NA-C1A	-4.82	104.54	106.71
10	bA	834	CLA	CHD-C1D-ND	-4.82	120.02	124.45
10	aA	854	CLA	C2C-C1C-NC	4.82	114.49	109.97
10	bA	854	CLA	C2C-C1C-NC	4.82	114.49	109.97
9	bA	801	CL0	CAA-C2A-C3A	-4.82	99.57	112.78
10	bA	832	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
10	aA	854	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
10	bA	854	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
10	cA	832	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
10	cA	854	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
10	bA	808	CLA	C4A-NA-C1A	-4.81	104.54	106.71
10	aB	804	CLA	C3C-C4C-NC	4.81	115.97	110.57
9	cA	801	CL0	CAA-C2A-C3A	-4.81	99.61	112.78
10	bB	812	CLA	C4A-NA-C1A	-4.81	104.55	106.71
10	cB	840	CLA	C4A-NA-C1A	-4.81	104.55	106.71
10	bA	824	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
10	aB	811	CLA	O2D-CGD-CBD	4.80	119.79	111.27
10	cL	204	CLA	C2C-C1C-NC	4.79	114.46	109.97
10	cA	820	CLA	C2C-C1C-NC	4.79	114.46	109.97
10	cA	824	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
10	aA	804	CLA	C4A-NA-C1A	-4.79	104.55	106.71
10	bL	204	CLA	C2C-C1C-NC	4.79	114.46	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	812	CLA	C4A-NA-C1A	-4.79	104.55	106.71
10	bL	205	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
10	cB	811	CLA	O2D-CGD-CBD	4.79	119.77	111.27
10	cA	805	CLA	CAA-C2A-C3A	-4.79	99.67	112.78
10	cA	816	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
10	bA	816	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
10	bB	824	CLA	C4A-NA-C1A	-4.78	104.56	106.71
10	cB	838	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
10	aA	805	CLA	CAA-C2A-C3A	-4.78	99.69	112.78
10	bB	811	CLA	O2D-CGD-CBD	4.78	119.76	111.27
10	cA	827	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
10	cA	810	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
10	aA	816	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
10	aB	838	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
10	aB	816	CLA	C4A-NA-C1A	-4.77	104.56	106.71
10	bA	805	CLA	CAA-C2A-C3A	-4.77	99.72	112.78
10	aL	204	CLA	C2C-C1C-NC	4.76	114.43	109.97
10	aA	802	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
10	cL	202	CLA	C1D-CHD-C4C	-4.76	115.79	126.06
10	aA	808	CLA	C4A-NA-C1A	-4.76	104.57	106.71
10	cA	802	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
10	cB	834	CLA	C4A-NA-C1A	-4.75	104.57	106.71
10	cB	840	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
10	aB	824	CLA	C4A-NA-C1A	-4.75	104.57	106.71
10	cB	812	CLA	C4A-NA-C1A	-4.75	104.57	106.71
10	bB	813	CLA	O2D-CGD-CBD	4.75	119.71	111.27
10	bB	838	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
10	aB	825	CLA	CHD-C1D-ND	-4.75	120.09	124.45
10	aB	840	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
10	bA	820	CLA	C2C-C1C-NC	4.75	114.42	109.97
10	aL	202	CLA	C1D-CHD-C4C	-4.75	115.82	126.06
10	aA	827	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
10	bA	824	CLA	C4A-NA-C1A	-4.74	104.57	106.71
10	aB	812	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
10	aA	820	CLA	C2C-C1C-NC	4.74	114.41	109.97
10	aA	810	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
10	bA	810	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
10	bB	840	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
10	bB	832	CLA	C4A-NA-C1A	-4.74	104.58	106.71
10	cA	804	CLA	C4A-NA-C1A	-4.74	104.58	106.71
10	cB	813	CLA	O2D-CGD-CBD	4.74	119.69	111.27
10	bL	202	CLA	C1D-CHD-C4C	-4.74	115.84	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	813	CLA	O2D-CGD-CBD	4.74	119.68	111.27
10	aL	205	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
10	bB	825	CLA	CHD-C1D-ND	-4.73	120.10	124.45
10	cA	809	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
10	cA	808	CLA	C4A-NA-C1A	-4.73	104.58	106.71
10	cA	817	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
10	bA	817	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
10	cL	205	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
10	bB	812	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
10	bA	802	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
10	cB	823	CLA	C4A-NA-C1A	-4.72	104.58	106.71
10	cB	824	CLA	C4A-NA-C1A	-4.72	104.59	106.71
10	bL	203	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
10	cL	203	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
10	aA	809	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
10	bA	827	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
10	bB	823	CLA	C4A-NA-C1A	-4.71	104.59	106.71
10	cB	836	CLA	C4A-NA-C1A	-4.71	104.59	106.71
10	bA	809	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
10	aL	203	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
10	cB	812	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
10	aB	839	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
10	aB	823	CLA	C4A-NA-C1A	-4.70	104.59	106.71
10	cB	825	CLA	CHD-C1D-ND	-4.70	120.13	124.45
10	bB	834	CLA	C4A-NA-C1A	-4.70	104.59	106.71
9	bA	801	CL0	CMD-C2D-C1D	4.70	133.00	124.71
10	cA	803	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
10	aA	841	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
10	bB	832	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
10	cB	816	CLA	C4A-NA-C1A	-4.70	104.59	106.71
10	bB	839	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
10	aA	829	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
10	bB	803	CLA	C3C-C4C-NC	4.70	115.84	110.57
10	cB	839	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
10	cA	841	CLA	C3D-C2D-C1D	-4.69	99.42	105.83
10	aA	817	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
10	cA	829	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
10	bA	841	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
10	aB	803	CLA	C3C-C4C-NC	4.68	115.82	110.57
10	cB	832	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
10	cA	806	CLA	C4A-NA-C1A	-4.68	104.60	106.71
10	bA	818	CLA	C3D-C2D-C1D	-4.68	99.44	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	843	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
9	aA	801	CL0	CMD-C2D-C1D	4.68	132.96	124.71
10	cB	826	CLA	C2C-C1C-NC	4.67	114.35	109.97
9	cA	801	CL0	CMD-C2D-C1D	4.67	132.95	124.71
10	aB	832	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
10	cA	825	CLA	C2C-C1C-NC	4.67	114.35	109.97
10	bA	803	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
10	cA	805	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
10	aB	810	CLA	CHD-C1D-ND	-4.66	120.17	124.45
10	cA	818	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
10	bA	829	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
10	aA	805	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
10	cB	803	CLA	C3C-C4C-NC	4.66	115.80	110.57
10	bB	819	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
10	aA	825	CLA	C2C-C1C-NC	4.66	114.34	109.97
10	bB	811	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
10	bB	817	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
10	aA	803	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
10	aB	824	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
10	aA	818	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
10	cA	825	CLA	C4A-NA-C1A	-4.66	104.61	106.71
10	aB	811	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
10	aB	826	CLA	C2C-C1C-NC	4.65	114.33	109.97
10	cB	817	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
10	aA	825	CLA	C4A-NA-C1A	-4.65	104.62	106.71
10	bB	835	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
10	bA	825	CLA	C2C-C1C-NC	4.65	114.33	109.97
10	bB	810	CLA	CHD-C1D-ND	-4.65	120.18	124.45
10	aB	819	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
10	cA	843	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
10	bB	826	CLA	C2C-C1C-NC	4.64	114.32	109.97
10	aA	843	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
10	cB	819	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
10	cB	811	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
10	aA	824	CLA	C4A-NA-C1A	-4.63	104.62	106.71
10	aB	817	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
10	aB	835	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
10	bA	805	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
10	cB	835	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
10	bB	824	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
10	aB	838	CLA	C2C-C1C-NC	4.62	114.30	109.97
10	cB	824	CLA	C3D-C2D-C1D	-4.62	99.53	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	806	CLA	C4A-NA-C1A	-4.62	104.63	106.71
10	aB	836	CLA	C4A-NA-C1A	-4.62	104.63	106.71
10	cB	810	CLA	CHD-C1D-ND	-4.61	120.21	124.45
10	cB	803	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
10	bB	802	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
10	bB	803	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
10	bA	825	CLA	C4A-NA-C1A	-4.60	104.64	106.71
10	bB	820	CLA	C4A-NA-C1A	-4.60	104.64	106.71
10	bB	836	CLA	C4A-NA-C1A	-4.60	104.64	106.71
10	aB	822	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
10	aA	842	CLA	O2D-CGD-CBD	4.60	119.44	111.27
10	bA	842	CLA	O2D-CGD-CBD	4.60	119.44	111.27
10	aB	840	CLA	C4A-NA-C1A	-4.60	104.64	106.71
10	cA	842	CLA	O2D-CGD-CBD	4.59	119.43	111.27
10	aB	802	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
10	bB	816	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
10	bB	831	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
10	cA	824	CLA	C4A-NA-C1A	-4.59	104.64	106.71
10	cA	826	CLA	C4A-NA-C1A	-4.59	104.64	106.71
10	cB	816	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
10	aB	816	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
10	cB	822	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
10	cB	820	CLA	C4A-NA-C1A	-4.58	104.64	106.71
10	cA	832	CLA	O2D-CGD-CBD	4.58	119.41	111.27
10	aB	831	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
10	cB	802	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
10	aB	803	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
10	bB	807	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
10	aA	813	CLA	O2D-CGD-CBD	4.58	119.41	111.27
10	bB	838	CLA	C2C-C1C-NC	4.58	114.26	109.97
10	aA	826	CLA	C4A-NA-C1A	-4.58	104.65	106.71
10	bA	813	CLA	O2D-CGD-CBD	4.58	119.40	111.27
10	cA	813	CLA	O2D-CGD-CBD	4.57	119.40	111.27
10	cA	814	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
10	cA	835	CLA	C4A-NA-C1A	-4.57	104.65	106.71
10	bA	832	CLA	O2D-CGD-CBD	4.57	119.38	111.27
10	cB	838	CLA	C2C-C1C-NC	4.56	114.25	109.97
10	bA	835	CLA	C4A-NA-C1A	-4.56	104.65	106.71
10	cB	819	CLA	C1C-C2C-C3C	-4.56	102.16	106.96
10	cB	807	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
10	aB	833	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
10	bB	806	CLA	C2C-C1C-NC	4.56	114.24	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	831	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
10	aA	814	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
10	cA	826	CLA	C2C-C1C-NC	4.56	114.24	109.97
10	aA	826	CLA	C2C-C1C-NC	4.55	114.24	109.97
10	aB	807	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
10	aA	832	CLA	O2D-CGD-CBD	4.55	119.36	111.27
10	aB	819	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
10	bB	841	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
10	aB	820	CLA	C4A-NA-C1A	-4.55	104.66	106.71
10	cB	841	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
10	bB	819	CLA	C1C-C2C-C3C	-4.55	102.18	106.96
10	aB	841	CLA	C1C-C2C-C3C	-4.55	102.18	106.96
10	cA	806	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
10	cB	833	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
10	aA	835	CLA	C4A-NA-C1A	-4.54	104.67	106.71
10	bA	814	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
10	aB	806	CLA	C2C-C1C-NC	4.54	114.22	109.97
10	bA	854	CLA	C4A-NA-C1A	-4.54	104.67	106.71
10	bB	833	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
10	bA	815	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
10	bA	813	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
10	bB	822	CLA	C1C-C2C-C3C	-4.53	102.20	106.96
10	aA	815	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
10	cB	802	CLA	O2D-CGD-CBD	4.52	119.31	111.27
10	aB	834	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
10	bA	829	CLA	C3C-C4C-NC	4.52	115.64	110.57
10	bB	834	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
10	bB	836	CLA	O2D-CGD-CBD	4.52	119.29	111.27
10	aA	806	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
10	cB	837	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
10	bA	806	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
10	bA	826	CLA	C2C-C1C-NC	4.51	114.20	109.97
10	aA	854	CLA	C4A-NA-C1A	-4.51	104.68	106.71
10	bB	802	CLA	CMB-C2B-C3B	4.51	133.11	124.68
10	cA	815	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
10	aB	826	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
10	bB	819	CLA	CBA-CAA-C2A	4.50	127.16	113.86
10	cB	831	CLA	O2D-CGD-CBD	4.50	119.27	111.27
10	cB	836	CLA	O2D-CGD-CBD	4.50	119.27	111.27
10	bA	856	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
10	cB	818	CLA	O2D-CGD-CBD	4.50	119.27	111.27
10	aA	829	CLA	C3C-C4C-NC	4.50	115.62	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	837	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
10	cB	806	CLA	C2C-C1C-NC	4.50	114.19	109.97
10	aB	819	CLA	CBA-CAA-C2A	4.50	127.13	113.86
10	cB	839	CLA	C4A-NA-C1A	-4.50	104.69	106.71
10	aB	802	CLA	O2D-CGD-CBD	4.50	119.26	111.27
10	aA	834	CLA	O2D-CGD-CBD	4.49	119.25	111.27
10	cA	813	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
10	bB	839	CLA	C4A-NA-C1A	-4.49	104.69	106.71
10	cB	802	CLA	CMB-C2B-C3B	4.49	133.08	124.68
10	cB	819	CLA	CBA-CAA-C2A	4.49	127.12	113.86
10	bA	834	CLA	O2D-CGD-CBD	4.49	119.25	111.27
10	cA	809	CLA	O2D-CGD-CBD	4.49	119.25	111.27
10	cA	834	CLA	O2D-CGD-CBD	4.49	119.25	111.27
10	bB	826	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
10	bA	806	CLA	C4A-NA-C1A	-4.49	104.69	106.71
10	cA	836	CLA	C4A-NA-C1A	-4.49	104.69	106.71
10	aB	802	CLA	CMB-C2B-C3B	4.49	133.07	124.68
10	cB	834	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
10	aB	836	CLA	O2D-CGD-CBD	4.49	119.24	111.27
10	cA	856	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
10	aB	818	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
10	bB	831	CLA	O2D-CGD-CBD	4.48	119.23	111.27
10	bB	804	CLA	O2D-CGD-O1D	-4.48	115.07	123.84
10	bB	802	CLA	O2D-CGD-CBD	4.48	119.23	111.27
10	aB	831	CLA	O2D-CGD-CBD	4.48	119.23	111.27
10	aA	813	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
10	aA	809	CLA	O2D-CGD-CBD	4.48	119.23	111.27
10	aA	836	CLA	C4A-NA-C1A	-4.48	104.69	106.71
10	cA	829	CLA	C3C-C4C-NC	4.48	115.59	110.57
10	cB	826	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
10	aB	837	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
10	cB	814	CLA	CAC-C3C-C4C	4.47	130.61	124.81
10	cB	804	CLA	O2D-CGD-O1D	-4.47	115.10	123.84
10	cA	839	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
10	aA	828	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
10	cB	823	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
10	aB	814	CLA	CAC-C3C-C4C	4.46	130.60	124.81
10	aB	804	CLA	O2D-CGD-O1D	-4.46	115.11	123.84
10	bB	818	CLA	O2D-CGD-CBD	4.46	119.20	111.27
10	aB	818	CLA	O2D-CGD-CBD	4.46	119.19	111.27
10	aB	839	CLA	C4A-NA-C1A	-4.46	104.70	106.71
10	cB	818	CLA	C3D-C2D-C1D	-4.46	99.75	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	826	CLA	C4A-NA-C1A	-4.46	104.70	106.71
10	bA	812	CLA	C3D-C4D-ND	4.46	117.44	110.24
10	bA	828	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
10	bB	823	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
10	aA	811	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
10	bA	836	CLA	C4A-NA-C1A	-4.45	104.70	106.71
10	cA	854	CLA	C4A-NA-C1A	-4.45	104.70	106.71
10	bB	818	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
10	bA	809	CLA	O2D-CGD-CBD	4.45	119.17	111.27
10	cA	842	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
10	cA	828	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
10	bA	842	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
10	bB	814	CLA	CAC-C3C-C4C	4.44	130.57	124.81
10	aA	812	CLA	C3D-C4D-ND	4.44	117.42	110.24
10	aA	856	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
10	cA	812	CLA	C3D-C4D-ND	4.44	117.42	110.24
10	cB	830	CLA	CHD-C4C-C3C	-4.44	118.32	124.84
10	bB	830	CLA	CHD-C4C-C3C	-4.43	118.32	124.84
10	aB	823	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
10	bA	839	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
10	cA	826	CLA	C3C-C4C-NC	4.43	115.54	110.57
10	aB	830	CLA	CHD-C4C-C3C	-4.43	118.33	124.84
10	bA	822	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
10	cA	822	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
10	cB	829	CLA	C4A-NA-C1A	-4.42	104.72	106.71
10	cA	811	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
10	aA	842	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
10	aA	822	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
10	aA	839	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
10	aA	826	CLA	C3C-C4C-NC	4.42	115.52	110.57
10	cB	834	CLA	C3D-C4D-ND	4.42	117.38	110.24
10	bA	811	CLA	C3D-C2D-C1D	-4.42	99.81	105.83
10	bA	826	CLA	C3C-C4C-NC	4.41	115.52	110.57
10	bB	834	CLA	C3D-C4D-ND	4.41	117.37	110.24
10	cA	820	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
9	cA	801	CL0	C3C-C4C-NC	4.40	115.51	110.57
10	bA	820	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
10	aA	820	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
10	aB	834	CLA	C3D-C4D-ND	4.40	117.35	110.24
9	bA	801	CL0	C3C-C4C-NC	4.39	115.50	110.57
10	cB	801	CLA	C3C-C4C-NC	4.39	115.50	110.57
10	aB	813	CLA	C4A-NA-C1A	-4.39	104.73	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bL	203	CLA	C4A-NA-C1A	-4.39	104.73	106.71
9	aA	801	CL0	C3C-C4C-NC	4.38	115.49	110.57
10	bA	822	CLA	C4A-NA-C1A	-4.38	104.73	106.71
10	bB	829	CLA	C4A-NA-C1A	-4.38	104.74	106.71
10	cA	804	CLA	C3D-C4D-ND	4.38	117.33	110.24
10	aB	814	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
10	bA	812	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
10	aA	820	CLA	O2D-CGD-CBD	4.37	119.04	111.27
10	cB	814	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
10	bB	840	CLA	C3C-C4C-NC	4.37	115.48	110.57
10	cA	820	CLA	O2D-CGD-CBD	4.37	119.04	111.27
10	cB	840	CLA	C3C-C4C-NC	4.37	115.47	110.57
10	aB	829	CLA	C4A-NA-C1A	-4.37	104.74	106.71
10	aA	808	CLA	C3C-C4C-NC	4.37	115.47	110.57
10	bB	813	CLA	C3C-C4C-NC	4.37	115.47	110.57
10	bA	803	CLA	C4A-NA-C1A	-4.37	104.74	106.71
10	cA	812	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
10	aB	801	CLA	C3C-C4C-NC	4.36	115.47	110.57
10	aB	840	CLA	C3C-C4C-NC	4.36	115.46	110.57
10	cL	204	CLA	C3D-C4D-ND	4.36	117.29	110.24
10	aB	825	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
10	cA	830	CLA	C4A-NA-C1A	-4.36	104.75	106.71
10	cB	813	CLA	C4A-NA-C1A	-4.36	104.75	106.71
10	bA	820	CLA	O2D-CGD-CBD	4.36	119.01	111.27
10	aA	812	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
10	aA	804	CLA	C3D-C4D-ND	4.36	117.28	110.24
10	cB	825	CLA	C3C-C4C-NC	4.36	115.46	110.57
10	bA	804	CLA	C3D-C4D-ND	4.36	117.28	110.24
10	aB	833	CLA	C4A-NA-C1A	-4.35	104.75	106.71
10	bB	825	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
10	bB	814	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
10	aB	813	CLA	C3D-C4D-ND	4.35	117.27	110.24
10	aA	822	CLA	C4A-NA-C1A	-4.35	104.75	106.71
10	bB	813	CLA	C3D-C4D-ND	4.35	117.27	110.24
10	bL	205	CLA	C3D-C4D-ND	4.35	117.27	110.24
10	cB	833	CLA	C4A-NA-C1A	-4.35	104.75	106.71
10	bA	830	CLA	C4A-NA-C1A	-4.34	104.75	106.71
10	aB	820	CLA	C3D-C4D-ND	4.34	117.26	110.24
10	bB	829	CLA	C3C-C4C-NC	4.34	115.44	110.57
10	bB	820	CLA	C3D-C4D-ND	4.34	117.26	110.24
10	bB	801	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
10	aB	825	CLA	C3C-C4C-NC	4.34	115.44	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	825	CLA	C3C-C4C-NC	4.34	115.44	110.57
10	aA	803	CLA	C4A-NA-C1A	-4.34	104.75	106.71
10	cB	801	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
10	aL	205	CLA	C3D-C4D-ND	4.34	117.26	110.24
10	bB	830	CLA	CAC-C3C-C4C	4.34	130.44	124.81
10	aL	203	CLA	C4A-NA-C1A	-4.34	104.76	106.71
10	cB	825	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
10	cA	815	CLA	C3D-C4D-ND	4.34	117.25	110.24
10	aB	801	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
10	aB	813	CLA	C3C-C4C-NC	4.33	115.43	110.57
10	aA	815	CLA	C3D-C4D-ND	4.33	117.25	110.24
10	cL	205	CLA	C3D-C4D-ND	4.33	117.25	110.24
9	bA	801	CL0	C1C-C2C-C3C	-4.33	102.40	106.96
10	bA	830	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
10	aL	204	CLA	C3D-C4D-ND	4.33	117.24	110.24
10	cB	820	CLA	C3D-C4D-ND	4.33	117.24	110.24
10	aA	822	CLA	C3C-C4C-NC	4.33	115.43	110.57
10	aB	829	CLA	C3C-C4C-NC	4.33	115.43	110.57
10	bB	833	CLA	C4A-NA-C1A	-4.33	104.76	106.71
10	cL	202	CLA	C3C-C4C-NC	4.33	115.42	110.57
10	bB	810	CLA	C1D-CHD-C4C	-4.33	116.72	126.06
10	cB	810	CLA	C1D-CHD-C4C	-4.33	116.72	126.06
10	bB	801	CLA	C3C-C4C-NC	4.33	115.42	110.57
10	cA	808	CLA	C3C-C4C-NC	4.33	115.42	110.57
10	bA	822	CLA	C3C-C4C-NC	4.33	115.42	110.57
10	cA	822	CLA	C3C-C4C-NC	4.32	115.42	110.57
10	cA	822	CLA	C4A-NA-C1A	-4.32	104.76	106.71
10	bA	815	CLA	C3D-C4D-ND	4.32	117.23	110.24
9	cA	801	CL0	C1C-C2C-C3C	-4.32	102.41	106.96
10	bL	202	CLA	C3C-C4C-NC	4.32	115.41	110.57
10	aB	810	CLA	C1D-CHD-C4C	-4.32	116.74	126.06
10	bB	813	CLA	C4A-NA-C1A	-4.32	104.77	106.71
10	cB	829	CLA	C3C-C4C-NC	4.32	115.41	110.57
10	cB	813	CLA	C3C-C4C-NC	4.32	115.41	110.57
10	bB	830	CLA	CMB-C2B-C3B	4.31	132.75	124.68
10	cB	827	CLA	C1D-CHD-C4C	-4.31	116.75	126.06
10	cB	830	CLA	CMB-C2B-C3B	4.31	132.75	124.68
10	aB	836	CLA	C3D-C2D-C1D	-4.31	99.94	105.83
10	bA	828	CLA	C3C-C4C-NC	4.31	115.41	110.57
10	bB	841	CLA	O2D-CGD-CBD	4.31	118.93	111.27
10	cA	830	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
10	bL	204	CLA	C3D-C4D-ND	4.31	117.21	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	827	CLA	C3C-C4C-NC	4.31	115.41	110.57
9	aA	801	CL0	C1C-C2C-C3C	-4.31	102.42	106.96
10	cL	203	CLA	C4A-NA-C1A	-4.31	104.77	106.71
10	aA	830	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
10	bB	809	CLA	C4A-NA-C1A	-4.31	104.77	106.71
10	cA	805	CLA	C4A-NA-C1A	-4.30	104.77	106.71
10	aB	840	CLA	O2D-CGD-CBD	4.30	118.91	111.27
10	bB	827	CLA	C1D-CHD-C4C	-4.30	116.78	126.06
10	aB	830	CLA	CAC-C3C-C4C	4.30	130.39	124.81
10	aL	203	CLA	C3D-C4D-ND	4.30	117.19	110.24
10	aB	830	CLA	CMB-C2B-C3B	4.30	132.72	124.68
10	aA	842	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
10	cB	837	CLA	C3C-C4C-NC	4.30	115.39	110.57
10	bB	836	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
10	aA	828	CLA	C3C-C4C-NC	4.30	115.39	110.57
10	aL	202	CLA	C3C-C4C-NC	4.30	115.39	110.57
10	cB	838	CLA	C3D-C4D-ND	4.30	117.19	110.24
10	cB	836	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
10	cA	834	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
10	cA	803	CLA	C4A-NA-C1A	-4.30	104.78	106.71
10	aB	841	CLA	O2D-CGD-CBD	4.29	118.89	111.27
10	cA	827	CLA	C3C-C4C-NC	4.29	115.38	110.57
10	aB	838	CLA	C3D-C4D-ND	4.29	117.18	110.24
10	aA	834	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
10	cB	840	CLA	O2D-CGD-CBD	4.29	118.89	111.27
10	cB	830	CLA	CAC-C3C-C4C	4.29	130.38	124.81
10	cA	842	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
10	bB	809	CLA	C3C-C4C-NC	4.29	115.38	110.57
10	bA	842	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
10	cB	813	CLA	C3D-C4D-ND	4.29	117.17	110.24
10	aB	827	CLA	C1D-CHD-C4C	-4.29	116.81	126.06
10	cB	841	CLA	O2D-CGD-CBD	4.29	118.88	111.27
10	cA	828	CLA	C3C-C4C-NC	4.28	115.37	110.57
10	bB	840	CLA	O2D-CGD-CBD	4.28	118.88	111.27
10	bA	808	CLA	C3C-C4C-NC	4.28	115.37	110.57
10	aA	825	CLA	CAA-C2A-C3A	-4.28	101.06	112.78
10	bL	203	CLA	C3D-C4D-ND	4.28	117.16	110.24
10	bA	825	CLA	CAA-C2A-C3A	-4.28	101.06	112.78
10	aB	813	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
10	aA	826	CLA	O2D-CGD-CBD	4.28	118.87	111.27
10	bA	823	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
10	aA	823	CLA	C3D-C2D-C1D	-4.28	99.99	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	827	CLA	C3C-C4C-NC	4.28	115.37	110.57
10	bB	811	CLA	C3C-C4C-NC	4.28	115.37	110.57
10	bA	834	CLA	C3D-C2D-C1D	-4.28	100.00	105.83
10	bA	840	CLA	C3D-C2D-C1D	-4.28	100.00	105.83
10	aA	835	CLA	C3D-C4D-ND	4.28	117.15	110.24
10	bB	837	CLA	C3C-C4C-NC	4.27	115.36	110.57
10	cA	825	CLA	CAA-C2A-C3A	-4.27	101.07	112.78
10	cA	841	CLA	C4A-NA-C1A	-4.27	104.78	106.71
10	aB	809	CLA	C4A-NA-C1A	-4.27	104.79	106.71
10	cA	823	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
10	cA	826	CLA	O2D-CGD-CBD	4.27	118.85	111.27
10	cA	840	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
10	cA	820	CLA	C3D-C4D-ND	4.27	117.14	110.24
10	bB	803	CLA	CAA-C2A-C3A	-4.27	101.09	112.78
10	bB	813	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
10	aA	820	CLA	C3D-C4D-ND	4.27	117.14	110.24
10	cA	806	CLA	C3D-C4D-ND	4.26	117.13	110.24
10	bA	806	CLA	C3D-C4D-ND	4.26	117.13	110.24
10	cB	809	CLA	C4A-NA-C1A	-4.26	104.79	106.71
10	bB	838	CLA	C3D-C4D-ND	4.26	117.13	110.24
10	cB	803	CLA	CAA-C2A-C3A	-4.26	101.11	112.78
10	cA	840	CLA	C3D-C4D-ND	4.26	117.13	110.24
10	cL	203	CLA	C3D-C4D-ND	4.26	117.13	110.24
10	bA	826	CLA	O2D-CGD-CBD	4.26	118.83	111.27
10	aA	843	CLA	C3D-C4D-ND	4.26	117.12	110.24
10	cB	813	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
10	cB	809	CLA	C3C-C4C-NC	4.26	115.34	110.57
10	cA	837	CLA	C4A-NA-C1A	-4.26	104.79	106.71
10	aB	827	CLA	C3C-C4C-NC	4.26	115.34	110.57
10	aB	809	CLA	C3C-C4C-NC	4.25	115.34	110.57
10	bB	827	CLA	C3C-C4C-NC	4.25	115.34	110.57
10	aB	803	CLA	CAA-C2A-C3A	-4.25	101.13	112.78
10	bA	843	CLA	C3D-C4D-ND	4.25	117.12	110.24
10	aA	830	CLA	C4A-NA-C1A	-4.25	104.79	106.71
10	aA	834	CLA	C3D-C4D-ND	4.25	117.11	110.24
10	bA	808	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
10	aB	811	CLA	C3C-C4C-NC	4.25	115.33	110.57
10	aA	840	CLA	C3D-C2D-C1D	-4.25	100.04	105.83
10	aA	806	CLA	C3D-C4D-ND	4.25	117.11	110.24
10	bA	819	CLA	C3D-C2D-C1D	-4.25	100.04	105.83
10	bB	834	CLA	O2D-CGD-CBD	4.24	118.81	111.27
10	bA	805	CLA	C4A-NA-C1A	-4.24	104.80	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	841	CLA	C4A-NA-C1A	-4.24	104.80	106.71
10	cA	835	CLA	C3D-C4D-ND	4.24	117.10	110.24
10	aA	840	CLA	C3D-C4D-ND	4.24	117.10	110.24
10	cA	819	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
10	bA	820	CLA	C3D-C4D-ND	4.24	117.10	110.24
10	bA	834	CLA	C3D-C4D-ND	4.24	117.09	110.24
10	cB	827	CLA	C3C-C4C-NC	4.24	115.32	110.57
10	aA	808	CLA	C3D-C2D-C1D	-4.23	100.05	105.83
14	bA	855	LHG	O4-P-O5	4.23	133.18	112.24
10	cA	843	CLA	C3D-C4D-ND	4.23	117.09	110.24
14	cA	855	LHG	O4-P-O5	4.23	133.17	112.24
10	cB	811	CLA	C3C-C4C-NC	4.23	115.32	110.57
10	cA	834	CLA	C3D-C4D-ND	4.23	117.08	110.24
10	bA	835	CLA	C3D-C4D-ND	4.23	117.08	110.24
10	aA	817	CLA	O2D-CGD-CBD	4.23	118.78	111.27
10	aB	807	CLA	C3D-C4D-ND	4.23	117.07	110.24
14	aA	855	LHG	O4-P-O5	4.22	133.12	112.24
10	bB	806	CLA	C3C-C4C-NC	4.22	115.31	110.57
10	aA	804	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
10	cA	854	CLA	C3D-C4D-ND	4.22	117.06	110.24
10	aA	837	CLA	C4A-NA-C1A	-4.22	104.81	106.71
10	aB	806	CLA	C3C-C4C-NC	4.22	115.30	110.57
10	cA	817	CLA	O2D-CGD-CBD	4.22	118.76	111.27
10	aB	820	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
10	bB	820	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
10	cB	834	CLA	O2D-CGD-CBD	4.21	118.76	111.27
10	cA	808	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
10	aA	819	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
10	bA	808	CLA	C3D-C4D-ND	4.21	117.05	110.24
10	bA	837	CLA	C4A-NA-C1A	-4.21	104.81	106.71
10	aB	834	CLA	O2D-CGD-CBD	4.21	118.75	111.27
10	aB	837	CLA	C3C-C4C-NC	4.21	115.29	110.57
10	bA	840	CLA	C3D-C4D-ND	4.21	117.05	110.24
10	bA	817	CLA	O2D-CGD-CBD	4.21	118.74	111.27
10	cB	824	CLA	O2D-CGD-CBD	4.20	118.74	111.27
10	aA	821	CLA	C4A-NA-C1A	-4.20	104.82	106.71
10	bB	805	CLA	CHD-C4C-C3C	-4.20	118.66	124.84
10	bA	842	CLA	C3D-C4D-ND	4.20	117.03	110.24
10	bB	811	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
10	cB	811	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
10	aB	805	CLA	CHD-C4C-C3C	-4.20	118.67	124.84
10	cB	806	CLA	C3C-C4C-NC	4.20	115.28	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	854	CLA	C3D-C4D-ND	4.19	117.02	110.24
10	aB	818	CLA	C3D-C4D-ND	4.19	117.02	110.24
10	cA	808	CLA	C3D-C4D-ND	4.19	117.02	110.24
10	cB	820	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
10	cB	807	CLA	C3D-C4D-ND	4.19	117.02	110.24
10	bB	818	CLA	C3D-C4D-ND	4.19	117.01	110.24
10	aB	811	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
10	aB	822	CLA	C3D-C4D-ND	4.19	117.01	110.24
10	aA	854	CLA	C3C-C4C-NC	4.19	115.27	110.57
10	aA	808	CLA	C3D-C4D-ND	4.19	117.01	110.24
10	cB	818	CLA	C3D-C4D-ND	4.19	117.01	110.24
10	aB	824	CLA	O2D-CGD-CBD	4.19	118.71	111.27
10	bB	824	CLA	O2D-CGD-CBD	4.19	118.70	111.27
10	aA	841	CLA	C4A-NA-C1A	-4.18	104.83	106.71
10	aA	856	CLA	C4A-NA-C1A	-4.18	104.83	106.71
10	cB	811	CLA	C4A-NA-C1A	-4.18	104.83	106.71
10	cB	822	CLA	C3D-C4D-ND	4.18	117.01	110.24
10	cA	804	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
10	bB	807	CLA	C3D-C4D-ND	4.18	117.00	110.24
10	aA	805	CLA	C4A-NA-C1A	-4.18	104.83	106.71
10	bB	835	CLA	C4A-NA-C1A	-4.18	104.83	106.71
10	aB	803	CLA	O2D-CGD-CBD	4.18	118.69	111.27
10	bB	822	CLA	C3D-C4D-ND	4.18	117.00	110.24
10	bB	839	CLA	C3D-C4D-ND	4.17	116.99	110.24
14	aA	852	LHG	O4-P-O5	4.17	132.87	112.24
10	bA	854	CLA	C3C-C4C-NC	4.17	115.25	110.57
10	bB	808	CLA	C3C-C4C-NC	4.17	115.25	110.57
10	aA	842	CLA	C3D-C4D-ND	4.17	116.99	110.24
10	bA	823	CLA	O2D-CGD-CBD	4.17	118.68	111.27
10	aB	829	CLA	C3D-C4D-ND	4.17	116.98	110.24
10	aB	837	CLA	C3D-C4D-ND	4.17	116.98	110.24
10	cB	833	CLA	C3D-C4D-ND	4.17	116.98	110.24
10	cB	805	CLA	CHD-C4C-C3C	-4.17	118.71	124.84
10	aB	839	CLA	C3D-C4D-ND	4.17	116.98	110.24
14	cA	852	LHG	O4-P-O5	4.17	132.84	112.24
10	aB	838	CLA	C4A-NA-C1A	-4.17	104.83	106.71
10	cA	856	CLA	C4A-NA-C1A	-4.17	104.83	106.71
14	bA	852	LHG	O4-P-O5	4.17	132.83	112.24
10	aA	816	CLA	C3C-C4C-NC	4.16	115.24	110.57
10	cA	854	CLA	C3C-C4C-NC	4.16	115.24	110.57
10	cA	808	CLA	C1D-CHD-C4C	-4.16	117.08	126.06
10	cA	816	CLA	C3C-C4C-NC	4.16	115.24	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	803	CLA	O2D-CGD-CBD	4.16	118.66	111.27
10	cB	829	CLA	C3D-C4D-ND	4.16	116.97	110.24
10	bA	854	CLA	C3D-C4D-ND	4.16	116.97	110.24
10	cA	823	CLA	O2D-CGD-CBD	4.16	118.66	111.27
10	aA	830	CLA	C3D-C4D-ND	4.16	116.96	110.24
10	cB	808	CLA	C3C-C4C-NC	4.16	115.23	110.57
10	bA	804	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
10	cA	842	CLA	C3D-C4D-ND	4.16	116.96	110.24
10	cB	803	CLA	O2D-CGD-CBD	4.15	118.65	111.27
10	aB	808	CLA	C3C-C4C-NC	4.15	115.23	110.57
10	bA	811	CLA	C3D-C4D-ND	4.15	116.96	110.24
10	aA	823	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
10	cB	839	CLA	C3D-C4D-ND	4.15	116.95	110.24
10	aA	823	CLA	O2D-CGD-CBD	4.15	118.64	111.27
10	aB	833	CLA	C3D-C4D-ND	4.15	116.95	110.24
10	cB	832	CLA	C3D-C4D-ND	4.15	116.95	110.24
10	bB	829	CLA	C3D-C4D-ND	4.15	116.95	110.24
10	cA	811	CLA	C3D-C4D-ND	4.15	116.95	110.24
10	bA	824	CLA	C3C-C4C-NC	4.15	115.22	110.57
10	cA	830	CLA	C3D-C4D-ND	4.14	116.94	110.24
10	bB	833	CLA	C3D-C4D-ND	4.14	116.94	110.24
10	cB	835	CLA	C4A-NA-C1A	-4.14	104.84	106.71
10	bA	830	CLA	C3D-C4D-ND	4.14	116.93	110.24
10	bA	823	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
10	aA	811	CLA	C3D-C4D-ND	4.14	116.93	110.24
10	bA	808	CLA	C1D-CHD-C4C	-4.14	117.14	126.06
10	bB	837	CLA	C3D-C4D-ND	4.14	116.93	110.24
10	cA	818	CLA	C3D-C4D-ND	4.14	116.93	110.24
10	cB	837	CLA	C3D-C4D-ND	4.13	116.93	110.24
10	bA	818	CLA	C3D-C4D-ND	4.13	116.92	110.24
10	aA	808	CLA	C1D-CHD-C4C	-4.13	117.15	126.06
10	bA	856	CLA	C4A-NA-C1A	-4.13	104.85	106.71
10	aA	824	CLA	C3C-C4C-NC	4.13	115.20	110.57
10	cA	821	CLA	C4A-NA-C1A	-4.13	104.85	106.71
10	aA	837	CLA	C3D-C4D-ND	4.13	116.92	110.24
10	aB	832	CLA	C3D-C4D-ND	4.13	116.92	110.24
10	aB	821	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
10	cB	838	CLA	C4A-NA-C1A	-4.13	104.85	106.71
10	cA	831	CLA	C3C-C4C-NC	4.13	115.20	110.57
10	aA	818	CLA	C3D-C4D-ND	4.13	116.91	110.24
10	bA	809	CLA	C3D-C4D-ND	4.12	116.91	110.24
10	cB	810	CLA	C3C-C4C-NC	4.12	115.19	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	821	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
10	cB	830	CLA	C3D-C4D-ND	4.12	116.90	110.24
10	cB	815	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
10	aA	818	CLA	CAA-C2A-C3A	-4.12	101.50	112.78
10	bA	821	CLA	C4A-NA-C1A	-4.12	104.86	106.71
10	bB	832	CLA	C3D-C4D-ND	4.12	116.90	110.24
10	bB	809	CLA	C3D-C4D-ND	4.12	116.90	110.24
10	bB	830	CLA	C3D-C4D-ND	4.12	116.90	110.24
10	bA	836	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
10	bA	824	CLA	CAC-C3C-C4C	4.11	130.15	124.81
10	bA	818	CLA	CAA-C2A-C3A	-4.11	101.52	112.78
10	cA	809	CLA	C3D-C4D-ND	4.11	116.89	110.24
10	bB	838	CLA	C4A-NA-C1A	-4.11	104.86	106.71
10	aB	815	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
10	cB	821	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
10	aB	809	CLA	C3D-C4D-ND	4.11	116.89	110.24
10	cA	837	CLA	C3D-C4D-ND	4.11	116.89	110.24
10	cA	836	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
10	bB	836	CLA	C3D-C4D-ND	4.11	116.88	110.24
10	bA	833	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
10	aB	802	CLA	CMD-C2D-C1D	4.11	131.95	124.71
10	cA	824	CLA	C3C-C4C-NC	4.11	115.18	110.57
10	cB	809	CLA	C3D-C4D-ND	4.11	116.88	110.24
10	cA	818	CLA	CAA-C2A-C3A	-4.11	101.53	112.78
10	aB	810	CLA	C3C-C4C-NC	4.11	115.18	110.57
10	aA	809	CLA	C3D-C4D-ND	4.11	116.88	110.24
10	aA	839	CLA	C3D-C4D-ND	4.11	116.88	110.24
10	aB	836	CLA	C3D-C4D-ND	4.11	116.88	110.24
10	bB	802	CLA	CMD-C2D-C1D	4.11	131.95	124.71
10	aB	824	CLA	C3D-C4D-ND	4.10	116.88	110.24
10	bA	837	CLA	C3D-C4D-ND	4.10	116.88	110.24
10	aA	831	CLA	C3C-C4C-NC	4.10	115.17	110.57
10	aB	816	CLA	C3C-C4C-NC	4.10	115.17	110.57
10	aB	817	CLA	O2D-CGD-CBD	4.10	118.56	111.27
10	cB	802	CLA	CMD-C2D-C1D	4.10	131.94	124.71
10	cA	835	CLA	C3D-C2D-C1D	-4.10	100.23	105.83
10	bA	831	CLA	C3C-C4C-NC	4.10	115.17	110.57
10	bA	816	CLA	C3C-C4C-NC	4.10	115.17	110.57
10	cA	833	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
10	cB	816	CLA	C3C-C4C-NC	4.10	115.17	110.57
10	aB	829	CLA	O2D-CGD-CBD	4.10	118.55	111.27
10	bB	815	CLA	C3D-C2D-C1D	-4.10	100.24	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	824	CLA	CAC-C3C-C4C	4.09	130.12	124.81
10	cB	836	CLA	C3D-C4D-ND	4.09	116.86	110.24
10	bA	839	CLA	C3D-C4D-ND	4.09	116.86	110.24
10	cA	817	CLA	C4A-NA-C1A	-4.09	104.87	106.71
10	bB	817	CLA	O2D-CGD-CBD	4.09	118.54	111.27
10	cA	823	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
10	bB	811	CLA	C4A-NA-C1A	-4.09	104.87	106.71
10	aA	833	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
10	aA	825	CLA	C3C-C4C-NC	4.09	115.16	110.57
10	aB	830	CLA	C3D-C4D-ND	4.09	116.85	110.24
10	bA	825	CLA	C3C-C4C-NC	4.09	115.15	110.57
10	aB	830	CLA	C3B-C4B-NB	4.09	114.49	109.21
10	cA	809	CLA	C1D-CHD-C4C	-4.09	117.24	126.06
10	bA	835	CLA	C3D-C2D-C1D	-4.09	100.26	105.83
10	cB	817	CLA	O2D-CGD-CBD	4.09	118.53	111.27
10	bB	824	CLA	C3D-C4D-ND	4.08	116.84	110.24
10	cA	816	CLA	C3D-C4D-ND	4.08	116.84	110.24
10	aB	826	CLA	C3D-C4D-ND	4.08	116.84	110.24
10	cB	824	CLA	C3D-C4D-ND	4.08	116.84	110.24
10	aA	836	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
10	aA	824	CLA	CAC-C3C-C4C	4.08	130.10	124.81
10	bB	829	CLA	O2D-CGD-CBD	4.08	118.51	111.27
10	bA	840	CLA	C3C-C4C-NC	4.07	115.14	110.57
10	bB	810	CLA	C3C-C4C-NC	4.07	115.14	110.57
10	aA	817	CLA	C4A-NA-C1A	-4.07	104.87	106.71
10	cB	830	CLA	C3B-C4B-NB	4.07	114.48	109.21
10	bB	826	CLA	C3D-C4D-ND	4.07	116.83	110.24
10	bB	816	CLA	C3C-C4C-NC	4.07	115.14	110.57
10	bB	830	CLA	C3B-C4B-NB	4.07	114.48	109.21
10	aA	819	CLA	C3D-C4D-ND	4.07	116.83	110.24
10	bA	821	CLA	C3C-C4C-NC	4.07	115.14	110.57
10	cB	829	CLA	O2D-CGD-CBD	4.07	118.50	111.27
10	cB	814	CLA	C3D-C4D-ND	4.07	116.83	110.24
10	aA	829	CLA	C3B-C4B-NB	4.07	114.47	109.21
10	cA	839	CLA	C3D-C4D-ND	4.07	116.82	110.24
10	cA	840	CLA	C3C-C4C-NC	4.07	115.13	110.57
10	bA	816	CLA	C3D-C4D-ND	4.07	116.82	110.24
10	bB	805	CLA	C4C-C3C-C2C	-4.06	100.97	106.90
10	cA	829	CLA	C3B-C4B-NB	4.06	114.46	109.21
10	aB	803	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
10	bB	803	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
10	bB	812	CLA	C3D-C4D-ND	4.06	116.80	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	826	CLA	C3D-C4D-ND	4.06	116.80	110.24
10	bA	841	CLA	C3C-C4C-NC	4.06	115.12	110.57
10	bA	828	CLA	CMB-C2B-C3B	4.06	132.27	124.68
10	aB	805	CLA	C2C-C1C-NC	4.06	113.77	109.97
10	bA	809	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
10	aA	816	CLA	C3D-C4D-ND	4.06	116.80	110.24
10	aB	814	CLA	C3D-C4D-ND	4.06	116.80	110.24
10	cA	819	CLA	C3D-C4D-ND	4.06	116.80	110.24
10	cA	838	CLA	C3D-C4D-ND	4.06	116.80	110.24
10	aA	835	CLA	C3D-C2D-C1D	-4.06	100.30	105.83
10	bA	802	CLA	C3C-C4C-NC	4.06	115.12	110.57
10	aA	838	CLA	C3D-C4D-ND	4.06	116.80	110.24
10	aB	841	CLA	C3D-C4D-ND	4.06	116.80	110.24
10	cB	803	CLA	C1D-CHD-C4C	-4.05	117.31	126.06
10	cB	805	CLA	C4C-C3C-C2C	-4.05	100.99	106.90
10	bB	841	CLA	C3D-C4D-ND	4.05	116.79	110.24
10	bA	829	CLA	C4A-NA-C1A	-4.05	104.88	106.71
10	cB	835	CLA	O2D-CGD-CBD	4.05	118.47	111.27
10	aB	812	CLA	C3D-C4D-ND	4.05	116.79	110.24
10	bA	832	CLA	C3D-C4D-ND	4.05	116.79	110.24
10	bA	821	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
10	bB	814	CLA	C3D-C4D-ND	4.05	116.79	110.24
10	cA	832	CLA	C3D-C4D-ND	4.05	116.79	110.24
10	cA	832	CLA	C3C-C4C-NC	4.05	115.11	110.57
10	cA	828	CLA	CMB-C2B-C3B	4.05	132.25	124.68
10	aA	828	CLA	CMB-C2B-C3B	4.05	132.25	124.68
10	cA	825	CLA	C3C-C4C-NC	4.05	115.11	110.57
10	bA	838	CLA	C3D-C4D-ND	4.05	116.78	110.24
9	aA	801	CL0	CHD-C1D-ND	-4.05	120.74	124.45
10	aA	809	CLA	C1D-CHD-C4C	-4.04	117.33	126.06
10	cB	841	CLA	C3D-C4D-ND	4.04	116.78	110.24
10	cB	812	CLA	C3D-C4D-ND	4.04	116.78	110.24
10	bA	829	CLA	C3B-C4B-NB	4.04	114.44	109.21
10	bA	819	CLA	C3D-C4D-ND	4.04	116.78	110.24
10	aA	832	CLA	C3C-C4C-NC	4.04	115.10	110.57
10	bA	832	CLA	C3C-C4C-NC	4.04	115.10	110.57
10	aA	832	CLA	C3D-C4D-ND	4.04	116.77	110.24
10	cB	815	CLA	C3D-C4D-ND	4.04	116.77	110.24
10	aB	805	CLA	C4C-C3C-C2C	-4.04	101.01	106.90
10	aB	835	CLA	C4A-NA-C1A	-4.04	104.89	106.71
10	cA	821	CLA	C3C-C4C-NC	4.04	115.10	110.57
10	cA	838	CLA	C3C-C4C-NC	4.03	115.10	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	829	CLA	C4A-NA-C1A	-4.03	104.89	106.71
10	aA	838	CLA	C3C-C4C-NC	4.03	115.09	110.57
10	bA	838	CLA	C3C-C4C-NC	4.03	115.09	110.57
10	cA	802	CLA	C3C-C4C-NC	4.03	115.09	110.57
10	aB	835	CLA	O2D-CGD-CBD	4.03	118.43	111.27
10	aA	821	CLA	C3C-C4C-NC	4.03	115.09	110.57
10	bA	817	CLA	C4A-NA-C1A	-4.03	104.89	106.71
10	cB	821	CLA	C3D-C4D-ND	4.03	116.75	110.24
10	aA	840	CLA	C3C-C4C-NC	4.03	115.09	110.57
10	aB	821	CLA	C3D-C4D-ND	4.02	116.75	110.24
10	cA	823	CLA	C3D-C4D-ND	4.02	116.75	110.24
10	bB	805	CLA	C2C-C1C-NC	4.02	113.74	109.97
10	bB	815	CLA	C3D-C4D-ND	4.02	116.74	110.24
10	cA	817	CLA	C3D-C4D-ND	4.02	116.74	110.24
10	cA	819	CLA	C3C-C4C-NC	4.02	115.08	110.57
10	cA	841	CLA	C3C-C4C-NC	4.02	115.08	110.57
9	cA	801	CL0	CHD-C1D-ND	-4.02	120.76	124.45
10	aA	841	CLA	C3C-C4C-NC	4.02	115.08	110.57
10	bA	817	CLA	C3D-C4D-ND	4.02	116.74	110.24
10	bB	835	CLA	O2D-CGD-CBD	4.02	118.41	111.27
10	bA	829	CLA	C3D-C4D-ND	4.02	116.73	110.24
10	aA	837	CLA	C3C-C4C-NC	4.02	115.08	110.57
10	cB	805	CLA	C2C-C1C-NC	4.02	113.73	109.97
10	cA	834	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
10	aA	814	CLA	C3C-C4C-NC	4.01	115.07	110.57
10	aA	817	CLA	C3D-C4D-ND	4.01	116.73	110.24
10	aA	802	CLA	C3C-C4C-NC	4.01	115.07	110.57
10	bA	823	CLA	C3D-C4D-ND	4.01	116.73	110.24
10	bA	836	CLA	C3C-C4C-NC	4.01	115.07	110.57
10	aA	834	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
10	aA	819	CLA	C3C-C4C-NC	4.01	115.07	110.57
10	cA	818	CLA	CMB-C2B-C3B	4.01	132.18	124.68
10	cA	837	CLA	C3C-C4C-NC	4.01	115.07	110.57
10	aA	802	CLA	C3D-C4D-ND	4.01	116.72	110.24
10	cA	821	CLA	C1C-C2C-C3C	-4.01	102.75	106.96
10	aB	815	CLA	C3D-C4D-ND	4.01	116.72	110.24
10	bA	837	CLA	C3C-C4C-NC	4.00	115.06	110.57
10	cA	829	CLA	C3D-C4D-ND	4.00	116.71	110.24
10	cA	814	CLA	C3C-C4C-NC	4.00	115.06	110.57
10	bA	814	CLA	C3D-C4D-ND	4.00	116.71	110.24
10	bB	821	CLA	C3C-C4C-NC	4.00	115.06	110.57
10	aA	805	CLA	C3D-C4D-ND	4.00	116.71	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	818	CLA	CMB-C2B-C3B	4.00	132.16	124.68
10	bB	810	CLA	CAA-C2A-C3A	-4.00	101.83	112.78
10	bA	814	CLA	C3C-C4C-NC	4.00	115.05	110.57
10	bA	815	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
10	bA	836	CLA	CMB-C2B-C3B	4.00	132.15	124.68
10	aB	810	CLA	CAA-C2A-C3A	-3.99	101.84	112.78
10	bA	802	CLA	C3D-C4D-ND	3.99	116.70	110.24
10	cA	814	CLA	C3D-C4D-ND	3.99	116.70	110.24
10	aA	814	CLA	C3D-C4D-ND	3.99	116.70	110.24
10	cA	831	CLA	C3D-C4D-ND	3.99	116.70	110.24
10	aB	811	CLA	C4A-NA-C1A	-3.99	104.91	106.71
10	cB	823	CLA	C3D-C4D-ND	3.99	116.69	110.24
10	cB	821	CLA	C3C-C4C-NC	3.99	115.05	110.57
10	aA	823	CLA	C3D-C4D-ND	3.99	116.69	110.24
10	aA	818	CLA	O2A-CGA-CBA	3.99	124.42	111.91
10	cB	810	CLA	CAA-C2A-C3A	-3.99	101.86	112.78
9	bA	801	CL0	CHD-C1D-ND	-3.99	120.79	124.45
10	bA	834	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
10	cA	818	CLA	O2A-CGA-CBA	3.99	124.42	111.91
10	bA	831	CLA	C3D-C4D-ND	3.99	116.69	110.24
10	bB	821	CLA	C3D-C4D-ND	3.99	116.69	110.24
10	bA	818	CLA	CMB-C2B-C3B	3.99	132.14	124.68
10	aA	829	CLA	C3D-C4D-ND	3.99	116.69	110.24
10	cA	805	CLA	C3D-C4D-ND	3.99	116.69	110.24
10	cA	829	CLA	C4A-NA-C1A	-3.99	104.91	106.71
10	aA	821	CLA	C1C-C2C-C3C	-3.99	102.77	106.96
10	bA	818	CLA	O2A-CGA-CBA	3.99	124.42	111.91
10	aA	839	CLA	O2D-CGD-CBD	3.98	118.35	111.27
10	cB	815	CLA	C1D-CHD-C4C	-3.98	117.46	126.06
10	cA	802	CLA	C3D-C4D-ND	3.98	116.68	110.24
10	aB	831	CLA	C3D-C4D-ND	3.98	116.68	110.24
10	aA	833	CLA	C3D-C4D-ND	3.98	116.68	110.24
10	bA	833	CLA	C3D-C4D-ND	3.98	116.68	110.24
10	bB	823	CLA	C3D-C4D-ND	3.98	116.67	110.24
10	aB	821	CLA	C3C-C4C-NC	3.98	115.03	110.57
10	bA	809	CLA	C3C-C4C-NC	3.98	115.03	110.57
10	bA	821	CLA	C3D-C4D-ND	3.98	116.67	110.24
10	bA	841	CLA	C3D-C4D-ND	3.98	116.67	110.24
10	cA	809	CLA	C3C-C4C-NC	3.97	115.03	110.57
10	cA	836	CLA	C3C-C4C-NC	3.97	115.03	110.57
10	cA	828	CLA	C1D-CHD-C4C	-3.97	117.49	126.06
10	bA	819	CLA	C3C-C4C-NC	3.97	115.03	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	836	CLA	C3C-C4C-NC	3.97	115.02	110.57
10	aL	202	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
10	bA	805	CLA	C3D-C4D-ND	3.97	116.66	110.24
10	aA	810	CLA	C3D-C4D-ND	3.97	116.66	110.24
10	aA	831	CLA	C3D-C4D-ND	3.97	116.66	110.24
10	cA	827	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
10	bA	828	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
10	cA	830	CLA	C3C-C4C-NC	3.97	115.02	110.57
10	bB	829	CLA	CHD-C1D-ND	-3.97	120.81	124.45
10	aA	836	CLA	CMB-C2B-C3B	3.96	132.10	124.68
10	aB	803	CLA	CMA-C3A-C2A	-3.96	97.83	113.83
10	aA	803	CLA	C3D-C4D-ND	3.96	116.65	110.24
10	cB	831	CLA	C3D-C4D-ND	3.96	116.65	110.24
10	bA	827	CLA	C1D-CHD-C4C	-3.96	117.51	126.06
10	aA	809	CLA	C3C-C4C-NC	3.96	115.01	110.57
10	cA	833	CLA	C3D-C4D-ND	3.96	116.64	110.24
10	bB	815	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
10	cA	821	CLA	C3D-C4D-ND	3.96	116.64	110.24
10	bL	202	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
10	bA	803	CLA	C3D-C4D-ND	3.96	116.64	110.24
10	cA	839	CLA	O2D-CGD-CBD	3.96	118.30	111.27
10	aA	834	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
10	cA	834	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
10	aA	830	CLA	C3C-C4C-NC	3.96	115.01	110.57
10	aA	827	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
10	cA	836	CLA	CMB-C2B-C3B	3.96	132.08	124.68
10	bA	822	CLA	C4-C3-C5	3.96	120.50	115.98
10	cB	803	CLA	CMA-C3A-C2A	-3.95	97.87	113.83
10	aA	821	CLA	C3D-C4D-ND	3.95	116.64	110.24
10	aA	836	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
10	aA	841	CLA	C3D-C4D-ND	3.95	116.63	110.24
10	bB	803	CLA	CMA-C3A-C2A	-3.95	97.89	113.83
10	aA	828	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
10	cL	202	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
10	cA	810	CLA	C3D-C4D-ND	3.95	116.63	110.24
10	cB	802	CLA	C3D-C4D-ND	3.95	116.63	110.24
10	bB	810	CLA	C3D-C4D-ND	3.95	116.63	110.24
10	aA	816	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
10	bA	834	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
10	bA	830	CLA	C3C-C4C-NC	3.95	115.00	110.57
10	cB	825	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
10	bA	839	CLA	O2D-CGD-CBD	3.95	118.28	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	823	CLA	C3D-C4D-ND	3.95	116.62	110.24
10	aA	815	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
10	bB	825	CLA	C1D-CHD-C4C	-3.94	117.55	126.06
10	bB	837	CLA	C1D-CHD-C4C	-3.94	117.55	126.06
10	aB	810	CLA	C3D-C4D-ND	3.94	116.62	110.24
10	aB	815	CLA	C1D-CHD-C4C	-3.94	117.55	126.06
10	bA	805	CLA	C3C-C4C-NC	3.94	114.99	110.57
10	cA	836	CLA	C1D-CHD-C4C	-3.94	117.55	126.06
10	bA	834	CLA	C3C-C4C-NC	3.94	114.99	110.57
10	cB	837	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
10	bB	801	CLA	C3D-C4D-ND	3.94	116.61	110.24
10	bA	810	CLA	C3D-C4D-ND	3.94	116.61	110.24
10	aA	813	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
10	bA	803	CLA	C3C-C4C-NC	3.94	114.99	110.57
10	bB	806	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
10	cA	813	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
10	cB	824	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
10	cB	808	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
10	cA	816	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
10	bB	835	CLA	C3D-C4D-ND	3.94	116.61	110.24
10	cB	801	CLA	C3D-C4D-ND	3.94	116.61	110.24
10	aB	808	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
10	aB	817	CLA	C3D-C4D-ND	3.94	116.61	110.24
10	bA	813	CLA	C3D-C4D-ND	3.94	116.61	110.24
10	aB	806	CLA	C3D-C4D-ND	3.94	116.61	110.24
10	aA	813	CLA	C3D-C4D-ND	3.94	116.60	110.24
10	cA	841	CLA	C3D-C4D-ND	3.94	116.60	110.24
10	aA	805	CLA	C3C-C4C-NC	3.93	114.98	110.57
10	cA	810	CLA	C3C-C4C-NC	3.93	114.98	110.57
10	cB	829	CLA	CHD-C1D-ND	-3.93	120.84	124.45
10	bB	831	CLA	C3D-C4D-ND	3.93	116.60	110.24
10	bA	813	CLA	C1D-CHD-C4C	-3.93	117.57	126.06
10	cA	834	CLA	C3C-C4C-NC	3.93	114.98	110.57
10	aB	821	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
9	cA	801	CL0	C3D-C4D-ND	3.93	116.60	110.24
10	cB	836	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
10	aB	825	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
10	bB	832	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
10	aB	837	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
10	cA	815	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
10	bA	816	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
9	bA	801	CL0	C3D-C4D-ND	3.93	116.59	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	803	CLA	C3C-C4C-NC	3.93	114.98	110.57
10	aB	836	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
10	cB	821	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
10	cB	806	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
10	bB	802	CLA	C3D-C4D-ND	3.93	116.59	110.24
10	cB	815	CLA	C3C-C4C-NC	3.93	114.97	110.57
10	aB	801	CLA	C3D-C4D-ND	3.93	116.59	110.24
10	aB	806	CLA	C1D-CHD-C4C	-3.93	117.59	126.06
10	bA	836	CLA	C1D-CHD-C4C	-3.93	117.59	126.06
10	aA	818	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
10	aB	818	CLA	CAA-C2A-C3A	-3.92	102.03	112.78
10	bA	824	CLA	C3D-C4D-ND	3.92	116.59	110.24
10	cA	803	CLA	C3D-C4D-ND	3.92	116.59	110.24
10	cA	805	CLA	C3C-C4C-NC	3.92	114.97	110.57
10	aB	802	CLA	C3D-C4D-ND	3.92	116.58	110.24
10	bA	810	CLA	C3C-C4C-NC	3.92	114.97	110.57
10	bB	815	CLA	C3C-C4C-NC	3.92	114.97	110.57
10	aA	843	CLA	C3C-C4C-NC	3.92	114.97	110.57
10	aA	856	CLA	C3D-C4D-ND	3.92	116.58	110.24
10	aB	815	CLA	C3C-C4C-NC	3.92	114.97	110.57
10	cB	817	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
10	cB	801	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
10	bB	818	CLA	CAA-C2A-C3A	-3.92	102.05	112.78
10	bA	813	CLA	C3B-C4B-NB	3.92	114.27	109.21
10	cB	810	CLA	C3D-C4D-ND	3.92	116.57	110.24
10	aA	813	CLA	C3B-C4B-NB	3.92	114.27	109.21
9	aA	801	CL0	C3D-C4D-ND	3.92	116.57	110.24
10	cB	835	CLA	C3D-C4D-ND	3.92	116.57	110.24
10	bB	817	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
10	aA	822	CLA	C4-C3-C5	3.91	120.46	115.98
10	bA	821	CLA	C1D-CHD-C4C	-3.91	117.61	126.06
10	bA	818	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
10	bB	817	CLA	C3D-C4D-ND	3.91	116.57	110.24
10	cB	818	CLA	CAA-C2A-C3A	-3.91	102.06	112.78
10	bB	808	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
10	aA	811	CLA	C3C-C4C-NC	3.91	114.96	110.57
10	aB	801	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
10	cA	832	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
10	cB	817	CLA	C3D-C4D-ND	3.91	116.57	110.24
10	bA	814	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
10	cA	813	CLA	C3D-C4D-ND	3.91	116.57	110.24
10	bB	806	CLA	C3D-C4D-ND	3.91	116.56	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	831	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
10	cB	832	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
10	cB	816	CLA	C3D-C4D-ND	3.91	116.56	110.24
10	bB	821	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
10	cA	822	CLA	C4-C3-C5	3.90	120.45	115.98
10	bB	824	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
10	aA	821	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
10	aA	836	CLA	C3B-C4B-NB	3.90	114.26	109.21
10	aA	816	CLA	C4A-NA-C1A	-3.90	104.95	106.71
10	cA	818	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
10	aA	802	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
10	aA	854	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
9	bA	801	CL0	C3D-C2D-C1D	-3.90	100.51	105.83
10	aB	817	CLA	C4A-NA-C1A	-3.90	104.95	106.71
10	aB	810	CLA	C3D-C2D-C1D	-3.90	100.51	105.83
10	aB	835	CLA	C3D-C4D-ND	3.90	116.55	110.24
10	aB	829	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
10	cA	821	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
10	aB	832	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
10	cB	813	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
10	aA	814	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
10	cB	810	CLA	C3D-C2D-C1D	-3.90	100.51	105.83
10	bB	816	CLA	C3D-C4D-ND	3.90	116.54	110.24
10	cB	840	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
10	bB	840	CLA	C1D-CHD-C4C	-3.90	117.66	126.06
10	aA	820	CLA	C4A-NA-C1A	-3.89	104.95	106.71
10	aB	803	CLA	C3D-C4D-ND	3.89	116.54	110.24
10	cB	803	CLA	C3D-C4D-ND	3.89	116.54	110.24
9	aA	801	CL0	C3D-C2D-C1D	-3.89	100.52	105.83
10	cA	807	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
10	aB	817	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
10	bB	836	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
10	cA	802	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
10	bA	832	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
9	cA	801	CL0	C3D-C2D-C1D	-3.89	100.52	105.83
10	cA	824	CLA	C3D-C4D-ND	3.89	116.53	110.24
10	aA	831	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
10	aA	803	CLA	C3C-C4C-NC	3.89	114.93	110.57
10	cA	813	CLA	C3B-C4B-NB	3.89	114.24	109.21
10	cA	836	CLA	C3B-C4B-NB	3.89	114.24	109.21
10	aB	824	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
10	bA	836	CLA	C3B-C4B-NB	3.89	114.24	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	856	CLA	C3D-C4D-ND	3.89	116.53	110.24
10	cB	806	CLA	C3D-C4D-ND	3.89	116.53	110.24
10	cA	815	CLA	C4A-NA-C1A	-3.89	104.96	106.71
10	bA	854	CLA	C1D-CHD-C4C	-3.89	117.68	126.06
10	cA	854	CLA	C1D-CHD-C4C	-3.89	117.68	126.06
10	bB	803	CLA	C3D-C4D-ND	3.88	116.52	110.24
10	bA	833	CLA	C4A-NA-C1A	-3.88	104.96	106.71
10	aA	825	CLA	C3D-C4D-ND	3.88	116.52	110.24
10	bB	832	CLA	C3C-C4C-NC	3.88	114.92	110.57
10	aB	813	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
10	bA	807	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
10	bB	813	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
10	bB	810	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
10	aA	824	CLA	C3D-C4D-ND	3.88	116.51	110.24
10	cA	814	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
10	aB	816	CLA	C3D-C4D-ND	3.88	116.51	110.24
10	cB	816	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
10	bA	826	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
10	cA	825	CLA	C3D-C4D-ND	3.88	116.51	110.24
10	bA	802	CLA	C1D-CHD-C4C	-3.88	117.70	126.06
10	bB	823	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
10	aB	840	CLA	C1D-CHD-C4C	-3.88	117.70	126.06
10	aA	829	CLA	CMB-C2B-C3B	3.87	131.93	124.68
10	aA	840	CLA	C1D-CHD-C4C	-3.87	117.70	126.06
10	aA	810	CLA	C3C-C4C-NC	3.87	114.92	110.57
9	aA	801	CL0	C3B-C4B-NB	3.87	114.22	109.21
9	bA	801	CL0	C3B-C4B-NB	3.87	114.22	109.21
10	aA	832	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
10	aA	839	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
10	cA	843	CLA	C3C-C4C-NC	3.87	114.91	110.57
10	aB	821	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
10	aA	833	CLA	C4A-NA-C1A	-3.87	104.97	106.71
10	cA	811	CLA	C3C-C4C-NC	3.87	114.91	110.57
10	bB	821	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
10	cA	856	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
10	bA	828	CLA	O2D-CGD-CBD	3.87	118.14	111.27
10	cB	804	CLA	C3D-C4D-ND	3.87	116.49	110.24
10	bB	801	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
10	bA	843	CLA	C3C-C4C-NC	3.86	114.91	110.57
10	aB	804	CLA	C3D-C4D-ND	3.86	116.49	110.24
10	cA	818	CLA	C1D-CHD-C4C	-3.86	117.72	126.06
10	aA	823	CLA	C1D-CHD-C4C	-3.86	117.72	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	cA	801	CL0	C3B-C4B-NB	3.86	114.20	109.21
10	cA	827	CLA	C3D-C4D-ND	3.86	116.48	110.24
10	cA	828	CLA	C3D-C4D-ND	3.86	116.48	110.24
10	aA	834	CLA	C3C-C4C-NC	3.86	114.90	110.57
10	bA	856	CLA	C3D-C4D-ND	3.86	116.48	110.24
10	bA	829	CLA	CMB-C2B-C3B	3.86	131.90	124.68
10	bA	841	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
10	bA	831	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
10	cA	826	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
10	aA	828	CLA	O2D-CGD-CBD	3.86	118.13	111.27
10	bA	856	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
10	cA	839	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
10	bA	828	CLA	C3D-C4D-ND	3.86	116.48	110.24
10	bA	840	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
10	bB	829	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
10	cB	829	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
10	aB	832	CLA	C3C-C4C-NC	3.86	114.90	110.57
10	aB	841	CLA	C3C-C4C-NC	3.86	114.89	110.57
10	bB	841	CLA	C3C-C4C-NC	3.86	114.89	110.57
10	cA	828	CLA	O2D-CGD-CBD	3.86	118.12	111.27
10	aA	826	CLA	C1D-CHD-C4C	-3.85	117.74	126.06
10	bB	807	CLA	C3C-C4C-NC	3.85	114.89	110.57
10	aA	843	CLA	C1C-C2C-C3C	-3.85	102.90	106.96
10	cA	840	CLA	C1D-CHD-C4C	-3.85	117.74	126.06
10	bA	827	CLA	C3D-C4D-ND	3.85	116.47	110.24
10	bA	818	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
10	bB	804	CLA	C3D-C4D-ND	3.85	116.47	110.24
10	aA	841	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
10	bA	825	CLA	C3D-C4D-ND	3.85	116.47	110.24
10	bB	816	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
10	aA	818	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
10	aB	816	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
10	cB	833	CLA	C1D-CHD-C4C	-3.85	117.75	126.06
10	cB	832	CLA	C3C-C4C-NC	3.85	114.89	110.57
10	bA	811	CLA	C3C-C4C-NC	3.85	114.89	110.57
10	cB	807	CLA	C3C-C4C-NC	3.85	114.89	110.57
10	cA	816	CLA	C4A-NA-C1A	-3.85	104.98	106.71
10	cA	823	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
10	cB	821	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
10	cA	829	CLA	CMB-C2B-C3B	3.85	131.87	124.68
10	cB	823	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
10	bA	823	CLA	C1D-CHD-C4C	-3.84	117.77	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	856	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
10	bL	205	CLA	C3C-C4C-NC	3.84	114.88	110.57
10	aB	829	CLA	CHD-C1D-ND	-3.84	120.93	124.45
10	aL	204	CLA	C3C-C4C-NC	3.84	114.87	110.57
10	cB	805	CLA	C3C-C4C-NC	3.84	114.87	110.57
10	aA	827	CLA	C3D-C4D-ND	3.84	116.44	110.24
10	aA	807	CLA	C1C-C2C-C3C	-3.83	102.92	106.96
10	aA	828	CLA	C3D-C4D-ND	3.83	116.44	110.24
10	bA	839	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
10	cA	843	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
10	aB	823	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
10	aB	807	CLA	C3C-C4C-NC	3.83	114.87	110.57
10	bA	830	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
10	cB	814	CLA	C3C-C4C-NC	3.83	114.86	110.57
10	aB	833	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
10	cA	841	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
10	bA	816	CLA	C4A-NA-C1A	-3.83	104.98	106.71
10	bA	843	CLA	C4A-NA-C1A	-3.83	104.98	106.71
10	aA	810	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
10	cL	205	CLA	C3C-C4C-NC	3.83	114.86	110.57
10	aA	838	CLA	CAA-CBA-CGA	-3.83	102.07	113.25
10	bA	807	CLA	C3D-C4D-ND	3.83	116.43	110.24
10	bA	822	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
10	bB	805	CLA	C3D-C4D-ND	3.83	116.43	110.24
10	cA	822	CLA	C1D-CHD-C4C	-3.83	117.81	126.06
10	cA	810	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
10	bA	843	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
10	bL	205	CLA	C4A-NA-C1A	-3.82	104.99	106.71
10	cB	841	CLA	C3C-C4C-NC	3.82	114.86	110.57
10	aB	839	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
10	cA	838	CLA	CAA-CBA-CGA	-3.82	102.08	113.25
10	aB	805	CLA	C3C-C4C-NC	3.82	114.86	110.57
10	cA	837	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
10	cA	830	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
10	bB	833	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
10	bB	841	CLA	C3B-C4B-NB	3.82	114.15	109.21
10	aA	837	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
10	aA	807	CLA	C3D-C4D-ND	3.82	116.42	110.24
10	cA	835	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
10	bA	810	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
10	cB	804	CLA	C1D-CHD-C4C	-3.82	117.83	126.06
10	bA	838	CLA	CAA-CBA-CGA	-3.82	102.10	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	822	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
10	cB	839	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
10	cA	805	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
10	bA	837	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
10	bB	812	CLA	C3C-C4C-NC	3.81	114.84	110.57
10	cL	204	CLA	C3C-C4C-NC	3.81	114.84	110.57
10	aB	814	CLA	C3C-C4C-NC	3.81	114.84	110.57
10	aA	830	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
10	aA	856	CLA	C3C-C4C-NC	3.81	114.84	110.57
10	cA	807	CLA	C3D-C4D-ND	3.81	116.40	110.24
10	bA	820	CLA	C4A-NA-C1A	-3.81	104.99	106.71
10	aB	828	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
10	aA	835	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
10	aB	804	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
10	bL	204	CLA	C3C-C4C-NC	3.81	114.84	110.57
10	cA	856	CLA	C3C-C4C-NC	3.81	114.84	110.57
10	bB	828	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
10	aA	820	CLA	C3C-C4C-NC	3.80	114.84	110.57
10	aB	841	CLA	C3B-C4B-NB	3.80	114.13	109.21
10	cA	820	CLA	C3C-C4C-NC	3.80	114.84	110.57
10	bB	804	CLA	C1D-CHD-C4C	-3.80	117.85	126.06
10	bB	839	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
10	cB	802	CLA	C3C-C4C-NC	3.80	114.83	110.57
10	aL	205	CLA	C3C-C4C-NC	3.80	114.83	110.57
10	bB	805	CLA	C3C-C4C-NC	3.80	114.83	110.57
10	bA	815	CLA	C4A-NA-C1A	-3.80	105.00	106.71
10	cB	817	CLA	C4A-NA-C1A	-3.80	105.00	106.71
10	bB	830	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
10	cB	828	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
10	aB	838	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
10	bB	838	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
10	bB	822	CLA	C3C-C4C-NC	3.79	114.83	110.57
10	cB	829	CLA	C3B-C4B-NB	3.79	114.11	109.21
10	cA	820	CLA	C4A-NA-C1A	-3.79	105.00	106.71
10	aB	805	CLA	C3D-C4D-ND	3.79	116.37	110.24
10	bA	835	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
10	bA	856	CLA	C3C-C4C-NC	3.79	114.82	110.57
10	cA	817	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
10	cA	819	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
10	cB	838	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
10	aA	815	CLA	C4A-NA-C1A	-3.79	105.00	106.71
10	bA	805	CLA	C1C-C2C-C3C	-3.79	102.97	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	812	CLA	C3C-C4C-NC	3.79	114.82	110.57
10	cB	841	CLA	C3B-C4B-NB	3.79	114.11	109.21
10	bB	817	CLA	C3C-C4C-NC	3.79	114.82	110.57
10	bA	817	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
10	bA	808	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
10	aA	813	CLA	C3C-C4C-NC	3.79	114.82	110.57
10	cB	830	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
10	aB	819	CLA	C3D-C4D-ND	3.79	116.36	110.24
10	bB	817	CLA	C4A-NA-C1A	-3.78	105.00	106.71
10	cB	805	CLA	C3D-C4D-ND	3.78	116.36	110.24
10	cA	838	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
10	bA	813	CLA	C3C-C4C-NC	3.78	114.81	110.57
10	cB	817	CLA	C3C-C4C-NC	3.78	114.81	110.57
10	bA	842	CLA	C3C-C4C-NC	3.78	114.81	110.57
10	aB	812	CLA	C3C-C4C-NC	3.78	114.81	110.57
10	bB	814	CLA	C3C-C4C-NC	3.78	114.81	110.57
10	cA	833	CLA	C4A-NA-C1A	-3.78	105.01	106.71
10	aB	802	CLA	C3C-C4C-NC	3.78	114.81	110.57
10	aB	835	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
9	cA	801	CL0	C1D-CHD-C4C	-3.77	117.92	126.06
10	aB	822	CLA	C3C-C4C-NC	3.77	114.80	110.57
10	bA	820	CLA	C3C-C4C-NC	3.77	114.80	110.57
10	bA	811	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
10	aB	830	CLA	C3D-C2D-C1D	-3.77	100.68	105.83
10	bA	819	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
10	aB	829	CLA	C3B-C4B-NB	3.77	114.08	109.21
9	bA	801	CL0	C1D-CHD-C4C	-3.77	117.93	126.06
10	aA	817	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
10	bA	818	CLA	C3B-C4B-NB	3.77	114.08	109.21
10	aA	838	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
10	aB	839	CLA	C3C-C4C-NC	3.77	114.80	110.57
10	aA	805	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
10	aA	819	CLA	C1D-CHD-C4C	-3.77	117.94	126.06
10	aA	818	CLA	C3B-C4B-NB	3.76	114.08	109.21
9	aA	801	CL0	C1D-CHD-C4C	-3.76	117.94	126.06
10	cB	801	CLA	C3B-C4B-NB	3.76	114.08	109.21
10	cB	822	CLA	C3C-C4C-NC	3.76	114.79	110.57
10	aB	802	CLA	C4A-NA-C1A	-3.76	105.01	106.71
10	cA	808	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
10	bB	830	CLA	C3D-C2D-C1D	-3.76	100.70	105.83
10	aB	830	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
10	cB	819	CLA	C3D-C4D-ND	3.76	116.32	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	838	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
10	aB	817	CLA	C3C-C4C-NC	3.76	114.79	110.57
10	cL	205	CLA	C4A-NA-C1A	-3.76	105.02	106.71
10	cA	818	CLA	C3B-C4B-NB	3.76	114.07	109.21
10	aB	838	CLA	C3C-C4C-NC	3.76	114.78	110.57
10	cA	811	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
10	bL	204	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
10	aA	811	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
10	cA	814	CLA	C4A-NA-C1A	-3.75	105.02	106.71
10	aB	801	CLA	C3B-C4B-NB	3.75	114.06	109.21
10	aA	822	CLA	C3D-C4D-ND	3.75	116.31	110.24
10	bA	832	CLA	C4A-NA-C1A	-3.75	105.02	106.71
10	aA	808	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
10	cA	822	CLA	C3D-C4D-ND	3.75	116.31	110.24
10	cA	843	CLA	C4A-NA-C1A	-3.75	105.02	106.71
10	bB	829	CLA	C3B-C4B-NB	3.75	114.06	109.21
10	aL	205	CLA	C4A-NA-C1A	-3.75	105.02	106.71
10	aB	806	CLA	CMC-C2C-C1C	3.75	130.74	125.04
10	cB	801	CLA	CMB-C2B-C3B	3.75	131.69	124.68
10	bB	802	CLA	C3C-C4C-NC	3.75	114.77	110.57
10	aA	832	CLA	C4A-NA-C1A	-3.74	105.02	106.71
10	bA	835	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
10	bB	825	CLA	C3D-C4D-ND	3.74	116.29	110.24
10	cA	813	CLA	C3C-C4C-NC	3.74	114.77	110.57
10	aA	819	CLA	C4A-NA-C1A	-3.74	105.02	106.71
10	bB	801	CLA	CMB-C2B-C3B	3.74	131.68	124.68
10	cA	812	CLA	C3C-C4C-NC	3.74	114.77	110.57
10	cA	813	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
10	cB	825	CLA	C3D-C4D-ND	3.74	116.29	110.24
10	cA	819	CLA	C4A-NA-C1A	-3.74	105.03	106.71
10	cB	839	CLA	C3C-C4C-NC	3.74	114.76	110.57
10	cB	840	CLA	C3D-C4D-ND	3.74	116.28	110.24
10	aB	840	CLA	C3D-C4D-ND	3.74	116.28	110.24
10	bA	829	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
10	aA	829	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
10	bA	825	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
10	bA	822	CLA	C3D-C4D-ND	3.73	116.28	110.24
10	cB	830	CLA	C3D-C2D-C1D	-3.73	100.74	105.83
10	bB	807	CLA	C3B-C4B-NB	3.73	114.04	109.21
10	bB	812	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
10	bB	840	CLA	C3D-C4D-ND	3.73	116.27	110.24
10	aA	842	CLA	C3C-C4C-NC	3.73	114.75	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	824	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
10	cB	832	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
10	bB	841	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
10	aB	801	CLA	CMB-C2B-C3B	3.73	131.66	124.68
10	cA	835	CLA	C3C-C4C-NC	3.73	114.75	110.57
10	aB	815	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
10	bA	806	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
10	cA	832	CLA	C4A-NA-C1A	-3.73	105.03	106.71
10	bB	835	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
10	aB	807	CLA	C3B-C4B-NB	3.73	114.03	109.21
10	cB	825	CLA	CAC-C3C-C4C	3.73	129.64	124.81
10	bB	819	CLA	C3D-C4D-ND	3.73	116.26	110.24
10	bB	801	CLA	C3B-C4B-NB	3.73	114.03	109.21
10	aB	832	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
10	aA	829	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
10	aB	812	CLA	C1D-CHD-C4C	-3.72	118.02	126.06
10	cA	825	CLA	C1D-CHD-C4C	-3.72	118.02	126.06
10	bA	812	CLA	C3C-C4C-NC	3.72	114.75	110.57
10	bA	833	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
10	bL	203	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
10	cA	831	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
10	cB	841	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
10	bB	839	CLA	C3C-C4C-NC	3.72	114.75	110.57
10	cA	829	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
10	aA	835	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
10	aB	834	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
10	aA	843	CLA	C4A-NA-C1A	-3.72	105.03	106.71
10	aB	824	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
10	cA	833	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
10	aB	825	CLA	C3D-C4D-ND	3.72	116.25	110.24
10	cA	835	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
10	bB	803	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
10	bB	834	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
10	cB	834	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
10	cB	835	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
10	bA	835	CLA	C3C-C4C-NC	3.72	114.74	110.57
10	cB	824	CLA	C1D-CHD-C4C	-3.71	118.04	126.06
10	aB	841	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
10	bA	809	CLA	CAA-C2A-C3A	-3.71	102.61	112.78
10	cB	812	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
10	cL	203	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
10	aA	813	CLA	C1C-C2C-C3C	-3.71	103.06	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	815	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
10	cB	807	CLA	C3B-C4B-NB	3.71	114.01	109.21
10	cB	803	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
10	bA	818	CLA	C3C-C4C-NC	3.71	114.73	110.57
10	bB	838	CLA	C3C-C4C-NC	3.71	114.73	110.57
10	cA	827	CLA	C3B-C4B-NB	3.71	114.00	109.21
10	aB	817	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
10	bB	806	CLA	CMC-C2C-C1C	3.71	130.68	125.04
10	cA	818	CLA	C3C-C4C-NC	3.71	114.73	110.57
10	cA	809	CLA	CAA-C2A-C3A	-3.71	102.63	112.78
10	bA	831	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
10	aB	803	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
10	cL	204	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
10	bA	839	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
10	bA	827	CLA	C3B-C4B-NB	3.70	114.00	109.21
10	aA	805	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
10	bB	825	CLA	CAC-C3C-C4C	3.70	129.61	124.81
10	cB	802	CLA	C4A-NA-C1A	-3.70	105.04	106.71
10	cB	817	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
10	cB	826	CLA	CMB-C2B-C3B	3.70	131.60	124.68
10	aA	817	CLA	C3C-C4C-NC	3.70	114.72	110.57
10	bB	832	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
10	aB	819	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
10	bB	828	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
10	aA	827	CLA	C3B-C4B-NB	3.70	113.99	109.21
10	aB	801	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
10	bB	823	CLA	C3C-C4C-NC	3.70	114.72	110.57
10	aA	825	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
10	cA	805	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
10	aA	815	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
10	aB	825	CLA	CAC-C3C-C4C	3.69	129.60	124.81
10	cA	840	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
10	cB	815	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
10	bA	819	CLA	C4A-NA-C1A	-3.69	105.05	106.71
10	aA	807	CLA	C3C-C4C-NC	3.69	114.71	110.57
10	bA	827	CLA	C4-C3-C5	3.69	121.48	115.27
10	bA	829	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
10	cA	829	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
10	aA	831	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
10	bA	813	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
10	aB	826	CLA	CMB-C2B-C3B	3.69	131.59	124.68
10	aA	818	CLA	C3C-C4C-NC	3.69	114.71	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	835	CLA	C3C-C4C-NC	3.69	114.71	110.57
10	bA	856	CLA	O2D-CGD-CBD	3.69	117.83	111.27
10	aA	809	CLA	CAA-C2A-C3A	-3.69	102.67	112.78
10	cA	842	CLA	C3C-C4C-NC	3.69	114.71	110.57
10	cB	823	CLA	C3C-C4C-NC	3.69	114.71	110.57
10	cA	833	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
10	aA	856	CLA	O2D-CGD-CBD	3.69	117.82	111.27
10	aB	835	CLA	C3C-C4C-NC	3.69	114.71	110.57
10	bB	836	CLA	C3C-C4C-NC	3.69	114.71	110.57
10	aB	828	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
10	cA	836	CLA	C3D-C4D-ND	3.69	116.20	110.24
10	aA	827	CLA	C4-C3-C5	3.69	121.47	115.27
10	aL	204	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
10	bA	802	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
10	bB	817	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
10	cA	839	CLA	C1D-CHD-C4C	-3.69	118.11	126.06
10	aB	836	CLA	C3C-C4C-NC	3.68	114.70	110.57
10	bB	823	CLA	C1D-CHD-C4C	-3.68	118.11	126.06
10	cB	806	CLA	CMC-C2C-C1C	3.68	130.65	125.04
10	bA	805	CLA	C3B-C4B-NB	3.68	113.97	109.21
10	cA	807	CLA	C3C-C4C-NC	3.68	114.70	110.57
10	aL	203	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
10	bB	826	CLA	CMB-C2B-C3B	3.68	131.56	124.68
10	cB	838	CLA	C3C-C4C-NC	3.68	114.70	110.57
10	aA	839	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
10	bA	840	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
10	cB	823	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
10	bB	802	CLA	C4A-NA-C1A	-3.68	105.05	106.71
10	bA	805	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
10	bA	815	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
10	aB	829	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
10	cA	806	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
10	cB	831	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
10	aA	833	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
10	aA	806	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
10	bA	807	CLA	C3C-C4C-NC	3.68	114.69	110.57
10	bB	831	CLA	C3C-C4C-NC	3.68	114.69	110.57
10	aB	823	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
10	bA	833	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
10	cA	827	CLA	C4A-NA-C1A	-3.67	105.05	106.71
10	aA	812	CLA	C3C-C4C-NC	3.67	114.69	110.57
10	aB	804	CLA	CMB-C2B-C3B	3.67	131.55	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	804	CLA	CMB-C2B-C3B	3.67	131.55	124.68
10	aA	803	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
10	cA	827	CLA	C4-C3-C5	3.67	121.45	115.27
10	aB	811	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
10	cA	815	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
10	cB	801	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
10	bA	826	CLA	C3D-C4D-ND	3.67	116.18	110.24
10	cB	822	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
10	aB	818	CLA	C3C-C4C-NC	3.67	114.69	110.57
10	bA	817	CLA	C3C-C4C-NC	3.67	114.69	110.57
10	bB	819	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
10	bB	839	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
10	aA	833	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
10	bB	801	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
10	bA	820	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
10	aB	823	CLA	C3C-C4C-NC	3.67	114.68	110.57
10	aB	819	CLA	C1-C2-C3	-3.67	119.70	126.04
10	aA	840	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
10	aA	826	CLA	C3D-C4D-ND	3.66	116.17	110.24
10	aA	820	CLA	C1D-CHD-C4C	-3.66	118.15	126.06
10	aA	802	CLA	C1C-C2C-C3C	-3.66	103.10	106.96
10	cA	856	CLA	O2D-CGD-CBD	3.66	117.78	111.27
10	bA	836	CLA	C3D-C4D-ND	3.66	116.16	110.24
10	cB	819	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
10	bB	829	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
10	cA	820	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
10	cA	826	CLA	C3D-C4D-ND	3.66	116.16	110.24
10	bB	822	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
10	bB	819	CLA	C1-C2-C3	-3.66	119.72	126.04
10	bB	808	CLA	C3D-C4D-ND	3.66	116.16	110.24
10	cB	839	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
10	cB	819	CLA	C1-C2-C3	-3.66	119.72	126.04
10	aA	805	CLA	C3B-C4B-NB	3.66	113.94	109.21
10	cA	811	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
10	bA	803	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
10	cA	803	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
10	aB	839	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
10	bA	819	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
10	cB	829	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
10	aB	822	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
10	bB	811	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
10	cB	804	CLA	CMB-C2B-C3B	3.66	131.52	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	aA	801	CL0	CMA-C3A-C2A	-3.65	99.09	113.83
10	aB	807	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
9	cA	801	CL0	CMA-C3A-C2A	-3.65	99.09	113.83
10	cB	820	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
10	aB	808	CLA	C3D-C4D-ND	3.65	116.14	110.24
10	bA	810	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
10	cB	808	CLA	C3D-C4D-ND	3.65	116.14	110.24
10	bB	833	CLA	C3C-C4C-NC	3.65	114.66	110.57
10	cB	811	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
10	cA	805	CLA	C3B-C4B-NB	3.65	113.93	109.21
10	aA	827	CLA	C4A-NA-C1A	-3.65	105.07	106.71
10	aA	836	CLA	C3D-C4D-ND	3.65	116.14	110.24
10	cB	835	CLA	C3C-C4C-NC	3.65	114.66	110.57
10	aB	831	CLA	C1C-C2C-C3C	-3.64	103.12	106.96
10	bA	856	CLA	C1C-C2C-C3C	-3.64	103.12	106.96
10	cB	818	CLA	C3C-C4C-NC	3.64	114.66	110.57
10	aB	809	CLA	CAC-C3C-C4C	3.64	129.54	124.81
10	aB	815	CLA	C4A-NA-C1A	-3.64	105.07	106.71
10	bB	815	CLA	C4A-NA-C1A	-3.64	105.07	106.71
10	bA	804	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
10	cA	817	CLA	C3C-C4C-NC	3.64	114.66	110.57
10	bA	827	CLA	C4A-NA-C1A	-3.64	105.07	106.71
10	bB	807	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
9	bA	801	CL0	CMA-C3A-C2A	-3.64	99.14	113.83
10	aA	819	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
10	aB	831	CLA	C3C-C4C-NC	3.64	114.65	110.57
10	bB	809	CLA	CAC-C3C-C4C	3.64	129.53	124.81
10	aB	835	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
10	cB	828	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
10	cA	804	CLA	C1D-CHD-C4C	-3.64	118.22	126.06
10	cB	818	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
10	bB	824	CLA	C3C-C4C-NC	3.63	114.64	110.57
10	aB	818	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
10	aB	833	CLA	C3C-C4C-NC	3.63	114.64	110.57
10	cB	836	CLA	C3C-C4C-NC	3.63	114.64	110.57
10	cB	807	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
10	bA	804	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
10	bA	811	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
10	cB	835	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
10	aA	804	CLA	CAA-C2A-C3A	-3.63	102.84	112.78
10	aA	804	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
10	aA	837	CLA	C1C-C2C-C3C	-3.63	103.14	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	856	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
10	cA	810	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
10	aA	810	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
10	bB	836	CLA	C1D-CHD-C4C	-3.63	118.24	126.06
10	bA	806	CLA	C3C-C4C-NC	3.62	114.64	110.57
10	aB	820	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
10	bB	835	CLA	C1D-CHD-C4C	-3.62	118.24	126.06
10	cB	833	CLA	C3C-C4C-NC	3.62	114.63	110.57
10	bA	804	CLA	CAA-C2A-C3A	-3.62	102.86	112.78
10	cA	806	CLA	C3C-C4C-NC	3.62	114.63	110.57
10	cB	822	CLA	C3B-C4B-NB	3.62	113.89	109.21
10	aB	811	CLA	C3B-C4B-NB	3.62	113.89	109.21
10	bB	818	CLA	C3C-C4C-NC	3.62	114.63	110.57
10	bB	831	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
10	cA	804	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
10	bB	820	CLA	C1C-C2C-C3C	-3.62	103.16	106.96
10	aB	836	CLA	C1D-CHD-C4C	-3.62	118.26	126.06
10	aA	807	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
10	aB	824	CLA	C3C-C4C-NC	3.61	114.62	110.57
10	bA	814	CLA	C4A-NA-C1A	-3.61	105.08	106.71
10	bA	810	CLA	C3B-C4B-NB	3.61	113.88	109.21
10	bA	822	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
10	cB	836	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
10	cA	804	CLA	CAA-C2A-C3A	-3.61	102.90	112.78
10	cA	831	CLA	CMB-C2B-C3B	3.61	131.43	124.68
10	aB	822	CLA	C3B-C4B-NB	3.61	113.87	109.21
10	aA	806	CLA	C3C-C4C-NC	3.61	114.62	110.57
10	bB	835	CLA	C3C-C4C-NC	3.61	114.62	110.57
10	bB	811	CLA	C3B-C4B-NB	3.61	113.87	109.21
10	cB	831	CLA	C3C-C4C-NC	3.61	114.61	110.57
10	bB	818	CLA	C1D-CHD-C4C	-3.60	118.28	126.06
10	cB	809	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
10	aA	811	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
10	cA	802	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
10	cB	824	CLA	C3C-C4C-NC	3.60	114.61	110.57
10	cA	819	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
10	cB	809	CLA	CAC-C3C-C4C	3.60	129.48	124.81
10	cB	811	CLA	C3B-C4B-NB	3.60	113.86	109.21
10	bB	822	CLA	C3B-C4B-NB	3.60	113.86	109.21
10	cB	815	CLA	C4A-NA-C1A	-3.60	105.09	106.71
10	aL	205	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
10	bA	807	CLA	C1D-CHD-C4C	-3.60	118.30	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	830	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
10	aA	814	CLA	C4A-NA-C1A	-3.59	105.09	106.71
10	cA	807	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
10	cB	827	CLA	C3B-C4B-NB	3.59	113.85	109.21
10	aA	856	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
10	aB	811	CLA	C3D-C4D-ND	3.59	116.05	110.24
10	cA	812	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
10	cA	822	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
10	bB	827	CLA	C3B-C4B-NB	3.59	113.85	109.21
10	bA	831	CLA	CMB-C2B-C3B	3.59	131.39	124.68
10	cA	810	CLA	C3B-C4B-NB	3.59	113.85	109.21
10	bB	808	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
10	bB	811	CLA	C3D-C4D-ND	3.59	116.04	110.24
10	bA	837	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
10	bB	809	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
10	aA	812	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
10	bA	812	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
13	cB	844	BCR	C3-C4-C5	-3.58	107.68	114.08
10	aB	836	CLA	C3B-C4B-NB	3.58	113.84	109.21
10	cB	830	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
10	cL	205	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
10	aB	809	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
10	aA	822	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
10	aB	830	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
13	bB	844	BCR	C3-C4-C5	-3.58	107.69	114.08
10	bB	834	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
10	aB	830	CLA	C3C-C4C-NC	3.58	114.58	110.57
10	bB	830	CLA	C3C-C4C-NC	3.58	114.58	110.57
10	aA	823	CLA	C3B-C4B-NB	3.58	113.83	109.21
10	aB	827	CLA	C3B-C4B-NB	3.57	113.83	109.21
10	cA	837	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
13	cA	847	BCR	C2-C1-C6	3.57	115.98	110.48
10	cB	827	CLA	C4A-NA-C1A	-3.57	105.10	106.71
10	aB	814	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
10	bA	812	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
10	cB	811	CLA	C3D-C4D-ND	3.57	116.01	110.24
10	cA	823	CLA	C3C-C4C-NC	3.57	114.58	110.57
10	bL	205	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
10	bB	834	CLA	CAC-C3C-C4C	3.57	129.44	124.81
10	cB	828	CLA	C3D-C4D-ND	3.57	116.01	110.24
10	cB	836	CLA	C3B-C4B-NB	3.57	113.82	109.21
10	cB	830	CLA	C3C-C4C-NC	3.57	114.57	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	bA	801	CL0	CMA-C3A-C4A	-3.57	102.19	111.77
10	aA	831	CLA	CMB-C2B-C3B	3.57	131.35	124.68
10	aB	807	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
10	aB	808	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
10	cB	807	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
10	bB	828	CLA	C3D-C4D-ND	3.56	116.00	110.24
10	cB	808	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
10	cB	813	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
10	aB	834	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
10	cB	834	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
10	aB	807	CLA	CAC-C3C-C4C	3.56	129.43	124.81
10	aA	827	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
13	bA	847	BCR	C2-C1-C6	3.56	115.96	110.48
10	cB	814	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
10	bB	836	CLA	C3B-C4B-NB	3.56	113.81	109.21
9	cA	801	CL0	CMA-C3A-C4A	-3.56	102.21	111.77
10	aA	804	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
10	cA	831	CLA	C3B-C4B-NB	3.55	113.81	109.21
13	aB	844	BCR	C3-C4-C5	-3.55	107.73	114.08
10	bB	807	CLA	CAC-C3C-C4C	3.55	129.42	124.81
10	cA	842	CLA	C3B-C4B-NB	3.55	113.80	109.21
9	aA	801	CL0	CMA-C3A-C4A	-3.55	102.23	111.77
13	aA	847	BCR	C2-C1-C6	3.55	115.95	110.48
10	cB	826	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
10	aA	817	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
10	aB	828	CLA	C3D-C4D-ND	3.55	115.98	110.24
10	bB	813	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
10	bA	827	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
10	cB	810	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
10	bB	807	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
10	aA	810	CLA	C3B-C4B-NB	3.54	113.79	109.21
10	cB	812	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
10	aB	815	CLA	C3B-C4B-NB	3.54	113.79	109.21
10	aA	812	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
10	aB	827	CLA	C4A-NA-C1A	-3.54	105.11	106.71
10	cA	823	CLA	C4A-NA-C1A	-3.54	105.11	106.71
10	bB	810	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
10	bA	838	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
10	aA	831	CLA	C3B-C4B-NB	3.54	113.79	109.21
10	bA	823	CLA	C3B-C4B-NB	3.54	113.79	109.21
10	cA	823	CLA	C3B-C4B-NB	3.54	113.79	109.21
10	aB	810	CLA	C1C-C2C-C3C	-3.54	103.24	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	812	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
10	bL	202	CLA	C3D-C4D-ND	3.54	115.96	110.24
10	bA	807	CLA	C4A-NA-C1A	-3.54	105.12	106.71
10	bA	833	CLA	C3C-C4C-NC	3.54	114.54	110.57
10	cB	808	CLA	O2D-CGD-CBD	3.54	117.55	111.27
10	bB	831	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
10	cB	831	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
10	bB	840	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
10	bB	814	CLA	C1D-CHD-C4C	-3.53	118.43	126.06
10	aA	834	CLA	C4A-NA-C1A	-3.53	105.12	106.71
10	aA	804	CLA	C3C-C4C-NC	3.53	114.53	110.57
10	cA	839	CLA	C3C-C4C-NC	3.53	114.53	110.57
10	aL	203	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
10	aA	833	CLA	C3C-C4C-NC	3.53	114.53	110.57
10	aB	834	CLA	CAC-C3C-C4C	3.53	129.39	124.81
10	cA	805	CLA	O2A-CGA-CBA	3.53	122.98	111.91
10	bB	812	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
10	cA	817	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
10	aA	805	CLA	O2A-CGA-CBA	3.53	122.98	111.91
10	aB	805	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
10	cA	843	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
10	bA	815	CLA	C3C-C4C-NC	3.53	114.53	110.57
10	bA	823	CLA	C3C-C4C-NC	3.53	114.53	110.57
10	bA	805	CLA	O2A-CGA-CBA	3.53	122.97	111.91
10	cB	802	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
10	bB	826	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
10	cB	834	CLA	CAC-C3C-C4C	3.52	129.38	124.81
10	aB	812	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
10	aB	808	CLA	O2D-CGD-CBD	3.52	117.53	111.27
10	cB	807	CLA	CAC-C3C-C4C	3.52	129.38	124.81
10	cL	204	CLA	CBC-CAC-C3C	-3.52	102.72	112.43
10	bB	815	CLA	C3B-C4B-NB	3.52	113.76	109.21
10	bB	805	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
10	aL	202	CLA	C3D-C4D-ND	3.52	115.93	110.24
10	bA	843	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
10	aA	843	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
10	aL	204	CLA	CBC-CAC-C3C	-3.52	102.73	112.43
10	bA	842	CLA	C3B-C4B-NB	3.52	113.76	109.21
10	aA	815	CLA	C3C-C4C-NC	3.52	114.52	110.57
10	cL	202	CLA	C3D-C4D-ND	3.52	115.93	110.24
10	aB	813	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
10	cA	807	CLA	C4A-NA-C1A	-3.52	105.12	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	811	CLA	CHC-C1C-C2C	-3.52	116.99	126.72
10	bL	203	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
10	aA	838	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
10	aA	823	CLA	C3C-C4C-NC	3.51	114.51	110.57
10	bA	804	CLA	C3C-C4C-NC	3.51	114.51	110.57
10	cA	815	CLA	C3C-C4C-NC	3.51	114.51	110.57
10	cA	804	CLA	C3C-C4C-NC	3.51	114.51	110.57
10	aB	828	CLA	C4A-NA-C1A	-3.51	105.13	106.71
10	aB	826	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
10	bL	204	CLA	CBC-CAC-C3C	-3.51	102.76	112.43
10	bB	808	CLA	O2D-CGD-CBD	3.51	117.50	111.27
10	cL	203	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
10	bA	831	CLA	C3B-C4B-NB	3.51	113.74	109.21
10	cB	828	CLA	C4A-NA-C1A	-3.51	105.13	106.71
10	cB	815	CLA	C3B-C4B-NB	3.51	113.74	109.21
10	bB	828	CLA	C1-O2A-CGA	3.51	125.64	116.44
10	cB	811	CLA	CHC-C1C-C2C	-3.51	117.03	126.72
10	aA	839	CLA	C3C-C4C-NC	3.51	114.50	110.57
10	cA	833	CLA	C3C-C4C-NC	3.51	114.50	110.57
10	bB	825	CLA	C3B-C4B-NB	3.50	113.74	109.21
10	cB	828	CLA	C1-O2A-CGA	3.50	125.64	116.44
10	aB	828	CLA	C1-O2A-CGA	3.50	125.64	116.44
10	cB	805	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
10	aA	807	CLA	C4A-NA-C1A	-3.50	105.13	106.71
10	aL	202	CLA	C1-O2A-CGA	3.50	125.64	116.44
10	aB	811	CLA	CHC-C1C-C2C	-3.50	117.03	126.72
10	aB	837	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
10	bB	802	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
10	aB	820	CLA	C3C-C4C-NC	3.50	114.50	110.57
10	aA	842	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
10	aA	842	CLA	C3B-C4B-NB	3.50	113.73	109.21
10	aB	831	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
10	cA	816	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
13	bI	101	BCR	C2-C1-C6	3.50	115.87	110.48
10	bL	202	CLA	C1-O2A-CGA	3.50	125.62	116.44
10	cB	837	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
10	aL	203	CLA	C3C-C4C-NC	3.50	114.49	110.57
10	cA	842	CLA	C1D-CHD-C4C	-3.49	118.52	126.06
10	bL	205	CLA	C1D-CHD-C4C	-3.49	118.52	126.06
10	cA	838	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
10	cB	840	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
10	bA	842	CLA	C1D-CHD-C4C	-3.49	118.52	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aL	205	CLA	C1D-CHD-C4C	-3.49	118.52	126.06
13	aI	101	BCR	C2-C1-C6	3.49	115.86	110.48
10	aA	827	CLA	CMB-C2B-C3B	3.49	131.21	124.68
10	bA	817	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
10	cL	205	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
10	cA	827	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
10	bA	839	CLA	C3C-C4C-NC	3.48	114.48	110.57
10	cB	825	CLA	C3B-C4B-NB	3.48	113.72	109.21
10	bB	807	CLA	O2A-CGA-CBA	3.48	122.84	111.91
10	aA	832	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
10	bA	816	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
13	cB	844	BCR	C2-C1-C6	3.48	115.84	110.48
10	bB	827	CLA	C4C-C3C-C2C	-3.48	101.83	106.90
10	aB	807	CLA	O2A-CGA-CBA	3.48	122.83	111.91
10	bB	837	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
13	cI	102	BCR	C2-C1-C6	3.48	115.83	110.48
10	aB	840	CLA	C1C-C2C-C3C	-3.47	103.30	106.96
10	bA	827	CLA	CMB-C2B-C3B	3.47	131.18	124.68
10	cA	827	CLA	CMB-C2B-C3B	3.47	131.18	124.68
13	aB	844	BCR	C2-C1-C6	3.47	115.83	110.48
10	bB	830	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
10	bA	825	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
10	cA	825	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
10	cL	202	CLA	C1-O2A-CGA	3.47	125.54	116.44
10	aB	830	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
10	aB	802	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
10	cB	807	CLA	O2A-CGA-CBA	3.47	122.78	111.91
10	bA	832	CLA	C1D-CHD-C4C	-3.46	118.58	126.06
10	cB	827	CLA	C3D-C4D-ND	3.46	115.84	110.24
10	cB	827	CLA	C4C-C3C-C2C	-3.46	101.85	106.90
10	cA	832	CLA	C1D-CHD-C4C	-3.46	118.59	126.06
10	cL	203	CLA	C3C-C4C-NC	3.46	114.45	110.57
10	cA	820	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
10	aA	823	CLA	C4A-NA-C1A	-3.46	105.15	106.71
10	bB	827	CLA	C3D-C4D-ND	3.46	115.83	110.24
10	bB	819	CLA	C3B-C4B-NB	3.45	113.67	109.21
10	bA	820	CLA	CMB-C2B-C3B	3.45	131.14	124.68
10	bL	203	CLA	C3C-C4C-NC	3.45	114.44	110.57
10	aL	205	CLA	C3B-C4B-NB	3.45	113.67	109.21
10	aB	820	CLA	CAC-C3C-C4C	3.45	129.29	124.81
10	aA	825	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
13	bB	844	BCR	C2-C1-C6	3.45	115.79	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	825	CLA	C3B-C4B-NB	3.45	113.67	109.21
10	aB	809	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
10	cB	830	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
10	aB	827	CLA	C3D-C4D-ND	3.45	115.81	110.24
10	cB	812	CLA	C3B-C4B-NB	3.45	113.67	109.21
10	aB	827	CLA	C4C-C3C-C2C	-3.45	101.87	106.90
10	bB	820	CLA	C3C-C4C-NC	3.45	114.44	110.57
10	aA	822	CLA	C3B-C4B-NB	3.44	113.66	109.21
10	cB	809	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
10	aA	816	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
10	cA	820	CLA	CMB-C2B-C3B	3.44	131.11	124.68
10	cA	828	CLA	C3B-C4B-NB	3.44	113.65	109.21
10	cB	806	CLA	CAA-C2A-C3A	-3.44	103.37	112.78
10	aA	843	CLA	C3B-C4B-NB	3.44	113.65	109.21
10	aB	819	CLA	C3B-C4B-NB	3.43	113.65	109.21
10	aA	820	CLA	CMB-C2B-C3B	3.43	131.10	124.68
10	bA	832	CLA	CAA-C2A-C3A	-3.43	103.38	112.78
10	bL	205	CLA	C3B-C4B-NB	3.43	113.65	109.21
10	cA	832	CLA	CAA-C2A-C3A	-3.43	103.38	112.78
10	cA	843	CLA	C3B-C4B-NB	3.43	113.65	109.21
10	cB	804	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
10	bB	827	CLA	C4A-NA-C1A	-3.43	105.16	106.71
10	bB	812	CLA	C3B-C4B-NB	3.43	113.64	109.21
10	cA	822	CLA	CMB-C2B-C3B	3.43	131.09	124.68
10	aB	806	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
10	bB	806	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
10	aB	829	CLA	C3D-C2D-C1D	-3.43	101.15	105.83
10	bB	826	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
10	bA	803	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
10	bB	809	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
10	bA	820	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
10	bA	828	CLA	C3B-C4B-NB	3.43	113.64	109.21
10	cA	803	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
10	aA	832	CLA	CAA-C2A-C3A	-3.42	103.40	112.78
10	cA	839	CLA	C3B-C4B-NB	3.42	113.64	109.21
10	aB	812	CLA	C3B-C4B-NB	3.42	113.64	109.21
10	aB	826	CLA	C1D-CHD-C4C	-3.42	118.67	126.06
10	bA	822	CLA	CMB-C2B-C3B	3.42	131.08	124.68
10	cB	826	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
10	aB	804	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
10	aA	828	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
10	bA	822	CLA	C3B-C4B-NB	3.42	113.63	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	822	CLA	C3B-C4B-NB	3.42	113.63	109.21
10	bB	829	CLA	C3D-C2D-C1D	-3.42	101.17	105.83
10	aA	820	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
10	aA	803	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
10	bA	839	CLA	C3B-C4B-NB	3.41	113.62	109.21
10	cA	834	CLA	C4A-NA-C1A	-3.41	105.17	106.71
10	cB	820	CLA	C3C-C4C-NC	3.41	114.40	110.57
10	cB	819	CLA	C3B-C4B-NB	3.41	113.62	109.21
10	bB	820	CLA	CAC-C3C-C4C	3.41	129.23	124.81
10	bB	831	CLA	CAC-C3C-C4C	3.41	129.23	124.81
10	bA	828	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
10	cL	205	CLA	C3B-C4B-NB	3.41	113.61	109.21
10	aA	822	CLA	CMB-C2B-C3B	3.41	131.05	124.68
14	cA	855	LHG	O8-C23-C24	3.40	120.31	111.38
10	cA	828	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
10	aA	828	CLA	C3B-C4B-NB	3.40	113.61	109.21
10	cB	810	CLA	O2A-CGA-O1A	-3.40	115.01	123.59
10	cB	829	CLA	C3D-C2D-C1D	-3.40	101.19	105.83
10	bB	816	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
10	bB	802	CLA	CAA-C2A-C3A	-3.40	103.47	112.78
10	bA	843	CLA	C3B-C4B-NB	3.40	113.60	109.21
10	aA	839	CLA	C3B-C4B-NB	3.40	113.60	109.21
10	aB	802	CLA	CAA-C2A-C3A	-3.40	103.48	112.78
10	bB	804	CLA	C4C-C3C-C2C	-3.40	101.95	106.90
10	bA	834	CLA	C4A-NA-C1A	-3.39	105.18	106.71
10	bB	828	CLA	C4A-NA-C1A	-3.39	105.18	106.71
10	bB	810	CLA	O2A-CGA-O1A	-3.39	115.03	123.59
10	bB	818	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
10	cB	802	CLA	CAA-C2A-C3A	-3.39	103.49	112.78
10	bA	824	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
14	aA	855	LHG	O8-C23-C24	3.39	120.27	111.38
10	aB	810	CLA	O2A-CGA-O1A	-3.39	115.04	123.59
10	bB	811	CLA	C4-C3-C5	3.39	120.97	115.27
10	aA	843	CLA	CAC-C3C-C4C	3.38	129.20	124.81
10	bB	820	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
10	bA	842	CLA	CAC-C3C-C4C	3.38	129.20	124.81
10	cB	801	CLA	CAC-C3C-C4C	3.38	129.20	124.81
10	cB	811	CLA	C4-C3-C5	3.38	120.96	115.27
10	bA	843	CLA	CAC-C3C-C4C	3.38	129.19	124.81
10	bA	829	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
10	aB	831	CLA	CAC-C3C-C4C	3.38	129.19	124.81
14	bA	855	LHG	O8-C23-C24	3.38	120.24	111.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	cI	103	BCR	C2-C1-C6	3.38	115.68	110.48
10	cB	820	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
10	cB	820	CLA	CAC-C3C-C4C	3.37	129.19	124.81
10	bB	828	CLA	C3B-C4B-NB	3.37	113.57	109.21
10	aB	838	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
10	cB	838	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
10	aA	824	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
10	aB	811	CLA	C4-C3-C5	3.37	120.94	115.27
10	cB	819	CLA	C3C-C4C-NC	3.37	114.35	110.57
10	cB	828	CLA	C3B-C4B-NB	3.37	113.57	109.21
10	aB	801	CLA	CAC-C3C-C4C	3.37	129.18	124.81
10	aB	816	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
10	cA	824	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
10	aB	820	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
10	bB	838	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
10	aA	807	CLA	C3B-C4B-NB	3.37	113.56	109.21
10	bA	807	CLA	C3B-C4B-NB	3.37	113.56	109.21
10	cA	802	CLA	C3B-C4B-NB	3.37	113.56	109.21
10	bB	804	CLA	C3B-C4B-NB	3.37	113.56	109.21
10	bA	840	CLA	CAA-C2A-C3A	-3.37	103.56	112.78
10	aA	842	CLA	CAC-C3C-C4C	3.36	129.17	124.81
10	bB	830	CLA	CHC-C1C-C2C	-3.36	117.42	126.72
10	cB	816	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
10	aB	828	CLA	C3B-C4B-NB	3.36	113.56	109.21
13	bL	207	BCR	C2-C1-C6	3.36	115.66	110.48
13	aL	207	BCR	C2-C1-C6	3.36	115.66	110.48
10	aA	829	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
10	aA	840	CLA	CAA-C2A-C3A	-3.36	103.58	112.78
10	aB	830	CLA	CHC-C1C-C2C	-3.36	117.43	126.72
10	cA	807	CLA	C3B-C4B-NB	3.36	113.55	109.21
10	cA	826	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
10	cA	802	CLA	C4A-NA-C1A	-3.36	105.20	106.71
10	cB	804	CLA	C3B-C4B-NB	3.36	113.55	109.21
10	aB	819	CLA	C3C-C4C-NC	3.36	114.33	110.57
13	cL	207	BCR	C2-C1-C6	3.36	115.65	110.48
10	bB	801	CLA	CAC-C3C-C4C	3.35	129.16	124.81
10	cB	831	CLA	CAC-C3C-C4C	3.35	129.16	124.81
10	cA	829	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
10	cA	840	CLA	CAA-C2A-C3A	-3.35	103.60	112.78
10	bA	823	CLA	C4A-NA-C1A	-3.35	105.20	106.71
10	cA	843	CLA	CAC-C3C-C4C	3.35	129.16	124.81
10	aB	804	CLA	C3B-C4B-NB	3.35	113.54	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	854	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
10	cB	830	CLA	CHC-C1C-C2C	-3.35	117.46	126.72
10	aB	819	CLA	CHC-C1C-C2C	-3.35	117.46	126.72
10	aA	806	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
10	aB	806	CLA	C4A-NA-C1A	-3.35	105.20	106.71
10	cA	842	CLA	CAC-C3C-C4C	3.35	129.15	124.81
10	bA	802	CLA	C3B-C4B-NB	3.35	113.53	109.21
10	bA	806	CLA	C1D-CHD-C4C	-3.35	118.84	126.06
10	aB	836	CLA	CAA-C2A-C3A	-3.34	103.62	112.78
10	cB	819	CLA	CHC-C1C-C2C	-3.34	117.47	126.72
10	bB	819	CLA	C3C-C4C-NC	3.34	114.32	110.57
10	cB	818	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
10	aA	802	CLA	C3B-C4B-NB	3.34	113.53	109.21
10	aB	818	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
10	bB	824	CLA	CAC-C3C-C4C	3.34	129.14	124.81
10	bB	836	CLA	CAA-C2A-C3A	-3.34	103.64	112.78
10	cB	836	CLA	CAA-C2A-C3A	-3.34	103.64	112.78
13	bI	102	BCR	C2-C1-C6	3.33	115.61	110.48
10	aA	854	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
13	aI	102	BCR	C2-C1-C6	3.33	115.61	110.48
10	cB	817	CLA	C3B-C4B-NB	3.33	113.52	109.21
10	cA	806	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
10	aA	826	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
10	aB	805	CLA	CAA-C2A-C3A	-3.33	103.66	112.78
10	bB	819	CLA	CHC-C1C-C2C	-3.33	117.51	126.72
10	bB	805	CLA	CAA-C2A-C3A	-3.33	103.66	112.78
10	cB	825	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
10	cB	805	CLA	CAA-C2A-C3A	-3.33	103.66	112.78
10	bA	826	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
10	bA	802	CLA	C4A-NA-C1A	-3.33	105.21	106.71
10	bA	854	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
10	cA	813	CLA	CMB-C2B-C3B	3.33	130.90	124.68
10	cB	803	CLA	C3B-C4B-NB	3.33	113.51	109.21
10	cB	818	CLA	CMB-C2B-C3B	3.32	130.90	124.68
10	aA	828	CLA	O2A-CGA-CBA	3.32	122.34	111.91
10	aA	832	CLA	C3B-C4B-NB	3.32	113.51	109.21
10	aA	813	CLA	CMB-C2B-C3B	3.32	130.90	124.68
10	aB	803	CLA	C3B-C4B-NB	3.32	113.51	109.21
10	cA	828	CLA	O2A-CGA-CBA	3.32	122.33	111.91
10	aB	825	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
10	bB	834	CLA	CMA-C3A-C4A	-3.32	102.85	111.77
10	cB	834	CLA	CMA-C3A-C4A	-3.32	102.85	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	803	CLA	C3B-C4B-NB	3.32	113.50	109.21
10	bB	803	CLA	CMA-C3A-C4A	-3.32	102.85	111.77
10	cB	828	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
10	bB	834	CLA	C3C-C4C-NC	3.32	114.29	110.57
10	cA	840	CLA	C4-C3-C5	3.32	119.78	115.98
10	aB	810	CLA	C3B-C4B-NB	3.32	113.50	109.21
10	cB	803	CLA	CMA-C3A-C4A	-3.32	102.86	111.77
10	cA	834	CLA	C3B-C4B-NB	3.31	113.50	109.21
10	bA	828	CLA	O2A-CGA-CBA	3.31	122.31	111.91
10	cB	824	CLA	CAC-C3C-C4C	3.31	129.11	124.81
10	cA	813	CLA	CHC-C1C-C2C	-3.31	117.56	126.72
10	aB	833	CLA	C3B-C4B-NB	3.31	113.49	109.21
10	cB	824	CLA	C3B-C4B-NB	3.31	113.49	109.21
10	aB	824	CLA	CAC-C3C-C4C	3.31	129.11	124.81
10	aA	834	CLA	C3B-C4B-NB	3.31	113.49	109.21
10	cB	833	CLA	C3B-C4B-NB	3.31	113.49	109.21
10	bA	828	CLA	CAC-C3C-C4C	3.31	129.10	124.81
10	aB	803	CLA	CMA-C3A-C4A	-3.31	102.88	111.77
10	bB	833	CLA	C3B-C4B-NB	3.31	113.49	109.21
10	cB	823	CLA	C3B-C4B-NB	3.31	113.48	109.21
10	aB	824	CLA	C3B-C4B-NB	3.31	113.48	109.21
10	bB	823	CLA	C3B-C4B-NB	3.31	113.48	109.21
10	bB	825	CLA	C4C-C3C-C2C	-3.30	102.08	106.90
10	cB	805	CLA	C3B-C4B-NB	3.30	113.48	109.21
10	aA	813	CLA	CHC-C1C-C2C	-3.30	117.58	126.72
10	aB	818	CLA	CMB-C2B-C3B	3.30	130.86	124.68
10	bA	813	CLA	CHC-C1C-C2C	-3.30	117.59	126.72
10	aB	813	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
10	bA	813	CLA	CMB-C2B-C3B	3.30	130.85	124.68
10	bB	818	CLA	CMB-C2B-C3B	3.30	130.85	124.68
10	aB	834	CLA	CMA-C3A-C4A	-3.30	102.91	111.77
10	bB	824	CLA	C3B-C4B-NB	3.30	113.47	109.21
10	bA	834	CLA	C3B-C4B-NB	3.30	113.47	109.21
10	aB	828	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
10	aB	841	CLA	CHC-C1C-C2C	-3.29	117.62	126.72
10	aB	817	CLA	C3B-C4B-NB	3.29	113.47	109.21
10	bB	828	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
10	bA	832	CLA	C3B-C4B-NB	3.29	113.46	109.21
10	bB	810	CLA	C4A-NA-C1A	-3.29	105.23	106.71
10	bA	802	CLA	CHC-C1C-C2C	-3.28	117.64	126.72
10	cA	856	CLA	C3B-C4B-NB	3.28	113.46	109.21
10	bL	204	CLA	O2D-CGD-O1D	-3.28	117.42	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cL	204	CLA	C1D-CHD-C4C	-3.28	118.97	126.06
10	bA	840	CLA	C4-C3-C5	3.28	119.74	115.98
10	cA	829	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
10	bL	204	CLA	C1D-CHD-C4C	-3.28	118.98	126.06
10	cA	814	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
10	bB	841	CLA	CHC-C1C-C2C	-3.28	117.64	126.72
10	bB	810	CLA	O2A-CGA-CBA	3.28	122.21	111.91
10	cA	828	CLA	CAC-C3C-C4C	3.28	129.07	124.81
10	bA	856	CLA	C3B-C4B-NB	3.28	113.45	109.21
10	bB	813	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
10	cB	826	CLA	C3C-C4C-NC	3.28	114.25	110.57
10	aL	204	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
10	aB	814	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
10	aB	805	CLA	C3B-C4B-NB	3.28	113.45	109.21
10	cB	810	CLA	O2A-CGA-CBA	3.28	122.19	111.91
10	bB	810	CLA	C3B-C4B-NB	3.28	113.45	109.21
10	aA	814	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
10	aA	829	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
10	bB	810	CLA	CBA-CAA-C2A	3.27	123.53	113.86
10	bA	814	CLA	C4C-C3C-C2C	-3.27	102.12	106.90
10	aB	806	CLA	C1C-C2C-C3C	-3.27	103.51	106.96
10	cB	813	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
10	aA	802	CLA	CHC-C1C-C2C	-3.27	117.67	126.72
10	bA	824	CLA	C1D-CHD-C4C	-3.27	119.00	126.06
10	cL	204	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
10	cB	810	CLA	CBA-CAA-C2A	3.27	123.52	113.86
10	cB	841	CLA	CHC-C1C-C2C	-3.27	117.67	126.72
10	bA	824	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
10	aB	810	CLA	CBA-CAA-C2A	3.27	123.52	113.86
10	aB	823	CLA	C3B-C4B-NB	3.27	113.44	109.21
10	aB	810	CLA	O2A-CGA-CBA	3.27	122.17	111.91
10	cB	810	CLA	C3B-C4B-NB	3.27	113.44	109.21
10	aA	840	CLA	C4-C3-C5	3.27	119.72	115.98
10	bB	802	CLA	CHB-C4A-NA	3.27	129.03	124.51
10	cA	824	CLA	C1D-CHD-C4C	-3.27	119.01	126.06
10	bB	806	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
10	bB	826	CLA	O2A-CGA-CBA	3.27	122.16	111.91
10	bA	829	CLA	O2D-CGD-O1D	-3.26	117.45	123.84
10	aL	204	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
10	aB	834	CLA	C3C-C4C-NC	3.26	114.23	110.57
10	cA	802	CLA	CHC-C1C-C2C	-3.26	117.69	126.72
10	cB	826	CLA	O2A-CGA-CBA	3.26	122.15	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	806	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
10	bB	817	CLA	C3B-C4B-NB	3.26	113.43	109.21
10	cA	821	CLA	C3B-C4B-NB	3.26	113.43	109.21
10	aB	826	CLA	O2A-CGA-CBA	3.26	122.14	111.91
10	aA	821	CLA	C3B-C4B-NB	3.26	113.43	109.21
10	aA	856	CLA	C3B-C4B-NB	3.26	113.43	109.21
10	aB	826	CLA	C3C-C4C-NC	3.26	114.23	110.57
10	aL	204	CLA	C4A-NA-C1A	-3.26	105.24	106.71
10	bB	821	CLA	C3B-C4B-NB	3.26	113.42	109.21
10	cA	832	CLA	C3B-C4B-NB	3.26	113.42	109.21
10	aA	841	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
10	cB	814	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
10	bA	821	CLA	C3B-C4B-NB	3.25	113.42	109.21
10	bB	826	CLA	C3C-C4C-NC	3.25	114.22	110.57
10	aA	828	CLA	CAC-C3C-C4C	3.25	129.03	124.81
10	cB	802	CLA	CHB-C4A-NA	3.25	129.01	124.51
10	bA	841	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
10	aB	804	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
10	cA	803	CLA	C3B-C4B-NB	3.25	113.41	109.21
10	cB	810	CLA	C4A-NA-C1A	-3.25	105.25	106.71
10	bA	803	CLA	C3B-C4B-NB	3.25	113.41	109.21
10	aA	808	CLA	O2D-CGD-CBD	3.25	117.04	111.27
10	aA	854	CLA	CHD-C4C-NC	3.25	129.32	124.20
10	aB	831	CLA	CAA-C2A-C3A	-3.25	103.88	112.78
10	bA	838	CLA	CAC-C3C-C4C	3.25	129.02	124.81
10	bB	814	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
10	cB	806	CLA	C3B-C4B-NB	3.24	113.40	109.21
10	bB	806	CLA	C4A-NA-C1A	-3.24	105.25	106.71
10	bB	831	CLA	CAA-C2A-C3A	-3.24	103.90	112.78
10	bB	814	CLA	C3B-C4B-NB	3.24	113.40	109.21
10	aB	802	CLA	CHB-C4A-NA	3.24	128.99	124.51
10	bB	804	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
10	bA	808	CLA	O2D-CGD-CBD	3.24	117.03	111.27
10	aA	802	CLA	C4A-NA-C1A	-3.24	105.25	106.71
10	aA	824	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
10	cA	842	CLA	CHC-C1C-C2C	-3.24	117.76	126.72
10	cA	854	CLA	CHD-C4C-NC	3.24	129.31	124.20
10	aA	854	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
10	cA	841	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
10	bA	854	CLA	CHD-C4C-NC	3.24	129.31	124.20
10	aA	824	CLA	C1D-CHD-C4C	-3.24	119.08	126.06
10	aA	823	CLA	CHC-C1C-C2C	-3.24	117.77	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	831	CLA	CAA-C2A-C3A	-3.24	103.92	112.78
10	cA	824	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
10	cA	824	CLA	C1C-C2C-C3C	-3.24	103.56	106.96
10	aB	806	CLA	C3B-C4B-NB	3.23	113.39	109.21
10	bA	842	CLA	CHC-C1C-C2C	-3.23	117.78	126.72
10	cA	823	CLA	CHC-C1C-C2C	-3.23	117.78	126.72
10	bA	815	CLA	CHC-C1C-C2C	-3.23	117.78	126.72
10	bA	854	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
10	aA	818	CLA	CHC-C1C-C2C	-3.23	117.78	126.72
10	aB	810	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
10	bB	805	CLA	C3B-C4B-NB	3.23	113.39	109.21
10	aA	838	CLA	CAC-C3C-C4C	3.23	129.00	124.81
10	aA	803	CLA	C3B-C4B-NB	3.23	113.39	109.21
10	cA	854	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
10	cA	811	CLA	C4A-NA-C1A	-3.23	105.25	106.71
10	cB	804	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
10	bA	823	CLA	CHC-C1C-C2C	-3.23	117.79	126.72
10	aA	842	CLA	CHC-C1C-C2C	-3.23	117.79	126.72
10	cA	827	CLA	O2A-CGA-CBA	3.23	122.04	111.91
10	aA	830	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
10	bA	818	CLA	CHC-C1C-C2C	-3.23	117.80	126.72
10	bA	833	CLA	CAA-C2A-C3A	-3.23	103.94	112.78
10	aA	803	CLA	CMB-C2B-C3B	3.23	130.72	124.68
10	bB	802	CLA	C1D-CHD-C4C	-3.23	119.10	126.06
10	cB	802	CLA	C1D-CHD-C4C	-3.23	119.10	126.06
10	bA	803	CLA	CMB-C2B-C3B	3.22	130.71	124.68
10	aA	827	CLA	O2A-CGA-CBA	3.22	122.03	111.91
10	bB	806	CLA	C3B-C4B-NB	3.22	113.38	109.21
10	bA	827	CLA	O2A-CGA-CBA	3.22	122.02	111.91
10	cA	808	CLA	O2D-CGD-CBD	3.22	117.00	111.27
10	aA	833	CLA	CAA-C2A-C3A	-3.22	103.95	112.78
10	bA	804	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
10	cA	818	CLA	CHC-C1C-C2C	-3.22	117.81	126.72
10	cB	810	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
13	cB	847	BCR	C2-C1-C6	3.22	115.44	110.48
10	cA	804	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
10	cB	814	CLA	C3B-C4B-NB	3.22	113.37	109.21
10	cA	838	CLA	CAC-C3C-C4C	3.22	128.99	124.81
10	aB	816	CLA	CAC-C3C-C4C	3.22	128.99	124.81
10	bA	842	CLA	C4A-NA-C1A	-3.22	105.26	106.71
10	bA	809	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
10	aA	802	CLA	CAC-C3C-C4C	3.22	128.99	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	816	CLA	CAC-C3C-C4C	3.22	128.98	124.81
10	aA	815	CLA	CHC-C1C-C2C	-3.22	117.82	126.72
10	cB	820	CLA	C3B-C4B-NB	3.22	113.37	109.21
10	aA	811	CLA	C4A-NA-C1A	-3.21	105.26	106.71
10	bA	815	CLA	C3B-C4B-NB	3.21	113.36	109.21
10	aB	820	CLA	CHC-C1C-C2C	-3.21	117.84	126.72
10	cA	815	CLA	C3B-C4B-NB	3.21	113.36	109.21
10	cA	830	CLA	C1D-CHD-C4C	-3.21	119.13	126.06
10	aB	802	CLA	C1D-CHD-C4C	-3.21	119.13	126.06
10	bB	810	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
10	aB	835	CLA	C3B-C4B-NB	3.21	113.36	109.21
10	cB	821	CLA	C3B-C4B-NB	3.21	113.36	109.21
10	cA	833	CLA	CAA-C2A-C3A	-3.21	103.99	112.78
10	aA	809	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
10	aB	816	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
10	bA	811	CLA	C4A-NA-C1A	-3.21	105.26	106.71
10	bB	837	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
10	cB	837	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
10	cB	834	CLA	C3C-C4C-NC	3.21	114.17	110.57
10	cA	803	CLA	CMB-C2B-C3B	3.21	130.68	124.68
10	aB	840	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
10	cB	820	CLA	CHC-C1C-C2C	-3.21	117.85	126.72
10	bB	820	CLA	CHC-C1C-C2C	-3.20	117.86	126.72
10	aA	804	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
13	aB	847	BCR	C2-C1-C6	3.20	115.41	110.48
10	bA	830	CLA	C1D-CHD-C4C	-3.20	119.15	126.06
10	aA	826	CLA	O2A-CGA-CBA	3.20	121.96	111.91
10	aB	821	CLA	C3B-C4B-NB	3.20	113.35	109.21
10	cA	809	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
10	cB	836	CLA	CHC-C1C-C2C	-3.20	117.87	126.72
10	cB	833	CLA	CAC-C3C-C4C	3.20	128.96	124.81
10	aB	814	CLA	C3B-C4B-NB	3.20	113.35	109.21
10	aA	835	CLA	CHC-C1C-C2C	-3.20	117.87	126.72
10	bA	814	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
10	cB	816	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
10	bL	204	CLA	C4A-NA-C1A	-3.20	105.27	106.71
10	aB	836	CLA	CHC-C1C-C2C	-3.20	117.88	126.72
10	bA	826	CLA	O2A-CGA-CBA	3.20	121.94	111.91
10	bA	841	CLA	CAC-C3C-C4C	3.20	128.96	124.81
10	cB	840	CLA	C4C-C3C-C2C	-3.20	102.24	106.90
10	cA	815	CLA	CHC-C1C-C2C	-3.20	117.88	126.72
10	aA	815	CLA	C3B-C4B-NB	3.20	113.34	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	826	CLA	O2A-CGA-CBA	3.19	121.93	111.91
10	cA	810	CLA	CAC-C3C-C4C	3.19	128.95	124.81
10	aA	824	CLA	C3B-C4B-NB	3.19	113.34	109.21
10	aA	841	CLA	CAC-C3C-C4C	3.19	128.95	124.81
10	cA	802	CLA	CAC-C3C-C4C	3.19	128.95	124.81
10	aA	824	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
10	cB	812	CLA	CHC-C1C-C2C	-3.19	117.90	126.72
10	bA	824	CLA	C3B-C4B-NB	3.19	113.33	109.21
10	cA	814	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
10	cA	827	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
10	aB	820	CLA	C3B-C4B-NB	3.19	113.33	109.21
10	bB	840	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
13	cB	847	BCR	C11-C10-C9	-3.19	122.76	127.31
10	cA	835	CLA	CHC-C1C-C2C	-3.19	117.91	126.72
10	cA	824	CLA	C3B-C4B-NB	3.19	113.33	109.21
10	bA	834	CLA	CHC-C1C-C2C	-3.19	117.91	126.72
10	bB	833	CLA	CAC-C3C-C4C	3.18	128.94	124.81
10	bB	836	CLA	CHC-C1C-C2C	-3.18	117.91	126.72
10	cB	805	CLA	CMB-C2B-C3B	3.18	130.63	124.68
10	bA	824	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
10	aA	835	CLA	C3B-C4B-NB	3.18	113.33	109.21
10	cA	834	CLA	CHC-C1C-C2C	-3.18	117.92	126.72
10	aB	833	CLA	CAC-C3C-C4C	3.18	128.94	124.81
10	bB	816	CLA	CAC-C3C-C4C	3.18	128.94	124.81
10	cA	841	CLA	CAC-C3C-C4C	3.18	128.94	124.81
10	bB	812	CLA	CHC-C1C-C2C	-3.18	117.92	126.72
10	aA	834	CLA	CHC-C1C-C2C	-3.18	117.92	126.72
10	cA	809	CLA	C3B-C4B-NB	3.18	113.32	109.21
10	aA	814	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
10	cB	808	CLA	CHD-C4C-NC	3.18	129.22	124.20
10	bA	827	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
10	bB	805	CLA	CMB-C2B-C3B	3.18	130.63	124.68
10	cB	822	CLA	CHC-C1C-C2C	-3.18	117.92	126.72
10	bA	810	CLA	CAC-C3C-C4C	3.18	128.94	124.81
10	aB	808	CLA	CHD-C4C-NC	3.18	129.21	124.20
10	bB	820	CLA	C3B-C4B-NB	3.18	113.32	109.21
13	bB	847	BCR	C2-C1-C6	3.18	115.37	110.48
10	aB	812	CLA	CHC-C1C-C2C	-3.18	117.93	126.72
10	aL	203	CLA	C3B-C4B-NB	3.18	113.32	109.21
10	bA	835	CLA	CHC-C1C-C2C	-3.18	117.93	126.72
10	cB	806	CLA	C4A-NA-C1A	-3.18	105.28	106.71
10	aB	822	CLA	CHC-C1C-C2C	-3.18	117.94	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	827	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
10	bB	816	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
10	bB	808	CLA	CHD-C4C-NC	3.17	129.20	124.20
10	cA	829	CLA	CHC-C1C-C2C	-3.17	117.95	126.72
10	aA	829	CLA	CHC-C1C-C2C	-3.17	117.95	126.72
10	bA	802	CLA	CAC-C3C-C4C	3.17	128.92	124.81
10	cB	814	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
10	aA	809	CLA	C3B-C4B-NB	3.17	113.31	109.21
10	bB	814	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
10	aB	837	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
10	aB	819	CLA	CMB-C2B-C3B	3.17	130.60	124.68
10	aB	814	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
10	bA	829	CLA	CHC-C1C-C2C	-3.17	117.96	126.72
10	bB	838	CLA	CHD-C4C-NC	3.17	129.19	124.20
10	cB	804	CLA	CAC-C3C-C4C	3.17	128.92	124.81
10	bB	809	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
10	bA	825	CLA	C4-C3-C5	3.16	120.59	115.27
13	aB	847	BCR	C11-C10-C9	-3.16	122.80	127.31
10	aB	835	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
10	bB	824	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
10	aB	805	CLA	CMB-C2B-C3B	3.16	130.59	124.68
10	aA	819	CLA	C3B-C4B-NB	3.16	113.30	109.21
10	cB	835	CLA	C3B-C4B-NB	3.16	113.30	109.21
10	cB	810	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
10	cA	825	CLA	CMC-C2C-C1C	3.16	129.85	125.04
10	cB	824	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
10	cA	856	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
10	cL	202	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
10	aB	824	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
10	bB	835	CLA	C3B-C4B-NB	3.16	113.29	109.21
10	cB	835	CLA	CHC-C1C-C2C	-3.16	117.99	126.72
10	aA	856	CLA	CHC-C1C-C2C	-3.16	117.99	126.72
10	aA	804	CLA	C4-C3-C5	3.16	120.58	115.27
13	bB	847	BCR	C11-C10-C9	-3.16	122.81	127.31
10	bA	856	CLA	CHC-C1C-C2C	-3.15	118.00	126.72
10	aB	809	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
10	bB	803	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
10	bB	819	CLA	CMB-C2B-C3B	3.15	130.58	124.68
10	bA	838	CLA	CBA-CAA-C2A	3.15	123.17	113.86
10	aA	838	CLA	CBA-CAA-C2A	3.15	123.17	113.86
10	cL	203	CLA	C3B-C4B-NB	3.15	113.28	109.21
10	aA	842	CLA	C4A-NA-C1A	-3.15	105.29	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bL	203	CLA	C3B-C4B-NB	3.15	113.28	109.21
10	bB	804	CLA	CAC-C3C-C4C	3.15	128.90	124.81
10	cA	830	CLA	CAC-C3C-C4C	3.15	128.90	124.81
10	cA	839	CLA	CAC-C3C-C4C	3.15	128.90	124.81
10	bB	810	CLA	CHC-C1C-C2C	-3.15	118.01	126.72
10	bA	809	CLA	C3B-C4B-NB	3.15	113.28	109.21
10	bA	835	CLA	C3B-C4B-NB	3.15	113.28	109.21
10	aA	810	CLA	CAC-C3C-C4C	3.15	128.90	124.81
10	cB	827	CLA	O2A-CGA-CBA	3.15	121.79	111.91
10	cB	838	CLA	CHD-C4C-NC	3.15	129.16	124.20
10	cB	819	CLA	CMB-C2B-C3B	3.15	130.57	124.68
10	cA	838	CLA	CBA-CAA-C2A	3.15	123.16	113.86
10	bA	819	CLA	C3B-C4B-NB	3.15	113.28	109.21
10	cA	842	CLA	C4A-NA-C1A	-3.15	105.29	106.71
10	aB	827	CLA	O2A-CGA-CBA	3.15	121.78	111.91
10	bB	827	CLA	O2A-CGA-CBA	3.15	121.78	111.91
10	aB	804	CLA	CAC-C3C-C4C	3.15	128.89	124.81
10	cA	809	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
10	cB	803	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
10	aB	838	CLA	CHD-C4C-NC	3.15	129.16	124.20
10	cA	814	CLA	CHC-C1C-C2C	-3.14	118.02	126.72
10	bB	835	CLA	CHC-C1C-C2C	-3.14	118.02	126.72
10	bA	839	CLA	CAC-C3C-C4C	3.14	128.89	124.81
10	aB	810	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
10	aB	803	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
10	bA	825	CLA	CMC-C2C-C1C	3.14	129.82	125.04
10	aB	833	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
10	aA	825	CLA	CMC-C2C-C1C	3.14	129.82	125.04
10	aA	830	CLA	CAC-C3C-C4C	3.14	128.88	124.81
10	aB	810	CLA	CAC-C3C-C4C	3.14	128.88	124.81
10	aA	825	CLA	C4-C3-C5	3.14	120.55	115.27
10	cB	822	CLA	CHD-C4C-NC	3.14	129.15	124.20
10	bA	809	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
10	bB	822	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
10	cA	841	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
10	bA	830	CLA	CAC-C3C-C4C	3.14	128.88	124.81
10	cB	824	CLA	CAA-C2A-C3A	-3.14	104.19	112.78
10	bA	822	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
10	cB	825	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
10	aA	814	CLA	CHC-C1C-C2C	-3.14	118.05	126.72
10	aB	825	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
10	bB	833	CLA	C4C-C3C-C2C	-3.14	102.33	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	822	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
10	cA	804	CLA	C4-C3-C5	3.14	120.55	115.27
10	aA	812	CLA	C3B-C4B-NB	3.13	113.26	109.21
10	aB	826	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
10	cB	810	CLA	CAC-C3C-C4C	3.13	128.88	124.81
10	bA	814	CLA	CHC-C1C-C2C	-3.13	118.05	126.72
10	bA	828	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
10	cA	819	CLA	C3B-C4B-NB	3.13	113.26	109.21
10	aA	809	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
10	cB	809	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
10	bB	825	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
10	cB	837	CLA	CAC-C3C-C4C	3.13	128.87	124.81
10	bL	202	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
10	cA	825	CLA	C4-C3-C5	3.13	120.54	115.27
10	aA	822	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
10	cB	833	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
10	cA	835	CLA	C3B-C4B-NB	3.13	113.26	109.21
10	aL	202	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
10	cB	810	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
10	bB	817	CLA	CAC-C3C-C4C	3.13	128.87	124.81
13	cI	102	BCR	C3-C4-C5	-3.13	108.49	114.08
10	bA	804	CLA	C4-C3-C5	3.13	120.53	115.27
10	aB	805	CLA	CHC-C1C-C2C	-3.13	118.07	126.72
10	cB	829	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
10	cB	833	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
10	bB	824	CLA	CAA-C2A-C3A	-3.13	104.22	112.78
10	aB	824	CLA	CAA-C2A-C3A	-3.12	104.23	112.78
10	aB	817	CLA	CHC-C1C-C2C	-3.12	118.08	126.72
10	bA	841	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
10	cA	806	CLA	C4-C3-C5	3.12	119.55	115.98
10	bA	812	CLA	C3B-C4B-NB	3.12	113.25	109.21
10	bA	806	CLA	CAC-C3C-C4C	3.12	128.86	124.81
10	bB	823	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
10	bA	833	CLA	C3B-C4B-NB	3.12	113.24	109.21
10	cB	829	CLA	C4-C3-C5	3.12	120.52	115.27
10	aB	810	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
10	bB	829	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
13	bI	101	BCR	C3-C4-C5	-3.12	108.51	114.08
10	bB	810	CLA	CAC-C3C-C4C	3.12	128.85	124.81
10	bB	833	CLA	CHC-C1C-C2C	-3.12	118.10	126.72
10	cB	839	CLA	C3B-C4B-NB	3.12	113.24	109.21
10	aB	810	CLA	C4A-NA-C1A	-3.12	105.31	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	841	CLA	C4C-C3C-C2C	-3.12	102.36	106.90
10	bB	833	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
10	bB	806	CLA	CHD-C4C-NC	3.11	129.11	124.20
10	cB	826	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
10	aA	839	CLA	CAC-C3C-C4C	3.11	128.85	124.81
10	bB	801	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
10	cA	806	CLA	CAC-C3C-C4C	3.11	128.85	124.81
10	aB	833	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
10	cB	813	CLA	C3B-C4B-NB	3.11	113.23	109.21
10	bB	827	CLA	CMB-C2B-C3B	3.11	130.50	124.68
10	bB	817	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
10	bB	839	CLA	C3B-C4B-NB	3.11	113.23	109.21
10	cA	812	CLA	C3B-C4B-NB	3.11	113.23	109.21
10	cB	806	CLA	CHD-C4C-NC	3.11	129.10	124.20
10	aB	801	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
10	aB	823	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
10	cB	833	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
10	cB	827	CLA	CHD-C4C-NC	3.11	129.10	124.20
10	aA	818	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
10	aB	833	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
10	aB	812	CLA	CAA-C2A-C3A	-3.11	104.27	112.78
10	aB	817	CLA	CAC-C3C-C4C	3.11	128.84	124.81
10	bA	807	CLA	CAC-C3C-C4C	3.10	128.84	124.81
10	bB	826	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
10	bB	810	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
10	aA	843	CLA	CHC-C1C-C2C	-3.10	118.14	126.72
10	bB	837	CLA	CAC-C3C-C4C	3.10	128.84	124.81
10	aB	829	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
13	aI	101	BCR	C3-C4-C5	-3.10	108.54	114.08
10	aB	802	CLA	C3B-C4B-NB	3.10	113.22	109.21
10	aA	805	CLA	CMB-C2B-C3B	3.10	130.48	124.68
10	bB	829	CLA	C4-C3-C5	3.10	120.49	115.27
10	bB	813	CLA	C3B-C4B-NB	3.10	113.22	109.21
10	bA	843	CLA	CHC-C1C-C2C	-3.10	118.14	126.72
10	aB	822	CLA	CHD-C4C-NC	3.10	129.09	124.20
10	cB	817	CLA	CHC-C1C-C2C	-3.10	118.15	126.72
10	aB	806	CLA	CHD-C4C-NC	3.10	129.09	124.20
10	cA	828	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
10	cB	823	CLA	CHC-C1C-C2C	-3.10	118.15	126.72
10	aB	813	CLA	C3B-C4B-NB	3.10	113.21	109.21
10	bA	818	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
10	aA	806	CLA	CAC-C3C-C4C	3.10	128.83	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	811	CLA	CHC-C1C-C2C	-3.09	118.16	126.72
10	cA	843	CLA	CHC-C1C-C2C	-3.09	118.16	126.72
10	cB	801	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
10	bB	812	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
10	bB	805	CLA	CHB-C4A-NA	3.09	128.79	124.51
10	cB	827	CLA	CMB-C2B-C3B	3.09	130.46	124.68
10	aA	828	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
10	bA	831	CLA	C4A-NA-C1A	-3.09	105.32	106.71
10	bB	822	CLA	CHD-C4C-NC	3.09	129.07	124.20
10	aB	838	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
10	cB	805	CLA	CHB-C4A-NA	3.09	128.79	124.51
10	aA	826	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
10	aB	829	CLA	C4-C3-C5	3.09	120.47	115.27
10	cA	838	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
10	aB	837	CLA	CAC-C3C-C4C	3.09	128.82	124.81
10	cB	812	CLA	CAA-C2A-C3A	-3.09	104.32	112.78
10	bB	802	CLA	C3B-C4B-NB	3.09	113.20	109.21
10	aA	839	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
10	cB	817	CLA	CAC-C3C-C4C	3.09	128.82	124.81
10	bB	805	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
10	cB	838	CLA	CAA-C2A-C3A	-3.09	104.33	112.78
10	bA	837	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
10	aA	837	CLA	C3B-C4B-NB	3.08	113.20	109.21
10	aB	839	CLA	C3B-C4B-NB	3.08	113.20	109.21
10	bA	805	CLA	CMB-C2B-C3B	3.08	130.45	124.68
10	aA	842	CLA	CMA-C3A-C2A	-3.08	101.39	113.83
10	cA	828	CLA	C1-C2-C3	-3.08	120.71	126.04
10	cA	818	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
10	aA	838	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
10	cA	805	CLA	CMB-C2B-C3B	3.08	130.45	124.68
10	aA	822	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
13	cB	846	BCR	C15-C16-C17	-3.08	117.16	123.47
10	cA	807	CLA	CAC-C3C-C4C	3.08	128.81	124.81
10	cB	805	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
10	aA	828	CLA	C1-C2-C3	-3.08	120.71	126.04
10	aB	805	CLA	CHB-C4A-NA	3.08	128.77	124.51
10	cB	832	CLA	C3B-C4B-NB	3.08	113.19	109.21
10	bB	838	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
10	aA	807	CLA	CAC-C3C-C4C	3.08	128.81	124.81
10	bB	801	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
10	cB	821	CLA	C4A-NA-C1A	-3.08	105.32	106.71
10	cA	839	CLA	CHC-C1C-C2C	-3.08	118.21	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	842	CLA	CMA-C3A-C2A	-3.08	101.41	113.83
10	bA	838	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
10	cA	837	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
10	cB	833	CLA	CAA-C2A-C3A	-3.08	104.36	112.78
10	bB	827	CLA	CHD-C4C-NC	3.08	129.05	124.20
10	aA	811	CLA	CHC-C1C-C2C	-3.08	118.21	126.72
10	aA	806	CLA	C4-C3-C5	3.07	119.50	115.98
10	cA	842	CLA	CMA-C3A-C2A	-3.07	101.43	113.83
10	cA	833	CLA	C3B-C4B-NB	3.07	113.18	109.21
10	aB	833	CLA	CAA-C2A-C3A	-3.07	104.36	112.78
10	bA	811	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
10	aA	819	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
10	bA	839	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
10	aB	809	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
10	bB	811	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
13	aB	846	BCR	C15-C16-C17	-3.07	117.19	123.47
10	cA	833	CLA	CHD-C4C-NC	3.07	129.04	124.20
10	aB	801	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
10	bB	825	CLA	CMB-C2B-C3B	3.07	130.42	124.68
10	cB	802	CLA	C3B-C4B-NB	3.07	113.17	109.21
10	bA	840	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
10	bA	828	CLA	C1-C2-C3	-3.07	120.74	126.04
10	aB	818	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
10	aA	833	CLA	C3B-C4B-NB	3.07	113.17	109.21
10	aB	827	CLA	CMB-C2B-C3B	3.07	130.41	124.68
10	aB	806	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
10	bB	833	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
10	bA	812	CLA	C1-C2-C3	-3.06	120.74	126.04
10	bB	806	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
10	bA	806	CLA	C4-C3-C5	3.06	119.49	115.98
10	aB	834	CLA	C3B-C4B-NB	3.06	113.17	109.21
10	aB	825	CLA	CMB-C2B-C3B	3.06	130.41	124.68
10	aA	812	CLA	C1-C2-C3	-3.06	120.75	126.04
10	bA	826	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
10	bA	819	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
10	aA	840	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
10	aA	805	CLA	CHD-C4C-NC	3.06	129.03	124.20
10	cB	801	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
10	aB	827	CLA	CHD-C4C-NC	3.06	129.03	124.20
13	bB	846	BCR	C15-C16-C17	-3.06	117.20	123.47
10	aB	832	CLA	C3B-C4B-NB	3.06	113.17	109.21
10	cB	821	CLA	CHC-C1C-C2C	-3.06	118.25	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	821	CLA	C4A-NA-C1A	-3.06	105.33	106.71
10	cB	801	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
10	bA	804	CLA	CAC-C3C-C4C	3.06	128.78	124.81
10	cB	816	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
10	aB	821	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
10	cL	204	CLA	C4A-NA-C1A	-3.06	105.33	106.71
10	aB	811	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
10	aA	837	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
10	cA	804	CLA	CAC-C3C-C4C	3.06	128.78	124.81
10	bA	822	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
10	bB	832	CLA	C3B-C4B-NB	3.06	113.16	109.21
10	bB	821	CLA	CHC-C1C-C2C	-3.05	118.27	126.72
10	aA	831	CLA	C4A-NA-C1A	-3.05	105.33	106.71
10	aB	801	CLA	CHC-C1C-C2C	-3.05	118.27	126.72
10	aA	819	CLA	CAC-C3C-C4C	3.05	128.77	124.81
10	bA	821	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
10	cA	819	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
10	bB	801	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
10	cB	807	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
10	cB	825	CLA	O2A-CGA-CBA	3.05	121.49	111.91
10	cB	825	CLA	CMB-C2B-C3B	3.05	130.39	124.68
10	aB	807	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
10	cA	805	CLA	CHD-C4C-NC	3.05	129.01	124.20
10	aA	816	CLA	C3B-C4B-NB	3.05	113.16	109.21
10	aB	802	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
10	aA	812	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
10	aA	838	CLA	O2A-CGA-CBA	3.05	121.48	111.91
10	cA	821	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
10	cB	811	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
10	cA	822	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
10	aA	808	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
9	aA	801	CL0	CHC-C1C-C2C	-3.05	118.29	126.72
10	aB	833	CLA	C4-C3-C5	3.05	120.40	115.27
11	aA	844	PQN	C11-C12-C13	-3.05	121.72	126.79
10	cA	826	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
10	aB	825	CLA	O2A-CGA-CBA	3.05	121.47	111.91
10	bB	825	CLA	O2A-CGA-CBA	3.05	121.47	111.91
10	cA	830	CLA	O2A-CGA-CBA	3.04	121.46	111.91
10	aA	814	CLA	C3B-C4B-NB	3.04	113.15	109.21
10	bA	816	CLA	C3B-C4B-NB	3.04	113.15	109.21
10	cA	819	CLA	CAC-C3C-C4C	3.04	128.76	124.81
10	cA	838	CLA	O2A-CGA-CBA	3.04	121.46	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	833	CLA	CHD-C4C-NC	3.04	129.00	124.20
10	aA	816	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
10	cB	809	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
10	bA	812	CLA	CAA-C2A-C3A	-3.04	104.44	112.78
10	cB	834	CLA	CHC-C1C-C2C	-3.04	118.30	126.72
10	aA	804	CLA	CAC-C3C-C4C	3.04	128.76	124.81
10	bA	838	CLA	O2A-CGA-CBA	3.04	121.46	111.91
10	aA	830	CLA	O2A-CGA-CBA	3.04	121.45	111.91
10	bB	807	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
10	cA	817	CLA	C4-C3-C5	3.04	120.39	115.27
10	cB	806	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
10	cL	202	CLA	C3B-C4B-NB	3.04	113.14	109.21
10	aB	834	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
10	aA	830	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
10	aB	839	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
10	aB	804	CLA	CMC-C2C-C1C	3.04	129.67	125.04
10	bB	839	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
10	cB	802	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
10	bA	830	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
10	bB	834	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
10	cB	839	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
10	aB	807	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
10	bL	202	CLA	C3B-C4B-NB	3.04	113.14	109.21
9	bA	801	CL0	CHC-C1C-C2C	-3.04	118.32	126.72
10	bA	805	CLA	CHD-C4C-NC	3.03	128.99	124.20
10	cA	816	CLA	C3B-C4B-NB	3.03	113.13	109.21
10	cA	836	CLA	C1-C2-C3	-3.03	120.80	126.04
10	cA	840	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
10	cB	818	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
10	bB	822	CLA	C4A-NA-C1A	-3.03	105.34	106.71
10	cA	831	CLA	C4A-NA-C1A	-3.03	105.34	106.71
10	bA	833	CLA	CHD-C4C-NC	3.03	128.98	124.20
10	cA	812	CLA	C1-C2-C3	-3.03	120.80	126.04
10	aA	821	CLA	CHC-C1C-C2C	-3.03	118.33	126.72
10	aB	807	CLA	CMB-C2B-C3B	3.03	130.35	124.68
10	bB	802	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
10	bA	837	CLA	C3B-C4B-NB	3.03	113.13	109.21
10	bA	819	CLA	CAC-C3C-C4C	3.03	128.74	124.81
9	cA	801	CL0	CHC-C1C-C2C	-3.03	118.33	126.72
10	aB	815	CLA	CHC-C1C-C2C	-3.03	118.33	126.72
10	bB	816	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
10	cB	834	CLA	C3B-C4B-NB	3.03	113.13	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	830	CLA	O2A-CGA-CBA	3.03	121.42	111.91
10	aB	816	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
10	cA	816	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
10	cA	810	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
10	bB	807	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
10	cB	807	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
10	cA	812	CLA	CAA-C2A-C3A	-3.03	104.48	112.78
10	bA	834	CLA	O2A-CGA-CBA	3.03	121.41	111.91
10	cA	817	CLA	CHD-C4C-NC	3.03	128.97	124.20
10	bB	826	CLA	C3B-C4B-NB	3.03	113.12	109.21
10	aA	842	CLA	CBC-CAC-C3C	-3.03	104.09	112.43
10	cA	830	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
10	bB	809	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
10	bA	833	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
10	bA	810	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
10	bA	825	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
10	aA	817	CLA	C4-C3-C5	3.03	120.36	115.27
10	cA	837	CLA	C3B-C4B-NB	3.03	113.12	109.21
10	cB	815	CLA	CHC-C1C-C2C	-3.02	118.35	126.72
10	cA	802	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
10	cA	814	CLA	C3B-C4B-NB	3.02	113.12	109.21
10	aB	827	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
10	cB	803	CLA	CMC-C2C-C1C	3.02	129.64	125.04
10	cA	825	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
10	cA	808	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
10	aA	818	CLA	CBA-CAA-C2A	3.02	122.78	113.86
10	aL	202	CLA	C3B-C4B-NB	3.02	113.12	109.21
10	cB	825	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
10	cB	804	CLA	CMC-C2C-C1C	3.02	129.64	125.04
11	aA	844	PQN	C14-C13-C15	3.02	120.35	115.27
10	aB	826	CLA	C3B-C4B-NB	3.02	113.11	109.21
10	cB	826	CLA	CAC-C3C-C4C	3.02	128.73	124.81
10	bB	825	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
10	bB	834	CLA	C3B-C4B-NB	3.02	113.11	109.21
11	bA	844	PQN	C11-C12-C13	-3.02	121.77	126.79
10	aA	834	CLA	O2A-CGA-CBA	3.02	121.38	111.91
10	bB	812	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
10	cA	842	CLA	CBC-CAC-C3C	-3.02	104.11	112.43
10	aA	833	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
10	aB	819	CLA	CAA-C2A-C3A	-3.02	104.52	112.78
10	bB	819	CLA	CAA-C2A-C3A	-3.02	104.52	112.78
10	bA	836	CLA	C1-C2-C3	-3.02	120.83	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	833	CLA	C4-C3-C5	3.02	120.34	115.27
10	aA	825	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
10	bA	820	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
10	cA	819	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
10	cB	819	CLA	CAA-C2A-C3A	-3.01	104.52	112.78
10	bA	811	CLA	C3B-C4B-NB	3.01	113.11	109.21
10	bL	205	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
10	bB	806	CLA	CAC-C3C-C4C	3.01	128.72	124.81
10	cA	818	CLA	CBA-CAA-C2A	3.01	122.76	113.86
10	bA	818	CLA	CBA-CAA-C2A	3.01	122.76	113.86
10	bB	807	CLA	CMB-C2B-C3B	3.01	130.32	124.68
10	bA	807	CLA	CMC-C2C-C1C	3.01	129.63	125.04
10	bB	815	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
10	cA	834	CLA	O2A-CGA-CBA	3.01	121.36	111.91
10	aB	821	CLA	C4A-NA-C1A	-3.01	105.35	106.71
11	cA	844	PQN	C11-C12-C13	-3.01	121.78	126.79
10	cB	818	CLA	C3B-C4B-NB	3.01	113.10	109.21
10	aA	820	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
10	aB	803	CLA	CMC-C2C-C1C	3.01	129.62	125.04
10	aA	811	CLA	C3B-C4B-NB	3.01	113.10	109.21
10	cA	820	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
10	bA	842	CLA	CBC-CAC-C3C	-3.01	104.14	112.43
10	cB	826	CLA	C3B-C4B-NB	3.01	113.10	109.21
10	cB	807	CLA	CMB-C2B-C3B	3.01	130.30	124.68
10	cA	833	CLA	CHC-C1C-C2C	-3.01	118.41	126.72
10	cA	854	CLA	O2A-CGA-CBA	3.01	121.34	111.91
10	bB	803	CLA	CMC-C2C-C1C	3.01	129.62	125.04
10	bB	832	CLA	CHD-C4C-NC	3.01	128.94	124.20
10	aA	819	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
10	aB	838	CLA	C3B-C4B-NB	3.01	113.09	109.21
10	bL	202	CLA	O2A-CGA-CBA	3.00	121.34	111.91
10	aA	854	CLA	O2A-CGA-CBA	3.00	121.34	111.91
10	cB	831	CLA	CHC-C1C-C2C	-3.00	118.41	126.72
10	cA	803	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
10	bA	816	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
10	aA	856	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
10	aL	202	CLA	O2A-CGA-CBA	3.00	121.33	111.91
10	bA	816	CLA	CHD-C4C-NC	3.00	128.93	124.20
10	aB	818	CLA	CAC-C3C-C4C	3.00	128.70	124.81
10	cL	205	CLA	CAC-C3C-C4C	3.00	128.70	124.81
10	cL	205	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
10	aA	806	CLA	O2A-CGA-CBA	3.00	121.32	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	806	CLA	O2A-CGA-CBA	3.00	121.32	111.91
10	cA	811	CLA	C3B-C4B-NB	3.00	113.09	109.21
10	bB	829	CLA	CMB-C2B-C3B	3.00	130.29	124.68
10	cB	829	CLA	CMB-C2B-C3B	3.00	130.29	124.68
10	bA	810	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
10	cB	839	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
10	bA	836	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
10	bA	806	CLA	O2A-CGA-CBA	3.00	121.31	111.91
10	cA	807	CLA	CMC-C2C-C1C	3.00	129.60	125.04
11	cA	844	PQN	C14-C13-C15	3.00	120.31	115.27
10	aA	816	CLA	CHD-C4C-NC	3.00	128.93	124.20
10	cA	836	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
10	bB	804	CLA	CMC-C2C-C1C	3.00	129.60	125.04
10	aA	836	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
10	bA	825	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
10	bB	814	CLA	O2A-CGA-CBA	2.99	121.30	111.91
10	bA	803	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
10	aB	832	CLA	CHD-C4C-NC	2.99	128.92	124.20
10	cL	202	CLA	O2A-CGA-CBA	2.99	121.30	111.91
10	cA	803	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
10	aA	836	CLA	C1-C2-C3	-2.99	120.87	126.04
10	cB	806	CLA	CAC-C3C-C4C	2.99	128.69	124.81
10	aA	810	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
10	aB	814	CLA	O2A-CGA-CBA	2.99	121.29	111.91
10	aB	829	CLA	CMB-C2B-C3B	2.99	130.27	124.68
10	aA	815	CLA	CHD-C4C-NC	2.99	128.91	124.20
10	bA	817	CLA	C4-C3-C5	2.99	120.30	115.27
10	aB	831	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
10	aB	806	CLA	CAC-C3C-C4C	2.99	128.69	124.81
10	aA	802	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
10	bB	818	CLA	C3B-C4B-NB	2.99	113.07	109.21
10	cB	812	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
10	bA	854	CLA	O2A-CGA-CBA	2.99	121.28	111.91
10	aB	839	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
10	bB	802	CLA	CHC-C1C-C2C	-2.99	118.46	126.72
10	aB	812	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
10	cB	814	CLA	O2A-CGA-CBA	2.99	121.28	111.91
10	bA	817	CLA	CHD-C4C-NC	2.99	128.91	124.20
10	bB	838	CLA	O2A-CGA-CBA	2.99	121.28	111.91
10	aB	825	CLA	C1C-C2C-C3C	-2.99	103.82	106.96
10	bA	814	CLA	C3B-C4B-NB	2.99	113.07	109.21
10	bB	808	CLA	C4C-C3C-C2C	-2.99	102.55	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	816	CLA	CHD-C4C-NC	2.99	128.91	124.20
10	cB	802	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
10	bB	818	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
10	bB	827	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
10	cB	832	CLA	CHD-C4C-NC	2.98	128.91	124.20
10	aA	826	CLA	CHD-C4C-NC	2.98	128.91	124.20
10	bA	802	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
10	cA	818	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
10	aB	809	CLA	C3B-C4B-NB	2.98	113.07	109.21
10	aB	827	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
10	bA	808	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
10	cA	856	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
10	cB	808	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
10	bA	826	CLA	CHD-C4C-NC	2.98	128.90	124.20
10	bB	827	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
10	cA	815	CLA	CHD-C4C-NC	2.98	128.90	124.20
10	bL	205	CLA	CAC-C3C-C4C	2.98	128.68	124.81
10	bB	839	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
10	aL	205	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
10	bA	856	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
10	cB	815	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
10	bB	833	CLA	C4-C3-C5	2.98	120.28	115.27
10	bA	812	CLA	CAC-C3C-C4C	2.98	128.68	124.81
10	cA	810	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
10	aA	816	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
11	bA	844	PQN	C14-C13-C15	2.98	120.28	115.27
10	cB	827	CLA	C1C-C2C-C3C	-2.98	103.83	106.96
10	cB	822	CLA	C4A-NA-C1A	-2.98	105.37	106.71
10	cB	818	CLA	CAC-C3C-C4C	2.98	128.67	124.81
10	aA	811	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
10	aA	817	CLA	CHD-C4C-NC	2.98	128.90	124.20
10	cB	811	CLA	CAC-C3C-C4C	2.98	128.67	124.81
10	aB	838	CLA	O2A-CGA-CBA	2.98	121.25	111.91
10	aA	803	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
10	aB	808	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
10	cB	827	CLA	CHC-C1C-C2C	-2.98	118.49	126.72
10	aA	810	CLA	CHC-C1C-C2C	-2.98	118.49	126.72
10	aA	807	CLA	CMC-C2C-C1C	2.98	129.57	125.04
10	aL	205	CLA	CAC-C3C-C4C	2.97	128.67	124.81
10	cA	854	CLA	C3B-C4B-NB	2.97	113.06	109.21
10	aA	837	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
10	bA	837	CLA	O2D-CGD-O1D	-2.97	118.02	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	831	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
10	bB	826	CLA	CAC-C3C-C4C	2.97	128.67	124.81
10	aA	803	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
10	cA	836	CLA	CAC-C3C-C4C	2.97	128.67	124.81
10	aB	808	CLA	CAA-C2A-C3A	-2.97	104.64	112.78
10	cB	838	CLA	O2A-CGA-CBA	2.97	121.23	111.91
10	cA	811	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
10	bA	819	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
10	aA	811	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
10	bB	808	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
10	bB	811	CLA	CAC-C3C-C4C	2.97	128.66	124.81
10	bB	809	CLA	C3B-C4B-NB	2.97	113.05	109.21
10	aA	843	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
10	cA	812	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
9	cA	801	CL0	CBC-CAC-C3C	-2.97	104.25	112.43
10	cA	837	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
10	cB	809	CLA	C3B-C4B-NB	2.97	113.05	109.21
10	aB	826	CLA	CAC-C3C-C4C	2.97	128.66	124.81
10	bB	837	CLA	C3B-C4B-NB	2.96	113.04	109.21
10	aB	802	CLA	CHC-C1C-C2C	-2.96	118.52	126.72
10	aA	836	CLA	CAC-C3C-C4C	2.96	128.66	124.81
10	bA	822	CLA	CHD-C4C-NC	2.96	128.87	124.20
10	aB	818	CLA	C3B-C4B-NB	2.96	113.04	109.21
10	cB	838	CLA	C3B-C4B-NB	2.96	113.04	109.21
10	cA	843	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
10	bA	843	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
10	bA	803	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
10	bA	811	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
10	aB	822	CLA	C4A-NA-C1A	-2.96	105.38	106.71
10	aA	811	CLA	CAC-C3C-C4C	2.96	128.65	124.81
10	aB	837	CLA	C3B-C4B-NB	2.96	113.04	109.21
10	cA	816	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
10	bA	836	CLA	CBC-CAC-C3C	-2.96	104.27	112.43
10	bA	815	CLA	CHD-C4C-NC	2.96	128.87	124.20
10	bB	840	CLA	CMB-C2B-C3B	2.96	130.21	124.68
10	aA	836	CLA	CBC-CAC-C3C	-2.96	104.27	112.43
10	bB	803	CLA	C4A-NA-C1A	-2.96	105.38	106.71
10	cA	811	CLA	CAC-C3C-C4C	2.96	128.65	124.81
10	cA	812	CLA	CAC-C3C-C4C	2.96	128.65	124.81
10	aA	822	CLA	CHD-C4C-NC	2.96	128.86	124.20
10	cA	822	CLA	CHD-C4C-NC	2.96	128.86	124.20
10	cB	808	CLA	CAA-C2A-C3A	-2.96	104.68	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	836	CLA	CAC-C3C-C4C	2.96	128.65	124.81
10	bB	815	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
10	cA	836	CLA	CBC-CAC-C3C	-2.96	104.28	112.43
10	bL	202	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
10	aL	202	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
10	cA	825	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
10	cB	811	CLA	CBC-CAC-C3C	-2.95	104.29	112.43
10	cA	841	CLA	C3B-C4B-NB	2.95	113.03	109.21
10	aB	811	CLA	CAC-C3C-C4C	2.95	128.64	124.81
10	aA	825	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
10	cB	839	CLA	CHC-C1C-C2C	-2.95	118.55	126.72
10	aB	839	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
9	aA	801	CL0	CBC-CAC-C3C	-2.95	104.30	112.43
10	bB	838	CLA	C3B-C4B-NB	2.95	113.02	109.21
10	aB	815	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
10	aA	818	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
10	cA	811	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
10	bA	828	CLA	CMC-C2C-C1C	2.95	129.53	125.04
10	bB	839	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
10	cA	809	CLA	CHD-C4C-NC	2.95	128.85	124.20
9	bA	801	CL0	CBC-CAC-C3C	-2.95	104.31	112.43
10	bA	811	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
10	cA	826	CLA	CHD-C4C-NC	2.95	128.85	124.20
10	bB	816	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
10	bA	818	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
10	bA	809	CLA	CHD-C4C-NC	2.94	128.84	124.20
10	bB	818	CLA	CAC-C3C-C4C	2.94	128.63	124.81
10	bA	804	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
10	aB	811	CLA	CBC-CAC-C3C	-2.94	104.32	112.43
10	aB	814	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
10	bA	821	CLA	CAA-C2A-C3A	-2.94	104.73	112.78
10	bA	812	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
10	bA	811	CLA	CAC-C3C-C4C	2.94	128.62	124.81
10	cL	202	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
10	cB	806	CLA	CMB-C2B-C3B	2.94	130.17	124.68
10	aA	804	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
10	aB	816	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
10	bA	816	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
10	aB	838	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
10	aA	821	CLA	CAA-C2A-C3A	-2.94	104.74	112.78
10	cB	816	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
10	aA	821	CLA	CHD-C4C-NC	2.94	128.83	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	809	CLA	CHD-C4C-NC	2.93	128.83	124.20
10	cA	821	CLA	CAA-C2A-C3A	-2.93	104.75	112.78
10	bA	839	CLA	O2A-CGA-CBA	2.93	121.11	111.91
10	aB	817	CLA	CHD-C4C-NC	2.93	128.82	124.20
10	aA	817	CLA	C3B-C4B-NB	2.93	113.00	109.21
10	bB	801	CLA	CHA-C1A-NA	-2.93	119.69	126.40
10	bA	817	CLA	C3B-C4B-NB	2.93	113.00	109.21
10	aA	812	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
10	bB	806	CLA	CMB-C2B-C3B	2.93	130.16	124.68
10	bB	811	CLA	CBC-CAC-C3C	-2.93	104.36	112.43
10	bB	817	CLA	CHD-C4C-NC	2.93	128.82	124.20
10	bA	854	CLA	C3B-C4B-NB	2.93	113.00	109.21
10	bA	813	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
10	cB	840	CLA	CMB-C2B-C3B	2.93	130.15	124.68
10	bA	831	CLA	CHD-C4C-NC	2.93	128.81	124.20
10	bA	803	CLA	CHC-C1C-C2C	-2.93	118.63	126.72
10	aA	813	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
10	aB	830	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
10	aA	814	CLA	CAC-C3C-C4C	2.93	128.61	124.81
10	cA	828	CLA	CMC-C2C-C1C	2.93	129.49	125.04
10	bB	830	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
10	cA	804	CLA	CHC-C1C-C2C	-2.92	118.63	126.72
10	cA	805	CLA	CHC-C1C-C2C	-2.92	118.63	126.72
10	aA	854	CLA	C3B-C4B-NB	2.92	112.99	109.21
10	aL	205	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
10	bA	832	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
10	bL	202	CLA	CHC-C1C-C2C	-2.92	118.63	126.72
10	cA	803	CLA	CHC-C1C-C2C	-2.92	118.63	126.72
10	cB	814	CLA	CHC-C1C-C2C	-2.92	118.63	126.72
10	aA	812	CLA	CAC-C3C-C4C	2.92	128.60	124.81
10	bB	838	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
10	bA	820	CLA	CHD-C4C-NC	2.92	128.81	124.20
10	aB	829	CLA	CAC-C3C-C4C	2.92	128.60	124.81
10	bL	204	CLA	C3B-C4B-NB	2.92	112.99	109.21
10	bB	814	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
10	cA	831	CLA	CHD-C4C-NC	2.92	128.81	124.20
10	cL	204	CLA	C3B-C4B-NB	2.92	112.98	109.21
10	aB	801	CLA	CHA-C1A-NA	-2.92	119.71	126.40
10	bB	835	CLA	CHD-C4C-NC	2.92	128.80	124.20
10	aL	202	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
10	cB	825	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
10	bB	828	CLA	CMC-C2C-C1C	2.92	129.48	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	831	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
10	bA	804	CLA	C3B-C4B-NB	2.92	112.98	109.21
10	bA	832	CLA	C1-C2-C3	-2.92	121.00	126.04
10	bA	805	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
10	cA	839	CLA	O2A-CGA-CBA	2.92	121.06	111.91
10	cB	829	CLA	CAC-C3C-C4C	2.92	128.59	124.81
10	cB	840	CLA	CAC-C3C-C4C	2.92	128.59	124.81
10	aA	832	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
10	bB	832	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
10	cB	832	CLA	CHC-C1C-C2C	-2.92	118.66	126.72
10	bA	814	CLA	CAC-C3C-C4C	2.91	128.59	124.81
10	bA	841	CLA	C3B-C4B-NB	2.91	112.98	109.21
10	aB	840	CLA	CMB-C2B-C3B	2.91	130.13	124.68
10	cL	205	CLA	CHC-C1C-C2C	-2.91	118.66	126.72
10	cL	205	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
10	aB	836	CLA	CAC-C3C-C4C	2.91	128.59	124.81
10	aA	803	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
10	aB	832	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
10	bB	814	CLA	C1-C2-C3	-2.91	121.01	126.04
10	bB	829	CLA	CAC-C3C-C4C	2.91	128.59	124.81
10	cL	202	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
10	cB	835	CLA	CHD-C4C-NC	2.91	128.79	124.20
10	aA	805	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
10	cA	830	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
10	cB	837	CLA	C3B-C4B-NB	2.91	112.97	109.21
10	cB	818	CLA	O2A-CGA-CBA	2.91	121.04	111.91
10	aL	205	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
9	bA	801	CL0	O2D-CGD-O1D	-2.91	118.15	123.84
10	cB	801	CLA	CHA-C1A-NA	-2.91	119.74	126.40
10	aB	825	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
10	aA	828	CLA	CMC-C2C-C1C	2.91	129.47	125.04
10	cB	817	CLA	CHD-C4C-NC	2.91	128.78	124.20
10	cL	205	CLA	CAA-C2A-C3A	-2.91	104.82	112.78
10	aB	828	CLA	CMC-C2C-C1C	2.91	129.47	125.04
10	aB	818	CLA	O2A-CGA-CBA	2.91	121.03	111.91
10	aA	804	CLA	C3B-C4B-NB	2.91	112.97	109.21
13	bB	844	BCR	C24-C23-C22	-2.91	121.84	126.23
10	bL	205	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
10	cA	838	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
10	aA	831	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
10	cA	809	CLA	CHC-C1C-C2C	-2.91	118.69	126.72
10	aB	813	CLA	CHC-C1C-C2C	-2.90	118.69	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	813	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
10	aB	806	CLA	CMB-C2B-C3B	2.90	130.11	124.68
10	aA	839	CLA	O2A-CGA-CBA	2.90	121.02	111.91
10	bA	821	CLA	CHD-C4C-NC	2.90	128.78	124.20
10	bB	825	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
10	bB	836	CLA	CAC-C3C-C4C	2.90	128.58	124.81
10	bB	840	CLA	CAC-C3C-C4C	2.90	128.58	124.81
10	aA	830	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
10	cB	814	CLA	C1-C2-C3	-2.90	121.02	126.04
10	bA	831	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
10	bB	832	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
13	aB	846	BCR	C15-C14-C13	-2.90	123.17	127.31
10	bB	813	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
10	aB	839	CLA	CAC-C3C-C4C	2.90	128.57	124.81
10	aL	205	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
10	aA	809	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
10	bL	205	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
10	aB	840	CLA	CAC-C3C-C4C	2.90	128.57	124.81
13	cB	846	BCR	C15-C14-C13	-2.90	123.17	127.31
10	aL	204	CLA	C3B-C4B-NB	2.90	112.96	109.21
10	cB	816	CLA	C3B-C4B-NB	2.90	112.96	109.21
10	bA	809	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
10	cB	829	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
10	aA	832	CLA	O2A-CGA-CBA	2.90	121.01	111.91
10	cA	814	CLA	CAC-C3C-C4C	2.90	128.57	124.81
10	cA	813	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
10	aA	854	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
10	cB	830	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
10	cA	832	CLA	C1-C2-C3	-2.90	121.03	126.04
10	cB	839	CLA	CAC-C3C-C4C	2.90	128.57	124.81
10	aA	841	CLA	C3B-C4B-NB	2.90	112.96	109.21
10	bL	205	CLA	CAA-C2A-C3A	-2.90	104.85	112.78
10	aA	832	CLA	C1-C2-C3	-2.90	121.03	126.04
10	cA	854	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
10	bA	832	CLA	O2A-CGA-CBA	2.90	121.00	111.91
10	aA	831	CLA	CHD-C4C-NC	2.89	128.76	124.20
10	aB	835	CLA	CHD-C4C-NC	2.89	128.76	124.20
10	cA	832	CLA	O2A-CGA-CBA	2.89	120.99	111.91
10	bA	854	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
10	cA	806	CLA	CAA-C2A-C3A	-2.89	104.85	112.78
10	cA	821	CLA	CHD-C4C-NC	2.89	128.76	124.20
10	aB	829	CLA	CHC-C1C-C2C	-2.89	118.72	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	cA	801	CL0	O2D-CGD-O1D	-2.89	118.18	123.84
10	aB	832	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
10	cA	804	CLA	CHB-C4A-NA	2.89	128.51	124.51
10	aA	827	CLA	CAC-C3C-C4C	2.89	128.56	124.81
10	aB	818	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
10	bB	829	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
10	aB	814	CLA	C1-C2-C3	-2.89	121.04	126.04
10	bB	818	CLA	O2A-CGA-CBA	2.89	120.98	111.91
10	bA	832	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
10	cA	833	CLA	CHB-C4A-NA	2.89	128.51	124.51
9	aA	801	CL0	O2D-CGD-O1D	-2.89	118.19	123.84
10	bA	830	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
10	aA	833	CLA	CHB-C4A-NA	2.89	128.50	124.51
10	bB	818	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
10	cB	838	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
10	aA	832	CLA	CHC-C1C-C2C	-2.89	118.74	126.72
10	bB	839	CLA	CAC-C3C-C4C	2.89	128.56	124.81
10	aA	804	CLA	CHB-C4A-NA	2.89	128.50	124.51
10	aB	809	CLA	CMC-C2C-C1C	2.89	129.43	125.04
10	bA	806	CLA	CMC-C2C-C1C	2.89	129.43	125.04
10	bB	840	CLA	CMC-C2C-C1C	2.89	129.43	125.04
10	bA	831	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
10	cA	832	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
10	cA	804	CLA	C3B-C4B-NB	2.89	112.94	109.21
10	cA	820	CLA	CHD-C4C-NC	2.88	128.75	124.20
10	cL	202	CLA	CAC-C3C-C4C	2.88	128.55	124.81
10	bA	827	CLA	CAC-C3C-C4C	2.88	128.55	124.81
10	aB	803	CLA	C4A-NA-C1A	-2.88	105.41	106.71
10	cB	836	CLA	CAC-C3C-C4C	2.88	128.55	124.81
10	aA	834	CLA	CBC-CAC-C3C	-2.88	104.48	112.43
10	aA	841	CLA	CHD-C4C-NC	2.88	128.74	124.20
10	bA	831	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
10	aA	804	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
10	cA	832	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
10	bB	809	CLA	CMC-C2C-C1C	2.88	129.42	125.04
10	cA	818	CLA	C2A-C3A-C4A	-2.88	97.22	101.87
10	cB	809	CLA	CMC-C2C-C1C	2.88	129.42	125.04
10	bL	202	CLA	C4A-NA-C1A	-2.88	105.41	106.71
10	cA	806	CLA	CMC-C2C-C1C	2.88	129.42	125.04
10	aA	820	CLA	CHD-C4C-NC	2.88	128.74	124.20
10	cA	831	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
10	bA	834	CLA	CBC-CAC-C3C	-2.88	104.50	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	818	CLA	C2A-C3A-C4A	-2.88	97.22	101.87
10	cB	832	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
10	cB	818	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
10	aA	806	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
9	cA	801	CL0	O2A-CGA-CBA	2.88	120.93	111.91
10	bA	806	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
10	cA	834	CLA	CBC-CAC-C3C	-2.87	104.51	112.43
10	cA	807	CLA	CHC-C1C-C2C	-2.87	118.77	126.72
10	aA	806	CLA	CMC-C2C-C1C	2.87	129.42	125.04
10	cA	827	CLA	CAC-C3C-C4C	2.87	128.54	124.81
16	cB	848	LMG	O6-C1-O1	-2.87	103.17	109.97
10	bB	816	CLA	C3B-C4B-NB	2.87	112.92	109.21
10	aB	819	CLA	CHD-C4C-NC	2.87	128.73	124.20
10	bA	834	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
10	bA	837	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
9	aA	801	CL0	C4C-C3C-C2C	-2.87	102.71	106.90
16	bB	848	LMG	O6-C1-O1	-2.87	103.17	109.97
10	aL	202	CLA	CAC-C3C-C4C	2.87	128.53	124.81
10	cA	817	CLA	C3B-C4B-NB	2.87	112.92	109.21
10	cA	841	CLA	CHD-C4C-NC	2.87	128.73	124.20
10	aA	832	CLA	CHD-C4C-NC	2.87	128.72	124.20
10	bA	807	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
9	cA	801	CL0	C4C-C3C-C2C	-2.87	102.72	106.90
16	aB	848	LMG	O6-C1-O1	-2.87	103.18	109.97
10	cA	831	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
10	aA	817	CLA	CAC-C3C-C4C	2.87	128.53	124.81
10	cA	856	CLA	CAC-C3C-C4C	2.87	128.53	124.81
10	aB	816	CLA	C3B-C4B-NB	2.87	112.92	109.21
10	bA	805	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
10	bA	818	CLA	C2A-C3A-C4A	-2.87	97.24	101.87
10	bB	834	CLA	CMA-C3A-C2A	-2.87	102.27	113.83
9	aA	801	CL0	O2A-CGA-CBA	2.87	120.90	111.91
10	aA	829	CLA	CAC-C3C-C4C	2.87	128.53	124.81
9	bA	801	CL0	O2A-CGA-CBA	2.87	120.90	111.91
10	aB	834	CLA	CMA-C3A-C2A	-2.87	102.27	113.83
10	cA	837	CLA	CHC-C1C-C2C	-2.87	118.80	126.72
10	bA	821	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
10	bA	838	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
10	cB	828	CLA	CMC-C2C-C1C	2.86	129.40	125.04
10	cB	803	CLA	C4A-NA-C1A	-2.86	105.42	106.71
10	aA	805	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
10	bA	841	CLA	CHD-C4C-NC	2.86	128.72	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	832	CLA	CHD-C4C-NC	2.86	128.72	124.20
13	bB	846	BCR	C15-C14-C13	-2.86	123.22	127.31
10	bA	804	CLA	CHB-C4A-NA	2.86	128.47	124.51
10	bB	819	CLA	CHD-C4C-NC	2.86	128.71	124.20
10	cA	834	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
13	aB	844	BCR	C24-C23-C22	-2.86	121.91	126.23
10	cB	807	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
10	aA	817	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
10	aA	803	CLA	CHD-C4C-NC	2.86	128.71	124.20
10	aA	816	CLA	O2A-CGA-CBA	2.86	120.88	111.91
10	aA	807	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
10	bA	838	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
10	aA	831	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
10	aB	820	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
10	aA	837	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
10	cB	815	CLA	C1-C2-C3	-2.86	121.10	126.04
10	cA	835	CLA	CAC-C3C-C4C	2.86	128.52	124.81
10	cB	826	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
10	cB	834	CLA	CMA-C3A-C2A	-2.86	102.30	113.83
10	aA	805	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
10	cB	806	CLA	CBA-CAA-C2A	2.86	122.30	113.86
10	aA	838	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
10	cA	820	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
10	cA	834	CLA	C4-C3-C5	2.86	120.07	115.27
9	bA	801	CL0	C4C-C3C-C2C	-2.86	102.74	106.90
10	bA	837	CLA	CHD-C4C-NC	2.85	128.70	124.20
10	bB	806	CLA	CBA-CAA-C2A	2.85	122.29	113.86
10	bA	829	CLA	CAC-C3C-C4C	2.85	128.51	124.81
10	bL	202	CLA	CAC-C3C-C4C	2.85	128.51	124.81
10	cA	819	CLA	C4-C3-C5	2.85	120.07	115.27
13	cB	844	BCR	C24-C23-C22	-2.85	121.93	126.23
10	aB	806	CLA	CBA-CAA-C2A	2.85	122.28	113.86
10	bB	821	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
10	cA	830	CLA	C3B-C4B-NB	2.85	112.89	109.21
10	bB	817	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
10	aA	808	CLA	CMC-C2C-C1C	2.85	129.38	125.04
10	cA	837	CLA	CHD-C4C-NC	2.85	128.69	124.20
10	aA	841	CLA	C4-C3-C5	2.85	120.06	115.27
10	bA	829	CLA	C1-C2-C3	-2.85	121.11	126.04
10	cA	838	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
10	bB	808	CLA	C1-C2-C3	-2.85	121.12	126.04
10	cA	829	CLA	C1-C2-C3	-2.85	121.12	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	819	CLA	C4-C3-C5	2.85	120.06	115.27
10	bB	821	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
10	cA	821	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
10	cA	817	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
10	bA	838	CLA	C3B-C4B-NB	2.85	112.89	109.21
10	aA	830	CLA	C1-C2-C3	-2.85	122.14	126.75
10	aB	821	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
10	bB	815	CLA	C1-C2-C3	-2.85	121.12	126.04
10	bA	834	CLA	C4-C3-C5	2.85	120.06	115.27
10	cA	830	CLA	C1-C2-C3	-2.85	122.14	126.75
10	bB	831	CLA	C3B-C4B-NB	2.85	112.89	109.21
10	aA	835	CLA	CAC-C3C-C4C	2.85	128.50	124.81
10	cB	808	CLA	C1-C2-C3	-2.85	121.12	126.04
10	cA	841	CLA	C4-C3-C5	2.85	120.06	115.27
13	cB	847	BCR	C3-C4-C5	-2.85	109.00	114.08
10	aB	840	CLA	CMC-C2C-C1C	2.85	129.37	125.04
10	aB	815	CLA	C1-C2-C3	-2.85	121.12	126.04
10	bA	804	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
10	aA	831	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
10	cL	202	CLA	C4A-NA-C1A	-2.84	105.43	106.71
10	cA	808	CLA	CMC-C2C-C1C	2.84	129.37	125.04
10	cA	838	CLA	C3B-C4B-NB	2.84	112.89	109.21
10	cA	816	CLA	O2A-CGA-CBA	2.84	120.83	111.91
10	aA	834	CLA	C4-C3-C5	2.84	120.05	115.27
10	aA	856	CLA	CAC-C3C-C4C	2.84	128.50	124.81
10	bA	820	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
10	cL	205	CLA	C1-C2-C3	-2.84	121.13	126.04
10	aA	837	CLA	CHD-C4C-NC	2.84	128.68	124.20
10	aB	817	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
10	bA	805	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
10	cB	839	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
10	aB	826	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
10	cB	831	CLA	C3B-C4B-NB	2.84	112.88	109.21
10	aB	839	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
10	cA	805	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
10	cA	812	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
10	aA	813	CLA	C4A-NA-C1A	-2.84	105.43	106.71
10	aA	834	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
10	bA	817	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
10	bA	806	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
10	cB	840	CLA	CMC-C2C-C1C	2.84	129.36	125.04
10	bA	856	CLA	CAC-C3C-C4C	2.84	128.49	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bB	847	BCR	C3-C4-C5	-2.84	109.01	114.08
10	bB	826	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
10	aA	819	CLA	C4-C3-C5	2.84	120.05	115.27
10	aA	838	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
10	aA	820	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
10	cA	804	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
10	bB	820	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
10	cB	808	CLA	C3B-C4B-NB	2.84	112.88	109.21
10	cA	817	CLA	CAC-C3C-C4C	2.84	128.49	124.81
10	bB	807	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
10	cB	821	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
10	cB	826	CLA	C4-C3-C5	2.83	120.04	115.27
10	bA	816	CLA	O2A-CGA-CBA	2.83	120.80	111.91
10	cA	803	CLA	CHD-C4C-NC	2.83	128.67	124.20
10	cA	825	CLA	CHD-C4C-NC	2.83	128.67	124.20
10	cB	833	CLA	CHD-C4C-NC	2.83	128.67	124.20
10	cA	832	CLA	CHD-C4C-NC	2.83	128.67	124.20
10	cB	819	CLA	CHD-C4C-NC	2.83	128.67	124.20
10	aA	838	CLA	CHD-C4C-NC	2.83	128.67	124.20
10	aA	829	CLA	C1-C2-C3	-2.83	121.14	126.04
10	cA	838	CLA	CHD-C4C-NC	2.83	128.67	124.20
10	bA	806	CLA	C3B-C4B-NB	2.83	112.87	109.21
10	bA	817	CLA	CAC-C3C-C4C	2.83	128.48	124.81
10	bA	835	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
10	bB	839	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
10	bL	203	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
10	bA	833	CLA	CHB-C4A-NA	2.83	128.43	124.51
10	bA	803	CLA	CHD-C4C-NC	2.83	128.66	124.20
13	cA	849	BCR	C28-C27-C26	-2.83	109.03	114.08
10	aB	817	CLA	O2A-CGA-CBA	2.83	120.79	111.91
10	bB	817	CLA	O2A-CGA-CBA	2.83	120.78	111.91
13	aA	849	BCR	C28-C27-C26	-2.83	109.03	114.08
10	aB	818	CLA	C1-C2-C3	-2.83	121.15	126.04
10	bL	205	CLA	C1-C2-C3	-2.83	121.15	126.04
10	aA	817	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
10	aB	821	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
10	aA	807	CLA	CHD-C4C-NC	2.83	128.66	124.20
10	bA	835	CLA	CAC-C3C-C4C	2.83	128.48	124.81
10	aA	835	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
10	aA	821	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
10	cA	805	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
10	aA	812	CLA	CHC-C1C-C2C	-2.83	118.91	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	812	CLA	CHC-C1C-C2C	-2.83	118.91	126.72
10	aB	807	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
10	cL	203	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
10	bB	826	CLA	C4-C3-C5	2.82	120.02	115.27
10	cA	807	CLA	CHB-C4A-NA	2.82	128.42	124.51
10	cB	821	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
10	aA	830	CLA	C3B-C4B-NB	2.82	112.86	109.21
10	bA	807	CLA	CHD-C4C-NC	2.82	128.65	124.20
10	aB	808	CLA	CMC-C2C-C1C	2.82	129.34	125.04
10	cB	817	CLA	O2A-CGA-CBA	2.82	120.77	111.91
10	bA	841	CLA	C4-C3-C5	2.82	120.02	115.27
10	cB	808	CLA	CMC-C2C-C1C	2.82	129.34	125.04
10	aA	806	CLA	C3B-C4B-NB	2.82	112.86	109.21
10	bB	808	CLA	CMC-C2C-C1C	2.82	129.33	125.04
10	bA	817	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
10	bA	807	CLA	CHB-C4A-NA	2.82	128.41	124.51
10	cA	837	CLA	CAA-C2A-C3A	-2.82	105.06	112.78
10	aA	823	CLA	CHD-C4C-NC	2.82	128.65	124.20
10	cA	806	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
10	bA	825	CLA	CHD-C4C-NC	2.82	128.65	124.20
11	cB	842	PQN	C11-C12-C13	-2.82	122.10	126.79
10	aL	203	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
10	bA	828	CLA	CHD-C4C-NC	2.82	128.64	124.20
10	bA	830	CLA	C1-C2-C3	-2.82	122.19	126.75
10	aL	204	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
10	cA	835	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
13	bA	849	BCR	C28-C27-C26	-2.82	109.05	114.08
10	aL	205	CLA	C1-C2-C3	-2.82	121.17	126.04
10	cA	829	CLA	CAC-C3C-C4C	2.82	128.46	124.81
10	aA	808	CLA	C3B-C4B-NB	2.82	112.85	109.21
10	bB	818	CLA	C1-C2-C3	-2.82	121.17	126.04
10	bA	827	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
10	cA	817	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
10	bA	839	CLA	C4-C3-C5	2.81	120.00	115.27
10	cA	840	CLA	O2A-CGA-CBA	2.81	120.74	111.91
10	aA	806	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
10	cL	203	CLA	CAC-C3C-C4C	2.81	128.46	124.81
10	aB	833	CLA	CHD-C4C-NC	2.81	128.64	124.20
11	bB	842	PQN	C11-C12-C13	-2.81	122.11	126.79
10	aA	807	CLA	CHB-C4A-NA	2.81	128.40	124.51
10	cA	813	CLA	C4A-NA-C1A	-2.81	105.44	106.71
11	aB	842	PQN	C11-C12-C13	-2.81	122.11	126.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	816	CLA	C4-C3-C5	2.81	120.00	115.27
10	cB	817	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
10	aA	827	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
10	aA	816	CLA	C4-C3-C5	2.81	120.00	115.27
10	aB	826	CLA	C4-C3-C5	2.81	120.00	115.27
10	bA	837	CLA	CAA-C2A-C3A	-2.81	105.08	112.78
13	aB	847	BCR	C3-C4-C5	-2.81	109.06	114.08
10	bL	203	CLA	CAC-C3C-C4C	2.81	128.46	124.81
10	cA	839	CLA	C4-C3-C5	2.81	120.00	115.27
10	aB	831	CLA	C3B-C4B-NB	2.81	112.84	109.21
10	bA	808	CLA	CMC-C2C-C1C	2.81	129.32	125.04
10	bL	203	CLA	CHD-C4C-NC	2.81	128.63	124.20
10	aB	808	CLA	C3B-C4B-NB	2.81	112.84	109.21
10	cA	806	CLA	C3B-C4B-NB	2.81	112.84	109.21
10	aL	203	CLA	CAC-C3C-C4C	2.81	128.45	124.81
10	bB	838	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
10	cA	828	CLA	CHD-C4C-NC	2.81	128.63	124.20
10	aL	202	CLA	C4A-NA-C1A	-2.81	105.44	106.71
10	cA	816	CLA	C4-C3-C5	2.81	119.99	115.27
10	bA	803	CLA	CAC-C3C-C4C	2.81	128.45	124.81
10	bA	823	CLA	CHD-C4C-NC	2.81	128.62	124.20
10	aA	840	CLA	O2A-CGA-CBA	2.81	120.71	111.91
10	bB	808	CLA	C3B-C4B-NB	2.81	112.84	109.21
10	cA	807	CLA	CHD-C4C-NC	2.81	128.62	124.20
10	cB	815	CLA	CMB-C2B-C3B	2.80	129.93	124.68
10	bA	830	CLA	C3B-C4B-NB	2.80	112.83	109.21
10	aA	837	CLA	CAA-C2A-C3A	-2.80	105.10	112.78
10	cB	818	CLA	C1-C2-C3	-2.80	121.19	126.04
10	aB	838	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
10	bA	809	CLA	CAC-C3C-C4C	2.80	128.45	124.81
10	aA	838	CLA	C3B-C4B-NB	2.80	112.83	109.21
10	aA	808	CLA	CAC-C3C-C4C	2.80	128.45	124.81
10	aB	815	CLA	CMB-C2B-C3B	2.80	129.92	124.68
10	aA	822	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
10	bA	840	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
10	cB	820	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
10	bA	822	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
10	bB	833	CLA	CHD-C4C-NC	2.80	128.62	124.20
10	cL	203	CLA	CHD-C4C-NC	2.80	128.62	124.20
10	cA	835	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
10	bA	808	CLA	C3B-C4B-NB	2.80	112.83	109.21
10	cB	823	CLA	CAC-C3C-C4C	2.80	128.44	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	837	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
10	bA	838	CLA	CHD-C4C-NC	2.80	128.62	124.20
10	bB	834	CLA	CHB-C4A-NA	2.80	128.38	124.51
11	bA	844	PQN	C2M-C2-C3	-2.80	119.83	124.40
10	aA	840	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
10	cB	838	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
10	bB	819	CLA	C2A-C3A-C4A	-2.80	97.35	101.87
10	bB	831	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
10	aA	836	CLA	O2A-CGA-CBA	2.80	120.69	111.91
13	aL	206	BCR	C31-C1-C6	2.80	114.84	110.30
10	cA	809	CLA	CAC-C3C-C4C	2.80	128.44	124.81
10	aB	823	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
10	aA	825	CLA	CHD-C4C-NC	2.80	128.61	124.20
10	cA	840	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
10	bB	815	CLA	CMB-C2B-C3B	2.80	129.91	124.68
10	aB	841	CLA	O2A-CGA-CBA	2.79	120.68	111.91
10	cA	822	CLA	CHC-C1C-C2C	-2.79	118.99	126.72
10	aL	203	CLA	CHD-C4C-NC	2.79	128.61	124.20
10	cA	823	CLA	CHD-C4C-NC	2.79	128.61	124.20
13	bB	844	BCR	C28-C27-C26	-2.79	109.09	114.08
10	cA	827	CLA	CHC-C1C-C2C	-2.79	118.99	126.72
10	cA	808	CLA	C3B-C4B-NB	2.79	112.82	109.21
10	cA	841	CLA	O2A-CGA-CBA	2.79	120.67	111.91
10	aA	809	CLA	CAC-C3C-C4C	2.79	128.43	124.81
10	bA	840	CLA	O2A-CGA-CBA	2.79	120.67	111.91
10	cA	813	CLA	CHD-C4C-NC	2.79	128.60	124.20
10	aB	828	CLA	C1-C2-C3	-2.79	121.21	126.04
10	cL	204	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
10	aA	839	CLA	C4-C3-C5	2.79	119.97	115.27
10	cA	836	CLA	O2A-CGA-CBA	2.79	120.67	111.91
10	aB	821	CLA	CHD-C4C-NC	2.79	128.60	124.20
13	bM	101	BCR	C15-C16-C17	-2.79	117.76	123.47
10	bA	835	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
13	cL	206	BCR	C31-C1-C6	2.79	114.83	110.30
10	aB	808	CLA	C1-C2-C3	-2.79	121.22	126.04
10	cA	841	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
10	aA	826	CLA	C1-C2-C3	-2.79	121.22	126.04
10	cB	815	CLA	CHD-C4C-NC	2.79	128.60	124.20
10	cB	823	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
10	cA	841	CLA	CMC-C2C-C1C	2.79	129.28	125.04
9	bA	801	CL0	C1-C2-C3	-2.79	121.22	126.04
10	bA	819	CLA	O2A-CGA-CBA	2.79	120.65	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	839	CLA	CHD-C4C-NC	2.79	128.59	124.20
10	bA	820	CLA	C3B-C4B-NB	2.79	112.81	109.21
10	bA	836	CLA	O2A-CGA-CBA	2.79	120.65	111.91
10	aA	841	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
13	aL	206	BCR	C29-C30-C25	2.79	114.77	110.48
10	cB	828	CLA	C1-C2-C3	-2.79	121.22	126.04
10	bB	837	CLA	CHC-C1C-C2C	-2.79	119.02	126.72
13	cL	206	BCR	C29-C30-C25	2.79	114.77	110.48
10	bB	828	CLA	CHC-C1C-C2C	-2.79	119.02	126.72
10	cB	841	CLA	O2A-CGA-CBA	2.79	120.65	111.91
10	cA	803	CLA	CAC-C3C-C4C	2.78	128.42	124.81
10	cB	827	CLA	C4-C3-C5	2.78	119.95	115.27
10	aA	841	CLA	O2A-CGA-CBA	2.78	120.64	111.91
10	cB	817	CLA	CHB-C4A-NA	2.78	128.36	124.51
10	cB	834	CLA	CHB-C4A-NA	2.78	128.36	124.51
10	aB	837	CLA	CHC-C1C-C2C	-2.78	119.02	126.72
10	aA	836	CLA	CHD-C4C-NC	2.78	128.59	124.20
10	bA	841	CLA	O2A-CGA-CBA	2.78	120.64	111.91
10	bA	841	CLA	CHC-C1C-C2C	-2.78	119.03	126.72
10	aA	835	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
10	aA	828	CLA	CHD-C4C-NC	2.78	128.59	124.20
10	bB	823	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
13	cA	851	BCR	C27-C26-C25	2.78	126.77	122.73
10	bB	841	CLA	O2A-CGA-CBA	2.78	120.63	111.91
10	aB	827	CLA	C4-C3-C5	2.78	119.95	115.27
10	bB	824	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
10	cB	819	CLA	C2A-C3A-C4A	-2.78	97.38	101.87
10	aB	824	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
10	bB	836	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
13	bL	206	BCR	C31-C1-C6	2.78	114.81	110.30
10	aA	816	CLA	CMC-C2C-C1C	2.78	129.27	125.04
10	cB	826	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
10	cB	802	CLA	CAC-C3C-C4C	2.78	128.41	124.81
10	aB	840	CLA	C3B-C4B-NB	2.78	112.80	109.21
11	aA	844	PQN	C2M-C2-C3	-2.78	119.87	124.40
10	bB	828	CLA	O1D-CGD-CBD	-2.78	118.80	124.48
10	aB	832	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
10	aB	828	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
10	bA	823	CLA	CHB-C4A-NA	2.78	128.35	124.51
10	cA	816	CLA	CMC-C2C-C1C	2.78	129.27	125.04
10	cA	826	CLA	C1-C2-C3	-2.77	121.24	126.04
10	cA	820	CLA	C3B-C4B-NB	2.77	112.80	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	841	CLA	CMC-C2C-C1C	2.77	129.26	125.04
10	aA	821	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
10	aB	831	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
10	bL	204	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
10	cA	820	CLA	O2A-CGA-CBA	2.77	120.61	111.91
10	bB	823	CLA	CAC-C3C-C4C	2.77	128.41	124.81
10	cB	839	CLA	CHD-C4C-NC	2.77	128.57	124.20
10	cB	809	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
13	cB	844	BCR	C28-C27-C26	-2.77	109.13	114.08
10	bB	826	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
10	aA	819	CLA	O2A-CGA-CBA	2.77	120.61	111.91
10	bA	826	CLA	C1-C2-C3	-2.77	121.25	126.04
10	cA	819	CLA	O2A-CGA-CBA	2.77	120.61	111.91
13	aB	844	BCR	C28-C27-C26	-2.77	109.13	114.08
10	bB	838	CLA	O2A-CGA-O1A	-2.77	116.60	123.59
10	bB	809	CLA	CHC-C1C-C2C	-2.77	119.06	126.72
10	aB	823	CLA	CAC-C3C-C4C	2.77	128.41	124.81
13	bL	206	BCR	C29-C30-C25	2.77	114.75	110.48
10	bA	806	CLA	CHD-C4C-NC	2.77	128.57	124.20
10	bA	808	CLA	CHD-C4C-NC	2.77	128.57	124.20
11	cA	844	PQN	C2M-C2-C3	-2.77	119.88	124.40
10	bB	821	CLA	CHD-C4C-NC	2.77	128.57	124.20
10	bA	816	CLA	CMC-C2C-C1C	2.77	129.26	125.04
10	cA	837	CLA	CAC-C3C-C4C	2.77	128.40	124.81
10	cA	836	CLA	CHD-C4C-NC	2.77	128.57	124.20
10	bB	827	CLA	C4-C3-C5	2.77	119.93	115.27
10	aA	806	CLA	CHD-C4C-NC	2.77	128.57	124.20
10	aB	838	CLA	O2A-CGA-O1A	-2.77	116.61	123.59
10	aA	840	CLA	CHD-C4C-NC	2.77	128.56	124.20
10	aA	836	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
10	bA	808	CLA	CAC-C3C-C4C	2.77	128.40	124.81
9	cA	801	CL0	CMC-C2C-C1C	2.77	129.25	125.04
13	cM	101	BCR	C15-C16-C17	-2.77	117.81	123.47
10	bA	820	CLA	O2A-CGA-CBA	2.77	120.59	111.91
10	aB	836	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
10	aB	815	CLA	CHD-C4C-NC	2.77	128.56	124.20
10	bB	815	CLA	CHD-C4C-NC	2.77	128.56	124.20
10	bB	809	CLA	CAA-C2A-C3A	-2.77	105.20	112.78
10	cB	835	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
10	bA	829	CLA	O2A-CGA-CBA	2.77	120.59	111.91
10	aB	840	CLA	CHD-C4C-NC	2.77	128.56	124.20
10	aA	837	CLA	CAC-C3C-C4C	2.77	128.40	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	820	CLA	O2A-CGA-CBA	2.77	120.58	111.91
10	cA	808	CLA	CHD-C4C-NC	2.76	128.56	124.20
10	cB	821	CLA	CHD-C4C-NC	2.76	128.56	124.20
10	cB	840	CLA	CHD-C4C-NC	2.76	128.56	124.20
10	aB	819	CLA	C2A-C3A-C4A	-2.76	97.40	101.87
10	bB	803	CLA	CHD-C4C-NC	2.76	128.56	124.20
10	cB	828	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
9	cA	801	CL0	C1-C2-C3	-2.76	121.26	126.04
10	aA	803	CLA	CAC-C3C-C4C	2.76	128.40	124.81
10	bA	836	CLA	CMC-C2C-C1C	2.76	129.25	125.04
10	cB	803	CLA	CHD-C4C-NC	2.76	128.56	124.20
10	aA	817	CLA	CMC-C2C-C1C	2.76	129.25	125.04
10	bA	802	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
10	cA	824	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
10	cA	835	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
10	cA	817	CLA	O2A-CGA-CBA	2.76	120.57	111.91
10	aA	829	CLA	O2A-CGA-CBA	2.76	120.57	111.91
10	bB	829	CLA	CMA-C3A-C2A	-2.76	102.69	113.83
10	cB	829	CLA	CMA-C3A-C2A	-2.76	102.69	113.83
10	aB	803	CLA	CHD-C4C-NC	2.76	128.55	124.20
10	aB	839	CLA	CHD-C4C-NC	2.76	128.55	124.20
10	bB	812	CLA	CHD-C4C-NC	2.76	128.55	124.20
10	bB	840	CLA	CHD-C4C-NC	2.76	128.55	124.20
10	aA	817	CLA	O2A-CGA-CBA	2.76	120.57	111.91
10	cA	816	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
10	aA	835	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
10	aB	828	CLA	O1D-CGD-CBD	-2.76	118.84	124.48
10	cB	809	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
10	cA	806	CLA	CHD-C4C-NC	2.76	128.55	124.20
10	cA	829	CLA	O2A-CGA-CBA	2.76	120.57	111.91
9	aA	801	CL0	C1-C2-C3	-2.76	121.27	126.04
10	cA	808	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
10	aA	817	CLA	CMB-C2B-C3B	2.76	129.84	124.68
10	bA	841	CLA	CMC-C2C-C1C	2.76	129.24	125.04
10	cA	836	CLA	CMC-C2C-C1C	2.76	129.24	125.04
10	bA	814	CLA	CMB-C2B-C3B	2.76	129.84	124.68
10	aA	813	CLA	CHD-C4C-NC	2.76	128.55	124.20
10	aA	820	CLA	C3B-C4B-NB	2.76	112.78	109.21
10	cA	817	CLA	CMB-C2B-C3B	2.76	129.84	124.68
10	aB	802	CLA	C4-C3-C5	2.76	119.91	115.27
10	bB	828	CLA	C1-C2-C3	-2.76	121.28	126.04
10	bB	840	CLA	C3B-C4B-NB	2.76	112.77	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	809	CLA	CAA-C2A-C3A	-2.76	105.23	112.78
10	bA	836	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
10	cA	836	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
10	aB	809	CLA	CHC-C1C-C2C	-2.76	119.10	126.72
10	aB	828	CLA	CHD-C4C-NC	2.76	128.55	124.20
13	bA	851	BCR	C27-C26-C25	2.76	126.73	122.73
10	bA	821	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
10	bB	817	CLA	CHB-C4A-NA	2.76	128.32	124.51
10	bA	817	CLA	O2A-CGA-CBA	2.76	120.55	111.91
10	cB	831	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
10	cA	807	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
10	cA	808	CLA	CAC-C3C-C4C	2.75	128.38	124.81
10	cB	832	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
10	bA	816	CLA	CHC-C1C-C2C	-2.75	119.10	126.72
10	bA	817	CLA	CMB-C2B-C3B	2.75	129.83	124.68
10	bA	837	CLA	CAC-C3C-C4C	2.75	128.38	124.81
13	aM	101	BCR	C15-C16-C17	-2.75	117.83	123.47
10	cB	840	CLA	C3B-C4B-NB	2.75	112.77	109.21
9	bA	801	CL0	CMC-C2C-C1C	2.75	129.23	125.04
13	cB	846	BCR	C27-C26-C25	2.75	126.73	122.73
10	aA	815	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
10	bA	813	CLA	CHD-C4C-NC	2.75	128.54	124.20
10	cB	828	CLA	O1D-CGD-CBD	-2.75	118.86	124.48
10	bB	808	CLA	CMB-C2B-C3B	2.75	129.82	124.68
10	aB	829	CLA	CMA-C3A-C2A	-2.75	102.73	113.83
10	cB	838	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
13	aA	851	BCR	C27-C26-C25	2.75	126.72	122.73
10	aB	835	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
10	cA	821	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
10	bL	204	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
13	aM	101	BCR	C2-C1-C6	2.75	114.71	110.48
13	bM	101	BCR	C2-C1-C6	2.75	114.71	110.48
10	cA	821	CLA	CMB-C2B-C3B	2.75	129.82	124.68
10	cB	802	CLA	C4-C3-C5	2.75	119.89	115.27
10	bA	824	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
10	aA	823	CLA	CHB-C4A-NA	2.75	128.31	124.51
10	aB	834	CLA	CHB-C4A-NA	2.75	128.31	124.51
10	bA	808	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
10	bA	835	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
10	bB	817	CLA	C4-C3-C5	2.75	119.89	115.27
10	aA	824	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
10	aB	808	CLA	CMB-C2B-C3B	2.75	129.82	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	817	CLA	CBC-CAC-C3C	-2.75	104.86	112.43
10	aB	802	CLA	CAC-C3C-C4C	2.75	128.37	124.81
10	cB	836	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
10	cB	801	CLA	O2A-CGA-CBA	2.75	120.52	111.91
9	aA	801	CL0	CMC-C2C-C1C	2.75	129.22	125.04
10	cB	827	CLA	CAA-C2A-C3A	-2.75	105.26	112.78
10	aB	826	CLA	C4C-C3C-C2C	-2.75	102.90	106.90
10	cL	204	CLA	CHC-C1C-C2C	-2.75	119.13	126.72
10	aA	836	CLA	CMC-C2C-C1C	2.74	129.22	125.04
10	bB	832	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
10	aB	801	CLA	O2A-CGA-CBA	2.74	120.52	111.91
13	aB	846	BCR	C27-C26-C25	2.74	126.72	122.73
10	cA	823	CLA	O2A-CGA-CBA	2.74	120.52	111.91
10	bB	837	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
10	aA	814	CLA	CMB-C2B-C3B	2.74	129.81	124.68
10	aB	827	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
10	aB	812	CLA	CHD-C4C-NC	2.74	128.52	124.20
10	bA	817	CLA	CBC-CAC-C3C	-2.74	104.87	112.43
10	cA	815	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
10	cA	802	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
10	cB	808	CLA	CMB-C2B-C3B	2.74	129.81	124.68
13	cA	848	BCR	C27-C26-C25	2.74	126.71	122.73
10	aA	816	CLA	CHC-C1C-C2C	-2.74	119.14	126.72
10	cL	204	CLA	O2A-CGA-CBA	2.74	120.51	111.91
10	cB	817	CLA	C4-C3-C5	2.74	119.88	115.27
10	aL	203	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
10	cB	828	CLA	CAC-C3C-C4C	2.74	128.36	124.81
10	aA	802	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
10	cB	824	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
10	bB	801	CLA	O2A-CGA-CBA	2.74	120.50	111.91
10	bA	821	CLA	CMB-C2B-C3B	2.74	129.80	124.68
10	bA	823	CLA	O2A-CGA-CBA	2.74	120.50	111.91
10	aA	808	CLA	CHD-C4C-NC	2.74	128.52	124.20
10	bA	828	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
10	aA	838	CLA	C1-C2-C3	-2.74	122.32	126.75
10	aB	819	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
10	cB	812	CLA	CHD-C4C-NC	2.74	128.51	124.20
10	bA	813	CLA	C4A-NA-C1A	-2.74	105.48	106.71
10	aA	834	CLA	CHD-C4C-NC	2.74	128.51	124.20
10	aA	821	CLA	CMB-C2B-C3B	2.74	129.80	124.68
10	cB	830	CLA	O2A-CGA-CBA	2.74	120.49	111.91
10	bA	815	CLA	C4C-C3C-C2C	-2.73	102.91	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	834	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
10	aA	808	CLA	CHC-C1C-C2C	-2.73	119.16	126.72
10	aA	841	CLA	CAA-C2A-C3A	-2.73	105.29	112.78
13	bB	846	BCR	C27-C26-C25	2.73	126.70	122.73
10	bA	836	CLA	CHD-C4C-NC	2.73	128.51	124.20
10	aB	830	CLA	O2A-CGA-CBA	2.73	120.48	111.91
10	bB	828	CLA	CAC-C3C-C4C	2.73	128.36	124.81
10	bA	807	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
13	bA	848	BCR	C40-C30-C25	2.73	114.73	110.30
10	aB	832	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
10	bB	835	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
10	bB	841	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
10	cA	823	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
13	aA	848	BCR	C27-C26-C25	2.73	126.70	122.73
10	cA	841	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
10	aA	807	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
10	bA	840	CLA	CHD-C4C-NC	2.73	128.51	124.20
10	cA	821	CLA	O2A-CGA-CBA	2.73	120.48	111.91
10	cA	840	CLA	CHD-C4C-NC	2.73	128.50	124.20
10	cA	817	CLA	CBC-CAC-C3C	-2.73	104.91	112.43
10	aA	823	CLA	O2A-CGA-CBA	2.73	120.47	111.91
10	aL	204	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
10	cB	841	CLA	CBC-CAC-C3C	-2.73	104.91	112.43
10	aL	203	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
10	bB	841	CLA	CBC-CAC-C3C	-2.73	104.91	112.43
10	aB	841	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
10	cB	837	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
10	cA	823	CLA	CHB-C4A-NA	2.73	128.28	124.51
10	bL	204	CLA	O2A-CGA-CBA	2.73	120.47	111.91
10	cB	841	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
10	bB	830	CLA	O2A-CGA-CBA	2.73	120.46	111.91
10	aA	840	CLA	C3B-C4B-NB	2.73	112.73	109.21
10	aL	204	CLA	O2A-CGA-CBA	2.73	120.46	111.91
10	bA	841	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
10	aA	828	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
10	cA	828	CLA	CHC-C1C-C2C	-2.72	119.18	126.72
10	aB	817	CLA	CHB-C4A-NA	2.72	128.28	124.51
10	aB	817	CLA	C4-C3-C5	2.72	119.85	115.27
10	cA	806	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
10	bB	827	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
10	bB	802	CLA	C4-C3-C5	2.72	119.85	115.27
13	cM	101	BCR	C2-C1-C6	2.72	114.67	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	821	CLA	O2A-CGA-CBA	2.72	120.45	111.91
10	bL	203	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
10	aA	821	CLA	O2A-CGA-CBA	2.72	120.44	111.91
10	cA	817	CLA	CMC-C2C-C1C	2.72	129.18	125.04
10	aA	811	CLA	C4-C3-C5	2.72	119.85	115.27
10	aA	807	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
10	bB	808	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
10	aB	808	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
10	bA	832	CLA	CHB-C4A-NA	2.72	128.27	124.51
10	aB	837	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
10	cB	841	CLA	CHD-C4C-NC	2.72	128.49	124.20
10	aB	841	CLA	CBC-CAC-C3C	-2.72	104.94	112.43
10	cB	808	CLA	CHC-C1C-C2C	-2.72	119.21	126.72
10	bB	832	CLA	CAA-C2A-C3A	-2.72	105.34	112.78
10	cA	834	CLA	CHD-C4C-NC	2.72	128.48	124.20
10	cA	814	CLA	CMB-C2B-C3B	2.71	129.76	124.68
10	aB	815	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
10	bB	827	CLA	OBD-CAD-C3D	-2.71	121.99	128.52
10	bB	804	CLA	O2A-CGA-CBA	2.71	120.42	111.91
10	cA	856	CLA	CAA-C2A-C3A	-2.71	105.35	112.78
10	bB	802	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
10	bB	802	CLA	CAC-C3C-C4C	2.71	128.33	124.81
10	cB	804	CLA	O2A-CGA-CBA	2.71	120.42	111.91
10	bB	828	CLA	CHD-C4C-NC	2.71	128.47	124.20
10	bA	829	CLA	C4-C3-C5	2.71	119.83	115.27
10	cB	815	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
10	cB	819	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
10	cB	832	CLA	CAA-C2A-C3A	-2.71	105.36	112.78
10	aA	806	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
10	cB	806	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
10	cL	203	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
13	bA	848	BCR	C27-C26-C25	2.71	126.66	122.73
10	bA	838	CLA	C1-C2-C3	-2.71	122.37	126.75
10	cL	203	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
10	bA	824	CLA	C4-C3-C5	2.71	119.82	115.27
10	cB	807	CLA	CHB-C4A-NA	2.71	128.25	124.51
10	bL	203	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
10	bB	841	CLA	CHD-C4C-NC	2.70	128.47	124.20
10	aA	819	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
13	aA	848	BCR	C40-C30-C25	2.70	114.68	110.30
10	aB	834	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
10	cA	824	CLA	C4-C3-C5	2.70	119.82	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	856	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
10	cA	832	CLA	CHB-C4A-NA	2.70	128.25	124.51
10	bA	806	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
10	bA	839	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
10	aB	807	CLA	CHB-C4A-NA	2.70	128.25	124.51
10	bA	817	CLA	CMC-C2C-C1C	2.70	129.15	125.04
10	bB	819	CLA	CAC-C3C-C4C	2.70	128.31	124.81
10	aA	835	CLA	CHD-C4C-NC	2.70	128.46	124.20
10	cA	838	CLA	C1-C2-C3	-2.70	122.38	126.75
10	aL	202	CLA	CAA-C2A-C1A	2.70	120.82	111.97
10	aB	819	CLA	CAC-C3C-C4C	2.70	128.31	124.81
10	bA	811	CLA	C4-C3-C5	2.70	119.81	115.27
10	bA	842	CLA	CMC-C2C-C1C	2.70	129.15	125.04
10	cL	202	CLA	CAA-C2A-C1A	2.70	120.82	111.97
10	bB	810	CLA	CHD-C4C-NC	2.70	128.46	124.20
10	cA	804	CLA	CHD-C4C-NC	2.70	128.46	124.20
10	cB	802	CLA	CBC-CAC-C3C	-2.70	104.99	112.43
10	cA	839	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
10	aA	824	CLA	C4-C3-C5	2.70	119.81	115.27
10	cA	829	CLA	C4-C3-C5	2.70	119.81	115.27
10	bB	815	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
10	aA	834	CLA	CAA-C2A-C3A	-2.70	105.39	112.78
10	bA	806	CLA	C1-C2-C3	-2.70	121.38	126.04
10	cB	819	CLA	CAC-C3C-C4C	2.70	128.31	124.81
10	bA	804	CLA	CHD-C4C-NC	2.70	128.45	124.20
10	cB	805	CLA	O2A-CGA-CBA	2.70	120.37	111.91
10	aB	804	CLA	O2A-CGA-CBA	2.70	120.37	111.91
10	cB	828	CLA	CHD-C4C-NC	2.70	128.45	124.20
10	bL	203	CLA	C1-C2-C3	-2.70	121.38	126.04
10	cA	811	CLA	C4-C3-C5	2.70	119.81	115.27
10	aA	832	CLA	CHB-C4A-NA	2.70	128.24	124.51
10	bA	807	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
10	cA	819	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
10	cB	834	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
10	aB	802	CLA	CBC-CAC-C3C	-2.69	105.00	112.43
10	bB	806	CLA	CBC-CAC-C3C	-2.69	105.00	112.43
10	bA	842	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
10	aA	816	CLA	CAC-C3C-C4C	2.69	128.31	124.81
10	bB	819	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
10	aB	805	CLA	O2A-CGA-CBA	2.69	120.36	111.91
10	aA	829	CLA	C4-C3-C5	2.69	119.80	115.27
10	cA	834	CLA	CAA-C2A-C3A	-2.69	105.41	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	856	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
10	bB	805	CLA	O2A-CGA-CBA	2.69	120.36	111.91
10	cB	827	CLA	OBD-CAD-C3D	-2.69	122.04	128.52
10	bL	202	CLA	CAA-C2A-C1A	2.69	120.79	111.97
10	aB	828	CLA	CAC-C3C-C4C	2.69	128.30	124.81
10	aB	827	CLA	OBD-CAD-C3D	-2.69	122.05	128.52
10	aB	806	CLA	CBC-CAC-C3C	-2.69	105.02	112.43
10	bA	835	CLA	CHD-C4C-NC	2.69	128.44	124.20
10	bB	807	CLA	CHB-C4A-NA	2.69	128.23	124.51
10	aA	811	CLA	CHB-C4A-NA	2.69	128.23	124.51
10	bA	811	CLA	CHD-C4C-NC	2.69	128.44	124.20
10	bA	819	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
10	bA	834	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
10	aA	804	CLA	CHD-C4C-NC	2.69	128.44	124.20
13	cA	848	BCR	C40-C30-C25	2.68	114.65	110.30
10	bB	820	CLA	O2A-CGA-CBA	2.68	120.33	111.91
10	cB	820	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
10	cL	204	CLA	CMC-C2C-C1C	2.68	129.12	125.04
10	aB	812	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
10	aA	854	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
10	aA	839	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
10	bA	823	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
10	bA	854	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
10	aB	841	CLA	CHD-C4C-NC	2.68	128.43	124.20
10	cA	816	CLA	CAC-C3C-C4C	2.68	128.29	124.81
10	cA	834	CLA	CAC-C3C-C4C	2.68	128.29	124.81
10	cB	839	CLA	O2A-CGA-CBA	2.68	120.31	111.91
10	aA	842	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
10	aA	842	CLA	CMC-C2C-C1C	2.68	129.12	125.04
10	bB	812	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
10	cA	807	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
10	bA	834	CLA	CHD-C4C-NC	2.68	128.42	124.20
10	aB	820	CLA	O2A-CGA-CBA	2.68	120.31	111.91
10	cB	803	CLA	C1-C2-C3	-2.68	121.42	126.04
10	aB	810	CLA	CHD-C4C-NC	2.67	128.42	124.20
10	cB	810	CLA	CHD-C4C-NC	2.67	128.42	124.20
10	bA	856	CLA	CHD-C4C-NC	2.67	128.42	124.20
10	bB	826	CLA	CHD-C4C-NC	2.67	128.42	124.20
10	bA	825	CLA	CAC-C3C-C4C	2.67	128.28	124.81
10	aB	820	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
10	bB	827	CLA	CAC-C3C-C4C	2.67	128.28	124.81
10	aB	823	CLA	CHD-C4C-NC	2.67	128.41	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	840	CLA	C3B-C4B-NB	2.67	112.67	109.21
10	cA	854	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
10	cB	805	CLA	O2D-CGD-CBD	2.67	116.02	111.27
10	bL	204	CLA	CMC-C2C-C1C	2.67	129.11	125.04
10	cB	838	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
10	aA	827	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
10	cB	820	CLA	O2A-CGA-CBA	2.67	120.29	111.91
10	bB	803	CLA	C1-C2-C3	-2.67	121.42	126.04
10	aL	203	CLA	C1-C2-C3	-2.67	121.43	126.04
10	cA	842	CLA	CMC-C2C-C1C	2.67	129.10	125.04
10	aA	806	CLA	C1-C2-C3	-2.67	121.43	126.04
10	cB	826	CLA	CHD-C4C-NC	2.67	128.41	124.20
10	cA	842	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
10	aB	803	CLA	C1-C2-C3	-2.67	121.43	126.04
10	bB	820	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
10	bA	840	CLA	C3B-C4B-NB	2.67	112.66	109.21
10	cB	827	CLA	CAC-C3C-C4C	2.67	128.27	124.81
10	bB	814	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
10	aB	826	CLA	CAA-C2A-C1A	-2.67	103.23	111.97
10	cA	811	CLA	CHD-C4C-NC	2.67	128.41	124.20
10	cA	835	CLA	CHD-C4C-NC	2.67	128.41	124.20
10	bA	813	CLA	CHB-C4A-NA	2.67	128.20	124.51
10	bA	816	CLA	CAC-C3C-C4C	2.67	128.27	124.81
10	aA	823	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
10	cA	841	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
10	aB	814	CLA	CAA-C2A-C3A	-2.67	105.48	112.78
10	aA	808	CLA	CBC-CAC-C3C	-2.67	105.08	112.43
10	aB	815	CLA	CHB-C4A-NA	2.67	128.20	124.51
10	bB	839	CLA	O2A-CGA-CBA	2.67	120.27	111.91
10	bA	841	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
10	aB	839	CLA	O2A-CGA-CBA	2.67	120.27	111.91
10	cA	827	CLA	CAA-C2A-C3A	-2.66	105.48	112.78
10	bA	815	CLA	CAA-C2A-C3A	-2.66	105.48	112.78
10	cA	856	CLA	CHD-C4C-NC	2.66	128.40	124.20
10	bB	811	CLA	O2A-CGA-CBA	2.66	120.27	111.91
10	aB	837	CLA	CHD-C4C-NC	2.66	128.40	124.20
10	cB	825	CLA	CHD-C4C-NC	2.66	128.40	124.20
10	bB	826	CLA	CAA-C2A-C1A	-2.66	103.25	111.97
10	cA	840	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
10	aL	204	CLA	CMC-C2C-C1C	2.66	129.09	125.04
10	cB	814	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
10	bA	834	CLA	CAC-C3C-C4C	2.66	128.26	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	812	CLA	CAC-C3C-C4C	2.66	128.26	124.81
10	aA	812	CLA	CHD-C4C-NC	2.66	128.40	124.20
10	aB	810	CLA	CHB-C4A-NA	2.66	128.19	124.51
13	bM	101	BCR	C31-C1-C6	2.66	114.61	110.30
10	aB	827	CLA	CAC-C3C-C4C	2.66	128.26	124.81
10	cA	815	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
13	cM	101	BCR	C31-C1-C6	2.66	114.61	110.30
10	cB	812	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
10	bB	805	CLA	O2D-CGD-CBD	2.66	115.99	111.27
10	cB	826	CLA	CAA-C2A-C1A	-2.66	103.27	111.97
10	bA	811	CLA	CHB-C4A-NA	2.66	128.19	124.51
10	cB	803	CLA	CHC-C1C-C2C	-2.66	119.38	126.72
10	aA	825	CLA	CAC-C3C-C4C	2.66	128.25	124.81
10	bB	838	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
10	cA	806	CLA	C1-C2-C3	-2.65	121.45	126.04
10	aB	811	CLA	O2A-CGA-CBA	2.65	120.23	111.91
10	cB	811	CLA	O2A-CGA-CBA	2.65	120.23	111.91
10	bA	807	CLA	CMB-C2B-C3B	2.65	129.64	124.68
13	aM	101	BCR	C31-C1-C6	2.65	114.60	110.30
10	cL	203	CLA	C1-C2-C3	-2.65	121.46	126.04
10	aA	815	CLA	CAA-C2A-C3A	-2.65	105.52	112.78
10	aA	856	CLA	CHD-C4C-NC	2.65	128.38	124.20
10	bB	825	CLA	CHD-C4C-NC	2.65	128.38	124.20
10	aB	805	CLA	O2D-CGD-CBD	2.65	115.98	111.27
10	bA	814	CLA	CHD-C4C-NC	2.65	128.38	124.20
10	aB	803	CLA	CHC-C1C-C2C	-2.65	119.39	126.72
10	aB	825	CLA	CHD-C4C-NC	2.65	128.38	124.20
10	cB	834	CLA	CHD-C4C-NC	2.65	128.38	124.20
10	aL	203	CLA	O2A-CGA-CBA	2.65	120.22	111.91
10	aB	836	CLA	CHD-C4C-NC	2.65	128.38	124.20
10	bB	833	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
10	aA	811	CLA	CHD-C4C-NC	2.65	128.37	124.20
10	bA	827	CLA	CHD-C4C-NC	2.65	128.37	124.20
10	bB	837	CLA	CHD-C4C-NC	2.65	128.37	124.20
10	cB	836	CLA	CHD-C4C-NC	2.65	128.37	124.20
10	cA	825	CLA	CAC-C3C-C4C	2.65	128.24	124.81
10	bA	808	CLA	CBC-CAC-C3C	-2.65	105.14	112.43
10	aA	841	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
10	cA	812	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
10	cL	203	CLA	CMB-C2B-C3B	2.65	129.63	124.68
10	cA	808	CLA	CBC-CAC-C3C	-2.65	105.14	112.43
10	bB	836	CLA	CHD-C4C-NC	2.65	128.37	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	831	CLA	CMC-C2C-C1C	2.64	129.07	125.04
10	bB	803	CLA	CHC-C1C-C2C	-2.64	119.41	126.72
10	bB	838	CLA	CHB-C4A-NA	2.64	128.17	124.51
10	bA	825	CLA	C1-C2-C3	-2.64	121.47	126.04
10	aB	826	CLA	CHD-C4C-NC	2.64	128.37	124.20
10	bA	812	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
10	cL	203	CLA	O2A-CGA-CBA	2.64	120.20	111.91
10	cB	818	CLA	CHB-C4A-NA	2.64	128.17	124.51
10	bA	827	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
10	cA	811	CLA	CHB-C4A-NA	2.64	128.16	124.51
10	cB	823	CLA	CHD-C4C-NC	2.64	128.37	124.20
10	cB	837	CLA	CHD-C4C-NC	2.64	128.37	124.20
10	aB	831	CLA	CMC-C2C-C1C	2.64	129.06	125.04
10	bA	840	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
10	bL	203	CLA	O2A-CGA-CBA	2.64	120.19	111.91
10	aL	205	CLA	CHD-C4C-NC	2.64	128.36	124.20
10	bB	823	CLA	CHD-C4C-NC	2.64	128.36	124.20
10	cB	831	CLA	CHD-C4C-NC	2.64	128.36	124.20
10	cA	825	CLA	C1-C2-C3	-2.64	121.48	126.04
10	aA	825	CLA	C1-C2-C3	-2.64	121.48	126.04
10	cA	824	CLA	CMC-C2C-C1C	2.64	129.06	125.04
10	aB	833	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
10	bB	815	CLA	CHB-C4A-NA	2.64	128.16	124.51
10	cA	812	CLA	CHD-C4C-NC	2.64	128.36	124.20
10	aA	840	CLA	CMB-C2B-C3B	2.64	129.61	124.68
10	aA	839	CLA	CAA-C2A-C3A	-2.63	105.56	112.78
10	bA	810	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
10	aL	205	CLA	O2A-CGA-CBA	2.63	120.17	111.91
10	aA	812	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
10	cB	838	CLA	CHB-C4A-NA	2.63	128.15	124.51
10	bA	839	CLA	CBC-CAC-C3C	-2.63	105.18	112.43
10	cB	833	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
10	cA	839	CLA	CBC-CAC-C3C	-2.63	105.18	112.43
10	cA	839	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
10	aA	840	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
10	bB	812	CLA	CMA-C3A-C2A	-2.63	103.22	113.83
10	bL	203	CLA	CMB-C2B-C3B	2.63	129.60	124.68
10	bA	812	CLA	CHD-C4C-NC	2.63	128.35	124.20
10	bB	804	CLA	CHA-C1A-NA	-2.63	120.38	126.40
10	aL	203	CLA	CMB-C2B-C3B	2.63	129.60	124.68
10	cA	813	CLA	CHB-C4A-NA	2.63	128.15	124.51
10	cB	824	CLA	CHD-C4C-NC	2.63	128.34	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	839	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
10	bL	205	CLA	O2A-CGA-CBA	2.63	120.15	111.91
10	aB	815	CLA	CAA-C2A-C3A	-2.63	105.59	112.78
10	bA	824	CLA	CMC-C2C-C1C	2.63	129.04	125.04
10	cA	807	CLA	CBA-CAA-C2A	2.63	121.61	113.86
10	aB	838	CLA	CHB-C4A-NA	2.63	128.14	124.51
10	bA	840	CLA	CMB-C2B-C3B	2.63	129.59	124.68
10	bB	831	CLA	CMC-C2C-C1C	2.63	129.04	125.04
9	aA	801	CL0	CHD-C4C-NC	2.63	128.34	124.20
10	cB	818	CLA	CHD-C4C-NC	2.63	128.34	124.20
10	cB	812	CLA	CAC-C3C-C4C	2.63	128.22	124.81
10	bA	856	CLA	CED-O2D-CGD	2.62	121.87	115.94
10	aA	824	CLA	CMC-C2C-C1C	2.62	129.03	125.04
10	aB	818	CLA	CHB-C4A-NA	2.62	128.14	124.51
10	cB	810	CLA	CHB-C4A-NA	2.62	128.14	124.51
10	cA	807	CLA	CMB-C2B-C3B	2.62	129.59	124.68
10	aB	824	CLA	CHD-C4C-NC	2.62	128.34	124.20
10	bB	824	CLA	CHD-C4C-NC	2.62	128.34	124.20
10	cL	205	CLA	CHD-C4C-NC	2.62	128.34	124.20
10	aB	838	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
10	aB	812	CLA	CMA-C3A-C2A	-2.62	103.25	113.83
10	cB	807	CLA	CMA-C3A-C2A	-2.62	103.25	113.83
11	aB	842	PQN	C14-C13-C15	2.62	119.68	115.27
10	bA	834	CLA	CHB-C4A-NA	2.62	128.14	124.51
10	cA	834	CLA	CHB-C4A-NA	2.62	128.13	124.51
10	cB	815	CLA	CHB-C4A-NA	2.62	128.13	124.51
10	aB	807	CLA	CMA-C3A-C2A	-2.62	103.26	113.83
10	bB	807	CLA	CMA-C3A-C2A	-2.62	103.26	113.83
10	bB	815	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
10	cA	840	CLA	CMB-C2B-C3B	2.62	129.58	124.68
9	cA	801	CL0	CHD-C4C-NC	2.62	128.33	124.20
10	bA	838	CLA	CMC-C2C-C1C	2.62	129.03	125.04
10	aA	807	CLA	CBA-CAA-C2A	2.62	121.59	113.86
10	aA	856	CLA	CED-O2D-CGD	2.62	121.86	115.94
10	bB	840	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
10	bB	818	CLA	CHB-C4A-NA	2.62	128.13	124.51
10	aB	812	CLA	CAC-C3C-C4C	2.62	128.21	124.81
10	cA	827	CLA	CHD-C4C-NC	2.62	128.33	124.20
10	cA	825	CLA	C3B-C4B-NB	2.62	112.59	109.21
10	aB	827	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
10	aA	834	CLA	CAC-C3C-C4C	2.62	128.21	124.81
10	bA	839	CLA	CAA-C2A-C3A	-2.62	105.61	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bL	205	CLA	CHD-C4C-NC	2.62	128.32	124.20
10	aB	818	CLA	CHD-C4C-NC	2.61	128.32	124.20
10	bA	832	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
10	cL	205	CLA	O2A-CGA-CBA	2.61	120.11	111.91
10	aA	814	CLA	CHD-C4C-NC	2.61	128.32	124.20
10	cA	806	CLA	CHB-C4A-NA	2.61	128.12	124.51
10	bB	815	CLA	CAC-C3C-C4C	2.61	128.20	124.81
10	bL	204	CLA	CHD-C4C-NC	2.61	128.32	124.20
10	aB	804	CLA	CHA-C1A-NA	-2.61	120.42	126.40
10	bB	834	CLA	CHD-C4C-NC	2.61	128.32	124.20
10	aB	806	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
11	bB	842	PQN	C14-C13-C15	2.61	119.66	115.27
10	aA	819	CLA	CMB-C2B-C3B	2.61	129.56	124.68
10	cB	812	CLA	CMA-C3A-C2A	-2.61	103.30	113.83
10	cB	801	CLA	CMC-C2C-C1C	2.61	129.01	125.04
10	aB	801	CLA	CMC-C2C-C1C	2.61	129.01	125.04
10	bB	840	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
9	bA	801	CL0	CHD-C4C-NC	2.61	128.31	124.20
10	aB	815	CLA	CAC-C3C-C4C	2.61	128.19	124.81
10	bA	854	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
10	cB	806	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
10	cB	819	CLA	CMC-C2C-C1C	2.61	129.01	125.04
10	bA	819	CLA	CMB-C2B-C3B	2.61	129.56	124.68
10	cA	810	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
10	cB	814	CLA	CMB-C2B-C3B	2.61	129.55	124.68
10	aB	831	CLA	CHD-C4C-NC	2.61	128.31	124.20
10	cB	815	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
10	aB	819	CLA	CMC-C2C-C1C	2.60	129.01	125.04
10	cA	830	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
10	aB	834	CLA	CHD-C4C-NC	2.60	128.31	124.20
10	aA	810	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
10	aA	834	CLA	CHB-C4A-NA	2.60	128.11	124.51
10	aA	807	CLA	CMB-C2B-C3B	2.60	129.55	124.68
10	cA	819	CLA	CMB-C2B-C3B	2.60	129.55	124.68
10	cB	827	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
10	bB	827	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
10	cA	856	CLA	CED-O2D-CGD	2.60	121.83	115.94
11	cB	842	PQN	C14-C13-C15	2.60	119.65	115.27
10	cB	804	CLA	CHA-C1A-NA	-2.60	120.44	126.40
10	bB	810	CLA	CHB-C4A-NA	2.60	128.11	124.51
10	cB	814	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
10	cB	840	CLA	CHC-C1C-C2C	-2.60	119.53	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	827	CLA	CHD-C4C-NC	2.60	128.30	124.20
10	bB	831	CLA	CHD-C4C-NC	2.60	128.30	124.20
10	cA	814	CLA	CHD-C4C-NC	2.60	128.30	124.20
10	cL	204	CLA	CHD-C4C-NC	2.60	128.30	124.20
10	cA	811	CLA	C1-C2-C3	-2.60	121.55	126.04
10	aA	813	CLA	CAC-C3C-C4C	2.60	128.18	124.81
10	bA	811	CLA	C1-C2-C3	-2.60	121.55	126.04
10	aB	808	CLA	CED-O2D-CGD	2.60	121.82	115.94
10	aA	854	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
10	bA	813	CLA	CAC-C3C-C4C	2.60	128.18	124.81
10	aA	811	CLA	C1-C2-C3	-2.60	121.55	126.04
10	bA	825	CLA	CMB-C2B-C3B	2.60	129.54	124.68
10	aA	832	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
10	bA	822	CLA	CMC-C2C-C1C	2.60	129.00	125.04
10	bB	806	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
10	cB	815	CLA	CAC-C3C-C4C	2.60	128.18	124.81
10	cA	854	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
10	aB	840	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
10	bA	807	CLA	CBA-CAA-C2A	2.60	121.53	113.86
10	bB	808	CLA	CED-O2D-CGD	2.60	121.81	115.94
10	cA	832	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
10	cB	808	CLA	CED-O2D-CGD	2.59	121.81	115.94
13	cA	848	BCR	C30-C25-C26	-2.59	118.96	122.61
10	bA	806	CLA	CHB-C4A-NA	2.59	128.10	124.51
10	cA	825	CLA	CMB-C2B-C3B	2.59	129.53	124.68
10	cA	814	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
10	aB	814	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
10	bA	814	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
10	aA	833	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
13	bA	850	BCR	C15-C16-C17	-2.59	118.17	123.47
10	aB	832	CLA	CMB-C2B-C3B	2.59	129.53	124.68
10	aA	830	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
10	aA	813	CLA	CHB-C4A-NA	2.59	128.09	124.51
10	bB	801	CLA	CMC-C2C-C1C	2.59	128.98	125.04
10	cB	817	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
13	cB	845	BCR	C27-C26-C25	2.59	126.49	122.73
10	aB	841	CLA	C4A-NA-C1A	-2.59	105.54	106.71
10	bB	810	CLA	CBC-CAC-C3C	-2.59	105.29	112.43
10	cB	820	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
10	aB	840	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
10	bB	814	CLA	CMB-C2B-C3B	2.59	129.52	124.68
10	aB	805	CLA	CHC-C1C-NC	2.59	128.13	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	817	CLA	CHB-C4A-NA	2.59	128.09	124.51
10	bA	833	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
10	aB	817	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
10	bA	811	CLA	O2A-CGA-CBA	2.59	120.03	111.91
10	aB	810	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
10	cB	841	CLA	C4A-NA-C1A	-2.59	105.54	106.71
10	cB	810	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
10	bA	830	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
10	aA	810	CLA	CMB-C2B-C3B	2.59	129.52	124.68
10	aA	825	CLA	CMB-C2B-C3B	2.59	129.52	124.68
10	aL	204	CLA	CHD-C4C-NC	2.59	128.28	124.20
10	aA	811	CLA	O2A-CGA-CBA	2.59	120.02	111.91
13	cA	850	BCR	C15-C16-C17	-2.59	118.18	123.47
13	aA	848	BCR	C30-C25-C26	-2.59	118.97	122.61
10	cA	840	CLA	C1-C2-C3	-2.59	121.57	126.04
10	aA	814	CLA	CAA-C2A-C3A	-2.58	105.70	112.78
10	aA	838	CLA	CMC-C2C-C1C	2.58	128.97	125.04
13	aI	102	BCR	C15-C14-C13	-2.58	123.62	127.31
13	aA	850	BCR	C15-C16-C17	-2.58	118.18	123.47
13	aI	102	BCR	C15-C16-C17	-2.58	118.18	123.47
10	aB	814	CLA	CMB-C2B-C3B	2.58	129.51	124.68
10	bA	825	CLA	C3B-C4B-NB	2.58	112.55	109.21
10	cA	823	CLA	CAC-C3C-C4C	2.58	128.16	124.81
10	aA	802	CLA	CHD-C4C-NC	2.58	128.27	124.20
10	bA	802	CLA	CBC-CAC-C3C	-2.58	105.31	112.43
10	cB	832	CLA	CMB-C2B-C3B	2.58	129.51	124.68
10	cA	843	CLA	CAA-C2A-C3A	-2.58	105.71	112.78
10	bB	818	CLA	CHD-C4C-NC	2.58	128.27	124.20
10	bA	831	CLA	CAA-C2A-C3A	-2.58	105.71	112.78
10	cA	810	CLA	CMB-C2B-C3B	2.58	129.50	124.68
10	aA	822	CLA	CMC-C2C-C1C	2.58	128.97	125.04
10	aA	856	CLA	CMB-C2B-C3B	2.58	129.50	124.68
10	cA	802	CLA	CBC-CAC-C3C	-2.58	105.32	112.43
10	cA	827	CLA	CHB-C4A-NA	2.58	128.08	124.51
10	bB	819	CLA	CMC-C2C-C1C	2.58	128.97	125.04
13	cI	103	BCR	C15-C16-C17	-2.58	118.19	123.47
10	aA	825	CLA	C3B-C4B-NB	2.58	112.54	109.21
13	bA	846	BCR	C11-C10-C9	-2.58	123.63	127.31
10	cA	813	CLA	CAC-C3C-C4C	2.58	128.15	124.81
10	cB	829	CLA	O2A-CGA-CBA	2.58	119.99	111.91
10	aA	806	CLA	CHB-C4A-NA	2.57	128.07	124.51
10	bB	832	CLA	CMB-C2B-C3B	2.57	129.49	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	820	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
10	cA	831	CLA	CMC-C2C-C1C	2.57	128.96	125.04
10	cB	816	CLA	CHD-C4C-NC	2.57	128.26	124.20
10	cA	811	CLA	O2A-CGA-CBA	2.57	119.98	111.91
10	cB	825	CLA	CMC-C2C-C1C	2.57	128.96	125.04
10	aA	817	CLA	CHB-C4A-NA	2.57	128.07	124.51
10	aA	810	CLA	CHD-C4C-NC	2.57	128.25	124.20
10	bA	839	CLA	CHD-C4C-NC	2.57	128.25	124.20
13	aA	851	BCR	C1-C6-C5	-2.57	118.99	122.61
10	bB	808	CLA	O2A-CGA-CBA	2.57	119.97	111.91
10	aA	831	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
10	bB	817	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
10	cB	841	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
10	aA	827	CLA	CHB-C4A-NA	2.57	128.06	124.51
10	bB	814	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
10	aB	816	CLA	CHD-C4C-NC	2.57	128.25	124.20
10	aA	802	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
10	cA	833	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
10	cB	831	CLA	CHB-C4A-NA	2.57	128.06	124.51
13	bI	102	BCR	C15-C16-C17	-2.57	118.21	123.47
13	cI	103	BCR	C15-C14-C13	-2.57	123.65	127.31
10	bA	810	CLA	CMB-C2B-C3B	2.57	129.48	124.68
13	bB	845	BCR	C27-C26-C25	2.57	126.46	122.73
10	cA	802	CLA	CHD-C4C-NC	2.57	128.25	124.20
10	cA	815	CLA	CBC-CAC-C3C	-2.57	105.36	112.43
10	bA	827	CLA	CHB-C4A-NA	2.57	128.06	124.51
10	aB	820	CLA	CAA-C2A-C3A	-2.56	105.75	112.78
10	aA	815	CLA	CBC-CAC-C3C	-2.56	105.36	112.43
10	bA	832	CLA	CMC-C2C-C1C	2.56	128.94	125.04
10	bB	829	CLA	O2A-CGA-CBA	2.56	119.96	111.91
13	aB	845	BCR	C27-C26-C25	2.56	126.45	122.73
10	aA	843	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
10	aB	829	CLA	O2A-CGA-CBA	2.56	119.95	111.91
10	aA	806	CLA	CMB-C2B-C3B	2.56	129.47	124.68
10	bA	843	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
10	cB	808	CLA	O2A-CGA-CBA	2.56	119.95	111.91
10	bA	831	CLA	CMC-C2C-C1C	2.56	128.94	125.04
10	bB	825	CLA	CMC-C2C-C1C	2.56	128.94	125.04
10	cB	840	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
10	bA	811	CLA	CMB-C2B-C3B	2.56	129.47	124.68
10	cA	831	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
10	aA	831	CLA	CMC-C2C-C1C	2.56	128.94	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	833	CLA	O2A-CGA-CBA	2.56	119.94	111.91
10	cA	856	CLA	CMB-C2B-C3B	2.56	129.47	124.68
10	bA	810	CLA	CHD-C4C-NC	2.56	128.24	124.20
10	cA	811	CLA	CMB-C2B-C3B	2.56	129.47	124.68
10	bA	856	CLA	CMB-C2B-C3B	2.56	129.47	124.68
10	cA	810	CLA	CHD-C4C-NC	2.56	128.24	124.20
10	bA	829	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
13	bI	102	BCR	C15-C14-C13	-2.56	123.66	127.31
10	bB	811	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
10	aB	808	CLA	O2A-CGA-CBA	2.56	119.93	111.91
13	bA	848	BCR	C30-C25-C26	-2.56	119.01	122.61
13	cA	851	BCR	C1-C6-C5	-2.56	119.01	122.61
10	aB	804	CLA	CHC-C1C-C2C	-2.56	119.65	126.72
10	aA	814	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
10	cB	804	CLA	CHC-C1C-C2C	-2.56	119.65	126.72
10	cA	803	CLA	CHB-C4A-NA	2.56	128.05	124.51
10	cA	806	CLA	CMB-C2B-C3B	2.56	129.46	124.68
10	bB	821	CLA	CHB-C4A-NA	2.55	128.04	124.51
10	cA	817	CLA	CHB-C4A-NA	2.55	128.04	124.51
10	cA	856	CLA	CHB-C4A-NA	2.55	128.04	124.51
10	aB	822	CLA	CHB-C4A-NA	2.55	128.04	124.51
10	bA	856	CLA	CHB-C4A-NA	2.55	128.04	124.51
10	bA	817	CLA	C1-C2-C3	-2.55	121.63	126.04
10	bB	841	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
10	aB	821	CLA	CHB-C4A-NA	2.55	128.04	124.51
10	bA	815	CLA	CBC-CAC-C3C	-2.55	105.39	112.43
10	bA	827	CLA	CMC-C2C-C1C	2.55	128.93	125.04
10	aB	841	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
10	aB	814	CLA	CMC-C2C-C1C	2.55	128.92	125.04
10	bB	816	CLA	CHD-C4C-NC	2.55	128.22	124.20
10	bA	823	CLA	CAC-C3C-C4C	2.55	128.12	124.81
10	bB	814	CLA	CMC-C2C-C1C	2.55	128.92	125.04
10	bA	854	CLA	CAC-C3C-C2C	2.55	131.89	127.53
13	aA	846	BCR	C11-C10-C9	-2.55	123.67	127.31
10	aB	816	CLA	CHB-C4A-NA	2.55	128.03	124.51
10	cA	818	CLA	CAA-CBA-CGA	2.55	120.69	113.25
10	bA	840	CLA	CAC-C3C-C4C	2.55	128.11	124.81
10	cB	823	CLA	CAA-C2A-C3A	-2.55	105.81	112.78
10	bA	819	CLA	CHB-C4A-NA	2.55	128.03	124.51
10	bB	828	CLA	CBA-CAA-C2A	2.55	121.38	113.86
10	aA	827	CLA	CMC-C2C-C1C	2.55	128.92	125.04
10	bA	826	CLA	CAA-C2A-C3A	-2.55	105.81	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	829	CLA	CAA-C2A-C3A	-2.55	105.81	112.78
10	bA	833	CLA	O2A-CGA-CBA	2.55	119.90	111.91
10	aA	817	CLA	C1-C2-C3	-2.55	121.64	126.04
10	bA	803	CLA	O1D-CGD-CBD	-2.54	119.28	124.48
10	aA	840	CLA	CAC-C3C-C4C	2.54	128.11	124.81
10	cA	840	CLA	CAC-C3C-C4C	2.54	128.11	124.81
10	aB	811	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
10	aB	817	CLA	CMC-C2C-C1C	2.54	128.91	125.04
10	aB	825	CLA	CMC-C2C-C1C	2.54	128.91	125.04
10	cA	838	CLA	CMC-C2C-C1C	2.54	128.91	125.04
10	aA	856	CLA	CHB-C4A-NA	2.54	128.03	124.51
10	bB	804	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
10	aB	837	CLA	O2A-CGA-CBA	2.54	119.89	111.91
10	cA	833	CLA	O2A-CGA-CBA	2.54	119.89	111.91
10	bA	818	CLA	CAA-CBA-CGA	2.54	120.68	113.25
10	bB	825	CLA	CHA-C1A-NA	-2.54	120.58	126.40
9	cA	801	CL0	CHB-C4A-NA	2.54	128.03	124.51
10	aL	204	CLA	CAC-C3C-C4C	2.54	128.11	124.81
13	cA	846	BCR	C11-C10-C9	-2.54	123.68	127.31
10	bB	805	CLA	CHC-C1C-NC	2.54	128.06	124.20
10	bA	843	CLA	CMB-C2B-C3B	2.54	129.43	124.68
10	cA	817	CLA	C1-C2-C3	-2.54	121.65	126.04
10	aA	826	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
10	aB	828	CLA	CBA-CAA-C2A	2.54	121.36	113.86
10	aA	854	CLA	CAC-C3C-C2C	2.54	131.87	127.53
10	cA	839	CLA	CHD-C4C-NC	2.54	128.21	124.20
10	aA	840	CLA	C1-C2-C3	-2.54	121.65	126.04
10	bA	806	CLA	CMB-C2B-C3B	2.54	129.43	124.68
10	bB	815	CLA	CBC-CAC-C3C	-2.54	105.43	112.43
10	bA	840	CLA	C1-C2-C3	-2.54	121.65	126.04
10	aA	819	CLA	CHB-C4A-NA	2.54	128.02	124.51
10	cB	821	CLA	CHB-C4A-NA	2.54	128.02	124.51
10	bB	815	CLA	O2A-CGA-CBA	2.54	119.87	111.91
10	aA	832	CLA	CMC-C2C-C1C	2.54	128.90	125.04
10	aB	838	CLA	CMB-C2B-C3B	2.54	129.42	124.68
10	cB	803	CLA	O2A-CGA-CBA	2.54	119.87	111.91
10	cB	814	CLA	CMC-C2C-C1C	2.54	128.90	125.04
10	bB	841	CLA	CAC-C3C-C4C	2.54	128.10	124.81
10	cA	826	CLA	CHC-C1C-C2C	-2.54	119.71	126.72
10	bL	203	CLA	CMC-C2C-C1C	2.54	128.90	125.04
10	cB	828	CLA	CBA-CAA-C2A	2.54	121.35	113.86
10	aB	823	CLA	CAA-C2A-C3A	-2.54	105.84	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	805	CLA	CHC-C1C-NC	2.54	128.05	124.20
10	cB	837	CLA	O2A-CGA-CBA	2.54	119.86	111.91
10	bL	204	CLA	C1-O2A-CGA	2.53	123.09	116.44
10	cB	816	CLA	CHB-C4A-NA	2.53	128.02	124.51
10	bB	803	CLA	O2A-CGA-CBA	2.53	119.86	111.91
10	cB	832	CLA	C4-C3-C5	2.53	119.53	115.27
10	cA	826	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
10	aA	829	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
10	cA	832	CLA	CMC-C2C-C1C	2.53	128.90	125.04
10	cA	819	CLA	CHB-C4A-NA	2.53	128.01	124.51
10	aB	837	CLA	C1-C2-C3	-2.53	121.66	126.04
10	aA	823	CLA	CAC-C3C-C4C	2.53	128.10	124.81
10	bB	831	CLA	CHB-C4A-NA	2.53	128.01	124.51
10	cA	822	CLA	CMC-C2C-C1C	2.53	128.90	125.04
10	bA	841	CLA	C1-C2-C3	-2.53	121.66	126.04
10	aA	839	CLA	CHD-C4C-NC	2.53	128.19	124.20
10	aA	818	CLA	CAA-CBA-CGA	2.53	120.65	113.25
10	cB	811	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
10	aL	204	CLA	C1-O2A-CGA	2.53	123.08	116.44
10	bB	819	CLA	CAA-CBA-CGA	2.53	120.65	113.25
10	bA	820	CLA	C1-C2-C3	-2.53	121.67	126.04
10	cA	854	CLA	CAC-C3C-C2C	2.53	131.86	127.53
10	aA	826	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
10	bB	823	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
10	cA	836	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
10	aB	803	CLA	O2A-CGA-CBA	2.53	119.85	111.91
10	aA	815	CLA	CAC-C3C-C4C	2.53	128.09	124.81
10	bA	805	CLA	CMC-C2C-C1C	2.53	128.89	125.04
10	cB	822	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
10	aA	811	CLA	CMB-C2B-C3B	2.53	129.41	124.68
10	cB	837	CLA	C1-C2-C3	-2.53	121.67	126.04
10	bB	816	CLA	CHB-C4A-NA	2.53	128.01	124.51
10	bA	802	CLA	CHD-C4C-NC	2.53	128.19	124.20
10	aB	825	CLA	CHA-C1A-NA	-2.53	120.61	126.40
10	aA	805	CLA	CMC-C2C-C1C	2.53	128.89	125.04
10	cA	805	CLA	CMC-C2C-C1C	2.53	128.89	125.04
10	cA	815	CLA	CAC-C3C-C4C	2.53	128.09	124.81
9	cA	801	CL0	CGD-CBD-CAD	-2.53	102.55	110.73
10	aA	822	CLA	O2A-CGA-CBA	2.53	119.84	111.91
10	bB	838	CLA	CMB-C2B-C3B	2.53	129.41	124.68
10	bA	826	CLA	CHC-C1C-C2C	-2.53	119.73	126.72
10	aB	841	CLA	CAC-C3C-C4C	2.53	128.09	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	814	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
10	cB	815	CLA	CBC-CAC-C3C	-2.53	105.47	112.43
10	aB	803	CLA	CHB-C4A-NA	2.53	128.01	124.51
10	aA	820	CLA	C1-C2-C3	-2.53	121.67	126.04
10	cB	822	CLA	CHB-C4A-NA	2.53	128.00	124.51
10	aB	815	CLA	O2A-CGA-CBA	2.53	119.83	111.91
13	bA	851	BCR	C1-C6-C5	-2.53	119.06	122.61
10	cB	819	CLA	CBC-CAC-C3C	-2.53	105.47	112.43
10	aA	805	CLA	CHB-C4A-NA	2.53	128.00	124.51
10	aB	835	CLA	CAC-C3C-C4C	2.52	128.09	124.81
10	cA	820	CLA	C1-C2-C3	-2.52	121.68	126.04
10	cA	841	CLA	C1-C2-C3	-2.52	121.68	126.04
10	aB	819	CLA	CBC-CAC-C3C	-2.52	105.47	112.43
10	bB	837	CLA	C1-C2-C3	-2.52	121.68	126.04
10	cB	841	CLA	C1-C2-C3	-2.52	121.68	126.04
10	bB	822	CLA	CHB-C4A-NA	2.52	128.00	124.51
10	cL	204	CLA	C1-O2A-CGA	2.52	123.06	116.44
9	bA	801	CL0	CGD-CBD-CAD	-2.52	102.56	110.73
10	aB	815	CLA	CBC-CAC-C3C	-2.52	105.47	112.43
10	aA	836	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
10	aB	831	CLA	CHB-C4A-NA	2.52	128.00	124.51
10	aB	819	CLA	CAA-CBA-CGA	2.52	120.62	113.25
10	bL	204	CLA	CAC-C3C-C4C	2.52	128.08	124.81
10	bB	837	CLA	O2A-CGA-CBA	2.52	119.82	111.91
10	cB	813	CLA	CMB-C2B-C3B	2.52	129.39	124.68
10	cA	818	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
10	cA	816	CLA	CHB-C4A-NA	2.52	127.99	124.51
10	bB	832	CLA	C4-C3-C5	2.52	119.51	115.27
13	bB	845	BCR	C7-C8-C9	-2.52	122.43	126.23
10	bB	819	CLA	CBC-CAC-C3C	-2.52	105.49	112.43
10	cB	825	CLA	CHA-C1A-NA	-2.52	120.63	126.40
10	cA	813	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
9	aA	801	CL0	CGD-CBD-CAD	-2.52	102.58	110.73
10	aB	822	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
10	aA	803	CLA	CHB-C4A-NA	2.52	127.99	124.51
10	bB	817	CLA	CMC-C2C-C1C	2.52	128.87	125.04
10	bB	814	CLA	O1D-CGD-CBD	-2.52	119.34	124.48
10	bB	803	CLA	CHB-C4A-NA	2.52	127.99	124.51
10	cB	815	CLA	O2A-CGA-CBA	2.51	119.80	111.91
10	bB	825	CLA	O1D-CGD-CBD	-2.51	119.34	124.48
10	cA	814	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
10	aB	832	CLA	CAC-C3C-C4C	2.51	128.07	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	841	CLA	C1-C2-C3	-2.51	121.70	126.04
10	bA	824	CLA	O1D-CGD-CBD	-2.51	119.34	124.48
10	cB	838	CLA	CMB-C2B-C3B	2.51	129.38	124.68
10	aA	841	CLA	C1-C2-C3	-2.51	121.70	126.04
10	bB	832	CLA	CAC-C3C-C4C	2.51	128.07	124.81
10	aB	803	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
10	bL	203	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
10	aA	803	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
10	cA	824	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
10	cL	203	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
10	cA	822	CLA	O2A-CGA-CBA	2.51	119.78	111.91
10	aA	813	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
10	cB	819	CLA	CAA-CBA-CGA	2.51	120.58	113.25
10	aB	837	CLA	CMC-C2C-C1C	2.51	128.86	125.04
10	cA	843	CLA	CMB-C2B-C3B	2.51	129.37	124.68
10	bA	822	CLA	CAC-C3C-C4C	2.51	128.06	124.81
10	bA	805	CLA	CHB-C4A-NA	2.51	127.98	124.51
10	cL	203	CLA	CMC-C2C-C1C	2.51	128.86	125.04
10	bB	822	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
10	aB	814	CLA	O1D-CGD-CBD	-2.51	119.36	124.48
10	cA	805	CLA	CHB-C4A-NA	2.51	127.98	124.51
10	aL	203	CLA	CAA-C2A-C3A	-2.51	105.92	112.78
10	bA	822	CLA	O2A-CGA-CBA	2.51	119.77	111.91
10	bB	813	CLA	CMB-C2B-C3B	2.51	129.37	124.68
10	aB	841	CLA	C1-C2-C3	-2.50	121.71	126.04
10	cA	803	CLA	O1D-CGD-CBD	-2.50	119.36	124.48
10	bB	837	CLA	CMC-C2C-C1C	2.50	128.85	125.04
10	bB	820	CLA	CHB-C4A-NA	2.50	127.97	124.51
10	cA	833	CLA	C1-C2-C3	-2.50	121.72	126.04
10	cA	815	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
10	bB	808	CLA	CAC-C3C-C4C	2.50	128.06	124.81
10	cB	841	CLA	CAC-C3C-C4C	2.50	128.06	124.81
10	aB	820	CLA	C4-C3-C5	2.50	119.48	115.27
10	cB	820	CLA	C4-C3-C5	2.50	119.48	115.27
10	aA	830	CLA	CHB-C4A-NA	2.50	127.97	124.51
10	bB	841	CLA	CHB-C4A-NA	2.50	127.97	124.51
9	bA	801	CL0	C4-C3-C5	2.50	119.48	115.27
10	aA	824	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
10	bB	803	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
10	cB	803	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
10	cA	841	CLA	CMB-C2B-C3B	2.50	129.36	124.68
10	bA	833	CLA	C1-C2-C3	-2.50	121.72	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	816	CLA	CHB-C4A-NA	2.50	127.97	124.51
10	bA	818	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
10	aB	806	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
9	bA	801	CL0	CHB-C4A-NA	2.50	127.97	124.51
10	aB	807	CLA	CHD-C4C-NC	2.50	128.14	124.20
10	cA	827	CLA	CMC-C2C-C1C	2.50	128.84	125.04
10	aA	815	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
10	bA	815	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
10	bA	813	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
10	aB	822	CLA	CMC-C2C-C1C	2.50	128.84	125.04
10	cB	817	CLA	CMC-C2C-C1C	2.50	128.84	125.04
10	aA	835	CLA	CBC-CAC-C3C	-2.50	105.55	112.43
10	bB	835	CLA	CMB-C2B-C3B	2.50	129.35	124.68
10	cB	813	CLA	CHD-C4C-NC	2.50	128.14	124.20
10	aB	832	CLA	C4-C3-C5	2.50	119.47	115.27
13	bL	207	BCR	C15-C16-C17	-2.50	118.36	123.47
10	bA	823	CLA	C1-C2-C3	-2.50	121.73	126.04
9	aA	801	CL0	C4-C3-C5	2.49	119.47	115.27
10	aB	838	CLA	CAC-C3C-C4C	2.49	128.05	124.81
10	bA	815	CLA	CAC-C3C-C4C	2.49	128.05	124.81
10	cB	822	CLA	CMC-C2C-C1C	2.49	128.84	125.04
10	cB	841	CLA	CHB-C4A-NA	2.49	127.96	124.51
10	aB	821	CLA	CAC-C3C-C4C	2.49	128.05	124.81
10	cB	808	CLA	CAC-C3C-C4C	2.49	128.04	124.81
10	aA	822	CLA	CAC-C3C-C4C	2.49	128.04	124.81
10	aB	816	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
10	aB	825	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
10	cB	837	CLA	CMC-C2C-C1C	2.49	128.83	125.04
10	aB	841	CLA	CHB-C4A-NA	2.49	127.96	124.51
10	bA	841	CLA	CMB-C2B-C3B	2.49	129.34	124.68
10	cB	835	CLA	CAC-C3C-C4C	2.49	128.04	124.81
10	aA	841	CLA	CMB-C2B-C3B	2.49	129.34	124.68
10	aA	843	CLA	CMB-C2B-C3B	2.49	129.34	124.68
10	aB	824	CLA	CMB-C2B-C3B	2.49	129.34	124.68
9	aA	801	CL0	CHB-C4A-NA	2.49	127.95	124.51
10	aB	820	CLA	CHB-C4A-NA	2.49	127.95	124.51
10	cA	835	CLA	CBC-CAC-C3C	-2.49	105.57	112.43
13	bB	843	BCR	C15-C16-C17	-2.49	118.37	123.47
10	cA	822	CLA	CAC-C3C-C4C	2.49	128.04	124.81
10	bA	836	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
10	bA	805	CLA	C1-C2-C3	-2.49	121.74	126.04
10	bB	817	CLA	CMB-C2B-C3B	2.49	129.33	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	833	CLA	CMB-C2B-C3B	2.49	129.33	124.68
10	aB	808	CLA	CAC-C3C-C4C	2.49	128.04	124.81
10	bA	812	CLA	C4-C3-C5	2.49	119.46	115.27
10	aA	833	CLA	CBC-CAC-C3C	-2.49	105.57	112.43
10	aB	833	CLA	CMB-C2B-C3B	2.49	129.33	124.68
10	bB	823	CLA	CMB-C2B-C3B	2.49	129.33	124.68
10	cB	825	CLA	O1D-CGD-CBD	-2.49	119.40	124.48
10	cA	823	CLA	CBC-CAC-C3C	-2.49	105.58	112.43
10	cB	824	CLA	CMB-C2B-C3B	2.49	129.33	124.68
10	aA	814	CLA	CHB-C4A-NA	2.49	127.95	124.51
10	aB	816	CLA	O1D-CGD-CBD	-2.49	119.40	124.48
10	bB	816	CLA	CAA-C2A-C3A	-2.49	105.97	112.78
10	bA	823	CLA	CBC-CAC-C3C	-2.49	105.58	112.43
10	cA	823	CLA	C1-C2-C3	-2.49	121.75	126.04
10	aL	203	CLA	CMC-C2C-C1C	2.48	128.82	125.04
10	aA	818	CLA	O1D-CGD-CBD	-2.48	119.40	124.48
10	cA	832	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
13	aB	847	BCR	C35-C13-C14	-2.48	119.44	122.92
10	cA	833	CLA	CBC-CAC-C3C	-2.48	105.58	112.43
13	aL	207	BCR	C27-C26-C25	2.48	126.34	122.73
16	aB	848	LMG	O1-C7-C8	-2.48	104.91	110.90
10	bA	803	CLA	CHB-C4A-NA	2.48	127.94	124.51
10	aA	821	CLA	CAC-C3C-C4C	2.48	128.03	124.81
10	cA	812	CLA	C4-C3-C5	2.48	119.45	115.27
10	bA	816	CLA	CHB-C4A-NA	2.48	127.94	124.51
10	cB	816	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
10	aB	835	CLA	CMB-C2B-C3B	2.48	129.32	124.68
10	aB	813	CLA	CHD-C4C-NC	2.48	128.11	124.20
13	cL	207	BCR	C27-C26-C25	2.48	126.33	122.73
9	aA	801	CL0	CMB-C2B-C1B	2.48	132.28	128.46
10	bB	806	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
10	cB	832	CLA	CAC-C3C-C4C	2.48	128.03	124.81
10	bB	820	CLA	C4-C3-C5	2.48	119.44	115.27
10	cA	821	CLA	CMC-C2C-C1C	2.48	128.81	125.04
10	bA	821	CLA	CMC-C2C-C1C	2.48	128.81	125.04
10	cB	814	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
10	bA	835	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
10	aB	821	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
10	bA	820	CLA	CHB-C4A-NA	2.48	127.94	124.51
10	bB	821	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
10	cB	823	CLA	CMB-C2B-C3B	2.48	129.31	124.68
10	cL	204	CLA	CAC-C3C-C4C	2.48	128.02	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	bA	801	CL0	CMB-C2B-C1B	2.48	132.27	128.46
10	aB	823	CLA	CMB-C2B-C3B	2.48	129.31	124.68
10	bA	839	CLA	CMB-C2B-C3B	2.48	129.31	124.68
10	bB	824	CLA	CMB-C2B-C3B	2.48	129.31	124.68
10	aB	813	CLA	CMB-C2B-C3B	2.48	129.31	124.68
10	bA	832	CLA	CBC-CAC-C3C	-2.48	105.61	112.43
10	bB	821	CLA	CAC-C3C-C4C	2.48	128.02	124.81
10	bA	814	CLA	CHB-C4A-NA	2.48	127.94	124.51
13	cL	207	BCR	C15-C16-C17	-2.48	118.40	123.47
9	cA	801	CL0	CMB-C2B-C1B	2.47	132.27	128.46
10	cB	821	CLA	CAA-C2A-C3A	-2.47	106.00	112.78
10	aA	823	CLA	CBC-CAC-C3C	-2.47	105.61	112.43
10	aA	805	CLA	C1-C2-C3	-2.47	121.76	126.04
10	aA	833	CLA	C1-C2-C3	-2.47	121.76	126.04
10	aB	817	CLA	CMB-C2B-C3B	2.47	129.31	124.68
10	bA	833	CLA	CBC-CAC-C3C	-2.47	105.61	112.43
10	bA	821	CLA	CAC-C3C-C4C	2.47	128.02	124.81
10	aB	801	CLA	CBC-CAC-C3C	-2.47	105.61	112.43
9	cA	801	CL0	C4-C3-C5	2.47	119.43	115.27
11	aA	844	PQN	C2M-C2-C1	2.47	120.37	116.27
10	bA	830	CLA	CHB-C4A-NA	2.47	127.93	124.51
10	cB	803	CLA	CHB-C4A-NA	2.47	127.93	124.51
10	cA	820	CLA	CAC-C3C-C4C	2.47	128.02	124.81
10	cB	818	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
11	bA	844	PQN	C2M-C2-C1	2.47	120.36	116.27
10	cB	817	CLA	CMB-C2B-C3B	2.47	129.30	124.68
10	aA	812	CLA	C4-C3-C5	2.47	119.43	115.27
10	bB	816	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
10	cB	816	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
10	cB	816	CLA	CMB-C2B-C3B	2.47	129.30	124.68
10	cB	835	CLA	CMB-C2B-C3B	2.47	129.30	124.68
10	cB	806	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
10	bB	838	CLA	CAC-C3C-C4C	2.47	128.01	124.81
16	cB	848	LMG	O1-C7-C8	-2.47	104.94	110.90
13	cB	847	BCR	C35-C13-C14	-2.47	119.47	122.92
10	aB	816	CLA	CMB-C2B-C3B	2.47	129.29	124.68
10	bB	833	CLA	CMB-C2B-C3B	2.47	129.29	124.68
11	cA	844	PQN	C2M-C2-C1	2.47	120.36	116.27
10	bA	830	CLA	CMA-C3A-C4A	-2.47	105.14	111.77
10	bB	841	CLA	C4A-NA-C1A	-2.47	105.60	106.71
13	aA	848	BCR	C31-C1-C6	2.47	114.30	110.30
10	aA	823	CLA	C1-C2-C3	-2.47	121.78	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	820	CLA	CHB-C4A-NA	2.47	127.92	124.51
10	cA	826	CLA	C3B-C4B-NB	2.47	112.40	109.21
10	bB	822	CLA	CMC-C2C-C1C	2.47	128.79	125.04
10	cB	801	CLA	CBC-CAC-C3C	-2.47	105.64	112.43
10	cA	842	CLA	CHD-C4C-NC	2.46	128.09	124.20
10	cA	832	CLA	CBC-CAC-C3C	-2.46	105.64	112.43
10	bB	801	CLA	C4-C3-C5	2.46	119.42	115.27
14	aA	852	LHG	C11-C10-C9	-2.46	101.92	114.42
13	bL	207	BCR	C27-C26-C25	2.46	126.31	122.73
10	aA	826	CLA	C3B-C4B-NB	2.46	112.39	109.21
10	aB	839	CLA	CMC-C2C-C1C	2.46	128.79	125.04
10	bB	816	CLA	CMB-C2B-C3B	2.46	129.29	124.68
10	aA	832	CLA	CBC-CAC-C3C	-2.46	105.64	112.43
10	cB	821	CLA	CAC-C3C-C4C	2.46	128.00	124.81
13	bA	846	BCR	C7-C8-C9	-2.46	122.52	126.23
10	aA	807	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
10	bL	202	CLA	CHA-C1A-NA	-2.46	120.76	126.40
10	bB	807	CLA	CHD-C4C-NC	2.46	128.08	124.20
13	cA	848	BCR	C31-C1-C6	2.46	114.29	110.30
10	aA	821	CLA	CMC-C2C-C1C	2.46	128.79	125.04
13	cM	101	BCR	C27-C26-C25	2.46	126.30	122.73
10	aA	830	CLA	CMA-C3A-C4A	-2.46	105.16	111.77
10	bB	801	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
13	bM	101	BCR	C27-C26-C25	2.46	126.30	122.73
10	bB	813	CLA	CHD-C4C-NC	2.46	128.08	124.20
16	bB	848	LMG	O1-C7-C8	-2.46	104.97	110.90
13	aL	207	BCR	C15-C16-C17	-2.46	118.44	123.47
14	cA	852	LHG	C11-C10-C9	-2.46	101.95	114.42
10	bA	820	CLA	CAC-C3C-C4C	2.46	128.00	124.81
10	bB	803	CLA	CAC-C3C-C4C	2.46	128.00	124.81
13	bA	848	BCR	C38-C26-C27	-2.46	108.90	113.62
10	aA	832	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
10	cA	830	CLA	CHB-C4A-NA	2.46	127.91	124.51
14	bA	852	LHG	C11-C10-C9	-2.46	101.95	114.42
13	cB	845	BCR	C7-C8-C9	-2.46	122.52	126.23
13	bB	847	BCR	C35-C13-C14	-2.46	119.48	122.92
10	aA	820	CLA	CAC-C3C-C4C	2.46	128.00	124.81
13	cB	843	BCR	C15-C16-C17	-2.46	118.44	123.47
10	bA	838	CLA	CHB-C4A-NA	2.46	127.91	124.51
10	aB	829	CLA	CHD-C4C-NC	2.45	128.07	124.20
10	cB	839	CLA	CMC-C2C-C1C	2.45	128.78	125.04
10	aA	842	CLA	CHD-C4C-NC	2.45	128.07	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	cA	846	BCR	C7-C8-C9	-2.45	122.53	126.23
13	aB	843	BCR	C15-C16-C17	-2.45	118.45	123.47
10	aA	820	CLA	CHB-C4A-NA	2.45	127.90	124.51
13	bB	847	BCR	C27-C26-C25	2.45	126.29	122.73
10	cA	839	CLA	CMB-C2B-C3B	2.45	129.27	124.68
10	aB	806	CLA	O2A-CGA-CBA	2.45	119.60	111.91
10	cA	830	CLA	CMA-C3A-C4A	-2.45	105.18	111.77
10	bA	807	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
13	bA	848	BCR	C31-C1-C6	2.45	114.27	110.30
10	aB	840	CLA	C1-C2-C3	-2.45	121.81	126.04
13	aA	848	BCR	C38-C26-C27	-2.45	108.91	113.62
13	cA	848	BCR	C38-C26-C27	-2.45	108.91	113.62
10	bB	835	CLA	CAC-C3C-C4C	2.45	127.99	124.81
10	cB	823	CLA	O2A-CGA-CBA	2.45	119.59	111.91
10	aA	839	CLA	CMB-C2B-C3B	2.45	129.26	124.68
10	bB	839	CLA	CMC-C2C-C1C	2.45	128.77	125.04
10	aA	828	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
10	bA	810	CLA	C1-O2A-CGA	2.45	122.86	116.44
10	cA	822	CLA	C1-C2-C3	-2.45	121.81	126.04
10	cB	801	CLA	C4-C3-C5	2.45	119.39	115.27
13	aB	845	BCR	C7-C8-C9	-2.45	122.54	126.23
10	cA	812	CLA	CMB-C2B-C3B	2.45	129.25	124.68
10	cB	807	CLA	CHD-C4C-NC	2.45	128.06	124.20
10	cB	829	CLA	CHD-C4C-NC	2.45	128.06	124.20
10	cA	820	CLA	CHB-C4A-NA	2.44	127.89	124.51
10	bB	807	CLA	C4-C3-C5	2.44	119.38	115.27
10	aA	824	CLA	O2A-CGA-CBA	2.44	119.58	111.91
10	cA	805	CLA	C11-C12-C13	-2.44	108.02	115.92
13	aB	849	BCR	C27-C26-C25	2.44	126.28	122.73
10	cB	806	CLA	CHB-C4A-NA	2.44	127.89	124.51
10	bA	832	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
10	aA	834	CLA	CMA-C3A-C4A	-2.44	105.21	111.77
10	aA	805	CLA	C11-C12-C13	-2.44	108.02	115.92
10	cA	805	CLA	C1-C2-C3	-2.44	121.82	126.04
10	bA	819	CLA	CHD-C4C-NC	2.44	128.05	124.20
10	cA	807	CLA	O1D-CGD-CBD	-2.44	119.49	124.48
10	aB	831	CLA	CMB-C2B-C3B	2.44	129.25	124.68
10	cA	830	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
13	aA	846	BCR	C7-C8-C9	-2.44	122.55	126.23
10	bA	834	CLA	CMA-C3A-C4A	-2.44	105.21	111.77
10	cA	819	CLA	CHD-C4C-NC	2.44	128.05	124.20
13	cA	849	BCR	C11-C10-C9	-2.44	123.83	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	831	CLA	CAC-C3C-C4C	2.44	127.97	124.81
10	cA	843	CLA	CHD-C4C-NC	2.44	128.05	124.20
13	aM	101	BCR	C27-C26-C25	2.44	126.27	122.73
10	aB	818	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
10	cL	202	CLA	CHA-C1A-NA	-2.44	120.81	126.40
10	cA	824	CLA	O2A-CGA-CBA	2.44	119.56	111.91
10	cB	840	CLA	C1-C2-C3	-2.44	121.83	126.04
10	cA	830	CLA	CMC-C2C-C1C	2.44	128.75	125.04
10	aB	823	CLA	O2A-CGA-CBA	2.44	119.55	111.91
10	bA	822	CLA	C1-C2-C3	-2.44	121.83	126.04
13	cA	847	BCR	C28-C27-C26	-2.44	109.73	114.08
10	bA	828	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
10	bA	805	CLA	C11-C12-C13	-2.43	108.05	115.92
10	aA	819	CLA	CHD-C4C-NC	2.43	128.04	124.20
10	cA	825	CLA	CHC-C1C-C2C	-2.43	119.99	126.72
10	aA	810	CLA	C1-O2A-CGA	2.43	122.83	116.44
10	aB	830	CLA	CMB-C2B-C1B	-2.43	124.72	128.46
10	cA	834	CLA	CMA-C3A-C4A	-2.43	105.23	111.77
10	cB	807	CLA	C4-C3-C5	2.43	119.36	115.27
10	cA	828	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
10	cB	830	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
10	aB	807	CLA	C4-C3-C5	2.43	119.36	115.27
13	bB	849	BCR	C27-C26-C25	2.43	126.26	122.73
10	bB	823	CLA	O2A-CGA-CBA	2.43	119.53	111.91
10	cA	814	CLA	CHB-C4A-NA	2.43	127.87	124.51
10	cA	838	CLA	CHB-C4A-NA	2.43	127.87	124.51
10	bA	854	CLA	CAA-CBA-CGA	-2.43	106.15	113.25
10	bB	827	CLA	CHB-C4A-NA	2.43	127.87	124.51
10	bA	830	CLA	CMC-C2C-C1C	2.43	128.74	125.04
10	bA	825	CLA	CHC-C1C-C2C	-2.43	120.00	126.72
10	bA	812	CLA	CMB-C2B-C3B	2.43	129.22	124.68
10	bA	824	CLA	O2A-CGA-CBA	2.43	119.53	111.91
10	aB	801	CLA	C4-C3-C5	2.43	119.36	115.27
10	aA	812	CLA	CMB-C2B-C3B	2.43	129.22	124.68
10	cB	831	CLA	CMB-C2B-C3B	2.43	129.22	124.68
10	bA	806	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
13	bA	850	BCR	C15-C14-C13	-2.43	123.84	127.31
10	aA	802	CLA	CHB-C4A-NA	2.43	127.87	124.51
13	aA	850	BCR	C15-C14-C13	-2.43	123.85	127.31
13	bA	849	BCR	C11-C10-C9	-2.43	123.85	127.31
10	bA	833	CLA	CMC-C2C-C1C	2.43	128.73	125.04
10	cA	806	CLA	O2D-CGD-O1D	-2.43	119.09	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	842	CLA	O2D-CGD-O1D	-2.43	119.10	123.84
10	cA	812	CLA	CHB-C4A-NA	2.42	127.86	124.51
10	bA	843	CLA	CHD-C4C-NC	2.42	128.02	124.20
13	bB	843	BCR	C27-C26-C25	2.42	126.25	122.73
13	cB	849	BCR	C27-C26-C25	2.42	126.25	122.73
10	bA	818	CLA	O2A-C1-C2	2.42	115.00	108.64
10	bA	816	CLA	CMB-C2B-C3B	2.42	129.21	124.68
10	cA	821	CLA	CAC-C3C-C4C	2.42	127.95	124.81
10	cB	838	CLA	CAC-C3C-C4C	2.42	127.95	124.81
13	aB	843	BCR	C27-C26-C25	2.42	126.25	122.73
10	cL	203	CLA	CBC-CAC-C3C	-2.42	105.75	112.43
10	aL	202	CLA	CHA-C1A-NA	-2.42	120.85	126.40
10	bL	203	CLA	CBC-CAC-C3C	-2.42	105.75	112.43
10	bB	806	CLA	CHB-C4A-NA	2.42	127.86	124.51
10	bA	830	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
10	cB	806	CLA	O2A-CGA-CBA	2.42	119.51	111.91
10	aA	810	CLA	CHB-C4A-NA	2.42	127.86	124.51
13	bA	847	BCR	C28-C27-C26	-2.42	109.75	114.08
10	bB	804	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
10	bB	806	CLA	O2A-CGA-CBA	2.42	119.50	111.91
13	aA	847	BCR	C28-C27-C26	-2.42	109.76	114.08
10	aA	830	CLA	CMC-C2C-C1C	2.42	128.72	125.04
10	cB	804	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
10	cB	803	CLA	CAC-C3C-C4C	2.42	127.95	124.81
10	bA	805	CLA	C4-C3-C5	2.42	119.34	115.27
10	bB	840	CLA	C1-C2-C3	-2.42	121.86	126.04
10	bB	831	CLA	CMB-C2B-C3B	2.42	129.20	124.68
13	bA	847	BCR	C3-C4-C5	-2.42	109.76	114.08
10	bB	829	CLA	CHD-C4C-NC	2.42	128.01	124.20
10	aB	803	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
10	aA	816	CLA	CMB-C2B-C3B	2.42	129.20	124.68
13	cB	847	BCR	C27-C26-C25	2.42	126.24	122.73
10	cB	809	CLA	O2A-CGA-CBA	2.42	119.49	111.91
10	bB	822	CLA	C4C-C3C-C2C	-2.42	103.38	106.90
13	cB	843	BCR	C27-C26-C25	2.42	126.24	122.73
10	aA	838	CLA	CHB-C4A-NA	2.42	127.85	124.51
10	aB	806	CLA	CHB-C4A-NA	2.42	127.85	124.51
10	bB	830	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
10	aA	833	CLA	O1D-CGD-CBD	-2.41	119.54	124.48
10	cA	816	CLA	CMB-C2B-C3B	2.41	129.20	124.68
10	cB	827	CLA	CHB-C4A-NA	2.41	127.85	124.51
10	cB	832	CLA	CMC-C2C-C1C	2.41	128.72	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	823	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
10	cA	823	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
10	bA	823	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
10	cB	825	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
10	aB	802	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
10	bA	812	CLA	CHB-C4A-NA	2.41	127.85	124.51
13	cA	847	BCR	C3-C4-C5	-2.41	109.77	114.08
10	aA	825	CLA	CHC-C1C-C2C	-2.41	120.05	126.72
10	aL	203	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
15	aA	853	LMT	C1'-O5'-C5'	2.41	118.42	113.69
15	cA	853	LMT	C1'-O5'-C5'	2.41	118.42	113.69
10	bA	842	CLA	CHD-C4C-NC	2.41	128.00	124.20
10	aA	822	CLA	C1-C2-C3	-2.41	121.87	126.04
10	bA	831	CLA	CAC-C3C-C4C	2.41	127.94	124.81
10	cA	854	CLA	CAA-CBA-CGA	-2.41	106.21	113.25
10	bB	822	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
10	cB	822	CLA	C4C-C3C-C2C	-2.41	103.38	106.90
10	cA	810	CLA	C1-O2A-CGA	2.41	122.77	116.44
10	aB	825	CLA	CAA-C2A-C3A	-2.41	106.18	112.78
10	aA	806	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
13	cA	850	BCR	C15-C14-C13	-2.41	123.87	127.31
10	aB	822	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
10	cA	802	CLA	CHB-C4A-NA	2.41	127.84	124.51
10	cB	804	CLA	C4-C3-C5	2.41	119.32	115.27
10	bB	818	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
13	aA	849	BCR	C11-C10-C9	-2.41	123.87	127.31
10	aA	830	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
13	aI	101	BCR	C38-C26-C27	-2.41	108.99	113.62
10	bL	205	CLA	C4-C3-C5	2.41	119.32	115.27
10	bA	826	CLA	C3B-C4B-NB	2.41	112.32	109.21
10	cB	832	CLA	CHB-C4A-NA	2.41	127.84	124.51
10	aB	830	CLA	C1-C2-C3	-2.41	121.88	126.04
13	cA	846	BCR	C27-C26-C25	2.41	126.22	122.73
10	aB	803	CLA	CAC-C3C-C4C	2.41	127.93	124.81
10	aA	854	CLA	CAA-CBA-CGA	-2.41	106.22	113.25
10	aA	810	CLA	O2A-CGA-CBA	2.41	119.46	111.91
13	aB	847	BCR	C27-C26-C25	2.41	126.22	122.73
13	cI	103	BCR	C27-C26-C25	2.41	126.22	122.73
10	bA	810	CLA	O2A-CGA-CBA	2.41	119.45	111.91
10	aA	839	CLA	CHB-C4A-NA	2.40	127.84	124.51
10	aA	818	CLA	O2A-C1-C2	2.40	114.95	108.64
10	bB	825	CLA	CAA-C2A-C3A	-2.40	106.19	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	837	CLA	CMC-C2C-C1C	2.40	128.70	125.04
13	bI	101	BCR	C38-C26-C27	-2.40	109.00	113.62
10	bB	809	CLA	O2A-CGA-CBA	2.40	119.45	111.91
10	aB	813	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
10	aB	804	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
10	bB	803	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
10	bB	803	CLA	CMB-C2B-C1B	2.40	132.16	128.46
10	cA	839	CLA	CHB-C4A-NA	2.40	127.83	124.51
10	aA	835	CLA	C4-C3-C5	2.40	119.31	115.27
10	aB	834	CLA	CMB-C2B-C3B	2.40	129.17	124.68
10	bA	835	CLA	C4-C3-C5	2.40	119.31	115.27
10	cA	810	CLA	CHB-C4A-NA	2.40	127.83	124.51
10	aB	809	CLA	O2A-CGA-CBA	2.40	119.44	111.91
10	cA	805	CLA	C4-C3-C5	2.40	119.31	115.27
10	bB	836	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
10	cA	822	CLA	CHB-C4A-NA	2.40	127.83	124.51
10	cB	822	CLA	O1D-CGD-CBD	-2.40	119.57	124.48
10	aA	837	CLA	CMC-C2C-C1C	2.40	128.69	125.04
10	aB	838	CLA	CMC-C2C-C1C	2.40	128.69	125.04
10	aA	836	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
10	cA	810	CLA	O2A-CGA-CBA	2.40	119.44	111.91
10	cB	828	CLA	CHA-C1A-NA	-2.40	120.90	126.40
10	aB	832	CLA	CMC-C2C-C1C	2.40	128.69	125.04
10	aB	832	CLA	CHB-C4A-NA	2.40	127.83	124.51
10	bB	832	CLA	CMC-C2C-C1C	2.40	128.69	125.04
10	cL	205	CLA	C4-C3-C5	2.40	119.31	115.27
10	aB	828	CLA	CHA-C1A-NA	-2.40	120.91	126.40
10	cA	824	CLA	CHD-C4C-NC	2.40	127.98	124.20
10	cB	802	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
10	cB	803	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
10	cA	832	CLA	CAC-C3C-C4C	2.40	127.92	124.81
16	aB	848	LMG	O7-C10-O9	-2.40	117.91	123.70
10	aB	836	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
13	bI	102	BCR	C27-C26-C25	2.40	126.21	122.73
13	cI	102	BCR	C38-C26-C27	-2.40	109.02	113.62
10	aA	842	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
10	cA	835	CLA	C4-C3-C5	2.39	119.30	115.27
13	cA	849	BCR	C29-C30-C25	2.39	114.16	110.48
10	aB	822	CLA	C4C-C3C-C2C	-2.39	103.41	106.90
10	aL	205	CLA	C4-C3-C5	2.39	119.29	115.27
10	aA	843	CLA	CHD-C4C-NC	2.39	127.97	124.20
10	bB	838	CLA	CMC-C2C-C1C	2.39	128.68	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	cA	801	CL0	CAC-C3C-C4C	2.39	127.91	124.81
10	aB	827	CLA	CHB-C4A-NA	2.39	127.82	124.51
10	aB	834	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
10	cA	836	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
10	aA	835	CLA	CMB-C2B-C3B	2.39	129.15	124.68
10	cA	818	CLA	O2A-C1-C2	2.39	114.92	108.64
13	bB	844	BCR	C29-C30-C25	2.39	114.16	110.48
10	cL	202	CLA	CMC-C2C-C1C	2.39	128.68	125.04
10	bB	834	CLA	CMB-C2B-C3B	2.39	129.15	124.68
10	cB	836	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
10	aB	804	CLA	C4-C3-C5	2.39	119.29	115.27
10	cA	833	CLA	CMC-C2C-C1C	2.39	128.68	125.04
10	aA	812	CLA	CAA-CBA-CGA	-2.39	106.28	113.25
15	bA	853	LMT	C1'-O5'-C5'	2.39	118.37	113.69
10	bA	820	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
10	cB	834	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
10	bB	832	CLA	CHB-C4A-NA	2.39	127.81	124.51
10	bB	806	CLA	CAA-C2A-C1A	2.39	119.79	111.97
10	bA	839	CLA	CHB-C4A-NA	2.39	127.81	124.51
16	cB	848	LMG	O7-C10-O9	-2.39	117.94	123.70
10	cB	813	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
10	aA	833	CLA	CMC-C2C-C1C	2.38	128.67	125.04
10	aA	831	CLA	CAC-C3C-C4C	2.38	127.90	124.81
10	bA	802	CLA	CHB-C4A-NA	2.38	127.81	124.51
10	bA	810	CLA	CHB-C4A-NA	2.38	127.81	124.51
10	bB	828	CLA	CHA-C1A-NA	-2.38	120.94	126.40
10	bL	202	CLA	CMC-C2C-C1C	2.38	128.67	125.04
16	bB	848	LMG	O7-C10-O9	-2.38	117.94	123.70
10	aA	808	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
10	cA	842	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
10	cA	831	CLA	C4-C3-C5	2.38	119.28	115.27
10	aA	815	CLA	CHB-C4A-NA	2.38	127.81	124.51
10	aL	202	CLA	CMC-C2C-C1C	2.38	128.66	125.04
10	aA	812	CLA	CHB-C4A-NA	2.38	127.80	124.51
10	aB	807	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
10	bA	824	CLA	CHD-C4C-NC	2.38	127.95	124.20
13	bA	849	BCR	C15-C16-C17	-2.38	118.60	123.47
16	aB	848	LMG	O3-C3-C2	-2.38	104.85	110.35
13	bA	846	BCR	C27-C26-C25	2.38	126.19	122.73
10	bB	828	CLA	C4-C3-C5	2.38	119.27	115.27
10	cB	803	CLA	CMB-C2B-C1B	2.38	132.12	128.46
13	cA	849	BCR	C15-C16-C17	-2.38	118.60	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	822	CLA	CHB-C4A-NA	2.38	127.80	124.51
9	bA	801	CL0	CAC-C3C-C4C	2.38	127.89	124.81
10	bA	833	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
10	bB	802	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
10	cA	820	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
10	cB	820	CLA	CHD-C4C-NC	2.38	127.95	124.20
10	cB	840	CLA	O2A-CGA-CBA	2.38	119.36	111.91
10	bA	808	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
10	aA	832	CLA	CAC-C3C-C4C	2.38	127.89	124.81
10	cB	807	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
13	aA	846	BCR	C27-C26-C25	2.37	126.18	122.73
10	cB	830	CLA	C1-C2-C3	-2.37	121.94	126.04
10	bA	836	CLA	CAA-C2A-C3A	-2.37	106.28	112.78
10	aA	841	CLA	CHB-C4A-NA	2.37	127.79	124.51
10	aB	803	CLA	CMB-C2B-C1B	2.37	132.11	128.46
10	bA	841	CLA	CHB-C4A-NA	2.37	127.79	124.51
10	cA	841	CLA	CHB-C4A-NA	2.37	127.79	124.51
10	bB	834	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
10	cB	838	CLA	CMC-C2C-C1C	2.37	128.65	125.04
10	cA	812	CLA	CAA-CBA-CGA	-2.37	106.32	113.25
10	aB	840	CLA	O2A-CGA-CBA	2.37	119.35	111.91
10	bA	812	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
10	cA	854	CLA	CMB-C2B-C3B	2.37	129.11	124.68
10	bA	826	CLA	OBD-CAD-C3D	-2.37	122.82	128.52
13	aA	849	BCR	C29-C30-C25	2.37	114.13	110.48
10	aB	806	CLA	CAA-C2A-C1A	2.37	119.74	111.97
10	bB	820	CLA	CHD-C4C-NC	2.37	127.94	124.20
10	cA	818	CLA	CHD-C4C-NC	2.37	127.94	124.20
10	bB	803	CLA	C4-C3-C5	2.37	119.25	115.27
10	bB	840	CLA	O2A-CGA-CBA	2.37	119.34	111.91
10	cA	833	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
10	bA	854	CLA	CMB-C2B-C3B	2.37	129.11	124.68
10	bA	832	CLA	CAC-C3C-C4C	2.37	127.88	124.81
10	aA	822	CLA	CHB-C4A-NA	2.37	127.79	124.51
10	bB	813	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
10	cA	837	CLA	CMC-C2C-C1C	2.37	128.64	125.04
10	bB	836	CLA	CBC-CAC-C3C	-2.37	105.91	112.43
10	cB	828	CLA	C4-C3-C5	2.37	119.25	115.27
10	cB	834	CLA	CMB-C2B-C3B	2.37	129.11	124.68
10	aA	826	CLA	OBD-CAD-C3D	-2.37	122.83	128.52
10	bA	837	CLA	CBC-CAC-C3C	-2.37	105.91	112.43
10	aA	830	CLA	CHD-C4C-NC	2.37	127.93	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	826	CLA	OBD-CAD-C3D	-2.37	122.83	128.52
13	aI	102	BCR	C27-C26-C25	2.37	126.17	122.73
10	aA	854	CLA	CMB-C2B-C3B	2.37	129.10	124.68
10	cB	803	CLA	C4-C3-C5	2.36	119.25	115.27
10	aA	856	CLA	O2A-CGA-CBA	2.36	119.33	111.91
13	aA	849	BCR	C15-C14-C13	-2.36	123.94	127.31
13	aA	850	BCR	C27-C26-C25	2.36	126.16	122.73
9	aA	801	CL0	CAC-C3C-C4C	2.36	127.88	124.81
10	aA	820	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
10	cB	806	CLA	CAA-C2A-C1A	2.36	119.72	111.97
10	cB	836	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
10	bB	804	CLA	C4-C3-C5	2.36	119.25	115.27
13	aA	847	BCR	C3-C4-C5	-2.36	109.86	114.08
10	bB	824	CLA	CMC-C2C-C1C	2.36	128.64	125.04
10	cB	838	CLA	C1-C2-C3	-2.36	121.96	126.04
10	bA	835	CLA	CMB-C2B-C3B	2.36	129.10	124.68
10	bB	807	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
10	aB	824	CLA	CMC-C2C-C1C	2.36	128.63	125.04
10	aB	836	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
13	aB	844	BCR	C29-C30-C25	2.36	114.11	110.48
10	aB	833	CLA	CAA-CBA-CGA	-2.36	106.36	113.25
10	bB	826	CLA	CMC-C2C-C1C	2.36	128.63	125.04
13	aA	849	BCR	C15-C16-C17	-2.36	118.64	123.47
10	bB	833	CLA	CAA-CBA-CGA	-2.36	106.36	113.25
10	bA	856	CLA	O2A-CGA-CBA	2.36	119.31	111.91
14	aA	855	LHG	C11-C10-C9	-2.36	102.45	114.42
10	aA	805	CLA	C4-C3-C5	2.36	119.24	115.27
10	cB	824	CLA	CMC-C2C-C1C	2.36	128.63	125.04
10	cB	826	CLA	CMC-C2C-C1C	2.36	128.63	125.04
10	cA	808	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
10	bB	828	CLA	CMB-C2B-C3B	2.36	129.09	124.68
16	bB	848	LMG	O3-C3-C2	-2.36	104.90	110.35
10	cB	828	CLA	CMB-C2B-C3B	2.36	129.09	124.68
14	bA	855	LHG	C11-C10-C9	-2.36	102.47	114.42
10	cA	835	CLA	CMB-C2B-C3B	2.36	129.09	124.68
10	bB	830	CLA	C1-C2-C3	-2.35	121.97	126.04
10	bB	820	CLA	CMB-C2B-C3B	2.35	129.08	124.68
10	cA	806	CLA	CBC-CAC-C3C	-2.35	105.94	112.43
13	cB	844	BCR	C29-C30-C25	2.35	114.11	110.48
10	cA	820	CLA	C4-C3-C5	2.35	119.23	115.27
10	cB	833	CLA	CAA-CBA-CGA	-2.35	106.37	113.25
10	cA	856	CLA	O2A-CGA-CBA	2.35	119.30	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	830	CLA	CHD-C4C-NC	2.35	127.91	124.20
10	aA	837	CLA	CBC-CAC-C3C	-2.35	105.94	112.43
10	bB	838	CLA	C1-C2-C3	-2.35	121.97	126.04
10	aA	810	CLA	C4-C3-C5	2.35	119.23	115.27
16	cB	848	LMG	O3-C3-C2	-2.35	104.91	110.35
10	cA	837	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
13	cB	845	BCR	C30-C25-C26	-2.35	119.30	122.61
10	cB	825	CLA	CHB-C4A-NA	2.35	127.76	124.51
10	bA	806	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
10	aA	835	CLA	C1-C2-C3	-2.35	121.98	126.04
10	aA	824	CLA	CHD-C4C-NC	2.35	127.91	124.20
10	aA	831	CLA	C4-C3-C5	2.35	119.22	115.27
10	aB	803	CLA	C4-C3-C5	2.35	119.22	115.27
10	bA	830	CLA	CHD-C4C-NC	2.35	127.90	124.20
13	bA	850	BCR	C27-C26-C25	2.35	126.14	122.73
10	aB	828	CLA	CMB-C2B-C3B	2.35	129.07	124.68
10	bA	826	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
13	bA	849	BCR	C15-C14-C13	-2.35	123.96	127.31
10	aB	820	CLA	CMB-C2B-C3B	2.35	129.07	124.68
10	aA	843	CLA	CHB-C4A-NA	2.35	127.75	124.51
14	cA	855	LHG	C11-C10-C9	-2.34	102.53	114.42
10	bA	842	CLA	C4-C3-C5	2.34	119.21	115.27
10	bA	805	CLA	CAC-C3C-C4C	2.34	127.85	124.81
10	cA	842	CLA	C4-C3-C5	2.34	119.21	115.27
10	bA	810	CLA	C4-C3-C5	2.34	119.21	115.27
10	aA	826	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
10	cA	816	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
10	aA	802	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
10	aB	838	CLA	C1-C2-C3	-2.34	122.00	126.04
10	cB	820	CLA	CMB-C2B-C3B	2.34	129.06	124.68
10	aA	806	CLA	CBC-CAC-C3C	-2.34	105.98	112.43
10	aB	830	CLA	CMC-C2C-C1C	2.34	128.60	125.04
10	cA	810	CLA	C4-C3-C5	2.34	119.21	115.27
10	bB	830	CLA	CMC-C2C-C1C	2.34	128.60	125.04
10	aA	816	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
13	bA	849	BCR	C29-C30-C25	2.34	114.08	110.48
10	bA	831	CLA	C4-C3-C5	2.34	119.20	115.27
10	cB	823	CLA	CHB-C4A-NA	2.34	127.75	124.51
10	cA	826	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
10	aB	820	CLA	CHD-C4C-NC	2.34	127.89	124.20
10	cB	834	CLA	CMD-C2D-C3D	-2.34	122.24	127.61
13	bI	101	BCR	C11-C10-C9	-2.34	123.97	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	804	CLA	C4-C3-C2	-2.34	117.68	123.68
10	aB	828	CLA	C4-C3-C5	2.34	119.20	115.27
10	bA	816	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
10	bA	815	CLA	CHB-C4A-NA	2.34	127.74	124.51
10	cA	843	CLA	CHB-C4A-NA	2.34	127.74	124.51
10	aA	823	CLA	C4-C3-C5	2.34	119.20	115.27
10	bA	823	CLA	C4-C3-C5	2.34	119.20	115.27
10	bB	829	CLA	CBC-CAC-C3C	-2.34	105.99	112.43
10	cA	815	CLA	CHB-C4A-NA	2.34	127.74	124.51
13	bB	845	BCR	C30-C25-C26	-2.33	119.33	122.61
10	aA	808	CLA	CAA-CBA-CGA	-2.33	106.31	112.51
10	aB	835	CLA	CHB-C4A-NA	2.33	127.74	124.51
10	aB	826	CLA	CMC-C2C-C1C	2.33	128.59	125.04
10	aB	804	CLA	CHD-C4C-NC	2.33	127.88	124.20
10	aA	820	CLA	C4-C3-C5	2.33	119.20	115.27
13	aB	845	BCR	C30-C25-C26	-2.33	119.33	122.61
10	aA	842	CLA	C4-C3-C5	2.33	119.19	115.27
16	bB	848	LMG	C40-C39-C38	-2.33	102.59	114.42
10	aB	823	CLA	C4-C3-C5	2.33	119.19	115.27
10	aB	806	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
10	cB	823	CLA	C4-C3-C5	2.33	119.19	115.27
10	bB	806	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
10	bA	835	CLA	C1-C2-C3	-2.33	122.01	126.04
16	aB	848	LMG	C40-C39-C38	-2.33	102.60	114.42
10	bA	802	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
10	aB	834	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
10	cA	835	CLA	C1-C2-C3	-2.33	122.02	126.04
10	cA	842	CLA	CMB-C2B-C1B	2.33	132.04	128.46
10	bA	822	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
10	cB	835	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
10	aA	842	CLA	CMB-C2B-C1B	2.33	132.04	128.46
13	cA	850	BCR	C27-C26-C25	2.33	126.11	122.73
16	cB	848	LMG	C40-C39-C38	-2.32	102.62	114.42
10	bB	835	CLA	CHB-C4A-NA	2.32	127.73	124.51
10	bB	834	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
10	aB	829	CLA	CBC-CAC-C3C	-2.32	106.02	112.43
10	cB	835	CLA	CHB-C4A-NA	2.32	127.73	124.51
10	cB	829	CLA	CBC-CAC-C3C	-2.32	106.02	112.43
10	aB	835	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
10	bA	807	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
10	cA	842	CLA	CHB-C4A-NA	2.32	127.72	124.51
10	cA	808	CLA	CAA-CBA-CGA	-2.32	106.34	112.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	804	CLA	C4-C3-C2	-2.32	117.72	123.68
10	cB	806	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
10	aB	825	CLA	CHB-C4A-NA	2.32	127.72	124.51
10	cA	809	CLA	CHB-C4A-NA	2.32	127.72	124.51
10	cA	817	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
10	aA	805	CLA	CAC-C3C-C4C	2.32	127.82	124.81
10	aA	818	CLA	CHD-C4C-NC	2.32	127.86	124.20
10	bB	835	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
10	bB	825	CLA	CHB-C4A-NA	2.32	127.72	124.51
10	aA	827	CLA	CHA-C1A-NA	-2.32	121.09	126.40
10	cA	822	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
10	bB	823	CLA	C4-C3-C5	2.32	119.17	115.27
10	bA	802	CLA	CMB-C2B-C3B	2.32	129.01	124.68
10	aA	809	CLA	CHB-C4A-NA	2.32	127.72	124.51
10	aA	833	CLA	CMB-C2B-C3B	2.32	129.01	124.68
13	aI	101	BCR	C11-C10-C9	-2.32	124.00	127.31
10	bA	808	CLA	CAA-CBA-CGA	-2.32	106.36	112.51
10	bA	815	CLA	CMB-C2B-C3B	2.32	129.01	124.68
10	aA	822	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
10	bB	827	CLA	C1-C2-C3	-2.31	122.04	126.04
10	aA	807	CLA	CBC-CAC-C3C	-2.31	106.05	112.43
10	aA	839	CLA	CMC-C2C-C1C	2.31	128.56	125.04
13	aM	101	BCR	C20-C21-C22	-2.31	124.01	127.31
10	aA	842	CLA	CHB-C4A-NA	2.31	127.71	124.51
10	cL	204	CLA	CHB-C4A-NA	2.31	127.71	124.51
10	bA	833	CLA	CMB-C2B-C3B	2.31	129.00	124.68
10	cA	815	CLA	CMB-C2B-C3B	2.31	129.00	124.68
13	cA	849	BCR	C15-C14-C13	-2.31	124.01	127.31
10	cB	804	CLA	CHD-C4C-NC	2.31	127.84	124.20
10	bL	203	CLA	C4-C3-C5	2.31	119.16	115.27
10	cA	823	CLA	C4-C3-C5	2.31	119.16	115.27
10	cA	802	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
10	cB	830	CLA	CMC-C2C-C1C	2.31	128.56	125.04
10	bB	804	CLA	C4-C3-C2	-2.31	117.76	123.68
10	cB	834	CLA	CMC-C2C-C1C	2.31	128.55	125.04
10	aA	837	CLA	C1-O2A-CGA	2.31	122.50	116.44
10	bA	803	CLA	CMC-C2C-C1C	2.31	128.55	125.04
10	cA	805	CLA	CAC-C3C-C4C	2.31	127.80	124.81
10	bA	820	CLA	C4-C3-C5	2.31	119.15	115.27
10	cA	827	CLA	CHA-C1A-NA	-2.31	121.12	126.40
10	aB	824	CLA	CBC-CAC-C3C	-2.31	106.08	112.43
10	cA	826	CLA	CMC-C2C-C1C	2.31	128.55	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	823	CLA	CHB-C4A-NA	2.31	127.70	124.51
10	bA	817	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
10	cA	833	CLA	CMB-C2B-C3B	2.30	128.99	124.68
10	bB	834	CLA	CMC-C2C-C1C	2.30	128.55	125.04
10	bA	818	CLA	CHD-C4C-NC	2.30	127.83	124.20
10	aB	827	CLA	C1-C2-C3	-2.30	122.06	126.04
10	cA	839	CLA	CMC-C2C-C1C	2.30	128.55	125.04
10	cA	837	CLA	C1-O2A-CGA	2.30	122.48	116.44
10	bB	839	CLA	CHB-C4A-NA	2.30	127.69	124.51
10	bA	839	CLA	CMC-C2C-C1C	2.30	128.54	125.04
10	bA	842	CLA	CHB-C4A-NA	2.30	127.69	124.51
10	cB	817	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
10	bA	837	CLA	C1-O2A-CGA	2.30	122.48	116.44
10	bB	804	CLA	CHD-C4C-NC	2.30	127.83	124.20
13	aB	845	BCR	C15-C16-C17	-2.30	118.76	123.47
10	cA	854	CLA	C4-C3-C5	2.30	119.14	115.27
10	bB	817	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
10	aA	817	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
13	bI	102	BCR	C3-C4-C5	-2.30	109.97	114.08
10	cB	827	CLA	C1-C2-C3	-2.30	122.07	126.04
10	bA	842	CLA	CMB-C2B-C1B	2.30	132.00	128.46
14	aA	852	LHG	O8-C23-C24	2.30	119.11	111.91
10	aA	815	CLA	CMB-C2B-C3B	2.30	128.97	124.68
10	aB	833	CLA	O2A-CGA-CBA	2.30	119.11	111.91
10	cA	821	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
14	cA	852	LHG	O8-C23-C24	2.29	119.11	111.91
16	aB	848	LMG	O1-C1-C2	-2.29	104.72	108.30
10	cA	813	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
10	aB	823	CLA	CHB-C4A-NA	2.29	127.68	124.51
10	cB	807	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
16	cB	848	LMG	O1-C1-C2	-2.29	104.72	108.30
10	cA	807	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
10	bA	854	CLA	C4-C3-C5	2.29	119.13	115.27
13	cI	102	BCR	C11-C10-C9	-2.29	124.04	127.31
13	aB	845	BCR	C33-C5-C6	-2.29	121.95	124.53
13	bB	845	BCR	C15-C16-C17	-2.29	118.78	123.47
10	bA	827	CLA	CHA-C1A-NA	-2.29	121.15	126.40
10	bB	807	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
10	aA	802	CLA	CMB-C2B-C3B	2.29	128.97	124.68
10	aB	817	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
10	aB	807	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
10	aA	826	CLA	CMC-C2C-C1C	2.29	128.53	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	821	CLA	CMC-C2C-C1C	2.29	128.53	125.04
10	aA	821	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
10	bA	843	CLA	CHB-C4A-NA	2.29	127.68	124.51
10	aB	809	CLA	CHD-C4C-NC	2.29	127.81	124.20
10	bB	830	CLA	C4-C3-C5	2.29	119.12	115.27
10	cB	821	CLA	CMB-C2B-C3B	2.29	128.96	124.68
10	bA	815	CLA	O2A-CGA-CBA	2.29	119.09	111.91
16	bB	848	LMG	O1-C1-C2	-2.29	104.73	108.30
10	cB	824	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
10	cA	802	CLA	CMB-C2B-C3B	2.29	128.96	124.68
10	bB	824	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
10	bA	804	CLA	CMB-C2B-C3B	2.29	128.96	124.68
10	cA	839	CLA	CED-O2D-CGD	2.29	121.11	115.94
10	aA	803	CLA	CMC-C2C-C1C	2.29	128.52	125.04
10	aB	834	CLA	CMC-C2C-C1C	2.29	128.52	125.04
10	cA	803	CLA	CMC-C2C-C1C	2.29	128.52	125.04
14	cA	852	LHG	C20-C19-C18	-2.29	102.81	114.42
10	cA	812	CLA	CMC-C2C-C1C	2.29	128.52	125.04
13	cI	103	BCR	C3-C4-C5	-2.29	109.99	114.08
10	bB	833	CLA	CHB-C4A-NA	2.29	127.67	124.51
10	aB	821	CLA	CMC-C2C-C1C	2.29	128.52	125.04
10	bB	818	CLA	C4-C3-C5	2.29	119.12	115.27
10	cB	833	CLA	O2A-CGA-CBA	2.29	119.08	111.91
10	cB	819	CLA	C4C-C3C-C2C	-2.29	103.56	106.90
10	aA	815	CLA	O2A-CGA-CBA	2.29	119.08	111.91
14	bA	852	LHG	O8-C23-C24	2.29	119.08	111.91
13	cB	845	BCR	C15-C16-C17	-2.29	118.79	123.47
10	aB	802	CLA	CHD-C4C-NC	2.29	127.81	124.20
14	bA	852	LHG	C20-C19-C18	-2.28	102.83	114.42
10	cA	815	CLA	O2A-CGA-CBA	2.28	119.08	111.91
13	cM	101	BCR	C20-C21-C22	-2.28	124.05	127.31
10	bA	812	CLA	CMC-C2C-C1C	2.28	128.52	125.04
14	aA	852	LHG	C20-C19-C18	-2.28	102.83	114.42
10	cB	811	CLA	CHA-C1A-NA	-2.28	121.17	126.40
10	bB	821	CLA	CMC-C2C-C1C	2.28	128.52	125.04
10	bB	833	CLA	O2A-CGA-CBA	2.28	119.07	111.91
11	cB	842	PQN	C2M-C2-C3	-2.28	120.68	124.40
10	bA	821	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
10	bB	802	CLA	CHD-C4C-NC	2.28	127.80	124.20
10	aA	854	CLA	C4-C3-C5	2.28	119.11	115.27
10	cB	818	CLA	C4-C3-C5	2.28	119.11	115.27
10	bA	839	CLA	CED-O2D-CGD	2.28	121.10	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	819	CLA	C4C-C3C-C2C	-2.28	103.57	106.90
10	cB	830	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
10	cB	818	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
13	bM	101	BCR	C20-C21-C22	-2.28	124.06	127.31
10	cB	810	CLA	C1-C2-C3	-2.28	122.10	126.04
10	cA	804	CLA	CMB-C2B-C3B	2.28	128.94	124.68
10	cB	802	CLA	CHD-C4C-NC	2.28	127.80	124.20
10	bA	809	CLA	CHB-C4A-NA	2.28	127.66	124.51
10	cB	839	CLA	CHB-C4A-NA	2.28	127.66	124.51
10	bB	821	CLA	CMB-C2B-C3B	2.28	128.94	124.68
10	bB	810	CLA	C1-C2-C3	-2.28	122.11	126.04
10	aB	818	CLA	C4-C3-C5	2.28	119.10	115.27
10	aA	813	CLA	CBC-CAC-C3C	-2.28	106.16	112.43
10	bB	819	CLA	C4C-C3C-C2C	-2.28	103.58	106.90
10	cB	833	CLA	CHB-C4A-NA	2.28	127.66	124.51
13	aI	102	BCR	C3-C4-C5	-2.28	110.01	114.08
10	bA	830	CLA	CBC-CAC-C3C	-2.28	106.16	112.43
10	bA	827	CLA	C1-O2A-CGA	2.27	122.41	116.44
10	bA	825	CLA	CHB-C4A-NA	2.27	127.66	124.51
16	cB	848	LMG	C38-C37-C36	-2.27	102.89	114.42
10	aA	831	CLA	CHB-C4A-NA	2.27	127.65	124.51
10	aB	833	CLA	CHB-C4A-NA	2.27	127.65	124.51
10	aB	839	CLA	CHB-C4A-NA	2.27	127.65	124.51
10	aA	839	CLA	CED-O2D-CGD	2.27	121.07	115.94
10	aB	830	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
10	aB	817	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
10	aA	830	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
13	bB	845	BCR	C33-C5-C6	-2.27	121.98	124.53
10	aB	838	CLA	CBA-CAA-C2A	2.27	120.56	113.86
10	aB	830	CLA	C4-C3-C5	2.27	119.09	115.27
10	cB	830	CLA	C4-C3-C5	2.27	119.09	115.27
13	cB	843	BCR	C7-C8-C9	-2.27	122.81	126.23
10	bA	813	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
10	aA	804	CLA	CMB-C2B-C3B	2.27	128.92	124.68
10	bB	809	CLA	CHD-C4C-NC	2.27	127.78	124.20
13	bI	101	BCR	C27-C26-C25	2.27	126.02	122.73
10	aL	203	CLA	C4-C3-C5	2.27	119.08	115.27
10	bA	819	CLA	O1D-CGD-CBD	-2.27	119.85	124.48
10	bB	830	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
10	bB	827	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
10	cA	830	CLA	CBC-CAC-C3C	-2.27	106.19	112.43
10	cB	817	CLA	CAA-C2A-C3A	-2.27	106.57	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	812	CLA	O1D-CGD-CBD	-2.27	119.85	124.48
10	cB	809	CLA	CHD-C4C-NC	2.27	127.77	124.20
10	cA	825	CLA	CHB-C4A-NA	2.26	127.64	124.51
10	cL	202	CLA	CHD-C4C-NC	2.26	127.77	124.20
10	cL	203	CLA	C4-C3-C5	2.26	119.08	115.27
10	aB	818	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
10	bA	826	CLA	CMC-C2C-C1C	2.26	128.48	125.04
10	bB	813	CLA	CHB-C4A-NA	2.26	127.64	124.51
10	bL	204	CLA	CHB-C4A-NA	2.26	127.64	124.51
10	aB	821	CLA	CMB-C2B-C3B	2.26	128.91	124.68
16	aB	848	LMG	C38-C37-C36	-2.26	102.94	114.42
10	aA	812	CLA	CMC-C2C-C1C	2.26	128.48	125.04
10	bB	829	CLA	CMC-C2C-C1C	2.26	128.48	125.04
10	cB	829	CLA	CMC-C2C-C1C	2.26	128.48	125.04
10	bB	817	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
10	aB	827	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
10	aB	810	CLA	C1-C2-C3	-2.26	122.13	126.04
16	bB	848	LMG	C38-C37-C36	-2.26	102.95	114.42
10	cB	838	CLA	CBA-CAA-C2A	2.26	120.53	113.86
10	bB	809	CLA	CHB-C4A-NA	2.26	127.64	124.51
10	bA	809	CLA	CMB-C2B-C3B	2.26	128.90	124.68
10	cB	806	CLA	C4-C3-C5	2.26	119.07	115.27
10	aA	812	CLA	O1D-CGD-CBD	-2.26	119.87	124.48
13	aB	843	BCR	C7-C8-C9	-2.26	122.83	126.23
10	aA	827	CLA	C1-O2A-CGA	2.26	122.36	116.44
10	aB	829	CLA	CMC-C2C-C1C	2.26	128.47	125.04
10	cB	820	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
10	cB	832	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
10	aA	825	CLA	CHB-C4A-NA	2.25	127.63	124.51
13	aI	101	BCR	C27-C26-C25	2.25	126.00	122.73
10	bA	831	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
10	bB	838	CLA	CBA-CAA-C2A	2.25	120.51	113.86
10	cB	827	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
10	aB	809	CLA	C11-C12-C13	-2.25	108.64	115.92
11	bB	842	PQN	C2M-C2-C3	-2.25	120.73	124.40
10	aB	806	CLA	C4-C3-C5	2.25	119.06	115.27
10	bA	812	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
10	cA	831	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
10	cA	827	CLA	C1-O2A-CGA	2.25	122.35	116.44
10	cA	834	CLA	CMA-C3A-C2A	-2.25	104.75	113.83
10	aB	820	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
10	bB	811	CLA	CHA-C1A-NA	-2.25	121.24	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bL	206	BCR	C15-C16-C17	-2.25	118.86	123.47
10	bB	832	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
10	aL	202	CLA	CHD-C4C-NC	2.25	127.75	124.20
10	bB	813	CLA	CAC-C3C-C4C	2.25	127.73	124.81
10	aB	832	CLA	O2A-CGA-CBA	2.25	118.97	111.91
10	bA	826	CLA	CHB-C4A-NA	2.25	127.62	124.51
10	cB	813	CLA	CHB-C4A-NA	2.25	127.62	124.51
10	aB	832	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
10	aA	842	CLA	O2A-CGA-CBA	2.25	118.97	111.91
10	bB	807	CLA	C1-C2-C3	-2.25	122.15	126.04
10	aA	831	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
10	aA	819	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
10	bB	809	CLA	C11-C12-C13	-2.25	108.65	115.92
10	bB	821	CLA	O2A-CGA-CBA	2.25	118.96	111.91
10	bB	839	CLA	CMB-C2B-C3B	2.25	128.88	124.68
10	aA	834	CLA	CMA-C3A-C2A	-2.25	104.76	113.83
10	bB	838	CLA	CBC-CAC-C3C	-2.25	106.24	112.43
10	bA	834	CLA	CMA-C3A-C2A	-2.25	104.76	113.83
10	aB	839	CLA	CMB-C2B-C3B	2.25	128.88	124.68
10	aB	813	CLA	CHB-C4A-NA	2.25	127.62	124.51
10	bB	806	CLA	C4-C3-C5	2.25	119.05	115.27
10	bB	818	CLA	CBC-CAC-C3C	-2.25	106.24	112.43
10	bB	820	CLA	CBC-CAC-C3C	-2.25	106.24	112.43
10	aB	811	CLA	CHA-C1A-NA	-2.25	121.25	126.40
10	aB	809	CLA	CHB-C4A-NA	2.25	127.62	124.51
10	aB	821	CLA	O2A-CGA-CBA	2.25	118.96	111.91
10	cB	821	CLA	O2A-CGA-CBA	2.25	118.96	111.91
10	cB	839	CLA	CMB-C2B-C3B	2.25	128.88	124.68
10	bB	841	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
11	aB	842	PQN	C2M-C2-C3	-2.25	120.74	124.40
10	bB	832	CLA	O2A-CGA-CBA	2.24	118.95	111.91
10	bA	835	CLA	O2A-CGA-CBA	2.24	118.95	111.91
10	cA	809	CLA	CMB-C2B-C3B	2.24	128.87	124.68
10	aA	840	CLA	CMC-C2C-C1C	2.24	128.45	125.04
10	aA	809	CLA	CMB-C2B-C3B	2.24	128.87	124.68
10	cA	827	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
10	bA	842	CLA	CED-O2D-CGD	2.24	121.00	115.94
10	bA	842	CLA	O2A-CGA-CBA	2.24	118.94	111.91
10	bA	827	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
10	cA	831	CLA	CHB-C4A-NA	2.24	127.61	124.51
10	cB	809	CLA	CHB-C4A-NA	2.24	127.61	124.51
13	cL	206	BCR	C15-C16-C17	-2.24	118.89	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	842	CLA	O2A-CGA-CBA	2.24	118.93	111.91
10	aB	801	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
10	aB	813	CLA	CAC-C3C-C4C	2.24	127.71	124.81
10	aA	837	CLA	C4-C3-C5	2.24	119.03	115.27
10	cA	819	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
10	cB	824	CLA	CHB-C4A-NA	2.24	127.60	124.51
10	aA	835	CLA	O2A-CGA-CBA	2.24	118.92	111.91
10	aB	837	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
10	cB	832	CLA	O2A-CGA-CBA	2.23	118.92	111.91
10	aB	838	CLA	CBC-CAC-C3C	-2.23	106.27	112.43
10	cA	835	CLA	O2A-CGA-CBA	2.23	118.92	111.91
10	aL	204	CLA	CHB-C4A-NA	2.23	127.60	124.51
10	aL	205	CLA	CHB-C4A-NA	2.23	127.60	124.51
10	cB	807	CLA	C1-C2-C3	-2.23	122.18	126.04
10	cB	801	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
10	cL	205	CLA	CHB-C4A-NA	2.23	127.60	124.51
13	cI	102	BCR	C27-C26-C25	2.23	125.97	122.73
10	bA	837	CLA	C4-C3-C5	2.23	119.02	115.27
13	aL	206	BCR	C15-C16-C17	-2.23	118.90	123.47
10	aB	809	CLA	C6-C7-C8	-2.23	108.71	115.92
10	cA	842	CLA	CED-O2D-CGD	2.23	120.98	115.94
10	cA	818	CLA	CAC-C3C-C4C	2.23	127.70	124.81
10	cA	804	CLA	O2A-CGA-CBA	2.23	118.91	111.91
10	aB	802	CLA	O2A-CGA-CBA	2.23	118.91	111.91
10	bA	819	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
13	bB	843	BCR	C7-C8-C9	-2.23	122.87	126.23
10	bA	804	CLA	O2A-CGA-CBA	2.23	118.90	111.91
10	cA	830	CLA	CMB-C2B-C3B	2.23	128.85	124.68
10	aA	816	CLA	C1-C2-C3	-2.23	122.19	126.04
10	bA	824	CLA	CHA-C1A-NA	-2.23	121.30	126.40
16	aB	848	LMG	O2-C2-C1	-2.23	104.64	110.05
10	cB	826	CLA	C1-O2A-CGA	2.23	122.29	116.44
10	cB	809	CLA	C11-C12-C13	-2.23	108.72	115.92
10	bA	840	CLA	CMC-C2C-C1C	2.23	128.43	125.04
10	bL	202	CLA	CHD-C4C-NC	2.23	127.71	124.20
10	aA	827	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
10	cB	838	CLA	CBC-CAC-C3C	-2.23	106.30	112.43
10	bB	810	CLA	C4-C3-C5	2.23	119.02	115.27
10	bB	820	CLA	C1-C2-C3	-2.23	122.19	126.04
10	aA	824	CLA	CHA-C1A-NA	-2.23	121.30	126.40
10	cA	840	CLA	CMC-C2C-C1C	2.22	128.43	125.04
10	aA	819	CLA	CAA-C2A-C3A	-2.22	106.69	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	cB	845	BCR	C33-C5-C6	-2.22	122.03	124.53
10	aA	838	CLA	C5-C3-C4	2.22	119.52	114.60
10	cB	813	CLA	CAC-C3C-C4C	2.22	127.69	124.81
10	aA	805	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
10	aB	826	CLA	C1-O2A-CGA	2.22	122.28	116.44
10	aA	842	CLA	CED-O2D-CGD	2.22	120.97	115.94
10	bA	831	CLA	CHB-C4A-NA	2.22	127.58	124.51
13	cB	845	BCR	C40-C30-C25	2.22	113.90	110.30
10	bB	837	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
10	bB	826	CLA	C1-O2A-CGA	2.22	122.27	116.44
10	cB	823	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
10	aA	830	CLA	CMB-C2B-C3B	2.22	128.83	124.68
10	aA	826	CLA	CHB-C4A-NA	2.22	127.58	124.51
10	bB	801	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
13	bA	847	BCR	C24-C23-C22	-2.22	122.88	126.23
10	bB	802	CLA	O2A-CGA-CBA	2.22	118.87	111.91
10	bA	830	CLA	CMB-C2B-C3B	2.22	128.83	124.68
10	cA	819	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
10	aB	810	CLA	C4-C3-C5	2.22	119.00	115.27
10	cA	816	CLA	C1-C2-C3	-2.22	122.21	126.04
10	bA	826	CLA	CAC-C3C-C4C	2.22	127.69	124.81
13	aB	845	BCR	C40-C30-C25	2.22	113.90	110.30
10	cA	838	CLA	CHA-C1A-NA	-2.22	121.32	126.40
10	cB	802	CLA	O2A-CGA-CBA	2.22	118.86	111.91
16	cB	848	LMG	O2-C2-C1	-2.22	104.66	110.05
10	aA	826	CLA	CAC-C3C-C4C	2.22	127.69	124.81
10	aB	830	CLA	CBC-CAC-C3C	-2.22	106.32	112.43
10	aA	826	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
10	bA	816	CLA	C1-C2-C3	-2.22	122.21	126.04
10	bL	205	CLA	CHB-C4A-NA	2.22	127.58	124.51
10	cA	824	CLA	CHA-C1A-NA	-2.21	121.33	126.40
13	cB	849	BCR	C2-C1-C6	2.21	113.89	110.48
13	aA	847	BCR	C24-C23-C22	-2.21	122.89	126.23
10	bB	835	CLA	CHA-C1A-NA	-2.21	121.33	126.40
10	aA	804	CLA	O2A-CGA-CBA	2.21	118.86	111.91
10	aA	842	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
10	cB	835	CLA	CHA-C1A-NA	-2.21	121.33	126.40
10	cA	826	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
10	bB	809	CLA	C6-C7-C8	-2.21	108.77	115.92
10	cA	805	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
10	bA	838	CLA	C5-C3-C4	2.21	119.49	114.60
13	cB	849	BCR	C31-C1-C6	2.21	113.89	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	810	CLA	C4-C3-C5	2.21	118.99	115.27
10	aB	807	CLA	C1-C2-C3	-2.21	122.22	126.04
10	bA	804	CLA	CMC-C2C-C1C	2.21	128.41	125.04
10	cA	837	CLA	C4-C3-C5	2.21	118.99	115.27
10	cA	826	CLA	CAC-C3C-C4C	2.21	127.68	124.81
10	bB	823	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
10	bB	826	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
10	aA	804	CLA	CMC-C2C-C1C	2.21	128.41	125.04
16	aB	848	LMG	C42-C41-C40	-2.21	103.20	114.42
10	aB	824	CLA	CHB-C4A-NA	2.21	127.57	124.51
13	bB	845	BCR	C40-C30-C25	2.21	113.88	110.30
16	bB	848	LMG	C42-C41-C40	-2.21	103.21	114.42
10	aB	826	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
10	cB	830	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
13	cA	847	BCR	C24-C23-C22	-2.21	122.90	126.23
10	aA	838	CLA	CHA-C1A-NA	-2.21	121.34	126.40
16	cB	848	LMG	C42-C41-C40	-2.21	103.22	114.42
10	cA	842	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
10	cB	841	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
10	bB	835	CLA	CBC-CAC-C3C	-2.21	106.35	112.43
10	cB	809	CLA	C6-C7-C8	-2.21	108.79	115.92
10	aB	814	CLA	CHD-C4C-NC	2.21	127.68	124.20
10	bB	814	CLA	CHD-C4C-NC	2.21	127.68	124.20
16	bB	848	LMG	O2-C2-C1	-2.21	104.69	110.05
10	bA	805	CLA	O1D-CGD-CBD	-2.20	119.97	124.48
10	cA	832	CLA	CMA-C3A-C4A	-2.20	105.85	111.77
10	bA	805	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
10	cB	806	CLA	C1-O2A-CGA	2.20	122.23	116.44
10	cA	838	CLA	C5-C3-C4	2.20	119.47	114.60
10	aB	835	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
10	cB	826	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
10	aB	835	CLA	CHA-C1A-NA	-2.20	121.35	126.40
10	cA	805	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
10	bA	826	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
10	aB	841	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
10	bB	836	CLA	CHB-C4A-NA	2.20	127.56	124.51
13	bB	849	BCR	C2-C1-C6	2.20	113.87	110.48
13	aB	849	BCR	C31-C1-C6	2.20	113.87	110.30
10	bB	819	CLA	O2A-CGA-CBA	2.20	118.81	111.91
10	bB	830	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
10	bA	825	CLA	O2A-CGA-CBA	2.20	118.81	111.91
10	bA	838	CLA	CHA-C1A-NA	-2.20	121.36	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bA	850	BCR	C24-C23-C22	-2.20	122.91	126.23
10	cB	837	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
10	bB	826	CLA	CHB-C4A-NA	2.20	127.55	124.51
10	bA	842	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
10	aA	829	CLA	CHD-C4C-NC	2.20	127.66	124.20
10	aB	823	CLA	O2D-CGD-O1D	-2.20	119.55	123.84
10	cB	835	CLA	CBC-CAC-C3C	-2.20	106.38	112.43
10	bL	205	CLA	CMC-C2C-C1C	2.20	128.38	125.04
9	cA	801	CL0	O2A-CGA-O1A	-2.19	118.05	123.59
10	cB	807	CLA	CMC-C2C-C1C	2.19	128.38	125.04
10	aA	805	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
10	aB	820	CLA	C1-C2-C3	-2.19	122.25	126.04
10	bB	834	CLA	CAA-C2A-C3A	-2.19	106.77	112.78
10	aA	842	CLA	C1-O2A-CGA	2.19	122.20	116.44
10	aB	836	CLA	CHB-C4A-NA	2.19	127.54	124.51
10	cA	825	CLA	O2A-CGA-CBA	2.19	118.79	111.91
9	bA	801	CL0	O2A-CGA-O1A	-2.19	118.06	123.59
10	aA	835	CLA	CHB-C4A-NA	2.19	127.54	124.51
10	aA	818	CLA	CAC-C3C-C4C	2.19	127.65	124.81
10	bA	818	CLA	CAC-C3C-C4C	2.19	127.65	124.81
10	aA	854	CLA	C1-C2-C3	-2.19	122.25	126.04
13	aA	850	BCR	C24-C23-C22	-2.19	122.93	126.23
10	bB	824	CLA	CHB-C4A-NA	2.19	127.54	124.51
10	cB	814	CLA	CHD-C4C-NC	2.19	127.65	124.20
10	bB	816	CLA	CMC-C2C-C1C	2.19	128.37	125.04
10	aB	819	CLA	O2A-CGA-CBA	2.19	118.77	111.91
10	aA	811	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
10	aA	834	CLA	CED-O2D-CGD	2.19	120.89	115.94
10	bA	832	CLA	CMA-C3A-C4A	-2.19	105.89	111.77
10	bA	829	CLA	CHD-C4C-NC	2.19	127.65	124.20
10	cA	826	CLA	CHB-C4A-NA	2.19	127.53	124.51
13	cA	850	BCR	C24-C23-C22	-2.19	122.93	126.23
10	aB	834	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
10	aA	832	CLA	CMA-C3A-C4A	-2.18	105.90	111.77
13	aB	849	BCR	C2-C1-C6	2.18	113.84	110.48
10	cA	829	CLA	CHD-C4C-NC	2.18	127.64	124.20
10	aA	825	CLA	O2A-CGA-CBA	2.18	118.76	111.91
10	bA	812	CLA	O2A-CGA-CBA	2.18	118.76	111.91
9	aA	801	CL0	O2A-CGA-O1A	-2.18	118.08	123.59
10	aB	806	CLA	C1-O2A-CGA	2.18	122.17	116.44
10	aA	834	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
10	cA	804	CLA	CMC-C2C-C1C	2.18	128.36	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	802	CLA	C1-C2-C3	-2.18	122.27	126.04
13	bA	846	BCR	C33-C5-C6	-2.18	122.08	124.53
10	cA	834	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
10	aA	812	CLA	O2A-CGA-CBA	2.18	118.76	111.91
13	aA	847	BCR	C29-C30-C25	2.18	113.84	110.48
10	aL	205	CLA	CMC-C2C-C1C	2.18	128.36	125.04
10	bL	204	CLA	CMB-C2B-C3B	2.18	128.76	124.68
10	aA	834	CLA	CMC-C2C-C1C	2.18	128.36	125.04
10	cB	819	CLA	O2A-CGA-CBA	2.18	118.75	111.91
10	bA	842	CLA	C1-O2A-CGA	2.18	122.16	116.44
10	aB	840	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
10	bA	829	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
10	bB	806	CLA	C1-O2A-CGA	2.18	122.16	116.44
14	cA	852	LHG	O8-C23-O10	-2.18	118.09	123.59
10	bB	815	CLA	C4-C3-C5	2.18	118.93	115.27
10	bB	840	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
10	cB	834	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
10	cA	834	CLA	CMC-C2C-C1C	2.18	128.35	125.04
10	bA	834	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
13	bA	847	BCR	C29-C30-C25	2.18	113.83	110.48
13	aA	848	BCR	C35-C13-C14	-2.18	119.88	122.92
13	cA	849	BCR	C24-C23-C22	-2.18	122.95	126.23
10	bA	811	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
10	bA	834	CLA	CMC-C2C-C1C	2.17	128.35	125.04
13	cA	847	BCR	C29-C30-C25	2.17	113.83	110.48
10	aB	837	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
10	aB	816	CLA	CMC-C2C-C1C	2.17	128.35	125.04
10	cA	811	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
13	aB	845	BCR	C38-C26-C27	-2.17	109.44	113.62
13	cA	848	BCR	C35-C13-C14	-2.17	119.88	122.92
10	aL	204	CLA	CMB-C2B-C3B	2.17	128.74	124.68
10	cA	834	CLA	CED-O2D-CGD	2.17	120.85	115.94
10	bB	824	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
10	cL	205	CLA	CMC-C2C-C1C	2.17	128.34	125.04
10	aA	834	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
10	cA	842	CLA	C1-O2A-CGA	2.17	122.14	116.44
10	aB	818	CLA	CMC-C2C-C1C	2.17	128.34	125.04
10	cA	834	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
10	cA	812	CLA	O2A-CGA-CBA	2.17	118.71	111.91
13	bB	849	BCR	C31-C1-C6	2.17	113.81	110.30
10	cB	820	CLA	C1-C2-C3	-2.17	122.29	126.04
10	aB	824	CLA	O2D-CGD-O1D	-2.17	119.60	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	820	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
10	cB	840	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
10	aA	820	CLA	O2D-CGD-O1D	-2.17	119.61	123.84
10	bB	840	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
10	bA	834	CLA	CED-O2D-CGD	2.16	120.83	115.94
13	bA	849	BCR	C33-C5-C6	-2.16	122.10	124.53
10	aB	815	CLA	C4-C3-C5	2.16	118.91	115.27
10	aB	801	CLA	C1-C2-C3	-2.16	122.30	126.04
10	aB	802	CLA	C1-C2-C3	-2.16	122.30	126.04
10	cB	816	CLA	CMC-C2C-C1C	2.16	128.33	125.04
10	aB	833	CLA	CBC-CAC-C3C	-2.16	106.47	112.43
10	bB	802	CLA	C1-C2-C3	-2.16	122.30	126.04
14	aA	852	LHG	O8-C23-O10	-2.16	118.14	123.59
10	bB	804	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
10	cB	824	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
10	cA	813	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
10	cB	815	CLA	C4-C3-C5	2.16	118.90	115.27
10	aA	829	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
13	bB	845	BCR	C38-C26-C27	-2.16	109.47	113.62
10	aB	805	CLA	C1-C2-C3	-2.16	122.31	126.04
14	bA	852	LHG	O8-C23-O10	-2.16	118.15	123.59
10	cB	801	CLA	C1-C2-C3	-2.16	122.31	126.04
10	aB	835	CLA	CMC-C2C-C1C	2.16	128.32	125.04
13	bA	848	BCR	C35-C13-C14	-2.16	119.90	122.92
10	cB	837	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
10	cA	829	CLA	CHB-C4A-NA	2.16	127.49	124.51
10	bA	820	CLA	O2D-CGD-O1D	-2.15	119.62	123.84
13	aA	849	BCR	C24-C23-C22	-2.15	122.98	126.23
10	aB	841	CLA	C4-C3-C5	2.15	118.89	115.27
13	cB	845	BCR	C38-C26-C27	-2.15	109.48	113.62
10	cB	833	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
10	aA	809	CLA	CMC-C2C-C1C	2.15	128.32	125.04
10	aB	807	CLA	CMC-C2C-C1C	2.15	128.32	125.04
10	bB	801	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
10	aA	828	CLA	CHA-C1A-NA	-2.15	121.47	126.40
10	cB	840	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
13	cA	849	BCR	C33-C5-C6	-2.15	122.11	124.53
10	aB	811	CLA	CMB-C2B-C3B	2.15	128.70	124.68
10	aA	817	CLA	CBA-CAA-C2A	2.15	120.21	113.86
10	aB	804	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
10	cA	822	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
10	cB	832	CLA	C1-O2A-CGA	2.15	122.08	116.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	820	CLA	CMC-C2C-C1C	2.15	128.31	125.04
10	cB	835	CLA	CMC-C2C-C1C	2.15	128.31	125.04
10	bA	822	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
10	bA	834	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
10	cA	829	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
10	bB	807	CLA	CMC-C2C-C1C	2.15	128.31	125.04
10	cA	835	CLA	CHB-C4A-NA	2.15	127.48	124.51
10	bB	801	CLA	C1-C2-C3	-2.15	122.33	126.04
13	cA	846	BCR	C33-C5-C6	-2.15	122.12	124.53
10	cB	804	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
10	cB	808	CLA	CHB-C4A-NA	2.15	127.48	124.51
10	bA	828	CLA	CHA-C1A-NA	-2.15	121.48	126.40
13	cM	101	BCR	C7-C8-C9	-2.14	122.99	126.23
10	bB	833	CLA	CBC-CAC-C3C	-2.14	106.52	112.43
10	aA	829	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
10	bA	835	CLA	CHB-C4A-NA	2.14	127.48	124.51
10	cB	826	CLA	CHB-C4A-NA	2.14	127.48	124.51
10	aB	839	CLA	CBC-CAC-C3C	-2.14	106.52	112.43
10	aA	813	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
10	bA	829	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
10	aA	816	CLA	CBC-CAC-C3C	-2.14	106.52	112.43
10	cA	814	CLA	O2A-CGA-CBA	2.14	120.92	114.03
10	cB	836	CLA	CHB-C4A-NA	2.14	127.48	124.51
10	cA	820	CLA	CMC-C2C-C1C	2.14	128.30	125.04
10	aB	801	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
10	bA	813	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
10	cA	816	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
10	cB	837	CLA	C4-C3-C5	2.14	118.87	115.27
10	aB	840	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
13	aA	849	BCR	C33-C5-C6	-2.14	122.12	124.53
10	cL	204	CLA	CMB-C2B-C3B	2.14	128.69	124.68
10	bB	835	CLA	CMC-C2C-C1C	2.14	128.30	125.04
10	bB	811	CLA	CMB-C2B-C3B	2.14	128.68	124.68
10	aA	820	CLA	CMC-C2C-C1C	2.14	128.30	125.04
10	bA	809	CLA	CMC-C2C-C1C	2.14	128.30	125.04
10	bB	832	CLA	C1-O2A-CGA	2.14	122.06	116.44
10	cA	828	CLA	CHA-C1A-NA	-2.14	121.50	126.40
10	aB	841	CLA	CMC-C2C-C1C	2.14	128.30	125.04
10	cB	818	CLA	CMC-C2C-C1C	2.14	128.30	125.04
10	cB	831	CLA	CED-O2D-CGD	2.14	120.78	115.94
10	aA	832	CLA	C4-C3-C5	2.14	118.87	115.27
10	cA	823	CLA	CBA-CAA-C2A	2.14	120.18	113.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	831	CLA	CED-O2D-CGD	2.14	120.78	115.94
10	bB	841	CLA	C4-C3-C5	2.14	118.87	115.27
10	bB	837	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
10	aB	837	CLA	C4-C3-C5	2.14	118.87	115.27
10	aA	822	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
13	bA	849	BCR	C24-C23-C22	-2.14	123.01	126.23
10	cA	854	CLA	CHB-C4A-NA	2.14	127.47	124.51
10	bB	830	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
10	cA	817	CLA	CBA-CAA-C2A	2.14	120.17	113.86
10	cA	809	CLA	CMC-C2C-C1C	2.14	128.29	125.04
10	aB	830	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
10	bB	818	CLA	CMC-C2C-C1C	2.14	128.29	125.04
10	bA	816	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
10	cB	801	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
10	cA	836	CLA	CHA-C1A-NA	-2.14	121.51	126.40
13	aM	101	BCR	C24-C23-C22	-2.13	123.01	126.23
10	bA	854	CLA	C1-C2-C3	-2.13	122.35	126.04
10	aB	822	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
10	cB	839	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
13	cB	847	BCR	C15-C14-C13	-2.13	124.26	127.31
10	cA	832	CLA	C4-C3-C5	2.13	118.86	115.27
10	bA	821	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
10	aB	831	CLA	CED-O2D-CGD	2.13	120.76	115.94
10	cA	854	CLA	C1-C2-C3	-2.13	122.35	126.04
10	bA	828	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
10	bB	805	CLA	C1-C2-C3	-2.13	122.36	126.04
10	bA	817	CLA	CBA-CAA-C2A	2.13	120.16	113.86
10	bA	814	CLA	O2A-CGA-CBA	2.13	120.88	114.03
10	aA	828	CLA	CHB-C4A-NA	2.13	127.46	124.51
10	aB	826	CLA	CHB-C4A-NA	2.13	127.46	124.51
10	cB	841	CLA	C4-C3-C5	2.13	118.86	115.27
14	aA	852	LHG	C18-C17-C16	-2.13	103.60	114.42
10	cB	805	CLA	C1-C2-C3	-2.13	122.36	126.04
10	cA	828	CLA	CHB-C4A-NA	2.13	127.46	124.51
10	bB	839	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
14	cA	852	LHG	C18-C17-C16	-2.13	103.61	114.42
10	cA	829	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
15	bA	853	LMT	C1'-C2'-C3'	2.13	114.43	110.00
10	bA	823	CLA	CBA-CAA-C2A	2.13	120.15	113.86
10	cB	830	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
15	aA	853	LMT	C1'-C2'-C3'	2.13	114.43	110.00
10	cB	841	CLA	CMC-C2C-C1C	2.13	128.28	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	823	CLA	CBA-CAA-C2A	2.13	120.15	113.86
10	aA	821	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
10	cB	810	CLA	CMC-C2C-C1C	2.13	128.28	125.04
10	aA	814	CLA	O2A-CGA-CBA	2.13	120.87	114.03
10	bA	829	CLA	CHB-C4A-NA	2.13	127.45	124.51
10	aB	832	CLA	C1-O2A-CGA	2.13	122.03	116.44
10	cB	837	CLA	CHA-C1A-NA	-2.13	121.53	126.40
10	cB	823	CLA	CHA-C1A-NA	-2.13	121.53	126.40
10	bA	820	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
10	cA	826	CLA	CMB-C2B-C3B	2.13	128.66	124.68
10	cB	811	CLA	CMB-C2B-C3B	2.13	128.66	124.68
10	bA	826	CLA	CMB-C2B-C3B	2.13	128.66	124.68
10	cA	833	CLA	CAC-C3C-C4C	2.13	127.57	124.81
10	bB	821	CLA	CBC-CAC-C3C	-2.13	106.57	112.43
14	bA	852	LHG	C18-C17-C16	-2.13	103.64	114.42
10	bB	822	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
10	aA	829	CLA	CHB-C4A-NA	2.12	127.45	124.51
10	aB	837	CLA	CHA-C1A-NA	-2.12	121.53	126.40
10	aA	826	CLA	CMB-C2B-C3B	2.12	128.65	124.68
13	bM	101	BCR	C7-C8-C9	-2.12	123.03	126.23
10	aA	833	CLA	CAC-C3C-C4C	2.12	127.56	124.81
10	bA	821	CLA	CHB-C4A-NA	2.12	127.45	124.51
10	aA	836	CLA	CHA-C1A-NA	-2.12	121.54	126.40
10	cA	836	CLA	CHB-C4A-NA	2.12	127.45	124.51
10	aA	828	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
10	bB	840	CLA	OBD-CAD-C3D	-2.12	123.42	128.52
10	bB	837	CLA	C4-C3-C5	2.12	118.84	115.27
10	aB	808	CLA	CHB-C4A-NA	2.12	127.44	124.51
10	bB	808	CLA	CHB-C4A-NA	2.12	127.44	124.51
10	aA	828	CLA	C4-C3-C5	2.12	118.84	115.27
10	bA	832	CLA	C4-C3-C5	2.12	118.84	115.27
10	bB	841	CLA	CMC-C2C-C1C	2.12	128.27	125.04
13	bB	847	BCR	C15-C14-C13	-2.12	124.28	127.31
10	bB	823	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
10	cB	821	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
10	cB	831	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
10	cA	835	CLA	CMC-C2C-C1C	2.12	128.26	125.04
10	bA	836	CLA	CHA-C1A-NA	-2.12	121.55	126.40
10	cA	821	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
10	cB	804	CLA	CHB-C4A-NA	2.12	127.44	124.51
10	aB	802	CLA	C1-O2A-CGA	2.12	122.00	116.44
10	aA	821	CLA	CHB-C4A-NA	2.12	127.44	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	831	CLA	CBC-CAC-C3C	-2.12	106.60	112.43
10	aB	823	CLA	CHA-C1A-NA	-2.12	121.55	126.40
10	aB	821	CLA	CBC-CAC-C3C	-2.12	106.60	112.43
10	cA	828	CLA	C4-C3-C5	2.12	118.83	115.27
10	bB	810	CLA	CMC-C2C-C1C	2.11	128.26	125.04
10	aB	823	CLA	CBC-CAC-C3C	-2.11	106.60	112.43
10	aB	840	CLA	OBD-CAD-C3D	-2.11	123.43	128.52
10	cA	818	CLA	CHB-C4A-NA	2.11	127.44	124.51
10	bA	810	CLA	CMC-C2C-C1C	2.11	128.26	125.04
10	bA	833	CLA	CAC-C3C-C4C	2.11	127.55	124.81
15	cA	853	LMT	C1'-C2'-C3'	2.11	114.40	110.00
10	aA	819	CLA	CMC-C2C-C1C	2.11	128.26	125.04
10	cA	821	CLA	CHB-C4A-NA	2.11	127.43	124.51
10	cA	828	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
10	bB	804	CLA	CHB-C4A-NA	2.11	127.43	124.51
13	cI	102	BCR	C15-C16-C17	-2.11	119.15	123.47
10	aB	831	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
10	cB	822	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
10	aA	835	CLA	CMC-C2C-C1C	2.11	128.25	125.04
10	aB	813	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
10	cB	811	CLA	CHD-C4C-NC	2.11	127.53	124.20
10	cA	820	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
13	cM	101	BCR	C24-C23-C22	-2.11	123.05	126.23
10	aB	811	CLA	CHD-C4C-NC	2.11	127.53	124.20
13	aB	847	BCR	C15-C14-C13	-2.11	124.30	127.31
10	bB	837	CLA	CHA-C1A-NA	-2.11	121.57	126.40
10	aA	818	CLA	CHB-C4A-NA	2.11	127.43	124.51
10	cB	823	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
10	bA	838	CLA	CMB-C2B-C3B	2.11	128.62	124.68
10	cL	204	CLA	C4-C3-C5	2.11	118.81	115.27
10	cB	813	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
10	bB	831	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
10	cB	840	CLA	OBD-CAD-C3D	-2.11	123.45	128.52
10	aA	828	CLA	CBC-CAC-C3C	-2.10	106.63	112.43
13	cM	101	BCR	C15-C14-C13	-2.10	124.31	127.31
10	cA	837	CLA	O2A-CGA-CBA	2.10	118.51	111.91
10	bB	823	CLA	CHA-C1A-NA	-2.10	121.58	126.40
13	bM	101	BCR	C24-C23-C22	-2.10	123.06	126.23
13	bM	101	BCR	C16-C15-C14	-2.10	119.16	123.47
10	cB	825	CLA	CGD-CBD-CAD	-2.10	103.92	110.73
10	bA	835	CLA	CMC-C2C-C1C	2.10	128.24	125.04
10	aA	838	CLA	CMB-C2B-C3B	2.10	128.61	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	cA	852	LHG	C27-C26-C25	-2.10	103.75	114.42
10	cB	815	CLA	CMC-C2C-C1C	2.10	128.24	125.04
14	bA	852	LHG	C27-C26-C25	-2.10	103.75	114.42
10	cB	812	CLA	CHB-C4A-NA	2.10	127.42	124.51
10	aA	820	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
10	bA	814	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
10	aA	806	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
10	cA	838	CLA	CMB-C2B-C3B	2.10	128.61	124.68
10	aB	805	CLA	CED-O2D-CGD	2.10	120.69	115.94
10	aA	817	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
10	aB	810	CLA	CMC-C2C-C1C	2.10	128.24	125.04
13	aI	101	BCR	C15-C16-C17	-2.10	119.17	123.47
14	aA	852	LHG	C27-C26-C25	-2.10	103.76	114.42
10	bB	812	CLA	CHB-C4A-NA	2.10	127.42	124.51
10	bB	823	CLA	CMC-C2C-C1C	2.10	128.24	125.04
10	bB	813	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
10	bA	828	CLA	CHB-C4A-NA	2.10	127.41	124.51
10	aA	837	CLA	O2A-CGA-CBA	2.10	118.49	111.91
10	bB	802	CLA	C1-O2A-CGA	2.10	121.95	116.44
10	aB	815	CLA	CMC-C2C-C1C	2.10	128.23	125.04
10	cA	817	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
10	bA	828	CLA	C4-C3-C5	2.10	118.80	115.27
10	bL	204	CLA	C4-C3-C5	2.10	118.80	115.27
13	aA	846	BCR	C33-C5-C6	-2.10	122.17	124.53
10	bA	811	CLA	CMC-C2C-C1C	2.09	128.23	125.04
10	bB	821	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
10	cA	810	CLA	CHA-C1A-NA	-2.09	121.61	126.40
10	bB	826	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
10	cA	810	CLA	CMC-C2C-C1C	2.09	128.22	125.04
10	aB	825	CLA	CGD-CBD-CAD	-2.09	103.96	110.73
10	bA	817	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
10	aA	854	CLA	CHB-C4A-NA	2.09	127.40	124.51
10	cB	826	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
10	bB	826	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
10	cB	821	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
10	cA	828	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
10	cB	802	CLA	C1-O2A-CGA	2.09	121.92	116.44
10	cA	811	CLA	CMC-C2C-C1C	2.09	128.22	125.04
10	bA	806	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
10	cB	814	CLA	CHA-C1A-NA	-2.09	121.62	126.40
13	bI	101	BCR	C15-C16-C17	-2.09	119.20	123.47
10	aA	816	CLA	CAA-C2A-C3A	-2.09	107.06	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	805	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
10	cA	819	CLA	CMC-C2C-C1C	2.09	128.22	125.04
10	aA	805	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
10	aA	810	CLA	CMC-C2C-C1C	2.09	128.22	125.04
10	bB	815	CLA	CMC-C2C-C1C	2.09	128.22	125.04
10	bB	811	CLA	CHD-C4C-NC	2.09	127.49	124.20
10	bA	816	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
13	cM	101	BCR	C16-C15-C14	-2.09	119.20	123.47
10	bB	805	CLA	CED-O2D-CGD	2.09	120.66	115.94
10	bA	803	CLA	CAA-C2A-C3A	-2.09	107.07	112.78
10	cA	806	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
13	aM	101	BCR	C7-C8-C9	-2.09	123.08	126.23
10	cA	840	CLA	CHB-C4A-NA	2.08	127.39	124.51
10	bA	854	CLA	CHB-C4A-NA	2.08	127.39	124.51
10	bB	814	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
10	aB	826	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
10	cL	202	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
10	cB	819	CLA	CAA-C2A-C1A	-2.08	105.15	111.97
10	aB	837	CLA	CBA-CAA-C2A	-2.08	107.72	113.86
10	bA	828	CLA	CBC-CAC-C3C	-2.08	106.69	112.43
10	bA	837	CLA	O2A-CGA-CBA	2.08	118.44	111.91
10	bB	830	CLA	CHB-C4A-NA	2.08	127.39	124.51
10	bA	818	CLA	C1-O2A-CGA	2.08	121.90	116.44
10	cB	820	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
10	aB	831	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
10	cB	831	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
10	bA	818	CLA	CHB-C4A-NA	2.08	127.39	124.51
13	bM	101	BCR	C15-C14-C13	-2.08	124.34	127.31
10	cB	810	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
10	bL	202	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
10	cA	816	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
10	cA	814	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
10	cB	805	CLA	CED-O2D-CGD	2.08	120.64	115.94
10	bB	837	CLA	CBA-CAA-C2A	-2.08	107.73	113.86
10	bB	814	CLA	CHA-C1A-NA	-2.08	121.64	126.40
10	cB	826	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
10	cA	805	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
13	cA	848	BCR	C1-C6-C5	-2.08	119.69	122.61
10	aB	820	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
10	aA	811	CLA	CMC-C2C-C1C	2.08	128.20	125.04
10	bB	825	CLA	CGD-CBD-CAD	-2.07	104.01	110.73
10	aA	807	CLA	CAA-C2A-C3A	-2.07	107.10	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	819	CLA	CAA-C2A-C1A	-2.07	105.18	111.97
10	aL	202	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
10	cB	810	CLA	CMB-C2B-C3B	2.07	128.56	124.68
10	aB	804	CLA	CHB-C4A-NA	2.07	127.38	124.51
10	bA	840	CLA	CHB-C4A-NA	2.07	127.38	124.51
10	cB	814	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
10	aB	826	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
10	aA	804	CLA	C6-C7-C8	-2.07	109.22	115.92
10	aA	837	CLA	CHB-C4A-NA	2.07	127.38	124.51
13	cM	101	BCR	C37-C22-C21	-2.07	120.02	122.92
10	aB	814	CLA	CHA-C1A-NA	-2.07	121.65	126.40
10	bA	819	CLA	CMC-C2C-C1C	2.07	128.19	125.04
10	bA	804	CLA	C6-C7-C8	-2.07	109.22	115.92
10	aB	814	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
10	bB	819	CLA	CAA-C2A-C1A	-2.07	105.19	111.97
10	cA	807	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
10	bL	205	CLA	CMB-C2B-C3B	2.07	128.55	124.68
10	cA	804	CLA	C6-C7-C8	-2.07	109.23	115.92
10	aA	809	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
10	aB	812	CLA	CHB-C4A-NA	2.07	127.37	124.51
10	cB	823	CLA	CMC-C2C-C1C	2.07	128.19	125.04
10	aA	836	CLA	CHB-C4A-NA	2.07	127.37	124.51
10	aB	823	CLA	CMC-C2C-C1C	2.07	128.19	125.04
10	cB	837	CLA	CBA-CAA-C2A	-2.07	107.76	113.86
10	aA	803	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
10	aA	810	CLA	CHA-C1A-NA	-2.07	121.67	126.40
10	cA	810	CLA	C1-C2-C3	-2.07	122.47	126.04
10	cA	809	CLA	O2D-CGD-O1D	-2.07	119.80	123.84
10	bA	836	CLA	CHB-C4A-NA	2.07	127.37	124.51
10	aB	836	CLA	CED-O2D-CGD	2.07	120.61	115.94
10	aA	810	CLA	C1-C2-C3	-2.06	122.47	126.04
13	aM	101	BCR	C16-C15-C14	-2.06	119.25	123.47
10	cB	836	CLA	CMC-C2C-C1C	2.06	128.18	125.04
10	bB	820	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
10	bA	810	CLA	CHA-C1A-NA	-2.06	121.67	126.40
10	bA	837	CLA	CHB-C4A-NA	2.06	127.36	124.51
10	aB	807	CLA	CBA-CAA-C2A	2.06	119.95	113.86
10	aB	821	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
10	bA	802	CLA	CMC-C2C-C1C	2.06	128.18	125.04
10	aL	204	CLA	C4-C3-C5	2.06	118.74	115.27
13	bA	848	BCR	C1-C6-C5	-2.06	119.71	122.61
10	bA	809	CLA	O2D-CGD-O1D	-2.06	119.81	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	808	CLA	C4-C3-C5	2.06	118.74	115.27
10	bL	203	CLA	CHB-C4A-NA	2.06	127.36	124.51
10	aA	814	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
10	aA	840	CLA	CHB-C4A-NA	2.06	127.36	124.51
10	aB	810	CLA	CMB-C2B-C3B	2.06	128.53	124.68
15	aA	853	LMT	C3'-C4'-C5'	-2.06	106.21	110.93
13	cL	206	BCR	C2-C1-C6	2.06	113.65	110.48
10	aB	825	CLA	C1-C2-C3	-2.06	122.48	126.04
10	cA	856	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
13	cB	849	BCR	C1-C6-C5	-2.06	119.72	122.61
10	cA	803	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
10	bB	810	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
10	aB	830	CLA	CHB-C4A-NA	2.06	127.35	124.51
10	cA	808	CLA	CMB-C2B-C3B	2.06	128.52	124.68
10	cB	836	CLA	CED-O2D-CGD	2.05	120.58	115.94
10	bB	836	CLA	CED-O2D-CGD	2.05	120.58	115.94
10	bB	809	CLA	C11-C10-C8	-2.05	109.28	115.92
10	bB	833	CLA	CHC-C1C-NC	2.05	127.32	124.20
10	cA	818	CLA	C1-O2A-CGA	2.05	121.83	116.44
10	bB	825	CLA	C1-C2-C3	-2.05	122.49	126.04
10	bB	834	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
10	bA	808	CLA	CMB-C2B-C3B	2.05	128.52	124.68
13	aM	101	BCR	C15-C14-C13	-2.05	124.38	127.31
10	bA	807	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
13	bB	849	BCR	C1-C6-C5	-2.05	119.72	122.61
13	aA	850	BCR	C2-C1-C6	2.05	113.64	110.48
10	aB	834	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
10	bB	807	CLA	CBA-CAA-C2A	2.05	119.91	113.86
10	cB	825	CLA	C1-C2-C3	-2.05	122.50	126.04
10	aA	827	CLA	CBC-CAC-C3C	-2.05	106.78	112.43
10	bA	810	CLA	C1-C2-C3	-2.05	122.50	126.04
10	aA	818	CLA	C1-O2A-CGA	2.05	121.82	116.44
10	aB	840	CLA	CED-O2D-CGD	2.05	120.57	115.94
10	cB	807	CLA	CBA-CAA-C2A	2.05	119.91	113.86
10	cB	809	CLA	C11-C10-C8	-2.05	109.30	115.92
10	cB	833	CLA	C1-C2-C3	-2.05	122.50	126.04
13	bA	846	BCR	C1-C6-C5	-2.05	119.73	122.61
10	bA	827	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
9	aA	801	CL0	C4A-NA-C1A	-2.05	105.79	106.71
13	bL	206	BCR	C2-C1-C6	2.05	113.63	110.48
10	cB	840	CLA	C4-C3-C5	2.05	118.71	115.27
10	aB	809	CLA	C11-C10-C8	-2.05	109.31	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	856	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
13	bM	101	BCR	C37-C22-C21	-2.04	120.06	122.92
15	bA	853	LMT	C3'-C4'-C5'	-2.04	106.24	110.93
13	aA	848	BCR	C1-C6-C5	-2.04	119.74	122.61
13	cA	850	BCR	C2-C1-C6	2.04	113.63	110.48
10	cA	843	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
10	aA	843	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
10	aB	812	CLA	O2A-CGA-CBA	2.04	120.59	114.03
13	bL	206	BCR	C15-C14-C13	-2.04	124.40	127.31
10	aL	205	CLA	CMB-C2B-C3B	2.04	128.50	124.68
13	aL	206	BCR	C2-C1-C6	2.04	113.62	110.48
10	cA	802	CLA	CMC-C2C-C1C	2.04	128.15	125.04
13	aB	843	BCR	C33-C5-C6	-2.04	122.24	124.53
15	cA	853	LMT	C3'-C4'-C5'	-2.04	106.25	110.93
13	aB	849	BCR	C1-C6-C5	-2.04	119.74	122.61
10	aB	833	CLA	C1-C2-C3	-2.04	122.52	126.04
10	aB	830	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
13	aM	101	BCR	C37-C22-C21	-2.04	120.07	122.92
10	cB	830	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
10	bB	830	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
10	aA	802	CLA	CMC-C2C-C1C	2.04	128.14	125.04
10	bL	202	CLA	CHB-C4A-NA	2.04	127.33	124.51
10	aB	806	CLA	CHA-C1A-NA	-2.04	121.73	126.40
10	aB	833	CLA	CHC-C1C-NC	2.04	127.29	124.20
10	cB	840	CLA	CED-O2D-CGD	2.04	120.54	115.94
10	cA	837	CLA	CHB-C4A-NA	2.04	127.33	124.51
10	aB	810	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
10	cB	812	CLA	O2A-CGA-CBA	2.04	120.57	114.03
10	bB	828	CLA	CHB-C4A-NA	2.04	127.33	124.51
13	aL	206	BCR	C15-C14-C13	-2.03	124.41	127.31
10	cA	813	CLA	O2A-CGA-CBA	2.03	120.57	114.03
10	aA	808	CLA	CMB-C2B-C3B	2.03	128.48	124.68
10	cA	837	CLA	C1-C2-C3	-2.03	122.53	126.04
10	bB	816	CLA	CHA-C1A-NA	-2.03	121.74	126.40
10	bB	836	CLA	CMC-C2C-C1C	2.03	128.14	125.04
10	bA	856	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
13	aL	206	BCR	C11-C10-C9	-2.03	124.41	127.31
10	bB	836	CLA	CMB-C2B-C3B	2.03	128.48	124.68
10	bB	817	CLA	C1-C2-C3	-2.03	122.53	126.04
10	bB	810	CLA	CMB-C2B-C3B	2.03	128.48	124.68
10	aB	841	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
13	bA	846	BCR	C15-C16-C17	-2.03	119.31	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	806	CLA	CHA-C1A-NA	-2.03	121.75	126.40
10	aB	836	CLA	CMC-C2C-C1C	2.03	128.13	125.04
10	cB	828	CLA	CHB-C4A-NA	2.03	127.32	124.51
13	cA	848	BCR	C15-C14-C13	-2.03	124.41	127.31
10	cB	834	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
10	cL	205	CLA	CMB-C2B-C3B	2.03	128.48	124.68
10	aB	832	CLA	CHA-C1A-NA	-2.03	121.75	126.40
10	cA	841	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
13	aA	846	BCR	C15-C16-C17	-2.03	119.32	123.47
10	aA	840	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
10	bB	840	CLA	CED-O2D-CGD	2.03	120.53	115.94
13	bA	850	BCR	C2-C1-C6	2.03	113.61	110.48
10	bA	838	CLA	CBC-CAC-C3C	-2.03	106.84	112.43
10	cB	806	CLA	CHA-C1A-NA	-2.03	121.75	126.40
10	aB	816	CLA	CHA-C1A-NA	-2.03	121.76	126.40
10	cB	829	CLA	CBA-CAA-C2A	2.03	119.84	113.86
10	aA	813	CLA	O2A-CGA-CBA	2.03	120.54	114.03
10	cA	832	CLA	CMA-C3A-C2A	-2.03	105.66	113.83
10	cB	833	CLA	CHC-C1C-NC	2.03	127.28	124.20
10	aA	838	CLA	CBC-CAC-C3C	-2.03	106.85	112.43
10	bA	813	CLA	O2A-CGA-CBA	2.03	120.54	114.03
10	aB	829	CLA	CBA-CAA-C2A	2.03	119.84	113.86
10	aB	808	CLA	CHA-C1A-NA	-2.03	121.76	126.40
10	aA	832	CLA	CMA-C3A-C2A	-2.02	105.66	113.83
10	cB	808	CLA	CHA-C1A-NA	-2.02	121.76	126.40
10	aA	803	CLA	CBC-CAC-C3C	-2.02	106.85	112.43
10	bA	803	CLA	CBC-CAC-C3C	-2.02	106.85	112.43
10	bA	811	CLA	CBC-CAC-C3C	-2.02	106.85	112.43
10	aB	836	CLA	CMB-C2B-C3B	2.02	128.46	124.68
10	bB	812	CLA	O2A-CGA-CBA	2.02	120.53	114.03
10	bB	840	CLA	C4-C3-C5	2.02	118.67	115.27
10	bA	832	CLA	CMA-C3A-C2A	-2.02	105.67	113.83
10	cB	827	CLA	CHA-C1A-NA	-2.02	121.77	126.40
10	cA	811	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
10	cL	203	CLA	CHB-C4A-NA	2.02	127.31	124.51
10	aB	808	CLA	C4-C3-C5	2.02	118.67	115.27
10	cB	830	CLA	CHB-C4A-NA	2.02	127.31	124.51
10	bB	808	CLA	CHA-C1A-NA	-2.02	121.77	126.40
13	bA	848	BCR	C15-C14-C13	-2.02	124.43	127.31
13	cA	851	BCR	C32-C1-C6	2.02	113.58	110.30
10	cA	838	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
13	cL	206	BCR	C1-C6-C5	-2.02	119.77	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	cL	206	BCR	C15-C14-C13	-2.02	124.43	127.31
10	cB	841	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
13	bA	851	BCR	C32-C1-C6	2.02	113.57	110.30
10	cA	803	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
13	bB	843	BCR	C33-C5-C6	-2.02	122.26	124.53
13	bL	206	BCR	C11-C10-C9	-2.02	124.43	127.31
10	cA	827	CLA	CBC-CAC-C3C	-2.02	106.87	112.43
10	bA	841	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
10	bA	843	CLA	CBC-CAC-C3C	-2.02	106.87	112.43
10	aB	805	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
10	aB	829	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
10	aA	811	CLA	CBC-CAC-C3C	-2.02	106.87	112.43
10	cB	832	CLA	CHA-C1A-NA	-2.02	121.78	126.40
10	aA	837	CLA	C1-C2-C3	-2.02	122.56	126.04
10	aL	202	CLA	CHB-C4A-NA	2.02	127.30	124.51
10	bB	829	CLA	CBA-CAA-C2A	2.01	119.81	113.86
13	cB	843	BCR	C33-C5-C6	-2.01	122.27	124.53
10	bA	840	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
13	bA	846	BCR	C20-C21-C22	-2.01	124.44	127.31
13	bL	206	BCR	C1-C6-C5	-2.01	119.78	122.61
10	aB	840	CLA	C4-C3-C5	2.01	118.66	115.27
10	bB	808	CLA	C4-C3-C5	2.01	118.66	115.27
10	bB	832	CLA	CHA-C1A-NA	-2.01	121.79	126.40
10	aB	828	CLA	CHB-C4A-NA	2.01	127.29	124.51
10	cB	807	CLA	C11-C10-C8	-2.01	109.42	115.92
13	cA	846	BCR	C1-C6-C5	-2.01	119.78	122.61
13	cA	846	BCR	C15-C16-C17	-2.01	119.36	123.47
10	bA	806	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
13	aA	851	BCR	C32-C1-C6	2.01	113.56	110.30
10	aB	814	CLA	C4-C3-C5	2.01	118.65	115.27
10	aB	817	CLA	C1-C2-C3	-2.01	122.57	126.04
10	bA	835	CLA	CAA-C2A-C1A	2.01	118.56	111.97
10	bA	837	CLA	C1-C2-C3	-2.01	122.57	126.04
10	cL	202	CLA	CMB-C2B-C3B	2.01	128.44	124.68
10	cB	805	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
10	bA	822	CLA	CHA-C1A-NA	-2.01	121.80	126.40
10	bB	819	CLA	CHA-C1A-NA	-2.01	121.80	126.40
10	aL	203	CLA	CHB-C4A-NA	2.01	127.29	124.51
10	cB	817	CLA	C1-C2-C3	-2.01	122.57	126.04
10	cA	835	CLA	CAA-C2A-C1A	2.01	118.56	111.97
13	bI	102	BCR	C7-C8-C9	-2.01	123.20	126.23
10	bA	833	CLA	O2A-CGA-O1A	-2.01	118.53	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	cA	846	BCR	C20-C21-C22	-2.01	124.44	127.31
10	aA	835	CLA	CAA-C2A-C1A	2.01	118.55	111.97
10	aB	819	CLA	CHA-C1A-NA	-2.01	121.80	126.40
13	aA	846	BCR	C20-C21-C22	-2.01	124.45	127.31
10	aA	817	CLA	CED-O2D-CGD	2.01	120.47	115.94
10	bB	841	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
10	aB	833	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
10	cL	202	CLA	CHB-C4A-NA	2.00	127.28	124.51
10	cB	829	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
10	cB	819	CLA	CHA-C1A-NA	-2.00	121.81	126.40
10	aB	807	CLA	C11-C10-C8	-2.00	109.44	115.92
10	aA	841	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
10	bB	814	CLA	C4-C3-C5	2.00	118.64	115.27
10	bB	805	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
10	cB	816	CLA	CHA-C1A-NA	-2.00	121.81	126.40
10	bB	829	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
10	bB	833	CLA	C1-C2-C3	-2.00	122.58	126.04
10	cA	822	CLA	CHA-C1A-NA	-2.00	121.81	126.40
10	aB	808	CLA	CBC-CAC-C3C	-2.00	106.91	112.43
10	cA	817	CLA	CED-O2D-CGD	2.00	120.47	115.94
10	aB	820	CLA	CHC-C1C-NC	2.00	127.24	124.20
10	cA	813	CLA	CHA-C1A-NA	-2.00	121.81	126.40
10	cA	840	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
10	bB	801	CLA	CHD-C4C-NC	2.00	127.36	124.20
10	bB	827	CLA	CHA-C1A-NA	-2.00	121.82	126.40
10	cB	831	CLA	CHA-C1A-NA	-2.00	121.82	126.40
13	aA	848	BCR	C2-C1-C6	2.00	113.56	110.48

All (255) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	aA	801	CL0	ND
9	aA	801	CL0	NC
9	aA	801	CL0	NA
9	bA	801	CL0	ND
9	bA	801	CL0	NC
9	bA	801	CL0	NA
9	cA	801	CL0	ND
9	cA	801	CL0	NC
9	cA	801	CL0	NA
10	aA	802	CLA	ND
10	aA	803	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	aA	804	CLA	ND
10	aA	805	CLA	ND
10	aA	806	CLA	ND
10	aA	807	CLA	ND
10	aA	808	CLA	ND
10	aA	809	CLA	ND
10	aA	810	CLA	ND
10	aA	811	CLA	ND
10	aA	812	CLA	ND
10	aA	813	CLA	ND
10	aA	814	CLA	ND
10	aA	815	CLA	ND
10	aA	818	CLA	ND
10	aA	819	CLA	ND
10	aA	820	CLA	ND
10	aA	821	CLA	ND
10	aA	822	CLA	ND
10	aA	823	CLA	ND
10	aA	824	CLA	ND
10	aA	825	CLA	ND
10	aA	826	CLA	ND
10	aA	827	CLA	ND
10	aA	828	CLA	ND
10	aA	829	CLA	ND
10	aA	830	CLA	ND
10	aA	831	CLA	ND
10	aA	832	CLA	ND
10	aA	833	CLA	ND
10	aA	834	CLA	ND
10	aA	835	CLA	ND
10	aA	836	CLA	ND
10	aA	837	CLA	ND
10	aA	838	CLA	ND
10	aA	839	CLA	ND
10	aA	840	CLA	ND
10	aA	841	CLA	ND
10	aA	842	CLA	ND
10	aA	843	CLA	ND
10	aA	856	CLA	ND
10	aB	801	CLA	ND
10	aB	802	CLA	ND
10	aB	803	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	aB	804	CLA	ND
10	aB	805	CLA	ND
10	aB	806	CLA	ND
10	aB	807	CLA	ND
10	aB	808	CLA	ND
10	aB	809	CLA	ND
10	aB	810	CLA	ND
10	aB	811	CLA	ND
10	aB	812	CLA	ND
10	aB	814	CLA	ND
10	aB	815	CLA	ND
10	aB	816	CLA	ND
10	aB	817	CLA	ND
10	aB	818	CLA	ND
10	aB	819	CLA	ND
10	aB	820	CLA	ND
10	aB	821	CLA	ND
10	aB	823	CLA	ND
10	aB	824	CLA	ND
10	aB	825	CLA	ND
10	aB	826	CLA	ND
10	aB	827	CLA	ND
10	aB	828	CLA	ND
10	aB	829	CLA	ND
10	aB	830	CLA	ND
10	aB	831	CLA	ND
10	aB	832	CLA	ND
10	aB	833	CLA	ND
10	aB	834	CLA	ND
10	aB	835	CLA	ND
10	aB	836	CLA	ND
10	aB	837	CLA	ND
10	aB	838	CLA	ND
10	aB	839	CLA	ND
10	aB	840	CLA	ND
10	aB	841	CLA	ND
10	aL	202	CLA	ND
10	aL	204	CLA	ND
10	bA	802	CLA	ND
10	bA	803	CLA	ND
10	bA	804	CLA	ND
10	bA	805	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	bA	806	CLA	ND
10	bA	807	CLA	ND
10	bA	808	CLA	ND
10	bA	809	CLA	ND
10	bA	810	CLA	ND
10	bA	811	CLA	ND
10	bA	812	CLA	ND
10	bA	813	CLA	ND
10	bA	814	CLA	ND
10	bA	815	CLA	ND
10	bA	818	CLA	ND
10	bA	819	CLA	ND
10	bA	820	CLA	ND
10	bA	821	CLA	ND
10	bA	822	CLA	ND
10	bA	823	CLA	ND
10	bA	824	CLA	ND
10	bA	825	CLA	ND
10	bA	826	CLA	ND
10	bA	827	CLA	ND
10	bA	828	CLA	ND
10	bA	829	CLA	ND
10	bA	830	CLA	ND
10	bA	831	CLA	ND
10	bA	832	CLA	ND
10	bA	833	CLA	ND
10	bA	834	CLA	ND
10	bA	835	CLA	ND
10	bA	836	CLA	ND
10	bA	837	CLA	ND
10	bA	838	CLA	ND
10	bA	839	CLA	ND
10	bA	840	CLA	ND
10	bA	841	CLA	ND
10	bA	842	CLA	ND
10	bA	843	CLA	ND
10	bA	856	CLA	ND
10	bB	801	CLA	ND
10	bB	802	CLA	ND
10	bB	803	CLA	ND
10	bB	804	CLA	ND
10	bB	805	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	bB	806	CLA	ND
10	bB	807	CLA	ND
10	bB	808	CLA	ND
10	bB	809	CLA	ND
10	bB	810	CLA	ND
10	bB	811	CLA	ND
10	bB	812	CLA	ND
10	bB	814	CLA	ND
10	bB	815	CLA	ND
10	bB	816	CLA	ND
10	bB	817	CLA	ND
10	bB	818	CLA	ND
10	bB	819	CLA	ND
10	bB	820	CLA	ND
10	bB	821	CLA	ND
10	bB	823	CLA	ND
10	bB	824	CLA	ND
10	bB	825	CLA	ND
10	bB	826	CLA	ND
10	bB	827	CLA	ND
10	bB	828	CLA	ND
10	bB	829	CLA	ND
10	bB	830	CLA	ND
10	bB	831	CLA	ND
10	bB	832	CLA	ND
10	bB	833	CLA	ND
10	bB	834	CLA	ND
10	bB	835	CLA	ND
10	bB	836	CLA	ND
10	bB	837	CLA	ND
10	bB	838	CLA	ND
10	bB	839	CLA	ND
10	bB	840	CLA	ND
10	bB	841	CLA	ND
10	bL	202	CLA	ND
10	bL	204	CLA	ND
10	cA	802	CLA	ND
10	cA	803	CLA	ND
10	cA	804	CLA	ND
10	cA	805	CLA	ND
10	cA	806	CLA	ND
10	cA	807	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	cA	808	CLA	ND
10	cA	809	CLA	ND
10	cA	810	CLA	ND
10	cA	811	CLA	ND
10	cA	812	CLA	ND
10	cA	813	CLA	ND
10	cA	814	CLA	ND
10	cA	815	CLA	ND
10	cA	818	CLA	ND
10	cA	819	CLA	ND
10	cA	820	CLA	ND
10	cA	821	CLA	ND
10	cA	822	CLA	ND
10	cA	823	CLA	ND
10	cA	824	CLA	ND
10	cA	825	CLA	ND
10	cA	826	CLA	ND
10	cA	827	CLA	ND
10	cA	828	CLA	ND
10	cA	829	CLA	ND
10	cA	830	CLA	ND
10	cA	831	CLA	ND
10	cA	832	CLA	ND
10	cA	833	CLA	ND
10	cA	834	CLA	ND
10	cA	835	CLA	ND
10	cA	836	CLA	ND
10	cA	837	CLA	ND
10	cA	838	CLA	ND
10	cA	839	CLA	ND
10	cA	840	CLA	ND
10	cA	841	CLA	ND
10	cA	842	CLA	ND
10	cA	843	CLA	ND
10	cA	856	CLA	ND
10	cB	801	CLA	ND
10	cB	802	CLA	ND
10	cB	803	CLA	ND
10	cB	804	CLA	ND
10	cB	805	CLA	ND
10	cB	806	CLA	ND
10	cB	807	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	cB	808	CLA	ND
10	cB	809	CLA	ND
10	cB	810	CLA	ND
10	cB	811	CLA	ND
10	cB	812	CLA	ND
10	cB	814	CLA	ND
10	cB	815	CLA	ND
10	cB	816	CLA	ND
10	cB	817	CLA	ND
10	cB	818	CLA	ND
10	cB	819	CLA	ND
10	cB	820	CLA	ND
10	cB	821	CLA	ND
10	cB	823	CLA	ND
10	cB	824	CLA	ND
10	cB	825	CLA	ND
10	cB	826	CLA	ND
10	cB	827	CLA	ND
10	cB	828	CLA	ND
10	cB	829	CLA	ND
10	cB	830	CLA	ND
10	cB	831	CLA	ND
10	cB	832	CLA	ND
10	cB	833	CLA	ND
10	cB	834	CLA	ND
10	cB	835	CLA	ND
10	cB	836	CLA	ND
10	cB	837	CLA	ND
10	cB	838	CLA	ND
10	cB	839	CLA	ND
10	cB	840	CLA	ND
10	cB	841	CLA	ND
10	cL	202	CLA	ND
10	cL	204	CLA	ND

All (3079) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	aA	805	CLA	C1A-C2A-CAA-CBA
10	aA	806	CLA	C2-C3-C5-C6
10	aA	806	CLA	C4-C3-C5-C6
10	aA	807	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aA	807	CLA	CHA-CBD-CGD-O2D
10	aA	809	CLA	CHA-CBD-CGD-O1D
10	aA	809	CLA	CHA-CBD-CGD-O2D
10	aA	810	CLA	C1A-C2A-CAA-CBA
10	aA	810	CLA	C3A-C2A-CAA-CBA
10	aA	810	CLA	CHA-CBD-CGD-O1D
10	aA	816	CLA	CHA-CBD-CGD-O1D
10	aA	816	CLA	CHA-CBD-CGD-O2D
10	aA	816	CLA	C4-C3-C5-C6
10	aA	817	CLA	C3A-C2A-CAA-CBA
10	aA	817	CLA	C2-C3-C5-C6
10	aA	817	CLA	C4-C3-C5-C6
10	aA	818	CLA	C1A-C2A-CAA-CBA
10	aA	818	CLA	CHA-CBD-CGD-O1D
10	aA	818	CLA	CHA-CBD-CGD-O2D
10	aA	821	CLA	CHA-CBD-CGD-O1D
10	aA	821	CLA	CHA-CBD-CGD-O2D
10	aA	822	CLA	CHA-CBD-CGD-O1D
10	aA	822	CLA	CHA-CBD-CGD-O2D
10	aA	822	CLA	CAD-CBD-CGD-O1D
10	aA	822	CLA	C2-C3-C5-C6
10	aA	823	CLA	C1A-C2A-CAA-CBA
10	aA	823	CLA	C3A-C2A-CAA-CBA
10	aA	823	CLA	CHA-CBD-CGD-O1D
10	aA	823	CLA	CHA-CBD-CGD-O2D
10	aA	825	CLA	C2-C3-C5-C6
10	aA	825	CLA	C4-C3-C5-C6
10	aA	827	CLA	C1A-C2A-CAA-CBA
10	aA	829	CLA	CHA-CBD-CGD-O1D
10	aA	829	CLA	CHA-CBD-CGD-O2D
10	aA	830	CLA	C2A-CAA-CBA-CGA
10	aA	831	CLA	C2-C3-C5-C6
10	aA	831	CLA	C4-C3-C5-C6
10	aA	835	CLA	C1A-C2A-CAA-CBA
10	aA	835	CLA	CHA-CBD-CGD-O1D
10	aA	835	CLA	CHA-CBD-CGD-O2D
10	aA	836	CLA	C2-C3-C5-C6
10	aA	838	CLA	C1A-C2A-CAA-CBA
10	aA	840	CLA	CHA-CBD-CGD-O1D
10	aA	840	CLA	CHA-CBD-CGD-O2D
10	aA	840	CLA	C2-C3-C5-C6
10	aA	840	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aA	841	CLA	C2-C3-C5-C6
10	aA	854	CLA	C3-C5-C6-C7
10	aA	856	CLA	CBD-CGD-O2D-CED
10	aB	803	CLA	CHA-CBD-CGD-O1D
10	aB	803	CLA	CHA-CBD-CGD-O2D
10	aB	804	CLA	C1A-C2A-CAA-CBA
10	aB	804	CLA	C3A-C2A-CAA-CBA
10	aB	806	CLA	C1A-C2A-CAA-CBA
10	aB	806	CLA	C3A-C2A-CAA-CBA
10	aB	807	CLA	C1A-C2A-CAA-CBA
10	aB	807	CLA	C3A-C2A-CAA-CBA
10	aB	811	CLA	C3A-C2A-CAA-CBA
10	aB	811	CLA	C2-C3-C5-C6
10	aB	811	CLA	C4-C3-C5-C6
10	aB	814	CLA	C1A-C2A-CAA-CBA
10	aB	814	CLA	C3A-C2A-CAA-CBA
10	aB	819	CLA	C1A-C2A-CAA-CBA
10	aB	819	CLA	C3A-C2A-CAA-CBA
10	aB	822	CLA	CHA-CBD-CGD-O1D
10	aB	822	CLA	CHA-CBD-CGD-O2D
10	aB	825	CLA	C1A-C2A-CAA-CBA
10	aB	825	CLA	C3A-C2A-CAA-CBA
10	aB	826	CLA	CHA-CBD-CGD-O1D
10	aB	826	CLA	CHA-CBD-CGD-O2D
10	aB	828	CLA	C1A-C2A-CAA-CBA
10	aB	828	CLA	C3A-C2A-CAA-CBA
10	aB	829	CLA	C1A-C2A-CAA-CBA
10	aB	829	CLA	C3A-C2A-CAA-CBA
10	aB	829	CLA	C2-C3-C5-C6
10	aB	829	CLA	C4-C3-C5-C6
10	aB	831	CLA	C2A-CAA-CBA-CGA
10	aB	833	CLA	C2-C3-C5-C6
10	aB	833	CLA	C4-C3-C5-C6
10	aB	835	CLA	CBD-CGD-O2D-CED
10	aL	204	CLA	C1A-C2A-CAA-CBA
10	bA	805	CLA	C1A-C2A-CAA-CBA
10	bA	806	CLA	C2-C3-C5-C6
10	bA	806	CLA	C4-C3-C5-C6
10	bA	807	CLA	C3A-C2A-CAA-CBA
10	bA	807	CLA	CHA-CBD-CGD-O2D
10	bA	809	CLA	CHA-CBD-CGD-O1D
10	bA	809	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bA	810	CLA	C1A-C2A-CAA-CBA
10	bA	810	CLA	C3A-C2A-CAA-CBA
10	bA	810	CLA	CHA-CBD-CGD-O1D
10	bA	816	CLA	CHA-CBD-CGD-O1D
10	bA	816	CLA	CHA-CBD-CGD-O2D
10	bA	817	CLA	C3A-C2A-CAA-CBA
10	bA	817	CLA	C2-C3-C5-C6
10	bA	817	CLA	C4-C3-C5-C6
10	bA	818	CLA	C1A-C2A-CAA-CBA
10	bA	818	CLA	CHA-CBD-CGD-O1D
10	bA	818	CLA	CHA-CBD-CGD-O2D
10	bA	821	CLA	CHA-CBD-CGD-O1D
10	bA	821	CLA	CHA-CBD-CGD-O2D
10	bA	822	CLA	CHA-CBD-CGD-O1D
10	bA	822	CLA	CHA-CBD-CGD-O2D
10	bA	822	CLA	CAD-CBD-CGD-O1D
10	bA	822	CLA	C2-C3-C5-C6
10	bA	823	CLA	C1A-C2A-CAA-CBA
10	bA	823	CLA	C3A-C2A-CAA-CBA
10	bA	823	CLA	CHA-CBD-CGD-O1D
10	bA	823	CLA	CHA-CBD-CGD-O2D
10	bA	825	CLA	C2-C3-C5-C6
10	bA	825	CLA	C4-C3-C5-C6
10	bA	827	CLA	C1A-C2A-CAA-CBA
10	bA	829	CLA	CHA-CBD-CGD-O1D
10	bA	829	CLA	CHA-CBD-CGD-O2D
10	bA	830	CLA	C2A-CAA-CBA-CGA
10	bA	831	CLA	C2-C3-C5-C6
10	bA	831	CLA	C4-C3-C5-C6
10	bA	835	CLA	C1A-C2A-CAA-CBA
10	bA	835	CLA	CHA-CBD-CGD-O1D
10	bA	835	CLA	CHA-CBD-CGD-O2D
10	bA	836	CLA	C2-C3-C5-C6
10	bA	838	CLA	C1A-C2A-CAA-CBA
10	bA	840	CLA	CHA-CBD-CGD-O1D
10	bA	840	CLA	CHA-CBD-CGD-O2D
10	bA	840	CLA	C2-C3-C5-C6
10	bA	840	CLA	C4-C3-C5-C6
10	bA	841	CLA	C2-C3-C5-C6
10	bA	854	CLA	C3-C5-C6-C7
10	bA	856	CLA	CBD-CGD-O2D-CED
10	bB	803	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bB	803	CLA	CHA-CBD-CGD-O2D
10	bB	804	CLA	C1A-C2A-CAA-CBA
10	bB	804	CLA	C3A-C2A-CAA-CBA
10	bB	806	CLA	C1A-C2A-CAA-CBA
10	bB	806	CLA	C3A-C2A-CAA-CBA
10	bB	807	CLA	C1A-C2A-CAA-CBA
10	bB	807	CLA	C3A-C2A-CAA-CBA
10	bB	811	CLA	C3A-C2A-CAA-CBA
10	bB	811	CLA	C2-C3-C5-C6
10	bB	811	CLA	C4-C3-C5-C6
10	bB	814	CLA	C1A-C2A-CAA-CBA
10	bB	814	CLA	C3A-C2A-CAA-CBA
10	bB	819	CLA	C1A-C2A-CAA-CBA
10	bB	819	CLA	C3A-C2A-CAA-CBA
10	bB	822	CLA	CHA-CBD-CGD-O1D
10	bB	822	CLA	CHA-CBD-CGD-O2D
10	bB	825	CLA	C1A-C2A-CAA-CBA
10	bB	825	CLA	C3A-C2A-CAA-CBA
10	bB	826	CLA	CHA-CBD-CGD-O1D
10	bB	826	CLA	CHA-CBD-CGD-O2D
10	bB	828	CLA	C1A-C2A-CAA-CBA
10	bB	828	CLA	C3A-C2A-CAA-CBA
10	bB	829	CLA	C1A-C2A-CAA-CBA
10	bB	829	CLA	C3A-C2A-CAA-CBA
10	bB	829	CLA	C2-C3-C5-C6
10	bB	829	CLA	C4-C3-C5-C6
10	bB	831	CLA	C2A-CAA-CBA-CGA
10	bB	833	CLA	C2-C3-C5-C6
10	bB	833	CLA	C4-C3-C5-C6
10	bB	835	CLA	CBD-CGD-O2D-CED
10	bL	204	CLA	C1A-C2A-CAA-CBA
10	cA	805	CLA	C1A-C2A-CAA-CBA
10	cA	806	CLA	C2-C3-C5-C6
10	cA	806	CLA	C4-C3-C5-C6
10	cA	807	CLA	C3A-C2A-CAA-CBA
10	cA	807	CLA	CHA-CBD-CGD-O2D
10	cA	809	CLA	CHA-CBD-CGD-O1D
10	cA	809	CLA	CHA-CBD-CGD-O2D
10	cA	810	CLA	C1A-C2A-CAA-CBA
10	cA	810	CLA	C3A-C2A-CAA-CBA
10	cA	810	CLA	CHA-CBD-CGD-O1D
10	cA	816	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cA	816	CLA	CHA-CBD-CGD-O2D
10	cA	817	CLA	C3A-C2A-CAA-CBA
10	cA	817	CLA	C2-C3-C5-C6
10	cA	817	CLA	C4-C3-C5-C6
10	cA	818	CLA	C1A-C2A-CAA-CBA
10	cA	818	CLA	CHA-CBD-CGD-O1D
10	cA	818	CLA	CHA-CBD-CGD-O2D
10	cA	821	CLA	CHA-CBD-CGD-O1D
10	cA	821	CLA	CHA-CBD-CGD-O2D
10	cA	822	CLA	CHA-CBD-CGD-O1D
10	cA	822	CLA	CHA-CBD-CGD-O2D
10	cA	822	CLA	CAD-CBD-CGD-O1D
10	cA	822	CLA	C2-C3-C5-C6
10	cA	823	CLA	C1A-C2A-CAA-CBA
10	cA	823	CLA	C3A-C2A-CAA-CBA
10	cA	823	CLA	CHA-CBD-CGD-O1D
10	cA	823	CLA	CHA-CBD-CGD-O2D
10	cA	825	CLA	C2-C3-C5-C6
10	cA	825	CLA	C4-C3-C5-C6
10	cA	827	CLA	C1A-C2A-CAA-CBA
10	cA	829	CLA	CHA-CBD-CGD-O1D
10	cA	829	CLA	CHA-CBD-CGD-O2D
10	cA	830	CLA	C2A-CAA-CBA-CGA
10	cA	831	CLA	C2-C3-C5-C6
10	cA	831	CLA	C4-C3-C5-C6
10	cA	835	CLA	C1A-C2A-CAA-CBA
10	cA	835	CLA	CHA-CBD-CGD-O1D
10	cA	835	CLA	CHA-CBD-CGD-O2D
10	cA	836	CLA	C2-C3-C5-C6
10	cA	838	CLA	C1A-C2A-CAA-CBA
10	cA	840	CLA	CHA-CBD-CGD-O1D
10	cA	840	CLA	CHA-CBD-CGD-O2D
10	cA	840	CLA	C2-C3-C5-C6
10	cA	840	CLA	C4-C3-C5-C6
10	cA	841	CLA	C2-C3-C5-C6
10	cA	854	CLA	C3-C5-C6-C7
10	cA	856	CLA	CBD-CGD-O2D-CED
10	cB	803	CLA	CHA-CBD-CGD-O1D
10	cB	803	CLA	CHA-CBD-CGD-O2D
10	cB	804	CLA	C1A-C2A-CAA-CBA
10	cB	804	CLA	C3A-C2A-CAA-CBA
10	cB	806	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cB	806	CLA	C3A-C2A-CAA-CBA
10	cB	807	CLA	C1A-C2A-CAA-CBA
10	cB	807	CLA	C3A-C2A-CAA-CBA
10	cB	811	CLA	C3A-C2A-CAA-CBA
10	cB	811	CLA	C2-C3-C5-C6
10	cB	811	CLA	C4-C3-C5-C6
10	cB	814	CLA	C1A-C2A-CAA-CBA
10	cB	814	CLA	C3A-C2A-CAA-CBA
10	cB	819	CLA	C1A-C2A-CAA-CBA
10	cB	819	CLA	C3A-C2A-CAA-CBA
10	cB	822	CLA	CHA-CBD-CGD-O1D
10	cB	822	CLA	CHA-CBD-CGD-O2D
10	cB	825	CLA	C1A-C2A-CAA-CBA
10	cB	825	CLA	C3A-C2A-CAA-CBA
10	cB	826	CLA	CHA-CBD-CGD-O1D
10	cB	826	CLA	CHA-CBD-CGD-O2D
10	cB	828	CLA	C1A-C2A-CAA-CBA
10	cB	828	CLA	C3A-C2A-CAA-CBA
10	cB	829	CLA	C1A-C2A-CAA-CBA
10	cB	829	CLA	C3A-C2A-CAA-CBA
10	cB	829	CLA	C2-C3-C5-C6
10	cB	829	CLA	C4-C3-C5-C6
10	cB	831	CLA	C2A-CAA-CBA-CGA
10	cB	833	CLA	C2-C3-C5-C6
10	cB	833	CLA	C4-C3-C5-C6
10	cB	835	CLA	CBD-CGD-O2D-CED
10	cL	204	CLA	C1A-C2A-CAA-CBA
13	aA	846	BCR	C1-C6-C7-C8
13	aA	846	BCR	C7-C8-C9-C10
13	aA	846	BCR	C7-C8-C9-C34
13	aA	846	BCR	C21-C22-C23-C24
13	aA	846	BCR	C37-C22-C23-C24
13	aA	847	BCR	C20-C21-C22-C37
13	aA	847	BCR	C21-C22-C23-C24
13	aA	847	BCR	C37-C22-C23-C24
13	aA	848	BCR	C6-C7-C8-C9
13	aA	848	BCR	C7-C8-C9-C34
13	aA	848	BCR	C10-C11-C12-C13
13	aA	848	BCR	C11-C12-C13-C14
13	aA	848	BCR	C11-C12-C13-C35
13	aA	848	BCR	C12-C13-C14-C15
13	aA	849	BCR	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	aA	849	BCR	C20-C21-C22-C23
13	aA	849	BCR	C20-C21-C22-C37
13	aA	849	BCR	C22-C23-C24-C25
13	aA	850	BCR	C1-C6-C7-C8
13	aA	850	BCR	C21-C22-C23-C24
13	aA	850	BCR	C37-C22-C23-C24
13	aA	851	BCR	C7-C8-C9-C34
13	aA	851	BCR	C18-C19-C20-C21
13	aA	851	BCR	C37-C22-C23-C24
13	aB	843	BCR	C1-C6-C7-C8
13	aB	843	BCR	C7-C8-C9-C10
13	aB	843	BCR	C7-C8-C9-C34
13	aB	843	BCR	C22-C23-C24-C25
13	aB	844	BCR	C1-C6-C7-C8
13	aB	844	BCR	C16-C17-C18-C36
13	aB	844	BCR	C21-C22-C23-C24
13	aB	845	BCR	C6-C7-C8-C9
13	aB	845	BCR	C7-C8-C9-C10
13	aB	845	BCR	C7-C8-C9-C34
13	aB	845	BCR	C37-C22-C23-C24
13	aB	846	BCR	C1-C6-C7-C8
13	aB	846	BCR	C7-C8-C9-C34
13	aB	846	BCR	C10-C11-C12-C13
13	aB	849	BCR	C12-C13-C14-C15
13	aB	849	BCR	C35-C13-C14-C15
13	aB	849	BCR	C14-C15-C16-C17
13	aB	849	BCR	C18-C19-C20-C21
13	aB	849	BCR	C37-C22-C23-C24
13	aB	849	BCR	C22-C23-C24-C25
13	aI	101	BCR	C6-C7-C8-C9
13	aI	101	BCR	C7-C8-C9-C10
13	aI	101	BCR	C7-C8-C9-C34
13	aI	101	BCR	C37-C22-C23-C24
13	aI	102	BCR	C6-C7-C8-C9
13	aI	102	BCR	C7-C8-C9-C10
13	aI	102	BCR	C7-C8-C9-C34
13	aI	102	BCR	C23-C24-C25-C30
13	aL	206	BCR	C7-C8-C9-C10
13	aL	206	BCR	C7-C8-C9-C34
13	aL	206	BCR	C23-C24-C25-C26
13	aL	207	BCR	C23-C24-C25-C30
13	aM	101	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	aM	101	BCR	C20-C21-C22-C37
13	aM	101	BCR	C37-C22-C23-C24
13	bA	846	BCR	C1-C6-C7-C8
13	bA	846	BCR	C7-C8-C9-C10
13	bA	846	BCR	C7-C8-C9-C34
13	bA	846	BCR	C21-C22-C23-C24
13	bA	846	BCR	C37-C22-C23-C24
13	bA	847	BCR	C20-C21-C22-C37
13	bA	847	BCR	C21-C22-C23-C24
13	bA	847	BCR	C37-C22-C23-C24
13	bA	848	BCR	C6-C7-C8-C9
13	bA	848	BCR	C7-C8-C9-C34
13	bA	848	BCR	C10-C11-C12-C13
13	bA	848	BCR	C11-C12-C13-C14
13	bA	848	BCR	C11-C12-C13-C35
13	bA	848	BCR	C12-C13-C14-C15
13	bA	849	BCR	C18-C19-C20-C21
13	bA	849	BCR	C20-C21-C22-C23
13	bA	849	BCR	C20-C21-C22-C37
13	bA	849	BCR	C22-C23-C24-C25
13	bA	850	BCR	C1-C6-C7-C8
13	bA	850	BCR	C21-C22-C23-C24
13	bA	850	BCR	C37-C22-C23-C24
13	bA	851	BCR	C7-C8-C9-C34
13	bA	851	BCR	C18-C19-C20-C21
13	bA	851	BCR	C37-C22-C23-C24
13	bB	843	BCR	C1-C6-C7-C8
13	bB	843	BCR	C7-C8-C9-C10
13	bB	843	BCR	C7-C8-C9-C34
13	bB	843	BCR	C22-C23-C24-C25
13	bB	844	BCR	C1-C6-C7-C8
13	bB	844	BCR	C16-C17-C18-C36
13	bB	844	BCR	C21-C22-C23-C24
13	bB	845	BCR	C6-C7-C8-C9
13	bB	845	BCR	C7-C8-C9-C10
13	bB	845	BCR	C7-C8-C9-C34
13	bB	845	BCR	C37-C22-C23-C24
13	bB	846	BCR	C1-C6-C7-C8
13	bB	846	BCR	C7-C8-C9-C34
13	bB	846	BCR	C10-C11-C12-C13
13	bB	849	BCR	C12-C13-C14-C15
13	bB	849	BCR	C35-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	bB	849	BCR	C14-C15-C16-C17
13	bB	849	BCR	C18-C19-C20-C21
13	bB	849	BCR	C37-C22-C23-C24
13	bB	849	BCR	C22-C23-C24-C25
13	bI	101	BCR	C6-C7-C8-C9
13	bI	101	BCR	C7-C8-C9-C10
13	bI	101	BCR	C7-C8-C9-C34
13	bI	101	BCR	C37-C22-C23-C24
13	bI	102	BCR	C6-C7-C8-C9
13	bI	102	BCR	C7-C8-C9-C10
13	bI	102	BCR	C7-C8-C9-C34
13	bI	102	BCR	C23-C24-C25-C30
13	bL	206	BCR	C7-C8-C9-C10
13	bL	206	BCR	C7-C8-C9-C34
13	bL	206	BCR	C23-C24-C25-C26
13	bL	207	BCR	C23-C24-C25-C30
13	bM	101	BCR	C7-C8-C9-C34
13	bM	101	BCR	C20-C21-C22-C37
13	bM	101	BCR	C37-C22-C23-C24
13	cA	846	BCR	C1-C6-C7-C8
13	cA	846	BCR	C7-C8-C9-C10
13	cA	846	BCR	C7-C8-C9-C34
13	cA	846	BCR	C21-C22-C23-C24
13	cA	846	BCR	C37-C22-C23-C24
13	cA	847	BCR	C20-C21-C22-C37
13	cA	847	BCR	C21-C22-C23-C24
13	cA	847	BCR	C37-C22-C23-C24
13	cA	848	BCR	C6-C7-C8-C9
13	cA	848	BCR	C7-C8-C9-C34
13	cA	848	BCR	C10-C11-C12-C13
13	cA	848	BCR	C11-C12-C13-C14
13	cA	848	BCR	C11-C12-C13-C35
13	cA	848	BCR	C12-C13-C14-C15
13	cA	849	BCR	C18-C19-C20-C21
13	cA	849	BCR	C20-C21-C22-C23
13	cA	849	BCR	C20-C21-C22-C37
13	cA	849	BCR	C22-C23-C24-C25
13	cA	850	BCR	C1-C6-C7-C8
13	cA	850	BCR	C21-C22-C23-C24
13	cA	850	BCR	C37-C22-C23-C24
13	cA	851	BCR	C7-C8-C9-C34
13	cA	851	BCR	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	cA	851	BCR	C37-C22-C23-C24
13	cB	843	BCR	C1-C6-C7-C8
13	cB	843	BCR	C7-C8-C9-C10
13	cB	843	BCR	C7-C8-C9-C34
13	cB	843	BCR	C22-C23-C24-C25
13	cB	844	BCR	C1-C6-C7-C8
13	cB	844	BCR	C16-C17-C18-C36
13	cB	844	BCR	C21-C22-C23-C24
13	cB	845	BCR	C6-C7-C8-C9
13	cB	845	BCR	C7-C8-C9-C10
13	cB	845	BCR	C7-C8-C9-C34
13	cB	845	BCR	C37-C22-C23-C24
13	cB	846	BCR	C1-C6-C7-C8
13	cB	846	BCR	C7-C8-C9-C34
13	cB	846	BCR	C10-C11-C12-C13
13	cB	849	BCR	C12-C13-C14-C15
13	cB	849	BCR	C35-C13-C14-C15
13	cB	849	BCR	C14-C15-C16-C17
13	cB	849	BCR	C18-C19-C20-C21
13	cB	849	BCR	C37-C22-C23-C24
13	cB	849	BCR	C22-C23-C24-C25
13	cI	102	BCR	C6-C7-C8-C9
13	cI	102	BCR	C7-C8-C9-C10
13	cI	102	BCR	C7-C8-C9-C34
13	cI	102	BCR	C37-C22-C23-C24
13	cI	103	BCR	C6-C7-C8-C9
13	cI	103	BCR	C7-C8-C9-C10
13	cI	103	BCR	C7-C8-C9-C34
13	cI	103	BCR	C23-C24-C25-C30
13	cL	206	BCR	C7-C8-C9-C10
13	cL	206	BCR	C7-C8-C9-C34
13	cL	206	BCR	C23-C24-C25-C26
13	cL	207	BCR	C23-C24-C25-C30
13	cM	101	BCR	C7-C8-C9-C34
13	cM	101	BCR	C20-C21-C22-C37
13	cM	101	BCR	C37-C22-C23-C24
14	aA	852	LHG	C1-C2-C3-O3
14	aA	852	LHG	C3-O3-P-O4
14	aA	855	LHG	C3-O3-P-O5
14	bA	852	LHG	C1-C2-C3-O3
14	bA	852	LHG	C3-O3-P-O4
14	bA	855	LHG	C3-O3-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	cA	852	LHG	C1-C2-C3-O3
14	cA	852	LHG	C3-O3-P-O4
14	cA	855	LHG	C3-O3-P-O5
15	aA	853	LMT	C2'-C1'-O1'-C1
15	aA	853	LMT	O5'-C1'-O1'-C1
15	bA	853	LMT	C2'-C1'-O1'-C1
15	bA	853	LMT	O5'-C1'-O1'-C1
15	cA	853	LMT	C2'-C1'-O1'-C1
15	cA	853	LMT	O5'-C1'-O1'-C1
10	aB	835	CLA	O1D-CGD-O2D-CED
10	bB	835	CLA	O1D-CGD-O2D-CED
10	cB	835	CLA	O1D-CGD-O2D-CED
10	aA	820	CLA	CBD-CGD-O2D-CED
10	aA	833	CLA	CBD-CGD-O2D-CED
10	aA	838	CLA	CBD-CGD-O2D-CED
10	aA	839	CLA	CBD-CGD-O2D-CED
10	aB	824	CLA	CBD-CGD-O2D-CED
10	bA	820	CLA	CBD-CGD-O2D-CED
10	bA	833	CLA	CBD-CGD-O2D-CED
10	bA	838	CLA	CBD-CGD-O2D-CED
10	bA	839	CLA	CBD-CGD-O2D-CED
10	bB	824	CLA	CBD-CGD-O2D-CED
10	cA	820	CLA	CBD-CGD-O2D-CED
10	cA	833	CLA	CBD-CGD-O2D-CED
10	cA	838	CLA	CBD-CGD-O2D-CED
10	cA	839	CLA	CBD-CGD-O2D-CED
10	cB	824	CLA	CBD-CGD-O2D-CED
10	aA	822	CLA	O1A-CGA-O2A-C1
10	bA	822	CLA	O1A-CGA-O2A-C1
10	cA	822	CLA	O1A-CGA-O2A-C1
14	aA	852	LHG	O10-C23-O8-C6
14	bA	852	LHG	O10-C23-O8-C6
14	cA	852	LHG	O10-C23-O8-C6
14	aA	855	LHG	C24-C23-O8-C6
14	bA	855	LHG	C24-C23-O8-C6
14	cA	855	LHG	C24-C23-O8-C6
10	aA	807	CLA	CBD-CGD-O2D-CED
10	aB	817	CLA	CBD-CGD-O2D-CED
10	aB	828	CLA	CBD-CGD-O2D-CED
10	aB	841	CLA	CBD-CGD-O2D-CED
10	bA	807	CLA	CBD-CGD-O2D-CED
10	bB	817	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bB	828	CLA	CBD-CGD-O2D-CED
10	bB	841	CLA	CBD-CGD-O2D-CED
10	cA	807	CLA	CBD-CGD-O2D-CED
10	cB	817	CLA	CBD-CGD-O2D-CED
10	cB	828	CLA	CBD-CGD-O2D-CED
10	cB	841	CLA	CBD-CGD-O2D-CED
10	aA	820	CLA	O1A-CGA-O2A-C1
10	aB	806	CLA	O1A-CGA-O2A-C1
10	aB	826	CLA	O1A-CGA-O2A-C1
10	bA	820	CLA	O1A-CGA-O2A-C1
10	bB	806	CLA	O1A-CGA-O2A-C1
10	bB	826	CLA	O1A-CGA-O2A-C1
10	cA	820	CLA	O1A-CGA-O2A-C1
10	cB	806	CLA	O1A-CGA-O2A-C1
10	cB	826	CLA	O1A-CGA-O2A-C1
14	aA	855	LHG	O10-C23-O8-C6
14	bA	855	LHG	O10-C23-O8-C6
14	cA	855	LHG	O10-C23-O8-C6
10	aA	816	CLA	CBD-CGD-O2D-CED
10	bA	816	CLA	CBD-CGD-O2D-CED
10	cA	816	CLA	CBD-CGD-O2D-CED
10	aA	856	CLA	O1D-CGD-O2D-CED
10	bA	856	CLA	O1D-CGD-O2D-CED
10	cA	856	CLA	O1D-CGD-O2D-CED
10	aA	811	CLA	C3-C5-C6-C7
10	aA	817	CLA	C3-C5-C6-C7
10	aA	831	CLA	C3-C5-C6-C7
10	aA	835	CLA	C3-C5-C6-C7
10	aA	837	CLA	C3-C5-C6-C7
10	aA	839	CLA	C3-C5-C6-C7
10	aB	804	CLA	C3-C5-C6-C7
10	aB	819	CLA	C3-C5-C6-C7
10	bA	811	CLA	C3-C5-C6-C7
10	bA	817	CLA	C3-C5-C6-C7
10	bA	831	CLA	C3-C5-C6-C7
10	bA	835	CLA	C3-C5-C6-C7
10	bA	837	CLA	C3-C5-C6-C7
10	bA	839	CLA	C3-C5-C6-C7
10	bB	804	CLA	C3-C5-C6-C7
10	bB	819	CLA	C3-C5-C6-C7
10	cA	811	CLA	C3-C5-C6-C7
10	cA	817	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cA	831	CLA	C3-C5-C6-C7
10	cA	835	CLA	C3-C5-C6-C7
10	cA	837	CLA	C3-C5-C6-C7
10	cA	839	CLA	C3-C5-C6-C7
10	cB	804	CLA	C3-C5-C6-C7
10	cB	819	CLA	C3-C5-C6-C7
10	aA	822	CLA	CBA-CGA-O2A-C1
10	aB	806	CLA	CBA-CGA-O2A-C1
10	bA	822	CLA	CBA-CGA-O2A-C1
10	bB	806	CLA	CBA-CGA-O2A-C1
10	cA	822	CLA	CBA-CGA-O2A-C1
10	cB	806	CLA	CBA-CGA-O2A-C1
10	aA	818	CLA	CBD-CGD-O2D-CED
10	aB	831	CLA	CBD-CGD-O2D-CED
10	bA	818	CLA	CBD-CGD-O2D-CED
10	bB	831	CLA	CBD-CGD-O2D-CED
10	cA	818	CLA	CBD-CGD-O2D-CED
10	cB	831	CLA	CBD-CGD-O2D-CED
10	aA	841	CLA	C4-C3-C5-C6
10	aB	806	CLA	C4-C3-C5-C6
10	aB	823	CLA	C4-C3-C5-C6
10	bA	816	CLA	C4-C3-C5-C6
10	bA	841	CLA	C4-C3-C5-C6
10	bB	806	CLA	C4-C3-C5-C6
10	bB	823	CLA	C4-C3-C5-C6
10	cA	816	CLA	C4-C3-C5-C6
10	cA	841	CLA	C4-C3-C5-C6
10	cB	806	CLA	C4-C3-C5-C6
10	cB	823	CLA	C4-C3-C5-C6
10	aA	816	CLA	C2-C3-C5-C6
10	aB	823	CLA	C2-C3-C5-C6
10	bA	816	CLA	C2-C3-C5-C6
10	bB	823	CLA	C2-C3-C5-C6
10	cA	816	CLA	C2-C3-C5-C6
10	cB	823	CLA	C2-C3-C5-C6
10	aA	822	CLA	CBD-CGD-O2D-CED
10	bA	822	CLA	CBD-CGD-O2D-CED
10	cA	822	CLA	CBD-CGD-O2D-CED
10	aA	811	CLA	C2A-CAA-CBA-CGA
10	aA	828	CLA	C2A-CAA-CBA-CGA
10	aB	811	CLA	C2A-CAA-CBA-CGA
10	aB	822	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aB	823	CLA	C2A-CAA-CBA-CGA
10	aB	840	CLA	C2A-CAA-CBA-CGA
10	bA	811	CLA	C2A-CAA-CBA-CGA
10	bA	828	CLA	C2A-CAA-CBA-CGA
10	bB	811	CLA	C2A-CAA-CBA-CGA
10	bB	822	CLA	C2A-CAA-CBA-CGA
10	bB	823	CLA	C2A-CAA-CBA-CGA
10	bB	840	CLA	C2A-CAA-CBA-CGA
10	cA	811	CLA	C2A-CAA-CBA-CGA
10	cA	828	CLA	C2A-CAA-CBA-CGA
10	cB	811	CLA	C2A-CAA-CBA-CGA
10	cB	822	CLA	C2A-CAA-CBA-CGA
10	cB	823	CLA	C2A-CAA-CBA-CGA
10	cB	840	CLA	C2A-CAA-CBA-CGA
10	aA	805	CLA	C3-C5-C6-C7
10	aB	817	CLA	C3-C5-C6-C7
10	bA	805	CLA	C3-C5-C6-C7
10	bB	817	CLA	C3-C5-C6-C7
10	cA	805	CLA	C3-C5-C6-C7
10	cB	817	CLA	C3-C5-C6-C7
11	aA	844	PQN	C13-C15-C16-C17
11	bA	844	PQN	C13-C15-C16-C17
11	cA	844	PQN	C13-C15-C16-C17
10	aA	820	CLA	CBA-CGA-O2A-C1
10	aA	823	CLA	CBA-CGA-O2A-C1
10	aA	830	CLA	CBA-CGA-O2A-C1
10	aB	804	CLA	CBA-CGA-O2A-C1
10	aB	826	CLA	CBA-CGA-O2A-C1
10	aB	830	CLA	CBA-CGA-O2A-C1
10	bA	820	CLA	CBA-CGA-O2A-C1
10	bA	823	CLA	CBA-CGA-O2A-C1
10	bA	830	CLA	CBA-CGA-O2A-C1
10	bB	804	CLA	CBA-CGA-O2A-C1
10	bB	826	CLA	CBA-CGA-O2A-C1
10	bB	830	CLA	CBA-CGA-O2A-C1
10	cA	820	CLA	CBA-CGA-O2A-C1
10	cA	823	CLA	CBA-CGA-O2A-C1
10	cA	830	CLA	CBA-CGA-O2A-C1
10	cB	804	CLA	CBA-CGA-O2A-C1
10	cB	826	CLA	CBA-CGA-O2A-C1
10	cB	830	CLA	CBA-CGA-O2A-C1
14	aA	852	LHG	C24-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	bA	852	LHG	C24-C23-O8-C6
14	cA	852	LHG	C24-C23-O8-C6
10	aA	839	CLA	O1D-CGD-O2D-CED
10	bA	839	CLA	O1D-CGD-O2D-CED
10	cA	839	CLA	O1D-CGD-O2D-CED
10	aB	833	CLA	CBD-CGD-O2D-CED
10	bB	833	CLA	CBD-CGD-O2D-CED
10	cB	833	CLA	CBD-CGD-O2D-CED
10	aB	804	CLA	O1A-CGA-O2A-C1
10	bB	804	CLA	O1A-CGA-O2A-C1
10	cB	804	CLA	O1A-CGA-O2A-C1
13	aA	848	BCR	C9-C10-C11-C12
13	aB	849	BCR	C15-C16-C17-C18
13	bA	848	BCR	C9-C10-C11-C12
13	bB	849	BCR	C15-C16-C17-C18
13	cA	848	BCR	C9-C10-C11-C12
13	cB	849	BCR	C15-C16-C17-C18
10	aB	802	CLA	CBD-CGD-O2D-CED
10	aB	822	CLA	CBD-CGD-O2D-CED
10	bB	802	CLA	CBD-CGD-O2D-CED
10	bB	822	CLA	CBD-CGD-O2D-CED
10	cB	802	CLA	CBD-CGD-O2D-CED
10	cB	822	CLA	CBD-CGD-O2D-CED
10	aA	820	CLA	O1D-CGD-O2D-CED
10	bA	820	CLA	O1D-CGD-O2D-CED
10	cA	820	CLA	O1D-CGD-O2D-CED
14	aA	852	LHG	O2-C2-C3-O3
14	bA	852	LHG	O2-C2-C3-O3
14	cA	852	LHG	O2-C2-C3-O3
10	aB	801	CLA	C3-C5-C6-C7
10	aB	802	CLA	C3-C5-C6-C7
10	aB	808	CLA	C3-C5-C6-C7
10	aB	815	CLA	C3-C5-C6-C7
10	aB	823	CLA	C3-C5-C6-C7
10	aL	202	CLA	C3-C5-C6-C7
10	bB	801	CLA	C3-C5-C6-C7
10	bB	802	CLA	C3-C5-C6-C7
10	bB	808	CLA	C3-C5-C6-C7
10	bB	815	CLA	C3-C5-C6-C7
10	bB	823	CLA	C3-C5-C6-C7
10	bL	202	CLA	C3-C5-C6-C7
10	cB	801	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cB	802	CLA	C3-C5-C6-C7
10	cB	808	CLA	C3-C5-C6-C7
10	cB	815	CLA	C3-C5-C6-C7
10	cB	823	CLA	C3-C5-C6-C7
10	cL	202	CLA	C3-C5-C6-C7
10	aA	810	CLA	CBA-CGA-O2A-C1
10	aA	842	CLA	CBA-CGA-O2A-C1
10	bA	810	CLA	CBA-CGA-O2A-C1
10	bA	842	CLA	CBA-CGA-O2A-C1
10	cA	810	CLA	CBA-CGA-O2A-C1
10	cA	842	CLA	CBA-CGA-O2A-C1
10	aB	830	CLA	O1A-CGA-O2A-C1
10	bB	830	CLA	O1A-CGA-O2A-C1
10	cB	830	CLA	O1A-CGA-O2A-C1
15	aA	853	LMT	O5B-C5B-C6B-O6B
15	bA	853	LMT	O5B-C5B-C6B-O6B
15	cA	853	LMT	O5B-C5B-C6B-O6B
10	aA	838	CLA	O1D-CGD-O2D-CED
10	bA	838	CLA	O1D-CGD-O2D-CED
10	cA	838	CLA	O1D-CGD-O2D-CED
10	aB	806	CLA	CBD-CGD-O2D-CED
10	bB	806	CLA	CBD-CGD-O2D-CED
10	cB	806	CLA	CBD-CGD-O2D-CED
10	aA	830	CLA	O1A-CGA-O2A-C1
10	cA	830	CLA	O1A-CGA-O2A-C1
10	aB	810	CLA	CBD-CGD-O2D-CED
14	aA	852	LHG	C2-C3-O3-P
14	bA	852	LHG	C2-C3-O3-P
14	cA	852	LHG	C2-C3-O3-P
10	aA	823	CLA	O1A-CGA-O2A-C1
10	bA	823	CLA	O1A-CGA-O2A-C1
10	bA	830	CLA	O1A-CGA-O2A-C1
10	cA	823	CLA	O1A-CGA-O2A-C1
10	aA	819	CLA	C4-C3-C5-C6
10	aA	827	CLA	C4-C3-C5-C6
10	bA	819	CLA	C4-C3-C5-C6
10	bA	827	CLA	C4-C3-C5-C6
10	cA	819	CLA	C4-C3-C5-C6
10	cA	827	CLA	C4-C3-C5-C6
10	aA	827	CLA	C2-C3-C5-C6
10	bA	827	CLA	C2-C3-C5-C6
10	cA	827	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bB	810	CLA	CBD-CGD-O2D-CED
10	cB	810	CLA	CBD-CGD-O2D-CED
10	aB	824	CLA	C2A-CAA-CBA-CGA
10	bB	824	CLA	C2A-CAA-CBA-CGA
10	cB	824	CLA	C2A-CAA-CBA-CGA
10	aA	810	CLA	O1A-CGA-O2A-C1
10	aA	842	CLA	O1A-CGA-O2A-C1
10	bA	810	CLA	O1A-CGA-O2A-C1
10	bA	842	CLA	O1A-CGA-O2A-C1
10	cA	810	CLA	O1A-CGA-O2A-C1
10	cA	842	CLA	O1A-CGA-O2A-C1
10	aA	827	CLA	CBA-CGA-O2A-C1
10	bA	827	CLA	CBA-CGA-O2A-C1
10	cA	827	CLA	CBA-CGA-O2A-C1
10	aB	824	CLA	O1D-CGD-O2D-CED
10	bB	824	CLA	O1D-CGD-O2D-CED
10	cB	824	CLA	O1D-CGD-O2D-CED
10	aA	827	CLA	O1A-CGA-O2A-C1
10	bA	827	CLA	O1A-CGA-O2A-C1
10	cA	827	CLA	O1A-CGA-O2A-C1
16	aB	848	LMG	C4-C5-C6-O5
16	bB	848	LMG	C4-C5-C6-O5
16	cB	848	LMG	C4-C5-C6-O5
10	aB	839	CLA	CBD-CGD-O2D-CED
10	bB	839	CLA	CBD-CGD-O2D-CED
10	cB	839	CLA	CBD-CGD-O2D-CED
10	aA	833	CLA	O1D-CGD-O2D-CED
10	bA	833	CLA	O1D-CGD-O2D-CED
10	cA	833	CLA	O1D-CGD-O2D-CED
10	aA	805	CLA	CBA-CGA-O2A-C1
10	aA	819	CLA	CBA-CGA-O2A-C1
10	aA	826	CLA	CBA-CGA-O2A-C1
10	aB	823	CLA	CBA-CGA-O2A-C1
10	aB	832	CLA	CBA-CGA-O2A-C1
10	bA	805	CLA	CBA-CGA-O2A-C1
10	bA	819	CLA	CBA-CGA-O2A-C1
10	bA	826	CLA	CBA-CGA-O2A-C1
10	bB	823	CLA	CBA-CGA-O2A-C1
10	bB	832	CLA	CBA-CGA-O2A-C1
10	cA	805	CLA	CBA-CGA-O2A-C1
10	cA	815	CLA	CBA-CGA-O2A-C1
10	cA	819	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cA	826	CLA	CBA-CGA-O2A-C1
10	cB	823	CLA	CBA-CGA-O2A-C1
10	cB	832	CLA	CBA-CGA-O2A-C1
10	aB	841	CLA	O1D-CGD-O2D-CED
10	bB	841	CLA	O1D-CGD-O2D-CED
10	cB	841	CLA	O1D-CGD-O2D-CED
10	aA	810	CLA	C8-C10-C11-C12
10	aA	820	CLA	C15-C16-C17-C18
10	bA	810	CLA	C8-C10-C11-C12
10	bA	820	CLA	C15-C16-C17-C18
10	cA	810	CLA	C8-C10-C11-C12
10	cA	820	CLA	C15-C16-C17-C18
10	aA	815	CLA	CBA-CGA-O2A-C1
10	bA	815	CLA	CBA-CGA-O2A-C1
10	aB	823	CLA	O1A-CGA-O2A-C1
10	bA	826	CLA	O1A-CGA-O2A-C1
10	bB	823	CLA	O1A-CGA-O2A-C1
10	cA	805	CLA	O1A-CGA-O2A-C1
10	cB	823	CLA	O1A-CGA-O2A-C1
16	bB	848	LMG	O6-C5-C6-O5
16	cB	848	LMG	O6-C5-C6-O5
10	aB	806	CLA	C2-C3-C5-C6
10	bB	806	CLA	C2-C3-C5-C6
10	cB	806	CLA	C2-C3-C5-C6
10	aA	818	CLA	C11-C12-C13-C14
10	aB	819	CLA	C11-C10-C8-C9
10	aB	828	CLA	C11-C10-C8-C9
10	bA	818	CLA	C11-C12-C13-C14
10	bB	819	CLA	C11-C10-C8-C9
10	bB	828	CLA	C11-C10-C8-C9
10	cA	818	CLA	C11-C12-C13-C14
10	cB	819	CLA	C11-C10-C8-C9
10	cB	828	CLA	C11-C10-C8-C9
10	cA	832	CLA	CBD-CGD-O2D-CED
10	aA	812	CLA	C10-C11-C12-C13
10	aL	205	CLA	C10-C11-C12-C13
10	bA	812	CLA	C10-C11-C12-C13
10	bL	205	CLA	C10-C11-C12-C13
10	cA	812	CLA	C10-C11-C12-C13
10	cL	205	CLA	C10-C11-C12-C13
10	aA	816	CLA	C2A-CAA-CBA-CGA
10	bA	816	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cA	816	CLA	C2A-CAA-CBA-CGA
13	aA	848	BCR	C37-C22-C23-C24
13	aA	849	BCR	C7-C8-C9-C34
13	aA	849	BCR	C37-C22-C23-C24
13	aA	850	BCR	C7-C8-C9-C34
13	aB	843	BCR	C37-C22-C23-C24
13	aB	844	BCR	C37-C22-C23-C24
13	aB	845	BCR	C11-C12-C13-C35
13	aL	206	BCR	C37-C22-C23-C24
13	aL	207	BCR	C36-C18-C19-C20
13	bA	848	BCR	C37-C22-C23-C24
13	bA	849	BCR	C7-C8-C9-C34
13	bA	849	BCR	C37-C22-C23-C24
13	bA	850	BCR	C7-C8-C9-C34
13	bB	843	BCR	C37-C22-C23-C24
13	bB	845	BCR	C11-C12-C13-C35
13	bL	206	BCR	C37-C22-C23-C24
13	bL	207	BCR	C36-C18-C19-C20
13	cA	848	BCR	C37-C22-C23-C24
13	cA	849	BCR	C7-C8-C9-C34
13	cA	849	BCR	C37-C22-C23-C24
13	cA	850	BCR	C7-C8-C9-C34
13	cB	843	BCR	C37-C22-C23-C24
13	cB	845	BCR	C11-C12-C13-C35
13	cL	206	BCR	C37-C22-C23-C24
13	cL	207	BCR	C36-C18-C19-C20
13	aA	848	BCR	C7-C8-C9-C10
13	aL	206	BCR	C21-C22-C23-C24
13	bA	848	BCR	C7-C8-C9-C10
13	bL	206	BCR	C21-C22-C23-C24
13	cA	848	BCR	C7-C8-C9-C10
13	cL	206	BCR	C21-C22-C23-C24
16	aB	848	LMG	O6-C5-C6-O5
16	aB	848	LMG	C28-C29-C30-C31
16	bB	848	LMG	C28-C29-C30-C31
16	cB	848	LMG	C28-C29-C30-C31
10	aA	805	CLA	O1A-CGA-O2A-C1
10	aA	819	CLA	O1A-CGA-O2A-C1
10	aA	826	CLA	O1A-CGA-O2A-C1
10	aB	832	CLA	O1A-CGA-O2A-C1
10	bA	805	CLA	O1A-CGA-O2A-C1
10	bA	819	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bB	832	CLA	O1A-CGA-O2A-C1
10	cA	819	CLA	O1A-CGA-O2A-C1
10	cA	826	CLA	O1A-CGA-O2A-C1
10	cB	832	CLA	O1A-CGA-O2A-C1
10	aA	812	CLA	C8-C10-C11-C12
10	aB	810	CLA	C5-C6-C7-C8
10	aB	838	CLA	C8-C10-C11-C12
10	bB	838	CLA	C8-C10-C11-C12
10	cA	812	CLA	C8-C10-C11-C12
10	cB	810	CLA	C5-C6-C7-C8
10	cB	838	CLA	C8-C10-C11-C12
10	aA	832	CLA	CBD-CGD-O2D-CED
10	bA	832	CLA	CBD-CGD-O2D-CED
10	aB	826	CLA	C3-C5-C6-C7
10	bB	826	CLA	C3-C5-C6-C7
10	cB	826	CLA	C3-C5-C6-C7
10	aA	829	CLA	C13-C15-C16-C17
10	aA	831	CLA	C10-C11-C12-C13
10	aB	802	CLA	C15-C16-C17-C18
10	aB	804	CLA	C5-C6-C7-C8
10	aB	827	CLA	C13-C15-C16-C17
10	aB	837	CLA	C8-C10-C11-C12
10	aB	838	CLA	C5-C6-C7-C8
10	aL	204	CLA	C8-C10-C11-C12
10	bA	812	CLA	C8-C10-C11-C12
10	bA	829	CLA	C13-C15-C16-C17
10	bA	831	CLA	C10-C11-C12-C13
10	bB	802	CLA	C15-C16-C17-C18
10	bB	804	CLA	C5-C6-C7-C8
10	bB	810	CLA	C5-C6-C7-C8
10	bB	827	CLA	C13-C15-C16-C17
10	bB	837	CLA	C8-C10-C11-C12
10	bB	838	CLA	C5-C6-C7-C8
10	bL	204	CLA	C8-C10-C11-C12
10	cA	829	CLA	C13-C15-C16-C17
10	cA	831	CLA	C10-C11-C12-C13
10	cB	802	CLA	C15-C16-C17-C18
10	cB	804	CLA	C5-C6-C7-C8
10	cB	827	CLA	C13-C15-C16-C17
10	cB	837	CLA	C8-C10-C11-C12
10	cB	838	CLA	C5-C6-C7-C8
10	cL	204	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bB	828	CLA	O1D-CGD-O2D-CED
10	aB	828	CLA	O1D-CGD-O2D-CED
10	cB	828	CLA	O1D-CGD-O2D-CED
10	aA	818	CLA	C13-C15-C16-C17
10	aA	823	CLA	C5-C6-C7-C8
10	aB	801	CLA	C10-C11-C12-C13
10	aB	817	CLA	C5-C6-C7-C8
10	aB	828	CLA	C13-C15-C16-C17
10	aB	838	CLA	C10-C11-C12-C13
10	bA	818	CLA	C13-C15-C16-C17
10	bA	823	CLA	C5-C6-C7-C8
10	bB	801	CLA	C10-C11-C12-C13
10	bB	817	CLA	C5-C6-C7-C8
10	bB	828	CLA	C13-C15-C16-C17
10	bB	838	CLA	C10-C11-C12-C13
10	cA	818	CLA	C13-C15-C16-C17
10	cA	823	CLA	C5-C6-C7-C8
10	cB	801	CLA	C10-C11-C12-C13
10	cB	817	CLA	C5-C6-C7-C8
10	cB	828	CLA	C13-C15-C16-C17
10	cB	838	CLA	C10-C11-C12-C13
10	aA	827	CLA	C8-C10-C11-C12
10	aB	830	CLA	C13-C15-C16-C17
10	bA	827	CLA	C8-C10-C11-C12
10	bB	830	CLA	C13-C15-C16-C17
10	cA	827	CLA	C8-C10-C11-C12
10	cB	830	CLA	C13-C15-C16-C17
10	aB	817	CLA	O1D-CGD-O2D-CED
10	bB	817	CLA	O1D-CGD-O2D-CED
10	cB	817	CLA	O1D-CGD-O2D-CED
10	aA	819	CLA	C2-C1-O2A-CGA
10	bA	819	CLA	C2-C1-O2A-CGA
10	cA	819	CLA	C2-C1-O2A-CGA
10	aA	841	CLA	C5-C6-C7-C8
10	aB	832	CLA	C15-C16-C17-C18
10	aB	837	CLA	C5-C6-C7-C8
10	bA	841	CLA	C5-C6-C7-C8
10	bB	832	CLA	C15-C16-C17-C18
10	bB	837	CLA	C5-C6-C7-C8
10	cA	841	CLA	C5-C6-C7-C8
10	cB	832	CLA	C15-C16-C17-C18
10	cB	837	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aB	820	CLA	CBD-CGD-O2D-CED
10	bB	820	CLA	CBD-CGD-O2D-CED
10	cB	820	CLA	CBD-CGD-O2D-CED
10	aA	826	CLA	C5-C6-C7-C8
10	aB	805	CLA	C8-C10-C11-C12
10	bA	826	CLA	C5-C6-C7-C8
10	bB	805	CLA	C8-C10-C11-C12
10	cA	826	CLA	C5-C6-C7-C8
10	cB	805	CLA	C8-C10-C11-C12
15	aA	853	LMT	C4B-C5B-C6B-O6B
15	bA	853	LMT	C4B-C5B-C6B-O6B
15	cA	853	LMT	C4B-C5B-C6B-O6B
10	aA	804	CLA	C11-C10-C8-C7
10	aB	818	CLA	C11-C10-C8-C7
10	bA	804	CLA	C11-C10-C8-C7
10	bB	818	CLA	C11-C10-C8-C7
10	cA	804	CLA	C11-C10-C8-C7
10	cB	818	CLA	C11-C10-C8-C7
10	aA	826	CLA	C3-C5-C6-C7
10	bA	826	CLA	C3-C5-C6-C7
10	cA	826	CLA	C3-C5-C6-C7
10	aA	815	CLA	O1A-CGA-O2A-C1
10	bA	815	CLA	O1A-CGA-O2A-C1
10	cA	815	CLA	O1A-CGA-O2A-C1
13	aB	843	BCR	C19-C20-C21-C22
13	aM	101	BCR	C19-C20-C21-C22
13	bB	843	BCR	C19-C20-C21-C22
13	bM	101	BCR	C19-C20-C21-C22
13	cB	843	BCR	C19-C20-C21-C22
13	cM	101	BCR	C19-C20-C21-C22
10	aB	825	CLA	C2A-CAA-CBA-CGA
10	bB	825	CLA	C2A-CAA-CBA-CGA
10	cB	825	CLA	C2A-CAA-CBA-CGA
10	aA	807	CLA	O1D-CGD-O2D-CED
10	bA	807	CLA	O1D-CGD-O2D-CED
10	cA	807	CLA	O1D-CGD-O2D-CED
10	aB	814	CLA	C13-C15-C16-C17
10	aB	819	CLA	C5-C6-C7-C8
10	aB	832	CLA	C8-C10-C11-C12
10	bA	835	CLA	C15-C16-C17-C18
10	bB	814	CLA	C13-C15-C16-C17
10	bB	819	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bB	832	CLA	C8-C10-C11-C12
10	cB	814	CLA	C13-C15-C16-C17
10	cB	819	CLA	C5-C6-C7-C8
10	cB	832	CLA	C8-C10-C11-C12
10	aA	835	CLA	C15-C16-C17-C18
10	cA	835	CLA	C15-C16-C17-C18
13	aA	846	BCR	C10-C11-C12-C13
13	aA	846	BCR	C18-C19-C20-C21
13	aA	848	BCR	C18-C19-C20-C21
13	aM	101	BCR	C18-C19-C20-C21
13	bA	846	BCR	C10-C11-C12-C13
13	bA	846	BCR	C18-C19-C20-C21
13	bA	848	BCR	C18-C19-C20-C21
13	bM	101	BCR	C18-C19-C20-C21
13	cA	846	BCR	C10-C11-C12-C13
13	cA	846	BCR	C18-C19-C20-C21
13	cA	848	BCR	C18-C19-C20-C21
13	cM	101	BCR	C18-C19-C20-C21
14	aA	855	LHG	O2-C2-C3-O3
14	bA	855	LHG	O2-C2-C3-O3
14	cA	855	LHG	O2-C2-C3-O3
10	aA	842	CLA	C15-C16-C17-C18
10	aL	203	CLA	C10-C11-C12-C13
10	aL	205	CLA	C5-C6-C7-C8
10	bA	842	CLA	C15-C16-C17-C18
10	bL	203	CLA	C10-C11-C12-C13
10	bL	205	CLA	C5-C6-C7-C8
10	cA	842	CLA	C15-C16-C17-C18
10	cL	203	CLA	C10-C11-C12-C13
10	cL	205	CLA	C5-C6-C7-C8
10	aA	812	CLA	C5-C6-C7-C8
10	aA	818	CLA	C10-C11-C12-C13
10	aA	827	CLA	C13-C15-C16-C17
10	aA	842	CLA	C8-C10-C11-C12
10	aB	805	CLA	C13-C15-C16-C17
10	bA	812	CLA	C5-C6-C7-C8
10	bA	818	CLA	C10-C11-C12-C13
10	bA	827	CLA	C13-C15-C16-C17
10	bA	841	CLA	C15-C16-C17-C18
10	bA	842	CLA	C8-C10-C11-C12
10	bB	805	CLA	C13-C15-C16-C17
10	cA	812	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cA	818	CLA	C10-C11-C12-C13
10	cA	827	CLA	C13-C15-C16-C17
10	cA	842	CLA	C8-C10-C11-C12
10	cB	805	CLA	C13-C15-C16-C17
10	cB	811	CLA	C5-C6-C7-C8
11	aA	844	PQN	C18-C20-C21-C22
11	bA	844	PQN	C18-C20-C21-C22
10	aA	816	CLA	O1D-CGD-O2D-CED
10	bA	816	CLA	O1D-CGD-O2D-CED
10	cA	816	CLA	O1D-CGD-O2D-CED
10	aA	812	CLA	C13-C15-C16-C17
10	aA	824	CLA	C5-C6-C7-C8
10	aA	837	CLA	C15-C16-C17-C18
10	aA	841	CLA	C15-C16-C17-C18
10	aB	807	CLA	C10-C11-C12-C13
10	aB	811	CLA	C5-C6-C7-C8
10	aB	827	CLA	C15-C16-C17-C18
10	bA	812	CLA	C13-C15-C16-C17
10	bA	824	CLA	C5-C6-C7-C8
10	bA	837	CLA	C15-C16-C17-C18
10	bB	807	CLA	C10-C11-C12-C13
10	bB	811	CLA	C5-C6-C7-C8
10	bB	827	CLA	C15-C16-C17-C18
10	cA	812	CLA	C13-C15-C16-C17
10	cA	824	CLA	C5-C6-C7-C8
10	cA	837	CLA	C15-C16-C17-C18
10	cA	841	CLA	C15-C16-C17-C18
10	cB	807	CLA	C10-C11-C12-C13
10	cB	827	CLA	C15-C16-C17-C18
11	cA	844	PQN	C18-C20-C21-C22
14	aA	852	LHG	C3-O3-P-O6
14	aA	855	LHG	C4-O6-P-O3
14	bA	852	LHG	C3-O3-P-O6
14	bA	855	LHG	C4-O6-P-O3
14	cA	852	LHG	C3-O3-P-O6
14	cA	855	LHG	C4-O6-P-O3
10	aA	819	CLA	C3-C5-C6-C7
10	aA	823	CLA	C3-C5-C6-C7
10	bA	819	CLA	C3-C5-C6-C7
10	bA	823	CLA	C3-C5-C6-C7
10	cA	819	CLA	C3-C5-C6-C7
10	cA	823	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bA	825	CLA	CBD-CGD-O2D-CED
10	cA	825	CLA	CBD-CGD-O2D-CED
10	aB	802	CLA	C13-C15-C16-C17
10	bB	802	CLA	C13-C15-C16-C17
10	cB	802	CLA	C13-C15-C16-C17
14	aA	855	LHG	C1-C2-C3-O3
14	bA	855	LHG	C1-C2-C3-O3
14	cA	855	LHG	C1-C2-C3-O3
10	aA	829	CLA	C4-C3-C5-C6
10	bA	829	CLA	C4-C3-C5-C6
10	cA	829	CLA	C4-C3-C5-C6
10	aA	819	CLA	C2-C3-C5-C6
10	bA	819	CLA	C2-C3-C5-C6
10	cA	819	CLA	C2-C3-C5-C6
10	aA	825	CLA	CBD-CGD-O2D-CED
10	aB	801	CLA	C2A-CAA-CBA-CGA
10	bB	801	CLA	C2A-CAA-CBA-CGA
10	cB	801	CLA	C2A-CAA-CBA-CGA
10	cA	834	CLA	CBA-CGA-O2A-C1
10	bA	818	CLA	O1D-CGD-O2D-CED
10	aA	818	CLA	O1D-CGD-O2D-CED
10	cA	818	CLA	O1D-CGD-O2D-CED
10	aB	826	CLA	C10-C11-C12-C13
10	bB	826	CLA	C10-C11-C12-C13
10	cB	826	CLA	C10-C11-C12-C13
13	aA	848	BCR	C20-C21-C22-C37
13	aA	850	BCR	C20-C21-C22-C37
13	aA	851	BCR	C20-C21-C22-C37
13	aB	843	BCR	C20-C21-C22-C37
13	aB	844	BCR	C20-C21-C22-C37
13	aB	846	BCR	C20-C21-C22-C37
13	aB	847	BCR	C35-C13-C14-C15
13	aB	847	BCR	C20-C21-C22-C37
13	bA	848	BCR	C20-C21-C22-C37
13	bA	850	BCR	C20-C21-C22-C37
13	bA	851	BCR	C20-C21-C22-C37
13	bB	843	BCR	C20-C21-C22-C37
13	bB	844	BCR	C20-C21-C22-C37
13	bB	846	BCR	C20-C21-C22-C37
13	bB	847	BCR	C35-C13-C14-C15
13	bB	847	BCR	C20-C21-C22-C37
13	cA	848	BCR	C20-C21-C22-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	cA	850	BCR	C20-C21-C22-C37
13	cA	851	BCR	C20-C21-C22-C37
13	cB	843	BCR	C20-C21-C22-C37
13	cB	844	BCR	C20-C21-C22-C37
13	cB	846	BCR	C20-C21-C22-C37
13	cB	847	BCR	C35-C13-C14-C15
13	cB	847	BCR	C20-C21-C22-C37
10	aA	825	CLA	C6-C7-C8-C9
10	bA	825	CLA	C6-C7-C8-C9
10	cA	825	CLA	C6-C7-C8-C9
11	aA	844	PQN	C26-C27-C28-C29
11	bA	844	PQN	C26-C27-C28-C29
11	cA	844	PQN	C26-C27-C28-C29
10	aA	834	CLA	CBA-CGA-O2A-C1
10	aB	814	CLA	CBA-CGA-O2A-C1
10	aB	833	CLA	CBA-CGA-O2A-C1
10	bA	834	CLA	CBA-CGA-O2A-C1
10	bB	814	CLA	CBA-CGA-O2A-C1
10	bB	833	CLA	CBA-CGA-O2A-C1
10	cB	814	CLA	CBA-CGA-O2A-C1
10	cB	833	CLA	CBA-CGA-O2A-C1
15	aA	853	LMT	C2-C3-C4-C5
15	bA	853	LMT	C2-C3-C4-C5
15	cA	853	LMT	C2-C3-C4-C5
10	aB	831	CLA	O1D-CGD-O2D-CED
10	bB	831	CLA	O1D-CGD-O2D-CED
10	cB	831	CLA	O1D-CGD-O2D-CED
14	aA	852	LHG	C9-C10-C11-C12
14	bA	852	LHG	C9-C10-C11-C12
14	cA	852	LHG	C9-C10-C11-C12
10	aA	818	CLA	C3-C5-C6-C7
10	aA	834	CLA	C3-C5-C6-C7
10	bA	818	CLA	C3-C5-C6-C7
10	bA	834	CLA	C3-C5-C6-C7
10	cA	818	CLA	C3-C5-C6-C7
10	cA	834	CLA	C3-C5-C6-C7
13	aA	846	BCR	C20-C21-C22-C23
13	aA	847	BCR	C20-C21-C22-C23
13	aA	848	BCR	C11-C10-C9-C8
13	aA	851	BCR	C11-C10-C9-C8
13	aB	843	BCR	C20-C21-C22-C23
13	aB	844	BCR	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	aB	849	BCR	C16-C17-C18-C19
13	aI	102	BCR	C11-C10-C9-C8
13	aM	101	BCR	C20-C21-C22-C23
13	bA	846	BCR	C20-C21-C22-C23
13	bA	847	BCR	C20-C21-C22-C23
13	bA	848	BCR	C11-C10-C9-C8
13	bA	851	BCR	C11-C10-C9-C8
13	bB	843	BCR	C20-C21-C22-C23
13	bB	844	BCR	C16-C17-C18-C19
13	bB	849	BCR	C16-C17-C18-C19
13	bI	102	BCR	C11-C10-C9-C8
13	bM	101	BCR	C20-C21-C22-C23
13	cA	846	BCR	C20-C21-C22-C23
13	cA	847	BCR	C20-C21-C22-C23
13	cA	848	BCR	C11-C10-C9-C8
13	cA	851	BCR	C11-C10-C9-C8
13	cB	843	BCR	C20-C21-C22-C23
13	cB	844	BCR	C16-C17-C18-C19
13	cB	849	BCR	C16-C17-C18-C19
13	cI	103	BCR	C11-C10-C9-C8
13	cM	101	BCR	C20-C21-C22-C23
10	aB	841	CLA	CBA-CGA-O2A-C1
10	bB	841	CLA	CBA-CGA-O2A-C1
10	cB	841	CLA	CBA-CGA-O2A-C1
10	aA	834	CLA	C5-C6-C7-C8
10	bA	834	CLA	C5-C6-C7-C8
10	cA	834	CLA	C5-C6-C7-C8
16	aB	848	LMG	C21-C22-C23-C24
16	bB	848	LMG	C21-C22-C23-C24
16	cB	848	LMG	C21-C22-C23-C24
10	bB	811	CLA	C16-C17-C18-C20
10	cB	811	CLA	C16-C17-C18-C20
10	aA	804	CLA	C4-C3-C5-C6
10	aA	824	CLA	C4-C3-C5-C6
10	aA	835	CLA	C4-C3-C5-C6
10	bA	804	CLA	C4-C3-C5-C6
10	bA	824	CLA	C4-C3-C5-C6
10	bA	835	CLA	C4-C3-C5-C6
10	cA	804	CLA	C4-C3-C5-C6
10	cA	824	CLA	C4-C3-C5-C6
10	cA	835	CLA	C4-C3-C5-C6
10	aA	824	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bA	824	CLA	C2-C3-C5-C6
10	cA	824	CLA	C2-C3-C5-C6
10	aA	827	CLA	C14-C13-C15-C16
10	aA	831	CLA	C14-C13-C15-C16
10	bA	827	CLA	C14-C13-C15-C16
10	bA	831	CLA	C14-C13-C15-C16
10	cA	827	CLA	C14-C13-C15-C16
10	cA	831	CLA	C14-C13-C15-C16
10	aB	833	CLA	O1D-CGD-O2D-CED
14	aA	852	LHG	C28-C29-C30-C31
14	aA	852	LHG	C30-C31-C32-C33
14	bA	852	LHG	C28-C29-C30-C31
14	bA	852	LHG	C30-C31-C32-C33
14	cA	852	LHG	C28-C29-C30-C31
14	cA	852	LHG	C30-C31-C32-C33
15	aA	853	LMT	C3-C4-C5-C6
15	bA	853	LMT	C3-C4-C5-C6
15	cA	853	LMT	C3-C4-C5-C6
13	aB	847	BCR	C7-C8-C9-C34
13	bB	844	BCR	C37-C22-C23-C24
13	bB	847	BCR	C7-C8-C9-C34
13	cB	844	BCR	C37-C22-C23-C24
13	cB	847	BCR	C7-C8-C9-C34
14	aA	855	LHG	O1-C1-C2-C3
14	bA	855	LHG	O1-C1-C2-C3
14	cA	855	LHG	O1-C1-C2-C3
13	aA	849	BCR	C21-C22-C23-C24
13	aB	847	BCR	C7-C8-C9-C10
13	aB	849	BCR	C21-C22-C23-C24
13	bA	849	BCR	C21-C22-C23-C24
13	bB	847	BCR	C7-C8-C9-C10
13	bB	849	BCR	C21-C22-C23-C24
13	cA	849	BCR	C21-C22-C23-C24
13	cB	847	BCR	C7-C8-C9-C10
13	cB	849	BCR	C21-C22-C23-C24
10	aA	812	CLA	C3-C5-C6-C7
10	bA	812	CLA	C3-C5-C6-C7
10	cA	812	CLA	C3-C5-C6-C7
10	bB	833	CLA	O1D-CGD-O2D-CED
10	cB	833	CLA	O1D-CGD-O2D-CED
10	aA	811	CLA	C5-C6-C7-C8
10	bA	811	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cA	811	CLA	C5-C6-C7-C8
10	aA	825	CLA	C6-C7-C8-C10
10	aB	811	CLA	C16-C17-C18-C19
10	aB	811	CLA	C16-C17-C18-C20
10	aB	827	CLA	C16-C17-C18-C19
10	bA	825	CLA	C6-C7-C8-C10
10	bB	811	CLA	C16-C17-C18-C19
10	bB	827	CLA	C16-C17-C18-C19
10	cA	825	CLA	C6-C7-C8-C10
10	cB	811	CLA	C16-C17-C18-C19
10	cB	827	CLA	C16-C17-C18-C19
10	aB	815	CLA	C5-C6-C7-C8
10	bB	815	CLA	C5-C6-C7-C8
10	cB	815	CLA	C5-C6-C7-C8
16	aB	848	LMG	C29-C30-C31-C32
16	bB	848	LMG	C29-C30-C31-C32
16	cB	848	LMG	C29-C30-C31-C32
10	aA	802	CLA	C3A-C2A-CAA-CBA
10	aA	812	CLA	C3A-C2A-CAA-CBA
10	aA	827	CLA	C3A-C2A-CAA-CBA
10	aA	835	CLA	C3A-C2A-CAA-CBA
10	aA	836	CLA	C3A-C2A-CAA-CBA
10	aA	840	CLA	C3A-C2A-CAA-CBA
10	aB	801	CLA	C3A-C2A-CAA-CBA
10	bA	802	CLA	C3A-C2A-CAA-CBA
10	bA	812	CLA	C3A-C2A-CAA-CBA
10	bA	827	CLA	C3A-C2A-CAA-CBA
10	bA	835	CLA	C3A-C2A-CAA-CBA
10	bA	836	CLA	C3A-C2A-CAA-CBA
10	bA	840	CLA	C3A-C2A-CAA-CBA
10	bB	801	CLA	C3A-C2A-CAA-CBA
10	cA	802	CLA	C3A-C2A-CAA-CBA
10	cA	812	CLA	C3A-C2A-CAA-CBA
10	cA	827	CLA	C3A-C2A-CAA-CBA
10	cA	835	CLA	C3A-C2A-CAA-CBA
10	cA	836	CLA	C3A-C2A-CAA-CBA
10	cA	840	CLA	C3A-C2A-CAA-CBA
10	cB	801	CLA	C3A-C2A-CAA-CBA
10	aB	811	CLA	C8-C10-C11-C12
10	bB	811	CLA	C8-C10-C11-C12
10	cB	811	CLA	C8-C10-C11-C12
14	bA	852	LHG	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	cA	852	LHG	C15-C16-C17-C18
11	aA	844	PQN	C26-C27-C28-C30
11	bA	844	PQN	C26-C27-C28-C30
11	cA	844	PQN	C26-C27-C28-C30
14	aA	852	LHG	C15-C16-C17-C18
10	aB	837	CLA	CBD-CGD-O2D-CED
10	bB	837	CLA	CBD-CGD-O2D-CED
10	cB	837	CLA	CBD-CGD-O2D-CED
10	aB	806	CLA	C3-C5-C6-C7
10	bB	806	CLA	C3-C5-C6-C7
10	cB	806	CLA	C3-C5-C6-C7
10	aA	832	CLA	C4-C3-C5-C6
10	bA	832	CLA	C4-C3-C5-C6
10	cA	832	CLA	C4-C3-C5-C6
10	aA	832	CLA	C2-C3-C5-C6
10	bA	832	CLA	C2-C3-C5-C6
10	cA	832	CLA	C2-C3-C5-C6
10	aA	838	CLA	C2A-CAA-CBA-CGA
10	bA	838	CLA	C2A-CAA-CBA-CGA
10	cA	838	CLA	C2A-CAA-CBA-CGA
16	aB	848	LMG	C40-C41-C42-C43
16	bB	848	LMG	C40-C41-C42-C43
16	cB	848	LMG	C40-C41-C42-C43
10	aB	822	CLA	O1D-CGD-O2D-CED
10	aA	834	CLA	O1A-CGA-O2A-C1
10	bA	834	CLA	O1A-CGA-O2A-C1
10	cA	834	CLA	O1A-CGA-O2A-C1
10	cB	822	CLA	O1D-CGD-O2D-CED
10	aA	804	CLA	C15-C16-C17-C18
10	bA	804	CLA	C15-C16-C17-C18
10	cA	804	CLA	C15-C16-C17-C18
10	aB	814	CLA	O1A-CGA-O2A-C1
10	aB	833	CLA	O1A-CGA-O2A-C1
10	bB	814	CLA	O1A-CGA-O2A-C1
10	bB	833	CLA	O1A-CGA-O2A-C1
10	cB	814	CLA	O1A-CGA-O2A-C1
10	cB	833	CLA	O1A-CGA-O2A-C1
10	aB	829	CLA	C5-C6-C7-C8
10	bB	829	CLA	C5-C6-C7-C8
10	cA	828	CLA	C5-C6-C7-C8
10	cB	829	CLA	C5-C6-C7-C8
10	bB	822	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	aA	852	LHG	C24-C25-C26-C27
14	aA	852	LHG	C32-C33-C34-C35
14	bA	852	LHG	C24-C25-C26-C27
14	bA	852	LHG	C32-C33-C34-C35
14	cA	852	LHG	C24-C25-C26-C27
14	cA	852	LHG	C32-C33-C34-C35
16	bB	848	LMG	C35-C36-C37-C38
16	cB	848	LMG	C35-C36-C37-C38
10	aA	824	CLA	C2-C1-O2A-CGA
10	aB	828	CLA	C2-C1-O2A-CGA
10	bA	824	CLA	C2-C1-O2A-CGA
10	bB	828	CLA	C2-C1-O2A-CGA
10	cA	824	CLA	C2-C1-O2A-CGA
10	cB	828	CLA	C2-C1-O2A-CGA
16	aB	848	LMG	C35-C36-C37-C38
10	aA	828	CLA	C5-C6-C7-C8
10	bA	828	CLA	C5-C6-C7-C8
10	aB	841	CLA	O1A-CGA-O2A-C1
10	bB	841	CLA	O1A-CGA-O2A-C1
10	cB	841	CLA	O1A-CGA-O2A-C1
10	aB	810	CLA	C3-C5-C6-C7
10	bB	810	CLA	C3-C5-C6-C7
10	cB	810	CLA	C3-C5-C6-C7
13	aA	846	BCR	C5-C6-C7-C8
13	aA	847	BCR	C23-C24-C25-C26
13	aA	847	BCR	C23-C24-C25-C30
13	aA	849	BCR	C1-C6-C7-C8
13	aA	849	BCR	C5-C6-C7-C8
13	aA	849	BCR	C23-C24-C25-C30
13	aA	850	BCR	C5-C6-C7-C8
13	aA	850	BCR	C23-C24-C25-C30
13	aA	851	BCR	C23-C24-C25-C26
13	aA	851	BCR	C23-C24-C25-C30
13	aB	843	BCR	C5-C6-C7-C8
13	aB	844	BCR	C5-C6-C7-C8
13	aB	845	BCR	C1-C6-C7-C8
13	aB	845	BCR	C5-C6-C7-C8
13	aB	846	BCR	C5-C6-C7-C8
13	aB	846	BCR	C23-C24-C25-C26
13	aB	846	BCR	C23-C24-C25-C30
13	aI	101	BCR	C1-C6-C7-C8
13	aI	101	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	aI	102	BCR	C23-C24-C25-C26
13	aL	206	BCR	C23-C24-C25-C30
13	aL	207	BCR	C23-C24-C25-C26
13	aM	101	BCR	C5-C6-C7-C8
13	aM	101	BCR	C23-C24-C25-C26
13	aM	101	BCR	C23-C24-C25-C30
13	bA	846	BCR	C5-C6-C7-C8
13	bA	847	BCR	C23-C24-C25-C26
13	bA	847	BCR	C23-C24-C25-C30
13	bA	849	BCR	C1-C6-C7-C8
13	bA	849	BCR	C5-C6-C7-C8
13	bA	849	BCR	C23-C24-C25-C30
13	bA	850	BCR	C5-C6-C7-C8
13	bA	850	BCR	C23-C24-C25-C30
13	bA	851	BCR	C23-C24-C25-C26
13	bA	851	BCR	C23-C24-C25-C30
13	bB	843	BCR	C5-C6-C7-C8
13	bB	844	BCR	C5-C6-C7-C8
13	bB	845	BCR	C1-C6-C7-C8
13	bB	845	BCR	C5-C6-C7-C8
13	bB	846	BCR	C5-C6-C7-C8
13	bB	846	BCR	C23-C24-C25-C26
13	bB	846	BCR	C23-C24-C25-C30
13	bI	101	BCR	C1-C6-C7-C8
13	bI	101	BCR	C5-C6-C7-C8
13	bI	102	BCR	C23-C24-C25-C26
13	bL	206	BCR	C23-C24-C25-C30
13	bL	207	BCR	C23-C24-C25-C26
13	bM	101	BCR	C5-C6-C7-C8
13	bM	101	BCR	C23-C24-C25-C26
13	bM	101	BCR	C23-C24-C25-C30
13	cA	846	BCR	C5-C6-C7-C8
13	cA	847	BCR	C23-C24-C25-C26
13	cA	847	BCR	C23-C24-C25-C30
13	cA	849	BCR	C1-C6-C7-C8
13	cA	849	BCR	C5-C6-C7-C8
13	cA	849	BCR	C23-C24-C25-C30
13	cA	850	BCR	C5-C6-C7-C8
13	cA	850	BCR	C23-C24-C25-C30
13	cA	851	BCR	C23-C24-C25-C26
13	cA	851	BCR	C23-C24-C25-C30
13	cB	843	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	cB	844	BCR	C5-C6-C7-C8
13	cB	845	BCR	C1-C6-C7-C8
13	cB	845	BCR	C5-C6-C7-C8
13	cB	846	BCR	C5-C6-C7-C8
13	cB	846	BCR	C23-C24-C25-C26
13	cB	846	BCR	C23-C24-C25-C30
13	cI	102	BCR	C1-C6-C7-C8
13	cI	102	BCR	C5-C6-C7-C8
13	cI	103	BCR	C23-C24-C25-C26
13	cL	206	BCR	C23-C24-C25-C30
13	cL	207	BCR	C23-C24-C25-C26
13	cM	101	BCR	C5-C6-C7-C8
13	cM	101	BCR	C23-C24-C25-C26
13	cM	101	BCR	C23-C24-C25-C30
10	aA	818	CLA	CBA-CGA-O2A-C1
10	bA	818	CLA	CBA-CGA-O2A-C1
10	cA	818	CLA	CBA-CGA-O2A-C1
10	aB	819	CLA	O1A-CGA-O2A-C1
10	bB	819	CLA	O1A-CGA-O2A-C1
10	cB	819	CLA	O1A-CGA-O2A-C1
10	aB	830	CLA	CBD-CGD-O2D-CED
10	bB	830	CLA	CBD-CGD-O2D-CED
11	aA	844	PQN	C15-C16-C17-C18
11	bA	844	PQN	C15-C16-C17-C18
11	cA	844	PQN	C15-C16-C17-C18
10	aA	833	CLA	C4-C3-C5-C6
10	bA	833	CLA	C4-C3-C5-C6
10	cA	833	CLA	C4-C3-C5-C6
10	aA	804	CLA	C2-C3-C5-C6
10	aA	820	CLA	C11-C12-C13-C15
10	aA	827	CLA	C12-C13-C15-C16
10	aA	833	CLA	C2-C3-C5-C6
10	aA	835	CLA	C2-C3-C5-C6
10	aL	205	CLA	C11-C12-C13-C15
10	bA	804	CLA	C2-C3-C5-C6
10	bA	820	CLA	C11-C12-C13-C15
10	bA	827	CLA	C12-C13-C15-C16
10	bA	833	CLA	C2-C3-C5-C6
10	bA	835	CLA	C2-C3-C5-C6
10	bL	205	CLA	C11-C12-C13-C15
10	cA	804	CLA	C2-C3-C5-C6
10	cA	820	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cA	827	CLA	C12-C13-C15-C16
10	cA	833	CLA	C2-C3-C5-C6
10	cA	835	CLA	C2-C3-C5-C6
10	cL	205	CLA	C11-C12-C13-C15
10	aL	202	CLA	O1A-CGA-O2A-C1
10	bL	202	CLA	O1A-CGA-O2A-C1
10	cL	202	CLA	O1A-CGA-O2A-C1
16	bB	848	LMG	C36-C37-C38-C39
10	aB	802	CLA	C10-C11-C12-C13
10	aL	203	CLA	C13-C15-C16-C17
10	bB	802	CLA	C10-C11-C12-C13
10	bL	203	CLA	C13-C15-C16-C17
10	cB	802	CLA	C10-C11-C12-C13
10	cL	203	CLA	C13-C15-C16-C17
10	cB	830	CLA	CBD-CGD-O2D-CED
10	aA	811	CLA	CBA-CGA-O2A-C1
10	aA	816	CLA	CBA-CGA-O2A-C1
10	aA	829	CLA	CBA-CGA-O2A-C1
10	aB	807	CLA	CBA-CGA-O2A-C1
10	aB	815	CLA	CBA-CGA-O2A-C1
10	aL	202	CLA	CBA-CGA-O2A-C1
10	bA	811	CLA	CBA-CGA-O2A-C1
10	bA	816	CLA	CBA-CGA-O2A-C1
10	bA	829	CLA	CBA-CGA-O2A-C1
10	bB	807	CLA	CBA-CGA-O2A-C1
10	bB	815	CLA	CBA-CGA-O2A-C1
10	bL	202	CLA	CBA-CGA-O2A-C1
10	cA	811	CLA	CBA-CGA-O2A-C1
10	cA	816	CLA	CBA-CGA-O2A-C1
10	cA	829	CLA	CBA-CGA-O2A-C1
10	cB	807	CLA	CBA-CGA-O2A-C1
10	cB	815	CLA	CBA-CGA-O2A-C1
10	cL	202	CLA	CBA-CGA-O2A-C1
16	aB	848	LMG	C36-C37-C38-C39
16	cB	848	LMG	C36-C37-C38-C39
10	aA	817	CLA	C2A-CAA-CBA-CGA
10	aA	823	CLA	C2A-CAA-CBA-CGA
10	aA	836	CLA	C2A-CAA-CBA-CGA
10	aL	203	CLA	C2A-CAA-CBA-CGA
10	bA	817	CLA	C2A-CAA-CBA-CGA
10	bA	823	CLA	C2A-CAA-CBA-CGA
10	bA	836	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bL	203	CLA	C2A-CAA-CBA-CGA
10	cA	817	CLA	C2A-CAA-CBA-CGA
10	cA	823	CLA	C2A-CAA-CBA-CGA
10	cA	836	CLA	C2A-CAA-CBA-CGA
10	cL	203	CLA	C2A-CAA-CBA-CGA
10	aB	818	CLA	C10-C11-C12-C13
10	bB	818	CLA	C10-C11-C12-C13
10	cB	818	CLA	C10-C11-C12-C13
14	aA	852	LHG	C12-C13-C14-C15
14	bA	852	LHG	C12-C13-C14-C15
14	cA	852	LHG	C12-C13-C14-C15
10	aA	822	CLA	O1D-CGD-O2D-CED
10	bA	822	CLA	O1D-CGD-O2D-CED
10	cA	822	CLA	O1D-CGD-O2D-CED
10	aA	820	CLA	C10-C11-C12-C13
10	bA	820	CLA	C10-C11-C12-C13
10	cA	820	CLA	C10-C11-C12-C13
16	aB	848	LMG	C41-C42-C43-C44
16	bB	848	LMG	C41-C42-C43-C44
16	cB	848	LMG	C41-C42-C43-C44
10	aL	205	CLA	CBA-CGA-O2A-C1
10	bL	205	CLA	CBA-CGA-O2A-C1
10	cL	205	CLA	CBA-CGA-O2A-C1
10	aA	842	CLA	C10-C11-C12-C13
10	bA	842	CLA	C10-C11-C12-C13
10	cA	842	CLA	C10-C11-C12-C13
14	aA	855	LHG	O7-C5-C6-O8
14	bA	855	LHG	O7-C5-C6-O8
14	cA	855	LHG	O7-C5-C6-O8
10	aA	829	CLA	C2-C3-C5-C6
10	aB	832	CLA	C2-C3-C5-C6
10	bA	829	CLA	C2-C3-C5-C6
10	bB	832	CLA	C2-C3-C5-C6
10	cA	829	CLA	C2-C3-C5-C6
10	cB	832	CLA	C2-C3-C5-C6
10	aA	810	CLA	C6-C7-C8-C9
10	aA	820	CLA	C11-C12-C13-C14
10	aB	801	CLA	C6-C7-C8-C9
10	bA	810	CLA	C6-C7-C8-C9
10	bA	820	CLA	C11-C12-C13-C14
10	bB	801	CLA	C6-C7-C8-C9
10	cA	810	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cA	820	CLA	C11-C12-C13-C14
10	cB	801	CLA	C6-C7-C8-C9
10	aL	204	CLA	C2A-CAA-CBA-CGA
10	bL	204	CLA	C2A-CAA-CBA-CGA
10	cL	204	CLA	C2A-CAA-CBA-CGA
13	aA	850	BCR	C11-C12-C13-C35
13	aB	849	BCR	C7-C8-C9-C34
13	bA	850	BCR	C11-C12-C13-C35
13	bB	849	BCR	C7-C8-C9-C34
13	cA	850	BCR	C11-C12-C13-C35
13	cB	849	BCR	C7-C8-C9-C34
13	bI	101	BCR	C21-C22-C23-C24
13	cI	102	BCR	C21-C22-C23-C24
10	aA	818	CLA	O1A-CGA-O2A-C1
10	aB	807	CLA	O1A-CGA-O2A-C1
10	aB	815	CLA	O1A-CGA-O2A-C1
10	bA	818	CLA	O1A-CGA-O2A-C1
10	bB	807	CLA	O1A-CGA-O2A-C1
10	bB	815	CLA	O1A-CGA-O2A-C1
10	cA	818	CLA	O1A-CGA-O2A-C1
10	cB	807	CLA	O1A-CGA-O2A-C1
10	cB	815	CLA	O1A-CGA-O2A-C1
10	aA	802	CLA	C1A-C2A-CAA-CBA
10	aA	807	CLA	C1A-C2A-CAA-CBA
10	aA	812	CLA	C1A-C2A-CAA-CBA
10	aA	817	CLA	C1A-C2A-CAA-CBA
10	aA	831	CLA	C1A-C2A-CAA-CBA
10	aA	834	CLA	C1A-C2A-CAA-CBA
10	aA	836	CLA	C1A-C2A-CAA-CBA
10	aA	840	CLA	C1A-C2A-CAA-CBA
10	aB	811	CLA	C1A-C2A-CAA-CBA
10	aB	812	CLA	C1A-C2A-CAA-CBA
10	aB	839	CLA	C1A-C2A-CAA-CBA
10	aB	841	CLA	C1A-C2A-CAA-CBA
10	aL	203	CLA	C1A-C2A-CAA-CBA
10	bA	802	CLA	C1A-C2A-CAA-CBA
10	bA	807	CLA	C1A-C2A-CAA-CBA
10	bA	812	CLA	C1A-C2A-CAA-CBA
10	bA	817	CLA	C1A-C2A-CAA-CBA
10	bA	831	CLA	C1A-C2A-CAA-CBA
10	bA	834	CLA	C1A-C2A-CAA-CBA
10	bA	836	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bA	840	CLA	C1A-C2A-CAA-CBA
10	bB	811	CLA	C1A-C2A-CAA-CBA
10	bB	812	CLA	C1A-C2A-CAA-CBA
10	bB	839	CLA	C1A-C2A-CAA-CBA
10	bB	841	CLA	C1A-C2A-CAA-CBA
10	bL	203	CLA	C1A-C2A-CAA-CBA
10	cA	802	CLA	C1A-C2A-CAA-CBA
10	cA	807	CLA	C1A-C2A-CAA-CBA
10	cA	812	CLA	C1A-C2A-CAA-CBA
10	cA	817	CLA	C1A-C2A-CAA-CBA
10	cA	831	CLA	C1A-C2A-CAA-CBA
10	cA	834	CLA	C1A-C2A-CAA-CBA
10	cA	836	CLA	C1A-C2A-CAA-CBA
10	cA	840	CLA	C1A-C2A-CAA-CBA
10	cB	811	CLA	C1A-C2A-CAA-CBA
10	cB	812	CLA	C1A-C2A-CAA-CBA
10	cB	839	CLA	C1A-C2A-CAA-CBA
10	cB	841	CLA	C1A-C2A-CAA-CBA
10	cL	203	CLA	C1A-C2A-CAA-CBA
10	aB	826	CLA	C16-C17-C18-C20
10	bB	826	CLA	C16-C17-C18-C20
16	aB	848	LMG	C17-C18-C19-C20
16	bB	848	LMG	C17-C18-C19-C20
16	cB	848	LMG	C17-C18-C19-C20
10	aB	820	CLA	C13-C15-C16-C17
10	bB	820	CLA	C13-C15-C16-C17
16	aB	848	LMG	C15-C16-C17-C18
16	bB	848	LMG	C15-C16-C17-C18
10	aB	814	CLA	C10-C11-C12-C13
10	bB	814	CLA	C10-C11-C12-C13
10	cB	814	CLA	C10-C11-C12-C13
10	cB	820	CLA	C13-C15-C16-C17
16	cB	848	LMG	C15-C16-C17-C18
10	cB	826	CLA	C16-C17-C18-C20
15	aA	853	LMT	C1-C2-C3-C4
15	bA	853	LMT	C1-C2-C3-C4
15	cA	853	LMT	C1-C2-C3-C4
10	aB	832	CLA	C4-C3-C5-C6
10	bB	832	CLA	C4-C3-C5-C6
10	cB	832	CLA	C4-C3-C5-C6
10	aB	811	CLA	C13-C15-C16-C17
10	bB	811	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cB	811	CLA	C13-C15-C16-C17
10	aA	816	CLA	O1A-CGA-O2A-C1
10	aA	829	CLA	O1A-CGA-O2A-C1
10	bA	816	CLA	O1A-CGA-O2A-C1
10	bA	829	CLA	O1A-CGA-O2A-C1
10	cA	816	CLA	O1A-CGA-O2A-C1
10	cA	829	CLA	O1A-CGA-O2A-C1
10	aB	813	CLA	C2A-CAA-CBA-CGA
10	bB	813	CLA	C2A-CAA-CBA-CGA
10	cB	813	CLA	C2A-CAA-CBA-CGA
10	cA	832	CLA	O1D-CGD-O2D-CED
10	aA	817	CLA	C6-C7-C8-C9
10	cA	817	CLA	C6-C7-C8-C9
10	aA	832	CLA	O1D-CGD-O2D-CED
10	bA	832	CLA	O1D-CGD-O2D-CED
10	bA	817	CLA	C6-C7-C8-C9
10	aA	811	CLA	O1A-CGA-O2A-C1
10	aL	205	CLA	O1A-CGA-O2A-C1
10	bA	811	CLA	O1A-CGA-O2A-C1
10	bL	205	CLA	O1A-CGA-O2A-C1
10	cA	811	CLA	O1A-CGA-O2A-C1
10	cL	205	CLA	O1A-CGA-O2A-C1
15	aA	853	LMT	C9-C10-C11-C12
15	cA	853	LMT	C9-C10-C11-C12
10	aB	814	CLA	C5-C6-C7-C8
10	bB	814	CLA	C5-C6-C7-C8
10	cB	814	CLA	C5-C6-C7-C8
15	bA	853	LMT	C9-C10-C11-C12
14	aA	855	LHG	O1-C1-C2-O2
14	bA	855	LHG	O1-C1-C2-O2
14	cA	855	LHG	O1-C1-C2-O2
14	aA	855	LHG	C10-C11-C12-C13
14	cA	855	LHG	C10-C11-C12-C13
14	bA	855	LHG	C10-C11-C12-C13
10	aB	802	CLA	O1D-CGD-O2D-CED
10	cB	802	CLA	O1D-CGD-O2D-CED
13	aA	851	BCR	C16-C17-C18-C36
13	aB	845	BCR	C20-C21-C22-C37
13	bA	851	BCR	C16-C17-C18-C36
13	bB	845	BCR	C20-C21-C22-C37
13	cA	851	BCR	C16-C17-C18-C36
13	cB	845	BCR	C20-C21-C22-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aB	809	CLA	C4-C3-C5-C6
10	bB	809	CLA	C4-C3-C5-C6
10	cB	809	CLA	C4-C3-C5-C6
10	bB	802	CLA	O1D-CGD-O2D-CED
10	aA	831	CLA	CBA-CGA-O2A-C1
10	aB	808	CLA	CBA-CGA-O2A-C1
10	bA	831	CLA	CBA-CGA-O2A-C1
10	bB	808	CLA	CBA-CGA-O2A-C1
10	cA	831	CLA	CBA-CGA-O2A-C1
10	cB	808	CLA	CBA-CGA-O2A-C1
10	aA	812	CLA	C15-C16-C17-C18
10	aL	204	CLA	C10-C11-C12-C13
10	bA	812	CLA	C15-C16-C17-C18
10	bL	204	CLA	C10-C11-C12-C13
10	cA	812	CLA	C15-C16-C17-C18
10	cL	204	CLA	C10-C11-C12-C13
16	aB	848	LMG	C23-C24-C25-C26
9	aA	801	CL0	C2-C1-O2A-CGA
9	bA	801	CL0	C2-C1-O2A-CGA
9	cA	801	CL0	C2-C1-O2A-CGA
10	aA	827	CLA	C2-C1-O2A-CGA
10	aB	804	CLA	C2-C1-O2A-CGA
10	bA	827	CLA	C2-C1-O2A-CGA
10	bB	804	CLA	C2-C1-O2A-CGA
10	cA	827	CLA	C2-C1-O2A-CGA
10	cB	804	CLA	C2-C1-O2A-CGA
16	bB	848	LMG	C23-C24-C25-C26
16	cB	848	LMG	C23-C24-C25-C26
10	bB	839	CLA	O1D-CGD-O2D-CED
10	cB	839	CLA	O1D-CGD-O2D-CED
16	aB	848	LMG	C34-C35-C36-C37
16	bB	848	LMG	C34-C35-C36-C37
16	cB	848	LMG	C34-C35-C36-C37
10	aB	839	CLA	O1D-CGD-O2D-CED
10	aA	854	CLA	CBA-CGA-O2A-C1
10	bA	854	CLA	CBA-CGA-O2A-C1
10	cA	854	CLA	CBA-CGA-O2A-C1
10	aB	806	CLA	O1D-CGD-O2D-CED
10	aB	828	CLA	C8-C10-C11-C12
10	bB	828	CLA	C8-C10-C11-C12
10	cB	828	CLA	C8-C10-C11-C12
10	bB	806	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cB	806	CLA	O1D-CGD-O2D-CED
10	aB	811	CLA	O1A-CGA-O2A-C1
10	bB	811	CLA	O1A-CGA-O2A-C1
10	cB	811	CLA	O1A-CGA-O2A-C1
10	aA	831	CLA	C13-C15-C16-C17
10	bA	831	CLA	C13-C15-C16-C17
10	cA	831	CLA	C13-C15-C16-C17
16	aB	848	LMG	C42-C43-C44-C45
16	bB	848	LMG	C42-C43-C44-C45
16	cB	848	LMG	C42-C43-C44-C45
10	aB	808	CLA	O1A-CGA-O2A-C1
10	bB	808	CLA	O1A-CGA-O2A-C1
10	cB	808	CLA	O1A-CGA-O2A-C1
10	aA	839	CLA	C4-C3-C5-C6
10	aB	817	CLA	C4-C3-C5-C6
10	bA	839	CLA	C4-C3-C5-C6
10	bB	817	CLA	C4-C3-C5-C6
10	cA	839	CLA	C4-C3-C5-C6
10	cB	817	CLA	C4-C3-C5-C6
16	bB	848	LMG	C16-C17-C18-C19
10	aA	828	CLA	C15-C16-C17-C18
10	aA	805	CLA	C12-C13-C15-C16
10	aA	810	CLA	C6-C7-C8-C10
10	aA	829	CLA	C12-C13-C15-C16
10	aA	833	CLA	C12-C13-C15-C16
10	aB	801	CLA	C6-C7-C8-C10
10	aB	817	CLA	C2-C3-C5-C6
10	aB	830	CLA	C6-C7-C8-C10
10	bA	805	CLA	C12-C13-C15-C16
10	bA	810	CLA	C6-C7-C8-C10
10	bA	829	CLA	C12-C13-C15-C16
10	bA	833	CLA	C12-C13-C15-C16
10	bB	801	CLA	C6-C7-C8-C10
10	bB	808	CLA	C11-C12-C13-C15
10	bB	817	CLA	C2-C3-C5-C6
10	bB	830	CLA	C6-C7-C8-C10
10	cA	805	CLA	C12-C13-C15-C16
10	cA	810	CLA	C6-C7-C8-C10
10	cA	829	CLA	C12-C13-C15-C16
10	cA	833	CLA	C12-C13-C15-C16
10	cB	801	CLA	C6-C7-C8-C10
10	cB	808	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cB	817	CLA	C2-C3-C5-C6
10	cB	830	CLA	C6-C7-C8-C10
16	aB	848	LMG	C16-C17-C18-C19
16	cB	848	LMG	C16-C17-C18-C19
10	aA	819	CLA	C6-C7-C8-C9
10	aA	829	CLA	C14-C13-C15-C16
10	aA	842	CLA	C11-C10-C8-C9
10	aB	805	CLA	C11-C12-C13-C14
10	aB	808	CLA	C11-C10-C8-C9
10	aB	808	CLA	C11-C12-C13-C14
10	aB	830	CLA	C6-C7-C8-C9
10	bA	819	CLA	C6-C7-C8-C9
10	bA	829	CLA	C14-C13-C15-C16
10	bA	842	CLA	C11-C10-C8-C9
10	bB	805	CLA	C11-C12-C13-C14
10	bB	808	CLA	C11-C10-C8-C9
10	bB	808	CLA	C11-C12-C13-C14
10	bB	830	CLA	C6-C7-C8-C9
10	cA	819	CLA	C6-C7-C8-C9
10	cA	829	CLA	C14-C13-C15-C16
10	cA	842	CLA	C11-C10-C8-C9
10	cB	805	CLA	C11-C12-C13-C14
10	cB	808	CLA	C11-C10-C8-C9
10	cB	808	CLA	C11-C12-C13-C14
10	cB	830	CLA	C6-C7-C8-C9
10	aA	825	CLA	CBA-CGA-O2A-C1
10	aB	819	CLA	CBA-CGA-O2A-C1
10	bA	825	CLA	CBA-CGA-O2A-C1
10	bB	819	CLA	CBA-CGA-O2A-C1
10	cA	825	CLA	CBA-CGA-O2A-C1
10	cB	819	CLA	CBA-CGA-O2A-C1
10	bA	828	CLA	C15-C16-C17-C18
10	cA	828	CLA	C15-C16-C17-C18
10	aA	807	CLA	C2A-CAA-CBA-CGA
10	bA	807	CLA	C2A-CAA-CBA-CGA
10	cA	807	CLA	C2A-CAA-CBA-CGA
13	aA	847	BCR	C7-C8-C9-C34
13	bA	847	BCR	C7-C8-C9-C34
13	cA	847	BCR	C7-C8-C9-C34
13	aI	101	BCR	C21-C22-C23-C24
13	aM	101	BCR	C21-C22-C23-C24
13	bM	101	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	cM	101	BCR	C21-C22-C23-C24
10	aL	204	CLA	C5-C6-C7-C8
10	bL	204	CLA	C5-C6-C7-C8
10	cL	204	CLA	C5-C6-C7-C8
10	aA	836	CLA	CBA-CGA-O2A-C1
10	aB	811	CLA	CBA-CGA-O2A-C1
10	bA	836	CLA	CBA-CGA-O2A-C1
10	bB	811	CLA	CBA-CGA-O2A-C1
10	cA	836	CLA	CBA-CGA-O2A-C1
10	cB	811	CLA	CBA-CGA-O2A-C1
10	bB	810	CLA	O1D-CGD-O2D-CED
10	aA	827	CLA	CAA-CBA-CGA-O2A
10	bA	827	CLA	CAA-CBA-CGA-O2A
10	cA	827	CLA	CAA-CBA-CGA-O2A
10	aB	810	CLA	O1D-CGD-O2D-CED
10	bB	821	CLA	CBA-CGA-O2A-C1
10	cB	821	CLA	CBA-CGA-O2A-C1
10	cB	810	CLA	O1D-CGD-O2D-CED
10	aB	808	CLA	C4-C3-C5-C6
10	aB	820	CLA	C4-C3-C5-C6
10	aL	205	CLA	C4-C3-C5-C6
10	bB	808	CLA	C4-C3-C5-C6
10	bB	820	CLA	C4-C3-C5-C6
10	bL	205	CLA	C4-C3-C5-C6
10	cB	808	CLA	C4-C3-C5-C6
10	cB	820	CLA	C4-C3-C5-C6
10	cL	205	CLA	C4-C3-C5-C6
10	aA	839	CLA	C2-C3-C5-C6
10	aB	808	CLA	C2-C3-C5-C6
10	aB	809	CLA	C2-C3-C5-C6
10	aL	205	CLA	C2-C3-C5-C6
10	bA	839	CLA	C2-C3-C5-C6
10	bB	808	CLA	C2-C3-C5-C6
10	bB	809	CLA	C2-C3-C5-C6
10	bL	205	CLA	C2-C3-C5-C6
10	cA	839	CLA	C2-C3-C5-C6
10	cB	808	CLA	C2-C3-C5-C6
10	cB	809	CLA	C2-C3-C5-C6
10	cL	205	CLA	C2-C3-C5-C6
14	aA	852	LHG	C16-C17-C18-C19
14	bA	852	LHG	C16-C17-C18-C19
14	cA	852	LHG	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aB	821	CLA	CBA-CGA-O2A-C1
10	bB	818	CLA	CAA-CBA-CGA-O2A
10	aA	805	CLA	C3A-C2A-CAA-CBA
10	aB	822	CLA	C3A-C2A-CAA-CBA
10	aL	204	CLA	C3A-C2A-CAA-CBA
10	bA	805	CLA	C3A-C2A-CAA-CBA
10	bB	822	CLA	C3A-C2A-CAA-CBA
10	bL	204	CLA	C3A-C2A-CAA-CBA
10	cA	805	CLA	C3A-C2A-CAA-CBA
10	cB	822	CLA	C3A-C2A-CAA-CBA
10	cL	204	CLA	C3A-C2A-CAA-CBA
13	aB	849	BCR	C13-C14-C15-C16
13	bB	849	BCR	C13-C14-C15-C16
13	cB	849	BCR	C13-C14-C15-C16
10	aA	817	CLA	CBA-CGA-O2A-C1
10	aA	824	CLA	CBA-CGA-O2A-C1
10	bA	817	CLA	CBA-CGA-O2A-C1
10	bA	824	CLA	CBA-CGA-O2A-C1
10	cA	817	CLA	CBA-CGA-O2A-C1
10	cA	824	CLA	CBA-CGA-O2A-C1
14	aA	852	LHG	C29-C30-C31-C32
14	bA	852	LHG	C29-C30-C31-C32
14	cA	852	LHG	C29-C30-C31-C32
14	cA	855	LHG	C11-C10-C9-C8
10	aB	818	CLA	CAA-CBA-CGA-O2A
10	cB	818	CLA	CAA-CBA-CGA-O2A
14	aA	855	LHG	C11-C10-C9-C8
14	bA	855	LHG	C11-C10-C9-C8
10	aA	842	CLA	C4-C3-C5-C6
10	aB	827	CLA	C4-C3-C5-C6
10	bA	842	CLA	C4-C3-C5-C6
10	bB	827	CLA	C4-C3-C5-C6
10	cA	842	CLA	C4-C3-C5-C6
10	cB	827	CLA	C4-C3-C5-C6
10	aA	831	CLA	O1A-CGA-O2A-C1
10	aA	854	CLA	O1A-CGA-O2A-C1
10	bA	831	CLA	O1A-CGA-O2A-C1
10	bA	854	CLA	O1A-CGA-O2A-C1
10	cA	854	CLA	O1A-CGA-O2A-C1
10	aA	825	CLA	O1D-CGD-O2D-CED
10	bA	825	CLA	O1D-CGD-O2D-CED
10	cA	825	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aB	820	CLA	C3-C5-C6-C7
10	bB	820	CLA	C3-C5-C6-C7
10	cB	820	CLA	C3-C5-C6-C7
14	aA	852	LHG	C11-C10-C9-C8
14	cA	852	LHG	C11-C10-C9-C8
14	bA	852	LHG	C11-C10-C9-C8
10	aA	825	CLA	O1A-CGA-O2A-C1
10	bA	825	CLA	O1A-CGA-O2A-C1
10	cA	825	CLA	O1A-CGA-O2A-C1
10	cA	831	CLA	O1A-CGA-O2A-C1
10	aA	831	CLA	C8-C10-C11-C12
10	bA	831	CLA	C8-C10-C11-C12
10	cA	831	CLA	C8-C10-C11-C12
15	aA	853	LMT	O1'-C1-C2-C3
15	bA	853	LMT	O1'-C1-C2-C3
15	cA	853	LMT	O1'-C1-C2-C3
10	aB	826	CLA	C16-C17-C18-C19
10	bB	826	CLA	C16-C17-C18-C19
10	aB	832	CLA	C2-C1-O2A-CGA
10	bB	832	CLA	C2-C1-O2A-CGA
10	cB	832	CLA	C2-C1-O2A-CGA
10	aA	820	CLA	C14-C13-C15-C16
10	aA	833	CLA	C14-C13-C15-C16
10	aA	841	CLA	C6-C7-C8-C9
10	aA	842	CLA	C14-C13-C15-C16
10	aB	805	CLA	C11-C10-C8-C9
10	bA	820	CLA	C14-C13-C15-C16
10	bA	833	CLA	C14-C13-C15-C16
10	bA	841	CLA	C6-C7-C8-C9
10	bA	842	CLA	C14-C13-C15-C16
10	bB	805	CLA	C11-C10-C8-C9
10	cA	820	CLA	C14-C13-C15-C16
10	cA	833	CLA	C14-C13-C15-C16
10	cA	841	CLA	C6-C7-C8-C9
10	cA	842	CLA	C14-C13-C15-C16
10	cB	805	CLA	C11-C10-C8-C9
10	aB	809	CLA	C15-C16-C17-C18
10	bB	809	CLA	C15-C16-C17-C18
10	cB	809	CLA	C15-C16-C17-C18
10	aA	822	CLA	C4-C3-C5-C6
10	bA	822	CLA	C4-C3-C5-C6
10	cA	822	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aB	829	CLA	C2A-CAA-CBA-CGA
10	bB	829	CLA	C2A-CAA-CBA-CGA
10	cB	829	CLA	C2A-CAA-CBA-CGA
10	aB	827	CLA	C16-C17-C18-C20
10	bB	827	CLA	C16-C17-C18-C20
10	cB	826	CLA	C16-C17-C18-C19
10	cB	827	CLA	C16-C17-C18-C20
13	aA	846	BCR	C23-C24-C25-C26
13	aA	846	BCR	C23-C24-C25-C30
13	aA	847	BCR	C1-C6-C7-C8
13	aA	849	BCR	C23-C24-C25-C26
13	aA	850	BCR	C23-C24-C25-C26
13	aA	851	BCR	C5-C6-C7-C8
13	aB	843	BCR	C23-C24-C25-C30
13	aB	844	BCR	C23-C24-C25-C26
13	aB	844	BCR	C23-C24-C25-C30
13	aB	847	BCR	C5-C6-C7-C8
13	aB	847	BCR	C23-C24-C25-C26
13	aB	847	BCR	C23-C24-C25-C30
13	aB	849	BCR	C23-C24-C25-C26
13	aL	206	BCR	C5-C6-C7-C8
13	aL	207	BCR	C5-C6-C7-C8
13	aM	101	BCR	C1-C6-C7-C8
13	bA	846	BCR	C23-C24-C25-C26
13	bA	846	BCR	C23-C24-C25-C30
13	bA	847	BCR	C1-C6-C7-C8
13	bA	849	BCR	C23-C24-C25-C26
13	bA	850	BCR	C23-C24-C25-C26
13	bA	851	BCR	C5-C6-C7-C8
13	bB	843	BCR	C23-C24-C25-C30
13	bB	844	BCR	C23-C24-C25-C26
13	bB	844	BCR	C23-C24-C25-C30
13	bB	847	BCR	C5-C6-C7-C8
13	bB	847	BCR	C23-C24-C25-C26
13	bB	847	BCR	C23-C24-C25-C30
13	bB	849	BCR	C23-C24-C25-C26
13	bL	206	BCR	C5-C6-C7-C8
13	bL	207	BCR	C5-C6-C7-C8
13	bM	101	BCR	C1-C6-C7-C8
13	cA	846	BCR	C23-C24-C25-C26
13	cA	846	BCR	C23-C24-C25-C30
13	cA	847	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	cA	849	BCR	C23-C24-C25-C26
13	cA	850	BCR	C23-C24-C25-C26
13	cA	851	BCR	C5-C6-C7-C8
13	cB	843	BCR	C23-C24-C25-C30
13	cB	844	BCR	C23-C24-C25-C26
13	cB	844	BCR	C23-C24-C25-C30
13	cB	847	BCR	C5-C6-C7-C8
13	cB	847	BCR	C23-C24-C25-C26
13	cB	847	BCR	C23-C24-C25-C30
13	cB	849	BCR	C23-C24-C25-C26
13	cL	206	BCR	C5-C6-C7-C8
13	cL	207	BCR	C5-C6-C7-C8
13	cM	101	BCR	C1-C6-C7-C8
10	aB	833	CLA	CAA-CBA-CGA-O2A
10	bB	833	CLA	CAA-CBA-CGA-O2A
10	cB	833	CLA	CAA-CBA-CGA-O2A
13	aA	851	BCR	C7-C8-C9-C10
13	bA	851	BCR	C7-C8-C9-C10
13	cA	851	BCR	C7-C8-C9-C10
10	aA	826	CLA	C13-C15-C16-C17
10	bA	826	CLA	C13-C15-C16-C17
10	cA	826	CLA	C13-C15-C16-C17
10	aA	817	CLA	O1A-CGA-O2A-C1
10	bA	817	CLA	O1A-CGA-O2A-C1
10	cA	817	CLA	O1A-CGA-O2A-C1
10	aA	819	CLA	C6-C7-C8-C10
10	aA	820	CLA	C12-C13-C15-C16
10	aA	842	CLA	C2-C3-C5-C6
10	aA	842	CLA	C12-C13-C15-C16
10	aB	805	CLA	C11-C12-C13-C15
10	aB	808	CLA	C11-C10-C8-C7
10	aB	808	CLA	C11-C12-C13-C15
10	aB	819	CLA	C11-C10-C8-C7
10	aB	832	CLA	C6-C7-C8-C10
10	aB	841	CLA	C11-C12-C13-C15
10	aL	204	CLA	C6-C7-C8-C10
10	bA	819	CLA	C6-C7-C8-C10
10	bA	820	CLA	C12-C13-C15-C16
10	bA	842	CLA	C2-C3-C5-C6
10	bA	842	CLA	C12-C13-C15-C16
10	bB	805	CLA	C11-C12-C13-C15
10	bB	808	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bB	819	CLA	C11-C10-C8-C7
10	bB	832	CLA	C6-C7-C8-C10
10	bB	841	CLA	C11-C12-C13-C15
10	bL	204	CLA	C6-C7-C8-C10
10	cA	819	CLA	C6-C7-C8-C10
10	cA	820	CLA	C12-C13-C15-C16
10	cA	842	CLA	C2-C3-C5-C6
10	cA	842	CLA	C12-C13-C15-C16
10	cB	805	CLA	C11-C12-C13-C15
10	cB	808	CLA	C11-C10-C8-C7
10	cB	819	CLA	C11-C10-C8-C7
10	cB	832	CLA	C6-C7-C8-C10
10	cB	841	CLA	C11-C12-C13-C15
10	cL	204	CLA	C6-C7-C8-C10
13	aA	848	BCR	C35-C13-C14-C15
13	aB	844	BCR	C35-C13-C14-C15
13	aL	207	BCR	C16-C17-C18-C36
13	aM	101	BCR	C16-C17-C18-C36
13	bA	848	BCR	C35-C13-C14-C15
13	bB	844	BCR	C35-C13-C14-C15
13	bL	207	BCR	C16-C17-C18-C36
13	bM	101	BCR	C16-C17-C18-C36
13	cA	848	BCR	C35-C13-C14-C15
13	cB	844	BCR	C35-C13-C14-C15
13	cL	207	BCR	C16-C17-C18-C36
13	cM	101	BCR	C16-C17-C18-C36
10	aL	203	CLA	C3-C5-C6-C7
10	aA	856	CLA	CBA-CGA-O2A-C1
10	bA	856	CLA	CBA-CGA-O2A-C1
10	cA	856	CLA	CBA-CGA-O2A-C1
10	aA	805	CLA	CAD-CBD-CGD-O2D
10	aA	822	CLA	CAD-CBD-CGD-O2D
10	aB	817	CLA	CAD-CBD-CGD-O2D
10	aB	823	CLA	CAD-CBD-CGD-O2D
10	aB	830	CLA	CAD-CBD-CGD-O2D
10	aB	832	CLA	CAD-CBD-CGD-O2D
10	aB	835	CLA	CAD-CBD-CGD-O2D
10	aL	202	CLA	CAD-CBD-CGD-O2D
10	bA	805	CLA	CAD-CBD-CGD-O2D
10	bA	822	CLA	CAD-CBD-CGD-O2D
10	bB	817	CLA	CAD-CBD-CGD-O2D
10	bB	823	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bB	830	CLA	CAD-CBD-CGD-O2D
10	bB	832	CLA	CAD-CBD-CGD-O2D
10	bB	835	CLA	CAD-CBD-CGD-O2D
10	bL	202	CLA	CAD-CBD-CGD-O2D
10	cA	805	CLA	CAD-CBD-CGD-O2D
10	cA	822	CLA	CAD-CBD-CGD-O2D
10	cB	817	CLA	CAD-CBD-CGD-O2D
10	cB	823	CLA	CAD-CBD-CGD-O2D
10	cB	830	CLA	CAD-CBD-CGD-O2D
10	cB	832	CLA	CAD-CBD-CGD-O2D
10	cB	835	CLA	CAD-CBD-CGD-O2D
10	cL	202	CLA	CAD-CBD-CGD-O2D
10	bL	203	CLA	C3-C5-C6-C7
10	cL	203	CLA	C3-C5-C6-C7
10	aA	804	CLA	C8-C10-C11-C12
10	cA	804	CLA	C8-C10-C11-C12
10	aA	823	CLA	C4-C3-C5-C6
10	bA	823	CLA	C4-C3-C5-C6
10	cA	823	CLA	C4-C3-C5-C6
16	cB	848	LMG	C19-C20-C21-C22
14	aA	852	LHG	C4-C5-C6-O8
14	bA	852	LHG	C4-C5-C6-O8
14	cA	852	LHG	C4-C5-C6-O8
10	aA	836	CLA	O1A-CGA-O2A-C1
10	aA	837	CLA	O1A-CGA-O2A-C1
10	bA	836	CLA	O1A-CGA-O2A-C1
10	bA	837	CLA	O1A-CGA-O2A-C1
10	cA	836	CLA	O1A-CGA-O2A-C1
10	cA	837	CLA	O1A-CGA-O2A-C1
16	aB	848	LMG	C19-C20-C21-C22
16	bB	848	LMG	C19-C20-C21-C22
10	bA	804	CLA	C8-C10-C11-C12
10	aB	815	CLA	C2A-CAA-CBA-CGA
10	bB	815	CLA	C2A-CAA-CBA-CGA
10	cB	815	CLA	C2A-CAA-CBA-CGA
10	aA	842	CLA	C13-C15-C16-C17
10	bA	842	CLA	C13-C15-C16-C17
10	cA	842	CLA	C13-C15-C16-C17
9	aA	801	CL0	C16-C17-C18-C20
9	bA	801	CL0	C16-C17-C18-C20
9	cA	801	CL0	C16-C17-C18-C20
14	aA	852	LHG	O9-C7-O7-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	bA	852	LHG	O9-C7-O7-C5
14	cA	852	LHG	O9-C7-O7-C5
10	aA	802	CLA	CHA-CBD-CGD-O1D
10	aA	802	CLA	CHA-CBD-CGD-O2D
10	aA	803	CLA	CHA-CBD-CGD-O1D
10	aA	804	CLA	CHA-CBD-CGD-O1D
10	aA	804	CLA	CHA-CBD-CGD-O2D
10	aA	807	CLA	CHA-CBD-CGD-O1D
10	aA	810	CLA	CHA-CBD-CGD-O2D
10	aA	814	CLA	CHA-CBD-CGD-O1D
10	aA	814	CLA	CHA-CBD-CGD-O2D
10	aA	854	CLA	CHA-CBD-CGD-O1D
10	aA	854	CLA	CHA-CBD-CGD-O2D
10	aB	804	CLA	CHA-CBD-CGD-O1D
10	aB	804	CLA	CHA-CBD-CGD-O2D
10	aB	807	CLA	CHA-CBD-CGD-O1D
10	aB	807	CLA	CHA-CBD-CGD-O2D
10	aB	810	CLA	CHA-CBD-CGD-O1D
10	aB	810	CLA	CHA-CBD-CGD-O2D
10	aB	825	CLA	CHA-CBD-CGD-O1D
10	aB	825	CLA	CHA-CBD-CGD-O2D
10	bA	802	CLA	CHA-CBD-CGD-O1D
10	bA	802	CLA	CHA-CBD-CGD-O2D
10	bA	803	CLA	CHA-CBD-CGD-O1D
10	bA	804	CLA	CHA-CBD-CGD-O1D
10	bA	804	CLA	CHA-CBD-CGD-O2D
10	bA	807	CLA	CHA-CBD-CGD-O1D
10	bA	810	CLA	CHA-CBD-CGD-O2D
10	bA	814	CLA	CHA-CBD-CGD-O1D
10	bA	814	CLA	CHA-CBD-CGD-O2D
10	bA	854	CLA	CHA-CBD-CGD-O1D
10	bA	854	CLA	CHA-CBD-CGD-O2D
10	bB	804	CLA	CHA-CBD-CGD-O1D
10	bB	804	CLA	CHA-CBD-CGD-O2D
10	bB	807	CLA	CHA-CBD-CGD-O1D
10	bB	807	CLA	CHA-CBD-CGD-O2D
10	bB	810	CLA	CHA-CBD-CGD-O1D
10	bB	810	CLA	CHA-CBD-CGD-O2D
10	bB	825	CLA	CHA-CBD-CGD-O1D
10	bB	825	CLA	CHA-CBD-CGD-O2D
10	cA	802	CLA	CHA-CBD-CGD-O1D
10	cA	802	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cA	803	CLA	CHA-CBD-CGD-O1D
10	cA	804	CLA	CHA-CBD-CGD-O1D
10	cA	804	CLA	CHA-CBD-CGD-O2D
10	cA	807	CLA	CHA-CBD-CGD-O1D
10	cA	810	CLA	CHA-CBD-CGD-O2D
10	cA	814	CLA	CHA-CBD-CGD-O1D
10	cA	814	CLA	CHA-CBD-CGD-O2D
10	cA	854	CLA	CHA-CBD-CGD-O1D
10	cA	854	CLA	CHA-CBD-CGD-O2D
10	cB	804	CLA	CHA-CBD-CGD-O1D
10	cB	804	CLA	CHA-CBD-CGD-O2D
10	cB	807	CLA	CHA-CBD-CGD-O1D
10	cB	807	CLA	CHA-CBD-CGD-O2D
10	cB	810	CLA	CHA-CBD-CGD-O1D
10	cB	810	CLA	CHA-CBD-CGD-O2D
10	cB	825	CLA	CHA-CBD-CGD-O1D
10	cB	825	CLA	CHA-CBD-CGD-O2D
10	bB	806	CLA	C6-C7-C8-C9
10	aA	816	CLA	C3-C5-C6-C7
10	bA	816	CLA	C3-C5-C6-C7
10	cA	816	CLA	C3-C5-C6-C7
10	aB	821	CLA	O1A-CGA-O2A-C1
10	bA	824	CLA	O1A-CGA-O2A-C1
10	bB	821	CLA	O1A-CGA-O2A-C1
10	cA	824	CLA	O1A-CGA-O2A-C1
10	cB	821	CLA	O1A-CGA-O2A-C1
10	aB	806	CLA	C6-C7-C8-C9
10	cB	806	CLA	C6-C7-C8-C9
13	aI	102	BCR	C20-C21-C22-C23
13	bI	102	BCR	C20-C21-C22-C23
13	cI	103	BCR	C20-C21-C22-C23
14	aA	852	LHG	O7-C5-C6-O8
14	bA	852	LHG	O7-C5-C6-O8
14	cA	852	LHG	O7-C5-C6-O8
10	aB	837	CLA	CBA-CGA-O2A-C1
10	bB	837	CLA	CBA-CGA-O2A-C1
10	cB	837	CLA	CBA-CGA-O2A-C1
10	aA	824	CLA	O1A-CGA-O2A-C1
10	aB	838	CLA	C4-C3-C5-C6
10	bB	838	CLA	C4-C3-C5-C6
10	cB	804	CLA	C4-C3-C5-C6
10	cB	838	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	aA	852	LHG	C26-C27-C28-C29
14	bA	852	LHG	C26-C27-C28-C29
14	cA	852	LHG	C26-C27-C28-C29
10	aB	830	CLA	O1D-CGD-O2D-CED
10	bB	830	CLA	O1D-CGD-O2D-CED
10	cA	827	CLA	C5-C6-C7-C8
11	bA	844	PQN	C25-C26-C27-C28
10	aB	804	CLA	C6-C7-C8-C9
10	aB	827	CLA	C14-C13-C15-C16
10	aB	832	CLA	C11-C12-C13-C14
10	aB	833	CLA	C11-C10-C8-C9
10	bB	804	CLA	C6-C7-C8-C9
10	bB	827	CLA	C14-C13-C15-C16
10	bB	832	CLA	C11-C12-C13-C14
10	bB	833	CLA	C11-C10-C8-C9
10	cB	804	CLA	C6-C7-C8-C9
10	cB	827	CLA	C14-C13-C15-C16
10	cB	832	CLA	C11-C12-C13-C14
10	cB	833	CLA	C11-C10-C8-C9
10	cB	820	CLA	O1D-CGD-O2D-CED
10	cB	830	CLA	O1D-CGD-O2D-CED
10	aA	856	CLA	O1A-CGA-O2A-C1
10	bA	856	CLA	O1A-CGA-O2A-C1
10	cA	856	CLA	O1A-CGA-O2A-C1
11	aA	844	PQN	C25-C26-C27-C28
11	cA	844	PQN	C25-C26-C27-C28
10	aA	823	CLA	C13-C15-C16-C17
10	bA	827	CLA	C5-C6-C7-C8
10	aB	820	CLA	O1D-CGD-O2D-CED
10	bB	820	CLA	O1D-CGD-O2D-CED
14	aA	852	LHG	C7-C8-C9-C10
14	bA	852	LHG	C7-C8-C9-C10
10	aA	827	CLA	C5-C6-C7-C8
10	bA	823	CLA	C13-C15-C16-C17
13	aB	849	BCR	C7-C8-C9-C10
13	bB	849	BCR	C7-C8-C9-C10
13	cB	849	BCR	C7-C8-C9-C10
10	aA	806	CLA	C1A-C2A-CAA-CBA
10	aA	808	CLA	C1A-C2A-CAA-CBA
10	aA	815	CLA	C1A-C2A-CAA-CBA
10	aA	856	CLA	C1A-C2A-CAA-CBA
10	bA	806	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bA	808	CLA	C1A-C2A-CAA-CBA
10	bA	815	CLA	C1A-C2A-CAA-CBA
10	bA	856	CLA	C1A-C2A-CAA-CBA
10	cA	806	CLA	C1A-C2A-CAA-CBA
10	cA	808	CLA	C1A-C2A-CAA-CBA
10	cA	815	CLA	C1A-C2A-CAA-CBA
10	cA	856	CLA	C1A-C2A-CAA-CBA
14	cA	852	LHG	C7-C8-C9-C10
10	cA	823	CLA	C13-C15-C16-C17
14	bA	852	LHG	C17-C18-C19-C20
10	cL	203	CLA	CBA-CGA-O2A-C1
10	bB	818	CLA	C11-C12-C13-C14
10	cB	818	CLA	C11-C12-C13-C14
14	aA	852	LHG	C17-C18-C19-C20
14	cA	852	LHG	C17-C18-C19-C20
10	aB	818	CLA	C11-C12-C13-C14
10	aB	804	CLA	C4-C3-C5-C6
10	bB	804	CLA	C4-C3-C5-C6
10	aA	810	CLA	C3-C5-C6-C7
10	aB	833	CLA	C3-C5-C6-C7
10	bA	810	CLA	C3-C5-C6-C7
10	bB	833	CLA	C3-C5-C6-C7
10	cA	810	CLA	C3-C5-C6-C7
10	cB	833	CLA	C3-C5-C6-C7
10	aB	820	CLA	C2-C3-C5-C6
10	aB	838	CLA	C2-C3-C5-C6
10	bB	838	CLA	C2-C3-C5-C6
10	cB	838	CLA	C2-C3-C5-C6
10	aB	837	CLA	O1A-CGA-O2A-C1
10	bB	837	CLA	O1A-CGA-O2A-C1
10	cB	820	CLA	O1A-CGA-O2A-C1
10	cB	837	CLA	O1A-CGA-O2A-C1
14	aA	855	LHG	C4-O6-P-O5
14	bA	855	LHG	C4-O6-P-O5
14	cA	855	LHG	C4-O6-P-O5
10	aL	203	CLA	CBA-CGA-O2A-C1
10	bL	203	CLA	CBA-CGA-O2A-C1
14	aA	852	LHG	O6-C4-C5-C6
14	bA	852	LHG	O6-C4-C5-C6
14	cA	852	LHG	O6-C4-C5-C6
10	aB	820	CLA	O1A-CGA-O2A-C1
10	bB	820	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aA	802	CLA	C2A-CAA-CBA-CGA
10	aA	803	CLA	CAD-CBD-CGD-O1D
10	aA	804	CLA	CAD-CBD-CGD-O1D
10	aA	812	CLA	CAD-CBD-CGD-O1D
10	aA	854	CLA	CAD-CBD-CGD-O1D
10	aB	804	CLA	CAD-CBD-CGD-O1D
10	aB	807	CLA	CAD-CBD-CGD-O1D
10	bA	803	CLA	CAD-CBD-CGD-O1D
10	bA	804	CLA	CAD-CBD-CGD-O1D
10	bA	812	CLA	CAD-CBD-CGD-O1D
10	bA	854	CLA	CAD-CBD-CGD-O1D
10	bB	804	CLA	CAD-CBD-CGD-O1D
10	bB	807	CLA	CAD-CBD-CGD-O1D
10	cA	803	CLA	CAD-CBD-CGD-O1D
10	cA	804	CLA	CAD-CBD-CGD-O1D
10	cA	812	CLA	CAD-CBD-CGD-O1D
10	cA	854	CLA	CAD-CBD-CGD-O1D
10	cB	804	CLA	CAD-CBD-CGD-O1D
10	cB	807	CLA	CAD-CBD-CGD-O1D
10	cB	814	CLA	CAD-CBD-CGD-O1D
9	aA	801	CL0	C15-C16-C17-C18
9	bA	801	CL0	C15-C16-C17-C18
9	cA	801	CL0	C15-C16-C17-C18
10	aB	820	CLA	CBA-CGA-O2A-C1
10	bB	820	CLA	CBA-CGA-O2A-C1
10	aA	812	CLA	C11-C12-C13-C15
10	aA	824	CLA	C11-C12-C13-C15
10	aA	829	CLA	C11-C12-C13-C15
10	aA	842	CLA	C11-C10-C8-C7
10	aB	805	CLA	C11-C10-C8-C7
10	aB	827	CLA	C12-C13-C15-C16
10	aB	829	CLA	C6-C7-C8-C10
10	aB	832	CLA	C11-C12-C13-C15
10	aB	833	CLA	C11-C10-C8-C7
10	aB	838	CLA	C12-C13-C15-C16
10	aB	841	CLA	C11-C10-C8-C7
10	aL	205	CLA	C6-C7-C8-C10
10	bA	812	CLA	C11-C12-C13-C15
10	bA	824	CLA	C11-C12-C13-C15
10	bA	829	CLA	C11-C12-C13-C15
10	bA	842	CLA	C11-C10-C8-C7
10	bB	805	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bB	827	CLA	C12-C13-C15-C16
10	bB	829	CLA	C6-C7-C8-C10
10	bB	832	CLA	C11-C12-C13-C15
10	bB	833	CLA	C11-C10-C8-C7
10	bB	838	CLA	C12-C13-C15-C16
10	bB	841	CLA	C11-C10-C8-C7
10	bL	205	CLA	C6-C7-C8-C10
10	cA	812	CLA	C11-C12-C13-C15
10	cA	824	CLA	C11-C12-C13-C15
10	cA	829	CLA	C11-C12-C13-C15
10	cA	842	CLA	C11-C10-C8-C7
10	cB	805	CLA	C11-C10-C8-C7
10	cB	827	CLA	C12-C13-C15-C16
10	cB	829	CLA	C6-C7-C8-C10
10	cB	832	CLA	C11-C12-C13-C15
10	cB	833	CLA	C11-C10-C8-C7
10	cB	838	CLA	C12-C13-C15-C16
10	cB	841	CLA	C11-C10-C8-C7
10	cL	205	CLA	C6-C7-C8-C10
14	aA	852	LHG	O6-C4-C5-O7
14	bA	852	LHG	O6-C4-C5-O7
14	cA	852	LHG	O6-C4-C5-O7
10	aB	805	CLA	C2C-C3C-CAC-CBC
10	aB	826	CLA	C15-C16-C17-C18
10	bB	826	CLA	C15-C16-C17-C18
10	cB	826	CLA	C15-C16-C17-C18
10	cB	820	CLA	CBA-CGA-O2A-C1
10	bB	805	CLA	C2C-C3C-CAC-CBC
10	cB	805	CLA	C2C-C3C-CAC-CBC
10	aL	203	CLA	O1A-CGA-O2A-C1
10	bL	203	CLA	O1A-CGA-O2A-C1
10	cL	203	CLA	O1A-CGA-O2A-C1
10	aA	821	CLA	C2A-CAA-CBA-CGA
10	bA	821	CLA	C2A-CAA-CBA-CGA
10	cA	802	CLA	C2A-CAA-CBA-CGA
10	cA	821	CLA	C2A-CAA-CBA-CGA
10	cA	827	CLA	C10-C11-C12-C13
14	aA	855	LHG	C4-C5-C6-O8
14	bA	855	LHG	C4-C5-C6-O8
14	cA	855	LHG	C4-C5-C6-O8
10	aA	827	CLA	C10-C11-C12-C13
10	bA	827	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aB	807	CLA	C4-C3-C5-C6
10	aB	815	CLA	C4-C3-C5-C6
10	bB	807	CLA	C4-C3-C5-C6
10	bB	815	CLA	C4-C3-C5-C6
10	cB	807	CLA	C4-C3-C5-C6
10	cB	815	CLA	C4-C3-C5-C6
10	aA	823	CLA	C2-C3-C5-C6
10	bA	823	CLA	C2-C3-C5-C6
10	bB	820	CLA	C2-C3-C5-C6
10	cA	823	CLA	C2-C3-C5-C6
10	cB	820	CLA	C2-C3-C5-C6
10	aA	825	CLA	C5-C6-C7-C8
10	bA	825	CLA	C5-C6-C7-C8
10	cA	825	CLA	C5-C6-C7-C8
10	aA	804	CLA	C11-C10-C8-C9
10	aA	805	CLA	C14-C13-C15-C16
10	aB	818	CLA	C11-C10-C8-C9
10	aB	832	CLA	C6-C7-C8-C9
10	aB	841	CLA	C11-C12-C13-C14
10	aL	204	CLA	C6-C7-C8-C9
10	bA	804	CLA	C11-C10-C8-C9
10	bB	818	CLA	C11-C10-C8-C9
10	bB	832	CLA	C6-C7-C8-C9
10	bB	841	CLA	C11-C12-C13-C14
10	bL	204	CLA	C6-C7-C8-C9
10	cA	804	CLA	C11-C10-C8-C9
10	cA	805	CLA	C14-C13-C15-C16
10	cB	818	CLA	C11-C10-C8-C9
10	cB	832	CLA	C6-C7-C8-C9
10	cB	841	CLA	C11-C12-C13-C14
10	cL	204	CLA	C6-C7-C8-C9
10	bA	802	CLA	C2A-CAA-CBA-CGA
10	cB	837	CLA	O1D-CGD-O2D-CED
10	bB	837	CLA	O1D-CGD-O2D-CED
10	aB	840	CLA	C16-C17-C18-C20
10	aB	837	CLA	O1D-CGD-O2D-CED
10	aB	807	CLA	C2-C3-C5-C6
10	aB	827	CLA	C2-C3-C5-C6
10	bB	807	CLA	C2-C3-C5-C6
10	cB	807	CLA	C2-C3-C5-C6
10	bB	840	CLA	C16-C17-C18-C20
10	cB	840	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aA	821	CLA	C1-C2-C3-C4
10	aA	856	CLA	C1-C2-C3-C4
10	bA	821	CLA	C1-C2-C3-C4
10	bA	856	CLA	C1-C2-C3-C4
10	cA	821	CLA	C1-C2-C3-C4
10	cA	856	CLA	C1-C2-C3-C4
10	aB	817	CLA	CAA-CBA-CGA-O2A
10	bB	817	CLA	CAA-CBA-CGA-O2A
10	cB	817	CLA	CAA-CBA-CGA-O2A
10	aA	827	CLA	C2A-CAA-CBA-CGA
10	aA	842	CLA	C2A-CAA-CBA-CGA
10	aB	802	CLA	C2A-CAA-CBA-CGA
10	bA	827	CLA	C2A-CAA-CBA-CGA
10	bA	842	CLA	C2A-CAA-CBA-CGA
10	bB	802	CLA	C2A-CAA-CBA-CGA
10	cA	827	CLA	C2A-CAA-CBA-CGA
10	cA	842	CLA	C2A-CAA-CBA-CGA
10	cB	802	CLA	C2A-CAA-CBA-CGA
10	aA	828	CLA	C2-C1-O2A-CGA
10	aA	829	CLA	C2-C1-O2A-CGA
10	aA	836	CLA	C2-C1-O2A-CGA
10	aB	807	CLA	C2-C1-O2A-CGA
10	aB	811	CLA	C2-C1-O2A-CGA
10	aB	818	CLA	C2-C1-O2A-CGA
10	aB	841	CLA	C2-C1-O2A-CGA
10	bA	828	CLA	C2-C1-O2A-CGA
10	bA	829	CLA	C2-C1-O2A-CGA
10	bA	836	CLA	C2-C1-O2A-CGA
10	bB	807	CLA	C2-C1-O2A-CGA
10	bB	811	CLA	C2-C1-O2A-CGA
10	bB	818	CLA	C2-C1-O2A-CGA
10	bB	841	CLA	C2-C1-O2A-CGA
10	cA	828	CLA	C2-C1-O2A-CGA
10	cA	829	CLA	C2-C1-O2A-CGA
10	cA	836	CLA	C2-C1-O2A-CGA
10	cB	807	CLA	C2-C1-O2A-CGA
10	cB	811	CLA	C2-C1-O2A-CGA
10	cB	818	CLA	C2-C1-O2A-CGA
10	cB	841	CLA	C2-C1-O2A-CGA
14	aA	852	LHG	C10-C11-C12-C13
14	cA	852	LHG	C10-C11-C12-C13
14	bA	852	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	aA	847	BCR	C5-C6-C7-C8
13	aB	843	BCR	C23-C24-C25-C26
13	aB	847	BCR	C1-C6-C7-C8
13	aB	849	BCR	C5-C6-C7-C8
13	aB	849	BCR	C23-C24-C25-C30
13	bA	847	BCR	C5-C6-C7-C8
13	bB	843	BCR	C23-C24-C25-C26
13	bB	847	BCR	C1-C6-C7-C8
13	bB	849	BCR	C5-C6-C7-C8
13	bB	849	BCR	C23-C24-C25-C30
13	cA	847	BCR	C5-C6-C7-C8
13	cB	843	BCR	C23-C24-C25-C26
13	cB	847	BCR	C1-C6-C7-C8
13	cB	849	BCR	C5-C6-C7-C8
13	cB	849	BCR	C23-C24-C25-C30
10	bB	827	CLA	C2-C3-C5-C6
10	cB	827	CLA	C2-C3-C5-C6
14	aA	852	LHG	C14-C15-C16-C17
14	bA	852	LHG	C14-C15-C16-C17
14	cA	852	LHG	C14-C15-C16-C17
10	aB	830	CLA	C10-C11-C12-C13
10	aA	841	CLA	C2A-CAA-CBA-CGA
10	bA	841	CLA	C2A-CAA-CBA-CGA
10	cA	841	CLA	C2A-CAA-CBA-CGA
10	cB	830	CLA	C10-C11-C12-C13
14	aA	855	LHG	C3-O3-P-O6
14	bA	855	LHG	C3-O3-P-O6
14	cA	855	LHG	C3-O3-P-O6
10	bB	830	CLA	C10-C11-C12-C13
10	aB	814	CLA	C4-C3-C5-C6
10	bB	814	CLA	C4-C3-C5-C6
10	cB	814	CLA	C4-C3-C5-C6
10	aA	841	CLA	C10-C11-C12-C13
10	aB	828	CLA	C12-C13-C15-C16
10	bB	828	CLA	C12-C13-C15-C16
10	cB	828	CLA	C12-C13-C15-C16
10	aA	824	CLA	C11-C12-C13-C14
10	aA	829	CLA	C11-C12-C13-C14
10	aB	829	CLA	C6-C7-C8-C9
10	aB	841	CLA	C11-C10-C8-C9
10	aL	205	CLA	C6-C7-C8-C9
10	bA	805	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bA	824	CLA	C11-C12-C13-C14
10	bA	829	CLA	C11-C12-C13-C14
10	bB	829	CLA	C6-C7-C8-C9
10	bB	841	CLA	C11-C10-C8-C9
10	bL	205	CLA	C6-C7-C8-C9
10	cA	824	CLA	C11-C12-C13-C14
10	cA	829	CLA	C11-C12-C13-C14
10	cB	829	CLA	C6-C7-C8-C9
10	cB	841	CLA	C11-C10-C8-C9
10	cL	205	CLA	C6-C7-C8-C9
10	bA	841	CLA	C10-C11-C12-C13
10	cA	841	CLA	C10-C11-C12-C13
10	bA	837	CLA	C8-C10-C11-C12
10	cA	837	CLA	C8-C10-C11-C12
10	aB	805	CLA	C2A-CAA-CBA-CGA
10	bB	805	CLA	C2A-CAA-CBA-CGA
10	cB	805	CLA	C2A-CAA-CBA-CGA
10	aA	837	CLA	C8-C10-C11-C12
10	aB	803	CLA	C8-C10-C11-C12
10	bB	803	CLA	C8-C10-C11-C12
10	cB	803	CLA	C8-C10-C11-C12
10	aB	823	CLA	C6-C7-C8-C10
10	bB	823	CLA	C6-C7-C8-C10
10	cB	823	CLA	C6-C7-C8-C10
10	aA	837	CLA	CBA-CGA-O2A-C1
10	bA	837	CLA	CBA-CGA-O2A-C1
10	cA	837	CLA	CBA-CGA-O2A-C1
10	aA	817	CLA	CAA-CBA-CGA-O2A
10	bA	817	CLA	CAA-CBA-CGA-O2A
10	cA	817	CLA	CAA-CBA-CGA-O2A
13	aA	846	BCR	C22-C23-C24-C25
13	bA	846	BCR	C22-C23-C24-C25
13	cA	846	BCR	C22-C23-C24-C25
10	aL	202	CLA	CBD-CGD-O2D-CED
10	bL	202	CLA	CBD-CGD-O2D-CED
13	aB	849	BCR	C19-C20-C21-C22
13	bB	849	BCR	C19-C20-C21-C22
13	cB	849	BCR	C19-C20-C21-C22
10	cL	202	CLA	CBD-CGD-O2D-CED
10	aB	820	CLA	C15-C16-C17-C18
10	cB	820	CLA	C15-C16-C17-C18
10	aB	818	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cB	818	CLA	O1A-CGA-O2A-C1
10	bB	807	CLA	CAA-CBA-CGA-O2A
10	cB	807	CLA	CAA-CBA-CGA-O2A
10	aA	811	CLA	C4-C3-C5-C6
10	aB	837	CLA	C4-C3-C5-C6
10	bA	811	CLA	C4-C3-C5-C6
10	bB	837	CLA	C4-C3-C5-C6
10	cA	811	CLA	C4-C3-C5-C6
10	bB	820	CLA	C15-C16-C17-C18
10	bA	832	CLA	O1A-CGA-O2A-C1
10	bB	818	CLA	O1A-CGA-O2A-C1
10	cA	832	CLA	O1A-CGA-O2A-C1
10	aB	807	CLA	CAA-CBA-CGA-O2A
10	aA	841	CLA	C2-C1-O2A-CGA
10	aB	823	CLA	C2-C1-O2A-CGA
10	bA	841	CLA	C2-C1-O2A-CGA
10	bB	823	CLA	C2-C1-O2A-CGA
10	cA	841	CLA	C2-C1-O2A-CGA
10	cB	823	CLA	C2-C1-O2A-CGA
10	aA	832	CLA	O1A-CGA-O2A-C1
10	aA	827	CLA	CAA-CBA-CGA-O1A
10	bA	827	CLA	CAA-CBA-CGA-O1A
10	cA	827	CLA	CAA-CBA-CGA-O1A
10	bA	828	CLA	CAA-CBA-CGA-O2A
10	aB	818	CLA	CBA-CGA-O2A-C1
10	cB	818	CLA	CBA-CGA-O2A-C1
10	cB	837	CLA	C4-C3-C5-C6
10	aB	815	CLA	C2-C3-C5-C6
10	bB	815	CLA	C2-C3-C5-C6
10	cB	815	CLA	C2-C3-C5-C6
10	aA	828	CLA	CAA-CBA-CGA-O2A
10	cA	828	CLA	CAA-CBA-CGA-O2A
10	aA	812	CLA	C11-C10-C8-C9
10	aA	826	CLA	C6-C7-C8-C9
10	aB	814	CLA	C11-C12-C13-C14
10	bA	812	CLA	C11-C10-C8-C9
10	bA	826	CLA	C6-C7-C8-C9
10	bB	814	CLA	C11-C12-C13-C14
10	cA	812	CLA	C11-C10-C8-C9
10	cA	826	CLA	C6-C7-C8-C9
10	cB	814	CLA	C11-C12-C13-C14
10	bB	818	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aA	820	CLA	C8-C10-C11-C12
10	bA	820	CLA	C8-C10-C11-C12
13	aA	846	BCR	C20-C21-C22-C37
13	aA	851	BCR	C11-C10-C9-C34
13	aB	845	BCR	C11-C10-C9-C34
13	aB	849	BCR	C16-C17-C18-C36
13	aI	102	BCR	C20-C21-C22-C37
13	aL	207	BCR	C20-C21-C22-C37
13	bA	846	BCR	C20-C21-C22-C37
13	bA	851	BCR	C11-C10-C9-C34
13	bB	845	BCR	C11-C10-C9-C34
13	bB	849	BCR	C16-C17-C18-C36
13	bI	102	BCR	C20-C21-C22-C37
13	bL	207	BCR	C20-C21-C22-C37
13	cA	846	BCR	C20-C21-C22-C37
13	cA	851	BCR	C11-C10-C9-C34
13	cB	845	BCR	C11-C10-C9-C34
13	cB	849	BCR	C16-C17-C18-C36
13	cI	103	BCR	C20-C21-C22-C37
13	cL	207	BCR	C20-C21-C22-C37
10	bA	808	CLA	CAA-CBA-CGA-O1A
10	cA	808	CLA	CAA-CBA-CGA-O1A
10	aA	833	CLA	C2A-CAA-CBA-CGA
10	bA	833	CLA	C2A-CAA-CBA-CGA
10	cA	833	CLA	C2A-CAA-CBA-CGA
10	cA	820	CLA	C8-C10-C11-C12
10	cA	838	CLA	O1A-CGA-O2A-C1
10	aA	838	CLA	O1A-CGA-O2A-C1
10	aB	835	CLA	CAA-CBA-CGA-O1A
10	bA	838	CLA	O1A-CGA-O2A-C1
10	aA	830	CLA	C1A-C2A-CAA-CBA
10	aB	801	CLA	C1A-C2A-CAA-CBA
10	aB	813	CLA	C1A-C2A-CAA-CBA
10	aB	820	CLA	C1A-C2A-CAA-CBA
10	aB	822	CLA	C1A-C2A-CAA-CBA
10	bA	830	CLA	C1A-C2A-CAA-CBA
10	bB	801	CLA	C1A-C2A-CAA-CBA
10	bB	813	CLA	C1A-C2A-CAA-CBA
10	bB	820	CLA	C1A-C2A-CAA-CBA
10	bB	822	CLA	C1A-C2A-CAA-CBA
10	cA	830	CLA	C1A-C2A-CAA-CBA
10	cB	801	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cB	813	CLA	C1A-C2A-CAA-CBA
10	cB	820	CLA	C1A-C2A-CAA-CBA
10	cB	822	CLA	C1A-C2A-CAA-CBA
9	aA	801	CL0	C12-C13-C15-C16
9	bA	801	CL0	C12-C13-C15-C16
9	cA	801	CL0	C12-C13-C15-C16
10	aA	835	CLA	C12-C13-C15-C16
10	aB	802	CLA	C12-C13-C15-C16
10	bA	835	CLA	C12-C13-C15-C16
10	bB	802	CLA	C12-C13-C15-C16
10	cA	835	CLA	C12-C13-C15-C16
10	cB	802	CLA	C12-C13-C15-C16
10	aA	808	CLA	CAA-CBA-CGA-O1A
10	aB	835	CLA	CAA-CBA-CGA-O2A
10	bB	835	CLA	CAA-CBA-CGA-O1A
10	cB	835	CLA	CAA-CBA-CGA-O1A
13	aB	847	BCR	C9-C10-C11-C12
13	bB	847	BCR	C9-C10-C11-C12
13	cB	847	BCR	C9-C10-C11-C12
10	bB	835	CLA	CAA-CBA-CGA-O2A
10	cB	835	CLA	CAA-CBA-CGA-O2A
11	aB	842	PQN	C26-C27-C28-C29
11	bB	842	PQN	C26-C27-C28-C29
11	cB	842	PQN	C26-C27-C28-C29
10	bA	811	CLA	C2-C3-C5-C6
10	cA	811	CLA	C2-C3-C5-C6
10	bA	832	CLA	CBA-CGA-O2A-C1
13	aA	851	BCR	C16-C17-C18-C19
13	aB	845	BCR	C11-C10-C9-C8
13	aB	845	BCR	C20-C21-C22-C23
13	bA	851	BCR	C16-C17-C18-C19
13	bB	845	BCR	C11-C10-C9-C8
13	bB	845	BCR	C20-C21-C22-C23
13	cA	851	BCR	C16-C17-C18-C19
13	cB	845	BCR	C11-C10-C9-C8
13	cB	845	BCR	C20-C21-C22-C23
10	aA	832	CLA	CBA-CGA-O2A-C1
10	cA	832	CLA	CBA-CGA-O2A-C1
10	cA	819	CLA	C5-C6-C7-C8
13	aA	849	BCR	C19-C20-C21-C22
13	bA	849	BCR	C19-C20-C21-C22
13	cA	849	BCR	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aB	824	CLA	CAA-CBA-CGA-O1A
10	bB	824	CLA	CAA-CBA-CGA-O1A
10	cB	824	CLA	CAA-CBA-CGA-O1A
10	aA	819	CLA	C5-C6-C7-C8
10	bA	819	CLA	C5-C6-C7-C8
10	cA	808	CLA	CAA-CBA-CGA-O2A
10	aB	820	CLA	C10-C11-C12-C13
10	bB	820	CLA	C10-C11-C12-C13
10	cB	808	CLA	C10-C11-C12-C13
10	cB	820	CLA	C10-C11-C12-C13
10	aA	820	CLA	C4-C3-C5-C6
10	aB	819	CLA	C4-C3-C5-C6
10	bA	820	CLA	C4-C3-C5-C6
10	bB	819	CLA	C4-C3-C5-C6
10	cA	820	CLA	C4-C3-C5-C6
10	cB	819	CLA	C4-C3-C5-C6
10	aA	811	CLA	C2-C1-O2A-CGA
10	bA	811	CLA	C2-C1-O2A-CGA
10	cA	811	CLA	C2-C1-O2A-CGA
10	aA	811	CLA	C2-C3-C5-C6
10	aB	814	CLA	C2-C3-C5-C6
10	aB	837	CLA	C2-C3-C5-C6
10	bB	814	CLA	C2-C3-C5-C6
10	bB	837	CLA	C2-C3-C5-C6
10	cB	814	CLA	C2-C3-C5-C6
10	cB	837	CLA	C2-C3-C5-C6
10	aB	808	CLA	C10-C11-C12-C13
10	bB	808	CLA	C10-C11-C12-C13
10	aB	813	CLA	CAA-CBA-CGA-O2A
10	aA	831	CLA	C11-C10-C8-C9
10	bA	812	CLA	C11-C12-C13-C14
10	bA	831	CLA	C11-C10-C8-C9
10	cA	812	CLA	C11-C12-C13-C14
10	cA	831	CLA	C11-C10-C8-C9
10	aA	808	CLA	CAA-CBA-CGA-O2A
10	bA	808	CLA	CAA-CBA-CGA-O2A
10	bB	813	CLA	CAA-CBA-CGA-O2A
10	cB	813	CLA	CAA-CBA-CGA-O2A
10	cB	832	CLA	C2A-CAA-CBA-CGA
10	aB	836	CLA	CAA-CBA-CGA-O2A
13	aA	848	BCR	C23-C24-C25-C26
13	aA	848	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	aA	851	BCR	C1-C6-C7-C8
13	aB	849	BCR	C1-C6-C7-C8
13	aI	101	BCR	C23-C24-C25-C30
13	aL	206	BCR	C1-C6-C7-C8
13	aL	207	BCR	C1-C6-C7-C8
13	bA	848	BCR	C23-C24-C25-C26
13	bA	848	BCR	C23-C24-C25-C30
13	bA	851	BCR	C1-C6-C7-C8
13	bB	849	BCR	C1-C6-C7-C8
13	bI	101	BCR	C23-C24-C25-C30
13	bL	206	BCR	C1-C6-C7-C8
13	bL	207	BCR	C1-C6-C7-C8
13	cA	848	BCR	C23-C24-C25-C26
13	cA	848	BCR	C23-C24-C25-C30
13	cA	851	BCR	C1-C6-C7-C8
13	cB	849	BCR	C1-C6-C7-C8
13	cI	102	BCR	C23-C24-C25-C30
13	cL	206	BCR	C1-C6-C7-C8
13	cL	207	BCR	C1-C6-C7-C8
10	aB	818	CLA	C8-C10-C11-C12
10	bB	818	CLA	C8-C10-C11-C12
10	cB	818	CLA	C8-C10-C11-C12
10	bB	836	CLA	CAA-CBA-CGA-O2A
10	cB	836	CLA	CAA-CBA-CGA-O2A
10	aB	826	CLA	C4-C3-C5-C6
10	bB	826	CLA	C4-C3-C5-C6
10	cB	826	CLA	C4-C3-C5-C6
13	aB	846	BCR	C7-C8-C9-C10
13	aB	847	BCR	C21-C22-C23-C24
13	bB	846	BCR	C7-C8-C9-C10
13	bB	847	BCR	C21-C22-C23-C24
13	cB	846	BCR	C7-C8-C9-C10
13	cB	847	BCR	C21-C22-C23-C24
10	aB	837	CLA	C11-C12-C13-C15
10	bB	837	CLA	C11-C12-C13-C15
10	cB	837	CLA	C11-C12-C13-C15
16	aB	848	LMG	C20-C21-C22-C23
16	bB	848	LMG	C20-C21-C22-C23
16	cB	848	LMG	C20-C21-C22-C23
10	aB	824	CLA	CAA-CBA-CGA-O2A
10	cB	824	CLA	CAA-CBA-CGA-O2A
10	aB	811	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cB	811	CLA	C3-C5-C6-C7
10	cA	805	CLA	C15-C16-C17-C18
10	aA	802	CLA	CAA-CBA-CGA-O2A
10	bB	824	CLA	CAA-CBA-CGA-O2A
10	cA	802	CLA	CAA-CBA-CGA-O2A
10	bB	832	CLA	C2A-CAA-CBA-CGA
10	aA	805	CLA	C15-C16-C17-C18
10	bA	805	CLA	C15-C16-C17-C18
10	bB	811	CLA	C3-C5-C6-C7
10	bA	802	CLA	CAA-CBA-CGA-O2A
10	aA	812	CLA	C11-C10-C8-C7
10	aA	820	CLA	C2-C3-C5-C6
10	aB	826	CLA	C2-C3-C5-C6
10	bA	812	CLA	C11-C10-C8-C7
10	bA	820	CLA	C2-C3-C5-C6
10	bB	826	CLA	C2-C3-C5-C6
10	cA	812	CLA	C11-C10-C8-C7
10	cA	820	CLA	C2-C3-C5-C6
10	cB	826	CLA	C2-C3-C5-C6
10	aB	831	CLA	CAA-CBA-CGA-O2A
10	cB	831	CLA	CAA-CBA-CGA-O2A
10	bA	854	CLA	C4C-C3C-CAC-CBC
10	cA	854	CLA	C4C-C3C-CAC-CBC
10	aL	205	CLA	C8-C10-C11-C12
10	bL	205	CLA	C8-C10-C11-C12
10	aB	818	CLA	CAA-CBA-CGA-O1A
10	bB	818	CLA	CAA-CBA-CGA-O1A
10	cB	818	CLA	CAA-CBA-CGA-O1A
10	aB	814	CLA	CAA-CBA-CGA-O2A
10	bB	814	CLA	CAA-CBA-CGA-O2A
10	cB	814	CLA	CAA-CBA-CGA-O2A
10	aA	854	CLA	C4C-C3C-CAC-CBC
10	bB	833	CLA	C10-C11-C12-C13
10	aA	802	CLA	CAA-CBA-CGA-O1A
10	cA	802	CLA	CAA-CBA-CGA-O1A
10	aB	833	CLA	C10-C11-C12-C13
10	cB	833	CLA	C10-C11-C12-C13
10	aB	832	CLA	C2A-CAA-CBA-CGA
10	cL	205	CLA	C8-C10-C11-C12
10	bB	823	CLA	C6-C7-C8-C9
10	cB	823	CLA	C6-C7-C8-C9
10	bA	802	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bB	831	CLA	CAA-CBA-CGA-O2A
10	aB	825	CLA	CAA-CBA-CGA-O2A
10	bB	825	CLA	CAA-CBA-CGA-O2A
16	aB	848	LMG	O7-C10-C11-C12
16	bB	848	LMG	O7-C10-C11-C12
16	cB	848	LMG	O7-C10-C11-C12
10	bB	832	CLA	CBD-CGD-O2D-CED
10	cB	832	CLA	CBD-CGD-O2D-CED
10	aA	818	CLA	C4-C3-C5-C6
10	aA	826	CLA	C4-C3-C5-C6
10	aB	810	CLA	C4-C3-C5-C6
10	bA	818	CLA	C4-C3-C5-C6
10	bA	826	CLA	C4-C3-C5-C6
10	bB	810	CLA	C4-C3-C5-C6
10	cA	818	CLA	C4-C3-C5-C6
10	cA	826	CLA	C4-C3-C5-C6
10	cB	810	CLA	C4-C3-C5-C6
10	aB	804	CLA	C2-C3-C5-C6
10	bB	804	CLA	C2-C3-C5-C6
10	bB	819	CLA	C2-C3-C5-C6
10	cB	804	CLA	C2-C3-C5-C6
10	aB	823	CLA	C6-C7-C8-C9
11	aB	842	PQN	C26-C27-C28-C30
11	bB	842	PQN	C26-C27-C28-C30
11	cB	842	PQN	C26-C27-C28-C30
10	aA	838	CLA	CBA-CGA-O2A-C1
10	bB	829	CLA	CBA-CGA-O2A-C1
10	cB	829	CLA	CBA-CGA-O2A-C1
10	cB	825	CLA	CAA-CBA-CGA-O2A
10	aA	812	CLA	C11-C12-C13-C14
10	aB	838	CLA	C14-C13-C15-C16
10	bB	838	CLA	C14-C13-C15-C16
10	cB	838	CLA	C14-C13-C15-C16
10	aB	817	CLA	C3A-C2A-CAA-CBA
10	bB	817	CLA	C3A-C2A-CAA-CBA
10	cB	817	CLA	C3A-C2A-CAA-CBA
10	aB	832	CLA	CBD-CGD-O2D-CED
10	aA	843	CLA	CAA-CBA-CGA-O2A
10	bA	843	CLA	CAA-CBA-CGA-O2A
10	cA	843	CLA	CAA-CBA-CGA-O2A
10	aA	808	CLA	CAD-CBD-CGD-O2D
10	aA	813	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	aB	821	CLA	CAD-CBD-CGD-O2D
10	bA	808	CLA	CAD-CBD-CGD-O2D
10	bA	813	CLA	CAD-CBD-CGD-O2D
10	bB	821	CLA	CAD-CBD-CGD-O2D
10	cA	808	CLA	CAD-CBD-CGD-O2D
10	cA	813	CLA	CAD-CBD-CGD-O2D
10	cB	821	CLA	CAD-CBD-CGD-O2D
10	aA	828	CLA	C10-C11-C12-C13
10	bA	828	CLA	C10-C11-C12-C13
10	cA	828	CLA	C10-C11-C12-C13
10	aB	829	CLA	CBA-CGA-O2A-C1
10	bA	838	CLA	CBA-CGA-O2A-C1
10	cA	838	CLA	CBA-CGA-O2A-C1
10	aA	834	CLA	C4-C3-C5-C6
10	aB	802	CLA	C4-C3-C5-C6
10	aL	203	CLA	C4-C3-C5-C6
10	bA	834	CLA	C4-C3-C5-C6
10	bB	802	CLA	C4-C3-C5-C6
10	bL	203	CLA	C4-C3-C5-C6
10	cA	834	CLA	C4-C3-C5-C6
10	cB	802	CLA	C4-C3-C5-C6
10	cL	203	CLA	C4-C3-C5-C6
10	aB	813	CLA	CAA-CBA-CGA-O1A
10	aB	836	CLA	CAA-CBA-CGA-O1A
10	bB	813	CLA	CAA-CBA-CGA-O1A
10	cB	813	CLA	CAA-CBA-CGA-O1A
10	bA	804	CLA	C13-C15-C16-C17
10	aB	819	CLA	C2-C3-C5-C6
10	aL	203	CLA	C2-C3-C5-C6
10	bL	203	CLA	C2-C3-C5-C6
10	cB	819	CLA	C2-C3-C5-C6
10	cL	203	CLA	C2-C3-C5-C6
10	aA	841	CLA	CAA-CBA-CGA-O2A
10	aB	823	CLA	CAA-CBA-CGA-O2A
10	bA	841	CLA	CAA-CBA-CGA-O2A
10	cA	841	CLA	CAA-CBA-CGA-O2A
10	cB	823	CLA	CAA-CBA-CGA-O2A
10	cB	829	CLA	O1A-CGA-O2A-C1
13	aA	849	BCR	C7-C8-C9-C10
13	bA	849	BCR	C7-C8-C9-C10
13	cA	849	BCR	C7-C8-C9-C10
10	bB	836	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cB	836	CLA	CAA-CBA-CGA-O1A
10	aB	838	CLA	O1A-CGA-O2A-C1
10	bB	829	CLA	O1A-CGA-O2A-C1
10	bB	838	CLA	O1A-CGA-O2A-C1
10	cB	838	CLA	O1A-CGA-O2A-C1
10	aA	804	CLA	C13-C15-C16-C17
10	cA	804	CLA	C13-C15-C16-C17
10	cB	803	CLA	C15-C16-C17-C18
10	aL	202	CLA	CAA-CBA-CGA-O2A
10	bB	823	CLA	CAA-CBA-CGA-O2A
10	bL	202	CLA	CAA-CBA-CGA-O2A
10	cL	202	CLA	CAA-CBA-CGA-O2A
10	bB	803	CLA	C15-C16-C17-C18
10	aA	831	CLA	O2A-C1-C2-C3
10	aB	823	CLA	O2A-C1-C2-C3
10	bA	831	CLA	O2A-C1-C2-C3
10	bB	806	CLA	O2A-C1-C2-C3
10	bB	823	CLA	O2A-C1-C2-C3
10	cA	831	CLA	O2A-C1-C2-C3
10	cB	823	CLA	O2A-C1-C2-C3
10	aB	829	CLA	O1A-CGA-O2A-C1
14	aA	852	LHG	O7-C7-C8-C9
14	bA	852	LHG	O7-C7-C8-C9
14	cA	852	LHG	O7-C7-C8-C9
10	aA	843	CLA	CAA-CBA-CGA-O1A
10	bA	843	CLA	CAA-CBA-CGA-O1A
10	cA	843	CLA	CAA-CBA-CGA-O1A
10	aA	803	CLA	CHA-CBD-CGD-O2D
10	aA	812	CLA	CHA-CBD-CGD-O1D
10	aA	824	CLA	CHA-CBD-CGD-O1D
10	aA	824	CLA	CHA-CBD-CGD-O2D
10	aA	833	CLA	CHA-CBD-CGD-O1D
10	aA	833	CLA	CHA-CBD-CGD-O2D
10	aB	806	CLA	CHA-CBD-CGD-O2D
10	aB	816	CLA	CHA-CBD-CGD-O1D
10	aB	816	CLA	CHA-CBD-CGD-O2D
10	aB	829	CLA	CHA-CBD-CGD-O1D
10	aB	829	CLA	CHA-CBD-CGD-O2D
10	aB	831	CLA	CHA-CBD-CGD-O2D
10	aB	833	CLA	CHA-CBD-CGD-O1D
10	aB	833	CLA	CHA-CBD-CGD-O2D
10	bA	803	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	bA	812	CLA	CHA-CBD-CGD-O1D
10	bA	824	CLA	CHA-CBD-CGD-O1D
10	bA	824	CLA	CHA-CBD-CGD-O2D
10	bA	833	CLA	CHA-CBD-CGD-O1D
10	bA	833	CLA	CHA-CBD-CGD-O2D
10	bB	806	CLA	CHA-CBD-CGD-O2D
10	bB	816	CLA	CHA-CBD-CGD-O1D
10	bB	816	CLA	CHA-CBD-CGD-O2D
10	bB	829	CLA	CHA-CBD-CGD-O1D
10	bB	829	CLA	CHA-CBD-CGD-O2D
10	bB	831	CLA	CHA-CBD-CGD-O2D
10	bB	833	CLA	CHA-CBD-CGD-O1D
10	bB	833	CLA	CHA-CBD-CGD-O2D
10	cA	803	CLA	CHA-CBD-CGD-O2D
10	cA	812	CLA	CHA-CBD-CGD-O1D
10	cA	824	CLA	CHA-CBD-CGD-O1D
10	cA	824	CLA	CHA-CBD-CGD-O2D
10	cA	833	CLA	CHA-CBD-CGD-O1D
10	cA	833	CLA	CHA-CBD-CGD-O2D
10	cB	806	CLA	CHA-CBD-CGD-O2D
10	cB	816	CLA	CHA-CBD-CGD-O1D
10	cB	816	CLA	CHA-CBD-CGD-O2D
10	cB	829	CLA	CHA-CBD-CGD-O1D
10	cB	829	CLA	CHA-CBD-CGD-O2D
10	cB	831	CLA	CHA-CBD-CGD-O2D
10	cB	833	CLA	CHA-CBD-CGD-O1D
10	cB	833	CLA	CHA-CBD-CGD-O2D
10	aB	803	CLA	C15-C16-C17-C18
10	aB	802	CLA	C2-C3-C5-C6
10	bB	802	CLA	C2-C3-C5-C6
10	cB	802	CLA	C2-C3-C5-C6
10	bB	831	CLA	CAA-CBA-CGA-O1A
10	aA	819	CLA	CAA-CBA-CGA-O2A
10	aB	811	CLA	CAA-CBA-CGA-O2A
10	bA	819	CLA	CAA-CBA-CGA-O2A
10	bB	811	CLA	CAA-CBA-CGA-O2A
10	cA	819	CLA	CAA-CBA-CGA-O2A
10	cB	811	CLA	CAA-CBA-CGA-O2A
14	aA	852	LHG	C35-C36-C37-C38
14	bA	852	LHG	C35-C36-C37-C38
10	aB	828	CLA	C10-C11-C12-C13
10	bB	828	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cB	828	CLA	C10-C11-C12-C13
10	aB	831	CLA	CAA-CBA-CGA-O1A
10	cB	831	CLA	CAA-CBA-CGA-O1A
14	cA	852	LHG	C35-C36-C37-C38
10	bA	833	CLA	C13-C15-C16-C17
14	aA	855	LHG	O7-C7-C8-C9
14	bA	855	LHG	O7-C7-C8-C9
14	cA	855	LHG	O7-C7-C8-C9
10	aB	817	CLA	C2A-CAA-CBA-CGA
10	bB	817	CLA	C2A-CAA-CBA-CGA
10	cB	817	CLA	C2A-CAA-CBA-CGA
10	aA	833	CLA	C13-C15-C16-C17
10	cA	833	CLA	C13-C15-C16-C17
10	bA	835	CLA	CAA-CBA-CGA-O2A
10	aA	826	CLA	C10-C11-C12-C13
10	bA	826	CLA	C10-C11-C12-C13
10	cA	826	CLA	C10-C11-C12-C13
10	aA	835	CLA	CAA-CBA-CGA-O2A
10	cA	835	CLA	CAA-CBA-CGA-O2A
10	aA	835	CLA	C14-C13-C15-C16
10	aB	802	CLA	C14-C13-C15-C16
10	aB	809	CLA	C6-C7-C8-C9
10	aB	818	CLA	C6-C7-C8-C9
10	aB	828	CLA	C14-C13-C15-C16
10	bA	835	CLA	C14-C13-C15-C16
10	bB	802	CLA	C14-C13-C15-C16
10	bB	809	CLA	C6-C7-C8-C9
10	bB	818	CLA	C6-C7-C8-C9
10	bB	828	CLA	C14-C13-C15-C16
10	cA	835	CLA	C14-C13-C15-C16
10	cB	802	CLA	C14-C13-C15-C16
10	cB	809	CLA	C6-C7-C8-C9
10	cB	818	CLA	C6-C7-C8-C9
10	cB	828	CLA	C14-C13-C15-C16
10	bB	833	CLA	CAA-CBA-CGA-O1A
14	aA	852	LHG	O8-C23-C24-C25
14	bA	852	LHG	O8-C23-C24-C25
10	aL	202	CLA	CAA-CBA-CGA-O1A
10	bL	202	CLA	CAA-CBA-CGA-O1A
10	cL	202	CLA	CAA-CBA-CGA-O1A
10	aB	837	CLA	C11-C12-C13-C14
10	bB	837	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cB	837	CLA	C11-C12-C13-C14
10	aA	837	CLA	CAA-CBA-CGA-O2A
10	bA	837	CLA	CAA-CBA-CGA-O2A
10	cA	837	CLA	CAA-CBA-CGA-O2A
14	cA	852	LHG	O8-C23-C24-C25
10	aB	833	CLA	CAA-CBA-CGA-O1A
10	cB	833	CLA	CAA-CBA-CGA-O1A
13	aA	846	BCR	C17-C18-C19-C20
13	aM	101	BCR	C7-C8-C9-C10
13	bA	846	BCR	C17-C18-C19-C20
13	bM	101	BCR	C7-C8-C9-C10
13	cA	846	BCR	C17-C18-C19-C20
13	cM	101	BCR	C7-C8-C9-C10
10	aA	824	CLA	C1A-C2A-CAA-CBA
10	bA	824	CLA	C1A-C2A-CAA-CBA
10	cA	824	CLA	C1A-C2A-CAA-CBA
10	aB	811	CLA	CAA-CBA-CGA-O1A
10	cB	811	CLA	CAA-CBA-CGA-O1A
10	bA	839	CLA	C5-C6-C7-C8
10	cA	839	CLA	C5-C6-C7-C8
10	aA	841	CLA	CAA-CBA-CGA-O1A
10	aB	814	CLA	CAA-CBA-CGA-O1A
10	bA	841	CLA	CAA-CBA-CGA-O1A
10	bB	811	CLA	CAA-CBA-CGA-O1A
10	bB	814	CLA	CAA-CBA-CGA-O1A
10	cA	841	CLA	CAA-CBA-CGA-O1A
10	aB	804	CLA	C2A-CAA-CBA-CGA
10	bB	804	CLA	C2A-CAA-CBA-CGA
10	cB	804	CLA	C2A-CAA-CBA-CGA
10	aA	854	CLA	C2C-C3C-CAC-CBC
10	aB	823	CLA	CAA-CBA-CGA-O1A
10	bB	823	CLA	CAA-CBA-CGA-O1A
10	cB	814	CLA	CAA-CBA-CGA-O1A
10	cB	823	CLA	CAA-CBA-CGA-O1A
10	aA	839	CLA	C5-C6-C7-C8
10	aB	825	CLA	CAA-CBA-CGA-O1A
10	bB	825	CLA	CAA-CBA-CGA-O1A
10	cA	854	CLA	C2C-C3C-CAC-CBC
10	aA	841	CLA	C16-C17-C18-C20
10	bA	854	CLA	C2C-C3C-CAC-CBC
10	aA	819	CLA	CAA-CBA-CGA-O1A
10	cB	825	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cB	808	CLA	CAA-CBA-CGA-O2A
9	cA	801	CL0	C3-C5-C6-C7
13	aA	848	BCR	C5-C6-C7-C8
13	aB	845	BCR	C23-C24-C25-C26
13	bA	848	BCR	C5-C6-C7-C8
13	bB	845	BCR	C23-C24-C25-C26
13	cA	848	BCR	C5-C6-C7-C8
13	cB	845	BCR	C23-C24-C25-C26
10	bA	819	CLA	CAA-CBA-CGA-O1A
10	cA	819	CLA	CAA-CBA-CGA-O1A
10	aB	808	CLA	CAA-CBA-CGA-O2A
10	bB	808	CLA	CAA-CBA-CGA-O2A
10	bL	203	CLA	C8-C10-C11-C12
10	bA	841	CLA	C16-C17-C18-C20
10	cA	841	CLA	C16-C17-C18-C20
16	bB	848	LMG	C14-C15-C16-C17
9	aA	801	CL0	C3-C5-C6-C7
16	cB	848	LMG	C14-C15-C16-C17
10	aB	805	CLA	C10-C11-C12-C13
10	bB	805	CLA	C10-C11-C12-C13
10	cB	805	CLA	C10-C11-C12-C13
16	aB	848	LMG	C14-C15-C16-C17
10	aB	810	CLA	C2-C3-C5-C6
10	bB	810	CLA	C2-C3-C5-C6
10	cB	810	CLA	C2-C3-C5-C6
10	cL	203	CLA	C8-C10-C11-C12
9	aA	801	CL0	CAD-CBD-CGD-O1D
9	bA	801	CL0	CAD-CBD-CGD-O1D
9	cA	801	CL0	CAD-CBD-CGD-O1D
10	aA	830	CLA	CAD-CBD-CGD-O1D
10	aB	814	CLA	CAD-CBD-CGD-O1D
10	aB	827	CLA	CAD-CBD-CGD-O1D
10	bA	830	CLA	CAD-CBD-CGD-O1D
10	bB	814	CLA	CAD-CBD-CGD-O1D
10	bB	827	CLA	CAD-CBD-CGD-O1D
10	cA	830	CLA	CAD-CBD-CGD-O1D
10	cB	827	CLA	CAD-CBD-CGD-O1D
10	aL	203	CLA	C8-C10-C11-C12
10	aA	812	CLA	C6-C7-C8-C9
10	aL	203	CLA	C11-C10-C8-C9
10	bA	812	CLA	C6-C7-C8-C9
10	bL	203	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cA	812	CLA	C6-C7-C8-C9
10	cL	203	CLA	C11-C10-C8-C9
11	aA	844	PQN	C24-C23-C25-C26
11	bA	844	PQN	C24-C23-C25-C26
11	cA	844	PQN	C24-C23-C25-C26
9	bA	801	CL0	C3-C5-C6-C7
10	aA	834	CLA	CAA-CBA-CGA-O2A
10	aA	838	CLA	CAA-CBA-CGA-O2A
10	aB	821	CLA	CAA-CBA-CGA-O2A
10	bA	834	CLA	CAA-CBA-CGA-O2A
10	bA	838	CLA	CAA-CBA-CGA-O2A
10	bB	821	CLA	CAA-CBA-CGA-O2A
10	cA	834	CLA	CAA-CBA-CGA-O2A
10	cA	838	CLA	CAA-CBA-CGA-O2A
10	aB	839	CLA	C2-C1-O2A-CGA
10	bB	839	CLA	C2-C1-O2A-CGA
10	cB	839	CLA	C2-C1-O2A-CGA
10	aB	805	CLA	CAA-CBA-CGA-O2A
10	aB	839	CLA	CAA-CBA-CGA-O2A
10	bB	805	CLA	CAA-CBA-CGA-O2A
10	bB	839	CLA	CAA-CBA-CGA-O2A
10	cB	821	CLA	CAA-CBA-CGA-O2A
10	cB	839	CLA	CAA-CBA-CGA-O2A
10	aB	814	CLA	C15-C16-C17-C18
10	bB	814	CLA	C15-C16-C17-C18
10	cB	814	CLA	C15-C16-C17-C18
10	aB	811	CLA	CBD-CGD-O2D-CED
10	bB	811	CLA	CBD-CGD-O2D-CED
10	cB	811	CLA	CBD-CGD-O2D-CED
10	aA	818	CLA	C11-C12-C13-C15
10	aA	827	CLA	C6-C7-C8-C10
10	aA	831	CLA	C11-C10-C8-C7
10	aA	838	CLA	C3A-C2A-CAA-CBA
10	aB	809	CLA	C6-C7-C8-C10
10	bA	818	CLA	C11-C12-C13-C15
10	bA	827	CLA	C6-C7-C8-C10
10	bA	831	CLA	C11-C10-C8-C7
10	bA	838	CLA	C3A-C2A-CAA-CBA
10	bB	809	CLA	C6-C7-C8-C10
10	cA	818	CLA	C11-C12-C13-C15
10	cA	827	CLA	C6-C7-C8-C10
10	cA	831	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	cA	838	CLA	C3A-C2A-CAA-CBA
10	cB	809	CLA	C6-C7-C8-C10
11	aA	844	PQN	C22-C23-C25-C26
11	bA	844	PQN	C22-C23-C25-C26
11	cA	844	PQN	C22-C23-C25-C26
10	cA	834	CLA	CAA-CBA-CGA-O1A
10	bB	810	CLA	CAA-CBA-CGA-O2A
10	cB	805	CLA	CAA-CBA-CGA-O2A
10	cB	810	CLA	CAA-CBA-CGA-O2A
10	bB	826	CLA	C5-C6-C7-C8
10	aA	856	CLA	O2A-C1-C2-C3
10	bA	856	CLA	O2A-C1-C2-C3
10	cA	856	CLA	O2A-C1-C2-C3
10	cB	826	CLA	C5-C6-C7-C8
10	aA	834	CLA	CAA-CBA-CGA-O1A
10	bA	834	CLA	CAA-CBA-CGA-O1A
10	aB	826	CLA	C5-C6-C7-C8
10	aA	835	CLA	CAA-CBA-CGA-O1A
10	aA	837	CLA	CAA-CBA-CGA-O1A
10	bA	835	CLA	CAA-CBA-CGA-O1A
10	bA	837	CLA	CAA-CBA-CGA-O1A
10	cA	835	CLA	CAA-CBA-CGA-O1A
10	cA	837	CLA	CAA-CBA-CGA-O1A
14	aA	852	LHG	O9-C7-C8-C9
14	bA	852	LHG	O9-C7-C8-C9
14	cA	852	LHG	O9-C7-C8-C9
10	aB	802	CLA	CBA-CGA-O2A-C1
10	bB	802	CLA	CBA-CGA-O2A-C1
10	cB	802	CLA	CBA-CGA-O2A-C1
10	aB	802	CLA	CAA-CBA-CGA-O2A
10	aB	809	CLA	CAA-CBA-CGA-O2A
10	aB	810	CLA	CAA-CBA-CGA-O2A
10	aB	838	CLA	CAA-CBA-CGA-O2A
10	bB	809	CLA	CAA-CBA-CGA-O2A
10	bB	838	CLA	CAA-CBA-CGA-O2A
10	cB	802	CLA	CAA-CBA-CGA-O2A
10	cB	809	CLA	CAA-CBA-CGA-O2A
10	cB	838	CLA	CAA-CBA-CGA-O2A
10	aB	808	CLA	C15-C16-C17-C18
10	bB	808	CLA	C15-C16-C17-C18
10	cB	808	CLA	C15-C16-C17-C18
10	aA	838	CLA	CAA-CBA-CGA-O1A

Continued on next page...

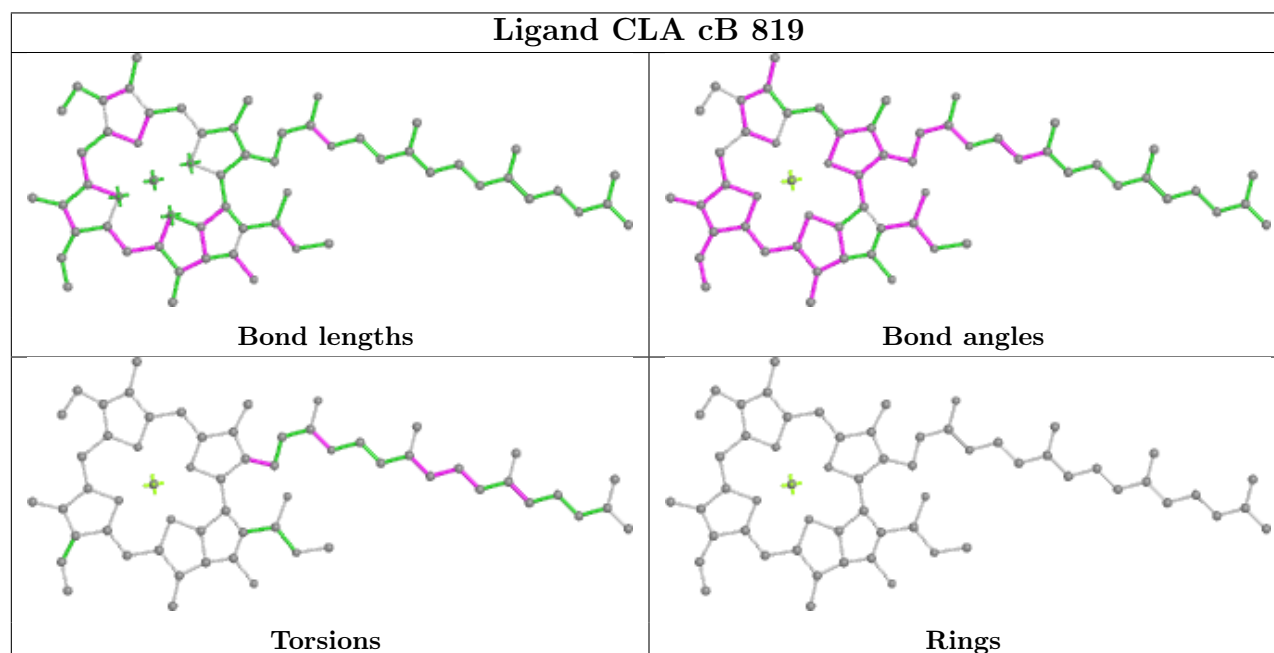
Continued from previous page...

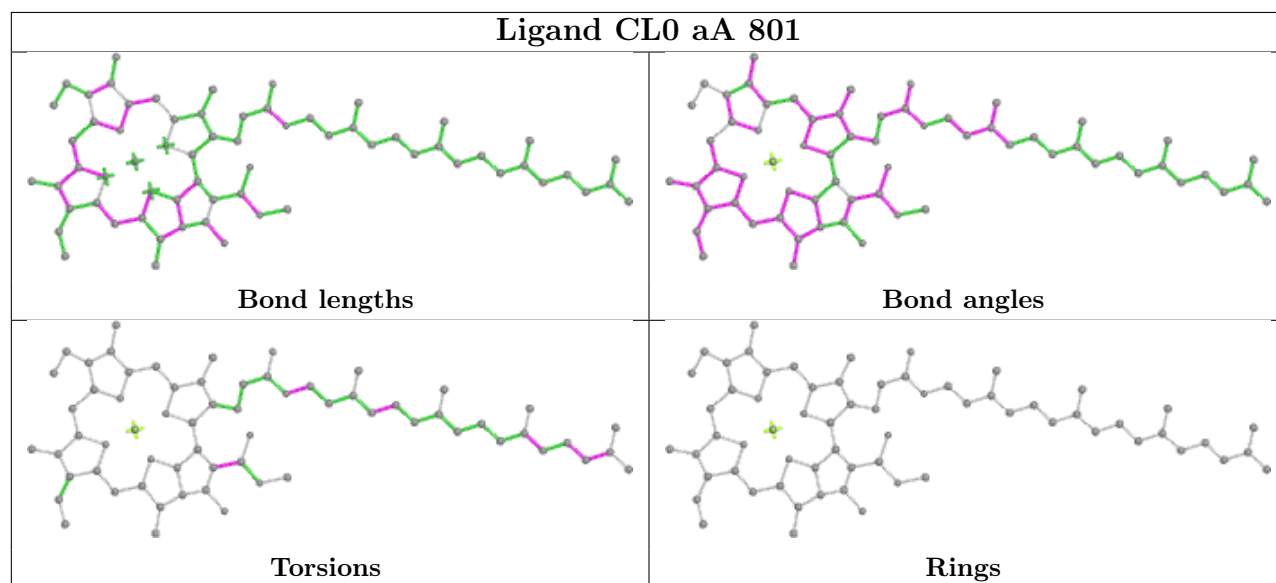
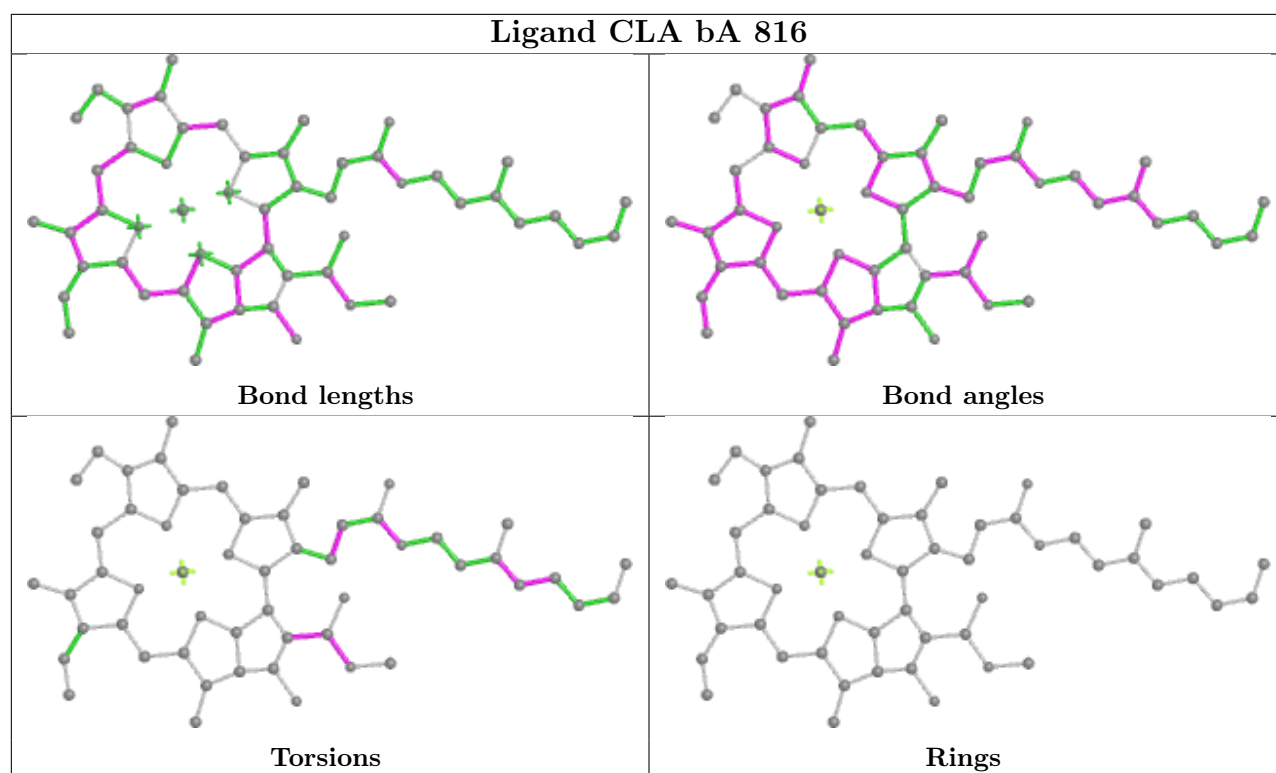
Mol	Chain	Res	Type	Atoms
10	bA	838	CLA	CAA-CBA-CGA-O1A
10	cA	838	CLA	CAA-CBA-CGA-O1A
10	aA	805	CLA	CAA-CBA-CGA-O2A
10	aL	205	CLA	CAA-CBA-CGA-O2A
10	bA	805	CLA	CAA-CBA-CGA-O2A
10	bB	802	CLA	CAA-CBA-CGA-O2A
10	bL	205	CLA	CAA-CBA-CGA-O2A
10	cA	805	CLA	CAA-CBA-CGA-O2A
10	cL	205	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

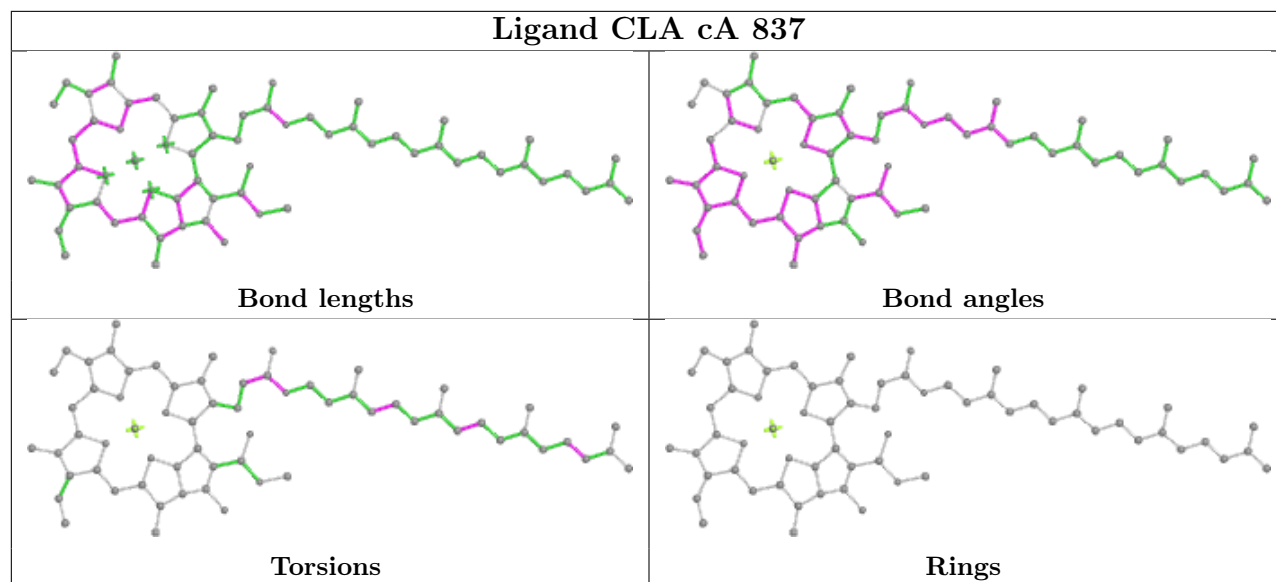
No monomer is involved in short contacts.

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.

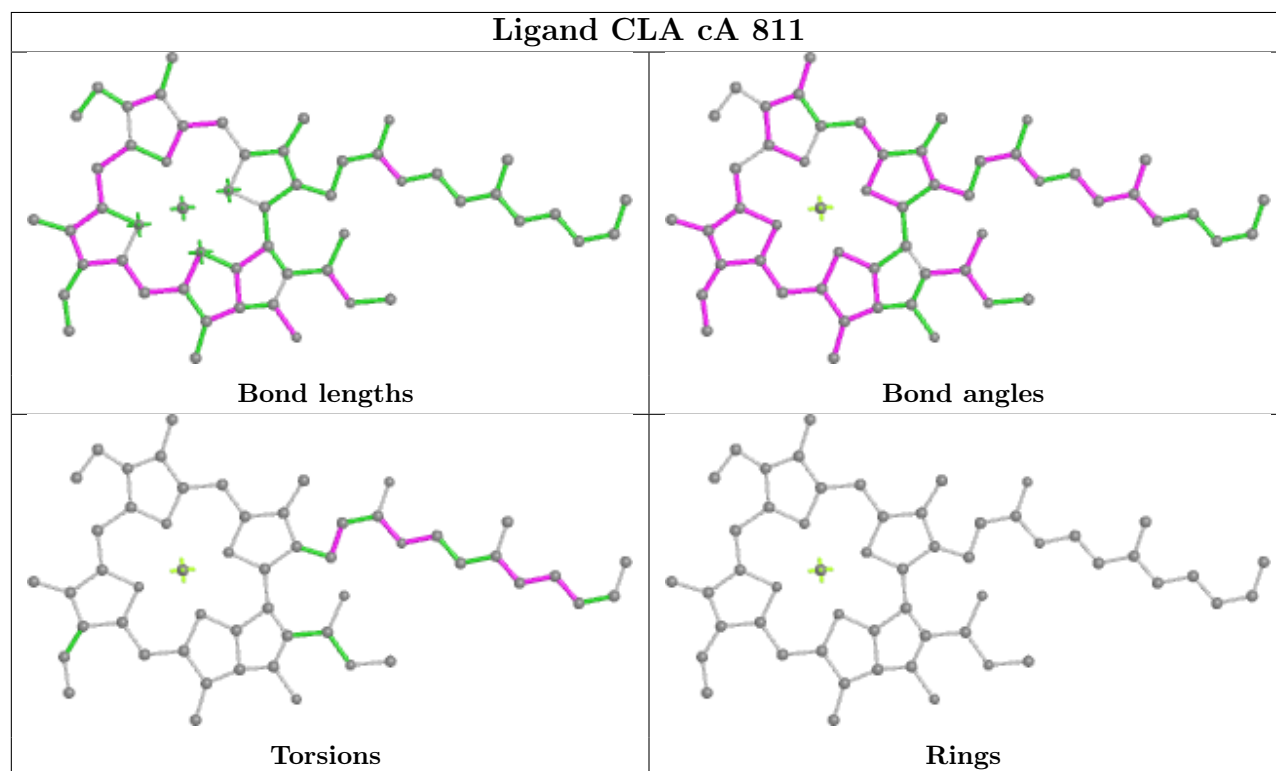


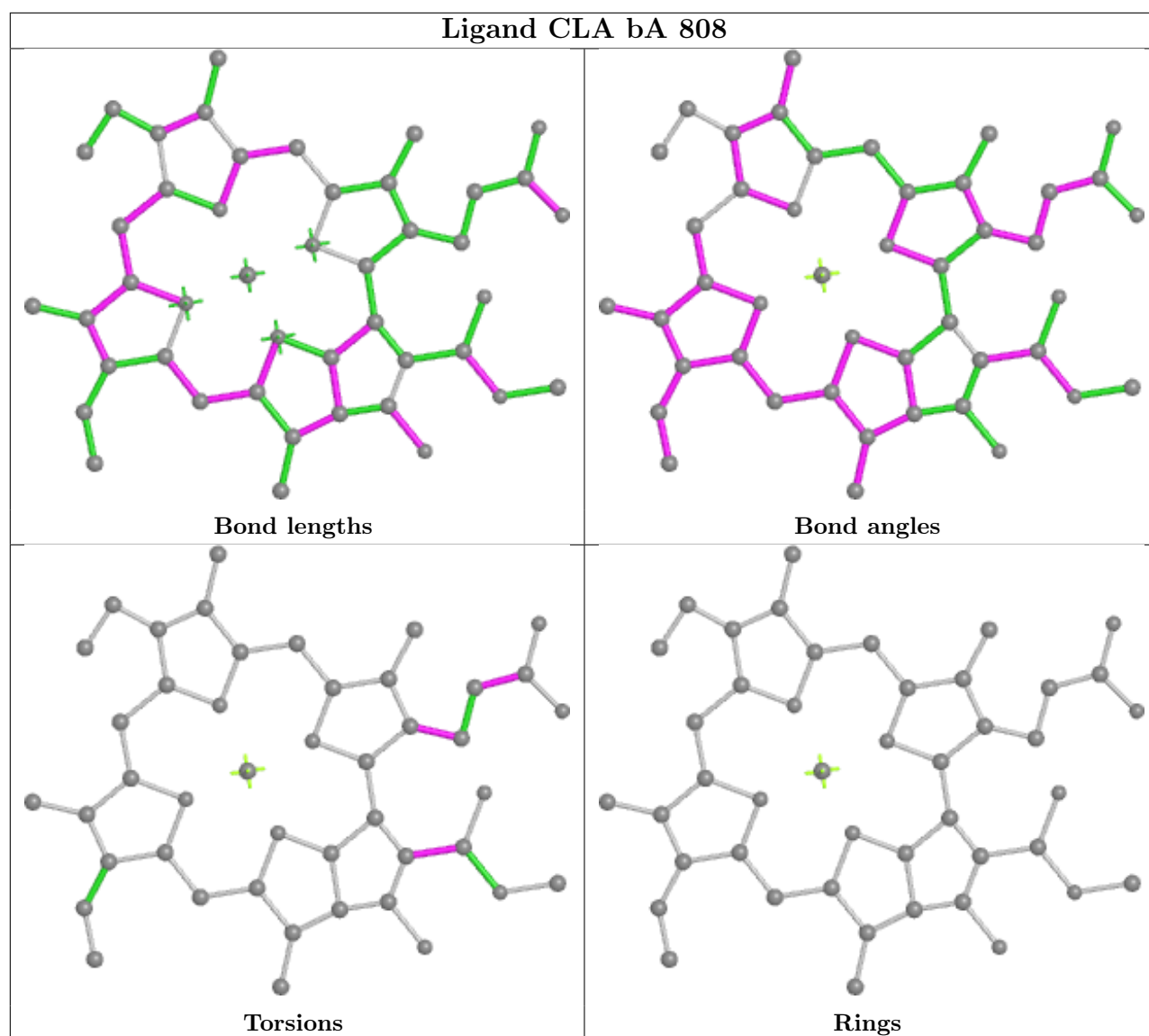


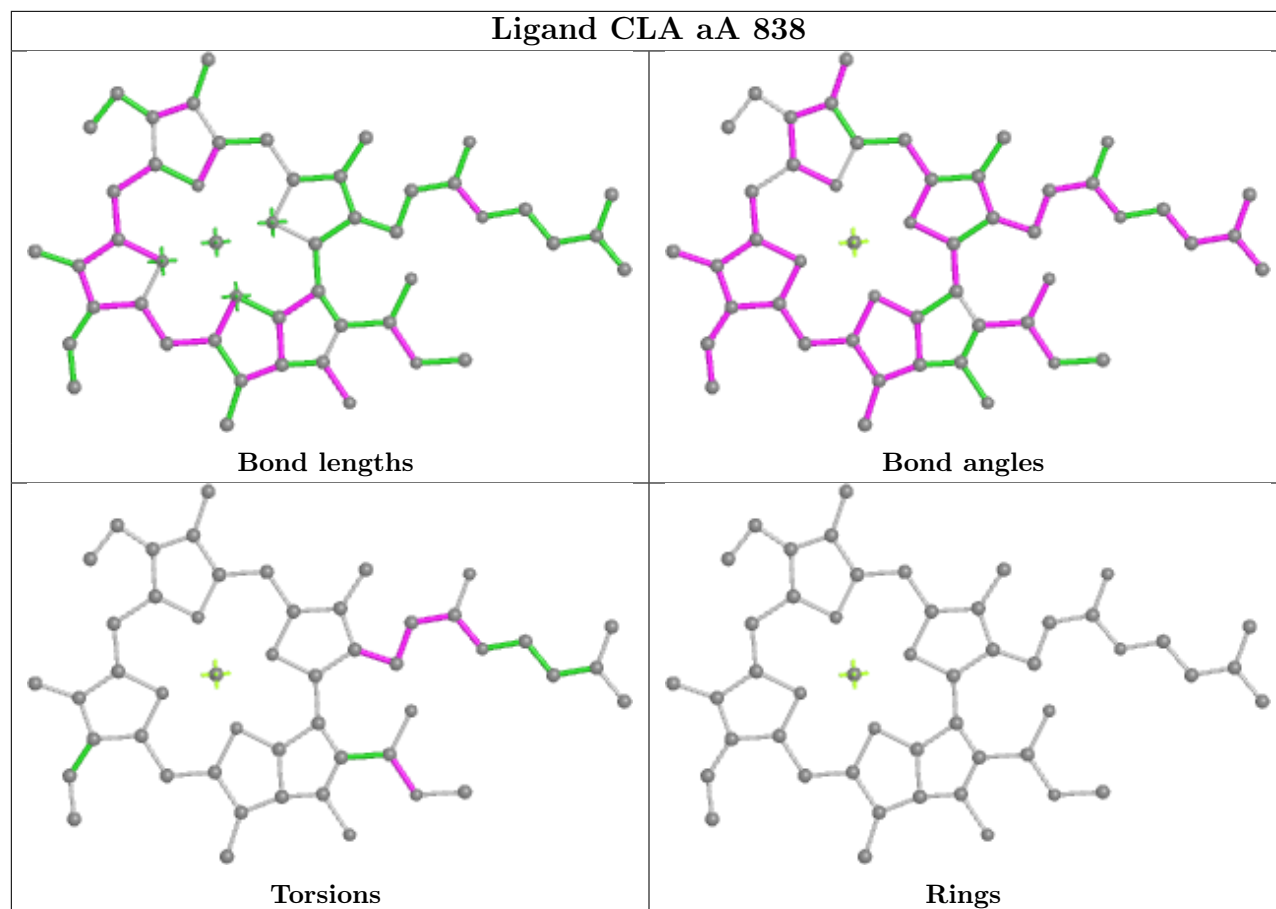
Ligand CLA cA 837



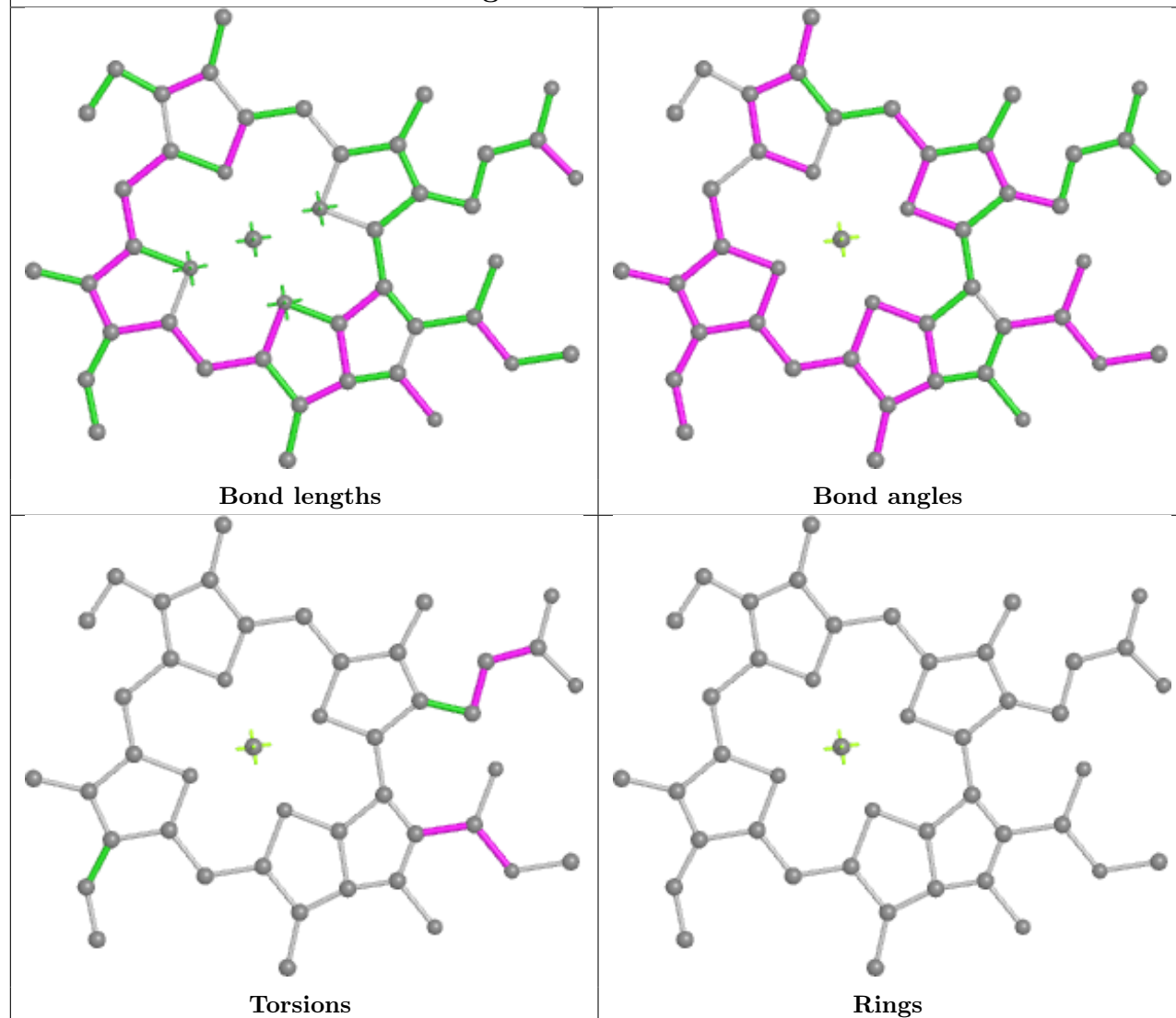
Ligand CLA cA 811



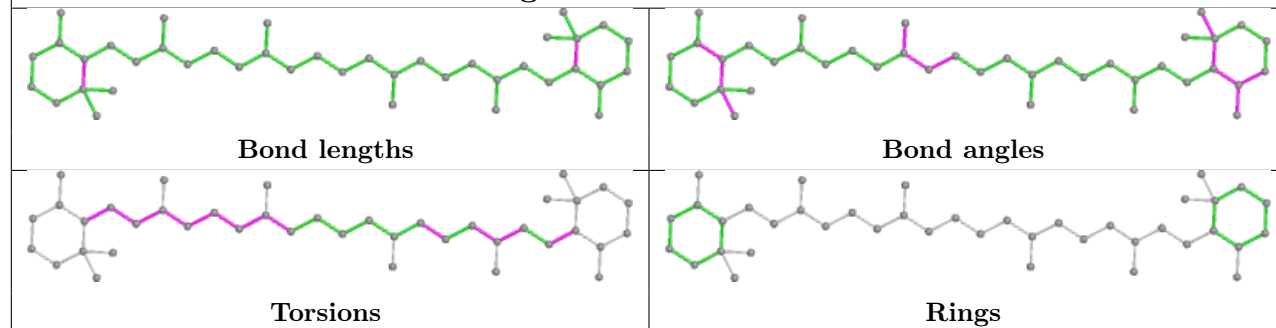


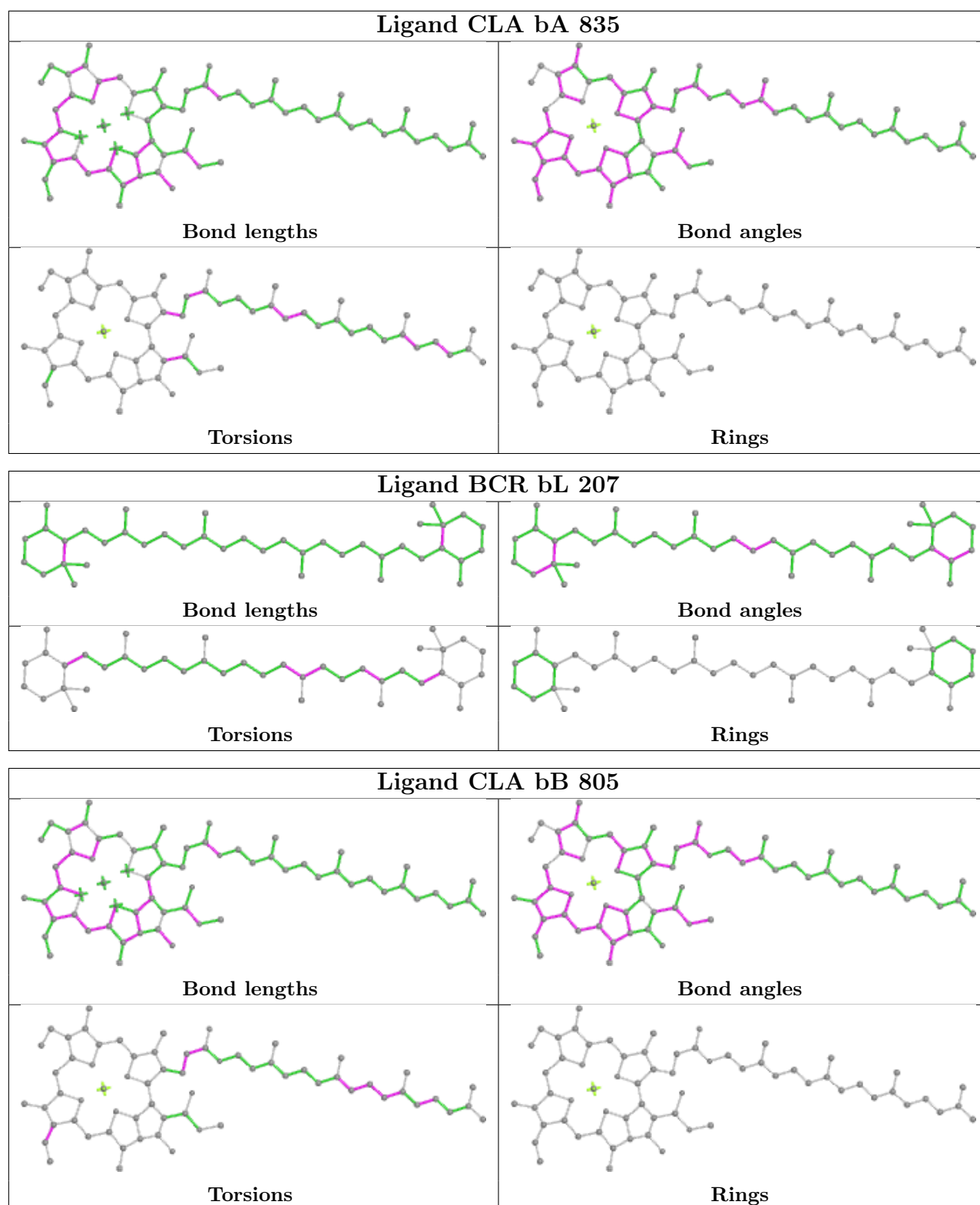


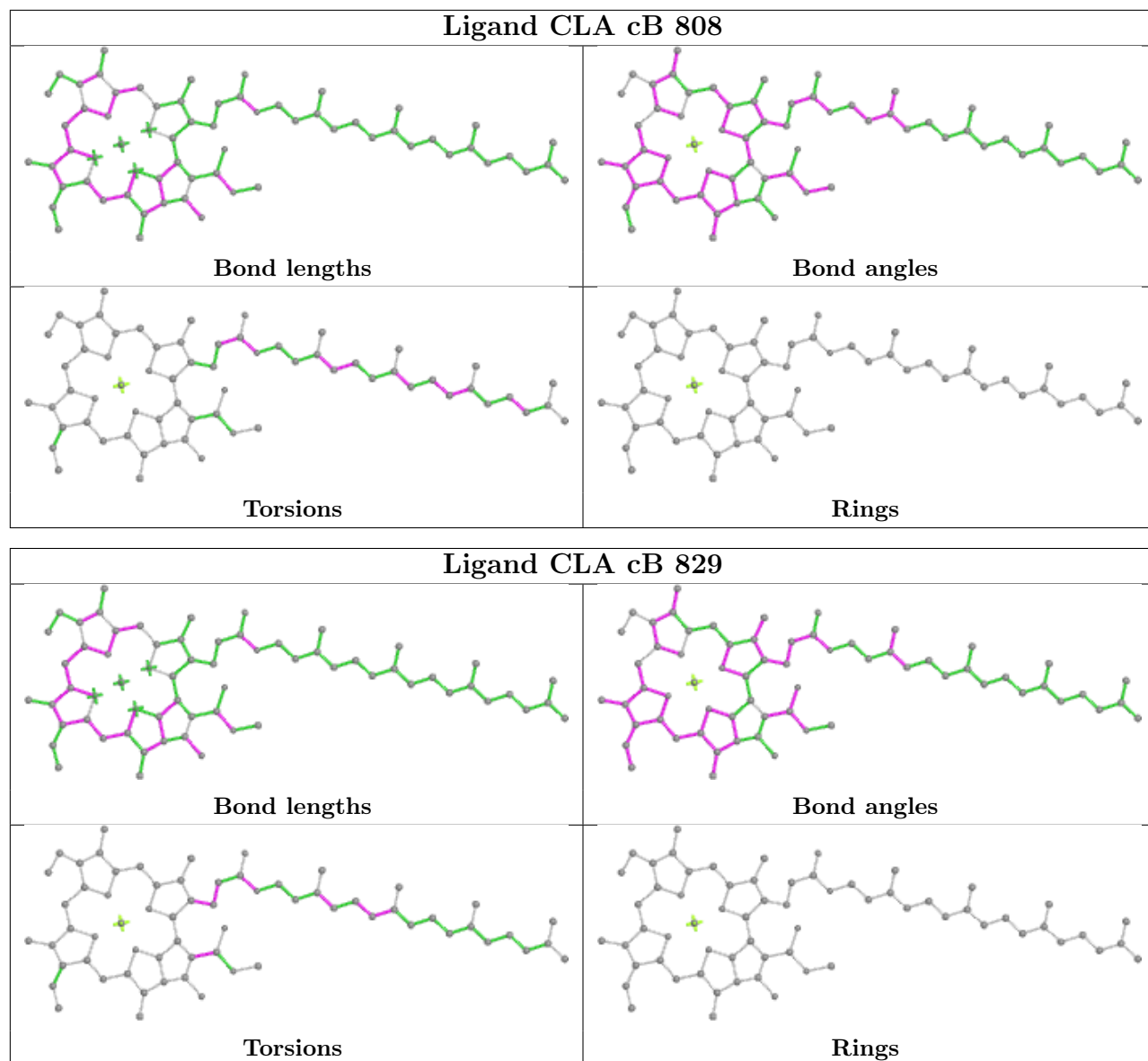
Ligand CLA aB 831



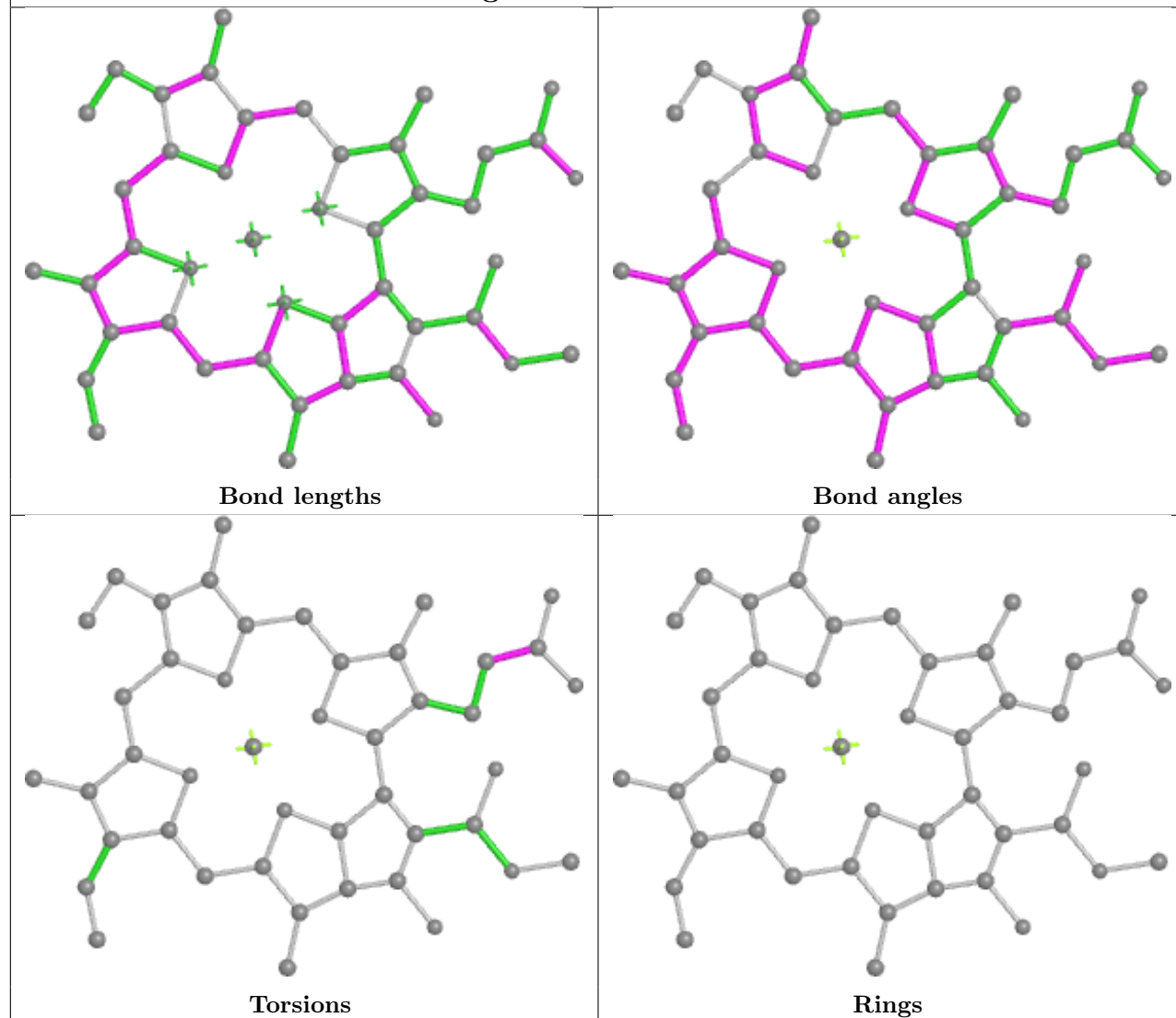
Ligand BCR bA 848



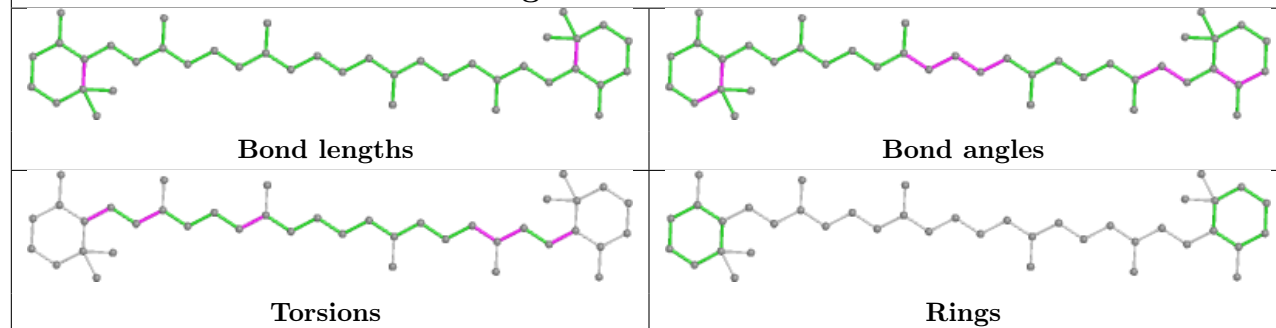




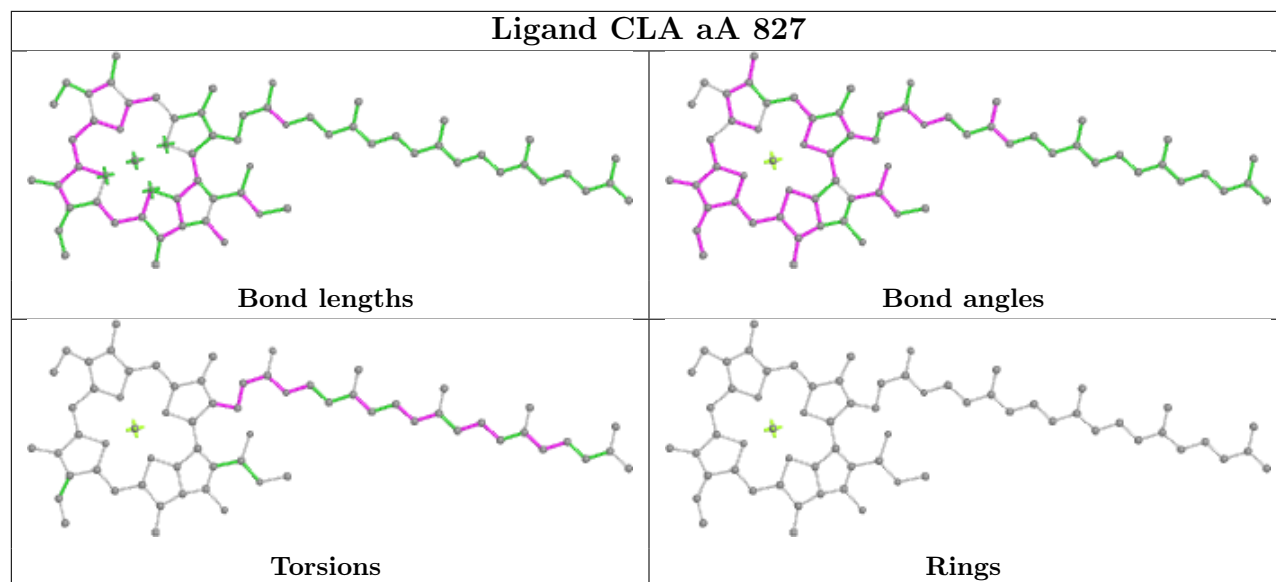
Ligand CLA aB 836



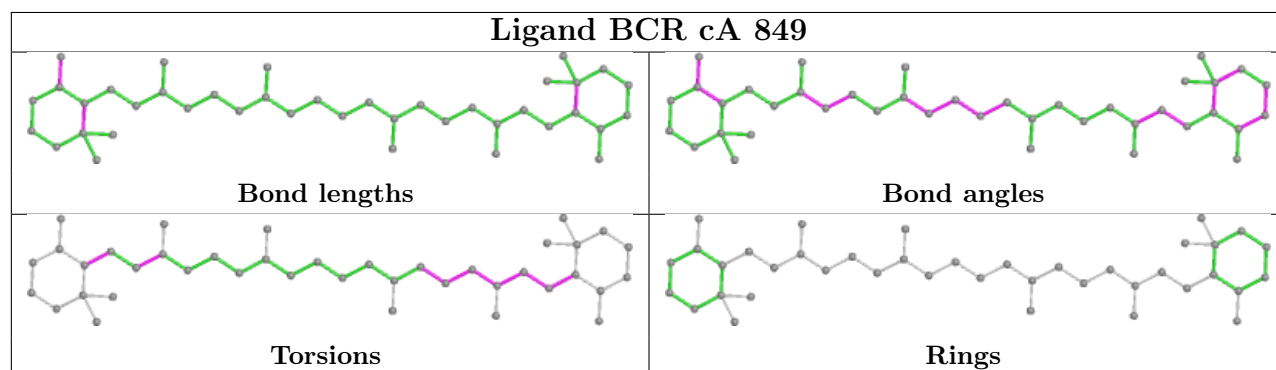
Ligand BCR cA 850



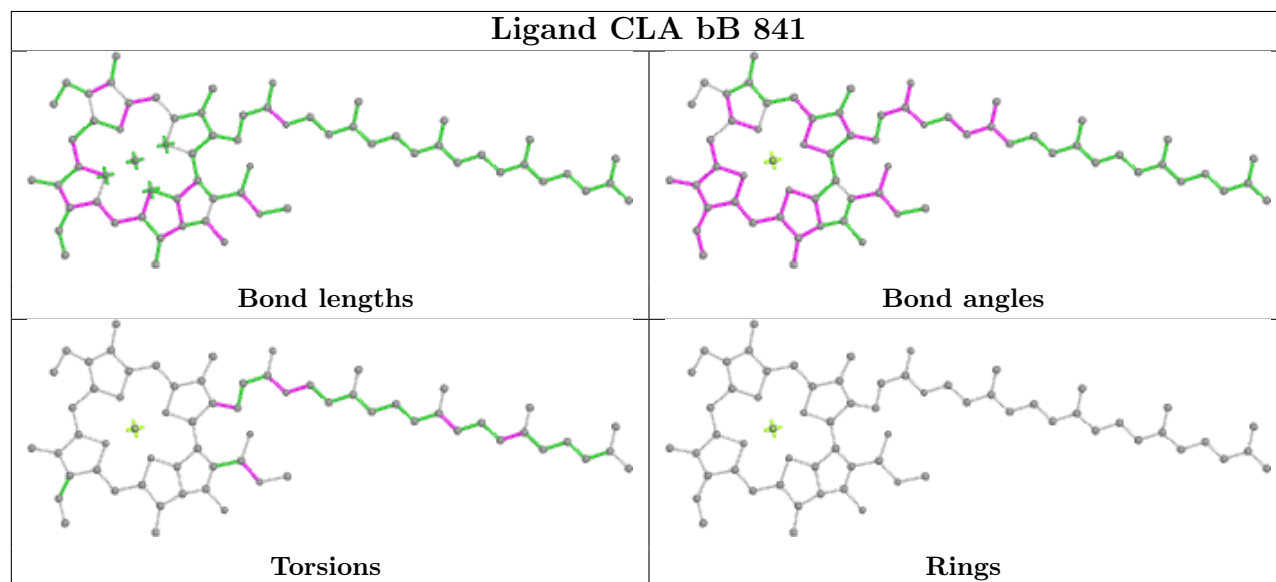
Ligand CLA aA 827

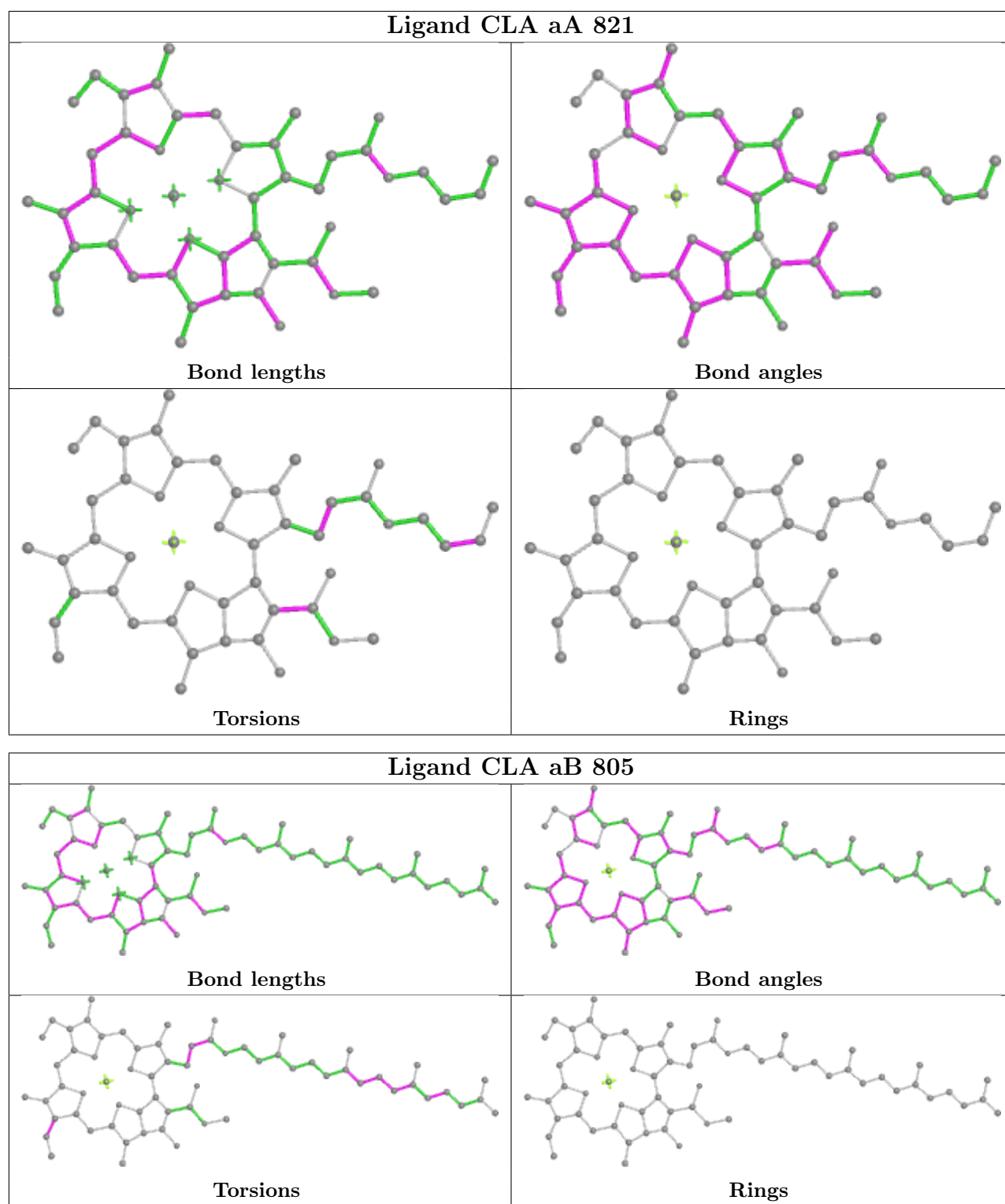


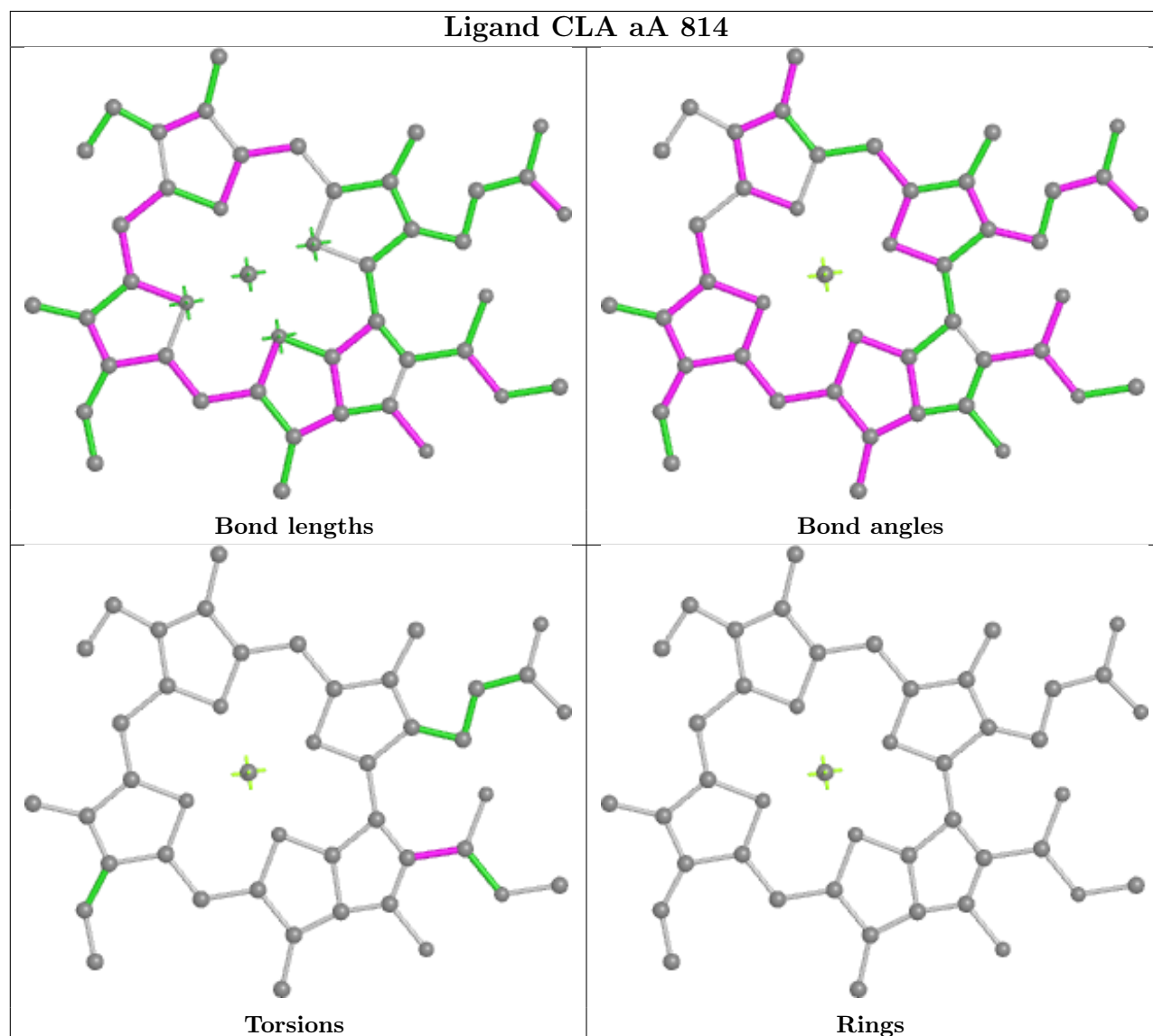
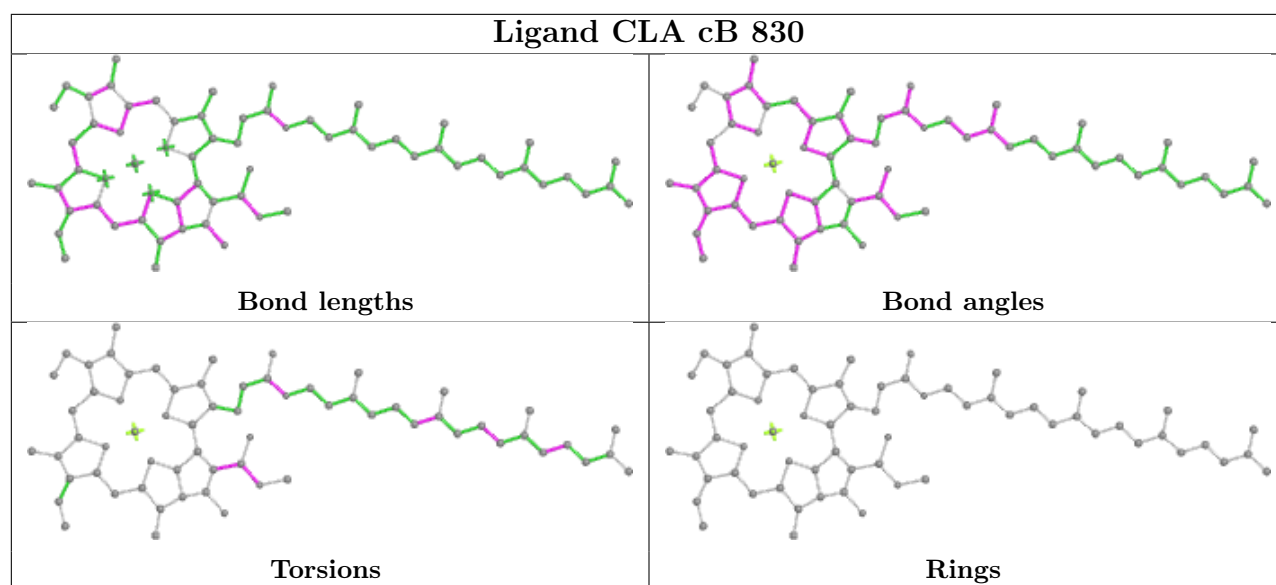
Ligand BCR cA 849

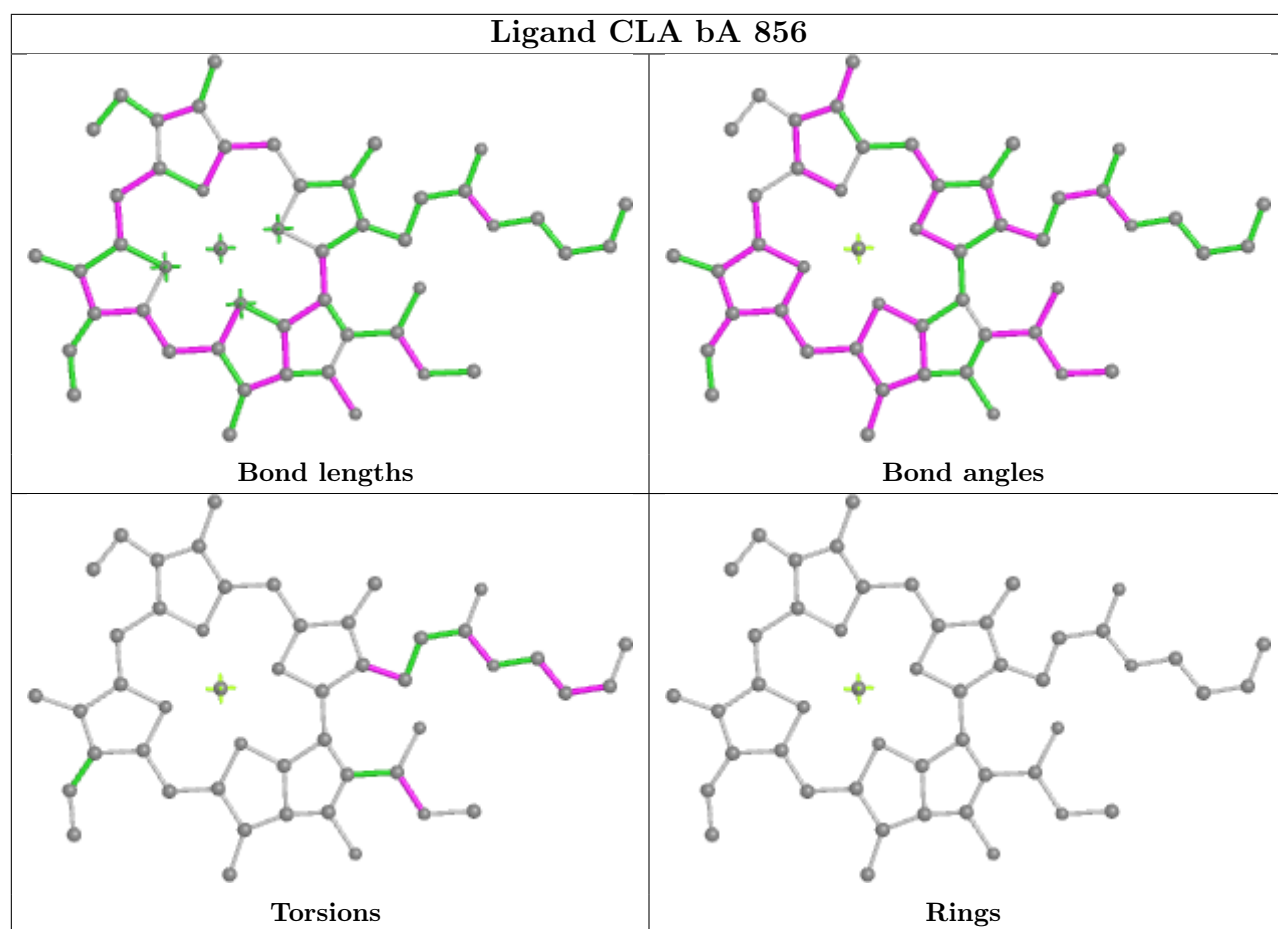


Ligand CLA bB 841

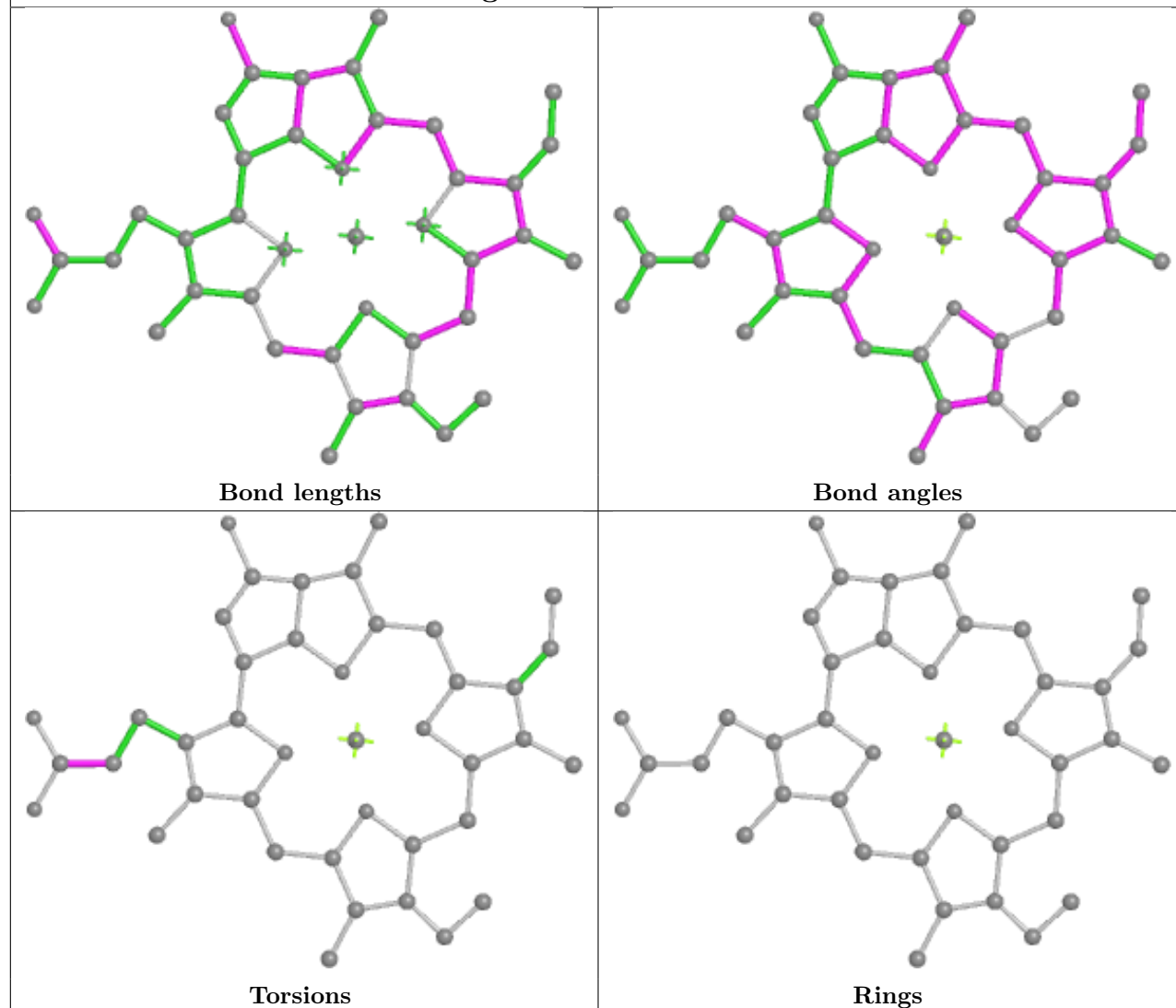




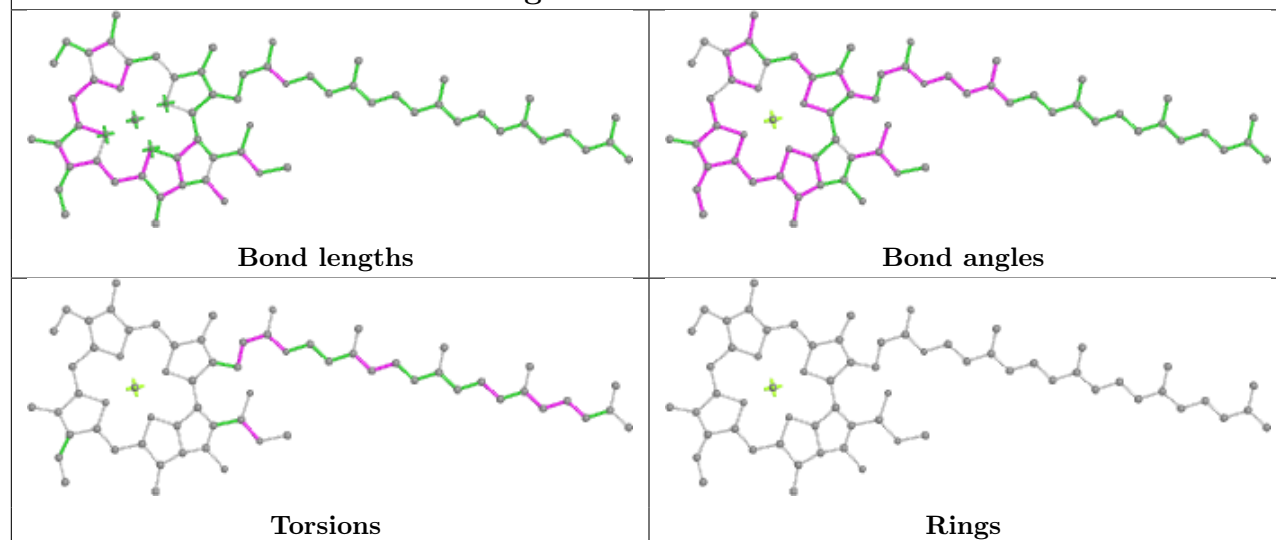


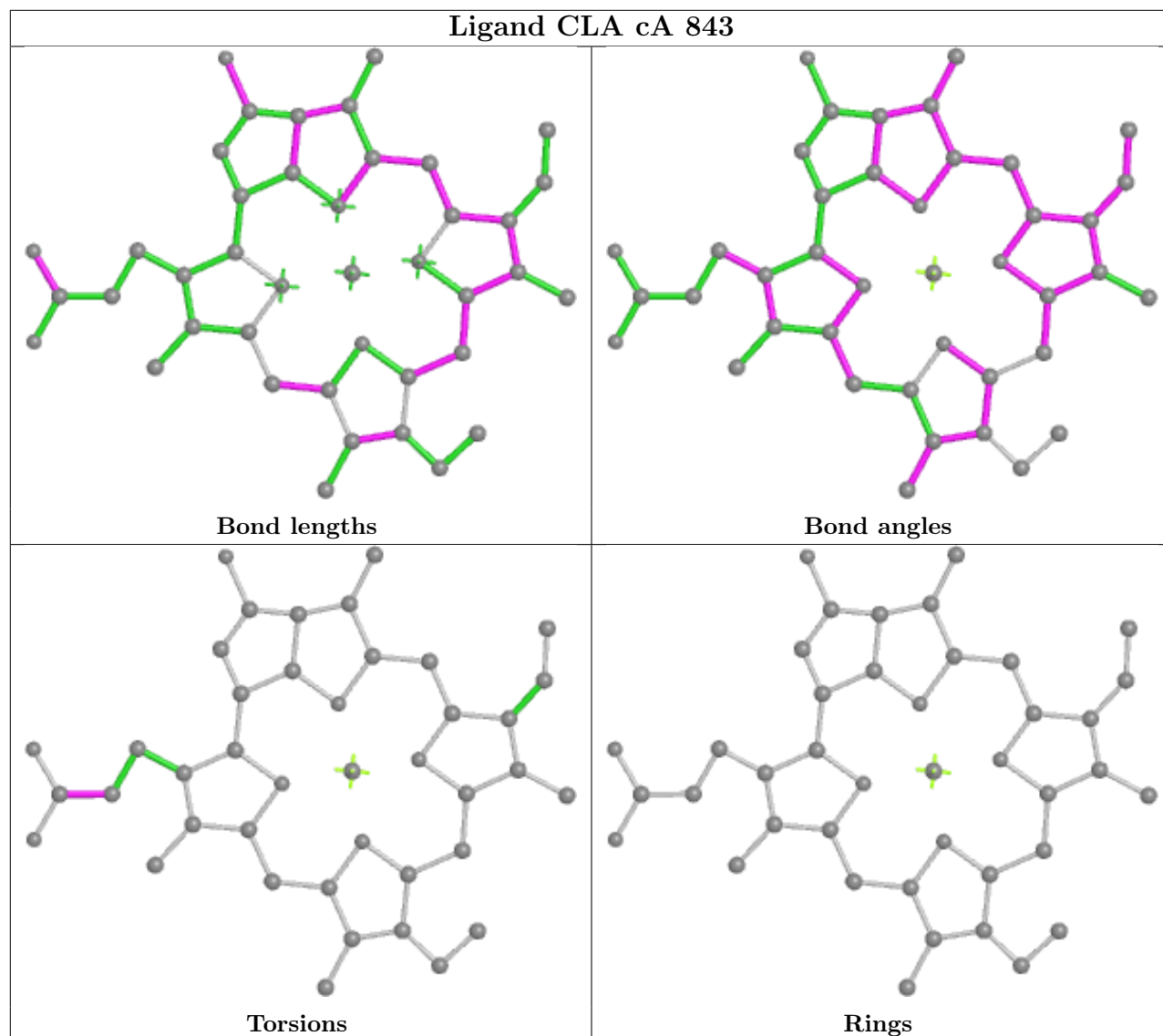


Ligand CLA aA 843

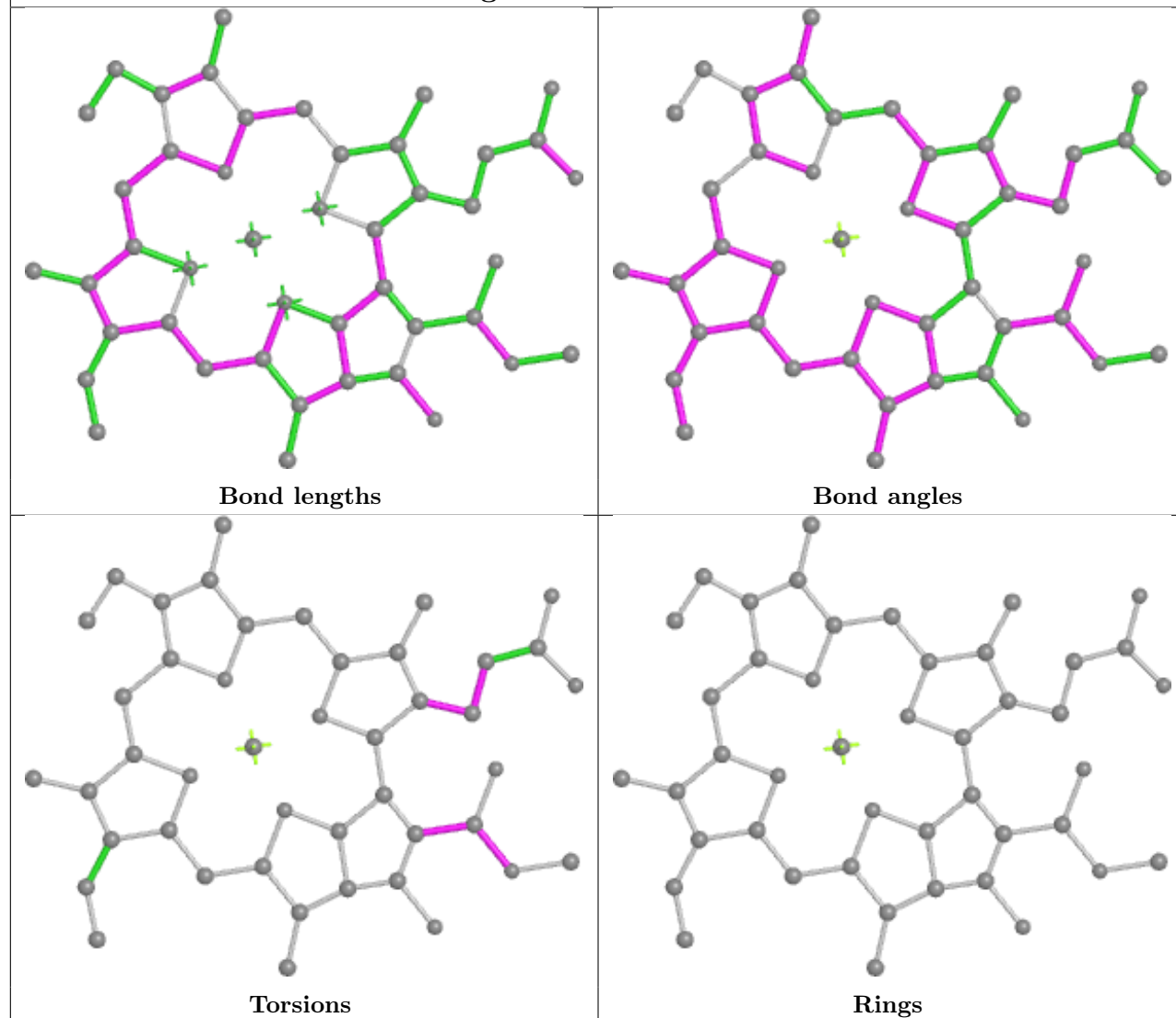


Ligand CLA cB 802

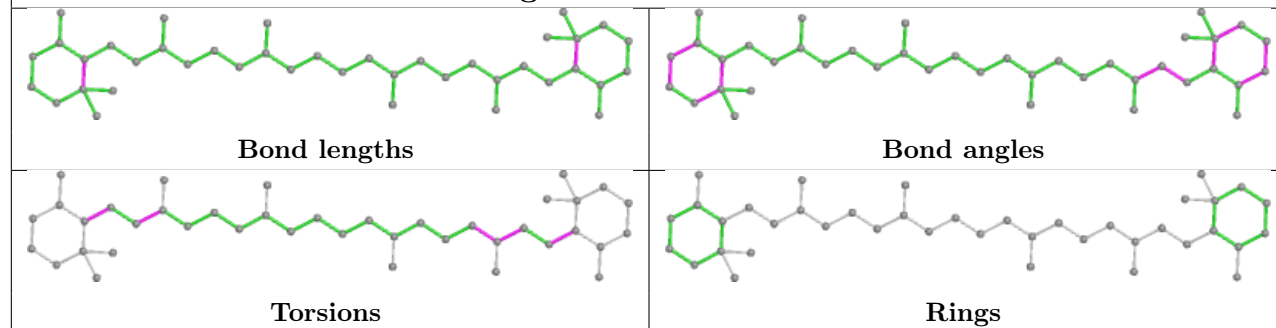


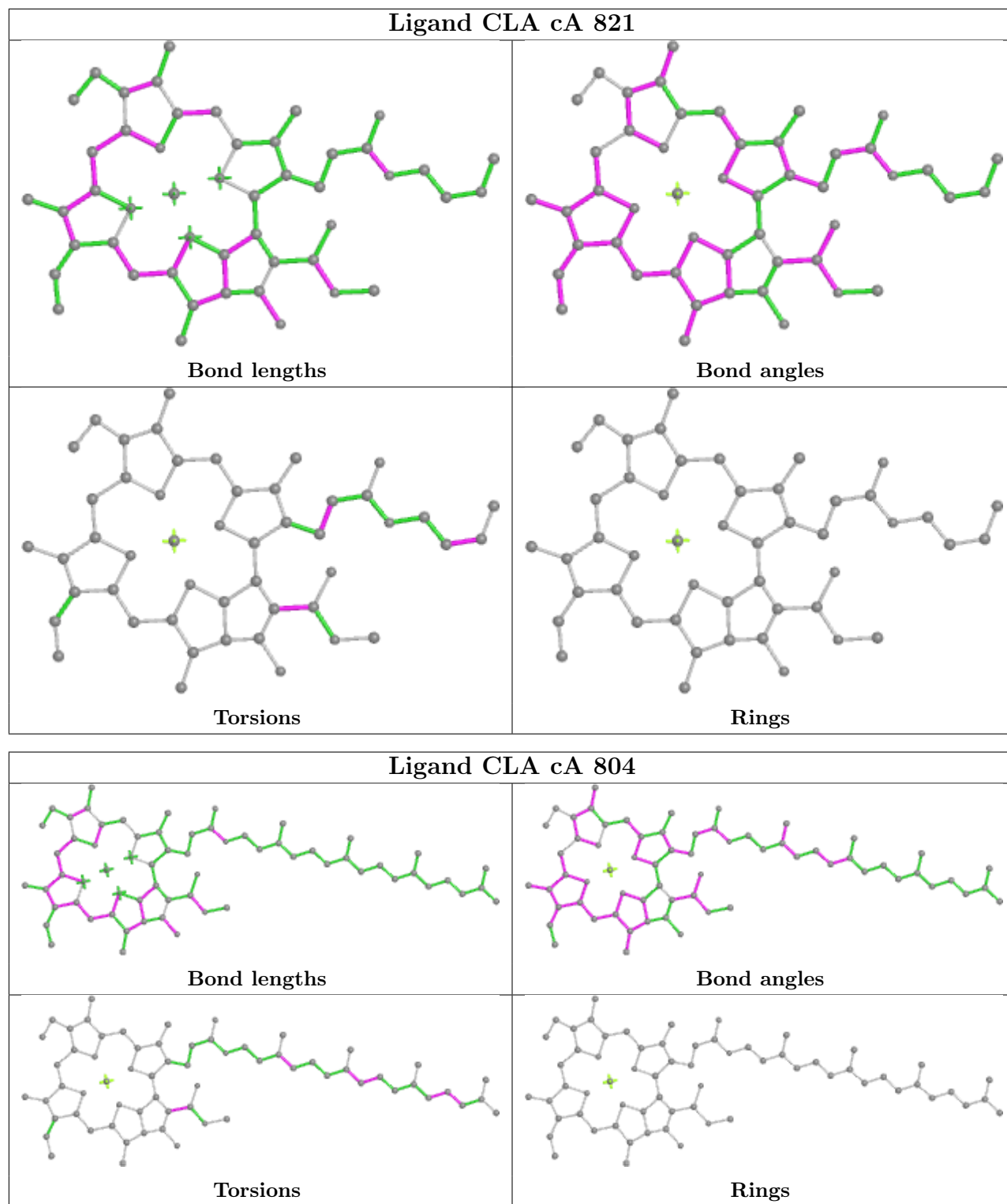


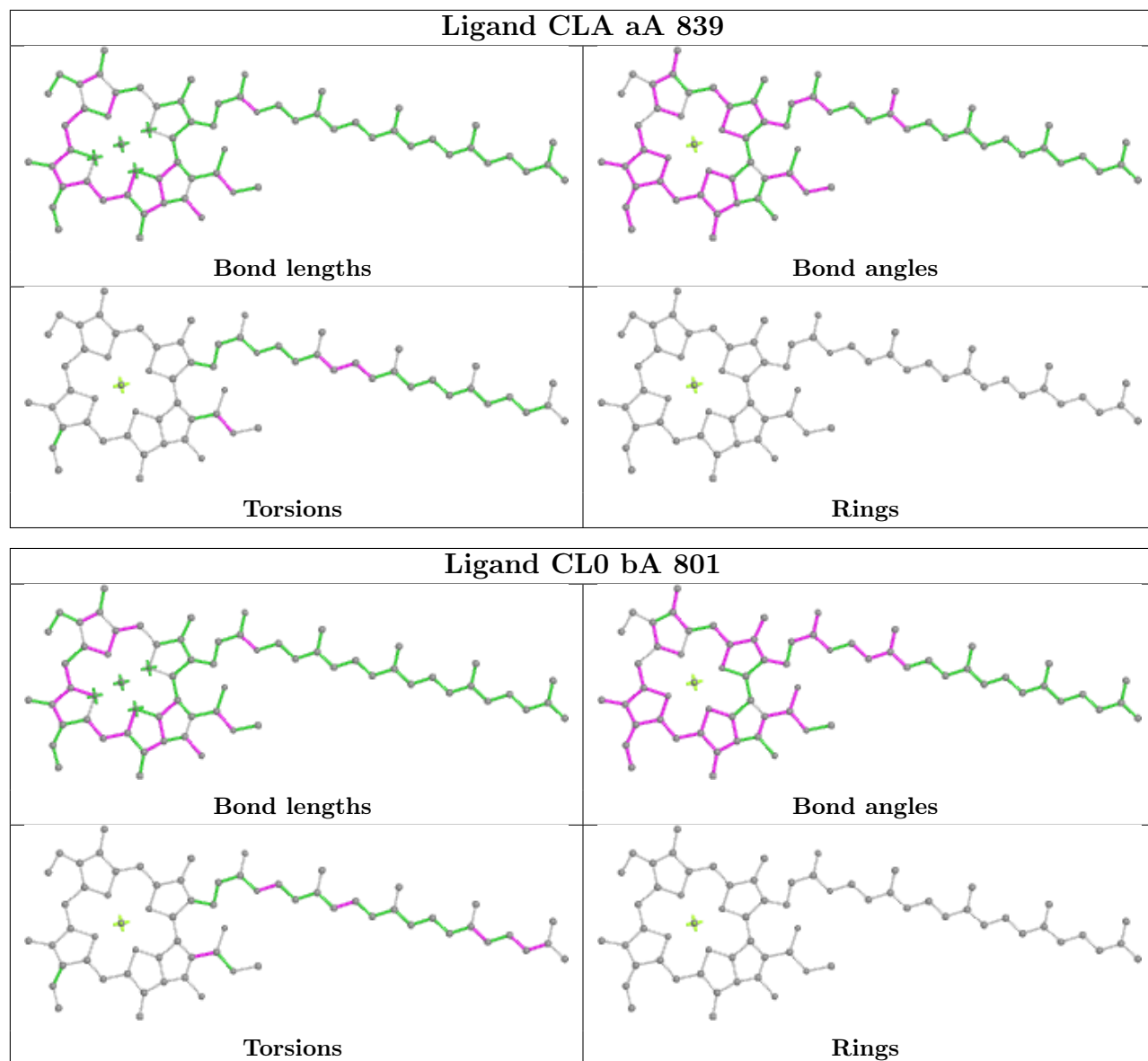
Ligand CLA bA 807



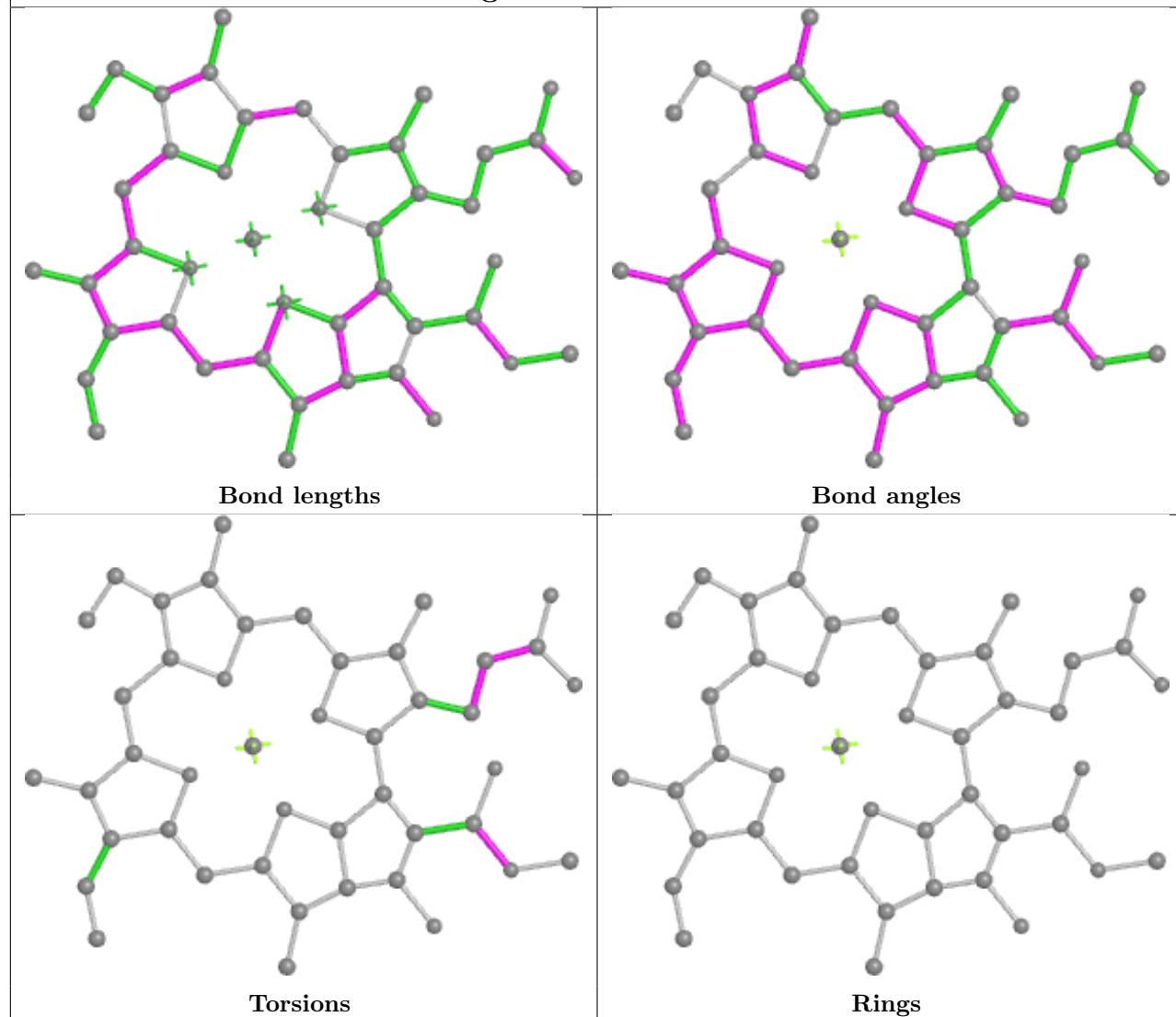
Ligand BCR bA 847



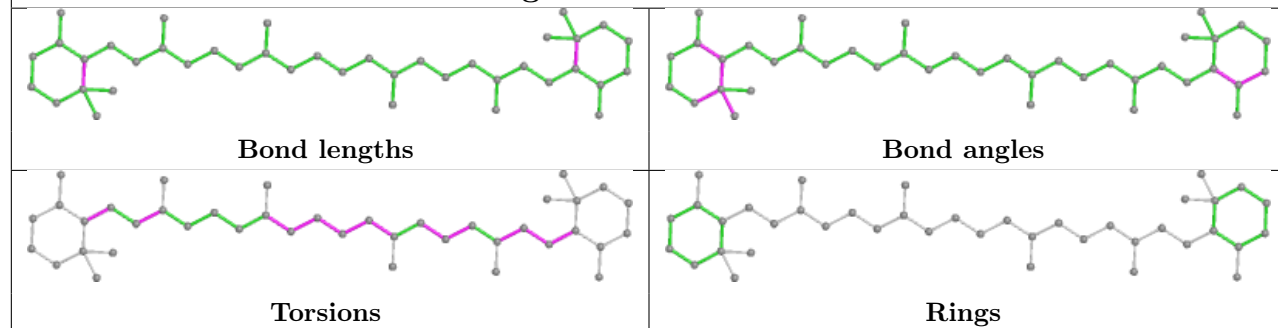


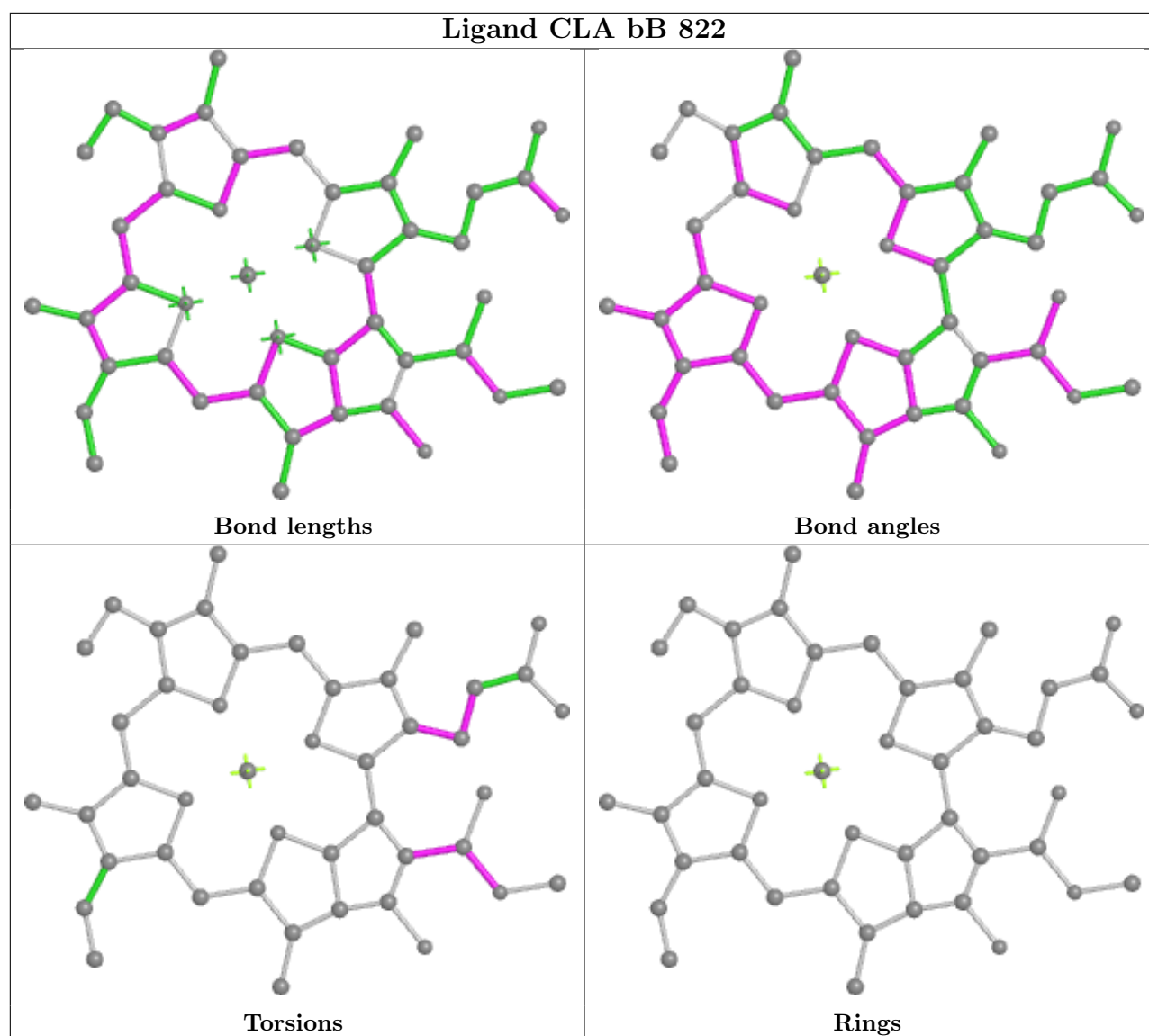


Ligand CLA aB 824

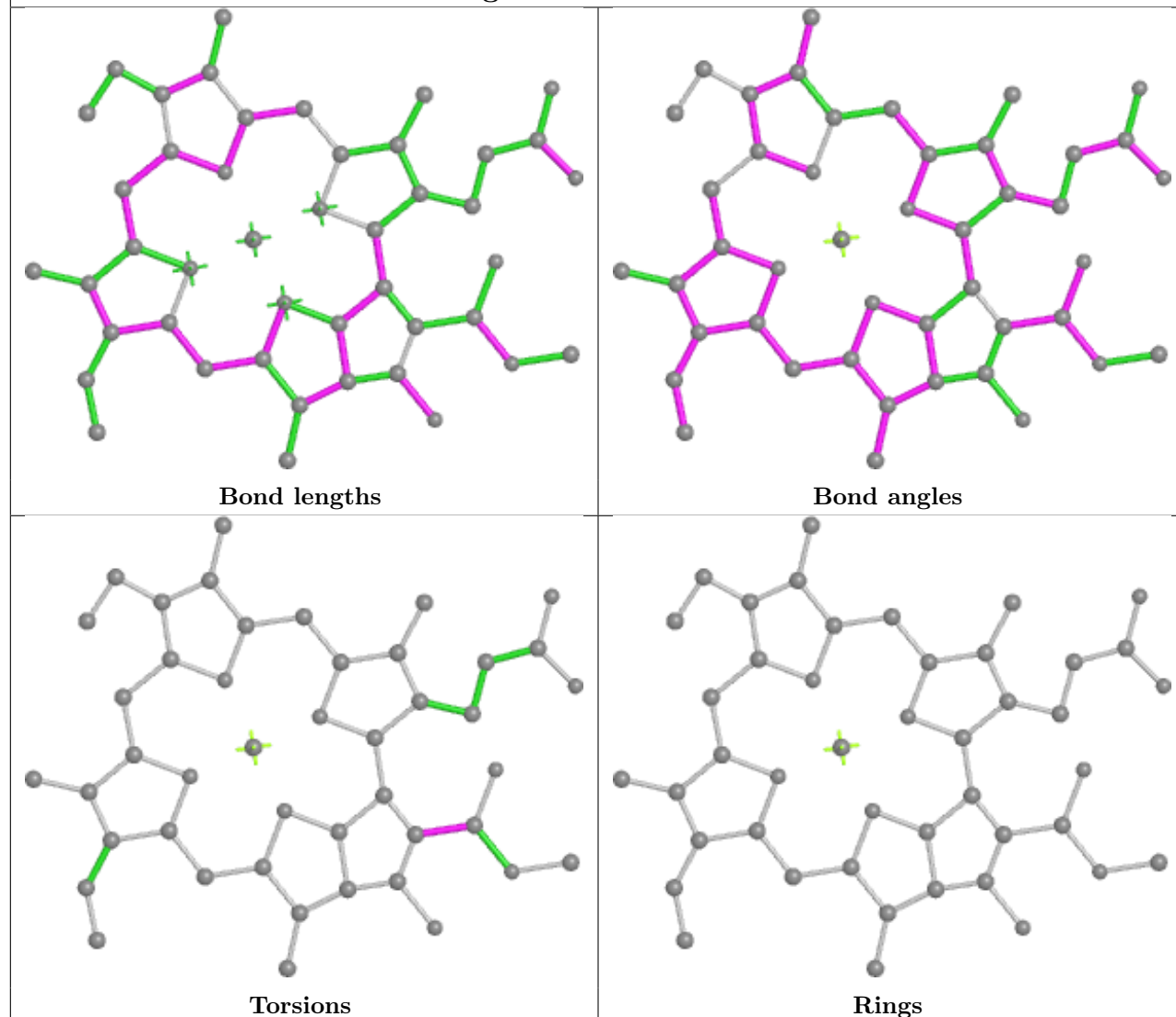


Ligand BCR aB 849

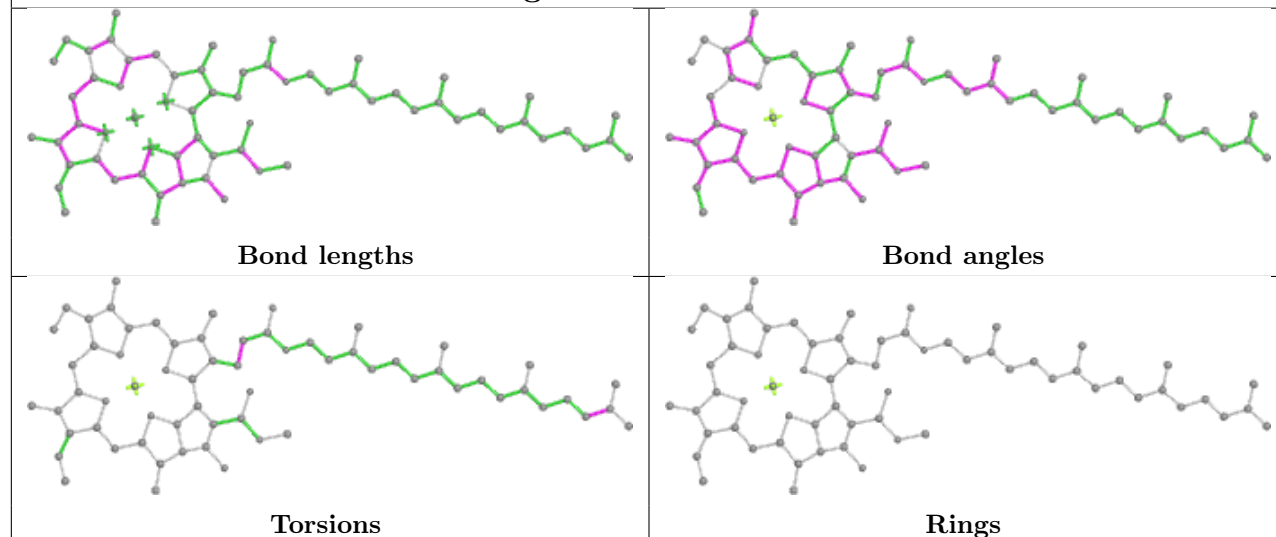


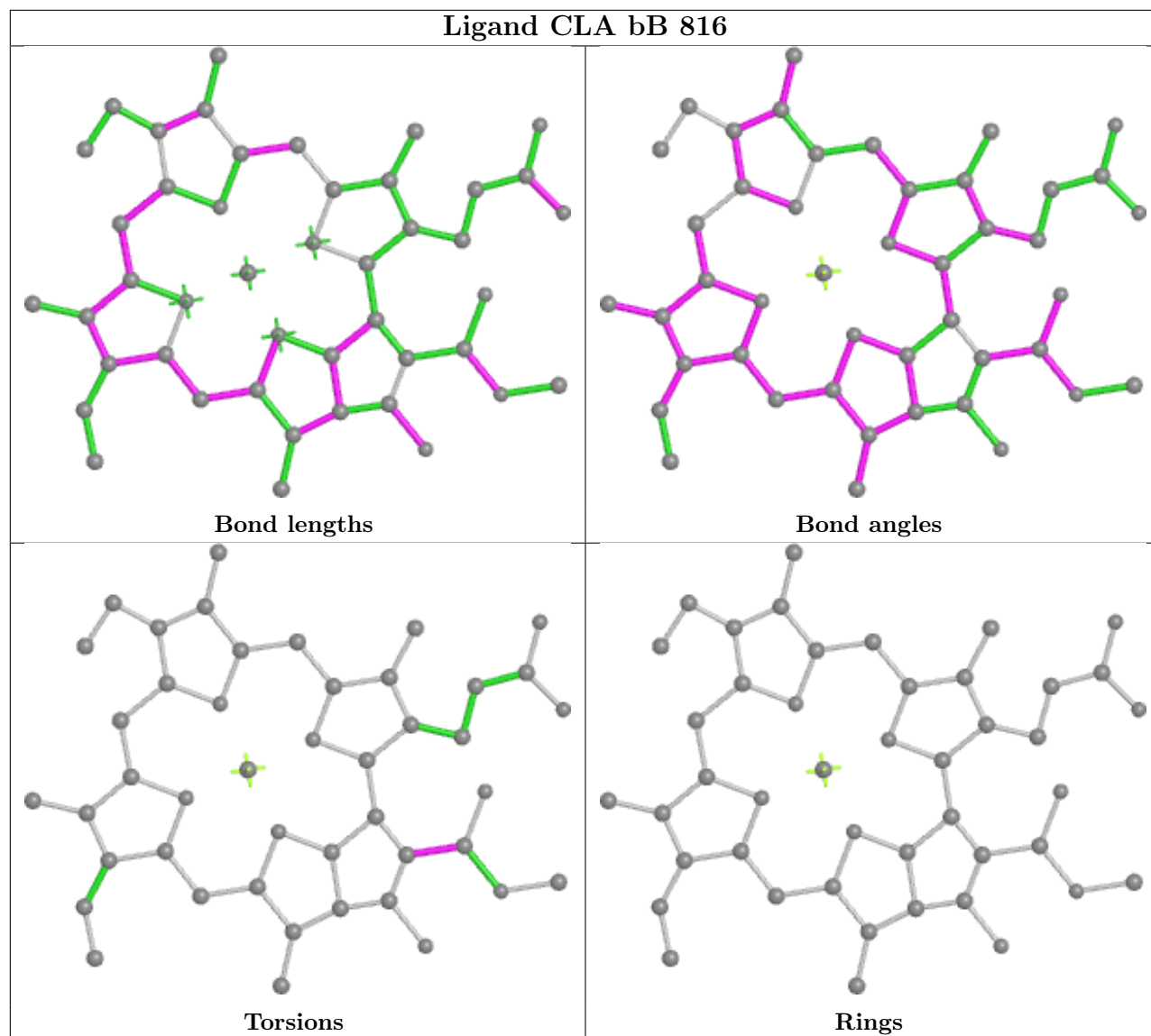
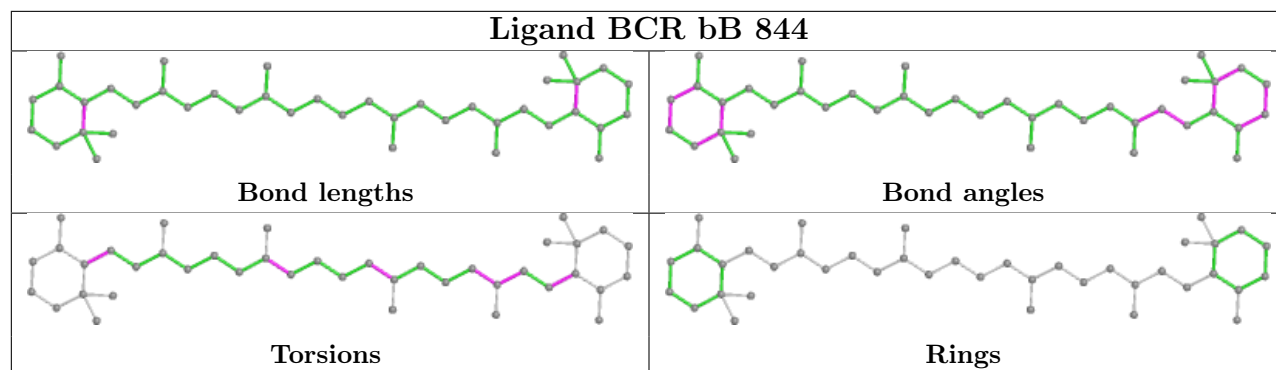


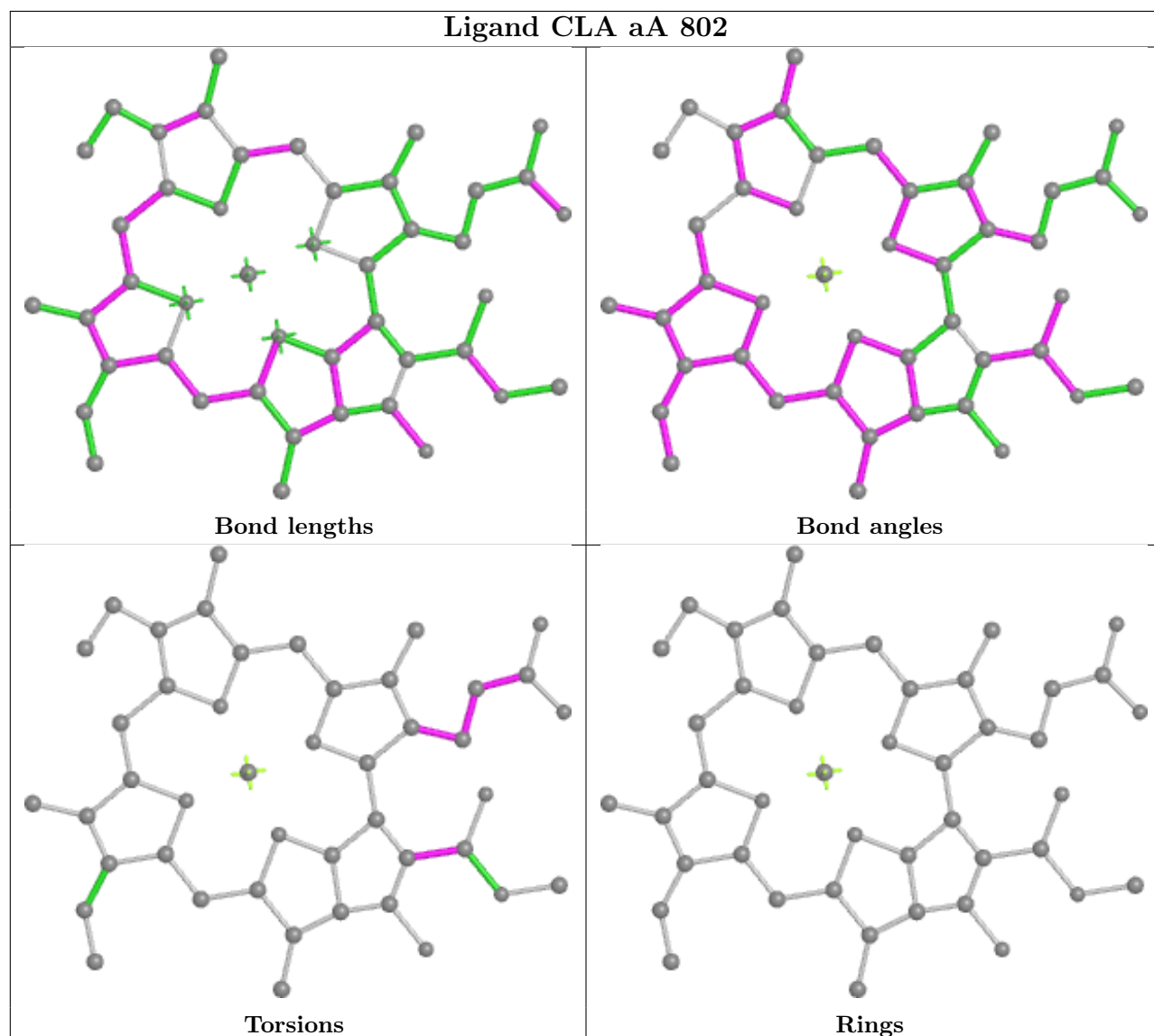
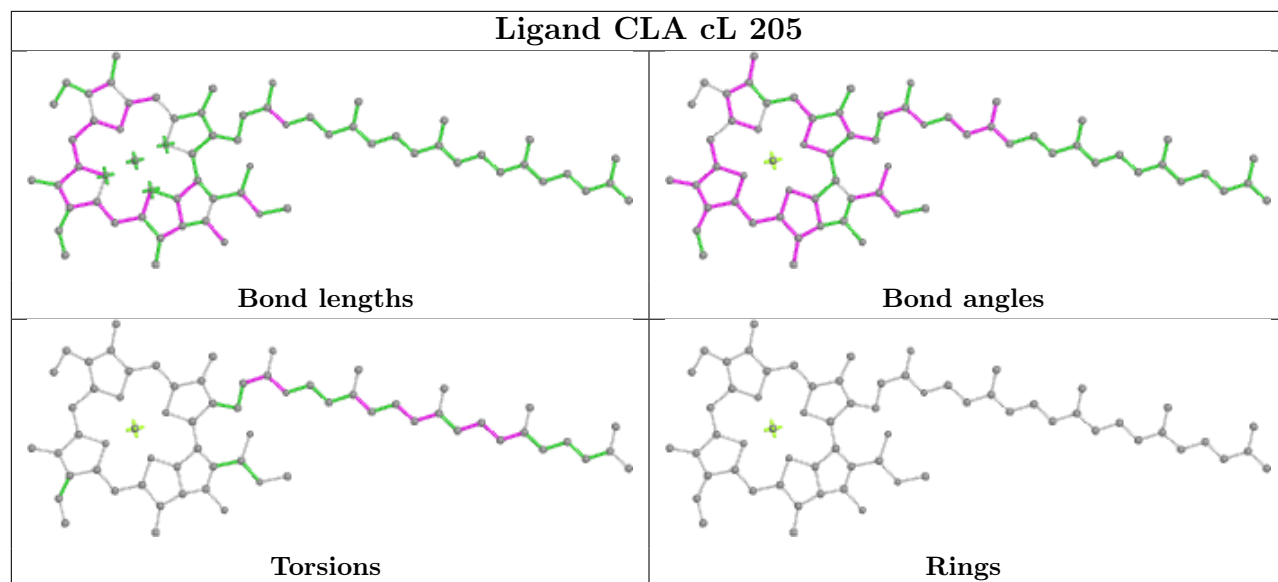
Ligand CLA cA 813

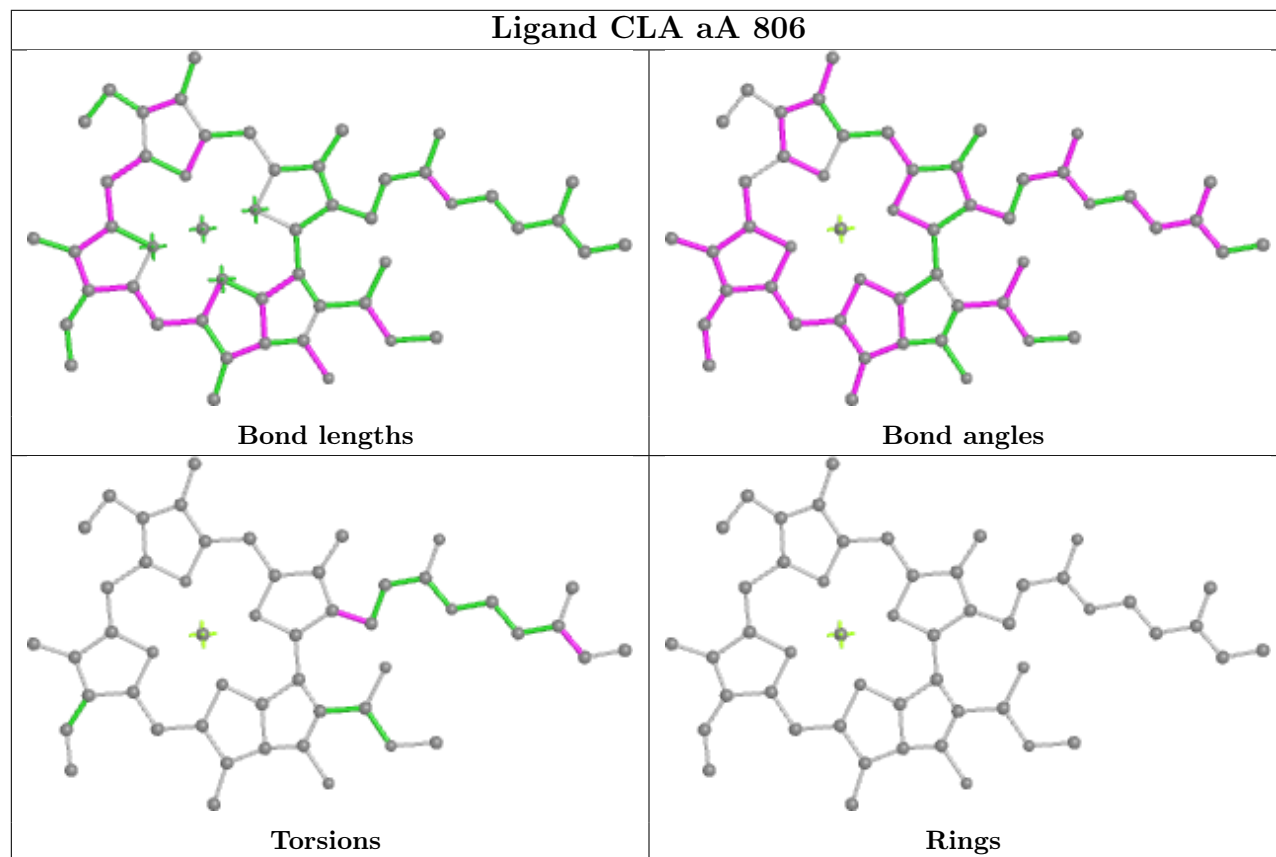
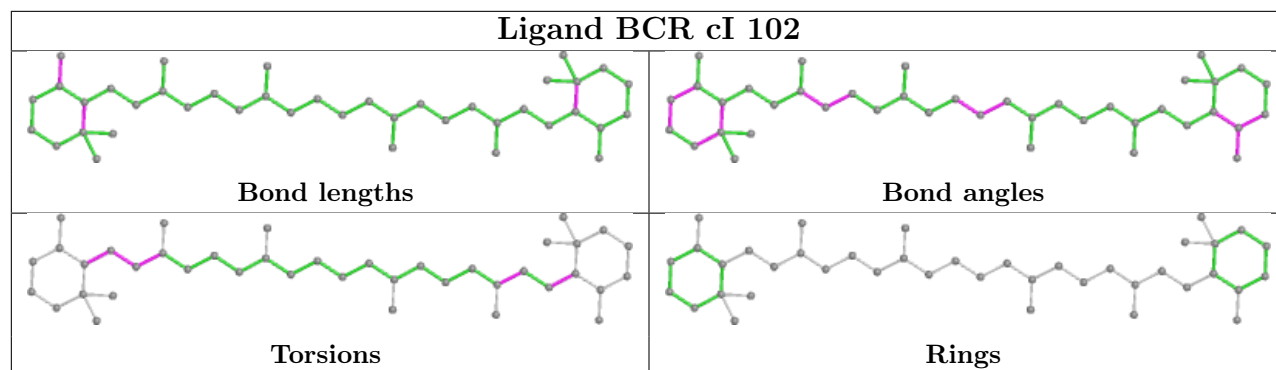
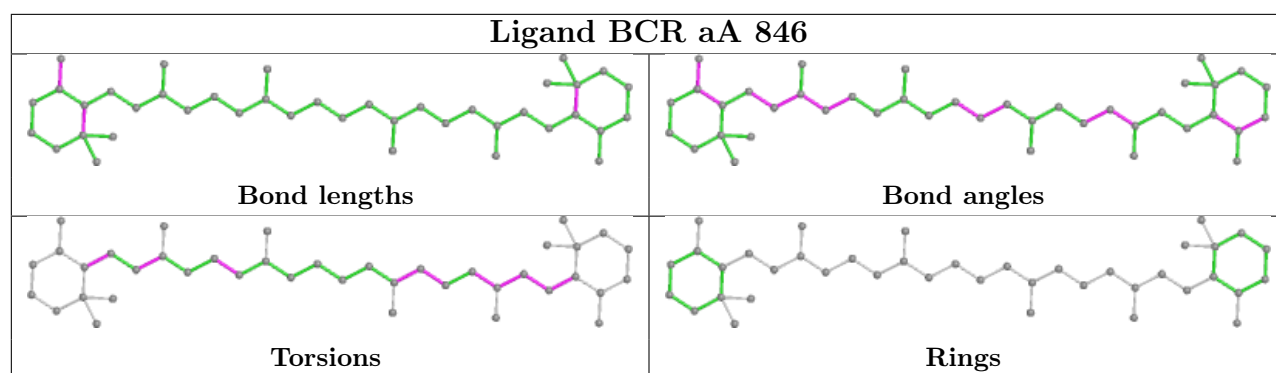


Ligand CLA aB 840

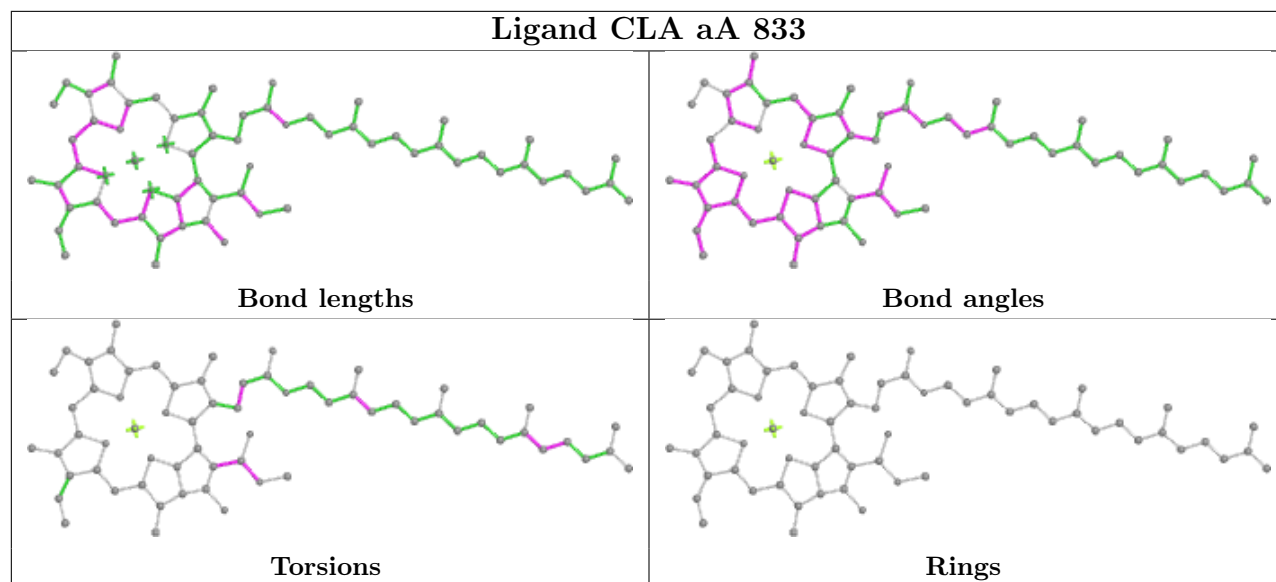




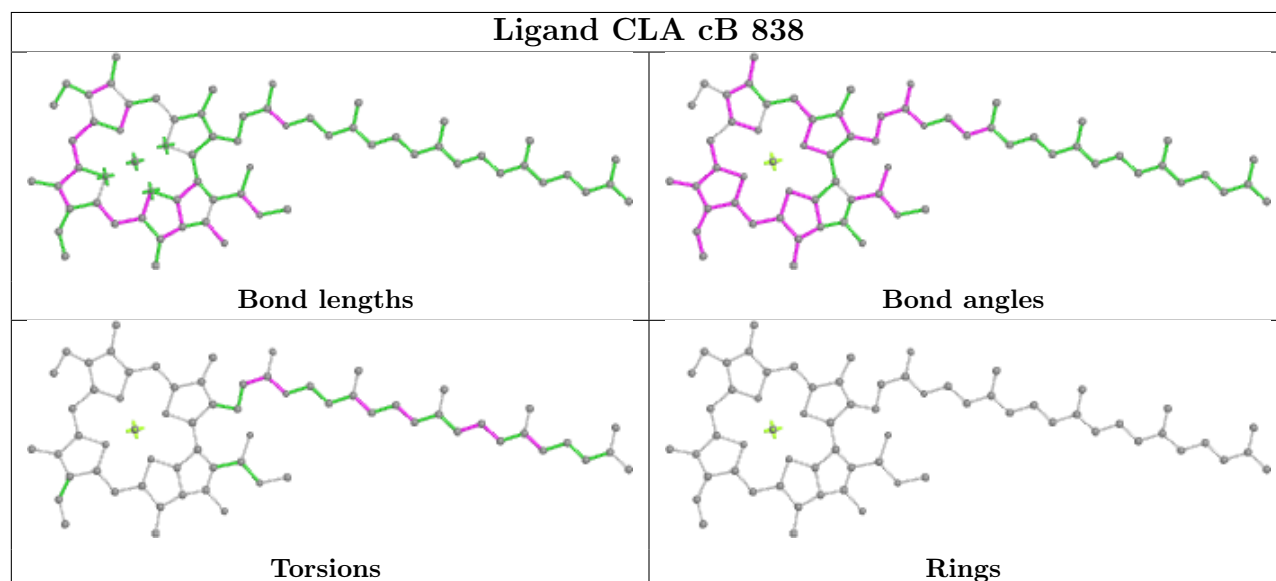




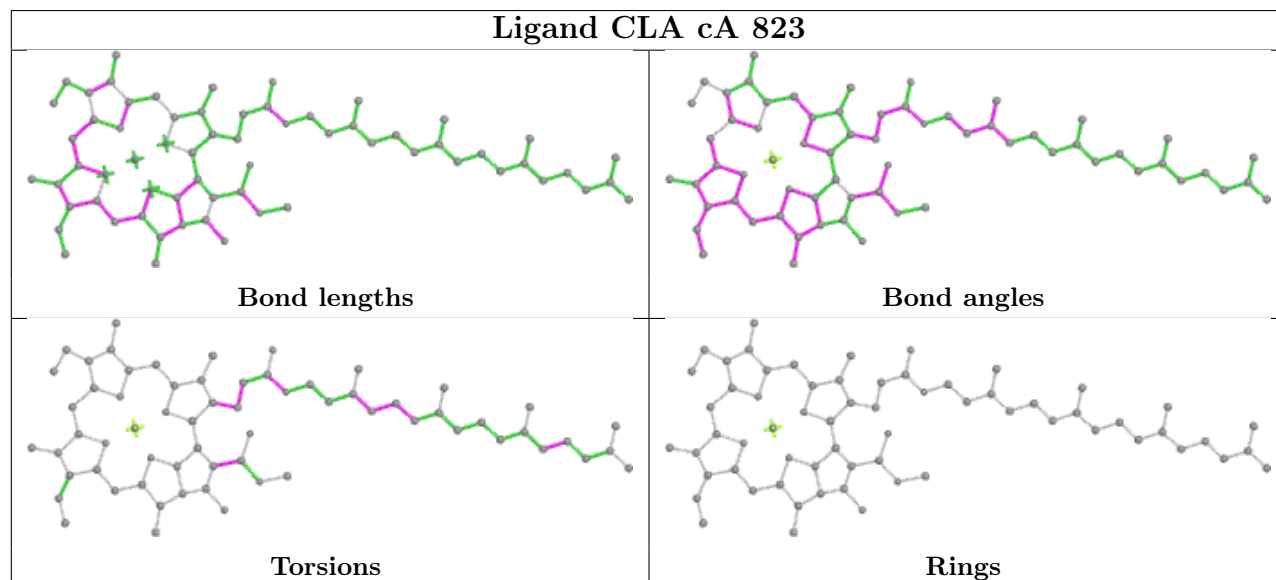
Ligand CLA aA 833

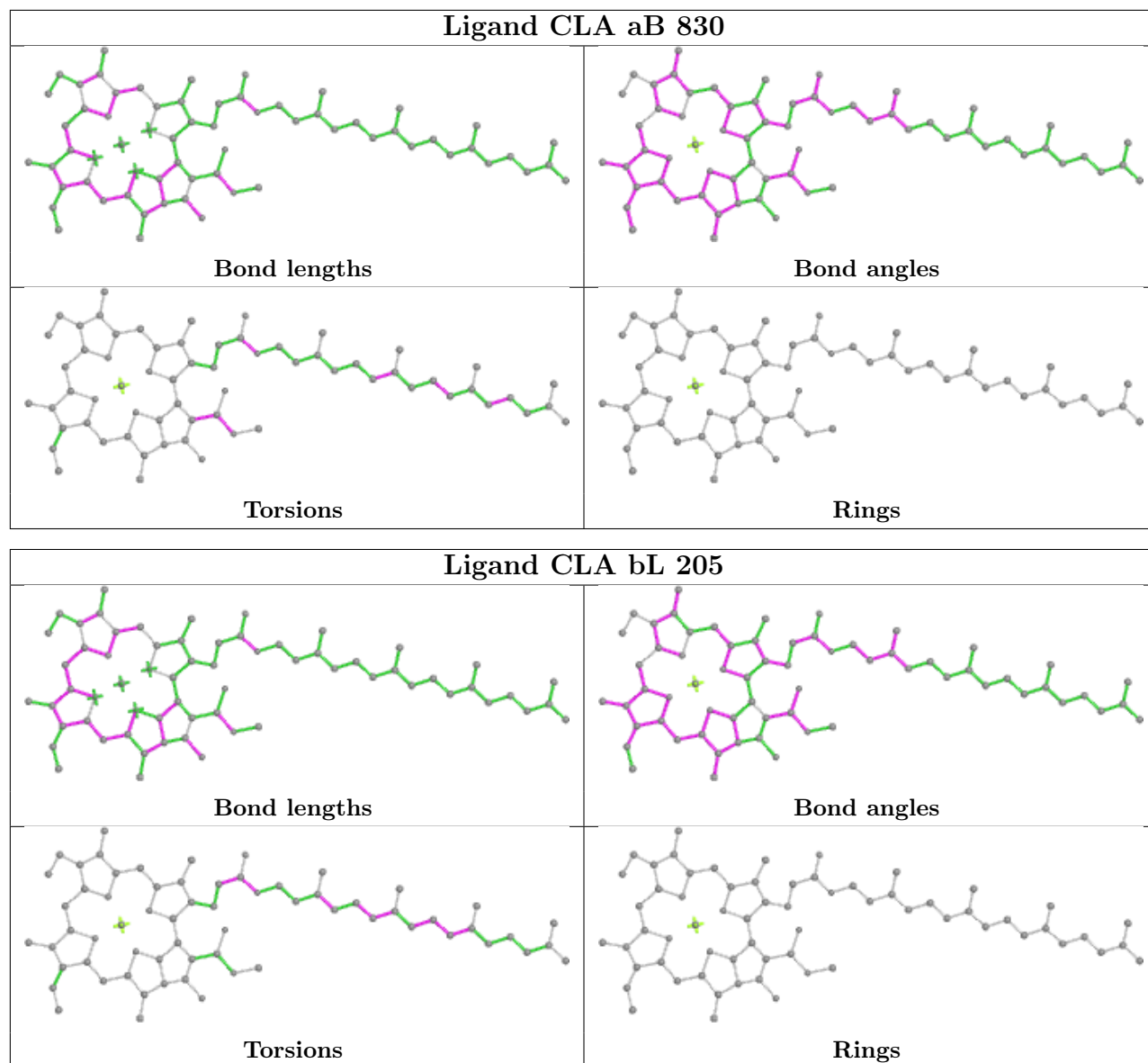


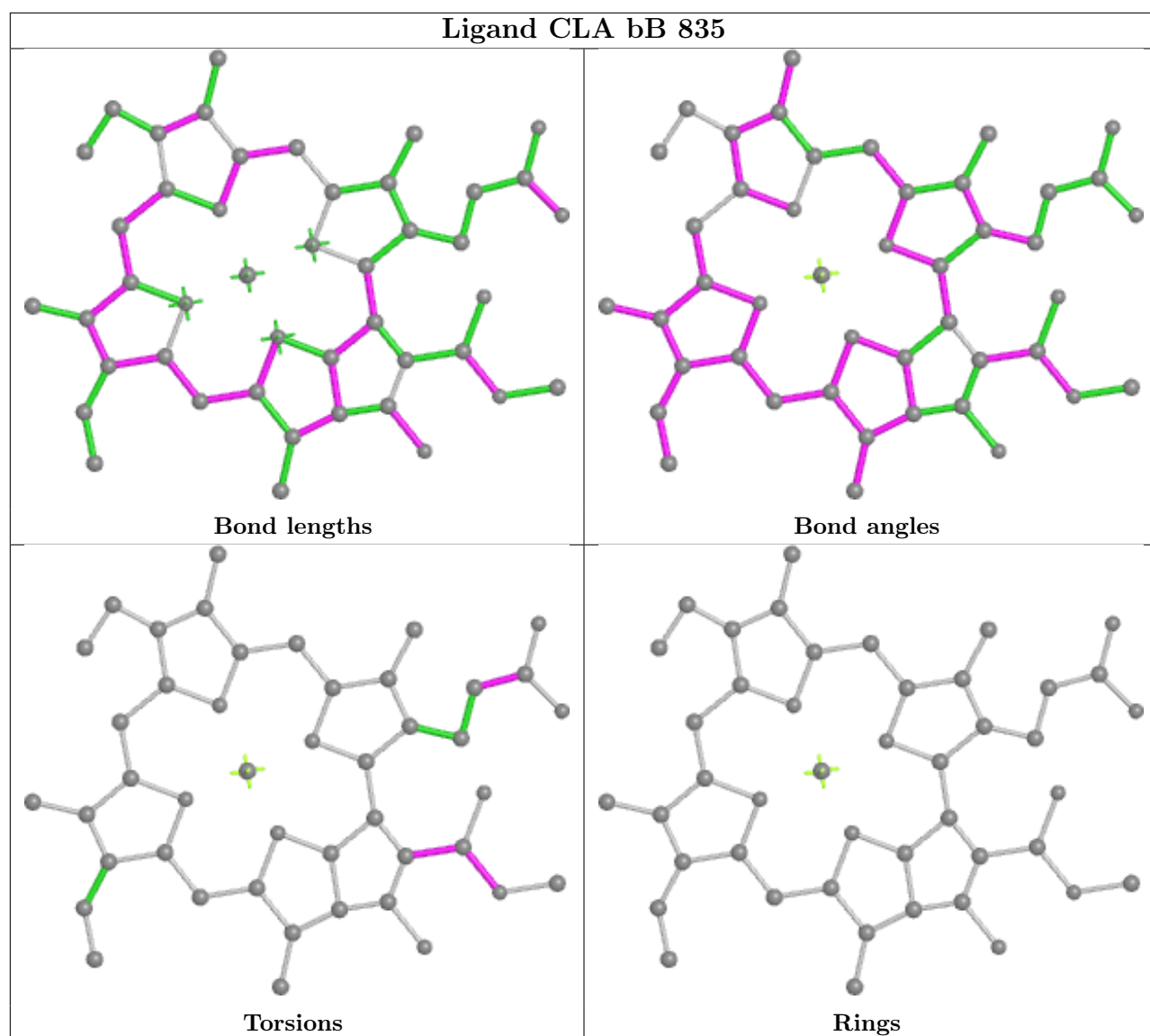
Ligand CLA cB 838

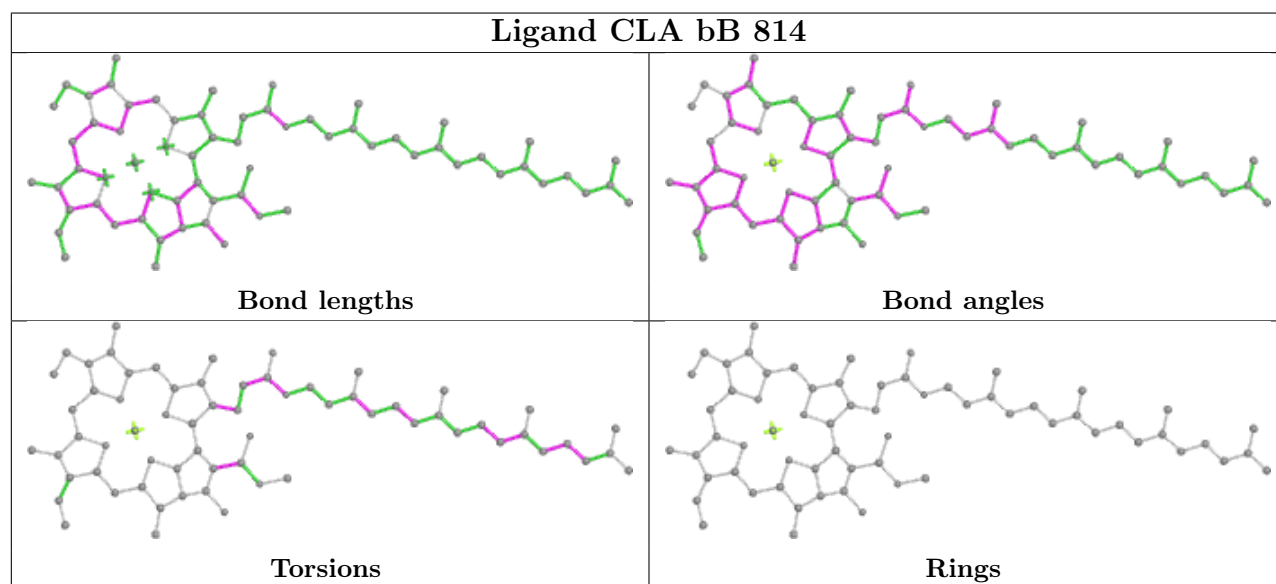
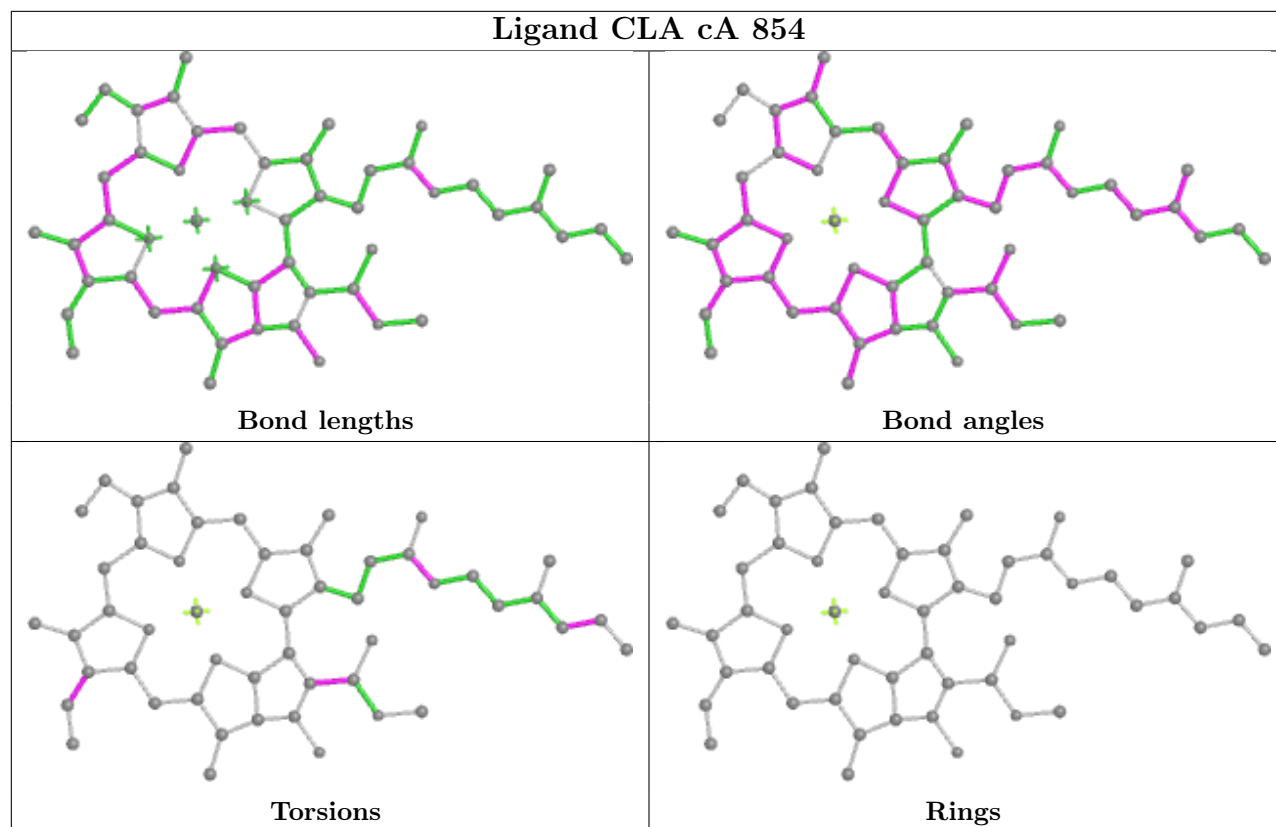


Ligand CLA cA 823

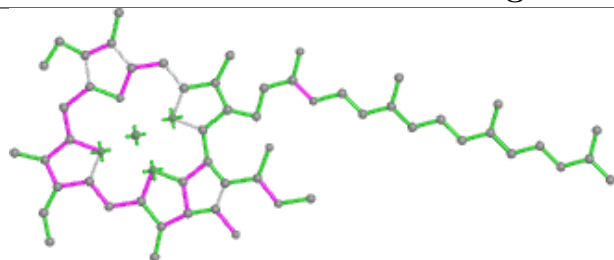




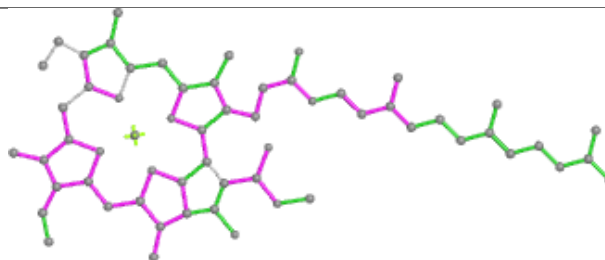




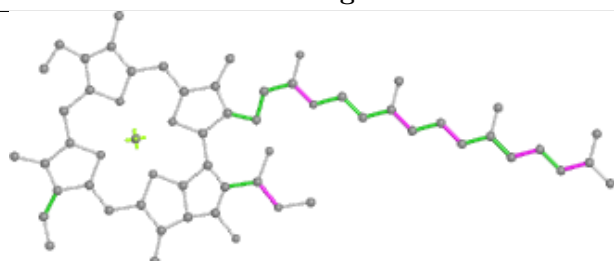
Ligand CLA cB 837



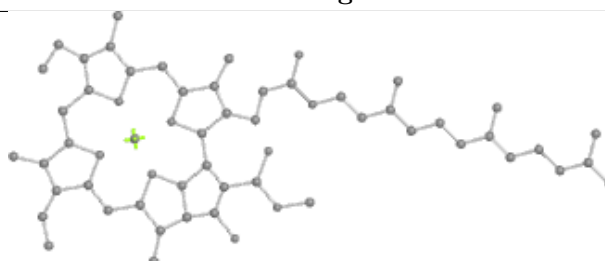
Bond lengths



Bond angles

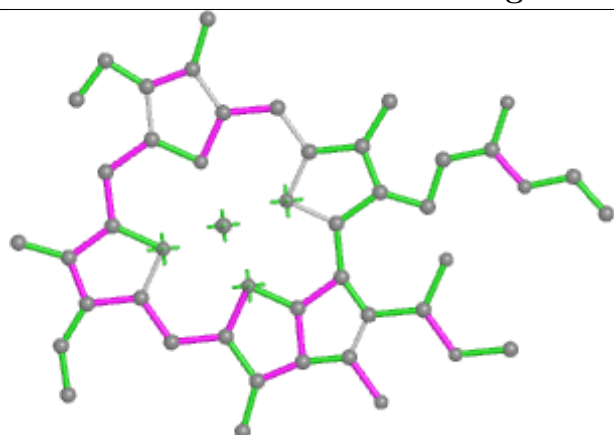


Torsions

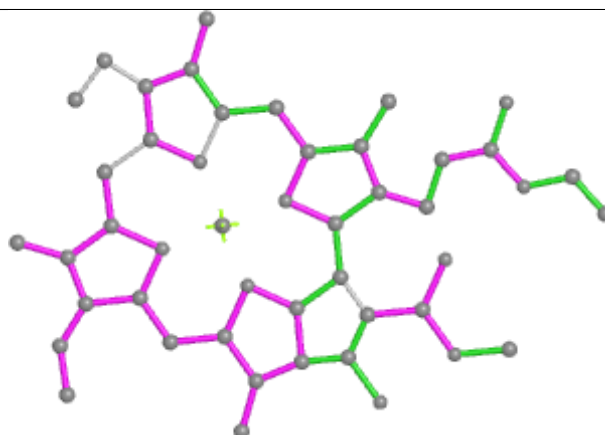


Rings

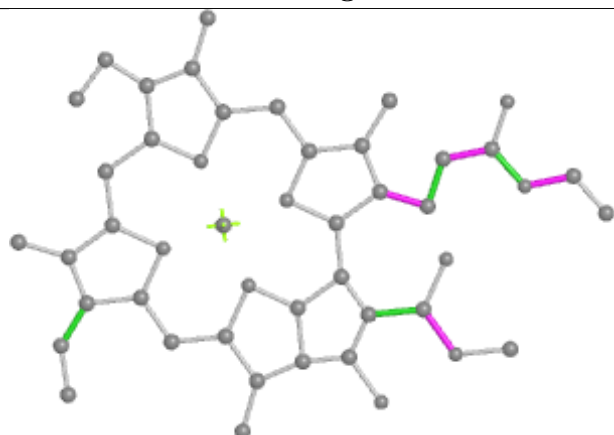
Ligand CLA aB 839



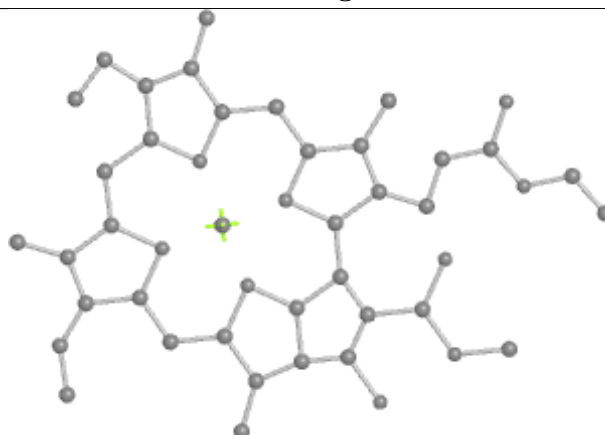
Bond lengths



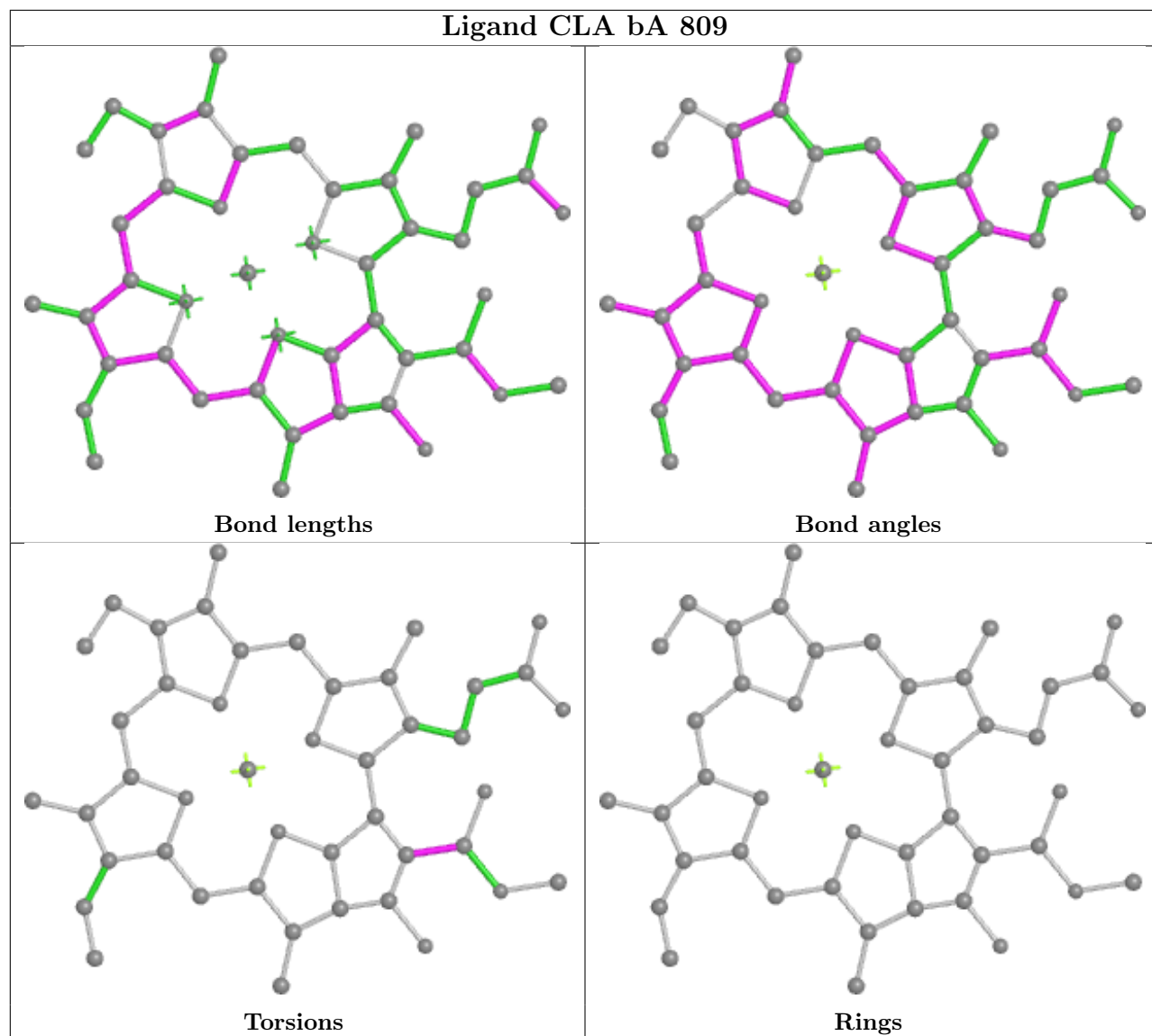
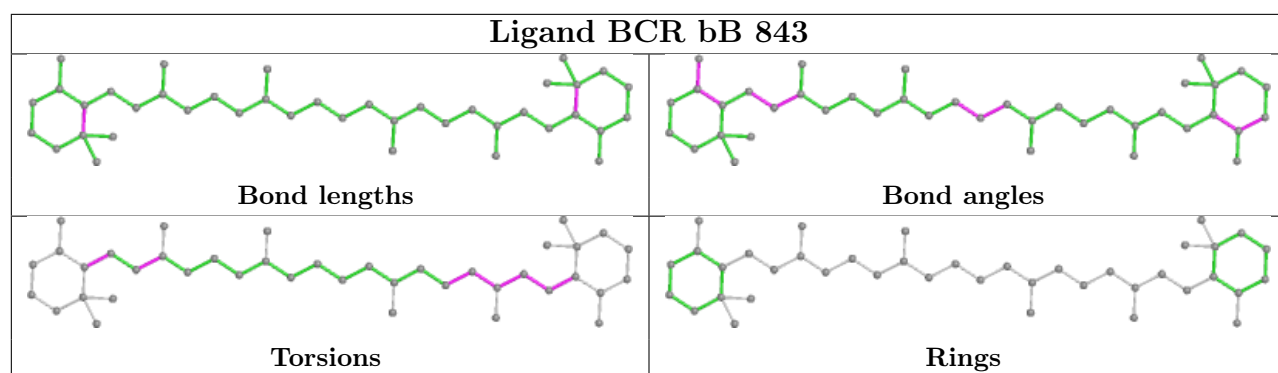
Bond angles

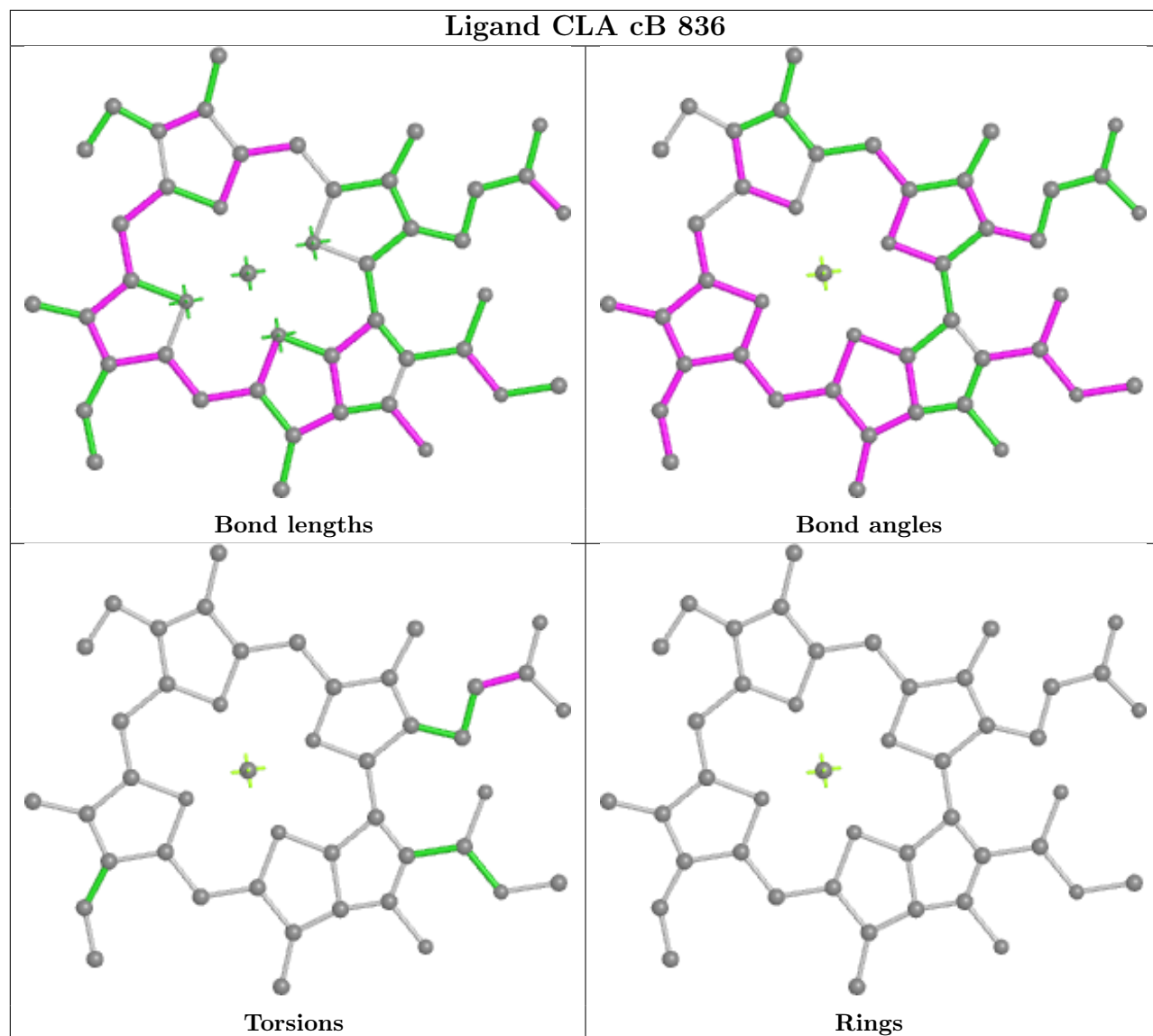


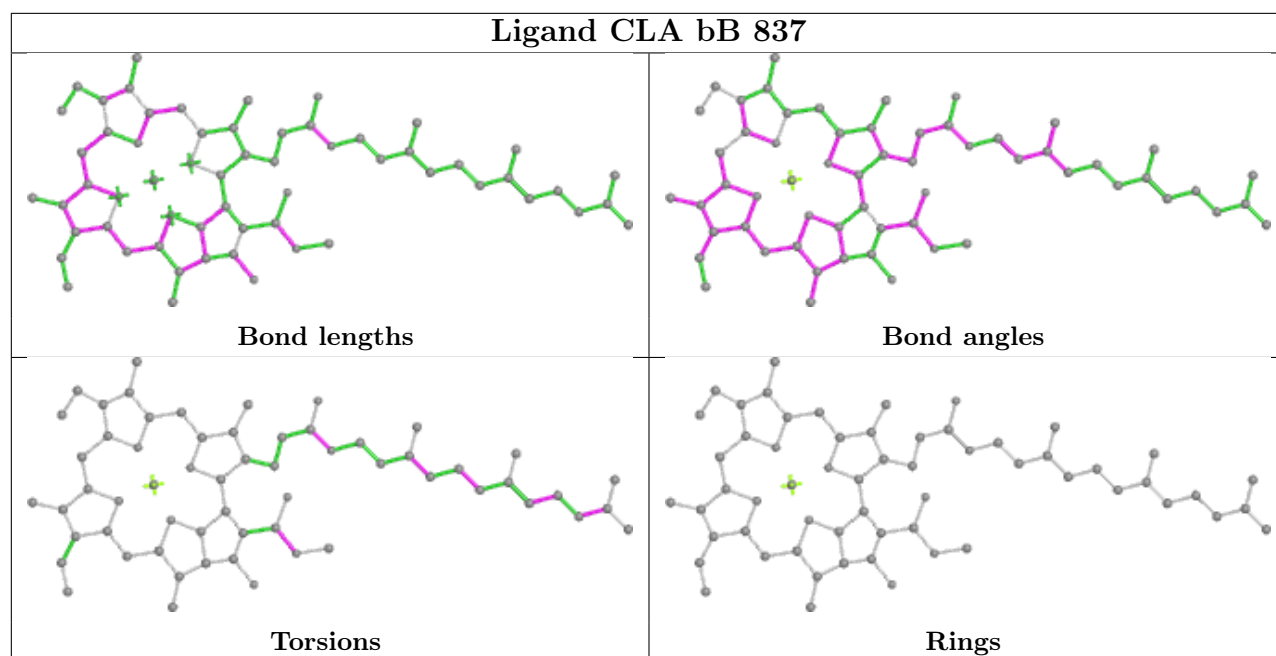
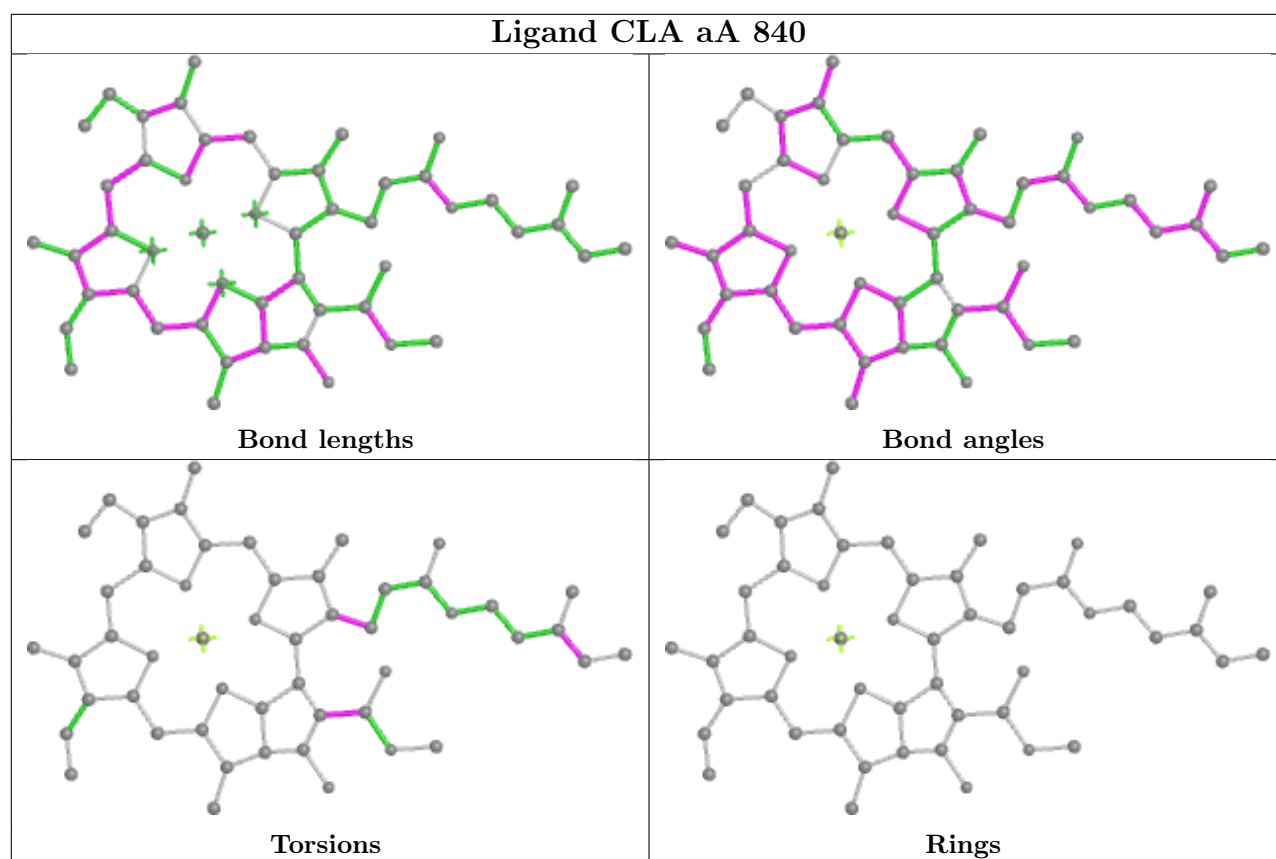
Torsions

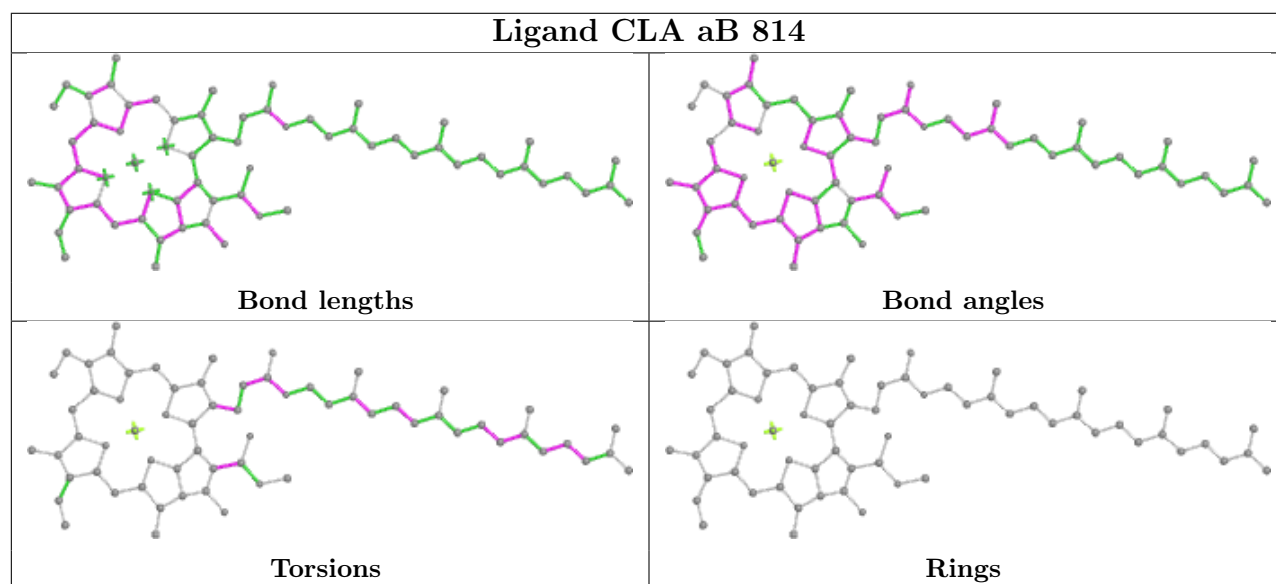
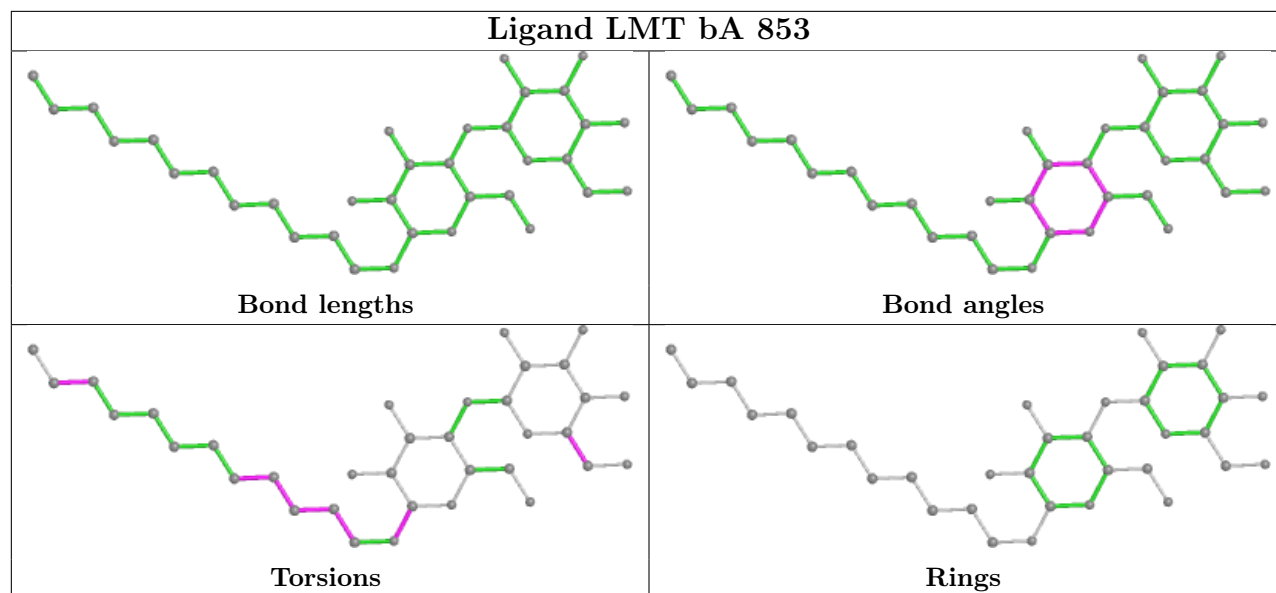


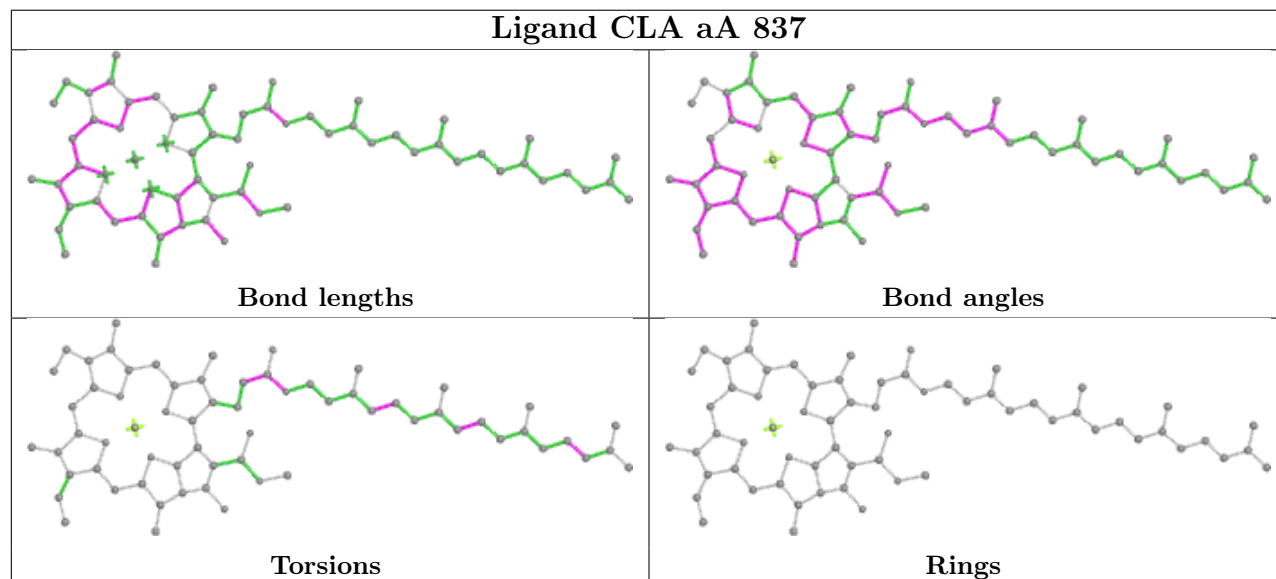
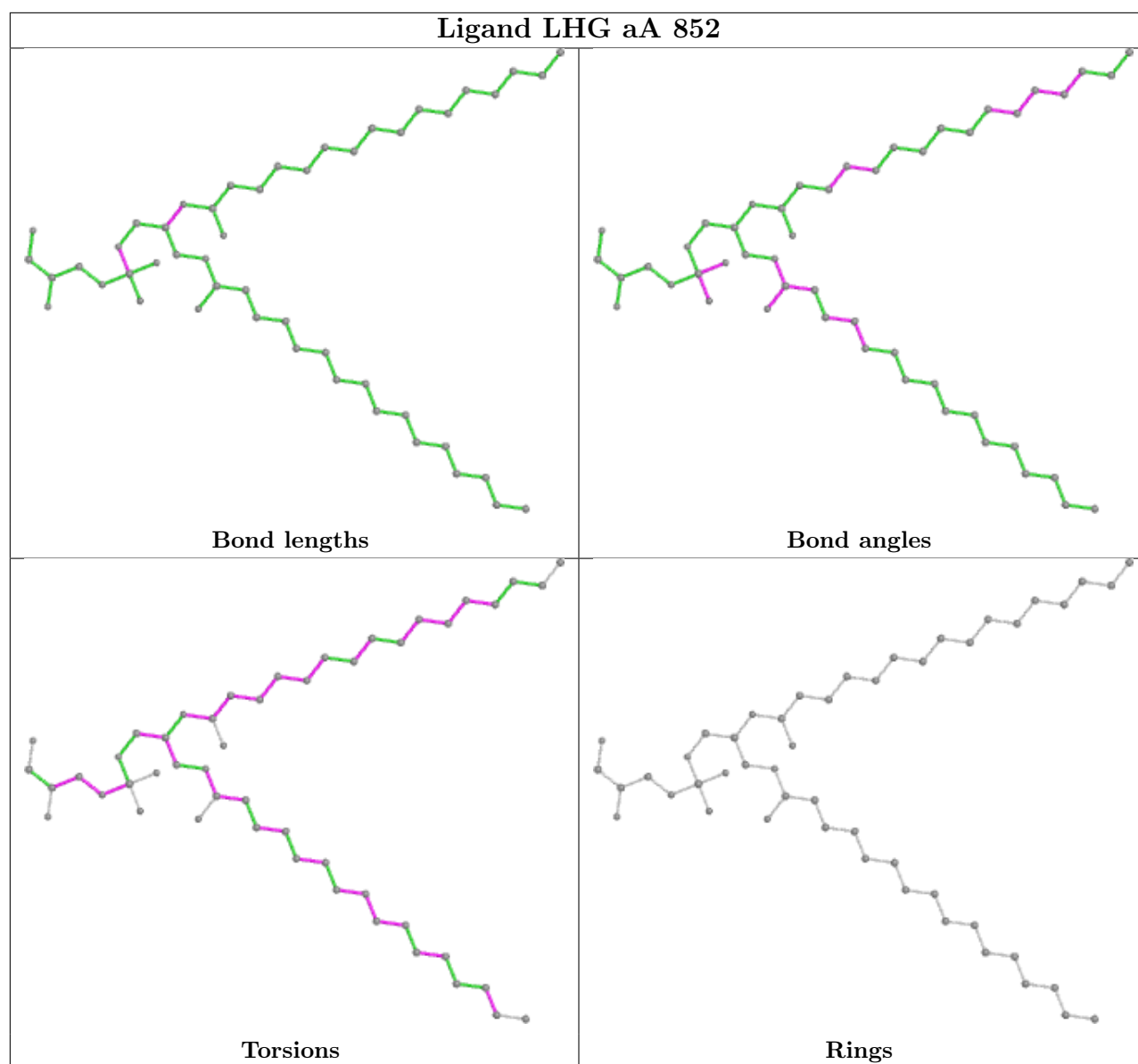
Rings



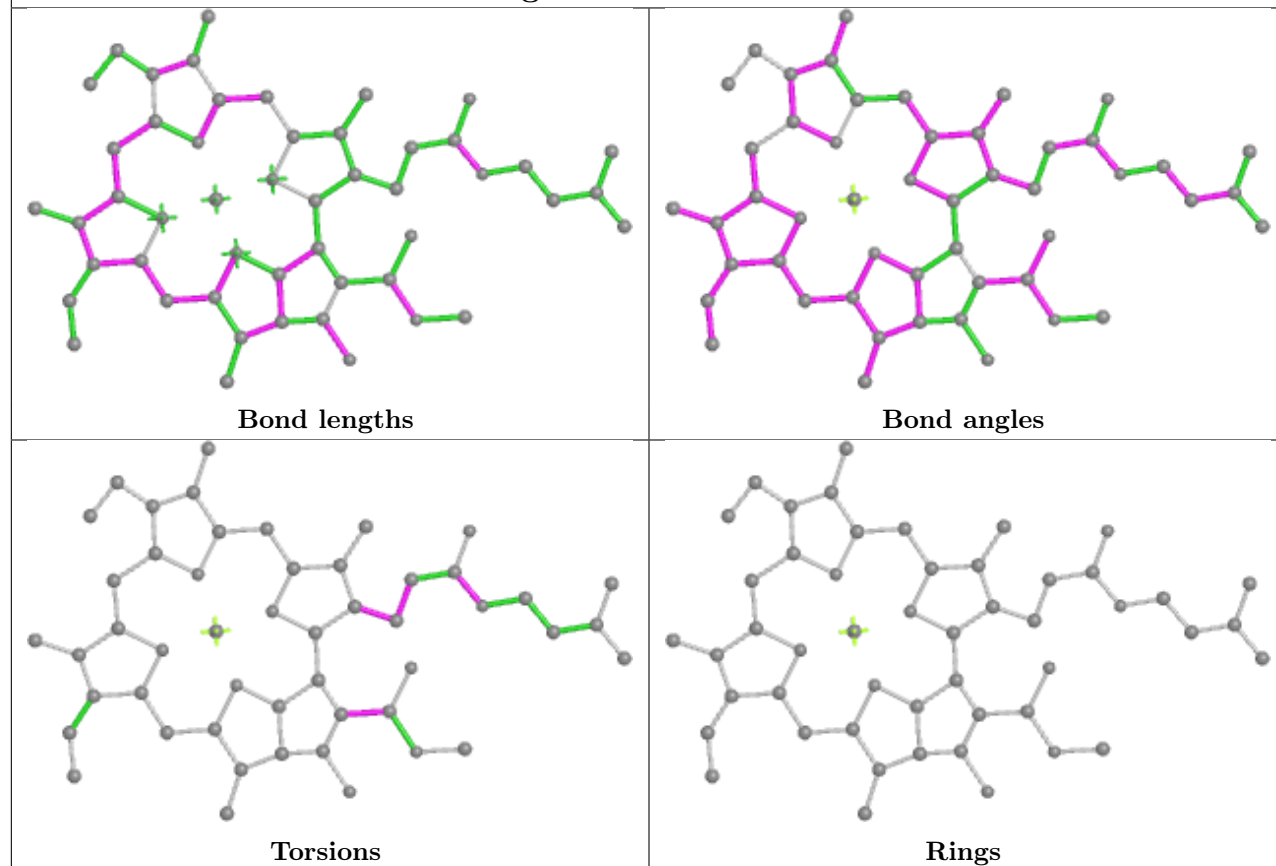




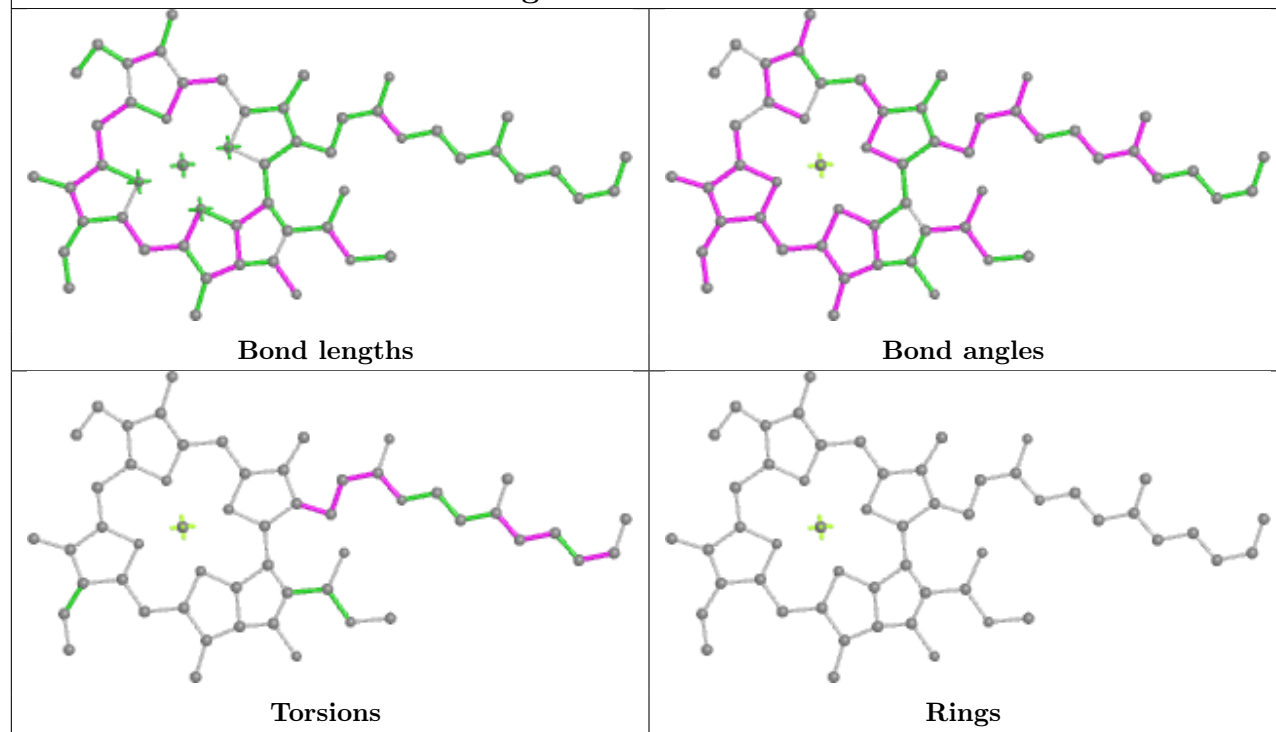




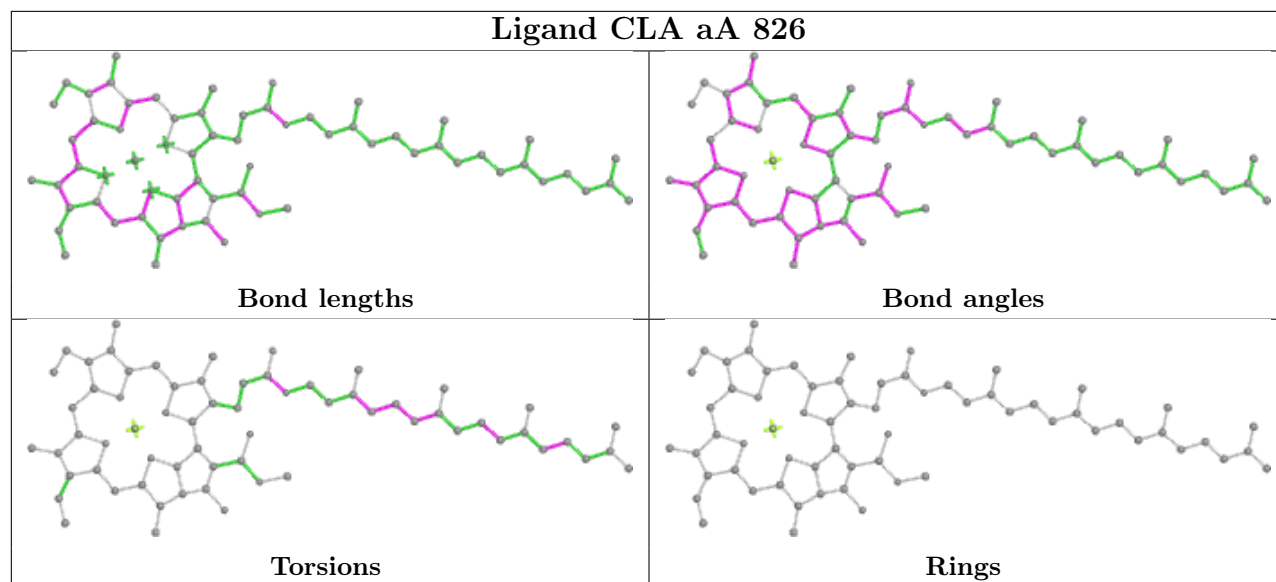
Ligand CLA bA 830



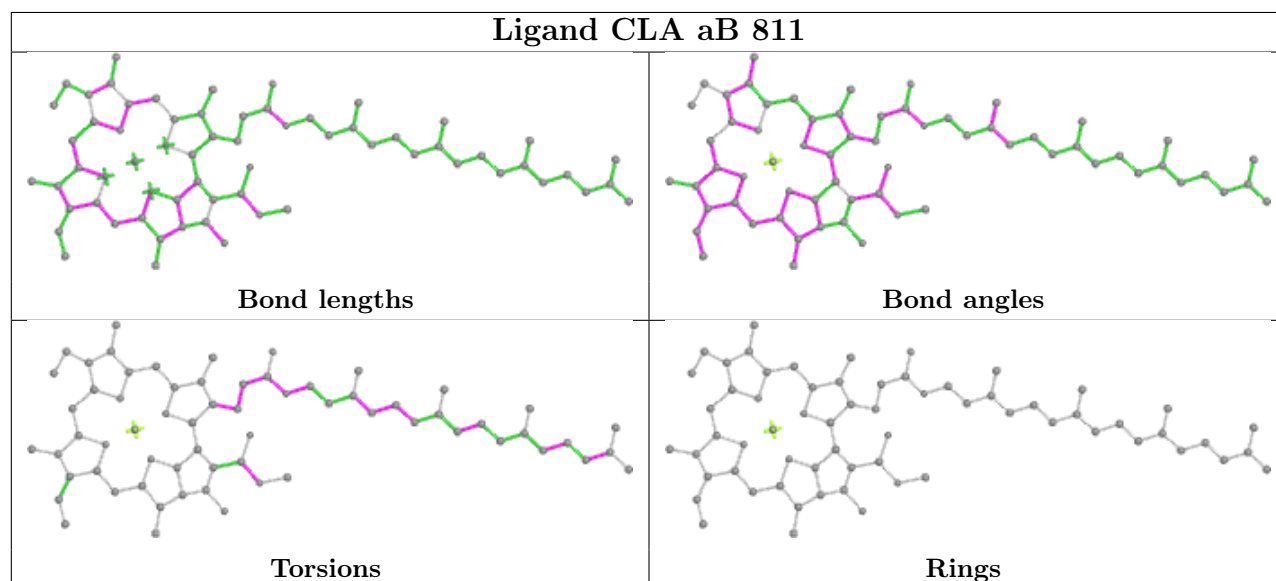
Ligand CLA bA 817



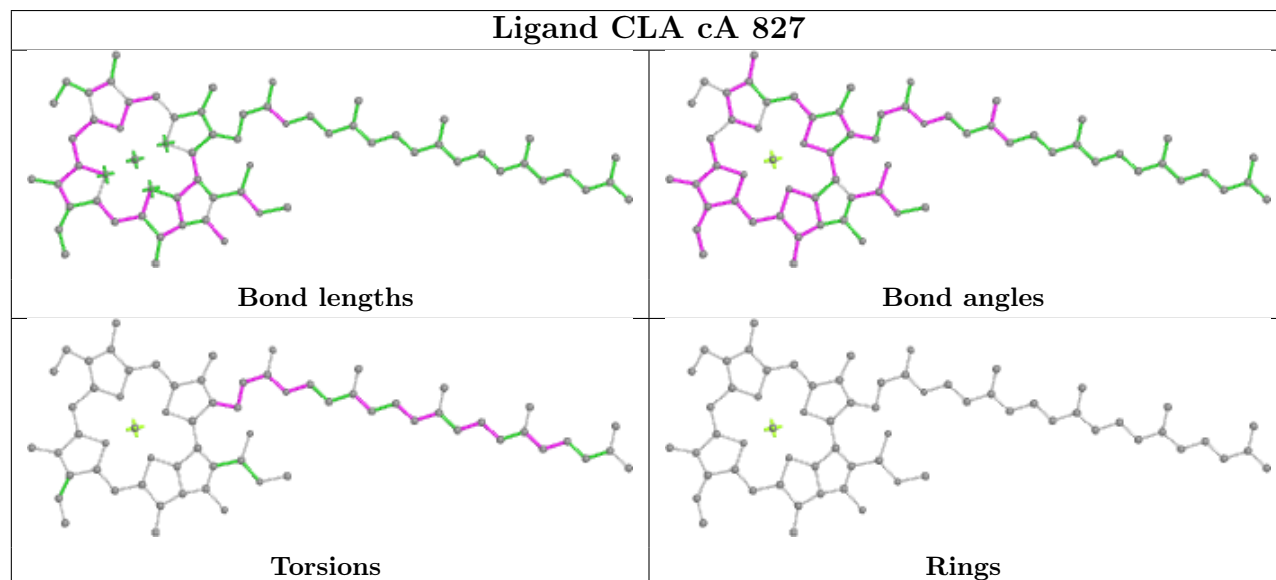
Ligand CLA aA 826

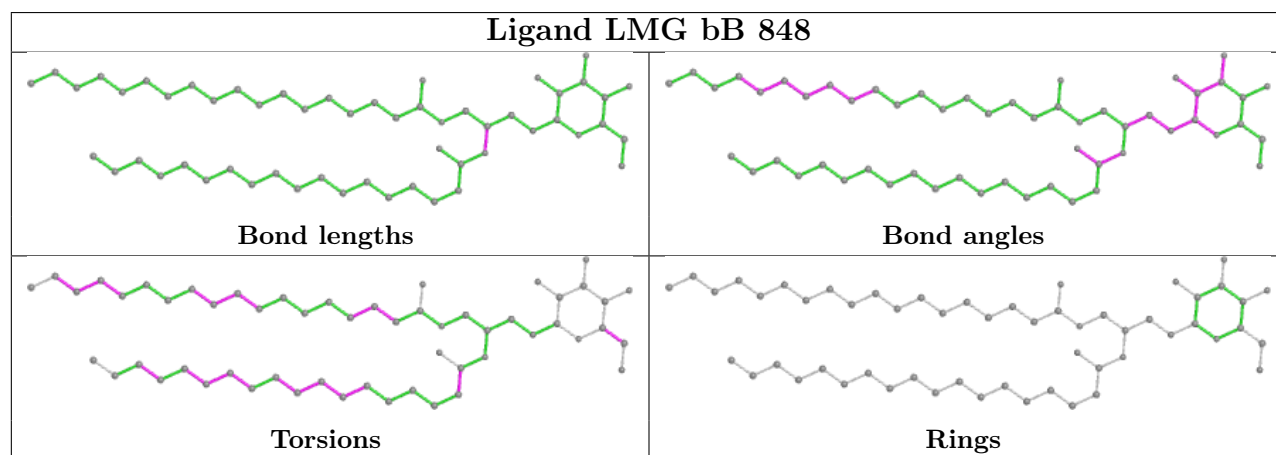
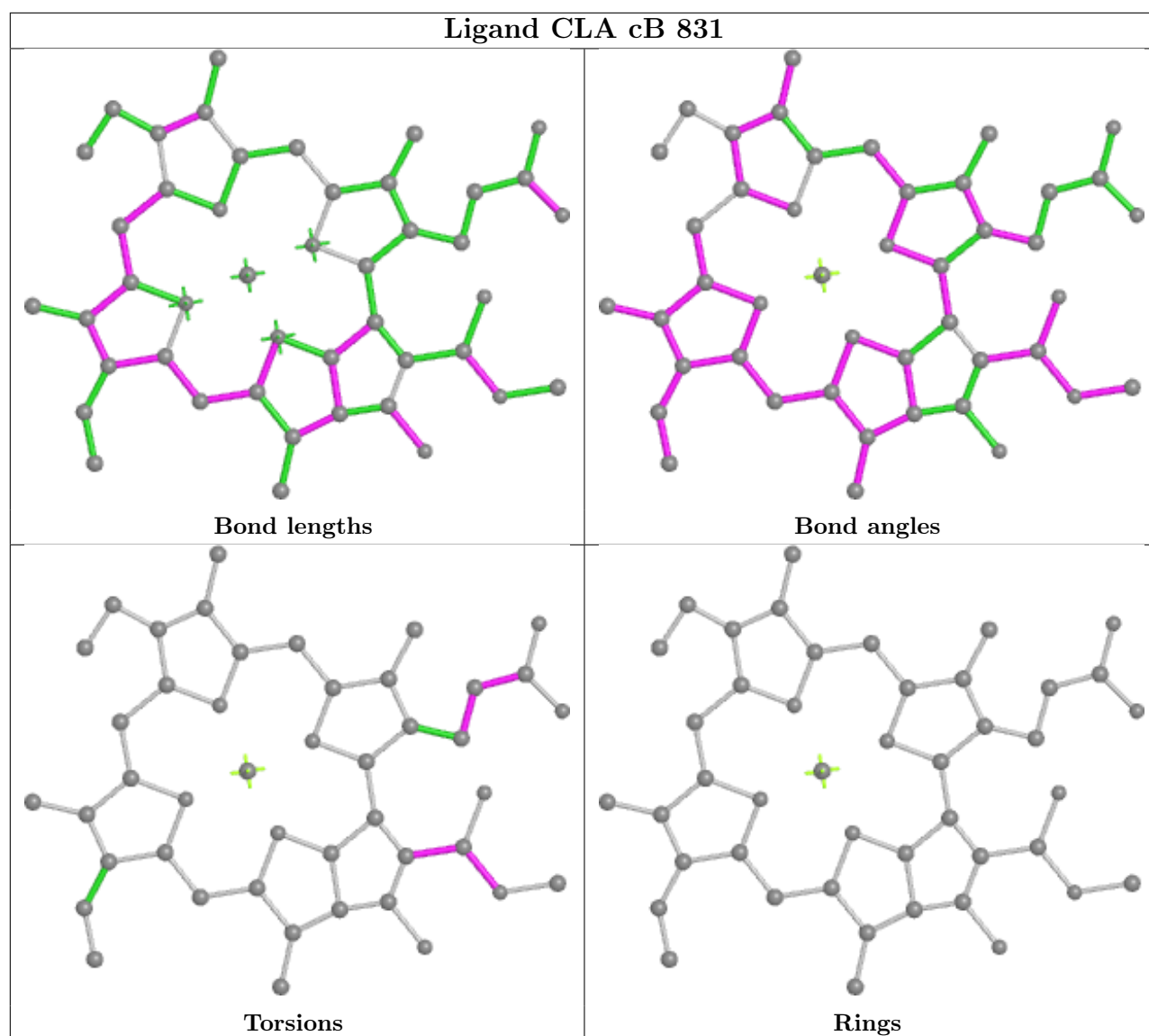


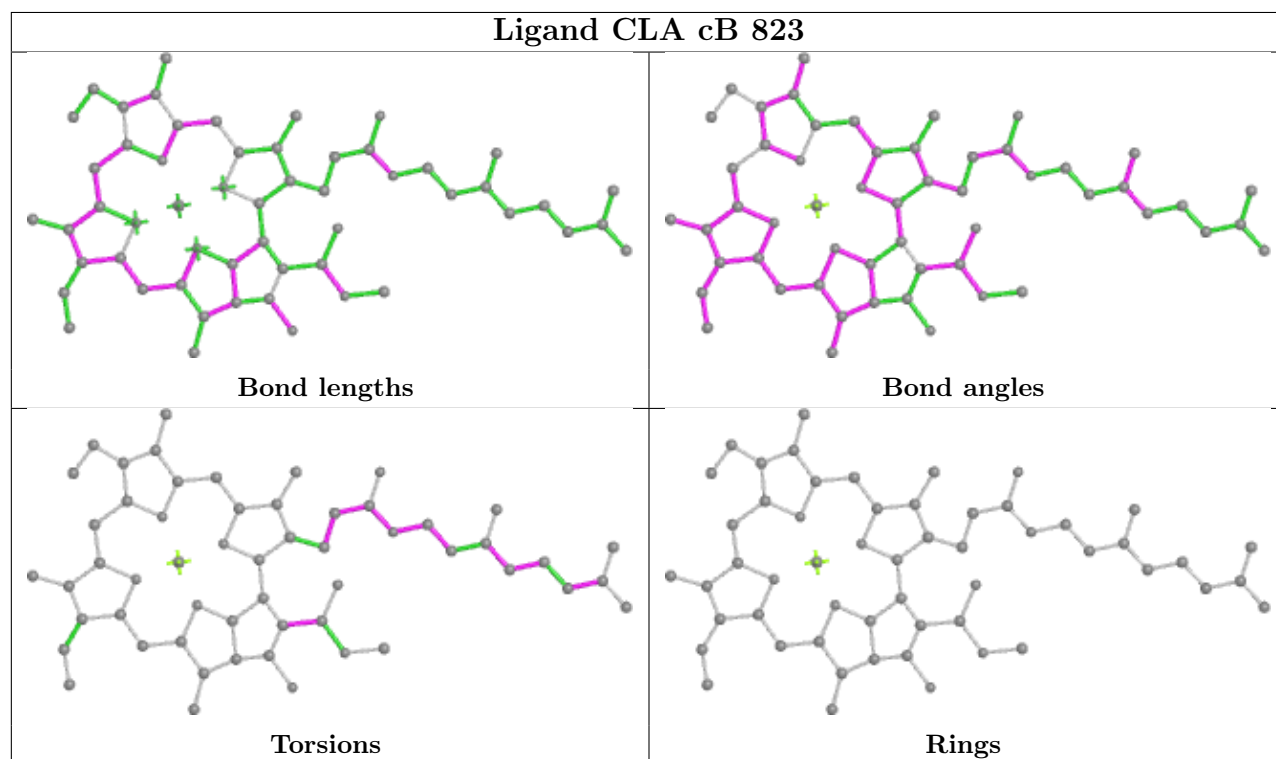
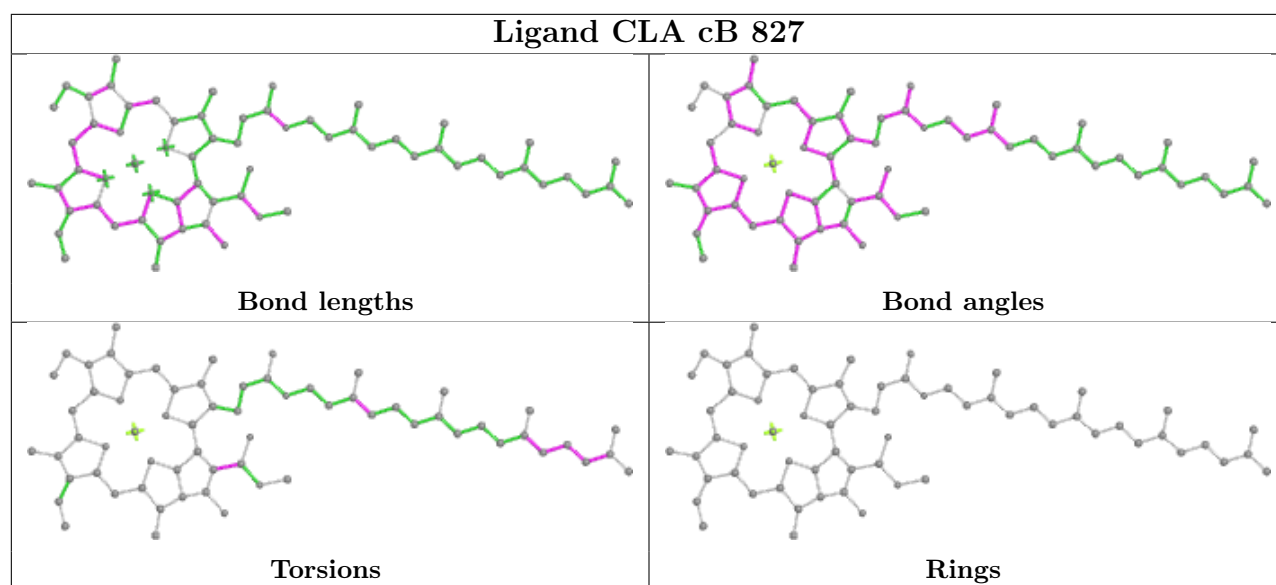
Ligand CLA aB 811

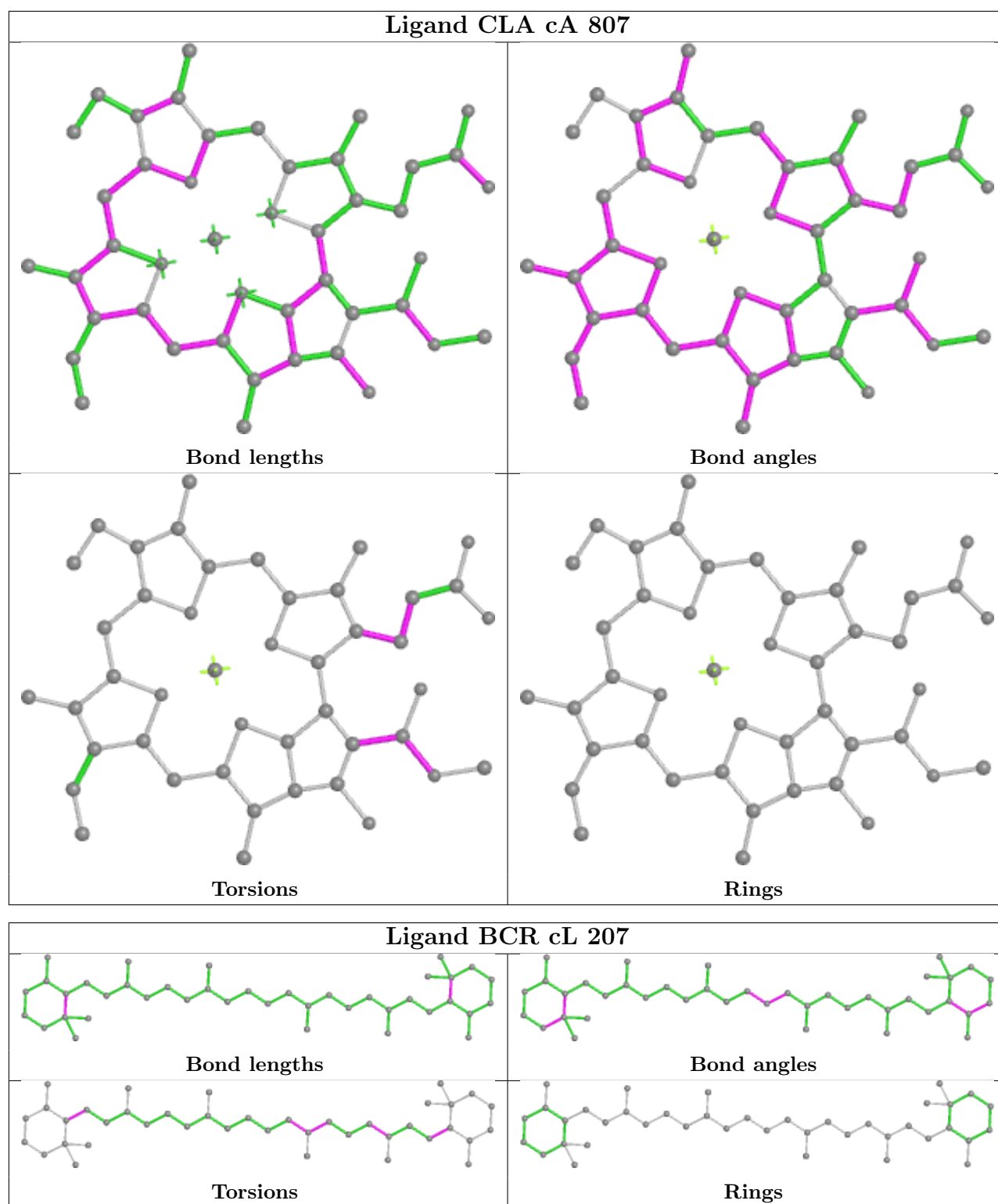


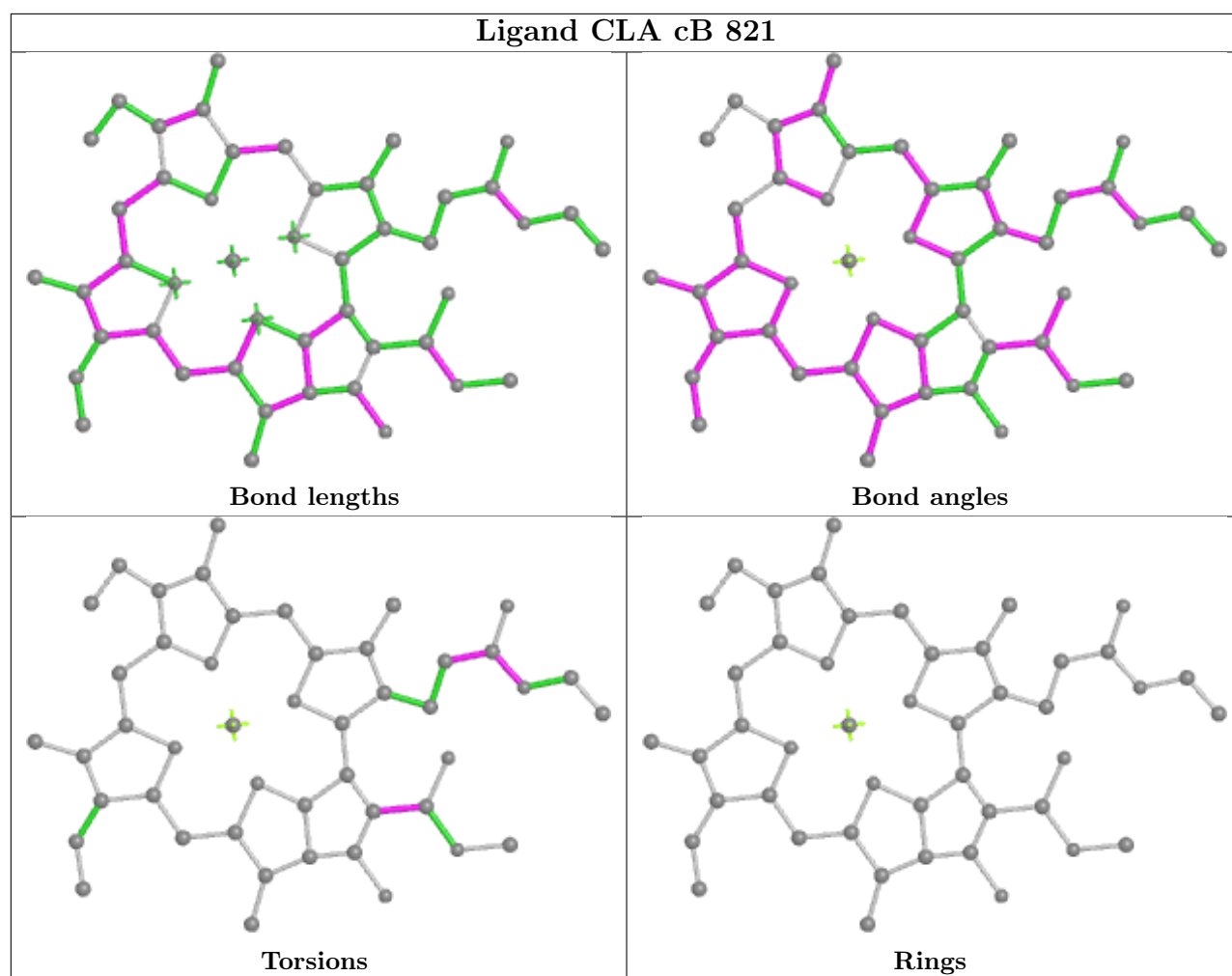
Ligand CLA cA 827



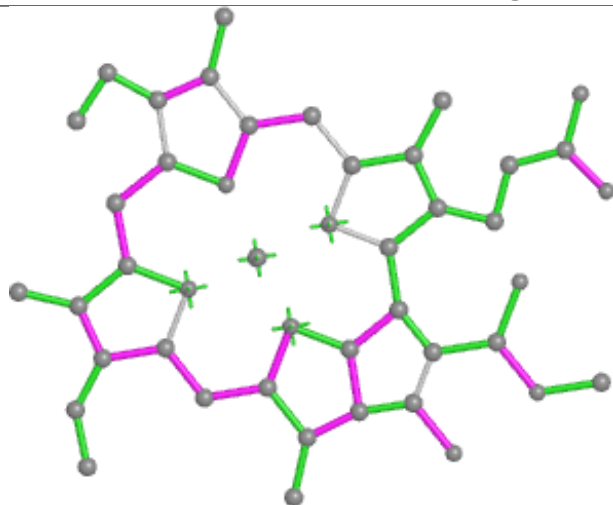




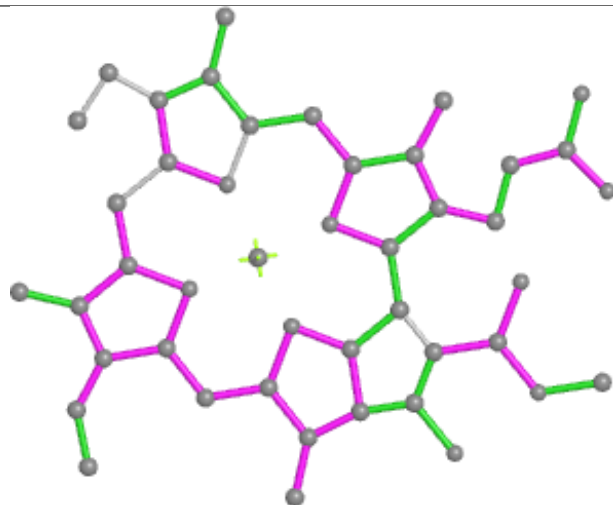




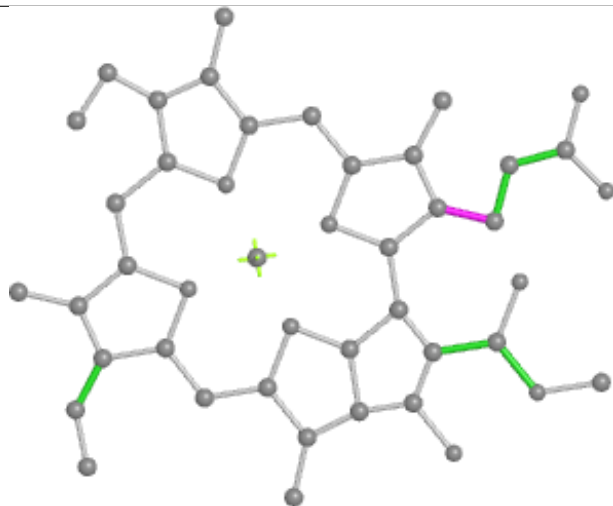
Ligand CLA cB 812



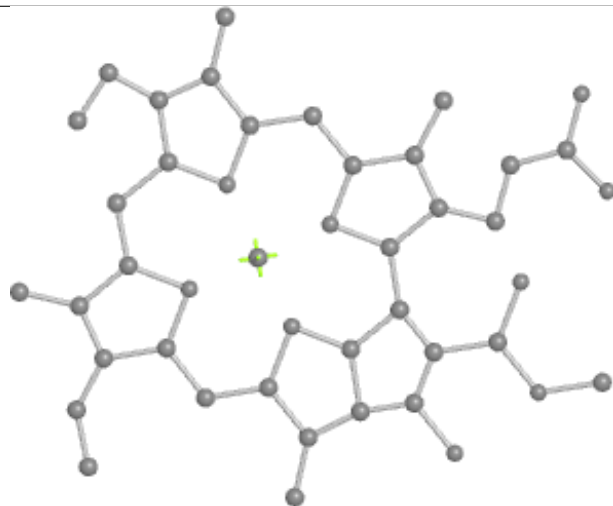
Bond lengths



Bond angles

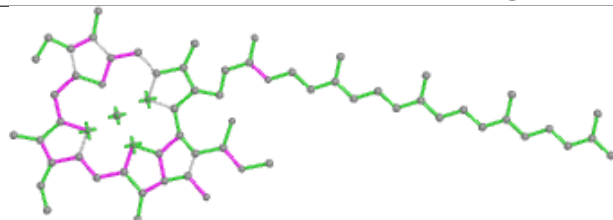


Torsions

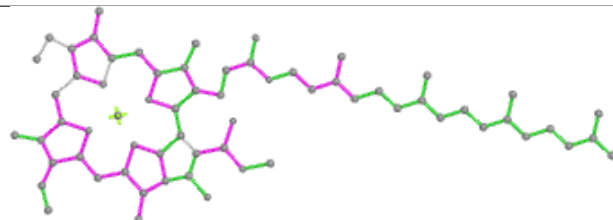


Rings

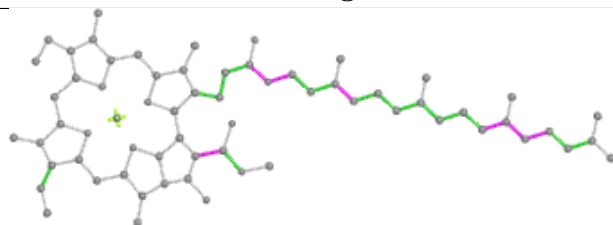
Ligand CLA ba 829



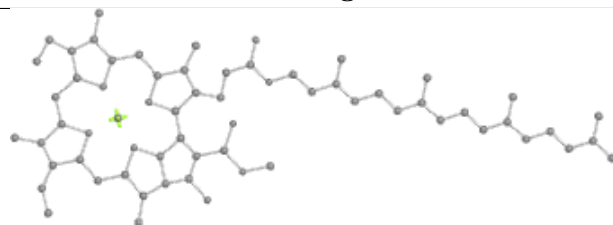
Bond lengths



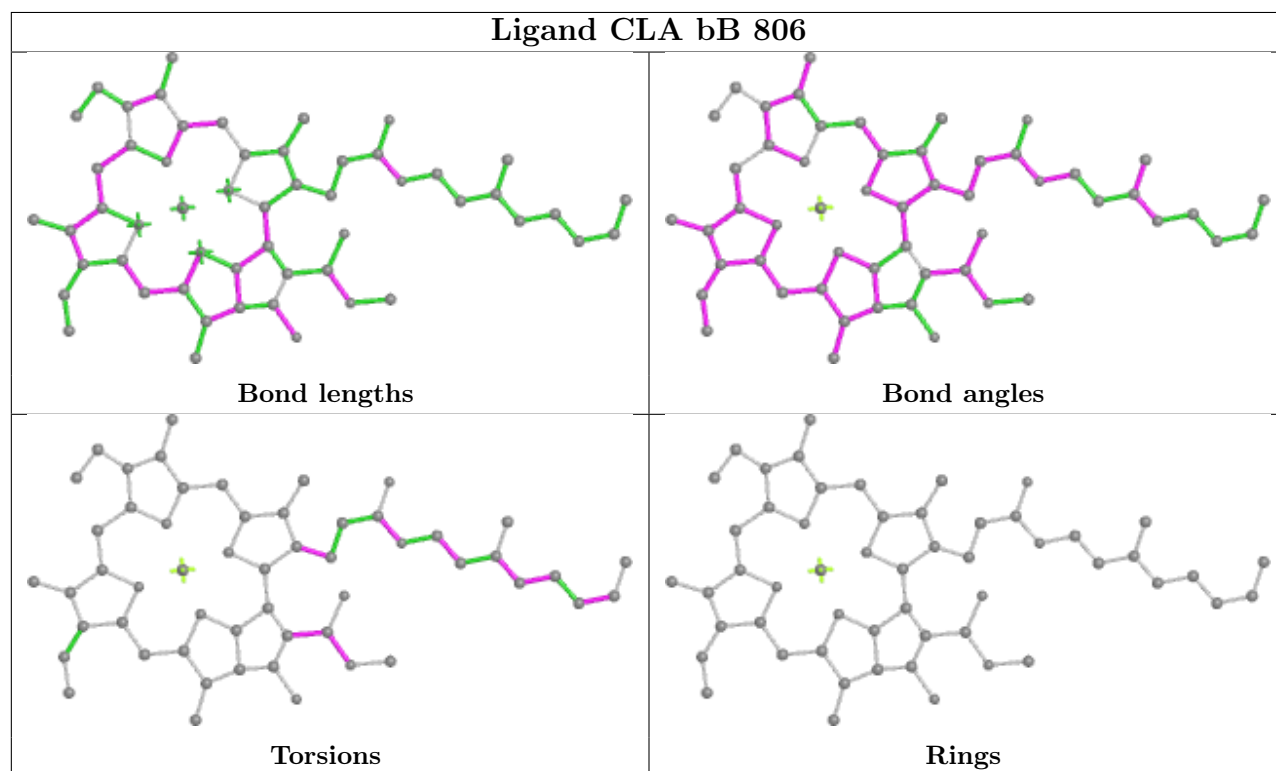
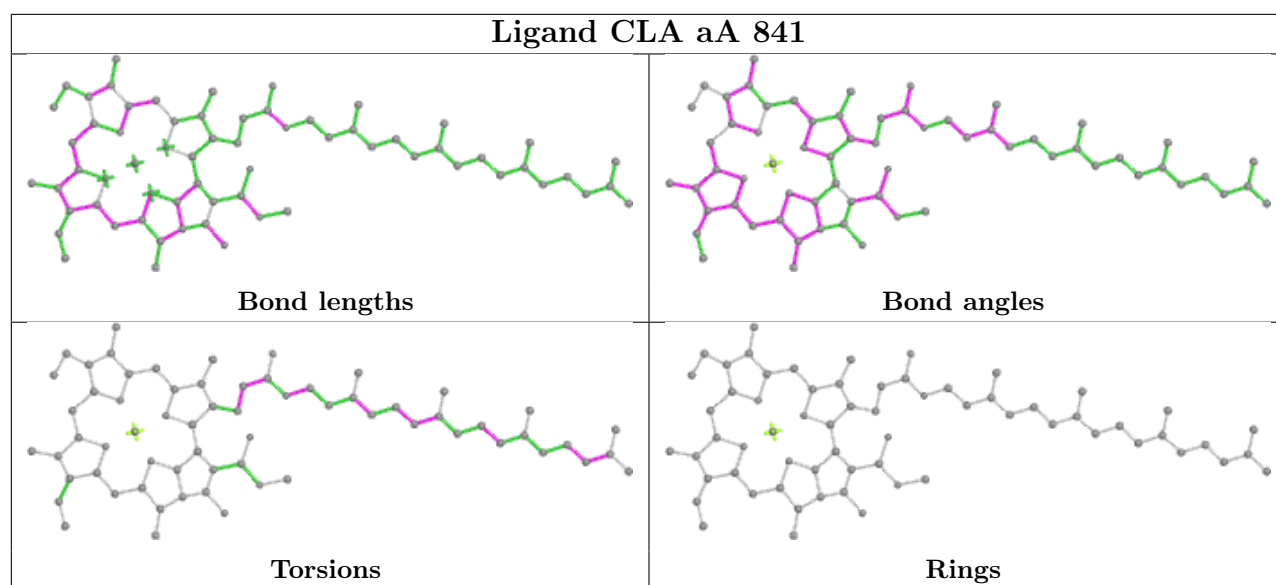
Bond angles



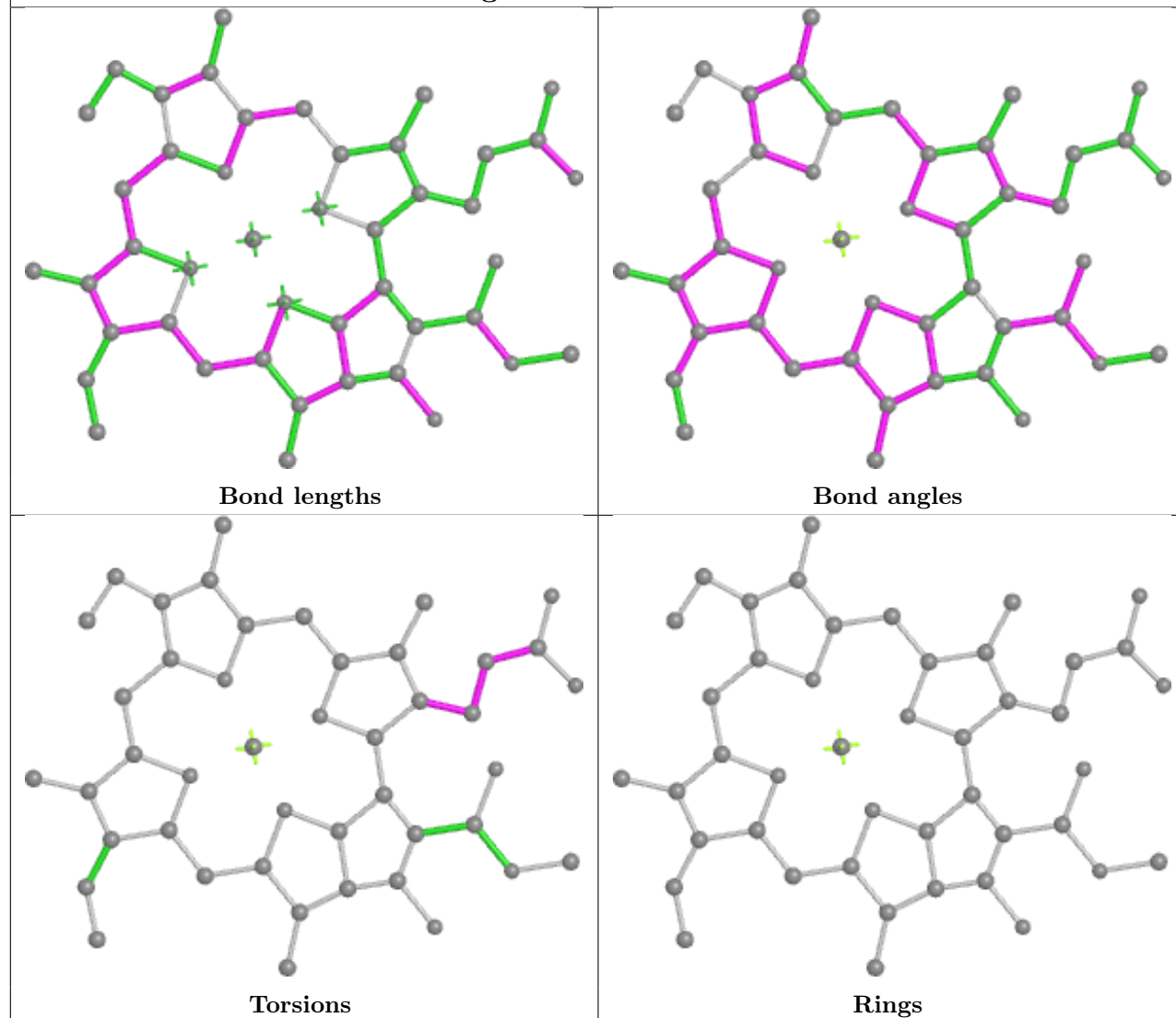
Torsions



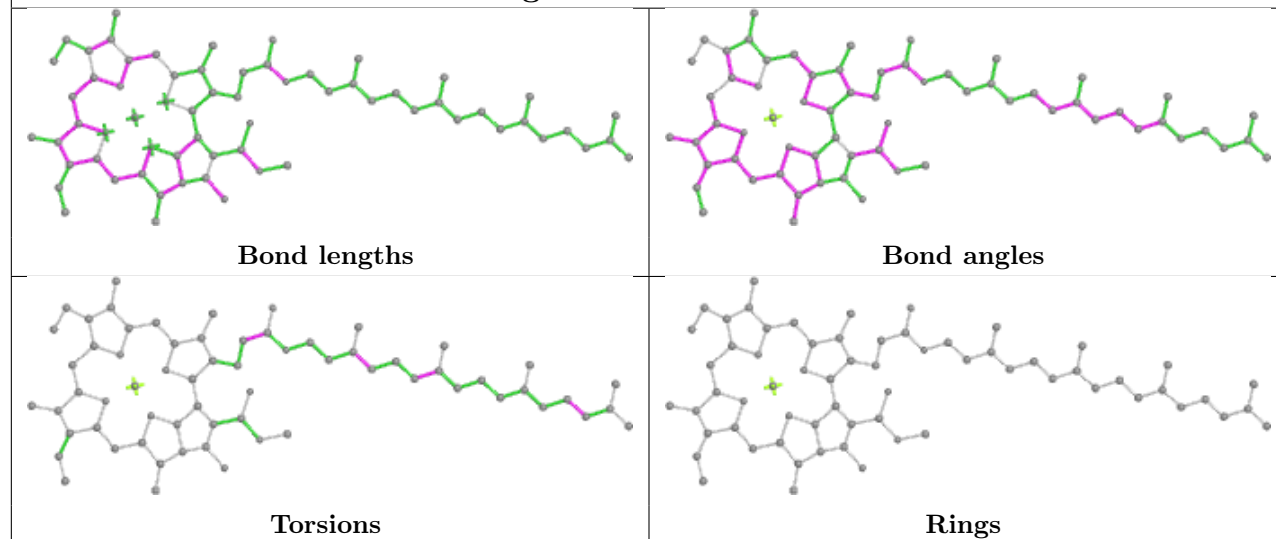
Rings

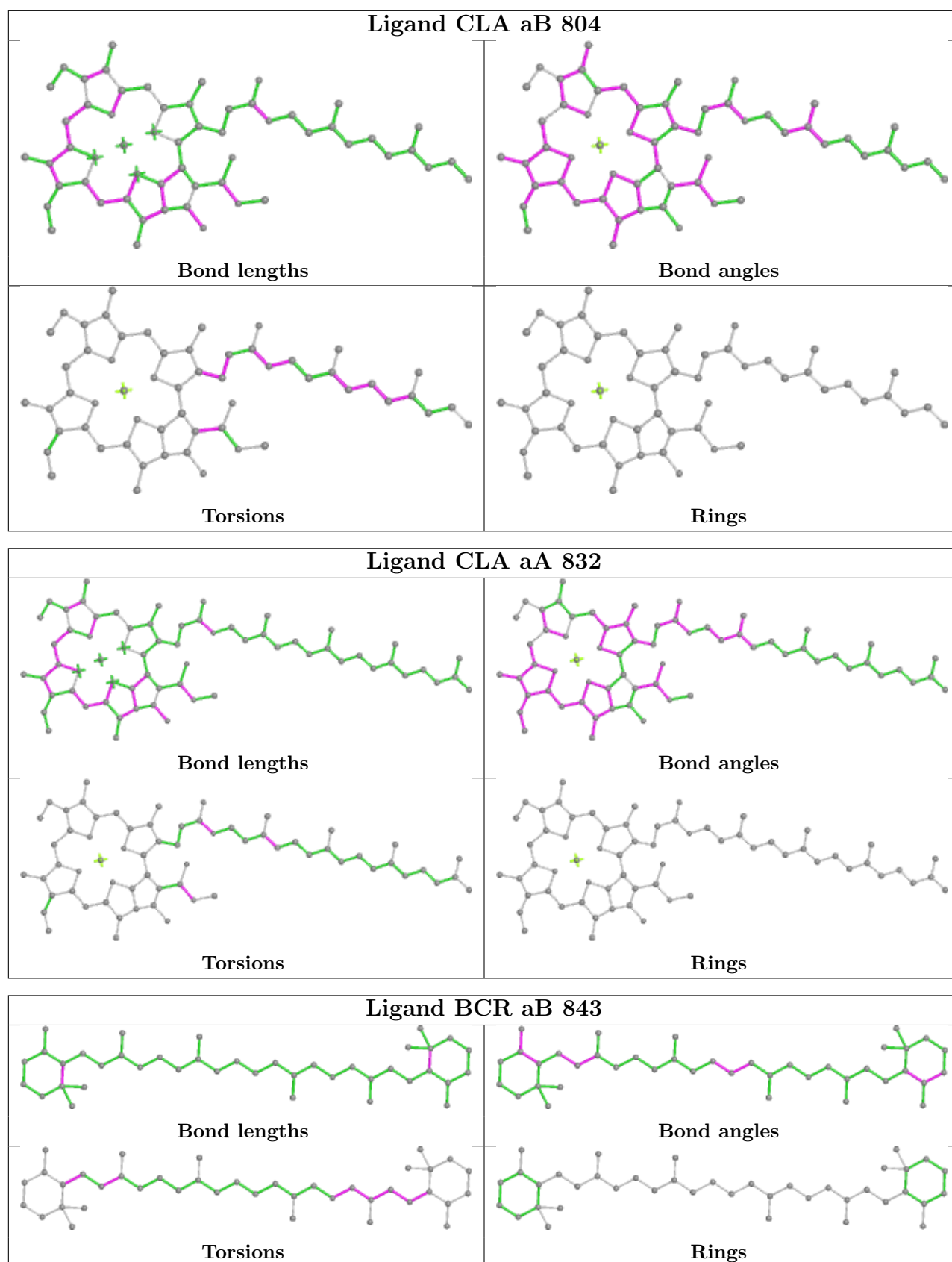


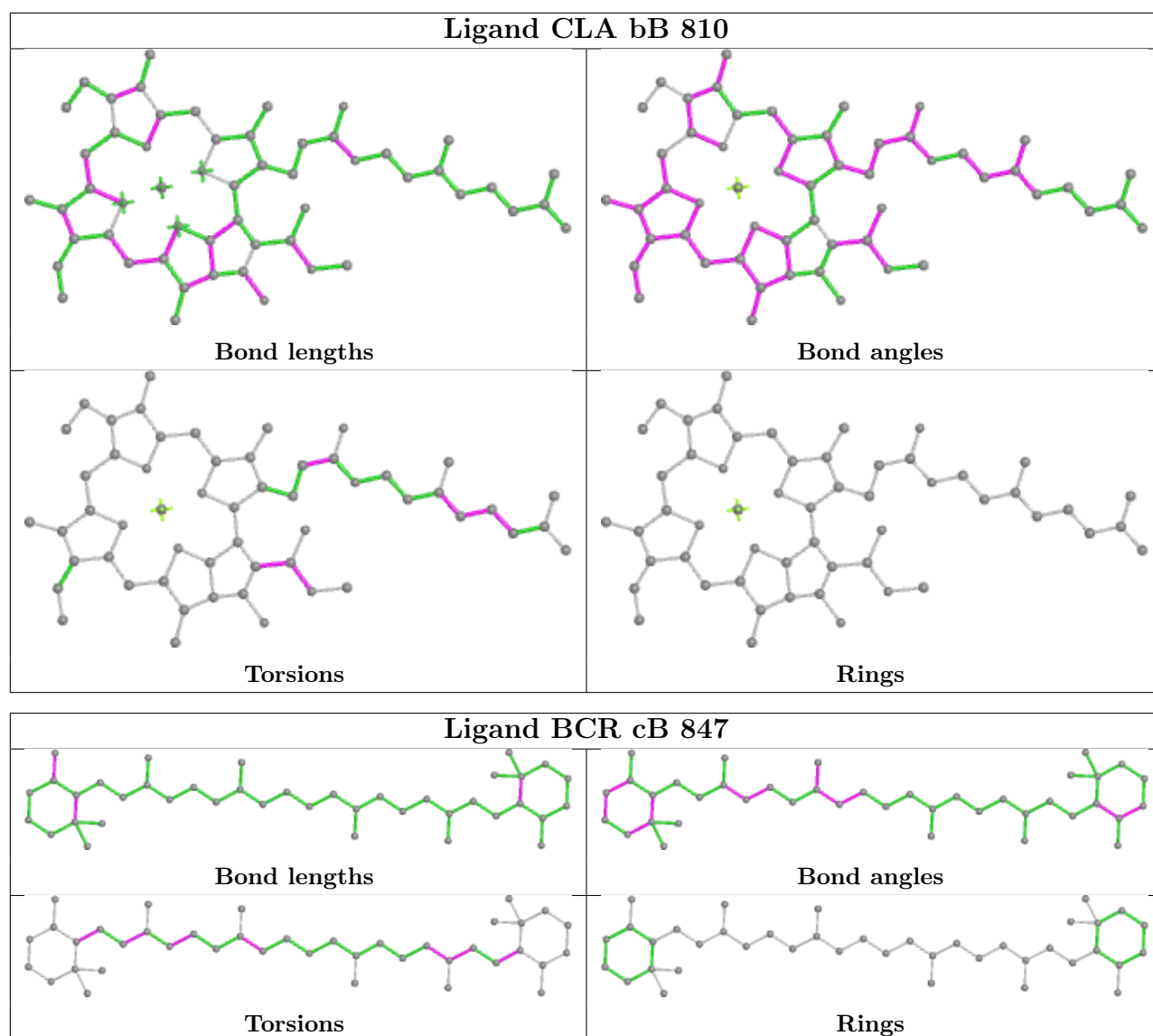
Ligand CLA bB 813

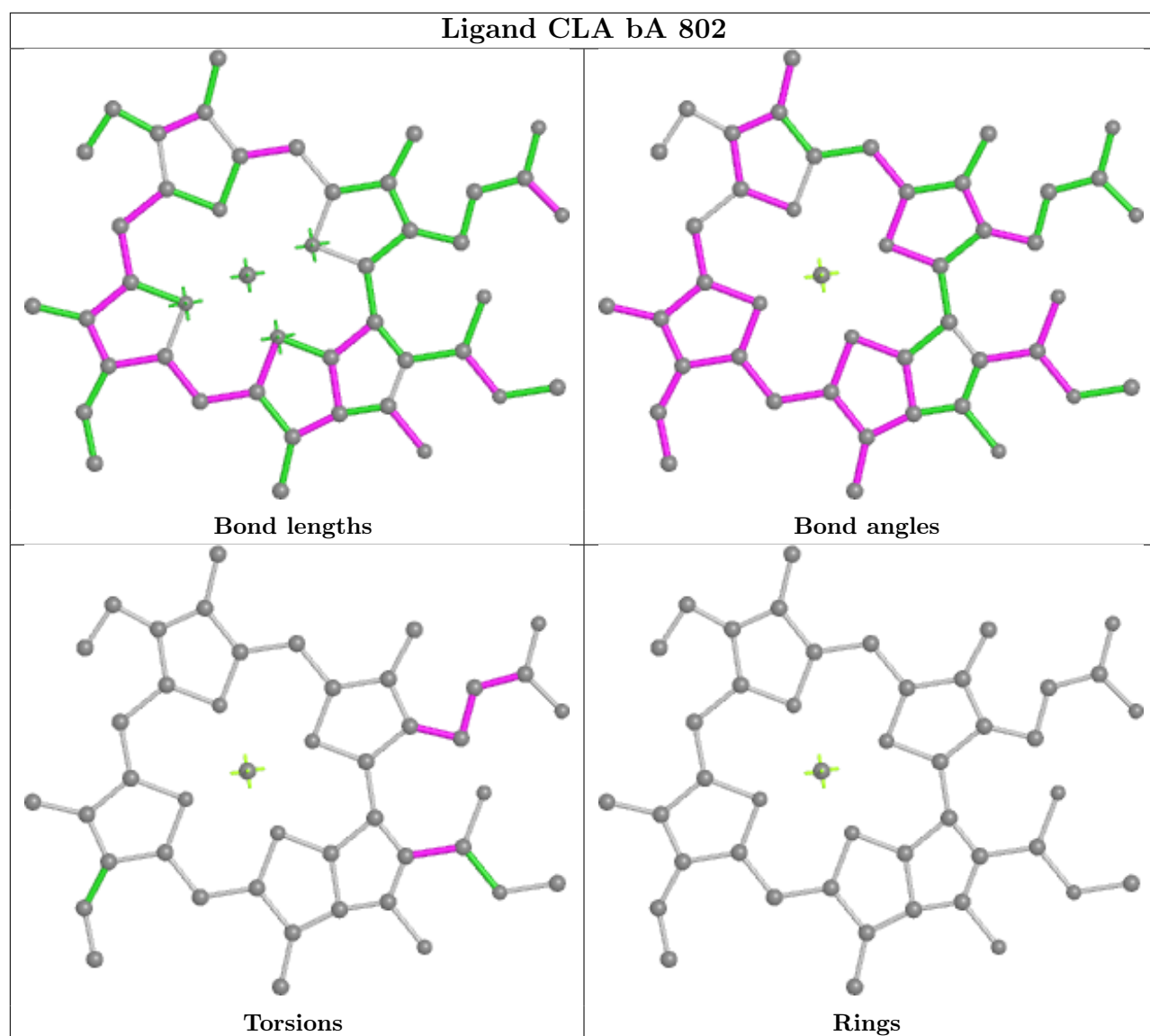


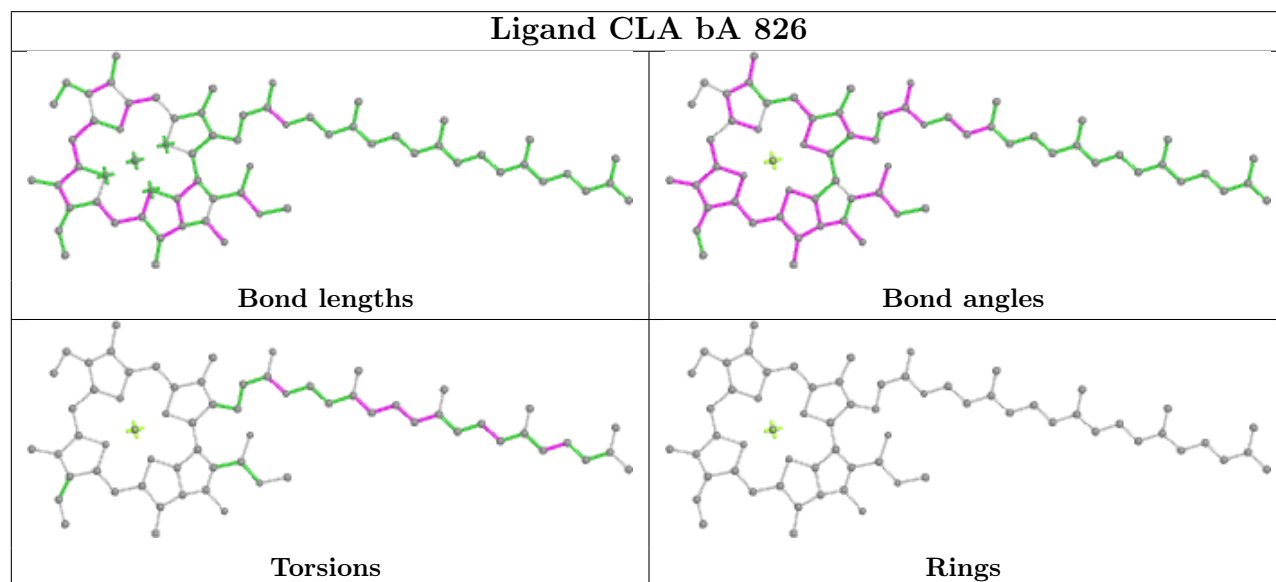
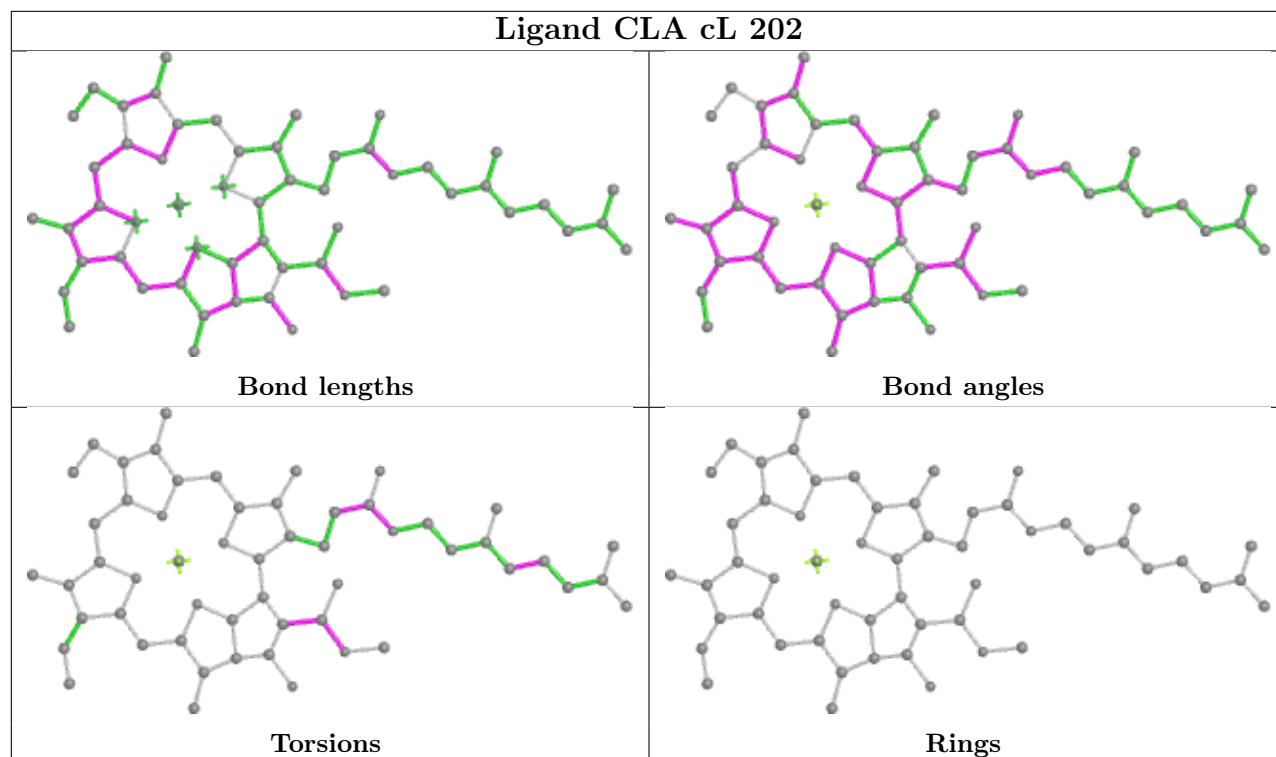
Ligand CLA bB 809

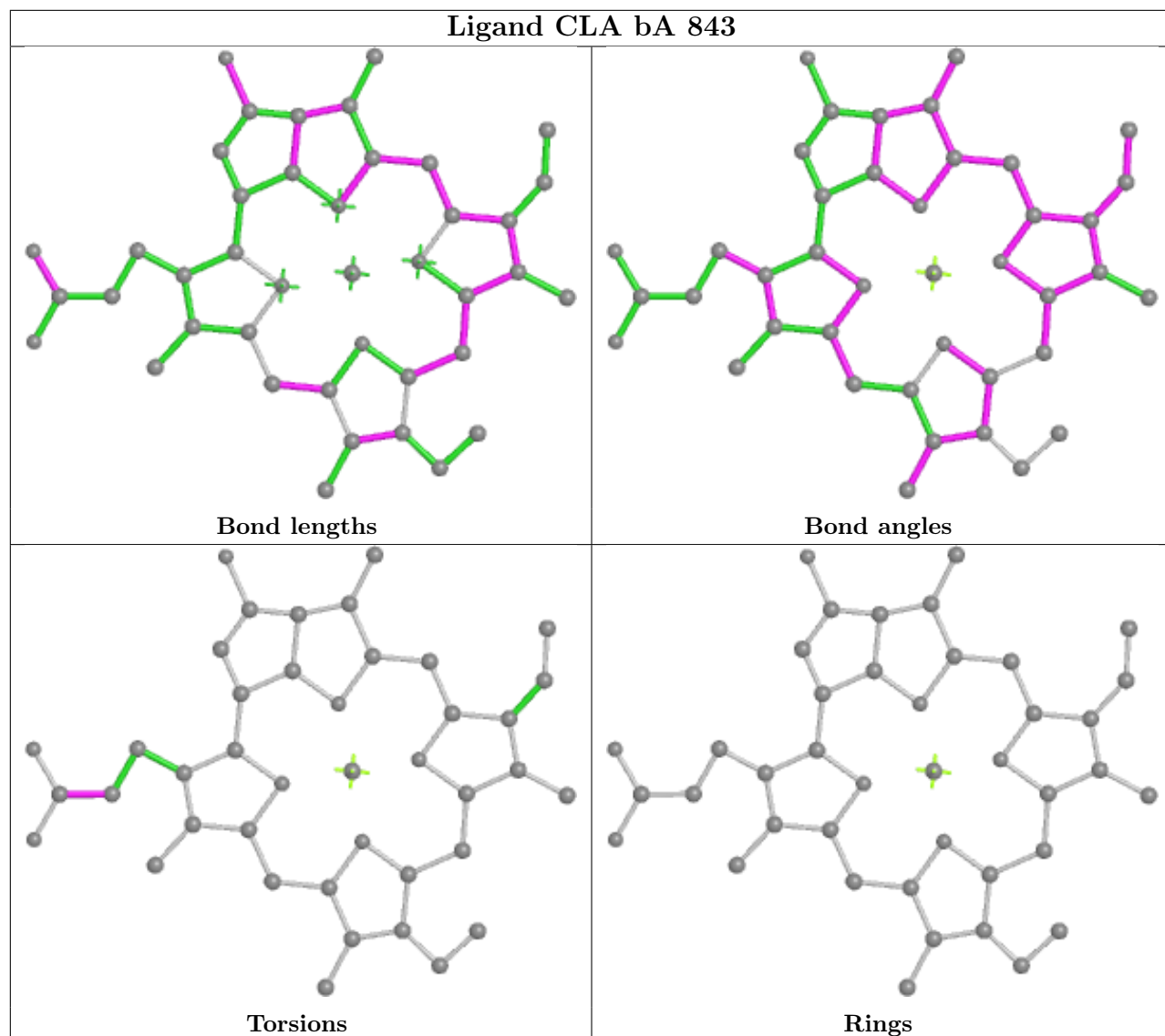


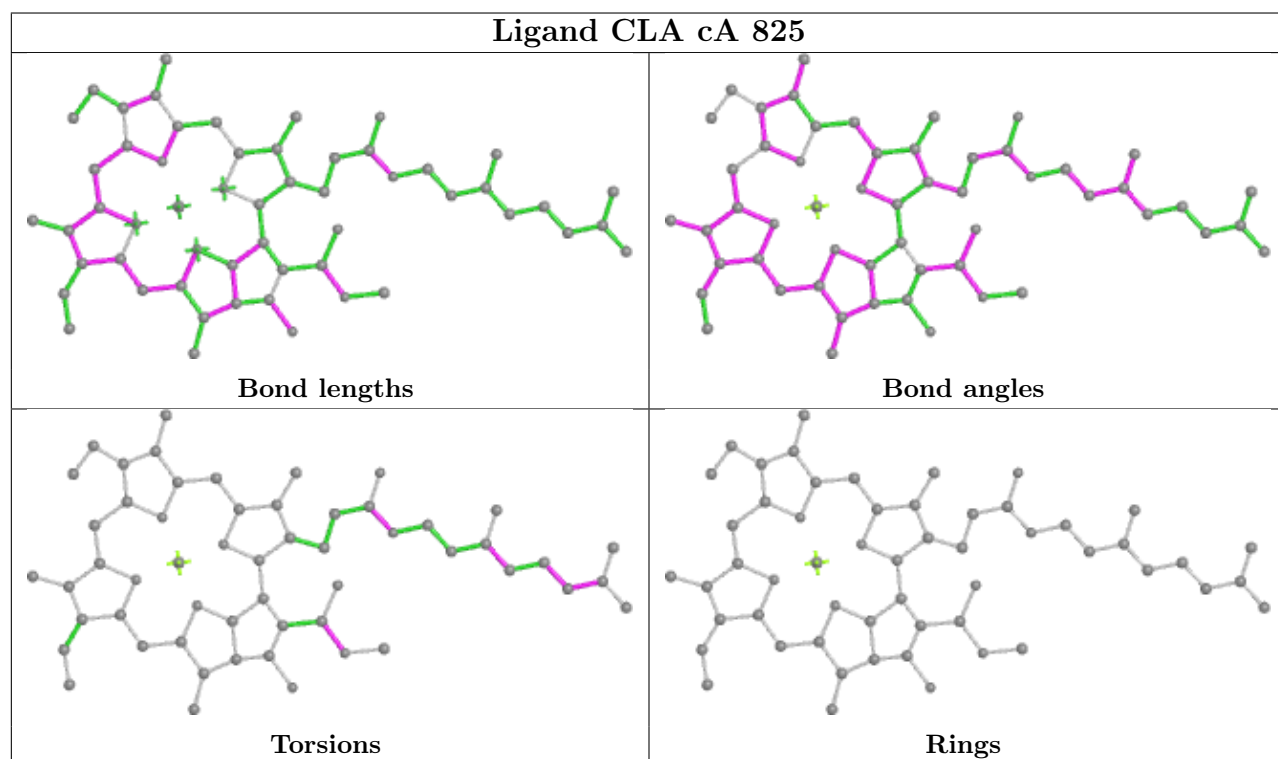
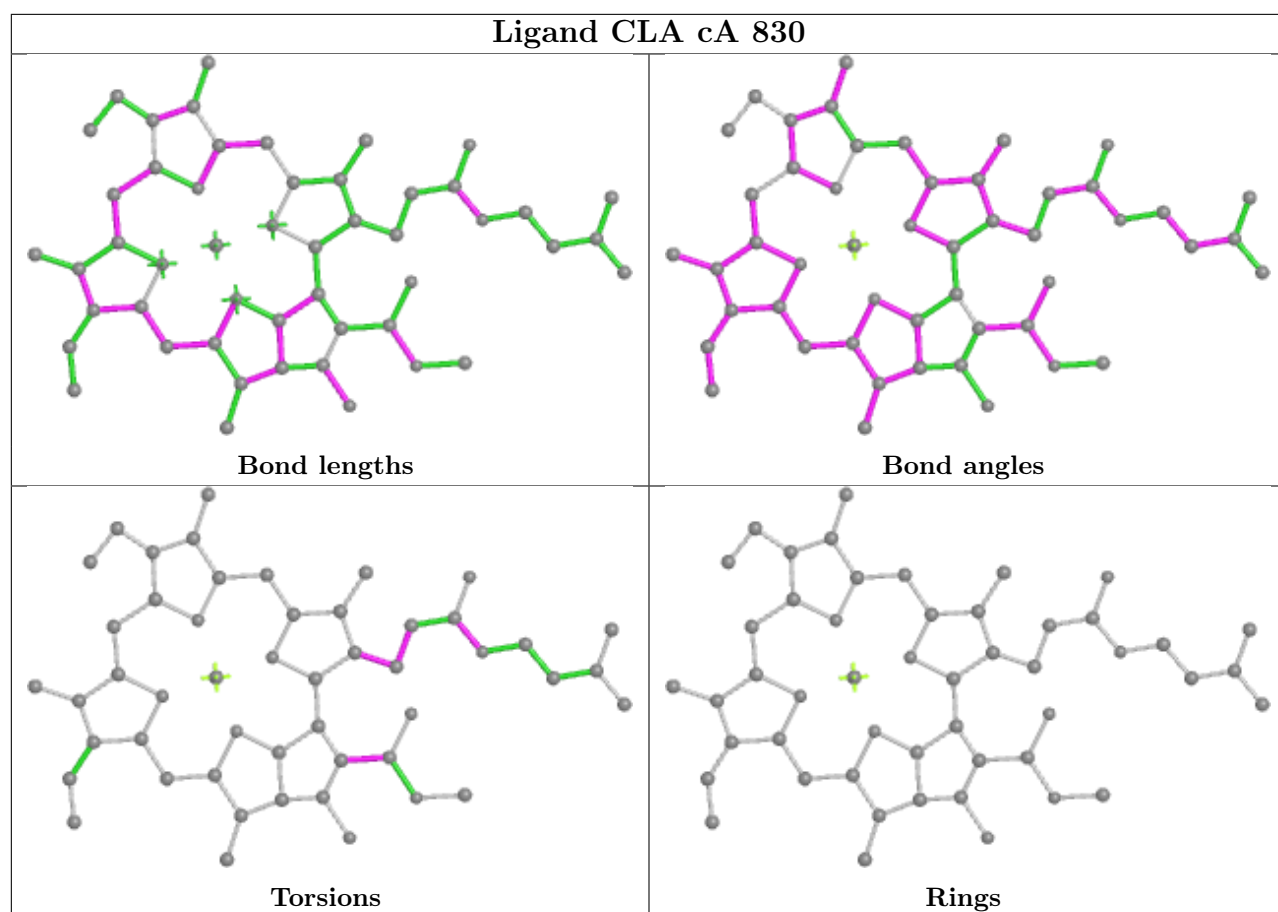


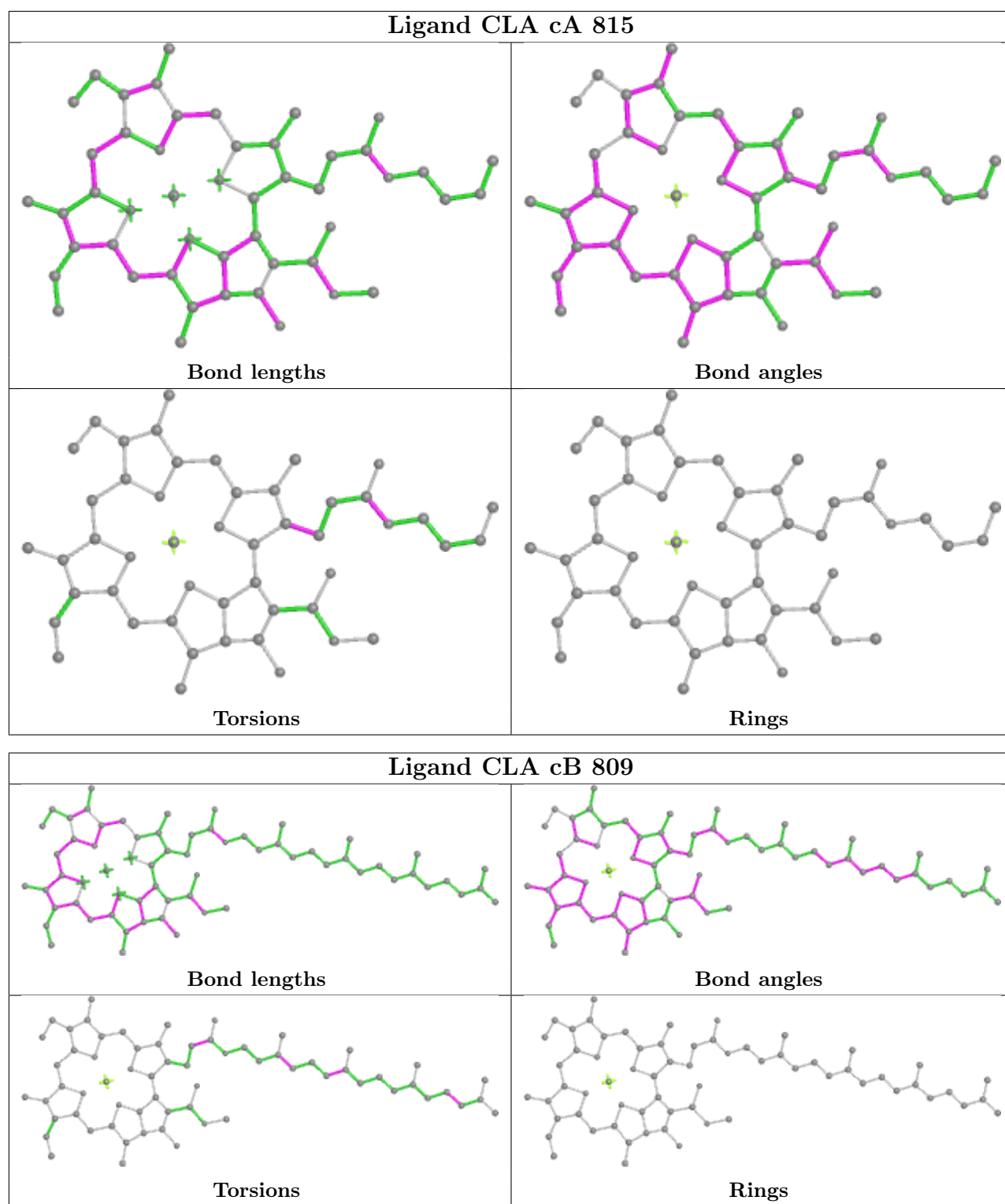


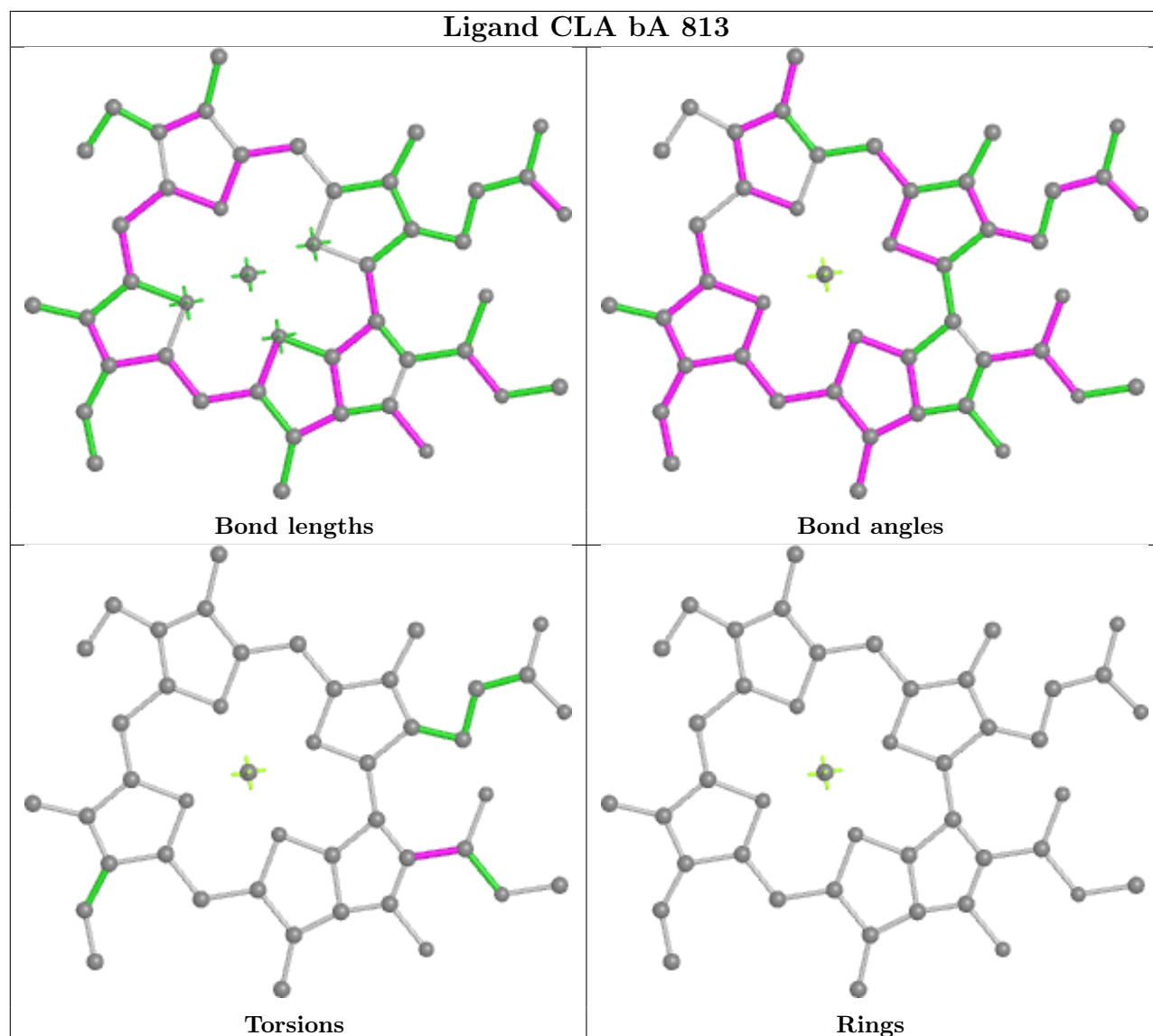
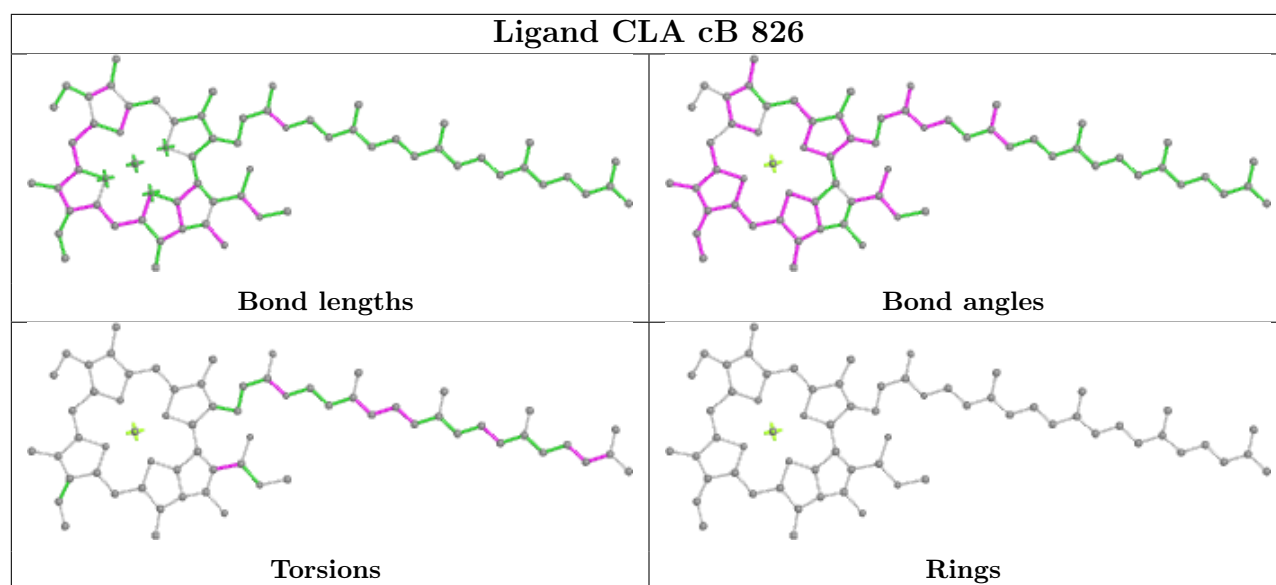


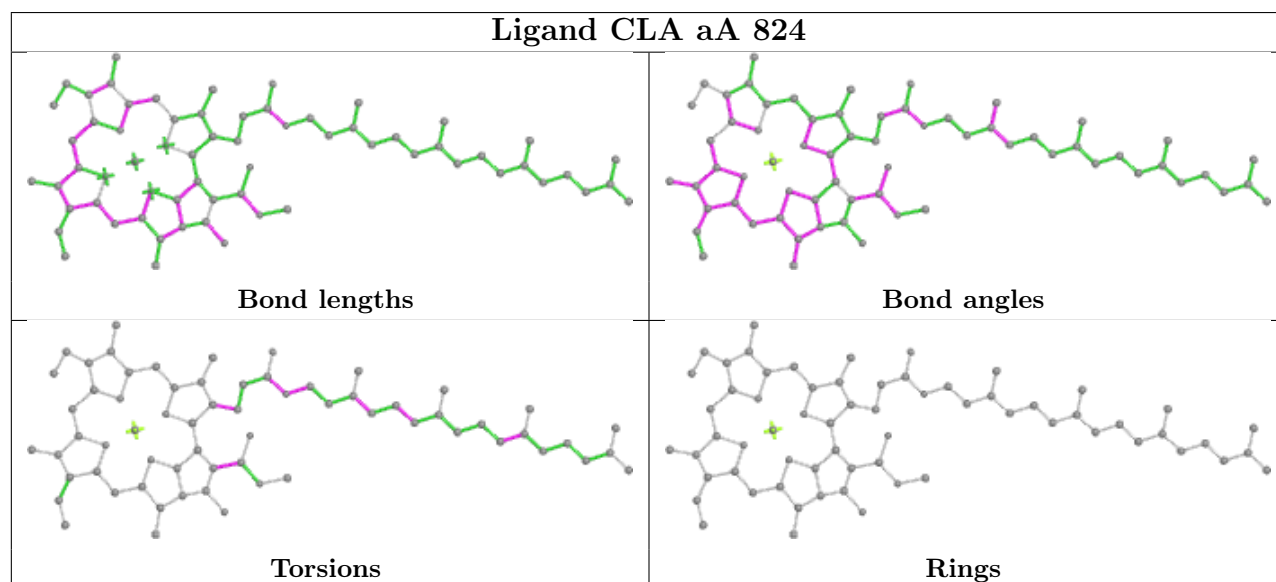
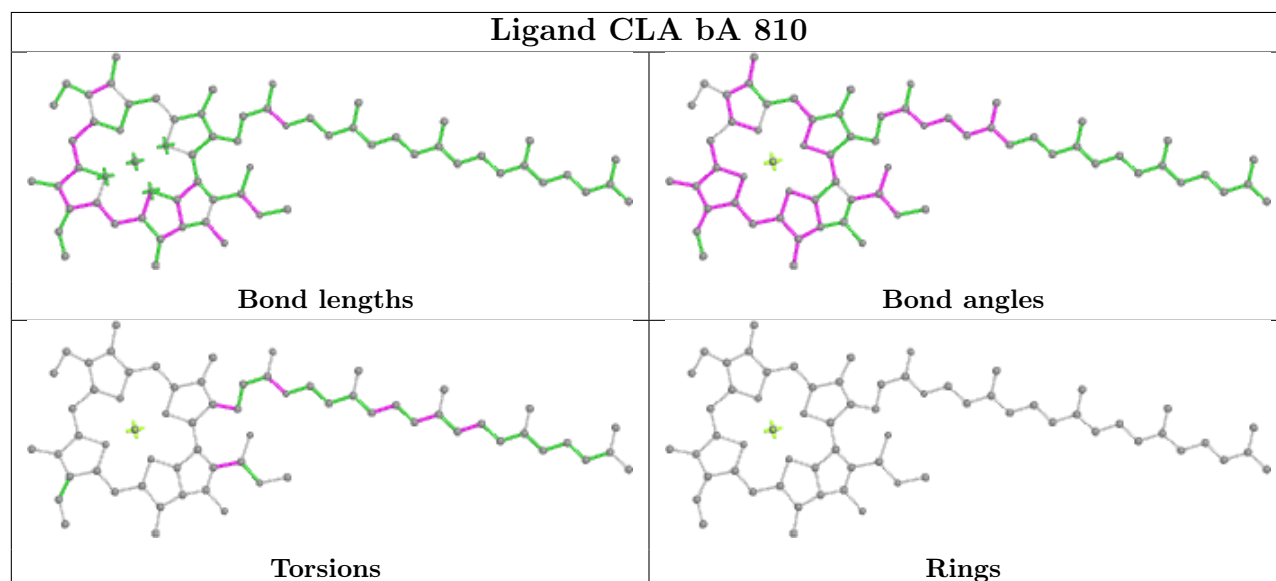
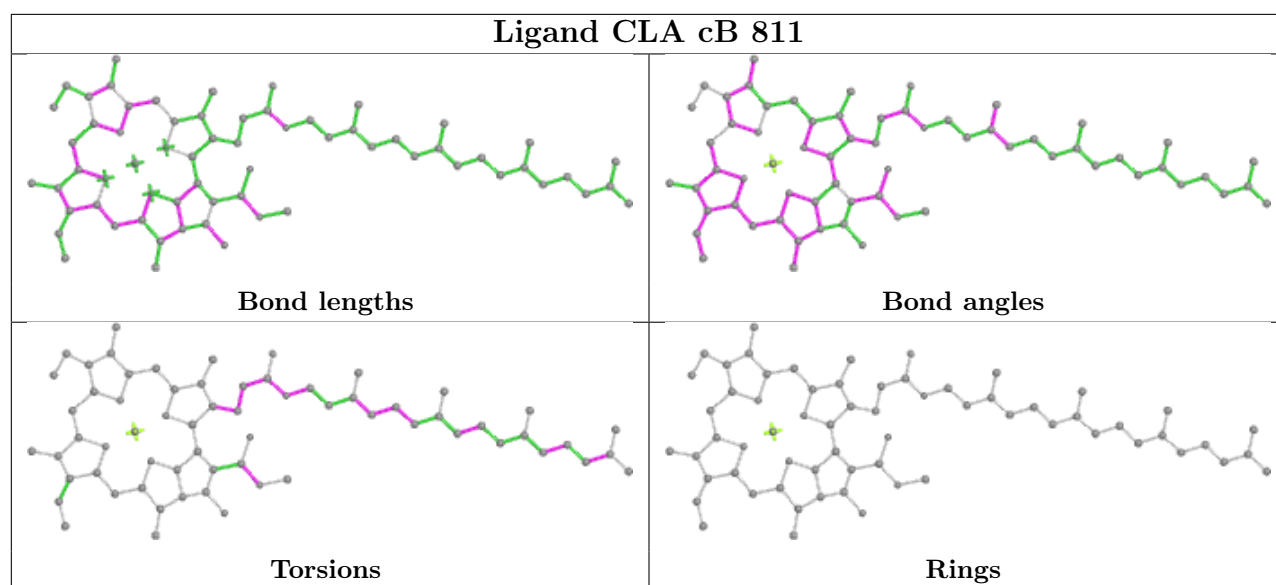




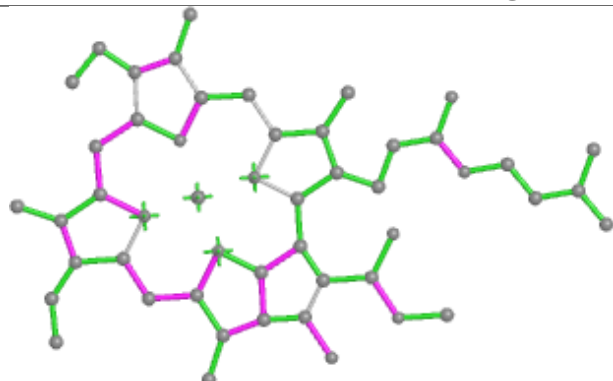




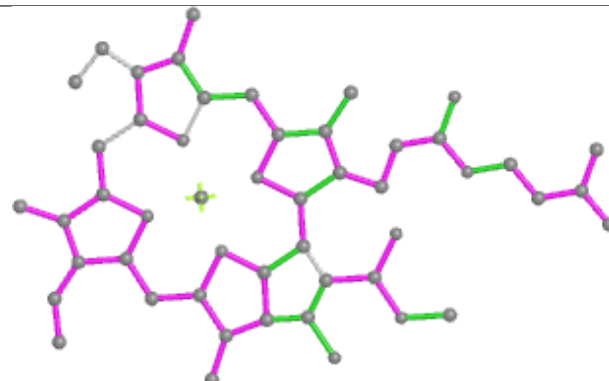




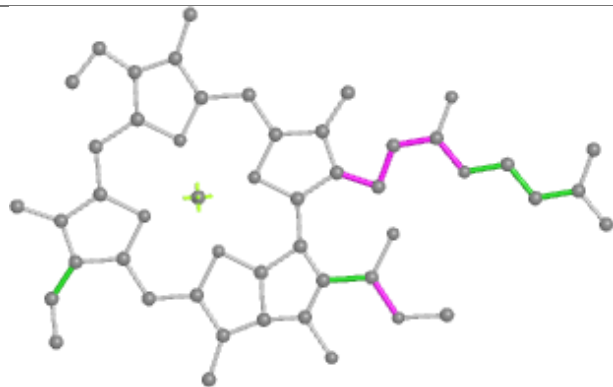
Ligand CLA bA 838



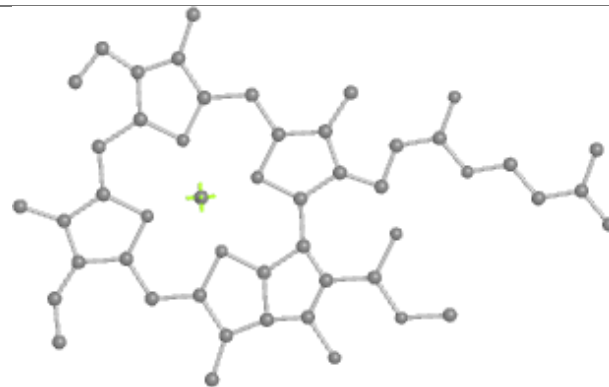
Bond lengths



Bond angles

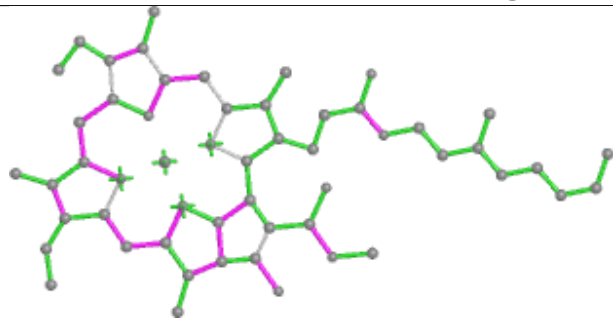


Torsions

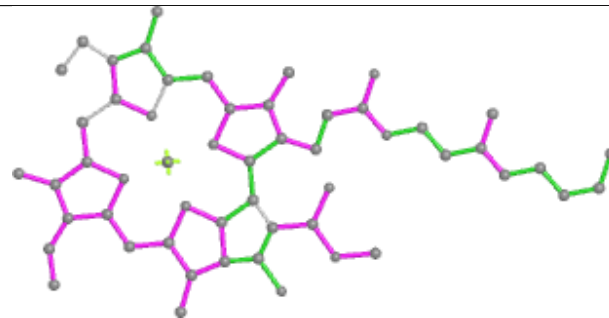


Rings

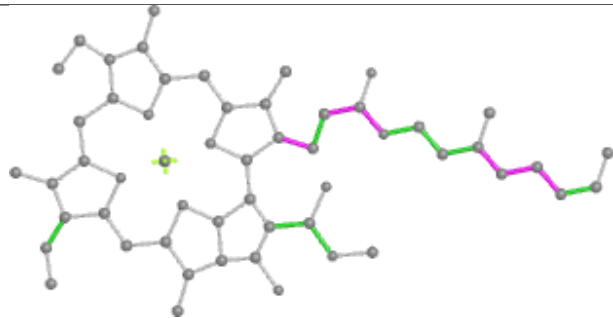
Ligand CLA bA 834



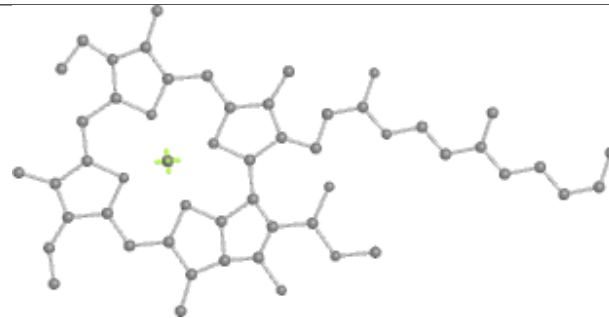
Bond lengths



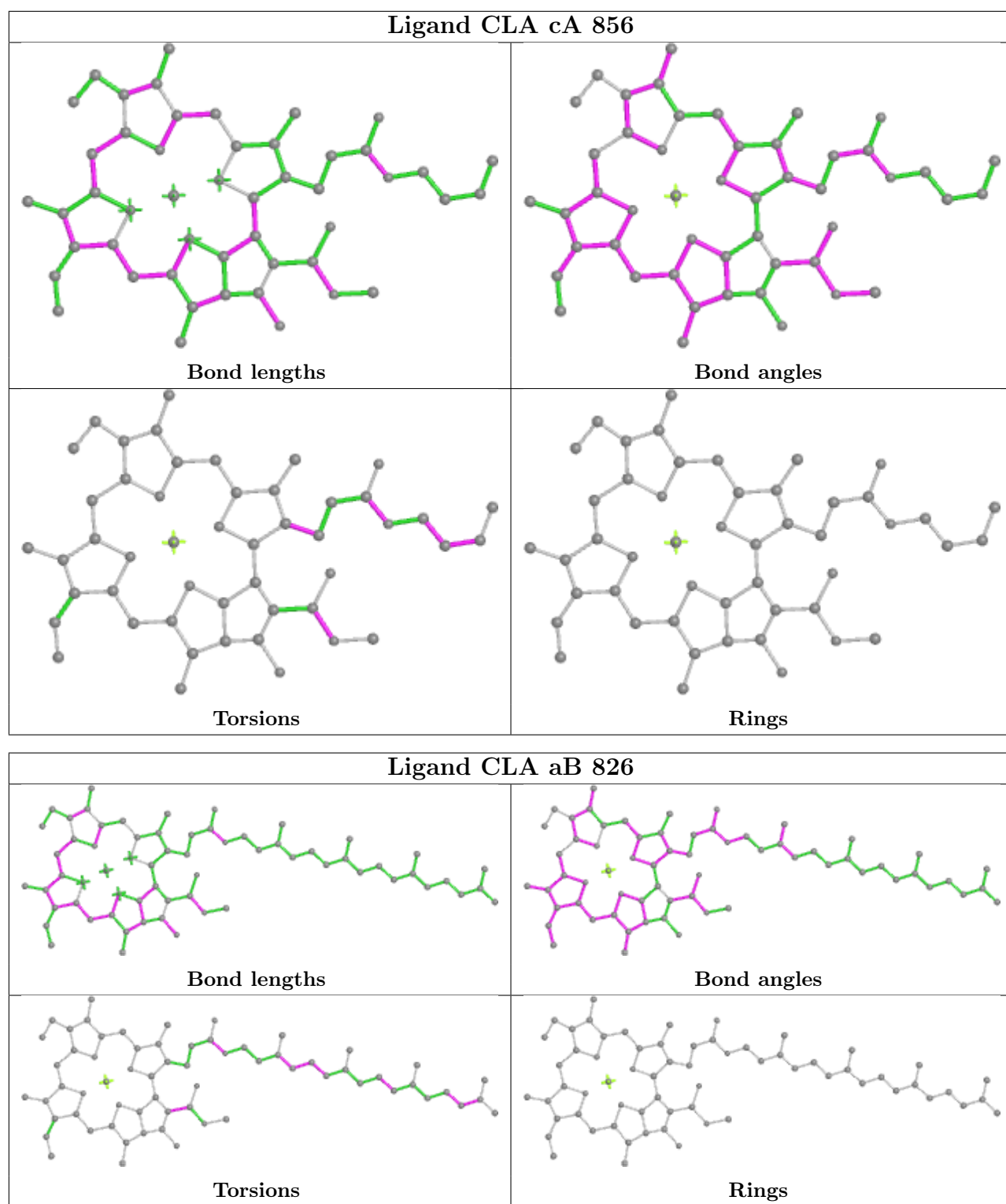
Bond angles

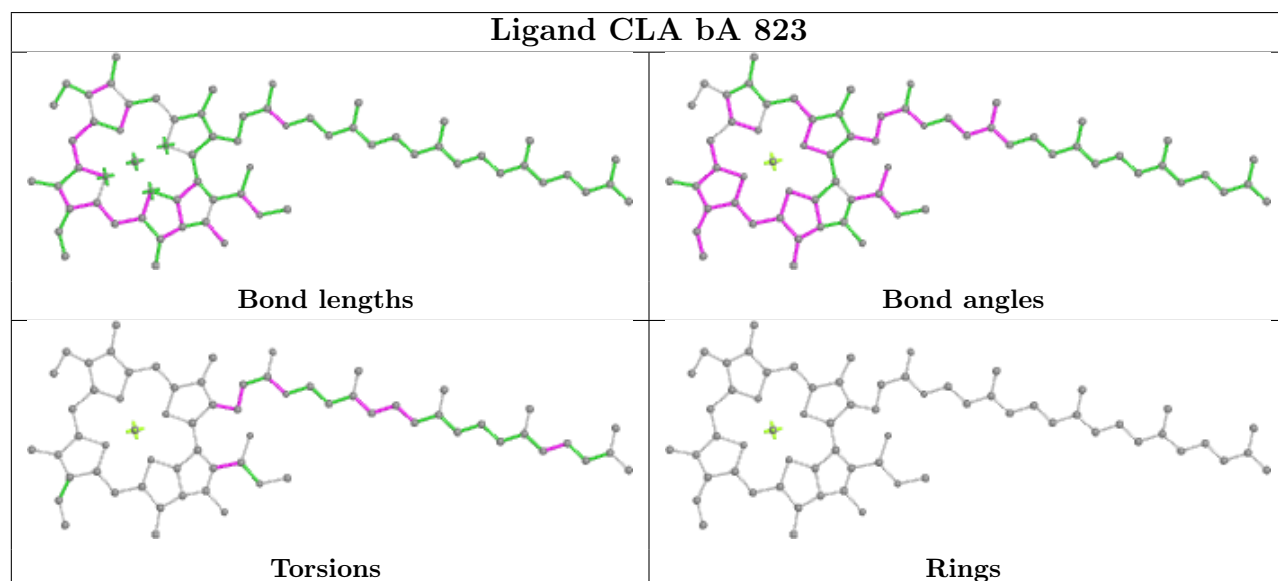
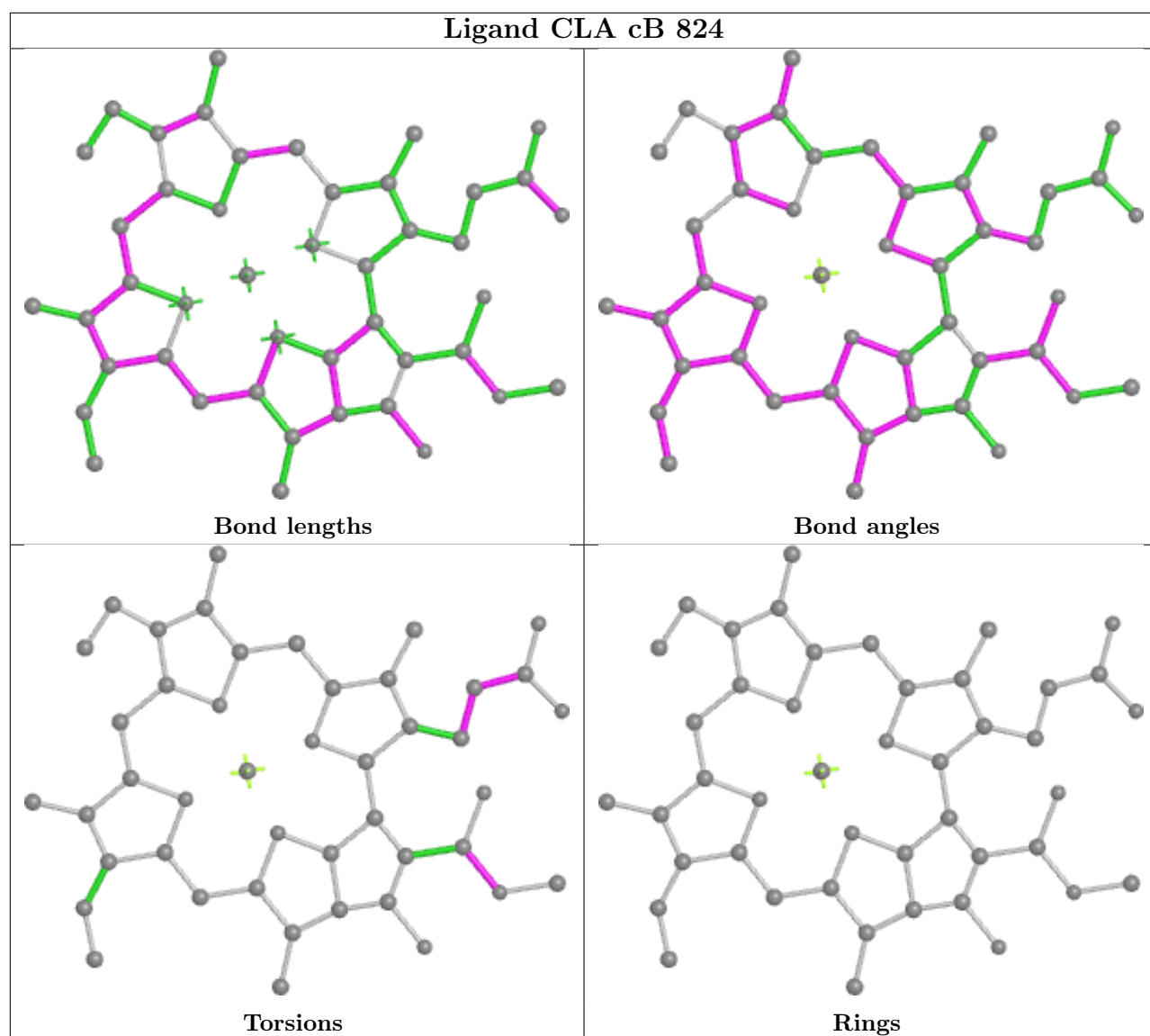


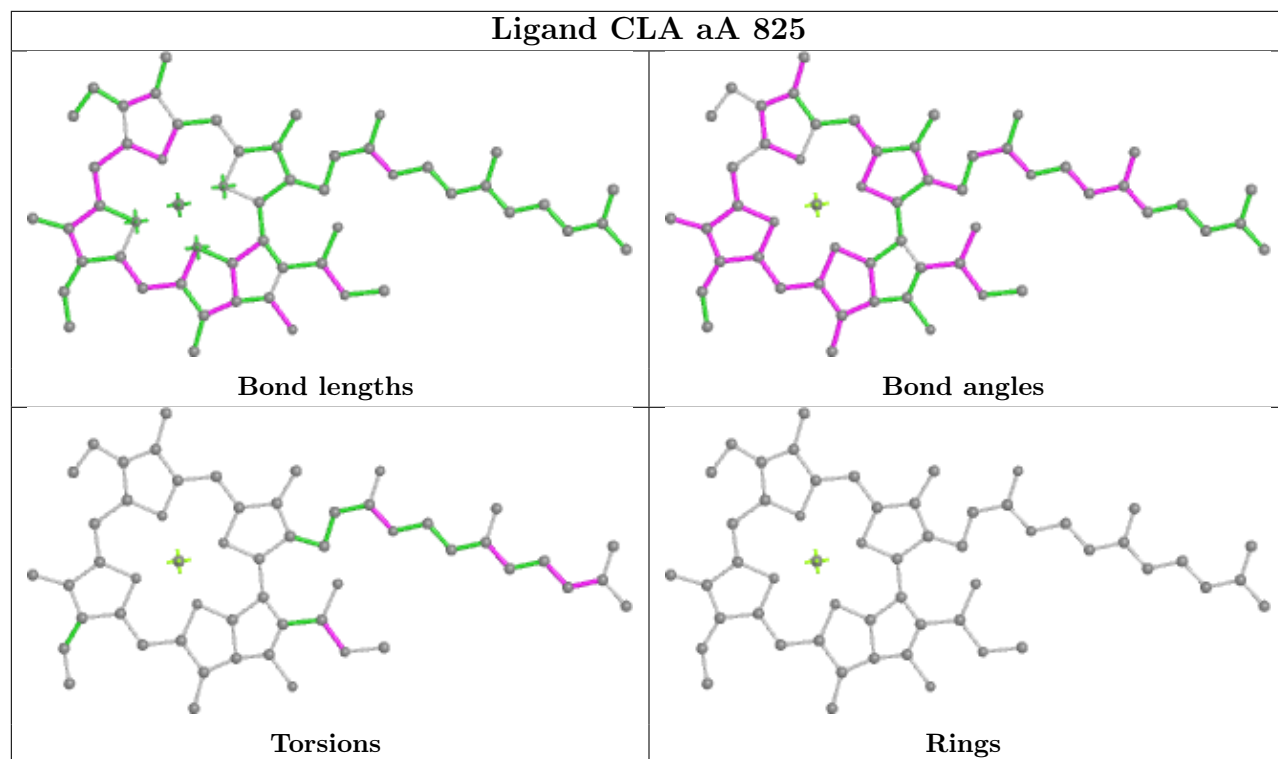
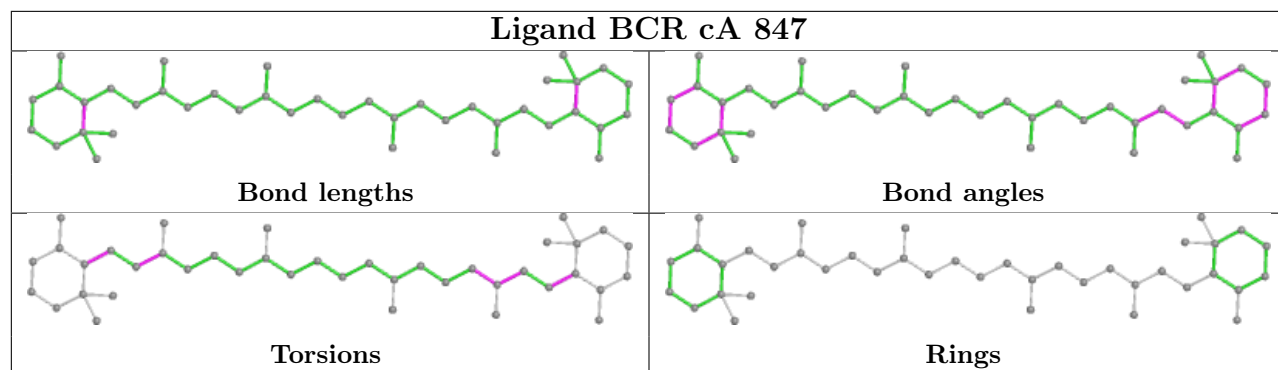
Torsions

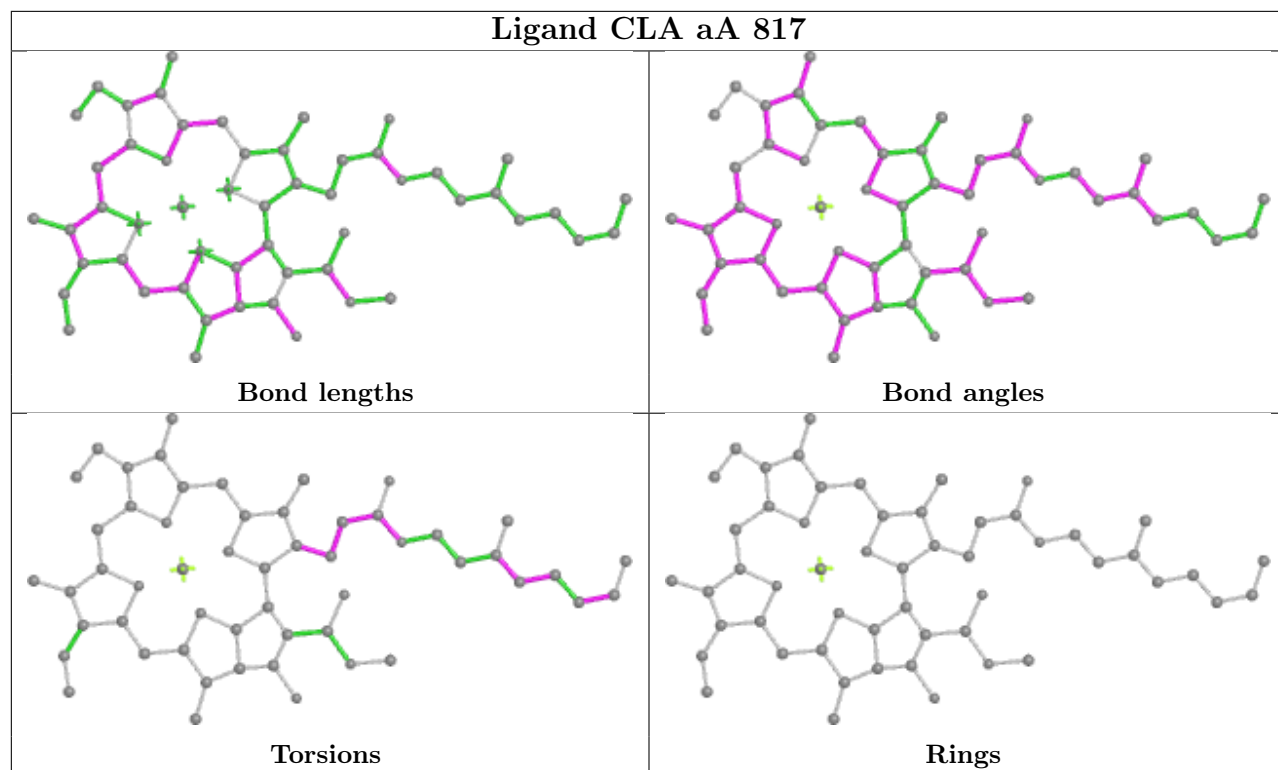


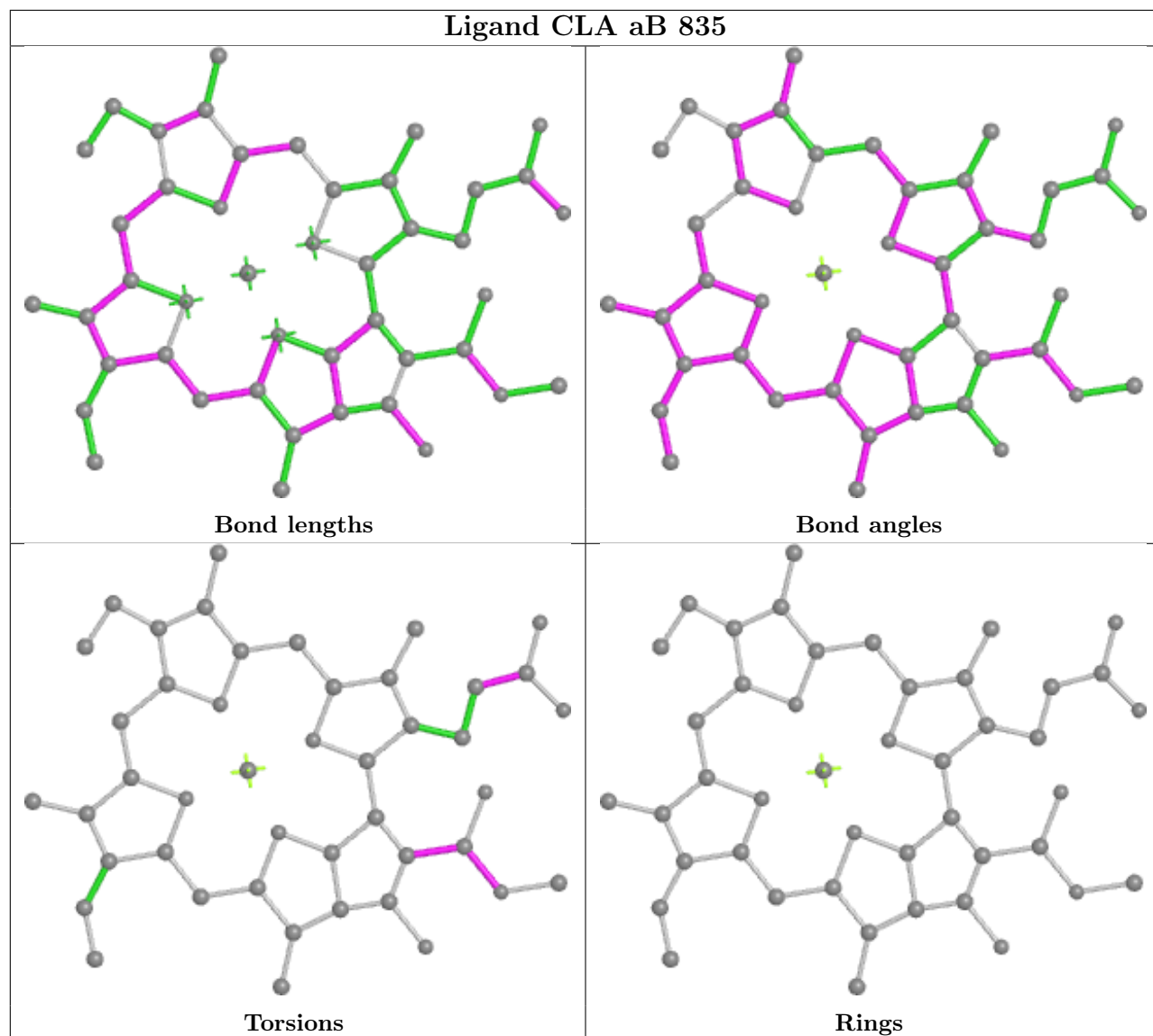
Rings

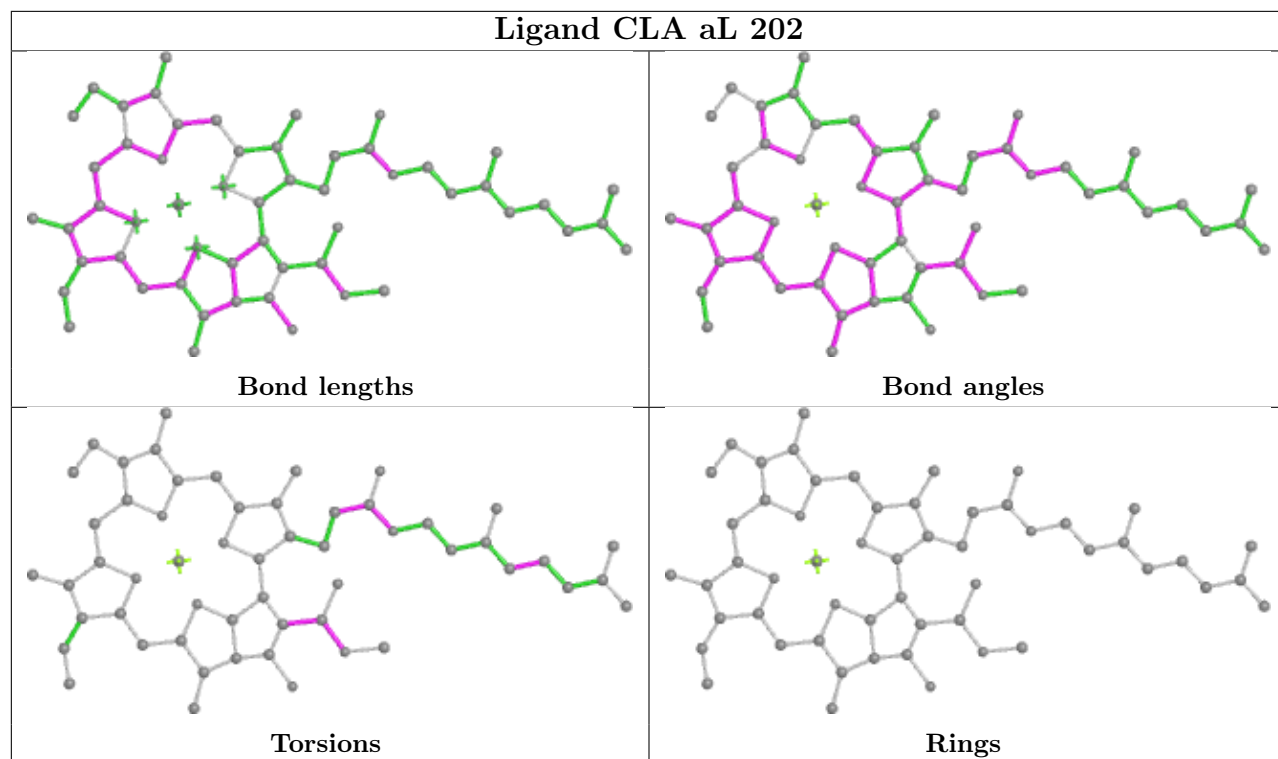


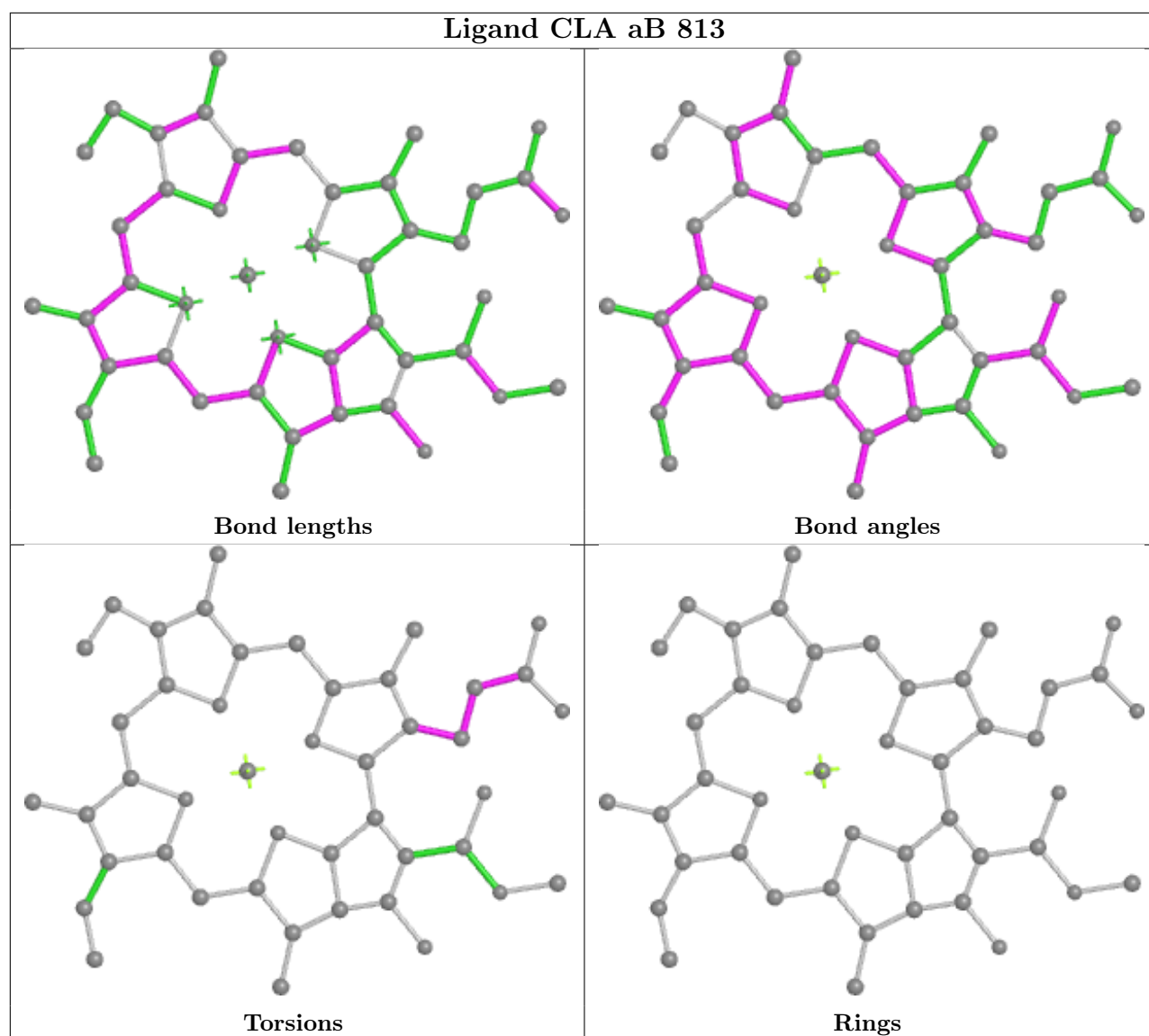


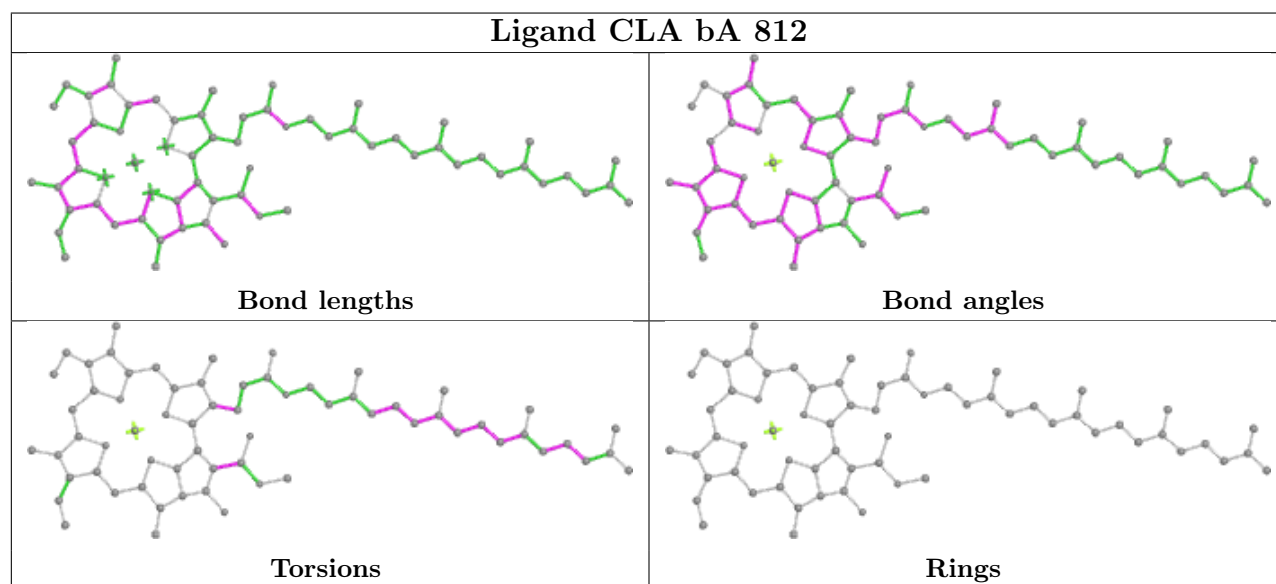
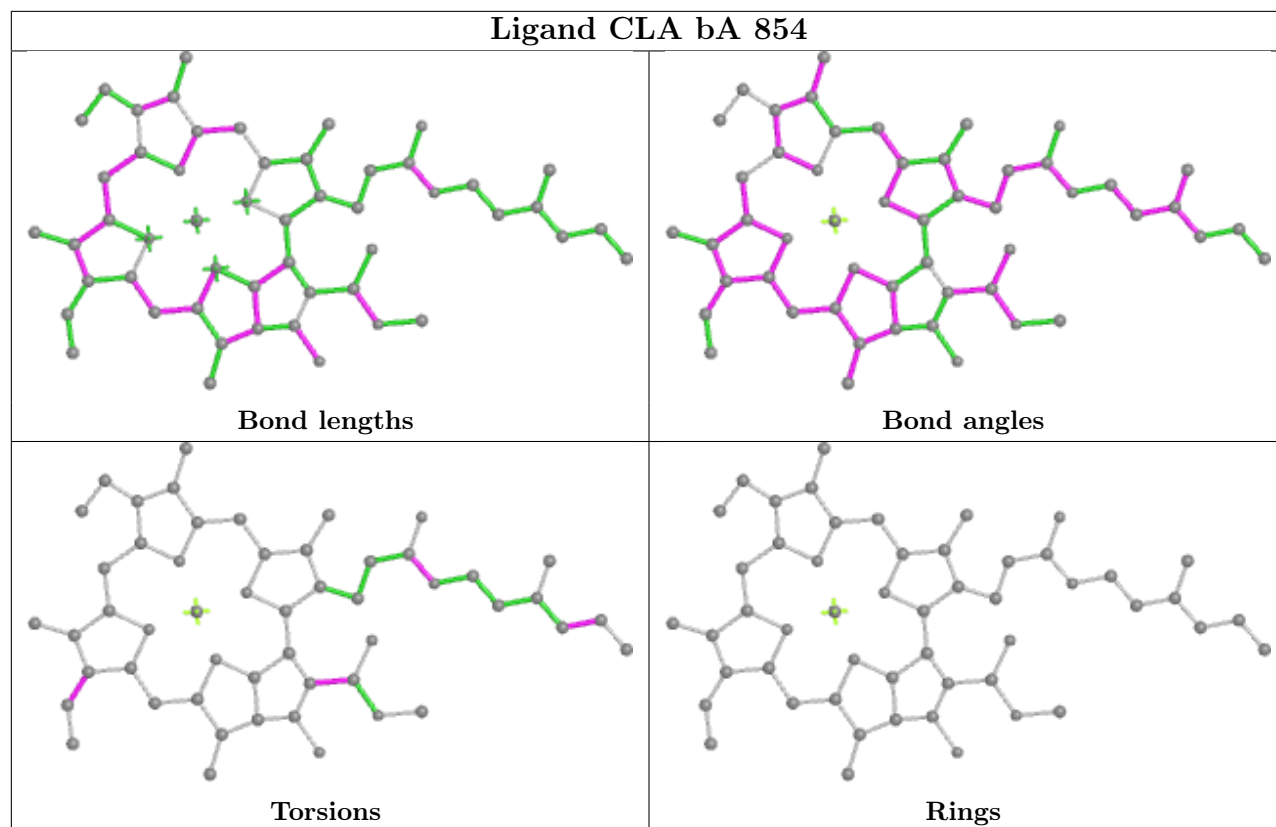


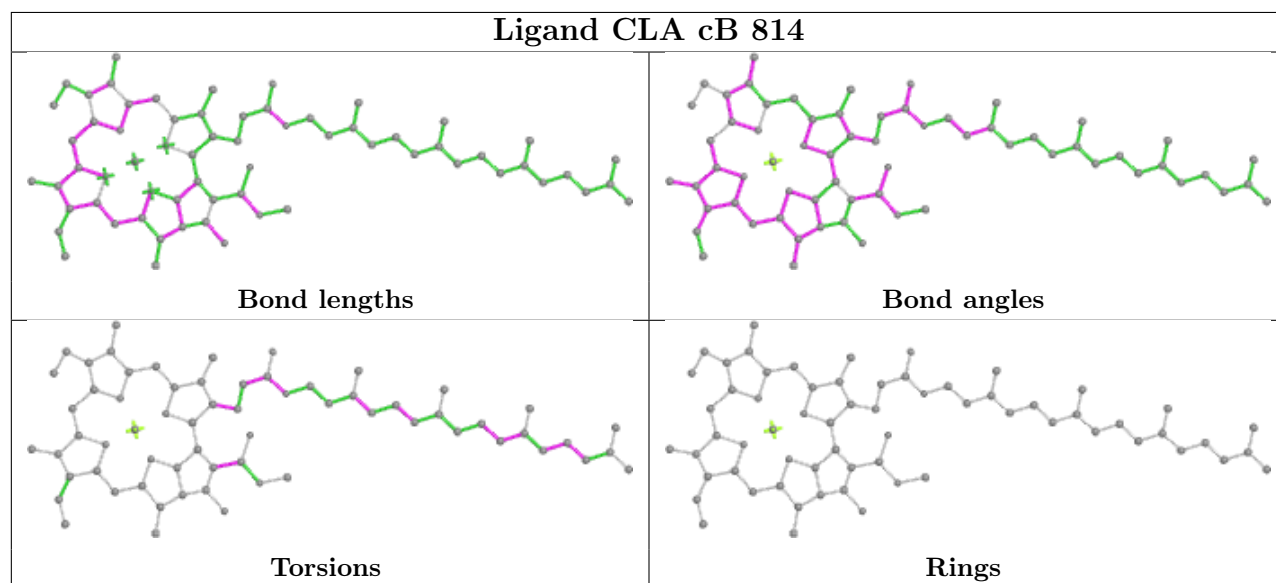
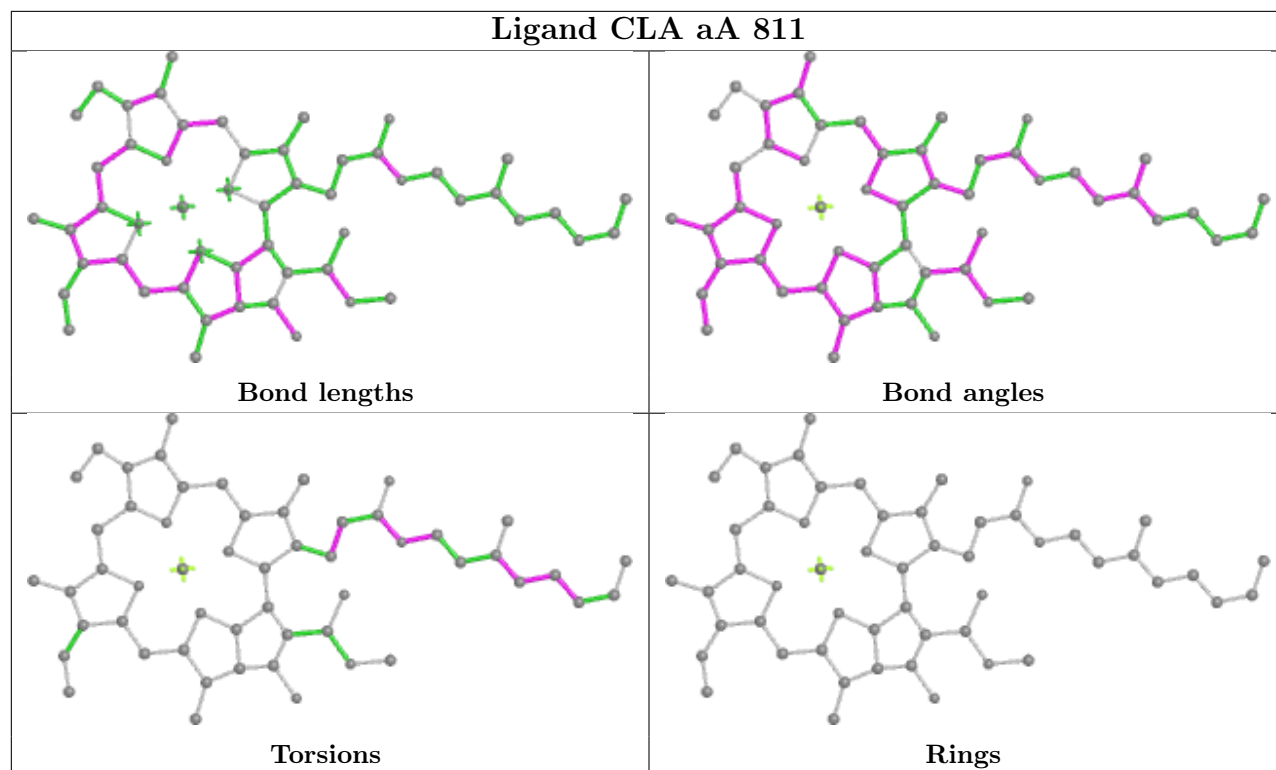


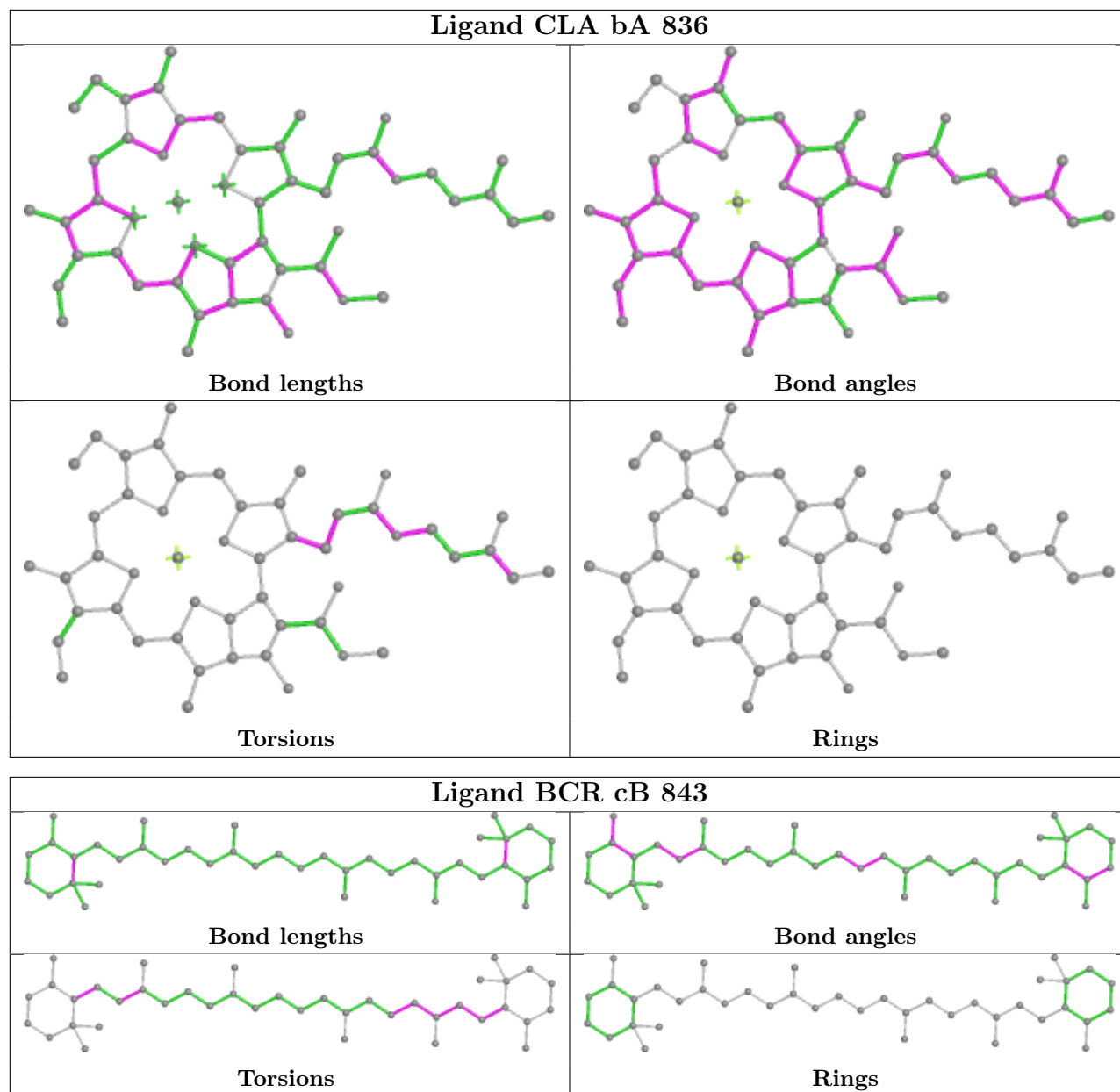




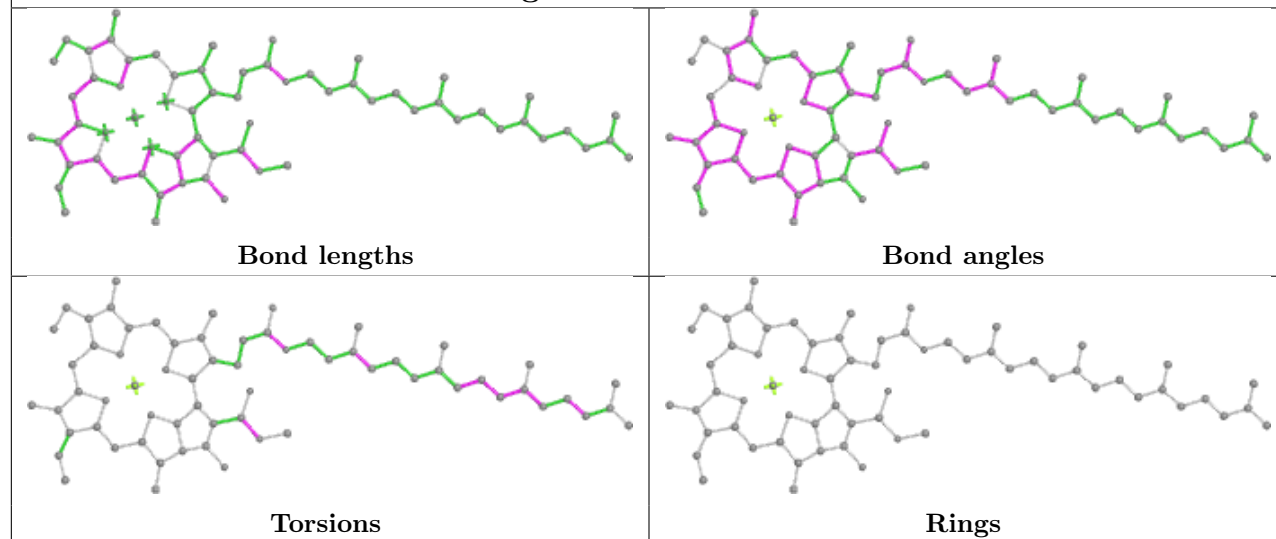




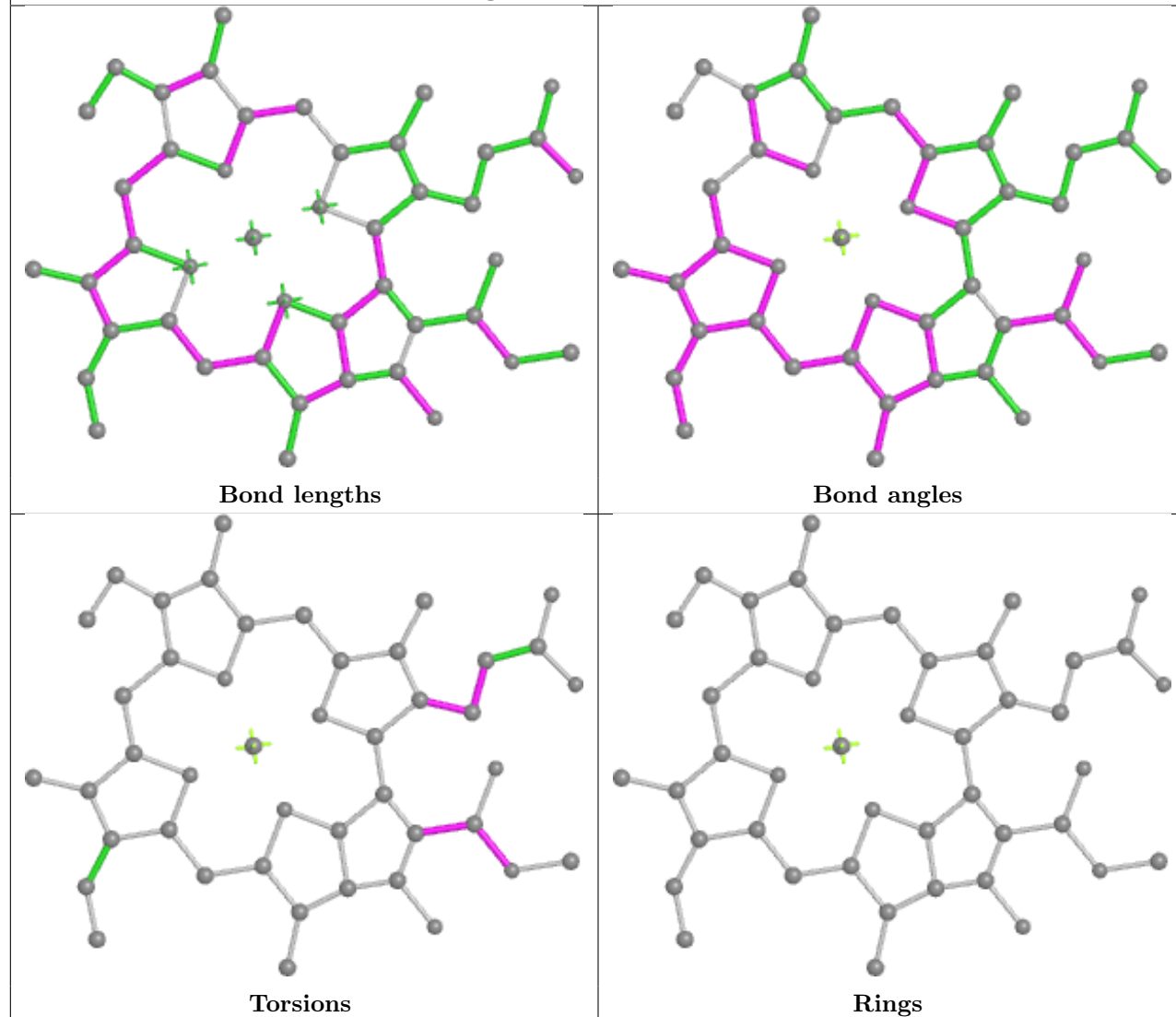


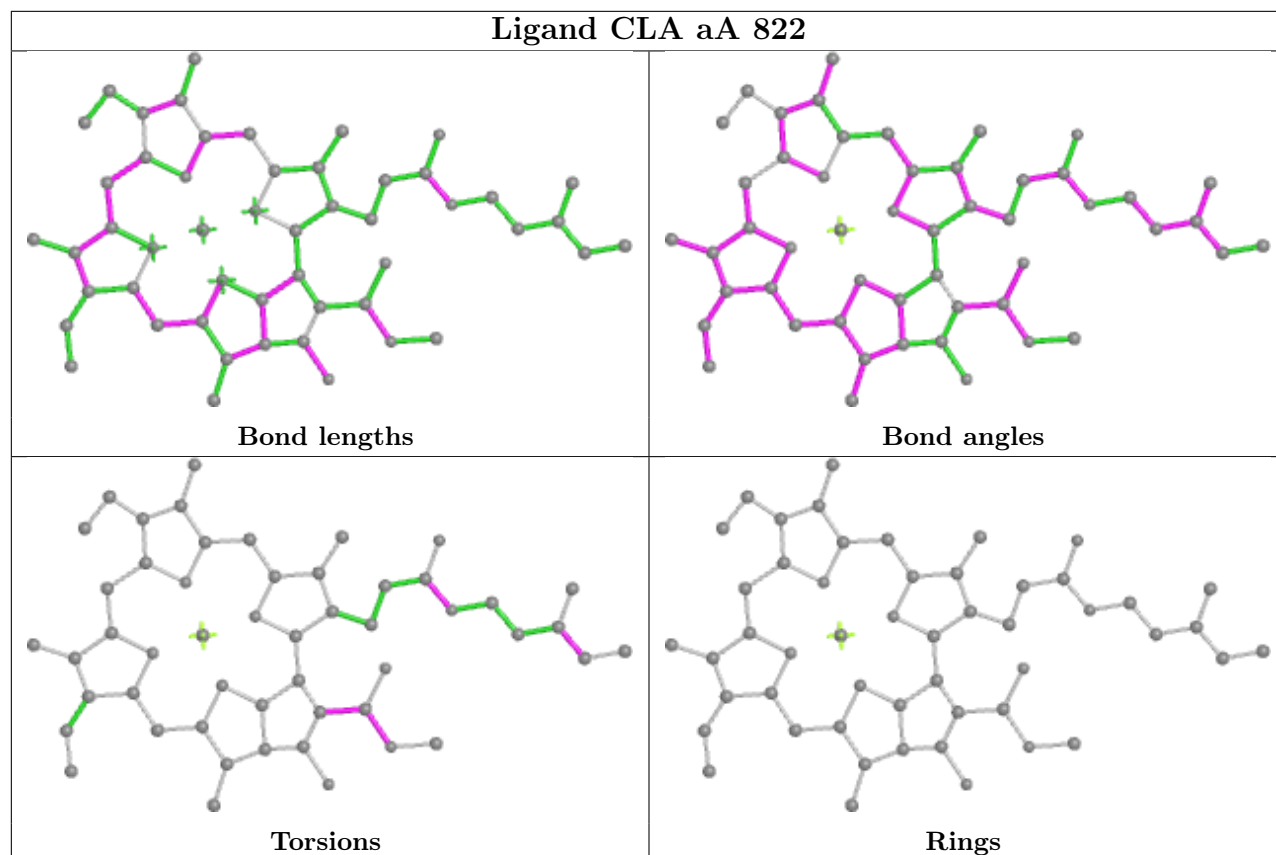
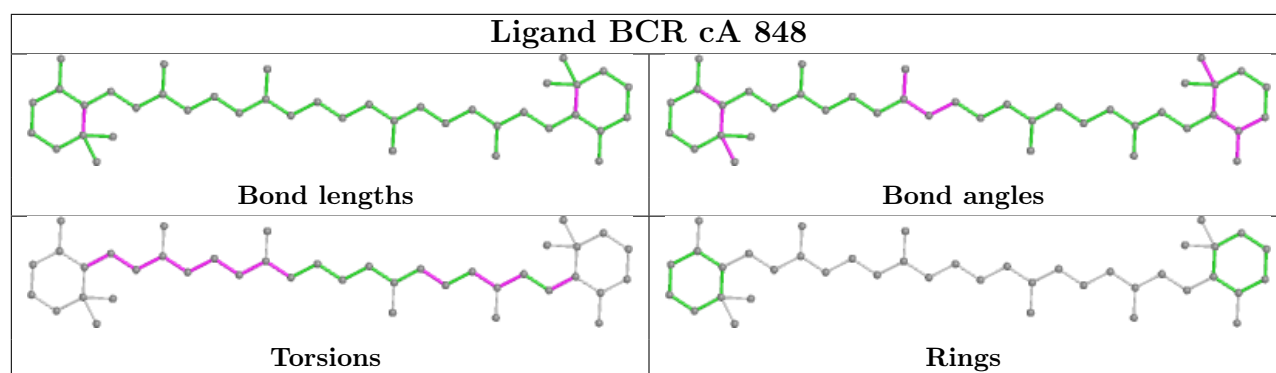


Ligand CLA bA 820

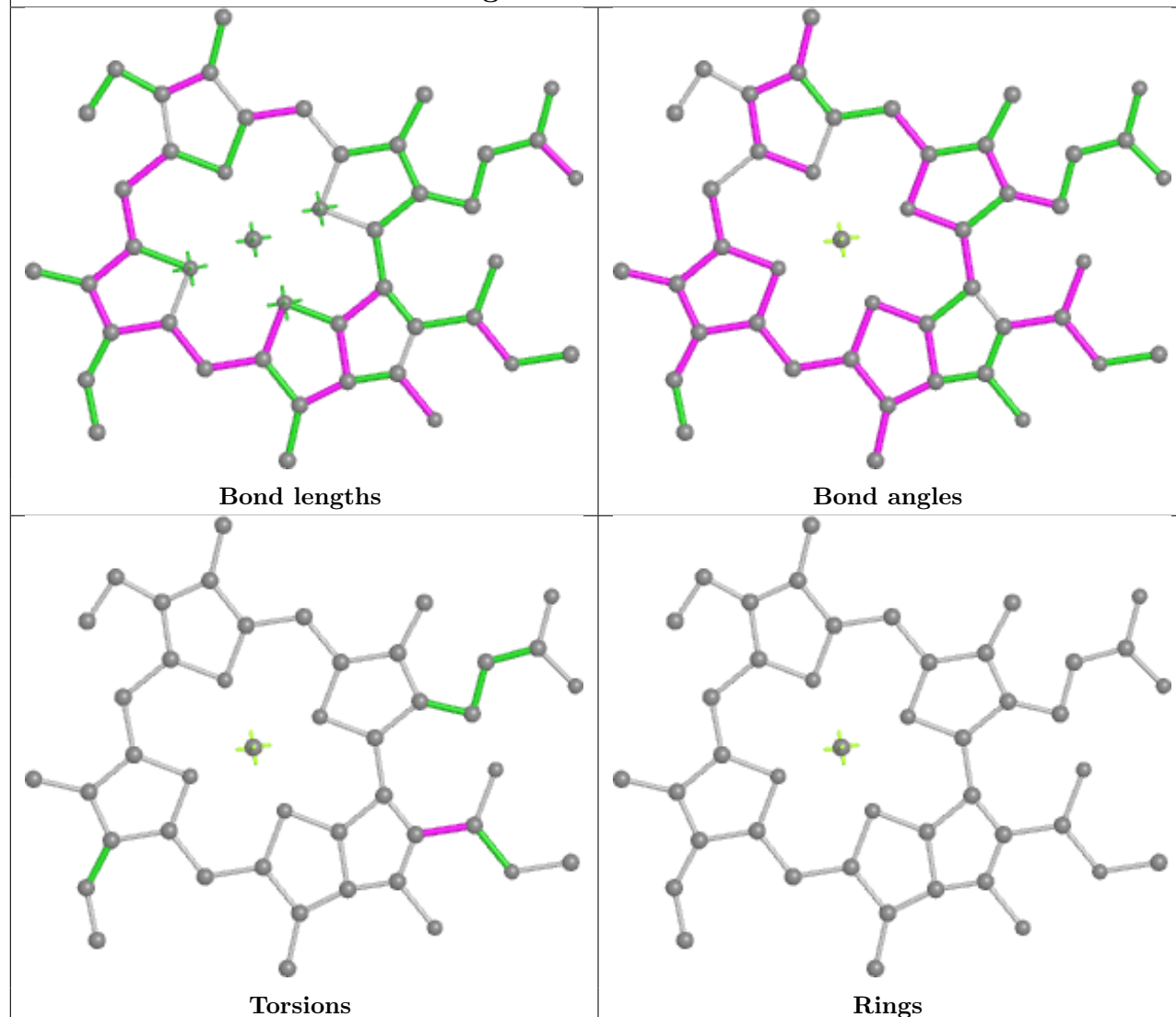


Ligand CLA aB 822

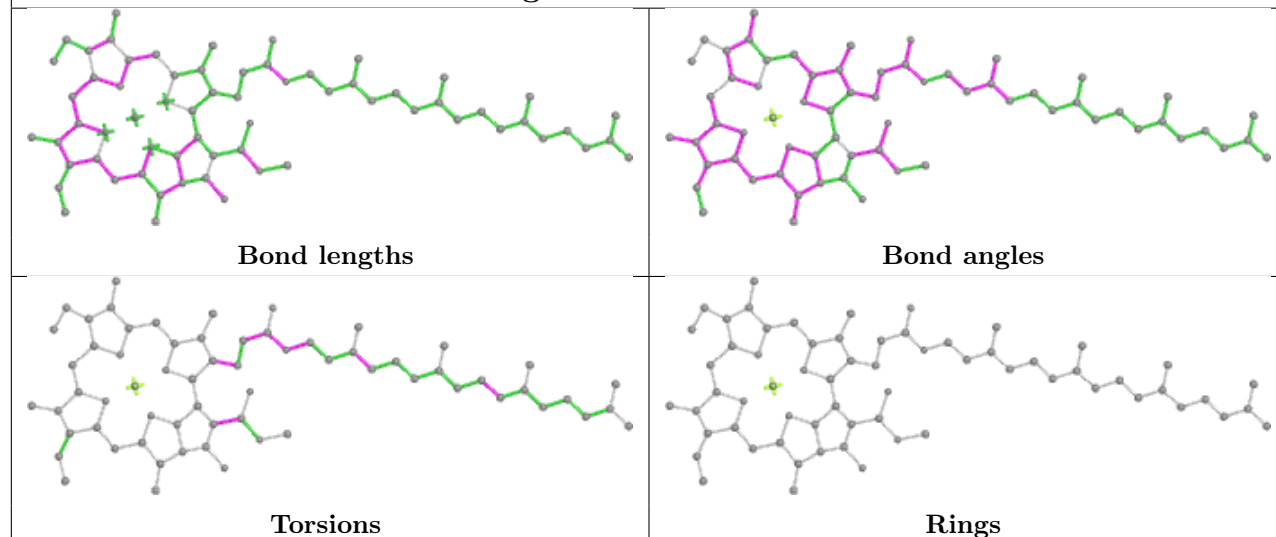


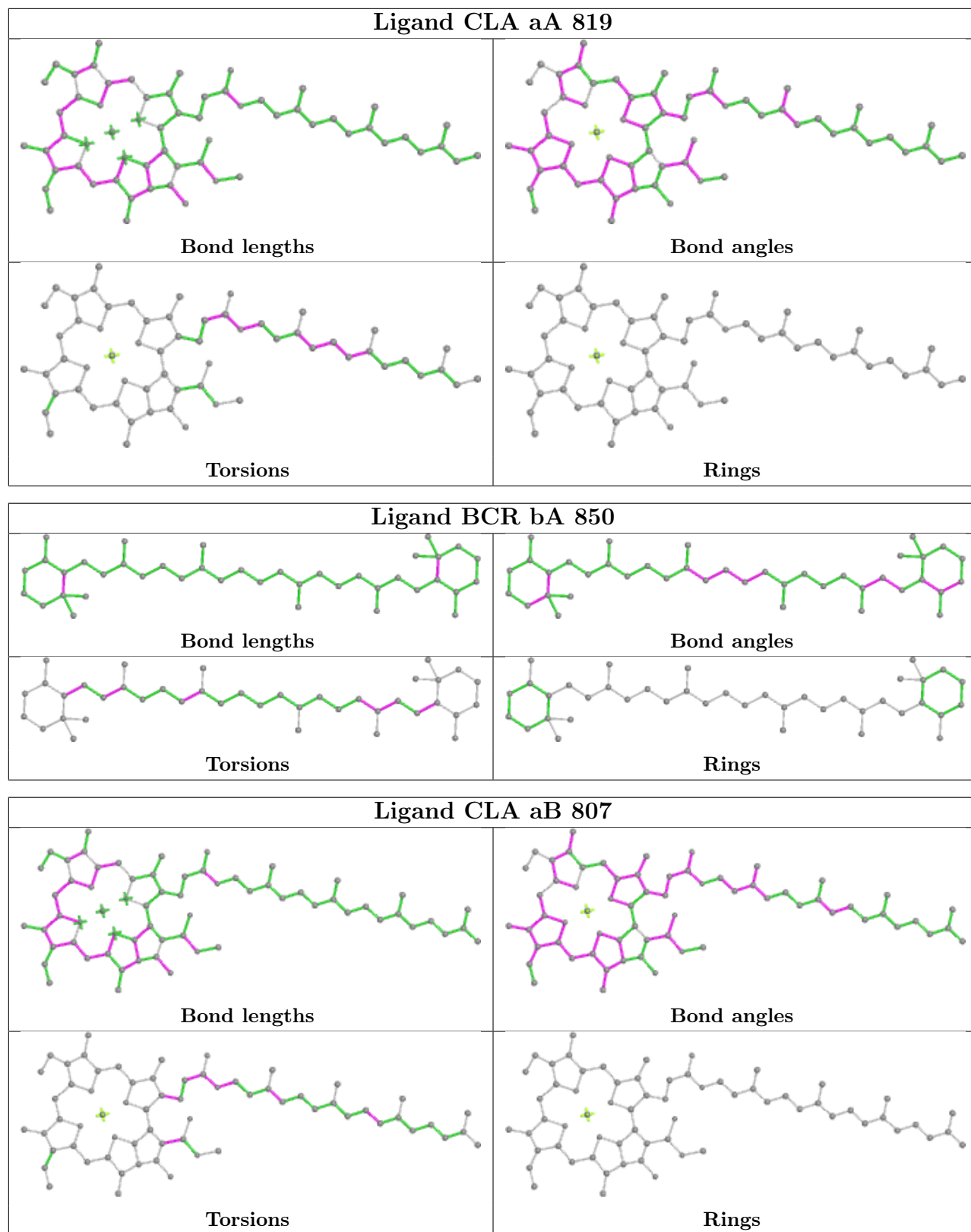


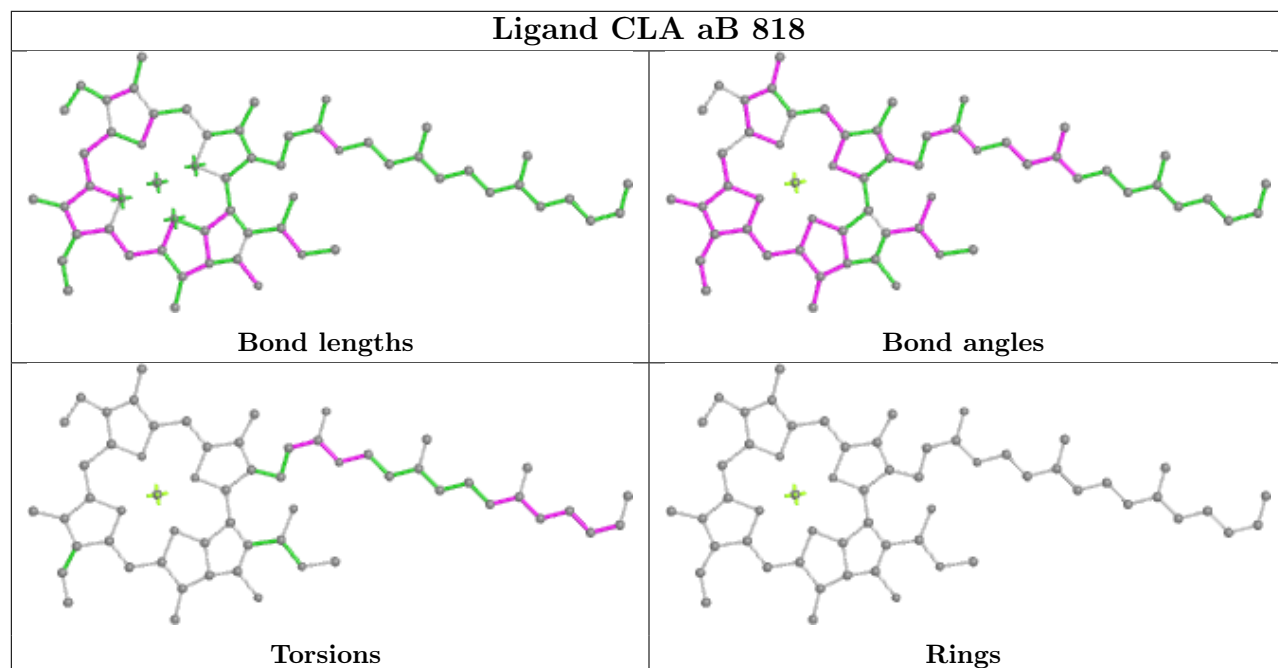
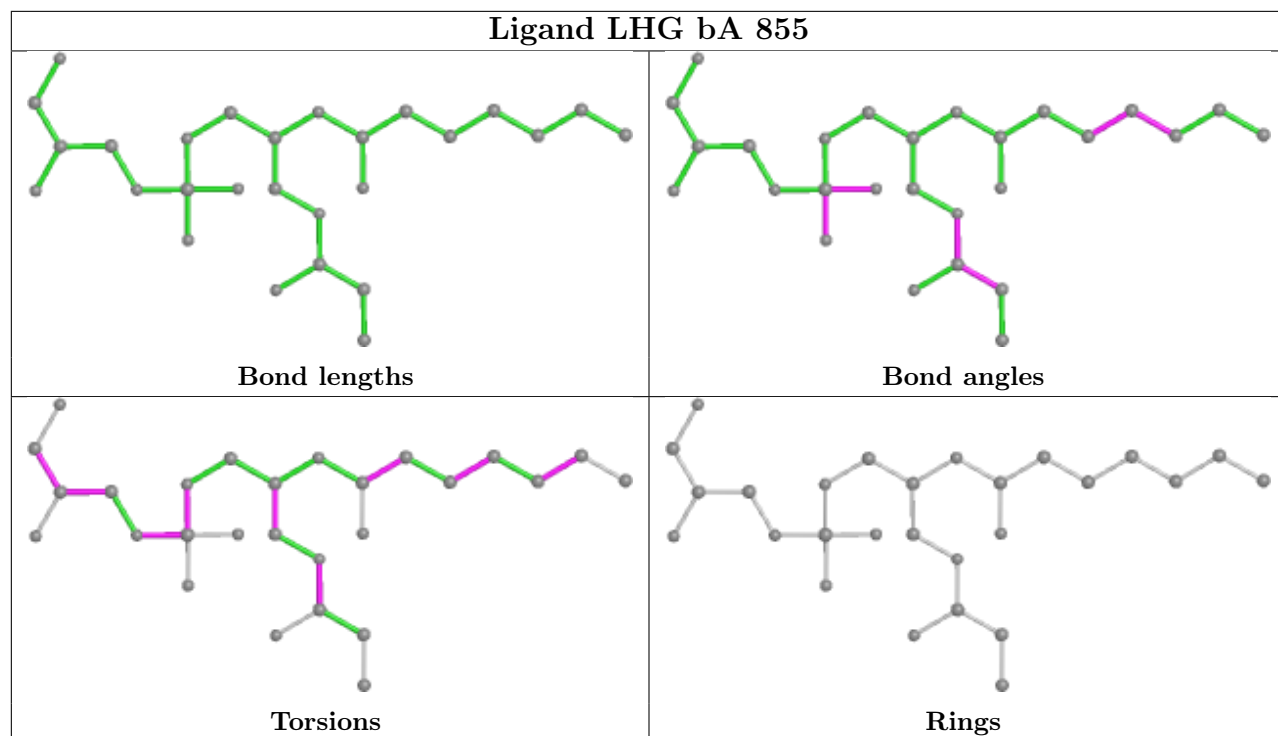
Ligand CLA aB 816

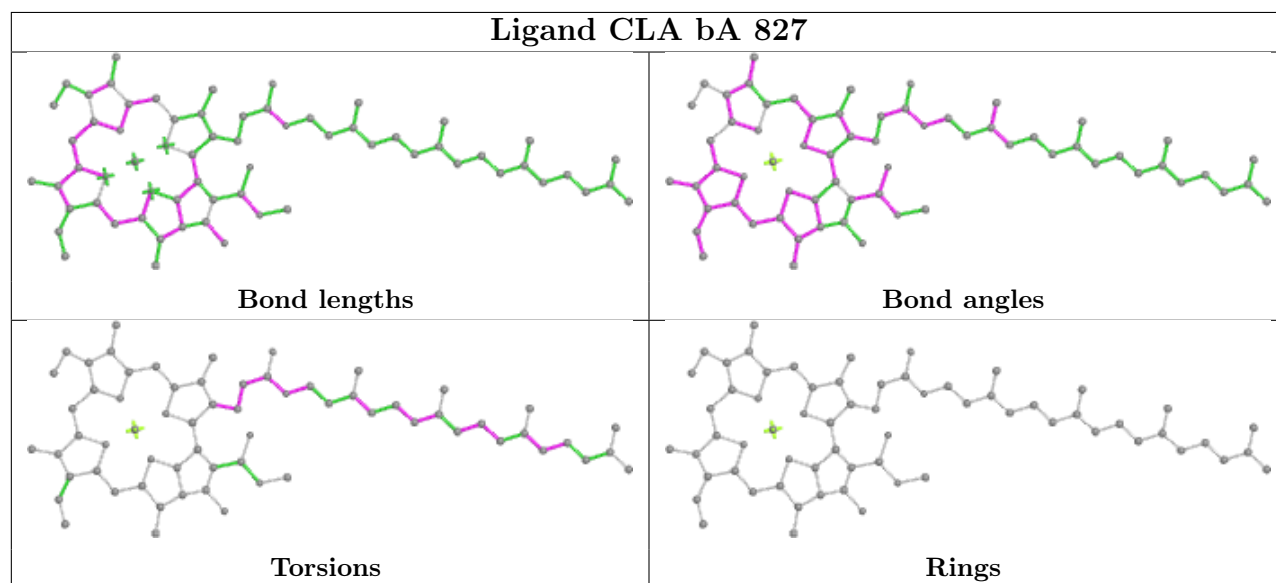
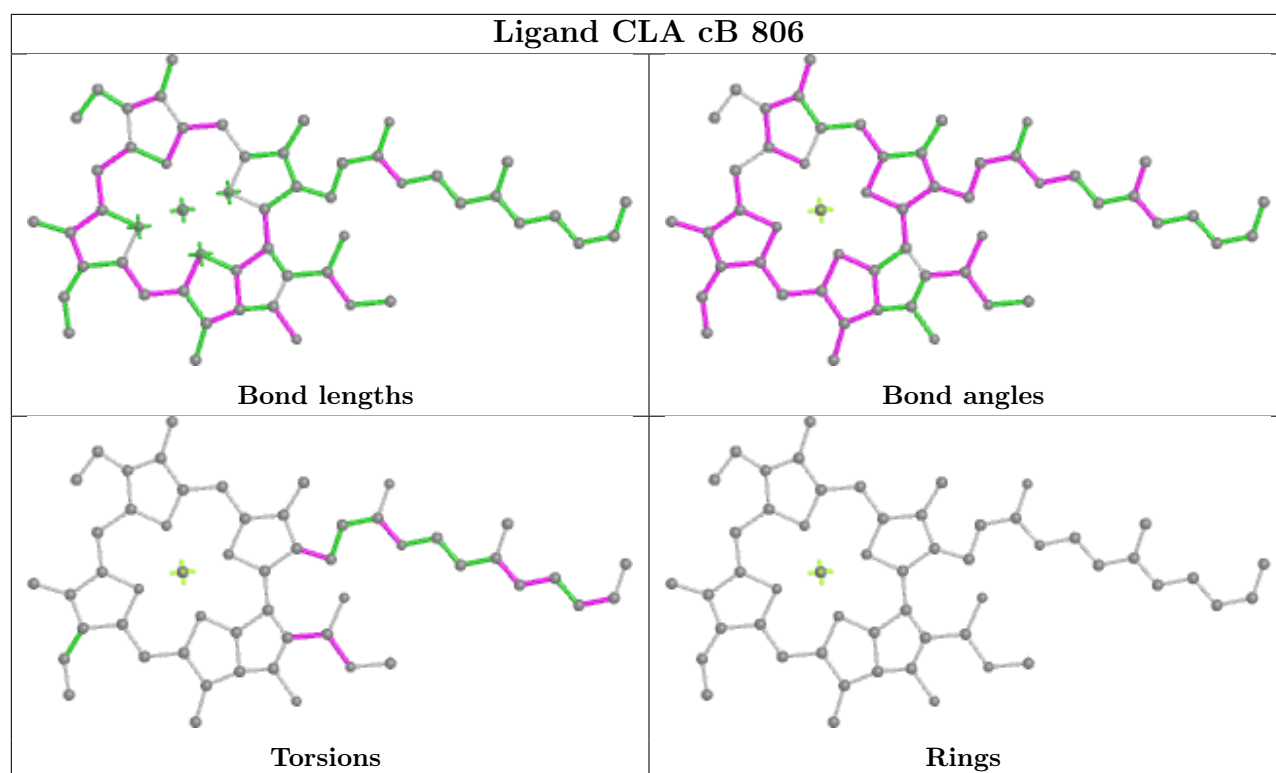


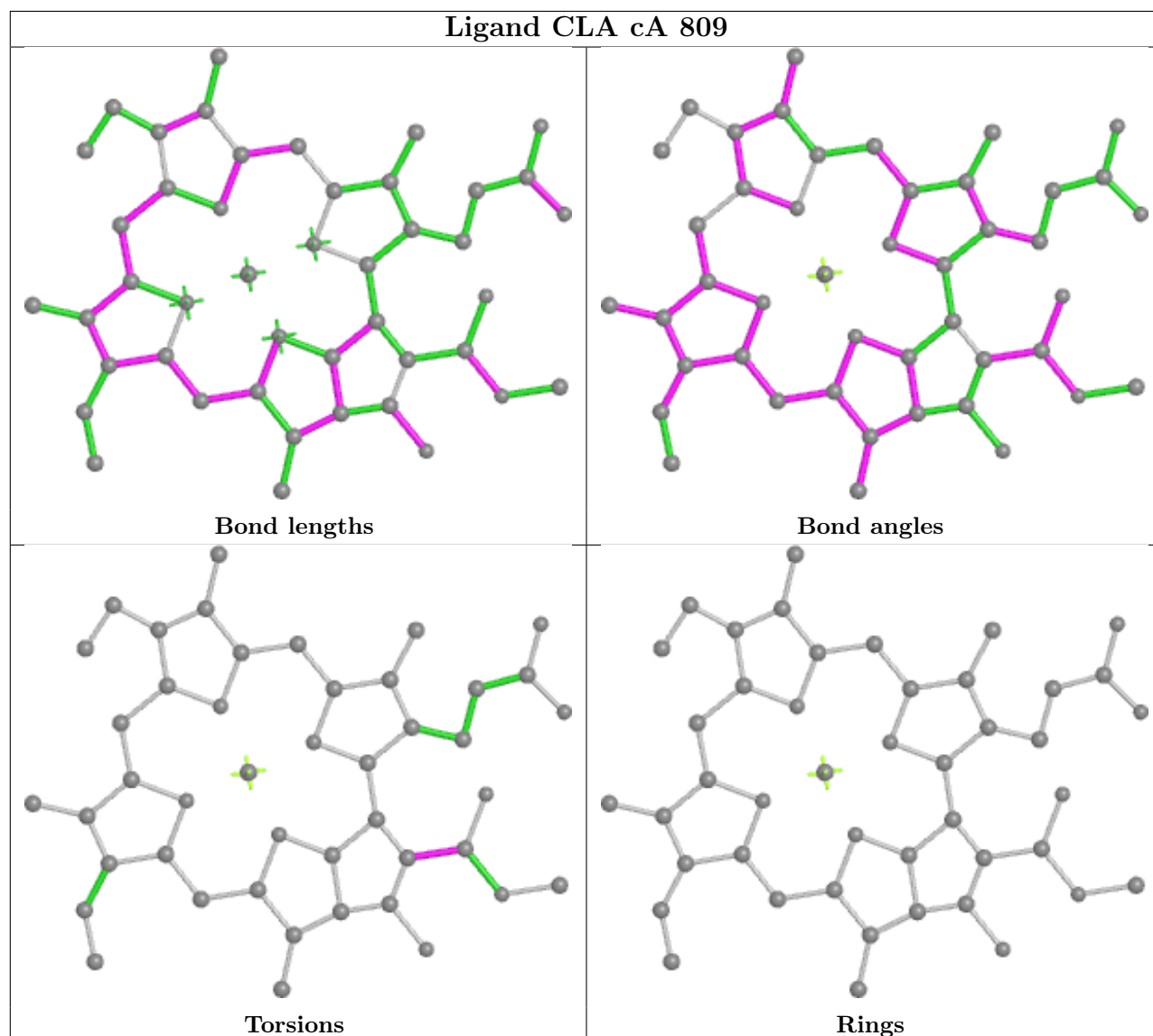
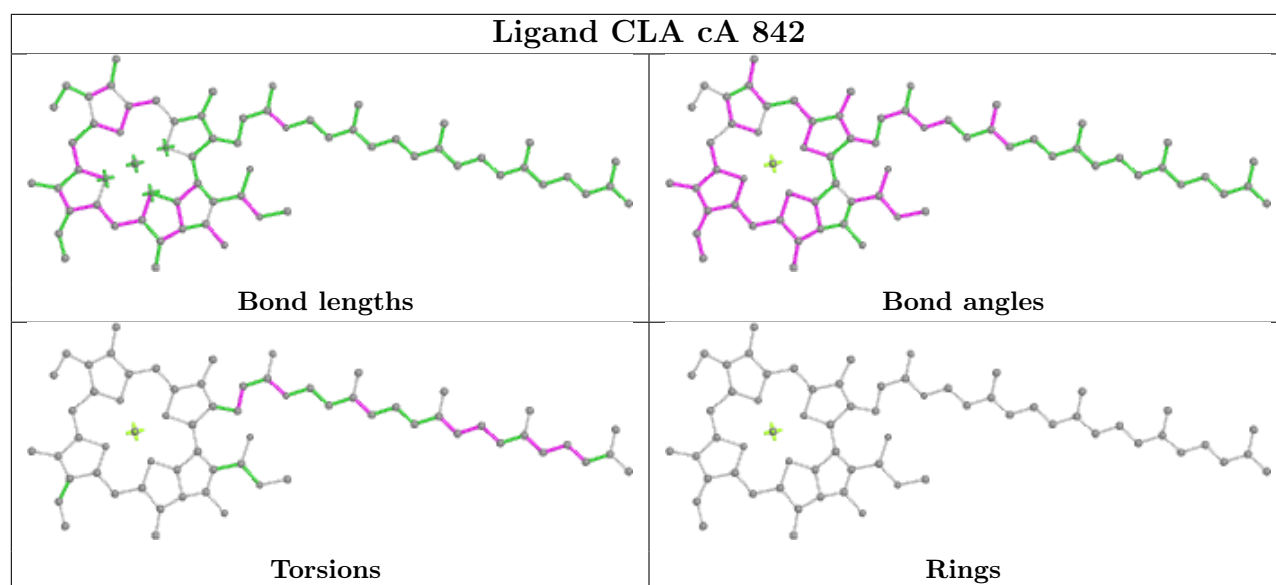
Ligand CLA bB 807

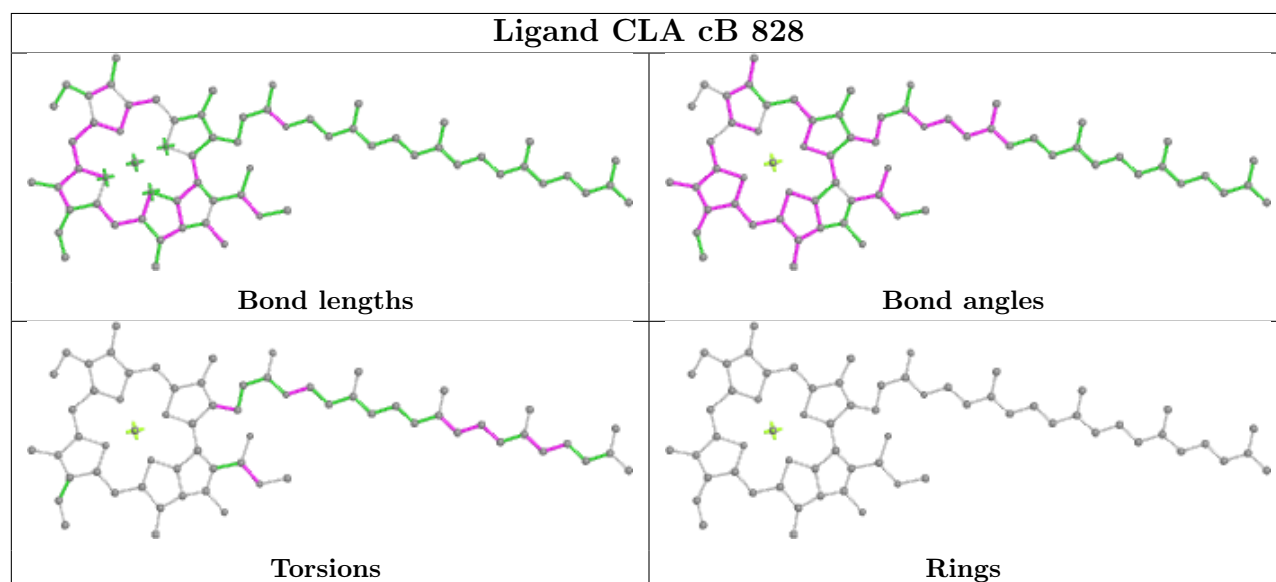
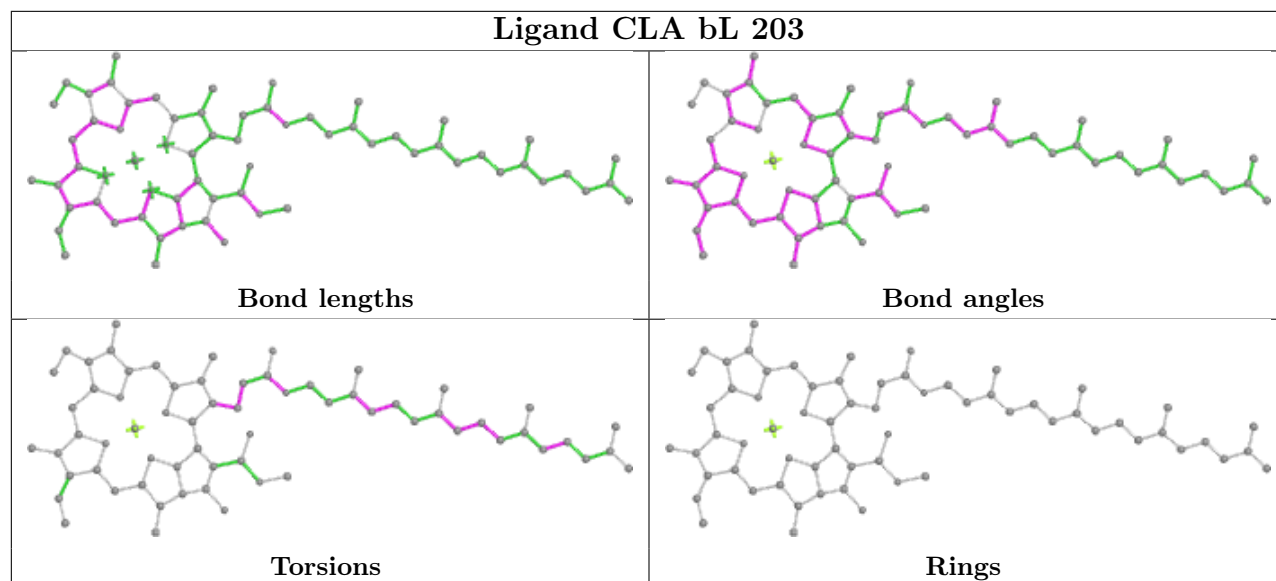
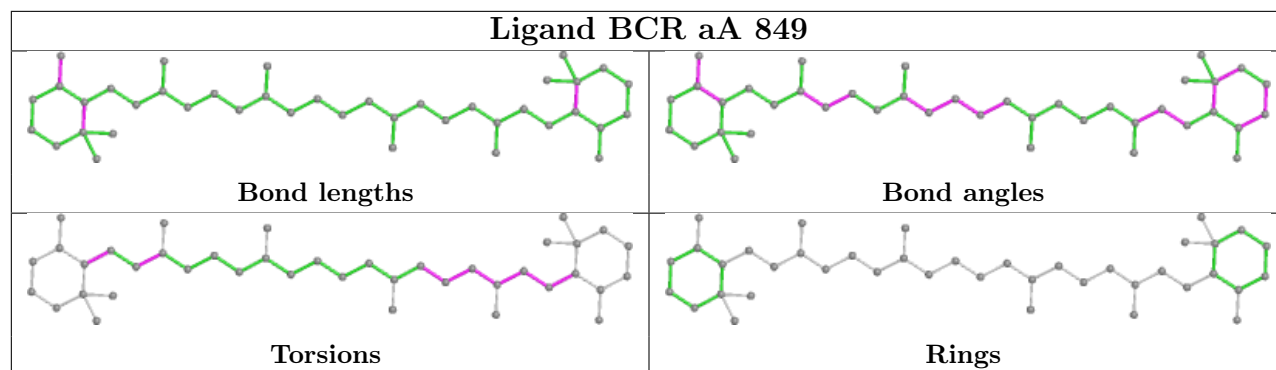




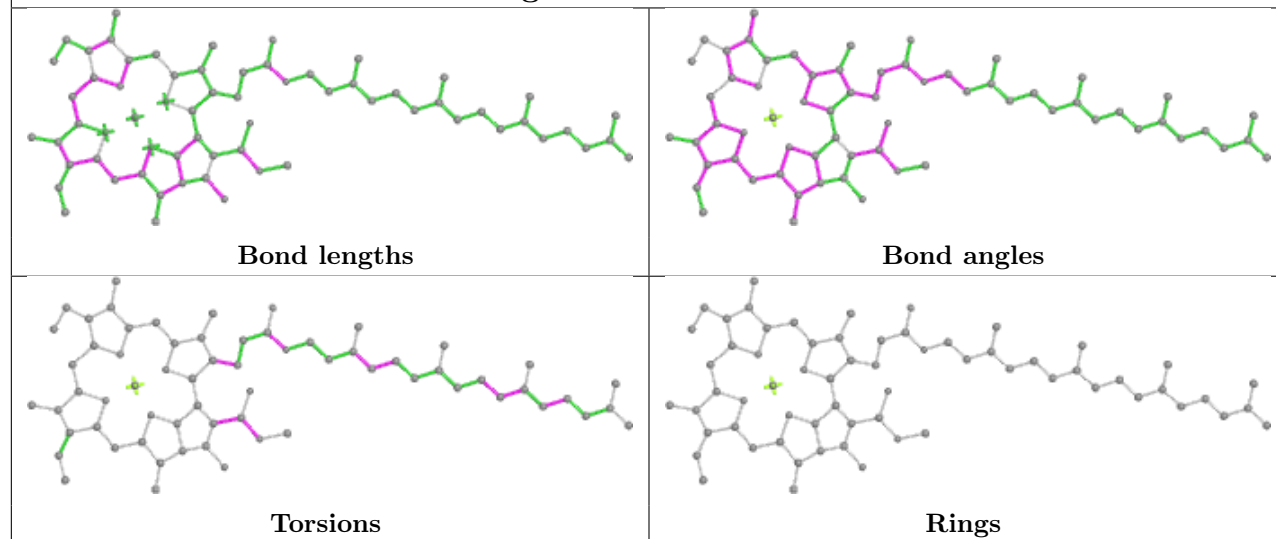




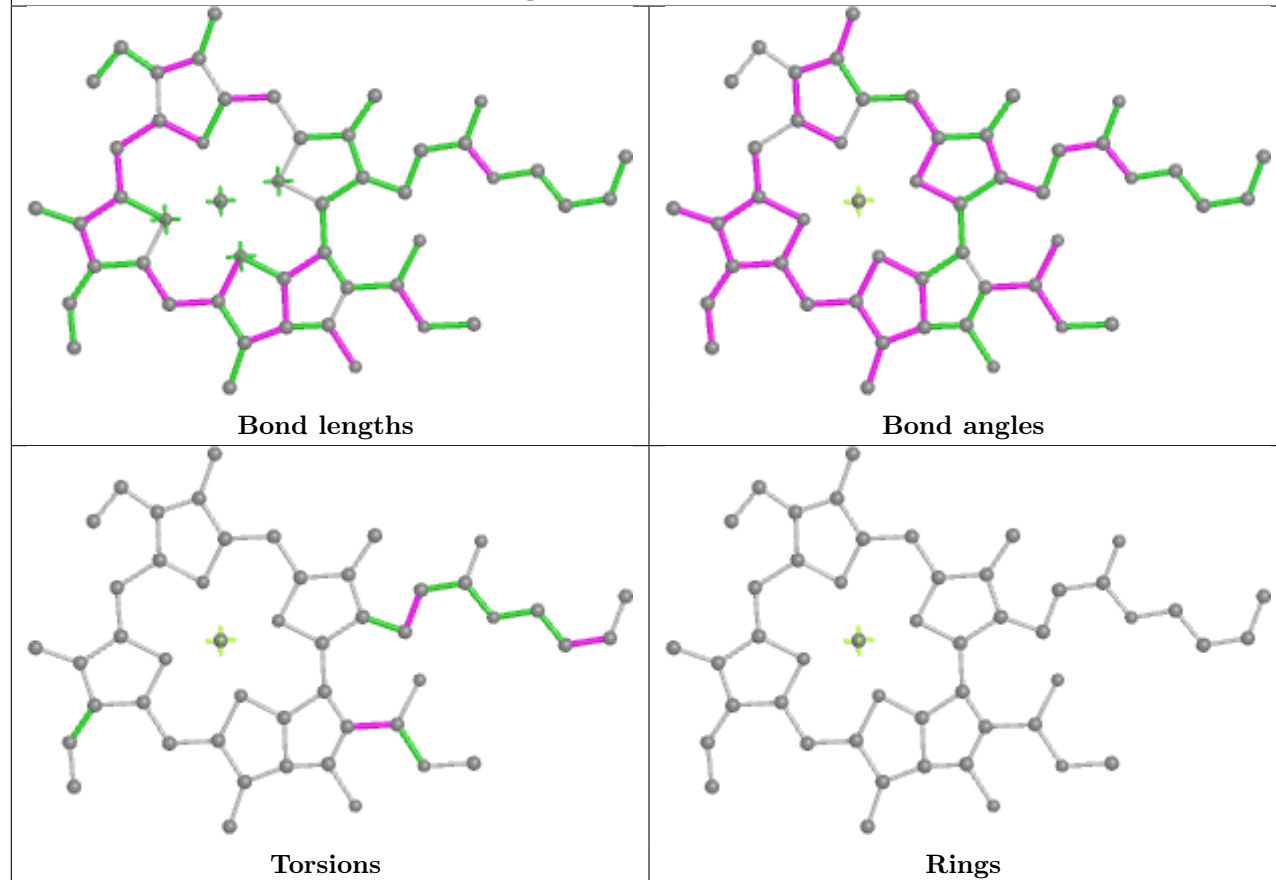


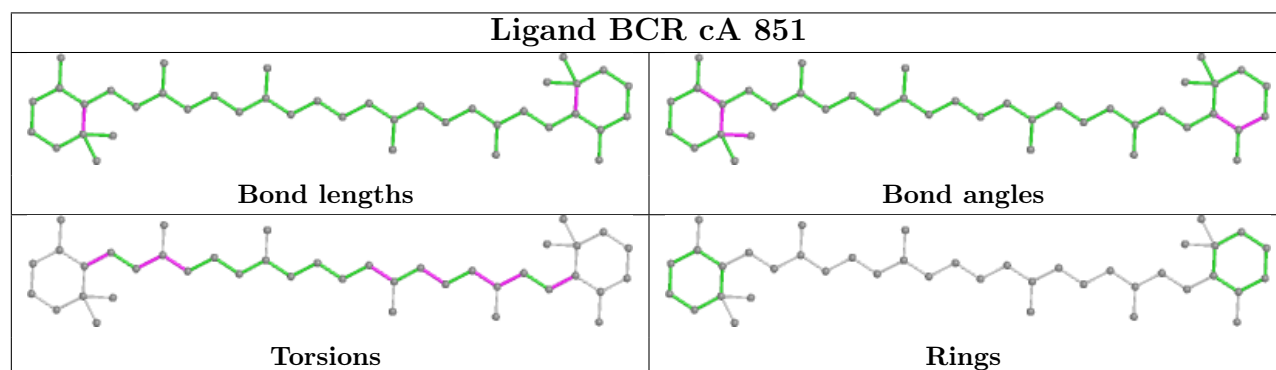
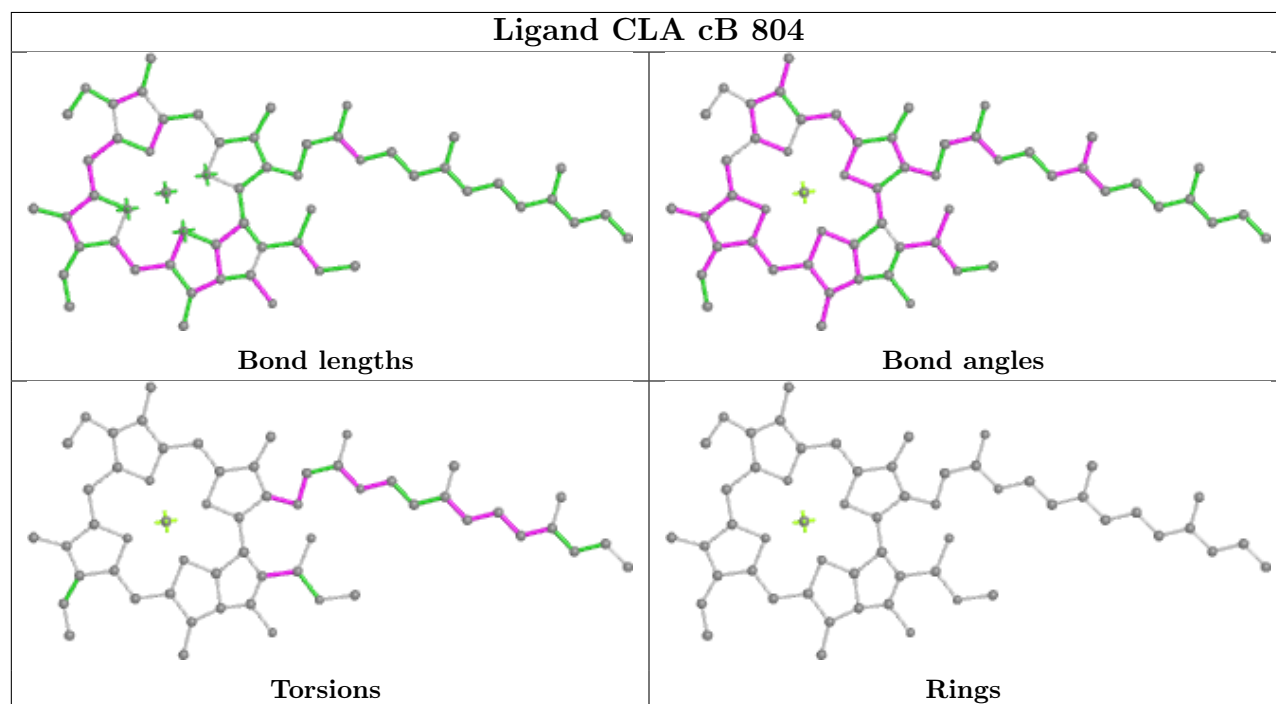
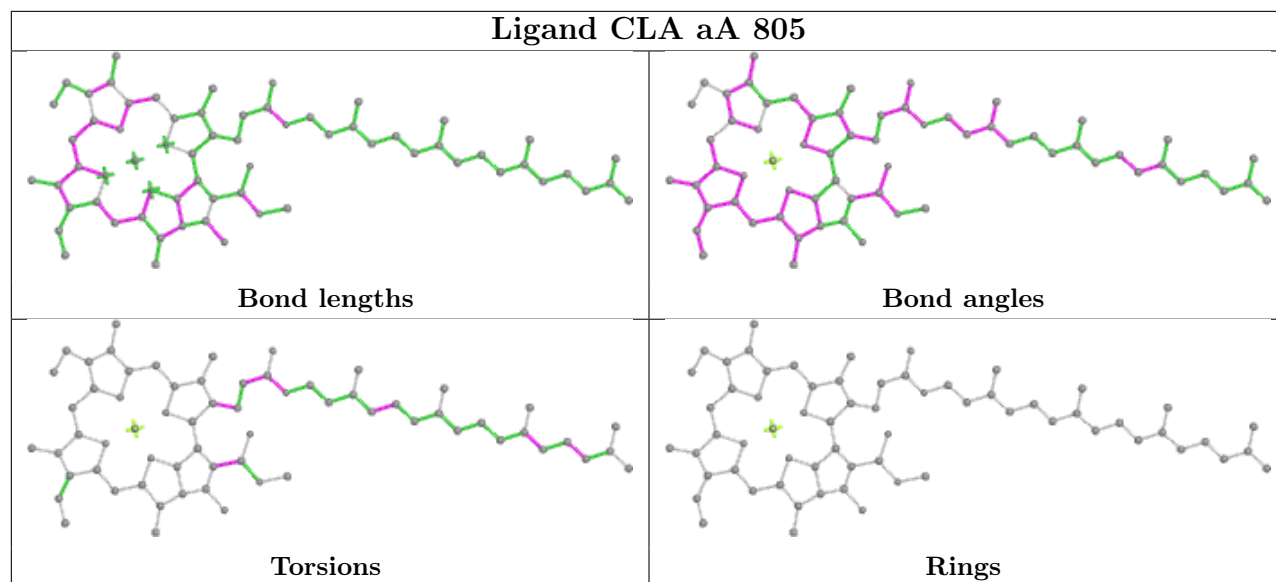


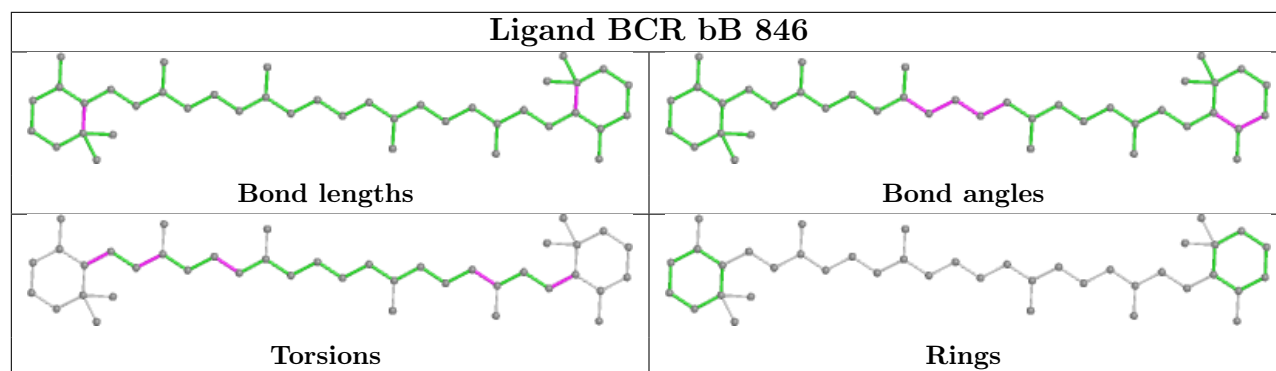
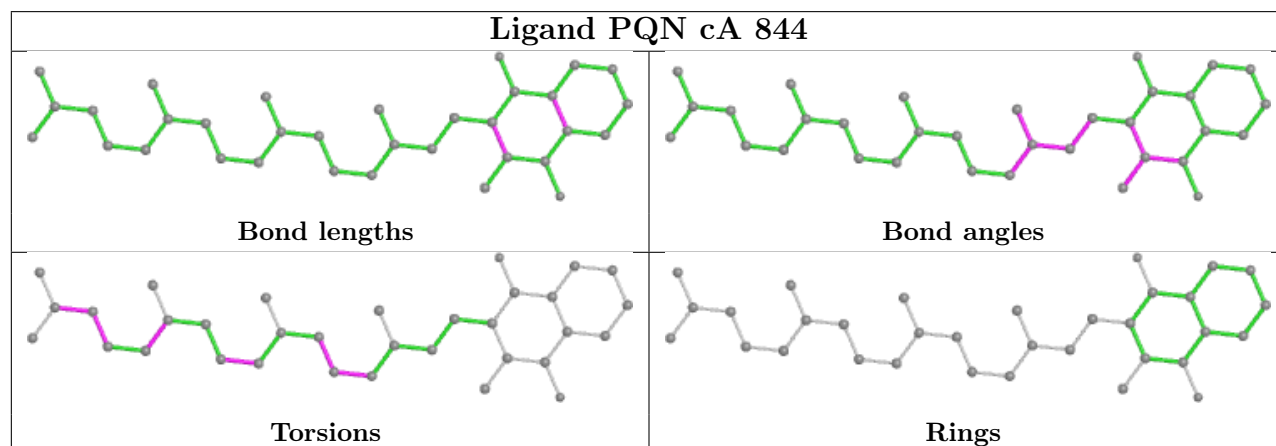
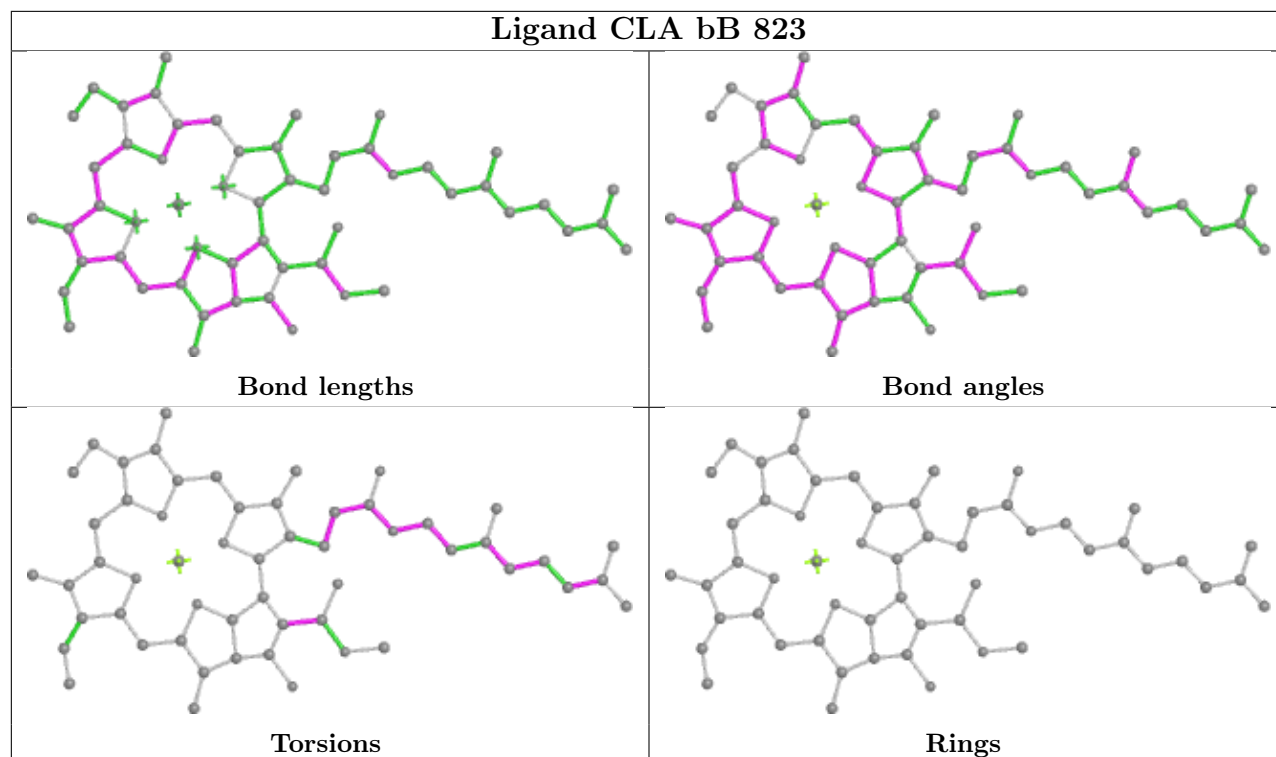
Ligand CLA bA 818



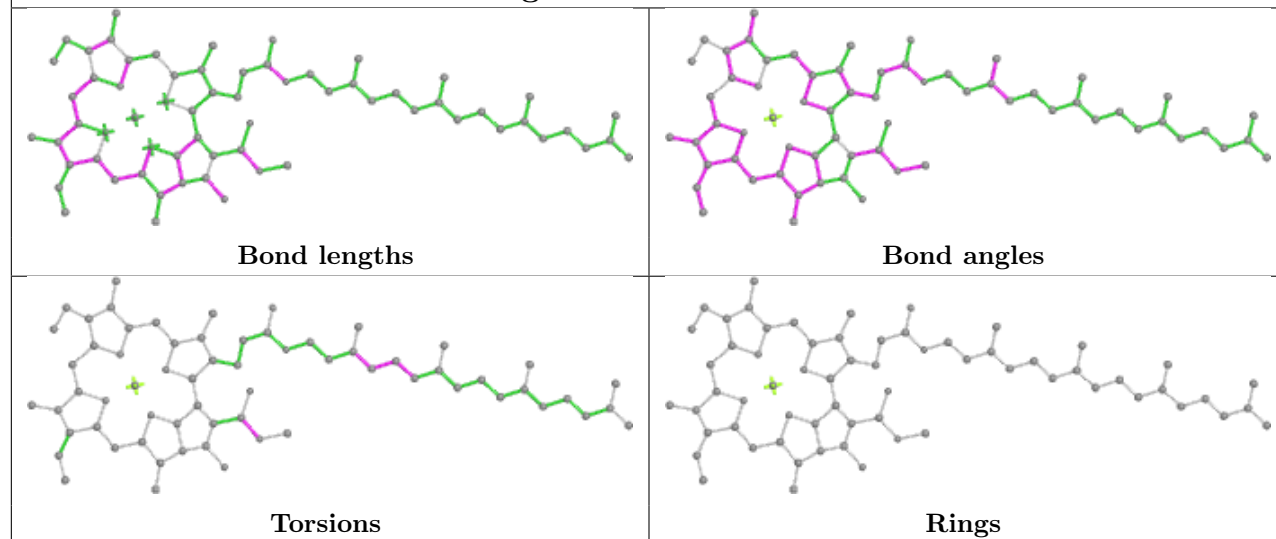
Ligand CLA bA 821



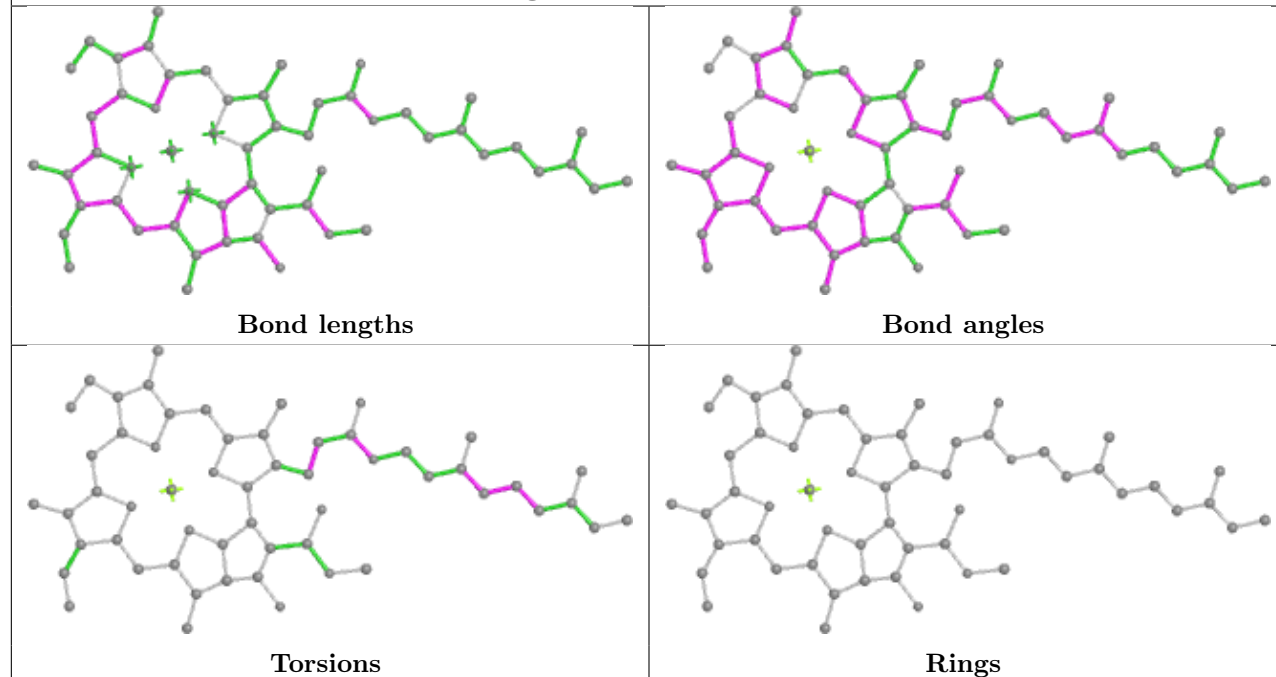




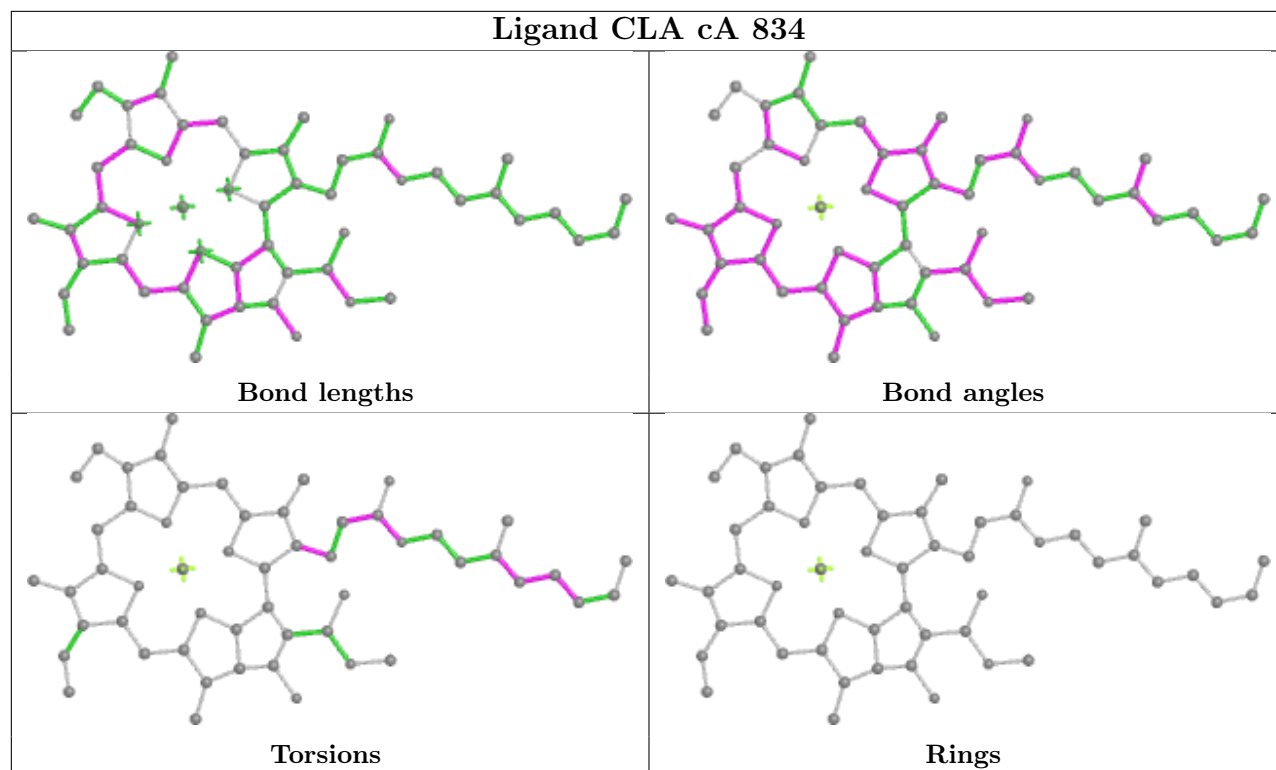
Ligand CLA bA 839



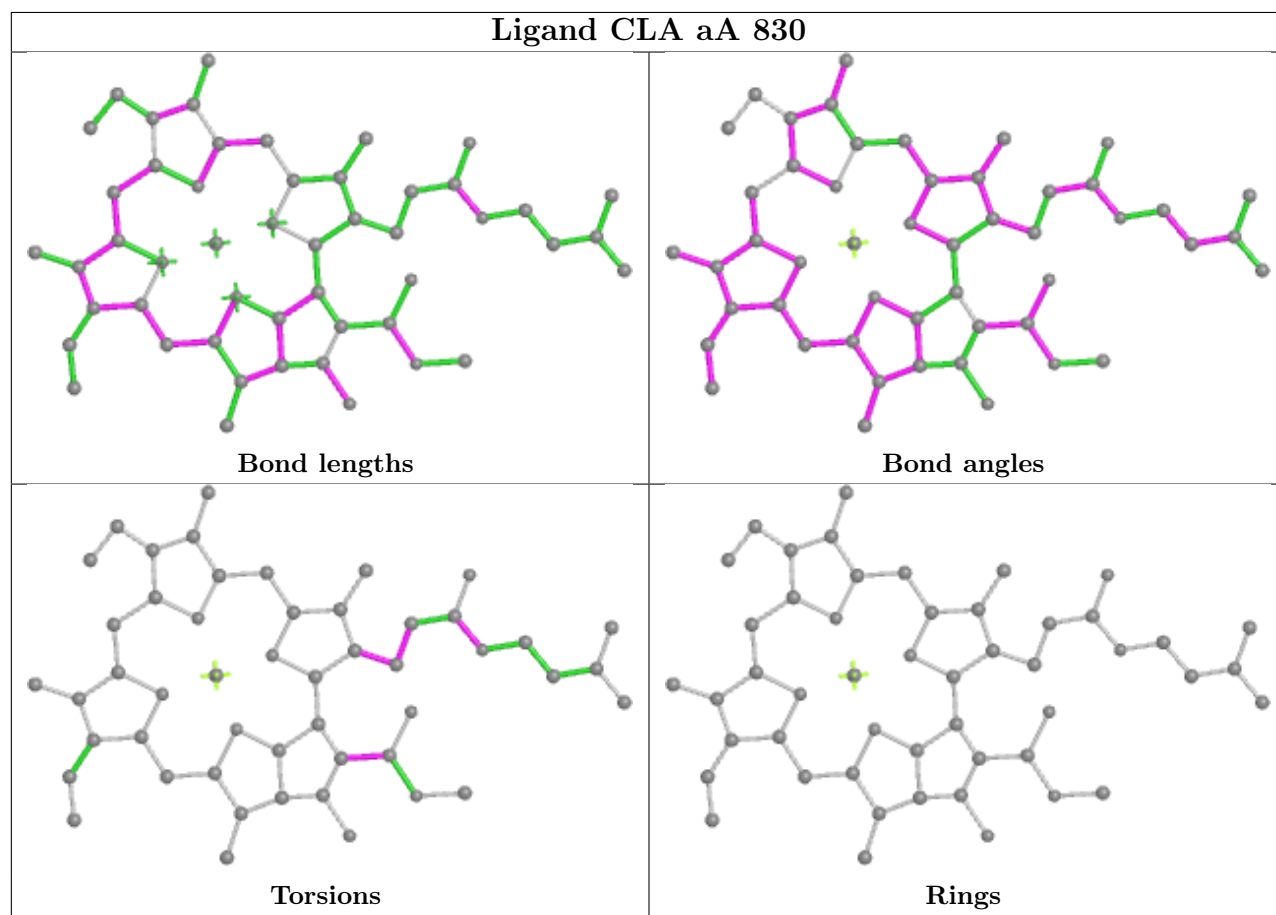
Ligand CLA aB 815



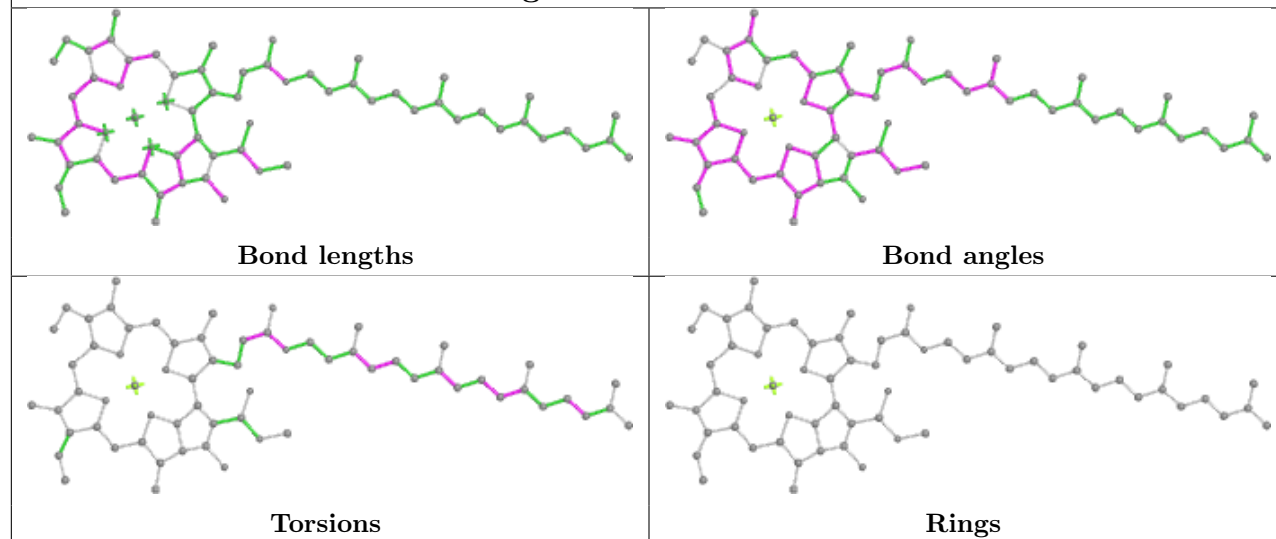
Ligand CLA cA 834



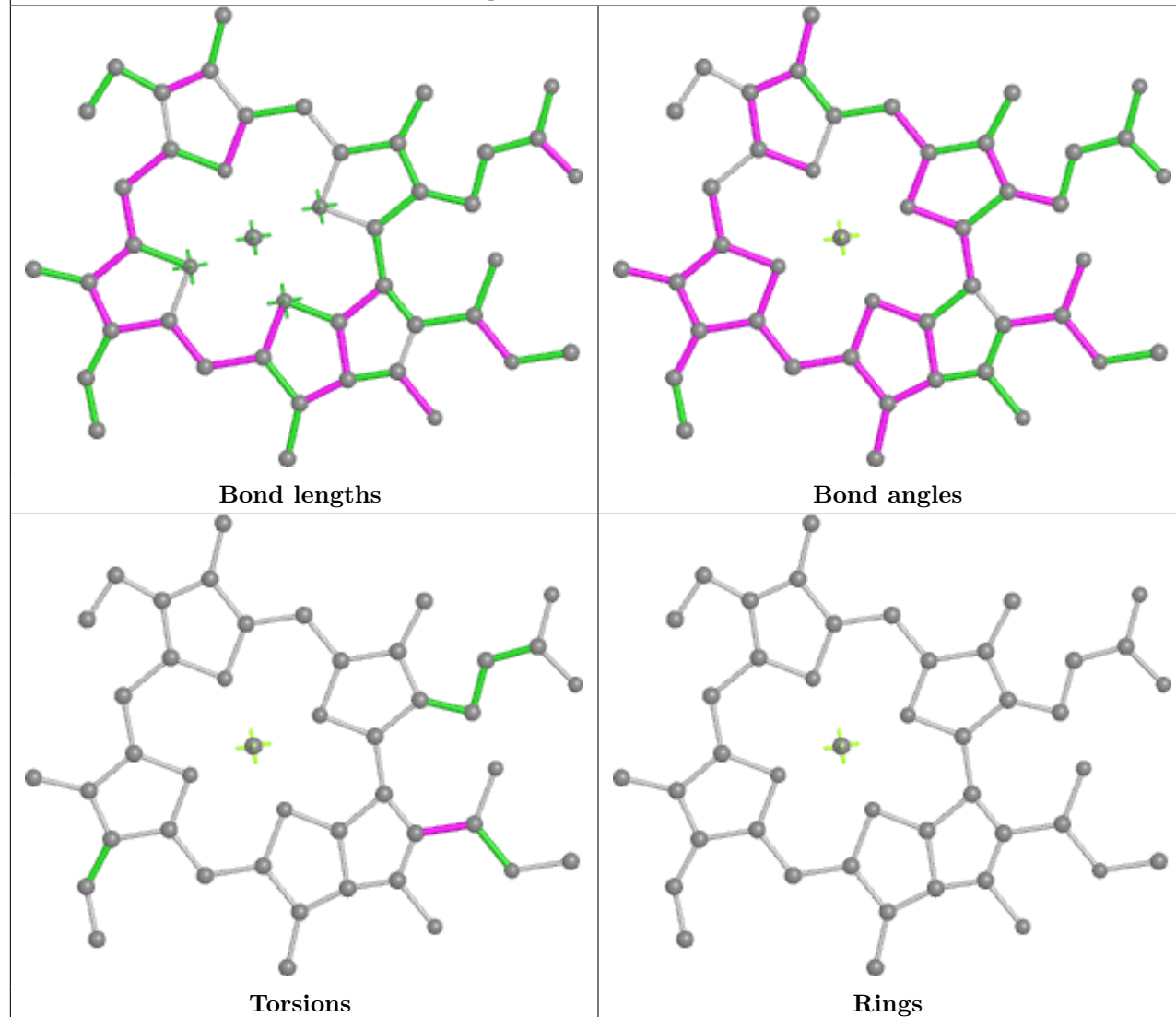
Ligand CLA aA 830

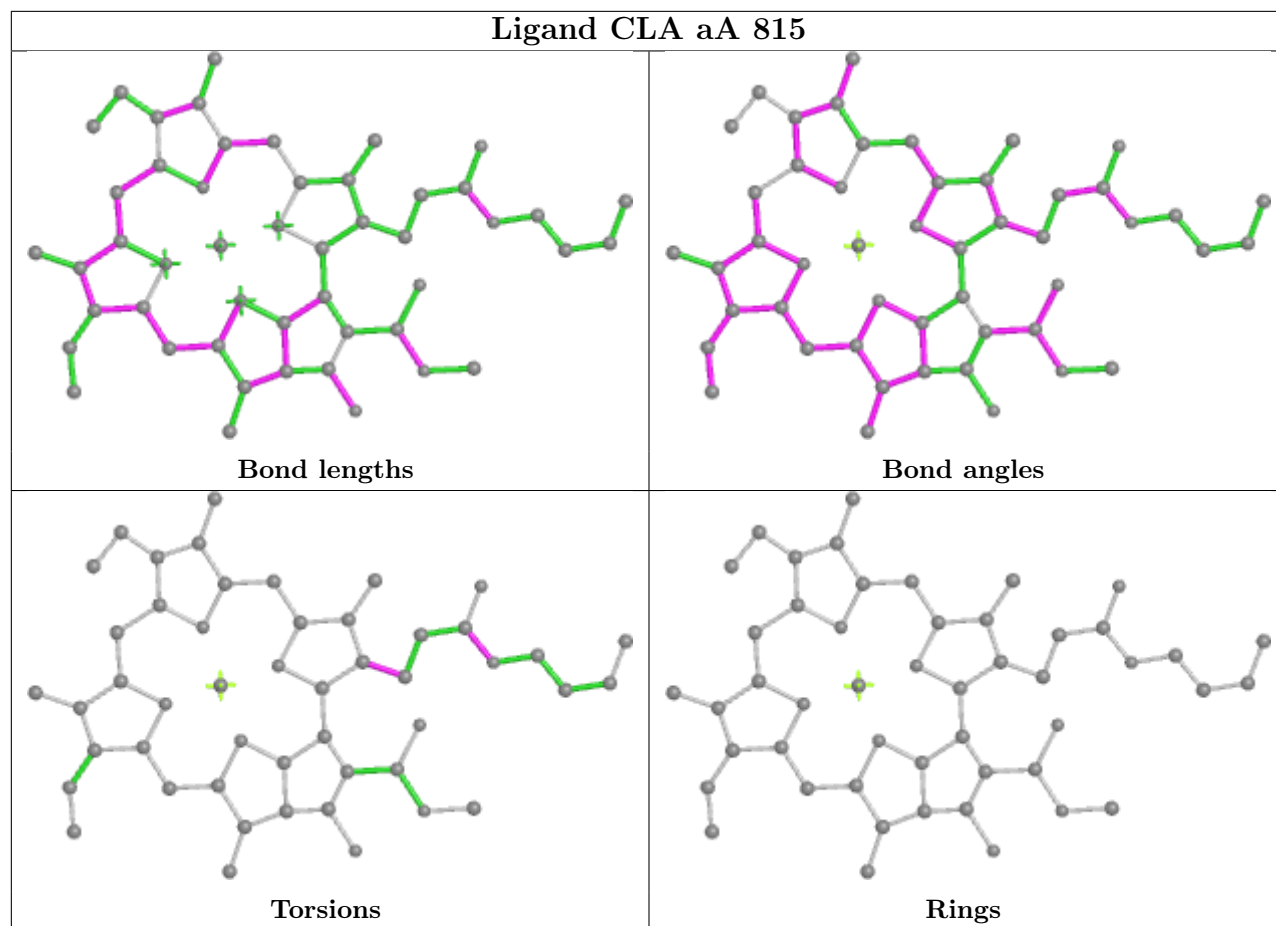


Ligand CLA bB 808

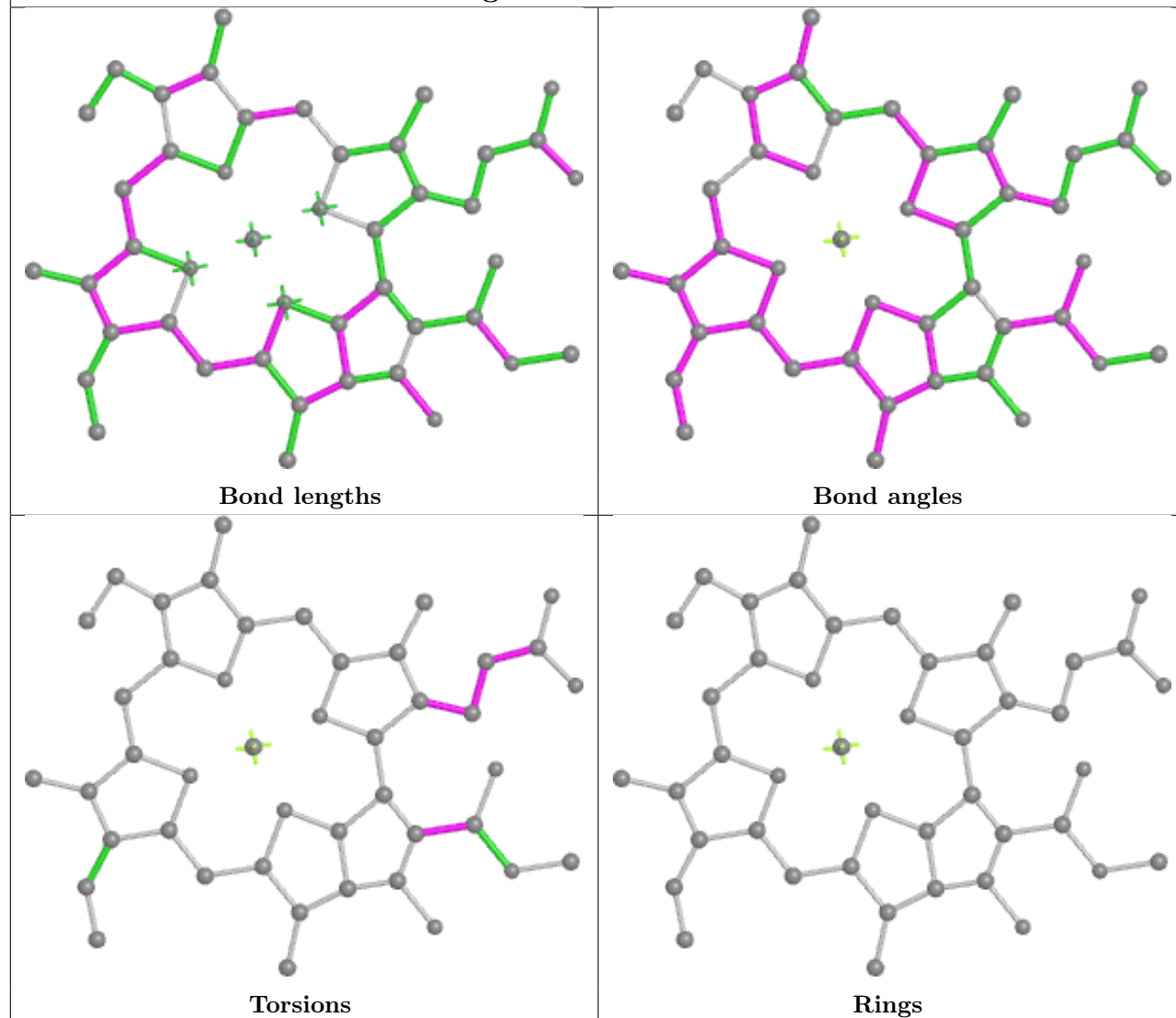


Ligand CLA cB 816

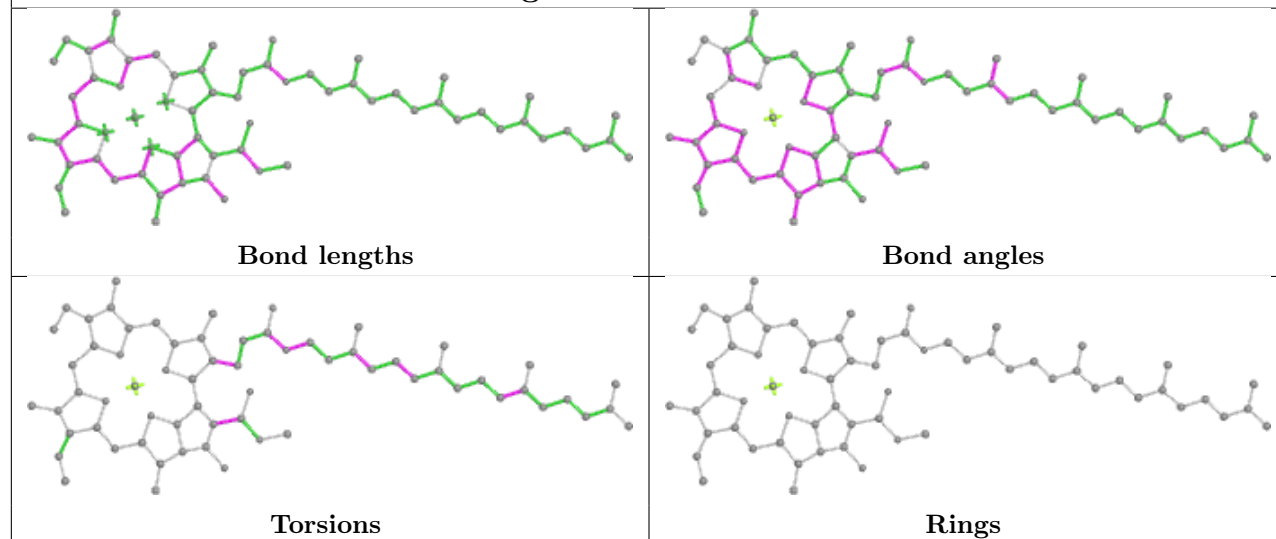


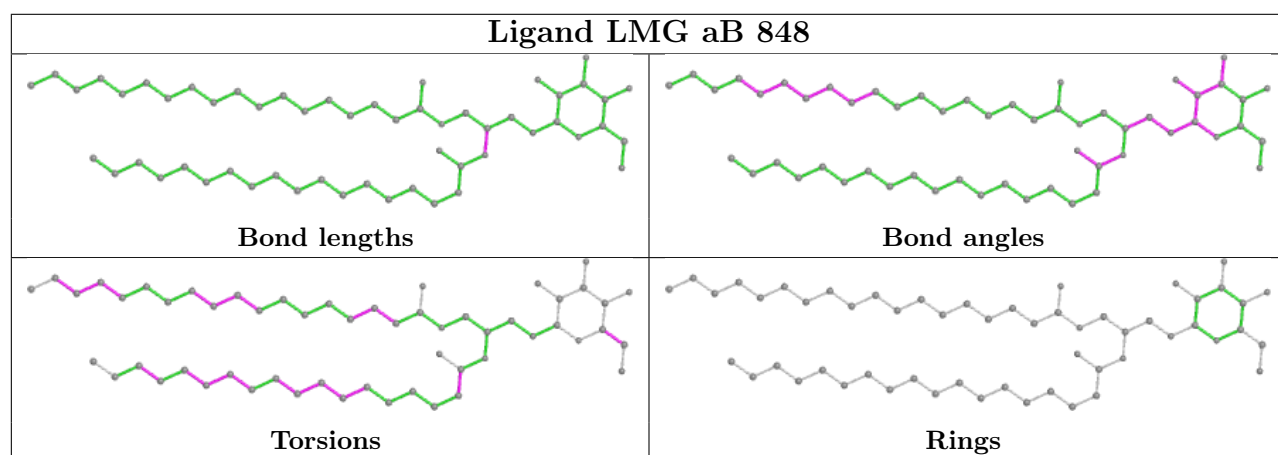
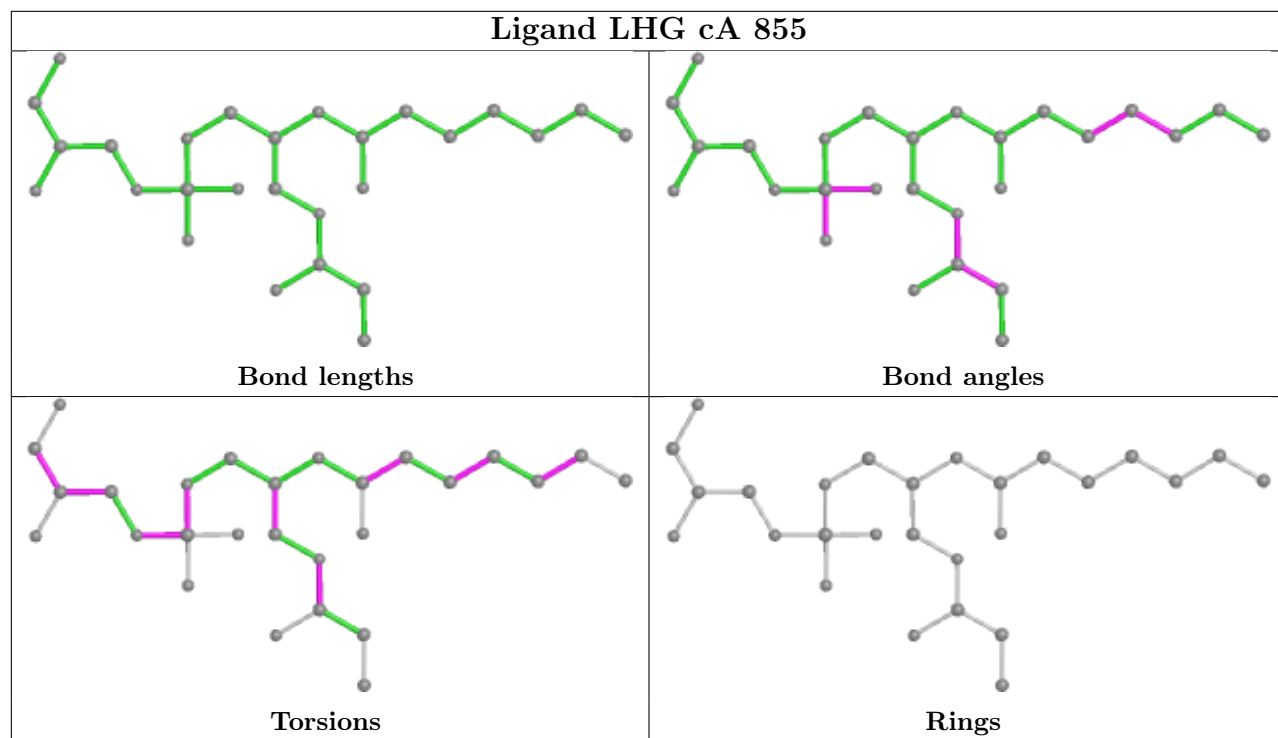
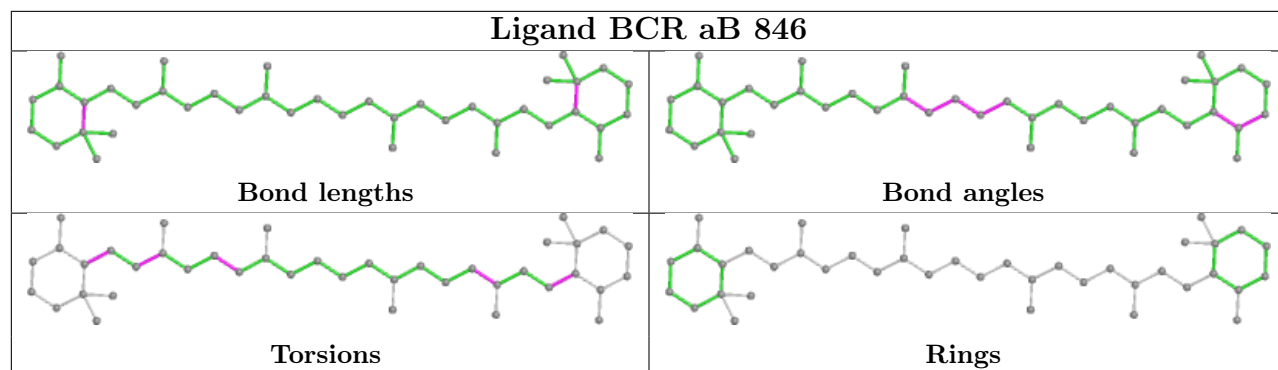


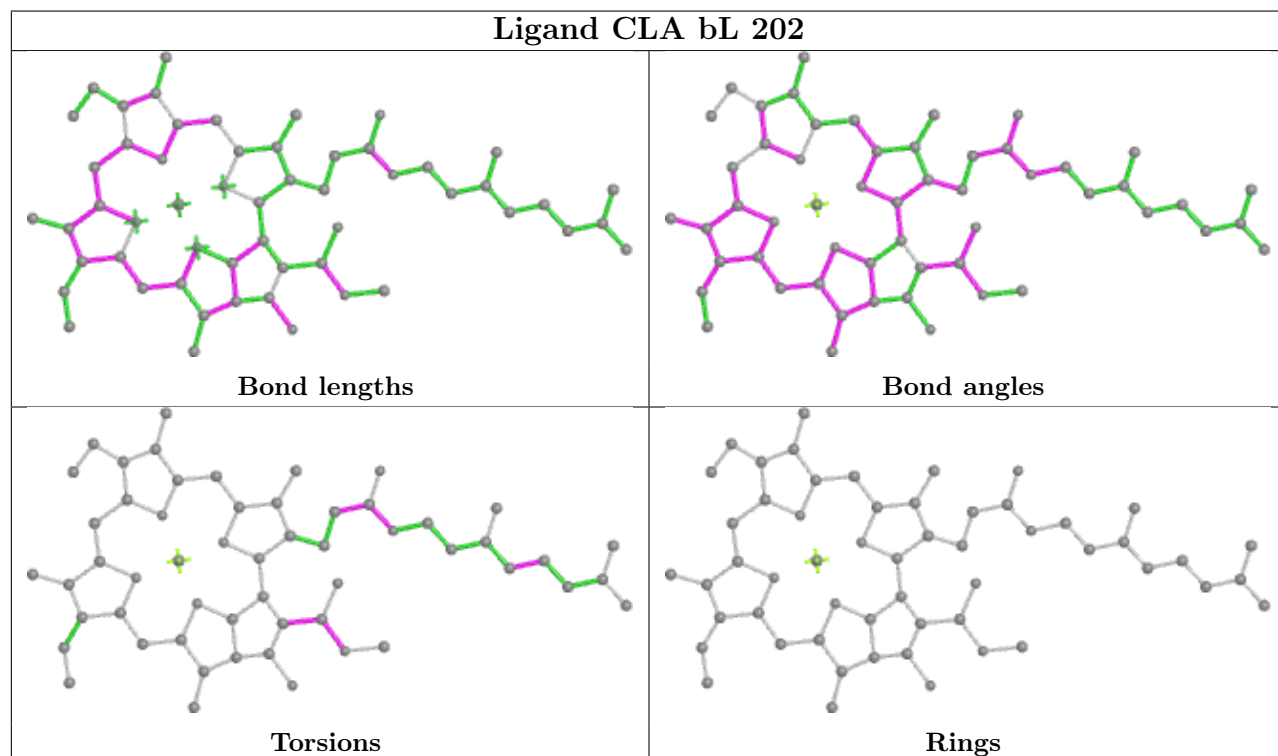
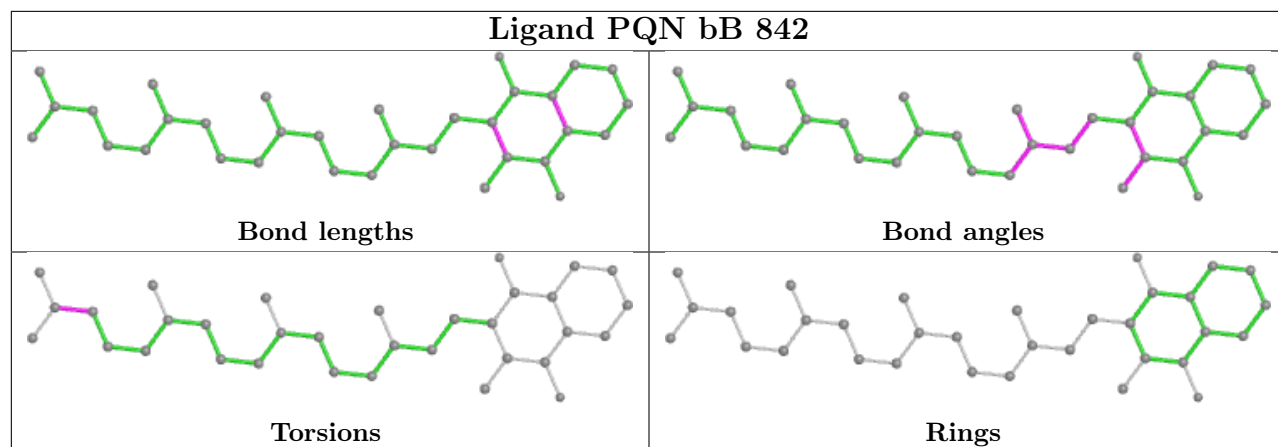
Ligand CLA cA 802

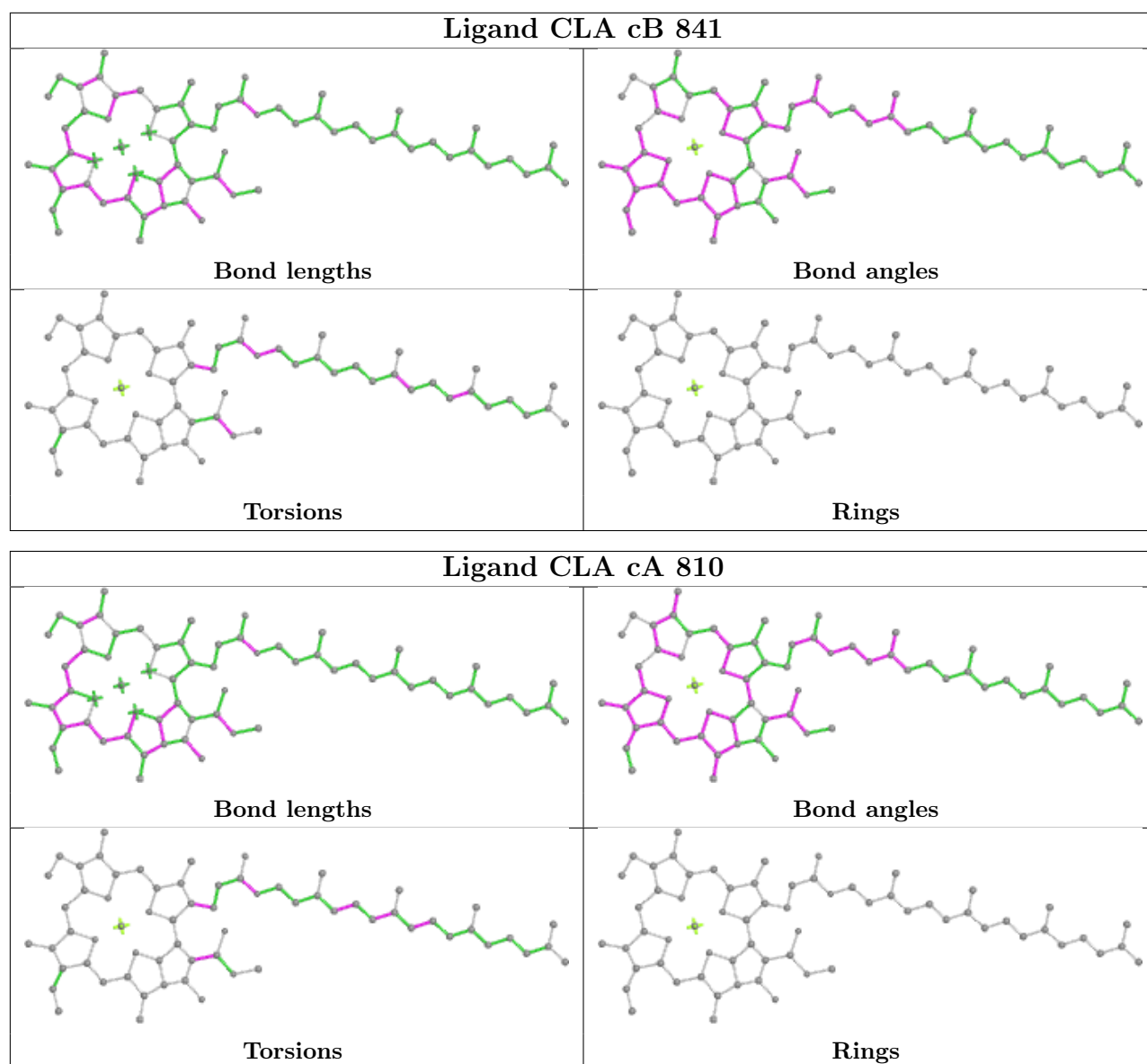


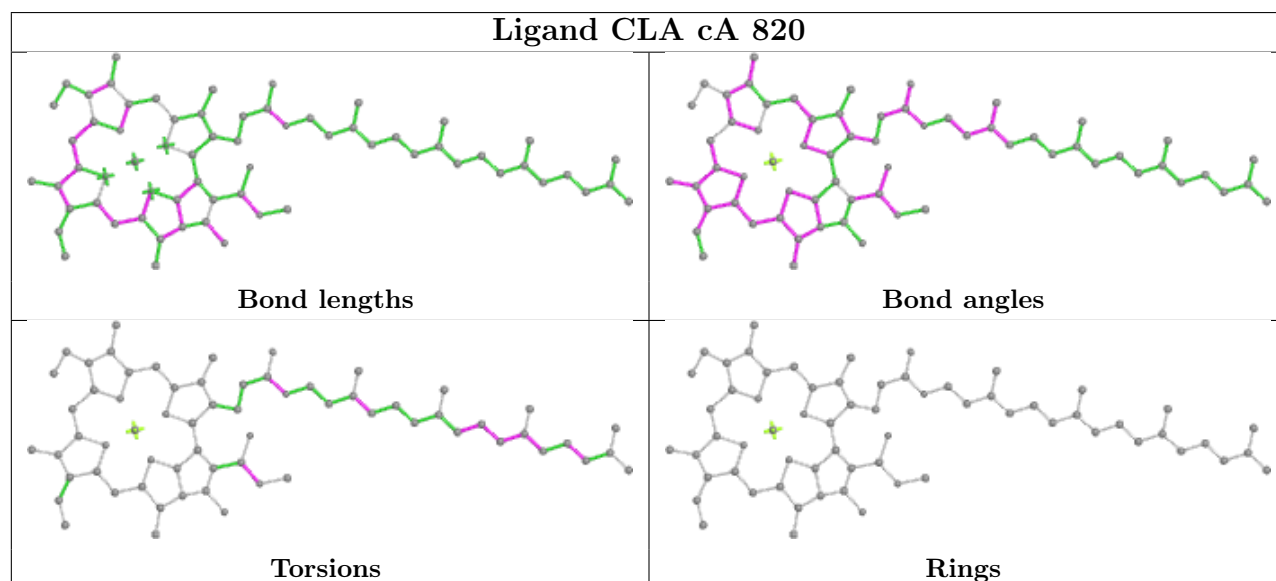
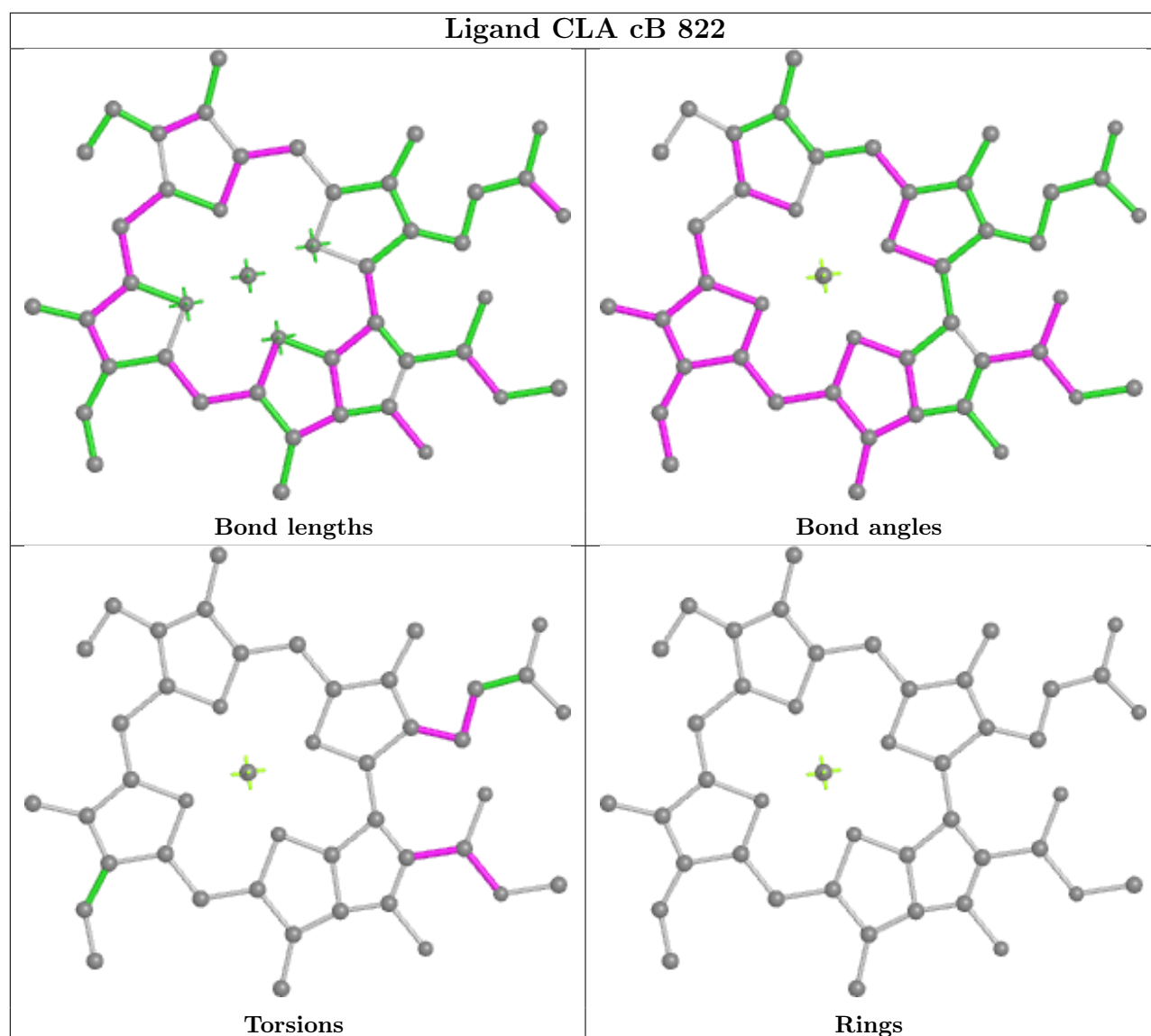
Ligand CLA bA 824

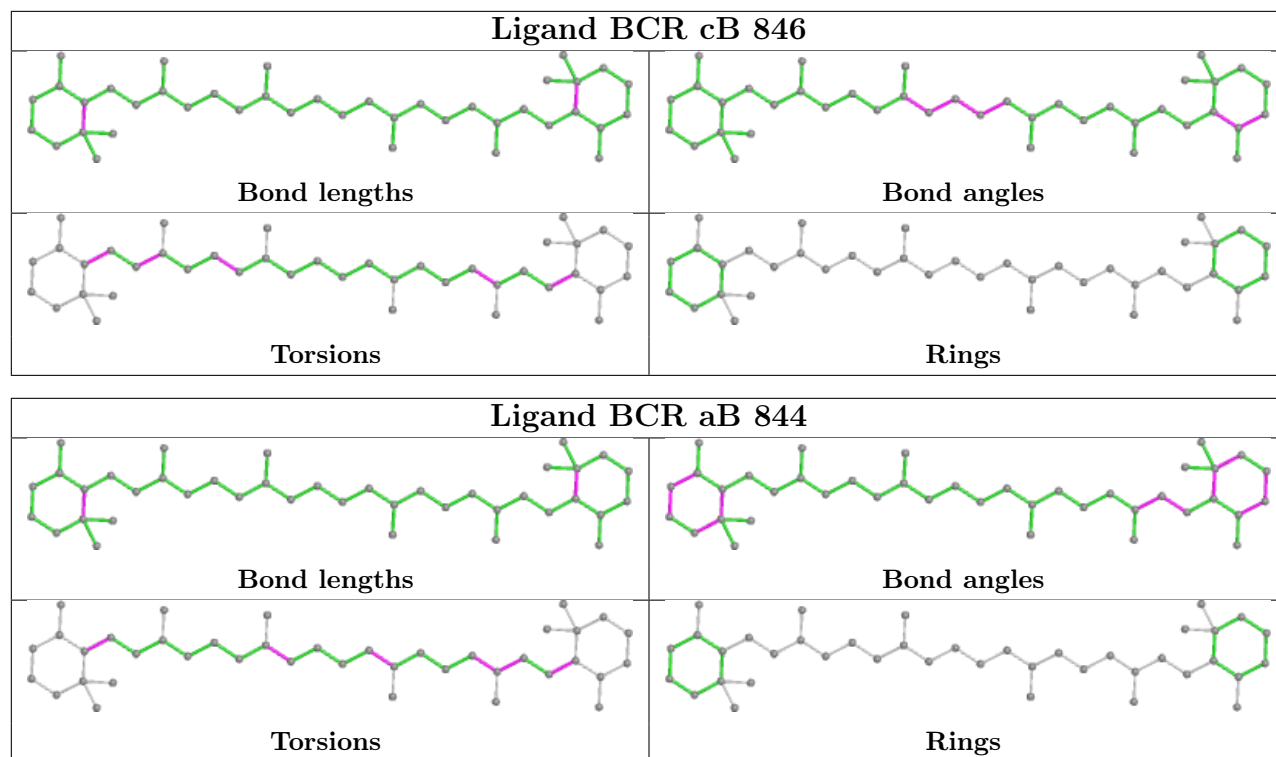


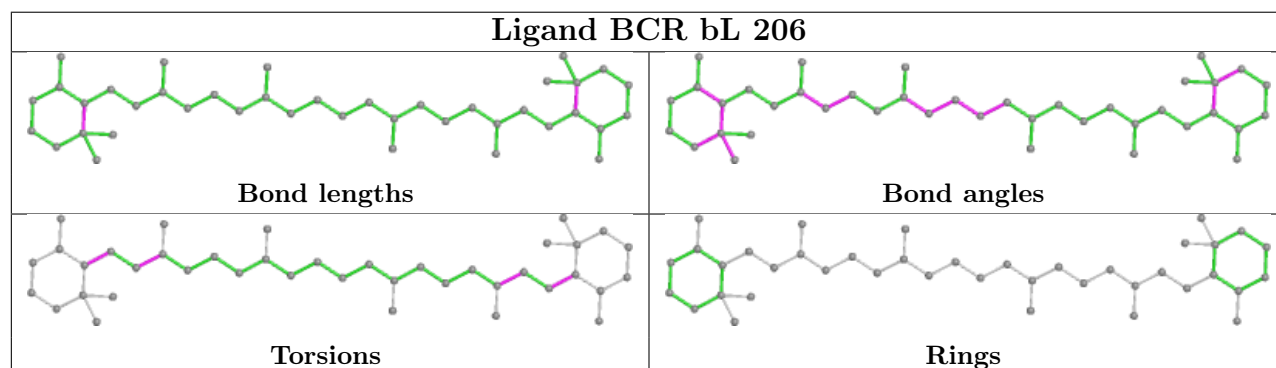
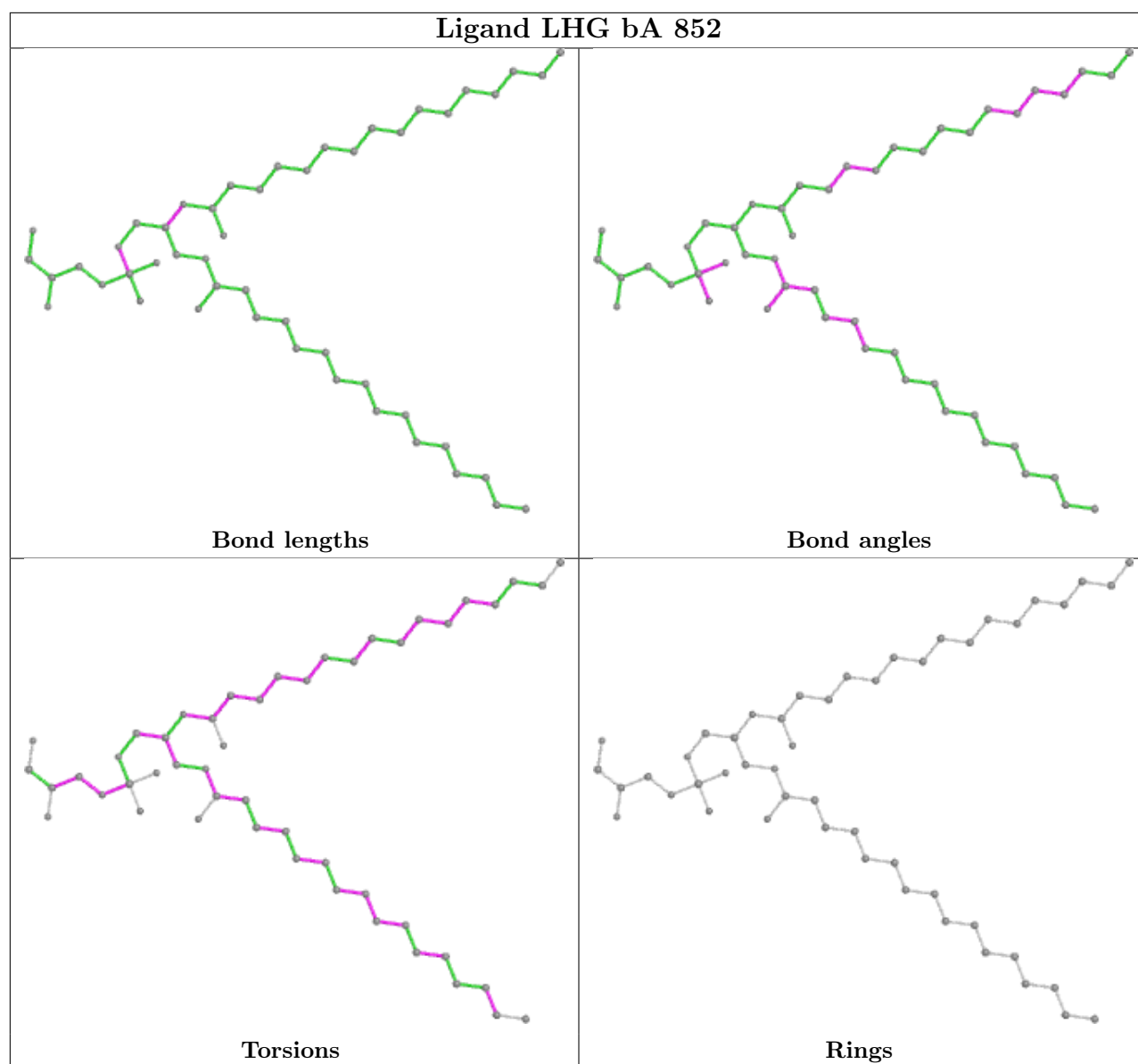


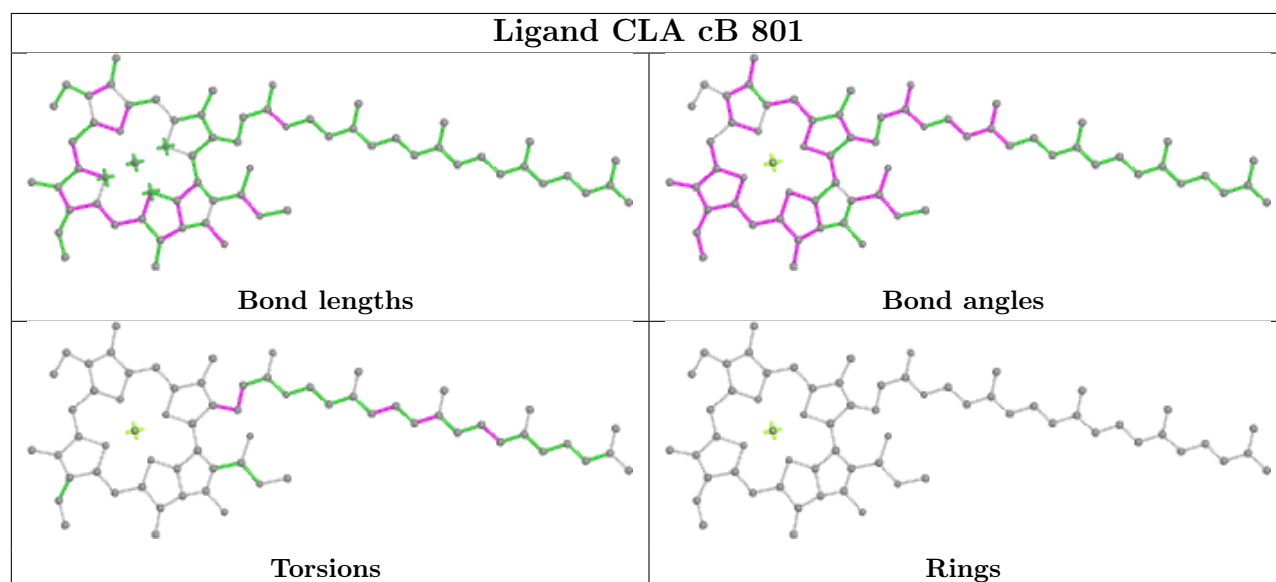
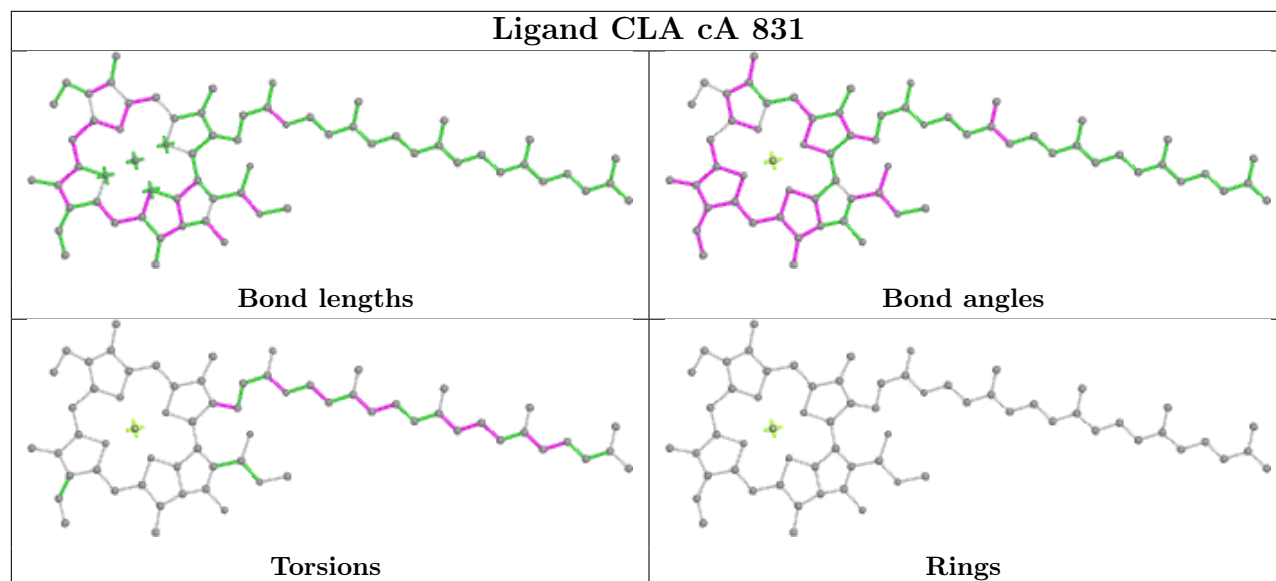
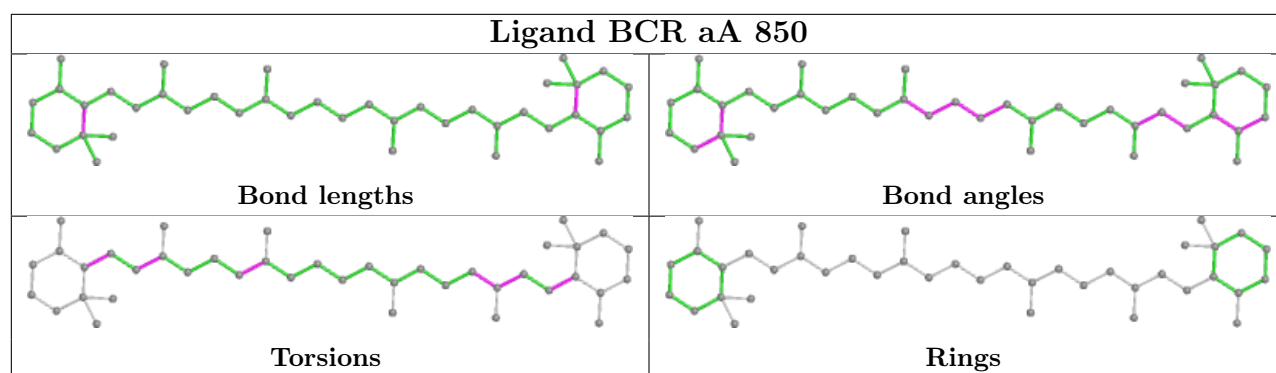




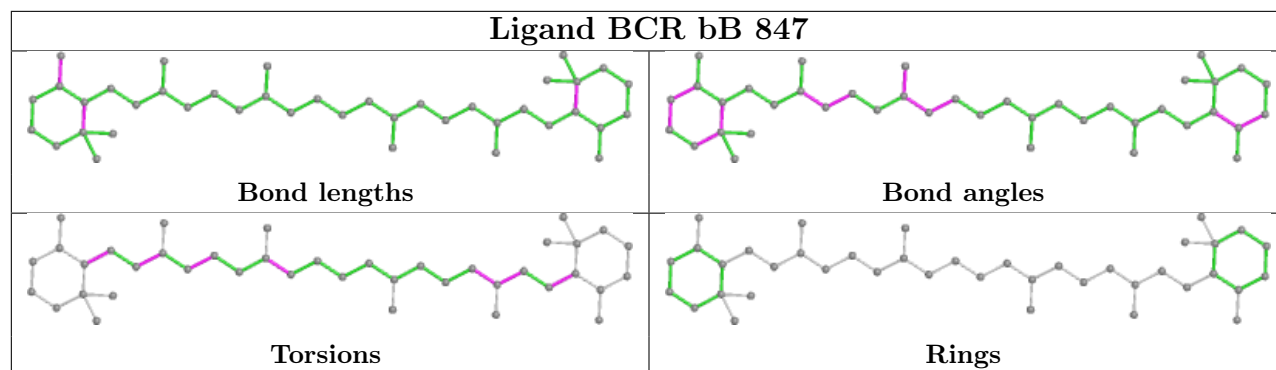




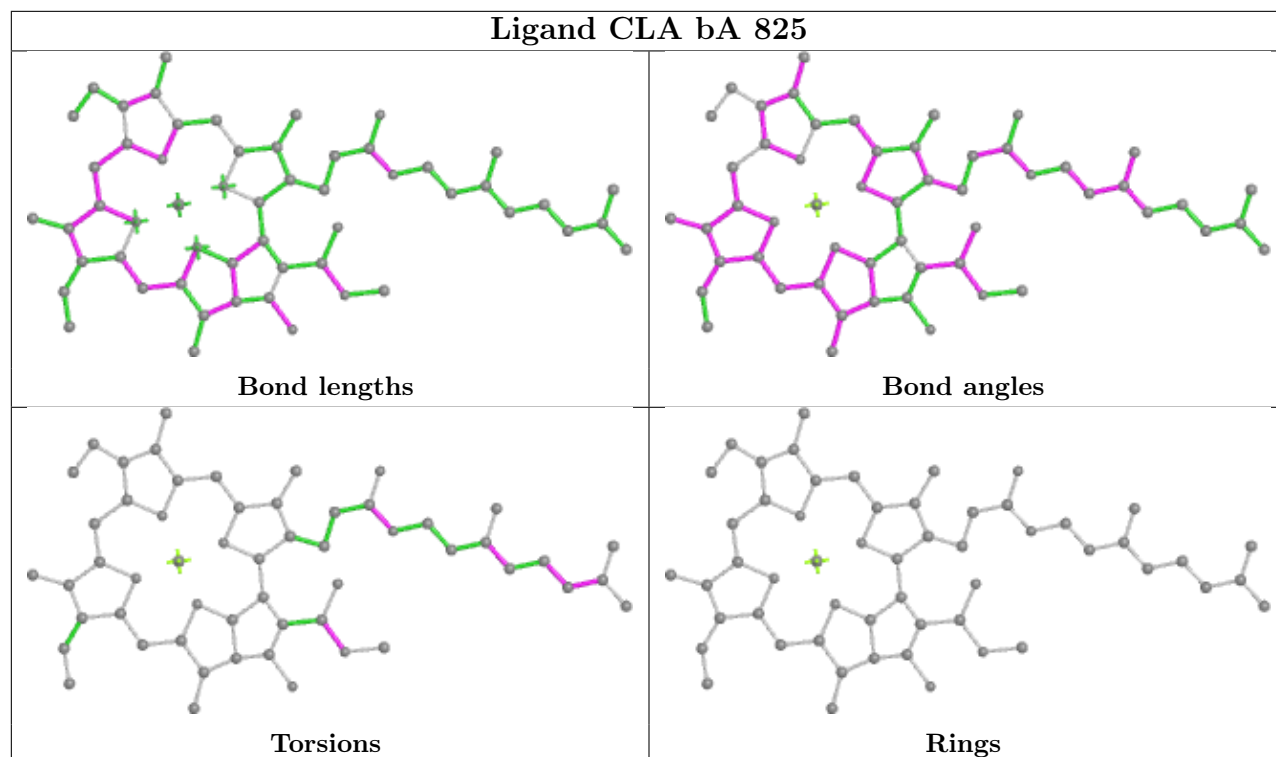




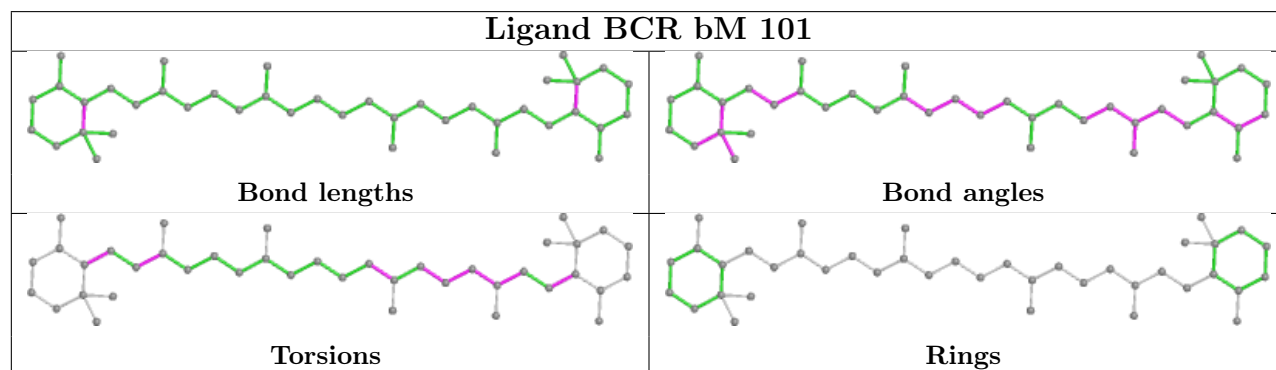
Ligand BCR bB 847

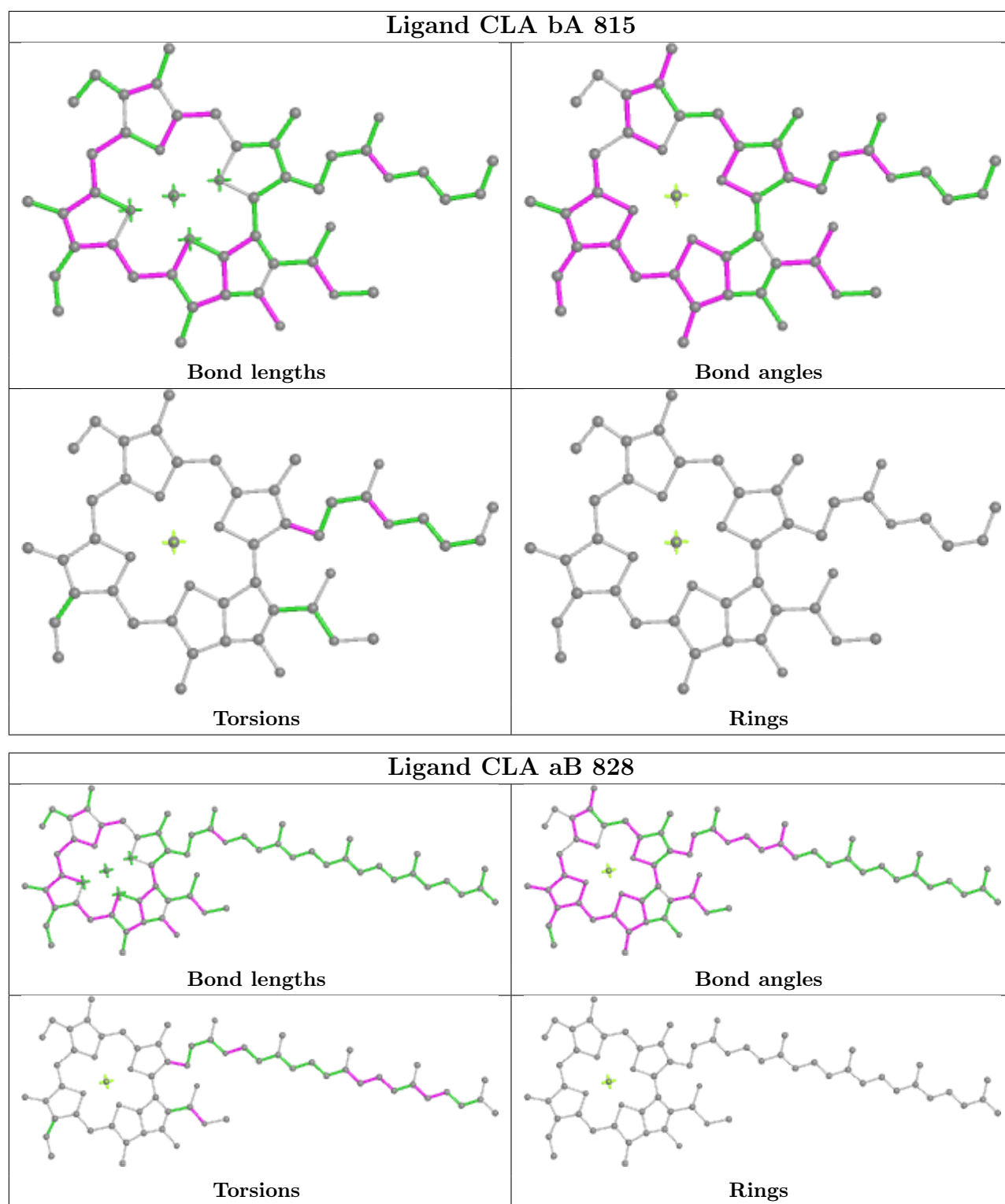


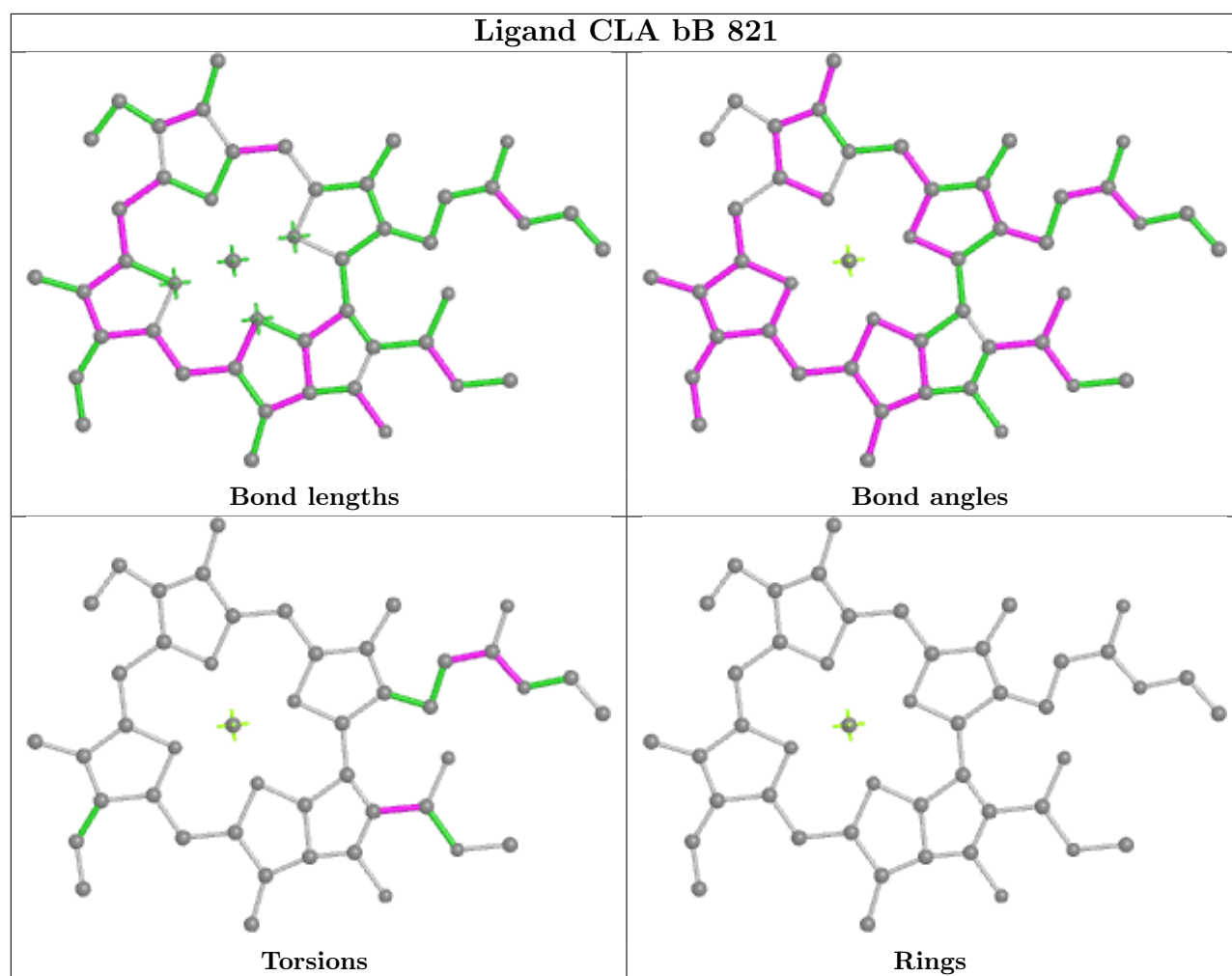
Ligand CLA bA 825

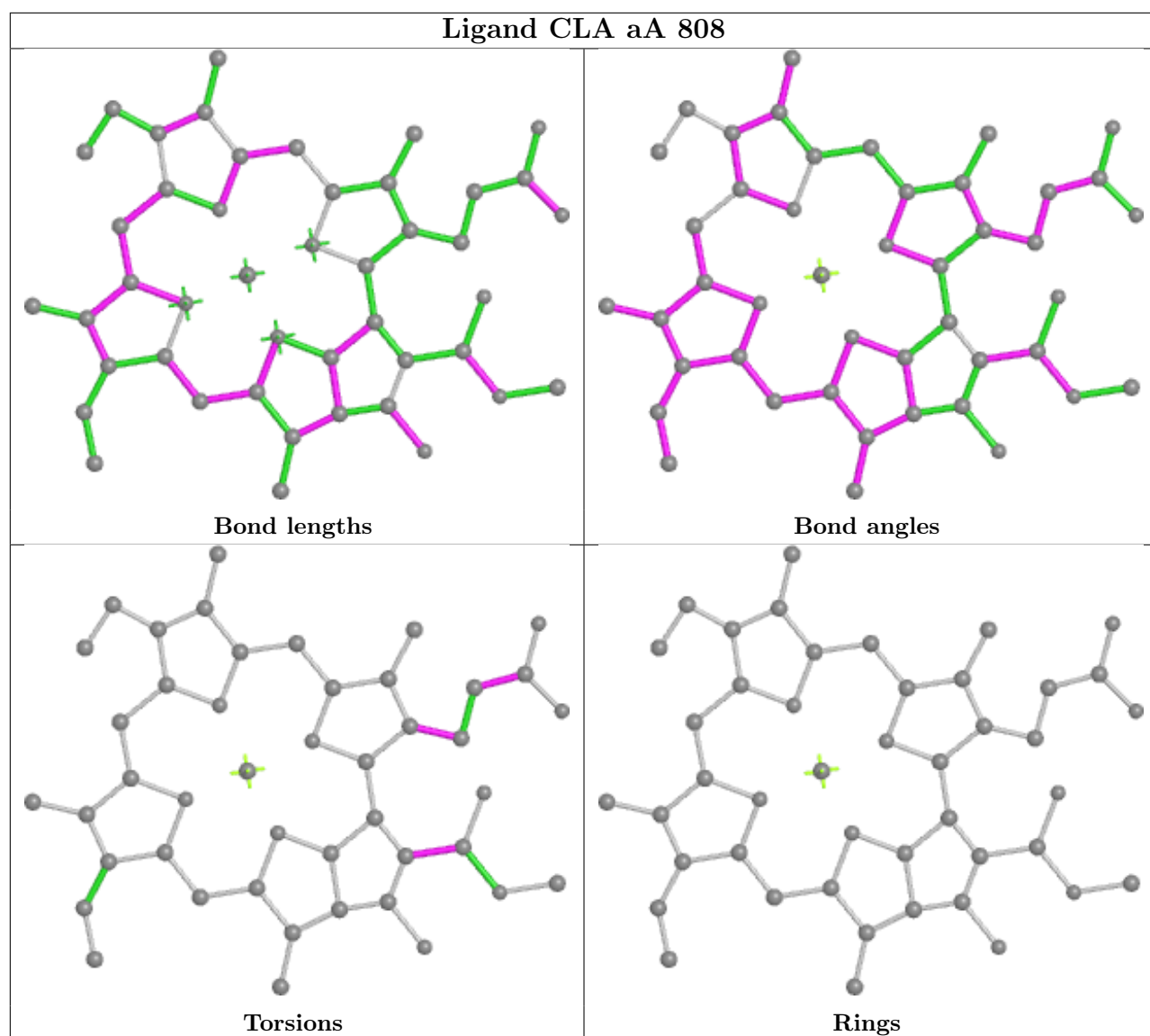


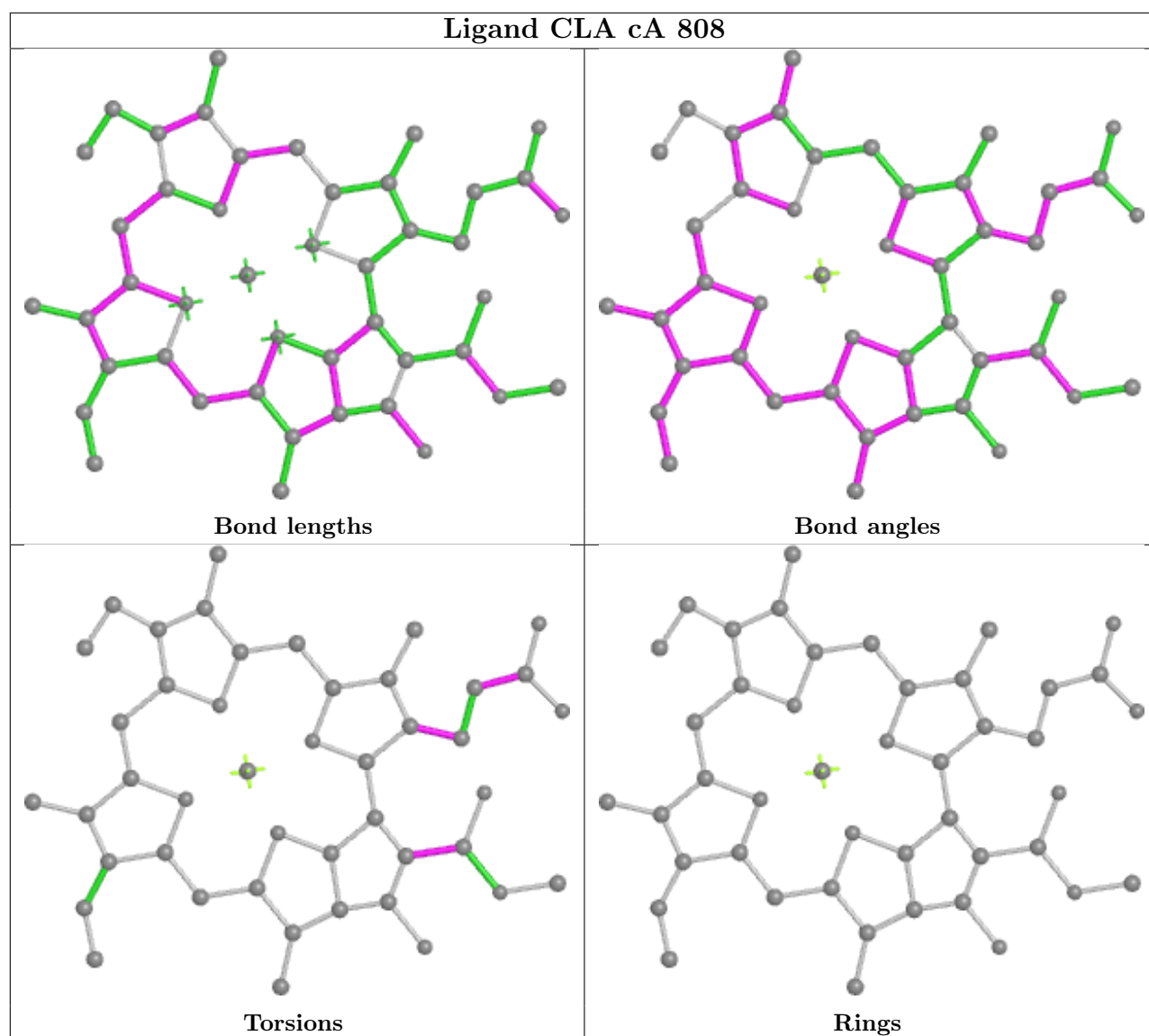
Ligand BCR bM 101

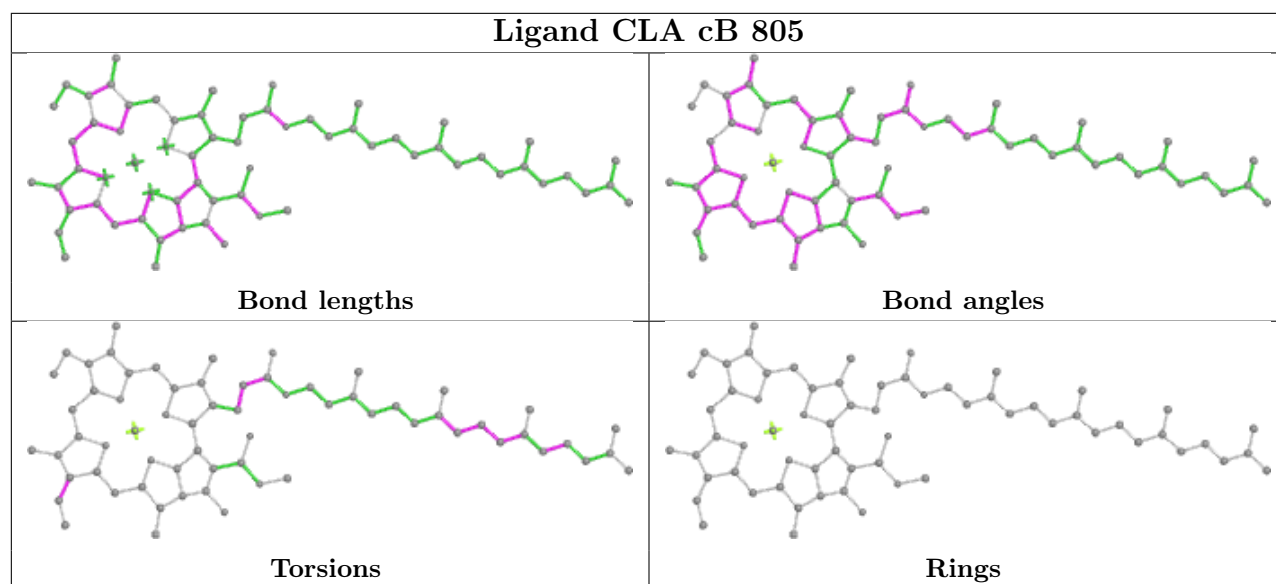
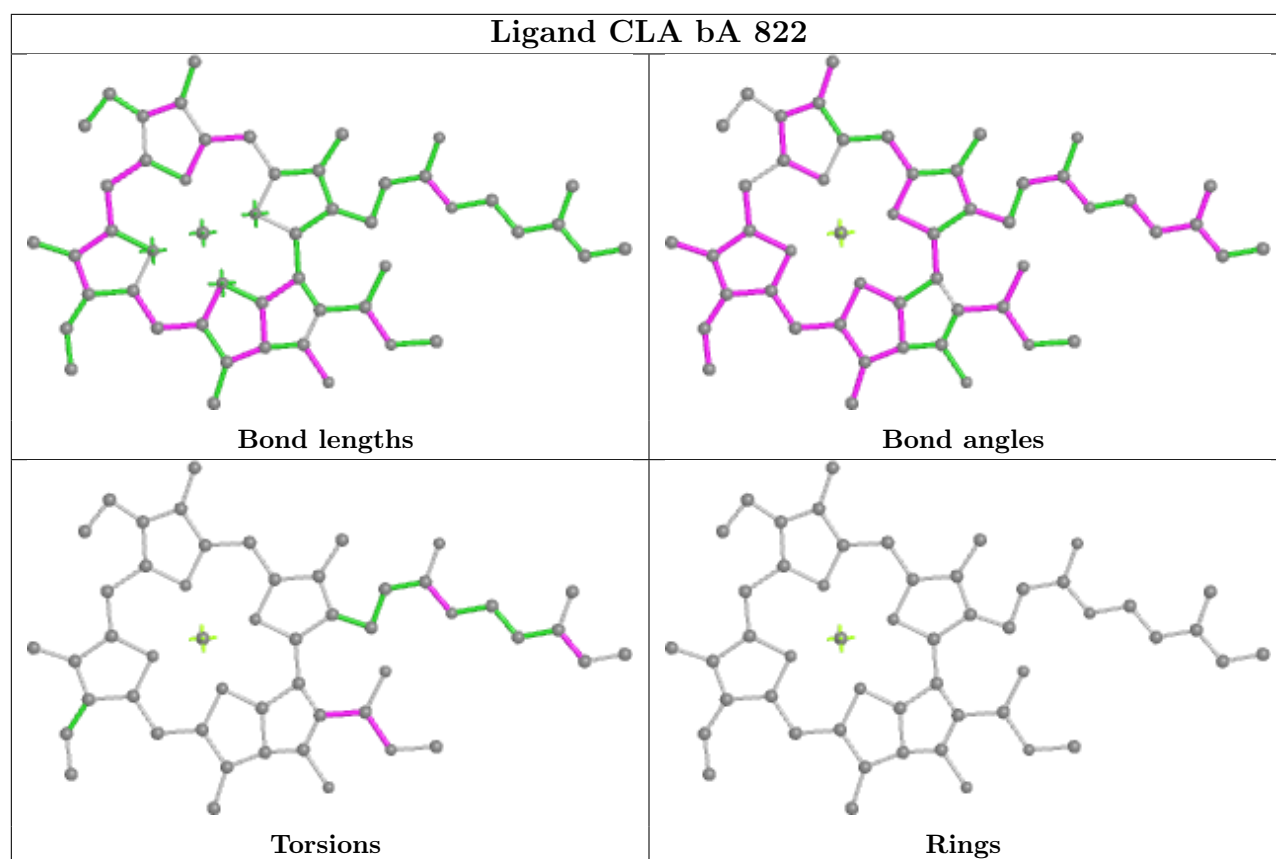




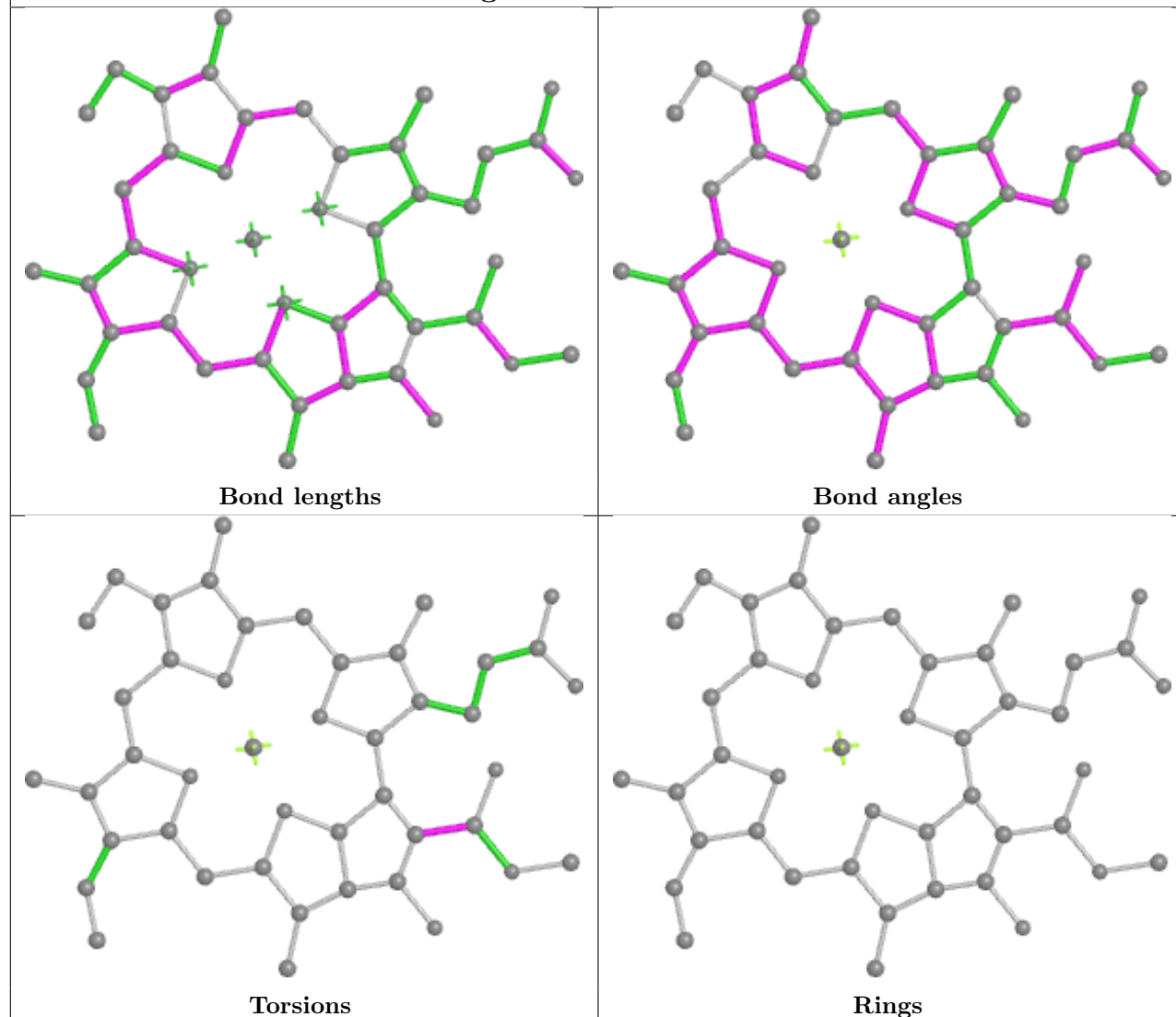




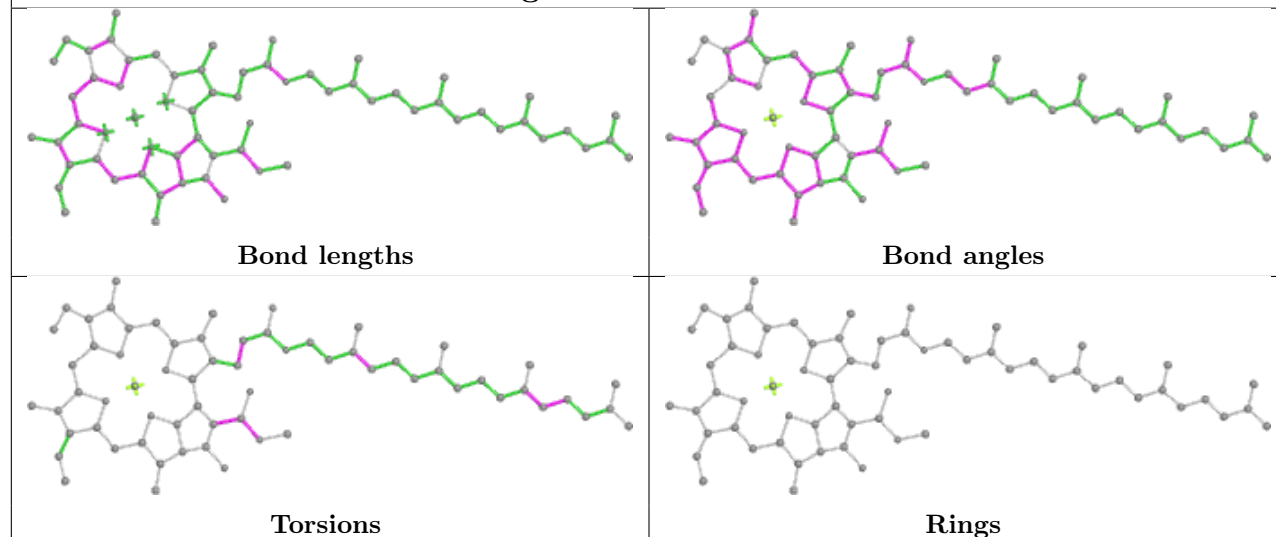


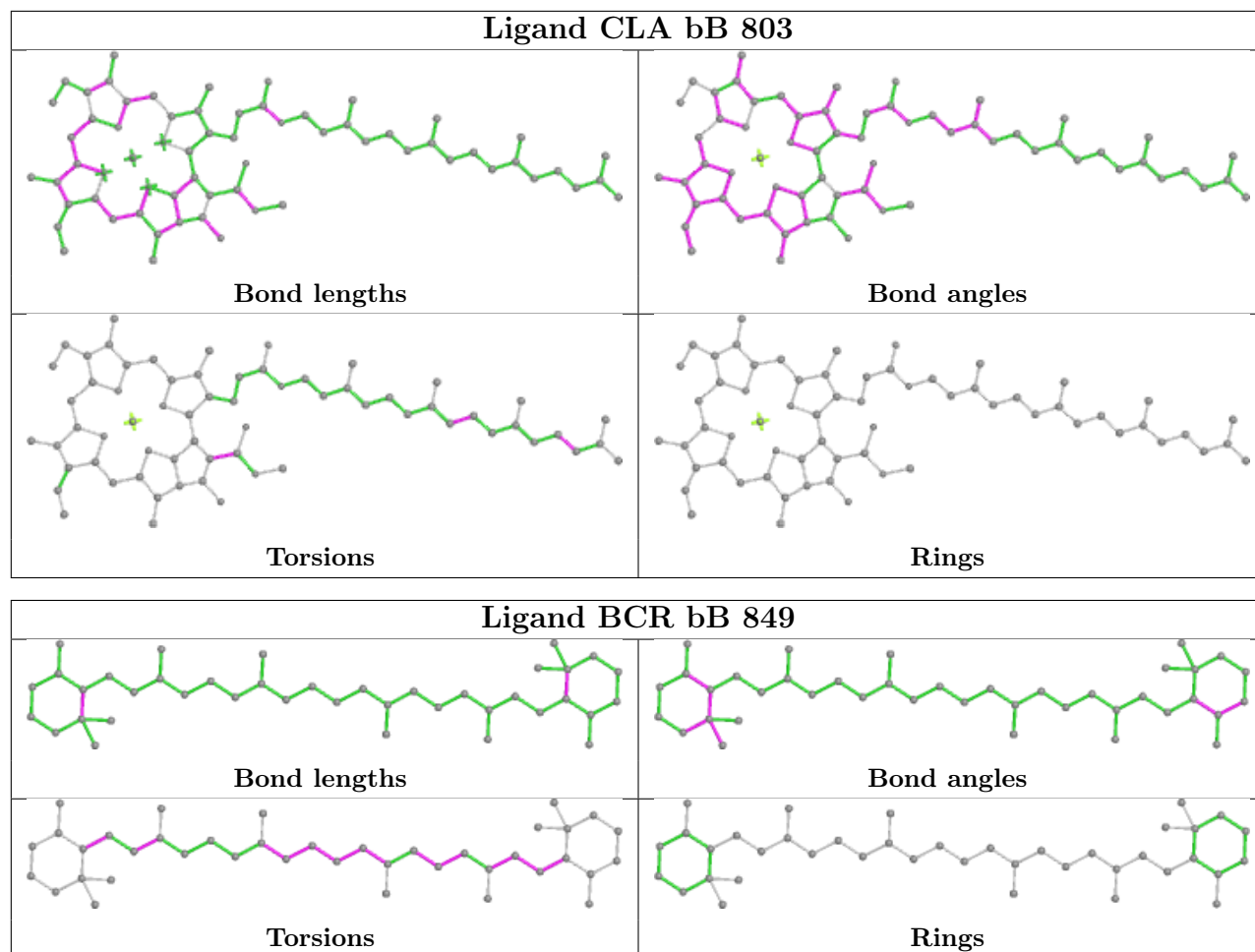


Ligand CLA bA 814

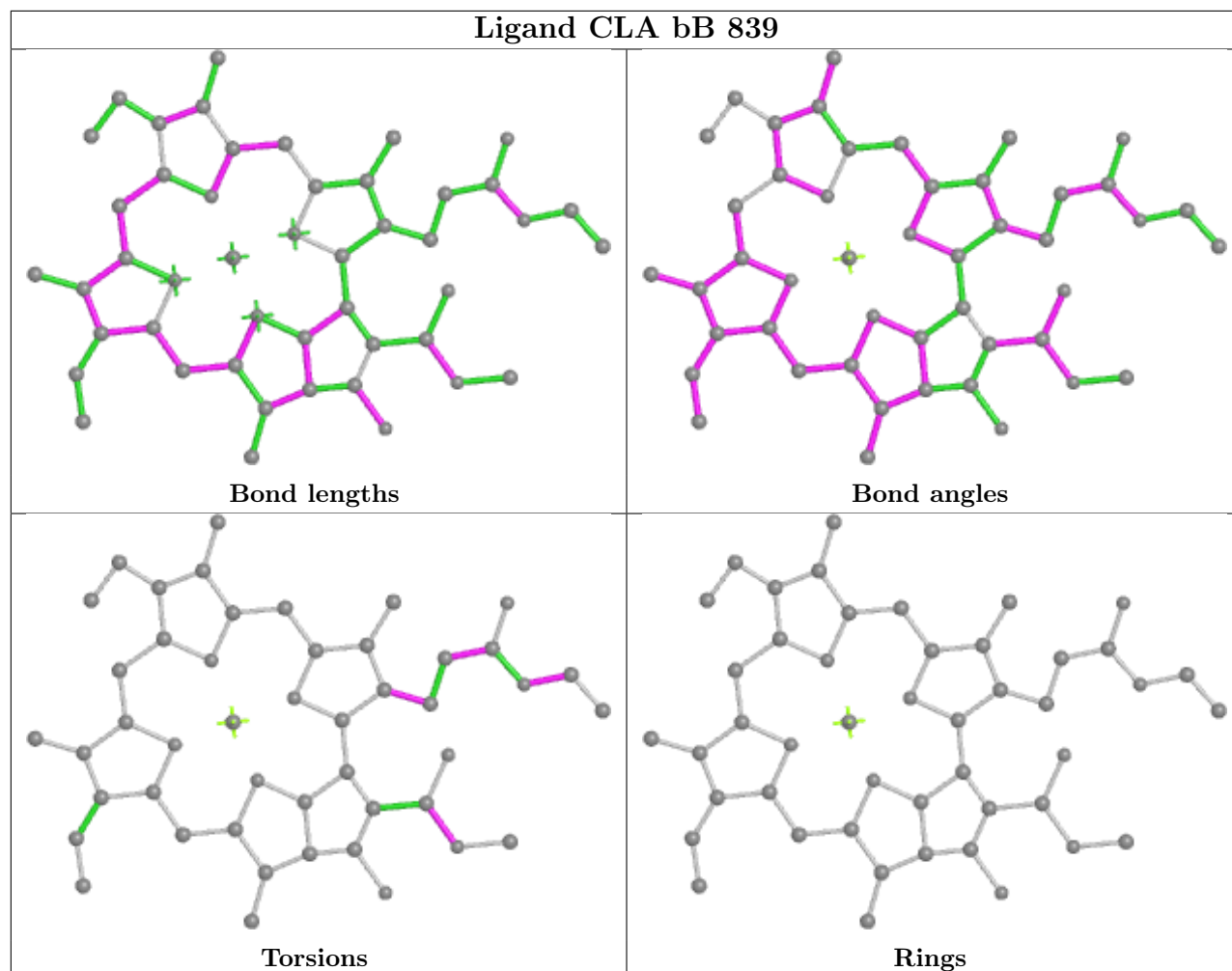


Ligand CLA bA 833

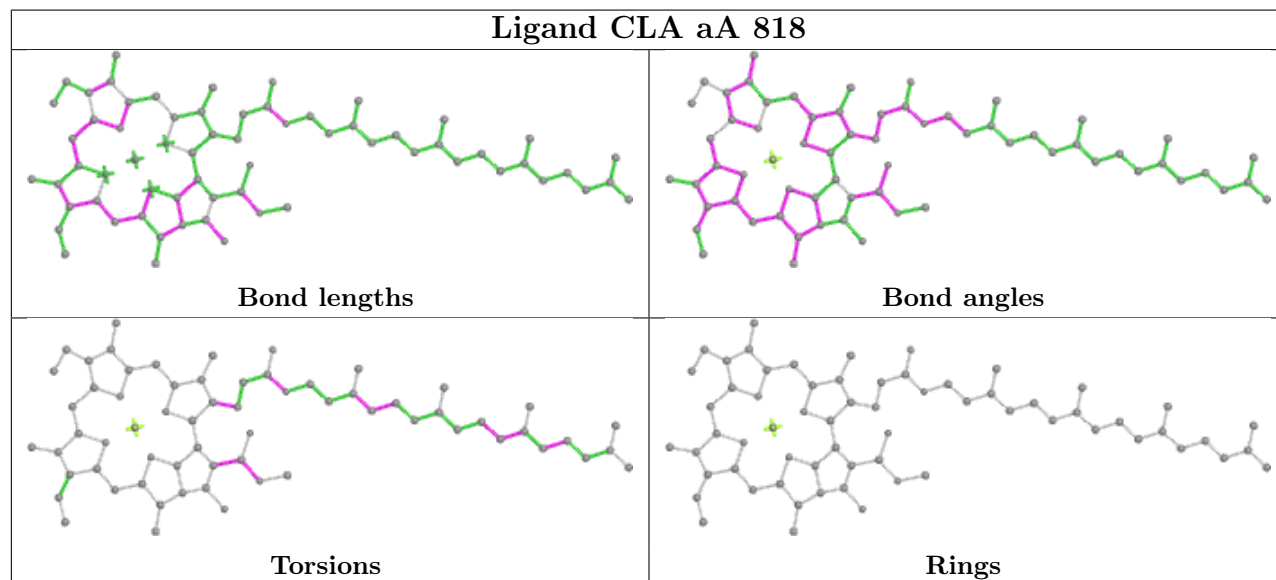


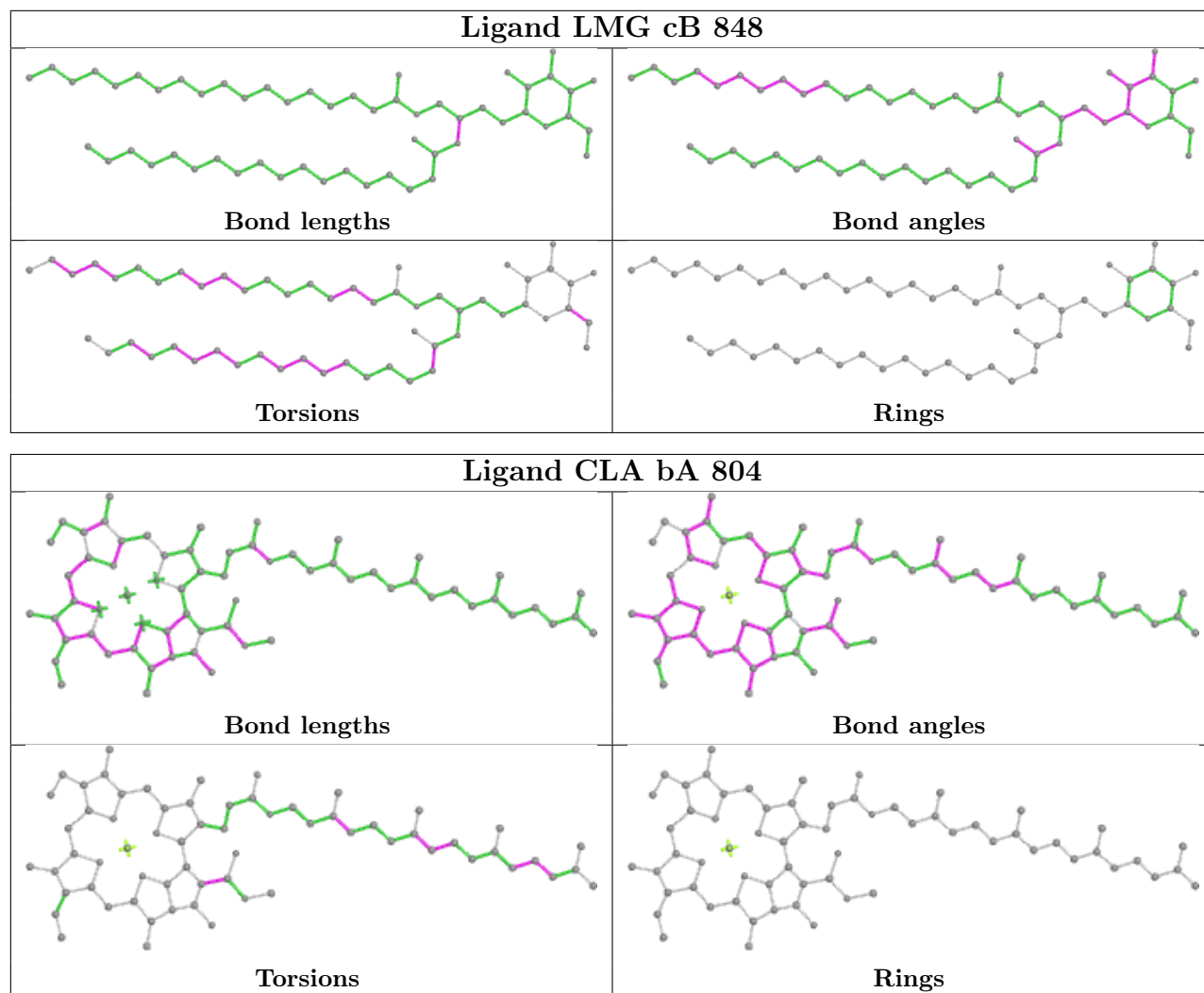


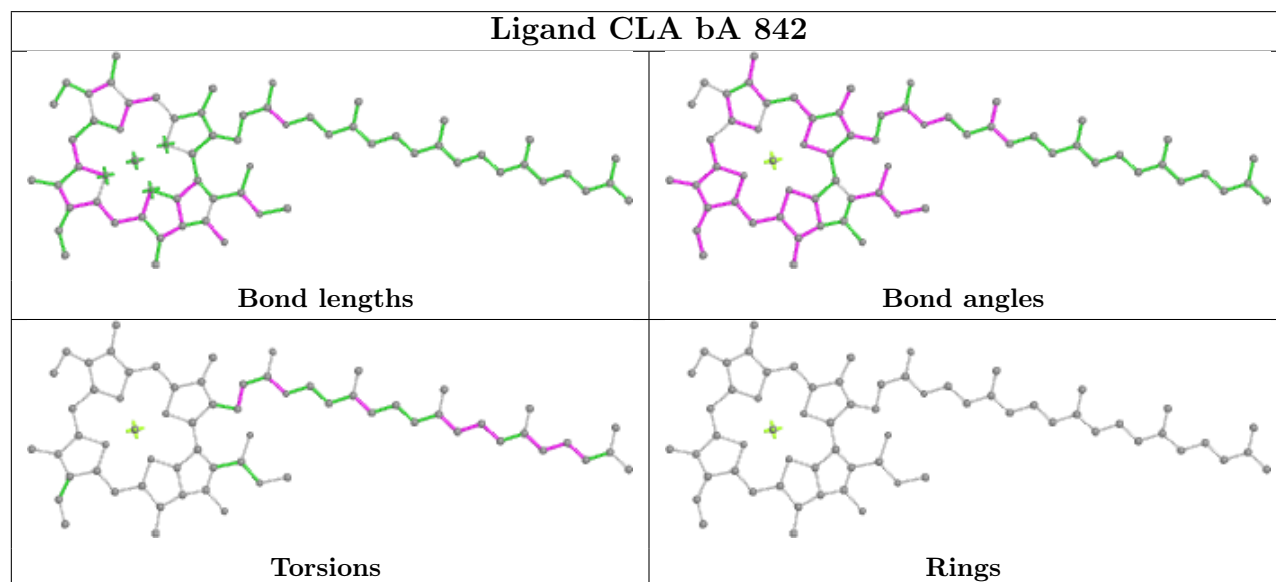
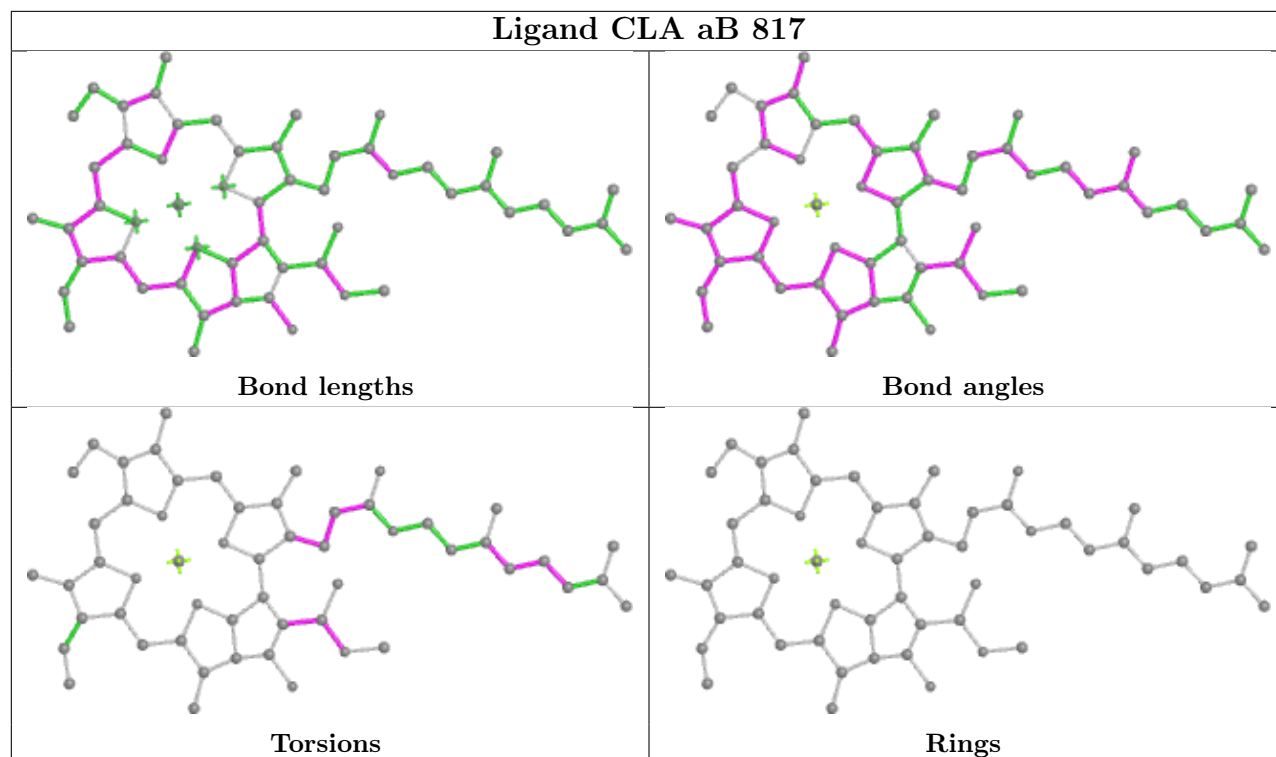
Ligand CLA bB 839

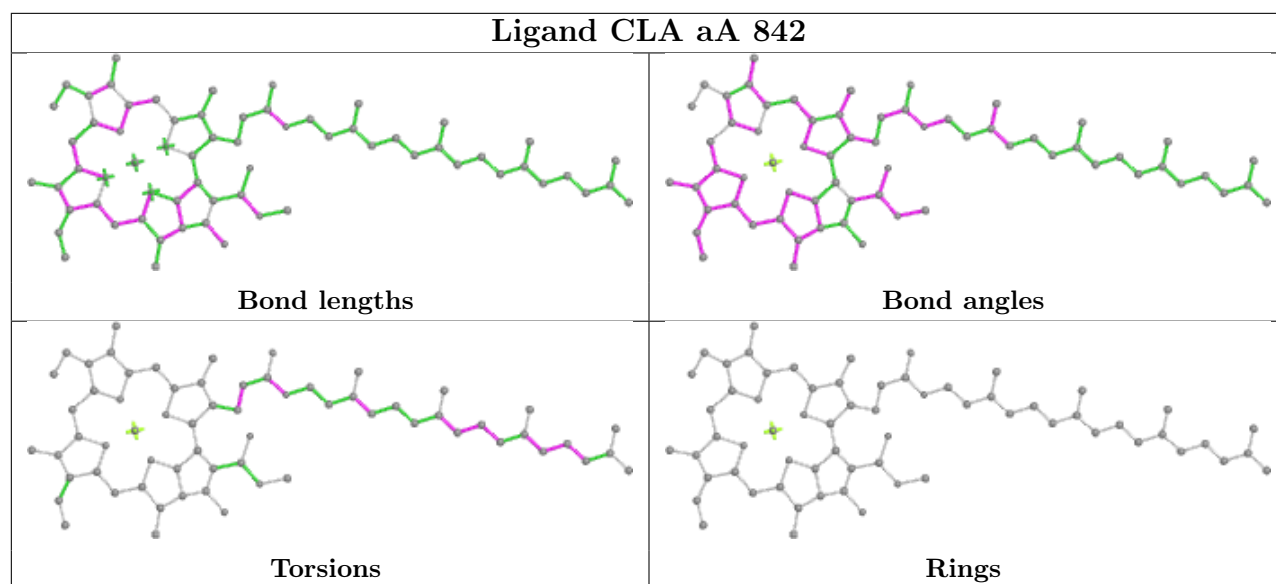
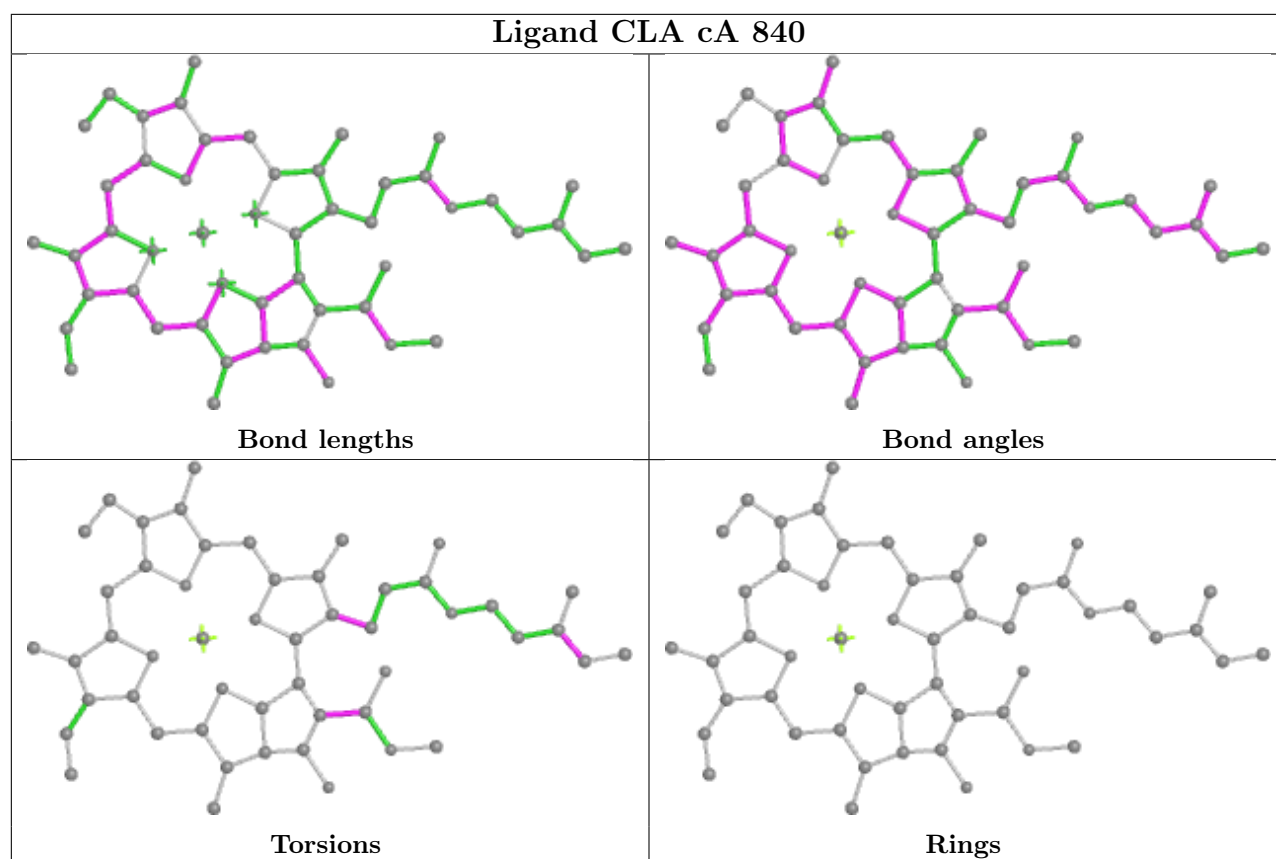


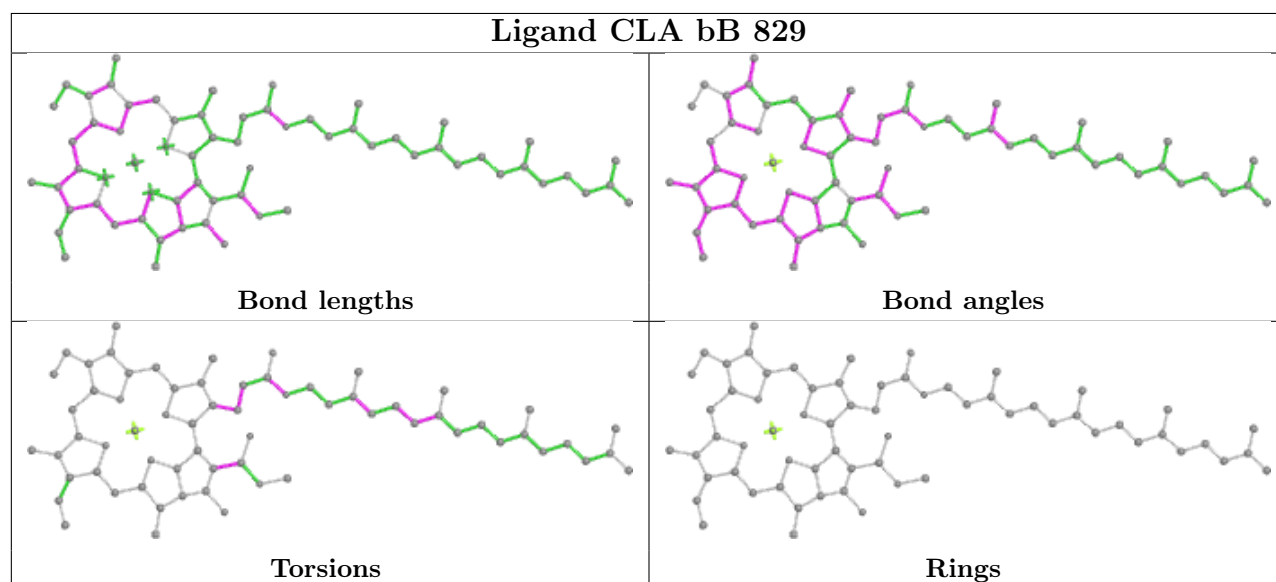
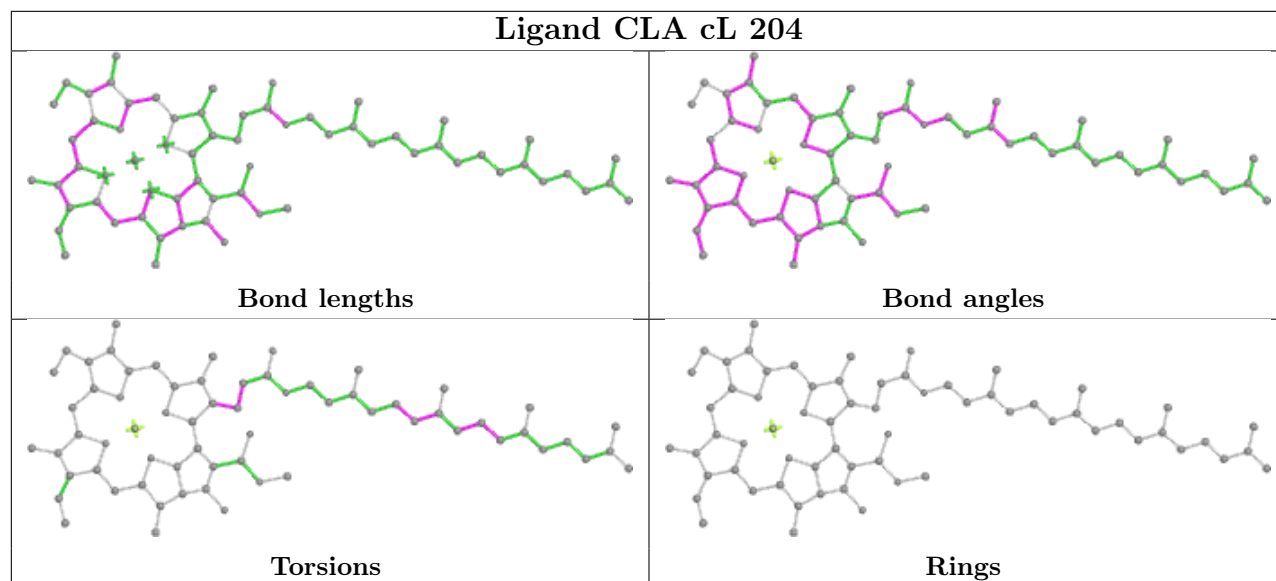
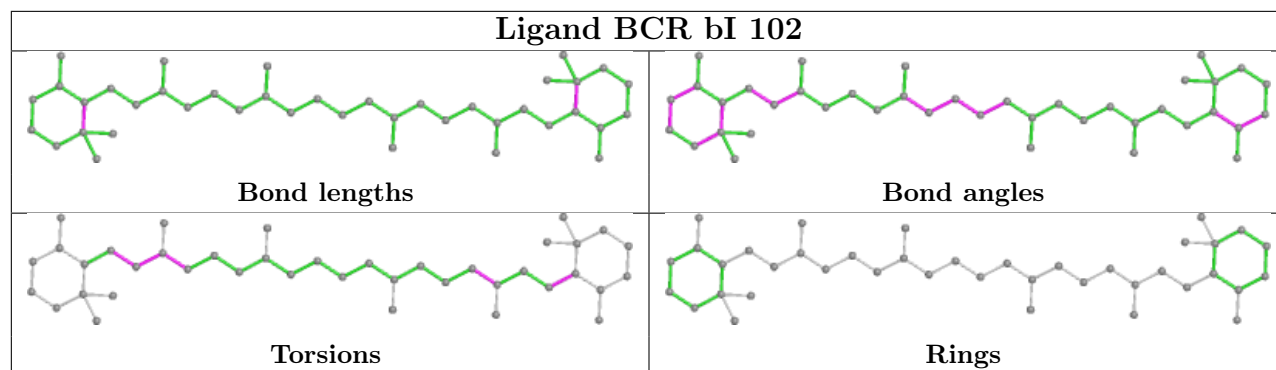
Ligand CLA aA 818

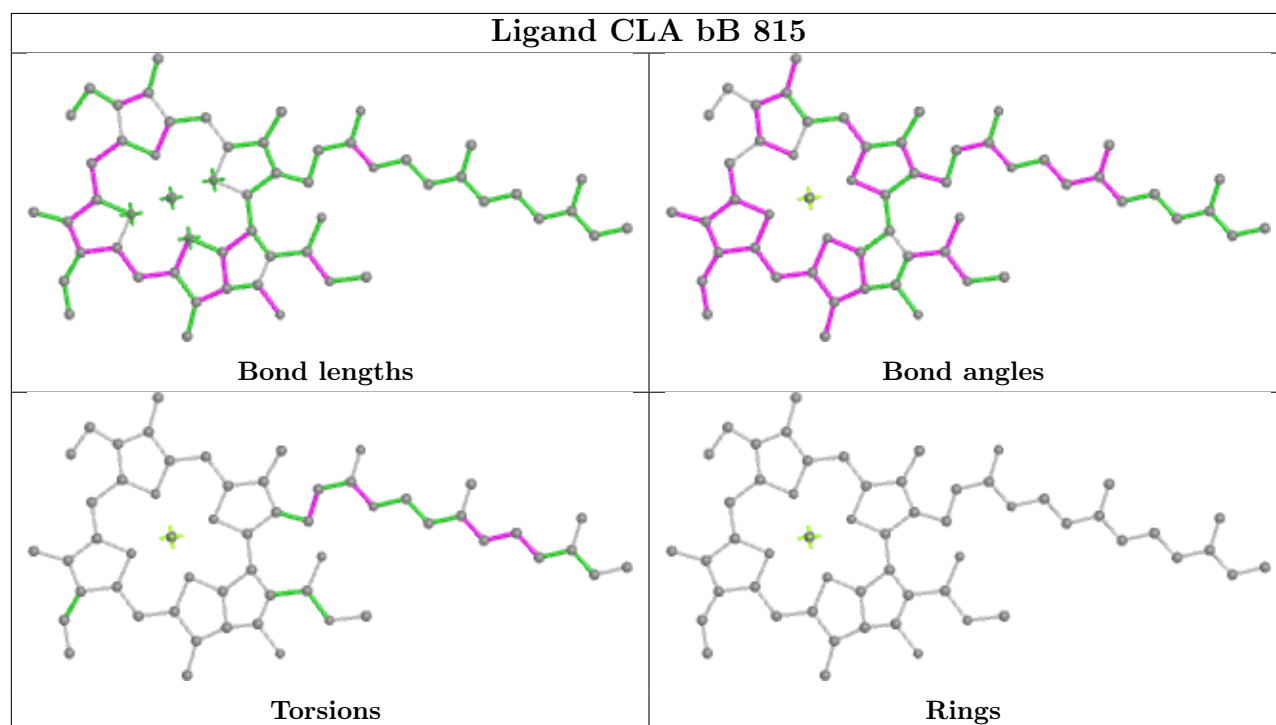
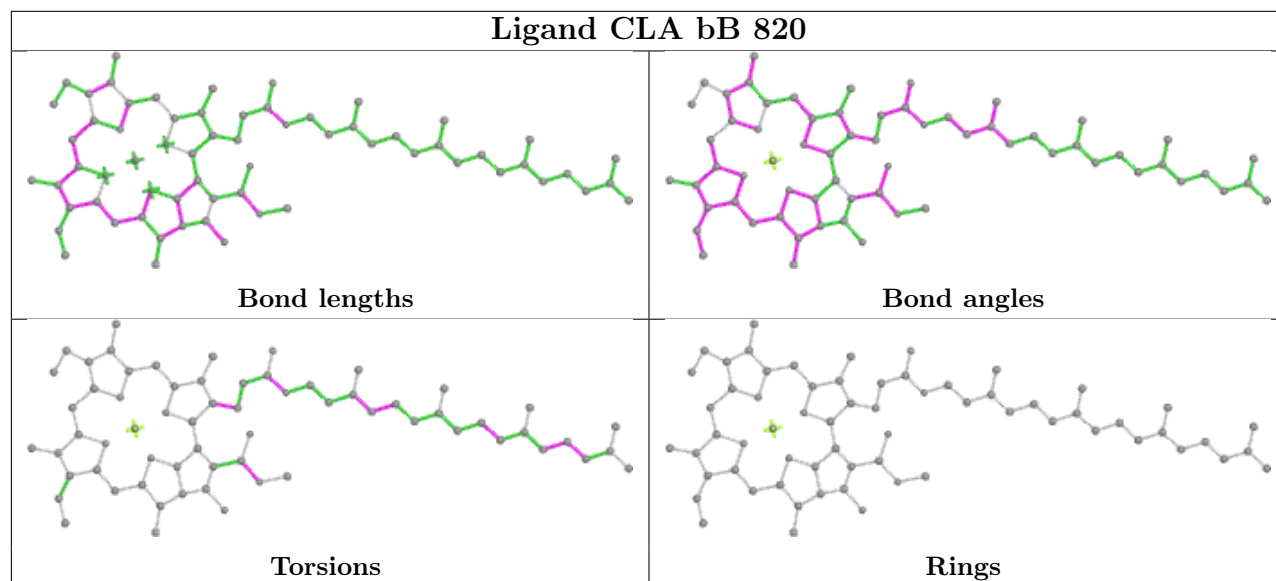
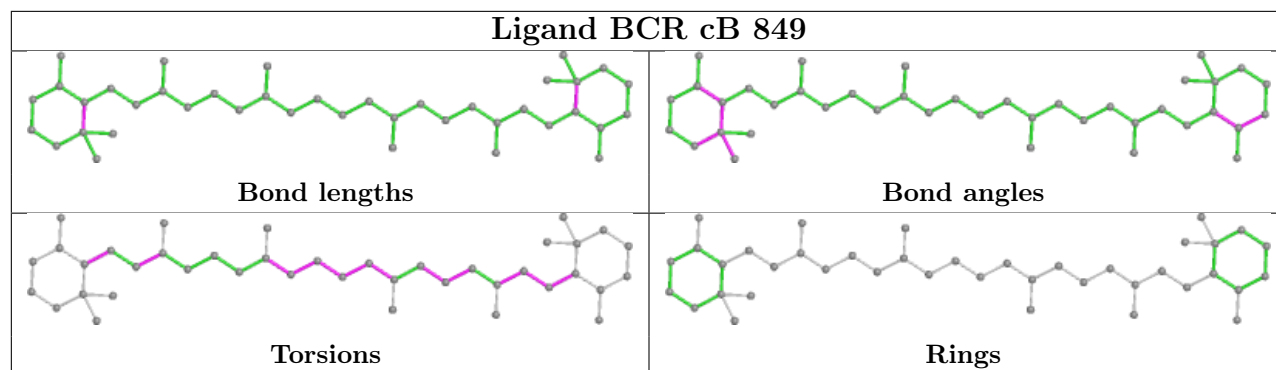




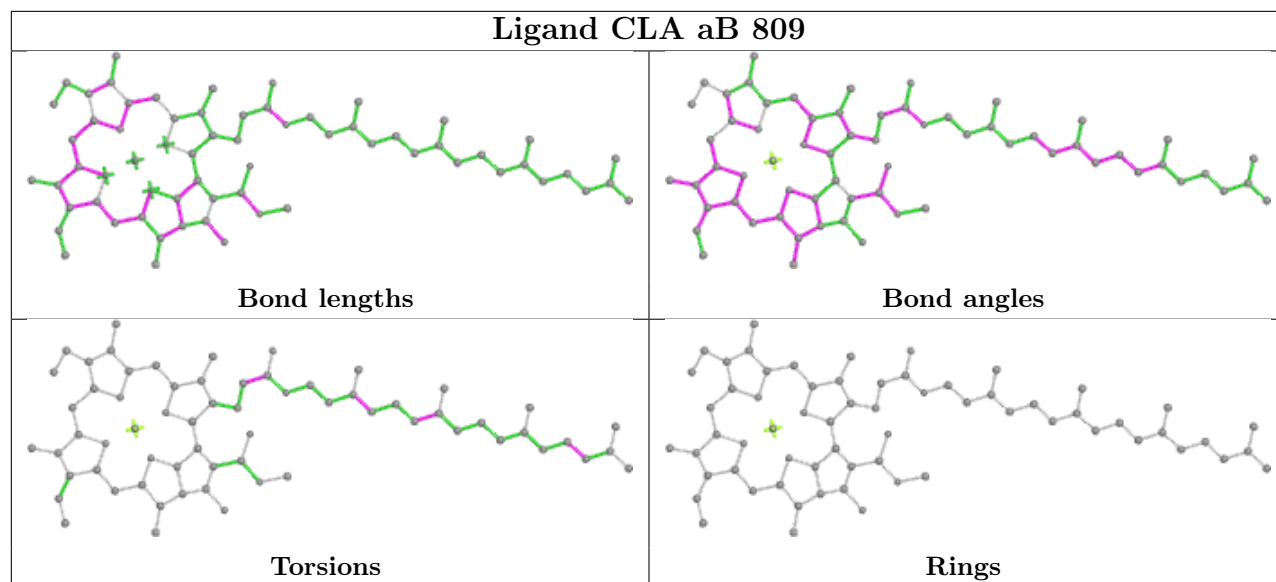




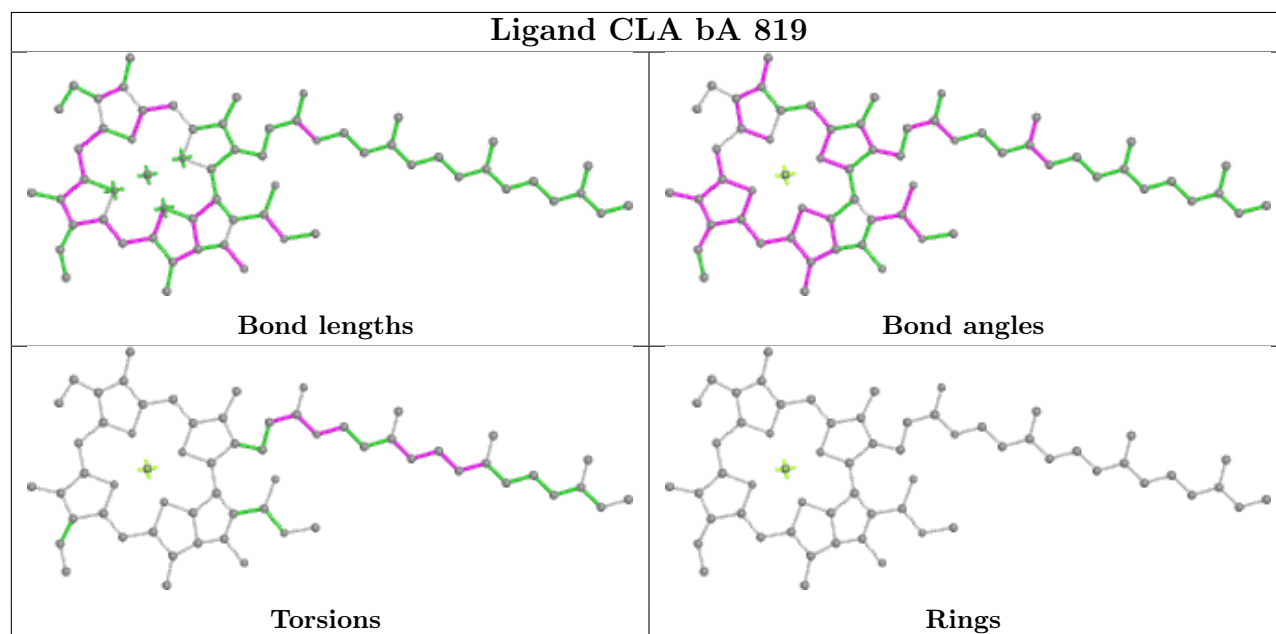


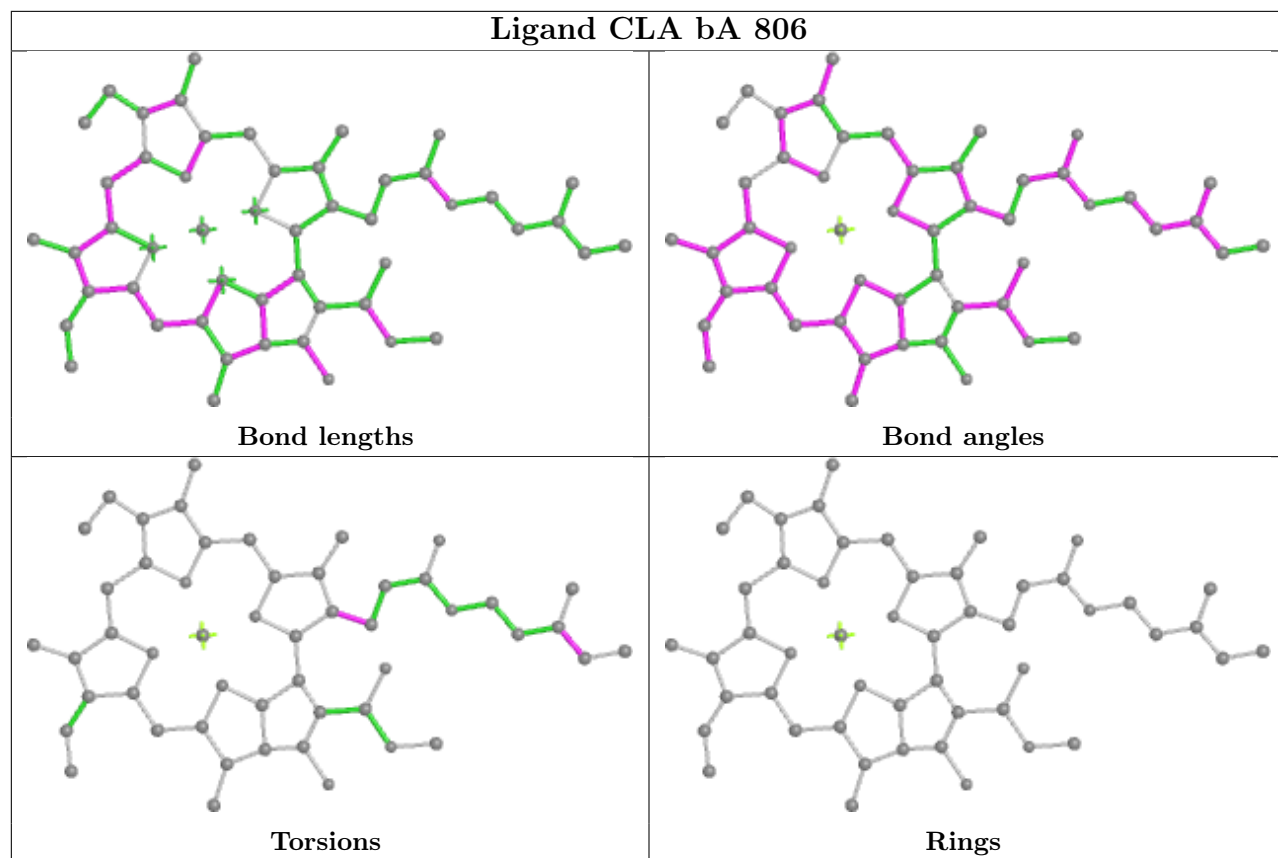


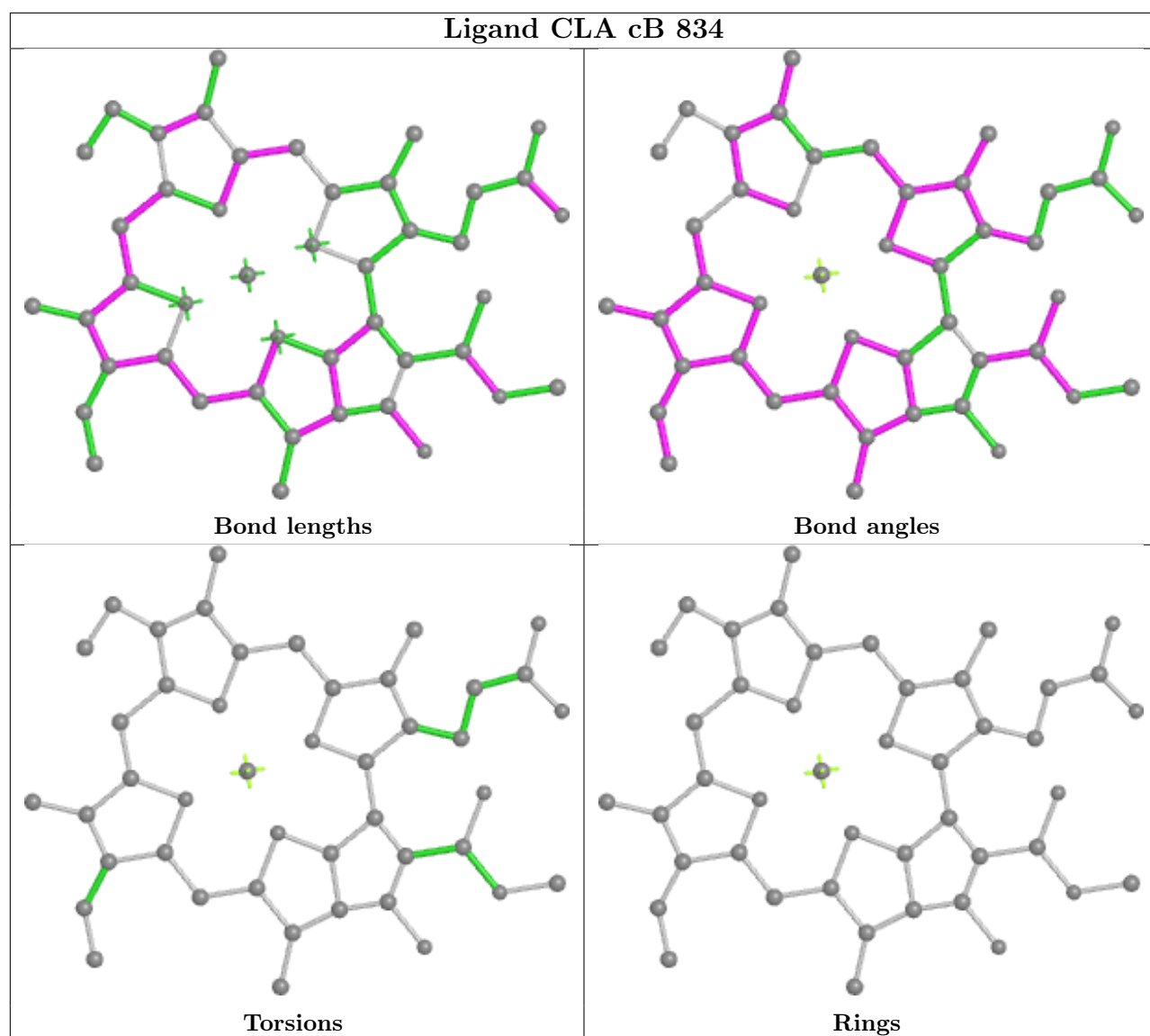
Ligand CLA aB 809



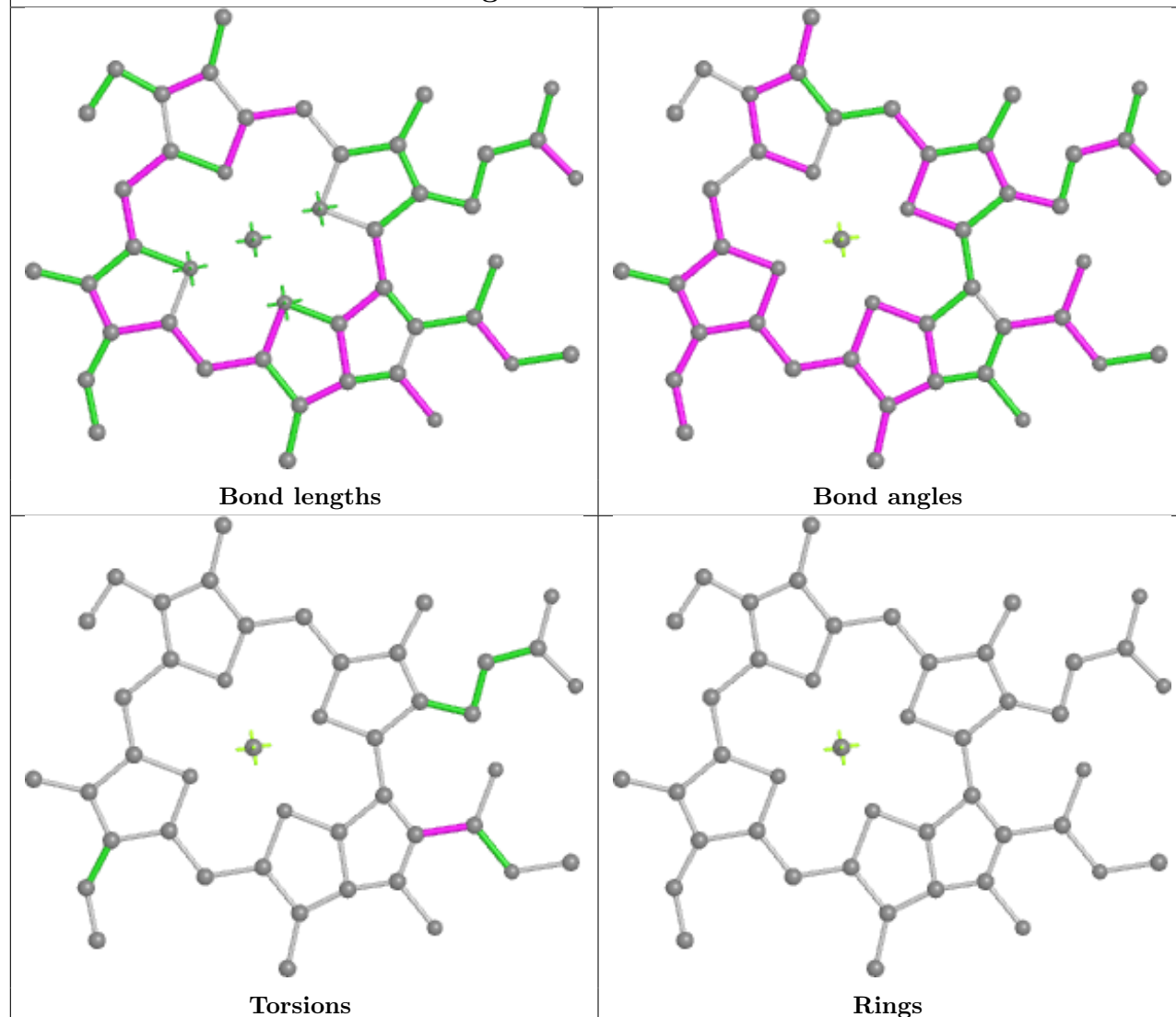
Ligand CLA bA 819



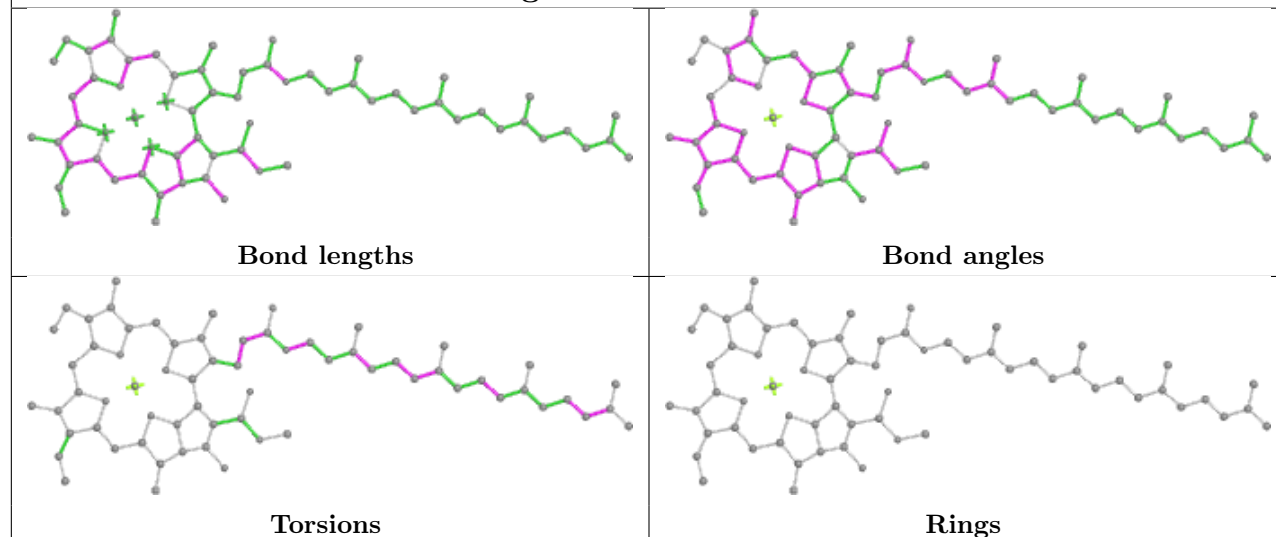


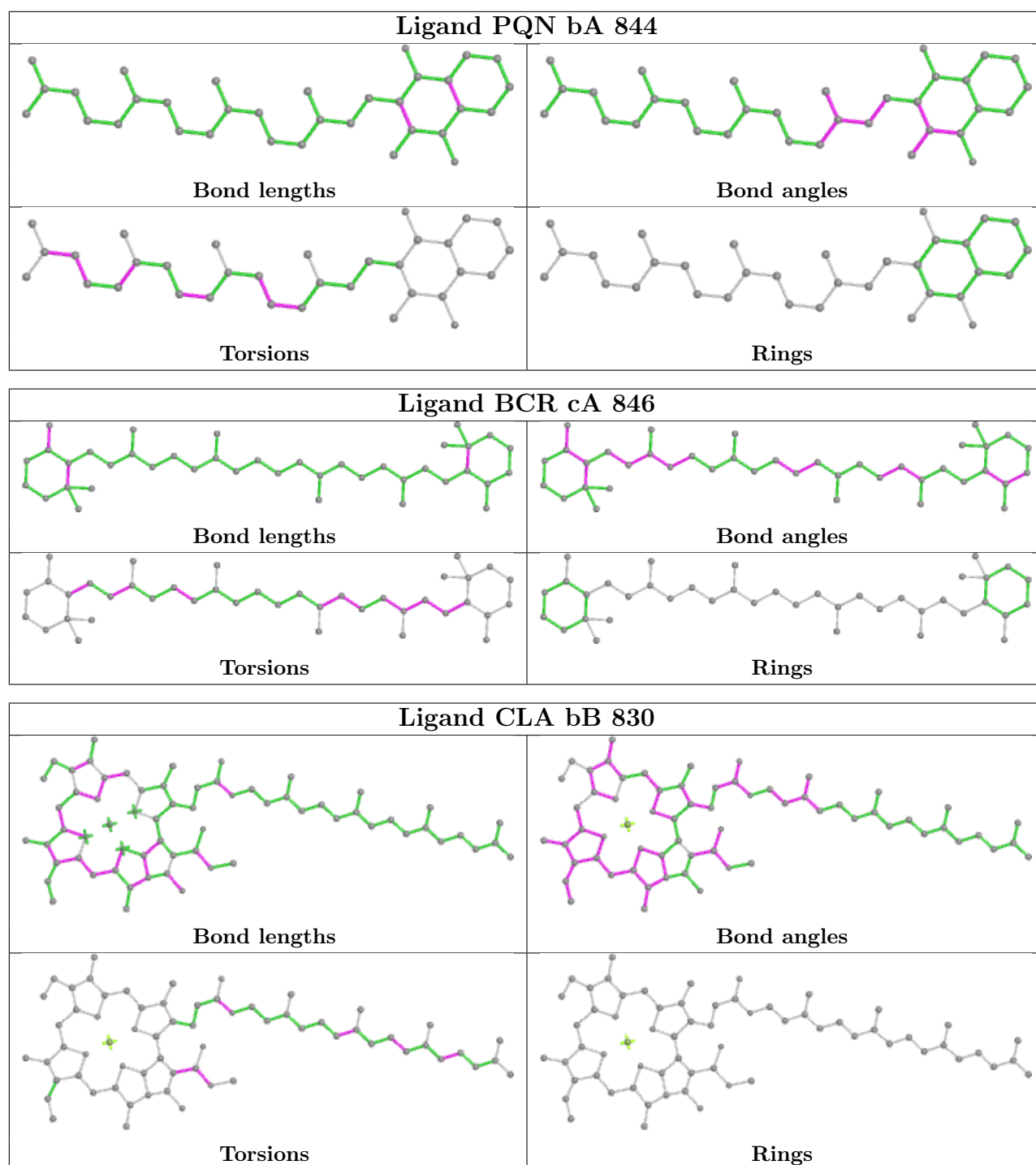


Ligand CLA aA 813

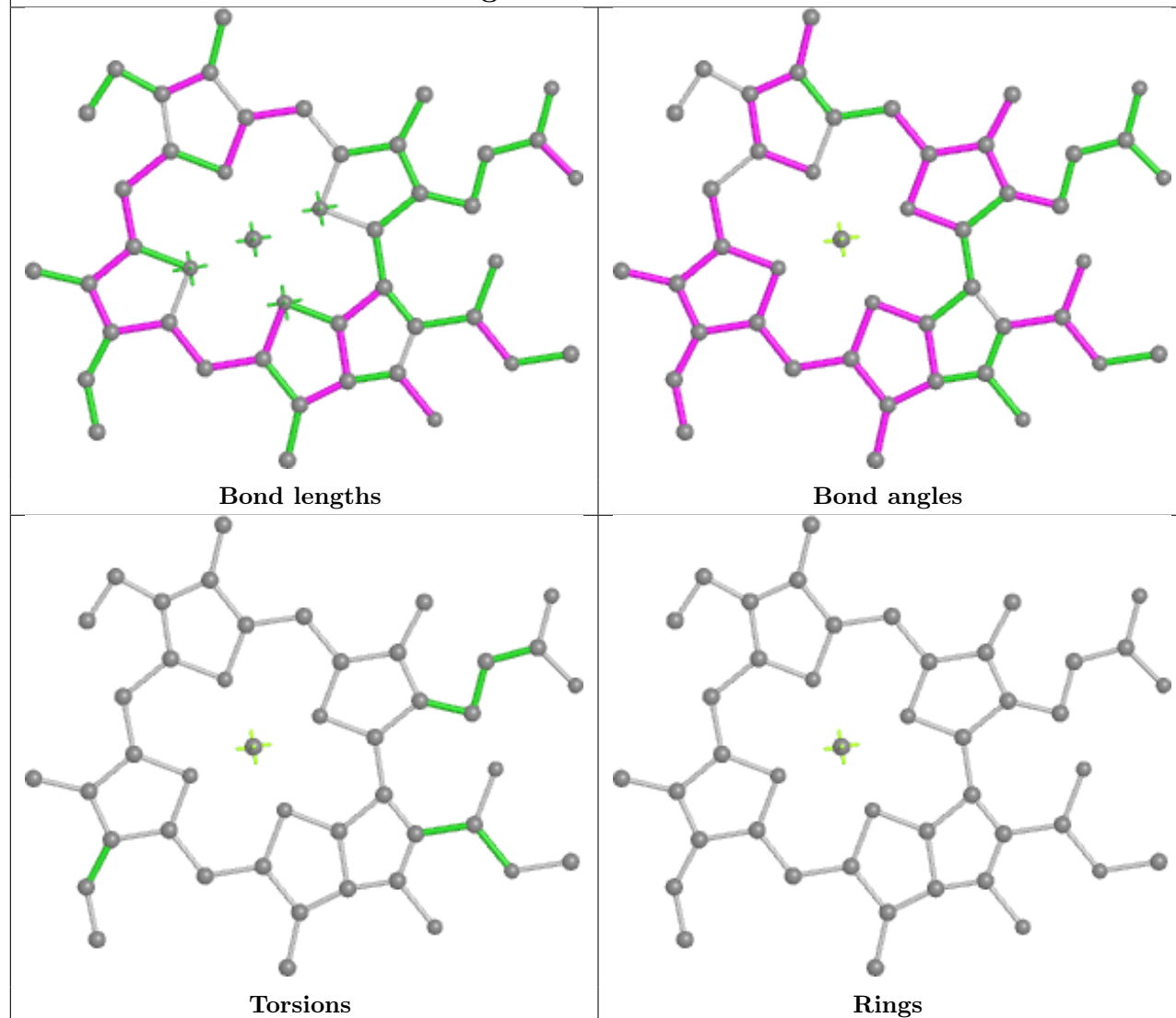


Ligand CLA bA 841

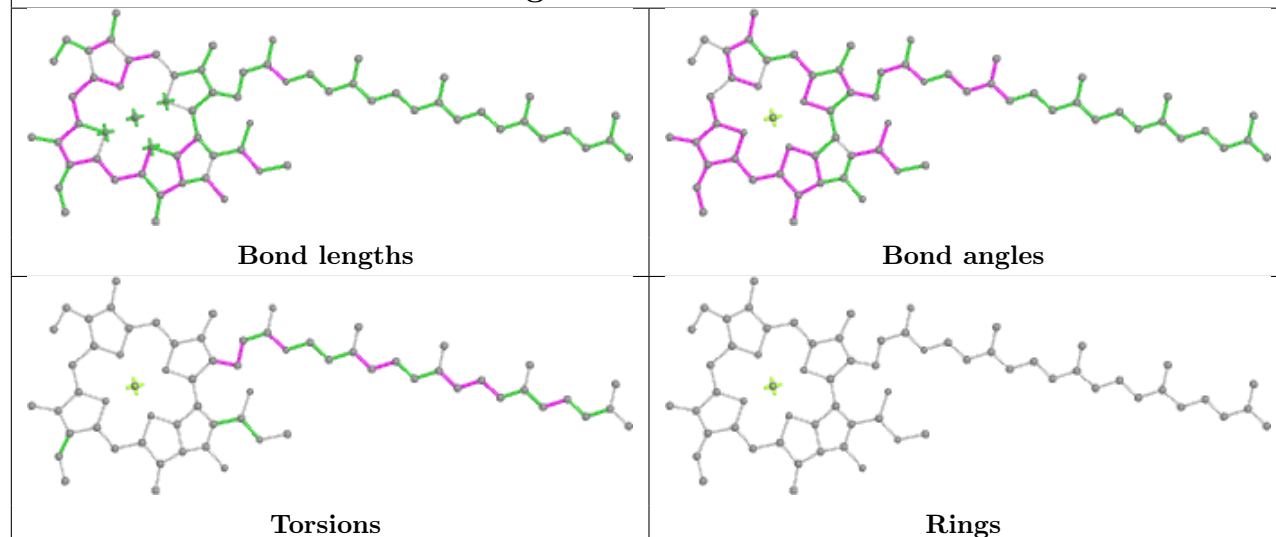




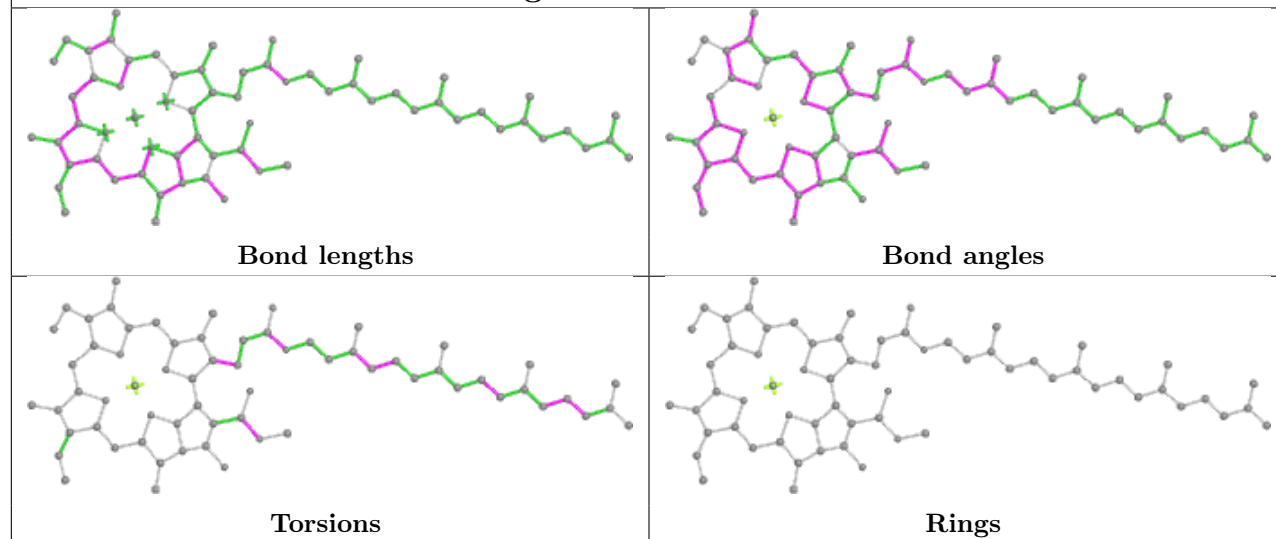
Ligand CLA bB 834



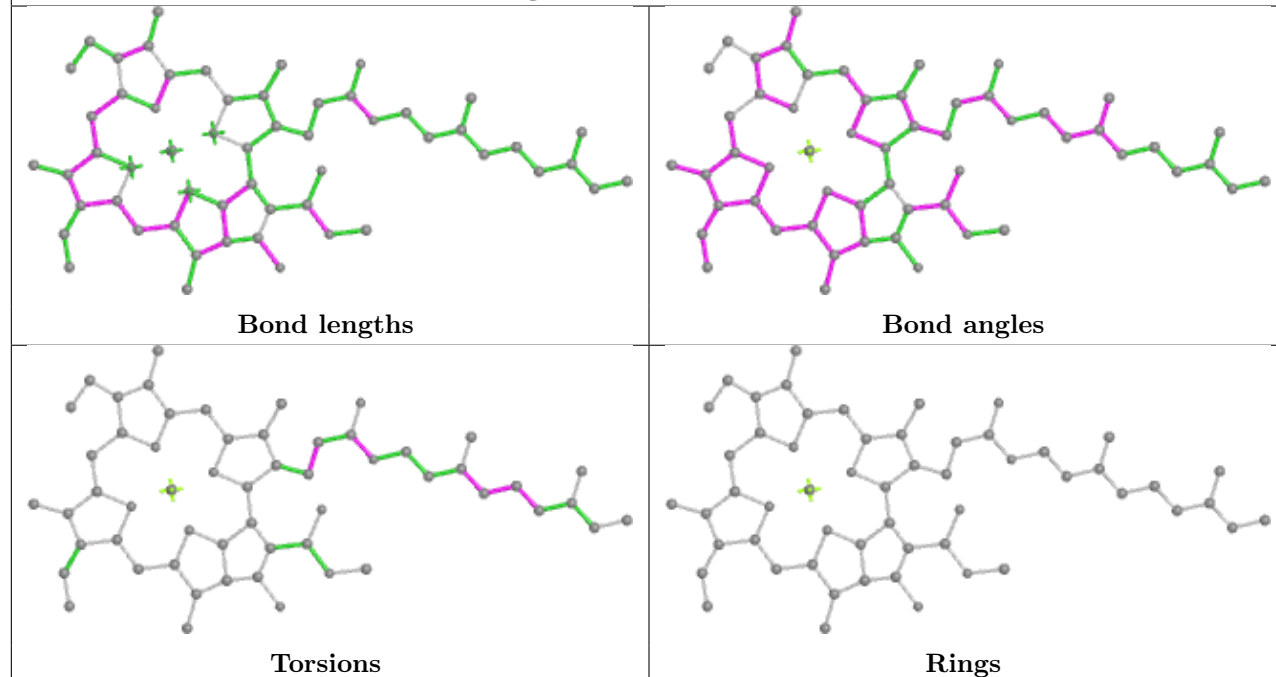
Ligand CLA cL 203



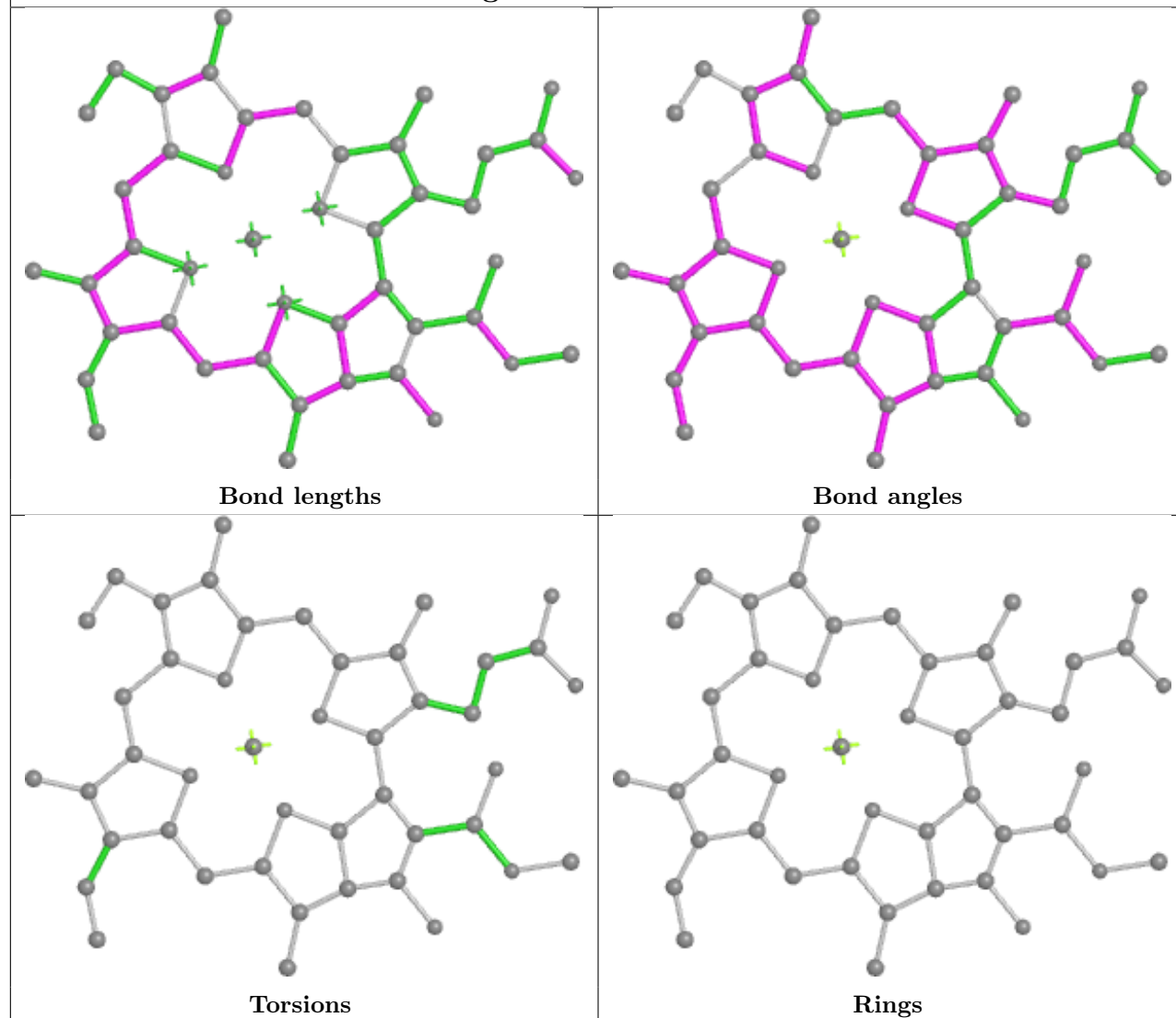
Ligand CLA cB 820



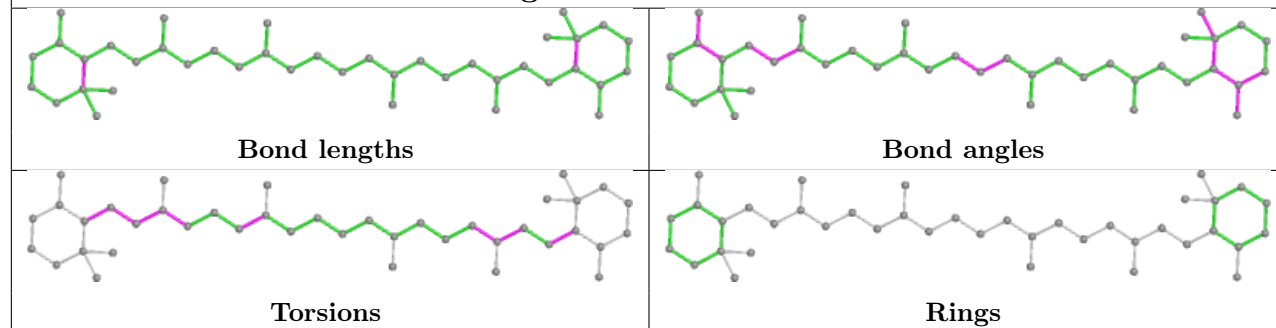
Ligand CLA cB 815

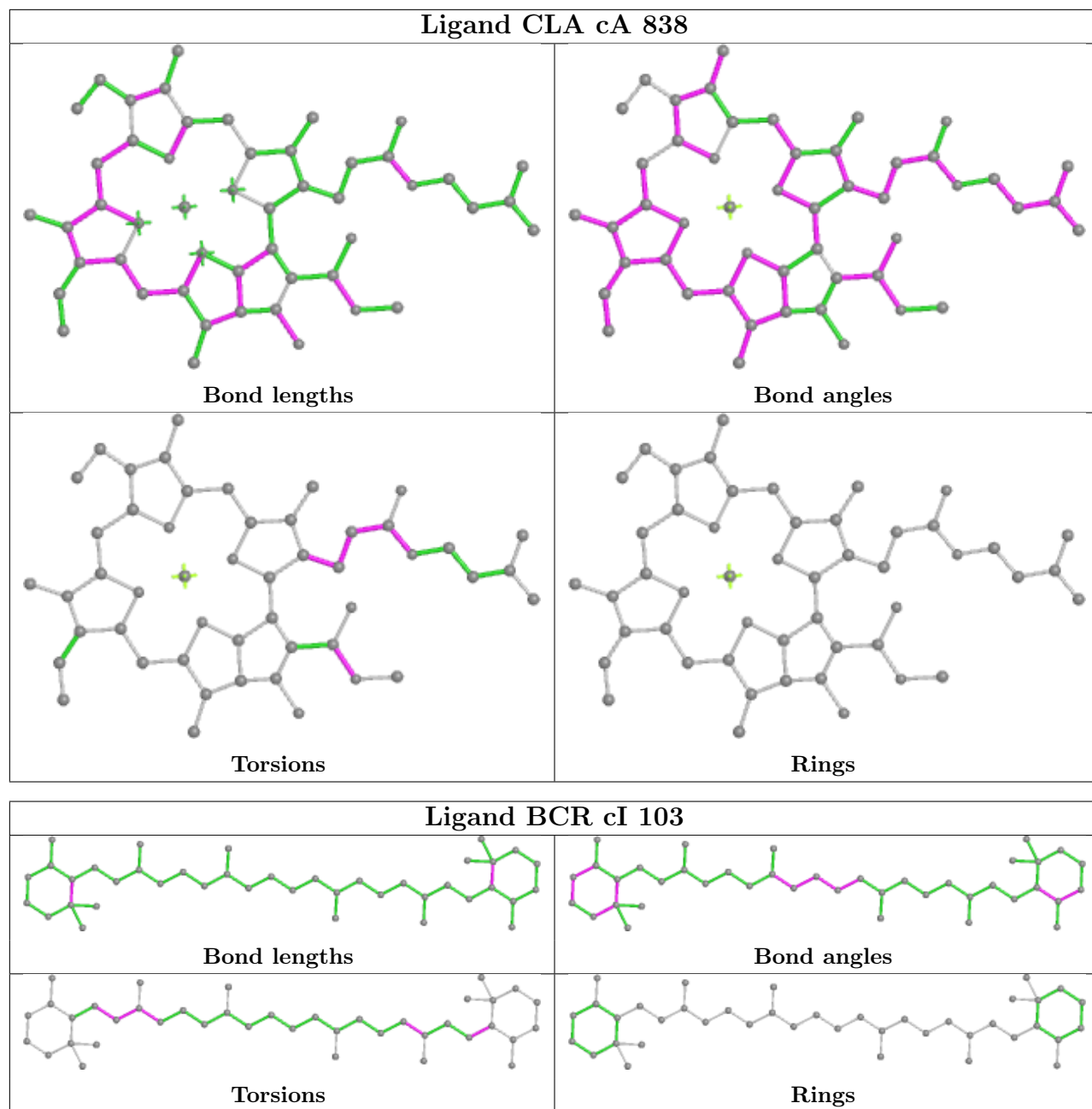


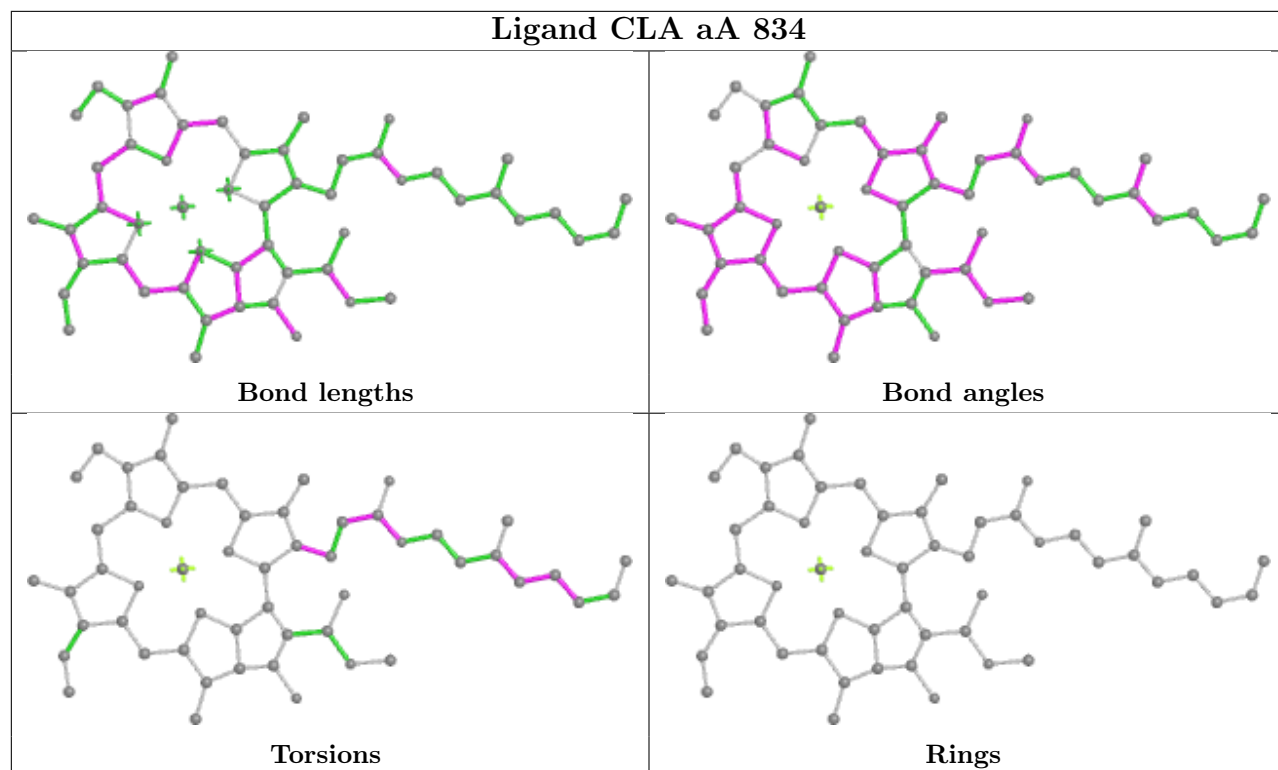
Ligand CLA aB 834



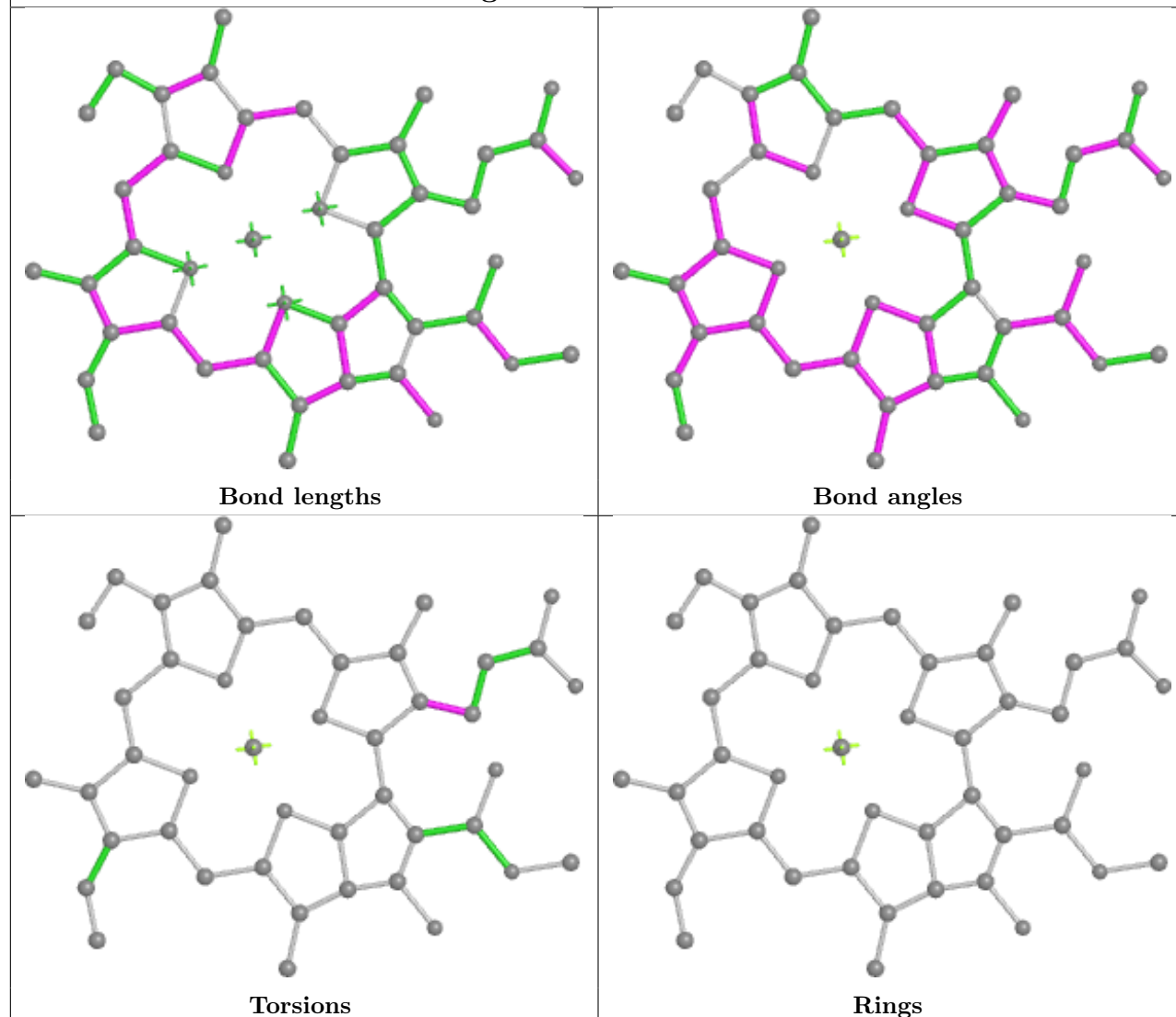
Ligand BCR bB 845



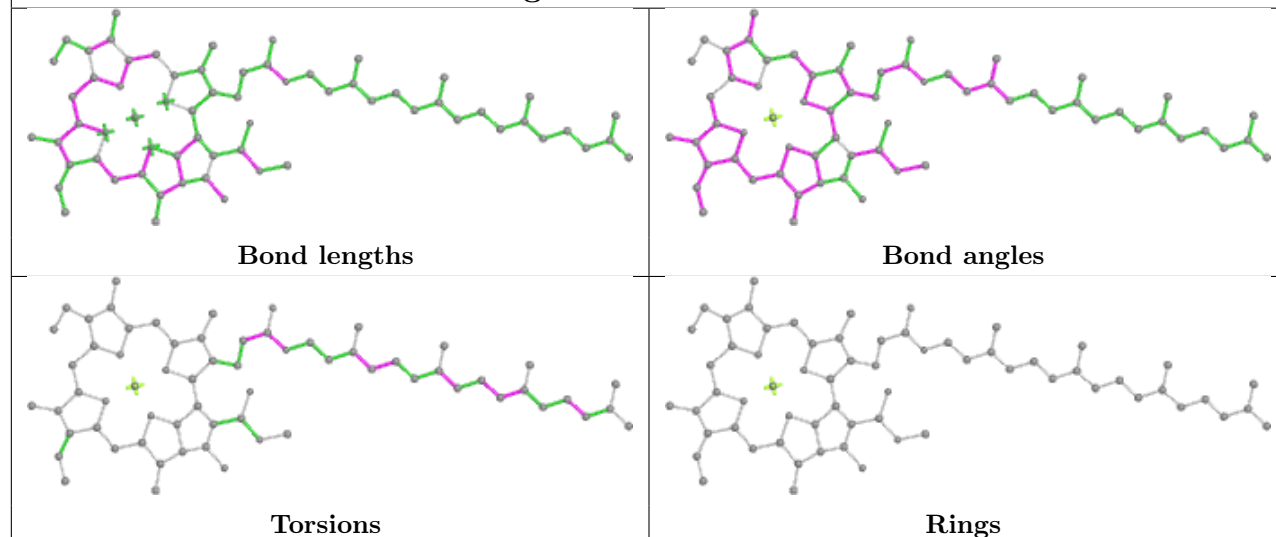


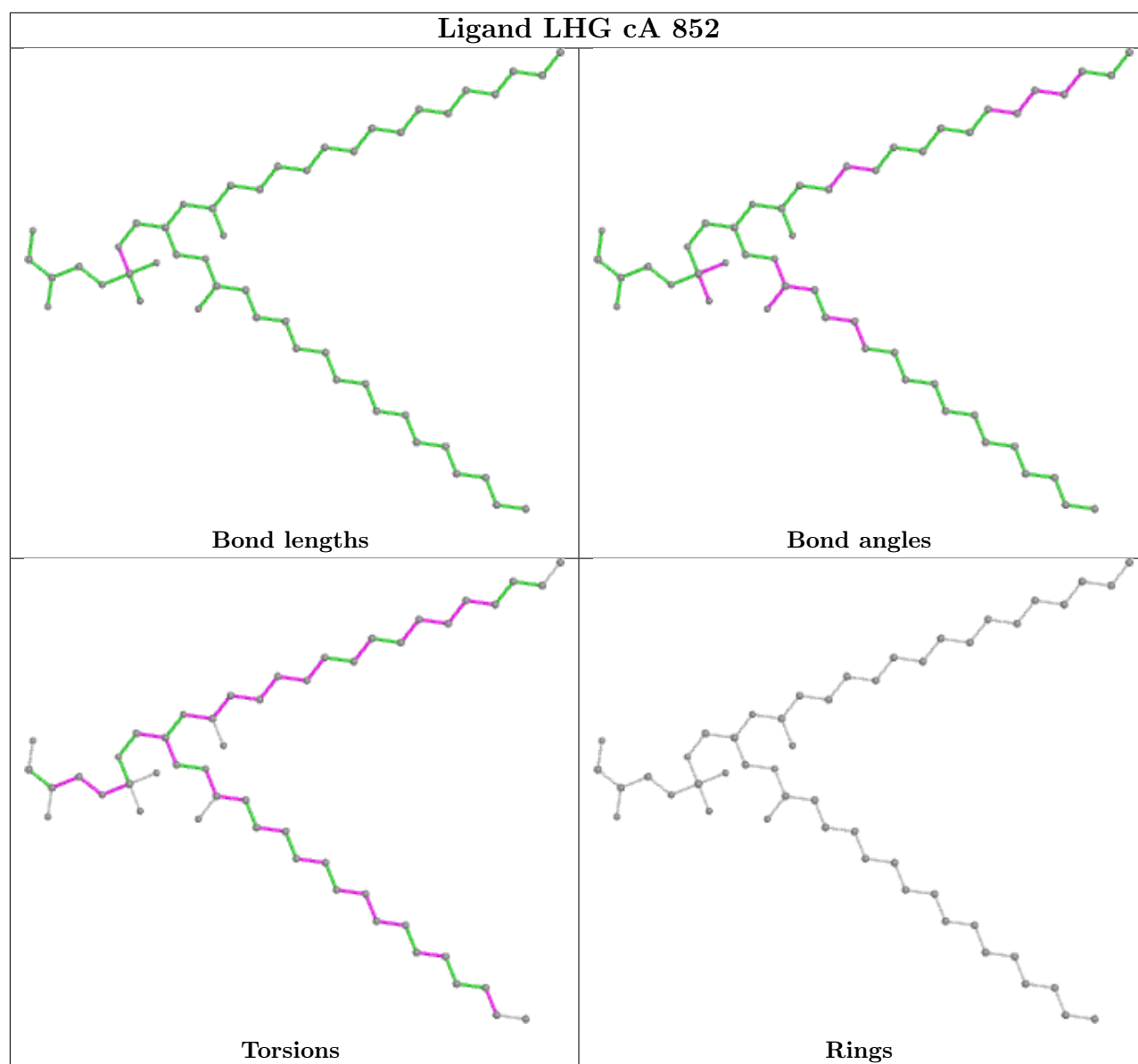


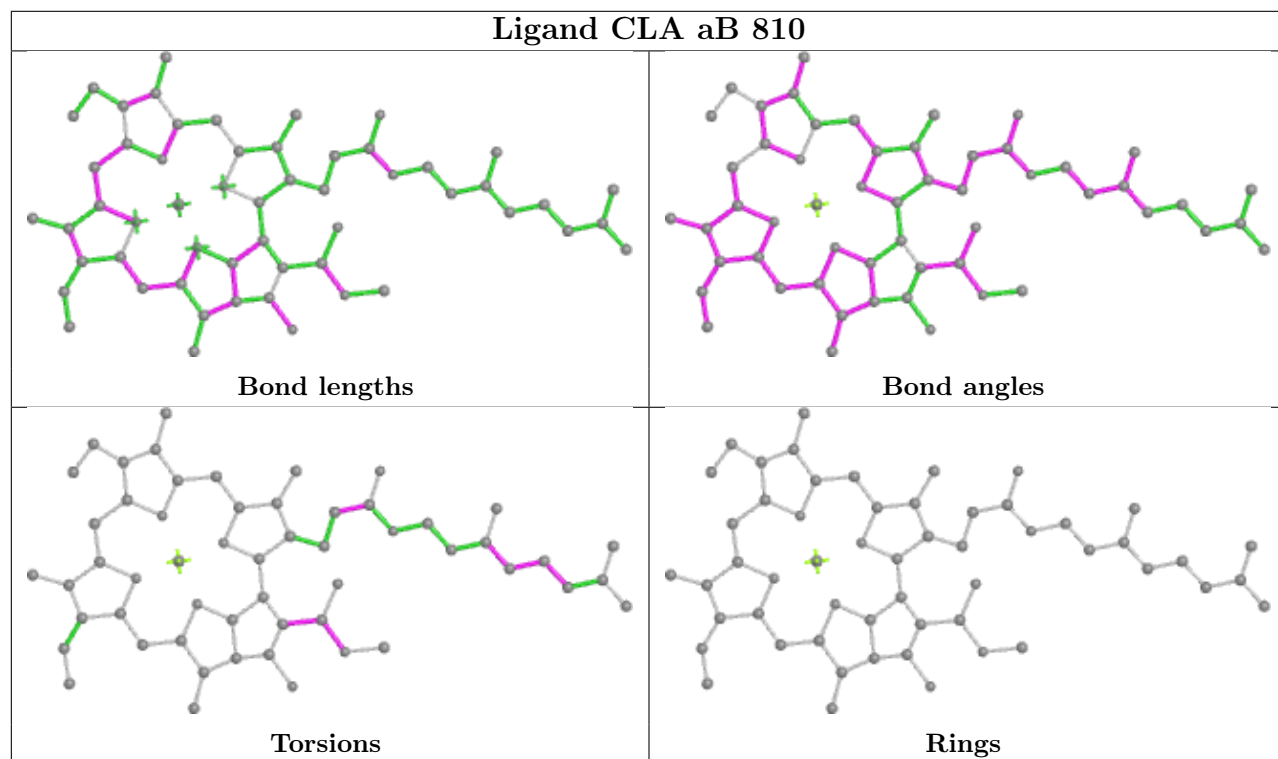
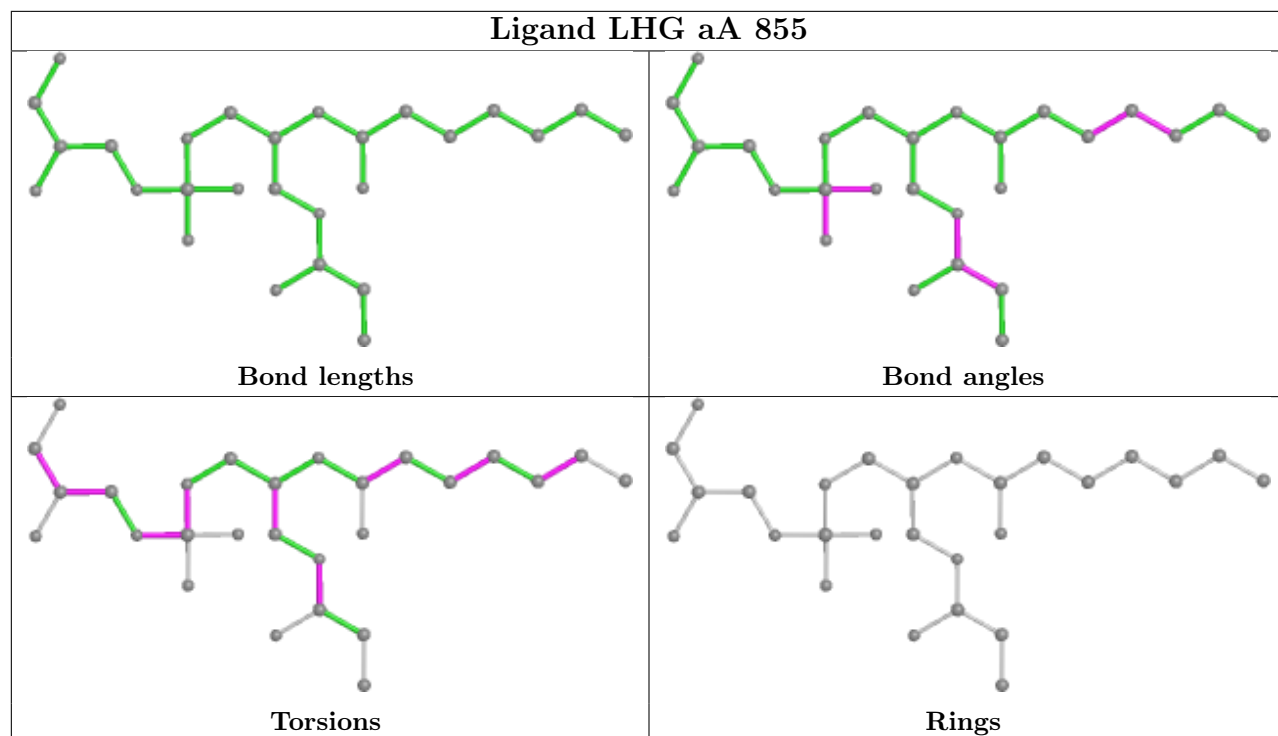
Ligand CLA bB 812

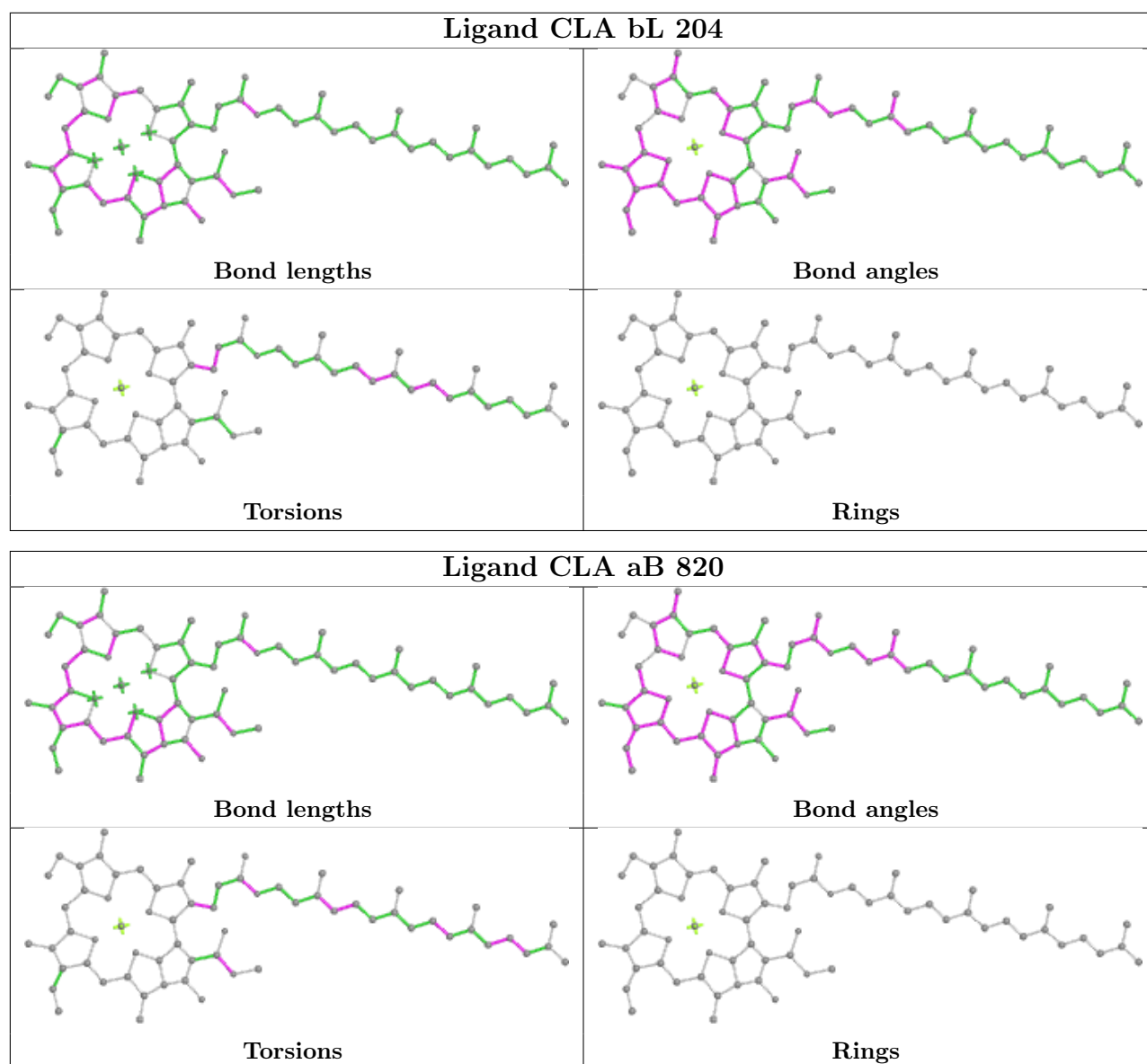


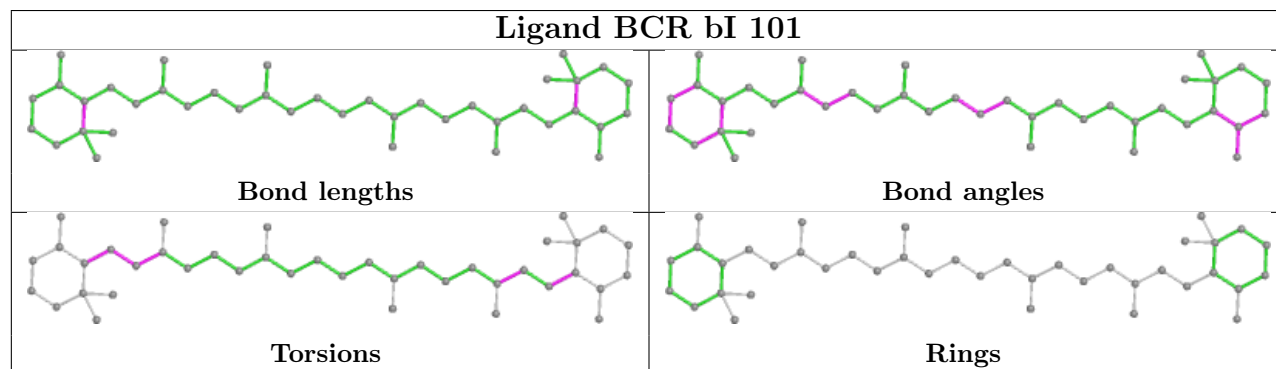
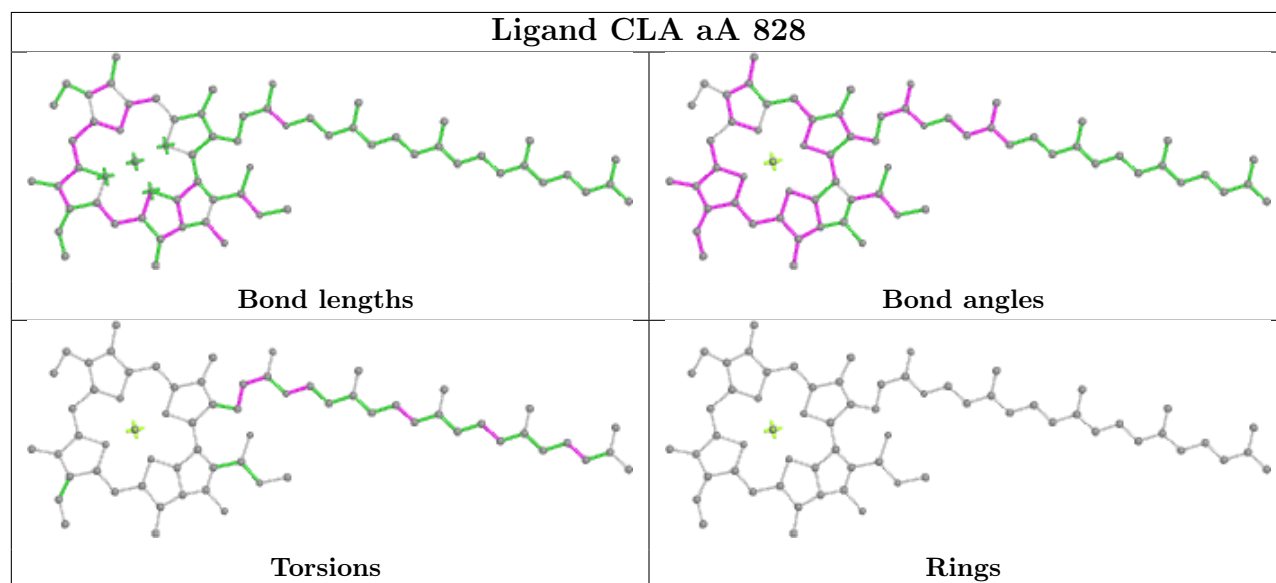
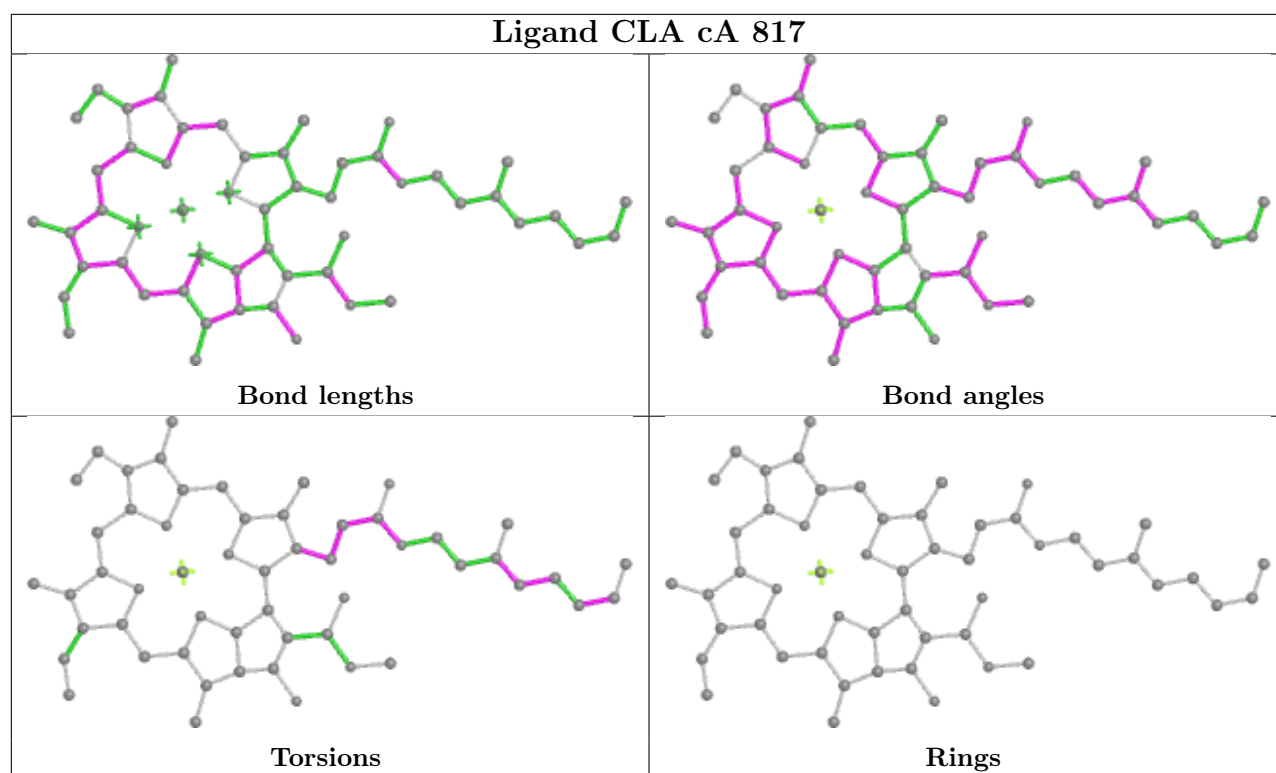
Ligand CLA aB 808

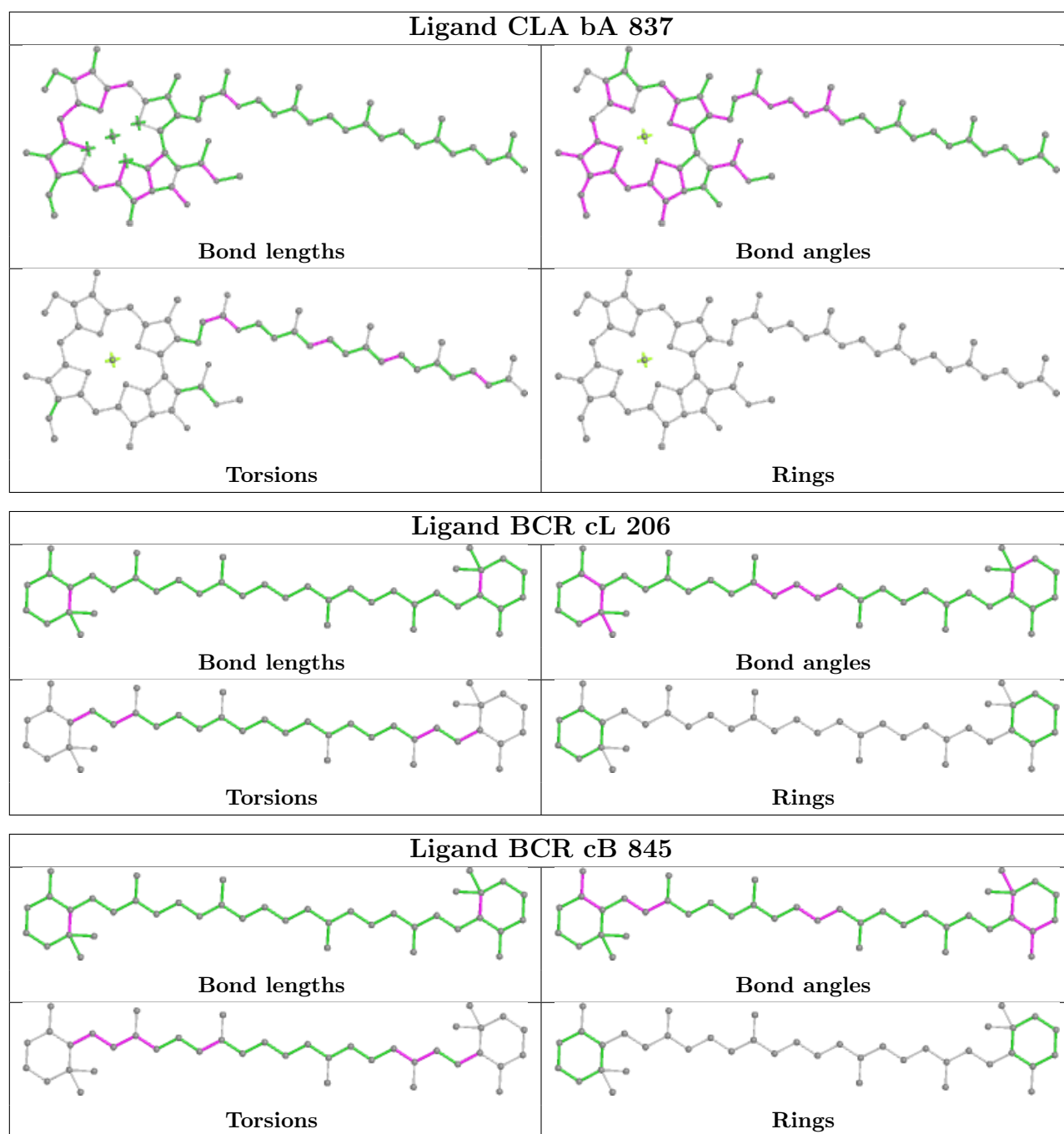




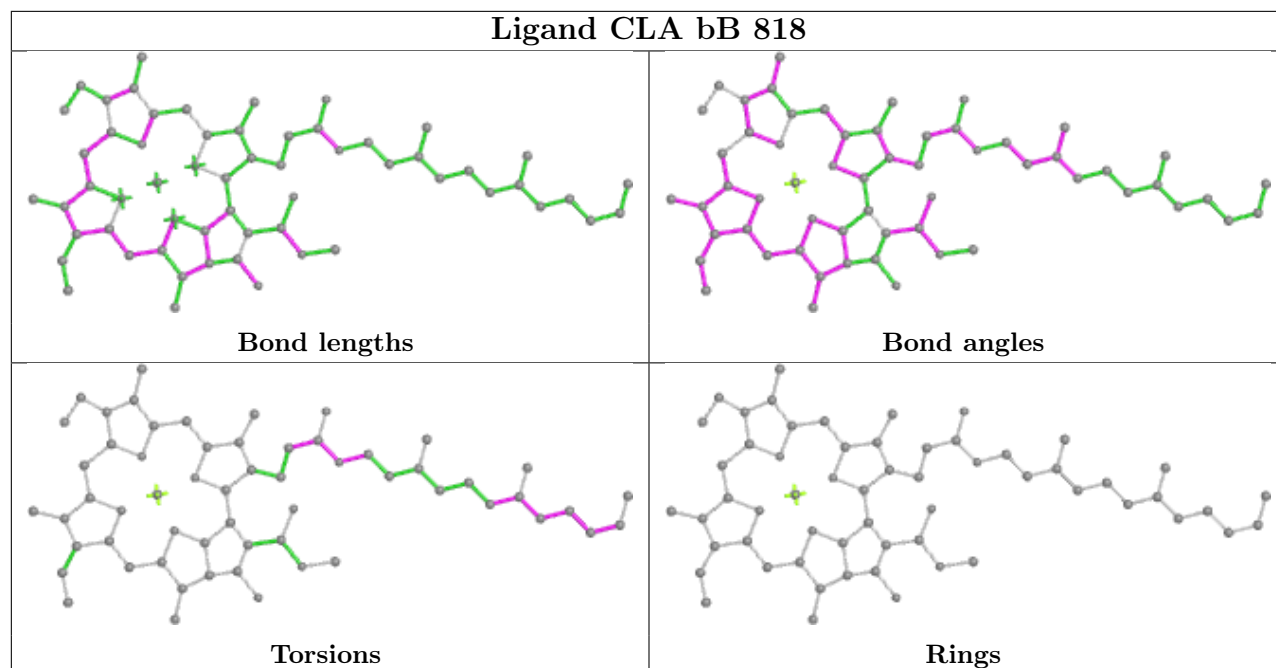




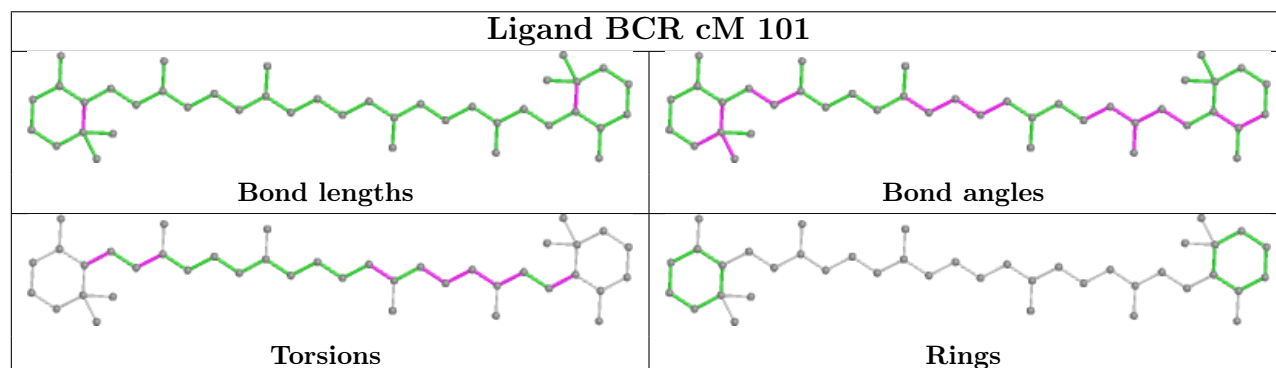




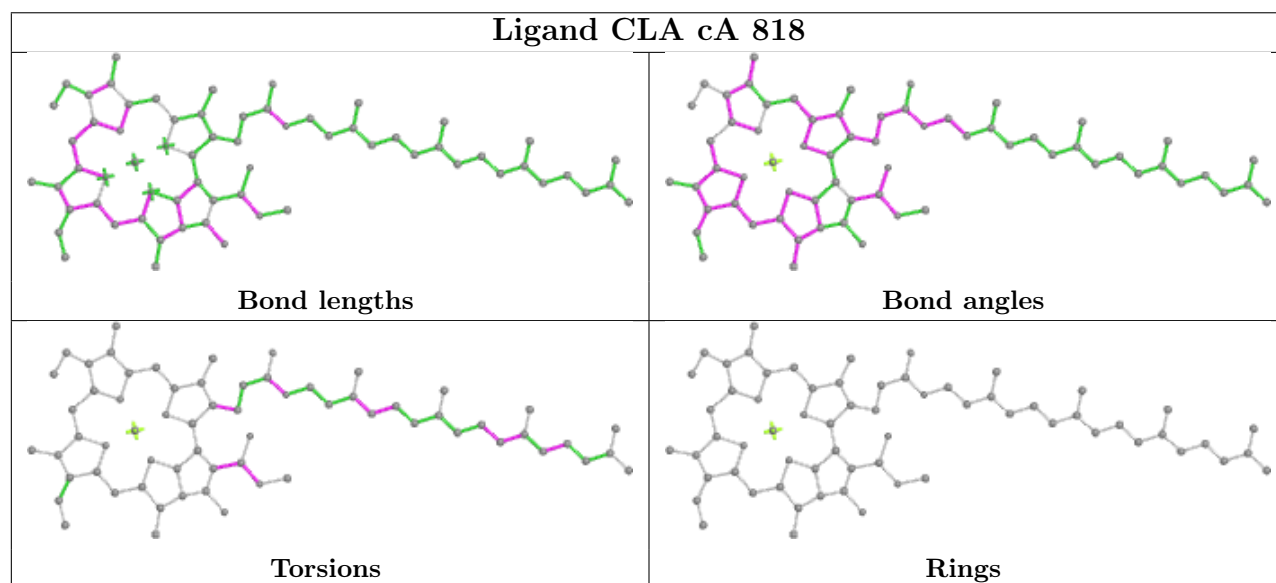
Ligand CLA bB 818

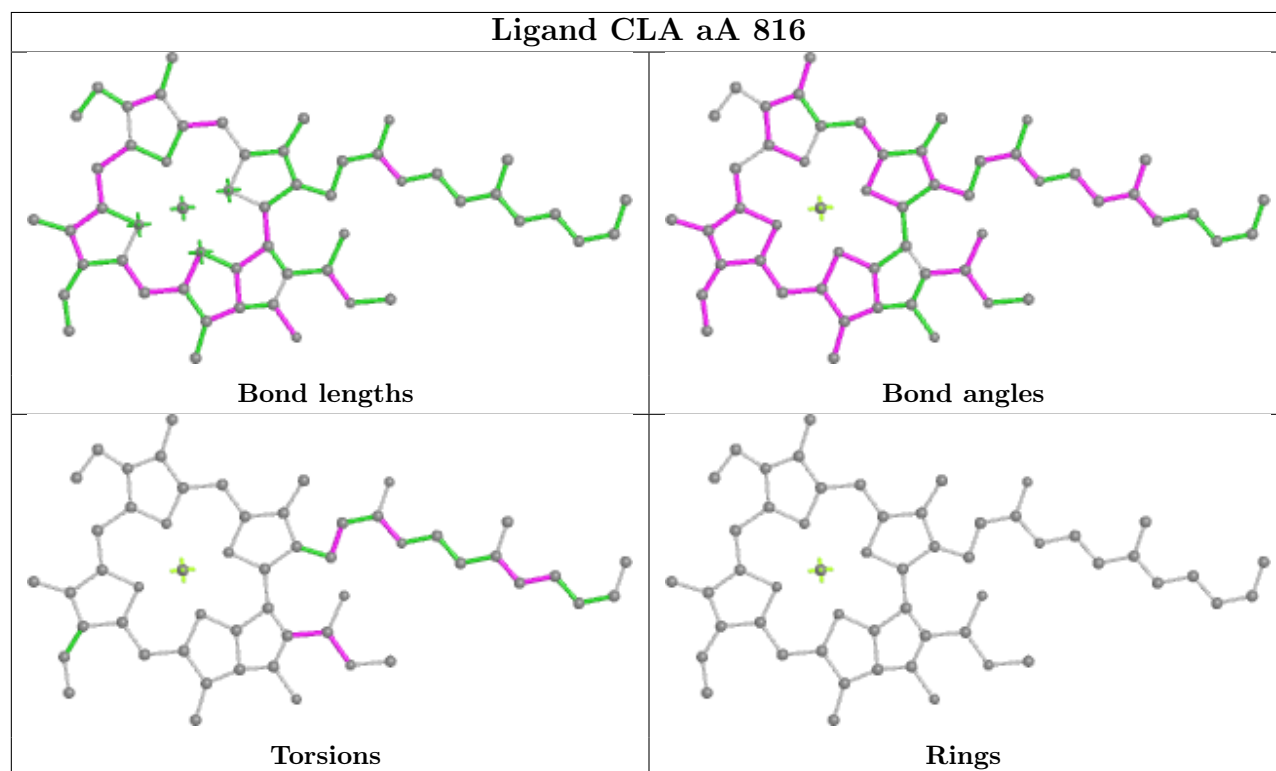
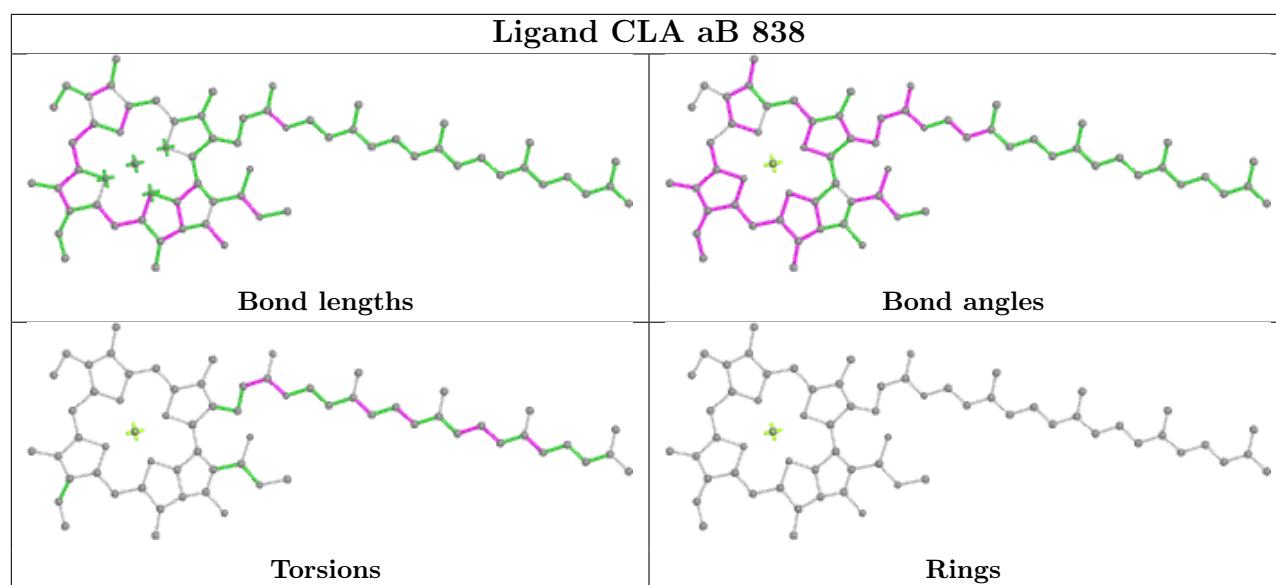


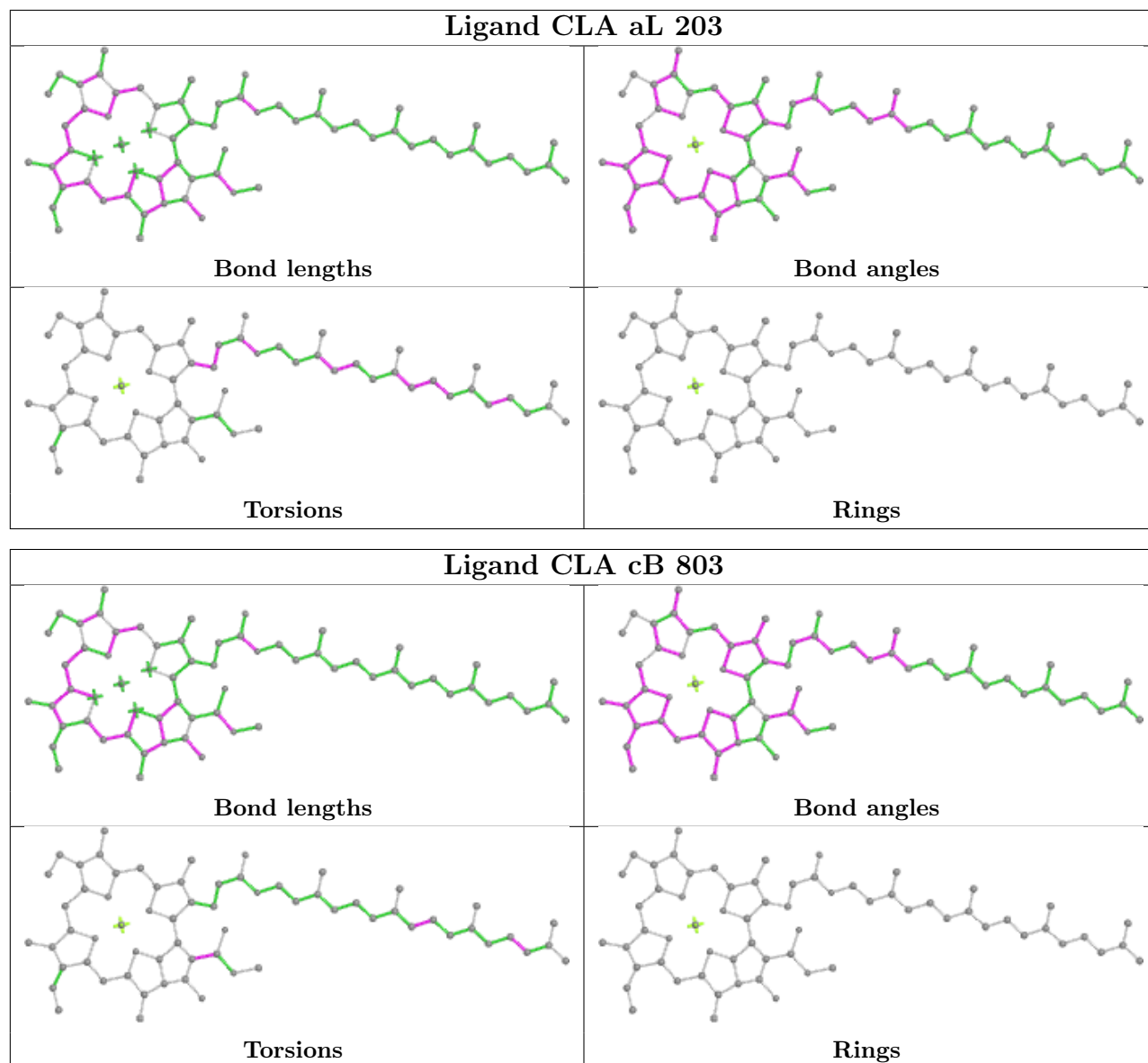
Ligand BCR cM 101



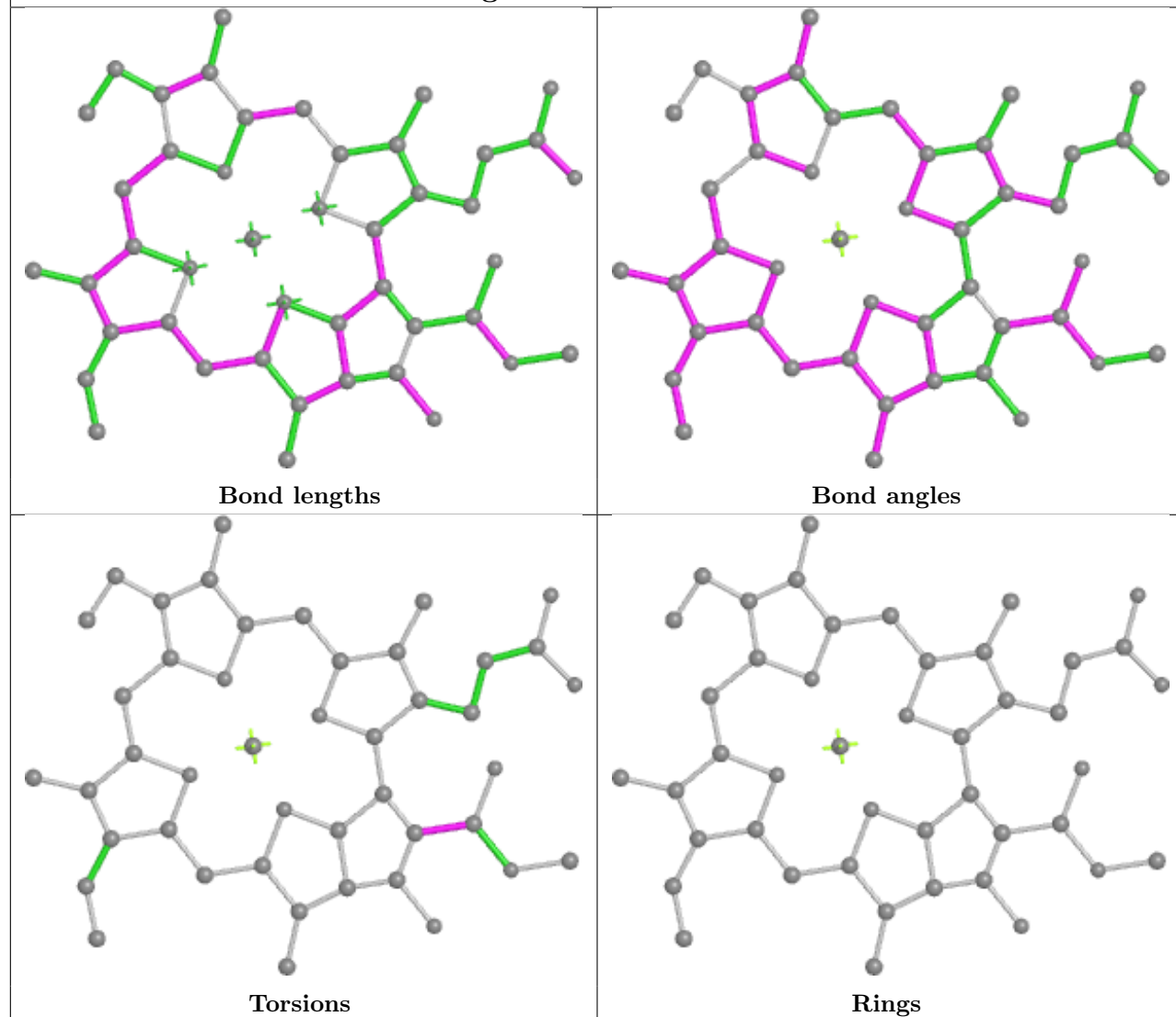
Ligand CLA cA 818



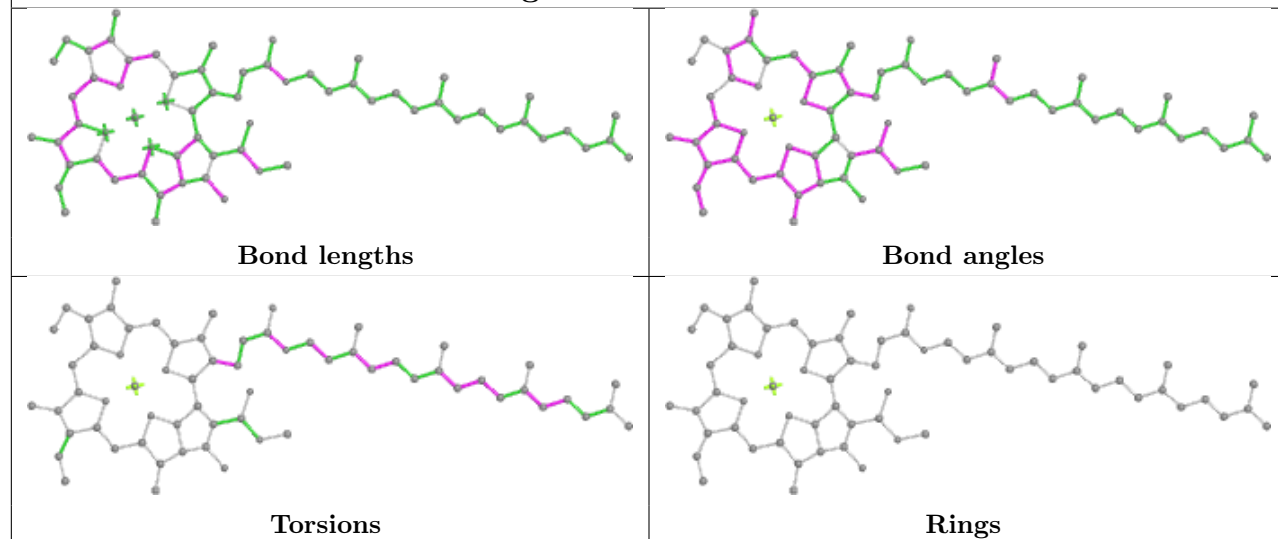




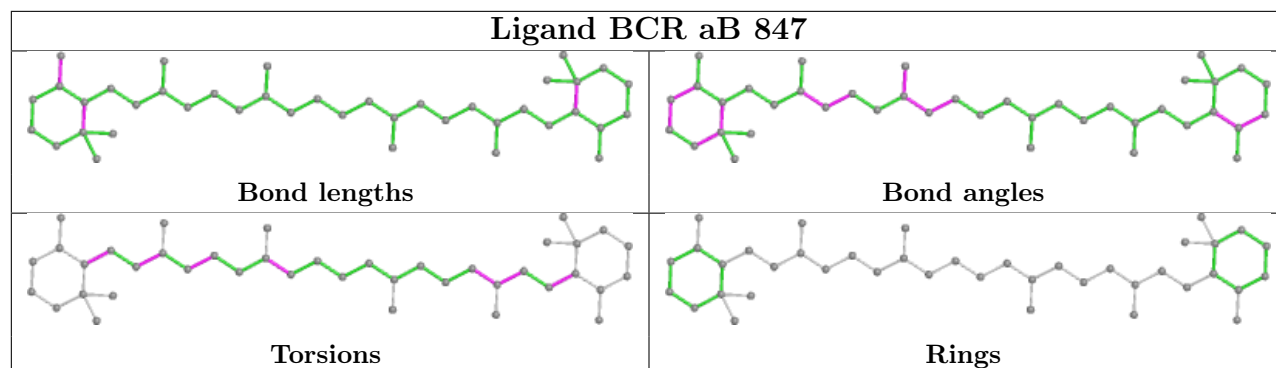
Ligand CLA cA 803



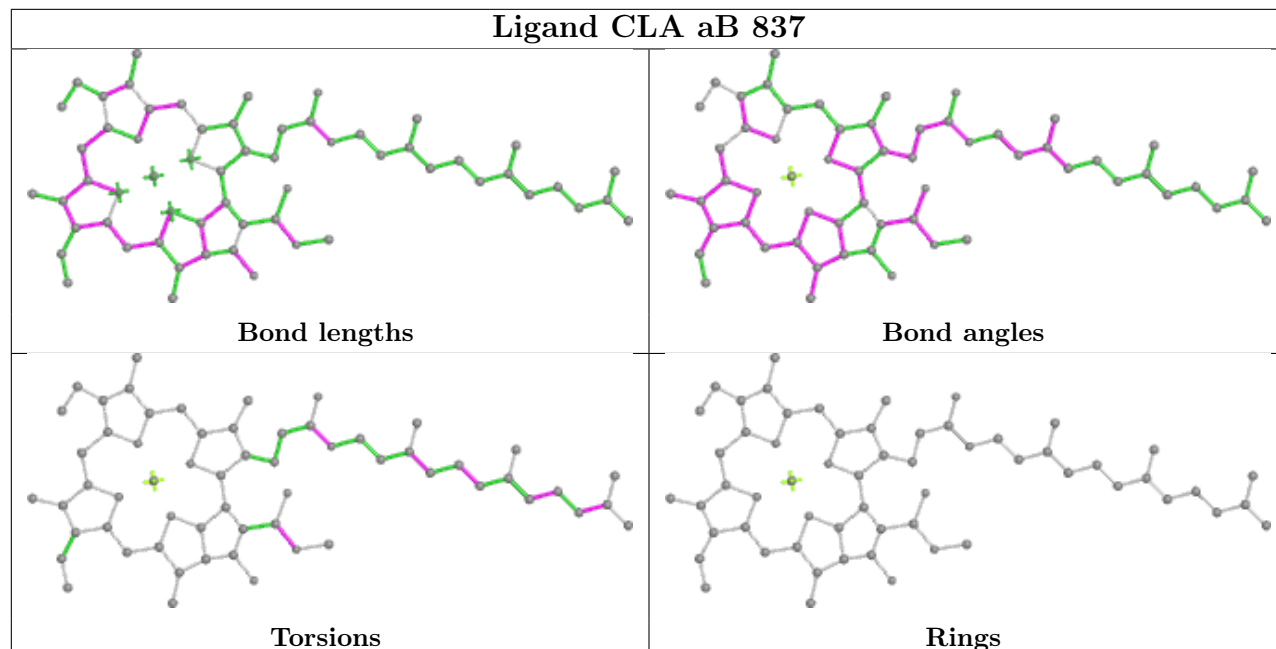
Ligand CLA bA 831



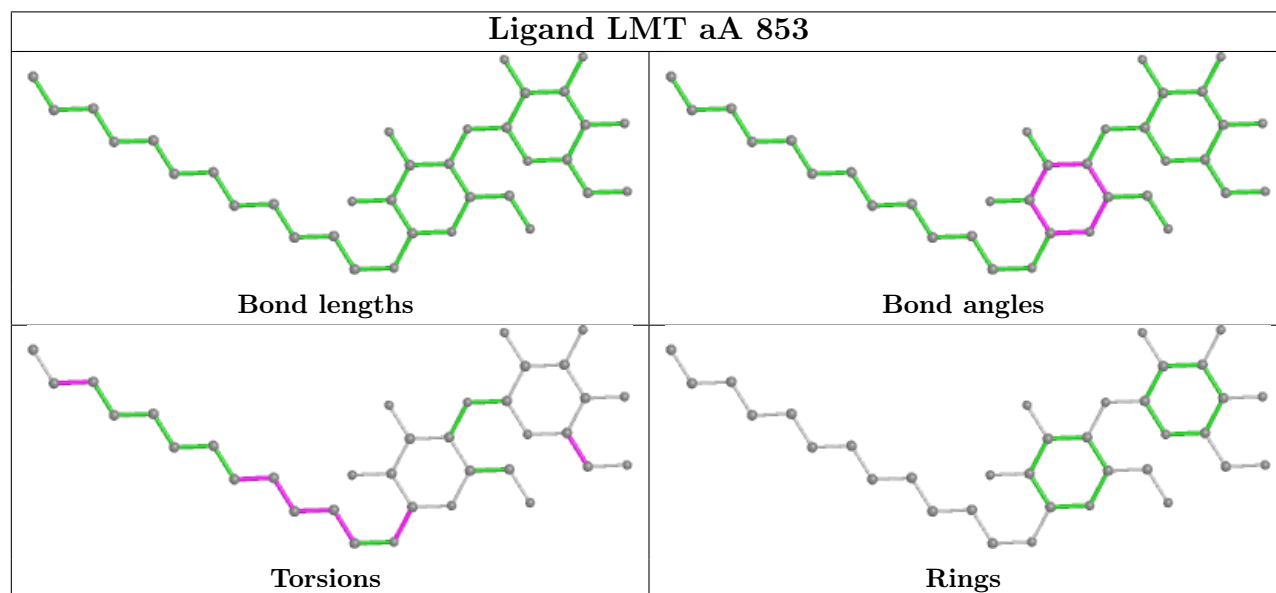
Ligand BCR aB 847

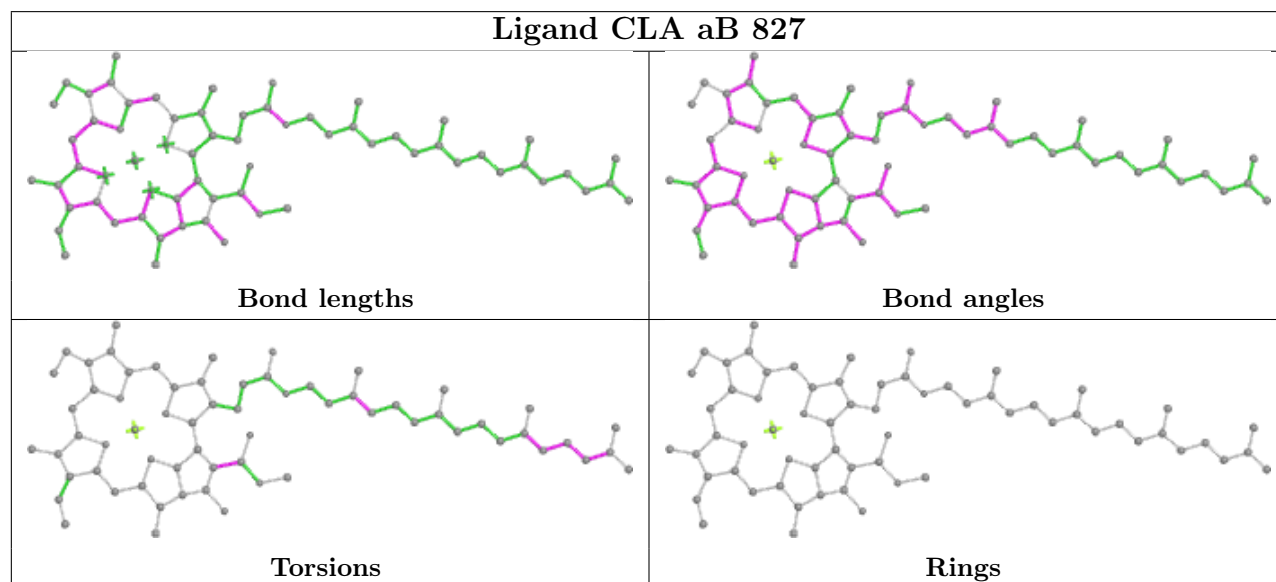
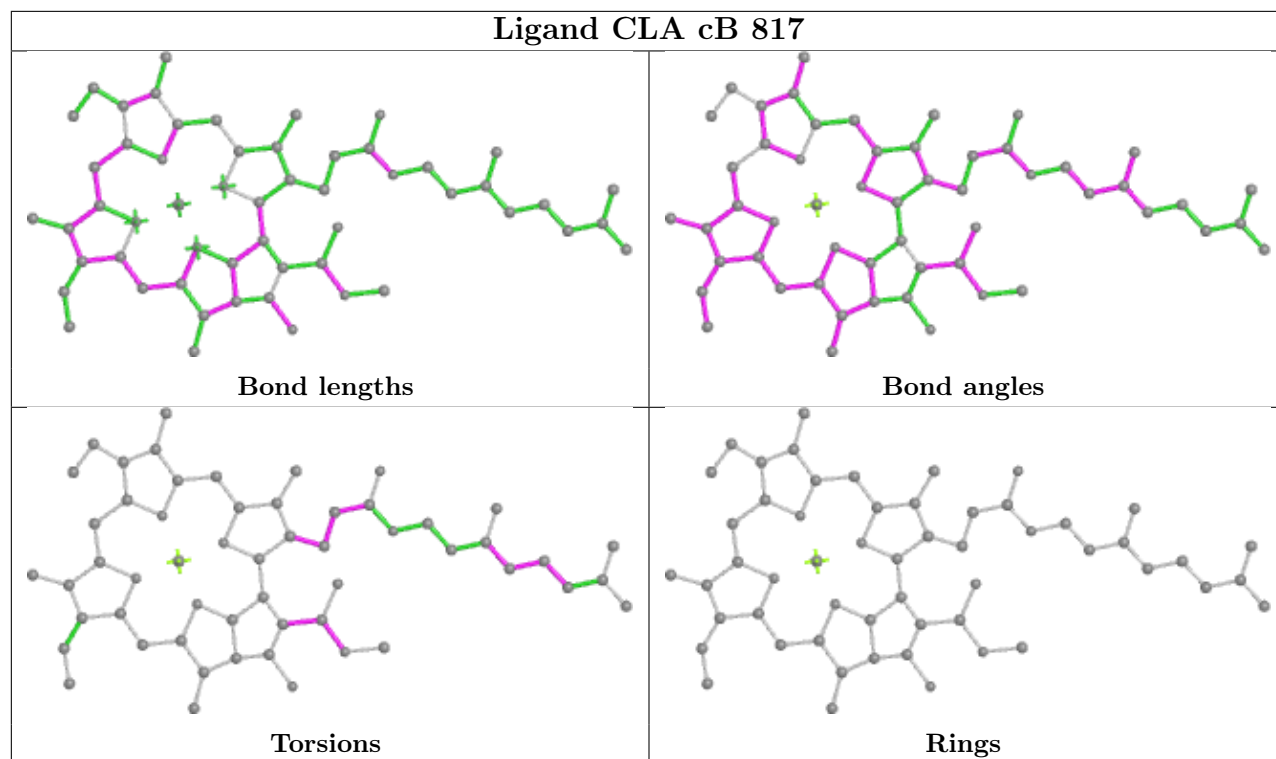


Ligand CLA aB 837

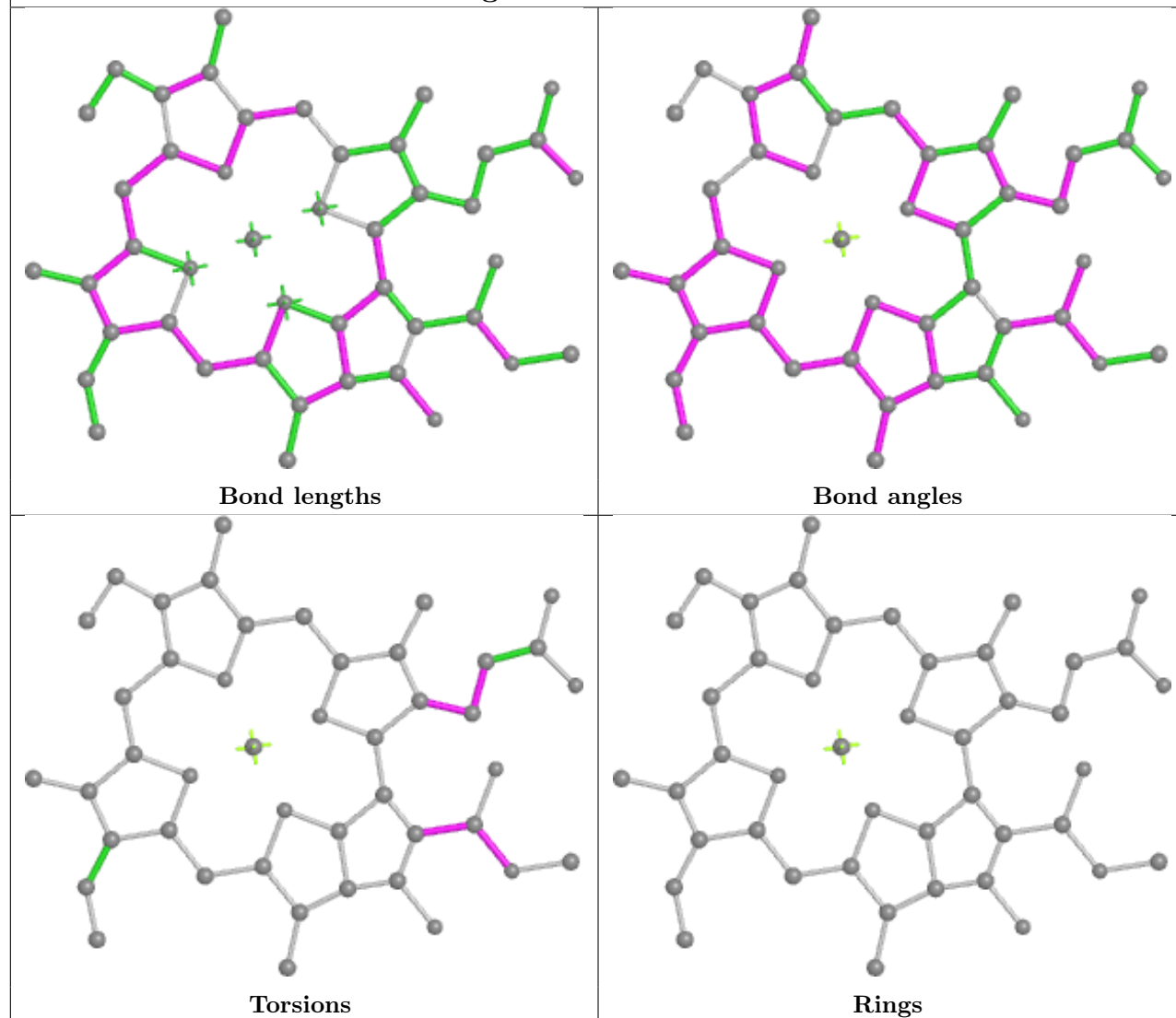


Ligand LMT aA 853

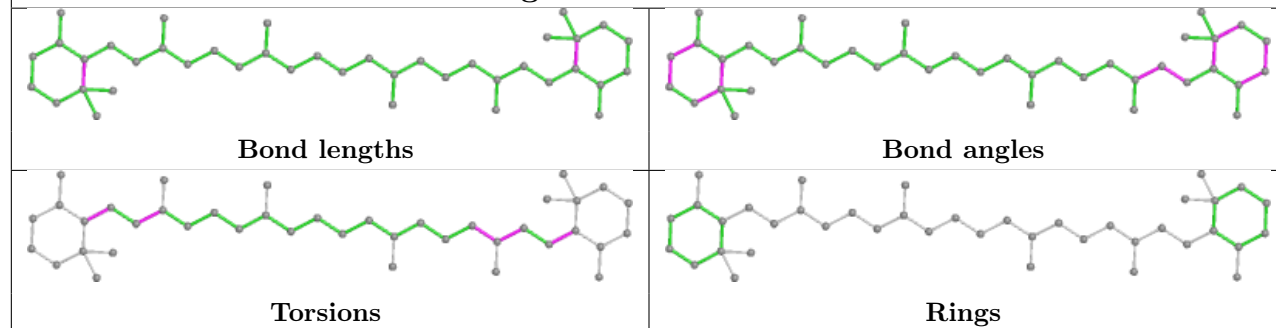


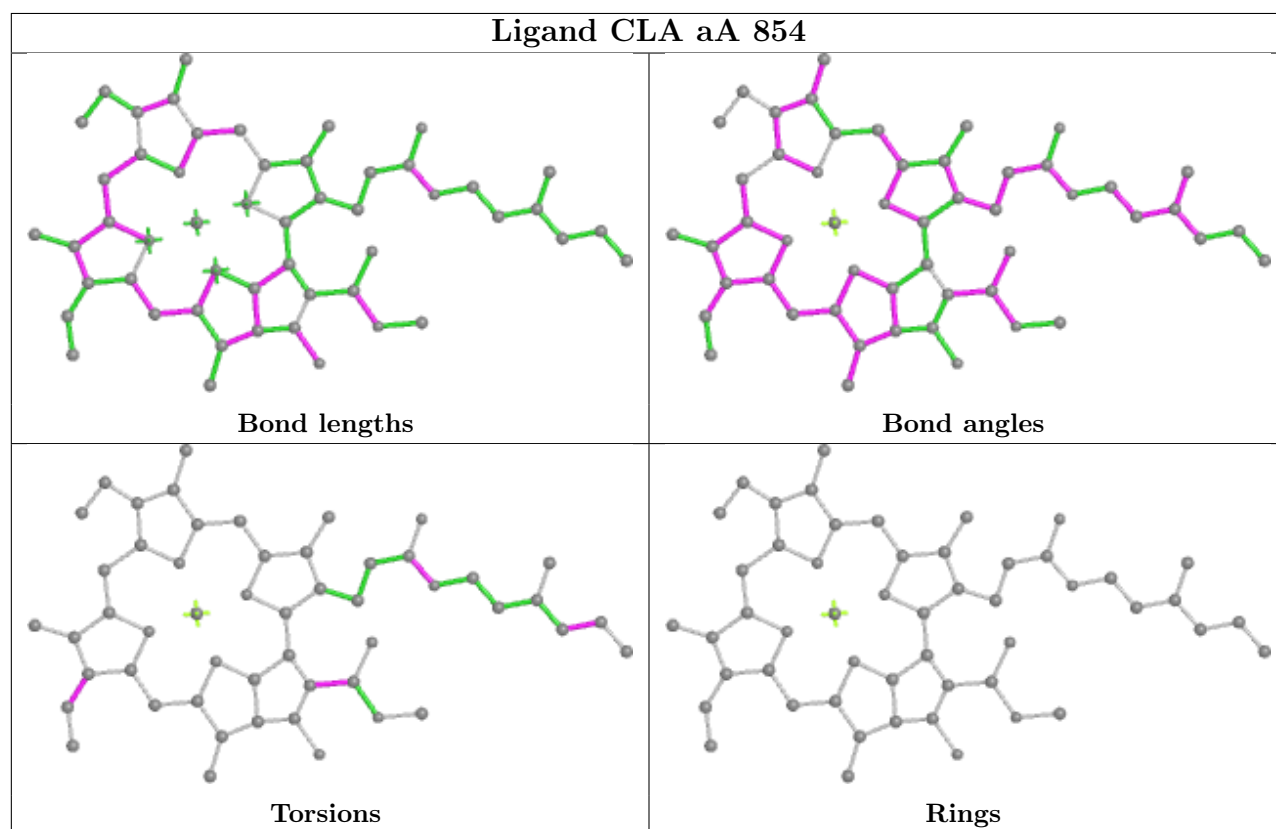
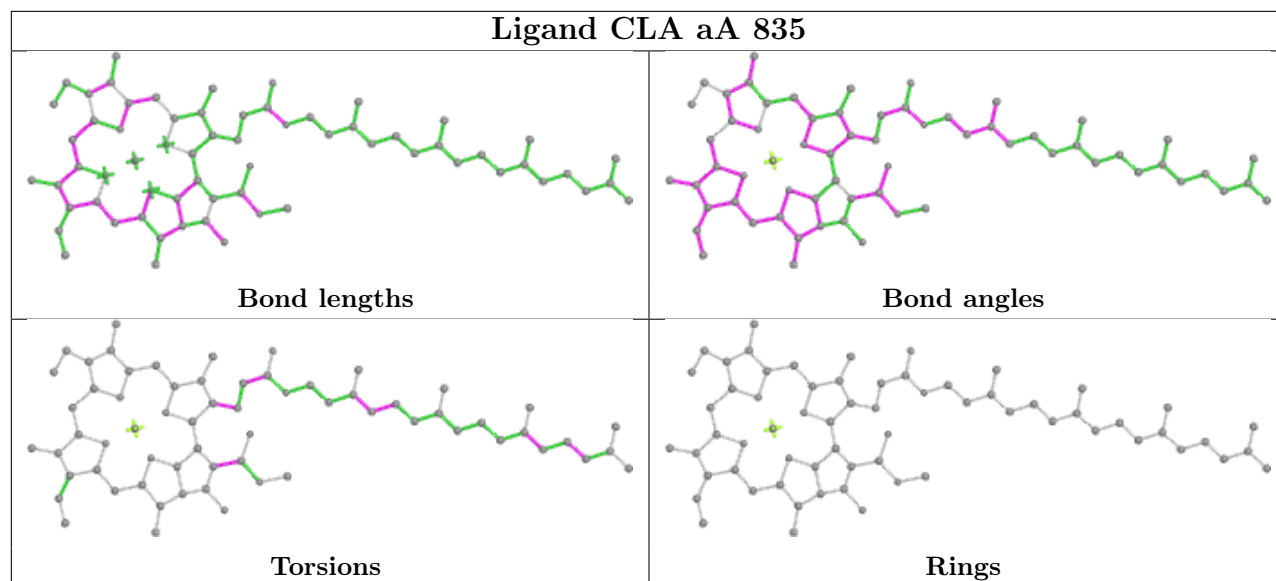
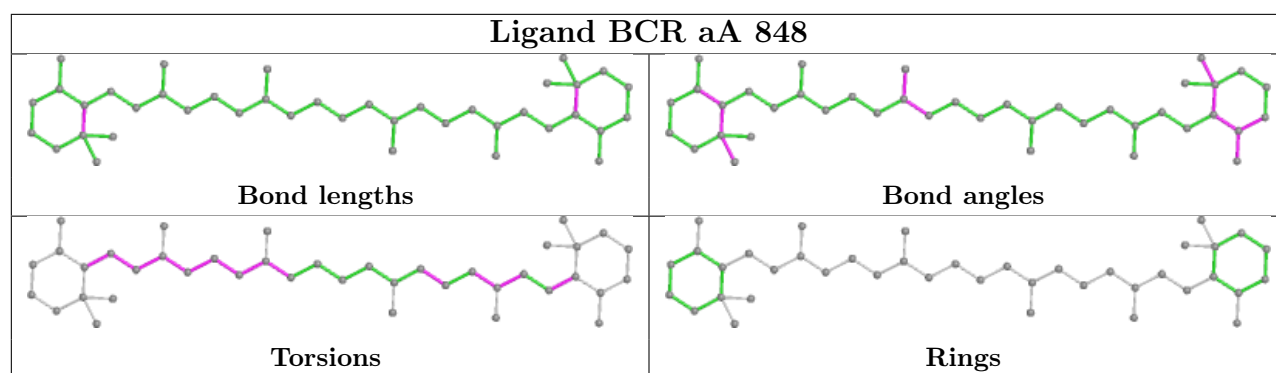


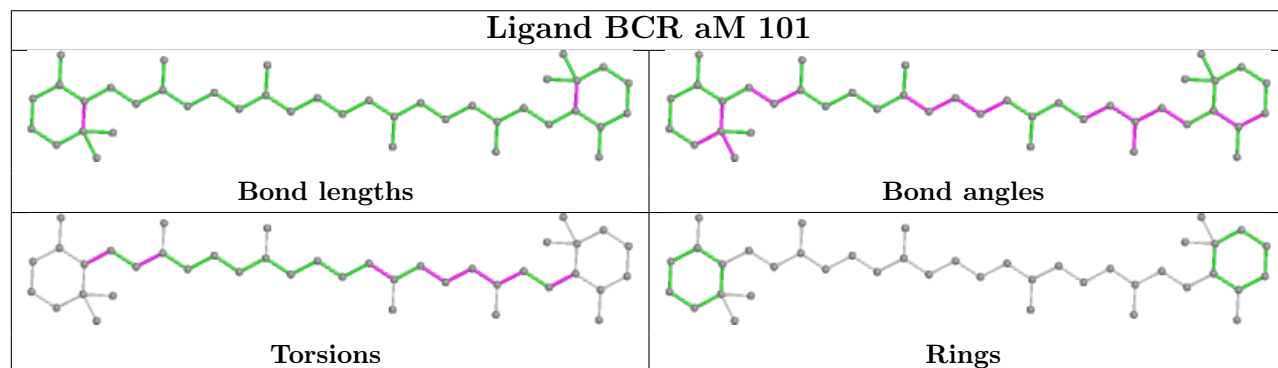
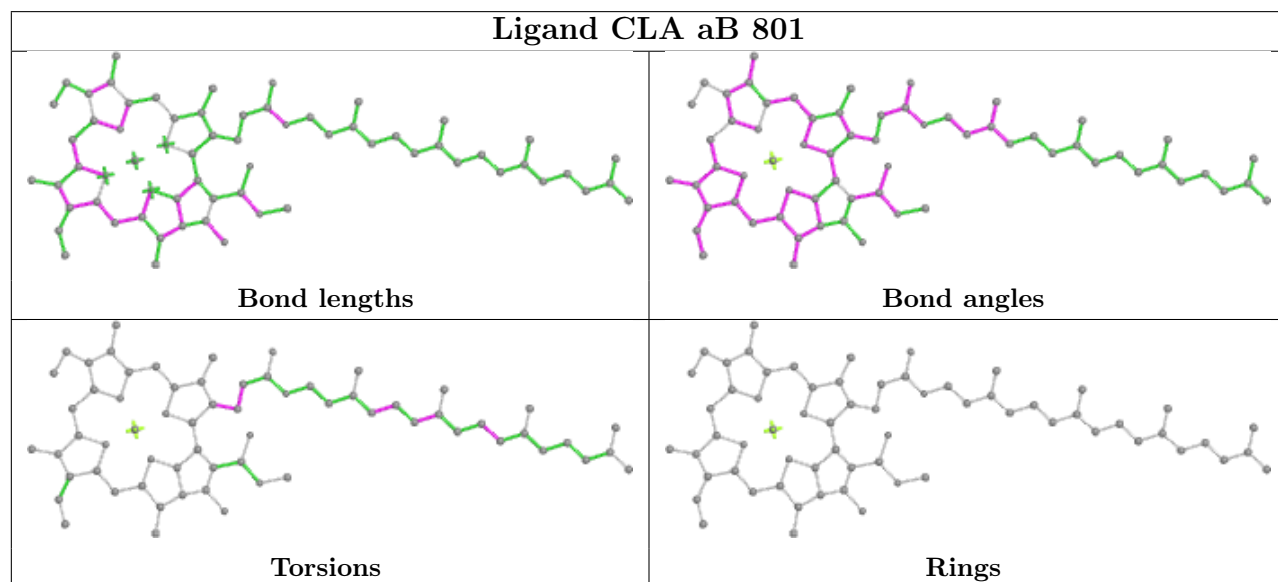
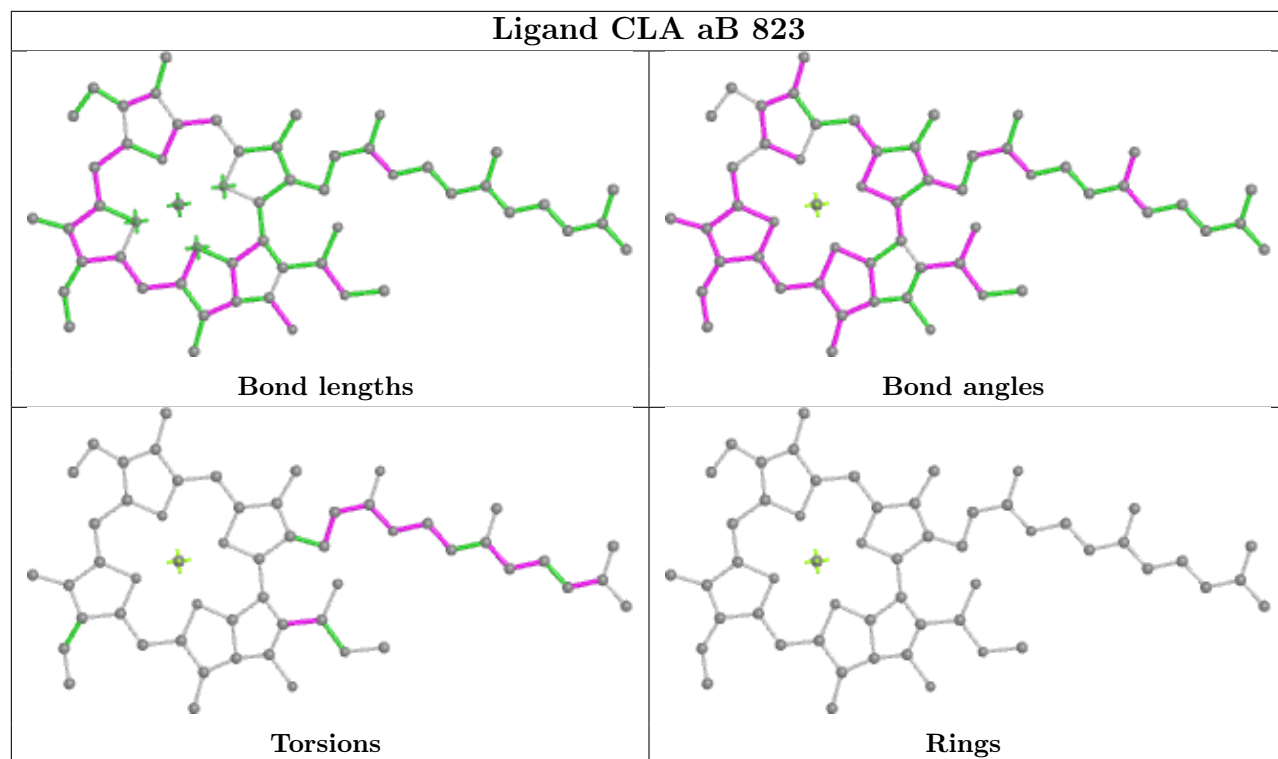
Ligand CLA aA 807

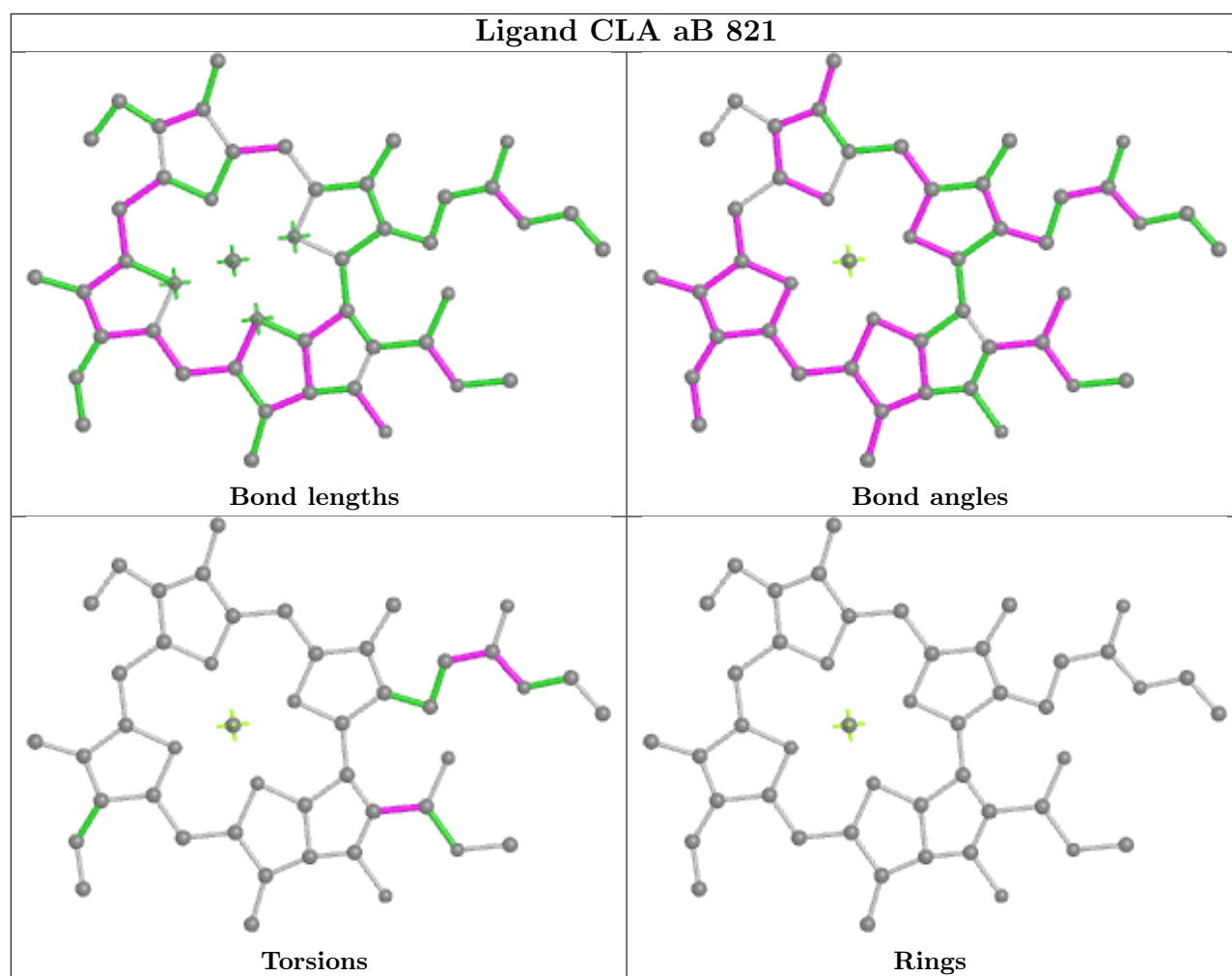


Ligand BCR aA 847

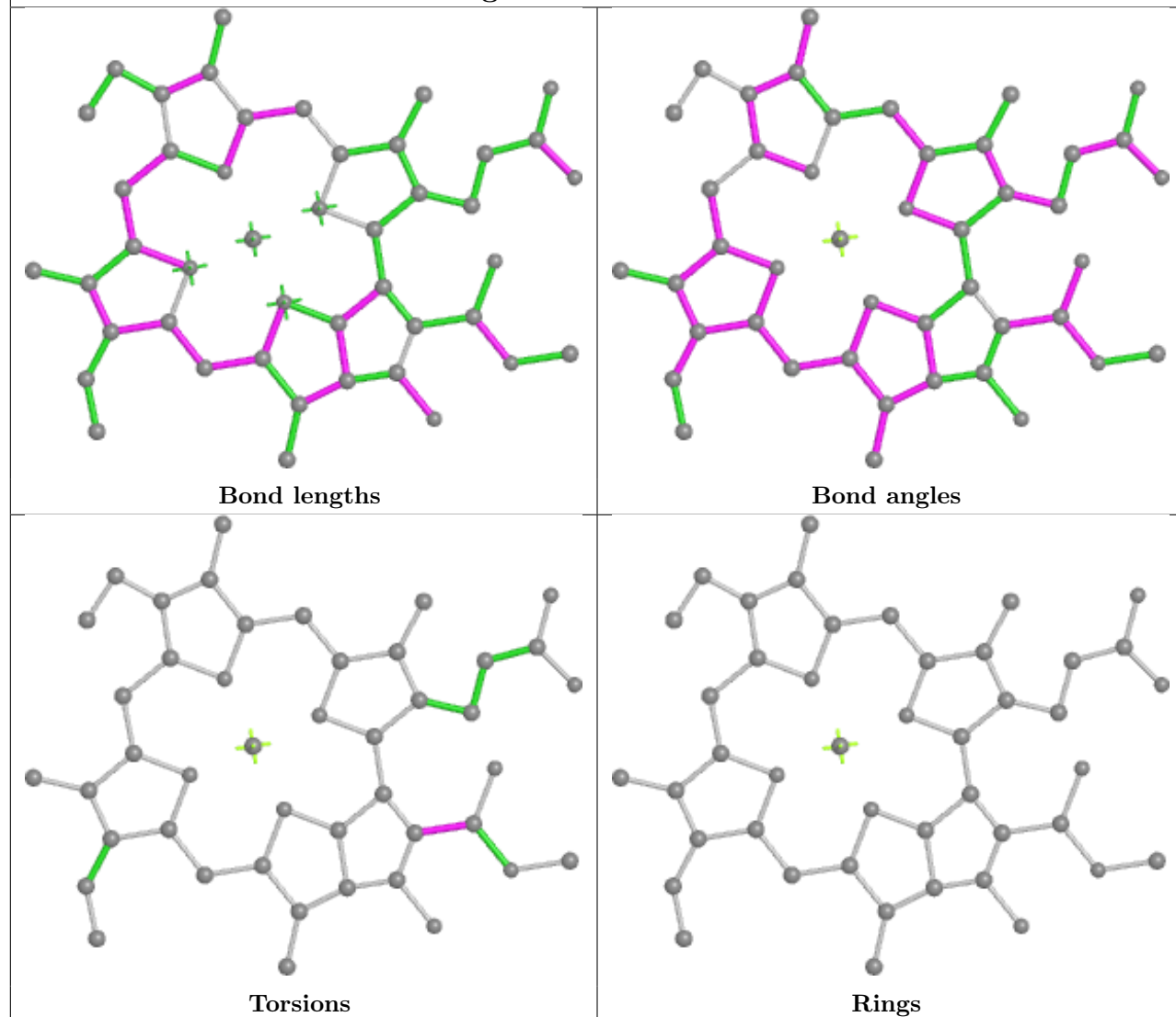




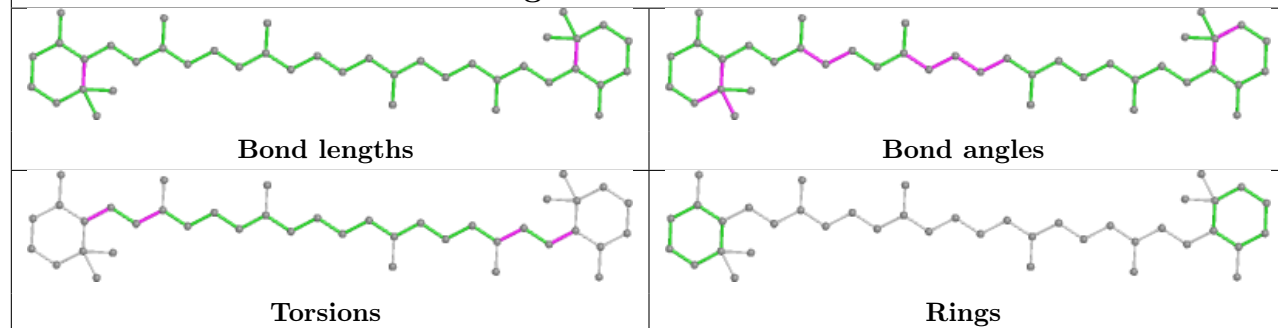




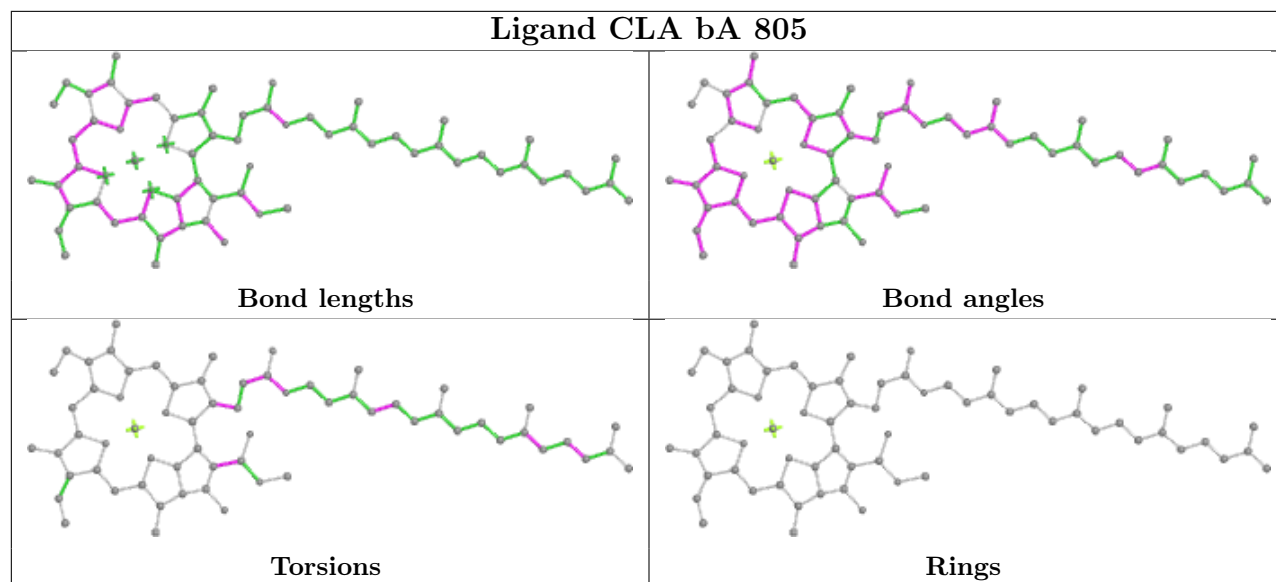
Ligand CLA cA 814



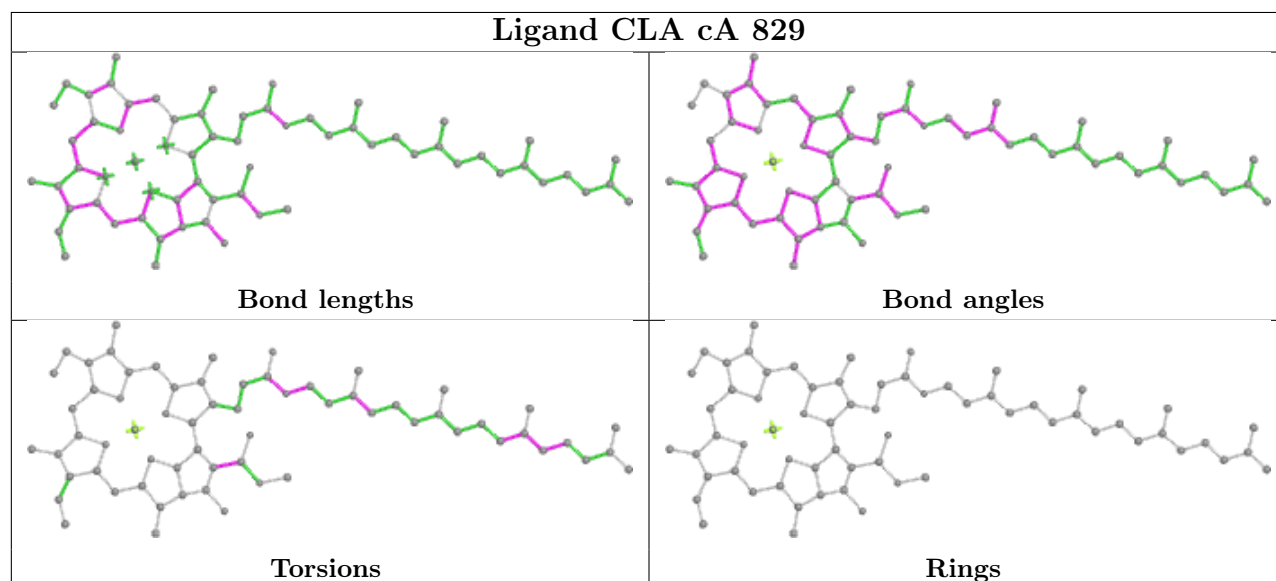
Ligand BCR aL 206



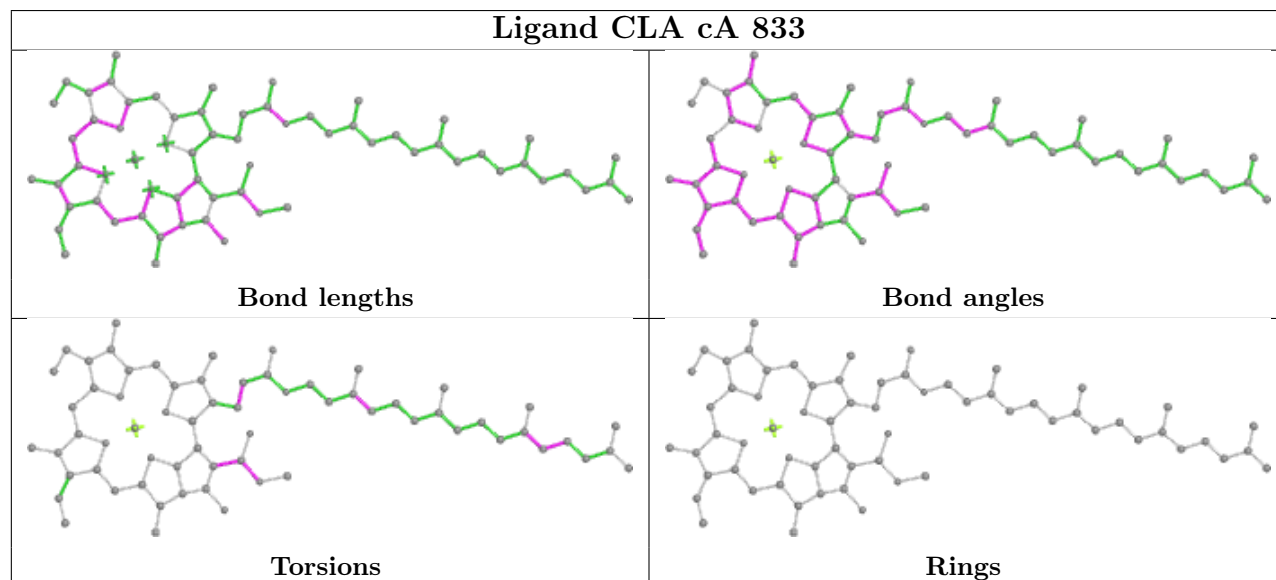
Ligand CLA bA 805

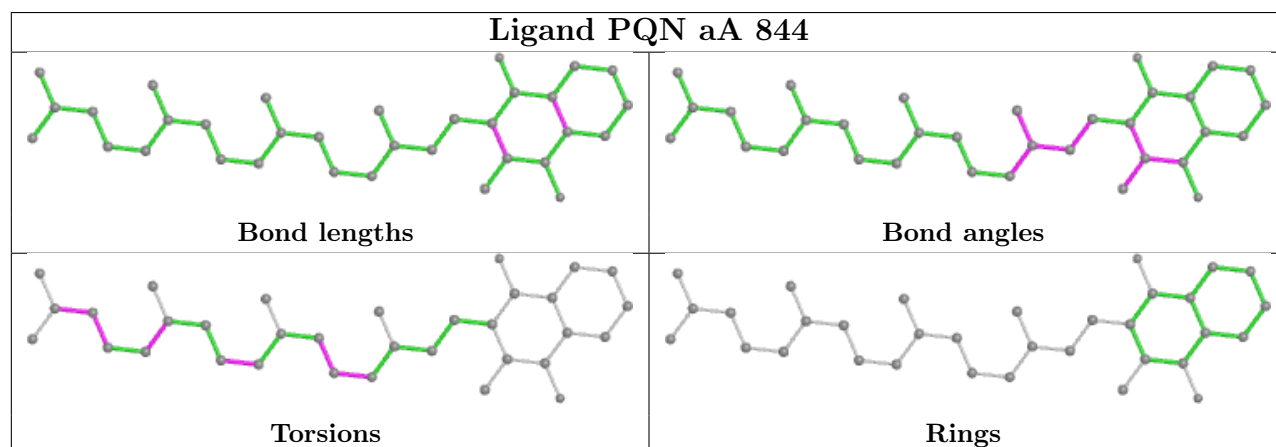
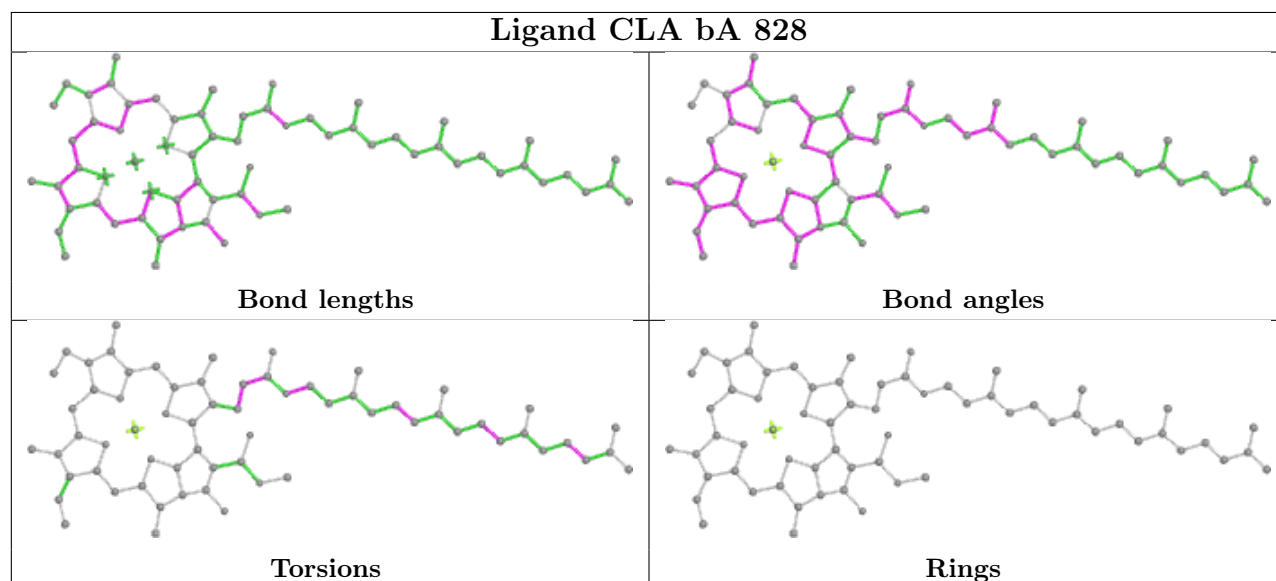
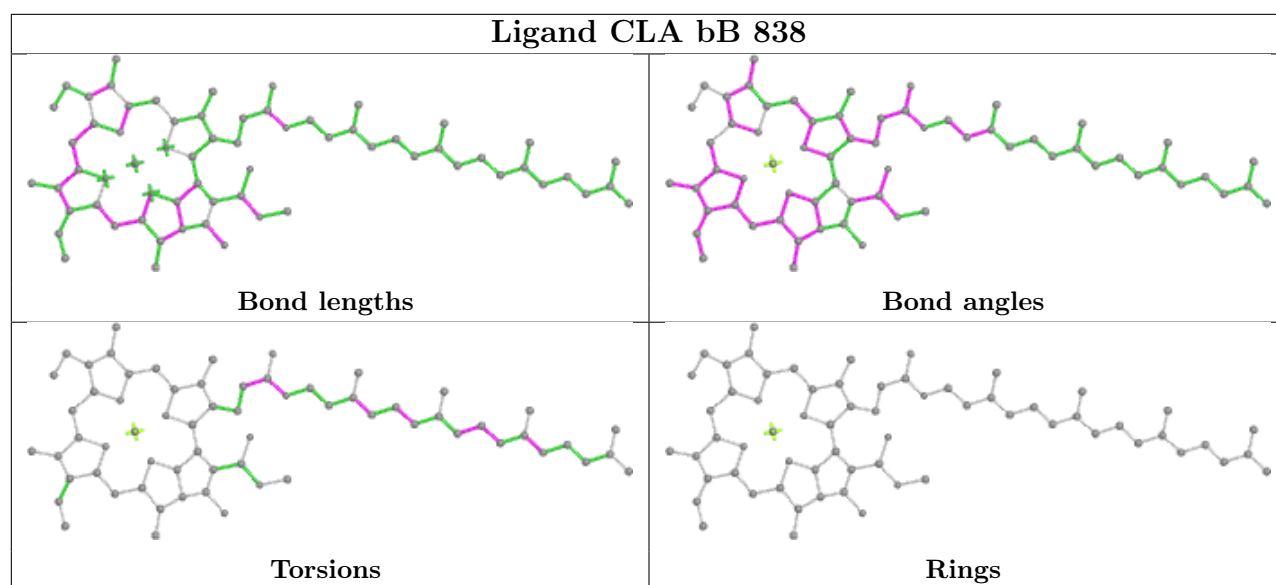


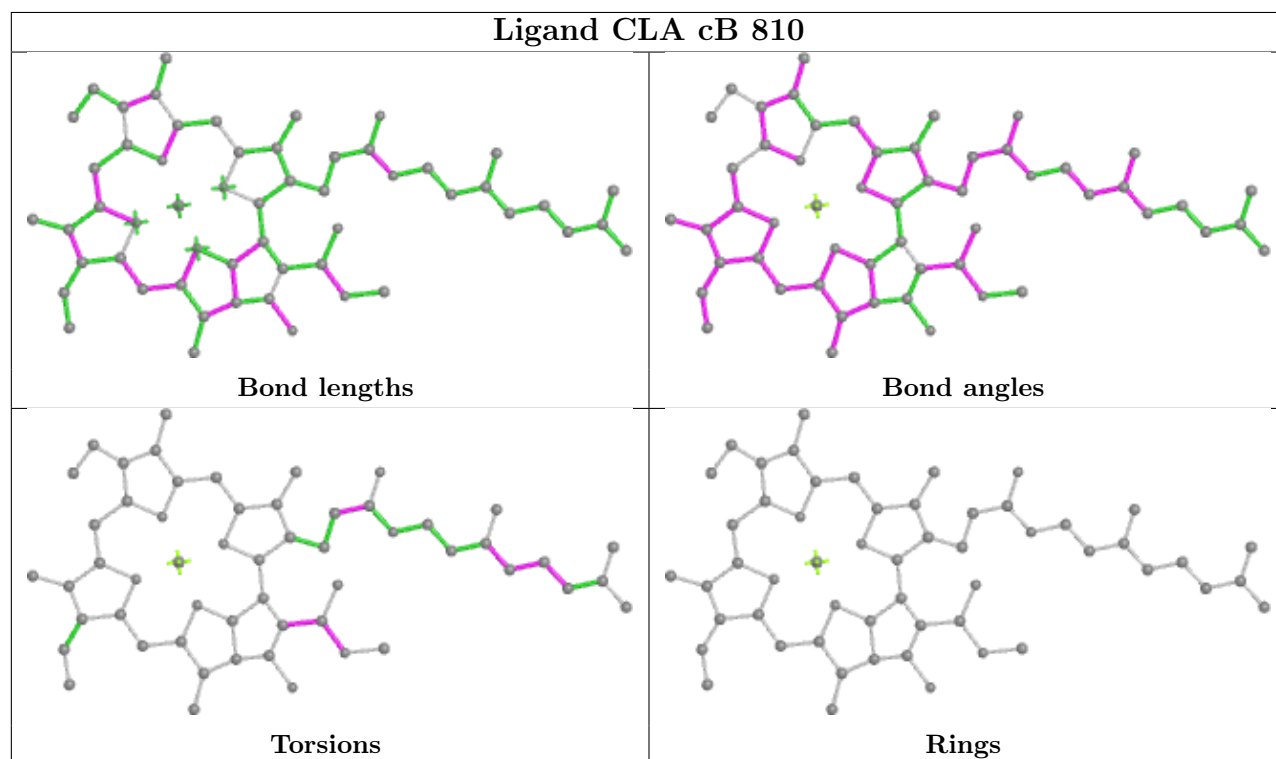
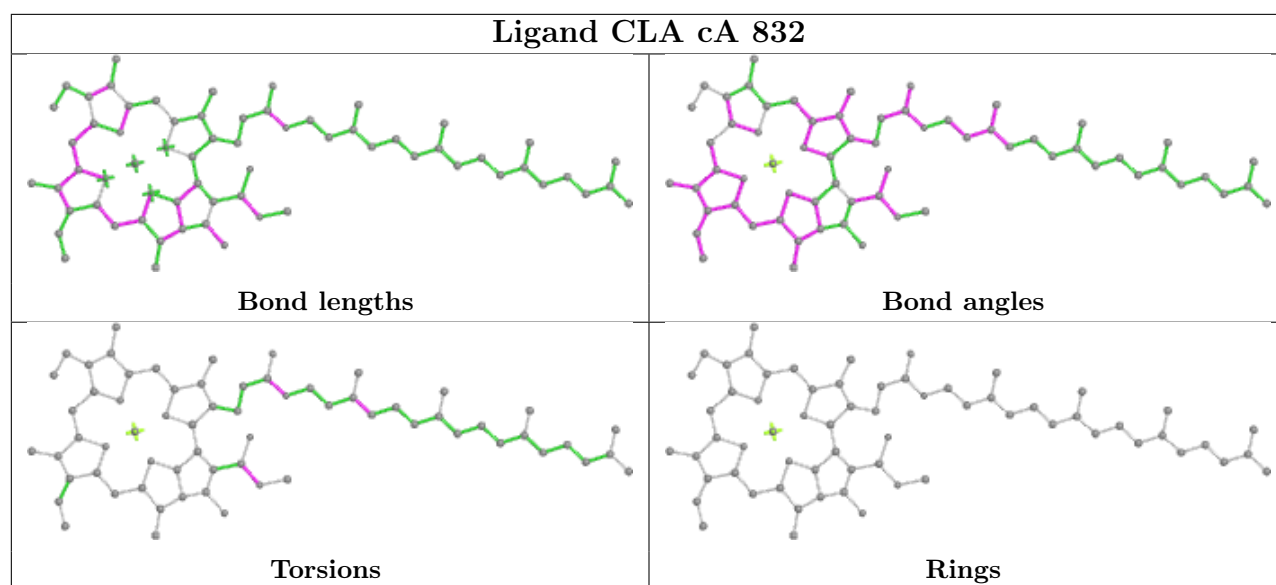
Ligand CLA cA 829



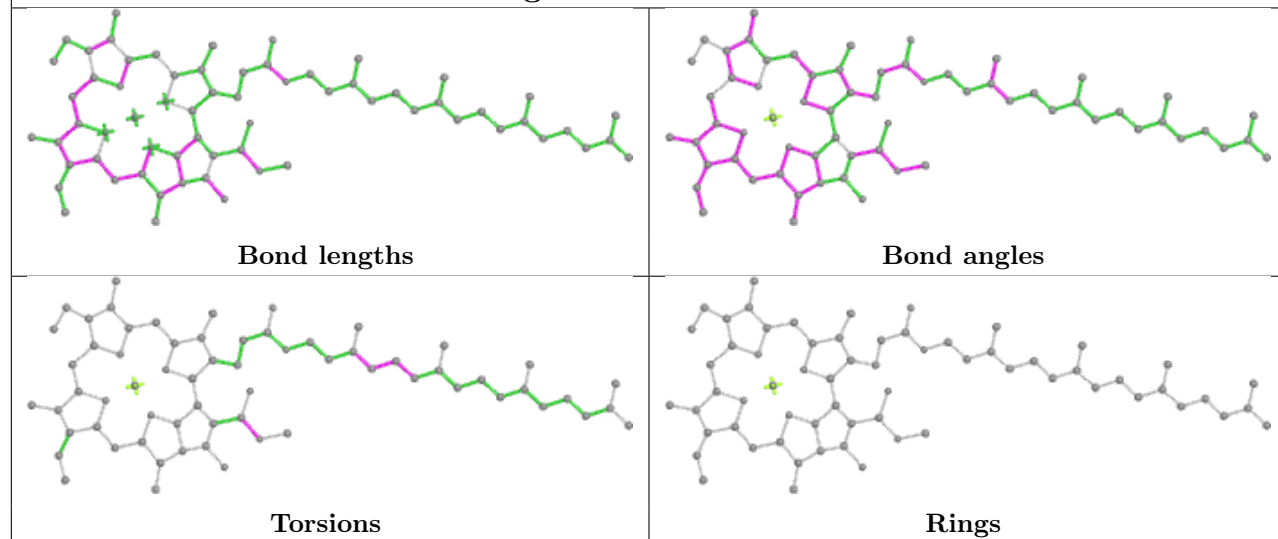
Ligand CLA cA 833



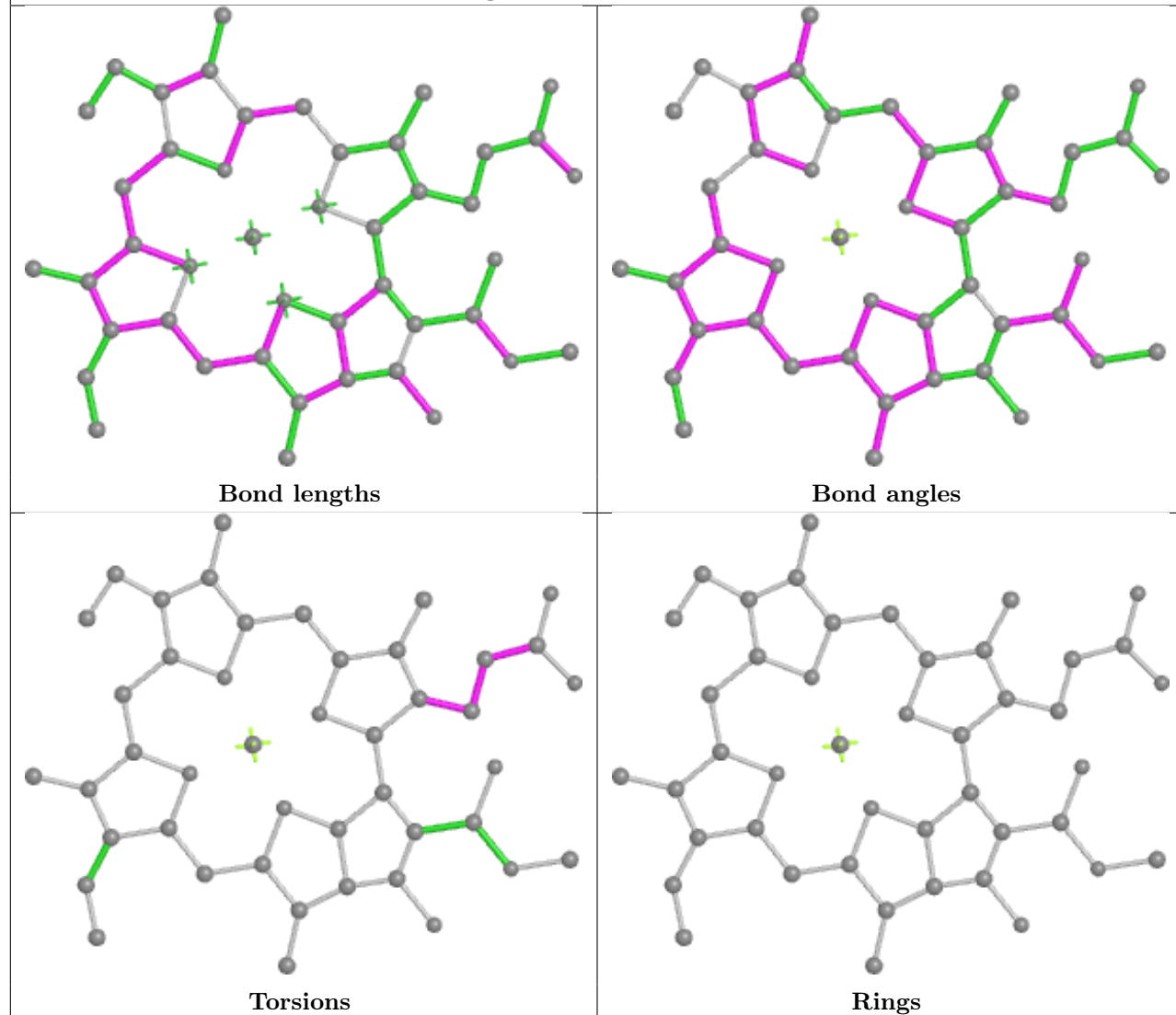


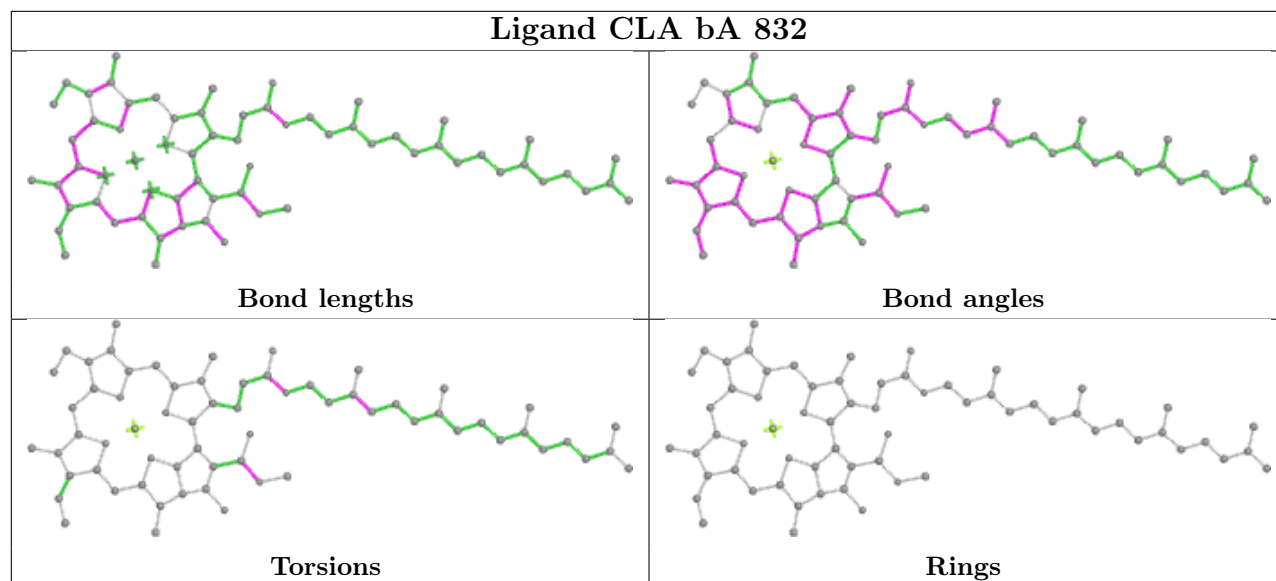
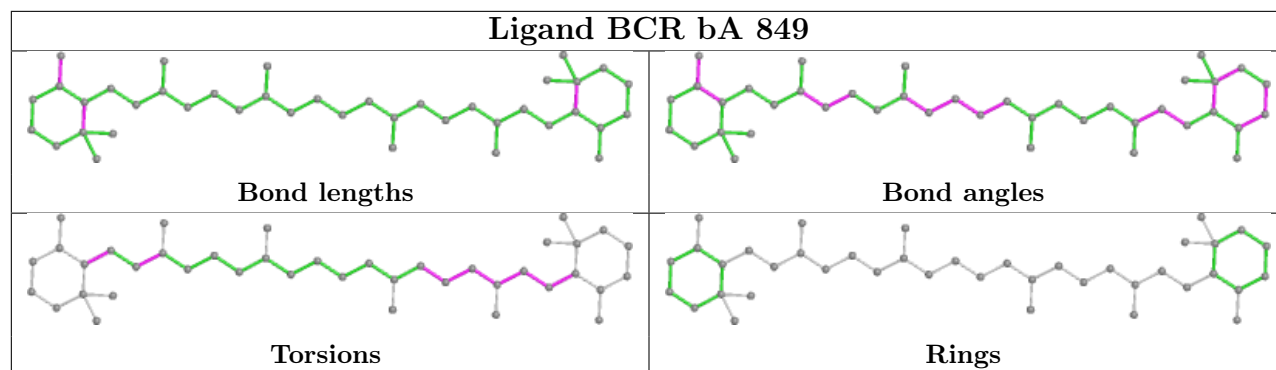


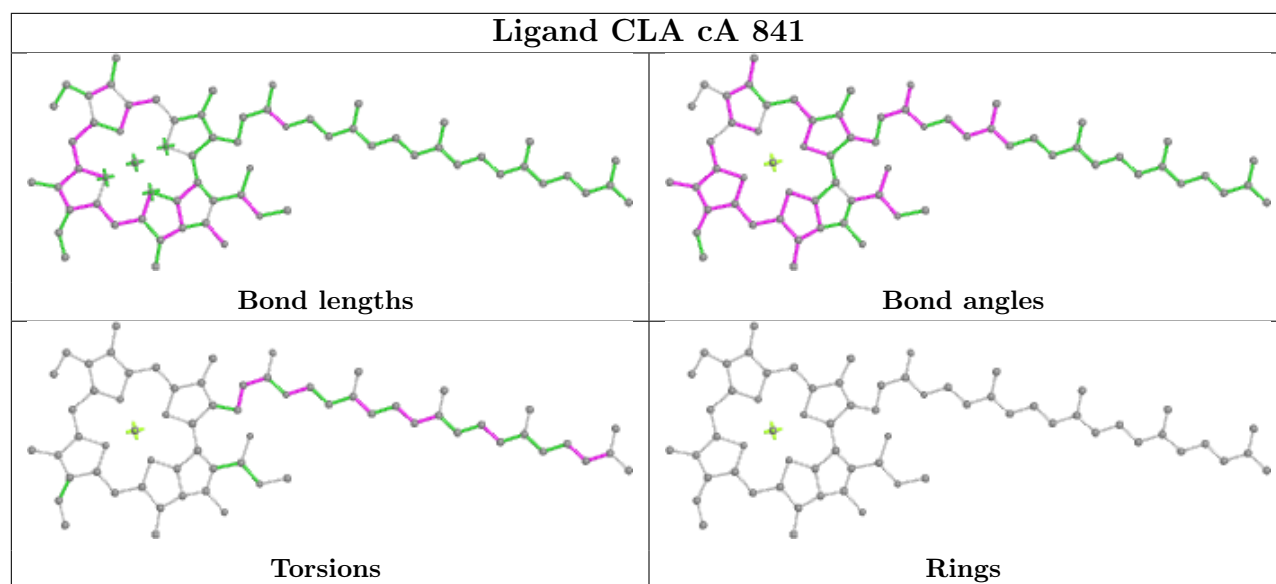
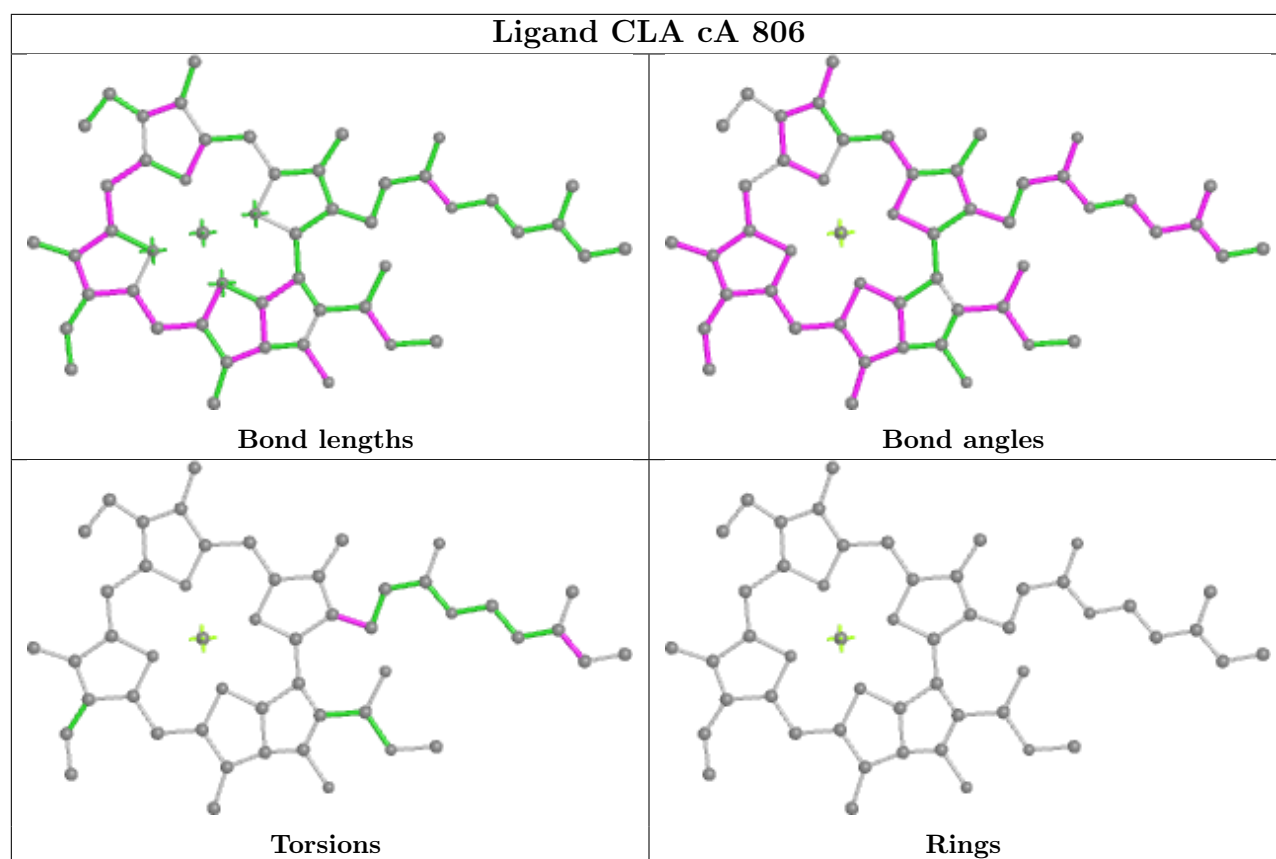
Ligand CLA cA 839



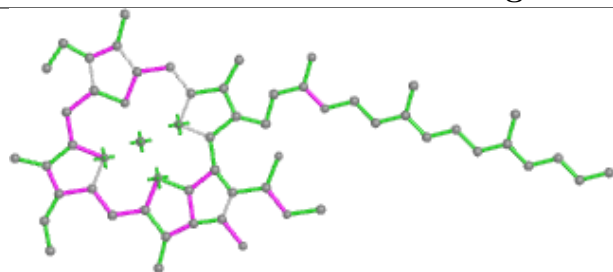
Ligand CLA cB 813



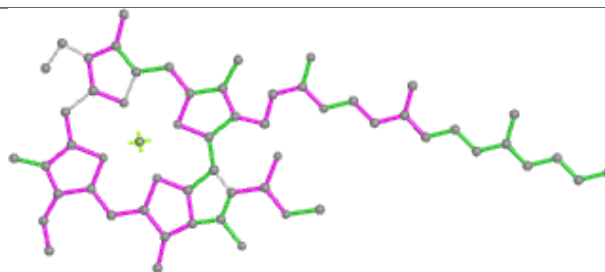




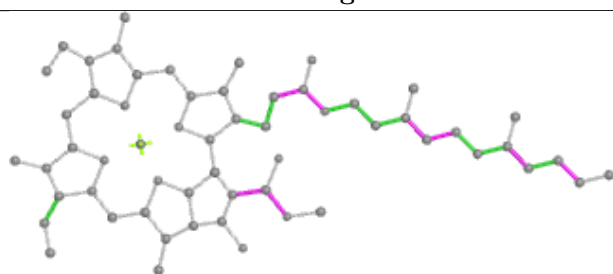
Ligand CLA aB 833



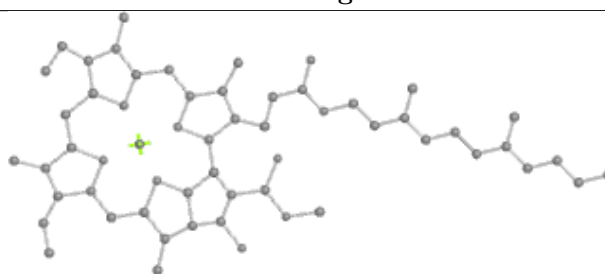
Bond lengths



Bond angles

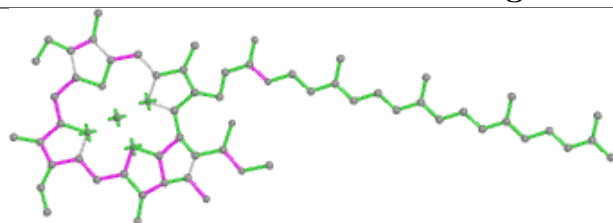


Torsions

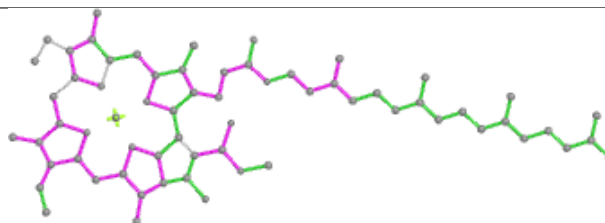


Rings

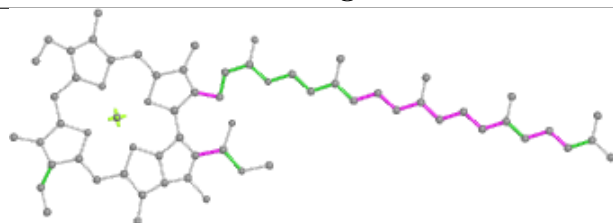
Ligand CLA cA 812



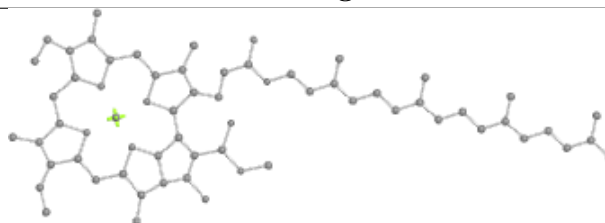
Bond lengths



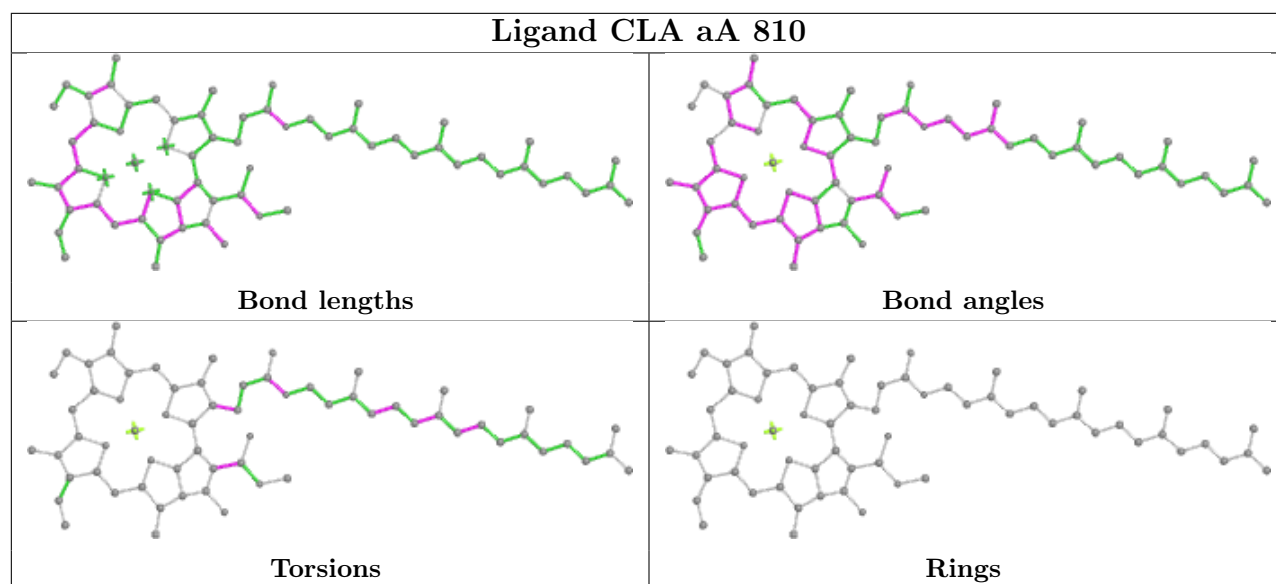
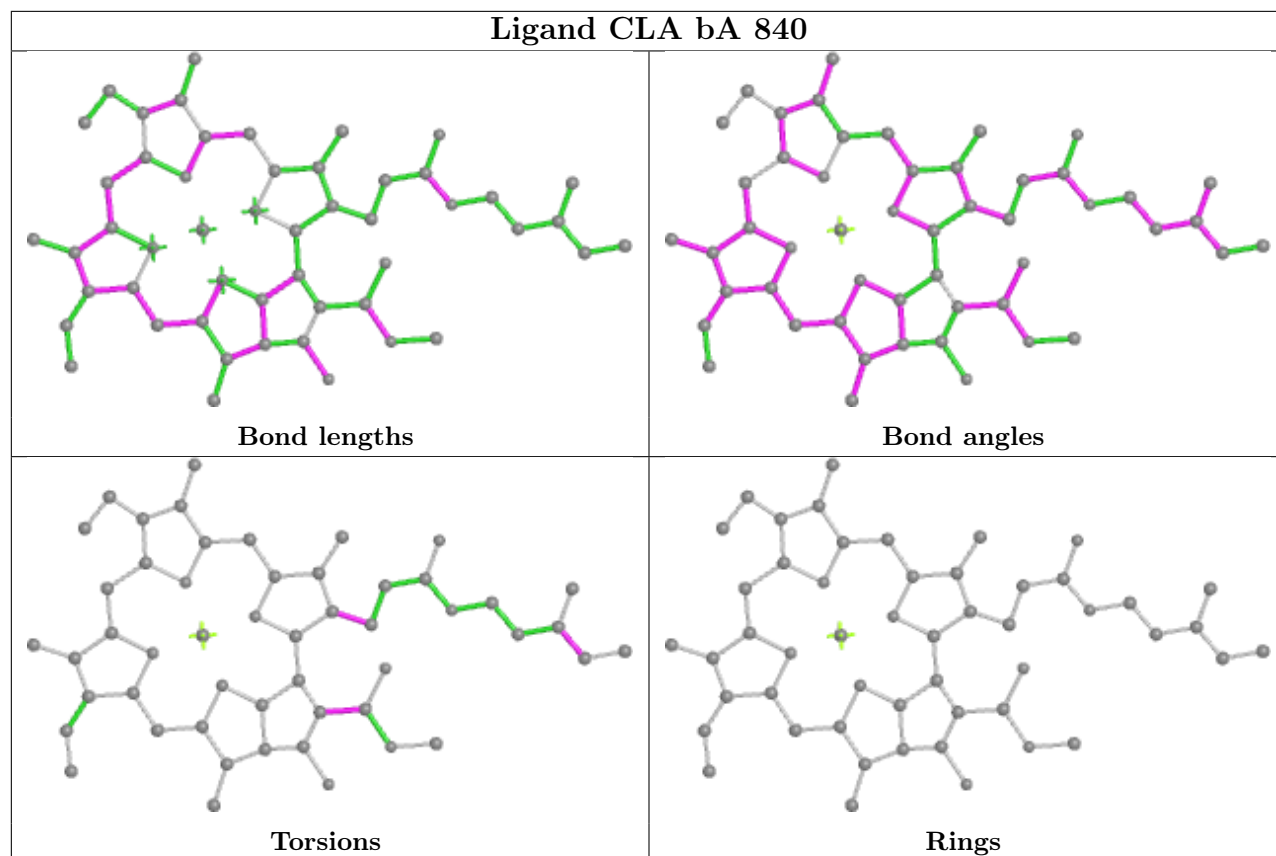
Bond angles



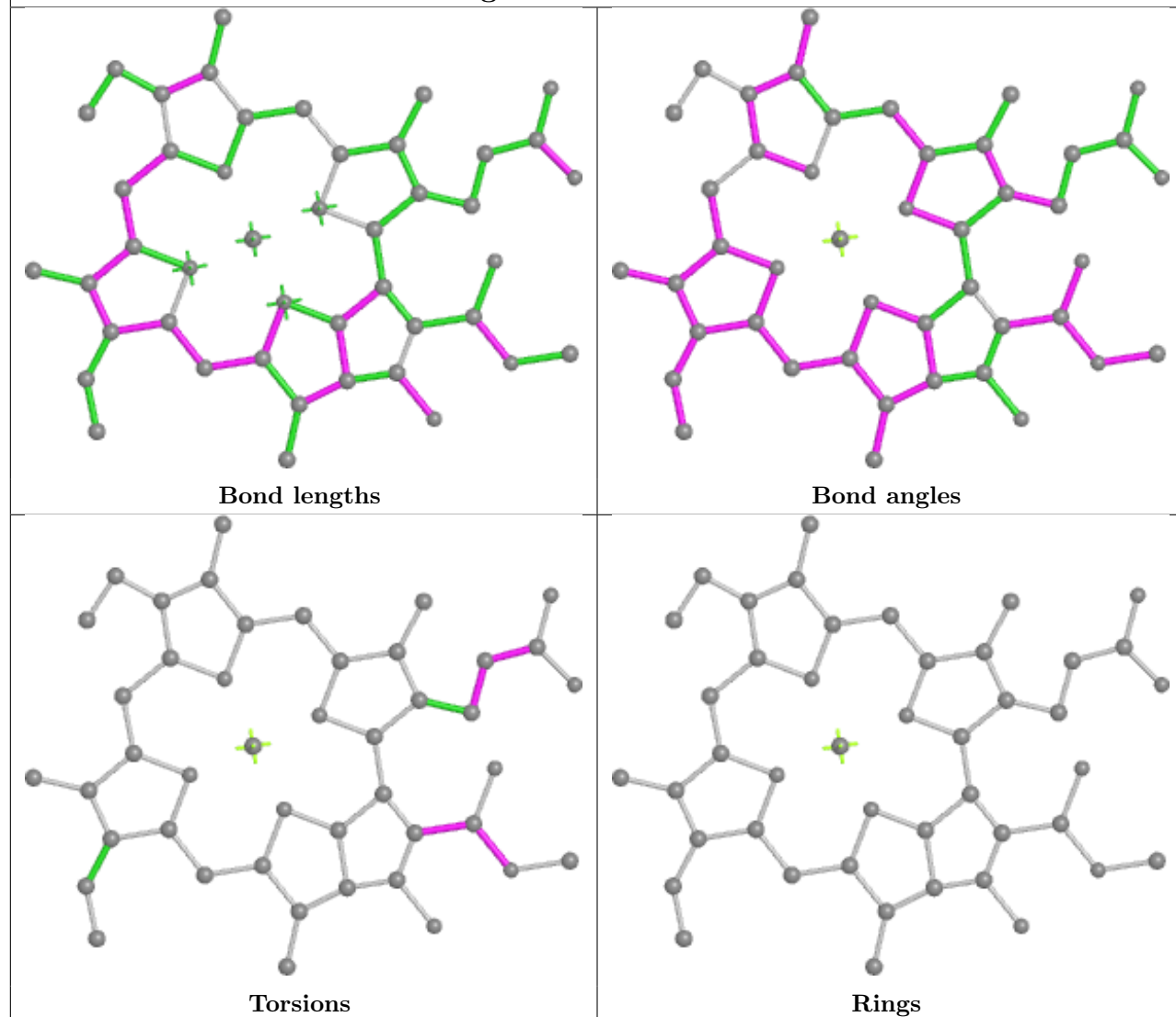
Torsions



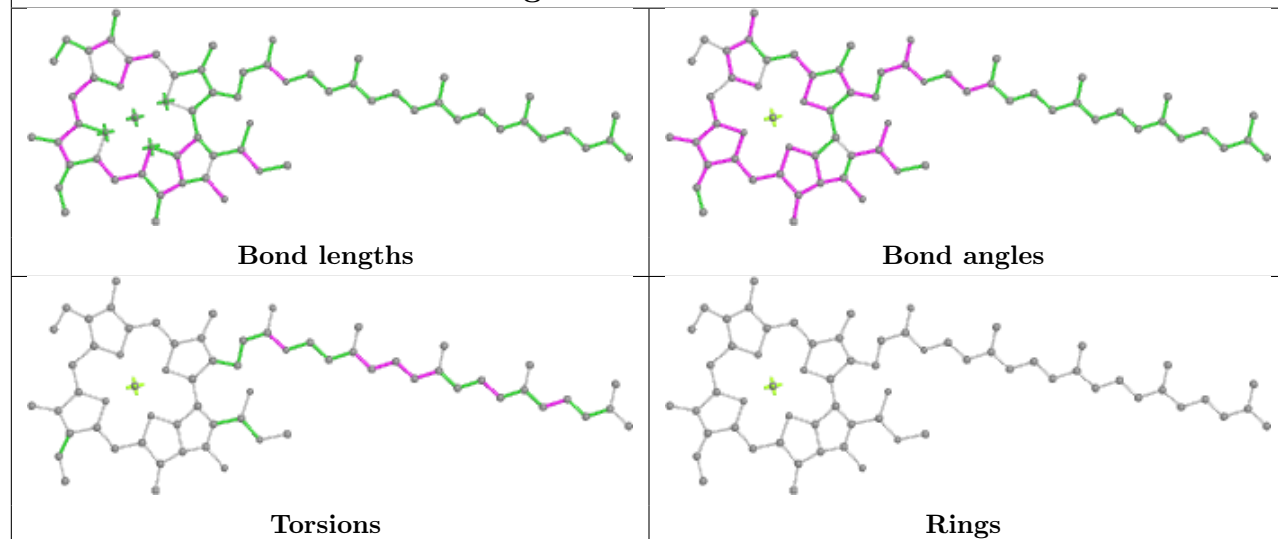
Rings

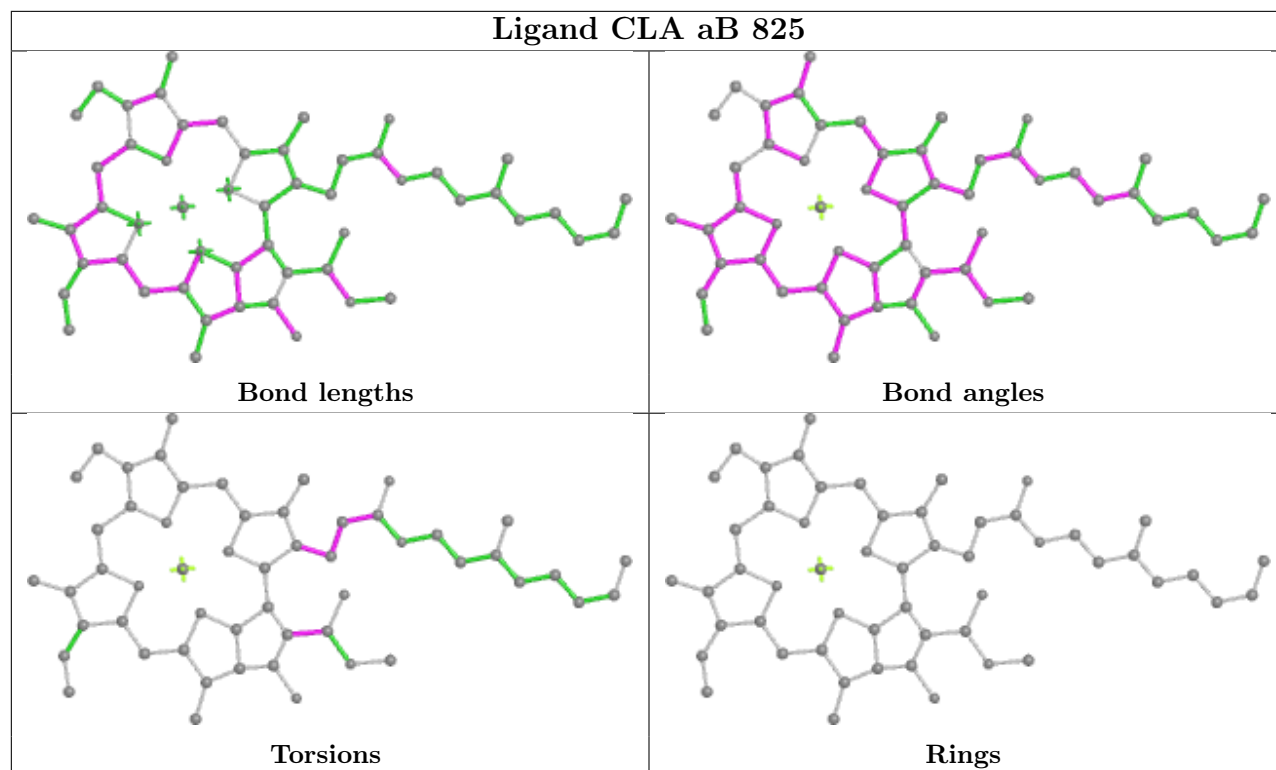


Ligand CLA bB 831

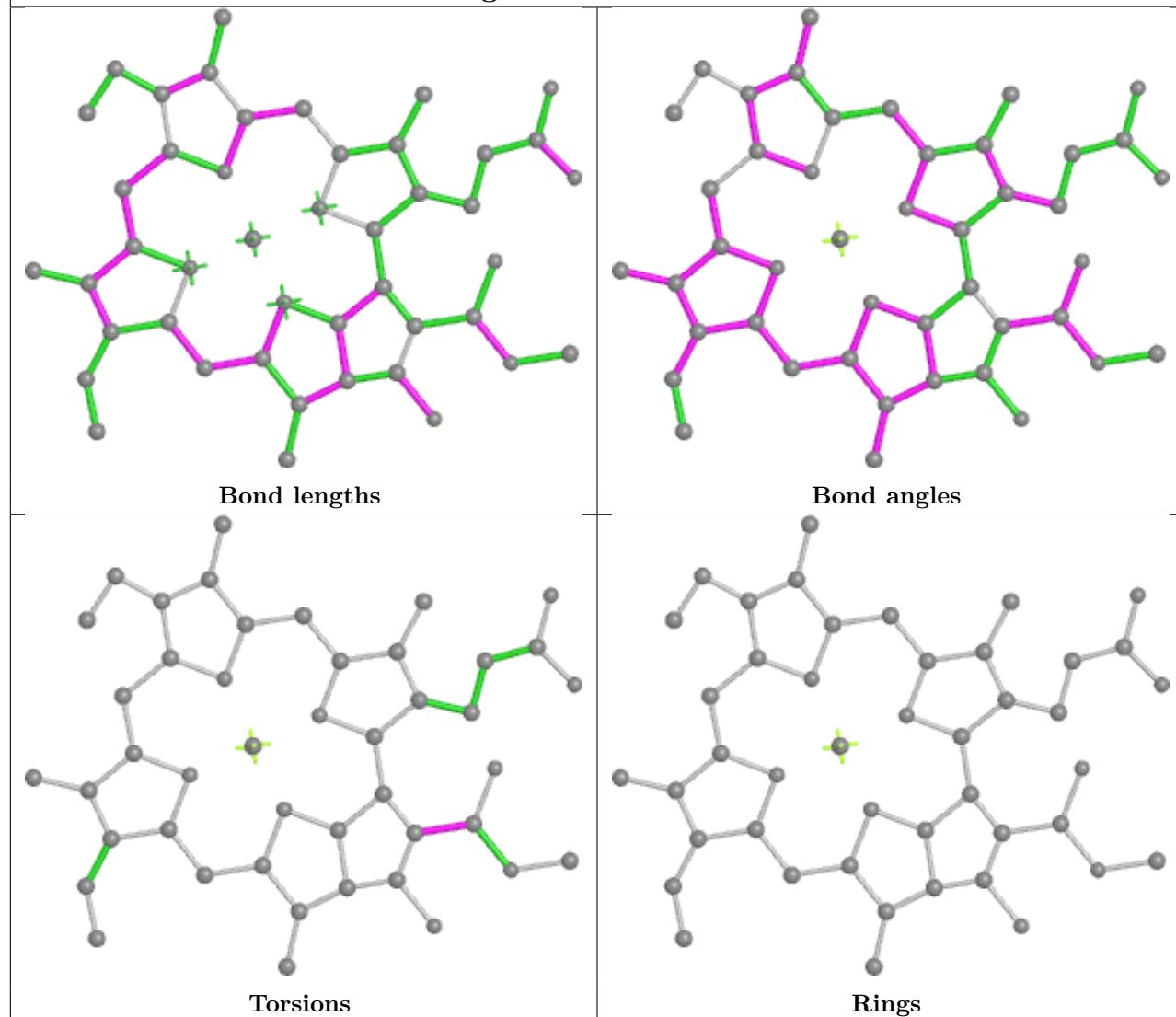


Ligand CLA cA 826

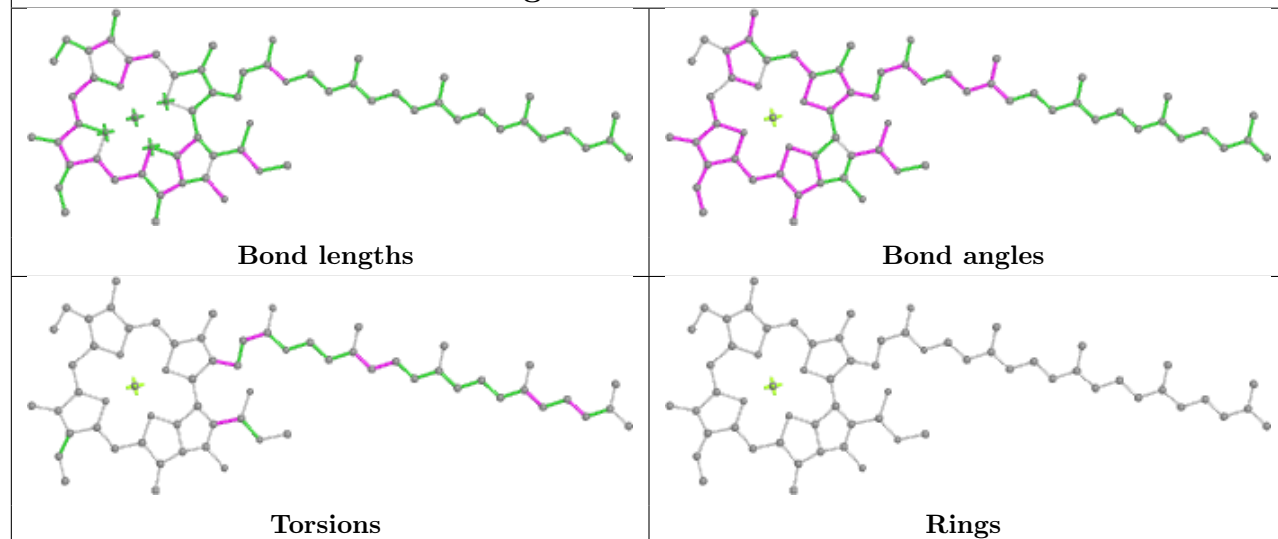


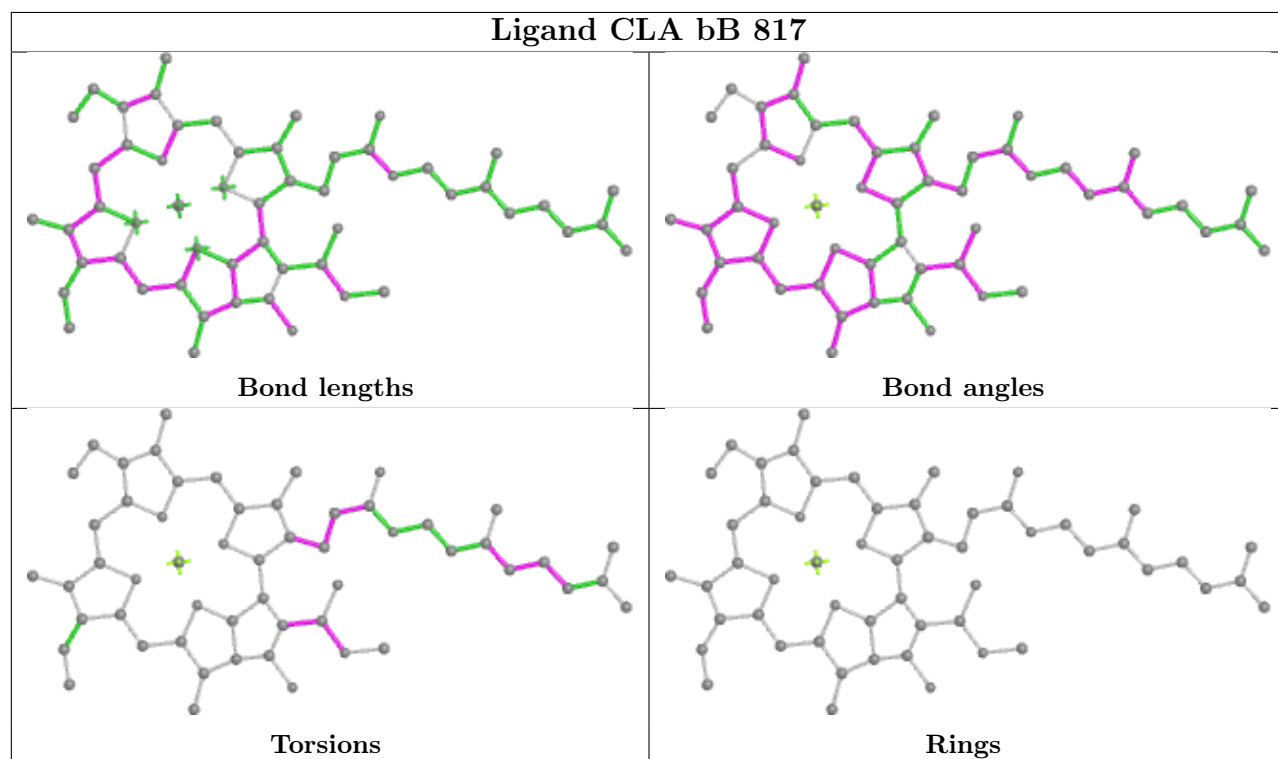
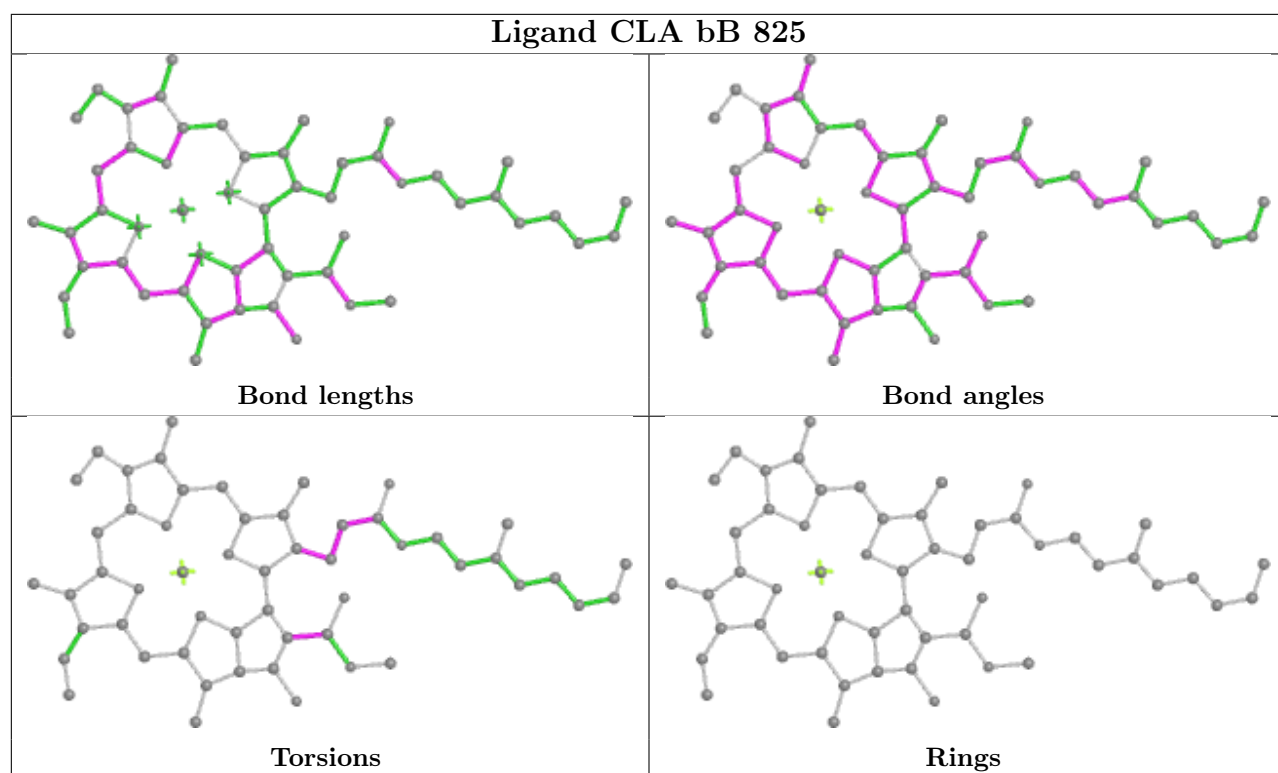


Ligand CLA aA 809

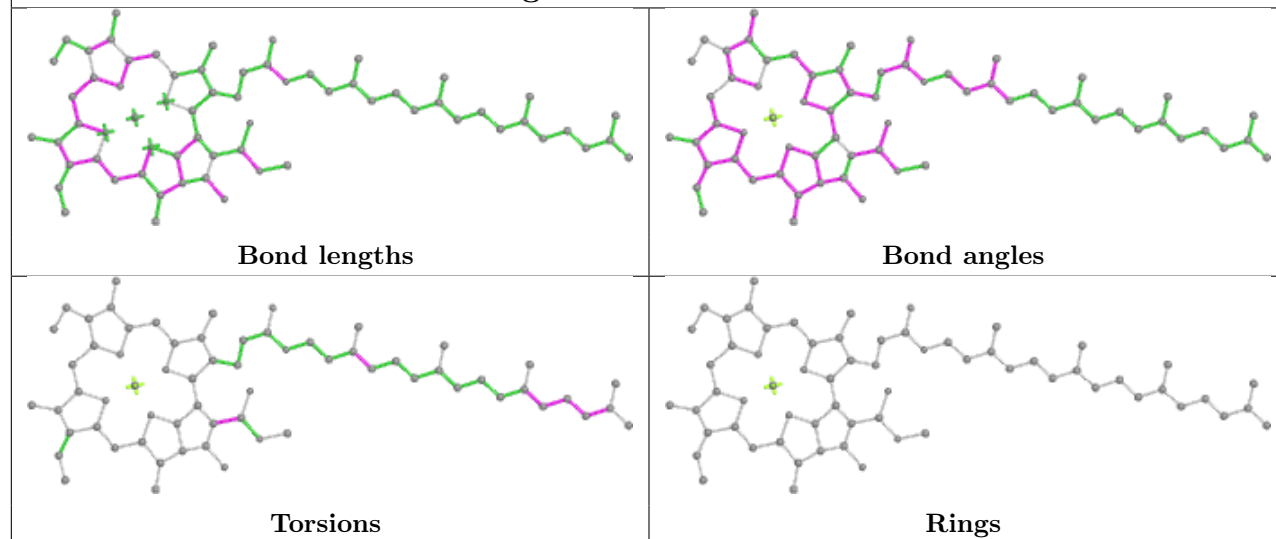


Ligand CLA cA 835

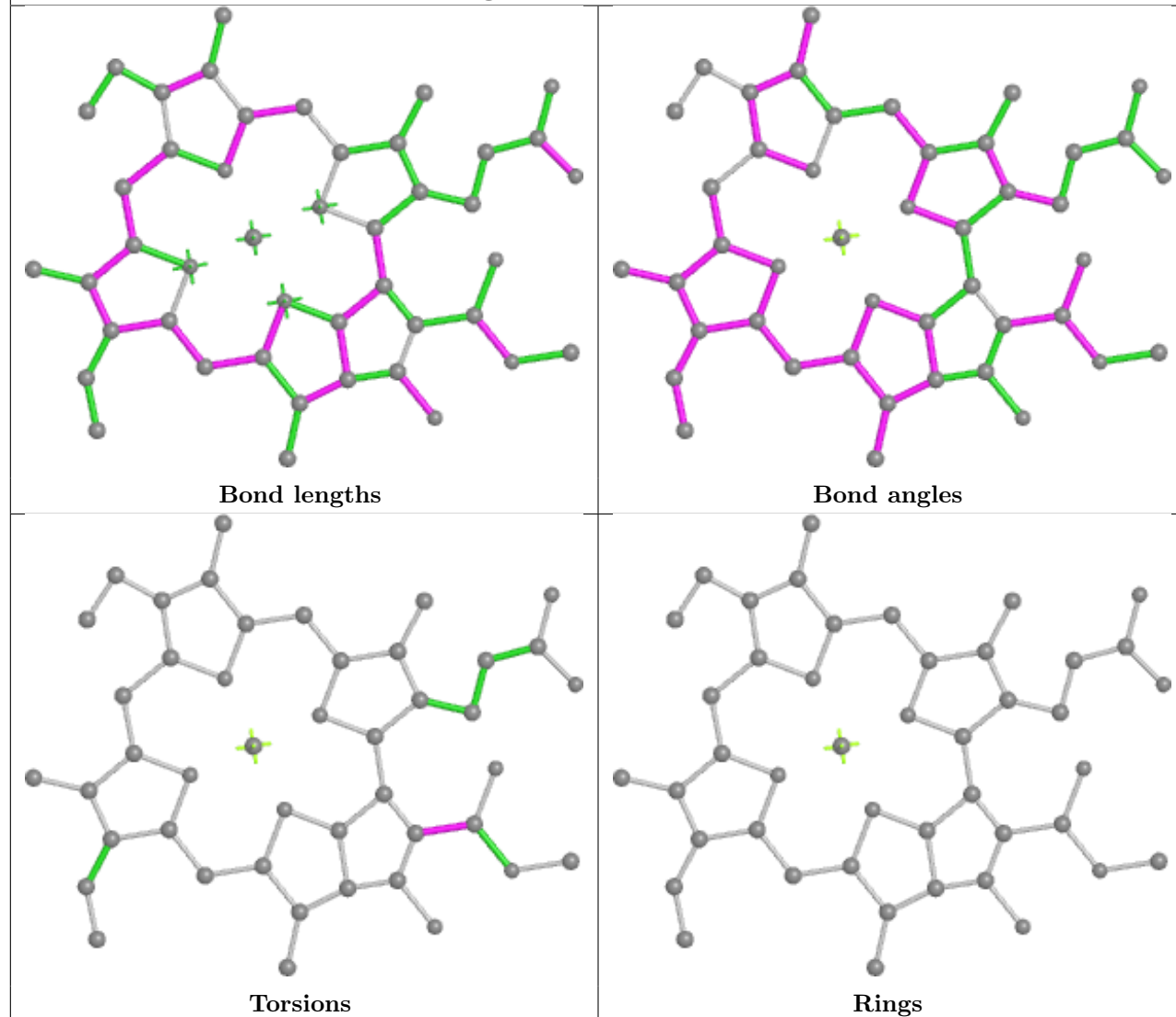


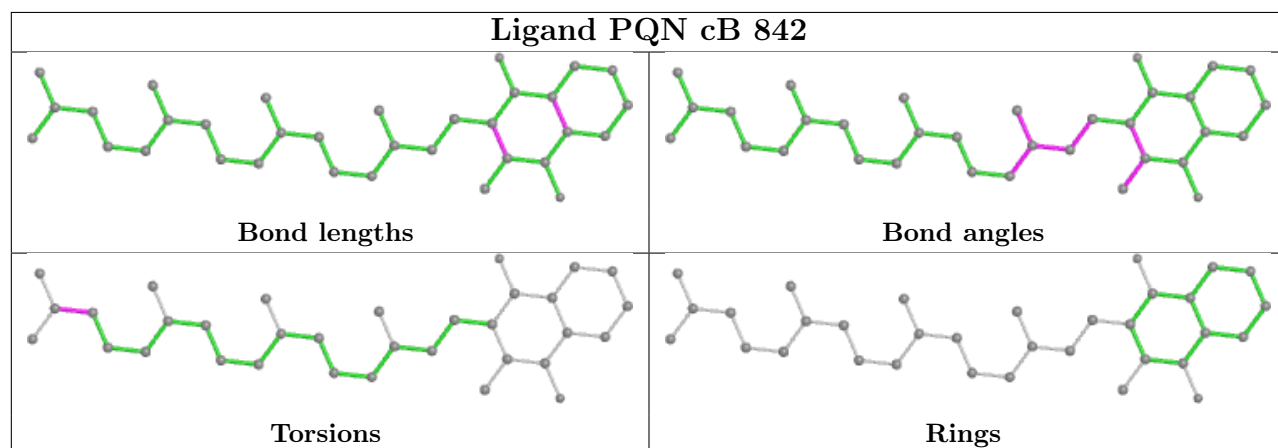
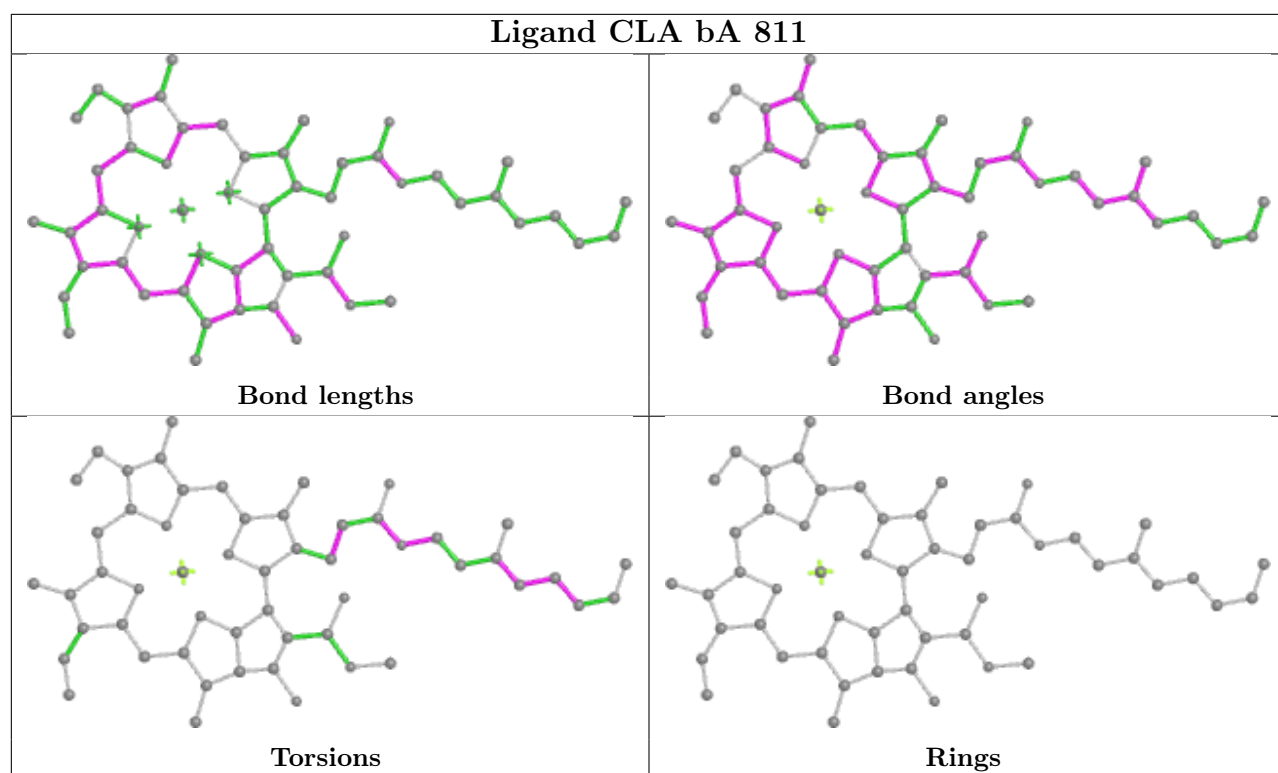


Ligand CLA bB 827

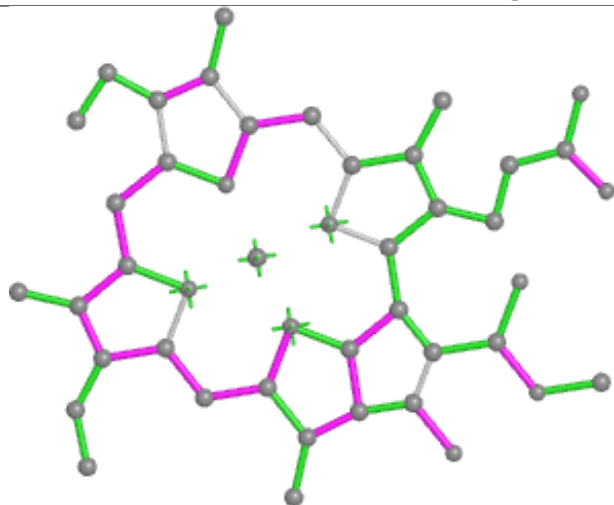


Ligand CLA bA 803

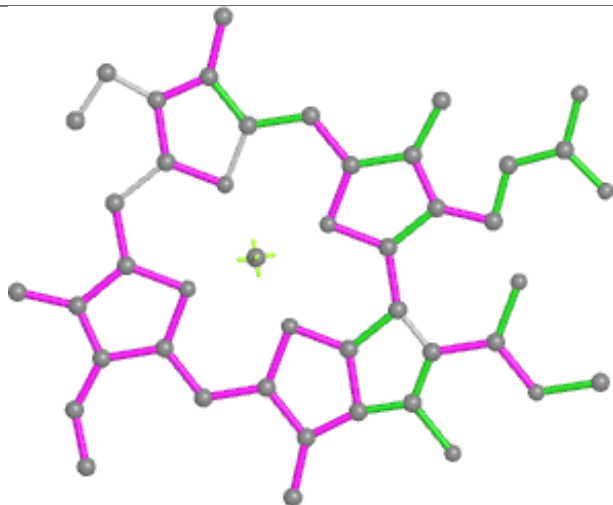




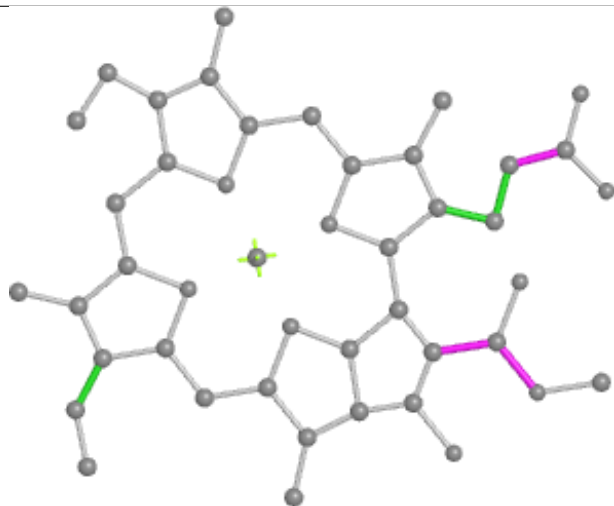
Ligand CLA cB 835



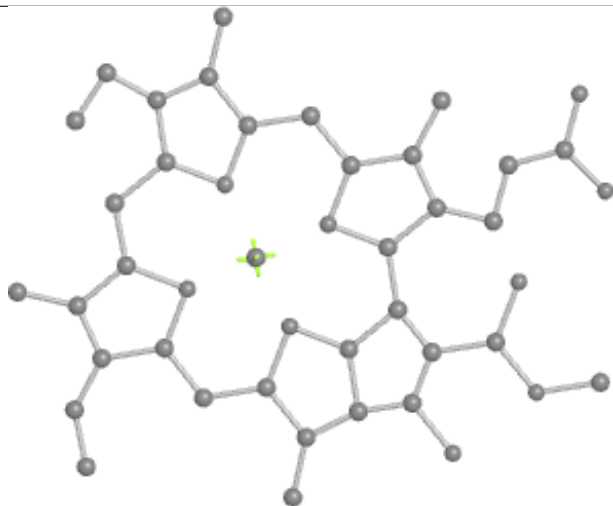
Bond lengths



Bond angles

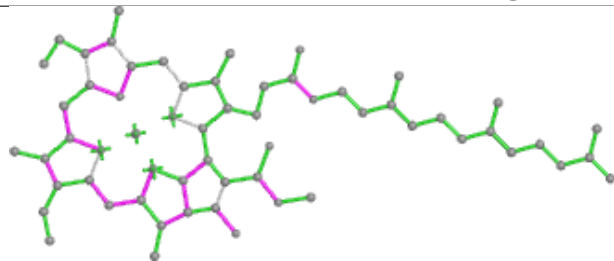


Torsions

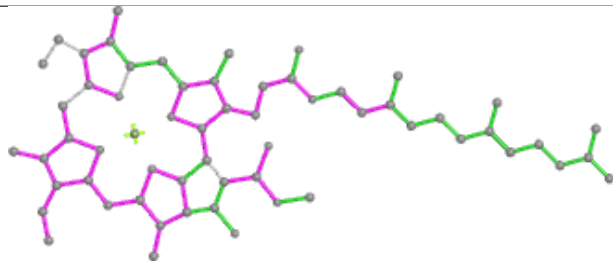


Rings

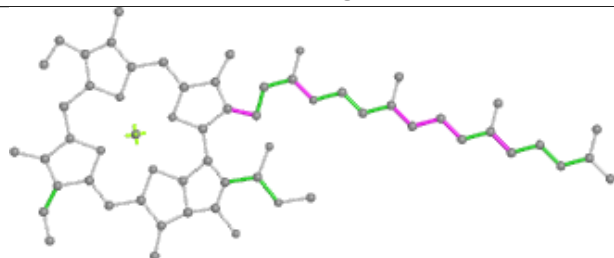
Ligand CLA bB 819



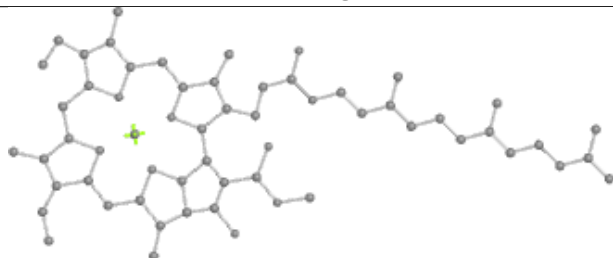
Bond lengths



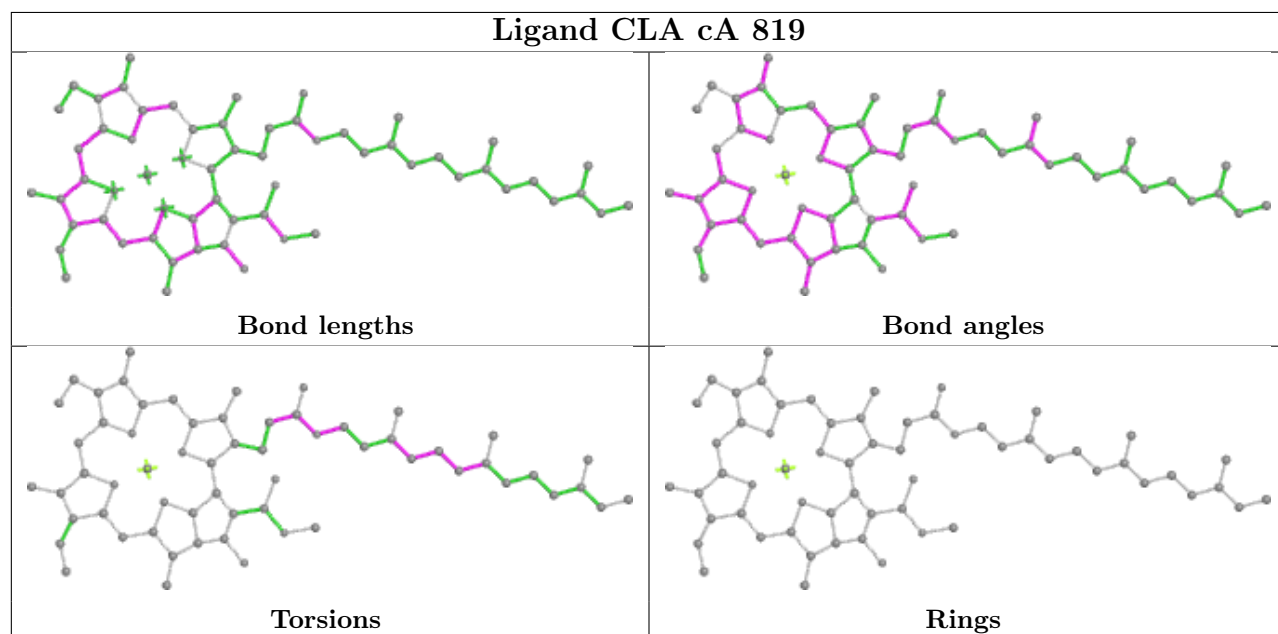
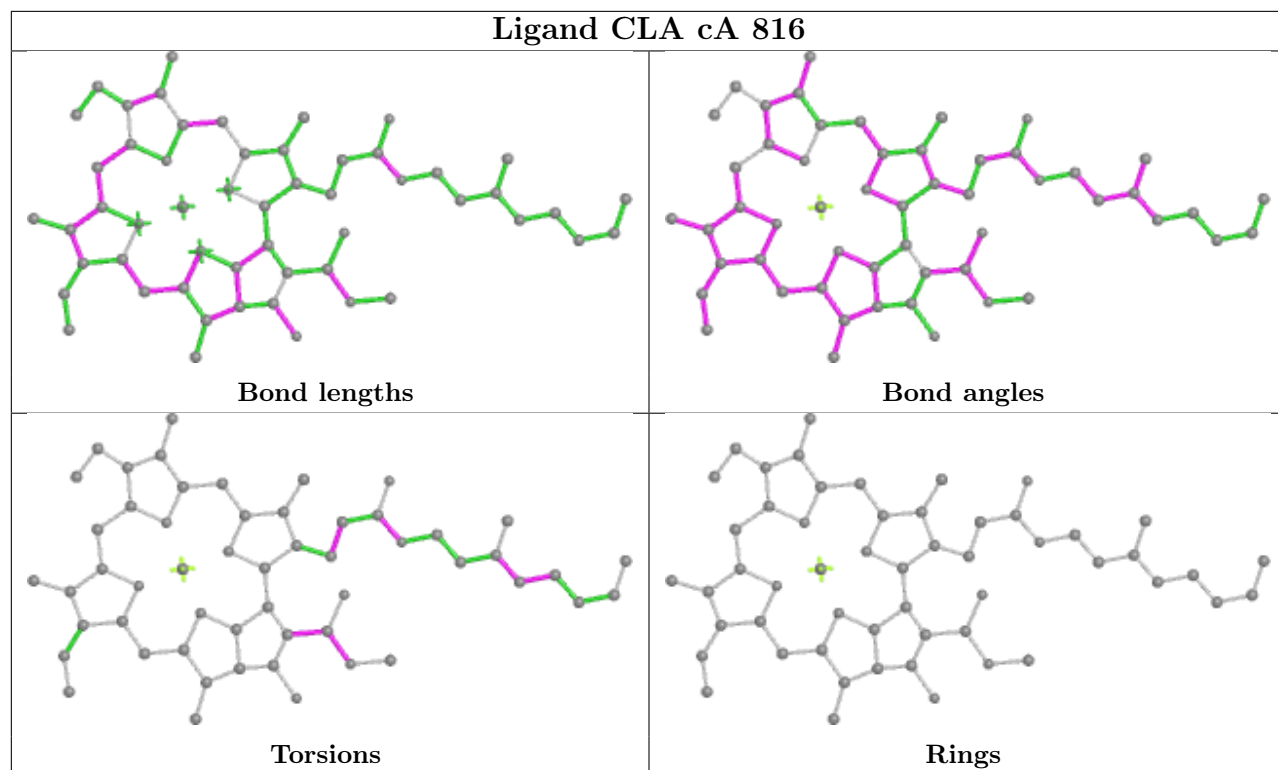
Bond angles



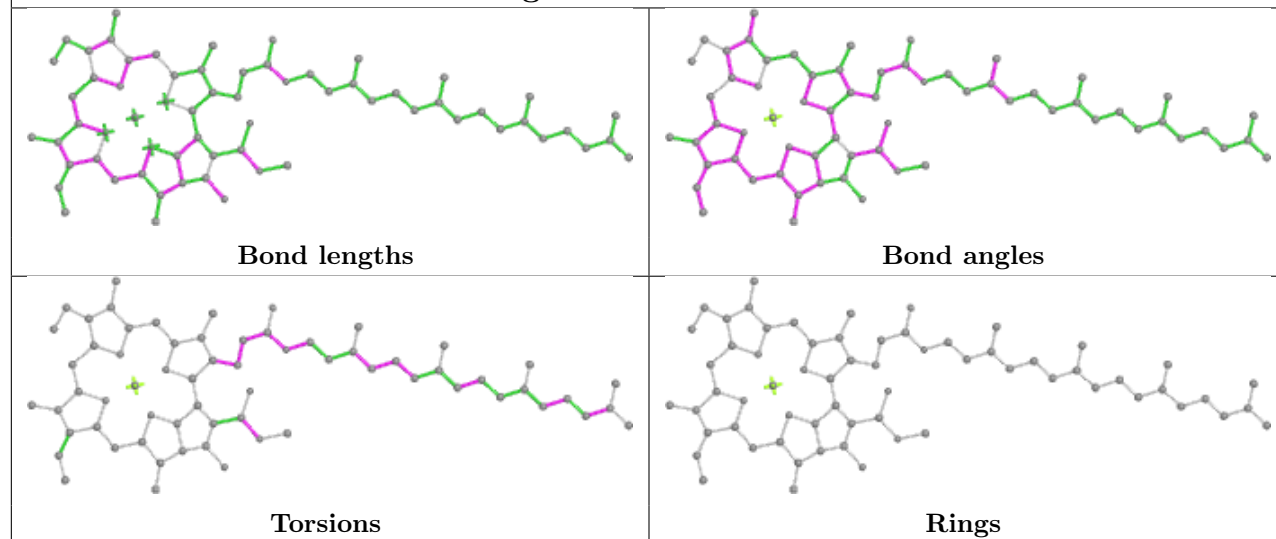
Torsions



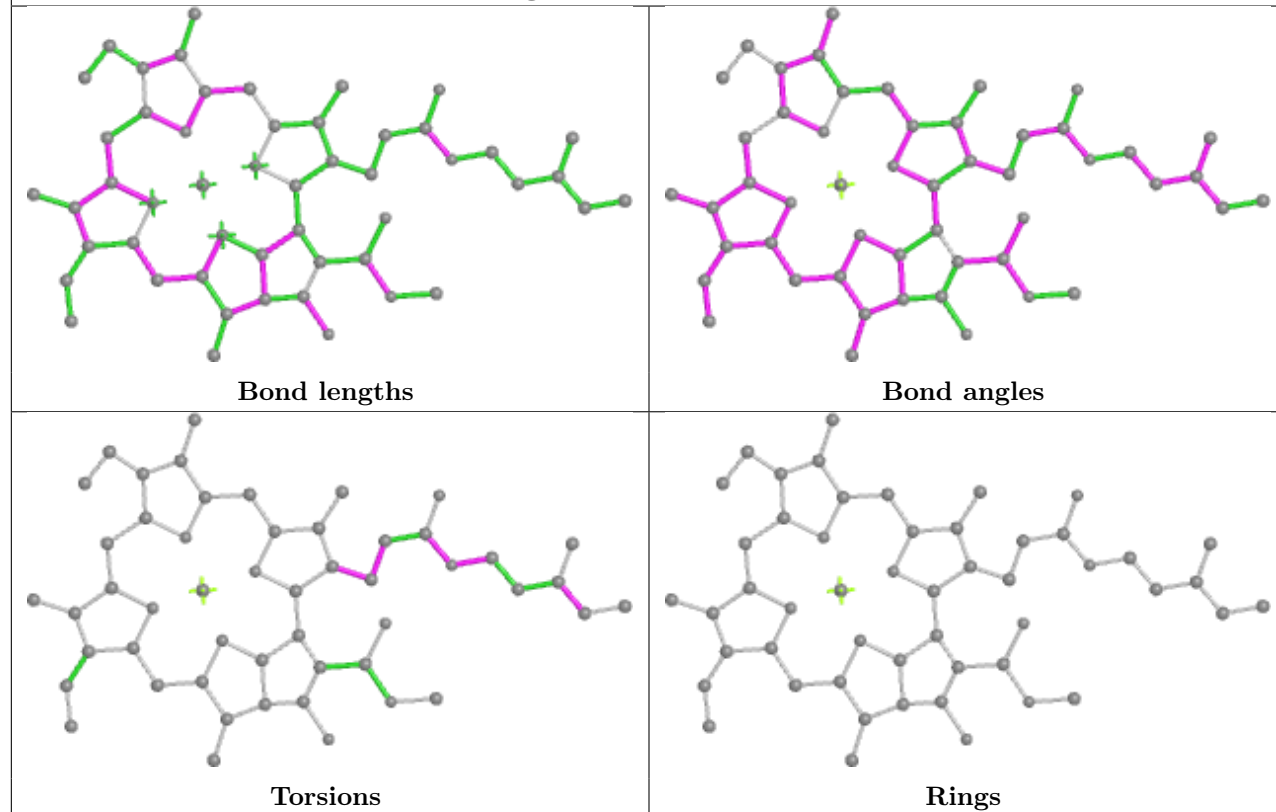
Rings

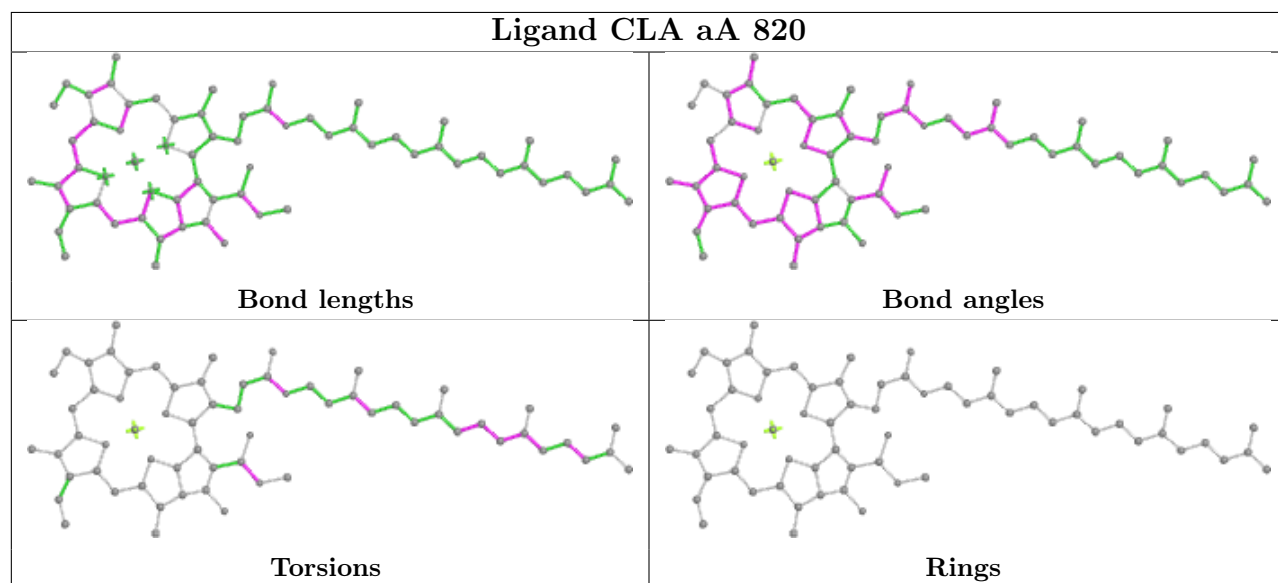
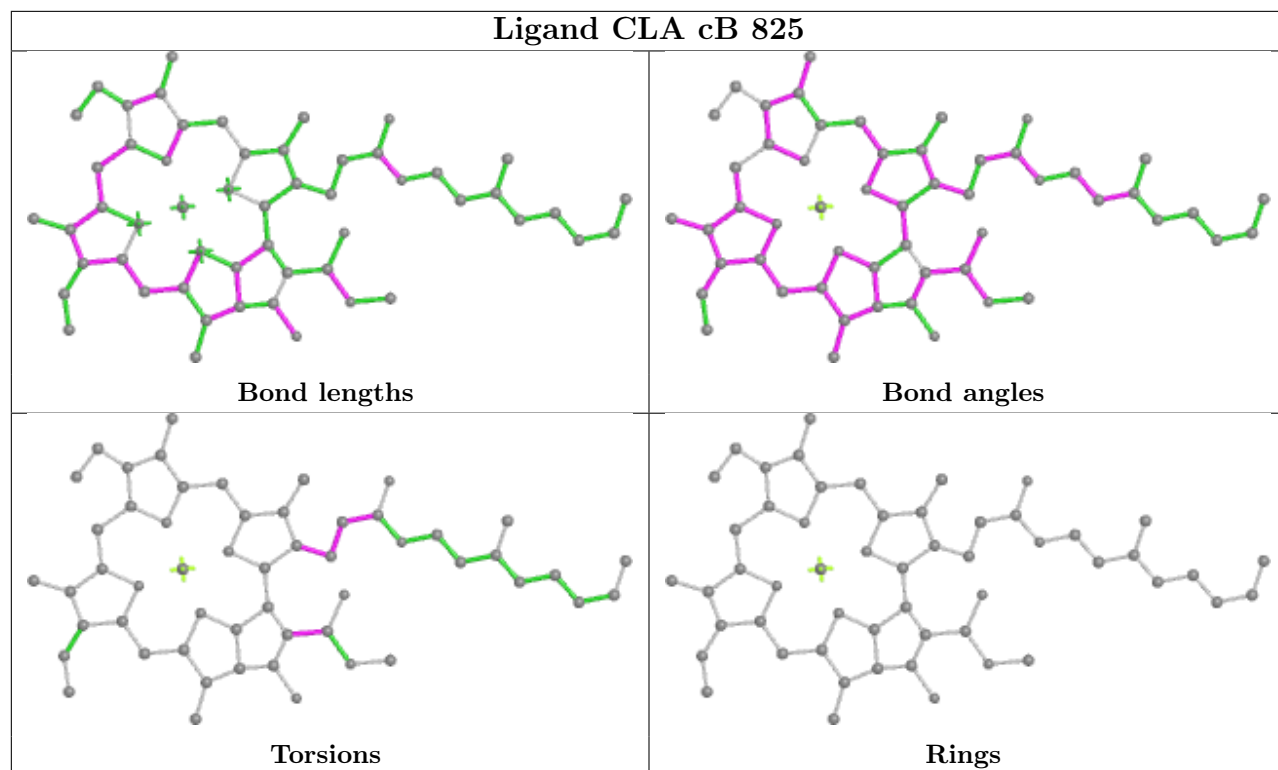


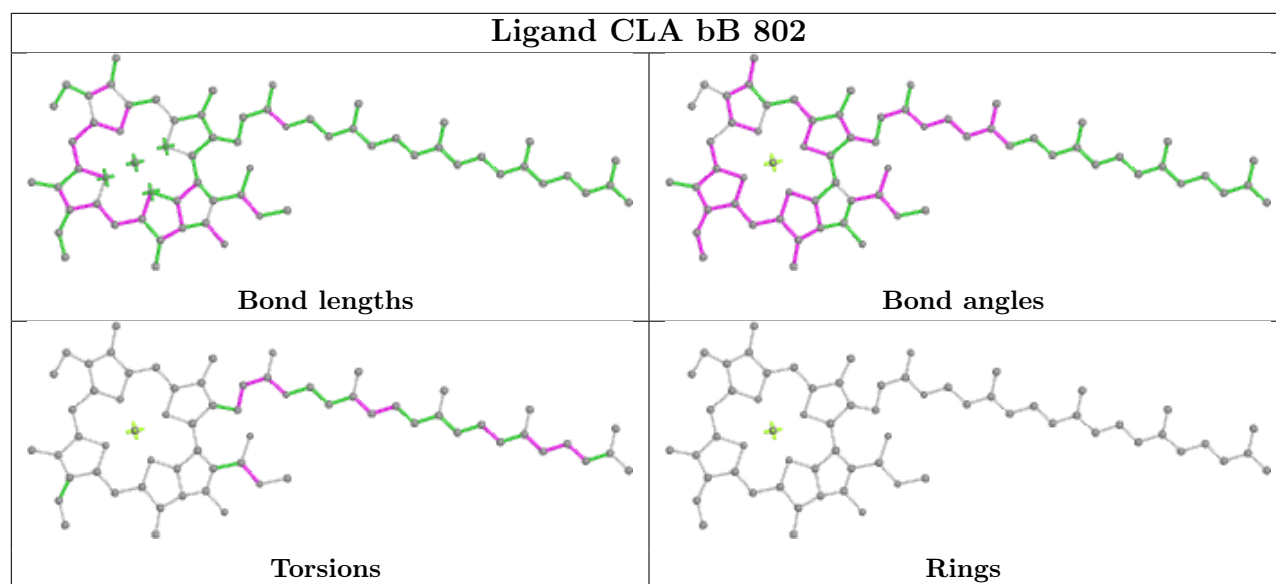
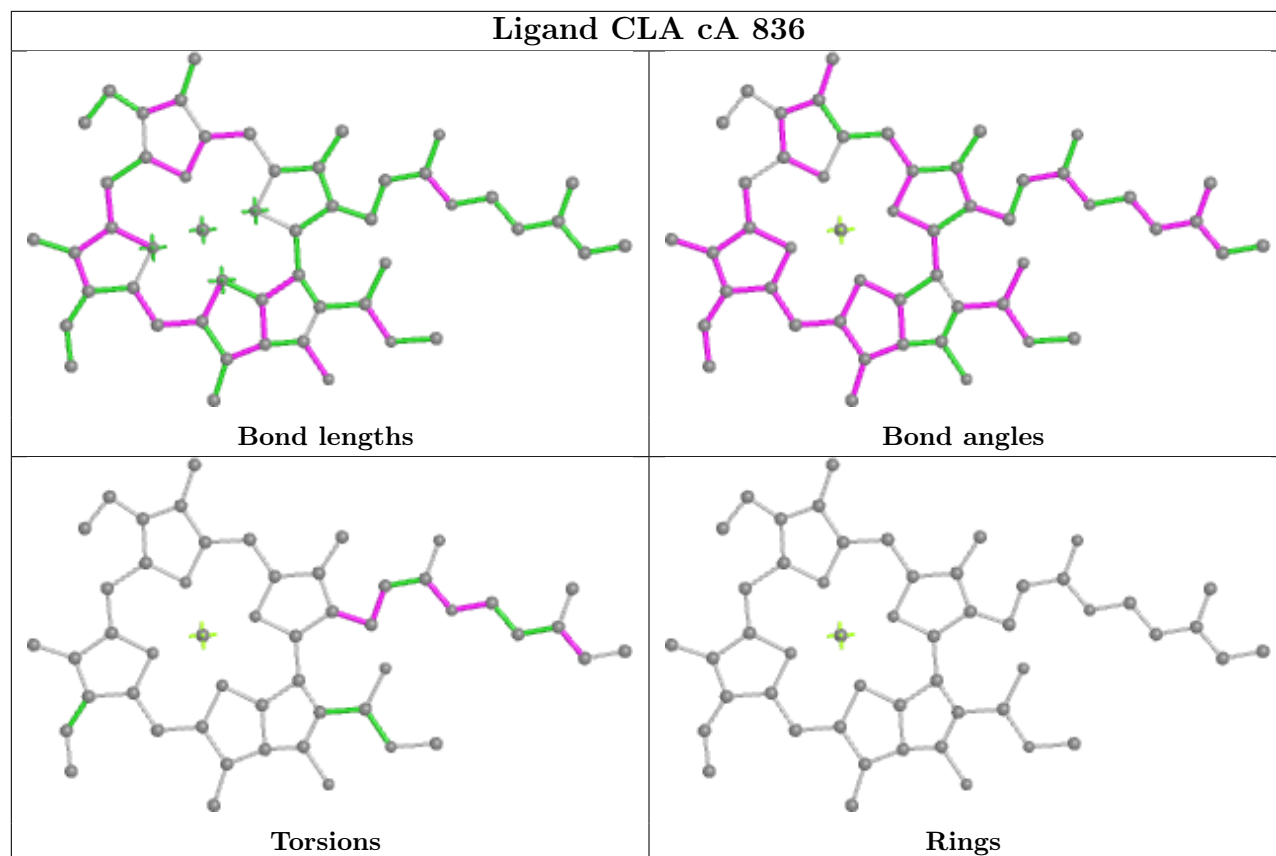
Ligand CLA bB 811

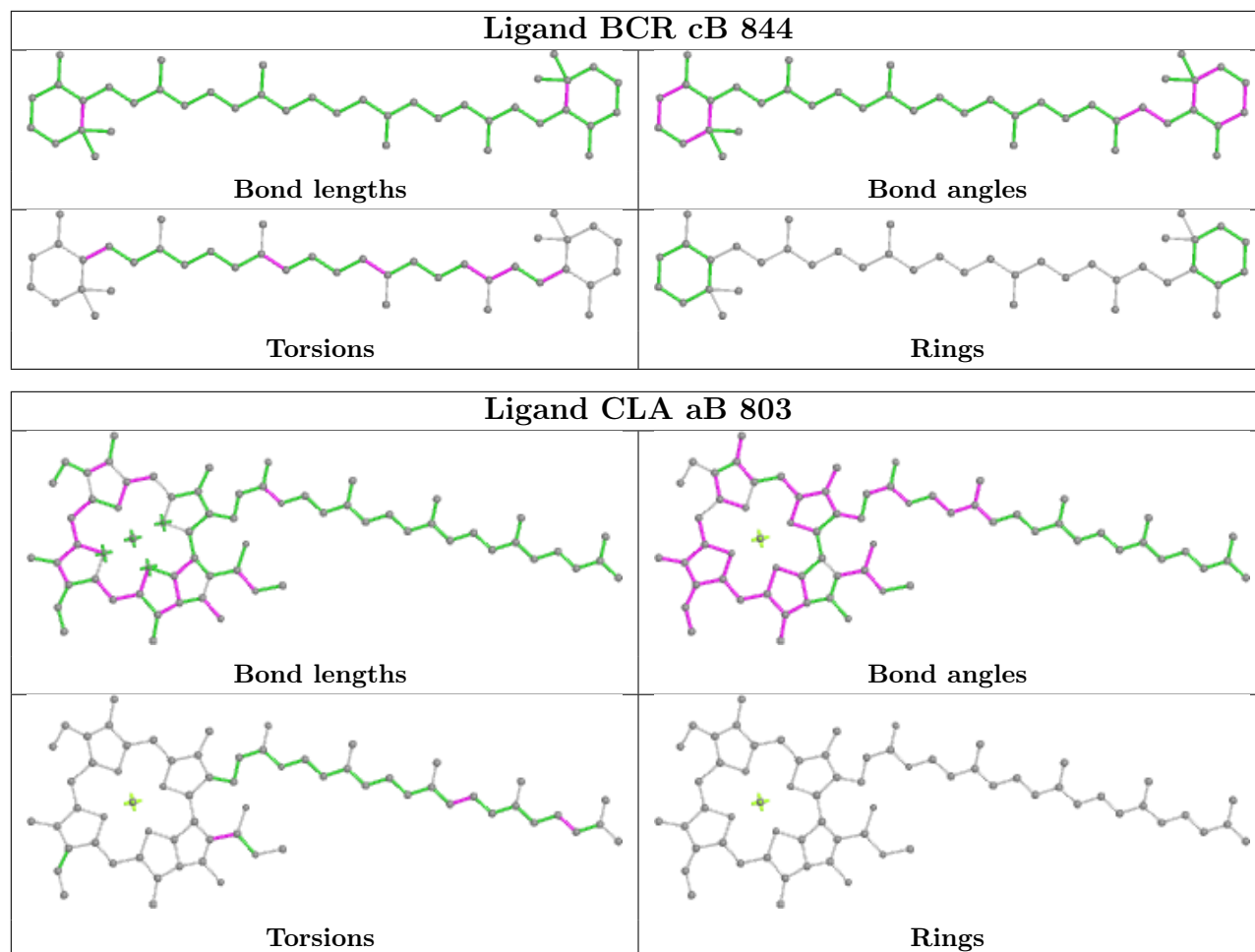


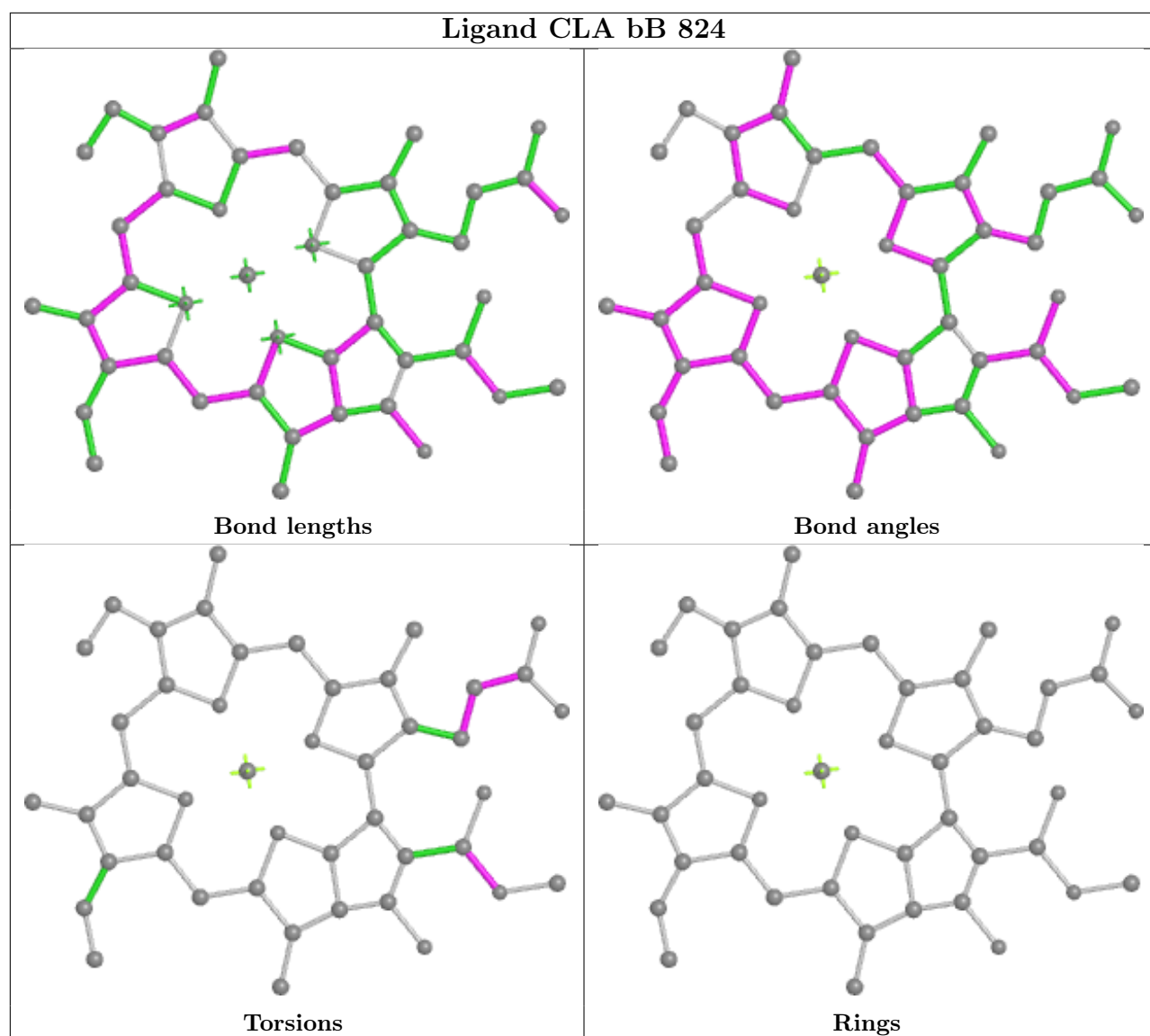
Ligand CLA aA 836



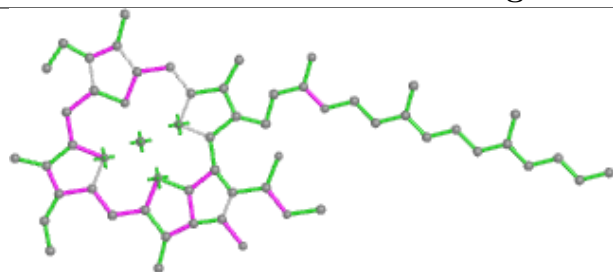




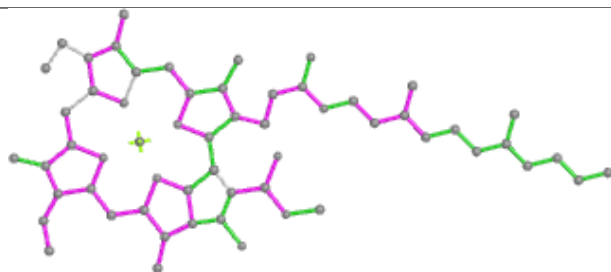




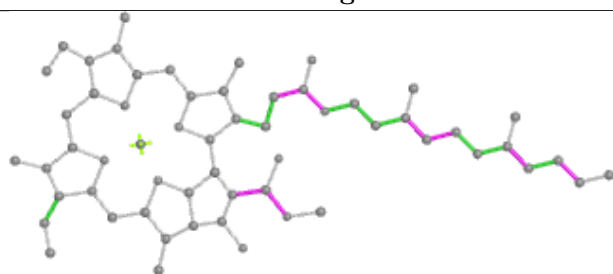
Ligand CLA cB 833



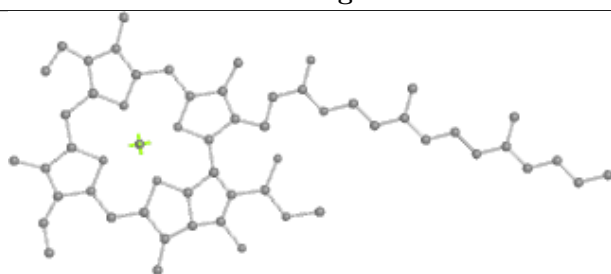
Bond lengths



Bond angles

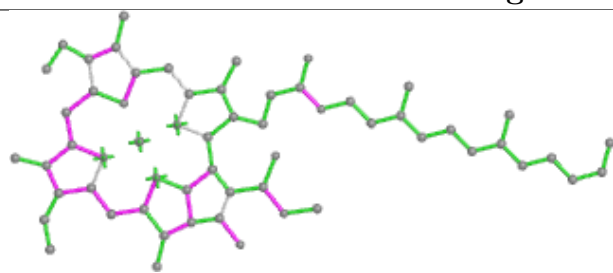


Torsions

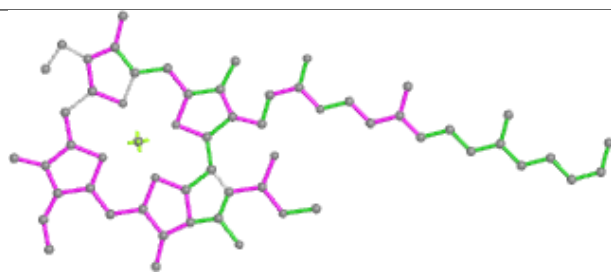


Rings

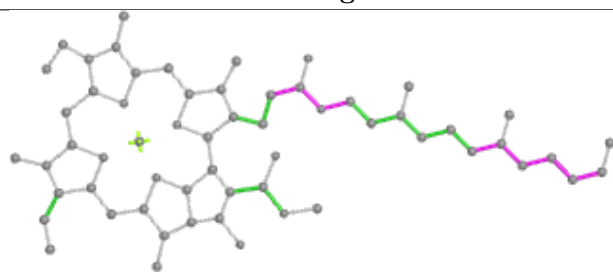
Ligand CLA cB 818



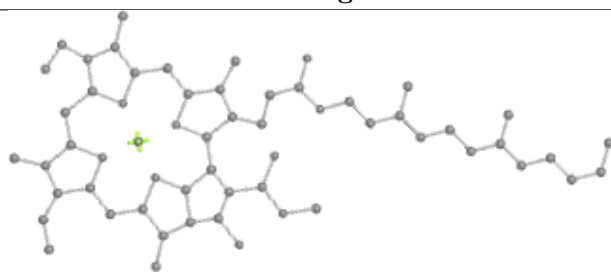
Bond lengths



Bond angles

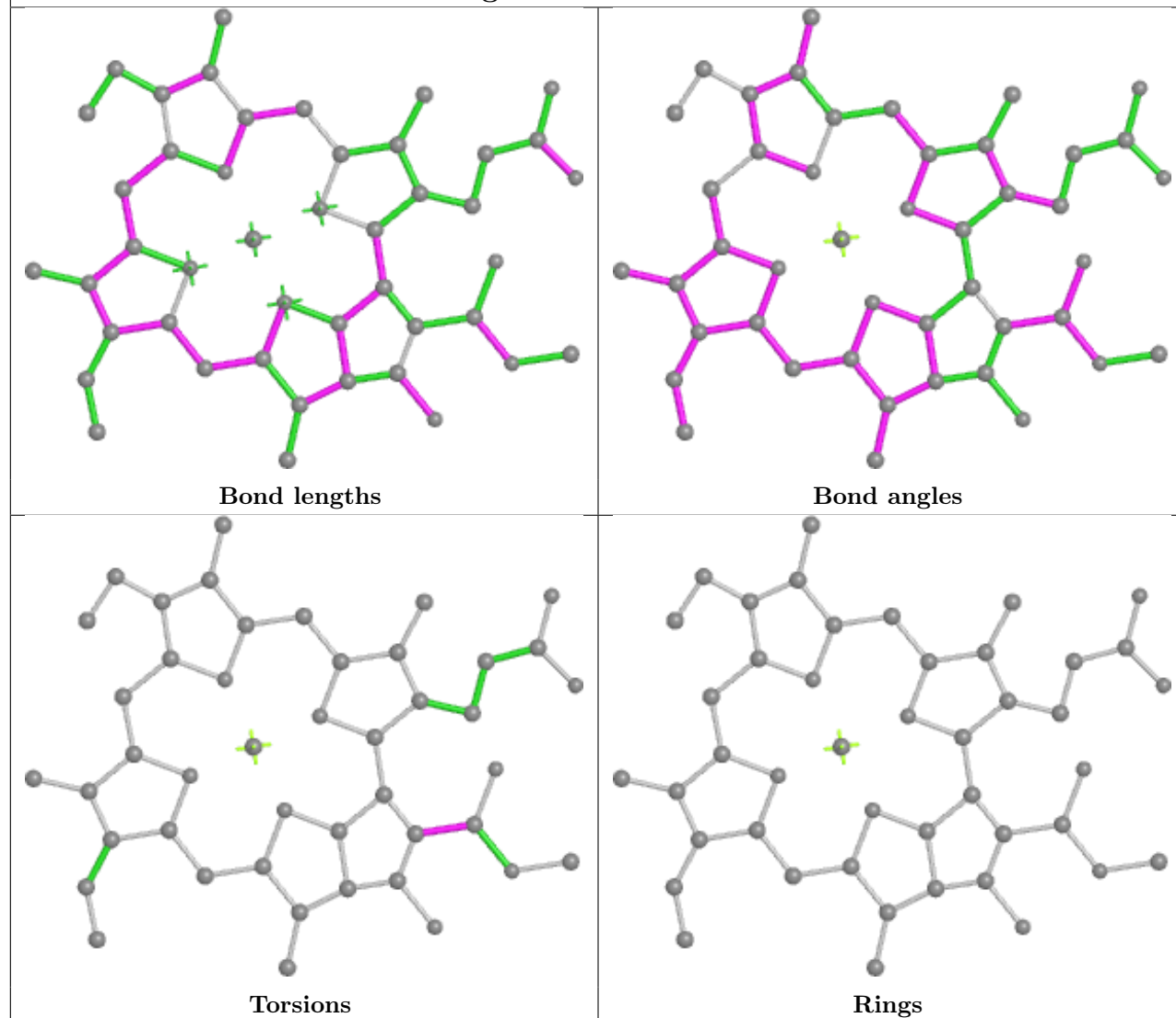


Torsions

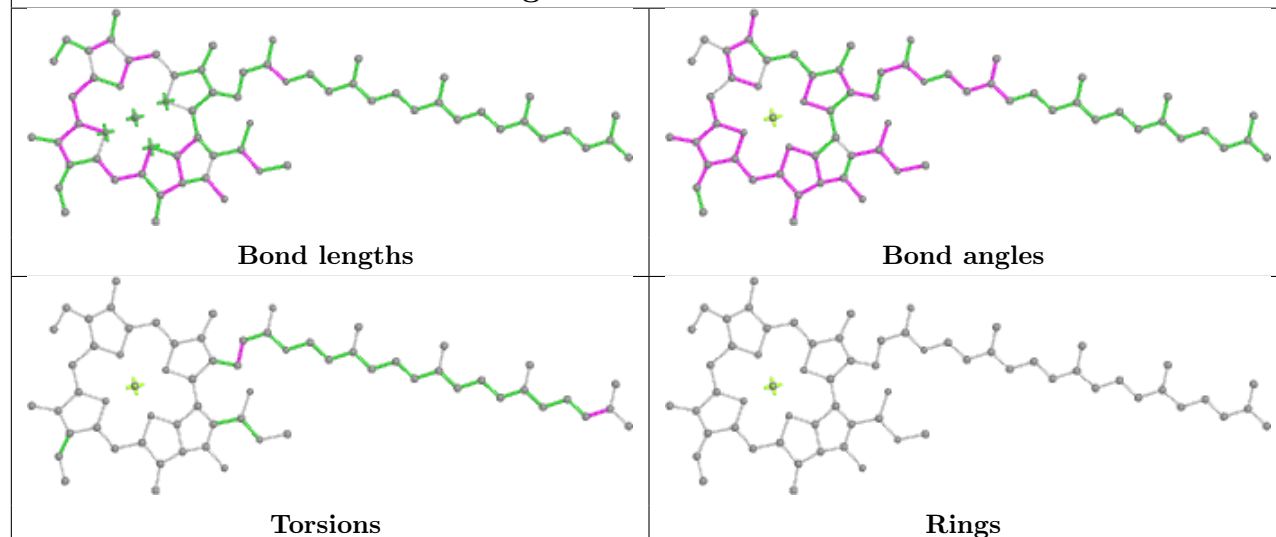


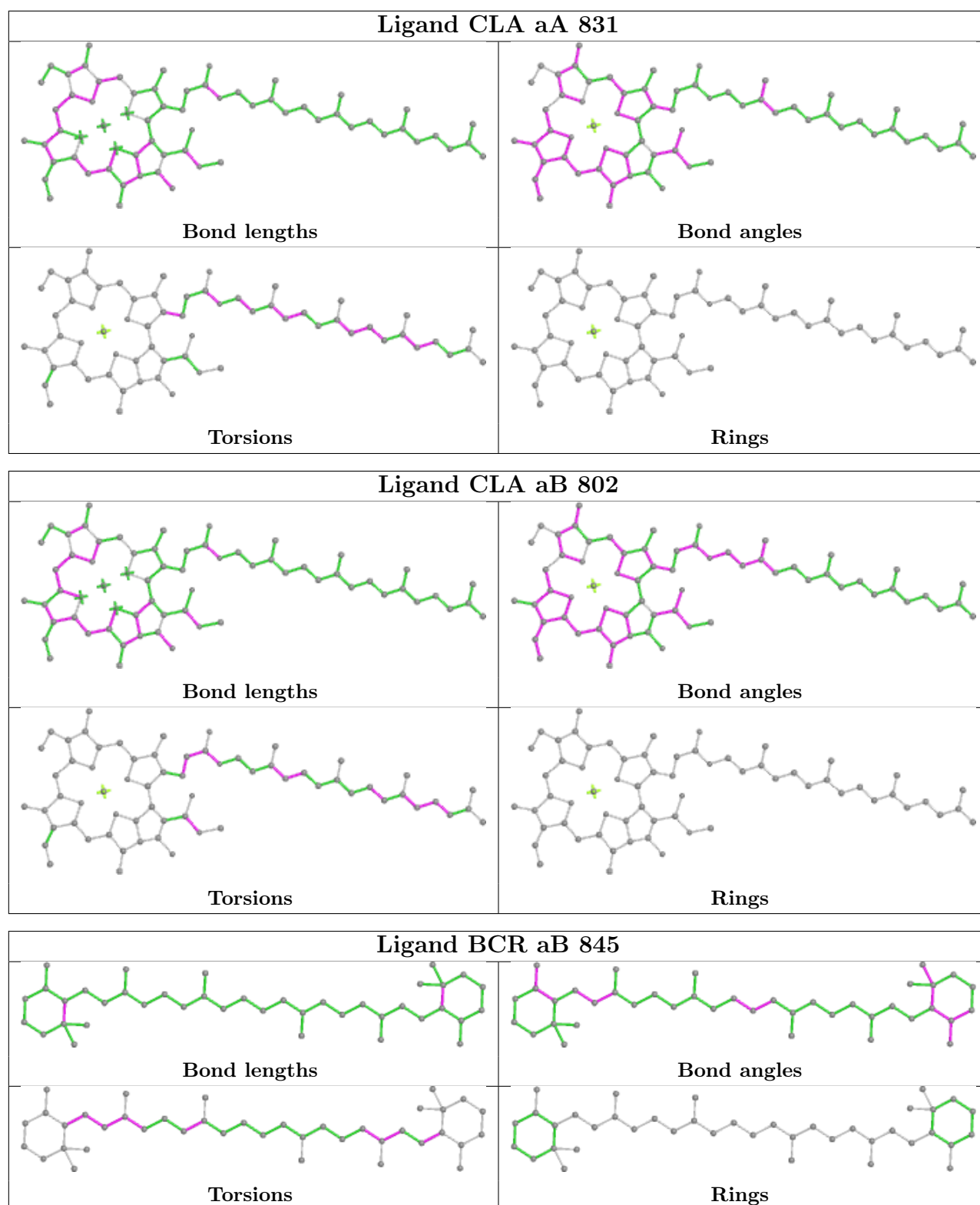
Rings

Ligand CLA aA 803

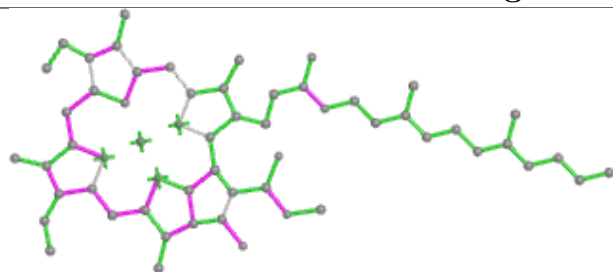


Ligand CLA bB 840

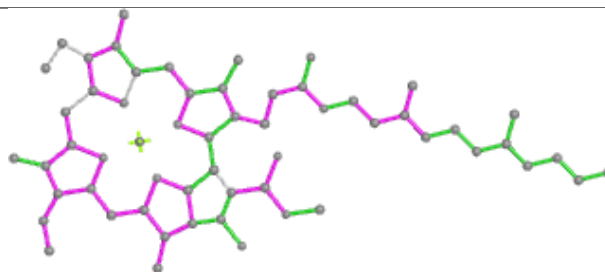




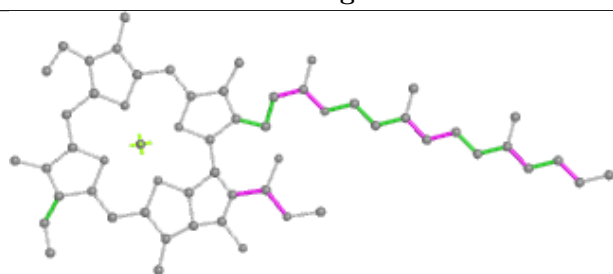
Ligand CLA bB 833



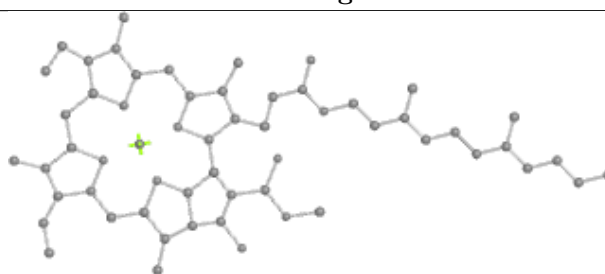
Bond lengths



Bond angles

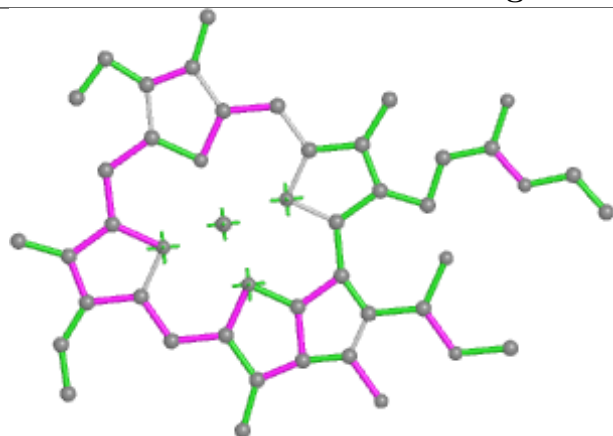


Torsions

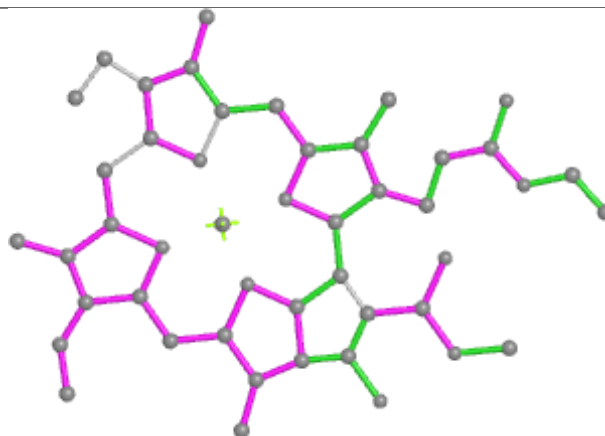


Rings

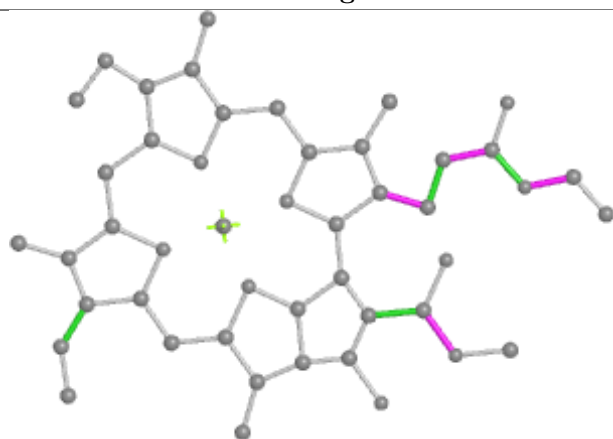
Ligand CLA cB 839



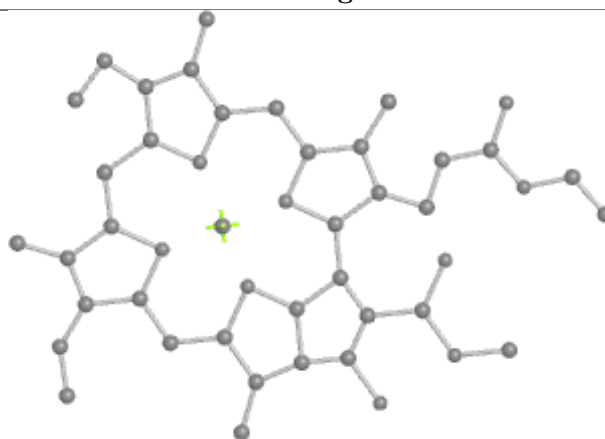
Bond lengths



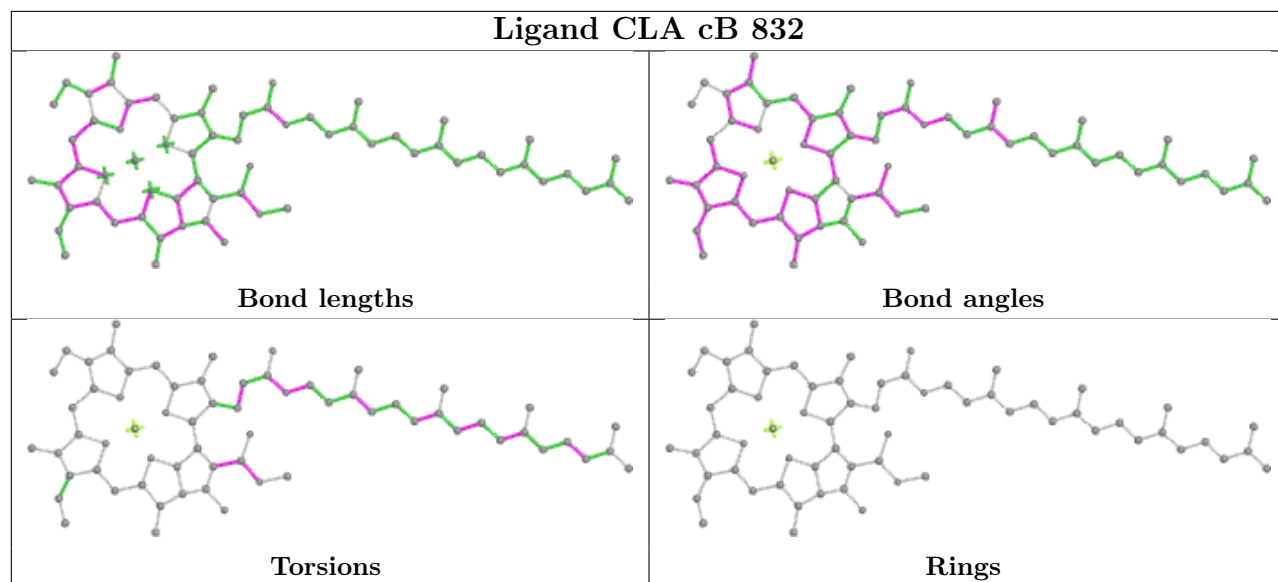
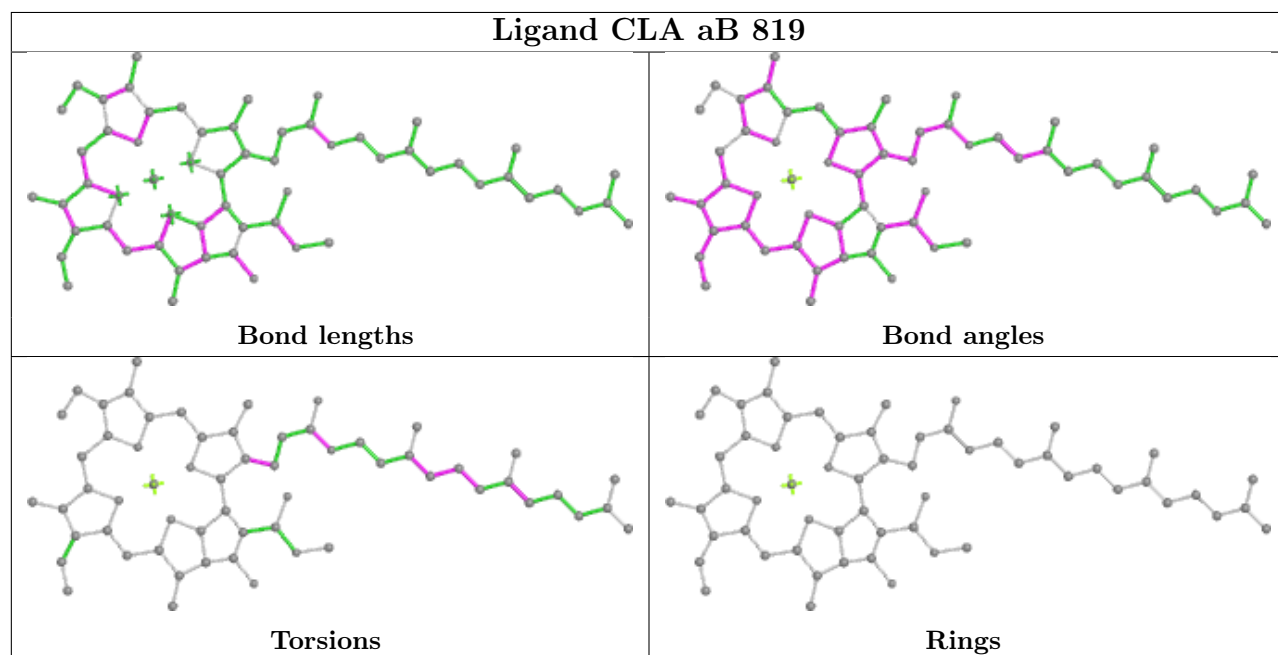
Bond angles



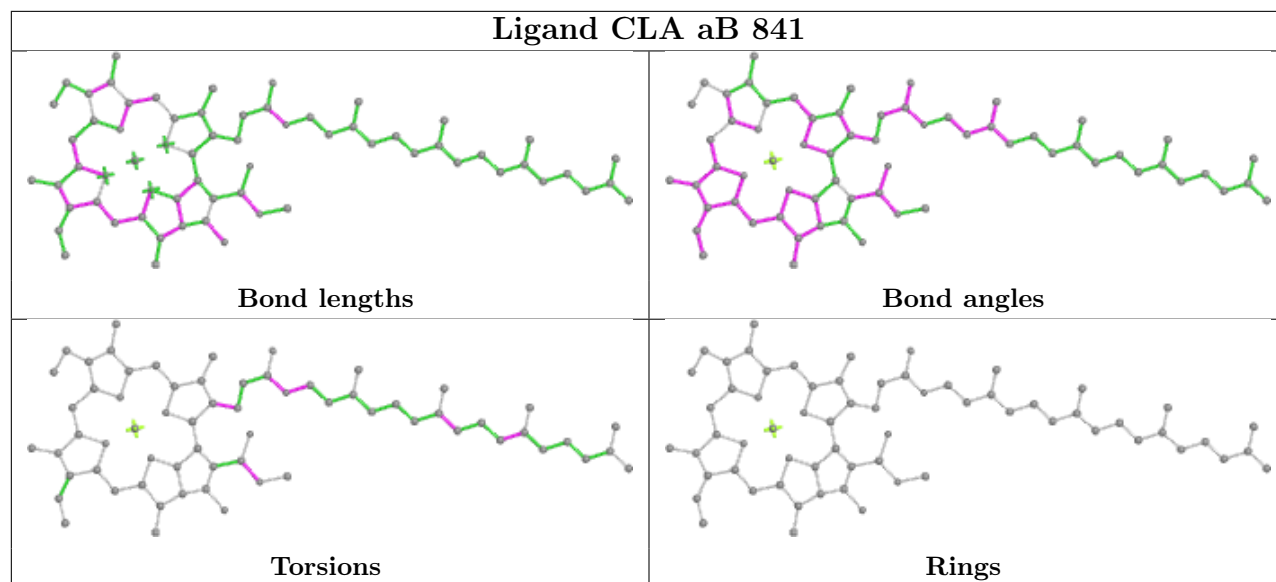
Torsions



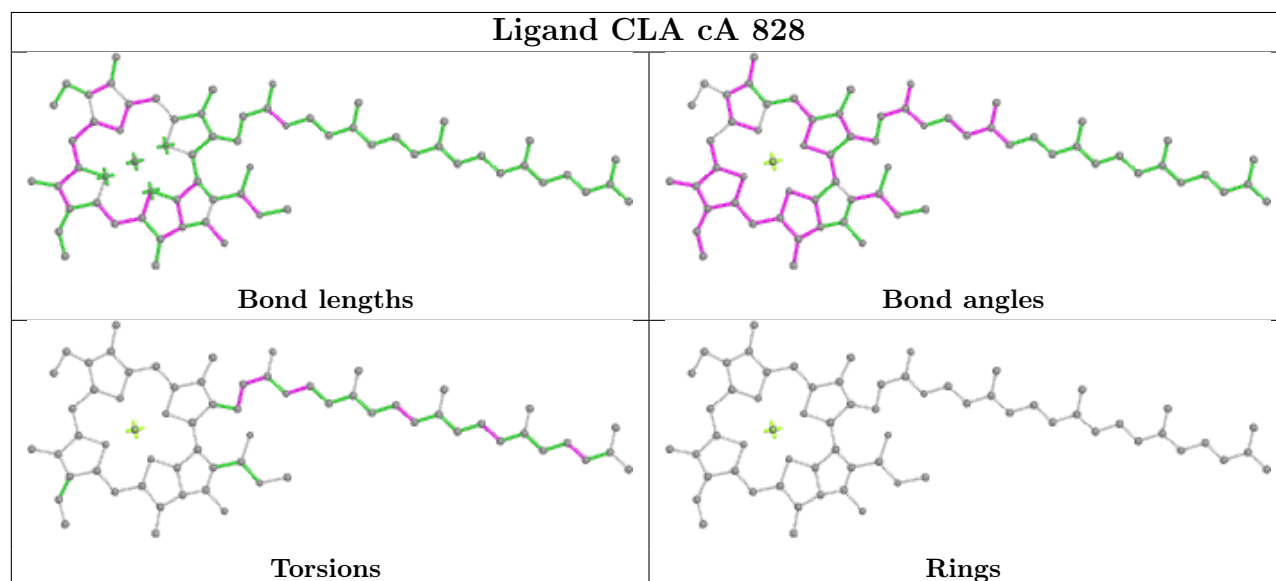
Rings

Ligand CLA cB 832**Ligand CLA aB 819**

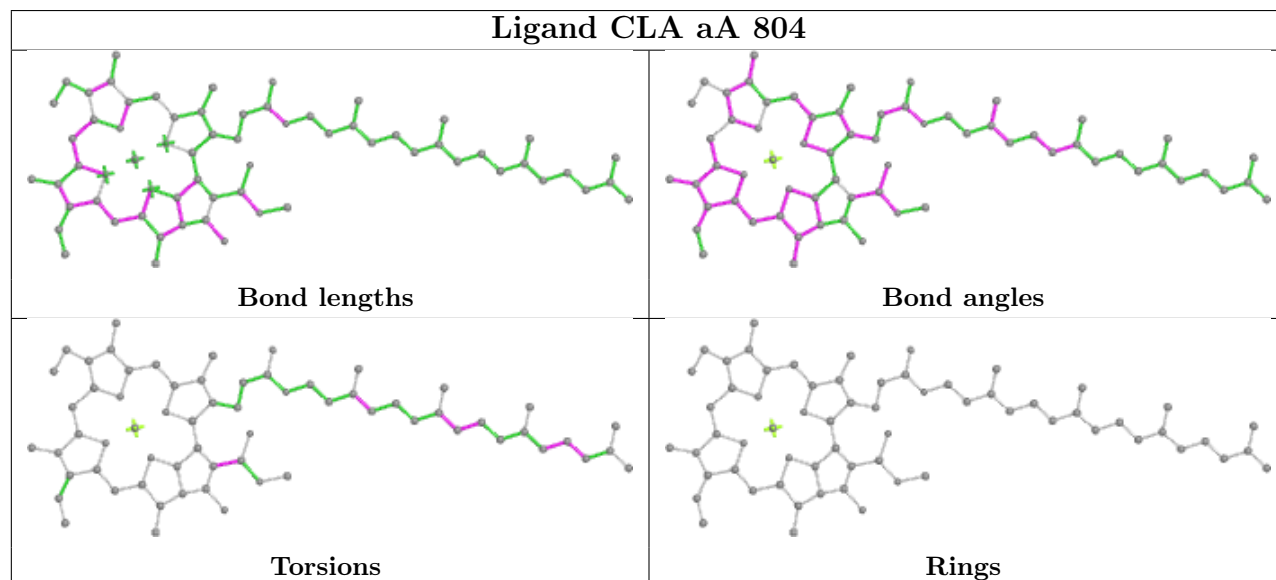
Ligand CLA aB 841



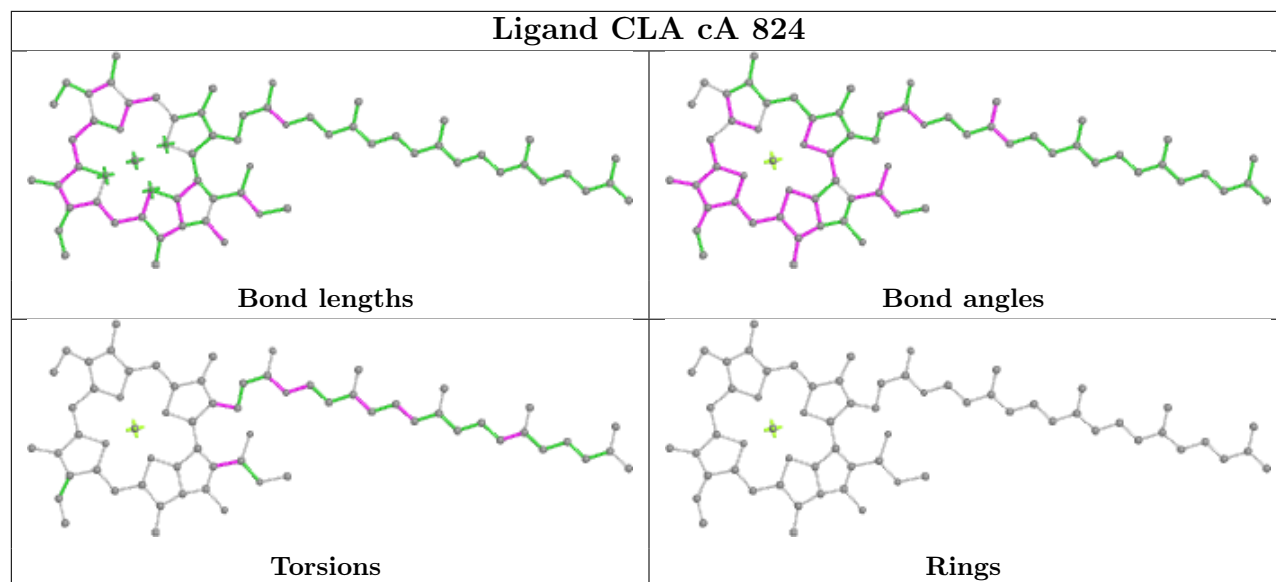
Ligand CLA cA 828



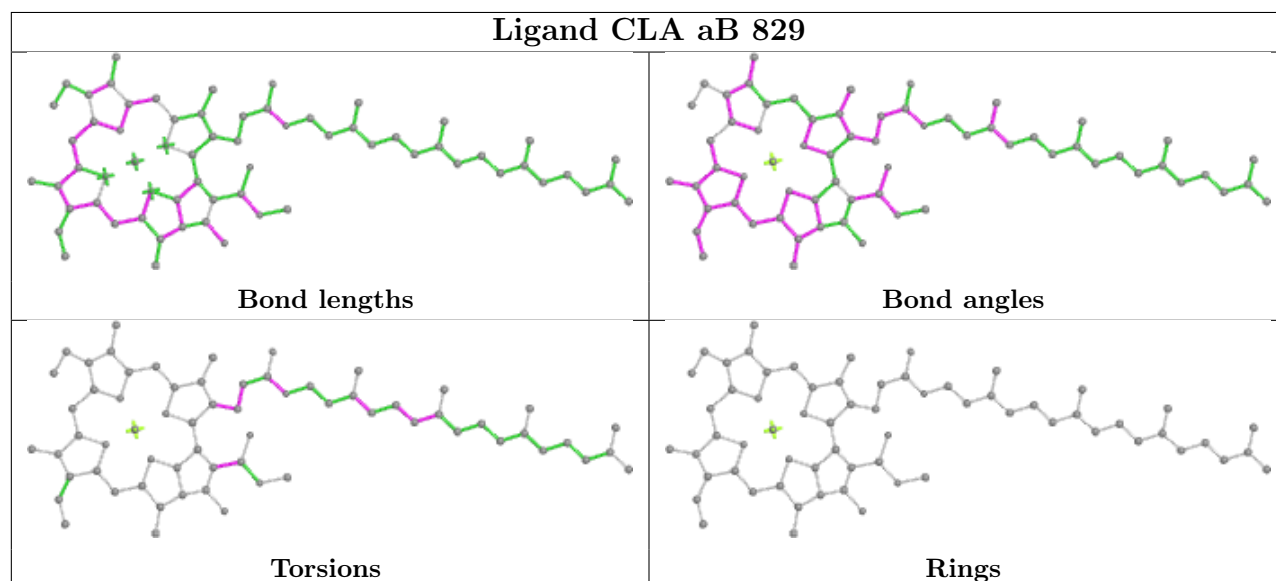
Ligand CLA aA 804



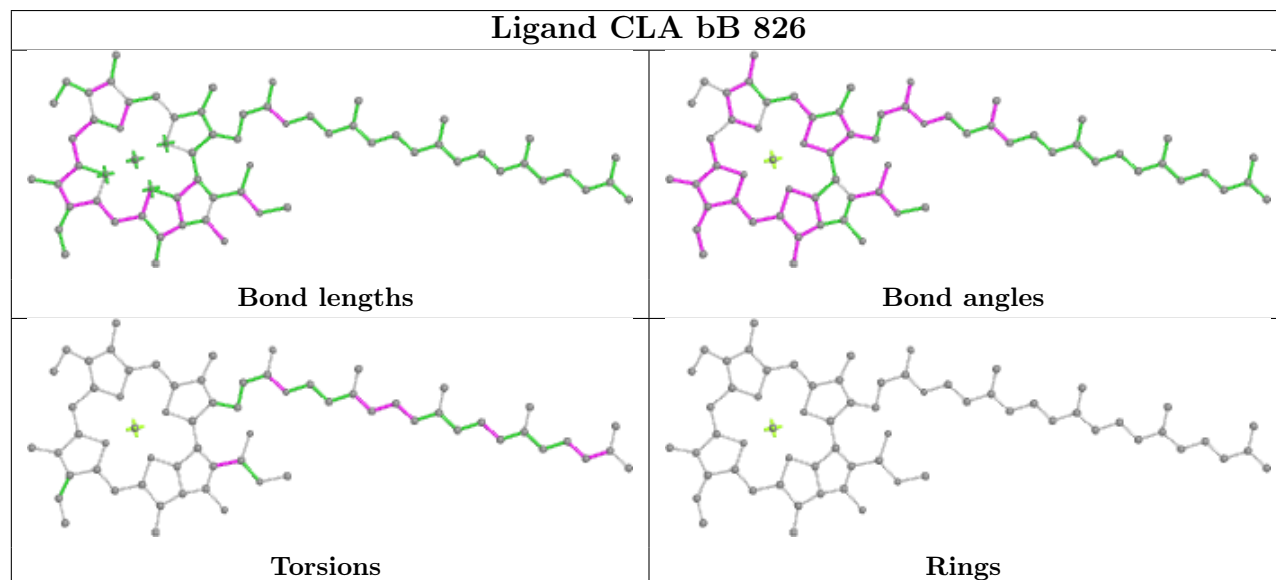
Ligand CLA cA 824



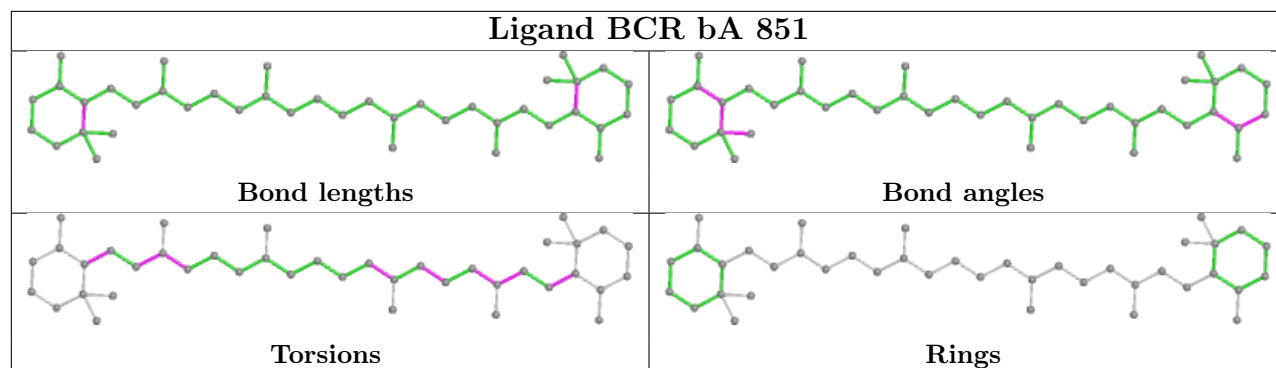
Ligand CLA aB 829



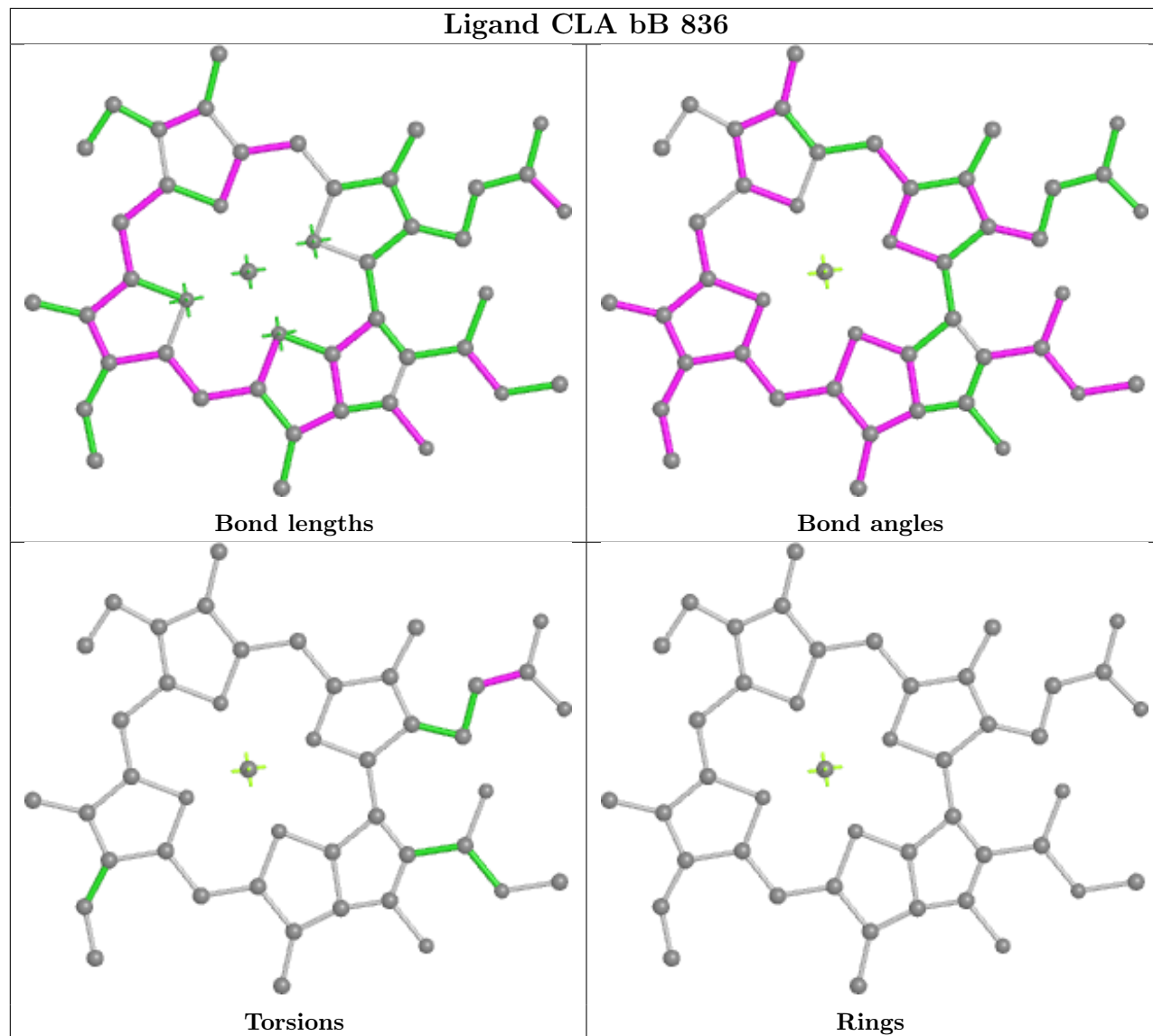
Ligand CLA bB 826



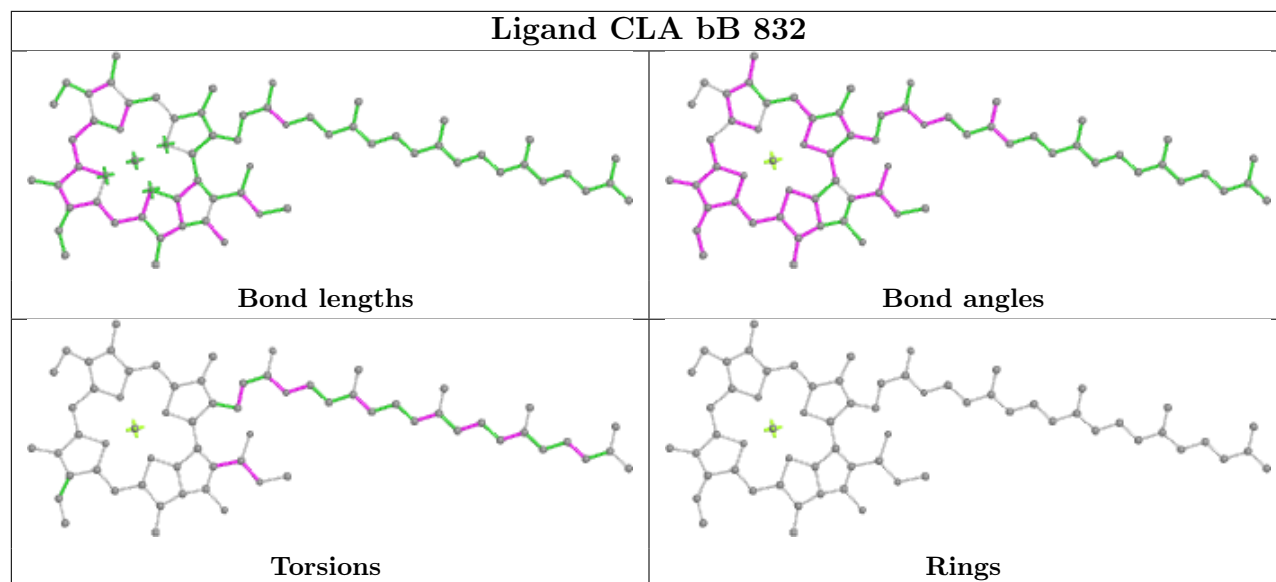
Ligand BCR bA 851



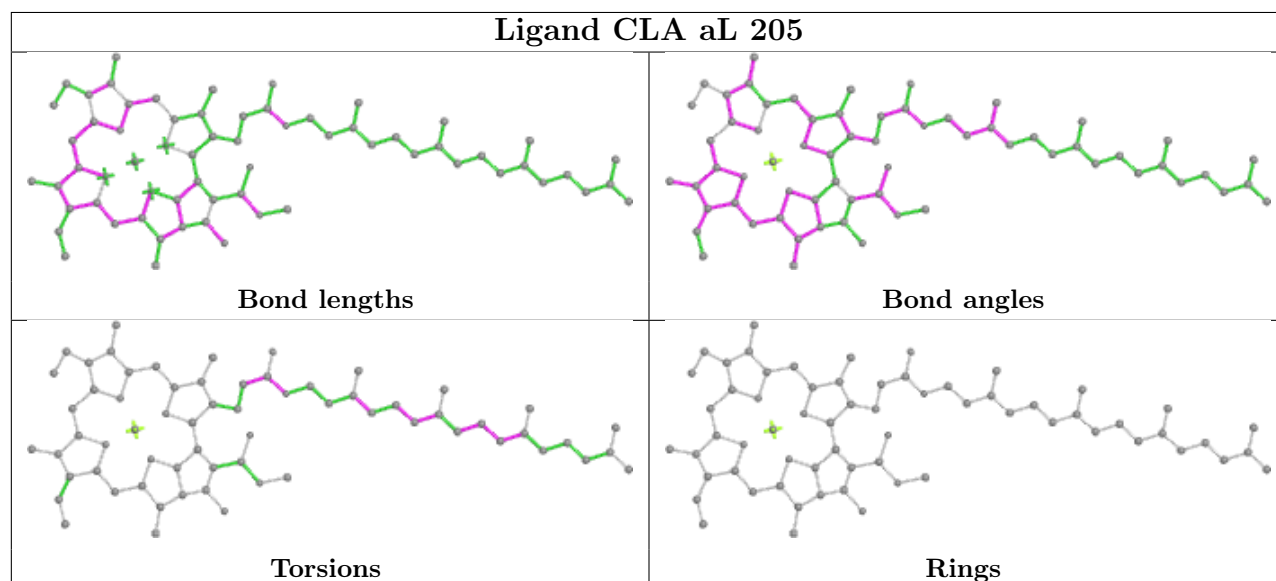
Ligand CLA bB 836



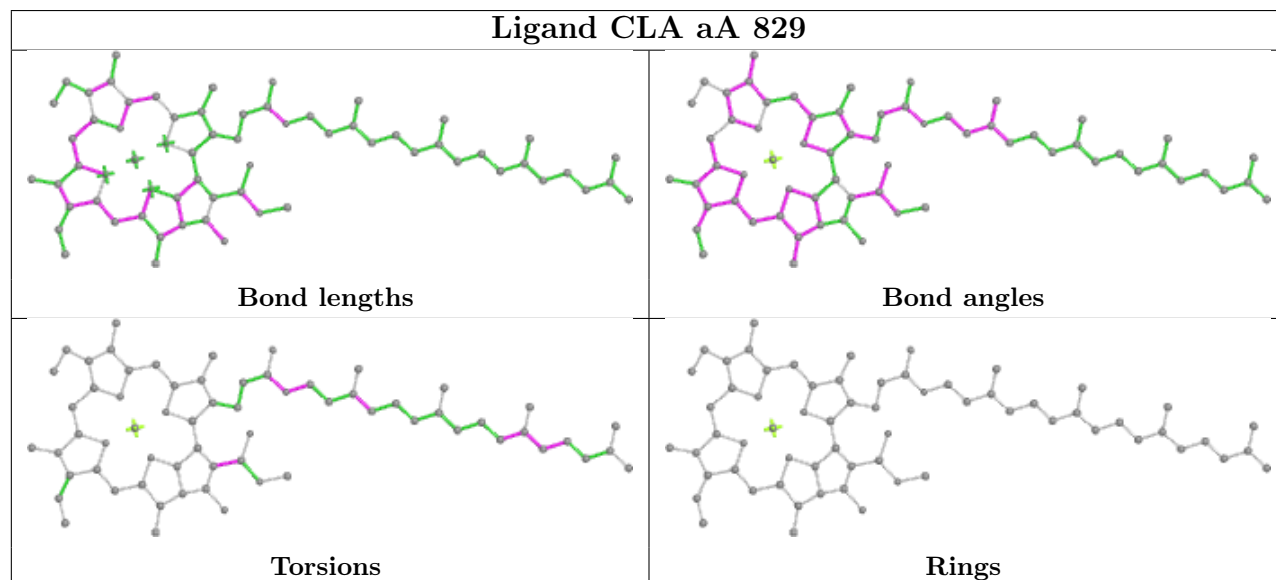
Ligand CLA bB 832

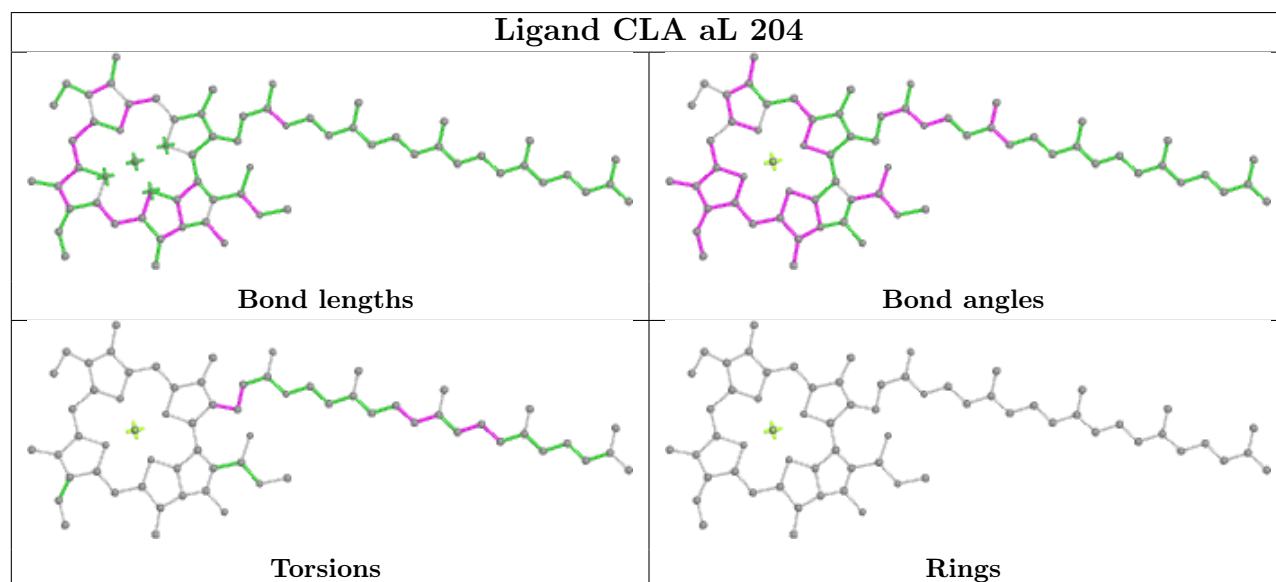
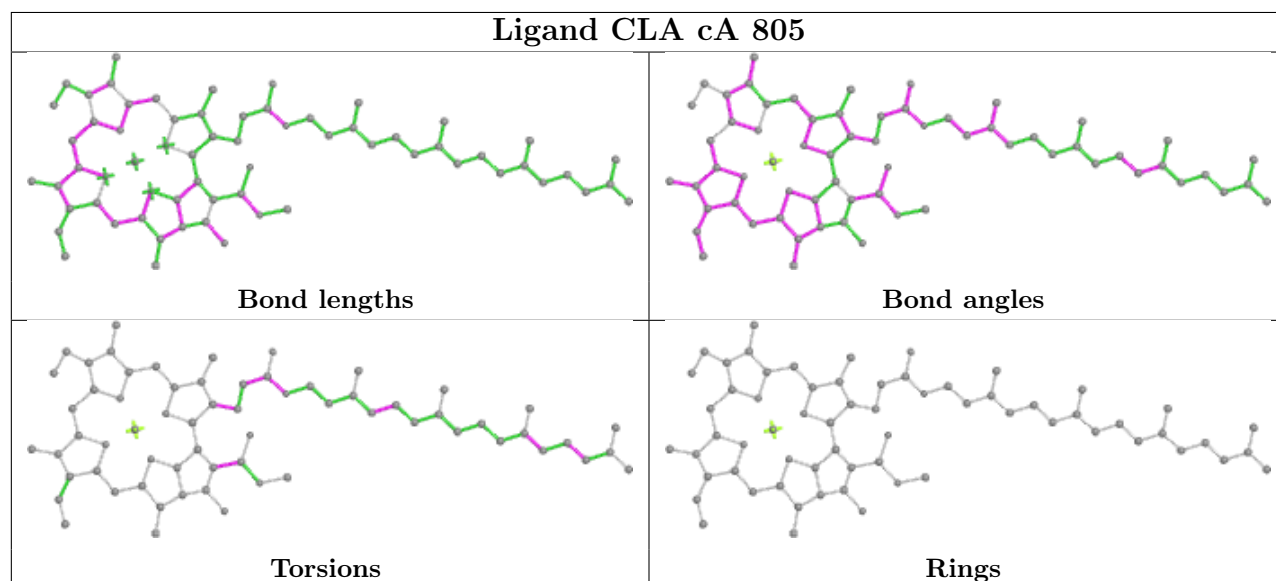
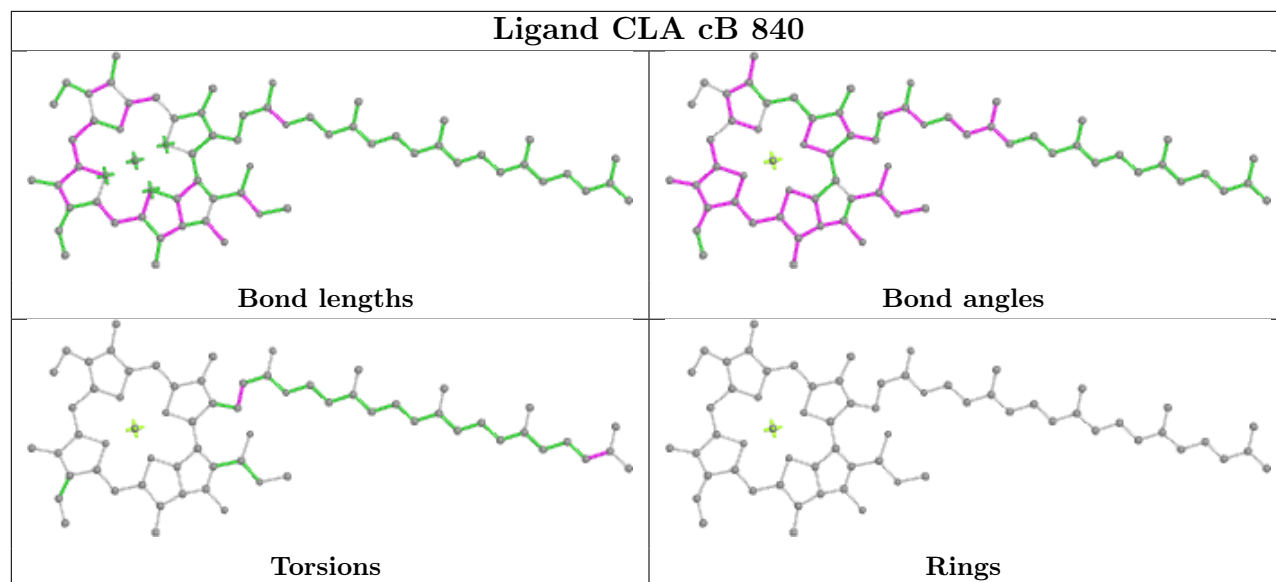


Ligand CLA aL 205

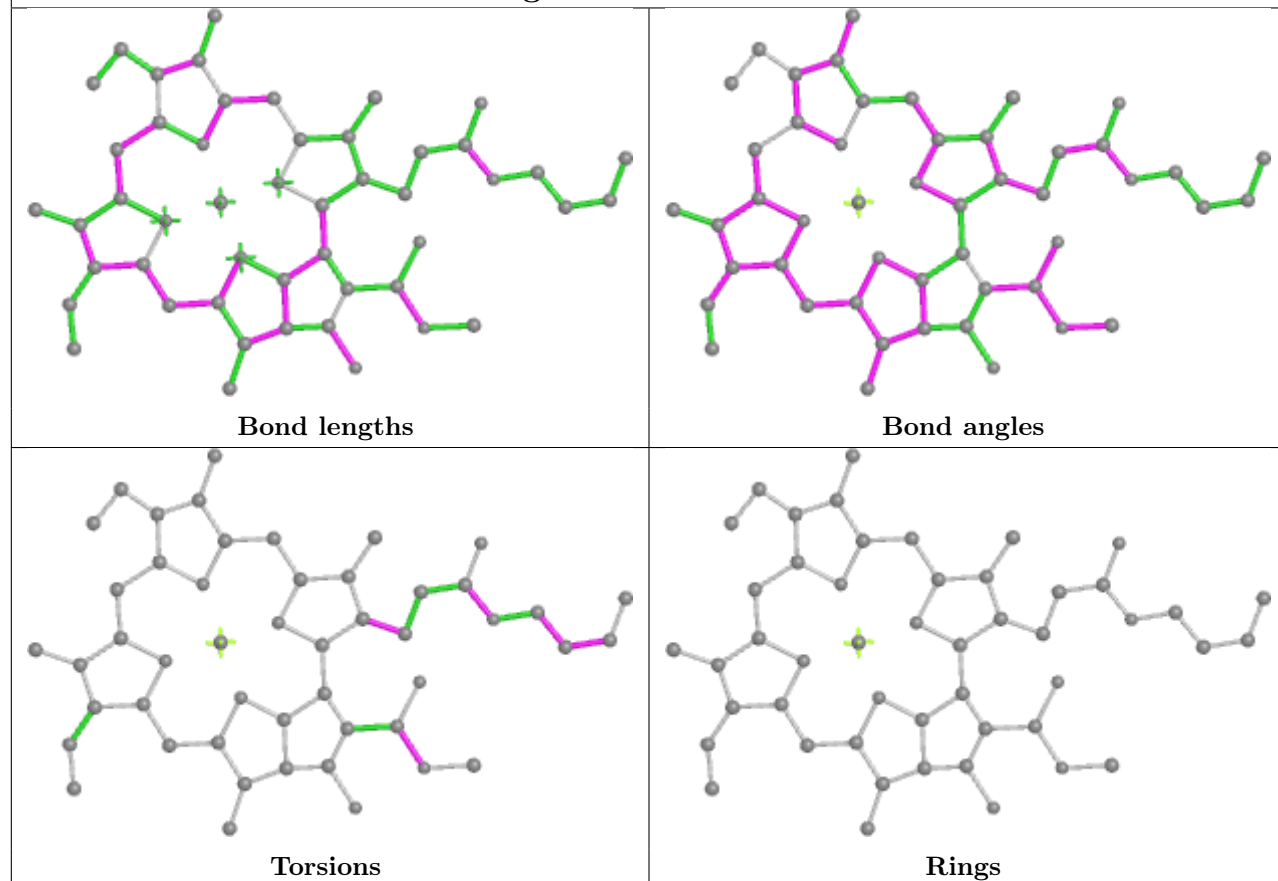


Ligand CLA aA 829

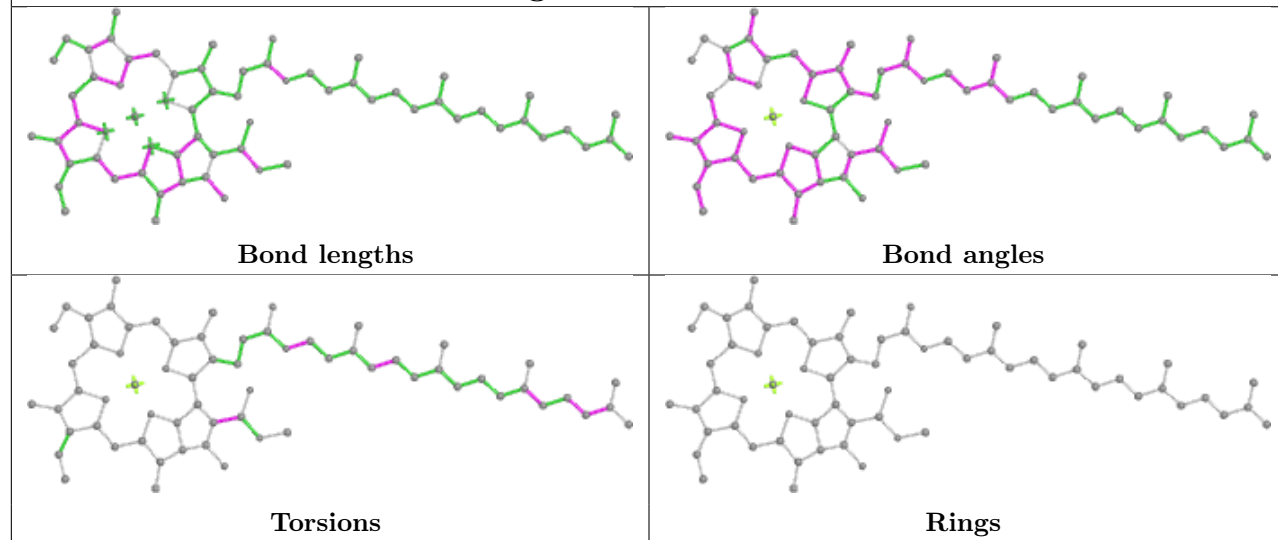


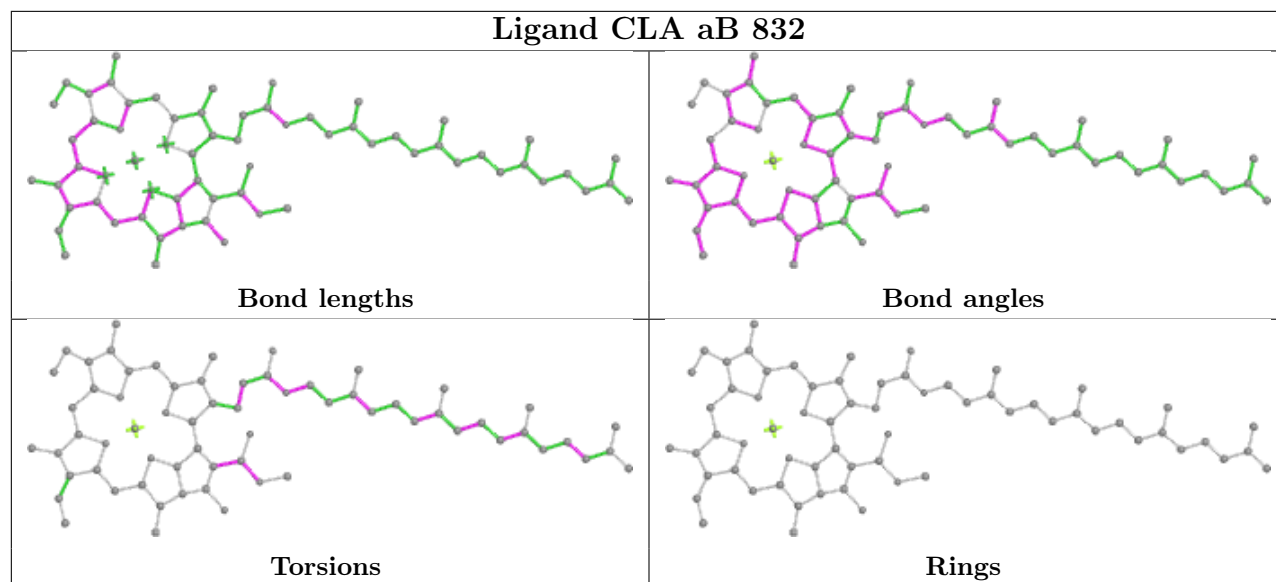
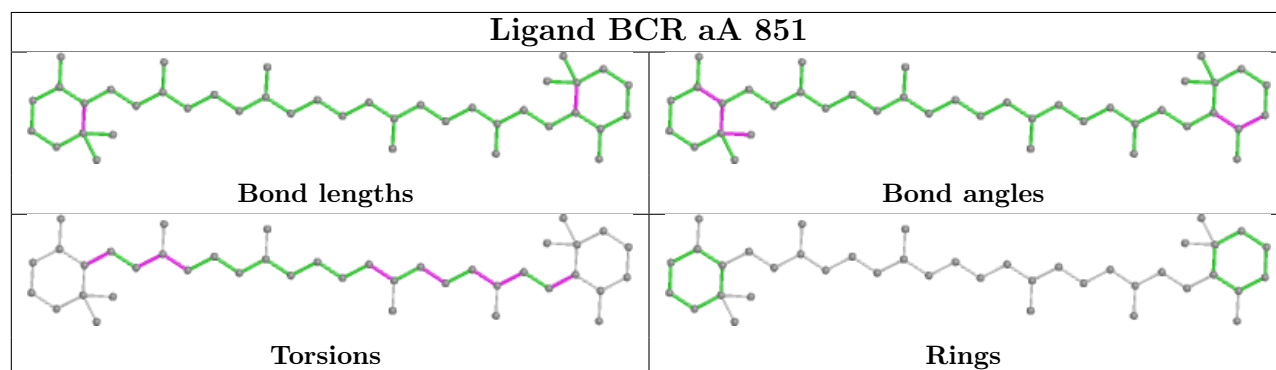
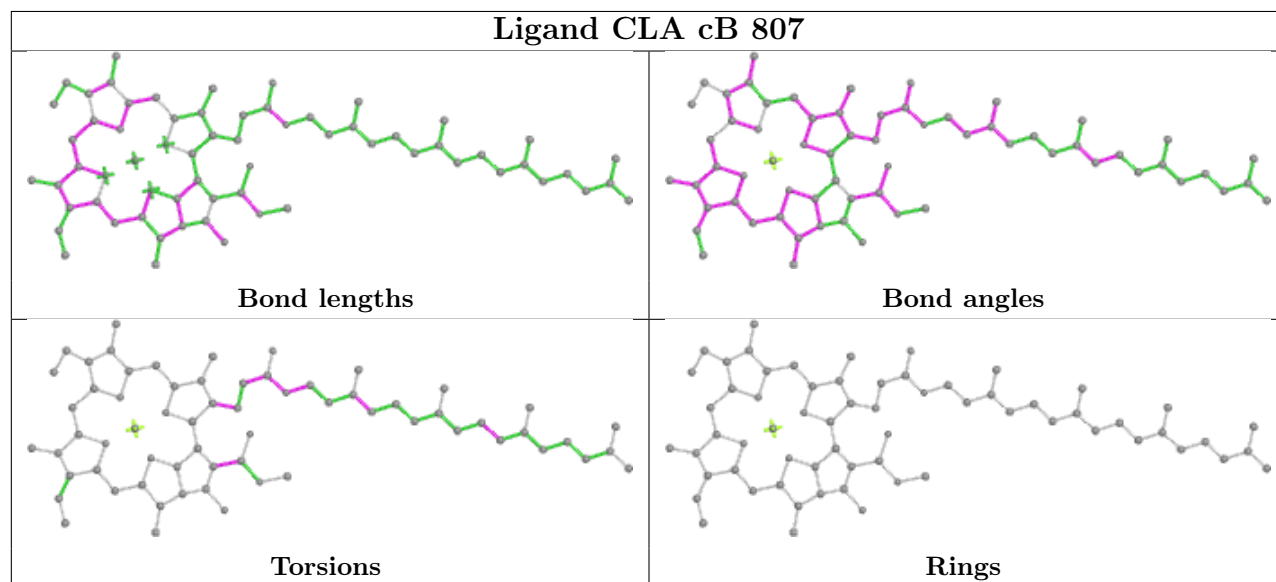


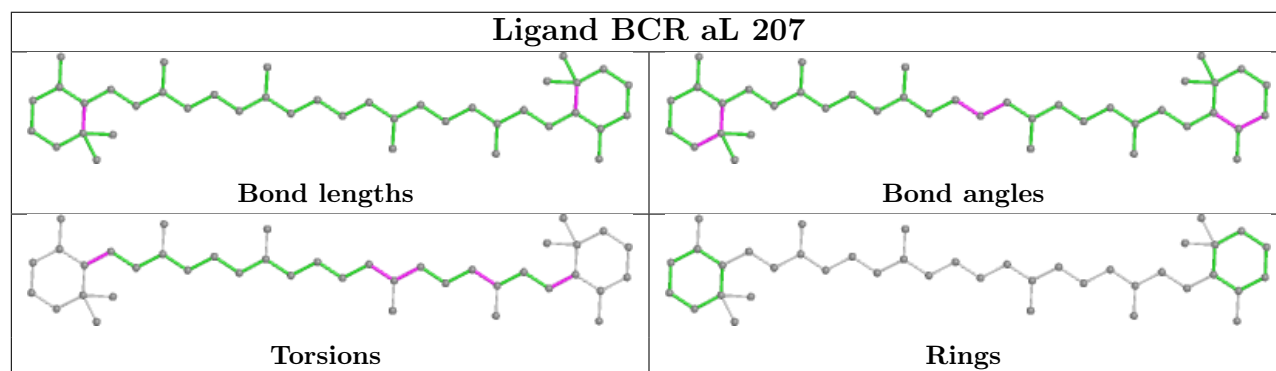
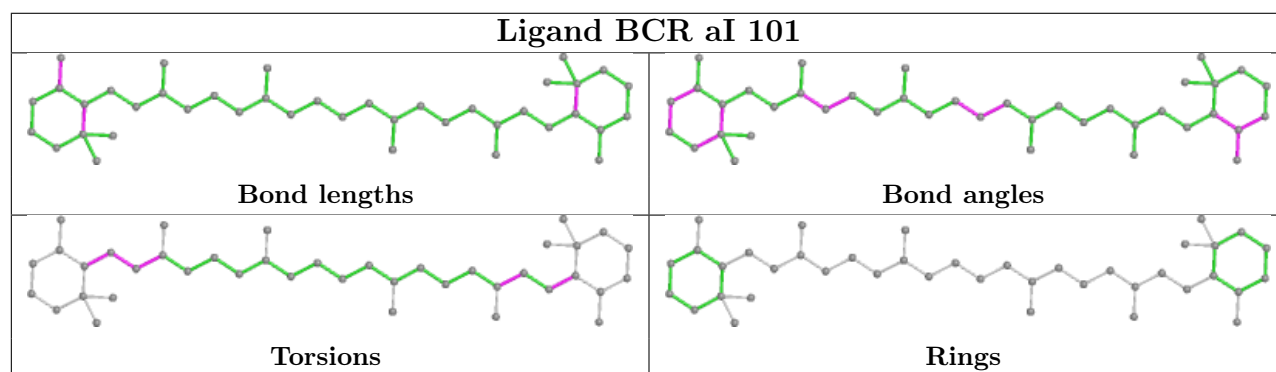
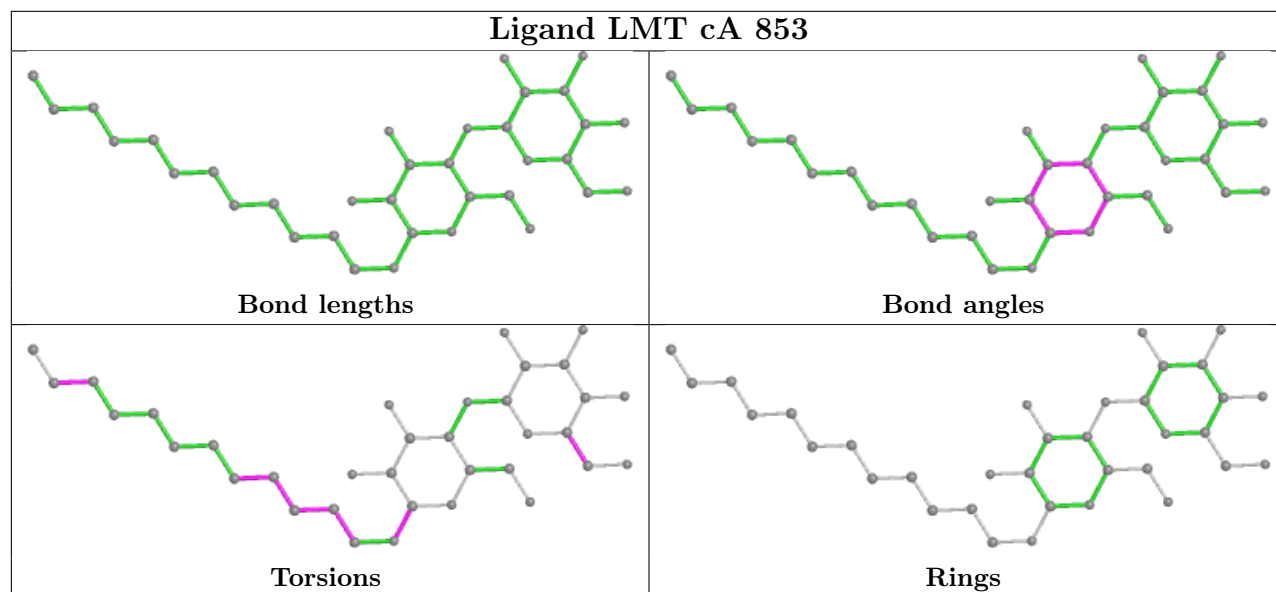
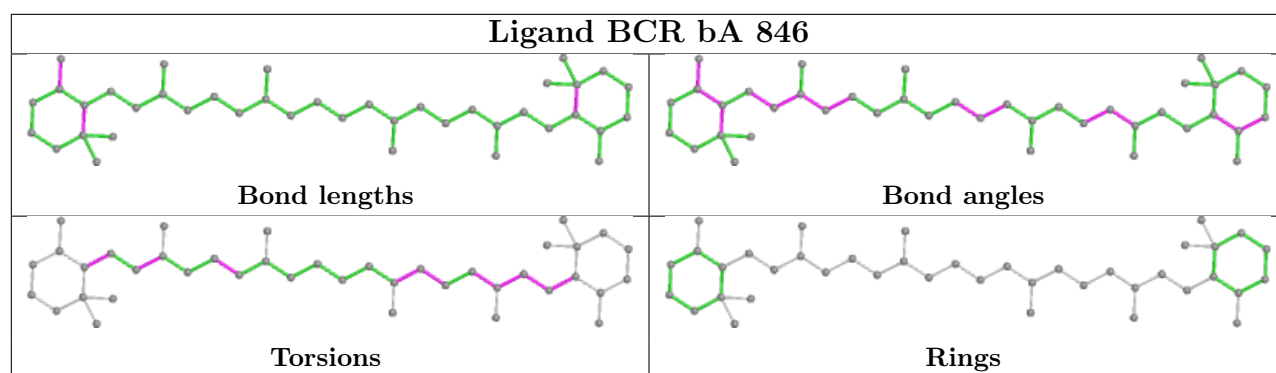
Ligand CLA aA 856

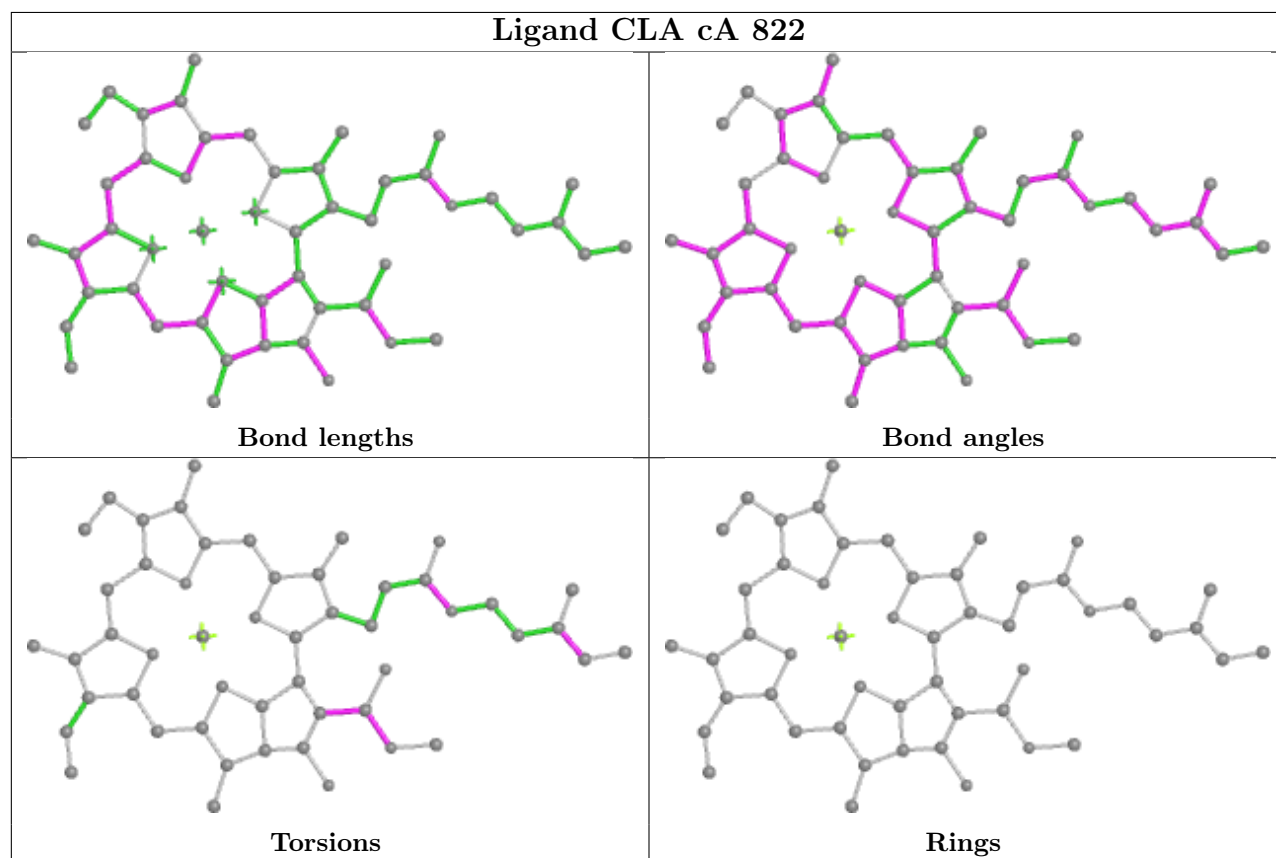
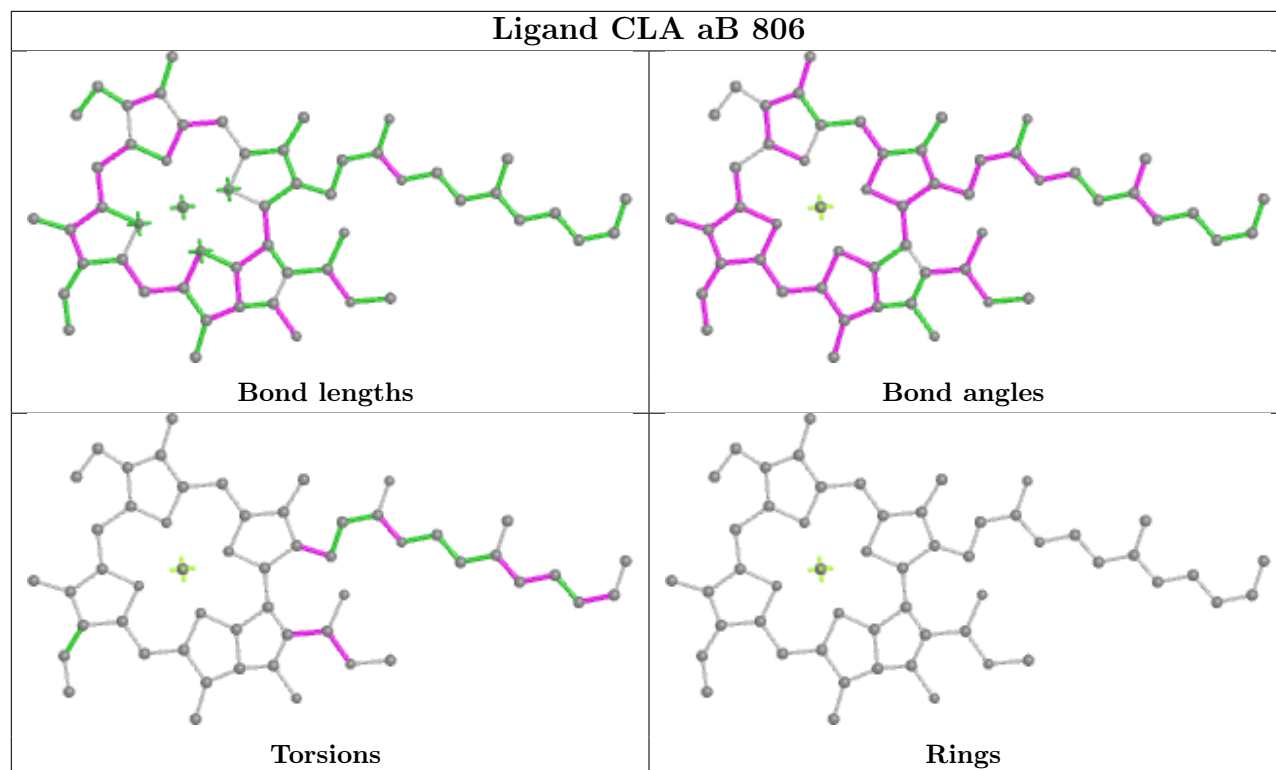


Ligand CL0 cA 801

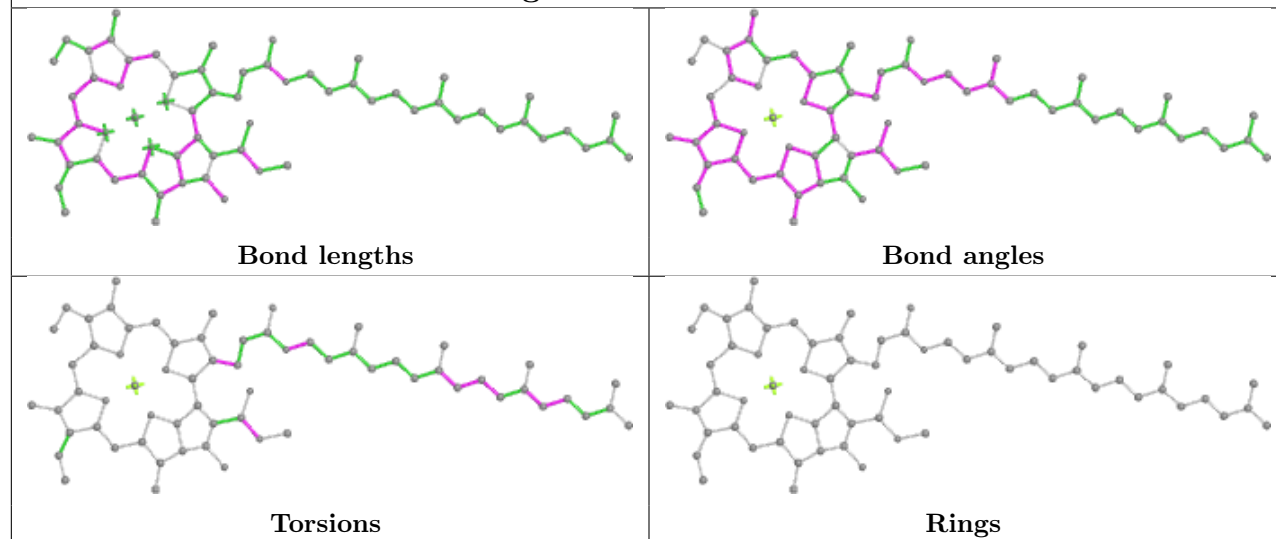


Ligand CLA aB 832**Ligand BCR aA 851****Ligand CLA cB 807**

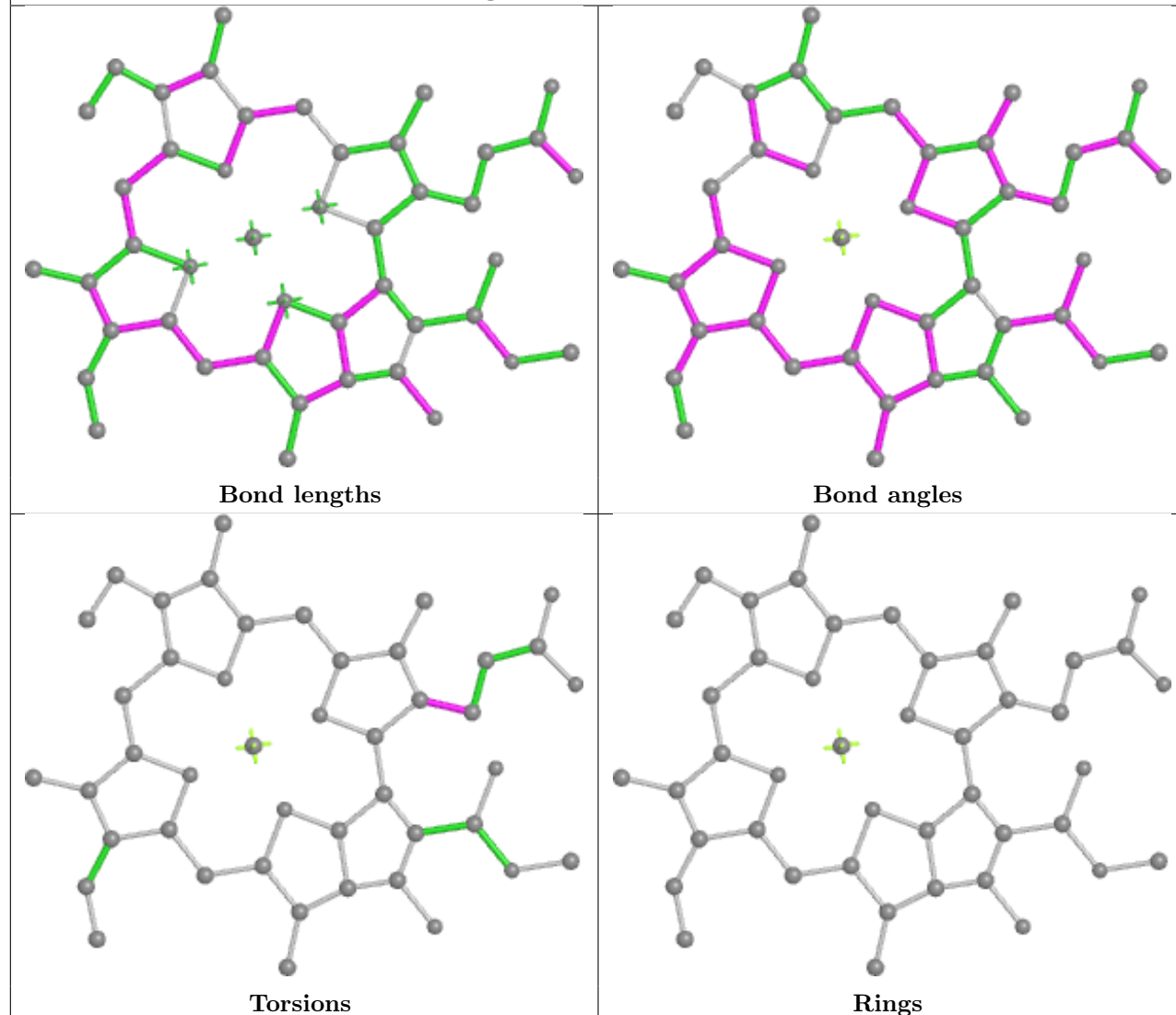


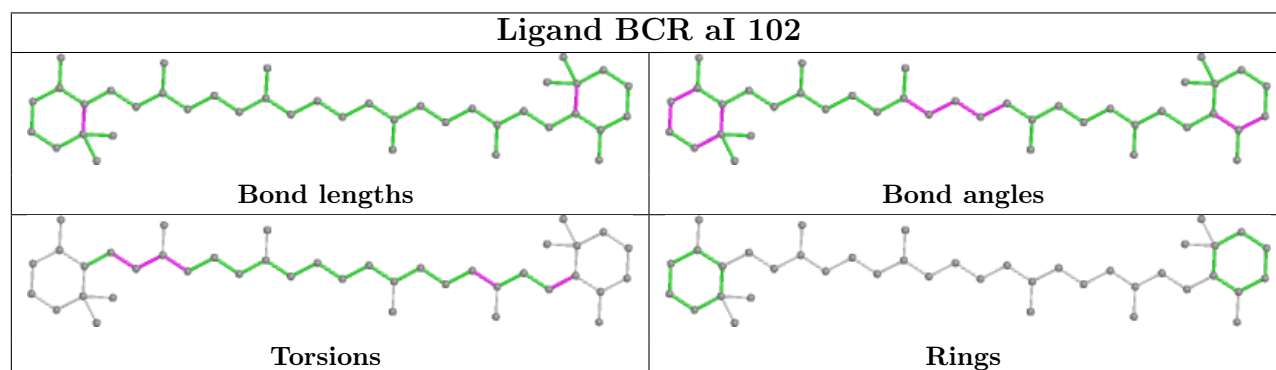
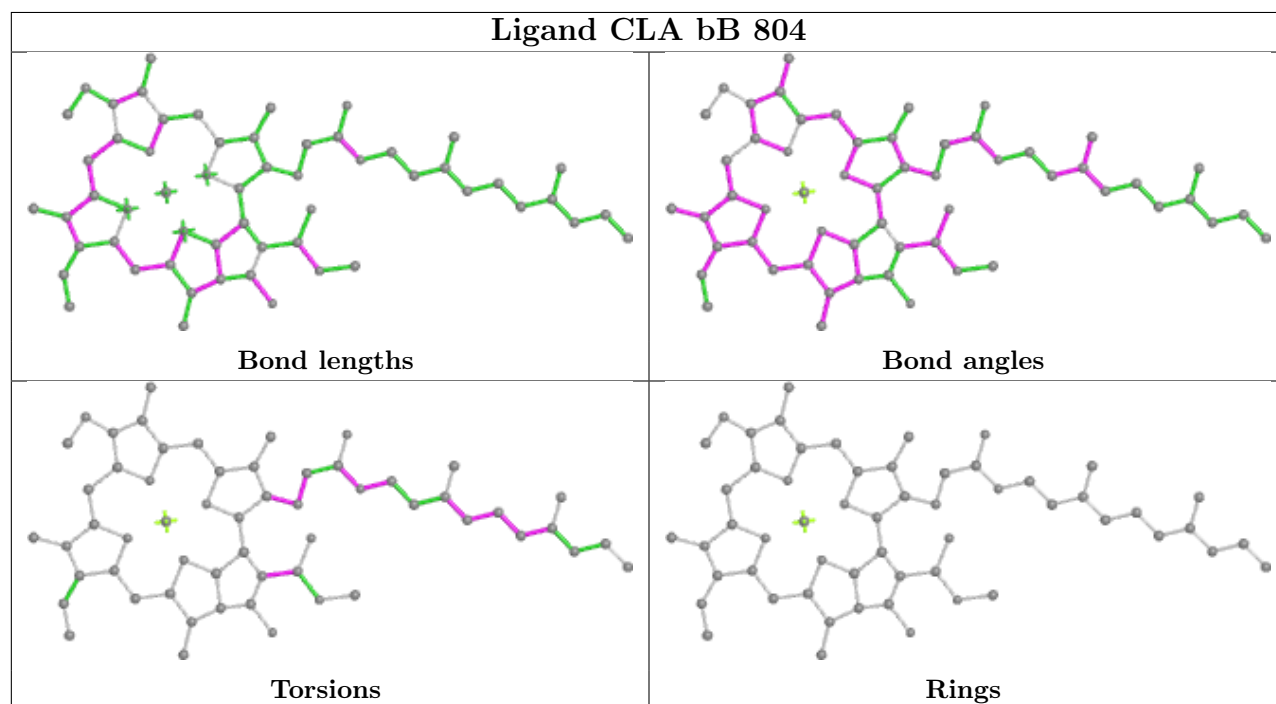
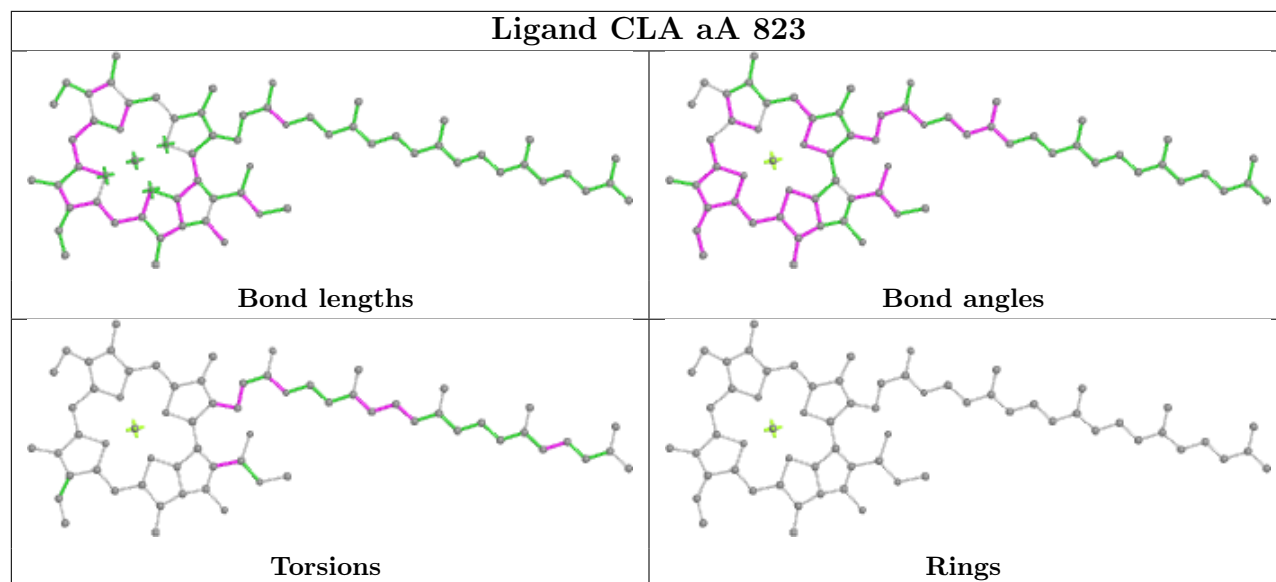


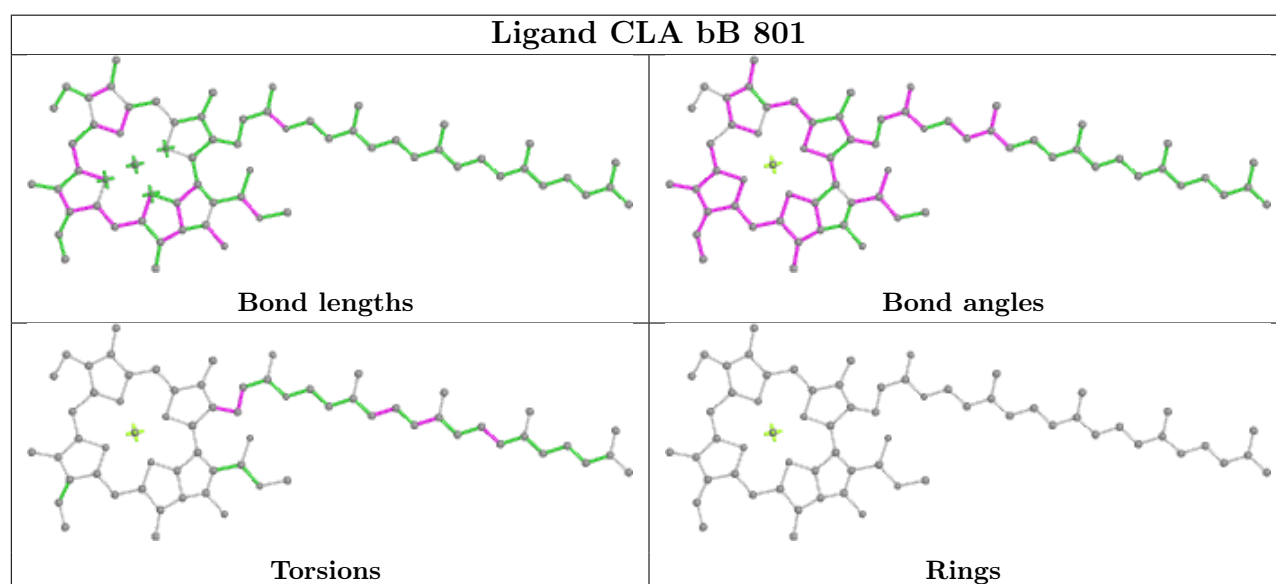
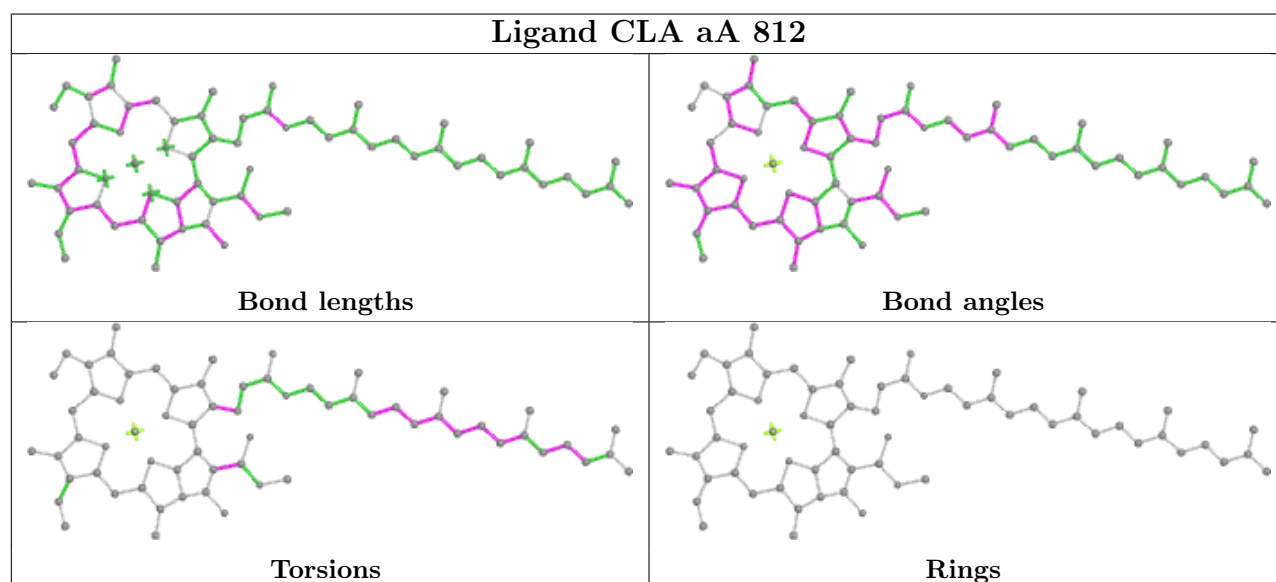
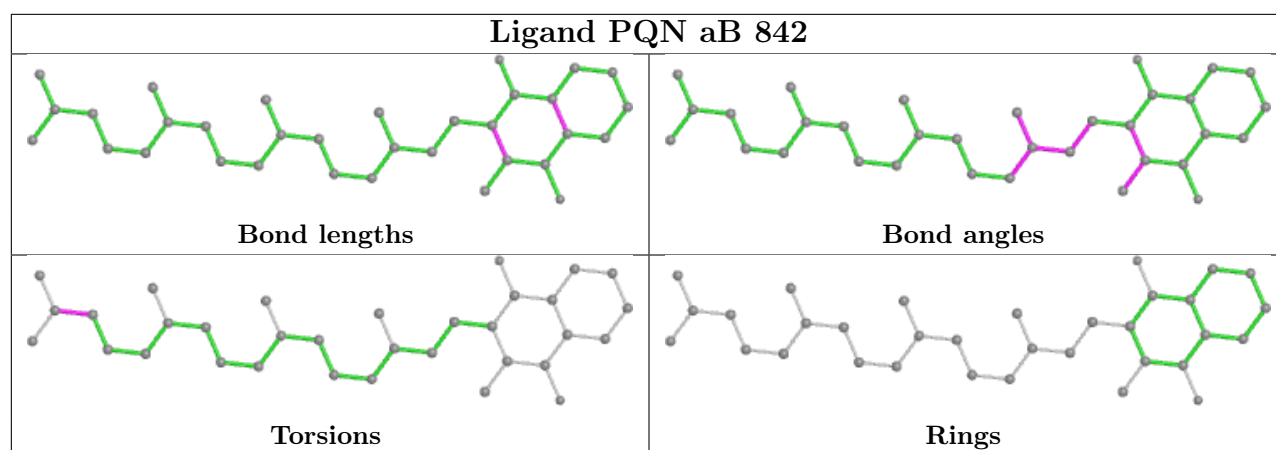
Ligand CLA bB 828



Ligand CLA aB 812







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.

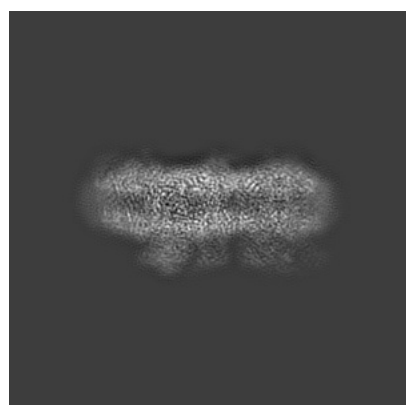
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0726. These allow visual inspection of the internal detail of the map and identification of artifacts.

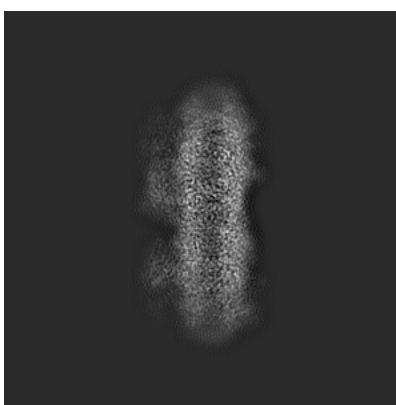
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

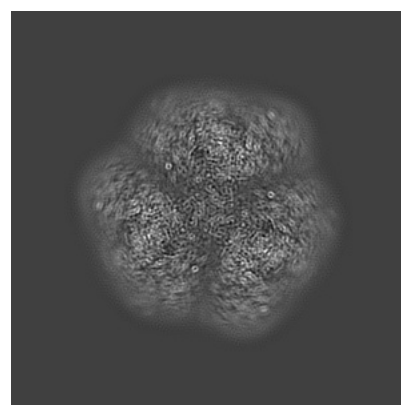
6.1.1 Primary map



X



Y

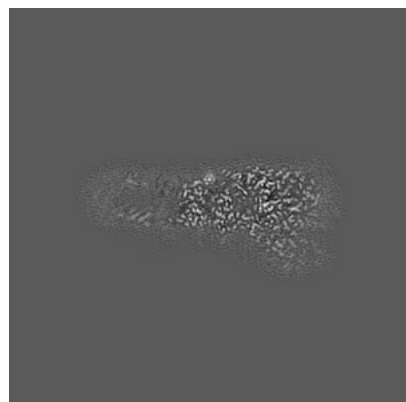


Z

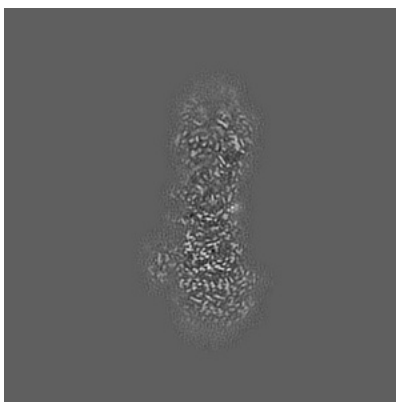
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

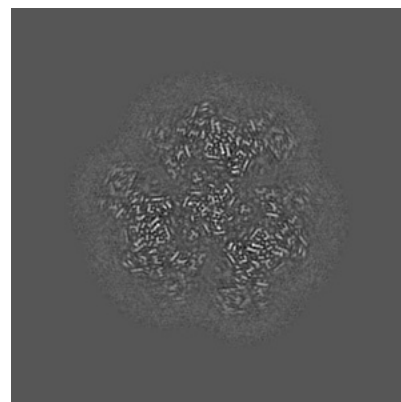
6.2.1 Primary map



X Index: 180



Y Index: 180

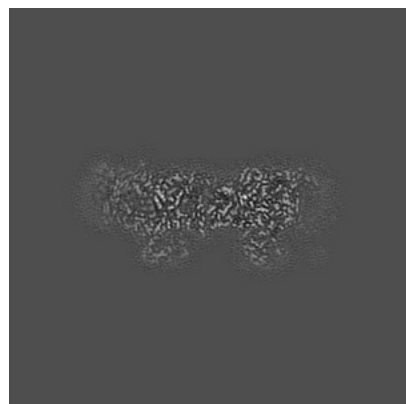


Z Index: 180

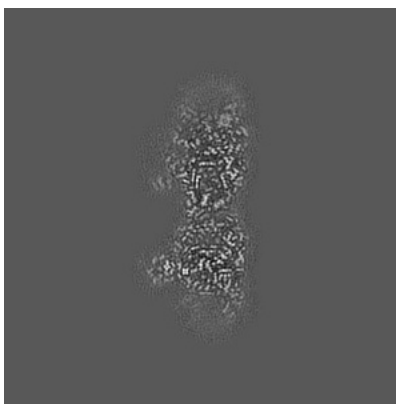
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

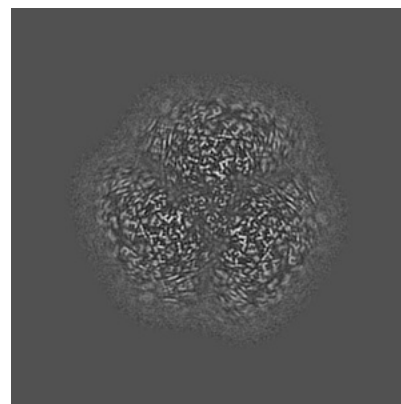
6.3.1 Primary map



X Index: 197



Y Index: 157

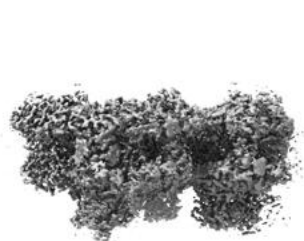


Z Index: 199

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

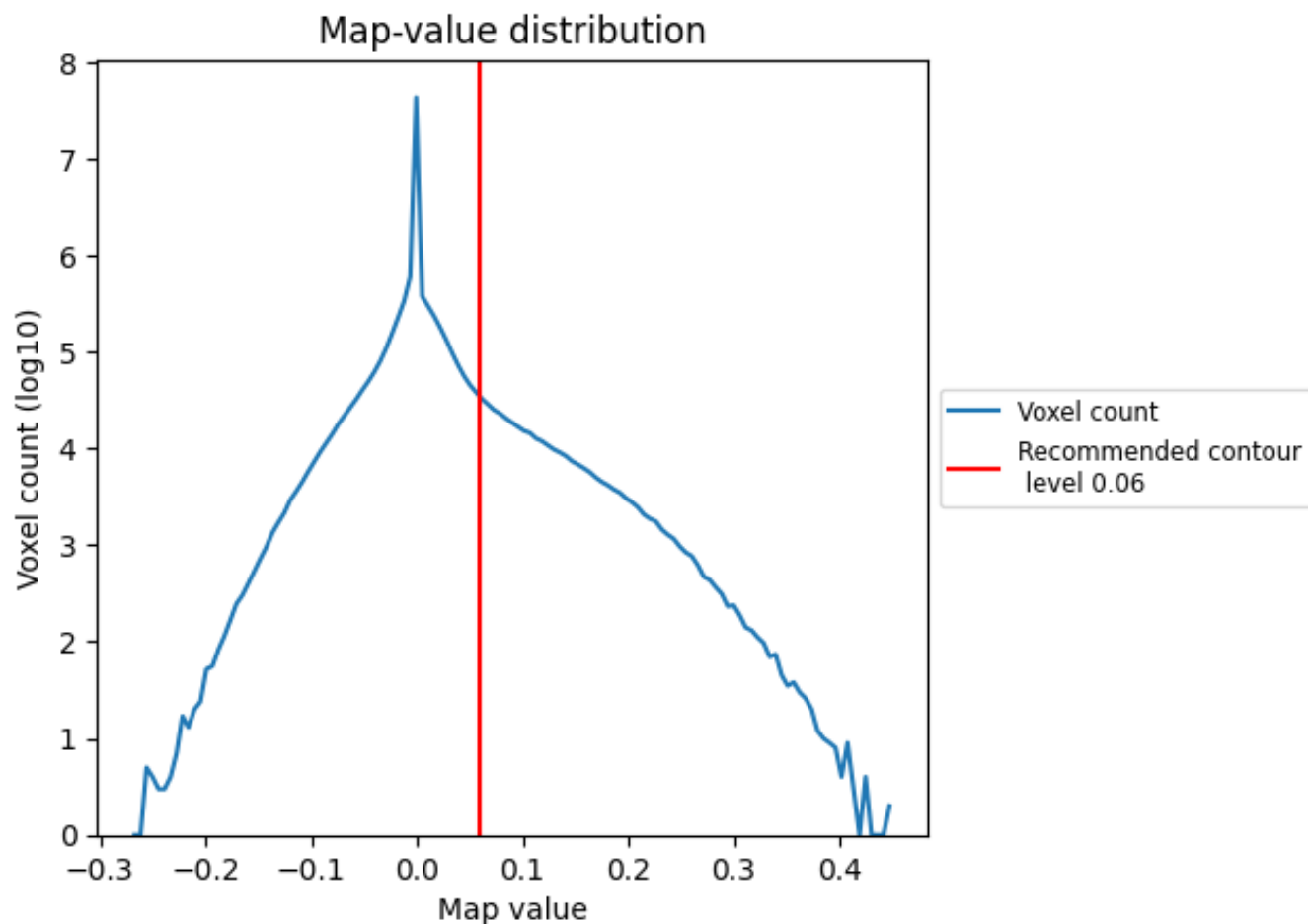
6.5 Mask visualisation

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

7 Map analysis [i](#)

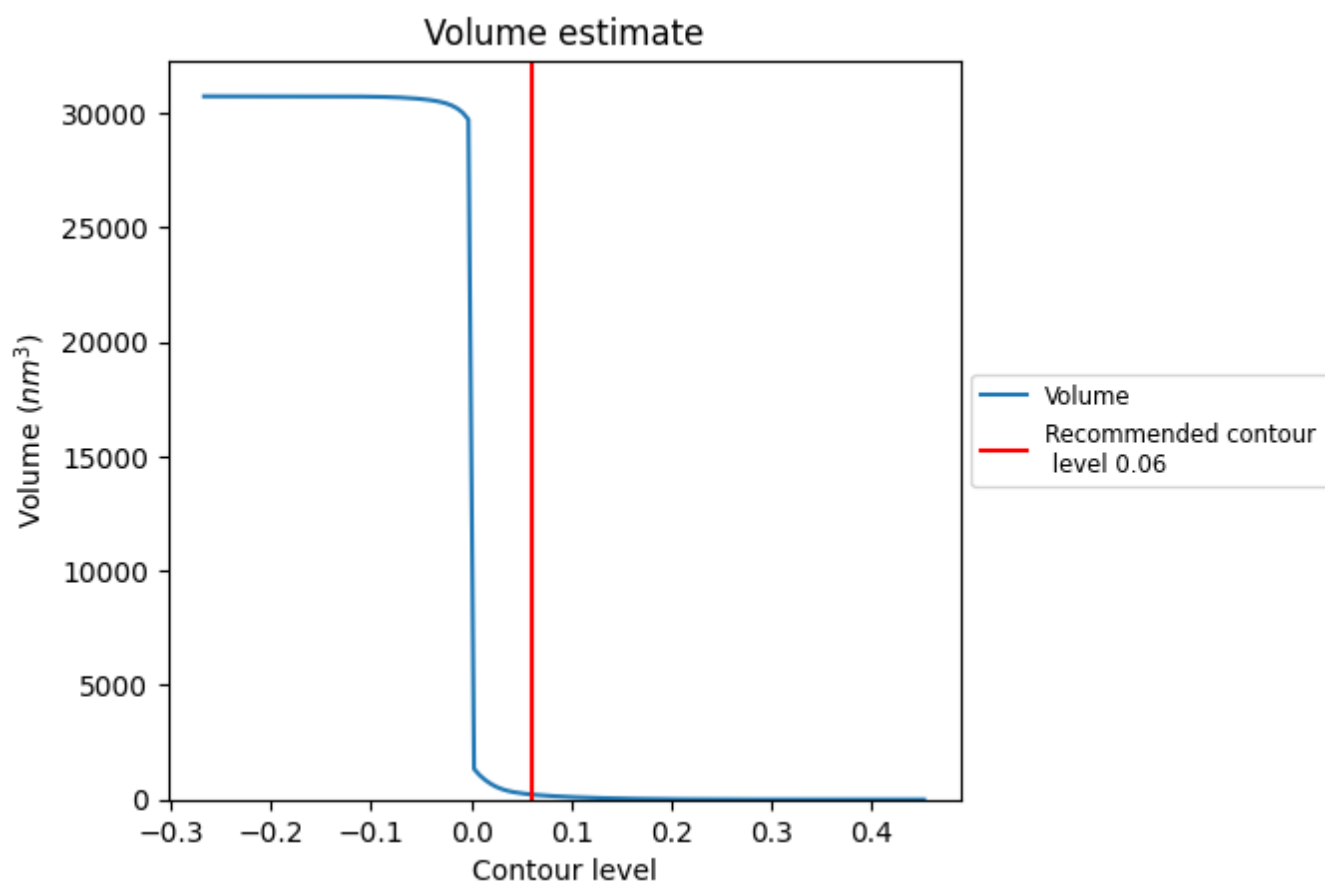
This section contains the results of statistical analysis of the map.

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.

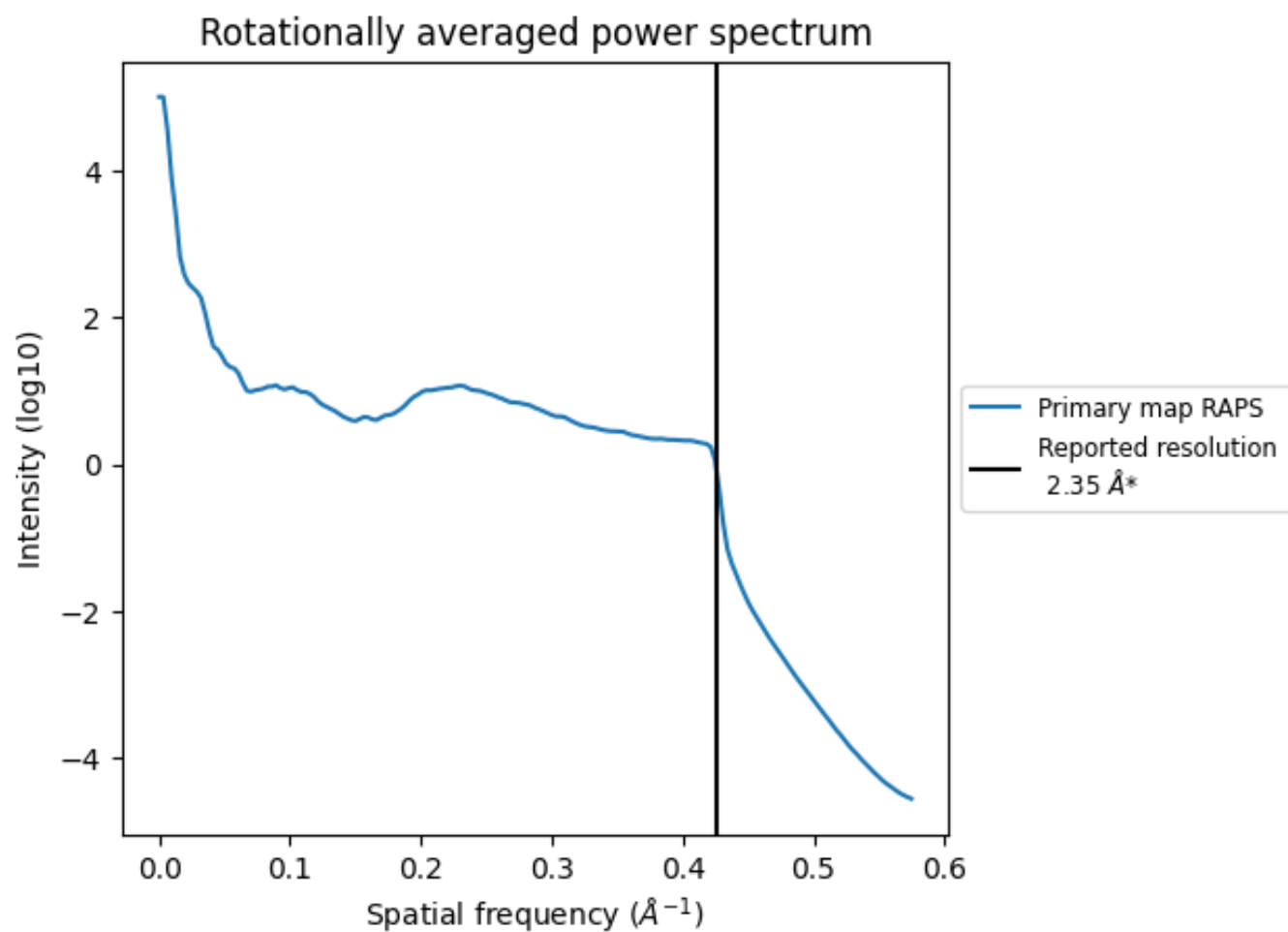
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 224 nm^3 ; this corresponds to an approximate mass of 202 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 ⓘ

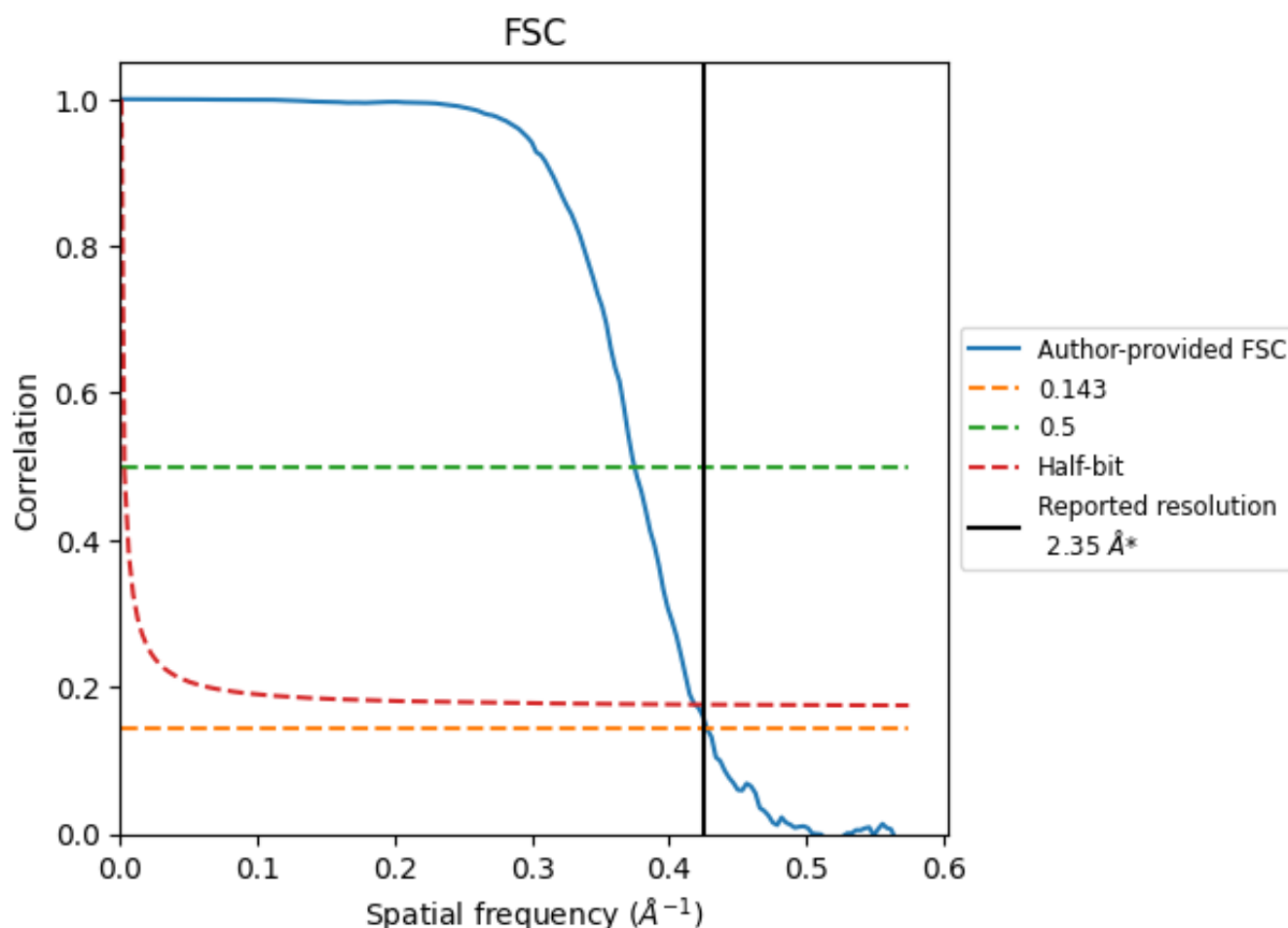


*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

8.2 Resolution estimates [i](#)

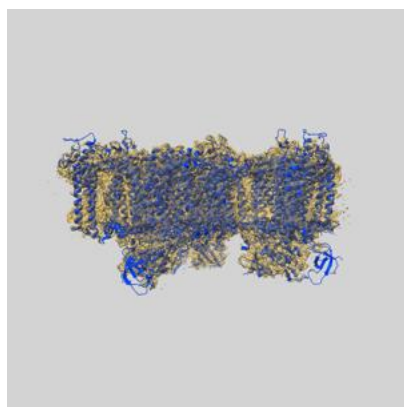
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.34	2.67	2.39
Unmasked-calculated*	-	-	-

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

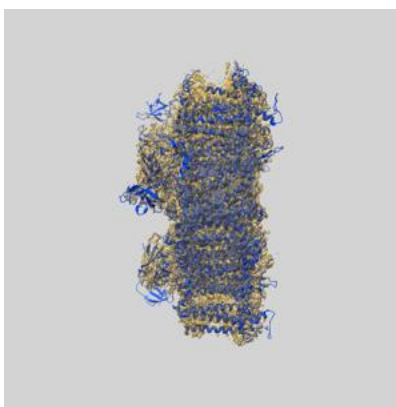
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0726 and PDB model 6KMW. Per-residue inclusion information can be found in section [3](#) on page [35](#).

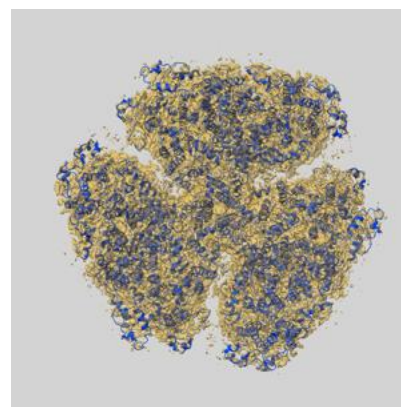
9.1 Map-model overlay [i](#)



X



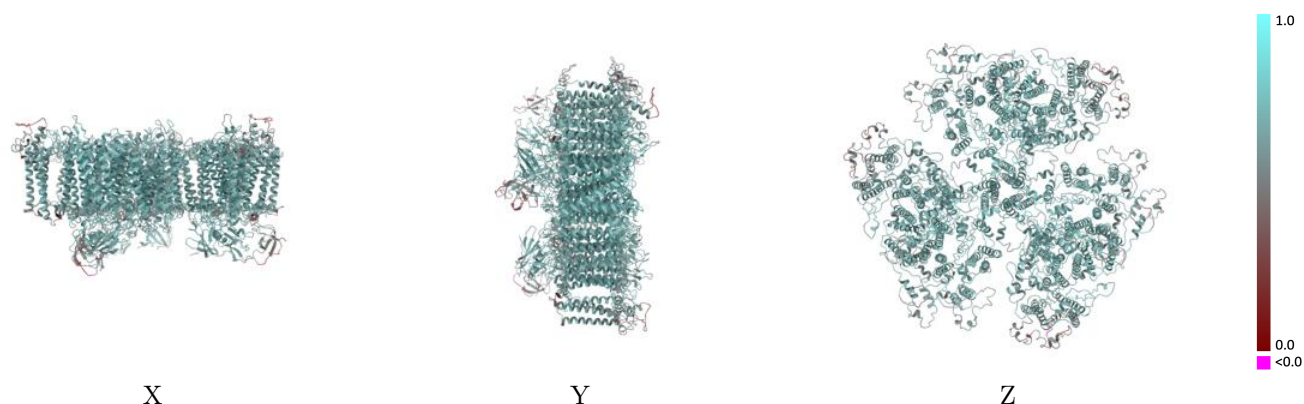
Y



Z

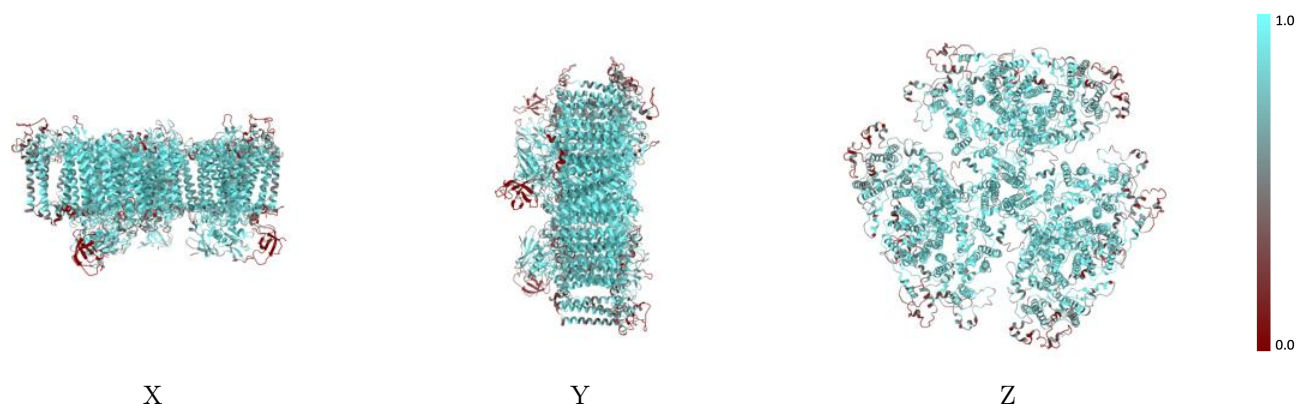
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



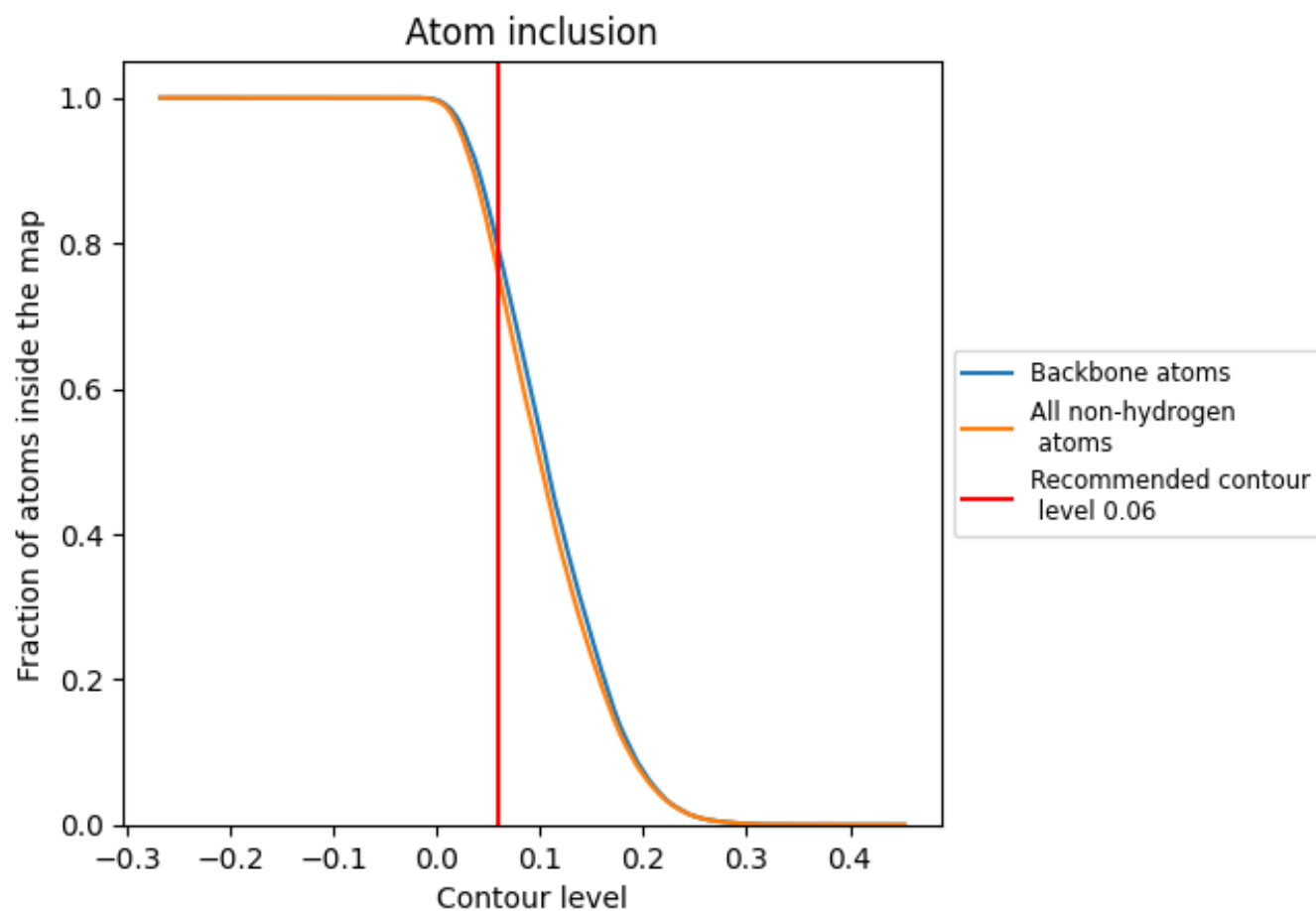
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 76% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7579	 0.6450
aA	 0.7318	 0.6360
aB	 0.7854	 0.6540
aC	 0.8211	 0.6660
aD	 0.7862	 0.6530
aE	 0.0998	 0.4610
aI	 0.9152	 0.7050
aL	 0.8676	 0.6930
aM	 0.8022	 0.6590
bA	 0.7317	 0.6370
bB	 0.7851	 0.6520
bC	 0.8261	 0.6650
bD	 0.7822	 0.6530
bE	 0.1164	 0.4620
bI	 0.9229	 0.7070
bL	 0.8655	 0.6920
bM	 0.7986	 0.6590
cA	 0.7301	 0.6350
cB	 0.7837	 0.6520
cC	 0.8294	 0.6620
cD	 0.7782	 0.6510
cE	 0.1081	 0.4530
cI	 0.9229	 0.7060
cL	 0.8676	 0.6920
cM	 0.8129	 0.6580

