



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 6, 2020 – 01:45 PM EST

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 PDB ID : 1JB0

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

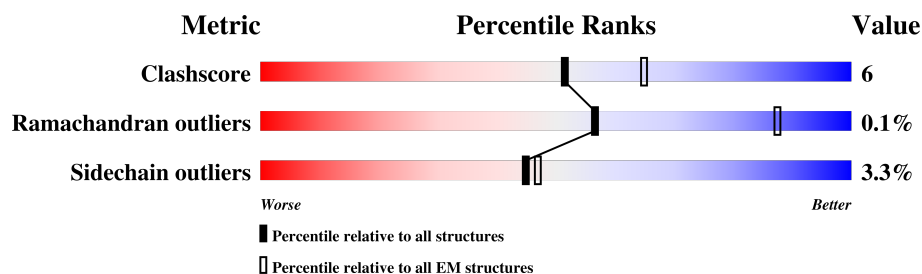
# 1 Overall quality at a glance

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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	aA	764	91% • 6%
1	bA	764	91% • 6%
1	cA	764	91% • 6%
2	aB	742	97% •
2	bB	742	97% •
2	cB	742	97% •
3	aC	81	98% ••
3	bC	81	98% ••
3	cC	81	98% ••

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Mol	Chain	Length	Quality of chain
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	-	-	-
10	CLA	aA	812	X	-	-	-
10	CLA	aA	813	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	aA	814	X	-	-	-
10	CLA	aA	815	X	-	-	-
10	CLA	aA	816	X	-	-	-
10	CLA	aA	817	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	854	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	aB	811	X	-	-	-
10	CLA	aB	812	X	-	-	-
10	CLA	aB	813	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	822	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	203	X	-	-	-
10	CLA	aL	204	X	-	-	-
10	CLA	aL	205	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
10	CLA	bA	814	X	-	-	-
10	CLA	bA	815	X	-	-	-
10	CLA	bA	816	X	-	-	-
10	CLA	bA	817	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	854	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	813	X	-	-	-
10	CLA	bB	814	X	-	-	-
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	822	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	203	X	-	-	-
10	CLA	bL	204	X	-	-	-
10	CLA	bL	205	X	-	-	-
10	CLA	cA	802	X	-	-	-
10	CLA	cA	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
10	CLA	cA	816	X	-	-	-
10	CLA	cA	817	X	-	-	-
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	854	X	-	-	-
10	CLA	cA	856	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	813	X	-	-	-
10	CLA	cB	814	X	-	-	-
10	CLA	cB	815	X	-	-	-
10	CLA	cB	816	X	-	-	-
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	822	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	cL	203	X	-	-	-
10	CLA	cL	204	X	-	-	-
10	CLA	cL	205	X	-	-	-
9	CL0	aA	801	X	-	-	-
9	CL0	bA	801	X	-	-	-
9	CL0	cA	801	X	-	-	-

## 2 Entry composition

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		

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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		

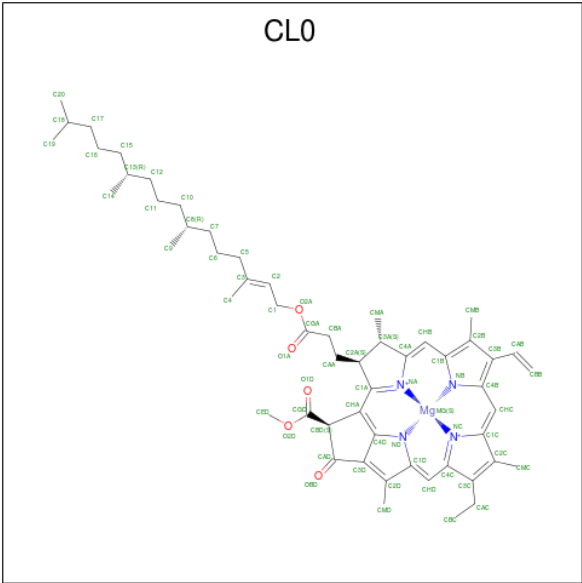
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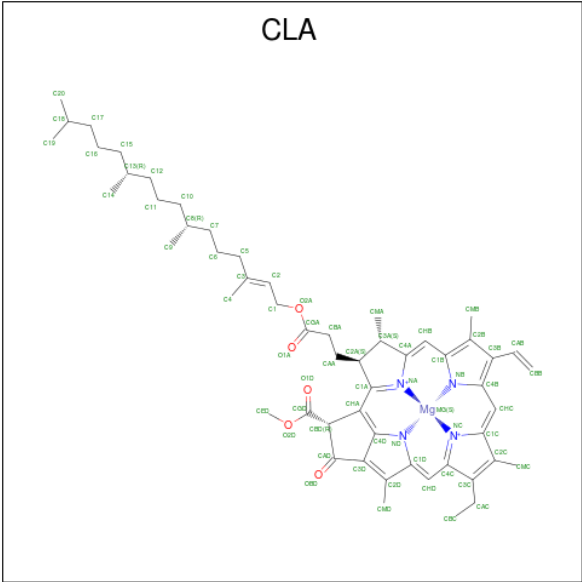
Mol	Chain	Residues	Atoms					AltConf	Trace
8	cM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		

- Molecule 9 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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	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	

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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	

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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	

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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	

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

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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	

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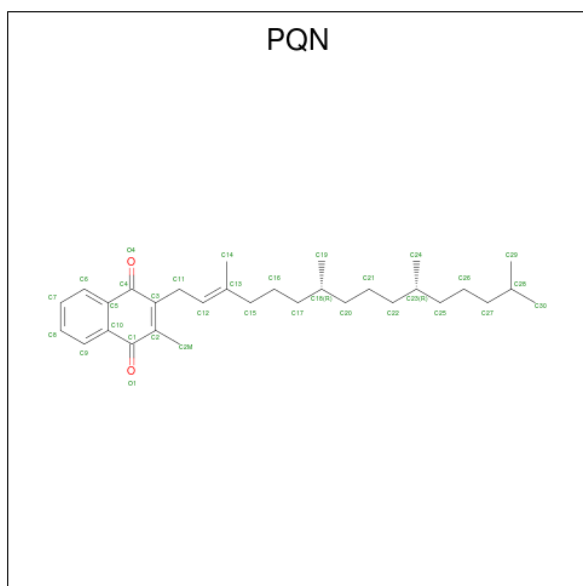
Mol	Chain	Residues	Atoms					AltConf
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total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

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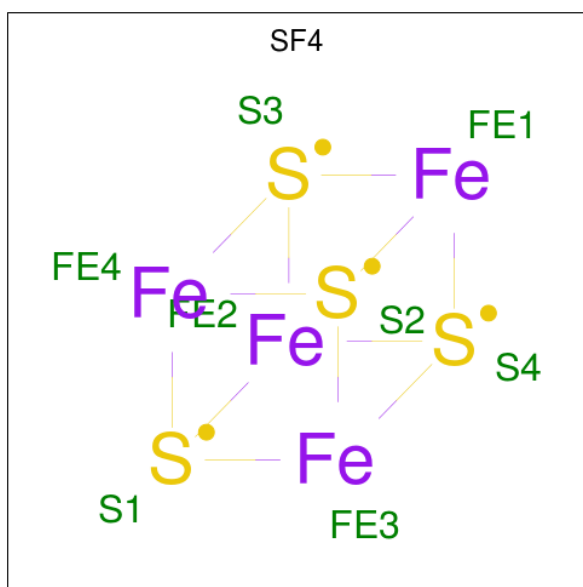
Mol	Chain	Residues	Atoms					AltConf
10	cL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	

- 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	

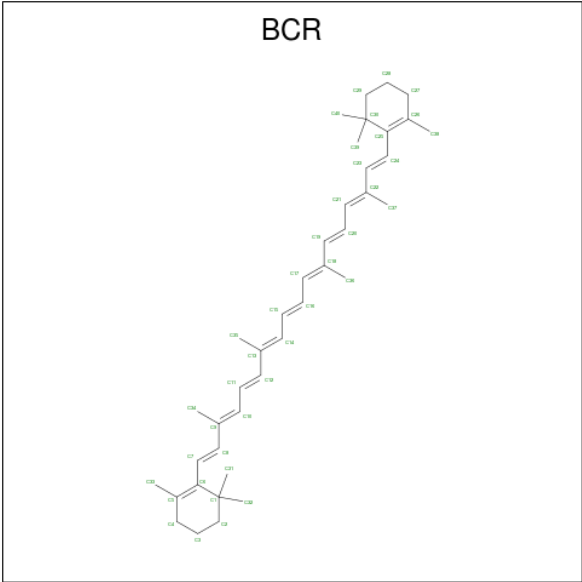
- Molecule 12 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



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:  $C_{40}H_{56}$ ).





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	

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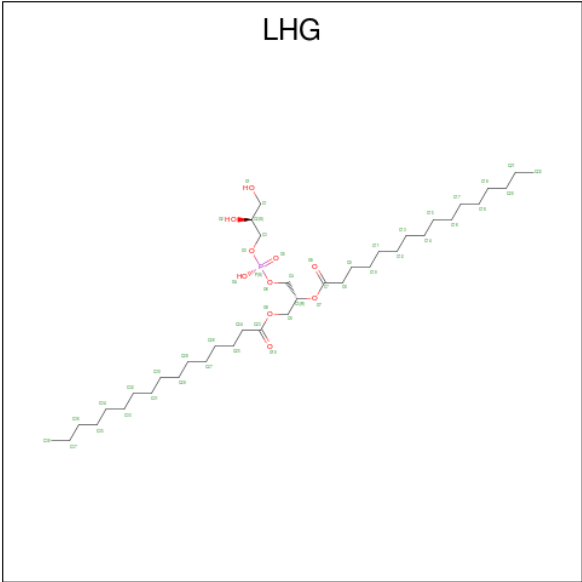
Mol	Chain	Residues	Atoms		AltConf
13	aL	1	Total 80	C 80	0
13	aL	1	Total 80	C 80	0
13	aM	1	Total 40	C 40	0
13	bA	1	Total 240	C 240	0
13	bA	1	Total 240	C 240	0
13	bA	1	Total 240	C 240	0
13	bA	1	Total 240	C 240	0
13	bA	1	Total 240	C 240	0
13	bA	1	Total 240	C 240	0
13	bB	1	Total 240	C 240	0
13	bB	1	Total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

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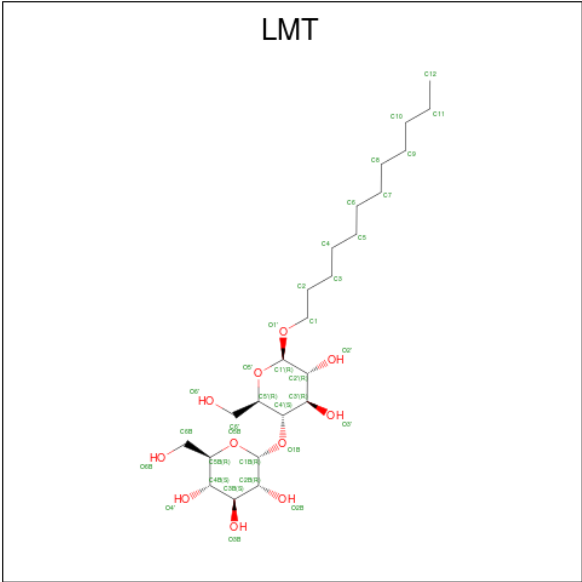
Mol	Chain	Residues	Atoms	AltConf
13	cA	1	Total C 240 240	0
13	cA	1	Total C 240 240	0
13	cA	1	Total C 240 240	0
13	cA	1	Total C 240 240	0
13	cA	1	Total C 240 240	0
13	cB	1	Total C 240 240	0
13	cB	1	Total C 240 240	0
13	cB	1	Total C 240 240	0
13	cB	1	Total C 240 240	0
13	cB	1	Total C 240 240	0
13	cB	1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

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



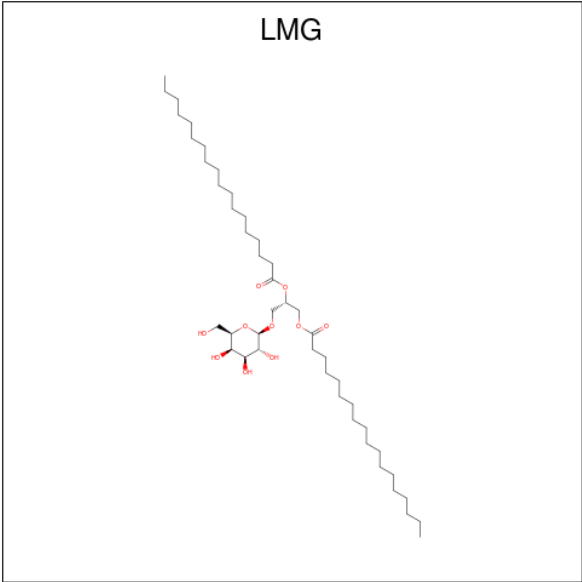
Mol	Chain	Residues	Atoms				AltConf
14	aA	1	Total	C	O	P	0
			76	54	20	2	
14	aA	1	Total	C	O	P	0
			76	54	20	2	
14	bA	1	Total	C	O	P	0
			76	54	20	2	
14	bA	1	Total	C	O	P	0
			76	54	20	2	
14	cA	1	Total	C	O	P	0
			76	54	20	2	
14	cA	1	Total	C	O	P	0
			76	54	20	2	

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



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

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



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	bL	4	Total	C	O	0
			56	52	4	
17	aL	4	Total	C	O	0
			56	52	4	
17	aI	1	Total	C		0
			9	9		
17	cI	1	Total	C		0
			9	9		
17	bI	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	bL	1	Total	Ca	0
			1	1	
18	aL	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	

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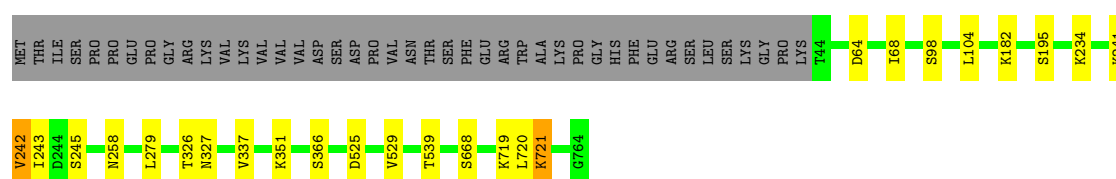
Mol	Chain	Residues	Atoms		AltConf
19	aD	12	Total 12	O 12	0
19	aI	1	Total 1	O 1	0
19	aL	30	Total 30	O 30	0
19	aM	1	Total 1	O 1	0
19	bA	63	Total 63	O 63	0
19	bB	85	Total 85	O 85	0
19	bC	17	Total 17	O 17	0
19	bD	12	Total 12	O 12	0
19	bI	1	Total 1	O 1	0
19	bL	30	Total 30	O 30	0
19	bM	1	Total 1	O 1	0
19	cA	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

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

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

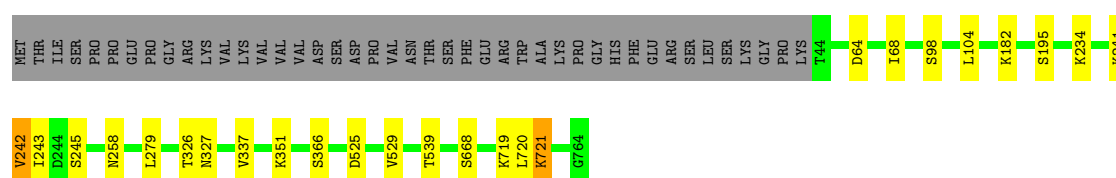
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain aA:  91% 6%



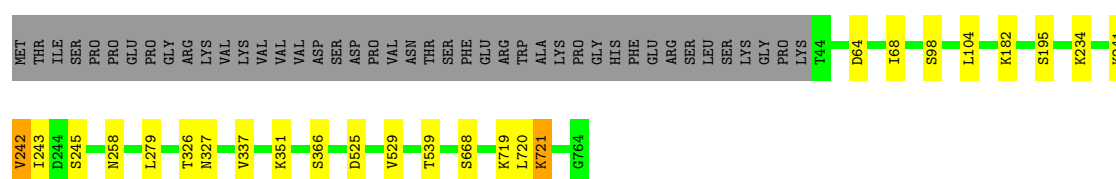
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain bA:  91% 6%



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain cA:  91% 6%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain aB:  97%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain bB:  97%





- Molecule 5: Photosystem I reaction center subunit IV

Chain aE:  84% 6% 10%




- Molecule 5: Photosystem I reaction center subunit IV

Chain bE:  84% 6% 10%



- Molecule 5: Photosystem I reaction center subunit IV

Chain cE:  84% 6% 10%



- Molecule 6: Photosystem I reaction center subunit VIII

Chain aI:  97% .



- Molecule 6: Photosystem I reaction center subunit VIII

Chain bI:  97% .




- Molecule 6: Photosystem I reaction center subunit VIII

Chain cI:  97% .



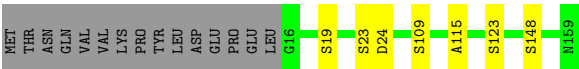
- Molecule 7: Photosystem I reaction center subunit XI

Chain aL:  86% . 9%

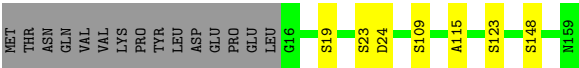
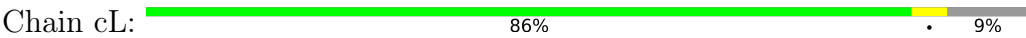


- Molecule 7: Photosystem I reaction center subunit XI

Chain bL:  86% . 9%



• Molecule 7: Photosystem I reaction center subunit XI



• Molecule 8: Photosystem I reaction center subunit XII



• Molecule 8: Photosystem I reaction center subunit XII



• Molecule 8: Photosystem I reaction center subunit XII



## 4 Experimental information

Property	Value	Source
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	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
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

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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

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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

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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%)	53	65
1	bA	719/764 (94%)	691 (96%)	27 (4%)	1 (0%)	53	65
1	cA	719/764 (94%)	691 (96%)	27 (4%)	1 (0%)	53	65
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%)	24	25
7	bL	142/159 (89%)	138 (97%)	3 (2%)	1 (1%)	24	25
7	cL	142/159 (89%)	138 (97%)	3 (2%)	1 (1%)	24	25

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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%)	56	65

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%)	37	45
1	bA	574/614 (94%)	553 (96%)	21 (4%)	37	45
1	cA	574/614 (94%)	553 (96%)	21 (4%)	37	45
2	aB	597/598 (100%)	581 (97%)	16 (3%)	48	58
2	bB	597/598 (100%)	581 (97%)	16 (3%)	48	58
2	cB	597/598 (100%)	581 (97%)	16 (3%)	48	58
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%)	36	44
4	bD	80/115 (70%)	77 (96%)	3 (4%)	36	44
4	cD	80/115 (70%)	77 (96%)	3 (4%)	36	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	aE	54/61 (88%)	51 (94%)	3 (6%)	23	25
5	bE	54/61 (88%)	51 (94%)	3 (6%)	23	25
5	cE	54/61 (88%)	51 (94%)	3 (6%)	23	25
6	aI	32/32 (100%)	31 (97%)	1 (3%)	43	52
6	bI	32/32 (100%)	31 (97%)	1 (3%)	43	52
6	cI	32/32 (100%)	31 (97%)	1 (3%)	43	52
7	aL	108/123 (88%)	102 (94%)	6 (6%)	23	25
7	bL	108/123 (88%)	102 (94%)	6 (6%)	23	25
7	cL	108/123 (88%)	102 (94%)	6 (6%)	23	25
8	aM	27/27 (100%)	26 (96%)	1 (4%)	37	45
8	bM	27/27 (100%)	26 (96%)	1 (4%)	37	45
8	cM	27/27 (100%)	26 (96%)	1 (4%)	37	45
All	All	4620/4917 (94%)	4467 (97%)	153 (3%)	45	50

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

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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

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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

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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

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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

Some 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

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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 carbohydrates 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	$\# Z  > 2$
9	CL0	aA	801	1	57,73,73	1.86	12 (21%)	66,113,113	2.29	25 (37%)
10	CLA	aA	802	1	34,53,73	2.45	12 (35%)	37,89,113	2.63	18 (48%)
10	CLA	aA	803	1	34,53,73	2.48	13 (38%)	37,89,113	2.68	19 (51%)
10	CLA	aA	804	1	57,73,73	1.89	13 (22%)	66,113,113	2.16	20 (30%)
10	CLA	aA	805	1	57,73,73	1.94	13 (22%)	66,113,113	2.26	24 (36%)
10	CLA	aA	806	1	43,59,73	2.24	13 (30%)	49,96,113	2.38	22 (44%)
10	CLA	aA	807	1	34,53,73	2.39	13 (38%)	37,89,113	2.64	19 (51%)
10	CLA	aA	808	1	34,53,73	2.38	12 (35%)	37,89,113	2.56	15 (40%)
10	CLA	aA	809	1	34,53,73	2.41	11 (32%)	37,89,113	2.62	17 (45%)
10	CLA	aA	810	1	57,73,73	1.98	13 (22%)	66,113,113	2.13	21 (31%)
10	CLA	aA	811	1	46,62,73	2.17	13 (28%)	52,99,113	2.28	21 (40%)
10	CLA	aA	812	1	57,73,73	1.96	13 (22%)	66,113,113	2.14	22 (33%)
10	CLA	aA	813	1	34,53,73	2.46	12 (35%)	37,89,113	2.58	17 (45%)
10	CLA	aA	814	1	34,53,73	2.42	12 (35%)	37,89,113	2.58	17 (45%)
10	CLA	aA	815	-	41,57,73	2.32	13 (31%)	46,93,113	2.36	18 (39%)
10	CLA	aA	816	1	46,62,73	2.15	13 (28%)	52,99,113	2.38	22 (42%)
10	CLA	aA	817	1	46,62,73	2.16	12 (26%)	52,99,113	2.28	22 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	aA	818	1	57,73,73	1.98	11 (19%)	66,113,113	2.37	22 (33%)
10	CLA	aA	819	1	53,69,73	2.06	13 (24%)	61,108,113	2.15	20 (32%)
10	CLA	aA	820	-	57,73,73	1.96	12 (21%)	66,113,113	2.00	21 (31%)
10	CLA	aA	821	1	41,57,73	2.33	12 (29%)	46,93,113	2.53	20 (43%)
10	CLA	aA	822	1	43,59,73	2.27	12 (27%)	49,96,113	2.50	21 (42%)
10	CLA	aA	823	1	57,73,73	1.92	14 (24%)	66,113,113	2.05	19 (28%)
10	CLA	aA	824	-	57,73,73	1.90	13 (22%)	66,113,113	2.15	18 (27%)
10	CLA	aA	825	-	47,63,73	2.08	12 (25%)	54,101,113	2.35	21 (38%)
10	CLA	aA	826	1	57,73,73	1.90	12 (21%)	66,113,113	2.08	21 (31%)
10	CLA	aA	827	1	57,73,73	1.96	14 (24%)	66,113,113	2.19	22 (33%)
10	CLA	aA	828	1	57,73,73	1.93	12 (21%)	66,113,113	2.17	22 (33%)
10	CLA	aA	829	1	57,73,73	1.94	13 (22%)	66,113,113	2.26	21 (31%)
10	CLA	aA	830	1	42,58,73	2.21	13 (30%)	48,95,113	2.40	21 (43%)
10	CLA	aA	831	1	57,73,73	1.93	12 (21%)	66,113,113	2.09	19 (28%)
10	CLA	aA	832	1	57,73,73	1.88	13 (22%)	66,113,113	2.11	23 (34%)
10	CLA	aA	833	1	57,73,73	1.88	12 (21%)	66,113,113	2.20	21 (31%)
10	CLA	aA	834	1	46,62,73	2.13	12 (26%)	52,99,113	2.34	23 (44%)
10	CLA	aA	835	1	57,73,73	1.94	13 (22%)	66,113,113	2.10	22 (33%)
10	CLA	aA	836	1	43,59,73	2.16	13 (30%)	49,96,113	6.08	25 (51%)
10	CLA	aA	837	1	57,73,73	1.85	13 (22%)	66,113,113	2.12	21 (31%)
10	CLA	aA	838	1	42,58,73	2.18	14 (33%)	48,95,113	2.79	24 (50%)
10	CLA	aA	839	1	57,73,73	1.96	13 (22%)	66,113,113	2.06	20 (30%)
10	CLA	aA	840	-	43,59,73	2.32	13 (30%)	49,96,113	2.48	21 (42%)
10	CLA	aA	841	-	57,73,73	1.95	13 (22%)	66,113,113	2.11	20 (30%)
10	CLA	aA	842	-	57,73,73	1.86	13 (22%)	66,113,113	2.11	23 (34%)
10	CLA	aA	843	-	30,49,73	2.45	11 (36%)	31,83,113	2.58	15 (48%)
11	PQN	aA	844	-	34,34,34	1.36	2 (5%)	42,45,45	1.17	4 (9%)
12	SF4	aA	845	1,2	0,12,12	0.00	-	-	-	-
13	BCR	aA	846	-	41,41,41	1.10	3 (7%)	56,56,56	1.23	5 (8%)
13	BCR	aA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.28	5 (8%)
13	BCR	aA	848	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	7 (12%)
13	BCR	aA	849	-	41,41,41	1.10	3 (7%)	56,56,56	1.26	7 (12%)
13	BCR	aA	850	-	41,41,41	1.12	2 (4%)	56,56,56	1.18	5 (8%)
13	BCR	aA	851	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	3 (5%)
14	LHG	aA	852	-	48,48,48	0.66	1 (2%)	51,54,54	1.22	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	LMT	aA	853	-	36,36,36	0.45	0	47,47,47	0.90	3 (6%)
10	CLA	aA	854	-	44,60,73	2.22	13 (29%)	50,97,113	2.41	20 (40%)
14	LHG	aA	855	-	26,26,48	0.82	0	29,32,54	1.32	3 (10%)
10	CLA	aA	856	2	41,57,73	2.34	13 (31%)	46,93,113	2.31	18 (39%)
10	CLA	aB	801	-	57,73,73	1.87	13 (22%)	66,113,113	2.37	23 (34%)
10	CLA	aB	802	-	57,73,73	1.93	12 (21%)	66,113,113	2.08	20 (30%)
10	CLA	aB	803	2	57,73,73	1.87	13 (22%)	66,113,113	2.20	23 (34%)
10	CLA	aB	804	-	49,65,73	2.07	12 (24%)	56,103,113	2.57	23 (41%)
10	CLA	aB	805	-	57,73,73	1.89	14 (24%)	66,113,113	1.89	16 (24%)
10	CLA	aB	806	2	46,62,73	2.16	13 (28%)	52,99,113	2.42	25 (48%)
10	CLA	aB	807	2	57,73,73	1.89	14 (24%)	66,113,113	2.22	24 (36%)
10	CLA	aB	808	2	57,73,73	1.88	13 (22%)	66,113,113	2.10	21 (31%)
10	CLA	aB	809	2	57,73,73	1.90	14 (24%)	66,113,113	2.15	20 (30%)
10	CLA	aB	810	2	47,63,73	2.02	12 (25%)	54,101,113	2.47	23 (42%)
10	CLA	aB	811	2	57,73,73	1.84	13 (22%)	66,113,113	2.22	19 (28%)
10	CLA	aB	812	2	34,53,73	2.35	11 (32%)	37,89,113	2.63	16 (43%)
10	CLA	aB	813	2	34,53,73	2.46	12 (35%)	37,89,113	2.55	16 (43%)
10	CLA	aB	814	2	57,73,73	1.94	14 (24%)	66,113,113	2.20	21 (31%)
10	CLA	aB	815	2	48,64,73	2.12	13 (27%)	55,102,113	2.27	21 (38%)
10	CLA	aB	816	2	34,53,73	2.38	12 (35%)	37,89,113	2.69	19 (51%)
10	CLA	aB	817	2	47,63,73	2.13	14 (29%)	54,101,113	2.24	21 (38%)
10	CLA	aB	818	2	51,67,73	2.09	14 (27%)	58,105,113	2.24	21 (36%)
10	CLA	aB	819	2	52,68,73	1.98	12 (23%)	60,107,113	2.41	24 (40%)
10	CLA	aB	820	-	57,73,73	1.97	13 (22%)	66,113,113	2.04	22 (33%)
10	CLA	aB	821	2	39,55,73	2.38	13 (33%)	44,91,113	2.44	20 (45%)
10	CLA	aB	822	2	34,53,73	2.47	12 (35%)	37,89,113	2.66	16 (43%)
10	CLA	aB	823	2	47,63,73	2.20	13 (27%)	54,101,113	2.26	21 (38%)
10	CLA	aB	824	2	34,53,73	2.46	12 (35%)	37,89,113	2.59	18 (48%)
10	CLA	aB	825	2	46,62,73	2.17	13 (28%)	52,99,113	2.49	22 (42%)
10	CLA	aB	826	-	57,73,73	1.98	13 (22%)	66,113,113	2.27	24 (36%)
10	CLA	aB	827	2	57,73,73	1.92	13 (22%)	66,113,113	2.21	21 (31%)
10	CLA	aB	828	2	57,73,73	1.89	12 (21%)	66,113,113	2.20	21 (31%)
10	CLA	aB	829	2	57,73,73	1.93	12 (21%)	66,113,113	2.08	19 (28%)
10	CLA	aB	830	2	57,73,73	1.92	13 (22%)	66,113,113	2.20	22 (33%)
10	CLA	aB	831	2	34,53,73	2.41	12 (35%)	37,89,113	2.59	19 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	aB	832	2	57,73,73	1.95	14 (24%)	66,113,113	2.11	22 (33%)
10	CLA	aB	833	2	50,66,73	2.10	13 (26%)	57,104,113	2.25	22 (38%)
10	CLA	aB	834	2	34,53,73	2.41	12 (35%)	37,89,113	2.59	20 (54%)
10	CLA	aB	835	-	34,53,73	2.42	12 (35%)	37,89,113	2.50	18 (48%)
10	CLA	aB	836	-	34,53,73	2.46	12 (35%)	37,89,113	2.61	18 (48%)
10	CLA	aB	837	2	52,68,73	2.00	14 (26%)	60,107,113	2.31	21 (35%)
10	CLA	aB	838	2	57,73,73	1.93	12 (21%)	66,113,113	2.12	22 (33%)
10	CLA	aB	839	2	39,55,73	2.30	13 (33%)	44,91,113	2.50	19 (43%)
10	CLA	aB	840	-	57,73,73	1.87	13 (22%)	66,113,113	2.06	20 (30%)
10	CLA	aB	841	2	57,73,73	1.87	13 (22%)	66,113,113	2.09	20 (30%)
11	PQN	aB	842	-	34,34,34	1.34	2 (5%)	42,45,45	1.02	2 (4%)
13	BCR	aB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	4 (7%)
13	BCR	aB	844	-	41,41,41	1.04	2 (4%)	56,56,56	1.32	5 (8%)
13	BCR	aB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
13	BCR	aB	846	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	3 (5%)
13	BCR	aB	847	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	6 (10%)
16	LMG	aB	848	-	55,55,55	0.76	1 (1%)	63,63,63	1.35	9 (14%)
13	BCR	aB	849	-	41,41,41	1.01	2 (4%)	56,56,56	1.16	4 (7%)
12	SF4	aC	101	3	0,12,12	0.00	-	-		
12	SF4	aC	102	3	0,12,12	0.00	-	-		
13	BCR	aI	101	-	41,41,41	1.06	3 (7%)	56,56,56	1.27	6 (10%)
13	BCR	aI	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	5 (8%)
10	CLA	aL	202	2	47,63,73	2.05	14 (29%)	54,101,113	2.35	20 (37%)
10	CLA	aL	203	7	57,73,73	1.92	13 (22%)	66,113,113	2.03	21 (31%)
10	CLA	aL	204	7	57,73,73	1.89	11 (19%)	66,113,113	2.05	20 (30%)
10	CLA	aL	205	-	57,73,73	1.91	14 (24%)	66,113,113	2.08	19 (28%)
13	BCR	aL	206	-	41,41,41	1.01	2 (4%)	56,56,56	1.29	6 (10%)
13	BCR	aL	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	3 (5%)
13	BCR	aM	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	11 (19%)
9	CL0	bA	801	1	57,73,73	1.87	11 (19%)	66,113,113	2.29	24 (36%)
10	CLA	bA	802	1	34,53,73	2.44	12 (35%)	37,89,113	2.63	18 (48%)
10	CLA	bA	803	1	34,53,73	2.48	13 (38%)	37,89,113	2.69	19 (51%)
10	CLA	bA	804	1	57,73,73	1.89	13 (22%)	66,113,113	2.17	20 (30%)
10	CLA	bA	805	1	57,73,73	1.95	13 (22%)	66,113,113	2.26	24 (36%)
10	CLA	bA	806	1	43,59,73	2.25	13 (30%)	49,96,113	2.39	22 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	bA	807	1	34,53,73	2.40	13 (38%)	37,89,113	2.65	19 (51%)
10	CLA	bA	808	1	34,53,73	2.37	12 (35%)	37,89,113	2.55	15 (40%)
10	CLA	bA	809	1	34,53,73	2.41	12 (35%)	37,89,113	2.61	17 (45%)
10	CLA	bA	810	1	57,73,73	1.99	13 (22%)	66,113,113	2.14	21 (31%)
10	CLA	bA	811	1	46,62,73	2.17	13 (28%)	52,99,113	2.28	21 (40%)
10	CLA	bA	812	1	57,73,73	1.96	13 (22%)	66,113,113	2.15	22 (33%)
10	CLA	bA	813	1	34,53,73	2.46	12 (35%)	37,89,113	2.57	17 (45%)
10	CLA	bA	814	1	34,53,73	2.42	12 (35%)	37,89,113	2.58	17 (45%)
10	CLA	bA	815	-	41,57,73	2.32	13 (31%)	46,93,113	2.36	18 (39%)
10	CLA	bA	816	1	46,62,73	2.15	13 (28%)	52,99,113	2.37	22 (42%)
10	CLA	bA	817	1	46,62,73	2.16	12 (26%)	52,99,113	2.27	22 (42%)
10	CLA	bA	818	1	57,73,73	1.97	11 (19%)	66,113,113	2.37	22 (33%)
10	CLA	bA	819	1	53,69,73	2.06	13 (24%)	61,108,113	2.15	20 (32%)
10	CLA	bA	820	-	57,73,73	1.96	13 (22%)	66,113,113	2.00	21 (31%)
10	CLA	bA	821	1	41,57,73	2.33	12 (29%)	46,93,113	2.54	20 (43%)
10	CLA	bA	822	1	43,59,73	2.27	12 (27%)	49,96,113	2.50	22 (44%)
10	CLA	bA	823	1	57,73,73	1.92	13 (22%)	66,113,113	2.05	19 (28%)
10	CLA	bA	824	-	57,73,73	1.90	13 (22%)	66,113,113	2.16	18 (27%)
10	CLA	bA	825	-	47,63,73	2.09	13 (27%)	54,101,113	2.35	21 (38%)
10	CLA	bA	826	1	57,73,73	1.90	12 (21%)	66,113,113	2.07	21 (31%)
10	CLA	bA	827	1	57,73,73	1.96	14 (24%)	66,113,113	2.19	22 (33%)
10	CLA	bA	828	1	57,73,73	1.94	12 (21%)	66,113,113	2.18	22 (33%)
10	CLA	bA	829	1	57,73,73	1.94	13 (22%)	66,113,113	2.26	21 (31%)
10	CLA	bA	830	1	42,58,73	2.21	13 (30%)	48,95,113	2.40	21 (43%)
10	CLA	bA	831	1	57,73,73	1.93	12 (21%)	66,113,113	2.09	19 (28%)
10	CLA	bA	832	1	57,73,73	1.89	13 (22%)	66,113,113	2.12	23 (34%)
10	CLA	bA	833	1	57,73,73	1.89	12 (21%)	66,113,113	2.20	21 (31%)
10	CLA	bA	834	1	46,62,73	2.14	12 (26%)	52,99,113	2.34	23 (44%)
10	CLA	bA	835	1	57,73,73	1.94	13 (22%)	66,113,113	2.10	22 (33%)
10	CLA	bA	836	1	43,59,73	2.16	13 (30%)	49,96,113	6.08	25 (51%)
10	CLA	bA	837	1	57,73,73	1.85	12 (21%)	66,113,113	2.11	21 (31%)
10	CLA	bA	838	1	42,58,73	2.17	12 (28%)	48,95,113	2.79	24 (50%)
10	CLA	bA	839	1	57,73,73	1.96	13 (22%)	66,113,113	2.06	20 (30%)
10	CLA	bA	840	-	43,59,73	2.32	13 (30%)	49,96,113	2.48	20 (40%)
10	CLA	bA	841	1	57,73,73	1.95	13 (22%)	66,113,113	2.11	20 (30%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	bA	842	-	57,73,73	1.86	13 (22%)	66,113,113	2.11	23 (34%)
10	CLA	bA	843	-	30,49,73	2.44	11 (36%)	31,83,113	2.58	15 (48%)
11	PQN	bA	844	-	34,34,34	1.37	2 (5%)	42,45,45	1.17	4 (9%)
12	SF4	bA	845	1,2	0,12,12	0.00	-	-		
13	BCR	bA	846	-	41,41,41	1.09	3 (7%)	56,56,56	1.23	6 (10%)
13	BCR	bA	847	-	41,41,41	1.02	2 (4%)	56,56,56	1.30	5 (8%)
13	BCR	bA	848	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	8 (14%)
13	BCR	bA	849	-	41,41,41	1.11	3 (7%)	56,56,56	1.26	7 (12%)
13	BCR	bA	850	-	41,41,41	1.11	2 (4%)	56,56,56	1.18	5 (8%)
13	BCR	bA	851	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	3 (5%)
14	LHG	bA	852	-	48,48,48	0.66	1 (2%)	51,54,54	1.22	7 (13%)
15	LMT	bA	853	-	36,36,36	0.45	0	47,47,47	0.90	3 (6%)
10	CLA	bA	854	-	44,60,73	2.22	12 (27%)	50,97,113	2.40	20 (40%)
14	LHG	bA	855	-	26,26,48	0.82	0	29,32,54	1.32	3 (10%)
10	CLA	bA	856	2	41,57,73	2.35	13 (31%)	46,93,113	2.32	18 (39%)
10	CLA	bB	801	-	57,73,73	1.86	13 (22%)	66,113,113	2.36	24 (36%)
10	CLA	bB	802	-	57,73,73	1.93	12 (21%)	66,113,113	2.08	20 (30%)
10	CLA	bB	803	2	57,73,73	1.88	13 (22%)	66,113,113	2.21	23 (34%)
10	CLA	bB	804	-	49,65,73	2.07	12 (24%)	56,103,113	2.57	23 (41%)
10	CLA	bB	805	-	57,73,73	1.88	14 (24%)	66,113,113	1.88	16 (24%)
10	CLA	bB	806	2	46,62,73	2.16	13 (28%)	52,99,113	2.41	25 (48%)
10	CLA	bB	807	2	57,73,73	1.89	14 (24%)	66,113,113	2.21	24 (36%)
10	CLA	bB	808	2	57,73,73	1.88	13 (22%)	66,113,113	2.10	21 (31%)
10	CLA	bB	809	2	57,73,73	1.90	14 (24%)	66,113,113	2.15	20 (30%)
10	CLA	bB	810	2	47,63,73	2.02	12 (25%)	54,101,113	2.48	23 (42%)
10	CLA	bB	811	2	57,73,73	1.85	13 (22%)	66,113,113	2.22	19 (28%)
10	CLA	bB	812	2	34,53,73	2.36	11 (32%)	37,89,113	2.64	16 (43%)
10	CLA	bB	813	2	34,53,73	2.45	12 (35%)	37,89,113	2.55	16 (43%)
10	CLA	bB	814	2	57,73,73	1.94	13 (22%)	66,113,113	2.19	21 (31%)
10	CLA	bB	815	2	48,64,73	2.12	13 (27%)	55,102,113	2.27	21 (38%)
10	CLA	bB	816	2	34,53,73	2.38	12 (35%)	37,89,113	2.69	19 (51%)
10	CLA	bB	817	2	47,63,73	2.13	14 (29%)	54,101,113	2.24	21 (38%)
10	CLA	bB	818	2	51,67,73	2.09	13 (25%)	58,105,113	2.23	21 (36%)
10	CLA	bB	819	2	52,68,73	1.98	12 (23%)	60,107,113	2.41	24 (40%)
10	CLA	bB	820	-	57,73,73	1.97	13 (22%)	66,113,113	2.05	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	bB	821	2	39,55,73	2.39	13 (33%)	44,91,113	2.45	20 (45%)
10	CLA	bB	822	2	34,53,73	2.46	12 (35%)	37,89,113	2.66	16 (43%)
10	CLA	bB	823	2	47,63,73	2.20	13 (27%)	54,101,113	2.26	21 (38%)
10	CLA	bB	824	2	34,53,73	2.45	12 (35%)	37,89,113	2.59	18 (48%)
10	CLA	bB	825	2	46,62,73	2.17	12 (26%)	52,99,113	2.49	22 (42%)
10	CLA	bB	826	-	57,73,73	1.99	13 (22%)	66,113,113	2.27	24 (36%)
10	CLA	bB	827	2	57,73,73	1.92	13 (22%)	66,113,113	2.20	22 (33%)
10	CLA	bB	828	2	57,73,73	1.89	12 (21%)	66,113,113	2.20	21 (31%)
10	CLA	bB	829	2	57,73,73	1.93	12 (21%)	66,113,113	2.08	19 (28%)
10	CLA	bB	830	2	57,73,73	1.92	13 (22%)	66,113,113	2.20	22 (33%)
10	CLA	bB	831	2	34,53,73	2.42	12 (35%)	37,89,113	2.59	19 (51%)
10	CLA	bB	832	2	57,73,73	1.95	14 (24%)	66,113,113	2.10	22 (33%)
10	CLA	bB	833	2	50,66,73	2.09	13 (26%)	57,104,113	2.25	22 (38%)
10	CLA	bB	834	2	34,53,73	2.42	12 (35%)	37,89,113	2.60	20 (54%)
10	CLA	bB	835	-	34,53,73	2.41	13 (38%)	37,89,113	2.49	18 (48%)
10	CLA	bB	836	-	34,53,73	2.47	12 (35%)	37,89,113	2.61	18 (48%)
10	CLA	bB	837	2	52,68,73	2.00	14 (26%)	60,107,113	2.31	21 (35%)
10	CLA	bB	838	2	57,73,73	1.93	12 (21%)	66,113,113	2.12	22 (33%)
10	CLA	bB	839	2	39,55,73	2.30	13 (33%)	44,91,113	2.50	19 (43%)
10	CLA	bB	840	-	57,73,73	1.87	13 (22%)	66,113,113	2.07	20 (30%)
10	CLA	bB	841	2	57,73,73	1.87	13 (22%)	66,113,113	2.09	20 (30%)
11	PQN	bB	842	-	34,34,34	1.34	2 (5%)	42,45,45	1.01	2 (4%)
13	BCR	bB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	4 (7%)
13	BCR	bB	844	-	41,41,41	1.04	2 (4%)	56,56,56	1.32	5 (8%)
13	BCR	bB	845	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	7 (12%)
13	BCR	bB	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	3 (5%)
13	BCR	bB	847	-	41,41,41	1.07	3 (7%)	56,56,56	1.30	6 (10%)
16	LMG	bB	848	-	55,55,55	0.77	1 (1%)	63,63,63	1.34	9 (14%)
13	BCR	bB	849	-	41,41,41	1.01	2 (4%)	56,56,56	1.15	4 (7%)
12	SF4	bC	101	3	0,12,12	0.00	-	-	-	-
12	SF4	bC	102	3	0,12,12	0.00	-	-	-	-
13	BCR	bI	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	6 (10%)
13	BCR	bI	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	6 (10%)
10	CLA	bL	202	2	47,63,73	2.04	14 (29%)	54,101,113	2.35	20 (37%)
10	CLA	bL	203	7	57,73,73	1.91	13 (22%)	66,113,113	2.03	21 (31%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	bL	204	7	57,73,73	1.89	11 (19%)	66,113,113	2.05	20 (30%)
10	CLA	bL	205	-	57,73,73	1.91	14 (24%)	66,113,113	2.08	19 (28%)
13	BCR	bL	206	-	41,41,41	1.01	2 (4%)	56,56,56	1.29	7 (12%)
13	BCR	bL	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.17	3 (5%)
13	BCR	bM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	11 (19%)
9	CL0	cA	801	1	57,73,73	1.87	12 (21%)	66,113,113	2.29	24 (36%)
10	CLA	cA	802	1	34,53,73	2.45	12 (35%)	37,89,113	2.63	18 (48%)
10	CLA	cA	803	1	34,53,73	2.49	13 (38%)	37,89,113	2.68	19 (51%)
10	CLA	cA	804	1	57,73,73	1.89	14 (24%)	66,113,113	2.16	20 (30%)
10	CLA	cA	805	1	57,73,73	1.95	13 (22%)	66,113,113	2.25	24 (36%)
10	CLA	cA	806	1	43,59,73	2.25	13 (30%)	49,96,113	2.39	22 (44%)
10	CLA	cA	807	1	34,53,73	2.39	13 (38%)	37,89,113	2.64	19 (51%)
10	CLA	cA	808	1	34,53,73	2.38	12 (35%)	37,89,113	2.55	15 (40%)
10	CLA	cA	809	1	34,53,73	2.42	12 (35%)	37,89,113	2.62	17 (45%)
10	CLA	cA	810	1	57,73,73	1.98	13 (22%)	66,113,113	2.14	21 (31%)
10	CLA	cA	811	1	46,62,73	2.17	13 (28%)	52,99,113	2.28	21 (40%)
10	CLA	cA	812	1	57,73,73	1.97	13 (22%)	66,113,113	2.15	22 (33%)
10	CLA	cA	813	1	34,53,73	2.46	12 (35%)	37,89,113	2.58	18 (48%)
10	CLA	cA	814	1	34,53,73	2.42	12 (35%)	37,89,113	2.58	17 (45%)
10	CLA	cA	815	-	41,57,73	2.32	12 (29%)	46,93,113	2.36	18 (39%)
10	CLA	cA	816	1	46,62,73	2.16	12 (26%)	52,99,113	2.38	22 (42%)
10	CLA	cA	817	1	46,62,73	2.16	13 (28%)	52,99,113	2.27	22 (42%)
10	CLA	cA	818	1	57,73,73	1.98	12 (21%)	66,113,113	2.37	22 (33%)
10	CLA	cA	819	1	53,69,73	2.05	13 (24%)	61,108,113	2.15	20 (32%)
10	CLA	cA	820	-	57,73,73	1.96	12 (21%)	66,113,113	2.00	21 (31%)
10	CLA	cA	821	1	41,57,73	2.33	12 (29%)	46,93,113	2.53	20 (43%)
10	CLA	cA	822	1	43,59,73	2.26	12 (27%)	49,96,113	2.50	22 (44%)
10	CLA	cA	823	1	57,73,73	1.92	13 (22%)	66,113,113	2.05	19 (28%)
10	CLA	cA	824	-	57,73,73	1.91	13 (22%)	66,113,113	2.15	18 (27%)
10	CLA	cA	825	-	47,63,73	2.09	14 (29%)	54,101,113	2.35	21 (38%)
10	CLA	cA	826	1	57,73,73	1.90	12 (21%)	66,113,113	2.08	21 (31%)
10	CLA	cA	827	1	57,73,73	1.96	14 (24%)	66,113,113	2.18	22 (33%)
10	CLA	cA	828	1	57,73,73	1.93	12 (21%)	66,113,113	2.17	22 (33%)
10	CLA	cA	829	1	57,73,73	1.94	13 (22%)	66,113,113	2.25	21 (31%)
10	CLA	cA	830	1	42,58,73	2.22	12 (28%)	48,95,113	2.41	21 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	cA	831	1	57,73,73	1.93	12 (21%)	66,113,113	2.09	19 (28%)
10	CLA	cA	832	1	57,73,73	1.89	13 (22%)	66,113,113	2.11	23 (34%)
10	CLA	cA	833	1	57,73,73	1.88	12 (21%)	66,113,113	2.19	21 (31%)
10	CLA	cA	834	1	46,62,73	2.14	12 (26%)	52,99,113	2.34	23 (44%)
10	CLA	cA	835	1	57,73,73	1.94	13 (22%)	66,113,113	2.10	22 (33%)
10	CLA	cA	836	1	43,59,73	2.17	13 (30%)	49,96,113	6.09	25 (51%)
10	CLA	cA	837	1	57,73,73	1.85	13 (22%)	66,113,113	2.11	21 (31%)
10	CLA	cA	838	1	42,58,73	2.18	14 (33%)	48,95,113	2.79	24 (50%)
10	CLA	cA	839	1	57,73,73	1.96	13 (22%)	66,113,113	2.06	20 (30%)
10	CLA	cA	840	-	43,59,73	2.32	13 (30%)	49,96,113	2.48	20 (40%)
10	CLA	cA	841	1	57,73,73	1.96	14 (24%)	66,113,113	2.11	20 (30%)
10	CLA	cA	842	-	57,73,73	1.86	13 (22%)	66,113,113	2.11	23 (34%)
10	CLA	cA	843	-	30,49,73	2.44	11 (36%)	31,83,113	2.58	15 (48%)
11	PQN	cA	844	-	34,34,34	1.37	2 (5%)	42,45,45	1.17	4 (9%)
12	SF4	cA	845	1,2	0,12,12	0.00	-	-		
13	BCR	cA	846	-	41,41,41	1.10	3 (7%)	56,56,56	1.23	6 (10%)
13	BCR	cA	847	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	5 (8%)
13	BCR	cA	848	-	41,41,41	1.01	2 (4%)	56,56,56	1.29	8 (14%)
13	BCR	cA	849	-	41,41,41	1.10	3 (7%)	56,56,56	1.27	7 (12%)
13	BCR	cA	850	-	41,41,41	1.11	2 (4%)	56,56,56	1.18	5 (8%)
13	BCR	cA	851	-	41,41,41	1.04	2 (4%)	56,56,56	1.21	3 (5%)
14	LHG	cA	852	-	48,48,48	0.66	1 (2%)	51,54,54	1.21	7 (13%)
15	LMT	cA	853	-	36,36,36	0.45	0	47,47,47	0.90	3 (6%)
10	CLA	cA	854	14	44,60,73	2.22	13 (29%)	50,97,113	2.40	20 (40%)
14	LHG	cA	855	10	26,26,48	0.82	0	29,32,54	1.32	3 (10%)
10	CLA	cA	856	2	41,57,73	2.35	13 (31%)	46,93,113	2.32	18 (39%)
10	CLA	cB	801	-	57,73,73	1.86	13 (22%)	66,113,113	2.36	23 (34%)
10	CLA	cB	802	-	57,73,73	1.94	12 (21%)	66,113,113	2.08	20 (30%)
10	CLA	cB	803	2	57,73,73	1.88	13 (22%)	66,113,113	2.20	23 (34%)
10	CLA	cB	804	-	49,65,73	2.07	12 (24%)	56,103,113	2.57	23 (41%)
10	CLA	cB	805	-	57,73,73	1.88	14 (24%)	66,113,113	1.88	16 (24%)
10	CLA	cB	806	2	46,62,73	2.16	13 (28%)	52,99,113	2.41	25 (48%)
10	CLA	cB	807	2	57,73,73	1.89	14 (24%)	66,113,113	2.21	24 (36%)
10	CLA	cB	808	2	57,73,73	1.88	13 (22%)	66,113,113	2.10	22 (33%)
10	CLA	cB	809	2	57,73,73	1.90	14 (24%)	66,113,113	2.15	20 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	cB	810	2	47,63,73	2.02	12 (25%)	54,101,113	2.48	24 (44%)
10	CLA	cB	811	2	57,73,73	1.85	13 (22%)	66,113,113	2.23	19 (28%)
10	CLA	cB	812	2	34,53,73	2.35	11 (32%)	37,89,113	2.64	16 (43%)
10	CLA	cB	813	2	34,53,73	2.46	13 (38%)	37,89,113	2.55	16 (43%)
10	CLA	cB	814	2	57,73,73	1.94	14 (24%)	66,113,113	2.20	21 (31%)
10	CLA	cB	815	2	48,64,73	2.12	13 (27%)	55,102,113	2.27	21 (38%)
10	CLA	cB	816	2	34,53,73	2.38	12 (35%)	37,89,113	2.69	19 (51%)
10	CLA	cB	817	2	47,63,73	2.13	14 (29%)	54,101,113	2.24	21 (38%)
10	CLA	cB	818	2	51,67,73	2.09	14 (27%)	58,105,113	2.23	21 (36%)
10	CLA	cB	819	2	52,68,73	1.98	12 (23%)	60,107,113	2.41	24 (40%)
10	CLA	cB	820	-	57,73,73	1.97	13 (22%)	66,113,113	2.04	21 (31%)
10	CLA	cB	821	2	39,55,73	2.38	13 (33%)	44,91,113	2.44	20 (45%)
10	CLA	cB	822	2	34,53,73	2.47	12 (35%)	37,89,113	2.66	16 (43%)
10	CLA	cB	823	2	47,63,73	2.20	13 (27%)	54,101,113	2.26	21 (38%)
10	CLA	cB	824	2	34,53,73	2.44	12 (35%)	37,89,113	2.59	18 (48%)
10	CLA	cB	825	2	46,62,73	2.18	13 (28%)	52,99,113	2.49	22 (42%)
10	CLA	cB	826	-	57,73,73	1.99	13 (22%)	66,113,113	2.28	24 (36%)
10	CLA	cB	827	2	57,73,73	1.92	13 (22%)	66,113,113	2.21	22 (33%)
10	CLA	cB	828	2	57,73,73	1.89	12 (21%)	66,113,113	2.19	21 (31%)
10	CLA	cB	829	2	57,73,73	1.93	13 (22%)	66,113,113	2.08	19 (28%)
10	CLA	cB	830	2	57,73,73	1.92	12 (21%)	66,113,113	2.20	22 (33%)
10	CLA	cB	831	2	34,53,73	2.42	12 (35%)	37,89,113	2.60	20 (54%)
10	CLA	cB	832	2	57,73,73	1.95	14 (24%)	66,113,113	2.10	22 (33%)
10	CLA	cB	833	2	50,66,73	2.09	13 (26%)	57,104,113	2.25	22 (38%)
10	CLA	cB	834	2	34,53,73	2.42	12 (35%)	37,89,113	2.58	20 (54%)
10	CLA	cB	835	-	34,53,73	2.41	12 (35%)	37,89,113	2.49	18 (48%)
10	CLA	cB	836	-	34,53,73	2.47	12 (35%)	37,89,113	2.60	18 (48%)
10	CLA	cB	837	2	52,68,73	2.00	14 (26%)	60,107,113	2.32	21 (35%)
10	CLA	cB	838	2	57,73,73	1.93	12 (21%)	66,113,113	2.11	22 (33%)
10	CLA	cB	839	2	39,55,73	2.30	14 (35%)	44,91,113	2.50	19 (43%)
10	CLA	cB	840	-	57,73,73	1.87	13 (22%)	66,113,113	2.07	20 (30%)
10	CLA	cB	841	2	57,73,73	1.87	13 (22%)	66,113,113	2.09	20 (30%)
11	PQN	cB	842	-	34,34,34	1.34	2 (5%)	42,45,45	1.01	2 (4%)
13	BCR	cB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.13	4 (7%)
13	BCR	cB	844	-	41,41,41	1.03	2 (4%)	56,56,56	1.32	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	BCR	cB	845	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	7 (12%)
13	BCR	cB	846	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	3 (5%)
13	BCR	cB	847	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	6 (10%)
16	LMG	cB	848	-	55,55,55	0.76	1 (1%)	63,63,63	1.35	9 (14%)
13	BCR	cB	849	-	41,41,41	1.01	2 (4%)	56,56,56	1.16	4 (7%)
12	SF4	cC	101	3	0,12,12	0.00	-	-	-	-
12	SF4	cC	102	3	0,12,12	0.00	-	-	-	-
13	BCR	cI	102	-	41,41,41	1.07	3 (7%)	56,56,56	1.27	6 (10%)
13	BCR	cI	103	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	5 (8%)
10	CLA	cL	202	2	47,63,73	2.05	14 (29%)	54,101,113	2.35	20 (37%)
10	CLA	cL	203	7	57,73,73	1.91	13 (22%)	66,113,113	2.02	21 (31%)
10	CLA	cL	204	7	57,73,73	1.89	11 (19%)	66,113,113	2.05	20 (30%)
10	CLA	cL	205	-	57,73,73	1.91	14 (24%)	66,113,113	2.08	19 (28%)
13	BCR	cL	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	6 (10%)
13	BCR	cL	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	3 (5%)
13	BCR	cM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	11 (19%)

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
9	CL0	aA	801	1	3/3/20/25	6/37/135/135	-
10	CLA	aA	802	1	2/2/16/25	5/11/111/135	-
10	CLA	aA	803	1	3/3/16/25	3/11/111/135	-
10	CLA	aA	804	1	3/3/20/25	10/37/135/135	-
10	CLA	aA	805	1	3/3/20/25	9/37/135/135	-
10	CLA	aA	806	1	3/3/17/25	3/21/119/135	-
10	CLA	aA	807	1	3/3/16/25	7/11/111/135	-
10	CLA	aA	808	1	3/3/16/25	2/11/111/135	-
10	CLA	aA	809	1	3/3/16/25	2/11/111/135	-
10	CLA	aA	810	1	3/3/20/25	10/37/135/135	-
10	CLA	aA	811	1	3/3/17/25	8/24/122/135	-
10	CLA	aA	812	1	3/3/20/25	15/37/135/135	-
10	CLA	aA	813	1	3/3/16/25	1/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	aA	814	1	3/3/16/25	2/11/111/135	-
10	CLA	aA	815	-	3/3/16/25	3/18/116/135	-
10	CLA	aA	816	1	2/2/17/25	10/24/122/135	-
10	CLA	aA	817	1	2/2/17/25	10/24/122/135	-
10	CLA	aA	818	1	2/2/20/25	13/37/135/135	-
10	CLA	aA	819	1	3/3/19/25	11/33/131/135	-
10	CLA	aA	820	-	3/3/20/25	13/37/135/135	-
10	CLA	aA	821	1	3/3/16/25	4/18/116/135	-
10	CLA	aA	822	1	2/2/17/25	10/21/119/135	-
10	CLA	aA	823	1	3/3/20/25	12/37/135/135	-
10	CLA	aA	824	-	3/3/20/25	11/37/135/135	-
10	CLA	aA	825	-	3/3/18/25	9/25/123/135	-
10	CLA	aA	826	1	3/3/20/25	8/37/135/135	-
10	CLA	aA	827	1	2/2/20/25	17/37/135/135	-
10	CLA	aA	828	1	3/3/20/25	6/37/135/135	-
10	CLA	aA	829	1	3/3/20/25	12/37/135/135	-
10	CLA	aA	830	1	3/3/17/25	5/19/117/135	-
10	CLA	aA	831	1	3/3/20/25	13/37/135/135	-
10	CLA	aA	832	1	3/3/20/25	6/37/135/135	-
10	CLA	aA	833	1	3/3/20/25	10/37/135/135	-
10	CLA	aA	834	1	3/3/17/25	8/24/122/135	-
10	CLA	aA	835	1	3/3/20/25	11/37/135/135	-
10	CLA	aA	836	1	3/3/17/25	7/21/119/135	-
10	CLA	aA	837	1	3/3/20/25	7/37/135/135	-
10	CLA	aA	838	1	3/3/17/25	9/19/117/135	-
10	CLA	aA	839	1	2/2/20/25	6/37/135/135	-
10	CLA	aA	840	-	3/3/17/25	6/21/119/135	-
10	CLA	aA	841	-	3/3/20/25	11/37/135/135	-
10	CLA	aA	842	-	3/3/20/25	14/37/135/135	-
10	CLA	aA	843	-	3/3/14/25	0/5/101/135	-
11	PQN	aA	844	-	-	8/23/43/43	0/2/2/2
12	SF4	aA	845	1,2	-	-	0/6/5/5
13	BCR	aA	846	-	-	14/29/63/63	0/2/2/2
13	BCR	aA	847	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCR	aA	848	-	-	16/29/63/63	0/2/2/2
13	BCR	aA	849	-	-	13/29/63/63	0/2/2/2
13	BCR	aA	850	-	-	9/29/63/63	0/2/2/2
13	BCR	aA	851	-	-	13/29/63/63	0/2/2/2
14	LHG	aA	852	-	-	31/53/53/53	-
15	LMT	aA	853	-	-	9/21/61/61	0/2/2/2
10	CLA	aA	854	-	2/2/17/25	8/22/120/135	-
14	LHG	aA	855	-	-	15/31/31/53	-
10	CLA	aA	856	2	3/3/16/25	7/18/116/135	-
10	CLA	aB	801	-	1/1/20/25	7/37/135/135	-
10	CLA	aB	802	-	3/3/20/25	12/37/135/135	-
10	CLA	aB	803	2	2/2/20/25	5/37/135/135	-
10	CLA	aB	804	-	1/1/18/25	14/28/126/135	-
10	CLA	aB	805	-	2/2/20/25	10/37/135/135	-
10	CLA	aB	806	2	3/3/17/25	11/24/122/135	-
10	CLA	aB	807	2	3/3/20/25	12/37/135/135	-
10	CLA	aB	808	2	3/3/20/25	12/37/135/135	-
10	CLA	aB	809	2	2/2/20/25	6/37/135/135	-
10	CLA	aB	810	2	2/2/18/25	8/25/123/135	-
10	CLA	aB	811	2	2/2/20/25	17/37/135/135	-
10	CLA	aB	812	2	3/3/16/25	1/11/111/135	-
10	CLA	aB	813	2	2/2/16/25	2/11/111/135	-
10	CLA	aB	814	2	3/3/20/25	14/37/135/135	-
10	CLA	aB	815	2	3/3/18/25	7/27/125/135	-
10	CLA	aB	816	2	3/3/16/25	2/11/111/135	-
10	CLA	aB	817	2	3/3/18/25	10/25/123/135	-
10	CLA	aB	818	2	3/3/18/25	11/30/128/135	-
10	CLA	aB	819	2	3/3/19/25	10/31/129/135	-
10	CLA	aB	820	-	3/3/20/25	11/37/135/135	-
10	CLA	aB	821	2	3/3/16/25	5/16/114/135	-
10	CLA	aB	822	2	2/2/16/25	7/11/111/135	-
10	CLA	aB	823	2	3/3/18/25	13/25/123/135	-
10	CLA	aB	824	2	3/3/16/25	3/11/111/135	-
10	CLA	aB	825	2	3/3/17/25	7/24/122/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	aB	826	-	3/3/20/25	11/37/135/135	-
10	CLA	aB	827	2	3/3/20/25	9/37/135/135	-
10	CLA	aB	828	2	1/1/20/25	11/37/135/135	-
10	CLA	aB	829	2	3/3/20/25	12/37/135/135	-
10	CLA	aB	830	2	3/3/20/25	9/37/135/135	-
10	CLA	aB	831	2	3/3/16/25	4/11/111/135	-
10	CLA	aB	832	2	3/3/20/25	14/37/135/135	-
10	CLA	aB	833	2	3/3/18/25	14/29/127/135	-
10	CLA	aB	834	2	3/3/16/25	0/11/111/135	-
10	CLA	aB	835	-	3/3/16/25	3/11/111/135	-
10	CLA	aB	836	-	2/2/16/25	1/11/111/135	-
10	CLA	aB	837	2	3/3/19/25	10/31/129/135	-
10	CLA	aB	838	2	3/3/20/25	9/37/135/135	-
10	CLA	aB	839	2	3/3/16/25	5/16/114/135	-
10	CLA	aB	840	-	3/3/20/25	2/37/135/135	-
10	CLA	aB	841	2	3/3/20/25	10/37/135/135	-
11	PQN	aB	842	-	-	2/23/43/43	0/2/2/2
13	BCR	aB	843	-	-	11/29/63/63	0/2/2/2
13	BCR	aB	844	-	-	10/29/63/63	0/2/2/2
13	BCR	aB	845	-	-	12/29/63/63	0/2/2/2
13	BCR	aB	846	-	-	8/29/63/63	0/2/2/2
13	BCR	aB	847	-	-	10/29/63/63	0/2/2/2
16	LMG	aB	848	-	-	19/50/70/70	0/1/1/1
13	BCR	aB	849	-	-	18/29/63/63	0/2/2/2
12	SF4	aC	101	3	-	-	0/6/5/5
12	SF4	aC	102	3	-	-	0/6/5/5
13	BCR	aI	101	-	-	8/29/63/63	0/2/2/2
13	BCR	aI	102	-	-	8/29/63/63	0/2/2/2
10	CLA	aL	202	2	3/3/18/25	7/25/123/135	-
10	CLA	aL	203	7	2/2/20/25	11/37/135/135	-
10	CLA	aL	204	7	3/3/20/25	8/37/135/135	-
10	CLA	aL	205	-	2/2/20/25	10/37/135/135	-
13	BCR	aL	206	-	-	8/29/63/63	0/2/2/2
13	BCR	aL	207	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCR	aM	101	-	-	13/29/63/63	0/2/2/2
9	CL0	bA	801	1	3/3/20/25	6/37/135/135	-
10	CLA	bA	802	1	2/2/16/25	5/11/111/135	-
10	CLA	bA	803	1	3/3/16/25	3/11/111/135	-
10	CLA	bA	804	1	3/3/20/25	10/37/135/135	-
10	CLA	bA	805	1	3/3/20/25	9/37/135/135	-
10	CLA	bA	806	1	3/3/17/25	3/21/119/135	-
10	CLA	bA	807	1	3/3/16/25	7/11/111/135	-
10	CLA	bA	808	1	3/3/16/25	2/11/111/135	-
10	CLA	bA	809	1	3/3/16/25	2/11/111/135	-
10	CLA	bA	810	1	3/3/20/25	10/37/135/135	-
10	CLA	bA	811	1	3/3/17/25	8/24/122/135	-
10	CLA	bA	812	1	3/3/20/25	15/37/135/135	-
10	CLA	bA	813	1	3/3/16/25	1/11/111/135	-
10	CLA	bA	814	1	3/3/16/25	2/11/111/135	-
10	CLA	bA	815	-	3/3/16/25	3/18/116/135	-
10	CLA	bA	816	1	2/2/17/25	10/24/122/135	-
10	CLA	bA	817	1	2/2/17/25	10/24/122/135	-
10	CLA	bA	818	1	2/2/20/25	13/37/135/135	-
10	CLA	bA	819	1	3/3/19/25	11/33/131/135	-
10	CLA	bA	820	-	3/3/20/25	13/37/135/135	-
10	CLA	bA	821	1	3/3/16/25	4/18/116/135	-
10	CLA	bA	822	1	2/2/17/25	10/21/119/135	-
10	CLA	bA	823	1	3/3/20/25	12/37/135/135	-
10	CLA	bA	824	-	3/3/20/25	11/37/135/135	-
10	CLA	bA	825	-	3/3/18/25	9/25/123/135	-
10	CLA	bA	826	1	3/3/20/25	8/37/135/135	-
10	CLA	bA	827	1	2/2/20/25	17/37/135/135	-
10	CLA	bA	828	1	3/3/20/25	6/37/135/135	-
10	CLA	bA	829	1	3/3/20/25	12/37/135/135	-
10	CLA	bA	830	1	3/3/17/25	5/19/117/135	-
10	CLA	bA	831	1	3/3/20/25	13/37/135/135	-
10	CLA	bA	832	1	3/3/20/25	6/37/135/135	-
10	CLA	bA	833	1	3/3/20/25	10/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bA	834	1	3/3/17/25	8/24/122/135	-
10	CLA	bA	835	1	3/3/20/25	11/37/135/135	-
10	CLA	bA	836	1	3/3/17/25	7/21/119/135	-
10	CLA	bA	837	1	3/3/20/25	7/37/135/135	-
10	CLA	bA	838	1	3/3/17/25	9/19/117/135	-
10	CLA	bA	839	1	2/2/20/25	6/37/135/135	-
10	CLA	bA	840	-	3/3/17/25	6/21/119/135	-
10	CLA	bA	841	1	3/3/20/25	11/37/135/135	-
10	CLA	bA	842	-	3/3/20/25	14/37/135/135	-
10	CLA	bA	843	-	3/3/14/25	0/5/101/135	-
11	PQN	bA	844	-	-	8/23/43/43	0/2/2/2
12	SF4	bA	845	1,2	-	-	0/6/5/5
13	BCR	bA	846	-	-	14/29/63/63	0/2/2/2
13	BCR	bA	847	-	-	9/29/63/63	0/2/2/2
13	BCR	bA	848	-	-	16/29/63/63	0/2/2/2
13	BCR	bA	849	-	-	13/29/63/63	0/2/2/2
13	BCR	bA	850	-	-	9/29/63/63	0/2/2/2
13	BCR	bA	851	-	-	13/29/63/63	0/2/2/2
14	LHG	bA	852	-	-	31/53/53/53	-
15	LMT	bA	853	-	-	9/21/61/61	0/2/2/2
10	CLA	bA	854	-	2/2/17/25	8/22/120/135	-
14	LHG	bA	855	-	-	15/31/31/53	-
10	CLA	bA	856	2	3/3/16/25	7/18/116/135	-
10	CLA	bB	801	-	1/1/20/25	7/37/135/135	-
10	CLA	bB	802	-	3/3/20/25	12/37/135/135	-
10	CLA	bB	803	2	2/2/20/25	5/37/135/135	-
10	CLA	bB	804	-	1/1/18/25	14/28/126/135	-
10	CLA	bB	805	-	2/2/20/25	10/37/135/135	-
10	CLA	bB	806	2	3/3/17/25	12/24/122/135	-
10	CLA	bB	807	2	3/3/20/25	12/37/135/135	-
10	CLA	bB	808	2	3/3/20/25	12/37/135/135	-
10	CLA	bB	809	2	2/2/20/25	6/37/135/135	-
10	CLA	bB	810	2	2/2/18/25	8/25/123/135	-
10	CLA	bB	811	2	2/2/20/25	17/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bB	812	2	3/3/16/25	1/11/111/135	-
10	CLA	bB	813	2	2/2/16/25	2/11/111/135	-
10	CLA	bB	814	2	3/3/20/25	14/37/135/135	-
10	CLA	bB	815	2	3/3/18/25	7/27/125/135	-
10	CLA	bB	816	2	3/3/16/25	2/11/111/135	-
10	CLA	bB	817	2	3/3/18/25	10/25/123/135	-
10	CLA	bB	818	2	3/3/18/25	11/30/128/135	-
10	CLA	bB	819	2	3/3/19/25	10/31/129/135	-
10	CLA	bB	820	-	3/3/20/25	11/37/135/135	-
10	CLA	bB	821	2	3/3/16/25	4/16/114/135	-
10	CLA	bB	822	2	2/2/16/25	7/11/111/135	-
10	CLA	bB	823	2	3/3/18/25	13/25/123/135	-
10	CLA	bB	824	2	3/3/16/25	3/11/111/135	-
10	CLA	bB	825	2	3/3/17/25	7/24/122/135	-
10	CLA	bB	826	-	3/3/20/25	11/37/135/135	-
10	CLA	bB	827	2	3/3/20/25	9/37/135/135	-
10	CLA	bB	828	2	1/1/20/25	11/37/135/135	-
10	CLA	bB	829	2	3/3/20/25	12/37/135/135	-
10	CLA	bB	830	2	3/3/20/25	9/37/135/135	-
10	CLA	bB	831	2	3/3/16/25	4/11/111/135	-
10	CLA	bB	832	2	3/3/20/25	14/37/135/135	-
10	CLA	bB	833	2	3/3/18/25	14/29/127/135	-
10	CLA	bB	834	2	3/3/16/25	0/11/111/135	-
10	CLA	bB	835	-	3/3/16/25	3/11/111/135	-
10	CLA	bB	836	-	2/2/16/25	1/11/111/135	-
10	CLA	bB	837	2	3/3/19/25	10/31/129/135	-
10	CLA	bB	838	2	3/3/20/25	9/37/135/135	-
10	CLA	bB	839	2	3/3/16/25	5/16/114/135	-
10	CLA	bB	840	-	3/3/20/25	2/37/135/135	-
10	CLA	bB	841	2	3/3/20/25	10/37/135/135	-
11	PQN	bB	842	-	-	2/23/43/43	0/2/2/2
13	BCR	bB	843	-	-	11/29/63/63	0/2/2/2
13	BCR	bB	844	-	-	10/29/63/63	0/2/2/2
13	BCR	bB	845	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCR	bB	846	-	-	8/29/63/63	0/2/2/2
13	BCR	bB	847	-	-	10/29/63/63	0/2/2/2
16	LMG	bB	848	-	-	19/50/70/70	0/1/1/1
13	BCR	bB	849	-	-	18/29/63/63	0/2/2/2
12	SF4	bC	101	3	-	-	0/6/5/5
12	SF4	bC	102	3	-	-	0/6/5/5
13	BCR	bI	101	-	-	8/29/63/63	0/2/2/2
13	BCR	bI	102	-	-	8/29/63/63	0/2/2/2
10	CLA	bL	202	2	3/3/18/25	7/25/123/135	-
10	CLA	bL	203	7	2/2/20/25	11/37/135/135	-
10	CLA	bL	204	7	3/3/20/25	8/37/135/135	-
10	CLA	bL	205	-	2/2/20/25	10/37/135/135	-
13	BCR	bL	206	-	-	8/29/63/63	0/2/2/2
13	BCR	bL	207	-	-	7/29/63/63	0/2/2/2
13	BCR	bM	101	-	-	13/29/63/63	0/2/2/2
9	CL0	cA	801	1	3/3/20/25	6/37/135/135	-
10	CLA	cA	802	1	2/2/16/25	5/11/111/135	-
10	CLA	cA	803	1	3/3/16/25	3/11/111/135	-
10	CLA	cA	804	1	3/3/20/25	10/37/135/135	-
10	CLA	cA	805	1	3/3/20/25	9/37/135/135	-
10	CLA	cA	806	1	3/3/17/25	3/21/119/135	-
10	CLA	cA	807	1	3/3/16/25	7/11/111/135	-
10	CLA	cA	808	1	3/3/16/25	2/11/111/135	-
10	CLA	cA	809	1	3/3/16/25	2/11/111/135	-
10	CLA	cA	810	1	3/3/20/25	10/37/135/135	-
10	CLA	cA	811	1	3/3/17/25	8/24/122/135	-
10	CLA	cA	812	1	3/3/20/25	15/37/135/135	-
10	CLA	cA	813	1	3/3/16/25	1/11/111/135	-
10	CLA	cA	814	1	3/3/16/25	2/11/111/135	-
10	CLA	cA	815	-	3/3/16/25	3/18/116/135	-
10	CLA	cA	816	1	2/2/17/25	10/24/122/135	-
10	CLA	cA	817	1	2/2/17/25	10/24/122/135	-
10	CLA	cA	818	1	2/2/20/25	13/37/135/135	-
10	CLA	cA	819	1	3/3/19/25	11/33/131/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cA	820	-	3/3/20/25	13/37/135/135	-
10	CLA	cA	821	1	3/3/16/25	4/18/116/135	-
10	CLA	cA	822	1	2/2/17/25	10/21/119/135	-
10	CLA	cA	823	1	3/3/20/25	12/37/135/135	-
10	CLA	cA	824	-	3/3/20/25	11/37/135/135	-
10	CLA	cA	825	-	3/3/18/25	9/25/123/135	-
10	CLA	cA	826	1	3/3/20/25	8/37/135/135	-
10	CLA	cA	827	1	2/2/20/25	17/37/135/135	-
10	CLA	cA	828	1	3/3/20/25	6/37/135/135	-
10	CLA	cA	829	1	3/3/20/25	12/37/135/135	-
10	CLA	cA	830	1	3/3/17/25	5/19/117/135	-
10	CLA	cA	831	1	3/3/20/25	13/37/135/135	-
10	CLA	cA	832	1	3/3/20/25	6/37/135/135	-
10	CLA	cA	833	1	3/3/20/25	10/37/135/135	-
10	CLA	cA	834	1	3/3/17/25	8/24/122/135	-
10	CLA	cA	835	1	3/3/20/25	11/37/135/135	-
10	CLA	cA	836	1	3/3/17/25	7/21/119/135	-
10	CLA	cA	837	1	3/3/20/25	7/37/135/135	-
10	CLA	cA	838	1	3/3/17/25	9/19/117/135	-
10	CLA	cA	839	1	2/2/20/25	6/37/135/135	-
10	CLA	cA	840	-	3/3/17/25	6/21/119/135	-
10	CLA	cA	841	1	3/3/20/25	11/37/135/135	-
10	CLA	cA	842	-	3/3/20/25	14/37/135/135	-
10	CLA	cA	843	-	3/3/14/25	0/5/101/135	-
11	PQN	cA	844	-	-	8/23/43/43	0/2/2/2
12	SF4	cA	845	1,2	-	-	0/6/5/5
13	BCR	cA	846	-	-	14/29/63/63	0/2/2/2
13	BCR	cA	847	-	-	9/29/63/63	0/2/2/2
13	BCR	cA	848	-	-	16/29/63/63	0/2/2/2
13	BCR	cA	849	-	-	13/29/63/63	0/2/2/2
13	BCR	cA	850	-	-	9/29/63/63	0/2/2/2
13	BCR	cA	851	-	-	13/29/63/63	0/2/2/2
14	LHG	cA	852	-	-	31/53/53/53	-
15	LMT	cA	853	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cA	854	14	2/2/17/25	8/22/120/135	-
14	LHG	cA	855	10	-	15/31/31/53	-
10	CLA	cA	856	2	3/3/16/25	7/18/116/135	-
10	CLA	cB	801	-	1/1/20/25	7/37/135/135	-
10	CLA	cB	802	-	3/3/20/25	12/37/135/135	-
10	CLA	cB	803	2	2/2/20/25	5/37/135/135	-
10	CLA	cB	804	-	1/1/18/25	14/28/126/135	-
10	CLA	cB	805	-	2/2/20/25	10/37/135/135	-
10	CLA	cB	806	2	3/3/17/25	11/24/122/135	-
10	CLA	cB	807	2	3/3/20/25	12/37/135/135	-
10	CLA	cB	808	2	3/3/20/25	12/37/135/135	-
10	CLA	cB	809	2	2/2/20/25	6/37/135/135	-
10	CLA	cB	810	2	2/2/18/25	8/25/123/135	-
10	CLA	cB	811	2	2/2/20/25	17/37/135/135	-
10	CLA	cB	812	2	3/3/16/25	1/11/111/135	-
10	CLA	cB	813	2	2/2/16/25	2/11/111/135	-
10	CLA	cB	814	2	3/3/20/25	14/37/135/135	-
10	CLA	cB	815	2	3/3/18/25	7/27/125/135	-
10	CLA	cB	816	2	3/3/16/25	2/11/111/135	-
10	CLA	cB	817	2	3/3/18/25	10/25/123/135	-
10	CLA	cB	818	2	3/3/18/25	11/30/128/135	-
10	CLA	cB	819	2	3/3/19/25	10/31/129/135	-
10	CLA	cB	820	-	3/3/20/25	11/37/135/135	-
10	CLA	cB	821	2	3/3/16/25	5/16/114/135	-
10	CLA	cB	822	2	2/2/16/25	7/11/111/135	-
10	CLA	cB	823	2	3/3/18/25	13/25/123/135	-
10	CLA	cB	824	2	3/3/16/25	3/11/111/135	-
10	CLA	cB	825	2	3/3/17/25	7/24/122/135	-
10	CLA	cB	826	-	3/3/20/25	11/37/135/135	-
10	CLA	cB	827	2	3/3/20/25	9/37/135/135	-
10	CLA	cB	828	2	1/1/20/25	11/37/135/135	-
10	CLA	cB	829	2	3/3/20/25	12/37/135/135	-
10	CLA	cB	830	2	3/3/20/25	9/37/135/135	-
10	CLA	cB	831	2	3/3/16/25	4/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cB	832	2	3/3/20/25	14/37/135/135	-
10	CLA	cB	833	2	3/3/18/25	14/29/127/135	-
10	CLA	cB	834	2	3/3/16/25	0/11/111/135	-
10	CLA	cB	835	-	3/3/16/25	3/11/111/135	-
10	CLA	cB	836	-	2/2/16/25	1/11/111/135	-
10	CLA	cB	837	2	3/3/19/25	10/31/129/135	-
10	CLA	cB	838	2	3/3/20/25	9/37/135/135	-
10	CLA	cB	839	2	3/3/16/25	5/16/114/135	-
10	CLA	cB	840	-	3/3/20/25	2/37/135/135	-
10	CLA	cB	841	2	3/3/20/25	10/37/135/135	-
11	PQN	cB	842	-	-	2/23/43/43	0/2/2/2
13	BCR	cB	843	-	-	11/29/63/63	0/2/2/2
13	BCR	cB	844	-	-	10/29/63/63	0/2/2/2
13	BCR	cB	845	-	-	12/29/63/63	0/2/2/2
13	BCR	cB	846	-	-	8/29/63/63	0/2/2/2
13	BCR	cB	847	-	-	10/29/63/63	0/2/2/2
16	LMG	cB	848	-	-	19/50/70/70	0/1/1/1
13	BCR	cB	849	-	-	18/29/63/63	0/2/2/2
12	SF4	cC	101	3	-	-	0/6/5/5
12	SF4	cC	102	3	-	-	0/6/5/5
13	BCR	cI	102	-	-	8/29/63/63	0/2/2/2
13	BCR	cI	103	-	-	8/29/63/63	0/2/2/2
10	CLA	cL	202	2	3/3/18/25	7/25/123/135	-
10	CLA	cL	203	7	2/2/20/25	11/37/135/135	-
10	CLA	cL	204	7	3/3/20/25	8/37/135/135	-
10	CLA	cL	205	-	2/2/20/25	10/37/135/135	-
13	BCR	cL	206	-	-	8/29/63/63	0/2/2/2
13	BCR	cL	207	-	-	7/29/63/63	0/2/2/2
13	BCR	cM	101	-	-	13/29/63/63	0/2/2/2

All (3560) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	828	CLA	C3B-C2B	6.54	1.49	1.40
10	bA	828	CLA	C3B-C2B	6.52	1.49	1.40
10	cA	828	CLA	C3B-C2B	6.52	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	836	CLA	C3B-C2B	6.39	1.49	1.40
10	bA	836	CLA	C3B-C2B	6.32	1.49	1.40
10	aA	836	CLA	C3B-C2B	6.32	1.49	1.40
10	aB	827	CLA	C3B-C2B	6.29	1.49	1.40
10	bA	813	CLA	C3B-C2B	6.29	1.49	1.40
10	aA	813	CLA	C3B-C2B	6.27	1.49	1.40
10	cB	827	CLA	C3B-C2B	6.25	1.49	1.40
10	cA	813	CLA	C3B-C2B	6.25	1.49	1.40
10	bB	827	CLA	C3B-C2B	6.25	1.49	1.40
10	aA	831	CLA	C3B-C2B	6.23	1.49	1.40
10	cA	831	CLA	C3B-C2B	6.22	1.49	1.40
10	aA	827	CLA	C3B-C2B	6.20	1.49	1.40
10	aA	822	CLA	C3B-C2B	6.19	1.49	1.40
10	cA	827	CLA	C3B-C2B	6.19	1.49	1.40
10	bA	831	CLA	C3B-C2B	6.18	1.49	1.40
10	cA	822	CLA	C3B-C2B	6.18	1.49	1.40
10	bA	827	CLA	C3B-C2B	6.18	1.49	1.40
11	cA	844	PQN	C3-C2	6.16	1.48	1.35
11	bA	844	PQN	C3-C2	6.16	1.48	1.35
11	aA	844	PQN	C3-C2	6.15	1.48	1.35
10	bA	822	CLA	C3B-C2B	6.14	1.48	1.40
10	bB	825	CLA	C3B-C2B	6.13	1.48	1.40
11	aB	842	PQN	C3-C2	6.09	1.48	1.35
10	aB	825	CLA	C3B-C2B	6.09	1.48	1.40
10	cB	825	CLA	C3B-C2B	6.08	1.48	1.40
11	cB	842	PQN	C3-C2	6.08	1.48	1.35
11	bB	842	PQN	C3-C2	6.08	1.48	1.35
10	bA	805	CLA	C3B-C2B	6.08	1.48	1.40
10	cA	803	CLA	C3B-C2B	6.08	1.48	1.40
10	cA	802	CLA	C3B-C2B	6.06	1.48	1.40
10	bA	803	CLA	C3B-C2B	6.03	1.48	1.40
10	aA	805	CLA	C3B-C2B	6.03	1.48	1.40
10	aB	826	CLA	C3B-C2B	6.02	1.48	1.40
10	cA	805	CLA	C3B-C2B	6.01	1.48	1.40
10	bB	826	CLA	C3B-C2B	6.01	1.48	1.40
10	aB	806	CLA	C3B-C2B	6.01	1.48	1.40
10	aA	802	CLA	C3B-C2B	6.00	1.48	1.40
10	bB	806	CLA	C3B-C2B	6.00	1.48	1.40
10	bA	802	CLA	C3B-C2B	6.00	1.48	1.40
10	cB	826	CLA	C3B-C2B	6.00	1.48	1.40
10	aA	803	CLA	C3B-C2B	6.00	1.48	1.40
10	cB	806	CLA	C3B-C2B	5.99	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	804	CLA	C3B-C2B	5.97	1.48	1.40
10	aA	821	CLA	C3B-C2B	5.95	1.48	1.40
10	aB	830	CLA	C3B-C2B	5.95	1.48	1.40
10	bA	821	CLA	C3B-C2B	5.95	1.48	1.40
10	cA	821	CLA	C3B-C2B	5.95	1.48	1.40
10	bB	830	CLA	C3B-C2B	5.92	1.48	1.40
10	aB	804	CLA	C3B-C2B	5.92	1.48	1.40
10	cB	830	CLA	C3B-C2B	5.91	1.48	1.40
10	aA	819	CLA	C3B-C2B	5.91	1.48	1.40
10	bB	821	CLA	C3B-C2B	5.90	1.48	1.40
10	bB	829	CLA	C3B-C2B	5.90	1.48	1.40
10	aB	815	CLA	C3B-C2B	5.90	1.48	1.40
10	aB	829	CLA	C3B-C2B	5.90	1.48	1.40
10	cB	829	CLA	C3B-C2B	5.90	1.48	1.40
10	cB	804	CLA	C3B-C2B	5.90	1.48	1.40
10	bA	819	CLA	C3B-C2B	5.89	1.48	1.40
10	cB	821	CLA	C3B-C2B	5.89	1.48	1.40
10	aB	821	CLA	C3B-C2B	5.88	1.48	1.40
10	bB	815	CLA	C3B-C2B	5.88	1.48	1.40
10	cB	815	CLA	C3B-C2B	5.88	1.48	1.40
10	cA	819	CLA	C3B-C2B	5.87	1.48	1.40
10	cB	813	CLA	C3B-C2B	5.82	1.48	1.40
10	bB	813	CLA	C3B-C2B	5.82	1.48	1.40
10	cB	823	CLA	C3B-C2B	5.81	1.48	1.40
10	bA	829	CLA	C3B-C2B	5.80	1.48	1.40
10	cB	840	CLA	C3B-C2B	5.80	1.48	1.40
10	aB	813	CLA	C3B-C2B	5.80	1.48	1.40
10	cB	802	CLA	C3B-C2B	5.80	1.48	1.40
10	aA	840	CLA	C3B-C2B	5.79	1.48	1.40
10	aB	828	CLA	C3B-C2B	5.78	1.48	1.40
10	bA	840	CLA	C3B-C2B	5.78	1.48	1.40
10	bB	823	CLA	C3B-C2B	5.78	1.48	1.40
10	bB	802	CLA	C3B-C2B	5.77	1.48	1.40
10	aB	802	CLA	C3B-C2B	5.77	1.48	1.40
10	aA	843	CLA	C3B-C2B	5.77	1.48	1.40
10	cA	829	CLA	C3B-C2B	5.77	1.48	1.40
10	aB	823	CLA	C3B-C2B	5.76	1.48	1.40
10	aB	824	CLA	C3B-C2B	5.76	1.48	1.40
10	bB	822	CLA	C3B-C2B	5.76	1.48	1.40
10	aB	822	CLA	C3B-C2B	5.75	1.48	1.40
10	aA	807	CLA	C3B-C2B	5.75	1.48	1.40
10	aA	829	CLA	C3B-C2B	5.75	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	814	CLA	C3B-C2B	5.75	1.48	1.40
10	cA	840	CLA	C3B-C2B	5.74	1.48	1.40
10	cB	824	CLA	C3B-C2B	5.74	1.48	1.40
10	aB	840	CLA	C3B-C2B	5.74	1.48	1.40
10	bB	828	CLA	C3B-C2B	5.74	1.48	1.40
10	cB	828	CLA	C3B-C2B	5.73	1.48	1.40
10	cA	843	CLA	C3B-C2B	5.73	1.48	1.40
10	aA	808	CLA	C3B-C2B	5.73	1.48	1.40
10	aA	814	CLA	C3B-C2B	5.72	1.48	1.40
10	bB	840	CLA	C3B-C2B	5.72	1.48	1.40
10	aB	822	CLA	OBD-CAD	5.72	1.30	1.22
10	bA	814	CLA	C3B-C2B	5.71	1.48	1.40
10	bB	822	CLA	OBD-CAD	5.71	1.30	1.22
10	bA	856	CLA	C3B-C2B	5.71	1.48	1.40
10	bA	807	CLA	C3B-C2B	5.71	1.48	1.40
10	cB	822	CLA	OBD-CAD	5.70	1.30	1.22
10	bA	843	CLA	C3B-C2B	5.70	1.48	1.40
10	cA	808	CLA	C3B-C2B	5.70	1.48	1.40
10	cB	822	CLA	C3B-C2B	5.70	1.48	1.40
10	bB	824	CLA	C3B-C2B	5.69	1.48	1.40
10	aA	856	CLA	C3B-C2B	5.69	1.48	1.40
10	cA	807	CLA	C3B-C2B	5.68	1.48	1.40
10	cA	856	CLA	C3B-C2B	5.68	1.48	1.40
10	aB	801	CLA	C3B-C2B	5.68	1.48	1.40
10	bB	814	CLA	C3B-C2B	5.68	1.48	1.40
10	aB	833	CLA	C3B-C2B	5.67	1.48	1.40
10	bA	841	CLA	C3B-C2B	5.67	1.48	1.40
10	bA	817	CLA	C3B-C2B	5.67	1.48	1.40
10	aA	841	CLA	C3B-C2B	5.67	1.48	1.40
10	cA	817	CLA	C3B-C2B	5.67	1.48	1.40
10	aB	814	CLA	C3B-C2B	5.66	1.48	1.40
10	cB	801	CLA	C3B-C2B	5.66	1.48	1.40
10	cB	807	CLA	C3B-C2B	5.66	1.48	1.40
10	bA	808	CLA	C3B-C2B	5.66	1.48	1.40
10	aB	807	CLA	C3B-C2B	5.66	1.48	1.40
10	cA	825	CLA	C3B-C2B	5.66	1.48	1.40
10	aB	838	CLA	C3B-C2B	5.65	1.48	1.40
10	cA	841	CLA	C3B-C2B	5.65	1.48	1.40
10	cB	832	CLA	C3B-C2B	5.65	1.48	1.40
10	bB	833	CLA	C3B-C2B	5.64	1.48	1.40
10	bB	838	CLA	C3B-C2B	5.64	1.48	1.40
10	bB	807	CLA	C3B-C2B	5.63	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	833	CLA	C3B-C2B	5.63	1.48	1.40
10	bA	810	CLA	C3B-C2B	5.63	1.48	1.40
10	aA	817	CLA	C3B-C2B	5.63	1.48	1.40
10	cB	814	CLA	C3B-C2B	5.63	1.48	1.40
10	cB	805	CLA	C3B-C2B	5.62	1.48	1.40
10	cB	838	CLA	C3B-C2B	5.62	1.48	1.40
10	aA	818	CLA	C3B-C2B	5.62	1.48	1.40
10	aB	832	CLA	C3B-C2B	5.61	1.48	1.40
10	cB	836	CLA	C3B-C2B	5.60	1.48	1.40
10	bA	818	CLA	C3B-C2B	5.60	1.48	1.40
10	cA	818	CLA	C3C-C2C	5.60	1.48	1.36
10	bB	832	CLA	C3B-C2B	5.60	1.48	1.40
10	bB	801	CLA	C3B-C2B	5.59	1.48	1.40
10	cA	818	CLA	C3B-C2B	5.59	1.48	1.40
10	bB	836	CLA	C3B-C2B	5.59	1.48	1.40
10	aB	805	CLA	C3B-C2B	5.59	1.48	1.40
10	bB	805	CLA	C3B-C2B	5.58	1.48	1.40
10	cB	834	CLA	C3B-C2B	5.58	1.48	1.40
10	cA	810	CLA	C3B-C2B	5.58	1.48	1.40
10	aA	811	CLA	C3B-C2B	5.57	1.48	1.40
10	aA	818	CLA	C3C-C2C	5.57	1.48	1.36
10	bA	825	CLA	C3B-C2B	5.57	1.48	1.40
10	bB	818	CLA	C3B-C2B	5.57	1.48	1.40
10	cB	818	CLA	C3B-C2B	5.57	1.48	1.40
10	bA	818	CLA	C3C-C2C	5.56	1.48	1.36
10	aA	810	CLA	C3B-C2B	5.56	1.48	1.40
10	bA	815	CLA	C3B-C2B	5.55	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	5.54	1.48	1.40
10	aB	834	CLA	C3B-C2B	5.54	1.48	1.40
10	cB	839	CLA	C3B-C2B	5.54	1.48	1.40
10	bB	839	CLA	C3B-C2B	5.54	1.48	1.40
10	aB	836	CLA	C3B-C2B	5.53	1.48	1.40
10	aL	203	CLA	C3B-C2B	5.53	1.48	1.40
10	bA	811	CLA	C3B-C2B	5.53	1.48	1.40
10	bA	812	CLA	C3B-C2B	5.53	1.48	1.40
10	bB	834	CLA	C3B-C2B	5.53	1.48	1.40
10	aB	818	CLA	C3B-C2B	5.53	1.48	1.40
10	aA	839	CLA	C3B-C2B	5.53	1.48	1.40
10	bB	808	CLA	C3B-C2B	5.52	1.48	1.40
10	aA	815	CLA	C3C-C2C	5.52	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	815	CLA	C3C-C2C	5.52	1.48	1.36
10	bA	816	CLA	C3B-C2B	5.51	1.48	1.40
10	cA	816	CLA	C3B-C2B	5.51	1.48	1.40
10	cA	812	CLA	C3B-C2B	5.51	1.48	1.40
10	aA	816	CLA	C3B-C2B	5.51	1.48	1.40
10	cL	203	CLA	C3B-C2B	5.51	1.48	1.40
10	bL	203	CLA	C3B-C2B	5.50	1.48	1.40
10	aA	815	CLA	C3B-C2B	5.50	1.48	1.40
10	aB	808	CLA	C3B-C2B	5.49	1.48	1.40
10	cA	815	CLA	C3B-C2B	5.49	1.48	1.40
10	cA	839	CLA	C3B-C2B	5.49	1.48	1.40
10	bA	839	CLA	C3B-C2B	5.49	1.48	1.40
10	aL	205	CLA	C3B-C2B	5.49	1.48	1.40
10	cB	808	CLA	C3B-C2B	5.48	1.48	1.40
10	cA	815	CLA	C3C-C2C	5.48	1.48	1.36
10	bA	840	CLA	C3C-C2C	5.46	1.48	1.36
10	aB	839	CLA	C3B-C2B	5.46	1.48	1.40
10	aA	840	CLA	C3C-C2C	5.46	1.48	1.36
10	bA	854	CLA	C3C-C2C	5.45	1.48	1.36
10	cA	854	CLA	C3C-C2C	5.45	1.48	1.36
10	cA	809	CLA	C3B-C2B	5.44	1.47	1.40
10	aB	813	CLA	C3C-C2C	5.44	1.48	1.36
10	aA	854	CLA	C3C-C2C	5.44	1.48	1.36
10	bB	813	CLA	C3C-C2C	5.43	1.48	1.36
10	cA	835	CLA	C3B-C2B	5.43	1.47	1.40
10	aL	202	CLA	C3B-C2B	5.43	1.47	1.40
10	bL	205	CLA	C3B-C2B	5.42	1.47	1.40
10	cB	813	CLA	C3C-C2C	5.42	1.48	1.36
10	cA	840	CLA	C3C-C2C	5.42	1.48	1.36
10	bA	854	CLA	C3B-C2B	5.42	1.47	1.40
10	cL	205	CLA	C3B-C2B	5.42	1.47	1.40
10	aA	835	CLA	C3B-C2B	5.42	1.47	1.40
10	aB	817	CLA	C3B-C2B	5.42	1.47	1.40
10	bA	835	CLA	C3B-C2B	5.41	1.47	1.40
10	cB	817	CLA	C3B-C2B	5.41	1.47	1.40
10	bA	810	CLA	C3C-C2C	5.40	1.48	1.36
10	aB	835	CLA	C3C-C2C	5.40	1.48	1.36
10	cL	202	CLA	C3B-C2B	5.40	1.47	1.40
10	bA	820	CLA	C3B-C2B	5.40	1.47	1.40
10	bA	809	CLA	C3B-C2B	5.40	1.47	1.40
10	cB	826	CLA	C3C-C2C	5.39	1.48	1.36
10	aA	826	CLA	C3C-C2C	5.39	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	854	CLA	C3B-C2B	5.39	1.47	1.40
10	aA	820	CLA	C3B-C2B	5.38	1.47	1.40
10	cB	835	CLA	C3C-C2C	5.38	1.48	1.36
10	cA	826	CLA	C3C-C2C	5.38	1.48	1.36
10	aA	854	CLA	C3B-C2B	5.38	1.47	1.40
10	bA	812	CLA	C3C-C2C	5.38	1.48	1.36
10	cA	856	CLA	O2D-CGD	5.38	1.46	1.33
10	bB	826	CLA	C3C-C2C	5.38	1.48	1.36
10	aA	819	CLA	C3C-C2C	5.38	1.48	1.36
10	cA	810	CLA	C3C-C2C	5.37	1.48	1.36
10	aA	843	CLA	C3C-C2C	5.37	1.48	1.36
10	bA	820	CLA	C3C-C2C	5.37	1.48	1.36
10	aA	810	CLA	C3C-C2C	5.37	1.48	1.36
10	cA	823	CLA	C3B-C2B	5.37	1.47	1.40
10	cA	820	CLA	C3B-C2B	5.37	1.47	1.40
10	aA	809	CLA	C3B-C2B	5.37	1.47	1.40
10	bA	823	CLA	C3B-C2B	5.36	1.47	1.40
10	cA	820	CLA	C3C-C2C	5.36	1.48	1.36
10	bA	843	CLA	C3C-C2C	5.36	1.48	1.36
10	bA	826	CLA	C3C-C2C	5.36	1.48	1.36
10	cA	843	CLA	C3C-C2C	5.36	1.48	1.36
10	bB	836	CLA	C3C-C2C	5.35	1.48	1.36
10	cA	806	CLA	C3B-C2B	5.35	1.47	1.40
10	cA	819	CLA	C3C-C2C	5.35	1.48	1.36
10	cB	836	CLA	C3C-C2C	5.35	1.48	1.36
10	bA	803	CLA	C3C-C2C	5.35	1.48	1.36
10	bB	834	CLA	C3C-C2C	5.35	1.48	1.36
10	bB	823	CLA	C3C-C2C	5.34	1.48	1.36
10	aB	818	CLA	C3C-C2C	5.34	1.48	1.36
10	bL	202	CLA	C3B-C2B	5.34	1.47	1.40
10	bB	817	CLA	C3B-C2B	5.34	1.47	1.40
10	cA	812	CLA	C3C-C2C	5.34	1.48	1.36
10	bA	856	CLA	O2D-CGD	5.34	1.46	1.33
10	bA	827	CLA	C3C-C2C	5.34	1.48	1.36
10	bB	835	CLA	C3C-C2C	5.34	1.48	1.36
10	cA	804	CLA	C3B-C2B	5.33	1.47	1.40
10	aB	836	CLA	C3C-C2C	5.33	1.48	1.36
10	aA	820	CLA	C3C-C2C	5.33	1.48	1.36
10	aA	823	CLA	C3B-C2B	5.33	1.47	1.40
10	aA	804	CLA	C3B-C2B	5.33	1.47	1.40
10	cB	823	CLA	C3C-C2C	5.33	1.48	1.36
10	bA	856	CLA	C3C-C2C	5.33	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	820	CLA	C3C-C2C	5.33	1.48	1.36
10	aA	812	CLA	C3C-C2C	5.33	1.48	1.36
10	bA	819	CLA	C3C-C2C	5.33	1.48	1.36
10	aB	823	CLA	C3C-C2C	5.33	1.48	1.36
10	cL	204	CLA	C3B-C2B	5.33	1.47	1.40
10	aB	834	CLA	C3C-C2C	5.33	1.48	1.36
10	cB	818	CLA	C3C-C2C	5.32	1.48	1.36
10	bB	818	CLA	C3C-C2C	5.32	1.48	1.36
10	cB	834	CLA	C3C-C2C	5.32	1.48	1.36
10	cB	816	CLA	C3B-C2B	5.32	1.47	1.40
10	aB	826	CLA	C3C-C2C	5.32	1.48	1.36
10	bA	822	CLA	C3C-C2C	5.32	1.48	1.36
10	aA	827	CLA	C3C-C2C	5.31	1.48	1.36
10	bA	806	CLA	C3B-C2B	5.31	1.47	1.40
10	aA	822	CLA	C3C-C2C	5.31	1.48	1.36
10	aA	803	CLA	C3C-C2C	5.31	1.48	1.36
9	cA	801	CL0	C3B-C2B	5.31	1.47	1.40
10	aB	819	CLA	C3B-C2B	5.31	1.47	1.40
10	aA	856	CLA	O2D-CGD	5.31	1.46	1.33
10	bB	820	CLA	C3C-C2C	5.30	1.47	1.36
10	cB	804	CLA	C3D-C2D	5.30	1.49	1.39
10	cA	856	CLA	C3C-C2C	5.30	1.47	1.36
10	aA	806	CLA	C3B-C2B	5.30	1.47	1.40
10	aA	829	CLA	C3C-C2C	5.30	1.47	1.36
10	aB	835	CLA	C3B-C2B	5.30	1.47	1.40
10	aA	814	CLA	C3C-C2C	5.29	1.47	1.36
9	bA	801	CL0	C3B-C2B	5.29	1.47	1.40
10	bB	816	CLA	C3B-C2B	5.29	1.47	1.40
10	aB	816	CLA	C3B-C2B	5.29	1.47	1.40
10	cB	820	CLA	C3C-C2C	5.29	1.47	1.36
10	aA	809	CLA	C3C-C2C	5.29	1.47	1.36
10	aB	804	CLA	C3D-C2D	5.29	1.49	1.39
10	cA	803	CLA	C3C-C2C	5.29	1.47	1.36
10	cA	806	CLA	C3C-C2C	5.29	1.47	1.36
9	aA	801	CL0	C3B-C2B	5.29	1.47	1.40
10	bA	823	CLA	C3C-C2C	5.29	1.47	1.36
10	aA	813	CLA	C3C-C2C	5.29	1.47	1.36
10	bA	813	CLA	C3C-C2C	5.29	1.47	1.36
10	cA	823	CLA	C3C-C2C	5.29	1.47	1.36
10	aA	823	CLA	C3C-C2C	5.29	1.47	1.36
10	bA	809	CLA	C3C-C2C	5.28	1.47	1.36
10	aB	832	CLA	C3C-C2C	5.28	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	806	CLA	C3C-C2C	5.28	1.47	1.36
10	cA	811	CLA	C3C-C2C	5.28	1.47	1.36
10	bA	804	CLA	C3B-C2B	5.28	1.47	1.40
10	bB	835	CLA	C3B-C2B	5.28	1.47	1.40
10	cA	827	CLA	C3C-C2C	5.28	1.47	1.36
10	bB	812	CLA	C3C-C2C	5.28	1.47	1.36
10	bA	811	CLA	C3C-C2C	5.28	1.47	1.36
10	cA	835	CLA	C3C-C2C	5.27	1.47	1.36
10	cA	829	CLA	C3C-C2C	5.27	1.47	1.36
10	aA	811	CLA	C3C-C2C	5.27	1.47	1.36
10	bB	809	CLA	C3B-C2B	5.27	1.47	1.40
10	cA	809	CLA	C3C-C2C	5.27	1.47	1.36
10	aA	856	CLA	C3C-C2C	5.27	1.47	1.36
10	cB	812	CLA	C3C-C2C	5.27	1.47	1.36
10	cA	822	CLA	C3C-C2C	5.26	1.47	1.36
10	aA	821	CLA	C3D-C2D	5.26	1.49	1.39
10	cA	813	CLA	C3C-C2C	5.26	1.47	1.36
10	aB	838	CLA	C3C-C2C	5.26	1.47	1.36
10	bA	814	CLA	C3C-C2C	5.26	1.47	1.36
10	aA	843	CLA	C3D-C2D	5.26	1.49	1.39
10	aB	816	CLA	C3C-C2C	5.26	1.47	1.36
10	aA	806	CLA	C3C-C2C	5.26	1.47	1.36
10	bB	804	CLA	C3D-C2D	5.26	1.49	1.39
10	bB	832	CLA	C3C-C2C	5.26	1.47	1.36
10	bA	835	CLA	C3C-C2C	5.26	1.47	1.36
10	bA	843	CLA	C3D-C2D	5.26	1.49	1.39
10	aL	204	CLA	C3B-C2B	5.26	1.47	1.40
10	cA	814	CLA	C3C-C2C	5.26	1.47	1.36
10	bA	829	CLA	C3C-C2C	5.26	1.47	1.36
10	bB	803	CLA	C3B-C2B	5.26	1.47	1.40
10	bB	815	CLA	C3C-C2C	5.25	1.47	1.36
10	bA	821	CLA	C3D-C2D	5.25	1.49	1.39
10	cB	819	CLA	C3B-C2B	5.25	1.47	1.40
10	aB	812	CLA	C3C-C2C	5.25	1.47	1.36
10	cB	832	CLA	C3C-C2C	5.25	1.47	1.36
10	bB	816	CLA	C3C-C2C	5.25	1.47	1.36
10	cB	816	CLA	C3C-C2C	5.25	1.47	1.36
10	bA	832	CLA	C3B-C2B	5.25	1.47	1.40
10	aB	815	CLA	C3C-C2C	5.25	1.47	1.36
10	bB	819	CLA	C3B-C2B	5.25	1.47	1.40
10	aB	841	CLA	C3B-C2B	5.25	1.47	1.40
10	cB	835	CLA	C3B-C2B	5.25	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	827	CLA	C3C-C2C	5.25	1.47	1.36
10	bB	821	CLA	C3C-C2C	5.25	1.47	1.36
10	aA	835	CLA	C3C-C2C	5.25	1.47	1.36
10	cB	815	CLA	C3C-C2C	5.25	1.47	1.36
10	bB	838	CLA	C3C-C2C	5.24	1.47	1.36
10	bB	831	CLA	C3C-C2C	5.24	1.47	1.36
10	bA	834	CLA	C3C-C2C	5.24	1.47	1.36
10	cA	834	CLA	C3C-C2C	5.24	1.47	1.36
10	aB	809	CLA	C3B-C2B	5.24	1.47	1.40
10	cB	831	CLA	C3B-C2B	5.24	1.47	1.40
10	bB	824	CLA	C3C-C2C	5.24	1.47	1.36
10	aA	817	CLA	C3C-C2C	5.24	1.47	1.36
10	bL	204	CLA	C3B-C2B	5.24	1.47	1.40
10	aB	824	CLA	C3C-C2C	5.23	1.47	1.36
10	aA	832	CLA	C3B-C2B	5.23	1.47	1.40
10	bB	841	CLA	C3B-C2B	5.23	1.47	1.40
10	aB	827	CLA	C3C-C2C	5.23	1.47	1.36
10	cB	831	CLA	C3C-C2C	5.23	1.47	1.36
10	cB	824	CLA	C3C-C2C	5.23	1.47	1.36
10	aB	821	CLA	C3C-C2C	5.23	1.47	1.36
10	cB	821	CLA	C3C-C2C	5.23	1.47	1.36
10	aA	839	CLA	C3C-C2C	5.23	1.47	1.36
10	aA	834	CLA	C3C-C2C	5.22	1.47	1.36
10	cA	843	CLA	C3D-C2D	5.22	1.49	1.39
10	cA	832	CLA	C3B-C2B	5.22	1.47	1.40
10	cL	203	CLA	C3C-C2C	5.22	1.47	1.36
10	cA	839	CLA	C3C-C2C	5.22	1.47	1.36
10	bB	831	CLA	C3B-C2B	5.22	1.47	1.40
10	aB	831	CLA	C3C-C2C	5.22	1.47	1.36
10	cB	822	CLA	C3C-C2C	5.22	1.47	1.36
10	bL	203	CLA	C3C-C2C	5.22	1.47	1.36
10	cA	821	CLA	C3D-C2D	5.21	1.49	1.39
10	bA	839	CLA	C3C-C2C	5.21	1.47	1.36
10	cA	817	CLA	C3C-C2C	5.21	1.47	1.36
10	bA	824	CLA	C3B-C2B	5.21	1.47	1.40
10	cA	824	CLA	C3B-C2B	5.21	1.47	1.40
10	cB	833	CLA	C3C-C2C	5.21	1.47	1.36
10	cB	838	CLA	C3C-C2C	5.21	1.47	1.36
10	aB	802	CLA	C3D-C2D	5.21	1.49	1.39
10	aA	824	CLA	C3B-C2B	5.20	1.47	1.40
10	aB	822	CLA	C3C-C2C	5.20	1.47	1.36
10	bB	802	CLA	C3D-C2D	5.20	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	809	CLA	C3B-C2B	5.20	1.47	1.40
10	aB	803	CLA	C3B-C2B	5.20	1.47	1.40
10	cB	827	CLA	C3C-C2C	5.20	1.47	1.36
10	aB	839	CLA	C3C-C2C	5.20	1.47	1.36
10	cA	856	CLA	C3D-C2D	5.20	1.49	1.39
10	aA	837	CLA	C3B-C2B	5.20	1.47	1.40
10	aB	831	CLA	C3B-C2B	5.19	1.47	1.40
10	cB	841	CLA	C3B-C2B	5.19	1.47	1.40
10	bB	839	CLA	C3C-C2C	5.19	1.47	1.36
10	cA	832	CLA	C3C-C2C	5.19	1.47	1.36
10	bB	822	CLA	C3C-C2C	5.19	1.47	1.36
10	aA	856	CLA	C3D-C2D	5.19	1.49	1.39
10	aL	205	CLA	C3C-C2C	5.19	1.47	1.36
10	bA	833	CLA	C3B-C2B	5.19	1.47	1.40
10	cB	807	CLA	C3C-C2C	5.19	1.47	1.36
10	bA	807	CLA	C3C-C2C	5.18	1.47	1.36
10	cL	205	CLA	C3C-C2C	5.18	1.47	1.36
10	bA	824	CLA	C3C-C2C	5.18	1.47	1.36
10	aL	203	CLA	C3C-C2C	5.18	1.47	1.36
10	bA	817	CLA	C3C-C2C	5.18	1.47	1.36
10	bB	833	CLA	C3C-C2C	5.18	1.47	1.36
10	cB	803	CLA	C3B-C2B	5.18	1.47	1.40
10	cA	807	CLA	C3C-C2C	5.18	1.47	1.36
10	bA	856	CLA	C3D-C2D	5.18	1.49	1.39
10	cB	802	CLA	C3D-C2D	5.18	1.49	1.39
10	aA	824	CLA	C3C-C2C	5.17	1.47	1.36
10	bA	832	CLA	C3C-C2C	5.17	1.47	1.36
10	bB	829	CLA	C3C-C2C	5.17	1.47	1.36
10	cB	822	CLA	O2D-CGD	5.17	1.46	1.33
10	aA	830	CLA	C3C-C2C	5.17	1.47	1.36
10	aB	833	CLA	C3C-C2C	5.17	1.47	1.36
10	aA	802	CLA	C3C-C2C	5.17	1.47	1.36
10	bA	821	CLA	C3C-C2C	5.17	1.47	1.36
10	bL	205	CLA	C3C-C2C	5.17	1.47	1.36
10	bB	836	CLA	C3D-C2D	5.17	1.49	1.39
10	aB	824	CLA	C3D-C2D	5.17	1.49	1.39
10	aB	829	CLA	C3C-C2C	5.17	1.47	1.36
10	aB	818	CLA	C3D-C2D	5.17	1.49	1.39
10	cA	802	CLA	C3C-C2C	5.17	1.47	1.36
10	bB	807	CLA	C3C-C2C	5.16	1.47	1.36
10	cA	824	CLA	C3C-C2C	5.16	1.47	1.36
10	aA	821	CLA	C3C-C2C	5.16	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	801	CLA	C3D-C2D	5.16	1.49	1.39
10	cA	830	CLA	C3C-C2C	5.16	1.47	1.36
10	aB	807	CLA	C3C-C2C	5.16	1.47	1.36
10	bA	802	CLA	C3C-C2C	5.16	1.47	1.36
10	bA	805	CLA	C3C-C2C	5.16	1.47	1.36
10	bA	830	CLA	C3C-C2C	5.16	1.47	1.36
10	aA	808	CLA	C3C-C2C	5.16	1.47	1.36
10	aA	832	CLA	C3C-C2C	5.16	1.47	1.36
10	cA	825	CLA	C3C-C2C	5.16	1.47	1.36
10	cB	814	CLA	C3D-C2D	5.16	1.49	1.39
10	cA	821	CLA	C3C-C2C	5.16	1.47	1.36
10	cA	833	CLA	C3B-C2B	5.15	1.47	1.40
10	cA	840	CLA	O2D-CGD	5.15	1.45	1.33
10	cB	839	CLA	C3C-C2C	5.15	1.47	1.36
10	cB	836	CLA	C3D-C2D	5.15	1.49	1.39
10	cB	829	CLA	C3C-C2C	5.15	1.47	1.36
10	bB	824	CLA	C3D-C2D	5.15	1.49	1.39
10	bA	804	CLA	C3C-C2C	5.15	1.47	1.36
10	cB	836	CLA	O2D-CGD	5.14	1.45	1.33
10	bA	837	CLA	C3B-C2B	5.14	1.47	1.40
10	cB	802	CLA	C3C-C2C	5.14	1.47	1.36
10	aA	805	CLA	C3C-C2C	5.14	1.47	1.36
10	aB	822	CLA	O2D-CGD	5.14	1.45	1.33
10	cA	837	CLA	C3B-C2B	5.14	1.47	1.40
10	aB	814	CLA	C3D-C2D	5.14	1.49	1.39
10	bA	825	CLA	C3C-C2C	5.14	1.47	1.36
10	bB	818	CLA	C3D-C2D	5.14	1.49	1.39
10	cA	805	CLA	C3C-C2C	5.14	1.47	1.36
10	cB	816	CLA	C3D-C2D	5.13	1.49	1.39
10	bB	802	CLA	C3C-C2C	5.13	1.47	1.36
10	cB	818	CLA	C3D-C2D	5.13	1.49	1.39
10	aB	801	CLA	C3D-C2D	5.13	1.49	1.39
10	bA	840	CLA	O2D-CGD	5.13	1.45	1.33
10	aA	807	CLA	C3C-C2C	5.13	1.47	1.36
10	aA	825	CLA	C3C-C2C	5.13	1.47	1.36
10	aB	836	CLA	C3D-C2D	5.13	1.49	1.39
10	aB	836	CLA	O2D-CGD	5.12	1.45	1.33
10	aB	816	CLA	C3D-C2D	5.12	1.49	1.39
10	cA	831	CLA	C3C-C2C	5.12	1.47	1.36
10	bA	833	CLA	C3C-C2C	5.12	1.47	1.36
10	bB	814	CLA	C3D-C2D	5.12	1.49	1.39
10	bA	831	CLA	C3C-C2C	5.12	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	808	CLA	C3C-C2C	5.12	1.47	1.36
10	cB	801	CLA	C3D-C2D	5.12	1.49	1.39
10	cA	833	CLA	C3C-C2C	5.12	1.47	1.36
10	aL	202	CLA	C3C-C2C	5.12	1.47	1.36
10	cL	202	CLA	C3C-C2C	5.12	1.47	1.36
10	cB	824	CLA	C3D-C2D	5.12	1.49	1.39
10	aA	837	CLA	C3C-C2C	5.12	1.47	1.36
10	bB	822	CLA	O2D-CGD	5.11	1.45	1.33
10	aA	839	CLA	O2D-CGD	5.11	1.45	1.33
10	bA	837	CLA	C3C-C2C	5.11	1.47	1.36
10	cB	823	CLA	O2D-CGD	5.11	1.45	1.33
10	bL	202	CLA	C3C-C2C	5.11	1.47	1.36
10	bB	816	CLA	C3D-C2D	5.11	1.49	1.39
10	aB	831	CLA	C3D-C2D	5.11	1.49	1.39
10	bA	821	CLA	O2D-CGD	5.11	1.45	1.33
10	aA	840	CLA	O2D-CGD	5.11	1.45	1.33
10	cA	826	CLA	C3B-C2B	5.11	1.47	1.40
10	bA	828	CLA	C3C-C2C	5.11	1.47	1.36
10	aA	829	CLA	C3D-C2D	5.11	1.49	1.39
10	cA	821	CLA	O2D-CGD	5.11	1.45	1.33
10	bB	836	CLA	O2D-CGD	5.11	1.45	1.33
10	aA	804	CLA	C3C-C2C	5.10	1.47	1.36
10	cA	804	CLA	C3C-C2C	5.10	1.47	1.36
10	cA	837	CLA	C3C-C2C	5.10	1.47	1.36
10	aA	821	CLA	O2D-CGD	5.10	1.45	1.33
10	aB	802	CLA	C3C-C2C	5.10	1.47	1.36
10	cA	839	CLA	C3D-C2D	5.10	1.49	1.39
10	aA	833	CLA	C3C-C2C	5.10	1.47	1.36
10	aB	823	CLA	O2D-CGD	5.10	1.45	1.33
10	aA	802	CLA	O2D-CGD	5.10	1.45	1.33
10	bA	802	CLA	O2D-CGD	5.10	1.45	1.33
10	cB	804	CLA	C3C-C2C	5.10	1.47	1.36
10	aA	833	CLA	C3B-C2B	5.10	1.47	1.40
10	bA	808	CLA	C3C-C2C	5.09	1.47	1.36
10	cA	841	CLA	C3C-C2C	5.09	1.47	1.36
10	bB	809	CLA	C3C-C2C	5.09	1.47	1.36
10	cB	811	CLA	C3C-C2C	5.09	1.47	1.36
10	cA	839	CLA	O2D-CGD	5.09	1.45	1.33
10	bB	837	CLA	C3B-C2B	5.09	1.47	1.40
10	bA	809	CLA	O2D-CGD	5.09	1.45	1.33
10	aB	833	CLA	C3D-C2D	5.09	1.49	1.39
10	aL	204	CLA	C3C-C2C	5.09	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	820	CLA	C3D-C2D	5.09	1.49	1.39
10	aB	809	CLA	C3C-C2C	5.09	1.47	1.36
10	bB	830	CLA	C3C-C2C	5.09	1.47	1.36
10	aB	817	CLA	C3C-C2C	5.09	1.47	1.36
10	bB	812	CLA	C3B-C2B	5.09	1.47	1.40
10	aB	821	CLA	C3D-C2D	5.09	1.49	1.39
10	cB	831	CLA	C3D-C2D	5.09	1.49	1.39
10	aA	841	CLA	C3C-C2C	5.09	1.47	1.36
10	aB	810	CLA	C3B-C2B	5.09	1.47	1.40
10	bB	831	CLA	C3D-C2D	5.09	1.49	1.39
10	bB	823	CLA	O2D-CGD	5.08	1.45	1.33
10	cB	812	CLA	C3B-C2B	5.08	1.47	1.40
10	cA	802	CLA	O2D-CGD	5.08	1.45	1.33
10	bB	820	CLA	C3D-C2D	5.08	1.49	1.39
10	aA	831	CLA	C3C-C2C	5.08	1.47	1.36
10	aA	809	CLA	O2D-CGD	5.08	1.45	1.33
10	bB	811	CLA	C3C-C2C	5.08	1.47	1.36
10	cA	830	CLA	C3B-C2B	5.08	1.47	1.40
10	cA	836	CLA	C3C-C2C	5.08	1.47	1.36
10	aA	839	CLA	C3D-C2D	5.08	1.49	1.39
10	aB	837	CLA	C3B-C2B	5.08	1.47	1.40
10	bA	839	CLA	O2D-CGD	5.08	1.45	1.33
10	aB	804	CLA	C3C-C2C	5.08	1.47	1.36
10	bL	204	CLA	C3C-C2C	5.08	1.47	1.36
10	cB	823	CLA	C3D-C2D	5.07	1.49	1.39
10	bB	833	CLA	C3D-C2D	5.07	1.49	1.39
10	cA	828	CLA	C3C-C2C	5.07	1.47	1.36
10	aA	828	CLA	C3C-C2C	5.07	1.47	1.36
10	aB	811	CLA	C3D-C2D	5.07	1.49	1.39
10	cA	829	CLA	C3D-C2D	5.07	1.49	1.39
10	bB	817	CLA	C3C-C2C	5.07	1.47	1.36
10	cA	834	CLA	C3D-C2D	5.07	1.49	1.39
10	bB	831	CLA	O2D-CGD	5.07	1.45	1.33
10	bA	834	CLA	C3D-C2D	5.07	1.49	1.39
10	bB	804	CLA	C3C-C2C	5.07	1.47	1.36
10	bB	810	CLA	C3B-C2B	5.07	1.47	1.40
10	aA	831	CLA	C3D-C2D	5.07	1.49	1.39
10	cB	837	CLA	C3C-C2C	5.07	1.47	1.36
10	cL	204	CLA	C3C-C2C	5.06	1.47	1.36
10	bA	836	CLA	C3C-C2C	5.06	1.47	1.36
10	aA	816	CLA	C3C-C2C	5.06	1.47	1.36
10	aB	811	CLA	C3C-C2C	5.06	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	818	CLA	C3D-C2D	5.06	1.49	1.39
10	bA	838	CLA	C3C-C2C	5.06	1.47	1.36
10	bA	829	CLA	C3D-C2D	5.06	1.49	1.39
10	aA	836	CLA	C3C-C2C	5.06	1.47	1.36
10	bA	816	CLA	C3C-C2C	5.06	1.47	1.36
10	cB	810	CLA	C3B-C2B	5.06	1.47	1.40
10	aA	826	CLA	C3B-C2B	5.06	1.47	1.40
10	bA	839	CLA	C3D-C2D	5.06	1.49	1.39
10	cB	809	CLA	C3C-C2C	5.06	1.47	1.36
10	cA	831	CLA	C3D-C2D	5.06	1.49	1.39
10	aB	837	CLA	C3C-C2C	5.06	1.47	1.36
10	cB	820	CLA	C3D-C2D	5.06	1.49	1.39
10	bB	837	CLA	C3C-C2C	5.06	1.47	1.36
10	bB	823	CLA	C3D-C2D	5.06	1.49	1.39
10	cB	808	CLA	C3C-C2C	5.06	1.47	1.36
10	bA	830	CLA	C3B-C2B	5.05	1.47	1.40
10	aB	831	CLA	O2D-CGD	5.05	1.45	1.33
10	aA	810	CLA	C3D-C2D	5.05	1.49	1.39
10	aB	812	CLA	C3B-C2B	5.05	1.47	1.40
10	bB	811	CLA	C3D-C2D	5.05	1.49	1.39
10	cA	816	CLA	C3C-C2C	5.05	1.47	1.36
10	cB	837	CLA	C3B-C2B	5.05	1.47	1.40
10	bB	814	CLA	C3C-C2C	5.05	1.47	1.36
10	cB	833	CLA	C3D-C2D	5.05	1.49	1.39
10	aA	854	CLA	O2D-CGD	5.05	1.45	1.33
10	cB	814	CLA	C3C-C2C	5.05	1.47	1.36
10	bA	826	CLA	C3B-C2B	5.05	1.47	1.40
10	cB	811	CLA	C3D-C2D	5.05	1.49	1.39
10	bA	841	CLA	C3C-C2C	5.05	1.47	1.36
10	cA	809	CLA	O2D-CGD	5.04	1.45	1.33
10	aA	834	CLA	C3D-C2D	5.04	1.49	1.39
10	bA	831	CLA	C3D-C2D	5.04	1.49	1.39
10	bB	808	CLA	C3C-C2C	5.04	1.47	1.36
10	cB	803	CLA	C3C-C2C	5.04	1.47	1.36
10	aB	823	CLA	C3D-C2D	5.04	1.49	1.39
10	bB	841	CLA	C3C-C2C	5.04	1.47	1.36
10	cA	810	CLA	C3D-C2D	5.04	1.49	1.39
10	bA	854	CLA	O2D-CGD	5.04	1.45	1.33
10	cB	817	CLA	C3C-C2C	5.04	1.47	1.36
10	bB	803	CLA	C3C-C2C	5.04	1.47	1.36
10	cA	803	CLA	C3D-C2D	5.04	1.49	1.39
10	bA	810	CLA	O2D-CGD	5.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	831	CLA	O2D-CGD	5.04	1.45	1.33
10	aB	830	CLA	C3C-C2C	5.04	1.47	1.36
10	aB	835	CLA	O2D-CGD	5.04	1.45	1.33
10	bB	808	CLA	O2D-CGD	5.04	1.45	1.33
10	aB	808	CLA	C3C-C2C	5.03	1.47	1.36
10	cA	854	CLA	O2D-CGD	5.03	1.45	1.33
10	aA	806	CLA	O2D-CGD	5.03	1.45	1.33
10	cA	818	CLA	C3D-C2D	5.03	1.49	1.39
10	aA	803	CLA	C3D-C2D	5.03	1.49	1.39
10	aA	814	CLA	O2D-CGD	5.03	1.45	1.33
10	bA	814	CLA	O2D-CGD	5.03	1.45	1.33
10	cB	820	CLA	O2D-CGD	5.03	1.45	1.33
10	aB	813	CLA	C3D-C2D	5.03	1.49	1.39
10	cB	821	CLA	C3D-C2D	5.03	1.49	1.39
10	cA	838	CLA	C3B-C2B	5.03	1.47	1.40
10	aB	818	CLA	O2D-CGD	5.03	1.45	1.33
10	aB	828	CLA	C3C-C2C	5.03	1.47	1.36
10	bA	810	CLA	C3D-C2D	5.03	1.49	1.39
10	bA	806	CLA	O2D-CGD	5.03	1.45	1.33
10	aA	838	CLA	C3B-C2B	5.02	1.47	1.40
10	bB	813	CLA	C3D-C2D	5.02	1.49	1.39
10	aB	814	CLA	C3C-C2C	5.02	1.47	1.36
10	aA	818	CLA	C3D-C2D	5.02	1.49	1.39
10	cA	834	CLA	O2D-CGD	5.02	1.45	1.33
10	aA	810	CLA	O2D-CGD	5.02	1.45	1.33
10	aB	803	CLA	C3C-C2C	5.02	1.47	1.36
10	cB	818	CLA	O2D-CGD	5.02	1.45	1.33
10	cB	835	CLA	O2D-CGD	5.02	1.45	1.33
10	aB	808	CLA	O2D-CGD	5.02	1.45	1.33
10	bA	803	CLA	C3D-C2D	5.02	1.49	1.39
10	bB	818	CLA	O2D-CGD	5.02	1.45	1.33
10	bA	834	CLA	O2D-CGD	5.01	1.45	1.33
10	cA	810	CLA	O2D-CGD	5.01	1.45	1.33
10	cA	814	CLA	O2D-CGD	5.01	1.45	1.33
10	cB	830	CLA	C3C-C2C	5.01	1.47	1.36
10	bB	828	CLA	C3C-C2C	5.01	1.47	1.36
10	cB	841	CLA	C3C-C2C	5.01	1.47	1.36
10	cA	806	CLA	O2D-CGD	5.01	1.45	1.33
10	aB	841	CLA	C3C-C2C	5.01	1.47	1.36
10	aA	838	CLA	C3C-C2C	5.01	1.47	1.36
10	aA	834	CLA	O2D-CGD	5.01	1.45	1.33
9	cA	801	CL0	C3C-C2C	5.01	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	842	CLA	C3D-C2D	5.01	1.49	1.39
10	aA	830	CLA	C3B-C2B	5.01	1.47	1.40
10	aB	826	CLA	C3D-C2D	5.01	1.49	1.39
10	cB	808	CLA	O2D-CGD	5.00	1.45	1.33
10	bB	826	CLA	C3D-C2D	5.00	1.49	1.39
9	bA	801	CL0	C3C-C2C	5.00	1.47	1.36
10	bB	821	CLA	C3D-C2D	5.00	1.49	1.39
10	aB	809	CLA	C3D-C2D	5.00	1.49	1.39
10	aA	804	CLA	O2D-CGD	4.99	1.45	1.33
10	bA	804	CLA	O2D-CGD	4.99	1.45	1.33
10	bA	842	CLA	C3D-C2D	4.99	1.49	1.39
10	cA	838	CLA	C3C-C2C	4.99	1.47	1.36
10	cA	804	CLA	O2D-CGD	4.99	1.45	1.33
10	cB	828	CLA	C3C-C2C	4.99	1.47	1.36
10	cB	826	CLA	C3D-C2D	4.99	1.49	1.39
10	bB	835	CLA	O2D-CGD	4.99	1.45	1.33
10	aB	806	CLA	C3C-C2C	4.99	1.47	1.36
10	bA	833	CLA	C3D-C2D	4.99	1.49	1.39
10	bA	838	CLA	C3B-C2B	4.99	1.47	1.40
10	cB	817	CLA	O2D-CGD	4.98	1.45	1.33
10	cA	815	CLA	O2D-CGD	4.98	1.45	1.33
10	aB	817	CLA	O2D-CGD	4.98	1.45	1.33
10	aA	803	CLA	O2D-CGD	4.98	1.45	1.33
10	bB	805	CLA	C3D-C2D	4.98	1.49	1.39
10	cB	809	CLA	C3D-C2D	4.98	1.49	1.39
10	aA	828	CLA	C3D-C2D	4.98	1.49	1.39
9	aA	801	CL0	C3C-C2C	4.98	1.47	1.36
10	aA	816	CLA	O2D-CGD	4.97	1.45	1.33
10	cB	817	CLA	C3D-C2D	4.97	1.49	1.39
10	bB	806	CLA	C3C-C2C	4.97	1.47	1.36
10	bB	840	CLA	C3C-C2C	4.97	1.47	1.36
10	bA	816	CLA	O2D-CGD	4.97	1.45	1.33
10	aB	833	CLA	O2D-CGD	4.97	1.45	1.33
10	bB	838	CLA	C3D-C2D	4.97	1.49	1.39
10	aB	838	CLA	C3D-C2D	4.97	1.49	1.39
10	cB	838	CLA	O2D-CGD	4.97	1.45	1.33
10	cA	814	CLA	C3D-C2D	4.97	1.49	1.39
10	aA	833	CLA	C3D-C2D	4.97	1.49	1.39
10	bA	820	CLA	O2D-CGD	4.97	1.45	1.33
10	bB	809	CLA	C3D-C2D	4.97	1.49	1.39
10	aA	820	CLA	O2D-CGD	4.97	1.45	1.33
10	bB	817	CLA	O2D-CGD	4.97	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	816	CLA	O2D-CGD	4.97	1.45	1.33
10	cA	820	CLA	O2D-CGD	4.97	1.45	1.33
10	aA	815	CLA	O2D-CGD	4.96	1.45	1.33
10	bA	812	CLA	C3D-C2D	4.96	1.49	1.39
10	cA	805	CLA	C3D-C2D	4.96	1.49	1.39
10	aB	820	CLA	O2D-CGD	4.96	1.45	1.33
10	cA	841	CLA	O2D-CGD	4.96	1.45	1.33
10	bA	815	CLA	O2D-CGD	4.96	1.45	1.33
10	cB	820	CLA	C3B-C2B	4.96	1.47	1.40
10	bA	803	CLA	O2D-CGD	4.96	1.45	1.33
10	bB	833	CLA	O2D-CGD	4.96	1.45	1.33
10	aA	842	CLA	C3D-C2D	4.96	1.49	1.39
10	cA	803	CLA	O2D-CGD	4.95	1.45	1.33
10	cB	838	CLA	C3D-C2D	4.95	1.49	1.39
10	bB	820	CLA	C3B-C2B	4.95	1.47	1.40
10	bA	817	CLA	O2D-CGD	4.95	1.45	1.33
10	aB	801	CLA	C3C-C2C	4.95	1.47	1.36
10	cB	840	CLA	C3C-C2C	4.95	1.47	1.36
10	cB	833	CLA	O2D-CGD	4.95	1.45	1.33
10	bA	841	CLA	O2D-CGD	4.95	1.45	1.33
10	bA	828	CLA	C3D-C2D	4.95	1.49	1.39
10	aA	823	CLA	O2D-CGD	4.95	1.45	1.33
10	cB	805	CLA	C3D-C2D	4.95	1.49	1.39
10	cB	806	CLA	C3C-C2C	4.95	1.47	1.36
10	aB	837	CLA	C3D-C2D	4.94	1.49	1.39
10	aB	840	CLA	C3C-C2C	4.94	1.47	1.36
10	cB	813	CLA	C3D-C2D	4.94	1.49	1.39
10	bB	838	CLA	O2D-CGD	4.94	1.45	1.33
10	bB	820	CLA	O2D-CGD	4.94	1.45	1.33
10	aB	821	CLA	O2D-CGD	4.94	1.45	1.33
10	cA	817	CLA	O2D-CGD	4.94	1.45	1.33
10	aA	811	CLA	C3D-C2D	4.94	1.49	1.39
10	cB	825	CLA	C3D-C2D	4.94	1.49	1.39
10	aA	820	CLA	C3D-C2D	4.94	1.49	1.39
10	cA	812	CLA	C3D-C2D	4.94	1.49	1.39
10	bA	819	CLA	C3D-C2D	4.94	1.49	1.39
10	bB	840	CLA	O2D-CGD	4.94	1.45	1.33
10	bB	825	CLA	C3D-C2D	4.94	1.49	1.39
10	aB	805	CLA	C3D-C2D	4.94	1.49	1.39
10	aB	817	CLA	C3D-C2D	4.94	1.49	1.39
10	bB	801	CLA	C3C-C2C	4.93	1.47	1.36
10	bA	811	CLA	C3D-C2D	4.93	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bL	205	CLA	C3D-C2D	4.93	1.49	1.39
10	aA	805	CLA	C3D-C2D	4.93	1.49	1.39
10	cA	823	CLA	O2D-CGD	4.93	1.45	1.33
10	bA	820	CLA	C3D-C2D	4.93	1.49	1.39
10	cB	819	CLA	C3D-C2D	4.93	1.49	1.39
10	bA	805	CLA	C3D-C2D	4.93	1.49	1.39
10	aA	819	CLA	C3D-C2D	4.93	1.49	1.39
10	cA	811	CLA	C3D-C2D	4.93	1.49	1.39
10	cB	811	CLA	C3B-C2B	4.93	1.47	1.40
10	cA	819	CLA	C3D-C2D	4.93	1.49	1.39
10	cB	801	CLA	C3C-C2C	4.93	1.47	1.36
10	cA	826	CLA	CHC-C1C	4.93	1.48	1.35
10	aB	824	CLA	O2D-CGD	4.93	1.45	1.33
10	bB	824	CLA	O2D-CGD	4.93	1.45	1.33
10	bB	821	CLA	O2D-CGD	4.93	1.45	1.33
10	aA	817	CLA	O2D-CGD	4.93	1.45	1.33
10	aB	820	CLA	C3B-C2B	4.93	1.47	1.40
10	aB	825	CLA	C3D-C2D	4.93	1.49	1.39
10	bA	813	CLA	C3D-C2D	4.93	1.49	1.39
10	aA	814	CLA	C3D-C2D	4.93	1.49	1.39
10	aB	819	CLA	C3D-C2D	4.92	1.49	1.39
10	bA	842	CLA	C3C-C2C	4.92	1.47	1.36
10	cB	832	CLA	C3D-C2D	4.92	1.49	1.39
10	bA	842	CLA	O2D-CGD	4.92	1.45	1.33
10	cA	806	CLA	C3D-C2D	4.92	1.49	1.39
10	bB	817	CLA	C3D-C2D	4.92	1.49	1.39
10	aB	832	CLA	C3D-C2D	4.92	1.49	1.39
10	cA	828	CLA	C3D-C2D	4.92	1.49	1.39
10	cA	820	CLA	C3D-C2D	4.92	1.49	1.39
10	cB	837	CLA	C3D-C2D	4.92	1.49	1.39
10	aA	822	CLA	O2D-CGD	4.92	1.45	1.33
10	bA	822	CLA	O2D-CGD	4.92	1.45	1.33
10	bB	837	CLA	C3D-C2D	4.92	1.49	1.39
10	cA	833	CLA	C3D-C2D	4.92	1.49	1.39
10	bA	823	CLA	O2D-CGD	4.91	1.45	1.33
10	cB	825	CLA	C3C-C2C	4.91	1.47	1.36
10	aA	802	CLA	C3D-C2D	4.91	1.49	1.39
10	aB	840	CLA	O2D-CGD	4.91	1.45	1.33
10	bB	811	CLA	C3B-C2B	4.91	1.47	1.40
10	cA	840	CLA	C3D-C2D	4.91	1.49	1.39
10	aA	841	CLA	O2D-CGD	4.91	1.45	1.33
10	cA	828	CLA	O2D-CGD	4.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	812	CLA	C3D-C2D	4.91	1.49	1.39
10	aA	842	CLA	C3C-C2C	4.91	1.47	1.36
10	cB	821	CLA	O2D-CGD	4.91	1.45	1.33
10	cA	815	CLA	C3D-C2D	4.91	1.49	1.39
10	cA	802	CLA	C3D-C2D	4.91	1.49	1.39
10	aA	826	CLA	CHC-C1C	4.91	1.48	1.35
10	aA	819	CLA	O2D-CGD	4.91	1.45	1.33
10	bB	819	CLA	C3D-C2D	4.91	1.49	1.39
10	cL	205	CLA	C3D-C2D	4.91	1.49	1.39
10	aB	812	CLA	O2D-CGD	4.91	1.45	1.33
10	bA	826	CLA	CHC-C1C	4.91	1.48	1.35
10	bA	811	CLA	O2D-CGD	4.91	1.45	1.33
10	cB	840	CLA	O2D-CGD	4.90	1.45	1.33
10	aA	842	CLA	O2D-CGD	4.90	1.45	1.33
10	aB	813	CLA	O2D-CGD	4.90	1.45	1.33
10	cB	829	CLA	O2D-CGD	4.90	1.45	1.33
10	cA	834	CLA	C3B-C2B	4.90	1.47	1.40
10	aB	838	CLA	O2D-CGD	4.90	1.45	1.33
10	bA	840	CLA	C3D-C2D	4.90	1.49	1.39
10	cA	827	CLA	O2D-CGD	4.90	1.45	1.33
10	aA	811	CLA	O2D-CGD	4.90	1.45	1.33
10	aA	827	CLA	O2D-CGD	4.90	1.45	1.33
10	aB	825	CLA	C3C-C2C	4.90	1.47	1.36
10	bB	832	CLA	C3D-C2D	4.90	1.49	1.39
10	bA	828	CLA	O2D-CGD	4.90	1.45	1.33
10	bA	830	CLA	C3D-C2D	4.90	1.49	1.39
10	cA	819	CLA	O2D-CGD	4.90	1.45	1.33
10	bB	825	CLA	C3C-C2C	4.89	1.47	1.36
10	cA	842	CLA	C3C-C2C	4.89	1.47	1.36
10	bA	826	CLA	O2D-CGD	4.89	1.45	1.33
10	cA	842	CLA	O2D-CGD	4.89	1.45	1.33
10	bB	812	CLA	O2D-CGD	4.89	1.45	1.33
10	aA	828	CLA	O2D-CGD	4.89	1.45	1.33
10	cB	828	CLA	O2D-CGD	4.89	1.45	1.33
10	cA	811	CLA	O2D-CGD	4.89	1.45	1.33
10	bA	803	CLA	CHC-C1C	4.89	1.48	1.35
10	bA	814	CLA	C3D-C2D	4.89	1.49	1.39
10	bA	827	CLA	O2D-CGD	4.89	1.45	1.33
10	cB	824	CLA	O2D-CGD	4.89	1.45	1.33
10	aB	826	CLA	CHC-C1C	4.89	1.48	1.35
10	bA	806	CLA	C3D-C2D	4.89	1.49	1.39
10	bA	815	CLA	C3D-C2D	4.89	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aL	205	CLA	C3D-C2D	4.89	1.49	1.39
10	cA	803	CLA	CHC-C1C	4.88	1.48	1.35
10	aB	812	CLA	C3D-C2D	4.88	1.49	1.39
10	bA	819	CLA	O2D-CGD	4.88	1.45	1.33
10	aA	806	CLA	C3D-C2D	4.88	1.49	1.39
10	bB	826	CLA	CHC-C1C	4.88	1.48	1.35
10	bB	811	CLA	O2D-CGD	4.88	1.45	1.33
10	cB	826	CLA	CHC-C1C	4.88	1.48	1.35
10	aA	813	CLA	C3D-C2D	4.88	1.49	1.39
10	bA	841	CLA	C3D-C2D	4.88	1.49	1.39
10	bA	802	CLA	C3D-C2D	4.88	1.49	1.39
10	aA	840	CLA	C3D-C2D	4.88	1.49	1.39
10	aB	829	CLA	O2D-CGD	4.88	1.45	1.33
10	cA	813	CLA	C3D-C2D	4.88	1.49	1.39
10	aA	815	CLA	C3D-C2D	4.87	1.49	1.39
10	aB	811	CLA	C3B-C2B	4.87	1.47	1.40
10	bB	819	CLA	O2D-CGD	4.87	1.45	1.33
10	cB	827	CLA	O2D-CGD	4.87	1.45	1.33
10	aB	827	CLA	O2D-CGD	4.87	1.45	1.33
10	cL	204	CLA	C3D-C2D	4.87	1.49	1.39
10	aA	803	CLA	CHC-C1C	4.87	1.48	1.35
10	aB	810	CLA	C3C-C2C	4.87	1.47	1.36
10	cA	830	CLA	C3D-C2D	4.87	1.49	1.39
10	bB	828	CLA	O2D-CGD	4.87	1.45	1.33
10	cB	811	CLA	O2D-CGD	4.87	1.45	1.33
10	cB	812	CLA	O2D-CGD	4.87	1.45	1.33
10	cB	813	CLA	O2D-CGD	4.86	1.45	1.33
10	bB	829	CLA	O2D-CGD	4.86	1.45	1.33
10	cA	841	CLA	C3D-C2D	4.86	1.49	1.39
10	cB	810	CLA	C3C-C2C	4.86	1.47	1.36
10	aB	841	CLA	C3D-C2D	4.86	1.49	1.39
10	cA	809	CLA	C3D-C2D	4.86	1.49	1.39
10	cB	819	CLA	O2D-CGD	4.86	1.45	1.33
10	bB	812	CLA	C3D-C2D	4.86	1.49	1.39
10	aA	841	CLA	C3D-C2D	4.86	1.49	1.39
10	bL	204	CLA	C3D-C2D	4.86	1.49	1.39
10	aB	811	CLA	O2D-CGD	4.86	1.45	1.33
10	aB	819	CLA	O2D-CGD	4.86	1.45	1.33
10	cA	822	CLA	O2D-CGD	4.86	1.45	1.33
10	aA	830	CLA	C3D-C2D	4.86	1.48	1.39
10	cA	826	CLA	O2D-CGD	4.85	1.45	1.33
10	aB	828	CLA	O2D-CGD	4.85	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	818	CLA	O2D-CGD	4.85	1.45	1.33
10	bB	827	CLA	O2D-CGD	4.85	1.45	1.33
10	bB	835	CLA	C3D-C2D	4.85	1.48	1.39
10	bB	813	CLA	O2D-CGD	4.85	1.45	1.33
10	bA	807	CLA	O2D-CGD	4.85	1.45	1.33
10	cA	813	CLA	O2D-CGD	4.85	1.45	1.33
10	bB	841	CLA	C3D-C2D	4.85	1.48	1.39
10	cA	807	CLA	O2D-CGD	4.85	1.45	1.33
10	cA	825	CLA	CHC-C1C	4.85	1.48	1.35
10	aL	203	CLA	C3D-C2D	4.84	1.48	1.39
10	cB	835	CLA	C3D-C2D	4.84	1.48	1.39
10	bL	203	CLA	C3D-C2D	4.84	1.48	1.39
10	bB	835	CLA	CHC-C1C	4.84	1.48	1.35
10	cA	806	CLA	CHC-C1C	4.84	1.48	1.35
10	aA	826	CLA	O2D-CGD	4.84	1.45	1.33
10	bA	809	CLA	C3D-C2D	4.84	1.48	1.39
10	cA	854	CLA	C3D-C2D	4.84	1.48	1.39
10	bA	806	CLA	CHC-C1C	4.83	1.48	1.35
10	bB	810	CLA	C3C-C2C	4.83	1.46	1.36
10	bA	818	CLA	O2D-CGD	4.83	1.45	1.33
10	aB	822	CLA	C3D-C2D	4.83	1.48	1.39
10	bA	813	CLA	O2D-CGD	4.83	1.45	1.33
10	bA	825	CLA	CHC-C1C	4.83	1.48	1.35
10	cB	819	CLA	C3C-C2C	4.83	1.46	1.36
10	aB	835	CLA	C3D-C2D	4.83	1.48	1.39
10	bA	807	CLA	C3D-C2D	4.83	1.48	1.39
10	aA	854	CLA	C3D-C2D	4.83	1.48	1.39
10	cA	824	CLA	O2D-CGD	4.83	1.45	1.33
10	aB	802	CLA	O2D-CGD	4.83	1.45	1.33
10	cA	818	CLA	O2D-CGD	4.83	1.45	1.33
10	aA	813	CLA	O2D-CGD	4.83	1.45	1.33
10	bB	837	CLA	O2D-CGD	4.83	1.45	1.33
10	aA	809	CLA	C3D-C2D	4.83	1.48	1.39
10	cB	837	CLA	O2D-CGD	4.82	1.45	1.33
10	cB	802	CLA	O2D-CGD	4.82	1.45	1.33
10	cA	820	CLA	CHC-C1C	4.82	1.48	1.35
10	bA	823	CLA	C3D-C2D	4.82	1.48	1.39
10	cB	807	CLA	O2D-CGD	4.82	1.45	1.33
10	aA	825	CLA	CHC-C1C	4.82	1.48	1.35
10	aA	806	CLA	CHC-C1C	4.82	1.48	1.35
10	cA	823	CLA	C3D-C2D	4.82	1.48	1.39
10	aB	835	CLA	CHC-C1C	4.82	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	816	CLA	C3D-C2D	4.82	1.48	1.39
10	cB	835	CLA	CHC-C1C	4.82	1.48	1.35
10	bB	822	CLA	C3D-C2D	4.82	1.48	1.39
10	aA	807	CLA	O2D-CGD	4.82	1.45	1.33
10	cB	822	CLA	C3D-C2D	4.82	1.48	1.39
10	aB	819	CLA	C3C-C2C	4.82	1.46	1.36
10	cB	841	CLA	C3D-C2D	4.82	1.48	1.39
10	cB	812	CLA	C3D-C2D	4.82	1.48	1.39
10	bB	802	CLA	O2D-CGD	4.82	1.45	1.33
10	aA	824	CLA	O2D-CGD	4.81	1.45	1.33
10	cA	808	CLA	O2D-CGD	4.81	1.45	1.33
10	aA	823	CLA	C3D-C2D	4.81	1.48	1.39
10	cA	854	CLA	CHC-C1C	4.81	1.48	1.35
10	bA	824	CLA	O2D-CGD	4.81	1.45	1.33
10	cA	824	CLA	CHC-C1C	4.81	1.48	1.35
10	aL	203	CLA	O2D-CGD	4.81	1.45	1.33
10	aA	834	CLA	C3B-C2B	4.81	1.47	1.40
10	cA	835	CLA	C3D-C2D	4.81	1.48	1.39
10	bA	854	CLA	C3D-C2D	4.81	1.48	1.39
10	aL	204	CLA	C3D-C2D	4.80	1.48	1.39
10	bB	819	CLA	C3C-C2C	4.80	1.46	1.36
10	cL	203	CLA	C3D-C2D	4.80	1.48	1.39
10	cB	815	CLA	C3D-C2D	4.80	1.48	1.39
10	cB	825	CLA	O2D-CGD	4.80	1.45	1.33
10	aB	806	CLA	CHC-C1C	4.80	1.48	1.35
10	cA	816	CLA	CHC-C1C	4.80	1.48	1.35
10	bB	839	CLA	C3D-C2D	4.80	1.48	1.39
10	cB	839	CLA	O2D-CGD	4.80	1.45	1.33
10	cA	805	CLA	O2D-CGD	4.80	1.45	1.33
10	cA	835	CLA	O2D-CGD	4.80	1.45	1.33
10	bA	835	CLA	O2D-CGD	4.80	1.45	1.33
10	bA	824	CLA	CHC-C1C	4.80	1.48	1.35
10	bA	854	CLA	CHC-C1C	4.80	1.48	1.35
10	aA	835	CLA	O2D-CGD	4.79	1.45	1.33
10	bA	834	CLA	C3B-C2B	4.79	1.47	1.40
10	bB	806	CLA	CHC-C1C	4.79	1.48	1.35
10	aA	854	CLA	CHC-C1C	4.79	1.48	1.35
10	bB	807	CLA	O2D-CGD	4.79	1.45	1.33
10	aA	835	CLA	C3D-C2D	4.79	1.48	1.39
10	cB	816	CLA	O2D-CGD	4.79	1.45	1.33
10	cA	809	CLA	CHC-C1C	4.79	1.48	1.35
10	bA	820	CLA	CHC-C1C	4.79	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	806	CLA	CHC-C1C	4.79	1.48	1.35
10	bB	825	CLA	O2D-CGD	4.79	1.45	1.33
10	cB	806	CLA	C3D-C2D	4.79	1.48	1.39
10	cA	807	CLA	C3D-C2D	4.79	1.48	1.39
10	aA	824	CLA	CHC-C1C	4.79	1.48	1.35
10	aB	825	CLA	O2D-CGD	4.79	1.45	1.33
10	cA	817	CLA	C3D-C2D	4.79	1.48	1.39
10	aB	807	CLA	O2D-CGD	4.78	1.45	1.33
10	aA	805	CLA	O2D-CGD	4.78	1.45	1.33
10	cA	831	CLA	O2D-CGD	4.78	1.45	1.33
10	aA	816	CLA	CHC-C1C	4.78	1.48	1.35
10	cA	812	CLA	CHC-C1C	4.78	1.48	1.35
10	bA	808	CLA	O2D-CGD	4.78	1.45	1.33
10	bA	831	CLA	O2D-CGD	4.78	1.45	1.33
10	aB	837	CLA	O2D-CGD	4.78	1.45	1.33
10	aB	839	CLA	O2D-CGD	4.78	1.45	1.33
10	cB	834	CLA	CHC-C1C	4.78	1.48	1.35
10	bB	804	CLA	CHC-C1C	4.78	1.48	1.35
10	aA	808	CLA	O2D-CGD	4.78	1.45	1.33
10	aA	807	CLA	C3D-C2D	4.78	1.48	1.39
10	bA	835	CLA	C3D-C2D	4.78	1.48	1.39
10	bA	816	CLA	C3D-C2D	4.78	1.48	1.39
10	aB	838	CLA	CHC-C1C	4.77	1.47	1.35
10	bA	816	CLA	CHC-C1C	4.77	1.47	1.35
10	aA	831	CLA	O2D-CGD	4.77	1.45	1.33
10	aB	818	CLA	CHC-C1C	4.77	1.47	1.35
10	aB	806	CLA	C3D-C2D	4.77	1.48	1.39
10	bB	841	CLA	O2D-CGD	4.77	1.45	1.33
10	bB	806	CLA	C3D-C2D	4.77	1.48	1.39
10	bB	834	CLA	CHC-C1C	4.77	1.47	1.35
10	bB	816	CLA	O2D-CGD	4.77	1.45	1.33
10	bB	815	CLA	C3D-C2D	4.77	1.48	1.39
10	aB	816	CLA	O2D-CGD	4.77	1.45	1.33
10	aA	812	CLA	CHC-C1C	4.77	1.47	1.35
10	bA	817	CLA	C3D-C2D	4.77	1.48	1.39
10	bB	818	CLA	CHC-C1C	4.77	1.47	1.35
10	cL	203	CLA	O2D-CGD	4.77	1.45	1.33
10	bB	839	CLA	O2D-CGD	4.76	1.45	1.33
10	aB	834	CLA	CHC-C1C	4.76	1.47	1.35
10	aB	810	CLA	O2D-CGD	4.76	1.45	1.33
10	aB	804	CLA	CHC-C1C	4.76	1.47	1.35
10	bA	809	CLA	CHC-C1C	4.76	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	841	CLA	O2D-CGD	4.76	1.45	1.33
10	bL	203	CLA	O2D-CGD	4.76	1.45	1.33
10	aA	817	CLA	CHC-C1C	4.76	1.47	1.35
10	aA	820	CLA	CHC-C1C	4.76	1.47	1.35
10	aB	815	CLA	C3D-C2D	4.76	1.48	1.39
10	bA	812	CLA	CHC-C1C	4.76	1.47	1.35
10	bB	838	CLA	CHC-C1C	4.76	1.47	1.35
10	aA	809	CLA	CHC-C1C	4.76	1.47	1.35
10	aB	820	CLA	CHC-C1C	4.76	1.47	1.35
10	aA	817	CLA	C3D-C2D	4.76	1.48	1.39
10	aA	822	CLA	CHC-C1C	4.76	1.47	1.35
10	bB	831	CLA	CHC-C1C	4.75	1.47	1.35
10	cB	838	CLA	CHC-C1C	4.75	1.47	1.35
10	bA	822	CLA	CHC-C1C	4.75	1.47	1.35
10	bA	840	CLA	CHC-C1C	4.75	1.47	1.35
10	aA	841	CLA	CHC-C1C	4.75	1.47	1.35
10	aB	831	CLA	CHC-C1C	4.75	1.47	1.35
10	bB	810	CLA	O2D-CGD	4.75	1.44	1.33
10	cA	822	CLA	CHC-C1C	4.75	1.47	1.35
10	cB	831	CLA	CHC-C1C	4.75	1.47	1.35
10	aB	839	CLA	C3D-C2D	4.75	1.48	1.39
10	cB	820	CLA	CHC-C1C	4.75	1.47	1.35
9	bA	801	CL0	O2D-CGD	4.74	1.44	1.33
10	bA	805	CLA	O2D-CGD	4.74	1.44	1.33
10	bL	204	CLA	O2D-CGD	4.74	1.44	1.33
10	cB	804	CLA	CHC-C1C	4.74	1.47	1.35
10	bA	837	CLA	C3D-C2D	4.74	1.48	1.39
10	cA	840	CLA	CHC-C1C	4.74	1.47	1.35
10	aA	832	CLA	C3D-C2D	4.74	1.48	1.39
10	bB	807	CLA	C3D-C2D	4.74	1.48	1.39
10	aA	816	CLA	C3D-C2D	4.74	1.48	1.39
10	cB	841	CLA	O2D-CGD	4.74	1.44	1.33
10	cA	841	CLA	CHC-C1C	4.74	1.47	1.35
10	aA	840	CLA	CHC-C1C	4.74	1.47	1.35
9	cA	801	CL0	O2D-CGD	4.73	1.44	1.33
10	aA	819	CLA	CHC-C1C	4.73	1.47	1.35
10	bB	830	CLA	O2D-CGD	4.73	1.44	1.33
10	aA	818	CLA	CHC-C1C	4.73	1.47	1.35
11	cA	844	PQN	C10-C5	4.73	1.48	1.40
10	aL	204	CLA	O2D-CGD	4.73	1.44	1.33
9	aA	801	CL0	O2D-CGD	4.73	1.44	1.33
10	cB	818	CLA	CHC-C1C	4.73	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	830	CLA	O2D-CGD	4.73	1.44	1.33
10	bA	819	CLA	CHC-C1C	4.73	1.47	1.35
10	cA	832	CLA	C3D-C2D	4.73	1.48	1.39
10	bA	817	CLA	CHC-C1C	4.73	1.47	1.35
10	bA	841	CLA	CHC-C1C	4.73	1.47	1.35
10	cB	810	CLA	O2D-CGD	4.73	1.44	1.33
10	bB	816	CLA	CHC-C1C	4.73	1.47	1.35
10	aB	815	CLA	O2D-CGD	4.73	1.44	1.33
10	cB	839	CLA	C3D-C2D	4.73	1.48	1.39
10	bA	818	CLA	CHC-C1C	4.73	1.47	1.35
11	bA	844	PQN	C10-C5	4.73	1.48	1.40
10	cB	807	CLA	C3D-C2D	4.72	1.48	1.39
10	cA	811	CLA	CHC-C1C	4.72	1.47	1.35
10	cA	837	CLA	O2D-CGD	4.72	1.44	1.33
10	cB	815	CLA	O2D-CGD	4.72	1.44	1.33
10	aB	805	CLA	C3C-C2C	4.72	1.46	1.36
10	bA	811	CLA	CHC-C1C	4.72	1.47	1.35
10	cA	837	CLA	C3D-C2D	4.72	1.48	1.39
10	aB	809	CLA	O2D-CGD	4.72	1.44	1.33
10	cL	204	CLA	O2D-CGD	4.72	1.44	1.33
10	bA	832	CLA	C3D-C2D	4.71	1.48	1.39
10	aA	811	CLA	CHC-C1C	4.71	1.47	1.35
10	aB	833	CLA	CHC-C1C	4.71	1.47	1.35
10	bB	820	CLA	CHC-C1C	4.71	1.47	1.35
10	aA	837	CLA	C3D-C2D	4.71	1.48	1.39
10	cA	819	CLA	CHC-C1C	4.71	1.47	1.35
10	cA	821	CLA	CHC-C1C	4.71	1.47	1.35
10	aL	204	CLA	CHC-C1C	4.71	1.47	1.35
10	bA	837	CLA	O2D-CGD	4.71	1.44	1.33
10	cB	813	CLA	CHC-C1C	4.71	1.47	1.35
10	bB	833	CLA	CHC-C1C	4.71	1.47	1.35
10	aA	821	CLA	CHC-C1C	4.71	1.47	1.35
10	cL	205	CLA	O2D-CGD	4.71	1.44	1.33
10	cB	805	CLA	C3C-C2C	4.70	1.46	1.36
10	bA	821	CLA	CHC-C1C	4.70	1.47	1.35
10	aB	830	CLA	O2D-CGD	4.70	1.44	1.33
10	cA	817	CLA	CHC-C1C	4.70	1.47	1.35
10	bB	815	CLA	O2D-CGD	4.70	1.44	1.33
10	cA	818	CLA	CHC-C1C	4.70	1.47	1.35
10	cB	816	CLA	CHC-C1C	4.70	1.47	1.35
10	bA	825	CLA	O2D-CGD	4.70	1.44	1.33
11	aA	844	PQN	C10-C5	4.70	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	809	CLA	O2D-CGD	4.70	1.44	1.33
10	aL	203	CLA	CHC-C1C	4.70	1.47	1.35
10	cA	813	CLA	CHC-C1C	4.70	1.47	1.35
10	cA	838	CLA	O2D-CGD	4.70	1.44	1.33
10	aA	837	CLA	O2D-CGD	4.70	1.44	1.33
10	bB	809	CLA	O2D-CGD	4.69	1.44	1.33
10	bL	203	CLA	CHC-C1C	4.69	1.47	1.35
9	bA	801	CL0	C3D-C2D	4.69	1.48	1.39
10	bL	204	CLA	CHC-C1C	4.69	1.47	1.35
10	cL	204	CLA	CHC-C1C	4.69	1.47	1.35
10	aB	807	CLA	C3D-C2D	4.69	1.48	1.39
10	cA	829	CLA	O2D-CGD	4.69	1.44	1.33
10	aL	205	CLA	O2D-CGD	4.69	1.44	1.33
10	bB	813	CLA	CHC-C1C	4.69	1.47	1.35
10	bA	815	CLA	CHC-C1C	4.69	1.47	1.35
10	bA	829	CLA	O2D-CGD	4.69	1.44	1.33
10	aB	808	CLA	CHC-C1C	4.69	1.47	1.35
10	bA	826	CLA	C3D-C2D	4.68	1.48	1.39
10	cB	825	CLA	CHC-C1C	4.68	1.47	1.35
10	aB	816	CLA	CHC-C1C	4.68	1.47	1.35
10	bB	805	CLA	C3C-C2C	4.68	1.46	1.36
10	aA	825	CLA	O2D-CGD	4.68	1.44	1.33
10	cB	836	CLA	CHC-C1C	4.68	1.47	1.35
10	bB	825	CLA	CHC-C1C	4.68	1.47	1.35
10	bA	828	CLA	CHC-C1C	4.68	1.47	1.35
10	bB	836	CLA	CHC-C1C	4.68	1.47	1.35
10	bA	804	CLA	CHC-C1C	4.68	1.47	1.35
10	cA	832	CLA	O2D-CGD	4.68	1.44	1.33
10	bB	826	CLA	O2D-CGD	4.68	1.44	1.33
10	aB	836	CLA	CHC-C1C	4.68	1.47	1.35
10	cB	815	CLA	CHC-C1C	4.68	1.47	1.35
10	cB	814	CLA	O2D-CGD	4.68	1.44	1.33
10	cB	826	CLA	O2D-CGD	4.67	1.44	1.33
10	bL	205	CLA	O2D-CGD	4.67	1.44	1.33
10	aB	813	CLA	CHC-C1C	4.67	1.47	1.35
10	aA	813	CLA	CHC-C1C	4.67	1.47	1.35
10	cB	833	CLA	CHC-C1C	4.67	1.47	1.35
10	bB	823	CLA	CHC-C1C	4.67	1.47	1.35
10	cL	203	CLA	CHC-C1C	4.67	1.47	1.35
10	aA	827	CLA	CHC-C1C	4.67	1.47	1.35
10	bA	810	CLA	CHC-C1C	4.67	1.47	1.35
10	aA	812	CLA	O2D-CGD	4.67	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	832	CLA	O2D-CGD	4.67	1.44	1.33
10	cA	828	CLA	CHC-C1C	4.67	1.47	1.35
10	cB	832	CLA	O2D-CGD	4.67	1.44	1.33
10	aB	814	CLA	O2D-CGD	4.67	1.44	1.33
10	aA	856	CLA	CHC-C1C	4.67	1.47	1.35
10	cA	856	CLA	CHC-C1C	4.67	1.47	1.35
10	aA	804	CLA	CHC-C1C	4.67	1.47	1.35
10	aB	826	CLA	O2D-CGD	4.66	1.44	1.33
10	aA	828	CLA	CHC-C1C	4.66	1.47	1.35
10	aB	815	CLA	CHC-C1C	4.66	1.47	1.35
10	aA	838	CLA	O2D-CGD	4.66	1.44	1.33
10	aA	829	CLA	O2D-CGD	4.66	1.44	1.33
9	cA	801	CL0	C3D-C2D	4.66	1.48	1.39
10	bB	808	CLA	CHC-C1C	4.66	1.47	1.35
10	cA	810	CLA	CHC-C1C	4.66	1.47	1.35
10	cA	826	CLA	C3D-C2D	4.66	1.48	1.39
10	aA	815	CLA	CHC-C1C	4.66	1.47	1.35
10	cA	825	CLA	O2D-CGD	4.66	1.44	1.33
10	bA	812	CLA	O2D-CGD	4.66	1.44	1.33
10	bB	815	CLA	CHC-C1C	4.66	1.47	1.35
10	bB	832	CLA	CHC-C1C	4.66	1.47	1.35
10	aA	832	CLA	O2D-CGD	4.66	1.44	1.33
10	cA	827	CLA	CHC-C1C	4.65	1.47	1.35
10	aB	825	CLA	CHC-C1C	4.65	1.47	1.35
10	aA	810	CLA	CHC-C1C	4.65	1.47	1.35
10	bA	838	CLA	O2D-CGD	4.65	1.44	1.33
10	bB	832	CLA	O2D-CGD	4.65	1.44	1.33
10	bA	839	CLA	CHC-C1C	4.65	1.47	1.35
10	bB	834	CLA	O2D-CGD	4.65	1.44	1.33
10	bA	827	CLA	CHC-C1C	4.65	1.47	1.35
10	cA	815	CLA	CHC-C1C	4.65	1.47	1.35
10	aB	823	CLA	CHC-C1C	4.65	1.47	1.35
10	cA	839	CLA	CHC-C1C	4.65	1.47	1.35
10	bA	856	CLA	CHC-C1C	4.65	1.47	1.35
10	aA	802	CLA	CHC-C1C	4.64	1.47	1.35
9	aA	801	CL0	C3D-C2D	4.64	1.48	1.39
10	cB	808	CLA	CHC-C1C	4.64	1.47	1.35
10	bL	205	CLA	CHC-C1C	4.64	1.47	1.35
10	aA	839	CLA	CHC-C1C	4.64	1.47	1.35
10	cB	827	CLA	C3D-C2D	4.64	1.48	1.39
10	cB	823	CLA	CHC-C1C	4.64	1.47	1.35
10	bA	813	CLA	CHC-C1C	4.64	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	825	CLA	C3D-C2D	4.64	1.48	1.39
10	cA	812	CLA	O2D-CGD	4.64	1.44	1.33
10	bB	814	CLA	O2D-CGD	4.64	1.44	1.33
10	aA	824	CLA	C3D-C2D	4.64	1.48	1.39
10	bB	808	CLA	C3D-C2D	4.64	1.48	1.39
10	bB	806	CLA	O2D-CGD	4.64	1.44	1.33
10	bA	824	CLA	C3D-C2D	4.64	1.48	1.39
10	cB	803	CLA	CHC-C1C	4.64	1.47	1.35
10	aA	807	CLA	CHC-C1C	4.64	1.47	1.35
10	aB	806	CLA	O2D-CGD	4.64	1.44	1.33
10	aB	808	CLA	C3D-C2D	4.64	1.48	1.39
10	aA	835	CLA	CHC-C1C	4.64	1.47	1.35
10	cA	838	CLA	C3D-C2D	4.64	1.48	1.39
10	bB	809	CLA	CHC-C1C	4.64	1.47	1.35
10	bA	835	CLA	CHC-C1C	4.64	1.47	1.35
10	cA	804	CLA	CHC-C1C	4.64	1.47	1.35
10	cB	832	CLA	CHC-C1C	4.63	1.47	1.35
10	bB	803	CLA	CHC-C1C	4.63	1.47	1.35
10	bA	802	CLA	CHC-C1C	4.63	1.47	1.35
10	bB	827	CLA	C3D-C2D	4.63	1.48	1.39
10	aL	205	CLA	CHC-C1C	4.63	1.47	1.35
10	aA	822	CLA	C3D-C2D	4.63	1.48	1.39
10	bA	807	CLA	CHC-C1C	4.63	1.47	1.35
10	aB	827	CLA	C3D-C2D	4.63	1.48	1.39
10	cA	835	CLA	CHC-C1C	4.63	1.47	1.35
10	aA	825	CLA	C3D-C2D	4.63	1.48	1.39
10	cB	809	CLA	CHC-C1C	4.63	1.47	1.35
10	cB	806	CLA	O2D-CGD	4.63	1.44	1.33
10	bA	825	CLA	C3D-C2D	4.63	1.48	1.39
10	cA	814	CLA	CHC-C1C	4.63	1.47	1.35
10	cB	836	CLA	OBD-CAD	4.63	1.28	1.22
10	cL	205	CLA	CHC-C1C	4.63	1.47	1.35
10	bB	824	CLA	CHC-C1C	4.62	1.47	1.35
10	cB	808	CLA	C3D-C2D	4.62	1.48	1.39
10	aB	809	CLA	CHC-C1C	4.62	1.47	1.35
10	bB	840	CLA	CHC-C1C	4.62	1.47	1.35
10	aA	826	CLA	C3D-C2D	4.62	1.48	1.39
10	aB	832	CLA	CHC-C1C	4.62	1.47	1.35
10	bB	821	CLA	CHC-C1C	4.62	1.47	1.35
10	aB	834	CLA	O2D-CGD	4.62	1.44	1.33
10	cA	802	CLA	CHC-C1C	4.62	1.47	1.35
10	aB	803	CLA	CHC-C1C	4.62	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	832	CLA	O2D-CGD	4.62	1.44	1.33
10	cA	830	CLA	CHC-C1C	4.62	1.47	1.35
10	cB	827	CLA	CHC-C1C	4.61	1.47	1.35
10	aA	808	CLA	CHC-C1C	4.61	1.47	1.35
10	bA	822	CLA	C3D-C2D	4.61	1.48	1.39
10	aA	838	CLA	C3D-C2D	4.61	1.48	1.39
10	cB	821	CLA	CHC-C1C	4.61	1.47	1.35
10	cA	807	CLA	CHC-C1C	4.61	1.47	1.35
10	bB	821	CLA	OBD-CAD	4.61	1.28	1.22
10	bA	808	CLA	CHC-C1C	4.61	1.47	1.35
10	cA	808	CLA	CHC-C1C	4.61	1.47	1.35
10	cA	842	CLA	C3B-C2B	4.61	1.46	1.40
10	bA	834	CLA	OBD-CAD	4.61	1.28	1.22
10	aB	824	CLA	CHC-C1C	4.61	1.47	1.35
10	cB	824	CLA	CHC-C1C	4.61	1.47	1.35
10	bA	814	CLA	CHC-C1C	4.60	1.47	1.35
10	bB	817	CLA	OBD-CAD	4.60	1.28	1.22
10	bB	820	CLA	OBD-CAD	4.60	1.28	1.22
10	aA	831	CLA	CHC-C1C	4.60	1.47	1.35
10	cB	840	CLA	CHC-C1C	4.60	1.47	1.35
10	aA	830	CLA	O2D-CGD	4.60	1.44	1.33
10	aB	827	CLA	CHC-C1C	4.60	1.47	1.35
10	cB	834	CLA	O2D-CGD	4.60	1.44	1.33
10	aB	802	CLA	CHC-C1C	4.60	1.47	1.35
10	cA	822	CLA	C3D-C2D	4.60	1.48	1.39
10	bA	830	CLA	O2D-CGD	4.60	1.44	1.33
10	cB	821	CLA	OBD-CAD	4.59	1.28	1.22
10	bA	838	CLA	C3D-C2D	4.59	1.48	1.39
10	aA	843	CLA	CHC-C1C	4.59	1.47	1.35
10	bA	842	CLA	C3B-C2B	4.59	1.46	1.40
10	aA	842	CLA	C3B-C2B	4.59	1.46	1.40
10	cA	824	CLA	C3D-C2D	4.59	1.48	1.39
10	cB	812	CLA	CHC-C1C	4.59	1.47	1.35
10	aB	810	CLA	C3D-C2D	4.59	1.48	1.39
10	cA	804	CLA	C3D-C2D	4.59	1.48	1.39
10	bB	802	CLA	CHC-C1C	4.59	1.47	1.35
10	aB	821	CLA	CHC-C1C	4.59	1.47	1.35
10	aA	805	CLA	CHC-C1C	4.59	1.47	1.35
10	cA	830	CLA	O2D-CGD	4.59	1.44	1.33
10	aA	836	CLA	O2D-CGD	4.58	1.44	1.33
10	aB	840	CLA	CHC-C1C	4.58	1.47	1.35
10	aB	839	CLA	CHC-C1C	4.58	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	802	CLA	CHC-C1C	4.58	1.47	1.35
10	bA	843	CLA	CHC-C1C	4.58	1.47	1.35
10	cB	810	CLA	C3D-C2D	4.58	1.48	1.39
10	aA	834	CLA	OBD-CAD	4.58	1.28	1.22
10	bB	836	CLA	OBD-CAD	4.58	1.28	1.22
10	aB	821	CLA	OBD-CAD	4.58	1.28	1.22
10	bA	832	CLA	CHC-C1C	4.58	1.47	1.35
10	bB	830	CLA	C3D-C2D	4.58	1.48	1.39
10	cA	843	CLA	CHC-C1C	4.58	1.47	1.35
10	cA	827	CLA	C3D-C2D	4.58	1.48	1.39
10	cB	817	CLA	OBD-CAD	4.58	1.28	1.22
10	bL	202	CLA	C3D-C2D	4.58	1.48	1.39
10	cL	202	CLA	C3D-C2D	4.58	1.48	1.39
10	bB	839	CLA	CHC-C1C	4.58	1.47	1.35
10	bB	827	CLA	CHC-C1C	4.57	1.47	1.35
10	aA	830	CLA	CHC-C1C	4.57	1.47	1.35
10	aL	202	CLA	C3D-C2D	4.57	1.48	1.39
10	cB	839	CLA	CHC-C1C	4.57	1.47	1.35
10	aA	814	CLA	CHC-C1C	4.57	1.47	1.35
10	bA	805	CLA	CHC-C1C	4.57	1.47	1.35
10	bB	823	CLA	OBD-CAD	4.57	1.28	1.22
10	aA	803	CLA	OBD-CAD	4.57	1.28	1.22
10	aA	804	CLA	C3D-C2D	4.57	1.48	1.39
10	cA	831	CLA	CHC-C1C	4.57	1.47	1.35
10	aB	817	CLA	OBD-CAD	4.57	1.28	1.22
10	bB	812	CLA	CHC-C1C	4.57	1.47	1.35
10	cB	830	CLA	C3D-C2D	4.57	1.48	1.39
10	bB	810	CLA	C3D-C2D	4.57	1.48	1.39
10	cA	833	CLA	O2D-CGD	4.57	1.44	1.33
10	cB	817	CLA	CHC-C1C	4.56	1.47	1.35
10	bA	833	CLA	O2D-CGD	4.56	1.44	1.33
10	bA	830	CLA	CHC-C1C	4.56	1.47	1.35
10	bA	803	CLA	OBD-CAD	4.56	1.28	1.22
10	aB	812	CLA	CHC-C1C	4.56	1.47	1.35
10	aB	836	CLA	OBD-CAD	4.56	1.28	1.22
10	cB	823	CLA	OBD-CAD	4.56	1.28	1.22
10	cA	836	CLA	O2D-CGD	4.56	1.44	1.33
10	cB	834	CLA	C3D-C2D	4.56	1.48	1.39
10	aB	830	CLA	C3D-C2D	4.56	1.48	1.39
10	aA	832	CLA	CHC-C1C	4.56	1.47	1.35
10	bB	817	CLA	CHC-C1C	4.56	1.47	1.35
10	aB	814	CLA	CHC-C1C	4.56	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	805	CLA	CHC-C1C	4.56	1.47	1.35
10	aB	817	CLA	CHC-C1C	4.56	1.47	1.35
10	aB	820	CLA	OBD-CAD	4.55	1.28	1.22
10	bA	836	CLA	O2D-CGD	4.55	1.44	1.33
10	bA	838	CLA	CHC-C1C	4.55	1.47	1.35
10	cB	820	CLA	OBD-CAD	4.55	1.28	1.22
10	cA	834	CLA	OBD-CAD	4.55	1.28	1.22
10	cA	832	CLA	CHC-C1C	4.55	1.47	1.35
10	bA	804	CLA	C3D-C2D	4.55	1.48	1.39
10	aB	823	CLA	OBD-CAD	4.55	1.28	1.22
10	aA	833	CLA	O2D-CGD	4.54	1.44	1.33
10	bA	837	CLA	CHC-C1C	4.54	1.47	1.35
10	cA	803	CLA	OBD-CAD	4.54	1.28	1.22
10	cA	838	CLA	CHC-C1C	4.54	1.47	1.35
10	aB	834	CLA	C3D-C2D	4.54	1.48	1.39
10	cA	815	CLA	OBD-CAD	4.54	1.28	1.22
10	bA	833	CLA	CHC-C1C	4.54	1.47	1.35
10	bA	836	CLA	C3D-C2D	4.54	1.48	1.39
10	bA	831	CLA	CHC-C1C	4.54	1.47	1.35
10	aA	833	CLA	CHC-C1C	4.53	1.47	1.35
10	cB	837	CLA	CHC-C1C	4.53	1.47	1.35
10	aA	838	CLA	CHC-C1C	4.53	1.47	1.35
10	bB	828	CLA	CHC-C1C	4.53	1.47	1.35
10	aA	836	CLA	C3D-C2D	4.53	1.48	1.39
10	bA	840	CLA	OBD-CAD	4.52	1.28	1.22
10	aA	840	CLA	OBD-CAD	4.52	1.28	1.22
10	aB	807	CLA	CHC-C1C	4.52	1.47	1.35
10	cB	829	CLA	CHC-C1C	4.52	1.47	1.35
10	aB	828	CLA	CHC-C1C	4.52	1.47	1.35
10	aA	837	CLA	CHC-C1C	4.52	1.47	1.35
10	cB	803	CLA	O2D-CGD	4.52	1.44	1.33
10	bB	807	CLA	CHC-C1C	4.52	1.47	1.35
10	bA	829	CLA	CHC-C1C	4.52	1.47	1.35
10	aA	827	CLA	C3D-C2D	4.52	1.48	1.39
10	bB	834	CLA	C3D-C2D	4.52	1.48	1.39
10	bB	805	CLA	O2D-CGD	4.52	1.44	1.33
10	cB	814	CLA	CHC-C1C	4.52	1.47	1.35
10	aA	816	CLA	OBD-CAD	4.52	1.28	1.22
10	cA	836	CLA	C3D-C2D	4.51	1.48	1.39
10	cA	809	CLA	OBD-CAD	4.51	1.28	1.22
10	cB	805	CLA	O2D-CGD	4.51	1.44	1.33
10	aB	837	CLA	CHC-C1C	4.51	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	813	CLA	OBD-CAD	4.51	1.28	1.22
10	aB	801	CLA	O2D-CGD	4.51	1.44	1.33
10	bB	803	CLA	O2D-CGD	4.51	1.44	1.33
10	cA	833	CLA	CHC-C1C	4.51	1.47	1.35
10	aA	815	CLA	OBD-CAD	4.51	1.28	1.22
10	aB	829	CLA	C3D-C2D	4.51	1.48	1.39
10	cB	807	CLA	CHC-C1C	4.51	1.47	1.35
10	aB	805	CLA	CHC-C1C	4.51	1.47	1.35
10	cB	828	CLA	CHC-C1C	4.51	1.47	1.35
10	bB	814	CLA	CHC-C1C	4.51	1.47	1.35
10	aB	829	CLA	CHC-C1C	4.51	1.47	1.35
10	aA	809	CLA	OBD-CAD	4.50	1.28	1.22
10	cB	813	CLA	OBD-CAD	4.50	1.28	1.22
10	bB	829	CLA	CHC-C1C	4.50	1.47	1.35
10	cB	801	CLA	O2D-CGD	4.50	1.44	1.33
10	cA	837	CLA	CHC-C1C	4.50	1.47	1.35
10	bB	813	CLA	OBD-CAD	4.50	1.28	1.22
10	aB	803	CLA	O2D-CGD	4.50	1.44	1.33
10	bB	837	CLA	CHC-C1C	4.50	1.47	1.35
10	cB	829	CLA	C3D-C2D	4.50	1.48	1.39
10	cA	829	CLA	CHC-C1C	4.50	1.47	1.35
10	bA	809	CLA	OBD-CAD	4.50	1.28	1.22
10	bB	801	CLA	O2D-CGD	4.49	1.44	1.33
10	cB	803	CLA	C3D-C2D	4.49	1.48	1.39
10	cA	840	CLA	OBD-CAD	4.49	1.28	1.22
10	bB	805	CLA	CHC-C1C	4.49	1.47	1.35
10	bB	829	CLA	C3D-C2D	4.49	1.48	1.39
10	bA	827	CLA	C3D-C2D	4.49	1.48	1.39
10	aA	829	CLA	CHC-C1C	4.49	1.47	1.35
10	cB	801	CLA	CHC-C1C	4.49	1.47	1.35
10	aA	813	CLA	OBD-CAD	4.49	1.28	1.22
10	aB	813	CLA	OBD-CAD	4.49	1.28	1.22
10	bA	816	CLA	OBD-CAD	4.49	1.28	1.22
10	bA	834	CLA	CHC-C1C	4.48	1.47	1.35
10	cB	805	CLA	CHC-C1C	4.48	1.47	1.35
10	aA	818	CLA	OBD-CAD	4.48	1.28	1.22
10	bB	803	CLA	C3D-C2D	4.48	1.48	1.39
10	aB	803	CLA	C3D-C2D	4.48	1.48	1.39
10	cA	816	CLA	OBD-CAD	4.48	1.28	1.22
10	bL	202	CLA	O2D-CGD	4.48	1.44	1.33
10	cL	202	CLA	O2D-CGD	4.48	1.44	1.33
10	aL	202	CLA	O2D-CGD	4.48	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aB	801	CLA	CHC-C1C	4.47	1.47	1.35
10	cB	828	CLA	C3D-C2D	4.47	1.48	1.39
10	aB	825	CLA	OBD-CAD	4.47	1.28	1.22
10	bB	832	CLA	OBD-CAD	4.47	1.28	1.22
10	aB	805	CLA	O2D-CGD	4.47	1.44	1.33
10	bB	830	CLA	CHC-C1C	4.47	1.47	1.35
10	cB	825	CLA	OBD-CAD	4.47	1.28	1.22
10	aB	830	CLA	CHC-C1C	4.47	1.47	1.35
10	cA	834	CLA	CHC-C1C	4.47	1.47	1.35
10	cB	830	CLA	CHC-C1C	4.46	1.47	1.35
10	bB	801	CLA	CHC-C1C	4.46	1.47	1.35
10	cB	832	CLA	OBD-CAD	4.46	1.28	1.22
10	aA	812	CLA	OBD-CAD	4.46	1.28	1.22
10	cB	825	CLA	O2A-CGA	4.46	1.46	1.33
10	cA	812	CLA	OBD-CAD	4.45	1.28	1.22
10	aA	834	CLA	CHC-C1C	4.45	1.47	1.35
10	bB	828	CLA	C3D-C2D	4.45	1.48	1.39
10	bB	825	CLA	OBD-CAD	4.45	1.28	1.22
10	bB	804	CLA	O2D-CGD	4.45	1.44	1.33
10	bA	823	CLA	CHC-C1C	4.45	1.47	1.35
10	aA	856	CLA	OBD-CAD	4.44	1.28	1.22
10	aB	832	CLA	OBD-CAD	4.44	1.28	1.22
10	cA	856	CLA	OBD-CAD	4.44	1.28	1.22
10	aB	828	CLA	C3D-C2D	4.44	1.48	1.39
10	cA	808	CLA	OBD-CAD	4.44	1.28	1.22
10	bA	812	CLA	OBD-CAD	4.44	1.28	1.22
10	cB	804	CLA	O2D-CGD	4.44	1.44	1.33
10	cA	806	CLA	OBD-CAD	4.44	1.28	1.22
10	cA	818	CLA	OBD-CAD	4.44	1.28	1.22
10	bA	822	CLA	OBD-CAD	4.43	1.28	1.22
10	aB	804	CLA	O2D-CGD	4.43	1.44	1.33
10	bB	825	CLA	O2A-CGA	4.43	1.46	1.33
10	bA	813	CLA	OBD-CAD	4.43	1.28	1.22
11	bB	842	PQN	C10-C5	4.43	1.48	1.40
10	cA	823	CLA	CHC-C1C	4.43	1.47	1.35
10	aB	825	CLA	O2A-CGA	4.43	1.46	1.33
10	aB	824	CLA	OBD-CAD	4.43	1.28	1.22
10	bA	815	CLA	OBD-CAD	4.43	1.28	1.22
10	cA	819	CLA	OBD-CAD	4.43	1.28	1.22
10	cB	831	CLA	OBD-CAD	4.42	1.28	1.22
10	bA	819	CLA	OBD-CAD	4.42	1.28	1.22
10	aA	823	CLA	CHC-C1C	4.42	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	835	CLA	OBD-CAD	4.42	1.28	1.22
10	cA	822	CLA	OBD-CAD	4.42	1.28	1.22
10	bA	818	CLA	OBD-CAD	4.42	1.28	1.22
10	bA	806	CLA	OBD-CAD	4.42	1.28	1.22
10	cA	820	CLA	OBD-CAD	4.42	1.28	1.22
10	bA	854	CLA	OBD-CAD	4.41	1.28	1.22
10	aA	822	CLA	OBD-CAD	4.41	1.28	1.22
11	aB	842	PQN	C10-C5	4.41	1.48	1.40
10	bB	831	CLA	OBD-CAD	4.41	1.28	1.22
10	bA	856	CLA	OBD-CAD	4.41	1.28	1.22
10	aB	835	CLA	OBD-CAD	4.40	1.28	1.22
10	aA	814	CLA	OBD-CAD	4.40	1.28	1.22
10	aB	831	CLA	OBD-CAD	4.40	1.28	1.22
10	cA	835	CLA	OBD-CAD	4.40	1.28	1.22
10	aB	815	CLA	OBD-CAD	4.40	1.28	1.22
10	aA	808	CLA	OBD-CAD	4.40	1.28	1.22
10	aA	836	CLA	CHC-C1C	4.39	1.46	1.35
10	cA	811	CLA	OBD-CAD	4.39	1.28	1.22
10	bA	839	CLA	OBD-CAD	4.39	1.28	1.22
10	aA	806	CLA	OBD-CAD	4.39	1.28	1.22
10	cB	824	CLA	OBD-CAD	4.39	1.28	1.22
10	cA	836	CLA	CHC-C1C	4.39	1.46	1.35
10	cA	814	CLA	OBD-CAD	4.39	1.28	1.22
10	aA	854	CLA	OBD-CAD	4.39	1.28	1.22
10	cB	815	CLA	OBD-CAD	4.38	1.28	1.22
11	cB	842	PQN	C10-C5	4.38	1.48	1.40
10	aA	819	CLA	OBD-CAD	4.38	1.28	1.22
10	bA	814	CLA	OBD-CAD	4.38	1.28	1.22
10	bA	835	CLA	OBD-CAD	4.38	1.28	1.22
10	bB	815	CLA	OBD-CAD	4.38	1.28	1.22
10	aA	830	CLA	O2A-CGA	4.37	1.46	1.33
10	bA	808	CLA	OBD-CAD	4.37	1.28	1.22
10	aA	807	CLA	OBD-CAD	4.37	1.28	1.22
10	bB	834	CLA	OBD-CAD	4.37	1.28	1.22
10	bA	836	CLA	CHC-C1C	4.37	1.46	1.35
10	cL	202	CLA	O2A-CGA	4.37	1.46	1.33
10	cB	834	CLA	OBD-CAD	4.37	1.28	1.22
10	cA	841	CLA	OBD-CAD	4.37	1.28	1.22
10	aA	810	CLA	OBD-CAD	4.36	1.28	1.22
10	cA	839	CLA	OBD-CAD	4.36	1.28	1.22
10	bB	824	CLA	OBD-CAD	4.36	1.28	1.22
10	aA	839	CLA	OBD-CAD	4.36	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	841	CLA	OBD-CAD	4.36	1.28	1.22
10	bA	807	CLA	OBD-CAD	4.36	1.28	1.22
10	cA	810	CLA	OBD-CAD	4.36	1.28	1.22
10	cA	830	CLA	O2A-CGA	4.36	1.46	1.33
10	aA	811	CLA	OBD-CAD	4.36	1.28	1.22
10	aL	202	CLA	O2A-CGA	4.36	1.46	1.33
10	aA	818	CLA	O2A-CGA	4.36	1.46	1.33
10	aA	842	CLA	CHC-C1C	4.35	1.46	1.35
10	aA	820	CLA	OBD-CAD	4.35	1.28	1.22
10	bA	808	CLA	C3D-C2D	4.35	1.48	1.39
10	cB	822	CLA	CHC-C1C	4.35	1.46	1.35
10	bA	811	CLA	OBD-CAD	4.35	1.28	1.22
10	cA	818	CLA	O2A-CGA	4.35	1.46	1.33
10	cA	854	CLA	OBD-CAD	4.35	1.28	1.22
10	aB	829	CLA	OBD-CAD	4.35	1.28	1.22
10	bA	842	CLA	CHC-C1C	4.34	1.46	1.35
10	aA	841	CLA	OBD-CAD	4.34	1.28	1.22
10	aA	808	CLA	C3D-C2D	4.34	1.48	1.39
10	cA	842	CLA	CHC-C1C	4.34	1.46	1.35
10	bA	830	CLA	O2A-CGA	4.34	1.46	1.33
10	aB	822	CLA	CHC-C1C	4.34	1.46	1.35
10	aA	829	CLA	OBD-CAD	4.34	1.28	1.22
10	cA	808	CLA	C3D-C2D	4.34	1.47	1.39
10	cB	835	CLA	OBD-CAD	4.34	1.28	1.22
10	bA	818	CLA	O2A-CGA	4.34	1.46	1.33
10	bB	837	CLA	O2A-CGA	4.33	1.46	1.33
10	cB	837	CLA	O2A-CGA	4.33	1.46	1.33
10	bL	202	CLA	O2A-CGA	4.33	1.46	1.33
10	cA	807	CLA	OBD-CAD	4.33	1.28	1.22
10	bB	833	CLA	OBD-CAD	4.33	1.28	1.22
10	aB	806	CLA	OBD-CAD	4.33	1.28	1.22
10	cL	202	CLA	CHC-C1C	4.33	1.46	1.35
10	cA	810	CLA	O2A-CGA	4.33	1.46	1.33
10	bA	820	CLA	OBD-CAD	4.33	1.28	1.22
10	aA	835	CLA	OBD-CAD	4.33	1.28	1.22
10	cB	829	CLA	OBD-CAD	4.33	1.28	1.22
10	bA	817	CLA	OBD-CAD	4.32	1.28	1.22
10	cB	806	CLA	OBD-CAD	4.32	1.28	1.22
10	bA	810	CLA	OBD-CAD	4.32	1.28	1.22
10	aL	202	CLA	CHC-C1C	4.32	1.46	1.35
10	cA	840	CLA	O2A-CGA	4.32	1.46	1.33
10	bA	840	CLA	O2A-CGA	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	822	CLA	CHC-C1C	4.32	1.46	1.35
9	bA	801	CL0	CHC-C1C	4.32	1.46	1.35
10	cB	818	CLA	OBD-CAD	4.31	1.28	1.22
10	bA	810	CLA	O2A-CGA	4.31	1.46	1.33
10	aA	840	CLA	O2A-CGA	4.31	1.46	1.33
10	aB	818	CLA	OBD-CAD	4.31	1.28	1.22
10	aA	810	CLA	O2A-CGA	4.31	1.46	1.33
9	cA	801	CL0	CHC-C1C	4.31	1.46	1.35
10	cB	833	CLA	OBD-CAD	4.31	1.28	1.22
10	bB	829	CLA	OBD-CAD	4.31	1.28	1.22
10	aB	834	CLA	OBD-CAD	4.31	1.28	1.22
10	bL	202	CLA	CHC-C1C	4.30	1.46	1.35
10	aB	837	CLA	O2A-CGA	4.30	1.46	1.33
10	bB	810	CLA	CHC-C1C	4.30	1.46	1.35
10	bB	806	CLA	OBD-CAD	4.30	1.28	1.22
10	aB	833	CLA	OBD-CAD	4.30	1.28	1.22
10	bB	828	CLA	O2A-CGA	4.30	1.46	1.33
10	cA	829	CLA	OBD-CAD	4.30	1.28	1.22
10	cB	828	CLA	O2A-CGA	4.30	1.46	1.33
10	aB	810	CLA	CHC-C1C	4.30	1.46	1.35
10	cB	820	CLA	O2A-CGA	4.30	1.46	1.33
10	cA	823	CLA	OBD-CAD	4.30	1.28	1.22
10	aB	829	CLA	O2A-CGA	4.30	1.46	1.33
10	aA	817	CLA	OBD-CAD	4.29	1.28	1.22
9	aA	801	CL0	CHC-C1C	4.29	1.46	1.35
10	aB	828	CLA	O2A-CGA	4.29	1.46	1.33
10	aA	854	CLA	O2A-CGA	4.29	1.46	1.33
10	bA	854	CLA	O2A-CGA	4.29	1.46	1.33
10	cB	810	CLA	CHC-C1C	4.29	1.46	1.35
10	cB	812	CLA	OBD-CAD	4.29	1.28	1.22
10	bB	818	CLA	OBD-CAD	4.29	1.28	1.22
10	aB	820	CLA	O2A-CGA	4.29	1.46	1.33
10	bB	812	CLA	OBD-CAD	4.28	1.28	1.22
10	bA	823	CLA	OBD-CAD	4.28	1.28	1.22
10	aB	812	CLA	OBD-CAD	4.28	1.28	1.22
10	aA	823	CLA	OBD-CAD	4.28	1.28	1.22
10	cB	802	CLA	OBD-CAD	4.27	1.28	1.22
10	cA	821	CLA	O2A-CGA	4.27	1.46	1.33
10	bB	820	CLA	O2A-CGA	4.27	1.46	1.33
10	cL	204	CLA	O2A-CGA	4.27	1.46	1.33
10	cB	829	CLA	O2A-CGA	4.27	1.46	1.33
10	bA	805	CLA	OBD-CAD	4.27	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	829	CLA	O2A-CGA	4.26	1.46	1.33
10	cA	817	CLA	OBD-CAD	4.26	1.28	1.22
10	bA	829	CLA	OBD-CAD	4.26	1.28	1.22
10	bB	833	CLA	O2A-CGA	4.26	1.46	1.33
10	aA	821	CLA	O2A-CGA	4.26	1.46	1.33
10	bA	822	CLA	O2A-CGA	4.26	1.46	1.33
10	cA	805	CLA	OBD-CAD	4.25	1.28	1.22
10	aL	204	CLA	O2A-CGA	4.25	1.46	1.33
10	aA	802	CLA	OBD-CAD	4.25	1.28	1.22
10	aB	819	CLA	OBD-CAD	4.25	1.28	1.22
10	cA	854	CLA	O2A-CGA	4.25	1.46	1.33
10	cA	822	CLA	O2A-CGA	4.25	1.46	1.33
10	bA	819	CLA	O2A-CGA	4.25	1.46	1.33
10	bA	821	CLA	O2A-CGA	4.25	1.45	1.33
10	cB	837	CLA	OBD-CAD	4.25	1.28	1.22
10	aA	819	CLA	O2A-CGA	4.24	1.45	1.33
10	cB	821	CLA	O2A-CGA	4.24	1.45	1.33
10	aA	822	CLA	O2A-CGA	4.24	1.45	1.33
10	bB	817	CLA	O2A-CGA	4.24	1.45	1.33
10	bB	839	CLA	O2A-CGA	4.24	1.45	1.33
10	bB	830	CLA	OBD-CAD	4.24	1.28	1.22
10	cA	819	CLA	O2A-CGA	4.24	1.45	1.33
10	cB	817	CLA	O2A-CGA	4.24	1.45	1.33
10	bA	802	CLA	OBD-CAD	4.24	1.28	1.22
10	bL	204	CLA	O2A-CGA	4.23	1.45	1.33
10	cB	830	CLA	OBD-CAD	4.23	1.28	1.22
10	bA	821	CLA	OBD-CAD	4.23	1.28	1.22
10	aB	840	CLA	O2A-CGA	4.23	1.45	1.33
10	cB	839	CLA	O2A-CGA	4.23	1.45	1.33
10	cB	833	CLA	O2A-CGA	4.23	1.45	1.33
10	aB	817	CLA	O2A-CGA	4.23	1.45	1.33
10	aB	833	CLA	O2A-CGA	4.23	1.45	1.33
10	bB	819	CLA	OBD-CAD	4.23	1.28	1.22
10	aB	837	CLA	OBD-CAD	4.22	1.28	1.22
10	aB	821	CLA	O2A-CGA	4.22	1.45	1.33
10	cB	819	CLA	CHC-C1C	4.22	1.46	1.35
10	bB	837	CLA	OBD-CAD	4.22	1.28	1.22
10	bB	821	CLA	O2A-CGA	4.22	1.45	1.33
10	cA	802	CLA	OBD-CAD	4.22	1.28	1.22
10	bB	840	CLA	O2A-CGA	4.22	1.45	1.33
10	cA	821	CLA	OBD-CAD	4.22	1.28	1.22
10	aB	839	CLA	O2A-CGA	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	833	CLA	O2A-CGA	4.22	1.45	1.33
10	aA	821	CLA	OBD-CAD	4.22	1.28	1.22
10	bB	819	CLA	CHC-C1C	4.22	1.46	1.35
10	aA	820	CLA	O2A-CGA	4.22	1.45	1.33
10	cB	804	CLA	O2A-CGA	4.21	1.45	1.33
10	cB	840	CLA	O2A-CGA	4.21	1.45	1.33
10	aB	803	CLA	OBD-CAD	4.21	1.28	1.22
10	cB	819	CLA	OBD-CAD	4.21	1.28	1.22
10	bB	802	CLA	OBD-CAD	4.21	1.28	1.22
10	aA	824	CLA	OBD-CAD	4.21	1.28	1.22
10	aA	815	CLA	O2A-CGA	4.21	1.45	1.33
10	aB	819	CLA	CHC-C1C	4.21	1.46	1.35
10	bA	820	CLA	O2A-CGA	4.21	1.45	1.33
10	aA	856	CLA	O2A-CGA	4.21	1.45	1.33
10	bA	856	CLA	O2A-CGA	4.20	1.45	1.33
10	bA	827	CLA	O2A-CGA	4.20	1.45	1.33
10	aA	823	CLA	O2A-CGA	4.20	1.45	1.33
10	aA	805	CLA	OBD-CAD	4.20	1.28	1.22
10	aA	833	CLA	O2A-CGA	4.20	1.45	1.33
10	aB	830	CLA	OBD-CAD	4.20	1.28	1.22
10	cA	820	CLA	O2A-CGA	4.20	1.45	1.33
10	bA	832	CLA	OBD-CAD	4.20	1.28	1.22
10	aA	827	CLA	O2A-CGA	4.20	1.45	1.33
10	cA	833	CLA	O2A-CGA	4.19	1.45	1.33
10	aA	833	CLA	OBD-CAD	4.19	1.28	1.22
10	bB	804	CLA	O2A-CGA	4.19	1.45	1.33
10	bA	815	CLA	O2A-CGA	4.19	1.45	1.33
10	cA	827	CLA	O2A-CGA	4.19	1.45	1.33
10	cA	830	CLA	OBD-CAD	4.19	1.28	1.22
10	aB	804	CLA	O2A-CGA	4.19	1.45	1.33
10	aL	204	CLA	OBD-CAD	4.19	1.28	1.22
10	cA	815	CLA	O2A-CGA	4.19	1.45	1.33
10	bB	803	CLA	OBD-CAD	4.18	1.28	1.22
10	bB	832	CLA	O2A-CGA	4.18	1.45	1.33
10	cA	824	CLA	OBD-CAD	4.18	1.28	1.22
10	cA	856	CLA	O2A-CGA	4.18	1.45	1.33
10	cL	204	CLA	OBD-CAD	4.18	1.28	1.22
10	cL	203	CLA	OBD-CAD	4.18	1.28	1.22
10	bA	823	CLA	O2A-CGA	4.18	1.45	1.33
10	cB	841	CLA	OBD-CAD	4.17	1.28	1.22
10	cA	823	CLA	O2A-CGA	4.17	1.45	1.33
10	cB	803	CLA	OBD-CAD	4.17	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aL	203	CLA	OBD-CAD	4.17	1.28	1.22
10	bL	205	CLA	OBD-CAD	4.17	1.28	1.22
10	bA	824	CLA	OBD-CAD	4.17	1.28	1.22
10	bA	826	CLA	O2A-CGA	4.16	1.45	1.33
10	cA	833	CLA	OBD-CAD	4.16	1.28	1.22
10	cA	835	CLA	O2A-CGA	4.16	1.45	1.33
10	cA	839	CLA	O2A-CGA	4.16	1.45	1.33
10	cB	841	CLA	O2A-CGA	4.16	1.45	1.33
10	bB	811	CLA	O2A-CGA	4.16	1.45	1.33
10	aB	811	CLA	CHC-C1C	4.16	1.46	1.35
10	bL	204	CLA	OBD-CAD	4.16	1.28	1.22
10	cB	815	CLA	O2A-CGA	4.16	1.45	1.33
10	cB	832	CLA	O2A-CGA	4.16	1.45	1.33
10	aB	832	CLA	O2A-CGA	4.16	1.45	1.33
10	aB	811	CLA	O2A-CGA	4.16	1.45	1.33
10	cL	205	CLA	OBD-CAD	4.16	1.28	1.22
10	cA	832	CLA	OBD-CAD	4.15	1.28	1.22
10	cB	811	CLA	O2A-CGA	4.15	1.45	1.33
10	aA	826	CLA	O2A-CGA	4.15	1.45	1.33
10	aA	835	CLA	O2A-CGA	4.15	1.45	1.33
10	cA	838	CLA	O2A-CGA	4.15	1.45	1.33
10	bL	203	CLA	OBD-CAD	4.15	1.28	1.22
10	aA	839	CLA	O2A-CGA	4.15	1.45	1.33
10	bA	835	CLA	O2A-CGA	4.15	1.45	1.33
10	aB	802	CLA	OBD-CAD	4.15	1.28	1.22
10	aB	815	CLA	O2A-CGA	4.15	1.45	1.33
10	bA	830	CLA	OBD-CAD	4.15	1.28	1.22
10	bA	833	CLA	OBD-CAD	4.15	1.28	1.22
10	bB	827	CLA	O2A-CGA	4.15	1.45	1.33
10	cA	816	CLA	O2A-CGA	4.15	1.45	1.33
10	cA	826	CLA	O2A-CGA	4.14	1.45	1.33
10	aB	841	CLA	O2A-CGA	4.14	1.45	1.33
10	cB	827	CLA	O2A-CGA	4.14	1.45	1.33
10	bB	841	CLA	O2A-CGA	4.14	1.45	1.33
10	aA	841	CLA	O2A-CGA	4.14	1.45	1.33
10	bB	826	CLA	O2A-CGA	4.13	1.45	1.33
10	aA	830	CLA	OBD-CAD	4.13	1.28	1.22
10	bA	839	CLA	O2A-CGA	4.13	1.45	1.33
10	aA	816	CLA	O2A-CGA	4.13	1.45	1.33
10	aB	826	CLA	O2A-CGA	4.13	1.45	1.33
10	cB	811	CLA	CHC-C1C	4.13	1.46	1.35
10	bB	811	CLA	CHC-C1C	4.13	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	815	CLA	O2A-CGA	4.13	1.45	1.33
10	cA	841	CLA	O2A-CGA	4.13	1.45	1.33
10	aB	841	CLA	OBD-CAD	4.13	1.28	1.22
10	aL	205	CLA	OBD-CAD	4.13	1.28	1.22
10	cA	834	CLA	O2A-CGA	4.13	1.45	1.33
10	aA	838	CLA	O2A-CGA	4.12	1.45	1.33
10	bA	816	CLA	O2A-CGA	4.12	1.45	1.33
10	bB	841	CLA	OBD-CAD	4.12	1.28	1.22
10	aA	832	CLA	OBD-CAD	4.12	1.28	1.22
10	aB	827	CLA	O2A-CGA	4.12	1.45	1.33
10	bA	827	CLA	OBD-CAD	4.12	1.28	1.22
10	aA	838	CLA	OBD-CAD	4.12	1.28	1.22
10	bA	838	CLA	O2A-CGA	4.12	1.45	1.33
10	bA	842	CLA	OBD-CAD	4.12	1.28	1.22
10	aB	823	CLA	O2A-CGA	4.12	1.45	1.33
10	bA	824	CLA	O2A-CGA	4.12	1.45	1.33
10	bA	841	CLA	O2A-CGA	4.12	1.45	1.33
10	cA	827	CLA	OBD-CAD	4.11	1.28	1.22
10	cA	836	CLA	O2A-CGA	4.11	1.45	1.33
10	cB	826	CLA	O2A-CGA	4.11	1.45	1.33
10	cB	802	CLA	O2A-CGA	4.11	1.45	1.33
10	cA	811	CLA	O2A-CGA	4.11	1.45	1.33
10	aA	834	CLA	O2A-CGA	4.11	1.45	1.33
10	aA	806	CLA	O2A-CGA	4.11	1.45	1.33
10	aB	840	CLA	C3D-C2D	4.11	1.47	1.39
10	bB	823	CLA	O2A-CGA	4.11	1.45	1.33
10	cB	840	CLA	C3D-C2D	4.10	1.47	1.39
10	aA	836	CLA	O2A-CGA	4.10	1.45	1.33
10	cA	806	CLA	O2A-CGA	4.10	1.45	1.33
10	cB	823	CLA	O2A-CGA	4.10	1.45	1.33
10	bA	806	CLA	O2A-CGA	4.10	1.45	1.33
10	bA	834	CLA	O2A-CGA	4.10	1.45	1.33
10	bB	840	CLA	C3D-C2D	4.10	1.47	1.39
10	bB	806	CLA	O2A-CGA	4.10	1.45	1.33
10	bB	838	CLA	O2A-CGA	4.10	1.45	1.33
10	aA	811	CLA	O2A-CGA	4.10	1.45	1.33
10	cA	824	CLA	O2A-CGA	4.10	1.45	1.33
10	aA	824	CLA	O2A-CGA	4.10	1.45	1.33
10	bA	836	CLA	O2A-CGA	4.10	1.45	1.33
10	cB	841	CLA	CHC-C1C	4.09	1.46	1.35
10	bB	802	CLA	O2A-CGA	4.09	1.45	1.33
10	aA	827	CLA	OBD-CAD	4.09	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	809	CLA	OBD-CAD	4.09	1.28	1.22
10	cB	806	CLA	O2A-CGA	4.09	1.45	1.33
10	cB	838	CLA	O2A-CGA	4.09	1.45	1.33
10	aB	814	CLA	OBD-CAD	4.08	1.28	1.22
10	bB	809	CLA	OBD-CAD	4.08	1.28	1.22
10	aB	809	CLA	OBD-CAD	4.08	1.28	1.22
10	bB	816	CLA	OBD-CAD	4.08	1.28	1.22
10	bA	838	CLA	OBD-CAD	4.08	1.28	1.22
10	aA	831	CLA	O2A-CGA	4.08	1.45	1.33
10	aB	838	CLA	O2A-CGA	4.08	1.45	1.33
10	aB	802	CLA	O2A-CGA	4.08	1.45	1.33
10	bB	809	CLA	O2A-CGA	4.08	1.45	1.33
10	aB	814	CLA	O2A-CGA	4.08	1.45	1.33
10	bB	814	CLA	OBD-CAD	4.08	1.28	1.22
10	aB	841	CLA	CHC-C1C	4.07	1.46	1.35
10	aB	806	CLA	O2A-CGA	4.07	1.45	1.33
10	cA	838	CLA	OBD-CAD	4.07	1.28	1.22
10	bA	811	CLA	O2A-CGA	4.07	1.45	1.33
10	aA	817	CLA	O2A-CGA	4.07	1.45	1.33
10	aB	809	CLA	O2A-CGA	4.07	1.45	1.33
10	cA	812	CLA	O2A-CGA	4.07	1.45	1.33
10	bB	826	CLA	OBD-CAD	4.07	1.28	1.22
10	aA	804	CLA	OBD-CAD	4.07	1.28	1.22
10	bA	817	CLA	O2A-CGA	4.07	1.45	1.33
10	cB	818	CLA	O2A-CGA	4.07	1.45	1.33
10	bB	814	CLA	O2A-CGA	4.07	1.45	1.33
10	aB	816	CLA	OBD-CAD	4.07	1.28	1.22
9	bA	801	CL0	OBD-CAD	4.07	1.28	1.22
10	bB	818	CLA	O2A-CGA	4.06	1.45	1.33
9	aA	801	CL0	OBD-CAD	4.06	1.28	1.22
10	cL	203	CLA	O2A-CGA	4.06	1.45	1.33
10	aB	818	CLA	O2A-CGA	4.06	1.45	1.33
10	cB	816	CLA	OBD-CAD	4.05	1.28	1.22
9	cA	801	CL0	OBD-CAD	4.05	1.28	1.22
10	bA	831	CLA	O2A-CGA	4.05	1.45	1.33
10	cB	814	CLA	OBD-CAD	4.05	1.28	1.22
10	cA	831	CLA	O2A-CGA	4.05	1.45	1.33
10	aA	842	CLA	OBD-CAD	4.05	1.28	1.22
10	cB	814	CLA	O2A-CGA	4.05	1.45	1.33
10	bB	841	CLA	CHC-C1C	4.05	1.46	1.35
10	aA	812	CLA	O2A-CGA	4.05	1.45	1.33
10	bA	812	CLA	O2A-CGA	4.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	843	CLA	OBD-CAD	4.04	1.28	1.22
10	cA	817	CLA	O2A-CGA	4.04	1.45	1.33
10	aL	203	CLA	O2A-CGA	4.04	1.45	1.33
10	cA	843	CLA	OBD-CAD	4.04	1.28	1.22
10	cB	809	CLA	O2A-CGA	4.04	1.45	1.33
10	cB	807	CLA	O2A-CGA	4.04	1.45	1.33
10	cB	826	CLA	OBD-CAD	4.03	1.28	1.22
10	aB	808	CLA	O2A-CGA	4.03	1.45	1.33
10	bA	837	CLA	O2A-CGA	4.02	1.45	1.33
10	cB	808	CLA	O2A-CGA	4.02	1.45	1.33
10	bB	803	CLA	O2A-CGA	4.02	1.45	1.33
10	bL	203	CLA	O2A-CGA	4.02	1.45	1.33
10	cA	842	CLA	OBD-CAD	4.02	1.28	1.22
10	bA	804	CLA	OBD-CAD	4.02	1.28	1.22
10	cA	837	CLA	O2A-CGA	4.02	1.45	1.33
10	aA	837	CLA	O2A-CGA	4.02	1.45	1.33
10	aA	805	CLA	O2A-CGA	4.01	1.45	1.33
10	aA	843	CLA	OBD-CAD	4.01	1.28	1.22
10	aB	805	CLA	O2A-CGA	4.01	1.45	1.33
10	aB	807	CLA	O2A-CGA	4.00	1.45	1.33
10	cB	803	CLA	O2A-CGA	4.00	1.45	1.33
10	bB	808	CLA	O2A-CGA	4.00	1.45	1.33
10	bB	805	CLA	O2A-CGA	4.00	1.45	1.33
10	cA	842	CLA	O2A-CGA	4.00	1.45	1.33
10	aA	842	CLA	O2A-CGA	4.00	1.45	1.33
10	aB	826	CLA	OBD-CAD	4.00	1.28	1.22
10	cA	805	CLA	O2A-CGA	3.99	1.45	1.33
10	bA	829	CLA	O2A-CGA	3.99	1.45	1.33
10	aB	803	CLA	O2A-CGA	3.99	1.45	1.33
10	bA	805	CLA	O2A-CGA	3.99	1.45	1.33
10	bA	842	CLA	O2A-CGA	3.99	1.45	1.33
10	aA	829	CLA	O2A-CGA	3.99	1.45	1.33
10	bB	807	CLA	O2A-CGA	3.99	1.45	1.33
10	aB	805	CLA	OBD-CAD	3.99	1.28	1.22
10	cA	829	CLA	O2A-CGA	3.98	1.45	1.33
10	cA	804	CLA	OBD-CAD	3.98	1.28	1.22
10	cB	805	CLA	O2A-CGA	3.98	1.45	1.33
10	cB	810	CLA	OBD-CAD	3.97	1.28	1.22
10	bA	831	CLA	OBD-CAD	3.97	1.28	1.22
10	cB	830	CLA	O2A-CGA	3.96	1.45	1.33
10	bB	830	CLA	O2A-CGA	3.96	1.45	1.33
10	bB	810	CLA	OBD-CAD	3.95	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	cA	801	CL0	O2A-CGA	3.95	1.45	1.33
10	aB	830	CLA	O2A-CGA	3.95	1.45	1.33
10	cB	805	CLA	OBD-CAD	3.95	1.27	1.22
10	aB	828	CLA	OBD-CAD	3.95	1.27	1.22
9	bA	801	CL0	O2A-CGA	3.94	1.45	1.33
10	bB	828	CLA	OBD-CAD	3.94	1.27	1.22
10	aB	810	CLA	OBD-CAD	3.94	1.27	1.22
9	aA	801	CL0	O2A-CGA	3.94	1.45	1.33
10	cB	819	CLA	O2A-CGA	3.93	1.45	1.33
10	bA	828	CLA	O2A-CGA	3.92	1.45	1.33
10	aA	828	CLA	O2A-CGA	3.92	1.45	1.33
10	cB	828	CLA	OBD-CAD	3.92	1.27	1.22
10	bA	832	CLA	O2A-CGA	3.91	1.44	1.33
10	bL	205	CLA	O2A-CGA	3.91	1.44	1.33
10	bB	810	CLA	O2A-CGA	3.91	1.44	1.33
10	cL	205	CLA	O2A-CGA	3.90	1.44	1.33
10	cB	810	CLA	O2A-CGA	3.90	1.44	1.33
10	aB	819	CLA	O2A-CGA	3.90	1.44	1.33
10	bB	819	CLA	O2A-CGA	3.90	1.44	1.33
10	aB	810	CLA	O2A-CGA	3.90	1.44	1.33
10	bB	805	CLA	OBD-CAD	3.90	1.27	1.22
10	cA	832	CLA	O2A-CGA	3.90	1.44	1.33
10	aL	205	CLA	O2A-CGA	3.89	1.44	1.33
10	aB	839	CLA	OBD-CAD	3.89	1.27	1.22
10	cA	831	CLA	OBD-CAD	3.89	1.27	1.22
10	cA	828	CLA	O2A-CGA	3.88	1.44	1.33
10	aA	832	CLA	O2A-CGA	3.88	1.44	1.33
10	bB	801	CLA	O2A-CGA	3.87	1.44	1.33
10	aA	831	CLA	OBD-CAD	3.86	1.27	1.22
10	bB	839	CLA	OBD-CAD	3.86	1.27	1.22
10	cB	839	CLA	OBD-CAD	3.85	1.27	1.22
10	bA	804	CLA	O2A-CGA	3.84	1.44	1.33
10	cA	804	CLA	O2A-CGA	3.84	1.44	1.33
10	aA	804	CLA	O2A-CGA	3.83	1.44	1.33
10	aB	801	CLA	O2A-CGA	3.83	1.44	1.33
10	cB	801	CLA	O2A-CGA	3.83	1.44	1.33
10	cA	825	CLA	O2A-CGA	3.78	1.44	1.33
10	aA	825	CLA	O2A-CGA	3.78	1.44	1.33
10	bA	825	CLA	O2A-CGA	3.77	1.44	1.33
10	bA	826	CLA	OBD-CAD	3.75	1.27	1.22
10	cA	826	CLA	OBD-CAD	3.73	1.27	1.22
10	aA	826	CLA	OBD-CAD	3.70	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	804	CLA	OBD-CAD	3.64	1.27	1.22
10	aB	804	CLA	OBD-CAD	3.62	1.27	1.22
10	bB	827	CLA	OBD-CAD	3.58	1.27	1.22
10	bB	804	CLA	OBD-CAD	3.58	1.27	1.22
10	cA	825	CLA	OBD-CAD	3.58	1.27	1.22
10	aA	825	CLA	OBD-CAD	3.54	1.27	1.22
10	cB	827	CLA	OBD-CAD	3.54	1.27	1.22
10	bB	808	CLA	OBD-CAD	3.53	1.27	1.22
10	aB	827	CLA	OBD-CAD	3.51	1.27	1.22
10	cB	838	CLA	OBD-CAD	3.50	1.27	1.22
10	bA	825	CLA	OBD-CAD	3.49	1.27	1.22
10	cB	811	CLA	OBD-CAD	3.49	1.27	1.22
10	aB	808	CLA	OBD-CAD	3.49	1.27	1.22
10	bB	838	CLA	OBD-CAD	3.48	1.27	1.22
10	cL	202	CLA	OBD-CAD	3.47	1.27	1.22
10	cB	808	CLA	OBD-CAD	3.46	1.27	1.22
13	aA	846	BCR	C1-C6	-3.46	1.49	1.53
10	aB	838	CLA	OBD-CAD	3.44	1.27	1.22
10	aL	202	CLA	OBD-CAD	3.44	1.27	1.22
10	bB	811	CLA	OBD-CAD	3.42	1.27	1.22
13	cA	846	BCR	C1-C6	-3.41	1.49	1.53
10	bL	202	CLA	OBD-CAD	3.40	1.27	1.22
13	bA	846	BCR	C1-C6	-3.39	1.49	1.53
10	cB	801	CLA	OBD-CAD	3.36	1.27	1.22
10	aB	811	CLA	OBD-CAD	3.35	1.27	1.22
10	cA	836	CLA	OBD-CAD	3.35	1.27	1.22
10	bB	801	CLA	OBD-CAD	3.34	1.27	1.22
10	aA	836	CLA	OBD-CAD	3.34	1.27	1.22
10	bA	836	CLA	OBD-CAD	3.33	1.27	1.22
10	aB	801	CLA	OBD-CAD	3.31	1.27	1.22
10	cA	837	CLA	OBD-CAD	3.29	1.27	1.22
10	bA	837	CLA	OBD-CAD	3.27	1.27	1.22
10	aA	837	CLA	OBD-CAD	3.27	1.27	1.22
10	bB	807	CLA	OBD-CAD	3.25	1.26	1.22
10	aB	807	CLA	OBD-CAD	3.23	1.26	1.22
10	cB	807	CLA	OBD-CAD	3.23	1.26	1.22
10	cA	828	CLA	OBD-CAD	3.22	1.26	1.22
13	cB	845	BCR	C1-C6	-3.20	1.49	1.53
10	bA	828	CLA	OBD-CAD	3.19	1.26	1.22
13	bB	843	BCR	C1-C6	-3.19	1.49	1.53
13	bB	846	BCR	C30-C25	-3.17	1.49	1.53
10	aB	840	CLA	OBD-CAD	3.17	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	828	CLA	OBD-CAD	3.16	1.26	1.22
13	cB	846	BCR	C30-C25	-3.16	1.49	1.53
13	cB	843	BCR	C1-C6	-3.14	1.49	1.53
10	cB	840	CLA	OBD-CAD	3.13	1.26	1.22
13	aB	843	BCR	C1-C6	-3.13	1.49	1.53
10	bB	840	CLA	OBD-CAD	3.13	1.26	1.22
13	bB	845	BCR	C1-C6	-3.13	1.49	1.53
13	aB	846	BCR	C30-C25	-3.12	1.49	1.53
13	cA	849	BCR	C1-C6	-3.10	1.49	1.53
13	aB	845	BCR	C1-C6	-3.09	1.49	1.53
13	aA	849	BCR	C1-C6	-3.08	1.49	1.53
13	bA	849	BCR	C1-C6	-3.08	1.49	1.53
10	aA	840	CLA	C4B-CHC	3.06	1.48	1.40
13	cM	101	BCR	C30-C25	-3.06	1.49	1.53
13	bM	101	BCR	C30-C25	-3.05	1.49	1.53
10	cA	840	CLA	C4B-CHC	3.05	1.48	1.40
13	aM	101	BCR	C30-C25	-3.04	1.49	1.53
10	bA	840	CLA	C4B-CHC	3.04	1.48	1.40
13	cA	850	BCR	C30-C25	-3.01	1.49	1.53
13	bA	850	BCR	C30-C25	-3.00	1.49	1.53
13	aA	850	BCR	C30-C25	-3.00	1.49	1.53
10	aA	826	CLA	C4B-CHC	2.99	1.48	1.40
13	bL	207	BCR	C30-C25	-2.97	1.49	1.53
9	bA	801	CL0	C1B-CHB	2.96	1.48	1.40
10	cA	826	CLA	C4B-CHC	2.96	1.48	1.40
9	cA	801	CL0	C1B-CHB	2.96	1.48	1.40
10	bA	808	CLA	C4B-CHC	2.95	1.48	1.40
9	aA	801	CL0	C1B-CHB	2.94	1.48	1.40
13	aL	207	BCR	C30-C25	-2.94	1.49	1.53
10	bA	826	CLA	C4B-CHC	2.94	1.47	1.40
10	aA	806	CLA	C1D-C2D	2.93	1.49	1.42
10	bB	834	CLA	C1D-C2D	2.93	1.49	1.42
10	bA	843	CLA	C1D-C2D	2.92	1.49	1.42
10	cA	808	CLA	C4B-CHC	2.92	1.47	1.40
10	cA	843	CLA	C1D-C2D	2.92	1.49	1.42
10	cA	806	CLA	C1D-C2D	2.91	1.49	1.42
10	aB	834	CLA	C4B-CHC	2.91	1.47	1.40
10	aB	834	CLA	C1D-C2D	2.91	1.49	1.42
10	aA	808	CLA	C4B-CHC	2.91	1.47	1.40
13	aM	101	BCR	C1-C6	-2.90	1.49	1.53
13	bM	101	BCR	C1-C6	-2.90	1.49	1.53
13	cL	207	BCR	C30-C25	-2.90	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	843	CLA	C1D-C2D	2.90	1.49	1.42
10	cB	834	CLA	C1D-C2D	2.90	1.49	1.42
10	bB	836	CLA	C1D-C2D	2.89	1.49	1.42
10	aB	836	CLA	C1D-C2D	2.89	1.49	1.42
10	bB	820	CLA	C1D-C2D	2.88	1.49	1.42
10	cB	836	CLA	C1D-C2D	2.88	1.49	1.42
10	bA	806	CLA	C1D-C2D	2.88	1.49	1.42
10	aB	840	CLA	C4B-CHC	2.87	1.47	1.40
13	cM	101	BCR	C1-C6	-2.87	1.49	1.53
10	cA	816	CLA	C4B-CHC	2.87	1.47	1.40
10	cA	802	CLA	C1D-C2D	2.87	1.49	1.42
13	cI	102	BCR	C1-C6	-2.87	1.49	1.53
10	bB	834	CLA	C4B-CHC	2.87	1.47	1.40
10	bA	816	CLA	C4B-CHC	2.87	1.47	1.40
10	aA	816	CLA	C4B-CHC	2.87	1.47	1.40
10	cB	834	CLA	C4B-CHC	2.87	1.47	1.40
10	aA	802	CLA	C1D-C2D	2.86	1.49	1.42
10	aA	815	CLA	C1D-C2D	2.86	1.49	1.42
10	cA	841	CLA	C4B-CHC	2.86	1.47	1.40
10	aB	820	CLA	C1D-C2D	2.86	1.49	1.42
10	cA	820	CLA	C4B-CHC	2.86	1.47	1.40
10	bA	820	CLA	C4B-CHC	2.86	1.47	1.40
10	aB	826	CLA	C4B-CHC	2.85	1.47	1.40
10	aA	820	CLA	C4B-CHC	2.85	1.47	1.40
10	bA	802	CLA	C1D-C2D	2.85	1.49	1.42
10	aA	817	CLA	C4B-CHC	2.85	1.47	1.40
10	bB	840	CLA	C4B-CHC	2.85	1.47	1.40
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	bA	841	CLA	C4B-CHC	2.85	1.47	1.40
10	bA	825	CLA	C4B-CHC	2.84	1.47	1.40
10	cA	817	CLA	C4B-CHC	2.84	1.47	1.40
10	cA	825	CLA	C4B-CHC	2.84	1.47	1.40
10	bA	803	CLA	C4B-CHC	2.84	1.47	1.40
10	cA	803	CLA	C4B-CHC	2.84	1.47	1.40
13	bI	101	BCR	C1-C6	-2.84	1.49	1.53
10	bA	817	CLA	C4B-CHC	2.84	1.47	1.40
10	bA	815	CLA	C1D-C2D	2.84	1.49	1.42
10	cB	818	CLA	C4B-CHC	2.84	1.47	1.40
10	cB	840	CLA	C4B-CHC	2.84	1.47	1.40
10	cB	832	CLA	C4B-CHC	2.84	1.47	1.40
10	cA	815	CLA	C1D-C2D	2.84	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	823	CLA	C1D-C2D	2.83	1.49	1.42
10	cB	820	CLA	C1D-C2D	2.83	1.49	1.42
10	aA	841	CLA	C4B-CHC	2.83	1.47	1.40
10	cB	823	CLA	C1D-C2D	2.83	1.49	1.42
10	aA	825	CLA	C4B-CHC	2.83	1.47	1.40
10	cA	812	CLA	C1D-C2D	2.83	1.49	1.42
10	cB	826	CLA	C4B-CHC	2.83	1.47	1.40
10	aB	823	CLA	C1D-C2D	2.83	1.49	1.42
10	aB	832	CLA	C4B-CHC	2.83	1.47	1.40
10	cB	835	CLA	C1D-C2D	2.83	1.49	1.42
10	aB	806	CLA	C4B-CHC	2.83	1.47	1.40
10	aA	819	CLA	C4B-CHC	2.83	1.47	1.40
10	aB	818	CLA	C4B-CHC	2.82	1.47	1.40
10	aA	803	CLA	C4B-CHC	2.82	1.47	1.40
10	bA	812	CLA	C1D-C2D	2.82	1.49	1.42
10	bB	806	CLA	C4B-CHC	2.82	1.47	1.40
10	bB	831	CLA	C1D-C2D	2.82	1.49	1.42
10	cB	806	CLA	C4B-CHC	2.82	1.47	1.40
10	cB	831	CLA	C1D-C2D	2.82	1.48	1.42
10	aB	813	CLA	C4B-CHC	2.82	1.47	1.40
10	aB	838	CLA	C4B-CHC	2.81	1.47	1.40
10	aA	812	CLA	C1D-C2D	2.81	1.48	1.42
10	bA	843	CLA	C4B-CHC	2.81	1.47	1.40
10	cA	811	CLA	C4B-CHC	2.81	1.47	1.40
10	aA	843	CLA	C4B-CHC	2.81	1.47	1.40
10	aB	835	CLA	C1D-C2D	2.81	1.48	1.42
10	bB	818	CLA	C4B-CHC	2.81	1.47	1.40
10	cB	813	CLA	C4B-CHC	2.81	1.47	1.40
10	bA	806	CLA	C4B-CHC	2.80	1.47	1.40
10	bB	832	CLA	C4B-CHC	2.80	1.47	1.40
10	aA	811	CLA	C4B-CHC	2.80	1.47	1.40
10	bA	811	CLA	C4B-CHC	2.80	1.47	1.40
10	cA	843	CLA	C4B-CHC	2.80	1.47	1.40
10	bB	837	CLA	C4B-CHC	2.80	1.47	1.40
10	cA	819	CLA	C4B-CHC	2.80	1.47	1.40
10	bB	838	CLA	C4B-CHC	2.80	1.47	1.40
10	aA	838	CLA	C4B-CHC	2.80	1.47	1.40
10	aB	837	CLA	C4B-CHC	2.80	1.47	1.40
10	cA	838	CLA	C4B-CHC	2.80	1.47	1.40
10	bB	813	CLA	C4B-CHC	2.80	1.47	1.40
10	cB	838	CLA	C4B-CHC	2.80	1.47	1.40
10	bB	826	CLA	C4B-CHC	2.80	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	838	CLA	C4B-CHC	2.79	1.47	1.40
13	aI	101	BCR	C1-C6	-2.79	1.50	1.53
10	bA	839	CLA	C1D-C2D	2.79	1.48	1.42
10	bA	819	CLA	C4B-CHC	2.79	1.47	1.40
10	cA	854	CLA	C4B-CHC	2.79	1.47	1.40
10	aA	804	CLA	C4B-CHC	2.79	1.47	1.40
10	cB	837	CLA	C4B-CHC	2.79	1.47	1.40
10	bA	842	CLA	C1B-CHB	2.79	1.47	1.40
10	cA	810	CLA	C1D-C2D	2.78	1.48	1.42
10	bB	835	CLA	C1D-C2D	2.78	1.48	1.42
10	bB	821	CLA	C4B-CHC	2.78	1.47	1.40
10	aA	842	CLA	C1B-CHB	2.78	1.47	1.40
10	cB	831	CLA	C4B-CHC	2.78	1.47	1.40
10	cB	833	CLA	C4B-CHC	2.78	1.47	1.40
10	aA	806	CLA	C4B-CHC	2.78	1.47	1.40
10	aA	854	CLA	C4B-CHC	2.77	1.47	1.40
10	cA	842	CLA	C1B-CHB	2.77	1.47	1.40
10	cB	805	CLA	C1C-NC	-2.77	1.33	1.37
10	aB	824	CLA	C1D-C2D	2.77	1.48	1.42
10	aA	814	CLA	C4B-CHC	2.77	1.47	1.40
10	cA	806	CLA	C4B-CHC	2.77	1.47	1.40
10	cB	839	CLA	C4B-CHC	2.77	1.47	1.40
10	bA	804	CLA	C4B-CHC	2.77	1.47	1.40
10	aB	831	CLA	C1D-C2D	2.77	1.48	1.42
10	aB	831	CLA	C4B-CHC	2.77	1.47	1.40
10	cB	808	CLA	C4B-CHC	2.77	1.47	1.40
10	bA	854	CLA	C4B-CHC	2.76	1.47	1.40
10	bB	824	CLA	C1D-C2D	2.76	1.48	1.42
10	bA	810	CLA	C1D-C2D	2.76	1.48	1.42
13	bB	849	BCR	C30-C25	-2.76	1.50	1.53
10	cB	821	CLA	C4B-CHC	2.76	1.47	1.40
10	aB	835	CLA	C4B-CHC	2.76	1.47	1.40
10	cA	804	CLA	C4B-CHC	2.76	1.47	1.40
10	aA	810	CLA	C1D-C2D	2.76	1.48	1.42
10	bB	831	CLA	C4B-CHC	2.76	1.47	1.40
10	aA	822	CLA	C4B-CHC	2.76	1.47	1.40
10	cA	814	CLA	C4B-CHC	2.76	1.47	1.40
10	aB	821	CLA	C4B-CHC	2.76	1.47	1.40
10	cA	839	CLA	C1D-C2D	2.76	1.48	1.42
10	aA	835	CLA	C4B-CHC	2.76	1.47	1.40
10	bB	839	CLA	C4B-CHC	2.76	1.47	1.40
10	cB	824	CLA	C1D-C2D	2.75	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	804	CLA	C4B-CHC	2.75	1.47	1.40
10	bA	822	CLA	C4B-CHC	2.75	1.47	1.40
10	cA	822	CLA	C4B-CHC	2.75	1.47	1.40
10	cB	826	CLA	C1D-C2D	2.75	1.48	1.42
13	aB	845	BCR	C30-C25	-2.75	1.50	1.53
10	bL	204	CLA	C4B-CHC	2.74	1.47	1.40
10	aB	804	CLA	C4B-CHC	2.74	1.47	1.40
10	bB	832	CLA	C1D-C2D	2.74	1.48	1.42
10	bB	833	CLA	C4B-CHC	2.74	1.47	1.40
10	cB	835	CLA	C4B-CHC	2.74	1.47	1.40
10	bA	835	CLA	C4B-CHC	2.74	1.47	1.40
10	bB	804	CLA	C4B-CHC	2.74	1.47	1.40
10	aA	839	CLA	C1D-C2D	2.74	1.48	1.42
10	aA	813	CLA	C1D-C2D	2.74	1.48	1.42
10	bA	813	CLA	C1D-C2D	2.74	1.48	1.42
10	cA	803	CLA	C1D-C2D	2.74	1.48	1.42
10	aB	833	CLA	C4B-CHC	2.74	1.47	1.40
10	aB	839	CLA	C4B-CHC	2.74	1.47	1.40
10	cA	813	CLA	C1D-C2D	2.74	1.48	1.42
10	aA	812	CLA	C4B-CHC	2.74	1.47	1.40
10	bA	815	CLA	C4B-CHC	2.74	1.47	1.40
13	aB	849	BCR	C30-C25	-2.73	1.50	1.53
10	aB	826	CLA	C1D-C2D	2.73	1.48	1.42
10	cA	824	CLA	C4B-CHC	2.73	1.47	1.40
10	bA	802	CLA	C4B-CHC	2.73	1.47	1.40
10	bB	826	CLA	C1D-C2D	2.73	1.48	1.42
13	cB	847	BCR	C30-C25	-2.73	1.50	1.53
10	cA	815	CLA	C4B-CHC	2.73	1.47	1.40
10	cA	802	CLA	C4B-CHC	2.73	1.47	1.40
10	cA	809	CLA	C4B-CHC	2.73	1.47	1.40
13	bB	845	BCR	C30-C25	-2.73	1.50	1.53
10	cA	835	CLA	C4B-CHC	2.73	1.47	1.40
13	aB	847	BCR	C30-C25	-2.73	1.50	1.53
10	bA	814	CLA	C4B-CHC	2.73	1.47	1.40
10	cL	204	CLA	C4B-CHC	2.73	1.47	1.40
10	bB	808	CLA	C4B-CHC	2.73	1.47	1.40
10	bB	823	CLA	C4B-CHC	2.73	1.47	1.40
10	aA	837	CLA	C4B-CHC	2.72	1.47	1.40
10	cB	824	CLA	C4B-CHC	2.72	1.47	1.40
10	aA	815	CLA	C4B-CHC	2.72	1.47	1.40
10	aA	809	CLA	C4B-CHC	2.72	1.47	1.40
10	aA	802	CLA	C4B-CHC	2.72	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	809	CLA	C4B-CHC	2.72	1.47	1.40
10	aB	814	CLA	C1D-C2D	2.72	1.48	1.42
10	aA	808	CLA	C1B-CHB	2.72	1.47	1.40
10	bA	803	CLA	C1D-C2D	2.72	1.48	1.42
10	aB	808	CLA	C4B-CHC	2.72	1.47	1.40
10	bA	808	CLA	C1B-CHB	2.72	1.47	1.40
10	aB	823	CLA	C4B-CHC	2.72	1.47	1.40
10	cA	837	CLA	C4B-CHC	2.72	1.47	1.40
10	aA	824	CLA	C4B-CHC	2.72	1.47	1.40
10	bA	837	CLA	C4B-CHC	2.72	1.47	1.40
10	bA	824	CLA	C4B-CHC	2.72	1.47	1.40
10	bA	812	CLA	C4B-CHC	2.72	1.47	1.40
10	aB	833	CLA	C1D-C2D	2.72	1.48	1.42
10	cB	823	CLA	C4B-CHC	2.71	1.47	1.40
10	aB	822	CLA	C1D-C2D	2.71	1.48	1.42
13	aA	850	BCR	C1-C6	-2.71	1.50	1.53
10	bB	824	CLA	C4B-CHC	2.71	1.47	1.40
10	aL	204	CLA	C4B-CHC	2.71	1.47	1.40
13	cA	850	BCR	C1-C6	-2.71	1.50	1.53
10	bB	835	CLA	C4B-CHC	2.71	1.47	1.40
10	bB	828	CLA	C1B-CHB	2.71	1.47	1.40
10	cA	812	CLA	C4B-CHC	2.71	1.47	1.40
10	cA	856	CLA	C4B-CHC	2.71	1.47	1.40
10	cB	816	CLA	C4B-CHC	2.71	1.47	1.40
10	cA	808	CLA	C1B-CHB	2.71	1.47	1.40
10	bA	835	CLA	C1D-C2D	2.71	1.48	1.42
10	aB	818	CLA	C1D-C2D	2.71	1.48	1.42
10	aB	828	CLA	C1B-CHB	2.70	1.47	1.40
10	cB	814	CLA	C1D-C2D	2.70	1.48	1.42
10	aA	803	CLA	C1D-C2D	2.70	1.48	1.42
10	cB	822	CLA	C1D-C2D	2.70	1.48	1.42
10	aB	824	CLA	C4B-CHC	2.70	1.47	1.40
10	bB	814	CLA	C1D-C2D	2.70	1.48	1.42
10	aB	816	CLA	C4B-CHC	2.70	1.47	1.40
10	bA	809	CLA	C1D-C2D	2.70	1.48	1.42
10	bB	827	CLA	C4B-CHC	2.70	1.47	1.40
10	cB	833	CLA	C1D-C2D	2.70	1.48	1.42
10	cB	832	CLA	C1D-C2D	2.70	1.48	1.42
10	aA	856	CLA	C4B-CHC	2.70	1.47	1.40
13	aA	851	BCR	C30-C25	-2.70	1.50	1.53
10	bA	856	CLA	C4B-CHC	2.70	1.47	1.40
10	cA	809	CLA	C1D-C2D	2.70	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	bA	850	BCR	C1-C6	-2.69	1.50	1.53
10	aB	827	CLA	C1B-CHB	2.69	1.47	1.40
10	bB	818	CLA	C1D-C2D	2.69	1.48	1.42
13	cB	849	BCR	C30-C25	-2.69	1.50	1.53
10	cB	818	CLA	C1D-C2D	2.69	1.48	1.42
10	bB	803	CLA	C1B-CHB	2.69	1.47	1.40
13	bA	851	BCR	C30-C25	-2.69	1.50	1.53
10	aB	827	CLA	C4B-CHC	2.68	1.47	1.40
10	bA	818	CLA	C1D-C2D	2.68	1.48	1.42
10	aA	818	CLA	C1D-C2D	2.68	1.48	1.42
10	aA	802	CLA	C1B-CHB	2.68	1.47	1.40
10	cB	827	CLA	C4B-CHC	2.68	1.47	1.40
10	cA	818	CLA	C1D-C2D	2.68	1.48	1.42
10	aA	814	CLA	C1D-C2D	2.68	1.48	1.42
10	cB	828	CLA	C1B-CHB	2.68	1.47	1.40
10	bB	827	CLA	C1B-CHB	2.68	1.47	1.40
10	aB	803	CLA	C1B-CHB	2.68	1.47	1.40
10	cA	814	CLA	C1D-C2D	2.68	1.48	1.42
10	aB	832	CLA	C1D-C2D	2.68	1.48	1.42
10	bB	816	CLA	C4B-CHC	2.68	1.47	1.40
10	cB	820	CLA	C4B-CHC	2.67	1.47	1.40
10	cA	843	CLA	C4C-C3C	2.67	1.49	1.45
10	bB	820	CLA	C4B-CHC	2.67	1.47	1.40
10	cB	827	CLA	C1B-CHB	2.67	1.47	1.40
10	bA	828	CLA	C4B-CHC	2.67	1.47	1.40
10	aA	835	CLA	C1D-C2D	2.67	1.48	1.42
10	aB	809	CLA	C4B-CHC	2.67	1.47	1.40
10	cA	835	CLA	C1D-C2D	2.67	1.48	1.42
10	cB	838	CLA	C1D-C2D	2.67	1.48	1.42
10	cB	809	CLA	C4B-CHC	2.67	1.47	1.40
10	cA	828	CLA	C4B-CHC	2.67	1.47	1.40
10	cB	825	CLA	C4B-CHC	2.67	1.47	1.40
10	cA	807	CLA	C4B-CHC	2.67	1.47	1.40
10	bB	822	CLA	C1D-C2D	2.67	1.48	1.42
10	bA	823	CLA	C1D-C2D	2.67	1.48	1.42
10	bA	807	CLA	C4B-CHC	2.66	1.47	1.40
10	cA	802	CLA	C1B-CHB	2.66	1.47	1.40
10	cB	830	CLA	C4C-C3C	2.66	1.49	1.45
13	bB	847	BCR	C30-C25	-2.66	1.50	1.53
10	cB	841	CLA	C1B-CHB	2.66	1.47	1.40
10	aB	836	CLA	C4B-CHC	2.66	1.47	1.40
10	cB	826	CLA	CHD-C4C	2.66	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	810	CLA	C4B-CHC	2.66	1.47	1.40
13	cI	103	BCR	C30-C25	-2.66	1.50	1.53
10	aA	809	CLA	C1D-C2D	2.66	1.48	1.42
10	bA	802	CLA	C1B-CHB	2.66	1.47	1.40
10	bB	838	CLA	C1D-C2D	2.66	1.48	1.42
10	aA	832	CLA	C4B-CHC	2.66	1.47	1.40
10	aB	820	CLA	C4B-CHC	2.66	1.47	1.40
10	bA	814	CLA	C1D-C2D	2.66	1.48	1.42
10	aB	812	CLA	C1D-C2D	2.66	1.48	1.42
10	aA	807	CLA	C4B-CHC	2.66	1.47	1.40
10	cB	803	CLA	C1B-CHB	2.66	1.47	1.40
10	bB	809	CLA	C4B-CHC	2.65	1.47	1.40
10	aB	826	CLA	CHD-C4C	2.65	1.48	1.41
10	bB	833	CLA	C1D-C2D	2.65	1.48	1.42
10	cA	810	CLA	C4B-CHC	2.65	1.47	1.40
10	aA	823	CLA	C1D-C2D	2.65	1.48	1.42
10	aB	825	CLA	C4B-CHC	2.65	1.47	1.40
10	bB	826	CLA	CHD-C4C	2.65	1.48	1.41
10	aB	838	CLA	C1D-C2D	2.65	1.48	1.42
10	cB	820	CLA	C4C-C3C	2.65	1.49	1.45
10	bA	827	CLA	C4B-CHC	2.65	1.47	1.40
10	aA	810	CLA	C4B-CHC	2.65	1.47	1.40
10	cA	856	CLA	C1D-C2D	2.65	1.48	1.42
10	cA	839	CLA	C4B-CHC	2.65	1.47	1.40
10	bB	825	CLA	C4B-CHC	2.65	1.47	1.40
10	cA	823	CLA	C1D-C2D	2.65	1.48	1.42
13	cA	851	BCR	C30-C25	-2.65	1.50	1.53
13	cB	845	BCR	C30-C25	-2.65	1.50	1.53
10	aL	203	CLA	C1D-C2D	2.65	1.48	1.42
10	cL	203	CLA	C1D-C2D	2.65	1.48	1.42
10	bL	203	CLA	C1D-C2D	2.65	1.48	1.42
10	aA	828	CLA	C4B-CHC	2.65	1.47	1.40
13	aI	102	BCR	C1-C6	-2.64	1.50	1.53
10	bA	841	CLA	C1B-CHB	2.64	1.47	1.40
10	cA	821	CLA	C1B-CHB	2.64	1.47	1.40
10	aA	840	CLA	C1D-C2D	2.64	1.48	1.42
10	bA	856	CLA	C1D-C2D	2.64	1.48	1.42
10	bA	821	CLA	C4B-CHC	2.64	1.47	1.40
10	bA	839	CLA	C4B-CHC	2.64	1.47	1.40
10	bB	830	CLA	C4C-C3C	2.64	1.49	1.45
13	aB	843	BCR	C30-C25	-2.64	1.50	1.53
13	bB	843	BCR	C30-C25	-2.64	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	812	CLA	C1D-C2D	2.64	1.48	1.42
10	cA	832	CLA	C4B-CHC	2.64	1.47	1.40
10	cB	829	CLA	C1B-CHB	2.64	1.47	1.40
10	bA	843	CLA	C4C-C3C	2.63	1.49	1.45
10	aA	854	CLA	C1D-C2D	2.63	1.48	1.42
10	aB	830	CLA	C4C-C3C	2.63	1.49	1.45
10	cA	830	CLA	C1D-C2D	2.63	1.48	1.42
10	cA	821	CLA	C4B-CHC	2.63	1.47	1.40
10	bA	821	CLA	C1B-CHB	2.63	1.47	1.40
10	bB	820	CLA	C4C-C3C	2.63	1.49	1.45
10	cB	812	CLA	C1D-C2D	2.63	1.48	1.42
10	cB	821	CLA	C1B-CHB	2.63	1.47	1.40
10	aA	843	CLA	C1B-CHB	2.63	1.47	1.40
10	aB	829	CLA	C1B-CHB	2.63	1.47	1.40
10	bA	834	CLA	C1B-CHB	2.63	1.47	1.40
10	cA	854	CLA	C1D-C2D	2.63	1.48	1.42
10	aA	843	CLA	C4C-C3C	2.63	1.49	1.45
10	bA	854	CLA	C1D-C2D	2.63	1.48	1.42
10	bA	805	CLA	C1B-CHB	2.63	1.47	1.40
10	aA	821	CLA	C4B-CHC	2.63	1.47	1.40
10	aA	805	CLA	C1B-CHB	2.63	1.47	1.40
10	cA	841	CLA	C1B-CHB	2.63	1.47	1.40
10	bA	832	CLA	C4B-CHC	2.63	1.47	1.40
10	cA	827	CLA	C4B-CHC	2.63	1.47	1.40
10	cA	805	CLA	C4B-CHC	2.63	1.47	1.40
10	aB	803	CLA	C4B-CHC	2.63	1.47	1.40
10	aA	821	CLA	C1B-CHB	2.63	1.47	1.40
10	bB	817	CLA	C1D-C2D	2.63	1.48	1.42
10	cA	827	CLA	C1D-C2D	2.62	1.48	1.42
10	aA	827	CLA	C4B-CHC	2.62	1.47	1.40
10	bL	202	CLA	C4B-CHC	2.62	1.47	1.40
10	aA	830	CLA	C4B-CHC	2.62	1.47	1.40
10	bB	829	CLA	C1B-CHB	2.62	1.47	1.40
10	bB	841	CLA	C1B-CHB	2.62	1.47	1.40
10	aA	805	CLA	C4B-CHC	2.62	1.47	1.40
10	aL	203	CLA	C4B-CHC	2.62	1.47	1.40
10	aB	817	CLA	C4B-CHC	2.62	1.47	1.40
10	aA	839	CLA	C4B-CHC	2.62	1.47	1.40
10	bA	805	CLA	C4B-CHC	2.62	1.47	1.40
10	aB	841	CLA	C1B-CHB	2.62	1.47	1.40
10	cB	803	CLA	C4B-CHC	2.62	1.47	1.40
10	bA	827	CLA	C1D-C2D	2.62	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	834	CLA	C1B-CHB	2.62	1.47	1.40
10	bB	836	CLA	C4B-CHC	2.62	1.47	1.40
10	cL	203	CLA	C4B-CHC	2.62	1.47	1.40
10	cB	836	CLA	C4B-CHC	2.62	1.47	1.40
10	cL	205	CLA	C1B-CHB	2.62	1.47	1.40
10	bL	203	CLA	C4B-CHC	2.62	1.47	1.40
10	bL	205	CLA	C1D-C2D	2.62	1.48	1.42
10	aA	841	CLA	C1B-CHB	2.62	1.47	1.40
10	aA	830	CLA	C1D-C2D	2.62	1.48	1.42
10	aA	834	CLA	C1B-CHB	2.61	1.47	1.40
10	cB	817	CLA	C1D-C2D	2.61	1.48	1.42
13	cI	103	BCR	C1-C6	-2.61	1.50	1.53
10	bA	840	CLA	C1D-C2D	2.61	1.48	1.42
10	aL	205	CLA	C1B-CHB	2.61	1.47	1.40
10	aA	817	CLA	C1D-C2D	2.61	1.48	1.42
10	bA	817	CLA	C1D-C2D	2.61	1.48	1.42
10	cA	805	CLA	C1B-CHB	2.61	1.47	1.40
10	bB	841	CLA	C1C-NC	-2.61	1.33	1.37
10	bB	803	CLA	C4B-CHC	2.61	1.47	1.40
10	cA	817	CLA	C1D-C2D	2.61	1.48	1.42
10	aB	821	CLA	C1B-CHB	2.61	1.47	1.40
10	aL	205	CLA	C1D-C2D	2.61	1.48	1.42
10	bB	821	CLA	C1B-CHB	2.61	1.47	1.40
10	cB	816	CLA	C1D-C2D	2.61	1.48	1.42
10	aL	202	CLA	C4B-CHC	2.61	1.47	1.40
10	cL	205	CLA	C1D-C2D	2.61	1.48	1.42
10	aA	856	CLA	C1D-C2D	2.61	1.48	1.42
13	aB	846	BCR	C1-C6	-2.61	1.50	1.53
10	cA	843	CLA	C1B-CHB	2.60	1.47	1.40
10	aB	815	CLA	C4B-CHC	2.60	1.47	1.40
13	bI	102	BCR	C1-C6	-2.60	1.50	1.53
10	bB	834	CLA	CHD-C4C	2.60	1.48	1.41
10	cA	805	CLA	C1D-C2D	2.60	1.48	1.42
10	cL	202	CLA	C4B-CHC	2.60	1.47	1.40
10	aB	834	CLA	CHD-C4C	2.60	1.48	1.41
10	cB	823	CLA	C1B-CHB	2.60	1.47	1.40
10	cA	815	CLA	C1B-CHB	2.60	1.47	1.40
10	cB	840	CLA	C1B-CHB	2.60	1.47	1.40
13	cA	846	BCR	C30-C25	-2.60	1.50	1.53
10	aB	823	CLA	C1B-CHB	2.60	1.47	1.40
10	cA	819	CLA	C1D-C2D	2.60	1.48	1.42
10	bB	813	CLA	C1B-CHB	2.60	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	bB	846	BCR	C1-C6	-2.60	1.50	1.53
10	bA	813	CLA	C4B-CHC	2.60	1.47	1.40
10	cB	841	CLA	C1C-NC	-2.59	1.33	1.37
10	aB	841	CLA	C1C-NC	-2.59	1.33	1.37
10	cA	824	CLA	C1B-CHB	2.59	1.47	1.40
10	aB	811	CLA	C1B-CHB	2.59	1.47	1.40
10	cA	840	CLA	C1D-C2D	2.59	1.48	1.42
10	bA	843	CLA	C1B-CHB	2.59	1.47	1.40
10	bB	816	CLA	C1D-C2D	2.59	1.48	1.42
10	cA	840	CLA	C1B-CHB	2.59	1.47	1.40
10	bA	830	CLA	C4B-CHC	2.59	1.47	1.40
10	bB	802	CLA	C4B-CHC	2.59	1.47	1.40
10	cB	813	CLA	C1B-CHB	2.59	1.47	1.40
10	aB	840	CLA	C1B-CHB	2.59	1.47	1.40
10	cB	834	CLA	CHD-C4C	2.59	1.48	1.41
10	cB	817	CLA	C4B-CHC	2.59	1.47	1.40
13	cB	843	BCR	C30-C25	-2.59	1.50	1.53
10	aB	837	CLA	C1B-CHB	2.59	1.47	1.40
10	aB	820	CLA	C4C-C3C	2.59	1.49	1.45
10	cA	813	CLA	C4B-CHC	2.58	1.47	1.40
10	bB	840	CLA	C1B-CHB	2.58	1.47	1.40
10	bL	205	CLA	C4B-CHC	2.58	1.47	1.40
10	cA	831	CLA	C4B-CHC	2.58	1.47	1.40
13	bA	846	BCR	C30-C25	-2.58	1.50	1.53
10	aB	824	CLA	C1B-CHB	2.58	1.47	1.40
10	aA	840	CLA	C1B-CHB	2.58	1.47	1.40
10	bA	824	CLA	C1B-CHB	2.58	1.47	1.40
10	aB	817	CLA	C1D-C2D	2.58	1.48	1.42
10	bL	205	CLA	C1B-CHB	2.58	1.47	1.40
10	aB	836	CLA	C1B-CHB	2.58	1.47	1.40
10	aL	205	CLA	C4B-CHC	2.58	1.47	1.40
10	aA	827	CLA	C1D-C2D	2.58	1.48	1.42
10	bA	830	CLA	C1D-C2D	2.58	1.48	1.42
10	cB	815	CLA	C4B-CHC	2.58	1.47	1.40
10	aA	813	CLA	C4B-CHC	2.58	1.47	1.40
10	cL	205	CLA	C4B-CHC	2.58	1.47	1.40
10	bB	817	CLA	C4B-CHC	2.58	1.47	1.40
10	cA	825	CLA	C1C-C2C	2.58	1.49	1.44
10	cB	822	CLA	C1B-CHB	2.58	1.47	1.40
10	cB	836	CLA	C1B-CHB	2.58	1.47	1.40
10	aA	815	CLA	C1B-CHB	2.58	1.47	1.40
13	aA	846	BCR	C30-C25	-2.57	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	821	CLA	C1D-C2D	2.57	1.48	1.42
10	bA	840	CLA	C1B-CHB	2.57	1.47	1.40
10	bB	815	CLA	C4B-CHC	2.57	1.47	1.40
10	aA	805	CLA	C1D-C2D	2.57	1.48	1.42
10	aB	822	CLA	C1B-CHB	2.57	1.47	1.40
10	bB	823	CLA	C1B-CHB	2.57	1.47	1.40
10	bB	820	CLA	CHD-C4C	2.57	1.48	1.41
10	bA	819	CLA	C1D-C2D	2.57	1.48	1.42
10	cA	830	CLA	C4B-CHC	2.57	1.47	1.40
10	aB	802	CLA	C4B-CHC	2.57	1.47	1.40
13	bI	102	BCR	C30-C25	-2.57	1.50	1.53
10	aB	820	CLA	CHD-C4C	2.57	1.48	1.41
10	bB	807	CLA	C1D-C2D	2.57	1.48	1.42
10	bA	825	CLA	C1C-C2C	2.57	1.49	1.44
10	bB	836	CLA	CHD-C4C	2.57	1.48	1.41
10	cA	821	CLA	C1D-C2D	2.57	1.48	1.42
10	bB	811	CLA	C1B-CHB	2.57	1.47	1.40
10	bB	836	CLA	C1B-CHB	2.57	1.47	1.40
10	aB	816	CLA	C1D-C2D	2.56	1.48	1.42
10	aB	836	CLA	CHD-C4C	2.56	1.48	1.41
10	cB	807	CLA	C1D-C2D	2.56	1.48	1.42
10	aA	831	CLA	C4B-CHC	2.56	1.46	1.40
10	aA	825	CLA	C1C-C2C	2.56	1.49	1.44
13	cB	846	BCR	C1-C6	-2.56	1.50	1.53
10	bB	831	CLA	CHD-C4C	2.56	1.48	1.41
10	bB	822	CLA	C1B-CHB	2.56	1.46	1.40
10	bB	823	CLA	CHD-C4C	2.56	1.48	1.41
10	bA	815	CLA	C1B-CHB	2.56	1.46	1.40
10	cA	807	CLA	C1D-C2D	2.56	1.48	1.42
10	cB	823	CLA	CHD-C4C	2.56	1.48	1.41
10	aB	813	CLA	C1B-CHB	2.56	1.46	1.40
10	bA	816	CLA	C1D-C2D	2.56	1.48	1.42
10	cB	802	CLA	C4B-CHC	2.56	1.46	1.40
10	aA	811	CLA	C1D-C2D	2.56	1.48	1.42
10	cB	837	CLA	C1B-CHB	2.56	1.46	1.40
10	aB	807	CLA	C1D-C2D	2.56	1.48	1.42
10	aB	824	CLA	C4C-C3C	2.56	1.49	1.45
10	aA	807	CLA	C1D-C2D	2.56	1.48	1.42
10	bA	831	CLA	C4B-CHC	2.56	1.46	1.40
10	aA	824	CLA	C1B-CHB	2.55	1.46	1.40
10	cB	811	CLA	C1B-CHB	2.55	1.46	1.40
10	cB	820	CLA	CHD-C4C	2.55	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	836	CLA	CHD-C4C	2.55	1.48	1.41
10	bB	834	CLA	C4C-C3C	2.55	1.49	1.45
10	aB	814	CLA	C1B-CHB	2.55	1.46	1.40
10	aA	829	CLA	C1B-CHB	2.55	1.46	1.40
13	aI	102	BCR	C30-C25	-2.55	1.50	1.53
10	cB	835	CLA	CHD-C4C	2.55	1.48	1.41
10	bA	811	CLA	C1D-C2D	2.55	1.48	1.42
13	bA	848	BCR	C30-C25	-2.55	1.50	1.53
10	aL	202	CLA	C1C-NC	-2.55	1.34	1.37
10	aB	835	CLA	CHD-C4C	2.55	1.48	1.41
13	bB	844	BCR	C30-C25	-2.55	1.50	1.53
10	bB	824	CLA	C1B-CHB	2.55	1.46	1.40
10	aB	805	CLA	C4B-CHC	2.55	1.46	1.40
10	cA	829	CLA	C1B-CHB	2.55	1.46	1.40
10	bB	837	CLA	C1B-CHB	2.54	1.46	1.40
10	bA	833	CLA	C4B-CHC	2.54	1.46	1.40
10	aB	823	CLA	CHD-C4C	2.54	1.48	1.41
10	cA	836	CLA	C1B-CHB	2.54	1.46	1.40
10	cB	807	CLA	C4B-CHC	2.54	1.46	1.40
10	aB	807	CLA	C4B-CHC	2.54	1.46	1.40
10	aA	837	CLA	C1B-CHB	2.54	1.46	1.40
10	bB	806	CLA	C1B-CHB	2.54	1.46	1.40
10	cB	824	CLA	C1B-CHB	2.54	1.46	1.40
10	cB	834	CLA	C4C-C3C	2.54	1.49	1.45
10	cB	814	CLA	C1B-CHB	2.54	1.46	1.40
10	aA	843	CLA	CHD-C4C	2.54	1.48	1.41
10	cB	814	CLA	C4B-CHC	2.54	1.46	1.40
10	aA	819	CLA	C1D-C2D	2.54	1.48	1.42
10	aB	814	CLA	C4C-C3C	2.54	1.49	1.45
10	cB	828	CLA	C4B-CHC	2.54	1.46	1.40
10	cA	816	CLA	C1D-C2D	2.54	1.48	1.42
10	cA	813	CLA	C1B-CHB	2.53	1.46	1.40
10	bL	202	CLA	C1C-NC	-2.53	1.34	1.37
10	bB	839	CLA	C1B-CHB	2.53	1.46	1.40
10	cL	202	CLA	C1C-NC	-2.53	1.34	1.37
10	cB	839	CLA	C1B-CHB	2.53	1.46	1.40
10	bB	814	CLA	C1B-CHB	2.53	1.46	1.40
10	bA	831	CLA	C1B-CHB	2.53	1.46	1.40
10	cA	833	CLA	C4B-CHC	2.53	1.46	1.40
10	aB	806	CLA	C1B-CHB	2.53	1.46	1.40
10	bA	805	CLA	C1D-C2D	2.53	1.48	1.42
10	bA	813	CLA	C1B-CHB	2.53	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	837	CLA	C1B-CHB	2.53	1.46	1.40
10	cA	811	CLA	C1D-C2D	2.53	1.48	1.42
10	aB	831	CLA	CHD-C4C	2.53	1.48	1.41
10	aA	816	CLA	C1D-C2D	2.53	1.48	1.42
10	bA	807	CLA	C1D-C2D	2.53	1.48	1.42
13	aA	848	BCR	C30-C25	-2.53	1.50	1.53
10	bB	835	CLA	CHD-C4C	2.53	1.48	1.41
10	bA	821	CLA	C1D-C2D	2.53	1.48	1.42
10	bB	830	CLA	C1D-C2D	2.53	1.48	1.42
10	aA	856	CLA	C1B-CHB	2.53	1.46	1.40
10	bA	829	CLA	C1B-CHB	2.53	1.46	1.40
10	bB	814	CLA	C4C-C3C	2.53	1.49	1.45
10	aA	834	CLA	C4B-CHC	2.53	1.46	1.40
10	cB	805	CLA	C4B-CHC	2.53	1.46	1.40
10	aA	820	CLA	C1D-C2D	2.52	1.48	1.42
10	aA	831	CLA	C1B-CHB	2.52	1.46	1.40
10	cB	831	CLA	CHD-C4C	2.52	1.48	1.41
10	bB	807	CLA	C4B-CHC	2.52	1.46	1.40
10	bA	834	CLA	C4B-CHC	2.52	1.46	1.40
10	aA	810	CLA	C4C-C3C	2.52	1.49	1.45
10	bB	819	CLA	C1D-C2D	2.52	1.48	1.42
10	cA	819	CLA	C1B-CHB	2.52	1.46	1.40
10	aA	836	CLA	C1B-CHB	2.52	1.46	1.40
10	aA	804	CLA	C1D-C2D	2.52	1.48	1.42
10	aA	813	CLA	C1B-CHB	2.52	1.46	1.40
10	aA	833	CLA	C4B-CHC	2.52	1.46	1.40
10	cB	809	CLA	C1B-CHB	2.52	1.46	1.40
10	cB	814	CLA	C4C-C3C	2.52	1.49	1.45
10	cA	810	CLA	C4C-C3C	2.52	1.49	1.45
10	aB	834	CLA	C4C-C3C	2.52	1.49	1.45
10	bB	814	CLA	C4B-CHC	2.52	1.46	1.40
10	cA	820	CLA	C1D-C2D	2.52	1.48	1.42
10	bB	824	CLA	CHD-C4C	2.51	1.48	1.41
10	aB	819	CLA	C1D-C2D	2.51	1.48	1.42
10	cA	834	CLA	C4B-CHC	2.51	1.46	1.40
10	bB	805	CLA	C4B-CHC	2.51	1.46	1.40
10	aB	814	CLA	C4B-CHC	2.51	1.46	1.40
10	bA	837	CLA	C1B-CHB	2.51	1.46	1.40
10	bA	826	CLA	C1B-CHB	2.51	1.46	1.40
10	cA	804	CLA	C1D-C2D	2.51	1.48	1.42
10	bA	811	CLA	C1B-CHB	2.51	1.46	1.40
10	bA	833	CLA	C1D-C2D	2.51	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	824	CLA	C4C-C3C	2.51	1.49	1.45
10	bA	820	CLA	C1D-C2D	2.51	1.48	1.42
10	cA	832	CLA	C1D-C2D	2.51	1.48	1.42
10	cA	839	CLA	CHD-C4C	2.51	1.48	1.41
10	cB	824	CLA	C4C-C3C	2.51	1.49	1.45
10	bA	836	CLA	C1B-CHB	2.51	1.46	1.40
10	aA	833	CLA	C1D-C2D	2.51	1.48	1.42
10	aB	824	CLA	CHD-C4C	2.51	1.48	1.41
10	cA	831	CLA	C1B-CHB	2.51	1.46	1.40
10	aA	826	CLA	C1B-CHB	2.51	1.46	1.40
10	bB	828	CLA	C4B-CHC	2.51	1.46	1.40
10	cB	830	CLA	C1B-CHB	2.51	1.46	1.40
10	bB	809	CLA	C1B-CHB	2.51	1.46	1.40
10	bA	843	CLA	CHD-C4C	2.51	1.48	1.41
10	bA	828	CLA	C1B-CHB	2.51	1.46	1.40
10	cA	856	CLA	C1B-CHB	2.50	1.46	1.40
10	cA	810	CLA	CHD-C4C	2.50	1.48	1.41
10	aA	828	CLA	C1B-CHB	2.50	1.46	1.40
10	bA	839	CLA	CHD-C4C	2.50	1.48	1.41
10	cA	843	CLA	CHD-C4C	2.50	1.48	1.41
10	cB	812	CLA	C1B-CHB	2.50	1.46	1.40
10	bA	810	CLA	CHD-C4C	2.50	1.48	1.41
10	aA	819	CLA	C1B-CHB	2.50	1.46	1.40
10	aB	828	CLA	C4B-CHC	2.50	1.46	1.40
10	cB	806	CLA	C1B-CHB	2.50	1.46	1.40
10	bA	804	CLA	C1D-C2D	2.50	1.48	1.42
10	bA	818	CLA	C4B-CHC	2.50	1.46	1.40
10	bA	803	CLA	C1B-CHB	2.50	1.46	1.40
10	cA	812	CLA	CHD-C4C	2.50	1.48	1.41
10	aA	818	CLA	C4B-CHC	2.50	1.46	1.40
10	cB	830	CLA	C1D-C2D	2.50	1.48	1.42
10	aB	830	CLA	C1D-C2D	2.50	1.48	1.42
10	cB	824	CLA	CHD-C4C	2.50	1.48	1.41
10	aB	839	CLA	C1B-CHB	2.50	1.46	1.40
10	cA	828	CLA	C1B-CHB	2.50	1.46	1.40
10	bA	819	CLA	C1B-CHB	2.50	1.46	1.40
10	bA	812	CLA	CHD-C4C	2.50	1.48	1.41
13	aB	844	BCR	C30-C25	-2.50	1.50	1.53
10	cL	204	CLA	C1B-CHB	2.50	1.46	1.40
13	bA	851	BCR	C1-C6	-2.50	1.50	1.53
10	cA	833	CLA	C1D-C2D	2.50	1.48	1.42
10	bA	818	CLA	CHD-C4C	2.50	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	818	CLA	CHD-C4C	2.50	1.48	1.41
10	aB	823	CLA	C4C-C3C	2.50	1.49	1.45
10	cA	818	CLA	CHD-C4C	2.49	1.48	1.41
10	aB	809	CLA	C1B-CHB	2.49	1.46	1.40
10	bA	832	CLA	C1D-C2D	2.49	1.48	1.42
10	aA	823	CLA	C4B-CHC	2.49	1.46	1.40
13	cB	844	BCR	C30-C25	-2.49	1.50	1.53
10	cB	829	CLA	C4B-CHC	2.49	1.46	1.40
10	cL	203	CLA	C1B-CHB	2.49	1.46	1.40
10	bA	856	CLA	C1B-CHB	2.49	1.46	1.40
10	bL	204	CLA	C1B-CHB	2.49	1.46	1.40
10	cA	854	CLA	C1B-CHB	2.49	1.46	1.40
10	cA	826	CLA	C1B-CHB	2.49	1.46	1.40
10	cA	838	CLA	C1D-C2D	2.49	1.48	1.42
10	bB	833	CLA	C1B-CHB	2.49	1.46	1.40
10	bA	806	CLA	CHD-C4C	2.49	1.48	1.41
10	cA	803	CLA	C1B-CHB	2.49	1.46	1.40
10	aA	835	CLA	C1B-CHB	2.49	1.46	1.40
10	bA	838	CLA	C1D-C2D	2.49	1.48	1.42
10	bL	203	CLA	C1B-CHB	2.49	1.46	1.40
10	aA	816	CLA	C1B-CHB	2.49	1.46	1.40
10	aA	810	CLA	CHD-C4C	2.48	1.48	1.41
10	aA	822	CLA	C1B-CHB	2.48	1.46	1.40
10	cB	813	CLA	C1D-C2D	2.48	1.48	1.42
10	cA	811	CLA	C1B-CHB	2.48	1.46	1.40
10	aA	832	CLA	C1D-C2D	2.48	1.48	1.42
10	bB	836	CLA	C4C-C3C	2.48	1.49	1.45
10	bA	854	CLA	C1B-CHB	2.48	1.46	1.40
10	aA	839	CLA	CHD-C4C	2.48	1.48	1.41
10	bA	810	CLA	C4C-C3C	2.48	1.49	1.45
13	cB	847	BCR	C1-C6	-2.48	1.50	1.53
13	aA	849	BCR	C30-C25	-2.48	1.50	1.53
10	aB	829	CLA	C4B-CHC	2.48	1.46	1.40
10	aB	836	CLA	C4C-C3C	2.48	1.49	1.45
13	cB	849	BCR	C1-C6	-2.48	1.50	1.53
10	aA	806	CLA	CHD-C4C	2.48	1.48	1.41
10	bA	822	CLA	C1B-CHB	2.48	1.46	1.40
10	bB	830	CLA	C1B-CHB	2.48	1.46	1.40
10	cB	837	CLA	C1D-C2D	2.48	1.48	1.42
10	cA	818	CLA	C4B-CHC	2.48	1.46	1.40
10	cB	835	CLA	C1B-CHB	2.48	1.46	1.40
10	aB	812	CLA	C1B-CHB	2.48	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	823	CLA	C4B-CHC	2.48	1.46	1.40
10	aB	830	CLA	C1B-CHB	2.47	1.46	1.40
10	aA	812	CLA	CHD-C4C	2.47	1.48	1.41
10	cA	803	CLA	CHD-C4C	2.47	1.48	1.41
10	aB	818	CLA	CHD-C4C	2.47	1.48	1.41
10	cB	819	CLA	C1D-C2D	2.47	1.48	1.42
10	aB	806	CLA	C1D-C2D	2.47	1.48	1.42
10	cB	812	CLA	C4B-CHC	2.47	1.46	1.40
10	cA	830	CLA	C1B-CHB	2.47	1.46	1.40
10	aA	811	CLA	C1B-CHB	2.47	1.46	1.40
13	cA	851	BCR	C1-C6	-2.47	1.50	1.53
13	bA	847	BCR	C1-C6	-2.47	1.50	1.53
10	bB	823	CLA	C4C-C3C	2.47	1.49	1.45
13	aA	851	BCR	C1-C6	-2.47	1.50	1.53
10	aL	204	CLA	C1B-CHB	2.47	1.46	1.40
10	cB	823	CLA	C4C-C3C	2.47	1.49	1.45
10	cA	802	CLA	CHD-C4C	2.47	1.48	1.41
10	cB	822	CLA	C4B-CHC	2.47	1.46	1.40
10	bB	812	CLA	C1B-CHB	2.47	1.46	1.40
10	bB	839	CLA	C1D-C2D	2.47	1.48	1.42
10	cA	827	CLA	C1B-CHB	2.47	1.46	1.40
10	cA	835	CLA	C1B-CHB	2.47	1.46	1.40
10	cB	808	CLA	C1B-CHB	2.47	1.46	1.40
10	aA	813	CLA	CHD-C4C	2.47	1.48	1.41
10	bB	813	CLA	C1D-C2D	2.47	1.48	1.42
10	bA	835	CLA	C1B-CHB	2.47	1.46	1.40
10	aB	812	CLA	C4B-CHC	2.46	1.46	1.40
10	aB	835	CLA	C1B-CHB	2.46	1.46	1.40
13	aB	849	BCR	C1-C6	-2.46	1.50	1.53
10	cB	818	CLA	CHD-C4C	2.46	1.48	1.41
10	aB	822	CLA	C4B-CHC	2.46	1.46	1.40
10	aA	838	CLA	C1D-C2D	2.46	1.48	1.42
10	aA	803	CLA	C1B-CHB	2.46	1.46	1.40
10	cA	816	CLA	C1B-CHB	2.46	1.46	1.40
13	cA	847	BCR	C1-C6	-2.46	1.50	1.53
10	bB	837	CLA	C1D-C2D	2.46	1.48	1.42
10	cB	834	CLA	C1B-CHB	2.46	1.46	1.40
10	bB	806	CLA	C1D-C2D	2.46	1.48	1.42
10	cA	809	CLA	C1B-CHB	2.46	1.46	1.40
10	cB	836	CLA	C4C-C3C	2.46	1.49	1.45
10	bA	803	CLA	CHD-C4C	2.46	1.48	1.41
10	cA	823	CLA	C4B-CHC	2.46	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	829	CLA	C4B-CHC	2.46	1.46	1.40
10	bB	812	CLA	CHD-C4C	2.46	1.48	1.41
10	cA	819	CLA	CHD-C4C	2.46	1.48	1.41
10	cA	822	CLA	C1B-CHB	2.46	1.46	1.40
13	aA	847	BCR	C1-C6	-2.46	1.50	1.53
10	aA	830	CLA	C1B-CHB	2.46	1.46	1.40
10	aA	814	CLA	C1B-CHB	2.46	1.46	1.40
10	aB	833	CLA	C1B-CHB	2.46	1.46	1.40
10	bA	802	CLA	CHD-C4C	2.46	1.48	1.41
10	bB	808	CLA	C1B-CHB	2.46	1.46	1.40
10	aA	803	CLA	CHD-C4C	2.46	1.48	1.41
10	aB	808	CLA	C1B-CHB	2.46	1.46	1.40
10	aL	203	CLA	C1B-CHB	2.46	1.46	1.40
10	bA	816	CLA	C1B-CHB	2.46	1.46	1.40
13	bA	849	BCR	C30-C25	-2.46	1.50	1.53
10	cB	806	CLA	C1D-C2D	2.46	1.48	1.42
10	cA	806	CLA	CHD-C4C	2.46	1.48	1.41
10	aB	833	CLA	CHD-C4C	2.46	1.48	1.41
10	bB	811	CLA	C1C-NC	-2.46	1.34	1.37
10	cB	833	CLA	C1B-CHB	2.45	1.46	1.40
10	bL	202	CLA	C1B-CHB	2.45	1.46	1.40
10	cB	810	CLA	C1C-NC	-2.45	1.34	1.37
10	aA	802	CLA	CHD-C4C	2.45	1.48	1.41
10	bB	830	CLA	CHD-C4C	2.45	1.48	1.41
10	cB	831	CLA	C4C-C3C	2.45	1.49	1.45
10	cA	817	CLA	C1B-CHB	2.45	1.46	1.40
10	cA	840	CLA	C1C-C2C	2.45	1.49	1.44
10	aA	809	CLA	C1B-CHB	2.45	1.46	1.40
10	bB	822	CLA	C4B-CHC	2.45	1.46	1.40
10	cB	814	CLA	CHD-C4C	2.45	1.48	1.41
10	aB	814	CLA	CHD-C4C	2.45	1.48	1.41
10	cB	833	CLA	CHD-C4C	2.45	1.48	1.41
10	aA	827	CLA	C1B-CHB	2.45	1.46	1.40
10	aA	819	CLA	C4C-C3C	2.45	1.49	1.45
10	aB	813	CLA	C1D-C2D	2.45	1.48	1.42
10	aA	854	CLA	C1B-CHB	2.45	1.46	1.40
10	bB	812	CLA	C4B-CHC	2.45	1.46	1.40
10	cB	839	CLA	C1D-C2D	2.45	1.48	1.42
10	aB	839	CLA	C1D-C2D	2.45	1.48	1.42
10	bB	818	CLA	CHD-C4C	2.45	1.48	1.41
10	aA	829	CLA	C4B-CHC	2.45	1.46	1.40
10	aA	817	CLA	C1B-CHB	2.45	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	812	CLA	C1B-CHB	2.44	1.46	1.40
10	bA	819	CLA	C4C-C3C	2.44	1.49	1.45
10	bA	840	CLA	C1C-C2C	2.44	1.49	1.44
10	bA	813	CLA	CHD-C4C	2.44	1.48	1.41
10	bB	816	CLA	C1B-CHB	2.44	1.46	1.40
10	aB	832	CLA	CHD-C4C	2.44	1.48	1.41
10	aL	202	CLA	C1B-CHB	2.44	1.46	1.40
13	cA	848	BCR	C30-C25	-2.44	1.50	1.53
10	bB	833	CLA	CHD-C4C	2.44	1.48	1.41
10	aB	834	CLA	C1B-CHB	2.44	1.46	1.40
10	cA	819	CLA	C4C-C3C	2.44	1.49	1.45
10	cB	815	CLA	C1D-C2D	2.44	1.48	1.42
10	cA	812	CLA	C1B-CHB	2.44	1.46	1.40
13	cA	849	BCR	C30-C25	-2.44	1.50	1.53
10	cB	838	CLA	CHD-C4C	2.44	1.48	1.41
10	bB	810	CLA	C1C-NC	-2.44	1.34	1.37
10	aB	812	CLA	CHD-C4C	2.44	1.48	1.41
10	cB	812	CLA	CHD-C4C	2.44	1.48	1.41
10	bB	832	CLA	CHD-C4C	2.44	1.48	1.41
10	bA	817	CLA	C1B-CHB	2.44	1.46	1.40
13	aB	847	BCR	C1-C6	-2.44	1.50	1.53
10	cB	811	CLA	C1C-NC	-2.44	1.34	1.37
10	bA	812	CLA	C1B-CHB	2.44	1.46	1.40
10	bB	815	CLA	C1D-C2D	2.44	1.48	1.42
10	cA	826	CLA	C1D-C2D	2.43	1.48	1.42
10	aA	814	CLA	CHD-C4C	2.43	1.48	1.41
10	bA	814	CLA	CHD-C4C	2.43	1.48	1.41
10	cA	829	CLA	C4B-CHC	2.43	1.46	1.40
10	aB	810	CLA	C1C-NC	-2.43	1.34	1.37
10	bA	815	CLA	CHD-C4C	2.43	1.48	1.41
10	bA	825	CLA	C1D-C2D	2.43	1.48	1.42
10	cA	842	CLA	C1D-C2D	2.43	1.48	1.42
10	bB	807	CLA	C1B-CHB	2.43	1.46	1.40
10	bA	814	CLA	C1B-CHB	2.43	1.46	1.40
10	bB	835	CLA	C1B-CHB	2.43	1.46	1.40
10	cA	822	CLA	C1C-C2C	2.43	1.49	1.44
10	cB	830	CLA	CHD-C4C	2.43	1.48	1.41
10	bA	842	CLA	C1D-C2D	2.43	1.48	1.42
10	bA	841	CLA	C1D-C2D	2.43	1.48	1.42
10	cA	856	CLA	CHD-C4C	2.43	1.48	1.41
10	cB	816	CLA	CHD-C4C	2.43	1.48	1.41
10	aB	838	CLA	CHD-C4C	2.43	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	837	CLA	C1D-C2D	2.43	1.48	1.42
10	aB	807	CLA	C1B-CHB	2.43	1.46	1.40
10	cB	832	CLA	CHD-C4C	2.43	1.48	1.41
10	bA	827	CLA	C1B-CHB	2.43	1.46	1.40
10	bA	830	CLA	C1B-CHB	2.43	1.46	1.40
13	bB	849	BCR	C1-C6	-2.43	1.50	1.53
10	cA	813	CLA	CHD-C4C	2.43	1.48	1.41
10	cA	814	CLA	C1B-CHB	2.43	1.46	1.40
10	cA	814	CLA	CHD-C4C	2.43	1.48	1.41
10	aB	837	CLA	C1D-C2D	2.43	1.48	1.42
10	aB	839	CLA	CHD-C4C	2.42	1.48	1.41
10	aB	825	CLA	C1B-CHB	2.42	1.46	1.40
10	cB	832	CLA	C1B-CHB	2.42	1.46	1.40
10	bA	819	CLA	CHD-C4C	2.42	1.48	1.41
10	cA	841	CLA	C1D-C2D	2.42	1.48	1.42
10	aA	841	CLA	C1D-C2D	2.42	1.48	1.42
10	bA	826	CLA	C1D-C2D	2.42	1.48	1.42
10	bA	826	CLA	C1C-C2C	2.42	1.49	1.44
10	bA	835	CLA	CHD-C4C	2.42	1.48	1.41
10	bB	816	CLA	CHD-C4C	2.42	1.48	1.41
10	aB	830	CLA	CHD-C4C	2.42	1.48	1.41
10	aA	815	CLA	CHD-C4C	2.42	1.48	1.41
10	bA	829	CLA	C4B-CHC	2.42	1.46	1.40
10	aA	840	CLA	C1C-C2C	2.42	1.49	1.44
10	bB	838	CLA	CHD-C4C	2.42	1.48	1.41
10	aB	816	CLA	CHD-C4C	2.42	1.48	1.41
10	cB	839	CLA	CHD-C4C	2.42	1.48	1.41
10	bA	817	CLA	CHD-C4C	2.42	1.48	1.41
10	bB	814	CLA	CHD-C4C	2.42	1.48	1.41
10	aB	816	CLA	C1B-CHB	2.42	1.46	1.40
10	cA	802	CLA	C4C-C3C	2.42	1.49	1.45
10	cA	815	CLA	CHD-C4C	2.42	1.48	1.41
10	aB	810	CLA	C4B-CHC	2.42	1.46	1.40
10	cB	807	CLA	C1B-CHB	2.42	1.46	1.40
10	bA	807	CLA	C1B-CHB	2.41	1.46	1.40
10	cA	817	CLA	CHD-C4C	2.41	1.48	1.41
10	aA	807	CLA	C1B-CHB	2.41	1.46	1.40
10	aB	811	CLA	C1C-NC	-2.41	1.34	1.37
10	bB	834	CLA	C1B-CHB	2.41	1.46	1.40
10	cA	835	CLA	CHD-C4C	2.41	1.48	1.41
10	bB	822	CLA	CHD-C4C	2.41	1.48	1.41
10	aA	856	CLA	CHD-C4C	2.41	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	809	CLA	C1D-C2D	2.41	1.48	1.42
10	bB	841	CLA	C4B-CHC	2.41	1.46	1.40
10	aB	832	CLA	C1B-CHB	2.41	1.46	1.40
10	cL	202	CLA	C1B-CHB	2.41	1.46	1.40
10	bB	840	CLA	C1C-NC	-2.41	1.34	1.37
10	cA	810	CLA	C1B-CHB	2.41	1.46	1.40
10	aA	825	CLA	C1D-C2D	2.41	1.48	1.42
10	aA	817	CLA	CHD-C4C	2.41	1.48	1.41
10	aA	832	CLA	C1B-CHB	2.41	1.46	1.40
10	cB	810	CLA	C4B-CHC	2.41	1.46	1.40
10	aA	835	CLA	CHD-C4C	2.41	1.48	1.41
10	bB	810	CLA	C4B-CHC	2.41	1.46	1.40
10	bB	821	CLA	C1D-C2D	2.41	1.48	1.42
10	cA	832	CLA	C1B-CHB	2.41	1.46	1.40
10	aB	838	CLA	C1B-CHB	2.41	1.46	1.40
10	aA	802	CLA	C4C-C3C	2.40	1.49	1.45
10	aB	840	CLA	C1C-NC	-2.40	1.34	1.37
10	bB	803	CLA	C1C-C2C	2.40	1.49	1.44
10	bA	856	CLA	CHD-C4C	2.40	1.48	1.41
10	bB	838	CLA	C1B-CHB	2.40	1.46	1.40
10	aA	819	CLA	CHD-C4C	2.40	1.48	1.41
10	bA	822	CLA	C1C-C2C	2.40	1.49	1.44
10	cB	825	CLA	C1B-CHB	2.40	1.46	1.40
10	bA	836	CLA	C4B-CHC	2.40	1.46	1.40
10	bB	831	CLA	C4C-C3C	2.40	1.49	1.45
10	cB	822	CLA	CHD-C4C	2.40	1.48	1.41
10	bB	825	CLA	C1B-CHB	2.40	1.46	1.40
10	cB	816	CLA	C1B-CHB	2.40	1.46	1.40
10	aL	203	CLA	CHD-C4C	2.40	1.48	1.41
10	cA	809	CLA	CHD-C4C	2.40	1.48	1.41
10	aA	836	CLA	C4B-CHC	2.40	1.46	1.40
10	cA	823	CLA	CHD-C4C	2.40	1.48	1.41
10	aB	831	CLA	C4C-C3C	2.40	1.49	1.45
10	cA	807	CLA	C1B-CHB	2.40	1.46	1.40
10	bA	809	CLA	C1B-CHB	2.40	1.46	1.40
10	aB	819	CLA	CHD-C4C	2.39	1.48	1.41
10	aA	826	CLA	C1D-C2D	2.39	1.48	1.42
10	aA	842	CLA	C1D-C2D	2.39	1.48	1.42
10	aB	841	CLA	C4B-CHC	2.39	1.46	1.40
10	bB	804	CLA	C1C-C2C	2.39	1.49	1.44
10	bA	832	CLA	C1B-CHB	2.39	1.46	1.40
10	aB	816	CLA	C4C-C3C	2.39	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	819	CLA	CHD-C4C	2.39	1.48	1.41
10	cB	841	CLA	C1D-C2D	2.39	1.48	1.42
10	cB	815	CLA	C1B-CHB	2.39	1.46	1.40
10	cA	837	CLA	C1D-C2D	2.39	1.48	1.42
10	bA	833	CLA	CHD-C4C	2.39	1.48	1.41
10	cA	825	CLA	C1D-C2D	2.39	1.48	1.42
10	cA	836	CLA	C4B-CHC	2.39	1.46	1.40
10	aB	803	CLA	C1C-C2C	2.39	1.49	1.44
10	aA	807	CLA	CHD-C4C	2.39	1.48	1.41
10	cA	842	CLA	C1C-NC	-2.39	1.34	1.37
10	bB	839	CLA	CHD-C4C	2.39	1.48	1.41
10	aB	822	CLA	CHD-C4C	2.39	1.48	1.41
13	aB	844	BCR	C1-C6	-2.39	1.50	1.53
10	bA	823	CLA	CHD-C4C	2.39	1.48	1.41
10	cB	840	CLA	C1C-NC	-2.39	1.34	1.37
10	bB	801	CLA	C1B-CHB	2.39	1.46	1.40
10	aA	826	CLA	C1C-C2C	2.39	1.49	1.44
13	cA	848	BCR	C1-C6	-2.39	1.50	1.53
10	cA	824	CLA	C4C-C3C	2.39	1.49	1.45
10	bA	839	CLA	C4C-C3C	2.38	1.49	1.45
10	bA	837	CLA	C1C-NC	-2.38	1.34	1.37
10	cB	803	CLA	C1C-C2C	2.38	1.49	1.44
10	bA	807	CLA	CHD-C4C	2.38	1.48	1.41
10	aB	807	CLA	CHD-C4C	2.38	1.48	1.41
10	aA	823	CLA	C1B-CHB	2.38	1.46	1.40
10	cA	811	CLA	CHD-C4C	2.38	1.48	1.41
10	bA	823	CLA	C1B-CHB	2.38	1.46	1.40
10	cA	823	CLA	C1B-CHB	2.38	1.46	1.40
10	aB	817	CLA	C1B-CHB	2.38	1.46	1.40
10	bB	819	CLA	CHD-C4C	2.38	1.48	1.41
10	aB	815	CLA	C1B-CHB	2.38	1.46	1.40
10	bA	841	CLA	CHD-C4C	2.38	1.48	1.41
10	aA	822	CLA	C1C-C2C	2.38	1.49	1.44
10	bB	832	CLA	C1B-CHB	2.38	1.46	1.40
10	aB	815	CLA	C1D-C2D	2.38	1.48	1.42
10	aA	810	CLA	C1B-CHB	2.38	1.46	1.40
10	cA	807	CLA	CHD-C4C	2.38	1.48	1.41
10	bA	821	CLA	CHD-C4C	2.38	1.48	1.41
10	bA	811	CLA	CHD-C4C	2.38	1.48	1.41
10	bA	810	CLA	C1B-CHB	2.38	1.46	1.40
10	aA	811	CLA	CHD-C4C	2.38	1.48	1.41
10	bB	818	CLA	C1B-CHB	2.37	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	cB	844	BCR	C1-C6	-2.37	1.50	1.53
10	cA	808	CLA	C1C-C2C	2.37	1.49	1.44
10	bA	840	CLA	CHD-C4C	2.37	1.48	1.41
9	aA	801	CL0	C4B-CHC	2.37	1.46	1.40
10	cA	833	CLA	CHD-C4C	2.37	1.48	1.41
10	aB	804	CLA	C1C-C2C	2.37	1.49	1.44
10	bA	825	CLA	C1B-CHB	2.37	1.46	1.40
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	aA	820	CLA	CHD-C4C	2.37	1.48	1.41
10	aA	833	CLA	CHD-C4C	2.37	1.48	1.41
10	bL	203	CLA	CHD-C4C	2.37	1.48	1.41
10	bA	809	CLA	CHD-C4C	2.37	1.48	1.41
10	bB	815	CLA	C1B-CHB	2.37	1.46	1.40
10	cB	817	CLA	C1B-CHB	2.37	1.46	1.40
10	bB	817	CLA	C1B-CHB	2.37	1.46	1.40
10	bA	837	CLA	C1D-C2D	2.37	1.47	1.42
10	cB	806	CLA	C1C-C2C	2.37	1.49	1.44
10	aB	818	CLA	C1B-CHB	2.37	1.46	1.40
10	cA	826	CLA	C1C-C2C	2.37	1.49	1.44
13	aA	848	BCR	C1-C6	-2.37	1.50	1.53
10	aB	820	CLA	C1B-CHB	2.37	1.46	1.40
10	cB	830	CLA	C4B-CHC	2.37	1.46	1.40
13	bB	847	BCR	C1-C6	-2.37	1.50	1.53
10	cB	838	CLA	C1B-CHB	2.37	1.46	1.40
10	cB	821	CLA	C1D-C2D	2.37	1.47	1.42
10	aA	809	CLA	CHD-C4C	2.37	1.48	1.41
10	aB	809	CLA	C1D-C2D	2.36	1.47	1.42
10	cB	801	CLA	C1B-CHB	2.36	1.46	1.40
10	cB	807	CLA	CHD-C4C	2.36	1.48	1.41
10	aB	801	CLA	C1D-C2D	2.36	1.47	1.42
10	cA	837	CLA	C1C-NC	-2.36	1.34	1.37
10	cB	804	CLA	C1C-C2C	2.36	1.49	1.44
13	bB	844	BCR	C1-C6	-2.36	1.50	1.53
10	aB	821	CLA	C1D-C2D	2.36	1.47	1.42
10	aB	841	CLA	C1D-C2D	2.36	1.47	1.42
10	cB	818	CLA	C1B-CHB	2.36	1.46	1.40
10	cA	842	CLA	C4B-CHC	2.36	1.46	1.40
10	bB	807	CLA	CHD-C4C	2.36	1.48	1.41
10	aA	823	CLA	CHD-C4C	2.36	1.48	1.41
10	cA	839	CLA	C4C-C3C	2.36	1.49	1.45
10	cA	840	CLA	CHD-C4C	2.36	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	840	CLA	CHD-C4C	2.36	1.48	1.41
10	cB	801	CLA	C4B-CHC	2.36	1.46	1.40
10	bA	802	CLA	C4C-C3C	2.36	1.49	1.45
10	bA	820	CLA	CHD-C4C	2.36	1.48	1.41
10	cL	203	CLA	CHD-C4C	2.36	1.48	1.41
10	cB	808	CLA	C1D-C2D	2.36	1.47	1.42
10	bA	808	CLA	C1C-C2C	2.35	1.49	1.44
10	bB	820	CLA	C1B-CHB	2.35	1.46	1.40
10	bB	809	CLA	C1D-C2D	2.35	1.47	1.42
10	cB	841	CLA	C4B-CHC	2.35	1.46	1.40
10	aA	841	CLA	CHD-C4C	2.35	1.47	1.41
10	bB	835	CLA	C4C-C3C	2.35	1.49	1.45
10	cA	820	CLA	CHD-C4C	2.35	1.47	1.41
10	bB	830	CLA	C4B-CHC	2.35	1.46	1.40
10	bB	816	CLA	C4C-C3C	2.35	1.49	1.45
10	cA	804	CLA	CHD-C4C	2.35	1.47	1.41
10	aA	839	CLA	C4C-C3C	2.35	1.49	1.45
9	bA	801	CL0	C4B-CHC	2.35	1.46	1.40
10	aB	830	CLA	C4B-CHC	2.35	1.46	1.40
10	bA	822	CLA	C1D-C2D	2.35	1.47	1.42
10	cA	841	CLA	CHD-C4C	2.35	1.47	1.41
10	bB	841	CLA	C1D-C2D	2.35	1.47	1.42
10	bA	824	CLA	C4C-C3C	2.35	1.49	1.45
10	bB	801	CLA	C1D-C2D	2.35	1.47	1.42
10	aB	801	CLA	C1B-CHB	2.35	1.46	1.40
10	aA	803	CLA	C4C-C3C	2.34	1.49	1.45
13	bL	206	BCR	C30-C25	-2.34	1.50	1.53
10	aA	831	CLA	C1D-C2D	2.34	1.47	1.42
10	cA	816	CLA	CHD-C4C	2.34	1.47	1.41
10	aB	801	CLA	C4B-CHC	2.34	1.46	1.40
10	cA	821	CLA	CHD-C4C	2.34	1.47	1.41
10	cA	825	CLA	C1B-CHB	2.34	1.46	1.40
10	aB	808	CLA	C1D-C2D	2.34	1.47	1.42
9	cA	801	CL0	C4B-CHC	2.34	1.46	1.40
10	aA	837	CLA	C1C-NC	-2.34	1.34	1.37
10	bB	808	CLA	C1D-C2D	2.34	1.47	1.42
10	bA	836	CLA	C1D-C2D	2.34	1.47	1.42
10	cA	822	CLA	C1D-C2D	2.34	1.47	1.42
10	bA	804	CLA	CHD-C4C	2.34	1.47	1.41
10	cA	806	CLA	C1B-CHB	2.34	1.46	1.40
10	aA	806	CLA	C1C-C2C	2.34	1.49	1.44
10	cB	816	CLA	C4C-C3C	2.34	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	819	CLA	C1B-CHB	2.34	1.46	1.40
10	bA	826	CLA	CHD-C4C	2.34	1.47	1.41
10	cA	806	CLA	C1C-C2C	2.34	1.49	1.44
10	bA	842	CLA	C4B-CHC	2.34	1.46	1.40
13	cL	206	BCR	C30-C25	-2.34	1.50	1.53
10	aA	824	CLA	C4C-C3C	2.34	1.49	1.45
13	aL	206	BCR	C30-C25	-2.34	1.50	1.53
13	bA	848	BCR	C1-C6	-2.34	1.50	1.53
10	aA	821	CLA	CHD-C4C	2.34	1.47	1.41
10	bB	813	CLA	CHD-C4C	2.34	1.47	1.41
10	aB	821	CLA	CHD-C4C	2.33	1.47	1.41
10	cA	803	CLA	C4C-C3C	2.33	1.49	1.45
10	aA	822	CLA	C1D-C2D	2.33	1.47	1.42
10	cA	826	CLA	CHD-C4C	2.33	1.47	1.41
10	cA	831	CLA	C1D-C2D	2.33	1.47	1.42
10	bB	806	CLA	C1C-C2C	2.33	1.49	1.44
10	bA	831	CLA	C1D-C2D	2.33	1.47	1.42
10	aA	804	CLA	CHD-C4C	2.33	1.47	1.41
10	bL	205	CLA	CHD-C4C	2.33	1.47	1.41
10	cB	813	CLA	CHD-C4C	2.33	1.47	1.41
10	cB	804	CLA	C1B-CHB	2.33	1.46	1.40
13	cI	102	BCR	C30-C25	-2.33	1.50	1.53
10	cA	818	CLA	C4C-C3C	2.33	1.49	1.45
10	cL	205	CLA	CHD-C4C	2.33	1.47	1.41
10	bB	801	CLA	C4B-CHC	2.33	1.46	1.40
10	bB	817	CLA	CHD-C4C	2.33	1.47	1.41
10	aA	808	CLA	C1C-C2C	2.33	1.49	1.44
10	cB	835	CLA	C4C-C3C	2.33	1.49	1.45
10	bA	856	CLA	C4C-C3C	2.33	1.49	1.45
10	cB	817	CLA	CHD-C4C	2.33	1.47	1.41
10	cB	801	CLA	C1D-C2D	2.32	1.47	1.42
10	aA	842	CLA	C1C-NC	-2.32	1.34	1.37
10	cB	802	CLA	CHD-C4C	2.32	1.47	1.41
10	aB	813	CLA	C4C-C3C	2.32	1.49	1.45
10	bB	804	CLA	C1B-CHB	2.32	1.46	1.40
10	cB	813	CLA	C4C-C3C	2.32	1.49	1.45
10	aB	813	CLA	CHD-C4C	2.32	1.47	1.41
10	bB	815	CLA	CHD-C4C	2.32	1.47	1.41
10	aA	818	CLA	C4C-C3C	2.32	1.49	1.45
10	bA	824	CLA	CHD-C4C	2.32	1.47	1.41
10	aA	803	CLA	C1C-C2C	2.32	1.49	1.44
10	aA	806	CLA	C1B-CHB	2.32	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	841	CLA	C1C-C2C	2.32	1.49	1.44
10	cA	836	CLA	C1D-C2D	2.32	1.47	1.42
10	bB	802	CLA	CHD-C4C	2.32	1.47	1.41
10	cA	854	CLA	CHD-C4C	2.32	1.47	1.41
10	aA	836	CLA	C1D-C2D	2.32	1.47	1.42
10	cB	831	CLA	C1C-C2C	2.32	1.49	1.44
10	aA	816	CLA	CHD-C4C	2.32	1.47	1.41
10	bA	842	CLA	C1C-NC	-2.32	1.34	1.37
10	bA	824	CLA	C1D-C2D	2.32	1.47	1.42
10	aB	804	CLA	C1B-CHB	2.32	1.46	1.40
10	bA	816	CLA	C1C-C2C	2.32	1.49	1.44
10	cA	803	CLA	C1C-C2C	2.31	1.49	1.44
10	aA	825	CLA	C1B-CHB	2.31	1.46	1.40
10	aA	826	CLA	CHD-C4C	2.31	1.47	1.41
10	cB	815	CLA	CHD-C4C	2.31	1.47	1.41
10	cB	819	CLA	C1B-CHB	2.31	1.46	1.40
10	aA	842	CLA	C4B-CHC	2.31	1.46	1.40
10	bB	821	CLA	CHD-C4C	2.31	1.47	1.41
10	aA	838	CLA	C1B-CHB	2.31	1.46	1.40
10	bA	816	CLA	CHD-C4C	2.31	1.47	1.41
10	aA	854	CLA	CHD-C4C	2.31	1.47	1.41
10	bA	820	CLA	C1B-CHB	2.31	1.46	1.40
10	aL	205	CLA	CHD-C4C	2.31	1.47	1.41
10	aB	819	CLA	C1B-CHB	2.31	1.46	1.40
10	aA	824	CLA	C1D-C2D	2.31	1.47	1.42
10	cB	821	CLA	CHD-C4C	2.31	1.47	1.41
10	bA	803	CLA	C4C-C3C	2.31	1.49	1.45
10	aB	807	CLA	C4C-C3C	2.31	1.49	1.45
10	aB	817	CLA	CHD-C4C	2.31	1.47	1.41
10	cA	816	CLA	C1C-C2C	2.31	1.49	1.44
10	bB	809	CLA	CHD-C4C	2.31	1.47	1.41
10	aA	806	CLA	C4C-C3C	2.31	1.49	1.45
10	cA	820	CLA	C1B-CHB	2.30	1.46	1.40
10	bA	806	CLA	C4C-C3C	2.30	1.49	1.45
10	aA	856	CLA	C4C-C3C	2.30	1.49	1.45
10	bA	806	CLA	C1B-CHB	2.30	1.46	1.40
10	cA	828	CLA	C1C-C2C	2.30	1.49	1.44
10	cA	856	CLA	C4C-C3C	2.30	1.49	1.45
10	cA	824	CLA	CHD-C4C	2.30	1.47	1.41
10	bA	834	CLA	CHD-C4C	2.30	1.47	1.41
13	bI	101	BCR	C30-C25	-2.30	1.50	1.53
10	aA	824	CLA	CHD-C4C	2.30	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	824	CLA	C1D-C2D	2.30	1.47	1.42
10	aA	830	CLA	CHD-C4C	2.30	1.47	1.41
10	bA	841	CLA	C1C-C2C	2.30	1.49	1.44
10	bA	854	CLA	CHD-C4C	2.30	1.47	1.41
10	cB	820	CLA	C1B-CHB	2.30	1.46	1.40
10	bA	838	CLA	CHD-C4C	2.29	1.47	1.41
10	cA	838	CLA	CHD-C4C	2.29	1.47	1.41
10	aA	820	CLA	C1B-CHB	2.29	1.46	1.40
10	aB	809	CLA	CHD-C4C	2.29	1.47	1.41
10	bA	834	CLA	C1D-C2D	2.29	1.47	1.42
10	aA	839	CLA	C1B-CHB	2.29	1.46	1.40
10	cL	204	CLA	CHD-C4C	2.29	1.47	1.41
10	cA	806	CLA	C4C-C3C	2.29	1.49	1.45
10	cA	830	CLA	CHD-C4C	2.29	1.47	1.41
10	bA	830	CLA	CHD-C4C	2.29	1.47	1.41
10	cB	801	CLA	CHD-C4C	2.29	1.47	1.41
10	aA	834	CLA	CHD-C4C	2.29	1.47	1.41
10	bA	839	CLA	C1B-CHB	2.29	1.46	1.40
10	aA	838	CLA	CHD-C4C	2.29	1.47	1.41
10	aA	840	CLA	C4C-C3C	2.29	1.49	1.45
10	aA	838	CLA	C1C-NC	-2.29	1.34	1.37
10	aB	802	CLA	CHD-C4C	2.29	1.47	1.41
10	cA	834	CLA	CHD-C4C	2.29	1.47	1.41
10	aA	832	CLA	CHD-C4C	2.29	1.47	1.41
10	aB	819	CLA	C4B-CHC	2.29	1.46	1.40
10	bA	803	CLA	C1C-C2C	2.29	1.49	1.44
10	aA	828	CLA	C1C-C2C	2.29	1.49	1.44
10	cB	839	CLA	C4C-C3C	2.28	1.49	1.45
10	bB	807	CLA	C4C-C3C	2.28	1.49	1.45
10	cA	822	CLA	CHD-C4C	2.28	1.47	1.41
10	aB	808	CLA	CHD-C4C	2.28	1.47	1.41
10	aB	815	CLA	CHD-C4C	2.28	1.47	1.41
10	bB	819	CLA	C4B-CHC	2.28	1.46	1.40
10	cB	809	CLA	CHD-C4C	2.28	1.47	1.41
13	aI	101	BCR	C30-C25	-2.28	1.50	1.53
10	aB	831	CLA	C1C-C2C	2.28	1.49	1.44
10	cB	819	CLA	C4B-CHC	2.28	1.46	1.40
10	bL	204	CLA	CHD-C4C	2.28	1.47	1.41
10	aB	832	CLA	C1C-C2C	2.28	1.49	1.44
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	cA	839	CLA	C1B-CHB	2.28	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bA	838	CLA	C1B-CHB	2.28	1.46	1.40
10	cA	838	CLA	C1C-NC	-2.28	1.34	1.37
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	bA	822	CLA	CHD-C4C	2.28	1.47	1.41
10	aB	801	CLA	CHD-C4C	2.28	1.47	1.41
10	aL	204	CLA	CHD-C4C	2.28	1.47	1.41
10	cA	838	CLA	C1B-CHB	2.28	1.46	1.40
10	bB	808	CLA	CHD-C4C	2.28	1.47	1.41
10	bA	825	CLA	CHD-C4C	2.27	1.47	1.41
10	bA	832	CLA	CHD-C4C	2.27	1.47	1.41
10	aB	821	CLA	C1C-C2C	2.27	1.49	1.44
10	bA	818	CLA	C4C-C3C	2.27	1.49	1.45
10	aA	827	CLA	CHD-C4C	2.27	1.47	1.41
10	aA	822	CLA	CHD-C4C	2.27	1.47	1.41
10	bL	202	CLA	C1D-C2D	2.27	1.47	1.42
13	aA	847	BCR	C30-C25	-2.27	1.50	1.53
10	cB	840	CLA	C1C-C2C	2.27	1.49	1.44
10	cB	808	CLA	CHD-C4C	2.27	1.47	1.41
10	aA	835	CLA	C4C-C3C	2.27	1.48	1.45
10	aA	812	CLA	C4C-C3C	2.27	1.48	1.45
10	bA	829	CLA	C1C-NC	-2.27	1.34	1.37
10	aA	834	CLA	C1D-C2D	2.27	1.47	1.42
10	aB	835	CLA	C4C-C3C	2.27	1.48	1.45
10	cA	812	CLA	C1C-C2C	2.27	1.49	1.44
10	cA	827	CLA	CHD-C4C	2.27	1.47	1.41
10	aL	202	CLA	C1D-C2D	2.27	1.47	1.42
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	829	CLA	C1C-NC	-2.27	1.34	1.37
10	cB	840	CLA	C1D-C2D	2.27	1.47	1.42
10	cA	832	CLA	CHD-C4C	2.27	1.47	1.41
10	cB	837	CLA	CHD-C4C	2.27	1.47	1.41
10	bB	810	CLA	C1B-CHB	2.27	1.46	1.40
10	cB	832	CLA	C1C-C2C	2.27	1.49	1.44
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	bA	838	CLA	C1C-NC	-2.26	1.34	1.37
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	827	CLA	C1C-C2C	2.26	1.48	1.44
10	cA	807	CLA	C1C-C2C	2.26	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	815	CLA	C4C-C3C	2.26	1.48	1.45
10	bB	837	CLA	CHD-C4C	2.26	1.47	1.41
10	cL	202	CLA	C1D-C2D	2.26	1.47	1.42
10	aA	810	CLA	C1C-C2C	2.26	1.48	1.44
10	bB	828	CLA	C1C-C2C	2.26	1.48	1.44
10	bA	819	CLA	C1C-C2C	2.26	1.48	1.44
10	bA	814	CLA	C4C-C3C	2.26	1.48	1.45
10	bB	840	CLA	C1D-C2D	2.26	1.47	1.42
10	cB	807	CLA	C4C-C3C	2.26	1.48	1.45
10	bB	826	CLA	C4C-C3C	2.26	1.48	1.45
10	aB	840	CLA	C1D-C2D	2.25	1.47	1.42
10	aA	805	CLA	CHD-C4C	2.25	1.47	1.41
10	cA	834	CLA	C1D-C2D	2.25	1.47	1.42
10	aB	840	CLA	C1C-C2C	2.25	1.48	1.44
10	cA	814	CLA	C4C-C3C	2.25	1.48	1.45
10	cA	840	CLA	C4C-C3C	2.25	1.48	1.45
10	cB	825	CLA	CHD-C4C	2.25	1.47	1.41
10	cA	804	CLA	C1B-CHB	2.25	1.46	1.40
10	cA	805	CLA	CHD-C4C	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	bA	805	CLA	CHD-C4C	2.25	1.47	1.41
10	cA	825	CLA	CHD-C4C	2.25	1.47	1.41
10	cA	829	CLA	C1C-NC	-2.25	1.34	1.37
10	aB	818	CLA	C4C-C3C	2.25	1.48	1.45
10	cB	831	CLA	C1B-CHB	2.25	1.46	1.40
10	bA	811	CLA	C4C-C3C	2.25	1.48	1.45
10	cB	818	CLA	C4C-C3C	2.25	1.48	1.45
10	bB	839	CLA	C4C-C3C	2.25	1.48	1.45
10	bA	840	CLA	C4C-C3C	2.25	1.48	1.45
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	bB	813	CLA	C4C-C3C	2.24	1.48	1.45
10	bB	825	CLA	CHD-C4C	2.24	1.47	1.41
10	cB	821	CLA	C1C-C2C	2.24	1.48	1.44
10	bB	831	CLA	C1C-C2C	2.24	1.48	1.44
10	cB	810	CLA	C1B-CHB	2.24	1.46	1.40
13	cA	847	BCR	C30-C25	-2.24	1.50	1.53
10	bA	827	CLA	CHD-C4C	2.24	1.47	1.41
10	cA	815	CLA	C4C-C3C	2.24	1.48	1.45
10	bA	815	CLA	C4C-C3C	2.24	1.48	1.45
10	bB	831	CLA	C1B-CHB	2.24	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	aB	816	CLA	C1C-C2C	2.24	1.48	1.44
10	bB	801	CLA	CHD-C4C	2.24	1.47	1.41
10	aB	837	CLA	CHD-C4C	2.24	1.47	1.41
10	aA	804	CLA	C1B-CHB	2.24	1.46	1.40
10	aA	825	CLA	CHD-C4C	2.24	1.47	1.41
10	bB	841	CLA	CHD-C4C	2.24	1.47	1.41
10	bA	804	CLA	C1B-CHB	2.24	1.46	1.40
10	bB	816	CLA	C1C-C2C	2.24	1.48	1.44
10	aA	828	CLA	CHD-C4C	2.24	1.47	1.41
10	aA	829	CLA	C1D-C2D	2.23	1.47	1.42
10	aB	837	CLA	C1C-NC	-2.23	1.34	1.37
10	aA	827	CLA	C1C-C2C	2.23	1.48	1.44
10	cA	827	CLA	C1C-C2C	2.23	1.48	1.44
10	bA	812	CLA	C1C-C2C	2.23	1.48	1.44
10	bA	829	CLA	C1D-C2D	2.23	1.47	1.42
10	aB	813	CLA	C1C-C2C	2.23	1.48	1.44
10	cA	828	CLA	CHD-C4C	2.23	1.47	1.41
10	aA	807	CLA	C1C-C2C	2.23	1.48	1.44
10	bB	818	CLA	C4C-C3C	2.23	1.48	1.45
10	bB	808	CLA	C1C-C2C	2.23	1.48	1.44
10	bB	805	CLA	C4C-C3C	2.23	1.48	1.45
10	aB	808	CLA	C1C-C2C	2.23	1.48	1.44
10	cA	835	CLA	C4C-C3C	2.23	1.48	1.45
10	bA	828	CLA	CHD-C4C	2.23	1.47	1.41
10	aA	811	CLA	C4C-C3C	2.22	1.48	1.45
10	cB	826	CLA	C4C-C3C	2.22	1.48	1.45
10	aB	810	CLA	C1B-CHB	2.22	1.46	1.40
10	cB	813	CLA	C1C-C2C	2.22	1.48	1.44
10	cA	829	CLA	C1D-C2D	2.22	1.47	1.42
10	aB	831	CLA	C1B-CHB	2.22	1.46	1.40
13	bA	847	BCR	C30-C25	-2.22	1.50	1.53
10	aB	839	CLA	C4C-C3C	2.22	1.48	1.45
10	bL	204	CLA	C1C-C2C	2.22	1.48	1.44
10	bA	837	CLA	CHD-C4C	2.22	1.47	1.41
10	bB	806	CLA	CHD-C4C	2.22	1.47	1.41
10	aA	837	CLA	CHD-C4C	2.22	1.47	1.41
10	cB	809	CLA	C4C-C3C	2.22	1.48	1.45
10	bA	812	CLA	C4C-C3C	2.22	1.48	1.45
10	bB	838	CLA	C1C-C2C	2.22	1.48	1.44
10	aB	814	CLA	C1C-NC	-2.22	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	808	CLA	C1C-C2C	2.22	1.48	1.44
10	cA	824	CLA	C1C-C2C	2.22	1.48	1.44
10	cA	819	CLA	C1C-C2C	2.22	1.48	1.44
10	cB	828	CLA	C1C-C2C	2.22	1.48	1.44
10	cB	825	CLA	C1D-C2D	2.22	1.47	1.42
10	bA	836	CLA	CHD-C4C	2.22	1.47	1.41
10	aA	819	CLA	C1C-C2C	2.22	1.48	1.44
10	aB	825	CLA	CHD-C4C	2.22	1.47	1.41
10	cA	811	CLA	C4C-C3C	2.22	1.48	1.45
10	bB	827	CLA	C1D-C2D	2.21	1.47	1.42
10	aB	825	CLA	C1D-C2D	2.21	1.47	1.42
10	aB	823	CLA	C1C-C2C	2.21	1.48	1.44
10	cB	812	CLA	C4C-C3C	2.21	1.48	1.45
10	aA	824	CLA	C1C-C2C	2.21	1.48	1.44
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	aA	836	CLA	CHD-C4C	2.21	1.47	1.41
10	aB	841	CLA	CHD-C4C	2.21	1.47	1.41
10	cB	837	CLA	C1C-NC	-2.21	1.34	1.37
10	cA	813	CLA	C4C-C3C	2.21	1.48	1.45
10	cB	804	CLA	CHD-C4C	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	cB	816	CLA	C1C-C2C	2.21	1.48	1.44
10	bL	205	CLA	C4C-C3C	2.21	1.48	1.45
10	cA	811	CLA	C1C-C2C	2.20	1.48	1.44
10	cB	823	CLA	C1C-C2C	2.20	1.48	1.44
10	cA	837	CLA	CHD-C4C	2.20	1.47	1.41
10	aA	814	CLA	C4C-C3C	2.20	1.48	1.45
10	cB	827	CLA	C1C-NC	-2.20	1.34	1.37
10	aB	829	CLA	CHD-C4C	2.20	1.47	1.41
10	cB	838	CLA	C1C-C2C	2.20	1.48	1.44
10	cA	831	CLA	CHD-C4C	2.20	1.47	1.41
10	bB	826	CLA	C1B-CHB	2.20	1.46	1.40
10	aB	828	CLA	C1C-NC	-2.20	1.34	1.37
10	bB	825	CLA	C1D-C2D	2.20	1.47	1.42
10	aB	809	CLA	C4C-C3C	2.20	1.48	1.45
10	bB	823	CLA	C1C-C2C	2.20	1.48	1.44
10	bA	804	CLA	C1C-NC	-2.20	1.34	1.37
10	cB	802	CLA	C1C-NC	-2.20	1.34	1.37
10	bB	835	CLA	C1C-C2C	2.20	1.48	1.44
10	bB	827	CLA	CHD-C4C	2.20	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	826	CLA	C1C-C2C	2.20	1.48	1.44
10	cA	836	CLA	CHD-C4C	2.20	1.47	1.41
10	cA	805	CLA	C1C-C2C	2.20	1.48	1.44
10	bA	842	CLA	CHD-C4C	2.20	1.47	1.41
10	cB	827	CLA	CHD-C4C	2.20	1.47	1.41
10	bA	831	CLA	CHD-C4C	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	826	CLA	C4C-C3C	2.20	1.48	1.45
13	aA	846	BCR	C33-C5	-2.20	1.47	1.50
10	aB	802	CLA	C1C-NC	-2.20	1.34	1.37
10	aB	804	CLA	CHD-C4C	2.20	1.47	1.41
10	bA	821	CLA	C1C-C2C	2.19	1.48	1.44
10	bB	828	CLA	C1C-NC	-2.19	1.34	1.37
14	aA	852	LHG	P-O6	2.19	1.68	1.59
10	cB	835	CLA	C1C-C2C	2.19	1.48	1.44
10	cA	821	CLA	C1C-C2C	2.19	1.48	1.44
14	bA	852	LHG	P-O6	2.19	1.68	1.59
10	cA	817	CLA	C1C-C2C	2.19	1.48	1.44
10	aB	827	CLA	C1D-C2D	2.19	1.47	1.42
10	cB	841	CLA	CHD-C4C	2.19	1.47	1.41
10	bB	837	CLA	C1C-NC	-2.19	1.34	1.37
14	cA	852	LHG	P-O6	2.19	1.68	1.59
13	bL	207	BCR	C1-C6	-2.19	1.50	1.53
9	aA	801	CL0	C1C-NC	-2.19	1.34	1.37
10	bB	821	CLA	C4C-C3C	2.19	1.48	1.45
10	bB	826	CLA	C1C-C2C	2.19	1.48	1.44
10	bA	829	CLA	CHD-C4C	2.19	1.47	1.41
10	aB	806	CLA	CHD-C4C	2.19	1.47	1.41
13	cL	207	BCR	C1-C6	-2.19	1.50	1.53
10	bA	805	CLA	C1C-C2C	2.19	1.48	1.44
10	aB	827	CLA	CHD-C4C	2.19	1.47	1.41
10	bB	829	CLA	CHD-C4C	2.19	1.47	1.41
10	cB	806	CLA	CHD-C4C	2.19	1.47	1.41
10	cL	202	CLA	CHD-C4C	2.19	1.47	1.41
10	aA	842	CLA	CHD-C4C	2.18	1.47	1.41
10	cB	805	CLA	C4C-C3C	2.18	1.48	1.45
10	bA	811	CLA	C1C-C2C	2.18	1.48	1.44
10	aA	831	CLA	CHD-C4C	2.18	1.47	1.41
10	bA	824	CLA	C1C-C2C	2.18	1.48	1.44
10	bB	814	CLA	C1C-NC	-2.18	1.34	1.37
10	aB	805	CLA	C4C-C3C	2.18	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aL	202	CLA	CHD-C4C	2.18	1.47	1.41
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	cB	826	CLA	C1B-CHB	2.18	1.45	1.40
10	aB	805	CLA	CHD-C4C	2.18	1.47	1.41
10	cB	821	CLA	C4C-C3C	2.18	1.48	1.45
10	aB	827	CLA	C1C-NC	-2.18	1.34	1.37
10	aB	838	CLA	C1C-C2C	2.18	1.48	1.44
10	aA	813	CLA	C4C-C3C	2.18	1.48	1.45
10	aB	817	CLA	C4C-C3C	2.18	1.48	1.45
10	bB	804	CLA	CHD-C4C	2.18	1.47	1.41
10	aB	826	CLA	C1B-CHB	2.18	1.45	1.40
10	bL	202	CLA	CHD-C4C	2.18	1.47	1.41
10	aA	811	CLA	C1C-C2C	2.17	1.48	1.44
10	bB	809	CLA	C4C-C3C	2.17	1.48	1.45
10	cL	204	CLA	C1C-C2C	2.17	1.48	1.44
10	bA	828	CLA	C1D-C2D	2.17	1.47	1.42
10	bA	813	CLA	C4C-C3C	2.17	1.48	1.45
10	aL	205	CLA	C4C-C3C	2.17	1.48	1.45
10	bB	805	CLA	CHD-C4C	2.17	1.47	1.41
10	cB	829	CLA	CHD-C4C	2.17	1.47	1.41
10	aA	830	CLA	C4C-C3C	2.17	1.48	1.45
10	aA	833	CLA	C1B-CHB	2.17	1.45	1.40
10	aA	828	CLA	C1D-C2D	2.16	1.47	1.42
13	aL	207	BCR	C1-C6	-2.16	1.50	1.53
10	cA	830	CLA	C4C-C3C	2.16	1.48	1.45
10	cB	827	CLA	C1D-C2D	2.16	1.47	1.42
10	bB	801	CLA	C1C-NC	-2.16	1.34	1.37
10	bA	817	CLA	C1C-C2C	2.16	1.48	1.44
10	bB	801	CLA	C4C-C3C	2.16	1.48	1.45
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	cA	842	CLA	CHD-C4C	2.16	1.47	1.41
10	cB	824	CLA	C1C-C2C	2.16	1.48	1.44
10	cA	832	CLA	C1C-C2C	2.16	1.48	1.44
10	cL	205	CLA	C4C-C3C	2.16	1.48	1.45
10	aB	833	CLA	C4C-C3C	2.16	1.48	1.45
10	cA	828	CLA	C1D-C2D	2.16	1.47	1.42
10	aB	801	CLA	C1C-NC	-2.16	1.34	1.37
10	cB	809	CLA	C1C-C2C	2.16	1.48	1.44
10	aA	821	CLA	C1C-C2C	2.16	1.48	1.44
10	bA	832	CLA	C1C-NC	-2.16	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	828	CLA	C1C-NC	-2.16	1.34	1.37
9	cA	801	CL0	C1C-NC	-2.16	1.34	1.37
10	cA	829	CLA	CHD-C4C	2.16	1.47	1.41
10	bB	818	CLA	C1C-C2C	2.16	1.48	1.44
10	bB	817	CLA	C4C-C3C	2.15	1.48	1.45
10	cA	829	CLA	C4C-C3C	2.15	1.48	1.45
10	aA	829	CLA	CHD-C4C	2.15	1.47	1.41
10	aL	204	CLA	C1C-C2C	2.15	1.48	1.44
13	aB	847	BCR	C33-C5	-2.15	1.47	1.50
10	cB	840	CLA	CHD-C4C	2.15	1.47	1.41
10	aB	826	CLA	C1C-C2C	2.15	1.48	1.44
10	cA	841	CLA	C4C-C3C	2.15	1.48	1.45
10	bA	830	CLA	C4C-C3C	2.15	1.48	1.45
10	bB	811	CLA	C4B-CHC	2.15	1.45	1.40
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	bA	833	CLA	C1B-CHB	2.15	1.45	1.40
10	cB	822	CLA	C1A-CHA	2.15	1.52	1.43
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	aB	811	CLA	C4B-CHC	2.15	1.45	1.40
10	cA	823	CLA	C1C-NC	-2.15	1.34	1.37
10	cB	801	CLA	C1C-NC	-2.15	1.34	1.37
10	cB	805	CLA	CHD-C4C	2.14	1.47	1.41
10	cB	815	CLA	C4C-C3C	2.14	1.48	1.45
10	aA	834	CLA	C1C-NC	-2.14	1.34	1.37
10	bB	833	CLA	C4C-C3C	2.14	1.48	1.45
10	aB	822	CLA	C1A-CHA	2.14	1.52	1.43
10	cB	814	CLA	C1C-NC	-2.14	1.34	1.37
10	aA	805	CLA	C1C-C2C	2.14	1.48	1.44
10	aA	807	CLA	C4C-C3C	2.14	1.48	1.45
13	bB	847	BCR	C33-C5	-2.14	1.47	1.50
10	bA	829	CLA	C4C-C3C	2.14	1.48	1.45
10	aA	832	CLA	C1C-C2C	2.14	1.48	1.44
10	aB	840	CLA	CHD-C4C	2.14	1.47	1.41
10	aB	821	CLA	C4C-C3C	2.14	1.48	1.45
10	bA	823	CLA	C1C-NC	-2.14	1.34	1.37
10	bB	829	CLA	C1C-C2C	2.14	1.48	1.44
10	bB	822	CLA	C1A-CHA	2.14	1.52	1.43
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	aA	808	CLA	CHD-C4C	2.14	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	833	CLA	C1B-CHB	2.14	1.45	1.40
10	cB	818	CLA	C1C-C2C	2.14	1.48	1.44
10	aA	829	CLA	C4C-C3C	2.13	1.48	1.45
10	bB	840	CLA	CHD-C4C	2.13	1.47	1.41
10	cA	834	CLA	C1C-NC	-2.13	1.34	1.37
10	cB	833	CLA	C4C-C3C	2.13	1.48	1.45
10	bA	820	CLA	C1C-C2C	2.13	1.48	1.44
10	bA	809	CLA	C1C-C2C	2.13	1.48	1.44
13	bA	846	BCR	C33-C5	-2.13	1.47	1.50
10	cB	803	CLA	C1D-C2D	2.13	1.47	1.42
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	cA	808	CLA	CHD-C4C	2.13	1.47	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	cB	811	CLA	C4B-CHC	2.13	1.45	1.40
10	aA	832	CLA	C1C-NC	-2.13	1.34	1.37
10	aB	836	CLA	C1C-C2C	2.13	1.48	1.44
10	bA	808	CLA	C1C-NC	-2.13	1.34	1.37
10	aB	808	CLA	C1C-NC	-2.13	1.34	1.37
16	cB	848	LMG	O7-C8	-2.13	1.41	1.46
10	bA	832	CLA	C1C-C2C	2.13	1.48	1.44
10	aA	833	CLA	C1C-NC	-2.12	1.34	1.37
10	cB	817	CLA	C4C-C3C	2.12	1.48	1.45
10	aA	817	CLA	C1C-C2C	2.12	1.48	1.44
10	cL	205	CLA	C1C-NC	-2.12	1.34	1.37
10	cB	825	CLA	C4C-C3C	2.12	1.48	1.45
10	bA	836	CLA	C1C-NC	-2.12	1.34	1.37
10	cB	836	CLA	C1C-C2C	2.12	1.48	1.44
10	cB	820	CLA	C1C-C2C	2.12	1.48	1.44
10	aB	839	CLA	C1C-C2C	2.12	1.48	1.44
10	bB	839	CLA	C1C-C2C	2.12	1.48	1.44
10	cA	805	CLA	C1C-NC	-2.12	1.34	1.37
10	bA	834	CLA	C1C-NC	-2.12	1.34	1.37
10	cA	836	CLA	C1C-NC	-2.12	1.34	1.37
10	bB	825	CLA	C4C-C3C	2.12	1.48	1.45
10	aL	205	CLA	C1C-NC	-2.12	1.34	1.37
16	bB	848	LMG	O7-C8	-2.12	1.41	1.46
10	aA	841	CLA	C4C-C3C	2.12	1.48	1.45
10	aB	807	CLA	C1C-NC	-2.12	1.34	1.37
10	cB	839	CLA	C1C-C2C	2.12	1.48	1.44
10	cB	833	CLA	C1C-NC	-2.12	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	836	CLA	C1C-NC	-2.12	1.34	1.37
10	cB	822	CLA	C1C-C2C	2.11	1.48	1.44
10	bA	808	CLA	CHD-C4C	2.11	1.47	1.41
10	aA	823	CLA	C1C-NC	-2.11	1.34	1.37
10	aB	803	CLA	C1D-C2D	2.11	1.47	1.42
10	aA	809	CLA	C1C-C2C	2.11	1.48	1.44
13	cA	846	BCR	C33-C5	-2.11	1.47	1.50
10	bB	834	CLA	C1C-C2C	2.11	1.48	1.44
10	bA	814	CLA	C1C-NC	-2.11	1.34	1.37
10	aB	809	CLA	C1C-C2C	2.11	1.48	1.44
10	aA	805	CLA	C1C-NC	-2.11	1.34	1.37
10	aA	835	CLA	C1C-C2C	2.11	1.48	1.44
10	bB	809	CLA	C1C-NC	-2.11	1.34	1.37
13	aL	206	BCR	C1-C6	-2.11	1.50	1.53
10	cB	834	CLA	C1C-C2C	2.11	1.48	1.44
10	cA	809	CLA	C1C-C2C	2.11	1.48	1.44
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	bB	820	CLA	C1C-C2C	2.11	1.48	1.44
10	bB	808	CLA	C1C-NC	-2.10	1.34	1.37
10	cA	832	CLA	C1C-NC	-2.10	1.34	1.37
10	cA	814	CLA	C1C-NC	-2.10	1.34	1.37
16	aB	848	LMG	O7-C8	-2.10	1.41	1.46
10	bB	833	CLA	C1C-NC	-2.10	1.34	1.37
10	aL	205	CLA	C1C-C2C	2.10	1.48	1.44
10	aB	834	CLA	C1C-C2C	2.10	1.48	1.44
10	cB	803	CLA	C1C-NC	-2.10	1.34	1.37
10	bL	205	CLA	C1C-NC	-2.10	1.34	1.37
10	cB	810	CLA	CHD-C4C	2.10	1.47	1.41
13	cL	206	BCR	C1-C6	-2.10	1.51	1.53
10	bB	837	CLA	C4C-C3C	2.10	1.48	1.45
10	cB	837	CLA	C1C-C2C	2.10	1.48	1.44
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	bB	832	CLA	C4C-C3C	2.10	1.48	1.45
10	aB	822	CLA	C1C-C2C	2.09	1.48	1.44
10	bB	803	CLA	C1D-C2D	2.09	1.47	1.42
10	aB	820	CLA	C1C-C2C	2.09	1.48	1.44
10	bB	815	CLA	C4C-C3C	2.09	1.48	1.45
10	aA	804	CLA	C4C-C3C	2.09	1.48	1.45
10	bA	833	CLA	C1C-NC	-2.09	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cB	805	CLA	C1D-C2D	2.09	1.47	1.42
10	cB	819	CLA	C1C-NC	-2.09	1.34	1.37
10	aA	808	CLA	C1D-C2D	2.09	1.47	1.42
10	cB	801	CLA	C4C-C3C	2.09	1.48	1.45
10	aB	818	CLA	C1C-C2C	2.09	1.48	1.44
10	aB	815	CLA	C1C-C2C	2.09	1.48	1.44
10	bB	811	CLA	CHD-C4C	2.09	1.47	1.41
10	cA	808	CLA	C1D-C2D	2.09	1.47	1.42
10	cL	205	CLA	C1C-C2C	2.09	1.48	1.44
10	bA	802	CLA	C1C-C2C	2.09	1.48	1.44
10	bB	827	CLA	C4C-C3C	2.08	1.48	1.45
10	cB	827	CLA	C4C-C3C	2.08	1.48	1.45
10	cA	807	CLA	C4C-C3C	2.08	1.48	1.45
13	cB	847	BCR	C33-C5	-2.08	1.47	1.50
10	cB	808	CLA	C1C-NC	-2.08	1.34	1.37
10	aB	811	CLA	CHD-C4C	2.08	1.47	1.41
10	cA	835	CLA	C1C-C2C	2.08	1.48	1.44
10	bB	837	CLA	C1C-C2C	2.08	1.48	1.44
10	cB	841	CLA	C4C-C3C	2.08	1.48	1.45
10	cB	815	CLA	C1C-C2C	2.08	1.48	1.44
10	cA	842	CLA	C4C-C3C	2.08	1.48	1.45
10	cB	802	CLA	C1B-CHB	2.08	1.45	1.40
10	bA	836	CLA	C1C-C2C	2.08	1.48	1.44
10	cA	813	CLA	C1A-CHA	2.08	1.51	1.43
10	aA	802	CLA	C1C-C2C	2.08	1.48	1.44
13	bL	206	BCR	C1-C6	-2.07	1.51	1.53
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	cA	823	CLA	C4C-C3C	2.07	1.48	1.45
10	bB	817	CLA	C1C-C2C	2.07	1.48	1.44
10	cA	808	CLA	C1C-NC	-2.07	1.34	1.37
10	cL	203	CLA	C1C-C2C	2.07	1.48	1.44
10	bA	808	CLA	C1D-C2D	2.07	1.47	1.42
10	cB	837	CLA	C4C-C3C	2.07	1.48	1.45
10	aA	842	CLA	C4C-C3C	2.07	1.48	1.45
10	aA	803	CLA	C1A-CHA	2.07	1.51	1.43
10	bA	804	CLA	C4C-C3C	2.07	1.48	1.45
10	bB	805	CLA	C1D-C2D	2.07	1.47	1.42
10	aB	810	CLA	CHD-C4C	2.07	1.47	1.41
10	aB	832	CLA	C1C-NC	-2.07	1.34	1.37
10	aA	839	CLA	C1C-C2C	2.07	1.48	1.44
10	bB	810	CLA	CHD-C4C	2.07	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	cA	827	CLA	C1C-NC	-2.07	1.34	1.37
10	aA	823	CLA	C4C-C3C	2.07	1.48	1.45
10	cB	809	CLA	C1C-NC	-2.07	1.34	1.37
10	cB	832	CLA	C4C-C3C	2.07	1.48	1.45
10	aL	203	CLA	C1C-C2C	2.06	1.48	1.44
10	cA	827	CLA	C1A-CHA	2.06	1.51	1.43
10	cA	804	CLA	C4C-C3C	2.06	1.48	1.45
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	cB	829	CLA	C4C-C3C	2.06	1.48	1.45
10	cA	833	CLA	C1C-NC	-2.06	1.34	1.37
10	bB	803	CLA	C1C-NC	-2.06	1.34	1.37
10	bB	828	CLA	C1A-CHA	2.06	1.51	1.43
10	cA	839	CLA	C1C-C2C	2.06	1.48	1.44
10	bB	804	CLA	C1D-C2D	2.06	1.47	1.42
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	cB	807	CLA	C1C-NC	-2.06	1.34	1.37
10	aA	814	CLA	C1C-NC	-2.06	1.34	1.37
10	bB	803	CLA	CHD-C4C	2.06	1.47	1.41
10	cA	807	CLA	C1A-CHA	2.06	1.51	1.43
10	bA	831	CLA	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
9	aA	801	CL0	C1C-C2C	2.06	1.48	1.44
10	aB	837	CLA	C4C-C3C	2.06	1.48	1.45
10	bB	815	CLA	C1C-C2C	2.06	1.48	1.44
10	cB	811	CLA	CHD-C4C	2.06	1.47	1.41
10	aB	837	CLA	C1C-C2C	2.06	1.48	1.44
10	aB	805	CLA	C1D-C2D	2.06	1.47	1.42
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	cB	817	CLA	C1A-CHA	2.06	1.51	1.43
10	cB	828	CLA	C1A-CHA	2.06	1.51	1.43
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	cL	202	CLA	C4C-C3C	2.05	1.48	1.45
13	bA	849	BCR	C33-C5	-2.05	1.47	1.50
10	bA	807	CLA	C1A-CHA	2.05	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	836	CLA	C1C-C2C	2.05	1.48	1.44
10	bA	835	CLA	C1C-C2C	2.05	1.48	1.44
10	aB	803	CLA	C1C-NC	-2.05	1.34	1.37
10	bA	813	CLA	C1A-CHA	2.05	1.51	1.43
10	bB	806	CLA	C1A-CHA	2.05	1.51	1.43
10	bA	827	CLA	C1A-CHA	2.05	1.51	1.43
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	807	CLA	C1C-C2C	2.05	1.48	1.44
10	aA	807	CLA	C1A-CHA	2.05	1.51	1.43
10	aA	854	CLA	C1C-C2C	2.05	1.48	1.44
10	aB	802	CLA	C1B-CHB	2.05	1.45	1.40
10	aA	827	CLA	C1A-CHA	2.05	1.51	1.43
10	bB	822	CLA	C1C-C2C	2.04	1.48	1.44
10	cA	831	CLA	C1C-C2C	2.04	1.48	1.44
10	cA	802	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	aA	831	CLA	C1C-C2C	2.04	1.48	1.44
10	bA	820	CLA	C4C-C3C	2.04	1.48	1.45
10	aB	827	CLA	C4C-C3C	2.04	1.48	1.45
9	bA	801	CL0	C1C-C2C	2.04	1.48	1.44
10	aB	828	CLA	C1A-CHA	2.04	1.51	1.43
10	bA	809	CLA	C4C-C3C	2.04	1.48	1.45
10	cB	829	CLA	C1C-NC	-2.04	1.34	1.37
10	bB	805	CLA	C1B-CHB	2.04	1.45	1.40
10	aB	803	CLA	CHD-C4C	2.04	1.47	1.41
10	bA	856	CLA	C1A-CHA	2.04	1.51	1.43
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	802	CLA	C1B-CHB	2.04	1.45	1.40
10	aA	854	CLA	C1C-NC	-2.04	1.34	1.37
10	aB	805	CLA	C1B-CHB	2.04	1.45	1.40
10	aB	817	CLA	C1C-C2C	2.04	1.48	1.44
10	aB	841	CLA	C4C-C3C	2.04	1.48	1.45
10	aB	832	CLA	C4C-C3C	2.03	1.48	1.45
10	cA	837	CLA	C1C-C2C	2.03	1.48	1.44
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	841	CLA	C1C-NC	-2.03	1.34	1.37
10	cB	805	CLA	C1B-CHB	2.03	1.45	1.40
10	aB	825	CLA	C1C-C2C	2.03	1.48	1.44
10	aL	202	CLA	C4C-C3C	2.03	1.48	1.45
10	aB	811	CLA	C1D-C2D	2.03	1.47	1.42
10	aB	818	CLA	C1C-NC	-2.03	1.34	1.37
10	bL	203	CLA	C4C-C3C	2.03	1.48	1.45
10	cB	803	CLA	CHD-C4C	2.03	1.47	1.41
10	bB	811	CLA	C1D-C2D	2.03	1.47	1.42
10	bA	830	CLA	C1C-C2C	2.03	1.48	1.44
10	aB	814	CLA	C1C-C2C	2.03	1.48	1.44
10	cB	805	CLA	C1A-CHA	2.03	1.51	1.43
13	aI	101	BCR	C33-C5	-2.03	1.47	1.50
10	aB	810	CLA	C1D-C2D	2.03	1.47	1.42
10	aB	802	CLA	C4C-C3C	2.03	1.48	1.45
10	aL	203	CLA	C4C-C3C	2.03	1.48	1.45
10	cA	825	CLA	C4C-C3C	2.03	1.48	1.45
10	cA	854	CLA	C1C-C2C	2.03	1.48	1.44
10	cB	810	CLA	C1D-C2D	2.03	1.47	1.42
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	cB	814	CLA	C1C-C2C	2.02	1.48	1.44
10	bL	202	CLA	C1C-C2C	2.02	1.48	1.44
10	aB	811	CLA	C4C-C3C	2.02	1.48	1.45
10	aL	202	CLA	C1C-C2C	2.02	1.48	1.44
10	bL	202	CLA	C4C-C3C	2.02	1.48	1.45
10	aA	837	CLA	C1C-C2C	2.02	1.48	1.44
10	bL	203	CLA	C1C-C2C	2.02	1.48	1.44
10	aB	804	CLA	C1D-C2D	2.02	1.47	1.42
10	cB	806	CLA	C1A-CHA	2.02	1.51	1.43
13	cI	102	BCR	C33-C5	-2.02	1.47	1.50
10	cB	804	CLA	C1D-C2D	2.02	1.47	1.42
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
10	aB	805	CLA	C1A-CHA	2.02	1.51	1.43
9	cA	801	CL0	C1C-C2C	2.01	1.48	1.44
9	aA	801	CL0	CHD-C4C	2.01	1.46	1.41
10	cB	813	CLA	C1C-NC	-2.01	1.34	1.37
10	bA	839	CLA	C1C-C2C	2.01	1.48	1.44
10	cA	817	CLA	C4C-C3C	2.01	1.48	1.45
10	aA	838	CLA	C1C-C2C	2.01	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	bB	832	CLA	C1C-NC	-2.01	1.34	1.37
10	cA	838	CLA	C4C-C3C	2.01	1.48	1.45
10	cB	825	CLA	C1C-C2C	2.01	1.48	1.44
10	cB	807	CLA	C1C-C2C	2.01	1.48	1.44
10	aA	830	CLA	C1C-C2C	2.01	1.48	1.44
10	bA	816	CLA	C1A-CHA	2.01	1.51	1.43
10	cA	838	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	cA	804	CLA	C1C-C2C	2.01	1.48	1.44
10	bA	815	CLA	C1C-C2C	2.01	1.48	1.44
10	cB	818	CLA	C1C-NC	-2.01	1.34	1.37
10	bB	835	CLA	C1A-CHA	2.01	1.51	1.43
9	cA	801	CL0	CHD-C4C	2.01	1.46	1.41
13	cA	849	BCR	C33-C5	-2.01	1.47	1.50
10	cL	203	CLA	C4C-C3C	2.01	1.48	1.45
10	cB	811	CLA	C1D-C2D	2.01	1.47	1.42
13	aA	849	BCR	C33-C5	-2.01	1.47	1.50
10	bB	810	CLA	C1D-C2D	2.01	1.47	1.42
10	cB	802	CLA	C4C-C3C	2.00	1.48	1.45
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	bB	811	CLA	C4C-C3C	2.00	1.48	1.45
10	aA	823	CLA	C1A-CHA	2.00	1.51	1.43
10	aA	815	CLA	C1C-C2C	2.00	1.48	1.44
10	cL	202	CLA	C1C-C2C	2.00	1.48	1.44
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 (5907) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	836	CLA	C4-C3-C5	-31.28	79.75	115.99
10	bA	836	CLA	C4-C3-C5	-31.26	79.77	115.99
10	aA	836	CLA	C4-C3-C5	-31.22	79.81	115.99
10	cA	836	CLA	C4-C3-C2	-16.94	79.65	123.68
10	aA	836	CLA	C4-C3-C2	-16.93	79.68	123.68
10	bA	836	CLA	C4-C3-C2	-16.93	79.69	123.68
10	aA	836	CLA	C5-C3-C2	15.60	159.48	120.50
10	bA	836	CLA	C5-C3-C2	15.59	159.45	120.50
10	cA	836	CLA	C5-C3-C2	15.56	159.38	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	838	CLA	CAA-C2A-C3A	-8.02	90.83	112.78
10	cA	838	CLA	CAA-C2A-C3A	-8.00	90.86	112.78
10	aA	838	CLA	CAA-C2A-C3A	-7.99	90.90	112.78
10	bB	804	CLA	O2D-CGD-CBD	7.75	124.81	111.25
10	aB	804	CLA	O2D-CGD-CBD	7.71	124.74	111.25
10	cB	804	CLA	O2D-CGD-CBD	7.71	124.74	111.25
10	bA	833	CLA	O2D-CGD-CBD	7.11	123.69	111.25
10	aA	833	CLA	O2D-CGD-CBD	7.10	123.67	111.25
10	cA	833	CLA	O2D-CGD-CBD	7.09	123.66	111.25
10	bA	824	CLA	O2D-CGD-CBD	6.95	123.42	111.25
10	cA	824	CLA	O2D-CGD-CBD	6.93	123.38	111.25
10	aA	824	CLA	O2D-CGD-CBD	6.92	123.36	111.25
10	bB	825	CLA	O2D-CGD-CBD	6.67	122.92	111.25
10	aB	825	CLA	O2D-CGD-CBD	6.65	122.89	111.25
10	cB	825	CLA	O2D-CGD-CBD	6.64	122.88	111.25
10	cA	818	CLA	O2D-CGD-CBD	6.63	122.86	111.25
10	aB	841	CLA	C2C-C1C-NC	6.63	116.18	109.97
10	bA	818	CLA	O2D-CGD-CBD	6.62	122.84	111.25
10	aA	818	CLA	O2D-CGD-CBD	6.62	122.83	111.25
10	cB	841	CLA	C2C-C1C-NC	6.60	116.16	109.97
10	bB	841	CLA	C2C-C1C-NC	6.59	116.15	109.97
10	cB	816	CLA	O2D-CGD-CBD	6.54	122.69	111.25
10	bB	811	CLA	C2C-C1C-NC	6.54	116.10	109.97
10	bA	803	CLA	O2D-CGD-CBD	6.53	122.67	111.25
10	aB	816	CLA	O2D-CGD-CBD	6.53	122.67	111.25
10	cA	803	CLA	O2D-CGD-CBD	6.53	122.67	111.25
10	bB	816	CLA	O2D-CGD-CBD	6.51	122.64	111.25
10	cB	811	CLA	C2C-C1C-NC	6.50	116.06	109.97
10	aA	803	CLA	O2D-CGD-CBD	6.50	122.62	111.25
10	aB	811	CLA	C2C-C1C-NC	6.49	116.06	109.97
10	aA	854	CLA	CHD-C4C-C3C	-6.49	115.41	124.87
10	aB	828	CLA	CHD-C4C-C3C	-6.48	115.42	124.87
10	bB	828	CLA	CHD-C4C-C3C	-6.48	115.43	124.87
10	cB	828	CLA	CHD-C4C-C3C	-6.47	115.43	124.87
10	bA	854	CLA	CHD-C4C-C3C	-6.46	115.44	124.87
10	cA	854	CLA	CHD-C4C-C3C	-6.46	115.45	124.87
10	bA	829	CLA	O2D-CGD-CBD	6.44	122.52	111.25
10	aA	829	CLA	O2D-CGD-CBD	6.42	122.49	111.25
10	cA	829	CLA	O2D-CGD-CBD	6.42	122.49	111.25
10	cB	814	CLA	C4A-NA-C1A	-6.42	103.82	106.71
10	bB	808	CLA	CHD-C4C-C3C	-6.40	115.54	124.87
10	cB	808	CLA	CHD-C4C-C3C	-6.39	115.55	124.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	808	CLA	CHD-C4C-C3C	-6.39	115.55	124.87
10	aA	826	CLA	CHD-C4C-C3C	-6.38	115.57	124.87
10	aA	816	CLA	O2D-CGD-CBD	6.38	122.41	111.25
10	bA	826	CLA	CHD-C4C-C3C	-6.37	115.57	124.87
10	cB	827	CLA	CHD-C4C-C3C	-6.37	115.58	124.87
10	bB	806	CLA	CHD-C4C-C3C	-6.37	115.58	124.87
10	cA	816	CLA	O2D-CGD-CBD	6.36	122.39	111.25
10	aB	814	CLA	C4A-NA-C1A	-6.36	103.85	106.71
10	bB	803	CLA	CHD-C4C-C3C	-6.36	115.60	124.87
10	bB	827	CLA	CHD-C4C-C3C	-6.35	115.61	124.87
10	aB	806	CLA	CHD-C4C-C3C	-6.35	115.61	124.87
10	cA	826	CLA	CHD-C4C-C3C	-6.35	115.61	124.87
10	cB	806	CLA	CHD-C4C-C3C	-6.34	115.62	124.87
10	aB	803	CLA	CHD-C4C-C3C	-6.34	115.62	124.87
10	aB	827	CLA	CHD-C4C-C3C	-6.34	115.63	124.87
10	bA	816	CLA	O2D-CGD-CBD	6.33	122.32	111.25
10	cB	803	CLA	CHD-C4C-C3C	-6.33	115.64	124.87
10	cB	837	CLA	C4A-NA-C1A	-6.33	103.86	106.71
10	bB	814	CLA	C4A-NA-C1A	-6.29	103.88	106.71
10	bA	822	CLA	CHD-C4C-C3C	-6.29	115.70	124.87
10	aA	822	CLA	CHD-C4C-C3C	-6.28	115.71	124.87
10	cA	822	CLA	CHD-C4C-C3C	-6.28	115.72	124.87
10	cB	810	CLA	O2D-CGD-CBD	6.25	122.20	111.25
10	bB	837	CLA	C4A-NA-C1A	-6.24	103.90	106.71
9	bA	801	CL0	C2C-C1C-NC	6.22	115.80	109.97
10	bB	810	CLA	O2D-CGD-CBD	6.21	122.13	111.25
10	aB	837	CLA	C4A-NA-C1A	-6.21	103.91	106.71
10	aB	810	CLA	O2D-CGD-CBD	6.21	122.12	111.25
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	aA	816	CLA	CHD-C4C-C3C	-6.20	115.83	124.87
10	aB	805	CLA	CAC-C3C-C4C	6.20	132.92	124.82
10	cB	805	CLA	CAC-C3C-C4C	6.20	132.92	124.82
10	bB	805	CLA	CAC-C3C-C4C	6.20	132.92	124.82
10	cL	204	CLA	O2D-CGD-CBD	6.19	122.09	111.25
10	cA	816	CLA	CHD-C4C-C3C	-6.19	115.85	124.87
10	bL	204	CLA	O2D-CGD-CBD	6.17	122.06	111.25
10	aB	801	CLA	C2C-C1C-NC	6.17	115.76	109.97
10	aL	204	CLA	O2D-CGD-CBD	6.17	122.05	111.25
9	aA	801	CL0	C2C-C1C-NC	6.17	115.75	109.97
10	cA	807	CLA	O2D-CGD-CBD	6.17	122.05	111.25
10	aB	826	CLA	O2D-CGD-CBD	6.17	122.05	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	807	CLA	O2D-CGD-CBD	6.17	122.04	111.25
10	aB	819	CLA	C2C-C1C-NC	6.16	115.75	109.97
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	bA	807	CLA	O2D-CGD-CBD	6.16	122.02	111.25
10	bA	816	CLA	CHD-C4C-C3C	-6.15	115.90	124.87
10	bB	826	CLA	O2D-CGD-CBD	6.15	122.02	111.25
10	cB	826	CLA	O2D-CGD-CBD	6.15	122.01	111.25
10	bA	828	CLA	CHD-C4C-C3C	-6.12	115.95	124.87
10	bA	842	CLA	C2C-C1C-NC	6.11	115.69	109.97
10	cB	840	CLA	CHD-C4C-C3C	-6.11	115.97	124.87
10	bB	840	CLA	CHD-C4C-C3C	-6.10	115.97	124.87
10	aB	840	CLA	CHD-C4C-C3C	-6.10	115.97	124.87
10	bB	801	CLA	C2C-C1C-NC	6.10	115.68	109.97
10	aA	805	CLA	CHD-C4C-C3C	-6.09	115.99	124.87
10	cA	831	CLA	CHD-C4C-C3C	-6.08	116.00	124.87
10	cA	828	CLA	CHD-C4C-C3C	-6.08	116.00	124.87
10	aA	808	CLA	CHD-C4C-C3C	-6.07	116.01	124.87
10	cA	805	CLA	CHD-C4C-C3C	-6.07	116.02	124.87
10	cA	808	CLA	CHD-C4C-C3C	-6.07	116.02	124.87
10	bA	831	CLA	CHD-C4C-C3C	-6.07	116.02	124.87
10	bL	202	CLA	C2C-C1C-NC	6.07	115.66	109.97
10	aA	828	CLA	CHD-C4C-C3C	-6.07	116.02	124.87
10	bA	805	CLA	CHD-C4C-C3C	-6.07	116.02	124.87
10	cA	842	CLA	C2C-C1C-NC	6.07	115.66	109.97
10	aB	814	CLA	O2D-CGD-CBD	6.07	121.87	111.25
10	aA	842	CLA	C2C-C1C-NC	6.06	115.65	109.97
10	bA	804	CLA	O2D-CGD-CBD	6.05	121.85	111.25
10	bB	814	CLA	O2D-CGD-CBD	6.05	121.84	111.25
10	aB	838	CLA	CHD-C4C-C3C	-6.04	116.06	124.87
10	cA	804	CLA	O2D-CGD-CBD	6.04	121.83	111.25
10	aL	202	CLA	C2C-C1C-NC	6.04	115.63	109.97
10	cB	822	CLA	CHD-C4C-C3C	-6.04	116.06	124.87
10	bA	808	CLA	CHD-C4C-C3C	-6.04	116.06	124.87
10	cB	814	CLA	O2D-CGD-CBD	6.04	121.83	111.25
10	cL	202	CLA	C2C-C1C-NC	6.04	115.63	109.97
10	aA	831	CLA	CHD-C4C-C3C	-6.04	116.06	124.87
10	aA	821	CLA	CHD-C4C-C3C	-6.03	116.08	124.87
10	bB	838	CLA	CHD-C4C-C3C	-6.03	116.08	124.87
10	bA	821	CLA	CHD-C4C-C3C	-6.03	116.08	124.87
10	bA	805	CLA	O2D-CGD-CBD	6.02	121.80	111.25
10	aA	804	CLA	O2D-CGD-CBD	6.02	121.78	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	822	CLA	CHD-C4C-C3C	-6.01	116.10	124.87
10	aB	822	CLA	CHD-C4C-C3C	-6.01	116.11	124.87
10	cA	805	CLA	O2D-CGD-CBD	6.01	121.76	111.25
10	aA	805	CLA	O2D-CGD-CBD	6.00	121.75	111.25
10	cA	809	CLA	CHD-C4C-C3C	-6.00	116.12	124.87
10	bA	809	CLA	CHD-C4C-C3C	-6.00	116.12	124.87
10	bB	832	CLA	CHD-C4C-C3C	-5.99	116.14	124.87
10	cB	838	CLA	CHD-C4C-C3C	-5.99	116.14	124.87
10	cA	821	CLA	CHD-C4C-C3C	-5.99	116.14	124.87
10	cB	825	CLA	CHD-C4C-C3C	-5.99	116.14	124.87
10	aB	804	CLA	CHD-C4C-C3C	-5.98	116.15	124.87
10	aA	809	CLA	CHD-C4C-C3C	-5.97	116.16	124.87
10	bA	841	CLA	CHD-C4C-C3C	-5.97	116.16	124.87
9	cA	801	CL0	CHD-C4C-C3C	-5.97	116.16	124.87
10	cB	804	CLA	CHD-C4C-C3C	-5.97	116.16	124.87
10	cB	826	CLA	C4A-NA-C1A	-5.97	104.02	106.71
9	aA	801	CL0	CHD-C4C-C3C	-5.97	116.17	124.87
10	aA	832	CLA	CHD-C4C-C3C	-5.96	116.17	124.87
10	bB	825	CLA	CHD-C4C-C3C	-5.96	116.18	124.87
10	aA	841	CLA	CHD-C4C-C3C	-5.96	116.18	124.87
10	aB	825	CLA	CHD-C4C-C3C	-5.96	116.18	124.87
10	bA	832	CLA	CHD-C4C-C3C	-5.96	116.18	124.87
10	aB	822	CLA	C2C-C1C-NC	5.96	115.55	109.97
10	aB	832	CLA	CHD-C4C-C3C	-5.96	116.19	124.87
9	bA	801	CL0	CHD-C4C-C3C	-5.95	116.19	124.87
10	bB	804	CLA	CHD-C4C-C3C	-5.95	116.19	124.87
10	cB	822	CLA	C2C-C1C-NC	5.95	115.55	109.97
10	cA	841	CLA	CHD-C4C-C3C	-5.95	116.19	124.87
10	bA	825	CLA	CHD-C4C-C3C	-5.95	116.20	124.87
10	cB	832	CLA	CHD-C4C-C3C	-5.94	116.21	124.87
10	bA	821	CLA	O2D-CGD-CBD	5.94	121.64	111.25
10	cA	825	CLA	CHD-C4C-C3C	-5.93	116.22	124.87
10	cA	832	CLA	CHD-C4C-C3C	-5.93	116.22	124.87
10	bB	822	CLA	C2C-C1C-NC	5.93	115.53	109.97
10	aA	825	CLA	CHD-C4C-C3C	-5.92	116.23	124.87
10	bA	837	CLA	CHD-C4C-C3C	-5.92	116.24	124.87
10	cB	837	CLA	CHD-C4C-C3C	-5.92	116.24	124.87
10	cA	838	CLA	CHD-C4C-C3C	-5.92	116.24	124.87
10	aA	838	CLA	CHD-C4C-C3C	-5.92	116.24	124.87
10	cA	837	CLA	CHD-C4C-C3C	-5.92	116.24	124.87
10	aA	837	CLA	CHD-C4C-C3C	-5.92	116.24	124.87
10	aA	843	CLA	C2C-C1C-NC	5.91	115.51	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	830	CLA	C2C-C1C-NC	5.91	115.51	109.97
10	cB	830	CLA	C2C-C1C-NC	5.91	115.51	109.97
10	cB	809	CLA	O2D-CGD-CBD	5.91	121.59	111.25
10	aB	809	CLA	O2D-CGD-CBD	5.91	121.59	111.25
10	aB	826	CLA	C4A-NA-C1A	-5.91	104.05	106.71
10	aB	830	CLA	C2C-C1C-NC	5.91	115.51	109.97
10	bB	837	CLA	CHD-C4C-C3C	-5.91	116.26	124.87
10	bA	827	CLA	CHD-C4C-C3C	-5.91	116.26	124.87
10	cA	821	CLA	O2D-CGD-CBD	5.90	121.58	111.25
10	bA	819	CLA	O2D-CGD-CBD	5.89	121.57	111.25
10	bB	809	CLA	O2D-CGD-CBD	5.89	121.56	111.25
10	aA	819	CLA	O2D-CGD-CBD	5.89	121.56	111.25
10	aA	821	CLA	O2D-CGD-CBD	5.89	121.56	111.25
10	cA	827	CLA	CHD-C4C-C3C	-5.88	116.29	124.87
10	bA	843	CLA	C2C-C1C-NC	5.88	115.48	109.97
10	aA	827	CLA	CHD-C4C-C3C	-5.88	116.29	124.87
10	bA	802	CLA	C2C-C1C-NC	5.88	115.48	109.97
10	bA	838	CLA	CHD-C4C-C3C	-5.88	116.29	124.87
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
10	cB	822	CLA	O2D-CGD-CBD	5.87	121.53	111.25
10	aB	837	CLA	CHD-C4C-C3C	-5.87	116.31	124.87
10	bB	821	CLA	O2D-CGD-CBD	5.87	121.53	111.25
10	aB	822	CLA	O2D-CGD-CBD	5.87	121.52	111.25
10	aB	806	CLA	O2D-CGD-CBD	5.87	121.52	111.25
10	cA	819	CLA	O2D-CGD-CBD	5.86	121.52	111.25
10	cA	843	CLA	C2C-C1C-NC	5.86	115.47	109.97
10	bB	822	CLA	O2D-CGD-CBD	5.86	121.51	111.25
10	aA	802	CLA	C2C-C1C-NC	5.86	115.46	109.97
10	bB	806	CLA	O2D-CGD-CBD	5.85	121.49	111.25
10	cB	806	CLA	O2D-CGD-CBD	5.85	121.49	111.25
10	cA	812	CLA	O2D-CGD-CBD	5.85	121.49	111.25
10	bA	829	CLA	C2C-C1C-NC	5.85	115.45	109.97
10	bA	803	CLA	CHD-C4C-C3C	-5.84	116.35	124.87
10	aA	840	CLA	CHD-C4C-C3C	-5.84	116.35	124.87
10	bA	840	CLA	CHD-C4C-C3C	-5.84	116.35	124.87
10	cA	803	CLA	CHD-C4C-C3C	-5.84	116.35	124.87
10	cB	821	CLA	O2D-CGD-CBD	5.84	121.47	111.25
10	cL	202	CLA	O2D-CGD-CBD	5.84	121.47	111.25
10	aA	803	CLA	CHD-C4C-C3C	-5.84	116.36	124.87
10	aB	821	CLA	O2D-CGD-CBD	5.84	121.46	111.25
10	cA	840	CLA	CHD-C4C-C3C	-5.83	116.36	124.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	817	CLA	CHD-C4C-C3C	-5.83	116.36	124.87
10	aB	821	CLA	CHD-C4C-C3C	-5.83	116.37	124.87
10	bA	812	CLA	O2D-CGD-CBD	5.83	121.45	111.25
10	cA	817	CLA	CHD-C4C-C3C	-5.83	116.37	124.87
10	bL	202	CLA	O2D-CGD-CBD	5.83	121.45	111.25
10	bB	821	CLA	CHD-C4C-C3C	-5.83	116.37	124.87
10	aL	202	CLA	O2D-CGD-CBD	5.83	121.45	111.25
10	aA	812	CLA	O2D-CGD-CBD	5.82	121.44	111.25
10	aA	817	CLA	CHD-C4C-C3C	-5.82	116.38	124.87
10	aA	836	CLA	CHD-C4C-C3C	-5.82	116.38	124.87
10	cB	810	CLA	CHD-C4C-C3C	-5.82	116.39	124.87
10	bA	820	CLA	CHD-C4C-C3C	-5.82	116.39	124.87
10	aB	817	CLA	CHD-C4C-C3C	-5.82	116.39	124.87
10	cA	802	CLA	C2C-C1C-NC	5.81	115.42	109.97
10	cB	821	CLA	CHD-C4C-C3C	-5.81	116.39	124.87
10	cA	829	CLA	C2C-C1C-NC	5.81	115.41	109.97
10	cA	836	CLA	CHD-C4C-C3C	-5.81	116.40	124.87
10	aB	837	CLA	O2D-CGD-CBD	5.81	121.42	111.25
10	cB	817	CLA	CHD-C4C-C3C	-5.81	116.40	124.87
10	bB	810	CLA	CHD-C4C-C3C	-5.81	116.40	124.87
10	bA	817	CLA	CHD-C4C-C3C	-5.81	116.40	124.87
10	aB	810	CLA	CHD-C4C-C3C	-5.80	116.41	124.87
10	cA	820	CLA	CHD-C4C-C3C	-5.80	116.41	124.87
10	cB	824	CLA	C2C-C1C-NC	5.80	115.40	109.97
10	cB	837	CLA	O2D-CGD-CBD	5.80	121.40	111.25
10	bA	836	CLA	CHD-C4C-C3C	-5.80	116.42	124.87
10	bB	837	CLA	O2D-CGD-CBD	5.79	121.39	111.25
10	cB	815	CLA	CHD-C4C-C3C	-5.79	116.42	124.87
10	aA	820	CLA	CHD-C4C-C3C	-5.79	116.42	124.87
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	bB	836	CLA	C2C-C1C-NC	5.79	115.39	109.97
10	aA	823	CLA	C2C-C1C-NC	5.79	115.39	109.97
10	cB	836	CLA	C2C-C1C-NC	5.79	115.39	109.97
10	aB	824	CLA	C2C-C1C-NC	5.79	115.39	109.97
10	bB	824	CLA	C2C-C1C-NC	5.78	115.39	109.97
10	cB	813	CLA	CHD-C4C-C3C	-5.77	116.45	124.87
10	bB	813	CLA	CHD-C4C-C3C	-5.77	116.45	124.87
10	aB	813	CLA	CHD-C4C-C3C	-5.77	116.45	124.87
10	cA	833	CLA	CHD-C4C-C3C	-5.77	116.46	124.87
10	bA	836	CLA	C2C-C1C-NC	5.77	115.37	109.97
10	bB	815	CLA	CHD-C4C-C3C	-5.76	116.46	124.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	833	CLA	CHD-C4C-C3C	-5.76	116.47	124.87
10	aB	815	CLA	CHD-C4C-C3C	-5.76	116.47	124.87
10	cA	823	CLA	C2C-C1C-NC	5.76	115.37	109.97
10	bA	834	CLA	C2C-C1C-NC	5.76	115.36	109.97
10	bA	833	CLA	CHD-C4C-C3C	-5.76	116.48	124.87
10	bB	801	CLA	C4A-NA-C1A	-5.75	104.12	106.71
10	aA	834	CLA	C2C-C1C-NC	5.75	115.36	109.97
10	bA	837	CLA	O2D-CGD-CBD	5.74	121.30	111.25
10	cA	836	CLA	C2C-C1C-NC	5.74	115.35	109.97
10	aB	829	CLA	CHD-C4C-C3C	-5.74	116.50	124.87
10	aB	801	CLA	C4A-NA-C1A	-5.73	104.13	106.71
10	cA	837	CLA	O2D-CGD-CBD	5.73	121.27	111.25
10	aA	818	CLA	C2C-C1C-NC	5.72	115.33	109.97
10	bA	818	CLA	C4A-NA-C1A	-5.72	104.13	106.71
10	aB	835	CLA	CHD-C4C-C3C	-5.72	116.53	124.87
10	aA	837	CLA	O2D-CGD-CBD	5.72	121.26	111.25
10	cB	829	CLA	CHD-C4C-C3C	-5.72	116.53	124.87
10	cA	834	CLA	CHD-C4C-C3C	-5.72	116.53	124.87
10	cA	834	CLA	C2C-C1C-NC	5.72	115.33	109.97
10	aA	836	CLA	C2C-C1C-NC	5.72	115.33	109.97
10	bB	829	CLA	CHD-C4C-C3C	-5.71	116.55	124.87
10	cB	835	CLA	CHD-C4C-C3C	-5.71	116.55	124.87
10	cA	818	CLA	C4A-NA-C1A	-5.70	104.14	106.71
10	aA	815	CLA	CHD-C4C-C3C	-5.69	116.57	124.87
10	cB	839	CLA	O2D-CGD-CBD	5.69	121.21	111.25
10	bA	814	CLA	CHD-C4C-C3C	-5.69	116.57	124.87
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	cB	816	CLA	CHD-C4C-C3C	-5.69	116.57	124.87
10	aB	816	CLA	CHD-C4C-C3C	-5.69	116.57	124.87
10	cA	838	CLA	O2D-CGD-CBD	5.69	121.20	111.25
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	bB	835	CLA	CHD-C4C-C3C	-5.68	116.58	124.87
10	aA	834	CLA	CHD-C4C-C3C	-5.68	116.58	124.87
10	bA	834	CLA	CHD-C4C-C3C	-5.68	116.59	124.87
10	cA	815	CLA	CHD-C4C-C3C	-5.68	116.59	124.87
10	cA	821	CLA	C2C-C1C-NC	5.67	115.28	109.97
10	bB	812	CLA	CHD-C4C-C3C	-5.67	116.60	124.87
10	aA	814	CLA	CHD-C4C-C3C	-5.67	116.61	124.87
10	bA	838	CLA	O2D-CGD-CBD	5.67	121.17	111.25
10	bA	815	CLA	CHD-C4C-C3C	-5.67	116.61	124.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	839	CLA	O2D-CGD-CBD	5.66	121.16	111.25
10	aA	807	CLA	CHD-C4C-C3C	-5.65	116.63	124.87
10	aB	839	CLA	O2D-CGD-CBD	5.65	121.14	111.25
10	cA	813	CLA	CHD-C4C-C3C	-5.65	116.63	124.87
10	bB	816	CLA	CHD-C4C-C3C	-5.65	116.63	124.87
10	aA	813	CLA	CHD-C4C-C3C	-5.65	116.63	124.87
10	bB	801	CLA	O2D-CGD-CBD	5.65	121.14	111.25
10	aB	801	CLA	O2D-CGD-CBD	5.65	121.14	111.25
10	cA	818	CLA	C2C-C1C-NC	5.65	115.26	109.97
10	cA	814	CLA	CHD-C4C-C3C	-5.64	116.64	124.87
10	bB	841	CLA	CHD-C4C-C3C	-5.64	116.64	124.87
10	bA	813	CLA	CHD-C4C-C3C	-5.64	116.65	124.87
10	bB	828	CLA	O2D-CGD-CBD	5.64	121.12	111.25
10	aA	802	CLA	CHD-C4C-C3C	-5.64	116.65	124.87
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	cA	802	CLA	CHD-C4C-C3C	-5.64	116.65	124.87
10	aB	839	CLA	CHD-C4C-C3C	-5.63	116.65	124.87
10	cB	841	CLA	CHD-C4C-C3C	-5.63	116.66	124.87
10	bA	807	CLA	CHD-C4C-C3C	-5.63	116.66	124.87
10	aA	821	CLA	C2C-C1C-NC	5.63	115.25	109.97
10	aA	838	CLA	O2D-CGD-CBD	5.63	121.11	111.25
10	bB	839	CLA	CHD-C4C-C3C	-5.63	116.66	124.87
10	cB	823	CLA	C2C-C1C-NC	5.63	115.25	109.97
10	cB	839	CLA	CHD-C4C-C3C	-5.63	116.66	124.87
10	cB	812	CLA	CHD-C4C-C3C	-5.63	116.66	124.87
10	cB	801	CLA	O2D-CGD-CBD	5.63	121.10	111.25
10	cA	813	CLA	C2C-C1C-NC	5.63	115.24	109.97
10	aB	812	CLA	CHD-C4C-C3C	-5.63	116.67	124.87
10	aA	811	CLA	CHD-C4C-C3C	-5.63	116.67	124.87
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	cA	807	CLA	CHD-C4C-C3C	-5.62	116.68	124.87
10	bA	811	CLA	CHD-C4C-C3C	-5.62	116.68	124.87
10	aB	828	CLA	O2D-CGD-CBD	5.62	121.08	111.25
10	aB	841	CLA	CHD-C4C-C3C	-5.62	116.68	124.87
10	bB	821	CLA	C2C-C1C-NC	5.62	115.23	109.97
10	bA	819	CLA	C2C-C1C-NC	5.62	115.23	109.97
10	cA	811	CLA	CHD-C4C-C3C	-5.61	116.68	124.87
10	bB	828	CLA	C2C-C1C-NC	5.61	115.23	109.97
10	bA	802	CLA	CHD-C4C-C3C	-5.61	116.68	124.87
10	cA	810	CLA	C4A-NA-C1A	-5.61	104.18	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	810	CLA	C2C-C1C-NC	5.61	115.22	109.97
10	cB	809	CLA	C2C-C1C-NC	5.61	115.22	109.97
10	cB	833	CLA	CHD-C4C-C3C	-5.60	116.70	124.87
10	bA	829	CLA	CHD-C4C-C3C	-5.60	116.70	124.87
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	aA	829	CLA	CHD-C4C-C3C	-5.60	116.71	124.87
10	cB	828	CLA	C2C-C1C-NC	5.60	115.21	109.97
10	cA	810	CLA	C2C-C1C-NC	5.60	115.21	109.97
10	aB	828	CLA	C2C-C1C-NC	5.59	115.21	109.97
10	aA	810	CLA	C2C-C1C-NC	5.59	115.21	109.97
10	bA	810	CLA	C4A-NA-C1A	-5.59	104.19	106.71
10	cB	828	CLA	O2D-CGD-CBD	5.59	121.03	111.25
10	bB	833	CLA	CHD-C4C-C3C	-5.59	116.72	124.87
10	aB	833	CLA	CHD-C4C-C3C	-5.59	116.72	124.87
10	cA	830	CLA	C2C-C1C-NC	5.59	115.20	109.97
10	cA	839	CLA	C2C-C1C-NC	5.58	115.20	109.97
10	bA	835	CLA	C2C-C1C-NC	5.58	115.20	109.97
10	aA	813	CLA	C2C-C1C-NC	5.58	115.20	109.97
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	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	C2C-C1C-NC	5.57	115.19	109.97
10	bB	809	CLA	C2C-C1C-NC	5.57	115.19	109.97
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	cA	829	CLA	CHD-C4C-C3C	-5.56	116.76	124.87
10	cA	856	CLA	CHD-C4C-C3C	-5.56	116.76	124.87
10	cB	813	CLA	C2C-C1C-NC	5.56	115.18	109.97
10	aA	839	CLA	C2C-C1C-NC	5.56	115.18	109.97
10	bA	856	CLA	CHD-C4C-C3C	-5.56	116.76	124.87
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	cA	840	CLA	O2D-CGD-CBD	5.56	120.98	111.25
10	aA	840	CLA	O2D-CGD-CBD	5.55	120.97	111.25
10	aA	830	CLA	C2C-C1C-NC	5.55	115.17	109.97
10	aA	856	CLA	CHD-C4C-C3C	-5.55	116.78	124.87
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	cA	810	CLA	CHD-C4C-C3C	-5.55	116.78	124.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	840	CLA	O2D-CGD-CBD	5.55	120.96	111.25
10	aA	831	CLA	C2C-C1C-NC	5.54	115.16	109.97
10	bA	810	CLA	CHD-C4C-C3C	-5.54	116.79	124.87
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	bA	806	CLA	CHD-C4C-C3C	-5.54	116.79	124.87
10	bL	205	CLA	CHD-C4C-C3C	-5.54	116.80	124.87
10	cL	205	CLA	CHD-C4C-C3C	-5.53	116.80	124.87
10	cL	202	CLA	CHD-C4C-C3C	-5.53	116.80	124.87
10	cA	831	CLA	C2C-C1C-NC	5.53	115.16	109.97
10	bA	856	CLA	C2C-C1C-NC	5.53	115.15	109.97
10	cA	823	CLA	CHD-C4C-C3C	-5.53	116.81	124.87
10	aL	205	CLA	CHD-C4C-C3C	-5.53	116.81	124.87
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	bA	814	CLA	O2D-CGD-CBD	5.52	120.92	111.25
10	cA	806	CLA	CHD-C4C-C3C	-5.52	116.82	124.87
10	aA	806	CLA	CHD-C4C-C3C	-5.52	116.82	124.87
10	bA	835	CLA	CHD-C4C-C3C	-5.52	116.82	124.87
10	aB	833	CLA	O2D-CGD-CBD	5.52	120.91	111.25
10	bA	824	CLA	CHD-C4C-C3C	-5.52	116.83	124.87
10	aA	810	CLA	CHD-C4C-C3C	-5.51	116.83	124.87
10	aA	835	CLA	CHD-C4C-C3C	-5.51	116.83	124.87
10	aA	823	CLA	CHD-C4C-C3C	-5.51	116.83	124.87
10	cA	822	CLA	O2D-CGD-CBD	5.51	120.90	111.25
10	aB	814	CLA	C2C-C1C-NC	5.51	115.13	109.97
10	bB	833	CLA	O2D-CGD-CBD	5.51	120.89	111.25
10	bL	204	CLA	CHD-C4C-C3C	-5.51	116.84	124.87
10	bB	839	CLA	C2C-C1C-NC	5.51	115.13	109.97
10	aA	815	CLA	C2C-C1C-NC	5.51	115.13	109.97
10	bA	823	CLA	CHD-C4C-C3C	-5.51	116.84	124.87
10	aA	814	CLA	O2D-CGD-CBD	5.51	120.89	111.25
10	cA	815	CLA	C2C-C1C-NC	5.51	115.13	109.97
10	aB	815	CLA	O2D-CGD-CBD	5.51	120.89	111.25
10	aB	813	CLA	C2C-C1C-NC	5.51	115.13	109.97
10	cA	835	CLA	CHD-C4C-C3C	-5.51	116.84	124.87
10	bB	809	CLA	CHD-C4C-C3C	-5.51	116.84	124.87
10	cA	824	CLA	CHD-C4C-C3C	-5.51	116.84	124.87
10	cB	815	CLA	O2D-CGD-CBD	5.50	120.88	111.25
10	aB	809	CLA	CHD-C4C-C3C	-5.50	116.84	124.87
10	aL	204	CLA	CHD-C4C-C3C	-5.50	116.85	124.87
10	cB	833	CLA	O2D-CGD-CBD	5.50	120.88	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	807	CLA	O2D-CGD-CBD	5.50	120.88	111.25
10	cL	204	CLA	CHD-C4C-C3C	-5.50	116.85	124.87
10	aL	202	CLA	CHD-C4C-C3C	-5.50	116.85	124.87
10	bB	837	CLA	C2C-C1C-NC	5.50	115.12	109.97
10	aA	822	CLA	O2D-CGD-CBD	5.49	120.86	111.25
10	cB	810	CLA	C2C-C1C-NC	5.49	115.11	109.97
10	aB	817	CLA	C2C-C1C-NC	5.49	115.11	109.97
10	bL	202	CLA	CHD-C4C-C3C	-5.49	116.87	124.87
10	cA	819	CLA	CHD-C4C-C3C	-5.49	116.87	124.87
10	cA	856	CLA	C2C-C1C-NC	5.49	115.11	109.97
10	bB	807	CLA	O2D-CGD-CBD	5.48	120.85	111.25
10	bB	815	CLA	O2D-CGD-CBD	5.48	120.85	111.25
10	aA	808	CLA	C2C-C1C-NC	5.48	115.11	109.97
10	bA	822	CLA	O2D-CGD-CBD	5.48	120.85	111.25
10	bB	810	CLA	C2C-C1C-NC	5.48	115.11	109.97
10	cA	812	CLA	CHD-C4C-C3C	-5.48	116.88	124.87
10	cA	814	CLA	O2D-CGD-CBD	5.48	120.84	111.25
10	bB	814	CLA	C2C-C1C-NC	5.48	115.10	109.97
10	cB	809	CLA	CHD-C4C-C3C	-5.48	116.88	124.87
10	bA	808	CLA	C2C-C1C-NC	5.47	115.10	109.97
10	aL	203	CLA	CHD-C4C-C3C	-5.47	116.89	124.87
10	aB	807	CLA	O2D-CGD-CBD	5.47	120.83	111.25
10	aA	824	CLA	CHD-C4C-C3C	-5.47	116.89	124.87
10	aA	819	CLA	CHD-C4C-C3C	-5.47	116.89	124.87
10	cA	808	CLA	C2C-C1C-NC	5.46	115.09	109.97
10	aB	823	CLA	CHD-C4C-C3C	-5.46	116.90	124.87
10	bA	825	CLA	O2D-CGD-CBD	5.46	120.81	111.25
10	aB	810	CLA	C2C-C1C-NC	5.46	115.09	109.97
10	bA	812	CLA	CHD-C4C-C3C	-5.46	116.91	124.87
10	aA	812	CLA	CHD-C4C-C3C	-5.46	116.91	124.87
10	bL	203	CLA	CHD-C4C-C3C	-5.45	116.92	124.87
10	aA	856	CLA	C2C-C1C-NC	5.45	115.08	109.97
10	aA	825	CLA	O2D-CGD-CBD	5.45	120.79	111.25
10	cB	814	CLA	C2C-C1C-NC	5.45	115.08	109.97
10	cL	203	CLA	CHD-C4C-C3C	-5.45	116.92	124.87
10	aB	836	CLA	CHD-C4C-C3C	-5.45	116.92	124.87
10	bB	836	CLA	CHD-C4C-C3C	-5.45	116.92	124.87
10	cA	825	CLA	O2D-CGD-CBD	5.45	120.79	111.25
10	bA	819	CLA	CHD-C4C-C3C	-5.45	116.92	124.87
10	bB	823	CLA	CHD-C4C-C3C	-5.45	116.92	124.87
10	bA	831	CLA	C2C-C1C-NC	5.45	115.08	109.97
10	cB	823	CLA	CHD-C4C-C3C	-5.45	116.92	124.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	819	CLA	CHD-C4C-C3C	-5.44	116.94	124.87
10	cB	817	CLA	C2C-C1C-NC	5.44	115.07	109.97
10	bA	838	CLA	C2C-C1C-NC	5.44	115.06	109.97
10	cB	807	CLA	C2C-C1C-NC	5.43	115.06	109.97
10	aB	807	CLA	C2C-C1C-NC	5.42	115.05	109.97
10	bB	819	CLA	CHD-C4C-C3C	-5.42	116.97	124.87
10	aB	827	CLA	O2D-CGD-CBD	5.42	120.73	111.25
10	cB	819	CLA	CHD-C4C-C3C	-5.41	116.98	124.87
10	cB	836	CLA	CHD-C4C-C3C	-5.41	116.98	124.87
10	bB	817	CLA	C2C-C1C-NC	5.41	115.04	109.97
10	aB	818	CLA	CHD-C4C-C3C	-5.41	116.99	124.87
10	cA	811	CLA	O2D-CGD-CBD	5.40	120.71	111.25
10	aB	807	CLA	CHD-C4C-C3C	-5.40	116.99	124.87
10	bB	819	CLA	C4A-NA-C1A	-5.40	104.28	106.71
10	cB	818	CLA	CHD-C4C-C3C	-5.40	117.00	124.87
10	cB	827	CLA	O2D-CGD-CBD	5.39	120.69	111.25
10	bB	831	CLA	CHD-C4C-C3C	-5.39	117.00	124.87
10	aA	841	CLA	O2D-CGD-CBD	5.39	120.69	111.25
10	bA	832	CLA	C2C-C1C-NC	5.39	115.02	109.97
10	cA	841	CLA	O2D-CGD-CBD	5.39	120.68	111.25
10	bA	811	CLA	O2D-CGD-CBD	5.39	120.68	111.25
10	aA	811	CLA	O2D-CGD-CBD	5.39	120.68	111.25
10	bB	824	CLA	CHD-C4C-C3C	-5.38	117.02	124.87
10	bB	807	CLA	C2C-C1C-NC	5.38	115.02	109.97
10	aA	838	CLA	C2C-C1C-NC	5.38	115.02	109.97
10	bB	807	CLA	CHD-C4C-C3C	-5.38	117.02	124.87
10	bA	841	CLA	O2D-CGD-CBD	5.38	120.67	111.25
10	cB	831	CLA	CHD-C4C-C3C	-5.38	117.02	124.87
10	cA	854	CLA	O2D-CGD-CBD	5.38	120.67	111.25
10	bB	827	CLA	O2D-CGD-CBD	5.38	120.66	111.25
10	aA	854	CLA	O2D-CGD-CBD	5.38	120.66	111.25
10	aA	804	CLA	CHD-C4C-C3C	-5.38	117.03	124.87
10	bA	833	CLA	C2C-C1C-NC	5.37	115.01	109.97
10	bA	804	CLA	CHD-C4C-C3C	-5.37	117.03	124.87
10	cA	804	CLA	CHD-C4C-C3C	-5.37	117.03	124.87
10	aB	831	CLA	CHD-C4C-C3C	-5.37	117.04	124.87
10	cA	838	CLA	C2C-C1C-NC	5.37	115.00	109.97
10	cA	843	CLA	CHD-C4C-C3C	-5.37	117.04	124.87
10	aB	824	CLA	CHD-C4C-C3C	-5.37	117.04	124.87
10	cB	815	CLA	C2C-C1C-NC	5.37	115.00	109.97
10	cB	824	CLA	CHD-C4C-C3C	-5.37	117.05	124.87
10	bA	831	CLA	O2D-CGD-CBD	5.36	120.64	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	831	CLA	O2D-CGD-CBD	5.36	120.64	111.25
10	aB	815	CLA	C2C-C1C-NC	5.36	115.00	109.97
10	bA	854	CLA	O2D-CGD-CBD	5.36	120.63	111.25
10	cB	807	CLA	CHD-C4C-C3C	-5.36	117.06	124.87
10	aA	843	CLA	CHD-C4C-C3C	-5.36	117.06	124.87
10	aA	830	CLA	CHD-C4C-C3C	-5.36	117.06	124.87
10	cA	832	CLA	C2C-C1C-NC	5.36	114.99	109.97
10	aA	831	CLA	O2D-CGD-CBD	5.35	120.62	111.25
10	cA	830	CLA	CHD-C4C-C3C	-5.35	117.07	124.87
10	cB	819	CLA	C4A-NA-C1A	-5.35	104.30	106.71
10	bB	815	CLA	C2C-C1C-NC	5.35	114.98	109.97
10	bA	843	CLA	CHD-C4C-C3C	-5.35	117.07	124.87
10	aB	819	CLA	C4A-NA-C1A	-5.34	104.31	106.71
10	aA	833	CLA	C2C-C1C-NC	5.33	114.97	109.97
10	aA	832	CLA	C2C-C1C-NC	5.33	114.97	109.97
10	bA	830	CLA	CHD-C4C-C3C	-5.33	117.10	124.87
10	cA	833	CLA	C2C-C1C-NC	5.33	114.97	109.97
10	bB	818	CLA	CHD-C4C-C3C	-5.33	117.10	124.87
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	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	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	cB	838	CLA	O2D-CGD-CBD	5.31	120.55	111.25
10	aB	835	CLA	C2C-C1C-NC	5.31	114.95	109.97
10	bB	832	CLA	C2C-C1C-NC	5.31	114.94	109.97
10	bB	838	CLA	O2D-CGD-CBD	5.31	120.54	111.25
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	aA	840	CLA	C2C-C1C-NC	5.31	114.94	109.97
10	aB	811	CLA	CHD-C4C-C3C	-5.30	117.14	124.87
10	aA	837	CLA	C2C-C1C-NC	5.30	114.94	109.97
10	bB	811	CLA	CHD-C4C-C3C	-5.30	117.14	124.87
10	aB	838	CLA	O2D-CGD-CBD	5.30	120.52	111.25
10	bA	814	CLA	C2C-C1C-NC	5.30	114.94	109.97
10	bA	827	CLA	C2C-C1C-NC	5.29	114.93	109.97
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	811	CLA	CHD-C4C-C3C	-5.29	117.15	124.87
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	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	cA	830	CLA	O2D-CGD-CBD	5.28	120.50	111.25
10	cA	835	CLA	O2D-CGD-CBD	5.28	120.50	111.25
10	aB	820	CLA	C2C-C1C-NC	5.28	114.92	109.97
10	aA	842	CLA	CHD-C4C-C3C	-5.28	117.17	124.87
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	835	CLA	O2D-CGD-CBD	5.28	120.49	111.25
10	bA	830	CLA	O2D-CGD-CBD	5.28	120.48	111.25
10	bA	812	CLA	C4A-NA-C1A	-5.28	104.33	106.71
10	cB	812	CLA	C2C-C1C-NC	5.27	114.91	109.97
10	bB	816	CLA	C2C-C1C-NC	5.27	114.91	109.97
10	bB	804	CLA	CAA-C2A-C3A	-5.27	98.34	112.78
10	bA	842	CLA	CHD-C4C-C3C	-5.27	117.18	124.87
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	aA	835	CLA	O2D-CGD-CBD	5.27	120.47	111.25
10	cB	834	CLA	C2C-C1C-NC	5.27	114.91	109.97
10	aB	801	CLA	CHD-C4C-C3C	-5.27	117.19	124.87
10	bA	807	CLA	C2C-C1C-NC	5.26	114.90	109.97
10	aA	830	CLA	O2D-CGD-CBD	5.26	120.46	111.25
10	cA	837	CLA	C2C-C1C-NC	5.26	114.90	109.97
10	aL	205	CLA	O2D-CGD-CBD	5.26	120.46	111.25
10	cA	842	CLA	CHD-C4C-C3C	-5.26	117.20	124.87
10	aB	812	CLA	C2C-C1C-NC	5.26	114.90	109.97
10	cA	836	CLA	O2D-CGD-CBD	5.26	120.45	111.25
10	cL	205	CLA	O2D-CGD-CBD	5.26	120.45	111.25
10	bL	205	CLA	C2C-C1C-NC	5.26	114.90	109.97
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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bL	205	CLA	O2D-CGD-CBD	5.25	120.43	111.25
10	bB	801	CLA	CHD-C4C-C3C	-5.25	117.22	124.87
10	bA	836	CLA	O2D-CGD-CBD	5.24	120.43	111.25
10	cL	205	CLA	C2C-C1C-NC	5.24	114.88	109.97
10	cB	801	CLA	CHD-C4C-C3C	-5.24	117.22	124.87
10	cB	835	CLA	C2C-C1C-NC	5.24	114.88	109.97
10	bB	812	CLA	C2C-C1C-NC	5.24	114.88	109.97
10	aA	836	CLA	O2D-CGD-CBD	5.24	120.42	111.25
10	aB	816	CLA	C2C-C1C-NC	5.24	114.88	109.97
10	bB	831	CLA	C2C-C1C-NC	5.24	114.88	109.97
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	cA	839	CLA	CHD-C4C-C3C	-5.22	117.26	124.87
10	aB	818	CLA	C4A-NA-C1A	-5.22	104.36	106.71
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	839	CLA	CHD-C4C-C3C	-5.21	117.27	124.87
10	cA	807	CLA	C2C-C1C-NC	5.21	114.85	109.97
10	aA	805	CLA	C2C-C1C-NC	5.20	114.84	109.97
10	cB	831	CLA	C4A-NA-C1A	-5.20	104.37	106.71
10	aA	839	CLA	CHD-C4C-C3C	-5.19	117.30	124.87
10	cA	818	CLA	CHD-C4C-C3C	-5.18	117.32	124.87
10	cB	826	CLA	CHD-C4C-C3C	-5.17	117.33	124.87
10	cB	812	CLA	O2D-CGD-CBD	5.17	120.29	111.25
10	bA	805	CLA	C2C-C1C-NC	5.16	114.81	109.97
10	bB	808	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	C4A-NA-C1A	-5.16	104.39	106.71
9	cA	801	CL0	O2D-CGD-CBD	5.15	120.27	111.25
9	aA	801	CL0	O2D-CGD-CBD	5.15	120.27	111.25
10	bB	826	CLA	CHD-C4C-C3C	-5.15	117.36	124.87
9	bA	801	CL0	O2D-CGD-CBD	5.15	120.27	111.25
10	aB	812	CLA	O2D-CGD-CBD	5.15	120.27	111.25
10	bB	812	CLA	O2D-CGD-CBD	5.15	120.26	111.25
10	aA	822	CLA	C2C-C1C-NC	5.15	114.79	109.97
10	aB	808	CLA	C4A-NA-C1A	-5.14	104.39	106.71
10	cB	802	CLA	CHD-C4C-C3C	-5.14	117.37	124.87
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	aA	802	CLA	O2D-CGD-CBD	5.13	120.24	111.25
10	bB	825	CLA	C4A-NA-C1A	-5.13	104.40	106.71
10	aB	804	CLA	C4A-NA-C1A	-5.13	104.40	106.71
10	bB	834	CLA	CHD-C4C-C3C	-5.13	117.39	124.87
10	aB	819	CLA	O2D-CGD-CBD	5.13	120.23	111.25
10	aB	802	CLA	CHD-C4C-C3C	-5.13	117.39	124.87
10	cB	819	CLA	O2D-CGD-CBD	5.13	120.23	111.25
10	cB	825	CLA	C2C-C1C-NC	5.13	114.78	109.97
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	aB	826	CLA	CHD-C4C-C3C	-5.13	117.39	124.87
10	cA	806	CLA	O2D-CGD-CBD	5.12	120.22	111.25
10	bB	807	CLA	C4A-NA-C1A	-5.12	104.40	106.71
10	aB	830	CLA	O2D-CGD-CBD	5.12	120.22	111.25
10	aB	840	CLA	C2C-C1C-NC	5.12	114.77	109.97
10	aB	807	CLA	C4A-NA-C1A	-5.12	104.41	106.71
10	cB	830	CLA	C4A-NA-C1A	-5.12	104.41	106.71
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	bA	806	CLA	O2D-CGD-CBD	5.11	120.19	111.25
10	aA	818	CLA	CHD-C4C-C3C	-5.11	117.42	124.87
10	aB	832	CLA	O2D-CGD-CBD	5.11	120.19	111.25
10	cA	805	CLA	C2C-C1C-NC	5.11	114.76	109.97
10	bA	802	CLA	O2D-CGD-CBD	5.11	120.19	111.25
10	bB	819	CLA	O2D-CGD-CBD	5.11	120.19	111.25
10	bA	818	CLA	CHD-C4C-C3C	-5.11	117.42	124.87
10	cB	818	CLA	C4A-NA-C1A	-5.10	104.41	106.71
10	bB	832	CLA	O2D-CGD-CBD	5.10	120.19	111.25
10	aA	806	CLA	O2D-CGD-CBD	5.10	120.18	111.25
10	cB	832	CLA	O2D-CGD-CBD	5.10	120.18	111.25
10	bB	802	CLA	CHD-C4C-C3C	-5.10	117.43	124.87
10	cA	802	CLA	O2D-CGD-CBD	5.10	120.18	111.25
10	bB	830	CLA	O2D-CGD-CBD	5.10	120.17	111.25
10	cB	825	CLA	C4A-NA-C1A	-5.10	104.41	106.71
10	cB	830	CLA	O2D-CGD-CBD	5.10	120.17	111.25
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	bA	815	CLA	O2D-CGD-CBD	5.09	120.16	111.25
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	cB	834	CLA	CHD-C4C-C3C	-5.08	117.46	124.87
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	aB	834	CLA	CHD-C4C-C3C	-5.08	117.46	124.87
10	cA	822	CLA	C2C-C1C-NC	5.08	114.73	109.97
10	aB	814	CLA	CHD-C4C-C3C	-5.08	117.47	124.87
10	cA	828	CLA	C2C-C1C-NC	5.07	114.72	109.97
10	cB	814	CLA	CHD-C4C-C3C	-5.07	117.47	124.87
10	cB	807	CLA	C4A-NA-C1A	-5.07	104.43	106.71
10	aA	815	CLA	O2D-CGD-CBD	5.07	120.12	111.25
10	bL	203	CLA	O2D-CGD-CBD	5.07	120.12	111.25
10	cA	804	CLA	C2C-C1C-NC	5.07	114.72	109.97
10	cA	815	CLA	O2D-CGD-CBD	5.06	120.11	111.25
10	cA	816	CLA	C2C-C1C-NC	5.06	114.71	109.97
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	bB	814	CLA	CHD-C4C-C3C	-5.05	117.50	124.87
10	aA	810	CLA	O2D-CGD-CBD	5.05	120.09	111.25
10	bL	203	CLA	C2C-C1C-NC	5.05	114.70	109.97
10	aA	806	CLA	C2C-C1C-NC	5.04	114.70	109.97
10	bA	812	CLA	C2C-C1C-NC	5.04	114.69	109.97
10	aL	203	CLA	O2D-CGD-CBD	5.03	120.06	111.25
10	bA	810	CLA	O2D-CGD-CBD	5.03	120.06	111.25
10	bA	824	CLA	C2C-C1C-NC	5.03	114.69	109.97
10	cL	203	CLA	O2D-CGD-CBD	5.03	120.05	111.25
10	cA	806	CLA	C2C-C1C-NC	5.03	114.68	109.97
10	bB	820	CLA	O2D-CGD-CBD	5.02	120.04	111.25
10	cA	810	CLA	O2D-CGD-CBD	5.02	120.04	111.25
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
10	bA	828	CLA	C4A-NA-C1A	-5.01	104.45	106.71
10	aA	812	CLA	C2C-C1C-NC	5.01	114.67	109.97
10	aB	820	CLA	O2D-CGD-CBD	5.01	120.02	111.25
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	823	CLA	O2D-CGD-CBD	5.00	120.01	111.25
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	823	CLA	O2D-CGD-CBD	5.00	119.99	111.25
10	aB	823	CLA	O2D-CGD-CBD	4.99	119.99	111.25
10	aL	203	CLA	C2C-C1C-NC	4.99	114.65	109.97
10	bA	827	CLA	O2D-CGD-CBD	4.99	119.98	111.25
10	cB	820	CLA	O2D-CGD-CBD	4.98	119.97	111.25
10	aB	820	CLA	CHD-C4C-C3C	-4.98	117.61	124.87
10	cA	827	CLA	O2D-CGD-CBD	4.97	119.96	111.25
10	bB	802	CLA	C2C-C1C-NC	4.97	114.63	109.97
10	aA	838	CLA	C4A-NA-C1A	-4.97	104.47	106.71
10	bB	820	CLA	CHD-C4C-C3C	-4.97	117.63	124.87
10	aA	827	CLA	O2D-CGD-CBD	4.97	119.94	111.25
10	bA	816	CLA	C2C-C1C-NC	4.96	114.62	109.97
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	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	bB	808	CLA	C2C-C1C-NC	4.95	114.61	109.97
10	cA	828	CLA	C4A-NA-C1A	-4.95	104.48	106.71
10	cB	820	CLA	CHD-C4C-C3C	-4.95	117.65	124.87
10	bB	801	CLA	CAA-C2A-C3A	-4.95	99.23	112.78
10	cB	828	CLA	C3C-C4C-NC	4.94	116.11	110.57
10	bB	804	CLA	C2C-C1C-NC	4.94	114.60	109.97
10	cB	833	CLA	C2C-C1C-NC	4.94	114.60	109.97
10	cB	801	CLA	CAA-C2A-C3A	-4.94	99.26	112.78
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	bB	833	CLA	C2C-C1C-NC	4.92	114.58	109.97
10	aA	817	CLA	C2C-C1C-NC	4.91	114.57	109.97
10	aB	818	CLA	C2C-C1C-NC	4.91	114.57	109.97
10	cL	202	CLA	C1D-CHD-C4C	-4.90	115.79	122.48
10	bA	804	CLA	C4A-NA-C1A	-4.89	104.51	106.71
10	aA	841	CLA	C2C-C1C-NC	4.88	114.55	109.97
10	aB	811	CLA	O2D-CGD-CBD	4.88	119.79	111.25
10	aL	202	CLA	C1D-CHD-C4C	-4.88	115.82	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	834	CLA	C4A-NA-C1A	-4.88	104.51	106.71
10	bB	818	CLA	C2C-C1C-NC	4.87	114.54	109.97
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	cB	811	CLA	O2D-CGD-CBD	4.87	119.77	111.25
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	811	CLA	O2D-CGD-CBD	4.86	119.76	111.25
10	cB	818	CLA	C2C-C1C-NC	4.86	114.53	109.97
10	bL	202	CLA	C1D-CHD-C4C	-4.86	115.84	122.48
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	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	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	bB	816	CLA	C4A-NA-C1A	-4.83	104.53	106.71
10	bB	813	CLA	O2D-CGD-CBD	4.83	119.71	111.25
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	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	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	cB	813	CLA	O2D-CGD-CBD	4.82	119.69	111.25
10	aB	813	CLA	O2D-CGD-CBD	4.82	119.68	111.25
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	cB	840	CLA	C4A-NA-C1A	-4.81	104.55	106.71
10	bB	812	CLA	C4A-NA-C1A	-4.81	104.55	106.71
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	aA	804	CLA	C4A-NA-C1A	-4.79	104.55	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bL	204	CLA	C2C-C1C-NC	4.79	114.46	109.97
10	aB	812	CLA	C4A-NA-C1A	-4.79	104.55	106.71
10	cA	805	CLA	CAA-C2A-C3A	-4.79	99.67	112.78
10	bB	824	CLA	C4A-NA-C1A	-4.78	104.56	106.71
10	aA	805	CLA	CAA-C2A-C3A	-4.78	99.69	112.78
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	808	CLA	C4A-NA-C1A	-4.76	104.57	106.71
10	cB	834	CLA	C4A-NA-C1A	-4.75	104.57	106.71
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	bA	820	CLA	C2C-C1C-NC	4.75	114.42	109.97
10	bA	824	CLA	C4A-NA-C1A	-4.74	104.57	106.71
10	aA	820	CLA	C2C-C1C-NC	4.74	114.41	109.97
10	cA	804	CLA	C4A-NA-C1A	-4.74	104.58	106.71
10	bB	832	CLA	C4A-NA-C1A	-4.74	104.58	106.71
10	cA	808	CLA	C4A-NA-C1A	-4.73	104.58	106.71
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	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	aB	823	CLA	C4A-NA-C1A	-4.70	104.59	106.71
10	bB	834	CLA	C4A-NA-C1A	-4.70	104.59	106.71
10	cB	816	CLA	C4A-NA-C1A	-4.70	104.59	106.71
10	bB	803	CLA	C3C-C4C-NC	4.70	115.84	110.57
10	aB	803	CLA	C3C-C4C-NC	4.68	115.82	110.57
10	aA	842	CLA	O2D-CGD-CBD	4.68	119.44	111.25
10	cA	806	CLA	C4A-NA-C1A	-4.68	104.60	106.71
10	bA	842	CLA	O2D-CGD-CBD	4.68	119.44	111.25
10	cA	842	CLA	O2D-CGD-CBD	4.67	119.43	111.25
10	cB	826	CLA	C2C-C1C-NC	4.67	114.35	109.97
10	cA	825	CLA	C2C-C1C-NC	4.67	114.35	109.97
10	cA	832	CLA	O2D-CGD-CBD	4.66	119.41	111.25
10	cB	803	CLA	C3C-C4C-NC	4.66	115.80	110.57
10	aA	813	CLA	O2D-CGD-CBD	4.66	119.41	111.25
10	aA	825	CLA	C2C-C1C-NC	4.66	114.34	109.97
10	bA	813	CLA	O2D-CGD-CBD	4.66	119.40	111.25
10	cA	825	CLA	C4A-NA-C1A	-4.66	104.61	106.71
10	cA	813	CLA	O2D-CGD-CBD	4.65	119.40	111.25
10	aB	826	CLA	C2C-C1C-NC	4.65	114.33	109.97
10	aA	825	CLA	C4A-NA-C1A	-4.65	104.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	825	CLA	C2C-C1C-NC	4.65	114.33	109.97
10	bA	832	CLA	O2D-CGD-CBD	4.65	119.38	111.25
10	bB	826	CLA	C2C-C1C-NC	4.64	114.32	109.97
10	aA	832	CLA	O2D-CGD-CBD	4.63	119.36	111.25
10	aA	824	CLA	C4A-NA-C1A	-4.63	104.62	106.71
10	aB	838	CLA	C2C-C1C-NC	4.62	114.30	109.97
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	802	CLA	O2D-CGD-CBD	4.60	119.31	111.25
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	bA	825	CLA	C4A-NA-C1A	-4.60	104.64	106.71
10	aB	840	CLA	C4A-NA-C1A	-4.60	104.64	106.71
10	bB	836	CLA	O2D-CGD-CBD	4.60	119.29	111.25
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	820	CLA	C4A-NA-C1A	-4.58	104.64	106.71
10	cB	831	CLA	O2D-CGD-CBD	4.58	119.27	111.25
10	cB	836	CLA	O2D-CGD-CBD	4.58	119.27	111.25
10	bB	838	CLA	C2C-C1C-NC	4.58	114.26	109.97
10	cB	818	CLA	O2D-CGD-CBD	4.58	119.27	111.25
10	aA	826	CLA	C4A-NA-C1A	-4.58	104.65	106.71
10	aB	802	CLA	O2D-CGD-CBD	4.57	119.26	111.25
10	cA	835	CLA	C4A-NA-C1A	-4.57	104.65	106.71
10	aA	834	CLA	O2D-CGD-CBD	4.57	119.25	111.25
10	bA	834	CLA	O2D-CGD-CBD	4.57	119.25	111.25
10	cA	834	CLA	O2D-CGD-CBD	4.57	119.25	111.25
10	cA	809	CLA	O2D-CGD-CBD	4.57	119.25	111.25
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	aB	836	CLA	O2D-CGD-CBD	4.56	119.24	111.25
10	bB	831	CLA	O2D-CGD-CBD	4.56	119.23	111.25
10	bB	802	CLA	O2D-CGD-CBD	4.56	119.23	111.25
10	aB	831	CLA	O2D-CGD-CBD	4.56	119.23	111.25
10	aB	822	CLA	C1C-C2C-C3C	-4.56	102.12	106.95
10	aA	809	CLA	O2D-CGD-CBD	4.56	119.23	111.25
10	bB	806	CLA	C2C-C1C-NC	4.56	114.24	109.97
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	820	CLA	C4A-NA-C1A	-4.55	104.66	106.71
10	cB	822	CLA	C1C-C2C-C3C	-4.54	102.13	106.95
10	aA	835	CLA	C4A-NA-C1A	-4.54	104.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	818	CLA	O2D-CGD-CBD	4.54	119.20	111.25
10	aB	818	CLA	O2D-CGD-CBD	4.54	119.19	111.25
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	bA	809	CLA	O2D-CGD-CBD	4.53	119.17	111.25
10	cB	819	CLA	C1C-C2C-C3C	-4.52	102.16	106.95
10	bA	829	CLA	C3C-C4C-NC	4.52	115.64	110.57
10	aB	819	CLA	C1C-C2C-C3C	-4.51	102.17	106.95
10	bB	841	CLA	C1C-C2C-C3C	-4.51	102.17	106.95
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	cB	841	CLA	C1C-C2C-C3C	-4.51	102.17	106.95
10	bB	819	CLA	C1C-C2C-C3C	-4.50	102.18	106.95
10	aB	841	CLA	C1C-C2C-C3C	-4.50	102.18	106.95
10	aA	829	CLA	C3C-C4C-NC	4.50	115.62	110.57
10	cB	806	CLA	C2C-C1C-NC	4.50	114.19	109.97
10	cB	839	CLA	C4A-NA-C1A	-4.50	104.69	106.71
10	bB	839	CLA	C4A-NA-C1A	-4.49	104.69	106.71
10	cB	830	CLA	CHD-C4C-C3C	-4.49	118.32	124.87
10	bB	830	CLA	CHD-C4C-C3C	-4.49	118.32	124.87
10	cA	836	CLA	C4A-NA-C1A	-4.49	104.69	106.71
10	bA	806	CLA	C4A-NA-C1A	-4.49	104.69	106.71
10	bB	822	CLA	C1C-C2C-C3C	-4.49	102.20	106.95
10	aB	830	CLA	CHD-C4C-C3C	-4.48	118.33	124.87
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	bB	819	CLA	CBA-CAA-C2A	4.47	127.16	113.85
10	aB	819	CLA	CBA-CAA-C2A	4.46	127.13	113.85
10	cB	819	CLA	CBA-CAA-C2A	4.46	127.12	113.85
10	aB	839	CLA	C4A-NA-C1A	-4.46	104.70	106.71
10	bA	826	CLA	C4A-NA-C1A	-4.46	104.70	106.71
10	cA	854	CLA	C4A-NA-C1A	-4.45	104.70	106.71
10	bA	836	CLA	C4A-NA-C1A	-4.45	104.70	106.71
10	aA	820	CLA	O2D-CGD-CBD	4.45	119.04	111.25
10	cA	820	CLA	O2D-CGD-CBD	4.45	119.04	111.25
10	bB	804	CLA	O2D-CGD-O1D	-4.43	115.07	123.83
10	bA	820	CLA	O2D-CGD-CBD	4.43	119.01	111.25
10	bB	802	CLA	CMB-C2B-C3B	4.43	133.11	124.80
10	cA	826	CLA	C3C-C4C-NC	4.43	115.54	110.57
10	cB	814	CLA	CAC-C3C-C4C	4.43	130.61	124.82
10	aB	814	CLA	CAC-C3C-C4C	4.42	130.60	124.82
10	cB	829	CLA	C4A-NA-C1A	-4.42	104.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	804	CLA	O2D-CGD-O1D	-4.42	115.10	123.83
10	cB	802	CLA	CMB-C2B-C3B	4.42	133.08	124.80
10	aA	826	CLA	C3C-C4C-NC	4.42	115.52	110.57
10	bA	826	CLA	C3C-C4C-NC	4.41	115.52	110.57
10	aB	804	CLA	O2D-CGD-O1D	-4.41	115.11	123.83
10	aB	802	CLA	CMB-C2B-C3B	4.41	133.07	124.80
9	cA	801	CL0	C3C-C4C-NC	4.40	115.51	110.57
10	bB	814	CLA	CAC-C3C-C4C	4.40	130.57	124.82
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
10	bB	841	CLA	O2D-CGD-CBD	4.39	118.93	111.25
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	aB	840	CLA	O2D-CGD-CBD	4.38	118.91	111.25
10	bB	840	CLA	C3C-C4C-NC	4.37	115.48	110.57
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	aB	841	CLA	O2D-CGD-CBD	4.36	118.89	111.25
10	aB	801	CLA	C3C-C4C-NC	4.36	115.47	110.57
10	cB	840	CLA	O2D-CGD-CBD	4.36	118.89	111.25
10	aB	840	CLA	C3C-C4C-NC	4.36	115.46	110.57
10	cB	841	CLA	O2D-CGD-CBD	4.36	118.88	111.25
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	bB	840	CLA	O2D-CGD-CBD	4.36	118.88	111.25
10	cB	825	CLA	C3C-C4C-NC	4.36	115.46	110.57
10	aA	826	CLA	O2D-CGD-CBD	4.35	118.87	111.25
10	aB	833	CLA	C4A-NA-C1A	-4.35	104.75	106.71
10	aA	822	CLA	C4A-NA-C1A	-4.35	104.75	106.71
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	cA	826	CLA	O2D-CGD-CBD	4.34	118.85	111.25
10	bB	829	CLA	C3C-C4C-NC	4.34	115.44	110.57
10	bB	825	CLA	C3C-C4C-NC	4.34	115.44	110.57
10	aB	825	CLA	C3C-C4C-NC	4.34	115.44	110.57
10	aA	803	CLA	C4A-NA-C1A	-4.34	104.75	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aL	203	CLA	C4A-NA-C1A	-4.34	104.76	106.71
10	aB	813	CLA	C3C-C4C-NC	4.33	115.43	110.57
10	bA	826	CLA	O2D-CGD-CBD	4.33	118.83	111.25
10	aB	829	CLA	C3C-C4C-NC	4.33	115.43	110.57
10	aA	822	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	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	bB	834	CLA	O2D-CGD-CBD	4.32	118.81	111.25
10	bL	202	CLA	C3C-C4C-NC	4.32	115.41	110.57
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	bA	828	CLA	C3C-C4C-NC	4.31	115.41	110.57
10	aA	827	CLA	C3C-C4C-NC	4.31	115.41	110.57
10	cL	203	CLA	C4A-NA-C1A	-4.31	104.77	106.71
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	aA	817	CLA	O2D-CGD-CBD	4.30	118.78	111.25
10	cB	837	CLA	C3C-C4C-NC	4.30	115.39	110.57
10	bB	830	CLA	CAC-C3C-C4C	4.30	130.44	124.82
10	aL	202	CLA	C3C-C4C-NC	4.30	115.39	110.57
10	aA	828	CLA	C3C-C4C-NC	4.30	115.39	110.57
10	cA	803	CLA	C4A-NA-C1A	-4.30	104.78	106.71
10	cA	817	CLA	O2D-CGD-CBD	4.29	118.76	111.25
9	bA	801	CL0	C1C-C2C-C3C	-4.29	102.40	106.95
10	cA	827	CLA	C3C-C4C-NC	4.29	115.38	110.57
10	bB	809	CLA	C3C-C4C-NC	4.29	115.38	110.57
10	cB	834	CLA	O2D-CGD-CBD	4.29	118.76	111.25
10	cA	828	CLA	C3C-C4C-NC	4.28	115.37	110.57
10	aB	834	CLA	O2D-CGD-CBD	4.28	118.75	111.25
9	cA	801	CL0	C1C-C2C-C3C	-4.28	102.41	106.95
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	bA	825	CLA	CAA-C2A-C3A	-4.28	101.06	112.78
10	bA	817	CLA	O2D-CGD-CBD	4.28	118.74	111.25
10	cB	824	CLA	O2D-CGD-CBD	4.28	118.74	111.25
10	bB	811	CLA	C3C-C4C-NC	4.28	115.37	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	827	CLA	C3C-C4C-NC	4.28	115.37	110.57
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
9	aA	801	CL0	C1C-C2C-C3C	-4.27	102.42	106.95
10	bB	803	CLA	CAA-C2A-C3A	-4.27	101.09	112.78
10	cB	809	CLA	C4A-NA-C1A	-4.26	104.79	106.71
10	aB	830	CLA	CAC-C3C-C4C	4.26	130.39	124.82
10	cB	803	CLA	CAA-C2A-C3A	-4.26	101.11	112.78
10	aB	824	CLA	O2D-CGD-CBD	4.26	118.71	111.25
10	bB	824	CLA	O2D-CGD-CBD	4.26	118.70	111.25
10	aA	842	CLA	C1C-C2C-C3C	-4.26	102.44	106.95
10	cB	809	CLA	C3C-C4C-NC	4.26	115.34	110.57
10	bB	805	CLA	CHD-C4C-C3C	-4.26	118.66	124.87
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	aA	830	CLA	C4A-NA-C1A	-4.25	104.79	106.71
10	aB	803	CLA	O2D-CGD-CBD	4.25	118.69	111.25
10	cB	830	CLA	CAC-C3C-C4C	4.25	130.38	124.82
10	aB	805	CLA	CHD-C4C-C3C	-4.25	118.67	124.87
10	cA	842	CLA	C1C-C2C-C3C	-4.25	102.45	106.95
10	bA	842	CLA	C1C-C2C-C3C	-4.25	102.45	106.95
10	aB	811	CLA	C3C-C4C-NC	4.25	115.33	110.57
10	bA	823	CLA	O2D-CGD-CBD	4.24	118.68	111.25
10	bA	805	CLA	C4A-NA-C1A	-4.24	104.80	106.71
10	bA	841	CLA	C4A-NA-C1A	-4.24	104.80	106.71
10	bB	830	CLA	CMB-C2B-C3B	4.24	132.75	124.80
10	cB	830	CLA	CMB-C2B-C3B	4.24	132.75	124.80
10	cB	827	CLA	C3C-C4C-NC	4.24	115.32	110.57
10	bB	803	CLA	O2D-CGD-CBD	4.24	118.66	111.25
10	cA	823	CLA	O2D-CGD-CBD	4.23	118.66	111.25
10	cB	811	CLA	C3C-C4C-NC	4.23	115.32	110.57
10	cB	803	CLA	O2D-CGD-CBD	4.23	118.65	111.25
10	aB	830	CLA	CMB-C2B-C3B	4.22	132.72	124.80
10	aA	823	CLA	O2D-CGD-CBD	4.22	118.64	111.25
10	bB	806	CLA	C3C-C4C-NC	4.22	115.31	110.57
10	cB	805	CLA	CHD-C4C-C3C	-4.22	118.71	124.87
10	aA	837	CLA	C4A-NA-C1A	-4.22	104.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	806	CLA	C3C-C4C-NC	4.22	115.30	110.57
10	bB	810	CLA	C1D-CHD-C4C	-4.22	116.72	122.48
10	cB	810	CLA	C1D-CHD-C4C	-4.21	116.72	122.48
10	bA	837	CLA	C4A-NA-C1A	-4.21	104.81	106.71
10	aB	837	CLA	C3C-C4C-NC	4.21	115.29	110.57
10	aA	821	CLA	C4A-NA-C1A	-4.20	104.82	106.71
10	aB	810	CLA	C1D-CHD-C4C	-4.20	116.74	122.48
10	cB	806	CLA	C3C-C4C-NC	4.20	115.28	110.57
10	cB	827	CLA	C1D-CHD-C4C	-4.19	116.75	122.48
10	aA	854	CLA	C3C-C4C-NC	4.19	115.27	110.57
10	aA	841	CLA	C4A-NA-C1A	-4.18	104.83	106.71
10	cB	811	CLA	C4A-NA-C1A	-4.18	104.83	106.71
10	aA	856	CLA	C4A-NA-C1A	-4.18	104.83	106.71
14	bA	855	LHG	O4-P-O5	4.18	133.18	112.21
14	cA	855	LHG	O4-P-O5	4.18	133.17	112.21
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	bB	827	CLA	C1D-CHD-C4C	-4.18	116.78	122.48
10	bB	808	CLA	C3C-C4C-NC	4.17	115.25	110.57
10	bA	854	CLA	C3C-C4C-NC	4.17	115.25	110.57
10	aB	817	CLA	O2D-CGD-CBD	4.17	118.56	111.25
14	aA	855	LHG	O4-P-O5	4.17	133.12	112.21
10	aB	829	CLA	O2D-CGD-CBD	4.17	118.55	111.25
10	cA	856	CLA	C4A-NA-C1A	-4.17	104.83	106.71
10	aB	838	CLA	C4A-NA-C1A	-4.17	104.83	106.71
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	816	CLA	C3C-C4C-NC	4.16	115.24	110.57
10	bB	817	CLA	O2D-CGD-CBD	4.16	118.54	111.25
10	bB	811	CLA	C1C-C2C-C3C	-4.16	102.54	106.95
10	cB	811	CLA	C1C-C2C-C3C	-4.16	102.54	106.95
10	cB	808	CLA	C3C-C4C-NC	4.16	115.23	110.57
10	cB	817	CLA	O2D-CGD-CBD	4.16	118.53	111.25
10	aB	808	CLA	C3C-C4C-NC	4.15	115.23	110.57
10	aB	827	CLA	C1D-CHD-C4C	-4.15	116.81	122.48
10	aB	811	CLA	C1C-C2C-C3C	-4.15	102.55	106.95
10	bB	829	CLA	O2D-CGD-CBD	4.15	118.51	111.25
10	bA	824	CLA	C3C-C4C-NC	4.15	115.22	110.57
10	cB	829	CLA	O2D-CGD-CBD	4.14	118.50	111.25
10	cB	835	CLA	C4A-NA-C1A	-4.14	104.84	106.71
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	821	CLA	C4A-NA-C1A	-4.13	104.85	106.71
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	cB	835	CLA	O2D-CGD-CBD	4.12	118.47	111.25
14	aA	852	LHG	O4-P-O5	4.12	132.87	112.21
10	cB	810	CLA	C3C-C4C-NC	4.12	115.19	110.57
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
14	cA	852	LHG	O4-P-O5	4.12	132.84	112.21
14	bA	852	LHG	O4-P-O5	4.11	132.83	112.21
10	aA	823	CLA	C1C-C2C-C3C	-4.11	102.59	106.95
10	bA	818	CLA	CAA-C2A-C3A	-4.11	101.52	112.78
10	bB	838	CLA	C4A-NA-C1A	-4.11	104.86	106.71
10	cA	824	CLA	C3C-C4C-NC	4.11	115.18	110.57
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	831	CLA	C3C-C4C-NC	4.10	115.17	110.57
10	aB	835	CLA	O2D-CGD-CBD	4.10	118.43	111.25
10	aB	816	CLA	C3C-C4C-NC	4.10	115.17	110.57
10	bA	831	CLA	C3C-C4C-NC	4.10	115.17	110.57
10	bA	823	CLA	C1C-C2C-C3C	-4.10	102.61	106.95
10	bA	816	CLA	C3C-C4C-NC	4.10	115.17	110.57
10	cB	816	CLA	C3C-C4C-NC	4.10	115.17	110.57
10	cA	817	CLA	C4A-NA-C1A	-4.09	104.87	106.71
10	bB	811	CLA	C4A-NA-C1A	-4.09	104.87	106.71
10	bB	835	CLA	O2D-CGD-CBD	4.09	118.41	111.25
10	aA	825	CLA	C3C-C4C-NC	4.09	115.16	110.57
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	bB	805	CLA	C4C-C3C-C2C	-4.08	100.97	106.89
10	bA	824	CLA	CAC-C3C-C4C	4.08	130.15	124.82
10	bA	836	CLA	C1C-C2C-C3C	-4.08	102.63	106.95
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	816	CLA	C3C-C4C-NC	4.07	115.14	110.57
10	cB	805	CLA	C4C-C3C-C2C	-4.07	100.99	106.89
10	bB	830	CLA	C3B-C4B-NB	4.07	114.48	109.21
10	bA	821	CLA	C3C-C4C-NC	4.07	115.14	110.57
10	aA	829	CLA	C3B-C4B-NB	4.07	114.47	109.21
10	cA	836	CLA	C1C-C2C-C3C	-4.07	102.64	106.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	833	CLA	C1C-C2C-C3C	-4.07	102.64	106.95
10	cA	840	CLA	C3C-C4C-NC	4.07	115.13	110.57
10	cA	829	CLA	C3B-C4B-NB	4.06	114.46	109.21
10	bA	841	CLA	C3C-C4C-NC	4.06	115.12	110.57
10	aB	805	CLA	C4C-C3C-C2C	-4.06	101.01	106.89
10	cA	833	CLA	C1C-C2C-C3C	-4.06	102.65	106.95
10	aB	805	CLA	C2C-C1C-NC	4.06	113.77	109.97
10	cA	824	CLA	CAC-C3C-C4C	4.06	130.12	124.82
10	bA	802	CLA	C3C-C4C-NC	4.06	115.12	110.57
10	aA	839	CLA	O2D-CGD-CBD	4.06	118.35	111.25
10	bA	829	CLA	C4A-NA-C1A	-4.05	104.88	106.71
10	cA	823	CLA	C1C-C2C-C3C	-4.05	102.66	106.95
10	cA	832	CLA	C3C-C4C-NC	4.05	115.11	110.57
10	aA	833	CLA	C1C-C2C-C3C	-4.05	102.66	106.95
10	cA	825	CLA	C3C-C4C-NC	4.05	115.11	110.57
10	bA	829	CLA	C3B-C4B-NB	4.04	114.44	109.21
10	aA	836	CLA	C1C-C2C-C3C	-4.04	102.67	106.95
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	824	CLA	CAC-C3C-C4C	4.04	130.10	124.82
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
10	aA	829	CLA	C4A-NA-C1A	-4.03	104.89	106.71
10	bA	838	CLA	C3C-C4C-NC	4.03	115.09	110.57
10	aA	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	aA	821	CLA	C3C-C4C-NC	4.03	115.09	110.57
10	cA	839	CLA	O2D-CGD-CBD	4.03	118.30	111.25
10	bA	817	CLA	C4A-NA-C1A	-4.03	104.89	106.71
10	aA	840	CLA	C3C-C4C-NC	4.03	115.09	110.57
10	bB	805	CLA	C2C-C1C-NC	4.02	113.74	109.97
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
10	aA	841	CLA	C3C-C4C-NC	4.02	115.08	110.57
10	bA	839	CLA	O2D-CGD-CBD	4.02	118.28	111.25
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	aA	814	CLA	C3C-C4C-NC	4.01	115.07	110.57
10	bA	821	CLA	C1C-C2C-C3C	-4.01	102.70	106.95
10	aA	802	CLA	C3C-C4C-NC	4.01	115.07	110.57
10	bA	836	CLA	C3C-C4C-NC	4.01	115.07	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	819	CLA	C3C-C4C-NC	4.01	115.07	110.57
10	cA	837	CLA	C3C-C4C-NC	4.01	115.07	110.57
10	bA	837	CLA	C3C-C4C-NC	4.00	115.06	110.57
10	cA	814	CLA	C3C-C4C-NC	4.00	115.06	110.57
10	bB	821	CLA	C3C-C4C-NC	4.00	115.06	110.57
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	aB	810	CLA	CAA-C2A-C3A	-3.99	101.84	112.78
10	aB	811	CLA	C4A-NA-C1A	-3.99	104.91	106.71
10	cB	821	CLA	C3C-C4C-NC	3.99	115.05	110.57
10	cB	810	CLA	CAA-C2A-C3A	-3.99	101.86	112.78
10	cA	829	CLA	C4A-NA-C1A	-3.99	104.91	106.71
10	bA	828	CLA	CMB-C2B-C3B	3.98	132.27	124.80
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	cA	834	CLA	C1C-C2C-C3C	-3.98	102.74	106.95
10	cA	828	CLA	CMB-C2B-C3B	3.98	132.25	124.80
10	aA	828	CLA	CMB-C2B-C3B	3.97	132.25	124.80
10	cA	836	CLA	C3C-C4C-NC	3.97	115.03	110.57
10	cA	809	CLA	C3C-C4C-NC	3.97	115.03	110.57
10	bA	819	CLA	C3C-C4C-NC	3.97	115.03	110.57
10	aA	834	CLA	C1C-C2C-C3C	-3.97	102.74	106.95
10	aA	836	CLA	C3C-C4C-NC	3.97	115.02	110.57
10	cA	821	CLA	C1C-C2C-C3C	-3.97	102.75	106.95
10	cA	830	CLA	C3C-C4C-NC	3.97	115.02	110.57
10	aA	809	CLA	C3C-C4C-NC	3.96	115.01	110.57
10	bA	815	CLA	C1C-C2C-C3C	-3.96	102.75	106.95
10	cA	808	CLA	C1D-CHD-C4C	-3.96	117.08	122.48
10	aA	830	CLA	C3C-C4C-NC	3.96	115.01	110.57
10	aB	803	CLA	CMA-C3A-C2A	-3.96	97.83	113.78
10	bA	834	CLA	C1C-C2C-C3C	-3.95	102.76	106.95
10	bA	830	CLA	C3C-C4C-NC	3.95	115.00	110.57
10	aA	821	CLA	C1C-C2C-C3C	-3.95	102.77	106.95
10	cB	803	CLA	CMA-C3A-C2A	-3.95	97.87	113.78
10	bA	805	CLA	C3C-C4C-NC	3.94	114.99	110.57
10	bB	803	CLA	CMA-C3A-C2A	-3.94	97.89	113.78
10	bA	834	CLA	C3C-C4C-NC	3.94	114.99	110.57
10	bA	803	CLA	C3C-C4C-NC	3.94	114.99	110.57
10	bA	828	CLA	O2D-CGD-CBD	3.94	118.14	111.25
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	cA	818	CLA	CMB-C2B-C3B	3.93	132.18	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	834	CLA	C3C-C4C-NC	3.93	114.98	110.57
10	aL	202	CLA	C1C-C2C-C3C	-3.93	102.78	106.95
10	cA	803	CLA	C3C-C4C-NC	3.93	114.98	110.57
10	aA	828	CLA	O2D-CGD-CBD	3.93	118.13	111.25
10	cB	815	CLA	C3C-C4C-NC	3.93	114.97	110.57
10	aA	818	CLA	CMB-C2B-C3B	3.93	132.16	124.80
10	aB	818	CLA	CAA-C2A-C3A	-3.92	102.03	112.78
10	cA	805	CLA	C3C-C4C-NC	3.92	114.97	110.57
10	cA	828	CLA	O2D-CGD-CBD	3.92	118.12	111.25
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	bL	202	CLA	C1C-C2C-C3C	-3.92	102.79	106.95
10	bA	836	CLA	CMB-C2B-C3B	3.92	132.15	124.80
10	aA	843	CLA	C3C-C4C-NC	3.92	114.97	110.57
10	aB	815	CLA	C3C-C4C-NC	3.92	114.97	110.57
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	aA	813	CLA	C3B-C4B-NB	3.92	114.27	109.21
10	bA	808	CLA	C1D-CHD-C4C	-3.91	117.14	122.48
10	cB	818	CLA	CAA-C2A-C3A	-3.91	102.06	112.78
10	bA	818	CLA	CMB-C2B-C3B	3.91	132.14	124.80
10	aA	811	CLA	C3C-C4C-NC	3.91	114.96	110.57
10	cL	202	CLA	C1C-C2C-C3C	-3.91	102.80	106.95
10	aA	815	CLA	C1C-C2C-C3C	-3.91	102.81	106.95
10	aA	808	CLA	C1D-CHD-C4C	-3.91	117.15	122.48
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	cB	824	CLA	C1C-C2C-C3C	-3.90	102.81	106.95
10	aB	817	CLA	C4A-NA-C1A	-3.90	104.95	106.71
10	aB	821	CLA	C1C-C2C-C3C	-3.90	102.82	106.95
10	cB	836	CLA	C1C-C2C-C3C	-3.90	102.82	106.95
10	aA	820	CLA	C4A-NA-C1A	-3.89	104.95	106.71
10	bA	822	CLA	C4-C3-C5	3.89	120.50	115.99
10	aA	818	CLA	O2A-CGA-CBA	3.89	124.42	111.93
10	cA	815	CLA	C1C-C2C-C3C	-3.89	102.83	106.95
10	cA	818	CLA	O2A-CGA-CBA	3.89	124.42	111.93
10	aA	836	CLA	CMB-C2B-C3B	3.89	132.10	124.80
10	cB	821	CLA	C1C-C2C-C3C	-3.89	102.83	106.95
10	aB	836	CLA	C1C-C2C-C3C	-3.89	102.83	106.95
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	818	CLA	O2A-CGA-CBA	3.89	124.42	111.93
10	bA	836	CLA	C3B-C4B-NB	3.89	114.24	109.21
10	aA	818	CLA	C1C-C2C-C3C	-3.89	102.83	106.95
10	cA	815	CLA	C4A-NA-C1A	-3.89	104.96	106.71
10	bA	833	CLA	C4A-NA-C1A	-3.88	104.96	106.71
10	bB	832	CLA	C3C-C4C-NC	3.88	114.92	110.57
10	cB	801	CLA	C1C-C2C-C3C	-3.88	102.84	106.95
10	cA	836	CLA	CMB-C2B-C3B	3.88	132.08	124.80
10	bA	818	CLA	C1C-C2C-C3C	-3.88	102.84	106.95
10	aB	801	CLA	C1C-C2C-C3C	-3.88	102.84	106.95
10	cA	832	CLA	C1C-C2C-C3C	-3.88	102.84	106.95
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	cA	843	CLA	C3C-C4C-NC	3.87	114.91	110.57
10	cA	831	CLA	C1C-C2C-C3C	-3.87	102.85	106.95
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	C1C-C2C-C3C	-3.87	102.85	106.95
10	bB	824	CLA	C1C-C2C-C3C	-3.87	102.85	106.95
10	cA	818	CLA	C1C-C2C-C3C	-3.87	102.85	106.95
10	bA	843	CLA	C3C-C4C-NC	3.86	114.91	110.57
9	cA	801	CL0	C3B-C4B-NB	3.86	114.20	109.21
10	aA	834	CLA	C3C-C4C-NC	3.86	114.90	110.57
10	cA	807	CLA	C1C-C2C-C3C	-3.86	102.86	106.95
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	bB	836	CLA	C1C-C2C-C3C	-3.86	102.86	106.95
10	bB	807	CLA	C3C-C4C-NC	3.85	114.89	110.57
10	bA	832	CLA	C1C-C2C-C3C	-3.85	102.87	106.95
10	aA	822	CLA	C4-C3-C5	3.85	120.46	115.99
10	aA	831	CLA	C1C-C2C-C3C	-3.85	102.87	106.95
10	aB	824	CLA	C1C-C2C-C3C	-3.85	102.87	106.95
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	bA	807	CLA	C1C-C2C-C3C	-3.85	102.88	106.95
10	cA	822	CLA	C4-C3-C5	3.84	120.45	115.99
10	bL	205	CLA	C3C-C4C-NC	3.84	114.88	110.57
10	bB	823	CLA	C1C-C2C-C3C	-3.84	102.88	106.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	805	CLA	C3C-C4C-NC	3.84	114.87	110.57
10	aL	204	CLA	C3C-C4C-NC	3.84	114.87	110.57
10	aA	839	CLA	C1C-C2C-C3C	-3.83	102.89	106.95
10	aA	832	CLA	C1C-C2C-C3C	-3.83	102.89	106.95
10	cA	809	CLA	C1D-CHD-C4C	-3.83	117.24	122.48
10	aB	807	CLA	C3C-C4C-NC	3.83	114.87	110.57
10	cB	814	CLA	C3C-C4C-NC	3.83	114.86	110.57
10	bB	801	CLA	C1C-C2C-C3C	-3.83	102.89	106.95
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	cL	205	CLA	C3C-C4C-NC	3.83	114.86	110.57
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	bA	831	CLA	C1C-C2C-C3C	-3.82	102.90	106.95
10	aB	805	CLA	C3C-C4C-NC	3.82	114.86	110.57
10	cA	839	CLA	C1C-C2C-C3C	-3.82	102.90	106.95
10	bB	841	CLA	C3B-C4B-NB	3.82	114.15	109.21
10	aA	843	CLA	C1C-C2C-C3C	-3.82	102.90	106.95
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	856	CLA	C3C-C4C-NC	3.81	114.84	110.57
10	bA	820	CLA	C4A-NA-C1A	-3.81	104.99	106.71
10	cB	823	CLA	C1C-C2C-C3C	-3.81	102.92	106.95
10	cA	856	CLA	C3C-C4C-NC	3.81	114.84	110.57
10	bL	204	CLA	C3C-C4C-NC	3.81	114.84	110.57
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	aA	829	CLA	CMB-C2B-C3B	3.80	131.93	124.80
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	aA	807	CLA	C1C-C2C-C3C	-3.80	102.92	106.95
10	bB	805	CLA	C3C-C4C-NC	3.80	114.83	110.57
10	aA	838	CLA	CAA-CBA-CGA	-3.80	102.07	113.26
10	cB	817	CLA	C4A-NA-C1A	-3.80	105.00	106.71
10	bA	815	CLA	C4A-NA-C1A	-3.80	105.00	106.71
10	bA	839	CLA	C1C-C2C-C3C	-3.80	102.93	106.95
10	cA	843	CLA	C1C-C2C-C3C	-3.80	102.93	106.95
10	aB	823	CLA	C1C-C2C-C3C	-3.79	102.93	106.95
10	bA	830	CLA	C1C-C2C-C3C	-3.79	102.93	106.95
10	bB	822	CLA	C3C-C4C-NC	3.79	114.83	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	838	CLA	CAA-CBA-CGA	-3.79	102.08	113.26
10	aB	803	CLA	C1D-CHD-C4C	-3.79	117.30	122.48
10	bB	803	CLA	C1D-CHD-C4C	-3.79	117.30	122.48
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	bA	856	CLA	C3C-C4C-NC	3.79	114.82	110.57
10	bA	809	CLA	C1D-CHD-C4C	-3.79	117.30	122.48
10	aA	815	CLA	C4A-NA-C1A	-3.79	105.00	106.71
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	aA	813	CLA	C3C-C4C-NC	3.79	114.82	110.57
10	bA	843	CLA	C1C-C2C-C3C	-3.79	102.94	106.95
10	aB	839	CLA	C1C-C2C-C3C	-3.79	102.94	106.95
10	bA	829	CLA	CMB-C2B-C3B	3.79	131.90	124.80
10	bA	838	CLA	CAA-CBA-CGA	-3.79	102.10	113.26
10	cB	803	CLA	C1D-CHD-C4C	-3.79	117.31	122.48
10	cA	830	CLA	C1C-C2C-C3C	-3.78	102.94	106.95
10	bB	817	CLA	C4A-NA-C1A	-3.78	105.00	106.71
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	cA	835	CLA	C1C-C2C-C3C	-3.78	102.94	106.95
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	cB	839	CLA	C1C-C2C-C3C	-3.78	102.95	106.95
10	cA	833	CLA	C4A-NA-C1A	-3.78	105.01	106.71
10	cA	805	CLA	C1C-C2C-C3C	-3.78	102.95	106.95
10	aB	802	CLA	C3C-C4C-NC	3.78	114.81	110.57
10	bA	820	CLA	C3C-C4C-NC	3.77	114.80	110.57
10	aB	822	CLA	C3C-C4C-NC	3.77	114.80	110.57
10	aA	830	CLA	C1C-C2C-C3C	-3.77	102.95	106.95
10	cA	829	CLA	CMB-C2B-C3B	3.77	131.87	124.80
10	aB	829	CLA	C3B-C4B-NB	3.77	114.08	109.21
10	aA	835	CLA	C1C-C2C-C3C	-3.77	102.95	106.95
10	aA	809	CLA	C1D-CHD-C4C	-3.77	117.33	122.48
10	bA	818	CLA	C3B-C4B-NB	3.77	114.08	109.21
10	aB	839	CLA	C3C-C4C-NC	3.77	114.80	110.57
10	bB	839	CLA	C1C-C2C-C3C	-3.76	102.96	106.95
10	aA	818	CLA	C3B-C4B-NB	3.76	114.08	109.21
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	802	CLA	C4A-NA-C1A	-3.76	105.01	106.71
10	bB	830	CLA	C1C-C2C-C3C	-3.76	102.97	106.95
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	bA	856	CLA	O2D-CGD-CBD	3.76	117.83	111.25
10	bA	835	CLA	C1C-C2C-C3C	-3.76	102.97	106.95
10	aB	806	CLA	CMC-C2C-C1C	3.75	130.74	125.03
10	cA	814	CLA	C4A-NA-C1A	-3.75	105.02	106.71
10	aA	856	CLA	O2D-CGD-CBD	3.75	117.82	111.25
10	aB	801	CLA	C3B-C4B-NB	3.75	114.06	109.21
10	bA	805	CLA	C1C-C2C-C3C	-3.75	102.97	106.95
10	bA	832	CLA	C4A-NA-C1A	-3.75	105.02	106.71
10	bA	808	CLA	C1C-C2C-C3C	-3.75	102.97	106.95
10	cB	830	CLA	C1C-C2C-C3C	-3.75	102.97	106.95
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	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	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	cA	812	CLA	C3C-C4C-NC	3.74	114.77	110.57
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	aB	835	CLA	C1C-C2C-C3C	-3.74	102.99	106.95
10	bB	807	CLA	C3B-C4B-NB	3.73	114.04	109.21
10	aA	842	CLA	C3C-C4C-NC	3.73	114.75	110.57
10	aA	805	CLA	C1C-C2C-C3C	-3.73	103.00	106.95
10	cA	856	CLA	O2D-CGD-CBD	3.73	117.78	111.25
10	cA	835	CLA	C3C-C4C-NC	3.73	114.75	110.57
10	cA	832	CLA	C4A-NA-C1A	-3.73	105.03	106.71
10	cA	808	CLA	C1C-C2C-C3C	-3.73	103.00	106.95
10	aB	830	CLA	C1C-C2C-C3C	-3.73	103.00	106.95
10	aB	807	CLA	C3B-C4B-NB	3.73	114.03	109.21
10	bB	801	CLA	C3B-C4B-NB	3.73	114.03	109.21
10	bA	812	CLA	C3C-C4C-NC	3.72	114.75	110.57
10	bB	839	CLA	C3C-C4C-NC	3.72	114.75	110.57
10	bL	204	CLA	C1C-C2C-C3C	-3.72	103.01	106.95
10	aA	843	CLA	C4A-NA-C1A	-3.72	105.03	106.71
10	bB	806	CLA	CMC-C2C-C1C	3.72	130.68	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	808	CLA	C1C-C2C-C3C	-3.72	103.01	106.95
10	bA	835	CLA	C3C-C4C-NC	3.72	114.74	110.57
10	bA	809	CLA	CAA-C2A-C3A	-3.71	102.61	112.78
10	cB	807	CLA	C3B-C4B-NB	3.71	114.01	109.21
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	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	cA	813	CLA	C1C-C2C-C3C	-3.70	103.02	106.95
10	bA	827	CLA	C3B-C4B-NB	3.70	114.00	109.21
10	cB	802	CLA	C4A-NA-C1A	-3.70	105.04	106.71
10	aA	817	CLA	C3C-C4C-NC	3.70	114.72	110.57
10	aA	829	CLA	C1C-C2C-C3C	-3.70	103.03	106.95
10	aA	827	CLA	C3B-C4B-NB	3.70	113.99	109.21
10	bB	823	CLA	C3C-C4C-NC	3.70	114.72	110.57
10	bA	819	CLA	C4A-NA-C1A	-3.69	105.05	106.71
10	cB	832	CLA	C1C-C2C-C3C	-3.69	103.03	106.95
10	aA	807	CLA	C3C-C4C-NC	3.69	114.71	110.57
10	bA	806	CLA	C1C-C2C-C3C	-3.69	103.04	106.95
10	aB	815	CLA	C1C-C2C-C3C	-3.69	103.04	106.95
10	cB	806	CLA	CMC-C2C-C1C	3.69	130.65	125.03
10	aA	818	CLA	C3C-C4C-NC	3.69	114.71	110.57
10	aA	835	CLA	C3C-C4C-NC	3.69	114.71	110.57
10	bB	835	CLA	C1C-C2C-C3C	-3.69	103.04	106.95
10	cB	825	CLA	CAC-C3C-C4C	3.69	129.64	124.82
10	aA	809	CLA	CAA-C2A-C3A	-3.69	102.67	112.78
10	cB	823	CLA	C3C-C4C-NC	3.69	114.71	110.57
10	cA	842	CLA	C3C-C4C-NC	3.69	114.71	110.57
10	aB	832	CLA	C1C-C2C-C3C	-3.69	103.04	106.95
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	bL	203	CLA	C1C-C2C-C3C	-3.69	103.04	106.95
10	aB	836	CLA	C3C-C4C-NC	3.68	114.70	110.57
10	aB	834	CLA	C1C-C2C-C3C	-3.68	103.05	106.95
10	bA	833	CLA	O2D-CGD-O1D	-3.68	116.56	123.83
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	bB	834	CLA	C1C-C2C-C3C	-3.68	103.05	106.95
10	bB	803	CLA	C1C-C2C-C3C	-3.68	103.05	106.95
10	cB	838	CLA	C3C-C4C-NC	3.68	114.70	110.57
10	cB	835	CLA	C1C-C2C-C3C	-3.68	103.05	106.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	834	CLA	C1C-C2C-C3C	-3.68	103.05	106.95
10	bB	802	CLA	C4A-NA-C1A	-3.68	105.05	106.71
10	cL	203	CLA	C1C-C2C-C3C	-3.68	103.05	106.95
10	cA	833	CLA	O2D-CGD-O1D	-3.68	116.57	123.83
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	aA	813	CLA	C1C-C2C-C3C	-3.68	103.06	106.95
10	bB	815	CLA	C1C-C2C-C3C	-3.68	103.06	106.95
10	cB	815	CLA	C1D-CHD-C4C	-3.67	117.46	122.48
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	cB	803	CLA	C1C-C2C-C3C	-3.67	103.06	106.95
10	aB	817	CLA	C1C-C2C-C3C	-3.67	103.06	106.95
10	cB	801	CLA	CMB-C2B-C3B	3.67	131.69	124.80
10	bA	817	CLA	C3C-C4C-NC	3.67	114.69	110.57
10	aB	818	CLA	C3C-C4C-NC	3.67	114.69	110.57
10	aB	803	CLA	C1C-C2C-C3C	-3.67	103.06	106.95
10	bB	825	CLA	CAC-C3C-C4C	3.67	129.61	124.82
10	bB	801	CLA	CMB-C2B-C3B	3.67	131.68	124.80
10	cL	204	CLA	C1C-C2C-C3C	-3.67	103.06	106.95
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	cB	817	CLA	C1C-C2C-C3C	-3.66	103.07	106.95
10	bB	832	CLA	C1C-C2C-C3C	-3.66	103.07	106.95
10	bB	828	CLA	C1C-C2C-C3C	-3.66	103.07	106.95
10	aB	825	CLA	CAC-C3C-C4C	3.66	129.60	124.82
10	cA	840	CLA	C1C-C2C-C3C	-3.66	103.07	106.95
10	cB	815	CLA	C1C-C2C-C3C	-3.66	103.07	106.95
10	bB	819	CLA	C1-C2-C3	-3.66	119.72	126.04
10	cA	829	CLA	C1C-C2C-C3C	-3.66	103.07	106.95
10	bA	829	CLA	C1C-C2C-C3C	-3.66	103.07	106.95
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	bA	813	CLA	C1C-C2C-C3C	-3.66	103.07	106.95
10	cA	828	CLA	C1D-CHD-C4C	-3.66	117.49	122.48
10	aB	801	CLA	CMB-C2B-C3B	3.66	131.66	124.80
10	aB	828	CLA	C1C-C2C-C3C	-3.65	103.08	106.95
10	aL	204	CLA	C1C-C2C-C3C	-3.65	103.08	106.95
10	bB	817	CLA	C1C-C2C-C3C	-3.65	103.08	106.95
10	bA	802	CLA	C1C-C2C-C3C	-3.65	103.08	106.95
10	bB	833	CLA	C3C-C4C-NC	3.65	114.66	110.57
10	cA	805	CLA	C3B-C4B-NB	3.65	113.93	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	827	CLA	C4A-NA-C1A	-3.65	105.07	106.71
10	cA	827	CLA	C1D-CHD-C4C	-3.65	117.50	122.48
10	cB	835	CLA	C3C-C4C-NC	3.65	114.66	110.57
10	bA	828	CLA	C1D-CHD-C4C	-3.65	117.50	122.48
10	aL	203	CLA	C1C-C2C-C3C	-3.65	103.09	106.95
9	aA	801	CL0	CMA-C3A-C2A	-3.65	99.09	113.78
9	cA	801	CL0	CMA-C3A-C2A	-3.64	99.09	113.78
10	cB	818	CLA	C3C-C4C-NC	3.64	114.66	110.57
10	bA	840	CLA	C1C-C2C-C3C	-3.64	103.09	106.95
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	cA	817	CLA	C3C-C4C-NC	3.64	114.66	110.57
10	aB	829	CLA	C1C-C2C-C3C	-3.64	103.09	106.95
10	cA	806	CLA	C1C-C2C-C3C	-3.64	103.09	106.95
10	cB	831	CLA	C1C-C2C-C3C	-3.64	103.09	106.95
10	bA	827	CLA	C4A-NA-C1A	-3.64	105.07	106.71
10	aA	806	CLA	C1C-C2C-C3C	-3.64	103.09	106.95
10	aB	831	CLA	C3C-C4C-NC	3.64	114.65	110.57
10	bA	827	CLA	C1D-CHD-C4C	-3.64	117.51	122.48
10	aA	833	CLA	O2D-CGD-O1D	-3.64	116.65	123.83
10	bB	815	CLA	C1D-CHD-C4C	-3.64	117.52	122.48
10	aA	834	CLA	C1D-CHD-C4C	-3.63	117.52	122.48
10	bB	824	CLA	C3C-C4C-NC	3.63	114.64	110.57
10	cA	834	CLA	C1D-CHD-C4C	-3.63	117.52	122.48
9	bA	801	CL0	CMA-C3A-C2A	-3.63	99.14	113.78
10	cB	836	CLA	C3C-C4C-NC	3.63	114.64	110.57
10	aB	833	CLA	C3C-C4C-NC	3.63	114.64	110.57
10	aA	827	CLA	C1D-CHD-C4C	-3.63	117.52	122.48
10	aA	840	CLA	C1C-C2C-C3C	-3.63	103.10	106.95
13	cB	844	BCR	C3-C4-C5	-3.63	107.68	113.99
10	aA	802	CLA	C1C-C2C-C3C	-3.63	103.10	106.95
10	aA	804	CLA	CAA-C2A-C3A	-3.63	102.84	112.78
10	cB	826	CLA	CMB-C2B-C3B	3.63	131.60	124.80
10	aA	836	CLA	C1D-CHD-C4C	-3.63	117.53	122.48
10	bB	829	CLA	C1C-C2C-C3C	-3.63	103.11	106.95
10	bA	806	CLA	C3C-C4C-NC	3.62	114.64	110.57
10	cA	811	CLA	C1C-C2C-C3C	-3.62	103.11	106.95
13	bB	844	BCR	C3-C4-C5	-3.62	107.69	113.99
10	cB	833	CLA	C3C-C4C-NC	3.62	114.63	110.57
10	bA	819	CLA	C1C-C2C-C3C	-3.62	103.11	106.95
10	cB	829	CLA	C1C-C2C-C3C	-3.62	103.11	106.95
10	bA	804	CLA	CAA-C2A-C3A	-3.62	102.86	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	828	CLA	C1D-CHD-C4C	-3.62	117.54	122.48
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	aB	826	CLA	CMB-C2B-C3B	3.62	131.59	124.80
10	aA	816	CLA	C1D-CHD-C4C	-3.62	117.54	122.48
10	bA	834	CLA	C1D-CHD-C4C	-3.62	117.54	122.48
10	cB	820	CLA	C1C-C2C-C3C	-3.62	103.12	106.95
10	cB	825	CLA	C1D-CHD-C4C	-3.62	117.54	122.48
10	bA	810	CLA	C1C-C2C-C3C	-3.61	103.12	106.95
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	bB	825	CLA	C1D-CHD-C4C	-3.61	117.55	122.48
10	bB	837	CLA	C1D-CHD-C4C	-3.61	117.55	122.48
10	bA	810	CLA	C3B-C4B-NB	3.61	113.88	109.21
10	aB	809	CLA	CAC-C3C-C4C	3.61	129.54	124.82
10	bA	856	CLA	C1C-C2C-C3C	-3.61	103.12	106.95
10	aB	831	CLA	C1C-C2C-C3C	-3.61	103.12	106.95
10	aB	815	CLA	C1D-CHD-C4C	-3.61	117.55	122.48
10	cA	804	CLA	CAA-C2A-C3A	-3.61	102.90	112.78
10	cA	836	CLA	C1D-CHD-C4C	-3.61	117.55	122.48
10	bB	826	CLA	CMB-C2B-C3B	3.61	131.56	124.80
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	837	CLA	C1D-CHD-C4C	-3.61	117.56	122.48
10	cB	831	CLA	C3C-C4C-NC	3.61	114.61	110.57
10	aA	819	CLA	C1C-C2C-C3C	-3.60	103.13	106.95
10	aA	813	CLA	C1D-CHD-C4C	-3.60	117.56	122.48
10	bB	809	CLA	CAC-C3C-C4C	3.60	129.53	124.82
10	bB	806	CLA	C1D-CHD-C4C	-3.60	117.56	122.48
10	cA	813	CLA	C1D-CHD-C4C	-3.60	117.56	122.48
10	cB	824	CLA	C3C-C4C-NC	3.60	114.61	110.57
10	cB	808	CLA	C1D-CHD-C4C	-3.60	117.56	122.48
10	cB	828	CLA	C1C-C2C-C3C	-3.60	103.13	106.95
10	cA	816	CLA	C1D-CHD-C4C	-3.60	117.56	122.48
10	cB	811	CLA	C3B-C4B-NB	3.60	113.86	109.21
10	aB	804	CLA	CMB-C2B-C3B	3.60	131.55	124.80
10	bB	804	CLA	CMB-C2B-C3B	3.60	131.55	124.80
10	cB	808	CLA	O2D-CGD-CBD	3.60	117.55	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	808	CLA	C1D-CHD-C4C	-3.60	117.56	122.48
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	bA	827	CLA	C4-C3-C5	3.60	121.48	115.29
13	aB	844	BCR	C3-C4-C5	-3.60	107.73	113.99
10	bA	811	CLA	C1C-C2C-C3C	-3.60	103.14	106.95
10	bA	804	CLA	C1C-C2C-C3C	-3.60	103.14	106.95
10	bA	813	CLA	C1D-CHD-C4C	-3.59	117.57	122.48
10	aA	814	CLA	C4A-NA-C1A	-3.59	105.09	106.71
10	cA	856	CLA	C1C-C2C-C3C	-3.59	103.14	106.95
10	aA	837	CLA	C1C-C2C-C3C	-3.59	103.14	106.95
10	cA	810	CLA	C1C-C2C-C3C	-3.59	103.14	106.95
10	cB	827	CLA	C3B-C4B-NB	3.59	113.85	109.21
10	aB	825	CLA	C1D-CHD-C4C	-3.59	117.58	122.48
10	aA	810	CLA	C1C-C2C-C3C	-3.59	103.14	106.95
10	aA	827	CLA	C4-C3-C5	3.59	121.47	115.29
10	bB	832	CLA	C1D-CHD-C4C	-3.59	117.58	122.48
10	aB	820	CLA	C1C-C2C-C3C	-3.59	103.15	106.95
10	bB	827	CLA	C3B-C4B-NB	3.59	113.85	109.21
10	aB	837	CLA	C1D-CHD-C4C	-3.59	117.58	122.48
10	cA	810	CLA	C3B-C4B-NB	3.59	113.85	109.21
10	bA	816	CLA	C1D-CHD-C4C	-3.59	117.58	122.48
10	aB	808	CLA	O2D-CGD-CBD	3.59	117.53	111.25
10	cB	806	CLA	C1D-CHD-C4C	-3.58	117.58	122.48
10	aB	836	CLA	C3B-C4B-NB	3.58	113.84	109.21
10	bB	831	CLA	C1C-C2C-C3C	-3.58	103.15	106.95
10	aB	806	CLA	C1D-CHD-C4C	-3.58	117.59	122.48
10	cA	804	CLA	C1C-C2C-C3C	-3.58	103.15	106.95
10	cB	804	CLA	CMB-C2B-C3B	3.58	131.52	124.80
10	bA	836	CLA	C1D-CHD-C4C	-3.58	117.59	122.48
10	bB	820	CLA	C1C-C2C-C3C	-3.58	103.16	106.95
10	cA	827	CLA	C4-C3-C5	3.58	121.45	115.29
10	bB	830	CLA	C3C-C4C-NC	3.58	114.58	110.57
10	aB	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	bA	822	CLA	C1C-C2C-C3C	-3.57	103.16	106.95
10	aB	827	CLA	C3B-C4B-NB	3.57	113.83	109.21
10	cB	827	CLA	C4A-NA-C1A	-3.57	105.10	106.71
10	cB	817	CLA	C1D-CHD-C4C	-3.57	117.60	122.48
10	bB	808	CLA	O2D-CGD-CBD	3.57	117.50	111.25
10	cA	823	CLA	C3C-C4C-NC	3.57	114.58	110.57
10	cB	836	CLA	C3B-C4B-NB	3.57	113.82	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	809	CLA	C1C-C2C-C3C	-3.57	103.17	106.95
10	aA	811	CLA	C1C-C2C-C3C	-3.57	103.17	106.95
10	cA	802	CLA	C1C-C2C-C3C	-3.57	103.17	106.95
10	cB	830	CLA	C3C-C4C-NC	3.57	114.57	110.57
9	bA	801	CL0	CMA-C3A-C4A	-3.57	102.19	111.77
10	cB	809	CLA	CAC-C3C-C4C	3.57	129.48	124.82
10	cA	819	CLA	C1C-C2C-C3C	-3.57	103.17	106.95
10	bB	817	CLA	C1D-CHD-C4C	-3.57	117.61	122.48
10	aL	205	CLA	C1C-C2C-C3C	-3.56	103.17	106.95
10	bA	821	CLA	C1D-CHD-C4C	-3.56	117.61	122.48
10	bB	808	CLA	C1D-CHD-C4C	-3.56	117.62	122.48
10	bA	814	CLA	C1D-CHD-C4C	-3.56	117.62	122.48
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	856	CLA	C1C-C2C-C3C	-3.56	103.18	106.95
10	cA	822	CLA	C1C-C2C-C3C	-3.55	103.18	106.95
13	cA	847	BCR	C2-C1-C6	3.55	115.98	110.48
10	cA	831	CLA	C3B-C4B-NB	3.55	113.81	109.21
10	cA	842	CLA	C3B-C4B-NB	3.55	113.80	109.21
10	cB	832	CLA	C1D-CHD-C4C	-3.55	117.63	122.48
10	bB	808	CLA	C1C-C2C-C3C	-3.55	103.19	106.95
9	aA	801	CL0	CMA-C3A-C4A	-3.55	102.23	111.77
10	bA	837	CLA	C1C-C2C-C3C	-3.55	103.19	106.95
10	bB	809	CLA	C1C-C2C-C3C	-3.55	103.19	106.95
10	cL	205	CLA	C1C-C2C-C3C	-3.55	103.19	106.95
10	aA	821	CLA	C1D-CHD-C4C	-3.55	117.64	122.48
10	aB	809	CLA	C1C-C2C-C3C	-3.55	103.19	106.95
10	aA	802	CLA	C1D-CHD-C4C	-3.55	117.64	122.48
10	aA	854	CLA	C1D-CHD-C4C	-3.55	117.64	122.48
10	aA	822	CLA	C1C-C2C-C3C	-3.55	103.19	106.95
10	aA	810	CLA	C3B-C4B-NB	3.54	113.79	109.21
10	aB	815	CLA	C3B-C4B-NB	3.54	113.79	109.21
10	cA	823	CLA	C4A-NA-C1A	-3.54	105.11	106.71
10	aB	827	CLA	C4A-NA-C1A	-3.54	105.11	106.71
13	bA	847	BCR	C2-C1-C6	3.54	115.96	110.48
10	aB	829	CLA	C1D-CHD-C4C	-3.54	117.65	122.48
10	cA	821	CLA	C1D-CHD-C4C	-3.54	117.65	122.48
10	cA	823	CLA	C3B-C4B-NB	3.54	113.79	109.21
10	bA	823	CLA	C3B-C4B-NB	3.54	113.79	109.21
10	aA	831	CLA	C3B-C4B-NB	3.54	113.79	109.21
10	cA	837	CLA	C1C-C2C-C3C	-3.54	103.20	106.95
10	aB	832	CLA	C1D-CHD-C4C	-3.54	117.65	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	813	CLA	C1D-CHD-C4C	-3.54	117.65	122.48
10	bA	807	CLA	C4A-NA-C1A	-3.54	105.12	106.71
10	bA	812	CLA	C1C-C2C-C3C	-3.54	103.20	106.95
10	aA	814	CLA	C1D-CHD-C4C	-3.54	117.65	122.48
10	bB	834	CLA	CAC-C3C-C4C	3.54	129.44	124.82
10	bA	833	CLA	C3C-C4C-NC	3.54	114.54	110.57
10	bL	205	CLA	C1C-C2C-C3C	-3.54	103.20	106.95
10	aA	834	CLA	C4A-NA-C1A	-3.53	105.12	106.71
10	cA	831	CLA	CMB-C2B-C3B	3.53	131.43	124.80
10	cB	840	CLA	C1D-CHD-C4C	-3.53	117.65	122.48
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	bB	840	CLA	C1D-CHD-C4C	-3.53	117.66	122.48
13	aA	847	BCR	C2-C1-C6	3.53	115.95	110.48
10	aB	808	CLA	C1C-C2C-C3C	-3.53	103.21	106.95
10	cB	807	CLA	C1C-C2C-C3C	-3.53	103.21	106.95
10	aB	807	CLA	C1C-C2C-C3C	-3.53	103.21	106.95
10	aA	833	CLA	C3C-C4C-NC	3.53	114.53	110.57
10	aB	817	CLA	C1D-CHD-C4C	-3.53	117.66	122.48
10	cB	813	CLA	C1C-C2C-C3C	-3.53	103.21	106.95
10	cB	808	CLA	C1C-C2C-C3C	-3.53	103.21	106.95
10	aB	807	CLA	CAC-C3C-C4C	3.53	129.43	124.82
10	cA	802	CLA	C1D-CHD-C4C	-3.53	117.66	122.48
10	bA	823	CLA	C3C-C4C-NC	3.53	114.53	110.57
10	bA	815	CLA	C3C-C4C-NC	3.53	114.53	110.57
10	aA	827	CLA	C1C-C2C-C3C	-3.53	103.21	106.95
10	bB	811	CLA	CHC-C1C-C2C	-3.52	116.99	126.71
10	aA	804	CLA	C1C-C2C-C3C	-3.52	103.22	106.95
10	bB	815	CLA	C3B-C4B-NB	3.52	113.76	109.21
10	bB	807	CLA	CAC-C3C-C4C	3.52	129.42	124.82
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	cA	854	CLA	C1D-CHD-C4C	-3.52	117.68	122.48
10	bA	854	CLA	C1D-CHD-C4C	-3.52	117.68	122.48
10	cB	826	CLA	C1C-C2C-C3C	-3.52	103.22	106.95
10	cA	807	CLA	C4A-NA-C1A	-3.52	105.12	106.71
10	aA	817	CLA	C1C-C2C-C3C	-3.52	103.22	106.95
10	bA	831	CLA	CMB-C2B-C3B	3.52	131.39	124.80
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	bB	813	CLA	C1C-C2C-C3C	-3.51	103.23	106.95
10	aB	813	CLA	C1D-CHD-C4C	-3.51	117.68	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	811	CLA	CHC-C1C-C2C	-3.51	117.03	126.71
10	cA	815	CLA	C3C-C4C-NC	3.51	114.51	110.57
10	bA	827	CLA	C1C-C2C-C3C	-3.51	103.23	106.95
10	cB	810	CLA	C1C-C2C-C3C	-3.51	103.23	106.95
10	cA	804	CLA	C3C-C4C-NC	3.51	114.51	110.57
10	bB	807	CLA	C1C-C2C-C3C	-3.51	103.23	106.95
10	bB	813	CLA	C1D-CHD-C4C	-3.51	117.69	122.48
10	aB	811	CLA	CHC-C1C-C2C	-3.51	117.03	126.71
10	cB	812	CLA	C1C-C2C-C3C	-3.51	103.23	106.95
10	aB	828	CLA	C4A-NA-C1A	-3.51	105.13	106.71
10	aA	812	CLA	C1C-C2C-C3C	-3.51	103.23	106.95
10	bB	810	CLA	C1C-C2C-C3C	-3.51	103.23	106.95
10	cA	814	CLA	C1D-CHD-C4C	-3.51	117.69	122.48
10	bA	831	CLA	C3B-C4B-NB	3.51	113.74	109.21
10	bA	838	CLA	C1C-C2C-C3C	-3.51	103.23	106.95
10	cB	816	CLA	C1D-CHD-C4C	-3.51	117.69	122.48
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	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	bA	826	CLA	C1D-CHD-C4C	-3.50	117.69	122.48
10	bB	825	CLA	C3B-C4B-NB	3.50	113.74	109.21
10	aB	810	CLA	C1C-C2C-C3C	-3.50	103.24	106.95
10	cA	812	CLA	C1C-C2C-C3C	-3.50	103.24	106.95
10	aA	807	CLA	C4A-NA-C1A	-3.50	105.13	106.71
10	bA	802	CLA	C1D-CHD-C4C	-3.50	117.70	122.48
10	aB	840	CLA	C1D-CHD-C4C	-3.50	117.70	122.48
10	aB	820	CLA	C3C-C4C-NC	3.50	114.50	110.57
10	aA	840	CLA	C1D-CHD-C4C	-3.50	117.70	122.48
10	bB	840	CLA	C1C-C2C-C3C	-3.50	103.24	106.95
10	aA	842	CLA	C3B-C4B-NB	3.50	113.73	109.21
10	aB	834	CLA	CAC-C3C-C4C	3.50	129.39	124.82
10	cL	204	CLA	CBC-CAC-C3C	-3.50	102.72	112.43
10	bB	827	CLA	C4C-C3C-C2C	-3.50	101.83	106.89
10	aL	203	CLA	C3C-C4C-NC	3.50	114.49	110.57
10	aB	821	CLA	C1D-CHD-C4C	-3.49	117.71	122.48
10	aL	204	CLA	CBC-CAC-C3C	-3.49	102.73	112.43
10	cA	817	CLA	C1C-C2C-C3C	-3.49	103.25	106.95
10	bB	812	CLA	C1C-C2C-C3C	-3.49	103.25	106.95
10	aA	831	CLA	CMB-C2B-C3B	3.49	131.35	124.80
10	bB	821	CLA	C1D-CHD-C4C	-3.49	117.71	122.48
10	cB	802	CLA	C1C-C2C-C3C	-3.49	103.25	106.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	834	CLA	CAC-C3C-C4C	3.49	129.38	124.82
10	cA	856	CLA	C1D-CHD-C4C	-3.49	117.72	122.48
10	bB	826	CLA	C1C-C2C-C3C	-3.49	103.25	106.95
10	cB	807	CLA	CAC-C3C-C4C	3.49	129.38	124.82
10	aB	812	CLA	C1C-C2C-C3C	-3.49	103.25	106.95
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	bL	204	CLA	CBC-CAC-C3C	-3.48	102.76	112.43
10	cA	818	CLA	C1D-CHD-C4C	-3.48	117.72	122.48
10	aB	813	CLA	C1C-C2C-C3C	-3.48	103.26	106.95
10	aA	823	CLA	C1D-CHD-C4C	-3.48	117.72	122.48
10	aA	838	CLA	C1C-C2C-C3C	-3.48	103.26	106.95
10	cB	827	CLA	C4C-C3C-C2C	-3.48	101.85	106.89
13	bI	101	BCR	C2-C1-C6	3.48	115.87	110.48
10	bA	841	CLA	C1D-CHD-C4C	-3.48	117.73	122.48
10	cA	826	CLA	C1D-CHD-C4C	-3.48	117.73	122.48
10	bA	856	CLA	C1D-CHD-C4C	-3.48	117.73	122.48
10	aB	826	CLA	C1C-C2C-C3C	-3.48	103.27	106.95
13	aI	101	BCR	C2-C1-C6	3.47	115.86	110.48
10	bB	829	CLA	C1D-CHD-C4C	-3.47	117.74	122.48
10	cB	829	CLA	C1D-CHD-C4C	-3.47	117.74	122.48
10	bA	840	CLA	C1D-CHD-C4C	-3.47	117.74	122.48
10	aA	826	CLA	C1D-CHD-C4C	-3.47	117.74	122.48
10	bB	802	CLA	C1C-C2C-C3C	-3.47	103.27	106.95
10	aB	837	CLA	C1C-C2C-C3C	-3.47	103.27	106.95
10	cA	840	CLA	C1D-CHD-C4C	-3.47	117.74	122.48
10	bA	818	CLA	C1D-CHD-C4C	-3.47	117.75	122.48
10	aA	841	CLA	C1D-CHD-C4C	-3.47	117.75	122.48
10	cA	816	CLA	C1C-C2C-C3C	-3.47	103.28	106.95
10	bB	816	CLA	C1D-CHD-C4C	-3.46	117.75	122.48
10	aB	827	CLA	C4C-C3C-C2C	-3.46	101.87	106.89
10	aA	818	CLA	C1D-CHD-C4C	-3.46	117.75	122.48
10	cB	837	CLA	C1C-C2C-C3C	-3.46	103.28	106.95
10	aB	816	CLA	C1D-CHD-C4C	-3.46	117.75	122.48
10	cB	833	CLA	C1D-CHD-C4C	-3.46	117.75	122.48
13	cB	844	BCR	C2-C1-C6	3.46	115.84	110.48
10	cL	203	CLA	C3C-C4C-NC	3.46	114.45	110.57
10	cA	838	CLA	C1C-C2C-C3C	-3.46	103.28	106.95
13	cI	102	BCR	C2-C1-C6	3.46	115.83	110.48
10	cB	840	CLA	C1C-C2C-C3C	-3.46	103.28	106.95
10	aA	823	CLA	C4A-NA-C1A	-3.46	105.15	106.71
10	bA	817	CLA	C1C-C2C-C3C	-3.46	103.29	106.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	823	CLA	C1D-CHD-C4C	-3.45	117.76	122.48
10	cB	821	CLA	C1D-CHD-C4C	-3.45	117.76	122.48
13	aB	844	BCR	C2-C1-C6	3.45	115.83	110.48
10	bB	819	CLA	C3B-C4B-NB	3.45	113.67	109.21
10	cA	827	CLA	C1C-C2C-C3C	-3.45	103.29	106.95
10	bL	203	CLA	C3C-C4C-NC	3.45	114.44	110.57
10	bA	823	CLA	C1D-CHD-C4C	-3.45	117.77	122.48
10	aL	205	CLA	C3B-C4B-NB	3.45	113.67	109.21
10	aB	825	CLA	C3B-C4B-NB	3.45	113.67	109.21
10	aA	856	CLA	C1D-CHD-C4C	-3.45	117.77	122.48
10	cB	804	CLA	C4C-C3C-C2C	-3.45	101.90	106.89
10	cB	812	CLA	C3B-C4B-NB	3.45	113.67	109.21
10	bA	816	CLA	C1C-C2C-C3C	-3.45	103.30	106.95
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	bB	837	CLA	C1C-C2C-C3C	-3.44	103.30	106.95
10	cA	805	CLA	O2A-CGA-CBA	3.44	122.98	111.93
10	aB	840	CLA	C1C-C2C-C3C	-3.44	103.30	106.95
10	aA	805	CLA	O2A-CGA-CBA	3.44	122.98	111.93
10	bA	805	CLA	O2A-CGA-CBA	3.44	122.97	111.93
10	aB	804	CLA	C4C-C3C-C2C	-3.44	101.91	106.89
10	cA	828	CLA	C3B-C4B-NB	3.44	113.65	109.21
10	bA	825	CLA	C1C-C2C-C3C	-3.44	103.31	106.95
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	cA	825	CLA	C1C-C2C-C3C	-3.43	103.31	106.95
10	aB	819	CLA	C3B-C4B-NB	3.43	113.65	109.21
10	bA	832	CLA	CAA-C2A-C3A	-3.43	103.38	112.78
13	bB	844	BCR	C2-C1-C6	3.43	115.79	110.48
10	aB	802	CLA	C1C-C2C-C3C	-3.43	103.31	106.95
10	bL	205	CLA	C3B-C4B-NB	3.43	113.65	109.21
10	bB	830	CLA	O2D-CGD-O1D	-3.43	117.05	123.83
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	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	841	CLA	C1D-CHD-C4C	-3.43	117.80	122.48
10	aB	833	CLA	C1D-CHD-C4C	-3.43	117.80	122.48
10	bB	806	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
10	aB	806	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
10	aB	830	CLA	O2D-CGD-O1D	-3.43	117.06	123.83
10	aA	810	CLA	C1D-CHD-C4C	-3.43	117.80	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	820	CLA	C1C-C2C-C3C	-3.43	103.32	106.95
10	bA	822	CLA	C1D-CHD-C4C	-3.43	117.80	122.48
10	bA	828	CLA	C3B-C4B-NB	3.43	113.64	109.21
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	cA	822	CLA	C1D-CHD-C4C	-3.42	117.81	122.48
10	aB	812	CLA	C3B-C4B-NB	3.42	113.64	109.21
10	cA	810	CLA	C1D-CHD-C4C	-3.42	117.81	122.48
10	bA	822	CLA	C3B-C4B-NB	3.42	113.63	109.21
10	cA	822	CLA	C3B-C4B-NB	3.42	113.63	109.21
10	aB	820	CLA	CAC-C3C-C4C	3.42	129.29	124.82
10	aA	825	CLA	C1C-C2C-C3C	-3.42	103.33	106.95
10	cA	837	CLA	C1D-CHD-C4C	-3.42	117.81	122.48
10	aA	827	CLA	CMB-C2B-C3B	3.42	131.21	124.80
10	bB	833	CLA	C1D-CHD-C4C	-3.42	117.82	122.48
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	aA	837	CLA	C1D-CHD-C4C	-3.41	117.82	122.48
10	bB	827	CLA	OBD-CAD-C3D	-3.41	121.99	128.04
10	bB	804	CLA	C4C-C3C-C2C	-3.41	101.95	106.89
10	cB	820	CLA	C3C-C4C-NC	3.41	114.40	110.57
10	cB	830	CLA	O2D-CGD-O1D	-3.41	117.09	123.83
10	cB	819	CLA	C3B-C4B-NB	3.41	113.62	109.21
10	bA	810	CLA	C1D-CHD-C4C	-3.41	117.82	122.48
10	cB	804	CLA	C1D-CHD-C4C	-3.41	117.83	122.48
10	aA	816	CLA	C1C-C2C-C3C	-3.41	103.34	106.95
10	aA	822	CLA	C1D-CHD-C4C	-3.41	117.83	122.48
10	cL	205	CLA	C3B-C4B-NB	3.41	113.61	109.21
14	cA	855	LHG	O8-C23-C24	3.40	120.31	111.38
10	aA	828	CLA	C3B-C4B-NB	3.40	113.61	109.21
10	bA	837	CLA	C1D-CHD-C4C	-3.40	117.83	122.48
10	bA	827	CLA	CMB-C2B-C3B	3.40	131.18	124.80
10	cA	827	CLA	CMB-C2B-C3B	3.40	131.18	124.80
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	bB	807	CLA	O2A-CGA-CBA	3.40	122.84	111.93
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	bA	829	CLA	C4C-C3C-C2C	-3.40	101.97	106.89
10	aB	828	CLA	C1D-CHD-C4C	-3.39	117.84	122.48
10	bB	828	CLA	C4A-NA-C1A	-3.39	105.18	106.71
10	bA	834	CLA	C4A-NA-C1A	-3.39	105.18	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	803	CLA	C1C-C2C-C3C	-3.39	103.35	106.95
10	aB	804	CLA	C1D-CHD-C4C	-3.39	117.85	122.48
10	aB	807	CLA	O2A-CGA-CBA	3.39	122.83	111.93
10	bA	820	CLA	C1C-C2C-C3C	-3.39	103.35	106.95
10	bB	828	CLA	C1D-CHD-C4C	-3.39	117.85	122.48
10	cA	803	CLA	C1C-C2C-C3C	-3.39	103.36	106.95
10	cB	802	CLA	CAA-C2A-C3A	-3.39	103.49	112.78
14	aA	855	LHG	O8-C23-C24	3.39	120.27	111.38
10	bB	804	CLA	C1D-CHD-C4C	-3.39	117.85	122.48
10	aA	828	CLA	C1C-C2C-C3C	-3.39	103.36	106.95
10	cB	827	CLA	OBD-CAD-C3D	-3.38	122.04	128.04
10	aA	820	CLA	C1C-C2C-C3C	-3.38	103.36	106.95
10	aB	827	CLA	OBD-CAD-C3D	-3.38	122.05	128.04
10	aA	803	CLA	C1C-C2C-C3C	-3.38	103.36	106.95
10	cB	807	CLA	O2A-CGA-CBA	3.38	122.78	111.93
10	bA	820	CLA	CMB-C2B-C3B	3.38	131.14	124.80
10	aA	829	CLA	C4C-C3C-C2C	-3.38	102.00	106.89
14	bA	855	LHG	O8-C23-C24	3.38	120.24	111.38
10	bB	831	CLA	CAC-C3C-C4C	3.38	129.23	124.82
10	bB	820	CLA	CAC-C3C-C4C	3.38	129.23	124.82
10	cB	828	CLA	C1D-CHD-C4C	-3.38	117.87	122.48
10	aB	838	CLA	C1D-CHD-C4C	-3.37	117.87	122.48
10	bA	828	CLA	C1C-C2C-C3C	-3.37	103.37	106.95
10	bB	838	CLA	C1D-CHD-C4C	-3.37	117.87	122.48
10	bB	828	CLA	C3B-C4B-NB	3.37	113.57	109.21
10	cA	826	CLA	C4C-C3C-C2C	-3.37	102.00	106.89
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	cA	829	CLA	C4C-C3C-C2C	-3.37	102.01	106.89
10	cA	828	CLA	C1C-C2C-C3C	-3.37	103.38	106.95
10	bB	830	CLA	CHC-C1C-C2C	-3.37	117.42	126.71
10	cA	819	CLA	C1D-CHD-C4C	-3.37	117.88	122.48
10	cB	838	CLA	C1D-CHD-C4C	-3.37	117.88	122.48
10	cA	817	CLA	C1D-CHD-C4C	-3.37	117.88	122.48
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	cA	820	CLA	CMB-C2B-C3B	3.37	131.11	124.80
10	bB	816	CLA	C1C-C2C-C3C	-3.37	103.38	106.95
10	bA	817	CLA	C1D-CHD-C4C	-3.37	117.89	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	830	CLA	CHC-C1C-C2C	-3.37	117.43	126.71
10	aB	828	CLA	C3B-C4B-NB	3.36	113.56	109.21
10	aA	820	CLA	CMB-C2B-C3B	3.36	131.10	124.80
10	bB	818	CLA	C1C-C2C-C3C	-3.36	103.39	106.95
10	aA	840	CLA	CAA-C2A-C3A	-3.36	103.58	112.78
13	cI	103	BCR	C2-C1-C6	3.36	115.68	110.48
10	cA	807	CLA	C3B-C4B-NB	3.36	113.55	109.21
10	cA	802	CLA	C4A-NA-C1A	-3.36	105.20	106.71
10	cA	838	CLA	C1D-CHD-C4C	-3.36	117.90	122.48
10	cB	830	CLA	CHC-C1C-C2C	-3.36	117.46	126.71
10	aB	819	CLA	CHC-C1C-C2C	-3.36	117.46	126.71
10	cA	822	CLA	CMB-C2B-C3B	3.36	131.09	124.80
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
10	aA	843	CLA	CAC-C3C-C4C	3.35	129.20	124.82
10	bA	824	CLA	O2D-CGD-O1D	-3.35	117.21	123.83
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	cB	801	CLA	CAC-C3C-C4C	3.35	129.20	124.82
10	bA	842	CLA	CAC-C3C-C4C	3.35	129.20	124.82
10	cB	819	CLA	CHC-C1C-C2C	-3.35	117.47	126.71
10	aB	804	CLA	C3B-C4B-NB	3.35	113.54	109.21
10	bA	822	CLA	CMB-C2B-C3B	3.35	131.08	124.80
10	aA	826	CLA	C4C-C3C-C2C	-3.35	102.04	106.89
10	aB	806	CLA	C4A-NA-C1A	-3.35	105.20	106.71
10	bA	843	CLA	CAC-C3C-C4C	3.35	129.19	124.82
10	cB	810	CLA	O2A-CGA-O1A	-3.35	115.01	123.56
10	bA	802	CLA	C3B-C4B-NB	3.35	113.53	109.21
10	aB	831	CLA	CAC-C3C-C4C	3.35	129.19	124.82
10	cB	825	CLA	C4C-C3C-C2C	-3.34	102.05	106.89
13	bL	207	BCR	C2-C1-C6	3.34	115.66	110.48
10	bA	826	CLA	C4C-C3C-C2C	-3.34	102.05	106.89
13	aL	207	BCR	C2-C1-C6	3.34	115.66	110.48
10	aB	836	CLA	CAA-C2A-C3A	-3.34	103.62	112.78
10	bB	819	CLA	C3C-C4C-NC	3.34	114.32	110.57
10	aA	802	CLA	C3B-C4B-NB	3.34	113.53	109.21
10	cB	820	CLA	CAC-C3C-C4C	3.34	129.19	124.82
9	cA	801	CL0	C1D-CHD-C4C	-3.34	117.92	122.48
10	bA	811	CLA	C1D-CHD-C4C	-3.34	117.92	122.48
10	cB	838	CLA	C1C-C2C-C3C	-3.34	103.41	106.95
10	aB	838	CLA	C1C-C2C-C3C	-3.34	103.41	106.95
10	bB	810	CLA	O2A-CGA-O1A	-3.34	115.03	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	801	CLA	CAC-C3C-C4C	3.34	129.18	124.82
13	cL	207	BCR	C2-C1-C6	3.34	115.65	110.48
10	aB	816	CLA	C1C-C2C-C3C	-3.34	103.41	106.95
10	bB	836	CLA	CAA-C2A-C3A	-3.34	103.64	112.78
10	bA	819	CLA	C1D-CHD-C4C	-3.34	117.92	122.48
10	aB	825	CLA	C4C-C3C-C2C	-3.34	102.06	106.89
10	bB	838	CLA	C1C-C2C-C3C	-3.34	103.41	106.95
10	cB	836	CLA	CAA-C2A-C3A	-3.34	103.64	112.78
10	bB	819	CLA	CHC-C1C-C2C	-3.34	117.51	126.71
10	aA	824	CLA	O2D-CGD-O1D	-3.34	117.24	123.83
10	aB	810	CLA	O2A-CGA-O1A	-3.34	115.04	123.56
9	bA	801	CL0	C1D-CHD-C4C	-3.33	117.93	122.48
10	cB	828	CLA	C4C-C3C-C2C	-3.33	102.06	106.89
10	aA	817	CLA	C1D-CHD-C4C	-3.33	117.93	122.48
10	cA	824	CLA	O2D-CGD-O1D	-3.33	117.25	123.83
10	cB	817	CLA	C3B-C4B-NB	3.33	113.52	109.21
10	aA	822	CLA	CMB-C2B-C3B	3.33	131.05	124.80
10	aA	838	CLA	C1D-CHD-C4C	-3.33	117.93	122.48
10	aA	842	CLA	CAC-C3C-C4C	3.33	129.17	124.82
10	aB	805	CLA	CAA-C2A-C3A	-3.33	103.66	112.78
10	bB	828	CLA	C1-O2A-CGA	3.33	125.64	116.54
10	cB	816	CLA	C1C-C2C-C3C	-3.33	103.42	106.95
10	cB	828	CLA	C1-O2A-CGA	3.33	125.64	116.54
10	bB	805	CLA	CAA-C2A-C3A	-3.33	103.66	112.78
10	aA	819	CLA	C1D-CHD-C4C	-3.33	117.94	122.48
10	aB	828	CLA	C1-O2A-CGA	3.33	125.64	116.54
10	cB	805	CLA	CAA-C2A-C3A	-3.33	103.66	112.78
10	aL	202	CLA	C1-O2A-CGA	3.33	125.64	116.54
10	bA	802	CLA	C4A-NA-C1A	-3.33	105.21	106.71
9	aA	801	CL0	C1D-CHD-C4C	-3.33	117.94	122.48
10	cB	803	CLA	C3B-C4B-NB	3.33	113.51	109.21
10	aA	832	CLA	C3B-C4B-NB	3.32	113.51	109.21
10	aB	803	CLA	C3B-C4B-NB	3.32	113.51	109.21
10	bB	801	CLA	CAC-C3C-C4C	3.32	129.16	124.82
10	cB	831	CLA	CAC-C3C-C4C	3.32	129.16	124.82
10	bL	202	CLA	C1-O2A-CGA	3.32	125.62	116.54
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
10	bB	825	CLA	C4C-C3C-C2C	-3.32	102.08	106.89
10	bA	838	CLA	C1D-CHD-C4C	-3.32	117.95	122.48
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	843	CLA	CAC-C3C-C4C	3.32	129.16	124.82
10	cA	813	CLA	CHC-C1C-C2C	-3.32	117.56	126.71
10	bB	834	CLA	C3C-C4C-NC	3.32	114.29	110.57
13	bI	102	BCR	C2-C1-C6	3.32	115.61	110.48
10	cA	854	CLA	C1C-C2C-C3C	-3.32	103.44	106.95
10	aB	810	CLA	C3B-C4B-NB	3.32	113.50	109.21
13	aI	102	BCR	C2-C1-C6	3.32	115.61	110.48
10	aB	813	CLA	C4C-C3C-C2C	-3.32	102.09	106.89
10	cA	811	CLA	C1D-CHD-C4C	-3.32	117.95	122.48
10	cA	842	CLA	CAC-C3C-C4C	3.32	129.15	124.82
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	aA	811	CLA	C1D-CHD-C4C	-3.31	117.95	122.48
10	cB	824	CLA	C3B-C4B-NB	3.31	113.49	109.21
10	aB	833	CLA	C3B-C4B-NB	3.31	113.49	109.21
10	aA	813	CLA	CHC-C1C-C2C	-3.31	117.58	126.71
10	cB	818	CLA	C1C-C2C-C3C	-3.31	103.44	106.95
10	cB	833	CLA	C3B-C4B-NB	3.31	113.49	109.21
10	aA	834	CLA	C3B-C4B-NB	3.31	113.49	109.21
10	bA	813	CLA	CHC-C1C-C2C	-3.31	117.59	126.71
10	aB	803	CLA	CMA-C3A-C4A	-3.31	102.88	111.77
10	aB	818	CLA	C1C-C2C-C3C	-3.31	103.44	106.95
10	aB	828	CLA	C4C-C3C-C2C	-3.31	102.10	106.89
10	aA	808	CLA	O2D-CGD-CBD	3.31	117.04	111.25
10	bB	824	CLA	CAC-C3C-C4C	3.31	129.14	124.82
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	bB	828	CLA	C4C-C3C-C2C	-3.31	102.10	106.89
10	bB	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	cB	805	CLA	C3B-C4B-NB	3.30	113.48	109.21
10	aA	854	CLA	C1C-C2C-C3C	-3.30	103.45	106.95
10	bA	808	CLA	O2D-CGD-CBD	3.30	117.03	111.25
10	bB	811	CLA	C4-C3-C5	3.30	120.97	115.29
10	cA	814	CLA	C4C-C3C-C2C	-3.30	102.11	106.89
10	aB	834	CLA	CMA-C3A-C4A	-3.30	102.91	111.77
10	aB	841	CLA	CHC-C1C-C2C	-3.30	117.62	126.71
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	bB	813	CLA	C4C-C3C-C2C	-3.30	102.12	106.89
10	bA	854	CLA	C1C-C2C-C3C	-3.30	103.46	106.95
10	cL	202	CLA	C1-O2A-CGA	3.29	125.54	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	835	CLA	C1D-CHD-C4C	-3.29	117.98	122.48
10	aA	814	CLA	C4C-C3C-C2C	-3.29	102.12	106.89
10	cB	811	CLA	C4-C3-C5	3.29	120.96	115.29
10	aB	817	CLA	C3B-C4B-NB	3.29	113.47	109.21
10	bA	802	CLA	CHC-C1C-C2C	-3.29	117.64	126.71
10	bA	814	CLA	C4C-C3C-C2C	-3.29	102.12	106.89
10	bA	832	CLA	C3B-C4B-NB	3.29	113.46	109.21
10	cB	813	CLA	C4C-C3C-C2C	-3.29	102.13	106.89
10	bB	841	CLA	CHC-C1C-C2C	-3.29	117.64	126.71
10	bA	824	CLA	C4C-C3C-C2C	-3.29	102.13	106.89
10	bB	810	CLA	C4A-NA-C1A	-3.29	105.23	106.71
10	aB	811	CLA	C4-C3-C5	3.28	120.94	115.29
10	cA	856	CLA	C3B-C4B-NB	3.28	113.46	109.21
10	cB	824	CLA	CAC-C3C-C4C	3.28	129.11	124.82
10	cA	808	CLA	O2D-CGD-CBD	3.28	117.00	111.25
10	bA	856	CLA	C3B-C4B-NB	3.28	113.45	109.21
10	bA	829	CLA	C1D-CHD-C4C	-3.28	118.00	122.48
10	aA	802	CLA	CHC-C1C-C2C	-3.28	117.67	126.71
10	bA	825	CLA	C1D-CHD-C4C	-3.28	118.00	122.48
10	cB	826	CLA	C3C-C4C-NC	3.28	114.25	110.57
10	aB	824	CLA	CAC-C3C-C4C	3.28	129.11	124.82
10	aB	805	CLA	C3B-C4B-NB	3.28	113.45	109.21
10	cB	841	CLA	CHC-C1C-C2C	-3.28	117.67	126.71
10	bA	828	CLA	CAC-C3C-C4C	3.28	129.10	124.82
10	bB	810	CLA	C3B-C4B-NB	3.28	113.45	109.21
10	bB	812	CLA	C1D-CHD-C4C	-3.28	118.01	122.48
10	bB	824	CLA	C1D-CHD-C4C	-3.27	118.01	122.48
10	bB	841	CLA	C1D-CHD-C4C	-3.27	118.01	122.48
10	cA	802	CLA	CHC-C1C-C2C	-3.27	117.69	126.71
10	aB	823	CLA	C3B-C4B-NB	3.27	113.44	109.21
10	cB	810	CLA	C3B-C4B-NB	3.27	113.44	109.21
10	bB	802	CLA	CHB-C4A-NA	3.27	129.03	124.51
10	aA	829	CLA	C1D-CHD-C4C	-3.27	118.02	122.48
10	cA	840	CLA	C4-C3-C5	3.26	119.78	115.99
10	aB	834	CLA	C3C-C4C-NC	3.26	114.23	110.57
10	aB	812	CLA	C1D-CHD-C4C	-3.26	118.02	122.48
10	cA	825	CLA	C1D-CHD-C4C	-3.26	118.02	122.48
10	cB	841	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
10	cA	831	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
10	cA	821	CLA	C3B-C4B-NB	3.26	113.43	109.21
10	bB	817	CLA	C3B-C4B-NB	3.26	113.43	109.21
10	cA	829	CLA	C1D-CHD-C4C	-3.26	118.03	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	835	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
10	aA	824	CLA	C4C-C3C-C2C	-3.26	102.17	106.89
10	aA	854	CLA	C4C-C3C-C2C	-3.26	102.17	106.89
10	aB	824	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
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	cA	813	CLA	CMB-C2B-C3B	3.25	130.90	124.80
10	cB	802	CLA	CHB-C4A-NA	3.25	129.01	124.51
10	cA	835	CLA	C1D-CHD-C4C	-3.25	118.04	122.48
10	bB	810	CLA	CBA-CAA-C2A	3.25	123.53	113.85
10	cB	818	CLA	CMB-C2B-C3B	3.25	130.90	124.80
10	cA	824	CLA	C4C-C3C-C2C	-3.25	102.18	106.89
10	aA	813	CLA	CMB-C2B-C3B	3.25	130.90	124.80
10	cA	803	CLA	C3B-C4B-NB	3.25	113.41	109.21
10	cB	810	CLA	CBA-CAA-C2A	3.25	123.52	113.85
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	cA	828	CLA	CAC-C3C-C4C	3.25	129.07	124.82
10	aA	854	CLA	CHD-C4C-NC	3.25	129.32	124.20
10	cB	824	CLA	C1D-CHD-C4C	-3.25	118.04	122.48
10	aB	831	CLA	CAA-C2A-C3A	-3.25	103.88	112.78
10	aB	841	CLA	C1D-CHD-C4C	-3.25	118.05	122.48
10	aB	810	CLA	CBA-CAA-C2A	3.25	123.52	113.85
10	bA	854	CLA	C4C-C3C-C2C	-3.25	102.19	106.89
10	bL	204	CLA	O2D-CGD-O1D	-3.25	117.42	123.83
10	aB	814	CLA	C1C-C2C-C3C	-3.25	103.51	106.95
10	cA	842	CLA	CHC-C1C-C2C	-3.25	117.76	126.71
10	cB	812	CLA	C1D-CHD-C4C	-3.25	118.05	122.48
10	cA	829	CLA	O2D-CGD-O1D	-3.25	117.42	123.83
10	cA	854	CLA	C4C-C3C-C2C	-3.25	102.19	106.89
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	aA	823	CLA	CHC-C1C-C2C	-3.24	117.77	126.71
10	bB	831	CLA	CAA-C2A-C3A	-3.24	103.90	112.78
10	aL	204	CLA	O2D-CGD-O1D	-3.24	117.43	123.83
10	aA	828	CLA	O2A-CGA-CBA	3.24	122.34	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	806	CLA	C1C-C2C-C3C	-3.24	103.51	106.95
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	aA	802	CLA	C4A-NA-C1A	-3.24	105.25	106.71
10	cA	854	CLA	CHD-C4C-NC	3.24	129.31	124.20
10	bA	842	CLA	CHC-C1C-C2C	-3.24	117.78	126.71
10	cA	828	CLA	O2A-CGA-CBA	3.24	122.33	111.93
10	cA	823	CLA	CHC-C1C-C2C	-3.24	117.78	126.71
10	bA	815	CLA	CHC-C1C-C2C	-3.24	117.78	126.71
10	bA	854	CLA	CHD-C4C-NC	3.24	129.31	124.20
10	aA	818	CLA	CHC-C1C-C2C	-3.24	117.78	126.71
10	aA	829	CLA	O2D-CGD-O1D	-3.24	117.44	123.83
10	cB	831	CLA	CAA-C2A-C3A	-3.24	103.92	112.78
10	cL	204	CLA	O2D-CGD-O1D	-3.24	117.44	123.83
10	bA	823	CLA	CHC-C1C-C2C	-3.24	117.79	126.71
10	bB	806	CLA	C1C-C2C-C3C	-3.23	103.52	106.95
10	aA	842	CLA	CHC-C1C-C2C	-3.23	117.79	126.71
10	aB	806	CLA	C3B-C4B-NB	3.23	113.39	109.21
10	bA	831	CLA	C1D-CHD-C4C	-3.23	118.06	122.48
10	bA	818	CLA	CHC-C1C-C2C	-3.23	117.80	126.71
10	bA	828	CLA	O2A-CGA-CBA	3.23	122.31	111.93
10	bA	840	CLA	C4-C3-C5	3.23	119.74	115.99
10	bB	805	CLA	C3B-C4B-NB	3.23	113.39	109.21
10	aA	803	CLA	C3B-C4B-NB	3.23	113.39	109.21
10	cB	806	CLA	C1C-C2C-C3C	-3.23	103.53	106.95
10	aB	818	CLA	CMB-C2B-C3B	3.23	130.86	124.80
10	cA	811	CLA	C4A-NA-C1A	-3.23	105.25	106.71
10	bA	839	CLA	C1D-CHD-C4C	-3.23	118.07	122.48
10	aA	805	CLA	C1D-CHD-C4C	-3.23	118.07	122.48
10	cA	818	CLA	CHC-C1C-C2C	-3.23	117.81	126.71
10	bA	829	CLA	O2D-CGD-O1D	-3.23	117.45	123.83
10	bA	833	CLA	CAA-C2A-C3A	-3.23	103.94	112.78
10	bA	813	CLA	CMB-C2B-C3B	3.23	130.85	124.80
10	bB	818	CLA	CMB-C2B-C3B	3.23	130.85	124.80
10	aA	841	CLA	C1C-C2C-C3C	-3.23	103.53	106.95
10	cB	814	CLA	C1C-C2C-C3C	-3.23	103.53	106.95
10	aB	819	CLA	C1D-CHD-C4C	-3.22	118.08	122.48
10	bB	806	CLA	C3B-C4B-NB	3.22	113.38	109.21
10	aA	815	CLA	CHC-C1C-C2C	-3.22	117.82	126.71
10	aB	816	CLA	C4C-C3C-C2C	-3.22	102.22	106.89
10	aA	833	CLA	CAA-C2A-C3A	-3.22	103.95	112.78
10	bB	837	CLA	C4C-C3C-C2C	-3.22	102.22	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	837	CLA	C4C-C3C-C2C	-3.22	102.22	106.89
10	aA	828	CLA	CAC-C3C-C4C	3.22	129.03	124.82
10	aB	801	CLA	C1D-CHD-C4C	-3.22	118.08	122.48
10	aB	840	CLA	C4C-C3C-C2C	-3.22	102.22	106.89
10	bA	841	CLA	C1C-C2C-C3C	-3.22	103.54	106.95
10	cB	814	CLA	C3B-C4B-NB	3.22	113.37	109.21
10	aB	804	CLA	C1C-C2C-C3C	-3.22	103.54	106.95
10	aA	825	CLA	C1D-CHD-C4C	-3.22	118.08	122.48
10	cA	805	CLA	C1D-CHD-C4C	-3.22	118.08	122.48
10	bA	842	CLA	C4A-NA-C1A	-3.22	105.26	106.71
10	aB	820	CLA	CHC-C1C-C2C	-3.22	117.84	126.71
10	aA	815	CLA	C1D-CHD-C4C	-3.22	118.09	122.48
10	bA	838	CLA	CAC-C3C-C4C	3.22	129.02	124.82
10	aA	840	CLA	C4-C3-C5	3.22	119.72	115.99
10	cB	820	CLA	C3B-C4B-NB	3.22	113.37	109.21
10	aA	831	CLA	C1D-CHD-C4C	-3.22	118.09	122.48
10	cB	816	CLA	C4C-C3C-C2C	-3.21	102.23	106.89
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	cB	840	CLA	C4C-C3C-C2C	-3.21	102.24	106.89
10	cB	820	CLA	CHC-C1C-C2C	-3.21	117.85	126.71
10	bB	814	CLA	C1C-C2C-C3C	-3.21	103.55	106.95
10	cA	815	CLA	C3B-C4B-NB	3.21	113.36	109.21
10	bB	820	CLA	CHC-C1C-C2C	-3.21	117.86	126.71
10	cB	821	CLA	C3B-C4B-NB	3.21	113.36	109.21
10	aB	835	CLA	C3B-C4B-NB	3.21	113.36	109.21
10	bB	804	CLA	C1C-C2C-C3C	-3.21	103.55	106.95
10	cA	833	CLA	CAA-C2A-C3A	-3.21	103.99	112.78
10	cA	833	CLA	C1D-CHD-C4C	-3.21	118.10	122.48
10	bA	811	CLA	C4A-NA-C1A	-3.21	105.26	106.71
10	cA	841	CLA	C1C-C2C-C3C	-3.21	103.55	106.95
10	cB	836	CLA	CHC-C1C-C2C	-3.21	117.87	126.71
10	cB	834	CLA	C3C-C4C-NC	3.21	114.17	110.57
10	aA	835	CLA	CHC-C1C-C2C	-3.21	117.87	126.71
10	aB	836	CLA	CHC-C1C-C2C	-3.20	117.88	126.71
13	cB	847	BCR	C2-C1-C6	3.20	115.44	110.48
10	cA	827	CLA	C4C-C3C-C2C	-3.20	102.25	106.89
10	cA	824	CLA	C1C-C2C-C3C	-3.20	103.56	106.95
10	bB	840	CLA	C4C-C3C-C2C	-3.20	102.25	106.89
10	aB	821	CLA	C3B-C4B-NB	3.20	113.35	109.21
10	cA	839	CLA	C1D-CHD-C4C	-3.20	118.11	122.48
10	cA	815	CLA	CHC-C1C-C2C	-3.20	117.88	126.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	810	CLA	O2A-CGA-CBA	3.20	122.21	111.93
10	bB	823	CLA	C1D-CHD-C4C	-3.20	118.11	122.48
10	aB	814	CLA	C3B-C4B-NB	3.20	113.35	109.21
10	aA	838	CLA	CAC-C3C-C4C	3.20	129.00	124.82
10	bL	204	CLA	C4A-NA-C1A	-3.20	105.27	106.71
10	cB	804	CLA	C1C-C2C-C3C	-3.20	103.56	106.95
10	bA	827	CLA	C4C-C3C-C2C	-3.20	102.26	106.89
10	cB	812	CLA	CHC-C1C-C2C	-3.20	117.90	126.71
10	cB	810	CLA	O2A-CGA-CBA	3.20	122.19	111.93
10	aA	815	CLA	C3B-C4B-NB	3.20	113.34	109.21
10	aB	810	CLA	O2D-CGD-O1D	-3.19	117.52	123.83
10	aA	839	CLA	C1D-CHD-C4C	-3.19	118.12	122.48
10	aA	824	CLA	C3B-C4B-NB	3.19	113.34	109.21
10	cB	823	CLA	C1D-CHD-C4C	-3.19	118.12	122.48
10	cA	835	CLA	CHC-C1C-C2C	-3.19	117.91	126.71
10	bA	805	CLA	C1D-CHD-C4C	-3.19	118.12	122.48
10	bA	834	CLA	CHC-C1C-C2C	-3.19	117.91	126.71
10	bB	836	CLA	CHC-C1C-C2C	-3.19	117.91	126.71
10	bA	815	CLA	C1D-CHD-C4C	-3.19	118.12	122.48
10	aA	827	CLA	C4C-C3C-C2C	-3.19	102.27	106.89
10	bB	816	CLA	C4C-C3C-C2C	-3.19	102.27	106.89
10	bA	824	CLA	C3B-C4B-NB	3.19	113.33	109.21
10	cA	834	CLA	CHC-C1C-C2C	-3.19	117.92	126.71
10	bB	812	CLA	CHC-C1C-C2C	-3.19	117.92	126.71
10	cA	838	CLA	CAC-C3C-C4C	3.19	128.99	124.82
10	aB	810	CLA	O2A-CGA-CBA	3.19	122.17	111.93
10	aA	834	CLA	CHC-C1C-C2C	-3.19	117.92	126.71
10	aB	816	CLA	CAC-C3C-C4C	3.19	128.99	124.82
13	aB	847	BCR	C2-C1-C6	3.19	115.41	110.48
10	aB	820	CLA	C3B-C4B-NB	3.19	113.33	109.21
10	cB	822	CLA	CHC-C1C-C2C	-3.19	117.92	126.71
10	aA	802	CLA	CAC-C3C-C4C	3.19	128.99	124.82
10	bA	809	CLA	C1C-C2C-C3C	-3.19	103.57	106.95
13	cB	847	BCR	C11-C10-C9	-3.19	122.76	127.31
10	bA	804	CLA	O2D-CGD-O1D	-3.19	117.54	123.83
10	aB	823	CLA	C1D-CHD-C4C	-3.19	118.13	122.48
10	bA	833	CLA	C1D-CHD-C4C	-3.19	118.13	122.48
10	cB	816	CLA	CAC-C3C-C4C	3.19	128.98	124.82
10	bB	826	CLA	O2A-CGA-CBA	3.19	122.16	111.93
10	cB	810	CLA	O2D-CGD-O1D	-3.19	117.54	123.83
10	cB	814	CLA	C4C-C3C-C2C	-3.19	102.28	106.89
10	cA	824	CLA	C3B-C4B-NB	3.19	113.33	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	814	CLA	C4C-C3C-C2C	-3.18	102.28	106.89
10	aB	812	CLA	CHC-C1C-C2C	-3.18	117.93	126.71
10	cA	804	CLA	O2D-CGD-O1D	-3.18	117.54	123.83
10	aA	835	CLA	C3B-C4B-NB	3.18	113.33	109.21
10	aB	837	CLA	C4C-C3C-C2C	-3.18	102.28	106.89
10	bA	835	CLA	CHC-C1C-C2C	-3.18	117.93	126.71
10	cB	826	CLA	O2A-CGA-CBA	3.18	122.15	111.93
10	aB	822	CLA	CHC-C1C-C2C	-3.18	117.94	126.71
10	aA	803	CLA	C1D-CHD-C4C	-3.18	118.14	122.48
10	cA	809	CLA	C3B-C4B-NB	3.18	113.32	109.21
10	aB	814	CLA	C4C-C3C-C2C	-3.18	102.28	106.89
10	cB	808	CLA	CHD-C4C-NC	3.18	129.22	124.20
10	aB	811	CLA	C1D-CHD-C4C	-3.18	118.14	122.48
10	aB	826	CLA	O2A-CGA-CBA	3.18	122.14	111.93
10	bB	809	CLA	C4C-C3C-C2C	-3.18	102.28	106.89
10	cB	801	CLA	C1D-CHD-C4C	-3.18	118.14	122.48
10	cA	815	CLA	C1D-CHD-C4C	-3.18	118.14	122.48
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
10	cB	822	CLA	C1D-CHD-C4C	-3.18	118.14	122.48
10	cA	829	CLA	CHC-C1C-C2C	-3.18	117.95	126.71
10	bB	819	CLA	C1D-CHD-C4C	-3.18	118.14	122.48
10	aA	829	CLA	CHC-C1C-C2C	-3.18	117.95	126.71
10	bB	839	CLA	C1D-CHD-C4C	-3.18	118.14	122.48
10	aA	809	CLA	C1C-C2C-C3C	-3.18	103.58	106.95
10	aL	203	CLA	C3B-C4B-NB	3.18	113.32	109.21
10	cB	806	CLA	C4A-NA-C1A	-3.18	105.28	106.71
10	aA	833	CLA	C1D-CHD-C4C	-3.18	118.14	122.48
10	bB	801	CLA	C1D-CHD-C4C	-3.18	118.14	122.48
10	bA	820	CLA	C1D-CHD-C4C	-3.18	118.14	122.48
10	cL	202	CLA	C4C-C3C-C2C	-3.17	102.29	106.89
10	bB	810	CLA	O2D-CGD-O1D	-3.17	117.56	123.83
10	bA	829	CLA	CHC-C1C-C2C	-3.17	117.96	126.71
10	bB	808	CLA	CHD-C4C-NC	3.17	129.20	124.20
10	cA	809	CLA	C1C-C2C-C3C	-3.17	103.59	106.95
10	aA	809	CLA	C3B-C4B-NB	3.17	113.31	109.21
10	cA	825	CLA	CMC-C2C-C1C	3.17	129.85	125.03
10	aA	820	CLA	C1D-CHD-C4C	-3.17	118.15	122.48
10	cB	833	CLA	CAC-C3C-C4C	3.17	128.96	124.82
10	aB	835	CLA	CHC-C1C-C2C	-3.17	117.97	126.71
10	aA	804	CLA	O2D-CGD-O1D	-3.17	117.57	123.83
10	aB	809	CLA	C4C-C3C-C2C	-3.17	102.30	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	803	CLA	C4C-C3C-C2C	-3.17	102.30	106.89
10	bB	824	CLA	CHC-C1C-C2C	-3.17	117.97	126.71
10	bA	814	CLA	C1C-C2C-C3C	-3.17	103.59	106.95
10	cB	810	CLA	CHC-C1C-C2C	-3.17	117.98	126.71
10	cB	819	CLA	C1D-CHD-C4C	-3.17	118.16	122.48
10	bA	841	CLA	CAC-C3C-C4C	3.17	128.96	124.82
10	cB	824	CLA	CHC-C1C-C2C	-3.17	117.98	126.71
10	cA	856	CLA	CHC-C1C-C2C	-3.17	117.98	126.71
10	bB	838	CLA	CHD-C4C-NC	3.17	129.19	124.20
10	aB	824	CLA	CHC-C1C-C2C	-3.16	117.98	126.71
10	cA	820	CLA	C1D-CHD-C4C	-3.16	118.16	122.48
13	aB	847	BCR	C11-C10-C9	-3.16	122.80	127.31
10	bB	822	CLA	C1D-CHD-C4C	-3.16	118.16	122.48
10	cB	835	CLA	CHC-C1C-C2C	-3.16	117.99	126.71
10	aA	856	CLA	CHC-C1C-C2C	-3.16	117.99	126.71
10	cA	810	CLA	CAC-C3C-C4C	3.16	128.95	124.82
13	bB	847	BCR	C2-C1-C6	3.16	115.37	110.48
10	aA	841	CLA	CAC-C3C-C4C	3.16	128.95	124.82
10	cB	835	CLA	C3B-C4B-NB	3.16	113.30	109.21
10	aA	819	CLA	C3B-C4B-NB	3.16	113.30	109.21
10	cB	803	CLA	C4C-C3C-C2C	-3.16	102.31	106.89
10	cA	809	CLA	C4C-C3C-C2C	-3.16	102.31	106.89
13	cI	102	BCR	C3-C4-C5	-3.16	108.49	113.99
10	bA	856	CLA	CHC-C1C-C2C	-3.16	118.00	126.71
10	cA	802	CLA	CAC-C3C-C4C	3.16	128.95	124.82
10	cB	839	CLA	C1D-CHD-C4C	-3.16	118.17	122.48
10	aA	824	CLA	C1C-C2C-C3C	-3.16	103.60	106.95
10	aB	803	CLA	C4C-C3C-C2C	-3.16	102.32	106.89
10	cA	814	CLA	C1C-C2C-C3C	-3.16	103.60	106.95
10	bA	803	CLA	C1D-CHD-C4C	-3.16	118.17	122.48
10	bB	835	CLA	C3B-C4B-NB	3.16	113.29	109.21
10	aB	833	CLA	C4C-C3C-C2C	-3.16	102.32	106.89
10	bB	810	CLA	CHC-C1C-C2C	-3.16	118.01	126.71
10	cA	803	CLA	C1D-CHD-C4C	-3.16	118.17	122.48
10	aB	839	CLA	C1D-CHD-C4C	-3.16	118.17	122.48
10	bB	811	CLA	C1D-CHD-C4C	-3.16	118.17	122.48
10	aB	822	CLA	C1D-CHD-C4C	-3.16	118.17	122.48
13	bB	847	BCR	C11-C10-C9	-3.16	122.81	127.31
10	aA	803	CLA	CMB-C2B-C3B	3.15	130.72	124.80
10	bB	833	CLA	CAC-C3C-C4C	3.15	128.94	124.82
10	bA	809	CLA	C4C-C3C-C2C	-3.15	102.32	106.89
10	cA	841	CLA	C4C-C3C-C2C	-3.15	102.32	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	824	CLA	C1C-C2C-C3C	-3.15	103.61	106.95
10	aB	807	CLA	C1D-CHD-C4C	-3.15	118.18	122.48
10	cA	841	CLA	CAC-C3C-C4C	3.15	128.94	124.82
10	bB	816	CLA	CAC-C3C-C4C	3.15	128.94	124.82
10	aB	833	CLA	CAC-C3C-C4C	3.15	128.94	124.82
10	cL	203	CLA	C3B-C4B-NB	3.15	113.28	109.21
10	bA	803	CLA	CMB-C2B-C3B	3.15	130.71	124.80
10	aA	842	CLA	C4A-NA-C1A	-3.15	105.29	106.71
10	bL	203	CLA	C3B-C4B-NB	3.15	113.28	109.21
10	bA	825	CLA	CMC-C2C-C1C	3.15	129.82	125.03
10	cA	814	CLA	CHC-C1C-C2C	-3.15	118.02	126.71
10	bB	833	CLA	C4C-C3C-C2C	-3.15	102.33	106.89
10	aA	814	CLA	C1C-C2C-C3C	-3.15	103.61	106.95
10	bA	835	CLA	C3B-C4B-NB	3.15	113.28	109.21
10	bA	809	CLA	C3B-C4B-NB	3.15	113.28	109.21
10	bB	835	CLA	CHC-C1C-C2C	-3.15	118.02	126.71
10	aB	810	CLA	CHC-C1C-C2C	-3.15	118.03	126.71
13	bI	101	BCR	C3-C4-C5	-3.15	108.51	113.99
10	bA	828	CLA	C4C-C3C-C2C	-3.15	102.33	106.89
10	bA	810	CLA	CAC-C3C-C4C	3.15	128.94	124.82
10	aA	825	CLA	CMC-C2C-C1C	3.15	129.82	125.03
10	cB	838	CLA	CHD-C4C-NC	3.15	129.16	124.20
10	aA	809	CLA	C4C-C3C-C2C	-3.15	102.33	106.89
10	bA	819	CLA	C3B-C4B-NB	3.15	113.28	109.21
10	cB	809	CLA	C4C-C3C-C2C	-3.15	102.33	106.89
10	cA	827	CLA	O2A-CGA-CBA	3.15	122.04	111.93
10	cA	842	CLA	C4A-NA-C1A	-3.15	105.29	106.71
10	bL	202	CLA	C4C-C3C-C2C	-3.15	102.33	106.89
10	cB	810	CLA	C4C-C3C-C2C	-3.15	102.33	106.89
10	aL	202	CLA	C4C-C3C-C2C	-3.15	102.33	106.89
10	aB	838	CLA	CHD-C4C-NC	3.15	129.16	124.20
10	cB	811	CLA	C1D-CHD-C4C	-3.15	118.19	122.48
10	aA	827	CLA	O2A-CGA-CBA	3.14	122.03	111.93
10	bB	822	CLA	CHC-C1C-C2C	-3.14	118.04	126.71
10	bA	827	CLA	O2A-CGA-CBA	3.14	122.02	111.93
10	aA	814	CLA	CHC-C1C-C2C	-3.14	118.05	126.71
10	bA	814	CLA	CHC-C1C-C2C	-3.14	118.05	126.71
10	cB	833	CLA	C4C-C3C-C2C	-3.14	102.34	106.89
10	cB	829	CLA	C4C-C3C-C2C	-3.14	102.34	106.89
10	bA	802	CLA	CAC-C3C-C4C	3.14	128.92	124.82
10	cB	822	CLA	CHD-C4C-NC	3.14	129.15	124.20
10	cB	824	CLA	CAA-C2A-C3A	-3.14	104.19	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	841	CLA	C4C-C3C-C2C	-3.14	102.35	106.89
10	bA	804	CLA	C1D-CHD-C4C	-3.14	118.20	122.48
10	aA	812	CLA	C3B-C4B-NB	3.13	113.26	109.21
10	cB	804	CLA	CAC-C3C-C4C	3.13	128.92	124.82
10	cA	819	CLA	C3B-C4B-NB	3.13	113.26	109.21
13	aI	101	BCR	C3-C4-C5	-3.13	108.54	113.99
10	cA	803	CLA	CMB-C2B-C3B	3.13	130.68	124.80
10	aB	810	CLA	C4C-C3C-C2C	-3.13	102.35	106.89
10	bB	829	CLA	C4C-C3C-C2C	-3.13	102.35	106.89
10	bB	807	CLA	C1D-CHD-C4C	-3.13	118.20	122.48
10	aB	805	CLA	CHC-C1C-C2C	-3.13	118.07	126.71
10	bA	838	CLA	CBA-CAA-C2A	3.13	123.17	113.85
10	aA	841	CLA	C4C-C3C-C2C	-3.13	102.36	106.89
10	aA	838	CLA	CBA-CAA-C2A	3.13	123.17	113.85
10	cA	835	CLA	C3B-C4B-NB	3.13	113.26	109.21
10	aB	817	CLA	CHC-C1C-C2C	-3.13	118.08	126.71
10	aB	835	CLA	C1D-CHD-C4C	-3.13	118.21	122.48
10	cA	838	CLA	CBA-CAA-C2A	3.13	123.16	113.85
10	bB	823	CLA	CHC-C1C-C2C	-3.13	118.09	126.71
10	bB	824	CLA	CAA-C2A-C3A	-3.13	104.22	112.78
10	bB	833	CLA	CHC-C1C-C2C	-3.12	118.10	126.71
10	aA	826	CLA	O2A-CGA-CBA	3.12	121.96	111.93
10	cA	804	CLA	C1D-CHD-C4C	-3.12	118.22	122.48
10	aB	824	CLA	CAA-C2A-C3A	-3.12	104.23	112.78
10	bA	812	CLA	C3B-C4B-NB	3.12	113.25	109.21
10	cB	818	CLA	C1D-CHD-C4C	-3.12	118.22	122.48
10	cA	830	CLA	CAC-C3C-C4C	3.12	128.90	124.82
10	bB	804	CLA	CAC-C3C-C4C	3.12	128.90	124.82
10	cA	839	CLA	CAC-C3C-C4C	3.12	128.90	124.82
10	bA	833	CLA	C3B-C4B-NB	3.12	113.24	109.21
10	aA	810	CLA	CAC-C3C-C4C	3.12	128.90	124.82
10	bA	826	CLA	O2A-CGA-CBA	3.12	121.94	111.93
10	bB	810	CLA	C4C-C3C-C2C	-3.12	102.37	106.89
10	aB	818	CLA	C1D-CHD-C4C	-3.12	118.22	122.48
10	aB	829	CLA	C4C-C3C-C2C	-3.12	102.38	106.89
10	aB	833	CLA	CHC-C1C-C2C	-3.12	118.11	126.71
10	cB	839	CLA	C3B-C4B-NB	3.12	113.24	109.21
10	bB	817	CLA	CHC-C1C-C2C	-3.12	118.12	126.71
10	cB	807	CLA	C1D-CHD-C4C	-3.12	118.22	122.48
10	aB	810	CLA	C4A-NA-C1A	-3.12	105.31	106.71
10	aB	804	CLA	CAC-C3C-C4C	3.12	128.89	124.82
10	cA	826	CLA	O2A-CGA-CBA	3.12	121.93	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	806	CLA	CHD-C4C-NC	3.11	129.11	124.20
10	cB	833	CLA	CHC-C1C-C2C	-3.11	118.12	126.71
10	aB	823	CLA	CHC-C1C-C2C	-3.11	118.12	126.71
10	cB	835	CLA	C1D-CHD-C4C	-3.11	118.23	122.48
10	cA	828	CLA	C4C-C3C-C2C	-3.11	102.38	106.89
10	bA	839	CLA	CAC-C3C-C4C	3.11	128.89	124.82
10	aA	804	CLA	C1D-CHD-C4C	-3.11	118.23	122.48
10	cB	805	CLA	CMB-C2B-C3B	3.11	130.63	124.80
10	cB	813	CLA	C3B-C4B-NB	3.11	113.23	109.21
10	aA	843	CLA	CHC-C1C-C2C	-3.11	118.14	126.71
10	bB	839	CLA	C3B-C4B-NB	3.11	113.23	109.21
10	aA	830	CLA	CAC-C3C-C4C	3.11	128.88	124.82
10	cA	812	CLA	C3B-C4B-NB	3.11	113.23	109.21
10	aB	810	CLA	CAC-C3C-C4C	3.11	128.88	124.82
10	bB	805	CLA	CMB-C2B-C3B	3.11	130.63	124.80
10	cB	806	CLA	CHD-C4C-NC	3.11	129.10	124.20
10	bB	836	CLA	C1D-CHD-C4C	-3.11	118.24	122.48
10	cB	827	CLA	CHD-C4C-NC	3.11	129.10	124.20
10	bA	830	CLA	CAC-C3C-C4C	3.11	128.88	124.82
10	bA	843	CLA	CHC-C1C-C2C	-3.11	118.14	126.71
10	aA	828	CLA	C4C-C3C-C2C	-3.11	102.39	106.89
10	cB	817	CLA	CHC-C1C-C2C	-3.11	118.15	126.71
10	aB	812	CLA	CAA-C2A-C3A	-3.11	104.27	112.78
10	cB	810	CLA	CAC-C3C-C4C	3.10	128.88	124.82
10	cA	838	CLA	C4C-C3C-C2C	-3.10	102.39	106.89
10	cB	823	CLA	CHC-C1C-C2C	-3.10	118.15	126.71
10	bB	835	CLA	C1D-CHD-C4C	-3.10	118.24	122.48
10	aB	802	CLA	C3B-C4B-NB	3.10	113.22	109.21
10	cB	837	CLA	CAC-C3C-C4C	3.10	128.87	124.82
10	cB	825	CLA	O2D-CGD-O1D	-3.10	117.70	123.83
10	bA	822	CLA	O2D-CGD-O1D	-3.10	117.70	123.83
10	bA	837	CLA	C4C-C3C-C2C	-3.10	102.40	106.89
10	bB	813	CLA	C3B-C4B-NB	3.10	113.22	109.21
10	cA	811	CLA	CHC-C1C-C2C	-3.10	118.16	126.71
10	cA	843	CLA	CHC-C1C-C2C	-3.10	118.16	126.71
10	aB	822	CLA	CHD-C4C-NC	3.10	129.09	124.20
10	aB	825	CLA	O2D-CGD-O1D	-3.10	117.71	123.83
10	cA	822	CLA	O2D-CGD-O1D	-3.10	117.71	123.83
10	cB	833	CLA	C1C-C2C-C3C	-3.10	103.67	106.95
10	aB	826	CLA	O2D-CGD-O1D	-3.10	117.71	123.83
10	aB	806	CLA	CHD-C4C-NC	3.10	129.09	124.20
10	bB	817	CLA	CAC-C3C-C4C	3.10	128.87	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	838	CLA	C4C-C3C-C2C	-3.10	102.40	106.89
10	aA	822	CLA	C4C-C3C-C2C	-3.10	102.40	106.89
10	bB	825	CLA	O2D-CGD-O1D	-3.10	117.71	123.83
10	aB	813	CLA	C3B-C4B-NB	3.10	113.21	109.21
10	aA	822	CLA	O2D-CGD-O1D	-3.10	117.72	123.83
10	aB	819	CLA	CMB-C2B-C3B	3.09	130.60	124.80
10	aA	839	CLA	CHC-C1C-C2C	-3.09	118.18	126.71
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	bB	805	CLA	CHC-C1C-C2C	-3.09	118.18	126.71
10	bB	801	CLA	C4C-C3C-C2C	-3.09	102.41	106.89
10	bA	838	CLA	C4C-C3C-C2C	-3.09	102.41	106.89
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	836	CLA	C1D-CHD-C4C	-3.09	118.26	122.48
10	cA	837	CLA	C4C-C3C-C2C	-3.09	102.41	106.89
10	aB	838	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
10	aA	807	CLA	C1D-CHD-C4C	-3.09	118.26	122.48
10	cB	805	CLA	CHB-C4A-NA	3.09	128.79	124.51
10	bA	806	CLA	CAC-C3C-C4C	3.09	128.86	124.82
10	aB	805	CLA	CMB-C2B-C3B	3.09	130.59	124.80
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	cB	805	CLA	CHC-C1C-C2C	-3.09	118.20	126.71
10	bB	810	CLA	CAC-C3C-C4C	3.09	128.85	124.82
10	cB	838	CLA	CAA-C2A-C3A	-3.09	104.33	112.78
10	aB	839	CLA	C3B-C4B-NB	3.08	113.20	109.21
10	aA	837	CLA	C3B-C4B-NB	3.08	113.20	109.21
10	bB	833	CLA	C1C-C2C-C3C	-3.08	103.68	106.95
10	bB	811	CLA	C4C-C3C-C2C	-3.08	102.42	106.89
10	cA	828	CLA	C1-C2-C3	-3.08	120.71	126.04
10	cA	839	CLA	CHC-C1C-C2C	-3.08	118.21	126.71
10	aB	801	CLA	C4C-C3C-C2C	-3.08	102.42	106.89
10	aA	839	CLA	CAC-C3C-C4C	3.08	128.85	124.82
10	aA	828	CLA	C1-C2-C3	-3.08	120.71	126.04
10	aA	811	CLA	CHC-C1C-C2C	-3.08	118.21	126.71
10	cB	836	CLA	C1D-CHD-C4C	-3.08	118.27	122.48
10	aB	805	CLA	CHB-C4A-NA	3.08	128.77	124.51
10	cA	806	CLA	CAC-C3C-C4C	3.08	128.85	124.82
10	bA	840	CLA	C4C-C3C-C2C	-3.08	102.43	106.89
10	bA	825	CLA	C4-C3-C5	3.08	120.59	115.29
10	bB	819	CLA	CMB-C2B-C3B	3.08	130.58	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	832	CLA	C3B-C4B-NB	3.08	113.19	109.21
10	aB	818	CLA	C4C-C3C-C2C	-3.08	102.43	106.89
10	bB	838	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
10	aB	806	CLA	C4C-C3C-C2C	-3.08	102.43	106.89
10	bA	811	CLA	CHC-C1C-C2C	-3.08	118.22	126.71
10	bB	806	CLA	C4C-C3C-C2C	-3.08	102.43	106.89
10	cB	826	CLA	O2D-CGD-O1D	-3.08	117.75	123.83
10	aA	819	CLA	CHC-C1C-C2C	-3.08	118.22	126.71
10	cB	821	CLA	C4A-NA-C1A	-3.08	105.32	106.71
10	bA	839	CLA	CHC-C1C-C2C	-3.08	118.23	126.71
10	aA	840	CLA	C4C-C3C-C2C	-3.08	102.43	106.89
10	bB	801	CLA	O2D-CGD-O1D	-3.08	117.75	123.83
10	cB	819	CLA	CMB-C2B-C3B	3.08	130.57	124.80
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	aB	833	CLA	C1C-C2C-C3C	-3.08	103.69	106.95
10	aB	817	CLA	CAC-C3C-C4C	3.08	128.84	124.82
10	cB	801	CLA	C4C-C3C-C2C	-3.07	102.44	106.89
10	aA	842	CLA	CMA-C3A-C2A	-3.07	101.39	113.78
10	bB	818	CLA	C1D-CHD-C4C	-3.07	118.28	122.48
10	cA	833	CLA	C3B-C4B-NB	3.07	113.18	109.21
10	bA	807	CLA	CAC-C3C-C4C	3.07	128.84	124.82
10	aB	833	CLA	CAA-C2A-C3A	-3.07	104.36	112.78
10	aB	801	CLA	O2D-CGD-O1D	-3.07	117.76	123.83
10	aA	804	CLA	C4-C3-C5	3.07	120.58	115.29
10	bB	837	CLA	CAC-C3C-C4C	3.07	128.84	124.82
10	aB	811	CLA	C4C-C3C-C2C	-3.07	102.44	106.89
10	aA	818	CLA	O2D-CGD-O1D	-3.07	117.76	123.83
10	aA	837	CLA	C4C-C3C-C2C	-3.07	102.44	106.89
10	cA	806	CLA	C4-C3-C5	3.07	119.55	115.99
10	cB	827	CLA	O2A-CGA-CBA	3.07	121.79	111.93
10	bA	822	CLA	C4C-C3C-C2C	-3.07	102.44	106.89
10	aB	827	CLA	O2A-CGA-CBA	3.07	121.78	111.93
10	bB	827	CLA	O2A-CGA-CBA	3.07	121.78	111.93
10	cA	833	CLA	CHD-C4C-NC	3.07	129.04	124.20
10	bB	826	CLA	O2D-CGD-O1D	-3.07	117.77	123.83
10	bA	819	CLA	CHC-C1C-C2C	-3.07	118.25	126.71
10	bA	842	CLA	CMA-C3A-C2A	-3.07	101.41	113.78
10	cB	801	CLA	CHC-C1C-C2C	-3.07	118.25	126.71
10	cB	802	CLA	C3B-C4B-NB	3.07	113.17	109.21
10	cB	821	CLA	CHC-C1C-C2C	-3.07	118.25	126.71
10	bA	828	CLA	C1-C2-C3	-3.07	120.74	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	802	CLA	C4C-C3C-C2C	-3.07	102.45	106.89
10	aA	806	CLA	CAC-C3C-C4C	3.07	128.83	124.82
10	aA	833	CLA	C3B-C4B-NB	3.07	113.17	109.21
10	bA	807	CLA	C1D-CHD-C4C	-3.07	118.30	122.48
10	aB	821	CLA	CHC-C1C-C2C	-3.07	118.26	126.71
10	bB	833	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
10	cA	842	CLA	CMA-C3A-C2A	-3.06	101.43	113.78
10	cB	811	CLA	C4C-C3C-C2C	-3.06	102.45	106.89
10	bA	812	CLA	C1-C2-C3	-3.06	120.74	126.04
10	aB	834	CLA	C3B-C4B-NB	3.06	113.17	109.21
10	cA	822	CLA	C4C-C3C-C2C	-3.06	102.45	106.89
10	aA	812	CLA	C1-C2-C3	-3.06	120.75	126.04
10	aA	808	CLA	C4C-C3C-C2C	-3.06	102.45	106.89
10	bB	830	CLA	C1D-CHD-C4C	-3.06	118.30	122.48
10	bA	818	CLA	O2D-CGD-O1D	-3.06	117.78	123.83
10	aA	805	CLA	CHD-C4C-NC	3.06	129.03	124.20
10	aB	827	CLA	CHD-C4C-NC	3.06	129.03	124.20
10	bB	821	CLA	CHC-C1C-C2C	-3.06	118.27	126.71
10	aB	832	CLA	C3B-C4B-NB	3.06	113.17	109.21
10	bB	821	CLA	C4A-NA-C1A	-3.06	105.33	106.71
10	aA	826	CLA	C1C-C2C-C3C	-3.06	103.71	106.95
10	aB	801	CLA	CHC-C1C-C2C	-3.06	118.27	126.71
10	bA	821	CLA	CHC-C1C-C2C	-3.06	118.28	126.71
10	cA	819	CLA	CHC-C1C-C2C	-3.06	118.28	126.71
10	bB	801	CLA	CHC-C1C-C2C	-3.06	118.28	126.71
10	cB	807	CLA	CHC-C1C-C2C	-3.06	118.28	126.71
10	cB	801	CLA	O2D-CGD-O1D	-3.06	117.79	123.83
10	aB	837	CLA	CAC-C3C-C4C	3.06	128.82	124.82
10	cL	204	CLA	C4A-NA-C1A	-3.06	105.33	106.71
10	aB	807	CLA	CHC-C1C-C2C	-3.06	118.28	126.71
10	cB	817	CLA	CAC-C3C-C4C	3.06	128.82	124.82
10	cA	807	CLA	C1D-CHD-C4C	-3.06	118.31	122.48
10	cA	821	CLA	CHC-C1C-C2C	-3.06	118.28	126.71
10	aA	825	CLA	C4-C3-C5	3.06	120.55	115.29
10	cB	806	CLA	C4C-C3C-C2C	-3.06	102.47	106.89
10	bB	832	CLA	C3B-C4B-NB	3.06	113.16	109.21
9	aA	801	CL0	CHC-C1C-C2C	-3.05	118.29	126.71
10	aA	831	CLA	C4A-NA-C1A	-3.05	105.33	106.71
10	cA	804	CLA	C4-C3-C5	3.05	120.55	115.29
10	cA	805	CLA	CHD-C4C-NC	3.05	129.01	124.20
10	cA	812	CLA	C1D-CHD-C4C	-3.05	118.31	122.48
10	cA	807	CLA	CAC-C3C-C4C	3.05	128.81	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	816	CLA	C3B-C4B-NB	3.05	113.16	109.21
10	cB	802	CLA	C4C-C3C-C2C	-3.05	102.47	106.89
10	aA	812	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
10	aB	807	CLA	C4C-C3C-C2C	-3.05	102.47	106.89
10	aA	807	CLA	CAC-C3C-C4C	3.05	128.81	124.82
10	cA	825	CLA	C4-C3-C5	3.05	120.54	115.29
10	cB	834	CLA	CHC-C1C-C2C	-3.05	118.30	126.71
10	cA	818	CLA	O2D-CGD-O1D	-3.05	117.81	123.83
10	cA	840	CLA	C4C-C3C-C2C	-3.05	102.47	106.89
10	cB	818	CLA	C4C-C3C-C2C	-3.05	102.47	106.89
10	bB	807	CLA	CHC-C1C-C2C	-3.05	118.31	126.71
11	aA	844	PQN	C11-C12-C13	-3.05	121.72	126.79
10	bB	802	CLA	C4C-C3C-C2C	-3.05	102.48	106.89
10	aB	804	CLA	CMC-C2C-C1C	3.05	129.67	125.03
10	aB	834	CLA	CHC-C1C-C2C	-3.05	118.31	126.71
10	aA	830	CLA	CHC-C1C-C2C	-3.05	118.31	126.71
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	810	CLA	C4C-C3C-C2C	-3.04	102.48	106.89
10	bA	804	CLA	C4-C3-C5	3.04	120.53	115.29
10	aA	833	CLA	CHD-C4C-NC	3.04	129.00	124.20
10	aA	812	CLA	C1D-CHD-C4C	-3.04	118.32	122.48
10	bA	812	CLA	C1D-CHD-C4C	-3.04	118.32	122.48
10	bB	807	CLA	C4C-C3C-C2C	-3.04	102.48	106.89
10	cB	807	CLA	C4C-C3C-C2C	-3.04	102.48	106.89
10	bA	812	CLA	CAA-C2A-C3A	-3.04	104.44	112.78
10	bB	834	CLA	CHC-C1C-C2C	-3.04	118.32	126.71
10	bA	830	CLA	CHC-C1C-C2C	-3.04	118.32	126.71
9	bA	801	CL0	CHC-C1C-C2C	-3.04	118.32	126.71
10	cL	202	CLA	C3B-C4B-NB	3.04	113.14	109.21
10	cB	830	CLA	C1D-CHD-C4C	-3.04	118.33	122.48
10	bA	810	CLA	C4C-C3C-C2C	-3.04	102.49	106.89
10	bA	825	CLA	C4C-C3C-C2C	-3.04	102.49	106.89
10	cA	802	CLA	C4C-C3C-C2C	-3.04	102.49	106.89
10	aA	821	CLA	CHC-C1C-C2C	-3.04	118.33	126.71
10	aB	839	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
10	bB	827	CLA	CMB-C2B-C3B	3.04	130.50	124.80
10	bB	839	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
9	cA	801	CL0	CHC-C1C-C2C	-3.04	118.33	126.71
10	aB	815	CLA	CHC-C1C-C2C	-3.04	118.33	126.71
10	cA	825	CLA	C4C-C3C-C2C	-3.04	102.49	106.89
10	cB	829	CLA	C4-C3-C5	3.04	120.52	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	839	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
10	aB	809	CLA	O2D-CGD-O1D	-3.04	117.83	123.83
10	cA	808	CLA	C4C-C3C-C2C	-3.04	102.49	106.89
10	bL	202	CLA	C3B-C4B-NB	3.04	113.14	109.21
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	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	aB	830	CLA	C1D-CHD-C4C	-3.03	118.34	122.48
10	cA	812	CLA	C1-C2-C3	-3.03	120.80	126.04
10	bA	826	CLA	C1C-C2C-C3C	-3.03	103.74	106.95
10	cA	830	CLA	CHC-C1C-C2C	-3.03	118.35	126.71
10	bA	837	CLA	C3B-C4B-NB	3.03	113.13	109.21
10	bB	812	CLA	C4C-C3C-C2C	-3.03	102.50	106.89
10	cB	834	CLA	C3B-C4B-NB	3.03	113.13	109.21
10	bA	833	CLA	CHC-C1C-C2C	-3.03	118.35	126.71
10	bB	834	CLA	C1D-CHD-C4C	-3.03	118.34	122.48
10	cB	815	CLA	CHC-C1C-C2C	-3.03	118.35	126.71
10	cB	803	CLA	CMC-C2C-C1C	3.03	129.64	125.03
10	aA	825	CLA	C4C-C3C-C2C	-3.03	102.50	106.89
10	bA	820	CLA	C4C-C3C-C2C	-3.03	102.50	106.89
10	cA	819	CLA	C4C-C3C-C2C	-3.03	102.50	106.89
10	bA	804	CLA	CAC-C3C-C4C	3.03	128.78	124.82
10	aA	805	CLA	CMB-C2B-C3B	3.03	130.48	124.80
10	cB	804	CLA	CMC-C2C-C1C	3.03	129.64	125.03
10	bL	205	CLA	C4C-C3C-C2C	-3.03	102.50	106.89
10	cA	812	CLA	CAA-C2A-C3A	-3.03	104.48	112.78
10	cA	817	CLA	CHD-C4C-NC	3.03	128.97	124.20
10	cA	804	CLA	CAC-C3C-C4C	3.03	128.78	124.82
10	bB	826	CLA	C3B-C4B-NB	3.03	113.12	109.21
10	cA	837	CLA	C3B-C4B-NB	3.03	113.12	109.21
10	cB	816	CLA	O2D-CGD-O1D	-3.03	117.86	123.83
10	aA	806	CLA	C4-C3-C5	3.02	119.50	115.99
10	cA	814	CLA	C3B-C4B-NB	3.02	113.12	109.21
10	aA	819	CLA	CAC-C3C-C4C	3.02	128.77	124.82
10	aA	820	CLA	C4C-C3C-C2C	-3.02	102.51	106.89
10	aB	814	CLA	C1D-CHD-C4C	-3.02	118.35	122.48
10	aA	833	CLA	CHC-C1C-C2C	-3.02	118.38	126.71
10	cA	820	CLA	C4C-C3C-C2C	-3.02	102.51	106.89
10	bA	807	CLA	CMC-C2C-C1C	3.02	129.63	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aL	202	CLA	C3B-C4B-NB	3.02	113.12	109.21
13	cB	846	BCR	C15-C16-C17	-3.02	117.16	123.51
10	cB	827	CLA	CMB-C2B-C3B	3.02	130.46	124.80
10	aB	826	CLA	C3B-C4B-NB	3.02	113.11	109.21
10	aA	819	CLA	C4C-C3C-C2C	-3.02	102.52	106.89
10	bB	829	CLA	C4-C3-C5	3.02	120.49	115.29
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	bB	815	CLA	CHC-C1C-C2C	-3.02	118.39	126.71
10	aB	803	CLA	CMC-C2C-C1C	3.02	129.62	125.03
10	bB	819	CLA	CAA-C2A-C3A	-3.02	104.52	112.78
10	aB	819	CLA	CAA-C2A-C3A	-3.02	104.52	112.78
10	cA	826	CLA	C1C-C2C-C3C	-3.02	103.75	106.95
10	bA	836	CLA	C1-C2-C3	-3.02	120.83	126.04
10	aA	856	CLA	C4C-C3C-C2C	-3.02	102.52	106.89
10	cB	819	CLA	CAA-C2A-C3A	-3.01	104.52	112.78
10	cA	819	CLA	CAC-C3C-C4C	3.01	128.76	124.82
10	bA	806	CLA	C4-C3-C5	3.01	119.49	115.99
10	bA	811	CLA	C3B-C4B-NB	3.01	113.11	109.21
10	cL	205	CLA	C4C-C3C-C2C	-3.01	102.53	106.89
10	bB	803	CLA	CMC-C2C-C1C	3.01	129.62	125.03
10	aA	804	CLA	CAC-C3C-C4C	3.01	128.76	124.82
10	bA	805	CLA	CMB-C2B-C3B	3.01	130.45	124.80
10	cA	833	CLA	CHC-C1C-C2C	-3.01	118.41	126.71
10	cA	805	CLA	CMB-C2B-C3B	3.01	130.45	124.80
10	cB	831	CLA	CHC-C1C-C2C	-3.01	118.41	126.71
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	809	CLA	O2D-CGD-O1D	-3.01	117.89	123.83
10	aA	816	CLA	O2D-CGD-O1D	-3.01	117.89	123.83
10	cB	818	CLA	C3B-C4B-NB	3.01	113.10	109.21
10	cB	834	CLA	C1D-CHD-C4C	-3.01	118.37	122.48
10	aB	834	CLA	C1D-CHD-C4C	-3.01	118.37	122.48
13	aB	846	BCR	C15-C16-C17	-3.01	117.19	123.51
10	aA	811	CLA	C3B-C4B-NB	3.01	113.10	109.21
10	bA	803	CLA	C4C-C3C-C2C	-3.01	102.53	106.89
10	aB	829	CLA	C4-C3-C5	3.01	120.47	115.29
10	cA	803	CLA	C4C-C3C-C2C	-3.01	102.53	106.89
10	cB	826	CLA	C3B-C4B-NB	3.01	113.10	109.21
10	bB	832	CLA	CHD-C4C-NC	3.01	128.94	124.20
10	aA	810	CLA	C4C-C3C-C2C	-3.01	102.54	106.89
10	cA	807	CLA	CMC-C2C-C1C	3.01	129.60	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	838	CLA	C3B-C4B-NB	3.01	113.09	109.21
10	aA	842	CLA	CBC-CAC-C3C	-3.00	104.09	112.43
10	bB	804	CLA	CMC-C2C-C1C	3.00	129.60	125.03
10	cB	814	CLA	C1D-CHD-C4C	-3.00	118.38	122.48
10	bA	810	CLA	CHC-C1C-C2C	-3.00	118.43	126.71
10	bA	836	CLA	CHC-C1C-C2C	-3.00	118.43	126.71
10	aA	802	CLA	C4C-C3C-C2C	-3.00	102.54	106.89
10	bA	819	CLA	CAC-C3C-C4C	3.00	128.74	124.82
10	cA	836	CLA	CHC-C1C-C2C	-3.00	118.43	126.71
10	aA	836	CLA	CHC-C1C-C2C	-3.00	118.43	126.71
10	cB	812	CLA	C4C-C3C-C2C	-3.00	102.54	106.89
10	bA	816	CLA	CHD-C4C-NC	3.00	128.93	124.20
10	aB	812	CLA	C4C-C3C-C2C	-3.00	102.54	106.89
10	aA	818	CLA	CBA-CAA-C2A	3.00	122.78	113.85
13	bB	846	BCR	C15-C16-C17	-3.00	117.20	123.51
10	bB	808	CLA	C4C-C3C-C2C	-3.00	102.55	106.89
10	bB	818	CLA	C4C-C3C-C2C	-3.00	102.55	106.89
10	cA	811	CLA	C3B-C4B-NB	3.00	113.09	109.21
10	cA	818	CLA	C4C-C3C-C2C	-3.00	102.55	106.89
10	bA	802	CLA	C4C-C3C-C2C	-3.00	102.55	106.89
10	bB	816	CLA	O2D-CGD-O1D	-3.00	117.91	123.83
10	bA	808	CLA	C4C-C3C-C2C	-3.00	102.55	106.89
10	cA	856	CLA	C4C-C3C-C2C	-3.00	102.55	106.89
10	cB	808	CLA	C4C-C3C-C2C	-3.00	102.55	106.89
10	aB	816	CLA	O2D-CGD-O1D	-3.00	117.91	123.83
10	aA	816	CLA	CHD-C4C-NC	3.00	128.93	124.20
10	cA	816	CLA	O2D-CGD-O1D	-3.00	117.91	123.83
10	bB	825	CLA	CMB-C2B-C3B	3.00	130.42	124.80
10	cA	842	CLA	CBC-CAC-C3C	-3.00	104.11	112.43
10	aB	831	CLA	CHC-C1C-C2C	-3.00	118.45	126.71
10	bA	856	CLA	C4C-C3C-C2C	-2.99	102.55	106.89
10	aL	205	CLA	C4C-C3C-C2C	-2.99	102.55	106.89
10	cB	815	CLA	C4C-C3C-C2C	-2.99	102.55	106.89
10	aB	827	CLA	C1C-C2C-C3C	-2.99	103.78	106.95
10	aA	816	CLA	C4C-C3C-C2C	-2.99	102.55	106.89
10	cA	818	CLA	CBA-CAA-C2A	2.99	122.76	113.85
10	aB	832	CLA	CHD-C4C-NC	2.99	128.92	124.20
10	bA	818	CLA	CBA-CAA-C2A	2.99	122.76	113.85
10	aB	827	CLA	CMB-C2B-C3B	2.99	130.41	124.80
10	bB	802	CLA	CHC-C1C-C2C	-2.99	118.46	126.71
10	aA	836	CLA	C1-C2-C3	-2.99	120.87	126.04
10	aA	811	CLA	C4C-C3C-C2C	-2.99	102.56	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	809	CLA	O2D-CGD-O1D	-2.99	117.92	123.83
10	aB	825	CLA	CMB-C2B-C3B	2.99	130.41	124.80
10	cB	825	CLA	C1C-C2C-C3C	-2.99	103.78	106.95
10	aA	803	CLA	C4C-C3C-C2C	-2.99	102.56	106.89
10	aB	808	CLA	C4C-C3C-C2C	-2.99	102.56	106.89
10	cB	802	CLA	CHC-C1C-C2C	-2.99	118.47	126.71
10	bB	827	CLA	CHC-C1C-C2C	-2.99	118.47	126.71
10	aA	815	CLA	CHD-C4C-NC	2.99	128.91	124.20
10	cB	826	CLA	CAC-C3C-C4C	2.99	128.73	124.82
10	bB	825	CLA	C1C-C2C-C3C	-2.99	103.78	106.95
10	aB	827	CLA	CHC-C1C-C2C	-2.99	118.47	126.71
10	bB	818	CLA	C3B-C4B-NB	2.99	113.07	109.21
10	bA	817	CLA	CHD-C4C-NC	2.99	128.91	124.20
10	cA	810	CLA	CHC-C1C-C2C	-2.99	118.48	126.71
10	bA	814	CLA	C3B-C4B-NB	2.99	113.07	109.21
10	bA	842	CLA	CBC-CAC-C3C	-2.99	104.14	112.43
10	bA	819	CLA	C4C-C3C-C2C	-2.99	102.57	106.89
10	cA	816	CLA	CHD-C4C-NC	2.99	128.91	124.20
10	bB	806	CLA	CAC-C3C-C4C	2.98	128.72	124.82
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	aB	809	CLA	C3B-C4B-NB	2.98	113.07	109.21
10	aA	807	CLA	CMC-C2C-C1C	2.98	129.57	125.03
10	bA	826	CLA	CHD-C4C-NC	2.98	128.90	124.20
10	cA	812	CLA	C4C-C3C-C2C	-2.98	102.57	106.89
10	aA	843	CLA	C4C-C3C-C2C	-2.98	102.57	106.89
10	cA	815	CLA	CHD-C4C-NC	2.98	128.90	124.20
10	cB	827	CLA	CHC-C1C-C2C	-2.98	118.49	126.71
10	aA	810	CLA	CHC-C1C-C2C	-2.98	118.49	126.71
10	cB	825	CLA	CMB-C2B-C3B	2.98	130.39	124.80
10	bB	831	CLA	CHC-C1C-C2C	-2.98	118.50	126.71
10	cB	822	CLA	C4A-NA-C1A	-2.98	105.37	106.71
10	aA	817	CLA	CHD-C4C-NC	2.98	128.90	124.20
10	cB	825	CLA	O2A-CGA-CBA	2.98	121.49	111.93
10	cA	843	CLA	C4C-C3C-C2C	-2.98	102.58	106.89
10	bA	843	CLA	C4C-C3C-C2C	-2.98	102.58	106.89
10	cA	854	CLA	C3B-C4B-NB	2.97	113.06	109.21
10	aA	838	CLA	O2A-CGA-CBA	2.97	121.48	111.93
10	cA	816	CLA	C4C-C3C-C2C	-2.97	102.58	106.89
10	aB	818	CLA	CAC-C3C-C4C	2.97	128.70	124.82
10	aB	808	CLA	CAA-C2A-C3A	-2.97	104.64	112.78
10	cL	205	CLA	CAC-C3C-C4C	2.97	128.70	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	825	CLA	O2A-CGA-CBA	2.97	121.47	111.93
10	aB	802	CLA	CHC-C1C-C2C	-2.97	118.52	126.71
10	bB	825	CLA	O2A-CGA-CBA	2.97	121.47	111.93
10	cA	803	CLA	O2D-CGD-O1D	-2.97	117.97	123.83
10	bB	808	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
10	bB	815	CLA	C4C-C3C-C2C	-2.97	102.59	106.89
10	cA	830	CLA	O2A-CGA-CBA	2.97	121.46	111.93
10	bA	816	CLA	O2D-CGD-O1D	-2.97	117.97	123.83
10	bB	809	CLA	C3B-C4B-NB	2.97	113.05	109.21
10	cA	838	CLA	O2A-CGA-CBA	2.97	121.46	111.93
10	aB	833	CLA	C4-C3-C5	2.97	120.40	115.29
10	bA	838	CLA	O2A-CGA-CBA	2.97	121.46	111.93
10	aA	830	CLA	O2A-CGA-CBA	2.97	121.45	111.93
10	bB	831	CLA	C1D-CHD-C4C	-2.97	118.43	122.48
10	cB	831	CLA	C1D-CHD-C4C	-2.97	118.43	122.48
10	cB	809	CLA	C3B-C4B-NB	2.97	113.05	109.21
10	bB	837	CLA	C3B-C4B-NB	2.96	113.04	109.21
10	bB	814	CLA	C1D-CHD-C4C	-2.96	118.43	122.48
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	cB	839	CLA	O2D-CGD-O1D	-2.96	117.98	123.83
10	aB	815	CLA	C4C-C3C-C2C	-2.96	102.60	106.89
10	cB	806	CLA	CAC-C3C-C4C	2.96	128.69	124.82
10	cA	811	CLA	C4C-C3C-C2C	-2.96	102.60	106.89
10	aA	818	CLA	C4C-C3C-C2C	-2.96	102.60	106.89
10	bA	811	CLA	C4C-C3C-C2C	-2.96	102.60	106.89
10	cA	817	CLA	C4-C3-C5	2.96	120.39	115.29
10	aB	822	CLA	C4A-NA-C1A	-2.96	105.38	106.71
10	aB	807	CLA	CMB-C2B-C3B	2.96	130.35	124.80
10	bA	825	CLA	O2D-CGD-O1D	-2.96	117.98	123.83
10	aB	806	CLA	CAC-C3C-C4C	2.96	128.69	124.82
10	aB	837	CLA	C3B-C4B-NB	2.96	113.04	109.21
10	aL	203	CLA	C1D-CHD-C4C	-2.96	118.44	122.48
10	bA	815	CLA	CHD-C4C-NC	2.96	128.87	124.20
10	bA	818	CLA	C4C-C3C-C2C	-2.96	102.61	106.89
10	cB	839	CLA	CHC-C1C-C2C	-2.96	118.55	126.71
10	bB	803	CLA	C4A-NA-C1A	-2.96	105.38	106.71
10	aB	839	CLA	CHC-C1C-C2C	-2.96	118.56	126.71
10	cA	822	CLA	CHD-C4C-NC	2.96	128.86	124.20
10	aA	822	CLA	CHD-C4C-NC	2.96	128.86	124.20
10	bA	828	CLA	CMC-C2C-C1C	2.96	129.53	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	825	CLA	C1C-C2C-C3C	-2.96	103.82	106.95
10	cB	808	CLA	CAA-C2A-C3A	-2.96	104.68	112.78
10	bA	830	CLA	O2A-CGA-CBA	2.96	121.42	111.93
10	cA	841	CLA	C3B-C4B-NB	2.95	113.03	109.21
10	bB	839	CLA	CHC-C1C-C2C	-2.95	118.57	126.71
10	aB	839	CLA	O2D-CGD-O1D	-2.95	118.00	123.83
10	bA	834	CLA	O2A-CGA-CBA	2.95	121.41	111.93
10	aB	805	CLA	C1D-CHD-C4C	-2.95	118.45	122.48
10	bA	812	CLA	C4C-C3C-C2C	-2.95	102.61	106.89
10	bB	827	CLA	C1C-C2C-C3C	-2.95	103.82	106.95
10	cA	843	CLA	C1D-CHD-C4C	-2.95	118.45	122.48
10	bL	205	CLA	CAC-C3C-C4C	2.95	128.68	124.82
10	bB	816	CLA	CHC-C1C-C2C	-2.95	118.57	126.71
10	bA	816	CLA	C4C-C3C-C2C	-2.95	102.62	106.89
10	bA	812	CLA	CAC-C3C-C4C	2.95	128.68	124.82
10	aB	838	CLA	C4C-C3C-C2C	-2.95	102.62	106.89
10	bB	838	CLA	C3B-C4B-NB	2.95	113.02	109.21
10	cB	818	CLA	CAC-C3C-C4C	2.95	128.67	124.82
10	cB	827	CLA	C1C-C2C-C3C	-2.95	103.83	106.95
10	cB	811	CLA	CAC-C3C-C4C	2.95	128.67	124.82
10	bA	826	CLA	OBD-CAD-C3D	-2.95	122.82	128.04
10	cA	809	CLA	CHD-C4C-NC	2.95	128.85	124.20
10	bB	839	CLA	O2D-CGD-O1D	-2.95	118.01	123.83
10	bA	804	CLA	CHC-C1C-C2C	-2.95	118.58	126.71
9	cA	801	CL0	CBC-CAC-C3C	-2.95	104.25	112.43
10	cA	826	CLA	CHD-C4C-NC	2.95	128.85	124.20
10	aL	205	CLA	CAC-C3C-C4C	2.95	128.67	124.82
10	aA	817	CLA	C4-C3-C5	2.95	120.36	115.29
10	aB	814	CLA	CHC-C1C-C2C	-2.94	118.59	126.71
10	bB	826	CLA	CAC-C3C-C4C	2.94	128.67	124.82
10	aA	826	CLA	OBD-CAD-C3D	-2.94	122.83	128.04
10	bA	809	CLA	CHD-C4C-NC	2.94	128.84	124.20
10	bB	805	CLA	C1D-CHD-C4C	-2.94	118.46	122.48
10	aB	816	CLA	CHC-C1C-C2C	-2.94	118.60	126.71
10	aA	804	CLA	CHC-C1C-C2C	-2.94	118.60	126.71
10	aA	812	CLA	C4C-C3C-C2C	-2.94	102.63	106.89
10	cA	836	CLA	CAC-C3C-C4C	2.94	128.67	124.82
10	aA	834	CLA	O2A-CGA-CBA	2.94	121.38	111.93
10	cA	826	CLA	OBD-CAD-C3D	-2.94	122.83	128.04
10	bA	843	CLA	C1D-CHD-C4C	-2.94	118.46	122.48
10	cB	816	CLA	CHC-C1C-C2C	-2.94	118.60	126.71
10	bB	807	CLA	CMB-C2B-C3B	2.94	130.32	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	837	CLA	O2D-CGD-O1D	-2.94	118.02	123.83
10	aA	837	CLA	O2D-CGD-O1D	-2.94	118.02	123.83
10	aA	843	CLA	C1D-CHD-C4C	-2.94	118.47	122.48
10	bA	813	CLA	C4C-C3C-C2C	-2.94	102.63	106.89
11	aA	844	PQN	C14-C13-C15	2.94	120.35	115.29
10	bB	811	CLA	CAC-C3C-C4C	2.94	128.66	124.82
10	aA	813	CLA	C4C-C3C-C2C	-2.94	102.63	106.89
10	aB	830	CLA	C4C-C3C-C2C	-2.94	102.63	106.89
10	aA	803	CLA	O2D-CGD-O1D	-2.94	118.03	123.83
10	bA	821	CLA	CAA-C2A-C3A	-2.94	104.73	112.78
10	bB	830	CLA	C4C-C3C-C2C	-2.94	102.63	106.89
10	bA	836	CLA	CBC-CAC-C3C	-2.94	104.27	112.43
10	bA	832	CLA	C4C-C3C-C2C	-2.94	102.64	106.89
10	aA	836	CLA	CBC-CAC-C3C	-2.94	104.27	112.43
10	cA	811	CLA	O2D-CGD-O1D	-2.94	118.03	123.83
10	aA	811	CLA	O2D-CGD-O1D	-2.94	118.03	123.83
10	bB	838	CLA	C4C-C3C-C2C	-2.94	102.64	106.89
10	aB	826	CLA	CAC-C3C-C4C	2.94	128.66	124.82
10	cB	833	CLA	C4-C3-C5	2.94	120.34	115.29
10	bL	203	CLA	C1D-CHD-C4C	-2.94	118.47	122.48
10	aA	821	CLA	CAA-C2A-C3A	-2.94	104.74	112.78
10	aA	821	CLA	CHD-C4C-NC	2.94	128.83	124.20
10	cA	834	CLA	O2A-CGA-CBA	2.94	121.36	111.93
10	aA	836	CLA	CAC-C3C-C4C	2.93	128.66	124.82
10	cB	807	CLA	CMB-C2B-C3B	2.93	130.30	124.80
10	cA	836	CLA	CBC-CAC-C3C	-2.93	104.28	112.43
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	cA	828	CLA	CMC-C2C-C1C	2.93	129.49	125.03
10	cA	837	CLA	O2D-CGD-O1D	-2.93	118.04	123.83
10	cB	811	CLA	CBC-CAC-C3C	-2.93	104.29	112.43
10	bA	803	CLA	CHC-C1C-C2C	-2.93	118.63	126.71
10	aA	811	CLA	CAC-C3C-C4C	2.93	128.65	124.82
10	aB	817	CLA	CHD-C4C-NC	2.93	128.82	124.20
10	cA	854	CLA	O2A-CGA-CBA	2.93	121.34	111.93
10	aA	817	CLA	C3B-C4B-NB	2.93	113.00	109.21
10	cA	805	CLA	CHC-C1C-C2C	-2.93	118.63	126.71
10	cA	804	CLA	CHC-C1C-C2C	-2.93	118.63	126.71
10	bL	202	CLA	O2A-CGA-CBA	2.93	121.34	111.93
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	832	CLA	C4C-C3C-C2C	-2.93	102.65	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	832	CLA	C4C-C3C-C2C	-2.93	102.65	106.89
10	bL	202	CLA	CHC-C1C-C2C	-2.93	118.63	126.71
10	cA	803	CLA	CHC-C1C-C2C	-2.93	118.63	126.71
10	aA	854	CLA	O2A-CGA-CBA	2.93	121.34	111.93
10	cB	814	CLA	CHC-C1C-C2C	-2.93	118.63	126.71
10	cA	811	CLA	CAC-C3C-C4C	2.93	128.65	124.82
9	aA	801	CL0	CBC-CAC-C3C	-2.93	104.30	112.43
10	bA	803	CLA	O2D-CGD-O1D	-2.93	118.05	123.83
10	cA	812	CLA	CAC-C3C-C4C	2.93	128.65	124.82
10	bB	817	CLA	CHD-C4C-NC	2.93	128.82	124.20
10	bA	811	CLA	O2D-CGD-O1D	-2.93	118.05	123.83
10	bA	854	CLA	C3B-C4B-NB	2.93	113.00	109.21
10	aL	202	CLA	O2A-CGA-CBA	2.93	121.33	111.93
10	bA	836	CLA	CAC-C3C-C4C	2.93	128.65	124.82
9	bA	801	CL0	CBC-CAC-C3C	-2.93	104.31	112.43
10	bB	828	CLA	CMC-C2C-C1C	2.93	129.48	125.03
10	bB	814	CLA	CHC-C1C-C2C	-2.93	118.64	126.71
10	bA	831	CLA	CHD-C4C-NC	2.93	128.81	124.20
10	bB	829	CLA	CMB-C2B-C3B	2.93	130.29	124.80
10	cB	829	CLA	CMB-C2B-C3B	2.93	130.29	124.80
10	aA	806	CLA	O2A-CGA-CBA	2.92	121.32	111.93
10	aA	854	CLA	C3B-C4B-NB	2.92	112.99	109.21
10	cA	806	CLA	O2A-CGA-CBA	2.92	121.32	111.93
10	aB	811	CLA	CAC-C3C-C4C	2.92	128.64	124.82
10	cB	825	CLA	CHC-C1C-C2C	-2.92	118.65	126.71
10	aL	202	CLA	CHC-C1C-C2C	-2.92	118.65	126.71
10	cA	830	CLA	C4C-C3C-C2C	-2.92	102.66	106.89
10	cA	831	CLA	CHC-C1C-C2C	-2.92	118.65	126.71
10	bA	820	CLA	CHD-C4C-NC	2.92	128.81	124.20
10	bA	805	CLA	CHC-C1C-C2C	-2.92	118.65	126.71
10	bA	806	CLA	O2A-CGA-CBA	2.92	121.31	111.93
10	bL	202	CLA	O2D-CGD-O1D	-2.92	118.06	123.83
10	cL	203	CLA	C1D-CHD-C4C	-2.92	118.49	122.48
10	aL	202	CLA	O2D-CGD-O1D	-2.92	118.06	123.83
10	cA	825	CLA	O2D-CGD-O1D	-2.92	118.06	123.83
10	bL	204	CLA	C3B-C4B-NB	2.92	112.99	109.21
10	cB	832	CLA	CHC-C1C-C2C	-2.92	118.66	126.71
10	aB	811	CLA	CBC-CAC-C3C	-2.92	104.32	112.43
10	cA	831	CLA	CHD-C4C-NC	2.92	128.81	124.20
10	aA	825	CLA	O2D-CGD-O1D	-2.92	118.06	123.83
10	bB	814	CLA	O2A-CGA-CBA	2.92	121.30	111.93
10	cL	204	CLA	C3B-C4B-NB	2.92	112.98	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cL	205	CLA	CHC-C1C-C2C	-2.92	118.66	126.71
10	aB	801	CLA	CHA-C1A-NA	-2.92	119.71	126.40
10	cL	202	CLA	O2A-CGA-CBA	2.92	121.30	111.93
10	bB	835	CLA	CHD-C4C-NC	2.92	128.80	124.20
10	aB	829	CLA	CMB-C2B-C3B	2.92	130.27	124.80
10	aA	803	CLA	CHC-C1C-C2C	-2.92	118.67	126.71
10	aB	832	CLA	CHC-C1C-C2C	-2.92	118.67	126.71
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	aA	830	CLA	C4C-C3C-C2C	-2.92	102.67	106.89
11	cA	844	PQN	C14-C13-C15	2.92	120.31	115.29
10	aA	828	CLA	CMC-C2C-C1C	2.92	129.47	125.03
10	cL	202	CLA	CHC-C1C-C2C	-2.92	118.67	126.71
10	aB	814	CLA	O2A-CGA-CBA	2.92	121.29	111.93
10	aA	805	CLA	CHC-C1C-C2C	-2.92	118.67	126.71
10	cB	805	CLA	C1D-CHD-C4C	-2.92	118.50	122.48
10	aB	828	CLA	CMC-C2C-C1C	2.91	129.47	125.03
10	bA	841	CLA	C3B-C4B-NB	2.91	112.98	109.21
10	aB	825	CLA	CHC-C1C-C2C	-2.91	118.68	126.71
10	bB	818	CLA	CAC-C3C-C4C	2.91	128.63	124.82
10	bA	854	CLA	O2A-CGA-CBA	2.91	121.28	111.93
10	cA	813	CLA	C4C-C3C-C2C	-2.91	102.67	106.89
10	cB	814	CLA	O2A-CGA-CBA	2.91	121.28	111.93
10	cB	830	CLA	C4C-C3C-C2C	-2.91	102.67	106.89
10	bB	814	CLA	C1-C2-C3	-2.91	121.01	126.04
10	bB	838	CLA	O2A-CGA-CBA	2.91	121.28	111.93
10	bL	205	CLA	CHC-C1C-C2C	-2.91	118.68	126.71
10	aA	831	CLA	CHC-C1C-C2C	-2.91	118.68	126.71
10	bA	817	CLA	C4-C3-C5	2.91	120.30	115.29
10	cA	809	CLA	CHC-C1C-C2C	-2.91	118.69	126.71
10	cB	813	CLA	CHC-C1C-C2C	-2.91	118.69	126.71
10	aB	813	CLA	CHC-C1C-C2C	-2.91	118.69	126.71
10	aA	842	CLA	C1D-CHD-C4C	-2.91	118.51	122.48
10	cB	835	CLA	CHD-C4C-NC	2.91	128.79	124.20
10	cB	837	CLA	C3B-C4B-NB	2.91	112.97	109.21
10	bB	825	CLA	CHC-C1C-C2C	-2.91	118.69	126.71
10	aB	831	CLA	C1D-CHD-C4C	-2.91	118.51	122.48
10	aL	205	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
10	bA	811	CLA	CAC-C3C-C4C	2.91	128.62	124.82
10	cB	801	CLA	CHA-C1A-NA	-2.91	119.74	126.40
10	bA	831	CLA	CHC-C1C-C2C	-2.91	118.69	126.71
10	bB	832	CLA	CHC-C1C-C2C	-2.91	118.69	126.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bB	844	BCR	C24-C23-C22	-2.91	121.84	126.21
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	bB	813	CLA	CHC-C1C-C2C	-2.91	118.69	126.71
10	aL	205	CLA	CHC-C1C-C2C	-2.91	118.69	126.71
10	bB	811	CLA	CBC-CAC-C3C	-2.91	104.36	112.43
10	aA	809	CLA	CHC-C1C-C2C	-2.91	118.70	126.71
10	aA	804	CLA	C3B-C4B-NB	2.91	112.97	109.21
10	cB	829	CLA	CHC-C1C-C2C	-2.91	118.70	126.71
10	bA	809	CLA	CHC-C1C-C2C	-2.91	118.70	126.71
10	aB	832	CLA	C4C-C3C-C2C	-2.90	102.68	106.89
10	cL	202	CLA	O2D-CGD-O1D	-2.90	118.09	123.83
10	bA	821	CLA	CHD-C4C-NC	2.90	128.78	124.20
10	aA	854	CLA	CHC-C1C-C2C	-2.90	118.70	126.71
10	cB	814	CLA	C1-C2-C3	-2.90	121.02	126.04
10	aB	838	CLA	O2A-CGA-CBA	2.90	121.25	111.93
13	aB	846	BCR	C15-C14-C13	-2.90	123.17	127.31
10	bB	833	CLA	C4-C3-C5	2.90	120.28	115.29
10	bA	830	CLA	C4C-C3C-C2C	-2.90	102.69	106.89
10	cA	842	CLA	C1D-CHD-C4C	-2.90	118.52	122.48
10	cA	854	CLA	CHC-C1C-C2C	-2.90	118.71	126.71
13	cB	846	BCR	C15-C14-C13	-2.90	123.17	127.31
10	bL	205	CLA	C1D-CHD-C4C	-2.90	118.52	122.48
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	cB	838	CLA	C4C-C3C-C2C	-2.90	102.69	106.89
11	bA	844	PQN	C14-C13-C15	2.90	120.28	115.29
10	bA	854	CLA	CHC-C1C-C2C	-2.90	118.72	126.71
10	bA	831	CLA	C4C-C3C-C2C	-2.90	102.69	106.89
10	cA	832	CLA	C4C-C3C-C2C	-2.90	102.69	106.89
10	bA	842	CLA	C1D-CHD-C4C	-2.90	118.52	122.48
10	aB	829	CLA	CHC-C1C-C2C	-2.90	118.72	126.71
10	cA	832	CLA	C1-C2-C3	-2.90	121.03	126.04
10	aL	205	CLA	C1D-CHD-C4C	-2.90	118.52	122.48
10	aA	841	CLA	C3B-C4B-NB	2.90	112.96	109.21
10	cB	838	CLA	O2A-CGA-CBA	2.90	121.23	111.93
10	aA	814	CLA	CAC-C3C-C4C	2.90	128.61	124.82
10	aB	818	CLA	CHC-C1C-C2C	-2.90	118.72	126.71
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	bB	829	CLA	CHC-C1C-C2C	-2.90	118.73	126.71
10	aA	831	CLA	CHD-C4C-NC	2.89	128.76	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	812	CLA	CAC-C3C-C4C	2.89	128.60	124.82
10	aB	835	CLA	CHD-C4C-NC	2.89	128.76	124.20
10	bA	832	CLA	CHC-C1C-C2C	-2.89	118.73	126.71
10	cA	806	CLA	CAA-C2A-C3A	-2.89	104.85	112.78
10	aA	804	CLA	C4C-C3C-C2C	-2.89	102.70	106.89
10	aB	829	CLA	CAC-C3C-C4C	2.89	128.60	124.82
10	aB	809	CLA	CMC-C2C-C1C	2.89	129.43	125.03
10	bB	840	CLA	CMC-C2C-C1C	2.89	129.43	125.03
10	bA	806	CLA	CMC-C2C-C1C	2.89	129.43	125.03
10	cA	821	CLA	CHD-C4C-NC	2.89	128.76	124.20
10	bB	818	CLA	CHC-C1C-C2C	-2.89	118.73	126.71
10	aA	832	CLA	CHC-C1C-C2C	-2.89	118.74	126.71
10	aL	205	CLA	O2D-CGD-O1D	-2.89	118.12	123.83
10	cA	804	CLA	CHB-C4A-NA	2.89	128.51	124.51
10	cA	831	CLA	C4C-C3C-C2C	-2.89	102.70	106.89
10	cB	832	CLA	C4C-C3C-C2C	-2.89	102.70	106.89
10	cL	205	CLA	C1D-CHD-C4C	-2.89	118.53	122.48
10	aB	814	CLA	C1-C2-C3	-2.89	121.04	126.04
10	cA	833	CLA	CHB-C4A-NA	2.89	128.51	124.51
10	aA	833	CLA	CHB-C4A-NA	2.89	128.50	124.51
10	cB	829	CLA	CAC-C3C-C4C	2.89	128.59	124.82
10	cB	840	CLA	CAC-C3C-C4C	2.89	128.59	124.82
10	bB	809	CLA	CMC-C2C-C1C	2.89	129.42	125.03
10	bB	840	CLA	CMB-C2B-C3B	2.89	130.21	124.80
10	cB	809	CLA	CMC-C2C-C1C	2.89	129.42	125.03
10	bA	834	CLA	C4C-C3C-C2C	-2.89	102.71	106.89
10	bA	814	CLA	CAC-C3C-C4C	2.89	128.59	124.82
10	cA	806	CLA	CMC-C2C-C1C	2.89	129.42	125.03
9	aA	801	CL0	C4C-C3C-C2C	-2.89	102.71	106.89
10	aA	804	CLA	CHB-C4A-NA	2.89	128.50	124.51
10	cA	804	CLA	C3B-C4B-NB	2.89	112.94	109.21
10	cA	832	CLA	CHC-C1C-C2C	-2.89	118.76	126.71
10	cA	820	CLA	CHD-C4C-NC	2.88	128.75	124.20
10	aB	836	CLA	CAC-C3C-C4C	2.88	128.59	124.82
9	cA	801	CL0	C4C-C3C-C2C	-2.88	102.72	106.89
10	aB	803	CLA	C4A-NA-C1A	-2.88	105.41	106.71
10	bB	829	CLA	CAC-C3C-C4C	2.88	128.59	124.82
10	cB	818	CLA	CHC-C1C-C2C	-2.88	118.76	126.71
10	aA	806	CLA	CMC-C2C-C1C	2.88	129.42	125.03
10	aA	841	CLA	CHD-C4C-NC	2.88	128.74	124.20
10	cA	807	CLA	CHC-C1C-C2C	-2.88	118.77	126.71
10	cL	205	CLA	O2D-CGD-O1D	-2.88	118.14	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	832	CLA	C1D-CHD-C4C	-2.88	118.55	122.48
10	cA	818	CLA	C2A-C3A-C4A	-2.88	97.22	101.87
10	bL	202	CLA	C4A-NA-C1A	-2.88	105.41	106.71
10	aA	805	CLA	C4C-C3C-C2C	-2.88	102.72	106.89
10	bA	837	CLA	CHC-C1C-C2C	-2.88	118.78	126.71
10	aA	820	CLA	CHD-C4C-NC	2.88	128.74	124.20
10	aA	818	CLA	C2A-C3A-C4A	-2.88	97.22	101.87
10	aA	806	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
9	bA	801	CL0	O2D-CGD-O1D	-2.88	118.15	123.83
10	bA	806	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
10	bB	840	CLA	CAC-C3C-C4C	2.88	128.58	124.82
10	bB	836	CLA	CAC-C3C-C4C	2.88	128.58	124.82
10	bA	807	CLA	CHC-C1C-C2C	-2.87	118.78	126.71
10	cA	834	CLA	C4C-C3C-C2C	-2.87	102.73	106.89
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	aB	839	CLA	CAC-C3C-C4C	2.87	128.57	124.82
10	cB	828	CLA	CMC-C2C-C1C	2.87	129.40	125.03
10	cA	838	CLA	O2D-CGD-O1D	-2.87	118.16	123.83
10	aB	840	CLA	CAC-C3C-C4C	2.87	128.57	124.82
10	aB	820	CLA	C4C-C3C-C2C	-2.87	102.73	106.89
10	aA	831	CLA	C4C-C3C-C2C	-2.87	102.73	106.89
10	cA	837	CLA	CHC-C1C-C2C	-2.87	118.80	126.71
13	cB	847	BCR	C3-C4-C5	-2.87	109.00	113.99
10	cA	814	CLA	CAC-C3C-C4C	2.87	128.57	124.82
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	cB	839	CLA	CAC-C3C-C4C	2.87	128.57	124.82
9	bA	801	CL0	C4C-C3C-C2C	-2.87	102.74	106.89
10	bL	205	CLA	O2D-CGD-O1D	-2.87	118.17	123.83
10	aB	816	CLA	C3B-C4B-NB	2.87	112.92	109.21
16	cB	848	LMG	O6-C1-O1	-2.87	103.17	109.94
10	bA	818	CLA	C2A-C3A-C4A	-2.87	97.24	101.87
16	bB	848	LMG	O6-C1-O1	-2.87	103.17	109.94
10	aA	817	CLA	CHC-C1C-C2C	-2.87	118.81	126.71
10	cB	806	CLA	CMB-C2B-C3B	2.87	130.17	124.80
10	cB	803	CLA	C4A-NA-C1A	-2.86	105.42	106.71
10	bA	841	CLA	CHD-C4C-NC	2.86	128.72	124.20
10	bB	821	CLA	C4C-C3C-C2C	-2.86	102.74	106.89
10	bA	832	CLA	CHD-C4C-NC	2.86	128.72	124.20
10	bB	817	CLA	C4C-C3C-C2C	-2.86	102.74	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	aB	848	LMG	O6-C1-O1	-2.86	103.18	109.94
10	aA	807	CLA	CHC-C1C-C2C	-2.86	118.82	126.71
10	bA	838	CLA	CHC-C1C-C2C	-2.86	118.82	126.71
13	bB	847	BCR	C3-C4-C5	-2.86	109.01	113.99
13	bB	846	BCR	C15-C14-C13	-2.86	123.22	127.31
10	aA	837	CLA	CHC-C1C-C2C	-2.86	118.82	126.71
10	aA	827	CLA	CAC-C3C-C4C	2.86	128.56	124.82
10	bA	804	CLA	CHB-C4A-NA	2.86	128.47	124.51
10	cB	826	CLA	CHC-C1C-C2C	-2.86	118.82	126.71
13	aB	844	BCR	C24-C23-C22	-2.86	121.91	126.21
10	aA	838	CLA	CHC-C1C-C2C	-2.86	118.82	126.71
10	aA	834	CLA	CBC-CAC-C3C	-2.86	104.48	112.43
10	cA	820	CLA	CHC-C1C-C2C	-2.86	118.82	126.71
10	bB	819	CLA	CHD-C4C-NC	2.86	128.71	124.20
10	aA	803	CLA	CHD-C4C-NC	2.86	128.71	124.20
9	cA	801	CL0	O2D-CGD-O1D	-2.86	118.18	123.83
10	bA	839	CLA	O2A-CGA-CBA	2.86	121.11	111.93
10	bA	804	CLA	C4C-C3C-C2C	-2.86	102.75	106.89
10	aA	808	CLA	CMC-C2C-C1C	2.86	129.38	125.03
10	bB	839	CLA	CAC-C3C-C4C	2.86	128.56	124.82
10	cB	815	CLA	C1-C2-C3	-2.86	121.10	126.04
10	bA	834	CLA	CBC-CAC-C3C	-2.86	104.50	112.43
10	bB	834	CLA	CMA-C3A-C2A	-2.86	102.27	113.78
10	bB	806	CLA	CMB-C2B-C3B	2.86	130.16	124.80
10	aB	834	CLA	CMA-C3A-C2A	-2.86	102.27	113.78
9	aA	801	CL0	O2D-CGD-O1D	-2.86	118.19	123.83
10	cL	202	CLA	CAC-C3C-C4C	2.86	128.55	124.82
10	cB	839	CLA	C4C-C3C-C2C	-2.86	102.75	106.89
10	bA	805	CLA	C4C-C3C-C2C	-2.86	102.75	106.89
10	aB	817	CLA	C4C-C3C-C2C	-2.86	102.75	106.89
10	bA	837	CLA	CHD-C4C-NC	2.85	128.70	124.20
10	bA	827	CLA	CAC-C3C-C4C	2.85	128.55	124.82
10	cA	838	CLA	CHC-C1C-C2C	-2.85	118.84	126.71
10	bA	832	CLA	C1D-CHD-C4C	-2.85	118.58	122.48
10	aB	839	CLA	C4C-C3C-C2C	-2.85	102.76	106.89
10	cB	840	CLA	CMB-C2B-C3B	2.85	130.15	124.80
10	cA	834	CLA	CBC-CAC-C3C	-2.85	104.51	112.43
10	cB	836	CLA	CAC-C3C-C4C	2.85	128.55	124.82
10	aB	840	CLA	CMC-C2C-C1C	2.85	129.37	125.03
10	cA	817	CLA	CHC-C1C-C2C	-2.85	118.84	126.71
13	cA	849	BCR	C28-C27-C26	-2.85	109.03	113.99
10	aA	834	CLA	C4C-C3C-C2C	-2.85	102.76	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	aA	849	BCR	C28-C27-C26	-2.85	109.03	113.99
13	cB	844	BCR	C24-C23-C22	-2.85	121.93	126.21
10	cA	808	CLA	CMC-C2C-C1C	2.85	129.37	125.03
10	cA	804	CLA	C4C-C3C-C2C	-2.85	102.76	106.89
10	cA	830	CLA	C3B-C4B-NB	2.85	112.89	109.21
10	cA	837	CLA	CHD-C4C-NC	2.85	128.69	124.20
10	bB	820	CLA	C4C-C3C-C2C	-2.85	102.76	106.89
10	bA	829	CLA	C1-C2-C3	-2.85	121.11	126.04
10	cB	821	CLA	C4C-C3C-C2C	-2.85	102.76	106.89
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
10	bA	831	CLA	O2D-CGD-O1D	-2.85	118.20	123.83
10	bA	820	CLA	CHC-C1C-C2C	-2.85	118.86	126.71
10	bA	838	CLA	C3B-C4B-NB	2.85	112.89	109.21
10	cA	832	CLA	C1D-CHD-C4C	-2.85	118.59	122.48
10	aA	830	CLA	C1-C2-C3	-2.85	122.14	126.75
10	bB	815	CLA	C1-C2-C3	-2.85	121.12	126.04
10	aB	826	CLA	CHC-C1C-C2C	-2.85	118.86	126.71
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	cB	840	CLA	CMC-C2C-C1C	2.85	129.36	125.03
10	cB	834	CLA	CMA-C3A-C2A	-2.85	102.30	113.78
10	cB	808	CLA	C1-C2-C3	-2.85	121.12	126.04
10	cA	812	CLA	CHC-C1C-C2C	-2.85	118.86	126.71
10	aB	815	CLA	C1-C2-C3	-2.85	121.12	126.04
10	cA	827	CLA	CAC-C3C-C4C	2.85	128.54	124.82
10	bA	817	CLA	CHC-C1C-C2C	-2.85	118.87	126.71
10	cL	202	CLA	C4A-NA-C1A	-2.84	105.43	106.71
10	bA	806	CLA	CHC-C1C-C2C	-2.84	118.87	126.71
10	cA	838	CLA	C3B-C4B-NB	2.84	112.89	109.21
10	bB	826	CLA	CHC-C1C-C2C	-2.84	118.87	126.71
10	cA	839	CLA	O2A-CGA-CBA	2.84	121.06	111.93
10	bB	839	CLA	C4C-C3C-C2C	-2.84	102.77	106.89
10	bA	835	CLA	C4C-C3C-C2C	-2.84	102.77	106.89
10	aA	820	CLA	CHC-C1C-C2C	-2.84	118.87	126.71
10	aL	202	CLA	CAC-C3C-C4C	2.84	128.53	124.82
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	840	CLA	CMB-C2B-C3B	2.84	130.13	124.80
10	cB	831	CLA	C3B-C4B-NB	2.84	112.88	109.21
10	aB	821	CLA	C4C-C3C-C2C	-2.84	102.78	106.89
10	aA	817	CLA	C4C-C3C-C2C	-2.84	102.78	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bA	849	BCR	C28-C27-C26	-2.84	109.05	113.99
10	aA	835	CLA	C4C-C3C-C2C	-2.84	102.78	106.89
10	aA	813	CLA	C4A-NA-C1A	-2.84	105.43	106.71
10	cA	856	CLA	CAC-C3C-C4C	2.84	128.53	124.82
10	aA	817	CLA	CAC-C3C-C4C	2.84	128.53	124.82
10	cA	805	CLA	C4C-C3C-C2C	-2.84	102.78	106.89
10	aA	829	CLA	CAC-C3C-C4C	2.84	128.53	124.82
10	cB	806	CLA	CBA-CAA-C2A	2.84	122.30	113.85
10	cB	808	CLA	C3B-C4B-NB	2.84	112.88	109.21
10	cB	818	CLA	O2A-CGA-CBA	2.84	121.04	111.93
10	cA	831	CLA	O2D-CGD-O1D	-2.84	118.23	123.83
10	bL	203	CLA	CHC-C1C-C2C	-2.84	118.89	126.71
10	bA	805	CLA	O2D-CGD-O1D	-2.83	118.23	123.83
10	cB	833	CLA	CHD-C4C-NC	2.83	128.67	124.20
10	cA	825	CLA	CHD-C4C-NC	2.83	128.67	124.20
10	cA	803	CLA	CHD-C4C-NC	2.83	128.67	124.20
10	aB	818	CLA	O2A-CGA-CBA	2.83	121.03	111.93
10	bB	806	CLA	CBA-CAA-C2A	2.83	122.29	113.85
10	cB	819	CLA	CHD-C4C-NC	2.83	128.67	124.20
10	cA	832	CLA	CHD-C4C-NC	2.83	128.67	124.20
13	aB	847	BCR	C3-C4-C5	-2.83	109.06	113.99
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	bA	817	CLA	C4C-C3C-C2C	-2.83	102.79	106.89
10	aB	806	CLA	CMB-C2B-C3B	2.83	130.11	124.80
10	bA	821	CLA	O2D-CGD-O1D	-2.83	118.24	123.83
10	bA	838	CLA	O2D-CGD-O1D	-2.83	118.24	123.83
10	cA	838	CLA	CHD-C4C-NC	2.83	128.67	124.20
10	aA	839	CLA	O2A-CGA-CBA	2.83	121.02	111.93
10	bA	806	CLA	C3B-C4B-NB	2.83	112.87	109.21
10	aB	806	CLA	CBA-CAA-C2A	2.83	122.28	113.85
10	aB	809	CLA	C1D-CHD-C4C	-2.83	118.61	122.48
10	aB	808	CLA	CMC-C2C-C1C	2.83	129.34	125.03
10	aA	812	CLA	CHC-C1C-C2C	-2.83	118.91	126.71
10	cA	835	CLA	C4C-C3C-C2C	-2.83	102.79	106.89
10	aL	204	CLA	C4C-C3C-C2C	-2.83	102.79	106.89
10	bA	812	CLA	CHC-C1C-C2C	-2.83	118.91	126.71
10	cB	808	CLA	CMC-C2C-C1C	2.83	129.34	125.03
10	bA	833	CLA	CHB-C4A-NA	2.83	128.43	124.51
10	cL	203	CLA	CHC-C1C-C2C	-2.83	118.91	126.71
10	bA	803	CLA	CHD-C4C-NC	2.83	128.66	124.20
10	cA	835	CLA	CAC-C3C-C4C	2.83	128.52	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	807	CLA	CHD-C4C-NC	2.83	128.66	124.20
10	bB	808	CLA	CMC-C2C-C1C	2.83	129.33	125.03
10	cB	807	CLA	O2D-CGD-O1D	-2.83	118.25	123.83
10	aA	832	CLA	O2A-CGA-CBA	2.83	121.01	111.93
10	cA	817	CLA	C4C-C3C-C2C	-2.83	102.80	106.89
10	bL	202	CLA	CAC-C3C-C4C	2.82	128.51	124.82
10	bA	829	CLA	CAC-C3C-C4C	2.82	128.51	124.82
10	cA	806	CLA	CHC-C1C-C2C	-2.82	118.92	126.71
10	cB	817	CLA	C4C-C3C-C2C	-2.82	102.80	106.89
10	aA	805	CLA	O2D-CGD-O1D	-2.82	118.25	123.83
10	cA	807	CLA	CHB-C4A-NA	2.82	128.42	124.51
10	aL	203	CLA	CHC-C1C-C2C	-2.82	118.93	126.71
10	bA	832	CLA	O2A-CGA-CBA	2.82	121.00	111.93
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	cA	832	CLA	O2A-CGA-CBA	2.82	120.99	111.93
10	aA	806	CLA	C3B-C4B-NB	2.82	112.86	109.21
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	bA	827	CLA	CHC-C1C-C2C	-2.82	118.94	126.71
10	aA	823	CLA	CHD-C4C-NC	2.82	128.65	124.20
10	cB	809	CLA	C1D-CHD-C4C	-2.82	118.63	122.48
10	bA	825	CLA	CHD-C4C-NC	2.82	128.65	124.20
10	aA	806	CLA	CHC-C1C-C2C	-2.82	118.94	126.71
10	aA	835	CLA	CAC-C3C-C4C	2.82	128.50	124.82
11	cB	842	PQN	C11-C12-C13	-2.82	122.10	126.79
10	bA	828	CLA	CHD-C4C-NC	2.82	128.64	124.20
13	bB	844	BCR	C28-C27-C26	-2.82	109.09	113.99
10	bA	830	CLA	C1-C2-C3	-2.82	122.19	126.75
10	bB	818	CLA	O2A-CGA-CBA	2.82	120.98	111.93
10	aL	205	CLA	C1-C2-C3	-2.82	121.17	126.04
10	bA	808	CLA	CMC-C2C-C1C	2.82	129.32	125.03
10	aA	827	CLA	CHC-C1C-C2C	-2.82	118.95	126.71
10	bB	821	CLA	O2D-CGD-O1D	-2.82	118.27	123.83
10	cA	821	CLA	O2D-CGD-O1D	-2.82	118.27	123.83
10	aA	808	CLA	C3B-C4B-NB	2.82	112.85	109.21
10	aB	821	CLA	O2D-CGD-O1D	-2.82	118.27	123.83
10	bB	818	CLA	C1-C2-C3	-2.82	121.17	126.04
10	aA	856	CLA	CAC-C3C-C4C	2.81	128.50	124.82
10	cB	820	CLA	C4C-C3C-C2C	-2.81	102.81	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	838	CLA	CHC-C1C-C2C	-2.81	118.95	126.71
10	aB	833	CLA	CHD-C4C-NC	2.81	128.64	124.20
10	aA	831	CLA	O2D-CGD-O1D	-2.81	118.28	123.83
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
10	bA	856	CLA	CAC-C3C-C4C	2.81	128.49	124.82
10	bA	837	CLA	CAA-C2A-C3A	-2.81	105.08	112.78
10	bB	831	CLA	C4C-C3C-C2C	-2.81	102.82	106.89
10	aB	823	CLA	C4C-C3C-C2C	-2.81	102.82	106.89
10	aB	831	CLA	C3B-C4B-NB	2.81	112.84	109.21
10	cA	805	CLA	O2D-CGD-O1D	-2.81	118.28	123.83
10	aB	838	CLA	CHC-C1C-C2C	-2.81	118.97	126.71
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	cA	817	CLA	CAC-C3C-C4C	2.81	128.49	124.82
10	cA	828	CLA	CHD-C4C-NC	2.81	128.63	124.20
10	aA	822	CLA	CHC-C1C-C2C	-2.81	118.97	126.71
10	aL	202	CLA	C4A-NA-C1A	-2.81	105.44	106.71
10	bA	840	CLA	CHC-C1C-C2C	-2.81	118.97	126.71
10	bA	822	CLA	CHC-C1C-C2C	-2.81	118.97	126.71
10	bA	823	CLA	CHD-C4C-NC	2.81	128.62	124.20
10	aA	838	CLA	O2D-CGD-O1D	-2.81	118.29	123.83
10	cL	204	CLA	C4C-C3C-C2C	-2.81	102.83	106.89
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	837	CLA	CHC-C1C-C2C	-2.80	118.98	126.71
10	aA	840	CLA	CHC-C1C-C2C	-2.80	118.98	126.71
10	cB	838	CLA	CHC-C1C-C2C	-2.80	118.98	126.71
10	bA	830	CLA	C3B-C4B-NB	2.80	112.83	109.21
10	bB	807	CLA	O2D-CGD-O1D	-2.80	118.29	123.83
10	aA	837	CLA	CAA-C2A-C3A	-2.80	105.10	112.78
9	cA	801	CL0	O2A-CGA-CBA	2.80	120.93	111.93
10	cB	818	CLA	C1-C2-C3	-2.80	121.19	126.04
10	bA	817	CLA	CAC-C3C-C4C	2.80	128.48	124.82
10	aA	838	CLA	C3B-C4B-NB	2.80	112.83	109.21
10	cA	840	CLA	CHC-C1C-C2C	-2.80	118.99	126.71
10	cB	823	CLA	C4C-C3C-C2C	-2.80	102.83	106.89
13	aL	206	BCR	C31-C1-C6	2.80	114.84	110.30
10	bB	833	CLA	CHD-C4C-NC	2.80	128.62	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	cA	822	CLA	CHC-C1C-C2C	-2.80	118.99	126.71
10	bA	838	CLA	CHD-C4C-NC	2.80	128.62	124.20
10	bA	835	CLA	CAC-C3C-C4C	2.80	128.48	124.82
10	bB	834	CLA	CHB-C4A-NA	2.80	128.38	124.51
10	cA	827	CLA	CHC-C1C-C2C	-2.80	118.99	126.71
10	bB	819	CLA	C2A-C3A-C4A	-2.80	97.35	101.87
10	aA	825	CLA	CHD-C4C-NC	2.80	128.61	124.20
10	bB	826	CLA	C1D-CHD-C4C	-2.80	118.66	122.48
10	cA	841	CLA	CMC-C2C-C1C	2.80	129.28	125.03
10	cA	841	CLA	CHC-C1C-C2C	-2.80	119.00	126.71
13	cB	844	BCR	C28-C27-C26	-2.80	109.13	113.99
13	cL	206	BCR	C31-C1-C6	2.79	114.83	110.30
10	aA	821	CLA	O2D-CGD-O1D	-2.79	118.31	123.83
9	aA	801	CL0	O2A-CGA-CBA	2.79	120.90	111.93
10	bB	809	CLA	C1D-CHD-C4C	-2.79	118.67	122.48
10	cA	823	CLA	CHD-C4C-NC	2.79	128.61	124.20
10	aL	203	CLA	CHD-C4C-NC	2.79	128.61	124.20
9	bA	801	CL0	O2A-CGA-CBA	2.79	120.90	111.93
13	aB	844	BCR	C28-C27-C26	-2.79	109.13	113.99
10	cA	808	CLA	C3B-C4B-NB	2.79	112.82	109.21
10	bB	823	CLA	C4C-C3C-C2C	-2.79	102.84	106.89
10	bB	824	CLA	C4C-C3C-C2C	-2.79	102.84	106.89
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	aB	824	CLA	C4C-C3C-C2C	-2.79	102.85	106.89
10	bB	836	CLA	C4C-C3C-C2C	-2.79	102.85	106.89
10	aB	807	CLA	O2D-CGD-O1D	-2.79	118.32	123.83
10	aA	841	CLA	CHC-C1C-C2C	-2.79	119.01	126.71
10	aB	821	CLA	CHD-C4C-NC	2.79	128.60	124.20
10	cB	821	CLA	O2D-CGD-O1D	-2.79	118.32	123.83
10	bA	835	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
10	cB	826	CLA	C4C-C3C-C2C	-2.79	102.85	106.89
10	aB	808	CLA	C1-C2-C3	-2.79	121.22	126.04
10	bB	837	CLA	CHC-C1C-C2C	-2.79	119.02	126.71
10	bB	828	CLA	CHC-C1C-C2C	-2.79	119.02	126.71
10	aA	826	CLA	C1-C2-C3	-2.79	121.22	126.04
10	aB	837	CLA	CHC-C1C-C2C	-2.79	119.02	126.71
10	cB	815	CLA	CHD-C4C-NC	2.79	128.60	124.20
10	cA	829	CLA	CAC-C3C-C4C	2.79	128.46	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	bA	801	CL0	C1-C2-C3	-2.79	121.22	126.04
10	aA	816	CLA	O2A-CGA-CBA	2.79	120.88	111.93
10	aB	826	CLA	C1D-CHD-C4C	-2.79	118.67	122.48
10	bA	841	CLA	CHC-C1C-C2C	-2.79	119.03	126.71
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	bL	204	CLA	C4C-C3C-C2C	-2.79	102.86	106.89
10	aA	821	CLA	C4C-C3C-C2C	-2.79	102.86	106.89
10	aB	831	CLA	C4C-C3C-C2C	-2.79	102.86	106.89
10	aA	816	CLA	CMC-C2C-C1C	2.79	129.27	125.03
10	cB	828	CLA	C1-C2-C3	-2.79	121.22	126.04
10	bB	826	CLA	C4C-C3C-C2C	-2.79	102.86	106.89
10	cL	203	CLA	CAC-C3C-C4C	2.79	128.46	124.82
10	cB	826	CLA	C1D-CHD-C4C	-2.78	118.68	122.48
10	cB	834	CLA	CHB-C4A-NA	2.78	128.36	124.51
10	cB	817	CLA	CHB-C4A-NA	2.78	128.36	124.51
10	cA	816	CLA	CMC-C2C-C1C	2.78	129.27	125.03
10	aA	836	CLA	CHD-C4C-NC	2.78	128.59	124.20
13	bL	206	BCR	C31-C1-C6	2.78	114.81	110.30
10	aA	841	CLA	CMC-C2C-C1C	2.78	129.26	125.03
10	bL	203	CLA	CAC-C3C-C4C	2.78	128.46	124.82
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	aB	828	CLA	CHC-C1C-C2C	-2.78	119.04	126.71
10	aA	836	CLA	C4C-C3C-C2C	-2.78	102.86	106.89
10	aL	203	CLA	CAC-C3C-C4C	2.78	128.45	124.82
10	cB	819	CLA	C2A-C3A-C4A	-2.78	97.38	101.87
10	aB	836	CLA	C4C-C3C-C2C	-2.78	102.86	106.89
10	cA	834	CLA	C4-C3-C5	2.78	120.07	115.29
10	cB	835	CLA	C4C-C3C-C2C	-2.78	102.87	106.89
10	bA	816	CLA	CMC-C2C-C1C	2.78	129.26	125.03
10	bA	803	CLA	CAC-C3C-C4C	2.78	128.45	124.82
10	cB	809	CLA	CHC-C1C-C2C	-2.78	119.05	126.71
10	aB	840	CLA	C3B-C4B-NB	2.78	112.80	109.21
10	bB	809	CLA	CHC-C1C-C2C	-2.78	119.06	126.71
10	cA	819	CLA	C4-C3-C5	2.78	120.07	115.29
10	bA	823	CLA	CHB-C4A-NA	2.78	128.35	124.51
10	bA	809	CLA	CAC-C3C-C4C	2.78	128.45	124.82
9	cA	801	CL0	CMC-C2C-C1C	2.77	129.25	125.03
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
10	aA	808	CLA	CAC-C3C-C4C	2.77	128.45	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	841	CLA	C4-C3-C5	2.77	120.06	115.29
10	cB	839	CLA	CHD-C4C-NC	2.77	128.57	124.20
10	bA	819	CLA	C4-C3-C5	2.77	120.06	115.29
10	cA	816	CLA	O2A-CGA-CBA	2.77	120.83	111.93
10	cB	823	CLA	CAC-C3C-C4C	2.77	128.44	124.82
10	bA	826	CLA	C1-C2-C3	-2.77	121.25	126.04
10	bA	834	CLA	C4-C3-C5	2.77	120.06	115.29
13	aL	206	BCR	C29-C30-C25	2.77	114.77	110.48
10	bA	808	CLA	CHD-C4C-NC	2.77	128.57	124.20
10	bA	806	CLA	CHD-C4C-NC	2.77	128.57	124.20
13	cL	206	BCR	C29-C30-C25	2.77	114.77	110.48
10	bB	821	CLA	CHD-C4C-NC	2.77	128.57	124.20
10	cA	841	CLA	C4-C3-C5	2.77	120.06	115.29
10	bA	836	CLA	CMC-C2C-C1C	2.77	129.25	125.03
10	cA	836	CLA	CHD-C4C-NC	2.77	128.57	124.20
10	aA	817	CLA	CMC-C2C-C1C	2.77	129.25	125.03
10	cB	828	CLA	CHC-C1C-C2C	-2.77	119.08	126.71
10	cA	809	CLA	CAC-C3C-C4C	2.77	128.44	124.82
10	cA	836	CLA	C4C-C3C-C2C	-2.77	102.88	106.89
10	bA	836	CLA	C4C-C3C-C2C	-2.77	102.88	106.89
10	aA	806	CLA	CHD-C4C-NC	2.77	128.57	124.20
10	bA	821	CLA	C4C-C3C-C2C	-2.77	102.88	106.89
10	aA	840	CLA	CHD-C4C-NC	2.77	128.56	124.20
10	cB	831	CLA	C4C-C3C-C2C	-2.77	102.88	106.89
10	aA	834	CLA	C4-C3-C5	2.77	120.05	115.29
10	cA	824	CLA	CHC-C1C-C2C	-2.77	119.08	126.71
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	cA	836	CLA	CMC-C2C-C1C	2.77	129.24	125.03
10	bA	841	CLA	CMC-C2C-C1C	2.77	129.24	125.03
10	aB	840	CLA	CHD-C4C-NC	2.77	128.56	124.20
10	aA	809	CLA	CAC-C3C-C4C	2.77	128.43	124.82
10	aA	815	CLA	C4C-C3C-C2C	-2.76	102.89	106.89
10	cB	821	CLA	CHD-C4C-NC	2.76	128.56	124.20
10	cA	808	CLA	CHD-C4C-NC	2.76	128.56	124.20
10	cB	840	CLA	CHD-C4C-NC	2.76	128.56	124.20
10	cA	816	CLA	CHC-C1C-C2C	-2.76	119.09	126.71
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	bA	816	CLA	O2A-CGA-CBA	2.76	120.80	111.93
9	cA	801	CL0	C1-C2-C3	-2.76	121.26	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	808	CLA	CHC-C1C-C2C	-2.76	119.09	126.71
10	aA	819	CLA	C4-C3-C5	2.76	120.05	115.29
10	cB	803	CLA	CHD-C4C-NC	2.76	128.56	124.20
13	cA	851	BCR	C27-C26-C25	2.76	126.77	122.74
10	aB	835	CLA	C4C-C3C-C2C	-2.76	102.89	106.89
10	cA	821	CLA	C4C-C3C-C2C	-2.76	102.89	106.89
10	bA	802	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
10	aB	809	CLA	CHC-C1C-C2C	-2.76	119.10	126.71
9	bA	801	CL0	CMC-C2C-C1C	2.76	129.23	125.03
10	aB	803	CLA	CHD-C4C-NC	2.76	128.55	124.20
10	bB	840	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	cB	826	CLA	C4-C3-C5	2.76	120.04	115.29
10	cB	809	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
10	bA	816	CLA	CHC-C1C-C2C	-2.76	119.10	126.71
10	cA	806	CLA	CHD-C4C-NC	2.76	128.55	124.20
10	cB	836	CLA	C4C-C3C-C2C	-2.76	102.89	106.89
9	aA	801	CL0	C1-C2-C3	-2.76	121.27	126.04
10	aB	817	CLA	O2A-CGA-CBA	2.76	120.79	111.93
10	bB	817	CLA	O2A-CGA-CBA	2.76	120.78	111.93
10	aB	826	CLA	C4C-C3C-C2C	-2.76	102.90	106.89
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	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
10	cA	803	CLA	CAC-C3C-C4C	2.76	128.42	124.82
13	bL	206	BCR	C29-C30-C25	2.76	114.75	110.48
10	aB	809	CLA	CAA-C2A-C3A	-2.76	105.23	112.78
10	aB	828	CLA	CHD-C4C-NC	2.76	128.55	124.20
10	bB	817	CLA	CHB-C4A-NA	2.76	128.32	124.51
10	bL	204	CLA	CHC-C1C-C2C	-2.75	119.12	126.71
10	cA	815	CLA	C4C-C3C-C2C	-2.75	102.90	106.89
9	aA	801	CL0	CMC-C2C-C1C	2.75	129.22	125.03
10	bA	824	CLA	CHC-C1C-C2C	-2.75	119.12	126.71
10	cB	840	CLA	C3B-C4B-NB	2.75	112.77	109.21
10	bA	808	CLA	CHC-C1C-C2C	-2.75	119.12	126.71
10	aA	836	CLA	CMC-C2C-C1C	2.75	129.22	125.03
10	aA	824	CLA	CHC-C1C-C2C	-2.75	119.12	126.71
10	aL	203	CLA	C4C-C3C-C2C	-2.75	102.90	106.89
10	bA	813	CLA	CHD-C4C-NC	2.75	128.54	124.20
10	cB	817	CLA	O2A-CGA-CBA	2.75	120.77	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	829	CLA	CMA-C3A-C2A	-2.75	102.69	113.78
10	cB	824	CLA	C4C-C3C-C2C	-2.75	102.91	106.89
10	cB	829	CLA	CMA-C3A-C2A	-2.75	102.69	113.78
10	cL	204	CLA	CHC-C1C-C2C	-2.75	119.13	126.71
10	cB	802	CLA	CAC-C3C-C4C	2.75	128.41	124.82
10	bB	826	CLA	C4-C3-C5	2.75	120.02	115.29
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	bB	834	CLA	C4C-C3C-C2C	-2.75	102.91	106.89
10	bA	815	CLA	C4C-C3C-C2C	-2.75	102.91	106.89
10	bA	841	CLA	C4-C3-C5	2.75	120.02	115.29
10	cB	827	CLA	CAA-C2A-C3A	-2.75	105.26	112.78
10	bB	823	CLA	CAC-C3C-C4C	2.75	128.41	124.82
10	aB	832	CLA	O2D-CGD-O1D	-2.75	118.41	123.83
10	aA	816	CLA	CHC-C1C-C2C	-2.75	119.14	126.71
10	cA	823	CLA	C4C-C3C-C2C	-2.74	102.92	106.89
10	bB	841	CLA	C4C-C3C-C2C	-2.74	102.92	106.89
10	bB	835	CLA	C4C-C3C-C2C	-2.74	102.92	106.89
10	aB	823	CLA	CAC-C3C-C4C	2.74	128.41	124.82
10	cA	840	CLA	O2A-CGA-CBA	2.74	120.74	111.93
10	aB	827	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
10	cA	837	CLA	CAC-C3C-C4C	2.74	128.40	124.82
10	aB	812	CLA	CHD-C4C-NC	2.74	128.52	124.20
10	bA	828	CLA	CHC-C1C-C2C	-2.74	119.15	126.71
10	aB	829	CLA	CMA-C3A-C2A	-2.74	102.73	113.78
10	cA	802	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
10	aB	841	CLA	C4C-C3C-C2C	-2.74	102.92	106.89
10	bA	808	CLA	CAC-C3C-C4C	2.74	128.40	124.82
10	bB	828	CLA	O1D-CGD-CBD	-2.74	118.80	124.48
10	aA	808	CLA	CHC-C1C-C2C	-2.74	119.16	126.71
10	cB	841	CLA	C4C-C3C-C2C	-2.74	102.92	106.89
10	aA	802	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
10	bA	839	CLA	C4-C3-C5	2.74	120.00	115.29
10	aA	837	CLA	CAC-C3C-C4C	2.74	128.40	124.82
10	aA	808	CLA	CHD-C4C-NC	2.74	128.52	124.20
13	bM	101	BCR	C15-C16-C17	-2.74	117.76	123.51
13	bA	851	BCR	C27-C26-C25	2.74	126.73	122.74
10	aA	838	CLA	C1-C2-C3	-2.74	122.32	126.75
10	cA	806	CLA	C4C-C3C-C2C	-2.74	102.93	106.89
10	cB	812	CLA	CHD-C4C-NC	2.74	128.51	124.20
10	bA	816	CLA	C4-C3-C5	2.74	120.00	115.29
13	bA	848	BCR	C40-C30-C25	2.74	114.73	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	813	CLA	C4A-NA-C1A	-2.74	105.48	106.71
10	aA	816	CLA	C4-C3-C5	2.74	120.00	115.29
10	aB	826	CLA	C4-C3-C5	2.74	120.00	115.29
10	aA	834	CLA	CHD-C4C-NC	2.74	128.51	124.20
10	aA	803	CLA	CAC-C3C-C4C	2.74	128.40	124.82
10	aA	840	CLA	O2A-CGA-CBA	2.74	120.71	111.93
10	cA	839	CLA	C4-C3-C5	2.74	120.00	115.29
13	aM	101	BCR	C2-C1-C6	2.73	114.71	110.48
13	bM	101	BCR	C2-C1-C6	2.73	114.71	110.48
10	aA	841	CLA	CAA-C2A-C3A	-2.73	105.29	112.78
13	cB	846	BCR	C27-C26-C25	2.73	126.73	122.74
10	aL	204	CLA	CHC-C1C-C2C	-2.73	119.17	126.71
10	bL	203	CLA	C4C-C3C-C2C	-2.73	102.93	106.89
10	bA	836	CLA	CHD-C4C-NC	2.73	128.51	124.20
10	cB	815	CLA	CMB-C2B-C3B	2.73	129.93	124.80
10	aB	832	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
10	cA	816	CLA	C4-C3-C5	2.73	119.99	115.29
10	cA	841	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
13	aA	851	BCR	C27-C26-C25	2.73	126.72	122.74
10	aA	807	CLA	C4C-C3C-C2C	-2.73	102.94	106.89
10	aB	815	CLA	CMB-C2B-C3B	2.73	129.92	124.80
10	bA	840	CLA	CHD-C4C-NC	2.73	128.51	124.20
10	aA	828	CLA	CHC-C1C-C2C	-2.73	119.18	126.71
10	cA	835	CLA	O2D-CGD-O1D	-2.73	118.44	123.83
10	cA	828	CLA	CHC-C1C-C2C	-2.73	119.18	126.71
10	cA	840	CLA	CHD-C4C-NC	2.73	128.50	124.20
10	aA	835	CLA	O2D-CGD-O1D	-2.73	118.44	123.83
10	cA	817	CLA	CMC-C2C-C1C	2.73	129.18	125.03
10	bB	820	CLA	C1D-CHD-C4C	-2.73	118.76	122.48
10	aA	817	CLA	CBC-CAC-C3C	-2.73	104.86	112.43
10	aA	836	CLA	O2A-CGA-CBA	2.73	120.69	111.93
10	cA	823	CLA	CHB-C4A-NA	2.73	128.28	124.51
10	cA	808	CLA	CAC-C3C-C4C	2.73	128.38	124.82
10	bA	837	CLA	CAC-C3C-C4C	2.73	128.38	124.82
10	aA	840	CLA	C3B-C4B-NB	2.73	112.73	109.21
13	aB	846	BCR	C27-C26-C25	2.73	126.72	122.74
10	bA	841	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
10	bB	838	CLA	O2A-CGA-O1A	-2.73	116.60	123.56
10	aB	817	CLA	CHB-C4A-NA	2.72	128.28	124.51
10	bB	815	CLA	CMB-C2B-C3B	2.72	129.91	124.80
10	aB	841	CLA	O2A-CGA-CBA	2.72	120.68	111.93
10	bB	827	CLA	CAA-C2A-C3A	-2.72	105.32	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	841	CLA	O2A-CGA-CBA	2.72	120.67	111.93
10	cA	807	CLA	O2D-CGD-O1D	-2.72	118.45	123.83
10	bB	808	CLA	CHC-C1C-C2C	-2.72	119.20	126.71
10	cB	832	CLA	O2D-CGD-O1D	-2.72	118.45	123.83
10	bA	840	CLA	O2A-CGA-CBA	2.72	120.67	111.93
10	aB	808	CLA	CHC-C1C-C2C	-2.72	119.20	126.71
10	aB	828	CLA	O1D-CGD-CBD	-2.72	118.84	124.48
13	cA	848	BCR	C27-C26-C25	2.72	126.71	122.74
10	cA	836	CLA	O2A-CGA-CBA	2.72	120.67	111.93
10	aB	838	CLA	O2A-CGA-O1A	-2.72	116.61	123.56
10	bA	817	CLA	CBC-CAC-C3C	-2.72	104.87	112.43
10	aA	806	CLA	C4C-C3C-C2C	-2.72	102.95	106.89
10	cB	805	CLA	O2D-CGD-CBD	2.72	116.02	111.25
10	cB	808	CLA	CHC-C1C-C2C	-2.72	119.21	126.71
10	aB	802	CLA	CAC-C3C-C4C	2.72	128.37	124.82
10	cL	203	CLA	C4C-C3C-C2C	-2.72	102.95	106.89
10	bA	832	CLA	CHB-C4A-NA	2.72	128.27	124.51
10	aA	839	CLA	C4-C3-C5	2.72	119.97	115.29
10	cB	841	CLA	CHD-C4C-NC	2.72	128.49	124.20
10	bA	819	CLA	O2A-CGA-CBA	2.72	120.65	111.93
10	bA	836	CLA	O2A-CGA-CBA	2.72	120.65	111.93
10	bA	835	CLA	O2D-CGD-O1D	-2.72	118.47	123.83
10	aB	834	CLA	C4C-C3C-C2C	-2.72	102.96	106.89
10	bB	832	CLA	CAA-C2A-C3A	-2.72	105.34	112.78
13	bB	846	BCR	C27-C26-C25	2.72	126.70	122.74
10	cB	841	CLA	O2A-CGA-CBA	2.72	120.65	111.93
10	cA	834	CLA	CHD-C4C-NC	2.72	128.48	124.20
10	bA	806	CLA	C4C-C3C-C2C	-2.71	102.96	106.89
10	bA	839	CLA	C4C-C3C-C2C	-2.71	102.96	106.89
10	aA	841	CLA	O2A-CGA-CBA	2.71	120.64	111.93
10	cB	828	CLA	O1D-CGD-CBD	-2.71	118.86	124.48
13	cM	101	BCR	C15-C16-C17	-2.71	117.81	123.51
13	aA	848	BCR	C27-C26-C25	2.71	126.70	122.74
10	bB	832	CLA	O2D-CGD-O1D	-2.71	118.47	123.83
10	bA	841	CLA	O2A-CGA-CBA	2.71	120.64	111.93
10	bB	837	CLA	O2D-CGD-O1D	-2.71	118.47	123.83
10	cB	820	CLA	C1D-CHD-C4C	-2.71	118.78	122.48
10	cB	828	CLA	CAC-C3C-C4C	2.71	128.36	124.82
10	cA	856	CLA	CAA-C2A-C3A	-2.71	105.35	112.78
10	cA	839	CLA	C4C-C3C-C2C	-2.71	102.96	106.89
10	bB	828	CLA	CHD-C4C-NC	2.71	128.47	124.20
10	bB	841	CLA	O2A-CGA-CBA	2.71	120.63	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	827	CLA	C4-C3-C5	2.71	119.95	115.29
10	cA	817	CLA	CBC-CAC-C3C	-2.71	104.91	112.43
10	cB	841	CLA	CBC-CAC-C3C	-2.71	104.91	112.43
10	bA	817	CLA	CMC-C2C-C1C	2.71	129.15	125.03
10	cB	832	CLA	CAA-C2A-C3A	-2.71	105.36	112.78
10	bB	841	CLA	CBC-CAC-C3C	-2.71	104.91	112.43
13	cM	101	BCR	C2-C1-C6	2.71	114.67	110.48
10	bA	838	CLA	C1-C2-C3	-2.71	122.37	126.75
10	bA	807	CLA	C4C-C3C-C2C	-2.71	102.97	106.89
13	aA	848	BCR	C40-C30-C25	2.71	114.68	110.30
10	cB	834	CLA	C4C-C3C-C2C	-2.71	102.97	106.89
10	bA	842	CLA	CMC-C2C-C1C	2.71	129.15	125.03
10	bA	842	CLA	C4C-C3C-C2C	-2.71	102.97	106.89
10	bB	805	CLA	O2D-CGD-CBD	2.71	115.99	111.25
10	aB	827	CLA	C4-C3-C5	2.71	119.95	115.29
10	bB	828	CLA	CAC-C3C-C4C	2.71	128.36	124.82
10	cB	807	CLA	CHB-C4A-NA	2.71	128.25	124.51
10	aB	819	CLA	O2D-CGD-O1D	-2.71	118.49	123.83
10	aB	820	CLA	C1D-CHD-C4C	-2.70	118.79	122.48
10	bB	841	CLA	CHD-C4C-NC	2.70	128.47	124.20
10	cA	820	CLA	O2A-CGA-CBA	2.70	120.61	111.93
10	cB	838	CLA	O2A-CGA-O1A	-2.70	116.65	123.56
10	bA	856	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
10	aA	819	CLA	O2A-CGA-CBA	2.70	120.61	111.93
10	cA	832	CLA	CHB-C4A-NA	2.70	128.25	124.51
10	cA	819	CLA	O2A-CGA-CBA	2.70	120.61	111.93
10	aB	807	CLA	CHB-C4A-NA	2.70	128.25	124.51
10	bA	807	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
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
13	aM	101	BCR	C15-C16-C17	-2.70	117.83	123.51
10	aA	807	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
10	aL	202	CLA	CAA-C2A-C1A	2.70	120.82	111.97
10	aB	805	CLA	O2D-CGD-CBD	2.70	115.98	111.25
10	cL	202	CLA	CAA-C2A-C1A	2.70	120.82	111.97
10	cA	804	CLA	CHD-C4C-NC	2.70	128.46	124.20
10	bB	810	CLA	CHD-C4C-NC	2.70	128.46	124.20
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	aL	203	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
10	bA	804	CLA	CHD-C4C-NC	2.70	128.45	124.20
10	aB	841	CLA	CBC-CAC-C3C	-2.70	104.94	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	820	CLA	O2A-CGA-CBA	2.70	120.59	111.93
10	bA	829	CLA	O2A-CGA-CBA	2.70	120.59	111.93
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	cB	837	CLA	O2D-CGD-O1D	-2.70	118.51	123.83
10	aA	820	CLA	O2A-CGA-CBA	2.70	120.58	111.93
10	bB	827	CLA	C4-C3-C5	2.70	119.93	115.29
10	aA	832	CLA	CHB-C4A-NA	2.70	128.24	124.51
10	aA	839	CLA	C4C-C3C-C2C	-2.69	102.99	106.89
10	cA	834	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
10	bA	823	CLA	C4C-C3C-C2C	-2.69	102.99	106.89
10	aA	856	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
10	cA	817	CLA	O2A-CGA-CBA	2.69	120.57	111.93
10	bB	802	CLA	CBC-CAC-C3C	-2.69	104.96	112.43
10	aA	829	CLA	O2A-CGA-CBA	2.69	120.57	111.93
10	bL	202	CLA	CAA-C2A-C1A	2.69	120.79	111.97
10	cL	204	CLA	CMC-C2C-C1C	2.69	129.12	125.03
10	aA	817	CLA	O2A-CGA-CBA	2.69	120.57	111.93
10	aA	842	CLA	C4C-C3C-C2C	-2.69	102.99	106.89
13	bA	848	BCR	C27-C26-C25	2.69	126.66	122.74
10	cA	829	CLA	O2A-CGA-CBA	2.69	120.57	111.93
10	cA	807	CLA	C4C-C3C-C2C	-2.69	103.00	106.89
10	bA	835	CLA	CHD-C4C-NC	2.69	128.44	124.20
10	cB	806	CLA	CBC-CAC-C3C	-2.69	104.96	112.43
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
13	cA	848	BCR	C40-C30-C25	2.69	114.65	110.30
10	aA	817	CLA	CMB-C2B-C3B	2.69	129.84	124.80
10	aB	837	CLA	O2D-CGD-O1D	-2.69	118.53	123.83
10	bA	814	CLA	CMB-C2B-C3B	2.69	129.84	124.80
10	bA	817	CLA	O2A-CGA-CBA	2.69	120.55	111.93
10	cA	817	CLA	CMB-C2B-C3B	2.69	129.84	124.80
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
10	aA	842	CLA	CMC-C2C-C1C	2.69	129.12	125.03
10	bB	802	CLA	CAC-C3C-C4C	2.68	128.33	124.82
10	aB	802	CLA	C4-C3-C5	2.68	119.91	115.29
10	bA	817	CLA	CMB-C2B-C3B	2.68	129.83	124.80
10	aB	815	CLA	O2D-CGD-O1D	-2.68	118.53	123.83
10	aA	854	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
10	cA	842	CLA	C4C-C3C-C2C	-2.68	103.01	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	854	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
10	bB	808	CLA	CMB-C2B-C3B	2.68	129.82	124.80
10	cB	802	CLA	CBC-CAC-C3C	-2.68	104.99	112.43
10	aB	841	CLA	CHD-C4C-NC	2.68	128.43	124.20
10	bL	204	CLA	CMC-C2C-C1C	2.68	129.11	125.03
10	aA	823	CLA	C4C-C3C-C2C	-2.68	103.01	106.89
10	cB	819	CLA	O2D-CGD-O1D	-2.68	118.54	123.83
10	cB	815	CLA	O2D-CGD-O1D	-2.68	118.54	123.83
10	cL	203	CLA	O2D-CGD-O1D	-2.68	118.54	123.83
10	cA	821	CLA	CMB-C2B-C3B	2.68	129.82	124.80
10	bA	834	CLA	CHD-C4C-NC	2.68	128.42	124.20
10	cA	842	CLA	CMC-C2C-C1C	2.68	129.10	125.03
10	cB	801	CLA	O2A-CGA-CBA	2.68	120.52	111.93
10	cB	803	CLA	C1-C2-C3	-2.68	121.42	126.04
10	aB	808	CLA	CMB-C2B-C3B	2.68	129.82	124.80
10	aB	801	CLA	O2A-CGA-CBA	2.68	120.52	111.93
10	aB	802	CLA	CBC-CAC-C3C	-2.67	105.00	112.43
10	cA	823	CLA	O2A-CGA-CBA	2.67	120.52	111.93
10	cB	802	CLA	C4-C3-C5	2.67	119.89	115.29
10	cB	810	CLA	CHD-C4C-NC	2.67	128.42	124.20
10	aB	810	CLA	CHD-C4C-NC	2.67	128.42	124.20
10	bB	806	CLA	CBC-CAC-C3C	-2.67	105.00	112.43
10	bL	203	CLA	O2D-CGD-O1D	-2.67	118.55	123.83
10	bB	819	CLA	CAC-C3C-C4C	2.67	128.31	124.82
10	bB	817	CLA	C4-C3-C5	2.67	119.89	115.29
10	bB	826	CLA	CHD-C4C-NC	2.67	128.42	124.20
10	bA	856	CLA	CHD-C4C-NC	2.67	128.42	124.20
10	aA	819	CLA	O2D-CGD-O1D	-2.67	118.55	123.83
10	aB	823	CLA	CHD-C4C-NC	2.67	128.41	124.20
10	cA	840	CLA	C3B-C4B-NB	2.67	112.67	109.21
10	aB	819	CLA	CAC-C3C-C4C	2.67	128.31	124.82
10	cA	854	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
10	aA	814	CLA	CMB-C2B-C3B	2.67	129.81	124.80
10	cL	204	CLA	O2A-CGA-CBA	2.67	120.51	111.93
10	aA	827	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
10	aL	204	CLA	CMC-C2C-C1C	2.67	129.09	125.03
10	cB	819	CLA	CAC-C3C-C4C	2.67	128.31	124.82
10	aB	806	CLA	CBC-CAC-C3C	-2.67	105.02	112.43
10	aA	806	CLA	C1D-CHD-C4C	-2.67	118.83	122.48
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	bB	801	CLA	O2A-CGA-CBA	2.67	120.50	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	808	CLA	CMB-C2B-C3B	2.67	129.81	124.80
10	bA	823	CLA	O2A-CGA-CBA	2.67	120.50	111.93
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	aB	803	CLA	C1-C2-C3	-2.67	121.43	126.04
10	bA	840	CLA	C3B-C4B-NB	2.67	112.66	109.21
10	bB	814	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
10	bB	815	CLA	O2D-CGD-O1D	-2.67	118.56	123.83
10	aB	826	CLA	CAA-C2A-C1A	-2.67	103.23	111.97
10	cA	835	CLA	CHD-C4C-NC	2.67	128.41	124.20
10	cA	811	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	821	CLA	CMB-C2B-C3B	2.67	129.80	124.80
10	cB	817	CLA	C4-C3-C5	2.67	119.88	115.29
10	aA	816	CLA	CAC-C3C-C4C	2.67	128.31	124.82
10	cB	830	CLA	O2A-CGA-CBA	2.67	120.49	111.93
10	aB	814	CLA	CAA-C2A-C3A	-2.67	105.48	112.78
10	bA	806	CLA	C1D-CHD-C4C	-2.67	118.84	122.48
10	aB	815	CLA	CHB-C4A-NA	2.67	128.20	124.51
10	cA	827	CLA	CAA-C2A-C3A	-2.66	105.48	112.78
10	aB	830	CLA	O2A-CGA-CBA	2.66	120.48	111.93
10	bA	815	CLA	CAA-C2A-C3A	-2.66	105.48	112.78
10	cA	819	CLA	O2D-CGD-O1D	-2.66	118.57	123.83
10	aA	821	CLA	CMB-C2B-C3B	2.66	129.80	124.80
10	cA	856	CLA	CHD-C4C-NC	2.66	128.40	124.20
10	aB	828	CLA	CAC-C3C-C4C	2.66	128.30	124.82
10	cB	825	CLA	CHD-C4C-NC	2.66	128.40	124.20
10	aB	837	CLA	CHD-C4C-NC	2.66	128.40	124.20
10	bB	826	CLA	CAA-C2A-C1A	-2.66	103.25	111.97
10	bB	819	CLA	O2D-CGD-O1D	-2.66	118.57	123.83
13	bM	101	BCR	C31-C1-C6	2.66	114.61	110.30
13	cM	101	BCR	C31-C1-C6	2.66	114.61	110.30
10	cA	821	CLA	O2A-CGA-CBA	2.66	120.48	111.93
10	cB	814	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
10	aA	812	CLA	CHD-C4C-NC	2.66	128.40	124.20
10	aA	823	CLA	O2A-CGA-CBA	2.66	120.47	111.93
10	cB	803	CLA	CHC-C1C-C2C	-2.66	119.38	126.71
10	aB	810	CLA	CHB-C4A-NA	2.66	128.19	124.51
10	cA	815	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
10	bL	204	CLA	O2A-CGA-CBA	2.66	120.47	111.93
10	bB	830	CLA	O2A-CGA-CBA	2.66	120.46	111.93
10	aL	204	CLA	O2A-CGA-CBA	2.66	120.46	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	826	CLA	CAA-C2A-C1A	-2.66	103.27	111.97
10	bA	819	CLA	O2D-CGD-O1D	-2.66	118.58	123.83
10	bA	811	CLA	CHB-C4A-NA	2.66	128.19	124.51
13	aM	101	BCR	C31-C1-C6	2.66	114.60	110.30
10	cA	806	CLA	C1-C2-C3	-2.65	121.45	126.04
10	aB	803	CLA	CHC-C1C-C2C	-2.65	119.39	126.71
10	bA	821	CLA	O2A-CGA-CBA	2.65	120.45	111.93
10	cB	820	CLA	O2D-CGD-O1D	-2.65	118.59	123.83
10	cB	831	CLA	CMC-C2C-C1C	2.65	129.07	125.03
10	aA	821	CLA	O2A-CGA-CBA	2.65	120.44	111.93
10	aB	812	CLA	O2D-CGD-O1D	-2.65	118.59	123.83
10	cA	816	CLA	CAC-C3C-C4C	2.65	128.29	124.82
10	cA	834	CLA	CAC-C3C-C4C	2.65	128.29	124.82
10	cL	203	CLA	C1-C2-C3	-2.65	121.46	126.04
10	aB	817	CLA	C4-C3-C5	2.65	119.85	115.29
10	aA	815	CLA	CAA-C2A-C3A	-2.65	105.52	112.78
10	bB	825	CLA	CHD-C4C-NC	2.65	128.38	124.20
10	aA	856	CLA	CHD-C4C-NC	2.65	128.38	124.20
10	bB	802	CLA	C4-C3-C5	2.65	119.85	115.29
10	bB	803	CLA	CHC-C1C-C2C	-2.65	119.41	126.71
10	bA	814	CLA	CHD-C4C-NC	2.65	128.38	124.20
10	cB	834	CLA	CHD-C4C-NC	2.65	128.38	124.20
10	aB	825	CLA	CHD-C4C-NC	2.65	128.38	124.20
10	aB	836	CLA	CHD-C4C-NC	2.65	128.38	124.20
10	bB	812	CLA	O2D-CGD-O1D	-2.65	118.60	123.83
10	aA	811	CLA	C4-C3-C5	2.65	119.85	115.29
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	bA	827	CLA	CHD-C4C-NC	2.65	128.37	124.20
10	aA	811	CLA	CHD-C4C-NC	2.65	128.37	124.20
10	aB	831	CLA	CMC-C2C-C1C	2.65	129.06	125.03
10	bA	825	CLA	CAC-C3C-C4C	2.65	128.28	124.82
10	aA	808	CLA	CBC-CAC-C3C	-2.65	105.08	112.43
10	bB	827	CLA	CAC-C3C-C4C	2.65	128.28	124.82
10	bB	836	CLA	CHD-C4C-NC	2.65	128.37	124.20
10	cA	824	CLA	CMC-C2C-C1C	2.64	129.06	125.03
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	bB	804	CLA	O2A-CGA-CBA	2.64	120.42	111.93
10	cA	806	CLA	C1D-CHD-C4C	-2.64	118.87	122.48
10	aB	826	CLA	CHD-C4C-NC	2.64	128.37	124.20
10	cA	814	CLA	CMB-C2B-C3B	2.64	129.76	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	804	CLA	O2A-CGA-CBA	2.64	120.42	111.93
10	aB	820	CLA	O2D-CGD-O1D	-2.64	118.61	123.83
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	cB	827	CLA	CAC-C3C-C4C	2.64	128.27	124.82
10	cB	838	CLA	O2D-CGD-O1D	-2.64	118.62	123.83
10	bA	816	CLA	CAC-C3C-C4C	2.64	128.27	124.82
10	bB	823	CLA	CHD-C4C-NC	2.64	128.36	124.20
10	aL	205	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	bA	829	CLA	C4-C3-C5	2.64	119.83	115.29
10	bB	820	CLA	O2D-CGD-O1D	-2.64	118.62	123.83
10	aA	825	CLA	C1-C2-C3	-2.64	121.48	126.04
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	cA	841	CLA	O2D-CGD-O1D	-2.64	118.62	123.83
10	bA	841	CLA	O2D-CGD-O1D	-2.63	118.63	123.83
10	bB	812	CLA	CAC-C3C-C4C	2.63	128.26	124.82
10	bA	834	CLA	CAC-C3C-C4C	2.63	128.26	124.82
10	bA	824	CLA	C4-C3-C5	2.63	119.82	115.29
10	aA	839	CLA	CAA-C2A-C3A	-2.63	105.56	112.78
10	bA	824	CLA	CMC-C2C-C1C	2.63	129.04	125.03
10	bB	831	CLA	CMC-C2C-C1C	2.63	129.04	125.03
10	cA	840	CLA	O2D-CGD-O1D	-2.63	118.63	123.83
10	aB	827	CLA	CAC-C3C-C4C	2.63	128.26	124.82
10	aA	824	CLA	CMC-C2C-C1C	2.63	129.03	125.03
10	cB	838	CLA	CHB-C4A-NA	2.63	128.15	124.51
10	cA	824	CLA	C4-C3-C5	2.63	119.82	115.29
10	cA	839	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
10	bA	812	CLA	CHD-C4C-NC	2.63	128.35	124.20
10	cB	805	CLA	O2A-CGA-CBA	2.63	120.37	111.93
10	bB	804	CLA	CHA-C1A-NA	-2.63	120.38	126.40
10	aB	804	CLA	O2A-CGA-CBA	2.63	120.37	111.93
10	aA	825	CLA	CAC-C3C-C4C	2.63	128.25	124.82
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
10	bA	808	CLA	CBC-CAC-C3C	-2.63	105.14	112.43
10	cB	812	CLA	O2D-CGD-O1D	-2.63	118.64	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	808	CLA	CBC-CAC-C3C	-2.63	105.14	112.43
10	bA	811	CLA	C4-C3-C5	2.63	119.81	115.29
10	bA	838	CLA	CMC-C2C-C1C	2.63	129.03	125.03
10	aB	815	CLA	CAA-C2A-C3A	-2.63	105.59	112.78
10	aA	824	CLA	C4-C3-C5	2.63	119.81	115.29
10	cA	829	CLA	C4-C3-C5	2.63	119.81	115.29
10	aB	838	CLA	CHB-C4A-NA	2.63	128.14	124.51
10	aB	805	CLA	O2A-CGA-CBA	2.63	120.36	111.93
10	cB	818	CLA	CHD-C4C-NC	2.63	128.34	124.20
9	aA	801	CL0	CHD-C4C-NC	2.63	128.34	124.20
10	bB	838	CLA	O2D-CGD-O1D	-2.62	118.65	123.83
10	bB	805	CLA	O2A-CGA-CBA	2.62	120.36	111.93
10	cB	810	CLA	CHB-C4A-NA	2.62	128.14	124.51
10	aB	818	CLA	CHB-C4A-NA	2.62	128.14	124.51
10	cA	811	CLA	C4-C3-C5	2.62	119.81	115.29
10	bB	840	CLA	CHC-C1C-C2C	-2.62	119.48	126.71
10	bB	824	CLA	CHD-C4C-NC	2.62	128.34	124.20
10	aB	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	bA	834	CLA	CHB-C4A-NA	2.62	128.14	124.51
10	aA	829	CLA	C4-C3-C5	2.62	119.80	115.29
10	bB	812	CLA	CMA-C3A-C2A	-2.62	103.22	113.78
10	cA	825	CLA	CAC-C3C-C4C	2.62	128.24	124.82
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	bB	815	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
9	cA	801	CL0	CHD-C4C-NC	2.62	128.33	124.20
10	cB	801	CLA	CMC-C2C-C1C	2.62	129.01	125.03
10	bB	818	CLA	CHB-C4A-NA	2.62	128.13	124.51
10	aB	801	CLA	CMC-C2C-C1C	2.62	129.01	125.03
10	bB	833	CLA	O2D-CGD-O1D	-2.62	118.66	123.83
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	aA	841	CLA	O2D-CGD-O1D	-2.62	118.66	123.83
10	cA	812	CLA	O2D-CGD-O1D	-2.62	118.66	123.83
10	bB	820	CLA	O2A-CGA-CBA	2.62	120.33	111.93
10	bA	839	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
10	bL	205	CLA	CHD-C4C-NC	2.62	128.32	124.20
10	cB	801	CLA	OBD-CAD-CBD	-2.62	122.07	125.91
10	aB	818	CLA	CHD-C4C-NC	2.61	128.32	124.20
10	cB	819	CLA	CMC-C2C-C1C	2.61	129.01	125.03
10	bA	812	CLA	O2D-CGD-O1D	-2.61	118.67	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	814	CLA	CHD-C4C-NC	2.61	128.32	124.20
10	bB	801	CLA	OBD-CAD-CBD	-2.61	122.07	125.91
10	cA	806	CLA	CHB-C4A-NA	2.61	128.12	124.51
10	aB	819	CLA	CMC-C2C-C1C	2.61	129.01	125.03
10	bL	204	CLA	CHD-C4C-NC	2.61	128.32	124.20
10	aB	812	CLA	CMA-C3A-C2A	-2.61	103.25	113.78
10	cB	807	CLA	CMA-C3A-C2A	-2.61	103.25	113.78
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	bA	839	CLA	CBC-CAC-C3C	-2.61	105.18	112.43
10	cB	839	CLA	O2A-CGA-CBA	2.61	120.31	111.93
10	cA	839	CLA	CBC-CAC-C3C	-2.61	105.18	112.43
10	bB	840	CLA	OBD-CAD-C3D	-2.61	123.42	128.04
10	aB	820	CLA	O2A-CGA-CBA	2.61	120.31	111.93
10	bB	807	CLA	CMA-C3A-C2A	-2.61	103.26	113.78
10	aB	807	CLA	CMA-C3A-C2A	-2.61	103.26	113.78
9	bA	801	CL0	CHD-C4C-NC	2.61	128.31	124.20
10	bA	840	CLA	O2D-CGD-O1D	-2.61	118.68	123.83
10	aA	839	CLA	CBC-CAC-C3C	-2.61	105.19	112.43
10	aB	833	CLA	O2D-CGD-O1D	-2.61	118.68	123.83
10	aB	831	CLA	CHD-C4C-NC	2.61	128.31	124.20
10	cB	840	CLA	CHC-C1C-C2C	-2.61	119.53	126.71
10	cB	815	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
10	bA	822	CLA	CMC-C2C-C1C	2.61	129.00	125.03
10	aB	834	CLA	CHD-C4C-NC	2.60	128.31	124.20
10	aA	834	CLA	CHB-C4A-NA	2.60	128.11	124.51
10	aA	833	CLA	C4C-C3C-C2C	-2.60	103.12	106.89
10	cB	820	CLA	O2A-CGA-CBA	2.60	120.29	111.93
10	bA	810	CLA	O2D-CGD-O1D	-2.60	118.69	123.83
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	aB	840	CLA	CHC-C1C-C2C	-2.60	119.54	126.71
10	cB	812	CLA	CMA-C3A-C2A	-2.60	103.30	113.78
10	aA	827	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	bB	831	CLA	CHD-C4C-NC	2.60	128.30	124.20
10	aA	812	CLA	O2D-CGD-O1D	-2.60	118.69	123.83
10	aB	840	CLA	OBD-CAD-C3D	-2.60	123.43	128.04
10	cA	811	CLA	C1-C2-C3	-2.60	121.55	126.04
10	cB	833	CLA	O2D-CGD-O1D	-2.60	118.69	123.83
10	bA	811	CLA	C1-C2-C3	-2.60	121.55	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	840	CLA	O2D-CGD-O1D	-2.60	118.70	123.83
10	bA	833	CLA	C4C-C3C-C2C	-2.60	103.12	106.89
10	aA	811	CLA	C1-C2-C3	-2.60	121.55	126.04
10	cB	812	CLA	CAC-C3C-C4C	2.60	128.22	124.82
10	bB	839	CLA	O2A-CGA-CBA	2.60	120.27	111.93
10	bB	801	CLA	CMC-C2C-C1C	2.60	128.98	125.03
10	aB	839	CLA	O2A-CGA-CBA	2.60	120.27	111.93
13	cA	848	BCR	C30-C25-C26	-2.60	118.96	122.59
10	bB	811	CLA	O2A-CGA-CBA	2.60	120.27	111.93
10	bA	806	CLA	CHB-C4A-NA	2.59	128.10	124.51
10	bA	856	CLA	CED-O2D-CGD	2.59	121.87	115.95
10	cA	814	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
10	aB	838	CLA	O2D-CGD-O1D	-2.59	118.71	123.83
10	aA	838	CLA	CMC-C2C-C1C	2.59	128.97	125.03
10	bA	814	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
10	aA	813	CLA	CHB-C4A-NA	2.59	128.09	124.51
10	aB	812	CLA	CAC-C3C-C4C	2.59	128.21	124.82
10	aA	834	CLA	CAC-C3C-C4C	2.59	128.21	124.82
10	aB	841	CLA	C4A-NA-C1A	-2.59	105.54	106.71
10	aB	801	CLA	OBD-CAD-CBD	-2.59	122.11	125.91
10	cB	820	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
10	aB	805	CLA	CHC-C1C-NC	2.59	128.13	124.20
13	aA	848	BCR	C30-C25-C26	-2.59	118.97	122.59
10	cB	840	CLA	OBD-CAD-C3D	-2.59	123.45	128.04
10	bA	817	CLA	CHB-C4A-NA	2.59	128.09	124.51
10	aA	856	CLA	CED-O2D-CGD	2.59	121.86	115.95
10	cB	841	CLA	C4A-NA-C1A	-2.59	105.54	106.71
10	aB	827	CLA	O2D-CGD-O1D	-2.59	118.72	123.83
10	aA	822	CLA	CMC-C2C-C1C	2.59	128.97	125.03
10	aB	811	CLA	O2A-CGA-CBA	2.59	120.23	111.93
10	bB	815	CLA	CAC-C3C-C4C	2.59	128.20	124.82
10	cB	811	CLA	O2A-CGA-CBA	2.59	120.23	111.93
10	aL	204	CLA	CHD-C4C-NC	2.59	128.28	124.20
10	bB	819	CLA	CMC-C2C-C1C	2.59	128.97	125.03
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
13	aI	102	BCR	C15-C14-C13	-2.58	123.62	127.31
10	bA	825	CLA	C3B-C4B-NB	2.58	112.55	109.21
10	aB	806	CLA	O2D-CGD-O1D	-2.58	118.73	123.83
10	aL	203	CLA	O2A-CGA-CBA	2.58	120.22	111.93
10	aB	815	CLA	CAC-C3C-C4C	2.58	128.19	124.82
10	aA	802	CLA	CHD-C4C-NC	2.58	128.27	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	807	CLA	CMB-C2B-C3B	2.58	129.64	124.80
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	bB	840	CLA	O2D-CGD-O1D	-2.58	118.73	123.83
10	cA	831	CLA	CMC-C2C-C1C	2.58	128.96	125.03
10	cA	833	CLA	C4C-C3C-C2C	-2.58	103.15	106.89
10	bA	831	CLA	CAA-C2A-C3A	-2.58	105.71	112.78
10	cB	825	CLA	CMC-C2C-C1C	2.58	128.96	125.03
10	cA	827	CLA	CHB-C4A-NA	2.58	128.08	124.51
10	cB	806	CLA	O2D-CGD-O1D	-2.58	118.74	123.83
10	bA	854	CLA	O2D-CGD-O1D	-2.58	118.74	123.83
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	810	CLA	O2D-CGD-O1D	-2.58	118.74	123.83
10	cL	203	CLA	O2A-CGA-CBA	2.58	120.20	111.93
10	cA	830	CLA	O2D-CGD-O1D	-2.58	118.75	123.83
10	cL	203	CLA	CMB-C2B-C3B	2.57	129.63	124.80
10	aA	810	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
10	cB	827	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
10	aA	813	CLA	CAC-C3C-C4C	2.57	128.18	124.82
10	aA	806	CLA	CHB-C4A-NA	2.57	128.07	124.51
10	bB	827	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
13	aA	851	BCR	C1-C6-C5	-2.57	118.99	122.59
10	bA	813	CLA	CAC-C3C-C4C	2.57	128.18	124.82
10	bB	820	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
10	cA	856	CLA	CED-O2D-CGD	2.57	121.83	115.95
10	cB	816	CLA	CHD-C4C-NC	2.57	128.26	124.20
10	bA	832	CLA	CMC-C2C-C1C	2.57	128.94	125.03
13	cB	845	BCR	C27-C26-C25	2.57	126.49	122.74
10	bL	203	CLA	O2A-CGA-CBA	2.57	120.19	111.93
10	cB	814	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
10	cB	815	CLA	CAC-C3C-C4C	2.57	128.18	124.82
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
10	aA	831	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
10	bB	810	CLA	CBC-CAC-C3C	-2.57	105.29	112.43
10	aA	854	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
10	bB	825	CLA	CMC-C2C-C1C	2.57	128.94	125.03
10	bA	831	CLA	CMC-C2C-C1C	2.57	128.94	125.03
10	bA	832	CLA	O2A-CGA-O1A	-2.57	117.00	123.56
10	aB	808	CLA	CED-O2D-CGD	2.57	121.82	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	841	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
10	aA	831	CLA	CMC-C2C-C1C	2.57	128.94	125.03
10	aB	810	CLA	CBC-CAC-C3C	-2.57	105.30	112.43
10	aA	827	CLA	CHB-C4A-NA	2.57	128.06	124.51
10	aB	816	CLA	CHD-C4C-NC	2.57	128.25	124.20
10	cL	204	CLA	C1D-CHD-C4C	-2.57	118.97	122.48
10	bB	806	CLA	O2D-CGD-O1D	-2.57	118.76	123.83
10	cB	810	CLA	CBC-CAC-C3C	-2.57	105.30	112.43
10	cB	831	CLA	CHB-C4A-NA	2.57	128.06	124.51
10	cA	854	CLA	O2D-CGD-O1D	-2.57	118.76	123.83
13	cI	103	BCR	C15-C14-C13	-2.57	123.65	127.31
10	bL	204	CLA	C1D-CHD-C4C	-2.57	118.98	122.48
10	cA	802	CLA	CHD-C4C-NC	2.57	128.25	124.20
10	bB	808	CLA	CED-O2D-CGD	2.57	121.81	115.95
10	aL	205	CLA	O2A-CGA-CBA	2.57	120.17	111.93
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	843	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
10	aA	840	CLA	CMB-C2B-C3B	2.56	129.61	124.80
10	cB	808	CLA	CED-O2D-CGD	2.56	121.81	115.95
10	aB	814	CLA	O2D-CGD-O1D	-2.56	118.77	123.83
10	bA	802	CLA	CBC-CAC-C3C	-2.56	105.31	112.43
10	bA	843	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
10	cA	831	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
10	aA	830	CLA	O2D-CGD-O1D	-2.56	118.77	123.83
10	aB	804	CLA	CHC-C1C-C2C	-2.56	119.65	126.71
10	cB	804	CLA	CHC-C1C-C2C	-2.56	119.65	126.71
10	cB	817	CLA	O2D-CGD-O1D	-2.56	118.77	123.83
10	bA	810	CLA	CHD-C4C-NC	2.56	128.24	124.20
10	bL	205	CLA	O2A-CGA-CBA	2.56	120.15	111.93
10	cA	802	CLA	CBC-CAC-C3C	-2.56	105.32	112.43
13	cA	851	BCR	C1-C6-C5	-2.56	119.01	122.59
13	bA	848	BCR	C30-C25-C26	-2.56	119.01	122.59
10	bA	827	CLA	CMC-C2C-C1C	2.56	128.93	125.03
10	aB	840	CLA	O2D-CGD-O1D	-2.56	118.78	123.83
10	aB	814	CLA	CMC-C2C-C1C	2.56	128.92	125.03
10	cA	810	CLA	CHD-C4C-NC	2.56	128.24	124.20
10	aB	817	CLA	O2D-CGD-O1D	-2.56	118.78	123.83
10	bA	829	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
10	bL	203	CLA	CMB-C2B-C3B	2.56	129.60	124.80
13	bI	102	BCR	C15-C14-C13	-2.56	123.66	127.31
10	aL	203	CLA	CMB-C2B-C3B	2.56	129.60	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	814	CLA	CMC-C2C-C1C	2.56	128.92	125.03
10	bA	830	CLA	O2D-CGD-O1D	-2.56	118.78	123.83
10	cA	823	CLA	CAC-C3C-C4C	2.56	128.16	124.82
10	cA	803	CLA	CHB-C4A-NA	2.56	128.05	124.51
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	aA	832	CLA	O2A-CGA-O1A	-2.55	117.03	123.56
10	cA	856	CLA	CHB-C4A-NA	2.55	128.04	124.51
10	bA	840	CLA	CMB-C2B-C3B	2.55	129.59	124.80
10	bA	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	817	CLA	C1-C2-C3	-2.55	121.63	126.04
10	aA	827	CLA	CMC-C2C-C1C	2.55	128.92	125.03
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	824	CLA	C1D-CHD-C4C	-2.55	119.00	122.48
10	cA	832	CLA	O2A-CGA-O1A	-2.55	117.04	123.56
10	cA	807	CLA	CMB-C2B-C3B	2.55	129.59	124.80
10	aB	825	CLA	CMC-C2C-C1C	2.55	128.91	125.03
10	cA	838	CLA	CMC-C2C-C1C	2.55	128.91	125.03
10	aB	817	CLA	CMC-C2C-C1C	2.55	128.91	125.03
10	aB	841	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
11	aB	842	PQN	C14-C13-C15	2.55	119.68	115.29
10	bB	816	CLA	CHD-C4C-NC	2.55	128.22	124.20
10	aA	802	CLA	CBC-CAC-C3C	-2.55	105.35	112.43
10	bA	854	CLA	CAC-C3C-C2C	2.55	131.89	127.53
13	bB	845	BCR	C27-C26-C25	2.55	126.46	122.74
10	cA	813	CLA	CAC-C3C-C4C	2.55	128.15	124.82
13	aA	846	BCR	C11-C10-C9	-2.55	123.67	127.31
10	cA	840	CLA	CMB-C2B-C3B	2.55	129.58	124.80
10	bB	804	CLA	CHC-C1C-C2C	-2.55	119.69	126.71
10	cA	815	CLA	CBC-CAC-C3C	-2.55	105.36	112.43
10	cL	205	CLA	O2A-CGA-CBA	2.55	120.11	111.93
10	aB	816	CLA	CHB-C4A-NA	2.55	128.03	124.51
13	aB	845	BCR	C27-C26-C25	2.55	126.45	122.74
10	cB	823	CLA	CAA-C2A-C3A	-2.55	105.81	112.78
10	aA	815	CLA	CBC-CAC-C3C	-2.55	105.36	112.43
10	bA	819	CLA	CHB-C4A-NA	2.55	128.03	124.51
10	cA	829	CLA	CAA-C2A-C3A	-2.55	105.81	112.78
10	bA	826	CLA	CAA-C2A-C3A	-2.55	105.81	112.78
10	aA	817	CLA	C1-C2-C3	-2.55	121.64	126.04
10	aA	826	CLA	CHC-C1C-C2C	-2.55	119.69	126.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	832	CLA	CMC-C2C-C1C	2.54	128.90	125.03
10	cB	814	CLA	CMC-C2C-C1C	2.54	128.90	125.03
10	aA	856	CLA	CHB-C4A-NA	2.54	128.03	124.51
10	cA	824	CLA	C1D-CHD-C4C	-2.54	119.01	122.48
10	bL	203	CLA	CMC-C2C-C1C	2.54	128.90	125.03
13	bA	850	BCR	C15-C16-C17	-2.54	118.17	123.51
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
13	cA	846	BCR	C11-C10-C9	-2.54	123.68	127.31
11	bB	842	PQN	C14-C13-C15	2.54	119.66	115.29
10	bB	805	CLA	CHC-C1C-NC	2.54	128.06	124.20
10	cA	832	CLA	CMC-C2C-C1C	2.54	128.90	125.03
10	cA	817	CLA	C1-C2-C3	-2.54	121.65	126.04
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	cA	826	CLA	CHC-C1C-C2C	-2.54	119.71	126.71
10	bB	817	CLA	O2D-CGD-O1D	-2.54	118.81	123.83
10	aA	819	CLA	CMB-C2B-C3B	2.54	129.56	124.80
10	aA	840	CLA	C1-C2-C3	-2.54	121.65	126.04
10	cA	822	CLA	CMC-C2C-C1C	2.54	128.90	125.03
10	bB	814	CLA	O2D-CGD-O1D	-2.54	118.82	123.83
10	aL	204	CLA	C1D-CHD-C4C	-2.54	119.02	122.48
10	bA	840	CLA	C1-C2-C3	-2.54	121.65	126.04
10	cB	821	CLA	CHB-C4A-NA	2.54	128.02	124.51
10	aA	819	CLA	CHB-C4A-NA	2.54	128.02	124.51
10	bA	805	CLA	CMC-C2C-C1C	2.54	128.89	125.03
13	cA	850	BCR	C15-C16-C17	-2.54	118.18	123.51
10	aA	805	CLA	CMC-C2C-C1C	2.54	128.89	125.03
10	cA	805	CLA	CMC-C2C-C1C	2.54	128.89	125.03
10	bA	819	CLA	CMB-C2B-C3B	2.54	129.56	124.80
10	aB	823	CLA	CAA-C2A-C3A	-2.54	105.84	112.78
10	cB	805	CLA	CHC-C1C-NC	2.54	128.05	124.20
10	cB	814	CLA	CMB-C2B-C3B	2.53	129.55	124.80
13	aI	102	BCR	C15-C16-C17	-2.53	118.18	123.51
13	aA	850	BCR	C15-C16-C17	-2.53	118.18	123.51
10	cB	816	CLA	CHB-C4A-NA	2.53	128.02	124.51
10	cA	826	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
10	bA	815	CLA	CBC-CAC-C3C	-2.53	105.39	112.43
10	aA	829	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
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
11	cB	842	PQN	C14-C13-C15	2.53	119.65	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	807	CLA	CMB-C2B-C3B	2.53	129.55	124.80
10	cA	819	CLA	CMB-C2B-C3B	2.53	129.55	124.80
10	cB	840	CLA	O2D-CGD-O1D	-2.53	118.83	123.83
10	bB	831	CLA	CHB-C4A-NA	2.53	128.01	124.51
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	bA	826	CLA	CHC-C1C-C2C	-2.53	119.73	126.71
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	bB	823	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
10	aA	826	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
10	cB	837	CLA	C1-C2-C3	-2.53	121.67	126.04
13	cI	103	BCR	C15-C16-C17	-2.53	118.19	123.51
10	bB	828	CLA	CBA-CAA-C2A	2.53	121.38	113.85
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	bB	811	CLA	O2D-CGD-O1D	-2.53	118.84	123.83
10	aB	825	CLA	CHA-C1A-NA	-2.53	120.61	126.40
13	bA	851	BCR	C1-C6-C5	-2.53	119.06	122.59
10	bA	825	CLA	CMB-C2B-C3B	2.53	129.54	124.80
9	cA	801	CL0	CGD-CBD-CAD	-2.53	102.55	110.73
10	aA	814	CLA	O2D-CGD-O1D	-2.53	118.84	123.83
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	aA	805	CLA	CHB-C4A-NA	2.53	128.00	124.51
10	cA	818	CLA	CAA-CBA-CGA	2.52	120.69	113.26
10	cA	841	CLA	C1-C2-C3	-2.52	121.68	126.04
10	cA	820	CLA	C1-C2-C3	-2.52	121.68	126.04
10	bA	823	CLA	CAC-C3C-C4C	2.52	128.12	124.82
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
9	bA	801	CL0	CGD-CBD-CAD	-2.52	102.56	110.73
10	aB	828	CLA	CBA-CAA-C2A	2.52	121.36	113.85
10	bB	817	CLA	CMC-C2C-C1C	2.52	128.87	125.03
10	aB	831	CLA	CHB-C4A-NA	2.52	128.00	124.51
10	bA	811	CLA	O2A-CGA-CBA	2.52	120.03	111.93
10	cA	825	CLA	CMB-C2B-C3B	2.52	129.53	124.80
10	bA	818	CLA	CAA-CBA-CGA	2.52	120.68	113.26
10	bB	815	CLA	CBC-CAC-C3C	-2.52	105.43	112.43
10	bA	840	CLA	CAC-C3C-C4C	2.52	128.11	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	811	CLA	O2A-CGA-CBA	2.52	120.02	111.93
10	aB	832	CLA	CMB-C2B-C3B	2.52	129.53	124.80
13	bI	102	BCR	C15-C16-C17	-2.52	118.21	123.51
10	cB	828	CLA	CBA-CAA-C2A	2.52	121.35	113.85
10	cA	816	CLA	CHB-C4A-NA	2.52	127.99	124.51
10	cA	840	CLA	CAC-C3C-C4C	2.52	128.11	124.82
10	aA	840	CLA	CAC-C3C-C4C	2.52	128.11	124.82
10	cB	825	CLA	CHA-C1A-NA	-2.52	120.63	126.40
10	bB	814	CLA	CMB-C2B-C3B	2.52	129.52	124.80
10	cA	813	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
13	bB	845	BCR	C7-C8-C9	-2.52	122.43	126.21
9	aA	801	CL0	CGD-CBD-CAD	-2.52	102.58	110.73
10	aB	837	CLA	CMC-C2C-C1C	2.52	128.86	125.03
10	aA	803	CLA	CHB-C4A-NA	2.52	127.99	124.51
10	aL	204	CLA	CAC-C3C-C4C	2.52	128.11	124.82
10	bB	803	CLA	CHB-C4A-NA	2.52	127.99	124.51
10	aB	811	CLA	O2D-CGD-O1D	-2.51	118.86	123.83
10	aA	825	CLA	CMB-C2B-C3B	2.51	129.52	124.80
10	aA	810	CLA	CMB-C2B-C3B	2.51	129.52	124.80
10	cL	203	CLA	CMC-C2C-C1C	2.51	128.86	125.03
10	aB	814	CLA	CMB-C2B-C3B	2.51	129.51	124.80
10	bB	841	CLA	C1-C2-C3	-2.51	121.70	126.04
10	aA	841	CLA	C1-C2-C3	-2.51	121.70	126.04
10	bA	803	CLA	O1D-CGD-CBD	-2.51	119.28	124.48
10	bB	837	CLA	CMC-C2C-C1C	2.51	128.85	125.03
10	bL	203	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
10	cB	829	CLA	O2A-CGA-CBA	2.51	119.99	111.93
10	cL	203	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
10	cB	832	CLA	CMB-C2B-C3B	2.51	129.51	124.80
10	aA	818	CLA	CAA-CBA-CGA	2.51	120.65	113.26
10	bB	841	CLA	CAC-C3C-C4C	2.51	128.10	124.82
10	aA	813	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
10	bB	819	CLA	CAA-CBA-CGA	2.51	120.65	113.26
10	cB	815	CLA	CBC-CAC-C3C	-2.51	105.47	112.43
10	cA	810	CLA	CMB-C2B-C3B	2.51	129.50	124.80
10	bA	805	CLA	CHB-C4A-NA	2.51	127.98	124.51
10	aA	856	CLA	CMB-C2B-C3B	2.51	129.50	124.80
10	cA	811	CLA	O2A-CGA-CBA	2.51	119.98	111.93
10	cB	819	CLA	CBC-CAC-C3C	-2.51	105.47	112.43
10	aA	823	CLA	CAC-C3C-C4C	2.51	128.10	124.82
10	cA	805	CLA	CHB-C4A-NA	2.51	127.98	124.51
10	aB	819	CLA	CBC-CAC-C3C	-2.51	105.47	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	827	CLA	CMC-C2C-C1C	2.51	128.84	125.03
10	aL	203	CLA	CAA-C2A-C3A	-2.51	105.92	112.78
10	bB	808	CLA	O2A-CGA-CBA	2.51	119.97	111.93
10	aB	815	CLA	CBC-CAC-C3C	-2.50	105.47	112.43
10	aB	841	CLA	C1-C2-C3	-2.50	121.71	126.04
10	aB	806	CLA	CHC-C1C-C2C	-2.50	119.81	126.71
10	cB	817	CLA	CMC-C2C-C1C	2.50	128.84	125.03
10	aB	822	CLA	CMC-C2C-C1C	2.50	128.84	125.03
10	aA	815	CLA	CAC-C3C-C4C	2.50	128.09	124.82
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	bB	832	CLA	CMB-C2B-C3B	2.50	129.49	124.80
10	cB	811	CLA	O2D-CGD-O1D	-2.50	118.89	123.83
10	cA	815	CLA	CAC-C3C-C4C	2.50	128.09	124.82
10	cB	822	CLA	CMC-C2C-C1C	2.50	128.84	125.03
10	bB	841	CLA	CHB-C4A-NA	2.50	127.97	124.51
10	aA	830	CLA	CHB-C4A-NA	2.50	127.97	124.51
10	aB	841	CLA	CAC-C3C-C4C	2.50	128.09	124.82
10	cA	836	CLA	O2D-CGD-O1D	-2.50	118.89	123.83
10	aB	819	CLA	CAA-CBA-CGA	2.50	120.62	113.26
13	bA	848	BCR	C38-C26-C27	-2.50	108.90	113.57
10	cB	822	CLA	O2D-CGD-O1D	-2.50	118.89	123.83
10	bA	833	CLA	C1-C2-C3	-2.50	121.72	126.04
10	aA	816	CLA	CHB-C4A-NA	2.50	127.97	124.51
10	bB	829	CLA	O2A-CGA-CBA	2.50	119.96	111.93
9	bA	801	CL0	CHB-C4A-NA	2.50	127.97	124.51
10	bB	819	CLA	CBC-CAC-C3C	-2.50	105.49	112.43
10	aB	835	CLA	CAC-C3C-C4C	2.50	128.09	124.82
10	aB	829	CLA	O2A-CGA-CBA	2.50	119.95	111.93
10	aB	807	CLA	CHD-C4C-NC	2.50	128.14	124.20
10	cB	837	CLA	CMC-C2C-C1C	2.50	128.83	125.03
10	bA	814	CLA	O2D-CGD-O1D	-2.50	118.90	123.83
10	cB	808	CLA	O2A-CGA-CBA	2.50	119.95	111.93
10	bA	813	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
10	aA	833	CLA	O2A-CGA-CBA	2.50	119.94	111.93
10	bA	810	CLA	CMB-C2B-C3B	2.50	129.48	124.80
10	cB	813	CLA	CHD-C4C-NC	2.50	128.14	124.20
10	bA	823	CLA	C1-C2-C3	-2.50	121.73	126.04
10	aA	824	CLA	C1D-CHD-C4C	-2.49	119.08	122.48
10	bL	204	CLA	CAC-C3C-C4C	2.49	128.08	124.82
10	cB	841	CLA	CHB-C4A-NA	2.49	127.96	124.51
10	aA	836	CLA	O2D-CGD-O1D	-2.49	118.91	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aB	808	CLA	O2A-CGA-CBA	2.49	119.93	111.93
13	aA	848	BCR	C38-C26-C27	-2.49	108.91	113.57
10	aA	806	CLA	CMB-C2B-C3B	2.49	129.47	124.80
10	aB	816	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
13	cA	848	BCR	C38-C26-C27	-2.49	108.91	113.57
10	aL	203	CLA	CMC-C2C-C1C	2.49	128.82	125.03
10	aB	841	CLA	CHB-C4A-NA	2.49	127.96	124.51
10	bA	811	CLA	CMB-C2B-C3B	2.49	129.47	124.80
10	aB	820	CLA	CHB-C4A-NA	2.49	127.95	124.51
9	aA	801	CL0	CHB-C4A-NA	2.49	127.95	124.51
10	cA	856	CLA	CMB-C2B-C3B	2.49	129.47	124.80
10	bA	805	CLA	C1-C2-C3	-2.49	121.74	126.04
10	cA	811	CLA	CMB-C2B-C3B	2.49	129.47	124.80
10	cB	819	CLA	CAA-CBA-CGA	2.49	120.58	113.26
10	aB	822	CLA	O2D-CGD-O1D	-2.49	118.92	123.83
10	bA	856	CLA	CMB-C2B-C3B	2.49	129.47	124.80
10	aB	832	CLA	CAC-C3C-C4C	2.49	128.07	124.82
10	aA	814	CLA	CHB-C4A-NA	2.49	127.95	124.51
10	cA	821	CLA	CMC-C2C-C1C	2.49	128.81	125.03
10	bA	821	CLA	CMC-C2C-C1C	2.49	128.81	125.03
10	bB	816	CLA	CAA-C2A-C3A	-2.49	105.97	112.78
10	bB	832	CLA	CAC-C3C-C4C	2.49	128.07	124.82
10	cA	823	CLA	C1-C2-C3	-2.49	121.75	126.04
10	bB	806	CLA	CHC-C1C-C2C	-2.48	119.86	126.71
10	cA	818	CLA	O1D-CGD-CBD	-2.48	119.33	124.48
10	cA	806	CLA	CMB-C2B-C3B	2.48	129.46	124.80
10	cA	814	CLA	O2D-CGD-O1D	-2.48	118.92	123.83
10	cA	805	CLA	C11-C12-C13	-2.48	108.02	115.77
13	aB	847	BCR	C35-C13-C14	-2.48	119.44	122.92
16	aB	848	LMG	O1-C7-C8	-2.48	104.91	110.90
10	bA	822	CLA	CAC-C3C-C4C	2.48	128.06	124.82
10	aA	805	CLA	C11-C12-C13	-2.48	108.02	115.77
10	bA	803	CLA	CHB-C4A-NA	2.48	127.94	124.51
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	bB	814	CLA	O1D-CGD-CBD	-2.48	119.34	124.48
10	aB	803	CLA	O2D-CGD-O1D	-2.48	118.93	123.83
10	bA	833	CLA	O2A-CGA-CBA	2.48	119.90	111.93
10	aB	813	CLA	CHD-C4C-NC	2.48	128.11	124.20
9	aA	801	CL0	CMB-C2B-C1B	2.48	132.28	128.46
10	aA	830	CLA	C1D-CHD-C4C	-2.48	119.09	122.48
10	bB	825	CLA	O1D-CGD-CBD	-2.48	119.34	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	833	CLA	O2A-CGA-CBA	2.48	119.89	111.93
10	aB	837	CLA	O2A-CGA-CBA	2.48	119.89	111.93
10	aA	835	CLA	CBC-CAC-C3C	-2.48	105.55	112.43
10	bB	822	CLA	O2D-CGD-O1D	-2.48	118.94	123.83
10	bA	824	CLA	O1D-CGD-CBD	-2.48	119.34	124.48
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
9	bA	801	CL0	CMB-C2B-C1B	2.48	132.27	128.46
10	bB	802	CLA	C1D-CHD-C4C	-2.48	119.10	122.48
10	cB	802	CLA	C1D-CHD-C4C	-2.48	119.10	122.48
10	aA	803	CLA	O1D-CGD-CBD	-2.48	119.35	124.48
10	cA	824	CLA	O1D-CGD-CBD	-2.48	119.35	124.48
10	cB	841	CLA	CAC-C3C-C4C	2.48	128.06	124.82
10	bB	808	CLA	CAC-C3C-C4C	2.48	128.06	124.82
10	bA	814	CLA	CHB-C4A-NA	2.48	127.94	124.51
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	bA	805	CLA	C11-C12-C13	-2.47	108.05	115.77
10	aA	833	CLA	C1-C2-C3	-2.47	121.76	126.04
10	aA	805	CLA	C1-C2-C3	-2.47	121.76	126.04
10	cA	815	CLA	O2D-CGD-O1D	-2.47	118.95	123.83
10	bB	815	CLA	O2A-CGA-CBA	2.47	119.87	111.93
10	bB	822	CLA	CMC-C2C-C1C	2.47	128.79	125.03
10	aB	814	CLA	O1D-CGD-CBD	-2.47	119.36	124.48
10	cB	806	CLA	CHC-C1C-C2C	-2.47	119.89	126.71
10	cB	803	CLA	O2A-CGA-CBA	2.47	119.87	111.93
10	cB	803	CLA	O2D-CGD-O1D	-2.47	118.95	123.83
10	bB	803	CLA	O2D-CGD-O1D	-2.47	118.95	123.83
10	cA	835	CLA	CBC-CAC-C3C	-2.47	105.57	112.43
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	cB	837	CLA	O2A-CGA-CBA	2.47	119.86	111.93
10	aB	839	CLA	CMC-C2C-C1C	2.47	128.79	125.03
10	bB	803	CLA	O2A-CGA-CBA	2.47	119.86	111.93
10	bA	843	CLA	CMB-C2B-C3B	2.47	129.43	124.80
13	aA	848	BCR	C31-C1-C6	2.47	114.30	110.30
10	aA	833	CLA	CBC-CAC-C3C	-2.47	105.57	112.43
10	cA	803	CLA	O1D-CGD-CBD	-2.47	119.36	124.48
10	aA	815	CLA	O2D-CGD-O1D	-2.47	118.95	123.83
10	bA	815	CLA	O2D-CGD-O1D	-2.47	118.95	123.83
10	aB	838	CLA	CAC-C3C-C4C	2.47	128.05	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	815	CLA	CAC-C3C-C4C	2.47	128.05	124.82
10	cA	823	CLA	CBC-CAC-C3C	-2.47	105.58	112.43
10	aA	821	CLA	CMC-C2C-C1C	2.47	128.79	125.03
16	cB	848	LMG	O1-C7-C8	-2.47	104.94	110.90
10	aB	821	CLA	CAC-C3C-C4C	2.47	128.05	124.82
10	bA	806	CLA	CMB-C2B-C3B	2.47	129.43	124.80
13	cB	847	BCR	C35-C13-C14	-2.47	119.47	122.92
10	cB	808	CLA	CAC-C3C-C4C	2.47	128.04	124.82
10	aA	824	CLA	O1D-CGD-CBD	-2.47	119.37	124.48
10	bA	823	CLA	CBC-CAC-C3C	-2.47	105.58	112.43
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
10	aA	822	CLA	CAC-C3C-C4C	2.47	128.04	124.82
10	bA	818	CLA	O1D-CGD-CBD	-2.47	119.37	124.48
10	aA	823	CLA	C1-C2-C3	-2.47	121.78	126.04
13	aL	207	BCR	C27-C26-C25	2.47	126.34	122.74
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	cB	832	CLA	C4-C3-C5	2.47	119.53	115.29
10	aB	803	CLA	O2A-CGA-CBA	2.47	119.85	111.93
10	aB	838	CLA	CMB-C2B-C3B	2.47	129.42	124.80
10	cA	833	CLA	CBC-CAC-C3C	-2.47	105.58	112.43
10	cB	835	CLA	CAC-C3C-C4C	2.47	128.04	124.82
10	cA	842	CLA	CHD-C4C-NC	2.46	128.09	124.20
13	cA	848	BCR	C31-C1-C6	2.46	114.29	110.30
13	cL	207	BCR	C27-C26-C25	2.46	126.33	122.74
10	cA	822	CLA	CAC-C3C-C4C	2.46	128.04	124.82
10	aA	822	CLA	O2A-CGA-CBA	2.46	119.84	111.93
10	aA	826	CLA	C3B-C4B-NB	2.46	112.39	109.21
10	aB	808	CLA	CAC-C3C-C4C	2.46	128.04	124.82
10	aB	815	CLA	O2A-CGA-CBA	2.46	119.83	111.93
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
10	cB	839	CLA	CMC-C2C-C1C	2.46	128.78	125.03
10	bA	836	CLA	O2D-CGD-O1D	-2.46	118.97	123.83
13	bA	846	BCR	C7-C8-C9	-2.46	122.52	126.21
10	aA	830	CLA	CMA-C3A-C4A	-2.46	105.16	111.77
10	bA	835	CLA	CBC-CAC-C3C	-2.46	105.60	112.43
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
10	aA	811	CLA	CMB-C2B-C3B	2.46	129.41	124.80
10	aB	825	CLA	O1D-CGD-CBD	-2.46	119.39	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	832	CLA	CBC-CAC-C3C	-2.46	105.61	112.43
10	aA	821	CLA	CAC-C3C-C4C	2.46	128.03	124.82
10	aA	823	CLA	CBC-CAC-C3C	-2.46	105.61	112.43
10	cA	830	CLA	CHB-C4A-NA	2.46	127.91	124.51
10	bB	838	CLA	CMB-C2B-C3B	2.46	129.41	124.80
10	bB	837	CLA	O2A-CGA-CBA	2.46	119.82	111.93
13	bB	847	BCR	C35-C13-C14	-2.46	119.48	122.92
10	cA	832	CLA	O2D-CGD-O1D	-2.46	118.98	123.83
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	bA	833	CLA	CBC-CAC-C3C	-2.45	105.61	112.43
13	cB	845	BCR	C7-C8-C9	-2.45	122.52	126.21
10	bB	839	CLA	CMC-C2C-C1C	2.45	128.77	125.03
10	aB	801	CLA	CBC-CAC-C3C	-2.45	105.61	112.43
10	cA	830	CLA	C1D-CHD-C4C	-2.45	119.13	122.48
10	cB	832	CLA	CAC-C3C-C4C	2.45	128.03	124.82
10	aA	842	CLA	CHD-C4C-NC	2.45	128.07	124.20
10	cB	825	CLA	O1D-CGD-CBD	-2.45	119.40	124.48
13	bA	848	BCR	C31-C1-C6	2.45	114.27	110.30
10	aB	802	CLA	C1D-CHD-C4C	-2.45	119.13	122.48
10	aA	820	CLA	CHB-C4A-NA	2.45	127.90	124.51
10	aB	816	CLA	O1D-CGD-CBD	-2.45	119.40	124.48
13	cA	846	BCR	C7-C8-C9	-2.45	122.53	126.21
10	cA	830	CLA	CMA-C3A-C4A	-2.45	105.18	111.77
10	cL	204	CLA	CAC-C3C-C4C	2.45	128.02	124.82
10	aA	818	CLA	O1D-CGD-CBD	-2.45	119.40	124.48
10	cB	815	CLA	O2A-CGA-CBA	2.45	119.80	111.93
10	bB	821	CLA	CAC-C3C-C4C	2.45	128.02	124.82
10	bB	832	CLA	C4-C3-C5	2.45	119.51	115.29
10	aB	840	CLA	C1-C2-C3	-2.45	121.81	126.04
13	cA	847	BCR	C28-C27-C26	-2.45	109.73	113.99
13	bL	207	BCR	C15-C16-C17	-2.45	118.36	123.51
13	aI	101	BCR	C38-C26-C27	-2.45	108.99	113.57
10	cB	813	CLA	CMB-C2B-C3B	2.45	129.39	124.80
10	cB	801	CLA	CBC-CAC-C3C	-2.45	105.64	112.43
10	cA	822	CLA	C1-C2-C3	-2.45	121.81	126.04
10	bA	821	CLA	CAC-C3C-C4C	2.45	128.02	124.82
13	bL	207	BCR	C27-C26-C25	2.45	126.31	122.74
10	cA	832	CLA	CBC-CAC-C3C	-2.45	105.64	112.43
10	cA	822	CLA	O2A-CGA-CBA	2.45	119.78	111.93
13	bI	101	BCR	C38-C26-C27	-2.45	109.00	113.57
10	cB	807	CLA	CHD-C4C-NC	2.45	128.06	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	829	CLA	CHD-C4C-NC	2.45	128.06	124.20
10	cA	820	CLA	CAC-C3C-C4C	2.45	128.02	124.82
13	aB	845	BCR	C7-C8-C9	-2.45	122.54	126.21
10	cA	820	CLA	CHB-C4A-NA	2.44	127.89	124.51
10	aA	832	CLA	CBC-CAC-C3C	-2.44	105.64	112.43
10	cB	814	CLA	O1D-CGD-CBD	-2.44	119.41	124.48
13	cM	101	BCR	C27-C26-C25	2.44	126.30	122.74
10	cA	830	CLA	CMC-C2C-C1C	2.44	128.75	125.03
13	bB	843	BCR	C15-C16-C17	-2.44	118.37	123.51
10	bB	838	CLA	CAC-C3C-C4C	2.44	128.01	124.82
10	cB	806	CLA	CHB-C4A-NA	2.44	127.89	124.51
10	aA	834	CLA	CMA-C3A-C4A	-2.44	105.21	111.77
10	cB	818	CLA	O2D-CGD-O1D	-2.44	119.01	123.83
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
13	bM	101	BCR	C27-C26-C25	2.44	126.30	122.74
10	bA	822	CLA	O2A-CGA-CBA	2.44	119.77	111.93
10	bB	801	CLA	CBC-CAC-C3C	-2.44	105.65	112.43
10	cA	830	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
10	bA	830	CLA	C1D-CHD-C4C	-2.44	119.15	122.48
10	cB	838	CLA	CMB-C2B-C3B	2.44	129.38	124.80
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
13	aA	846	BCR	C7-C8-C9	-2.44	122.55	126.21
10	cA	843	CLA	CHD-C4C-NC	2.44	128.05	124.20
10	cA	825	CLA	CHC-C1C-C2C	-2.44	119.99	126.71
10	cL	202	CLA	CHA-C1A-NA	-2.44	120.81	126.40
10	cA	843	CLA	CMB-C2B-C3B	2.44	129.37	124.80
10	cB	840	CLA	C1-C2-C3	-2.44	121.83	126.04
10	cB	821	CLA	CAC-C3C-C4C	2.44	128.00	124.82
13	cI	102	BCR	C38-C26-C27	-2.44	109.02	113.57
10	bA	830	CLA	CMC-C2C-C1C	2.44	128.74	125.03
10	bA	822	CLA	C1-C2-C3	-2.44	121.83	126.04
13	bB	847	BCR	C27-C26-C25	2.44	126.29	122.74
10	bB	816	CLA	O1D-CGD-CBD	-2.44	119.43	124.48
10	cB	816	CLA	O1D-CGD-CBD	-2.44	119.43	124.48
10	aA	819	CLA	CHD-C4C-NC	2.43	128.04	124.20
10	bB	813	CLA	CMB-C2B-C3B	2.43	129.37	124.80
10	aB	820	CLA	C4-C3-C5	2.43	119.48	115.29
10	cB	820	CLA	C4-C3-C5	2.43	119.48	115.29
13	bA	847	BCR	C28-C27-C26	-2.43	109.75	113.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	833	CLA	CMC-C2C-C1C	2.43	128.73	125.03
9	bA	801	CL0	C4-C3-C5	2.43	119.48	115.29
10	bA	825	CLA	CHC-C1C-C2C	-2.43	120.00	126.71
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
13	aA	847	BCR	C28-C27-C26	-2.43	109.76	113.99
10	cB	830	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
10	bA	820	CLA	CAC-C3C-C4C	2.43	128.00	124.82
10	bB	803	CLA	CAC-C3C-C4C	2.43	128.00	124.82
13	bA	847	BCR	C3-C4-C5	-2.43	109.76	113.99
10	aA	820	CLA	CAC-C3C-C4C	2.43	128.00	124.82
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	cA	841	CLA	CMB-C2B-C3B	2.43	129.36	124.80
10	bB	827	CLA	CHB-C4A-NA	2.43	127.87	124.51
13	cL	207	BCR	C15-C16-C17	-2.43	118.40	123.51
10	aA	807	CLA	O1D-CGD-CBD	-2.43	119.45	124.48
10	aA	832	CLA	O2D-CGD-O1D	-2.43	119.03	123.83
10	aB	832	CLA	C4-C3-C5	2.43	119.47	115.29
13	bA	850	BCR	C15-C14-C13	-2.43	123.84	127.31
9	aA	801	CL0	C4-C3-C5	2.43	119.47	115.29
11	aA	844	PQN	C2M-C2-C1	2.43	120.37	116.29
10	aA	802	CLA	CHB-C4A-NA	2.43	127.87	124.51
11	bA	844	PQN	C2M-C2-C1	2.43	120.36	116.29
13	bA	849	BCR	C11-C10-C9	-2.43	123.85	127.31
13	aA	850	BCR	C15-C14-C13	-2.43	123.85	127.31
10	bB	822	CLA	C4C-C3C-C2C	-2.43	103.38	106.89
10	aA	830	CLA	CMC-C2C-C1C	2.43	128.72	125.03
13	aB	849	BCR	C27-C26-C25	2.43	126.28	122.74
13	cA	847	BCR	C3-C4-C5	-2.43	109.77	113.99
10	bB	835	CLA	CMB-C2B-C3B	2.42	129.35	124.80
10	cA	812	CLA	CHB-C4A-NA	2.42	127.86	124.51
14	aA	852	LHG	C11-C10-C9	-2.42	101.92	114.44
10	bA	843	CLA	CHD-C4C-NC	2.42	128.02	124.20
10	bA	818	CLA	O2A-C1-C2	2.42	115.00	108.64
11	cA	844	PQN	C2M-C2-C1	2.42	120.36	116.29
10	bB	835	CLA	CAC-C3C-C4C	2.42	127.99	124.82
10	aL	202	CLA	CHA-C1A-NA	-2.42	120.85	126.40
13	aM	101	BCR	C27-C26-C25	2.42	126.27	122.74
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	832	CLA	CMC-C2C-C1C	2.42	128.72	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	810	CLA	CHB-C4A-NA	2.42	127.86	124.51
10	cB	822	CLA	C4C-C3C-C2C	-2.42	103.38	106.89
10	bA	812	CLA	C4-C3-C5	2.42	119.46	115.29
10	bA	841	CLA	CMB-C2B-C3B	2.42	129.34	124.80
10	bB	804	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
10	aA	841	CLA	CMB-C2B-C3B	2.42	129.34	124.80
10	aB	824	CLA	CMB-C2B-C3B	2.42	129.34	124.80
10	aA	843	CLA	CMB-C2B-C3B	2.42	129.34	124.80
10	cB	804	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
10	bB	840	CLA	C1-C2-C3	-2.42	121.86	126.04
10	bA	807	CLA	O1D-CGD-CBD	-2.42	119.47	124.48
14	cA	852	LHG	C11-C10-C9	-2.42	101.95	114.44
10	bB	829	CLA	CHD-C4C-NC	2.42	128.01	124.20
10	bB	817	CLA	CMB-C2B-C3B	2.42	129.33	124.80
10	cB	833	CLA	CMB-C2B-C3B	2.42	129.33	124.80
14	bA	852	LHG	C11-C10-C9	-2.42	101.95	114.44
10	aA	825	CLA	CHC-C1C-C2C	-2.42	120.05	126.71
10	bB	823	CLA	CMB-C2B-C3B	2.42	129.33	124.80
10	aB	833	CLA	CMB-C2B-C3B	2.42	129.33	124.80
10	cB	824	CLA	CMB-C2B-C3B	2.42	129.33	124.80
10	aB	806	CLA	CHB-C4A-NA	2.42	127.85	124.51
10	aA	838	CLA	CHB-C4A-NA	2.42	127.85	124.51
10	cA	812	CLA	C4-C3-C5	2.42	119.45	115.29
10	bB	830	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
10	bA	832	CLA	O2D-CGD-O1D	-2.41	119.06	123.83
10	cB	827	CLA	CHB-C4A-NA	2.41	127.85	124.51
10	cA	831	CLA	CAC-C3C-C4C	2.41	127.97	124.82
13	bB	849	BCR	C27-C26-C25	2.41	126.26	122.74
10	cB	825	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
10	bA	812	CLA	CHB-C4A-NA	2.41	127.85	124.51
13	aL	207	BCR	C15-C16-C17	-2.41	118.44	123.51
10	bB	820	CLA	C4-C3-C5	2.41	119.44	115.29
10	bA	842	CLA	CHD-C4C-NC	2.41	128.00	124.20
10	bA	837	CLA	CMC-C2C-C1C	2.41	128.70	125.03
10	aA	822	CLA	C1-C2-C3	-2.41	121.87	126.04
10	bA	854	CLA	CAA-CBA-CGA	-2.41	106.15	113.26
10	aB	818	CLA	O2D-CGD-O1D	-2.41	119.07	123.83
10	aB	835	CLA	CMB-C2B-C3B	2.41	129.32	124.80
13	cB	843	BCR	C15-C16-C17	-2.41	118.44	123.51
10	aB	825	CLA	CAA-C2A-C3A	-2.41	106.18	112.78
13	cA	850	BCR	C15-C14-C13	-2.41	123.87	127.31
10	cA	802	CLA	CHB-C4A-NA	2.41	127.84	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	aA	849	BCR	C11-C10-C9	-2.41	123.87	127.31
10	cA	807	CLA	O1D-CGD-CBD	-2.41	119.49	124.48
13	aB	843	BCR	C15-C16-C17	-2.41	118.45	123.51
10	aA	830	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
10	aA	837	CLA	CMC-C2C-C1C	2.41	128.69	125.03
10	aB	838	CLA	CMC-C2C-C1C	2.41	128.69	125.03
13	cB	849	BCR	C27-C26-C25	2.41	126.25	122.74
13	bB	843	BCR	C27-C26-C25	2.41	126.25	122.74
10	bA	826	CLA	C3B-C4B-NB	2.41	112.32	109.21
13	aB	843	BCR	C27-C26-C25	2.41	126.25	122.74
10	cB	823	CLA	CMB-C2B-C3B	2.41	129.31	124.80
10	cB	832	CLA	CHB-C4A-NA	2.41	127.84	124.51
10	aB	832	CLA	CMC-C2C-C1C	2.41	128.69	125.03
10	aB	830	CLA	C1-C2-C3	-2.41	121.88	126.04
10	bB	824	CLA	CMB-C2B-C3B	2.41	129.31	124.80
10	aB	823	CLA	CMB-C2B-C3B	2.41	129.31	124.80
10	bA	839	CLA	CMB-C2B-C3B	2.41	129.31	124.80
10	bB	832	CLA	CMC-C2C-C1C	2.41	128.69	125.03
10	cL	203	CLA	CBC-CAC-C3C	-2.41	105.75	112.43
9	cA	801	CL0	C4-C3-C5	2.40	119.43	115.29
10	aA	828	CLA	O2A-CGA-O1A	-2.40	117.42	123.56
10	aB	813	CLA	CMB-C2B-C3B	2.40	129.31	124.80
10	aA	839	CLA	CHB-C4A-NA	2.40	127.84	124.51
10	bL	203	CLA	CBC-CAC-C3C	-2.40	105.75	112.43
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
10	aB	804	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
10	aA	812	CLA	C4-C3-C5	2.40	119.43	115.29
10	bB	803	CLA	CMB-C2B-C1B	2.40	132.16	128.46
10	aB	817	CLA	CMB-C2B-C3B	2.40	129.31	124.80
10	cA	839	CLA	CHB-C4A-NA	2.40	127.83	124.51
10	aB	822	CLA	C4C-C3C-C2C	-2.40	103.41	106.89
10	cA	810	CLA	CHB-C4A-NA	2.40	127.83	124.51
10	cA	822	CLA	CHB-C4A-NA	2.40	127.83	124.51
10	bA	806	CLA	O2D-CGD-O1D	-2.40	119.09	123.83
10	aA	836	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
10	aB	803	CLA	CBC-CAC-C3C	-2.40	105.77	112.43
13	cB	847	BCR	C27-C26-C25	2.40	126.24	122.74
10	cB	828	CLA	CHA-C1A-NA	-2.40	120.90	126.40
10	cB	817	CLA	CMB-C2B-C3B	2.40	129.30	124.80
13	cB	843	BCR	C27-C26-C25	2.40	126.24	122.74
10	aB	832	CLA	CHB-C4A-NA	2.40	127.83	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cA	853	LMT	C1'-O5'-C5'	2.40	118.42	113.70
15	aA	853	LMT	C1'-O5'-C5'	2.40	118.42	113.70
10	bB	838	CLA	CMC-C2C-C1C	2.40	128.68	125.03
10	cA	806	CLA	O2D-CGD-O1D	-2.40	119.09	123.83
10	bL	204	CLA	C1-O2A-CGA	2.40	123.09	116.54
10	cB	838	CLA	CAC-C3C-C4C	2.40	127.95	124.82
10	cA	821	CLA	CAC-C3C-C4C	2.40	127.95	124.82
10	cB	835	CLA	CMB-C2B-C3B	2.40	129.30	124.80
10	cB	816	CLA	CMB-C2B-C3B	2.40	129.30	124.80
10	aB	828	CLA	CHA-C1A-NA	-2.40	120.91	126.40
10	bA	842	CLA	O2D-CGD-O1D	-2.40	119.10	123.83
10	bB	801	CLA	C4-C3-C5	2.40	119.42	115.29
10	cA	824	CLA	CHD-C4C-NC	2.40	127.98	124.20
10	aB	816	CLA	CMB-C2B-C3B	2.40	129.29	124.80
10	bB	833	CLA	CMB-C2B-C3B	2.40	129.29	124.80
10	cL	202	CLA	CMC-C2C-C1C	2.40	128.68	125.03
10	cA	833	CLA	CMC-C2C-C1C	2.39	128.68	125.03
10	aL	204	CLA	C1-O2A-CGA	2.39	123.08	116.54
10	aL	203	CLA	CBC-CAC-C3C	-2.39	105.78	112.43
10	cB	803	CLA	CAC-C3C-C4C	2.39	127.95	124.82
10	bA	828	CLA	O2A-CGA-O1A	-2.39	117.45	123.56
10	aA	833	CLA	CMC-C2C-C1C	2.39	128.67	125.03
10	cA	854	CLA	CAA-CBA-CGA	-2.39	106.21	113.26
10	bB	816	CLA	CMB-C2B-C3B	2.39	129.29	124.80
10	aA	843	CLA	CHD-C4C-NC	2.39	127.97	124.20
10	aB	827	CLA	CHB-C4A-NA	2.39	127.82	124.51
10	cA	836	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
10	cA	818	CLA	O2A-C1-C2	2.39	114.92	108.64
10	cA	828	CLA	O2A-CGA-O1A	-2.39	117.45	123.56
10	aB	806	CLA	O2A-CGA-CBA	2.39	119.60	111.93
10	bL	202	CLA	CMC-C2C-C1C	2.39	128.67	125.03
13	cA	846	BCR	C27-C26-C25	2.39	126.22	122.74
13	aB	847	BCR	C27-C26-C25	2.39	126.22	122.74
13	cI	103	BCR	C27-C26-C25	2.39	126.22	122.74
10	aL	202	CLA	CMC-C2C-C1C	2.39	128.66	125.03
10	cL	204	CLA	C1-O2A-CGA	2.39	123.06	116.54
10	aA	854	CLA	CAA-CBA-CGA	-2.39	106.22	113.26
10	bA	820	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
10	bB	832	CLA	CHB-C4A-NA	2.39	127.81	124.51
10	cA	823	CLA	O2D-CGD-O1D	-2.39	119.12	123.83
10	aA	823	CLA	O2D-CGD-O1D	-2.39	119.12	123.83
10	bB	806	CLA	CAA-C2A-C1A	2.39	119.79	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	823	CLA	O2D-CGD-O1D	-2.39	119.12	123.83
10	bA	839	CLA	CHB-C4A-NA	2.39	127.81	124.51
10	bA	831	CLA	CAC-C3C-C4C	2.39	127.94	124.82
10	bB	803	CLA	CBC-CAC-C3C	-2.39	105.81	112.43
10	cB	823	CLA	O2A-CGA-CBA	2.39	119.59	111.93
10	aB	802	CLA	O2D-CGD-O1D	-2.38	119.12	123.83
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	aA	833	CLA	O1D-CGD-CBD	-2.38	119.54	124.48
10	aA	824	CLA	O2A-CGA-CBA	2.38	119.58	111.93
10	aA	808	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
10	aA	815	CLA	CHB-C4A-NA	2.38	127.81	124.51
10	aA	806	CLA	O2D-CGD-O1D	-2.38	119.13	123.83
10	cA	839	CLA	CMB-C2B-C3B	2.38	129.27	124.80
10	bB	818	CLA	O2D-CGD-O1D	-2.38	119.13	123.83
10	cB	801	CLA	C4-C3-C5	2.38	119.39	115.29
10	aB	803	CLA	CAC-C3C-C4C	2.38	127.93	124.82
10	aA	812	CLA	CHB-C4A-NA	2.38	127.80	124.51
10	cB	838	CLA	CMC-C2C-C1C	2.38	128.65	125.03
10	bA	824	CLA	CHD-C4C-NC	2.38	127.95	124.20
13	cA	849	BCR	C29-C30-C25	2.38	114.16	110.48
10	cB	803	CLA	CBC-CAC-C3C	-2.38	105.82	112.43
13	bI	102	BCR	C27-C26-C25	2.38	126.21	122.74
10	bB	807	CLA	C4-C3-C5	2.38	119.38	115.29
10	cB	803	CLA	CMB-C2B-C1B	2.38	132.12	128.46
10	bB	822	CLA	O1D-CGD-CBD	-2.38	119.55	124.48
10	bA	822	CLA	CHB-C4A-NA	2.38	127.80	124.51
13	bB	844	BCR	C29-C30-C25	2.38	114.16	110.48
10	cA	820	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
10	aA	839	CLA	CMB-C2B-C3B	2.38	129.26	124.80
10	aB	822	CLA	O1D-CGD-CBD	-2.38	119.56	124.48
10	cB	820	CLA	CHD-C4C-NC	2.38	127.95	124.20
10	cA	824	CLA	O2A-CGA-CBA	2.38	119.56	111.93
10	bA	808	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
10	aB	813	CLA	O2D-CGD-O1D	-2.38	119.14	123.83
10	cA	812	CLA	CMB-C2B-C3B	2.37	129.25	124.80
10	aB	823	CLA	O2A-CGA-CBA	2.37	119.55	111.93
10	cA	837	CLA	CMC-C2C-C1C	2.37	128.64	125.03
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
13	aA	847	BCR	C3-C4-C5	-2.37	109.86	113.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	841	CLA	CHB-C4A-NA	2.37	127.79	124.51
10	bB	836	CLA	O2D-CGD-O1D	-2.37	119.14	123.83
15	bA	853	LMT	C1'-O5'-C5'	2.37	118.37	113.70
10	aB	834	CLA	CBC-CAC-C3C	-2.37	105.84	112.43
10	aB	803	CLA	CMB-C2B-C1B	2.37	132.11	128.46
10	cA	841	CLA	CHB-C4A-NA	2.37	127.79	124.51
10	bA	841	CLA	CHB-C4A-NA	2.37	127.79	124.51
10	cA	832	CLA	CAC-C3C-C4C	2.37	127.92	124.82
10	aB	831	CLA	CMB-C2B-C3B	2.37	129.25	124.80
10	aB	806	CLA	CAA-C2A-C1A	2.37	119.74	111.97
10	cA	818	CLA	CHD-C4C-NC	2.37	127.94	124.20
10	bB	820	CLA	CHD-C4C-NC	2.37	127.94	124.20
10	cB	802	CLA	O2D-CGD-O1D	-2.37	119.15	123.83
10	bB	824	CLA	CMC-C2C-C1C	2.37	128.64	125.03
10	cB	834	CLA	CBC-CAC-C3C	-2.37	105.85	112.43
10	aA	812	CLA	CAA-CBA-CGA	-2.37	106.28	113.26
10	bB	823	CLA	O2A-CGA-CBA	2.37	119.53	111.93
10	aB	836	CLA	O2D-CGD-O1D	-2.37	119.15	123.83
10	aB	824	CLA	CMC-C2C-C1C	2.37	128.63	125.03
16	aB	848	LMG	O3-C3-C2	-2.37	104.85	110.34
10	cB	822	CLA	O1D-CGD-CBD	-2.37	119.57	124.48
10	aA	822	CLA	CHB-C4A-NA	2.37	127.79	124.51
10	bA	824	CLA	O2A-CGA-CBA	2.37	119.53	111.93
10	aA	842	CLA	O2D-CGD-O1D	-2.37	119.16	123.83
10	cB	807	CLA	C4-C3-C5	2.37	119.36	115.29
10	bB	826	CLA	CMC-C2C-C1C	2.37	128.63	125.03
10	aA	830	CLA	CHD-C4C-NC	2.37	127.93	124.20
9	cA	801	CL0	CAC-C3C-C4C	2.37	127.91	124.82
10	cB	826	CLA	CMC-C2C-C1C	2.37	128.63	125.03
10	cB	824	CLA	CMC-C2C-C1C	2.37	128.63	125.03
10	aB	807	CLA	C4-C3-C5	2.36	119.36	115.29
13	aA	849	BCR	C15-C14-C13	-2.36	123.94	127.31
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
13	bA	846	BCR	C27-C26-C25	2.36	126.19	122.74
10	aB	801	CLA	C4-C3-C5	2.36	119.36	115.29
16	aB	848	LMG	O7-C10-O9	-2.36	117.91	123.71
10	cB	838	CLA	C1-C2-C3	-2.36	121.96	126.04
10	cB	836	CLA	O2D-CGD-O1D	-2.36	119.17	123.83
10	cB	806	CLA	O2A-CGA-CBA	2.36	119.51	111.93
10	aA	831	CLA	CAC-C3C-C4C	2.36	127.90	124.82
10	bB	806	CLA	O2A-CGA-CBA	2.36	119.50	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	808	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
10	bA	812	CLA	CMB-C2B-C3B	2.36	129.22	124.80
13	aA	846	BCR	C27-C26-C25	2.36	126.18	122.74
10	cB	813	CLA	O2D-CGD-O1D	-2.36	119.17	123.83
10	aA	812	CLA	CMB-C2B-C3B	2.36	129.22	124.80
10	cB	831	CLA	CMB-C2B-C3B	2.36	129.22	124.80
13	aA	849	BCR	C29-C30-C25	2.36	114.13	110.48
10	bB	834	CLA	CBC-CAC-C3C	-2.36	105.89	112.43
10	bB	830	CLA	C1-C2-C3	-2.35	121.97	126.04
10	cB	809	CLA	O2A-CGA-CBA	2.35	119.49	111.93
10	cA	830	CLA	CHD-C4C-NC	2.35	127.91	124.20
10	cA	842	CLA	O2D-CGD-O1D	-2.35	119.18	123.83
10	cA	812	CLA	CAA-CBA-CGA	-2.35	106.32	113.26
10	bB	838	CLA	C1-C2-C3	-2.35	121.97	126.04
9	bA	801	CL0	CAC-C3C-C4C	2.35	127.89	124.82
10	bA	805	CLA	C4-C3-C5	2.35	119.34	115.29
10	bA	816	CLA	CMB-C2B-C3B	2.35	129.21	124.80
10	bA	812	CLA	CAA-CBA-CGA	-2.35	106.33	113.26
13	cB	845	BCR	C30-C25-C26	-2.35	119.30	122.59
16	cB	848	LMG	O7-C10-O9	-2.35	117.94	123.71
10	aA	832	CLA	CAC-C3C-C4C	2.35	127.89	124.82
10	cB	825	CLA	CHB-C4A-NA	2.35	127.76	124.51
10	bB	836	CLA	CBC-CAC-C3C	-2.35	105.91	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	bB	802	CLA	O2D-CGD-O1D	-2.35	119.19	123.83
10	bA	837	CLA	CBC-CAC-C3C	-2.35	105.91	112.43
13	aI	102	BCR	C27-C26-C25	2.35	126.17	122.74
16	bB	848	LMG	O7-C10-O9	-2.35	117.94	123.71
10	bA	830	CLA	CHD-C4C-NC	2.35	127.90	124.20
13	aA	850	BCR	C27-C26-C25	2.35	126.16	122.74
10	aB	830	CLA	CMC-C2C-C1C	2.35	128.60	125.03
10	bB	831	CLA	CMB-C2B-C3B	2.35	129.20	124.80
13	aB	844	BCR	C29-C30-C25	2.35	114.11	110.48
10	bB	830	CLA	CMC-C2C-C1C	2.35	128.60	125.03
13	bA	849	BCR	C15-C14-C13	-2.35	123.96	127.31
10	bA	833	CLA	O1D-CGD-CBD	-2.35	119.62	124.48
10	aA	816	CLA	CMB-C2B-C3B	2.35	129.20	124.80
10	cB	836	CLA	CBC-CAC-C3C	-2.35	105.92	112.43
10	aA	843	CLA	CHB-C4A-NA	2.35	127.75	124.51
16	bB	848	LMG	O3-C3-C2	-2.34	104.90	110.34
10	aA	810	CLA	O2A-CGA-CBA	2.34	119.46	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	816	CLA	CMB-C2B-C3B	2.34	129.20	124.80
10	bA	810	CLA	O2A-CGA-CBA	2.34	119.45	111.93
10	cB	804	CLA	C4-C3-C5	2.34	119.32	115.29
10	aB	836	CLA	CBC-CAC-C3C	-2.34	105.92	112.43
10	bA	832	CLA	CAC-C3C-C4C	2.34	127.88	124.82
10	bB	809	CLA	O2A-CGA-CBA	2.34	119.45	111.93
10	aB	833	CLA	CAA-CBA-CGA	-2.34	106.36	113.26
13	cB	844	BCR	C29-C30-C25	2.34	114.11	110.48
10	bL	205	CLA	C4-C3-C5	2.34	119.32	115.29
10	aB	826	CLA	CMC-C2C-C1C	2.34	128.59	125.03
10	bB	833	CLA	CAA-CBA-CGA	-2.34	106.36	113.26
10	aB	838	CLA	C1-C2-C3	-2.34	122.00	126.04
10	aB	809	CLA	O2A-CGA-CBA	2.34	119.44	111.93
10	bB	813	CLA	O2D-CGD-O1D	-2.34	119.21	123.83
16	cB	848	LMG	O3-C3-C2	-2.34	104.91	110.34
9	aA	801	CL0	CAC-C3C-C4C	2.34	127.88	124.82
10	cA	810	CLA	O2A-CGA-CBA	2.34	119.44	111.93
10	aB	807	CLA	O2A-CGA-O1A	-2.34	117.59	123.56
10	cB	823	CLA	CHB-C4A-NA	2.34	127.75	124.51
10	aB	820	CLA	CHD-C4C-NC	2.34	127.89	124.20
10	cA	806	CLA	CBC-CAC-C3C	-2.34	105.94	112.43
10	aA	835	CLA	C4-C3-C5	2.34	119.31	115.29
13	bI	101	BCR	C11-C10-C9	-2.34	123.97	127.31
10	bA	835	CLA	C4-C3-C5	2.34	119.31	115.29
10	aA	837	CLA	CBC-CAC-C3C	-2.34	105.94	112.43
10	cB	833	CLA	CAA-CBA-CGA	-2.34	106.37	113.26
10	cA	833	CLA	O1D-CGD-CBD	-2.34	119.64	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
13	bA	849	BCR	C15-C16-C17	-2.34	118.60	123.51
13	bB	845	BCR	C30-C25-C26	-2.34	119.33	122.59
10	cA	805	CLA	C4-C3-C5	2.34	119.31	115.29
10	cA	815	CLA	CHB-C4A-NA	2.34	127.74	124.51
10	aB	835	CLA	CHB-C4A-NA	2.33	127.74	124.51
13	cA	849	BCR	C15-C16-C17	-2.33	118.60	123.51
10	cA	837	CLA	CBC-CAC-C3C	-2.33	105.95	112.43
10	aB	804	CLA	CHD-C4C-NC	2.33	127.88	124.20
13	aB	845	BCR	C30-C25-C26	-2.33	119.33	122.59
10	cB	807	CLA	O2A-CGA-O1A	-2.33	117.60	123.56
10	bA	806	CLA	CBC-CAC-C3C	-2.33	105.95	112.43
10	cL	205	CLA	C4-C3-C5	2.33	119.31	115.29
10	aB	834	CLA	CMB-C2B-C3B	2.33	129.17	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bA	850	BCR	C27-C26-C25	2.33	126.14	122.74
10	bA	835	CLA	C1-C2-C3	-2.33	122.01	126.04
10	cA	835	CLA	C4-C3-C5	2.33	119.30	115.29
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	aL	205	CLA	C4-C3-C5	2.33	119.29	115.29
13	bA	849	BCR	C29-C30-C25	2.33	114.08	110.48
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
10	bB	835	CLA	CHB-C4A-NA	2.32	127.73	124.51
10	cB	835	CLA	CHB-C4A-NA	2.32	127.73	124.51
10	aB	804	CLA	C4-C3-C5	2.32	119.29	115.29
10	aA	806	CLA	CBC-CAC-C3C	-2.32	105.98	112.43
10	aB	835	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
10	cA	842	CLA	CHB-C4A-NA	2.32	127.72	124.51
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
14	aA	855	LHG	C11-C10-C9	-2.32	102.45	114.44
10	bB	807	CLA	O2A-CGA-O1A	-2.32	117.63	123.56
10	aA	818	CLA	CHD-C4C-NC	2.32	127.86	124.20
10	aA	839	CLA	CMC-C2C-C1C	2.32	128.56	125.03
10	aA	835	CLA	CMB-C2B-C3B	2.32	129.15	124.80
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	bA	826	CLA	O2D-CGD-O1D	-2.32	119.25	123.83
10	bA	805	CLA	CAC-C3C-C4C	2.32	127.85	124.82
10	bB	829	CLA	CBC-CAC-C3C	-2.32	105.99	112.43
14	bA	855	LHG	C11-C10-C9	-2.32	102.47	114.44
10	aA	827	CLA	CHA-C1A-NA	-2.32	121.09	126.40
10	bB	834	CLA	CMB-C2B-C3B	2.32	129.15	124.80
10	cA	822	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
10	cA	831	CLA	C4-C3-C5	2.32	119.28	115.29
10	aA	809	CLA	CHB-C4A-NA	2.32	127.72	124.51
13	aA	849	BCR	C15-C16-C17	-2.32	118.64	123.51
10	cB	830	CLA	CMC-C2C-C1C	2.32	128.56	125.03
13	aI	101	BCR	C11-C10-C9	-2.32	124.00	127.31
10	cB	840	CLA	O2A-CGA-CBA	2.32	119.36	111.93
10	cB	834	CLA	CMC-C2C-C1C	2.32	128.55	125.03
10	aA	826	CLA	O2D-CGD-O1D	-2.31	119.26	123.83
10	aA	822	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
10	aA	802	CLA	O2D-CGD-O1D	-2.31	119.26	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	827	CLA	C1-C2-C3	-2.31	122.04	126.04
10	bA	803	CLA	CMC-C2C-C1C	2.31	128.55	125.03
10	bB	828	CLA	C4-C3-C5	2.31	119.27	115.29
10	bA	810	CLA	C1-O2A-CGA	2.31	122.86	116.54
10	cA	826	CLA	CMC-C2C-C1C	2.31	128.55	125.03
13	aM	101	BCR	C20-C21-C22	-2.31	124.01	127.31
10	cA	826	CLA	O2D-CGD-O1D	-2.31	119.27	123.83
10	bB	834	CLA	CMC-C2C-C1C	2.31	128.55	125.03
10	aB	840	CLA	O2A-CGA-CBA	2.31	119.35	111.93
10	cA	839	CLA	CMC-C2C-C1C	2.31	128.55	125.03
10	cA	816	CLA	O1D-CGD-CBD	-2.31	119.69	124.48
10	cL	204	CLA	CHB-C4A-NA	2.31	127.71	124.51
10	aA	842	CLA	CHB-C4A-NA	2.31	127.71	124.51
13	cA	849	BCR	C15-C14-C13	-2.31	124.01	127.31
13	cA	850	BCR	C27-C26-C25	2.31	126.11	122.74
10	cB	804	CLA	CHD-C4C-NC	2.31	127.84	124.20
10	aA	816	CLA	O1D-CGD-CBD	-2.31	119.70	124.48
10	bA	839	CLA	CMC-C2C-C1C	2.31	128.54	125.03
13	bI	102	BCR	C3-C4-C5	-2.31	109.97	113.99
10	bB	840	CLA	O2A-CGA-CBA	2.31	119.34	111.93
10	aB	829	CLA	CBC-CAC-C3C	-2.31	106.02	112.43
10	cB	829	CLA	CBC-CAC-C3C	-2.31	106.02	112.43
14	cA	855	LHG	C11-C10-C9	-2.31	102.53	114.44
10	bA	807	CLA	CBC-CAC-C3C	-2.31	106.03	112.43
10	cB	804	CLA	C4-C3-C2	-2.31	117.68	123.68
10	cA	827	CLA	CHA-C1A-NA	-2.31	121.12	126.40
10	bB	823	CLA	CHB-C4A-NA	2.31	127.70	124.51
10	bA	816	CLA	O1D-CGD-CBD	-2.30	119.70	124.48
10	aA	856	CLA	O2A-CGA-CBA	2.30	119.33	111.93
10	bB	803	CLA	C4-C3-C5	2.30	119.25	115.29
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	cB	828	CLA	C4-C3-C5	2.30	119.25	115.29
10	bA	802	CLA	O2D-CGD-O1D	-2.30	119.28	123.83
10	bB	839	CLA	CHB-C4A-NA	2.30	127.69	124.51
10	bA	842	CLA	CHB-C4A-NA	2.30	127.69	124.51
10	cB	803	CLA	C4-C3-C5	2.30	119.25	115.29
10	aA	810	CLA	C1-O2A-CGA	2.30	122.83	116.54
10	cA	854	CLA	CMB-C2B-C3B	2.30	129.11	124.80
10	bB	804	CLA	CHD-C4C-NC	2.30	127.83	124.20
10	aB	806	CLA	O1D-CGD-CBD	-2.30	119.72	124.48
10	bA	856	CLA	O2A-CGA-CBA	2.30	119.31	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	806	CLA	O1D-CGD-CBD	-2.30	119.72	124.48
10	cB	821	CLA	CMC-C2C-C1C	2.30	128.53	125.03
10	aA	826	CLA	CMC-C2C-C1C	2.30	128.53	125.03
10	bB	804	CLA	C4-C3-C5	2.30	119.25	115.29
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
10	bA	854	CLA	CMB-C2B-C3B	2.30	129.11	124.80
10	aA	807	CLA	CBC-CAC-C3C	-2.30	106.05	112.43
13	cI	103	BCR	C3-C4-C5	-2.30	109.99	113.99
10	cB	819	CLA	C4C-C3C-C2C	-2.30	103.56	106.89
10	cB	834	CLA	CMB-C2B-C3B	2.30	129.11	124.80
13	aB	845	BCR	C33-C5-C6	-2.30	121.95	124.51
10	aA	803	CLA	CMC-C2C-C1C	2.30	128.52	125.03
10	aB	834	CLA	CMC-C2C-C1C	2.30	128.52	125.03
10	aA	805	CLA	CAC-C3C-C4C	2.30	127.82	124.82
16	bB	848	LMG	C40-C39-C38	-2.29	102.59	114.44
10	cA	803	CLA	CMC-C2C-C1C	2.29	128.52	125.03
10	aA	854	CLA	CMB-C2B-C3B	2.29	129.10	124.80
10	cA	812	CLA	CMC-C2C-C1C	2.29	128.52	125.03
10	cA	856	CLA	O2A-CGA-CBA	2.29	119.30	111.93
10	aA	805	CLA	C4-C3-C5	2.29	119.24	115.29
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
10	cA	817	CLA	O2D-CGD-O1D	-2.29	119.30	123.83
10	aB	821	CLA	CMC-C2C-C1C	2.29	128.52	125.03
13	cI	102	BCR	C11-C10-C9	-2.29	124.04	127.31
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
16	aB	848	LMG	C40-C39-C38	-2.29	102.60	114.44
10	aB	804	CLA	C4-C3-C2	-2.29	117.72	123.68
10	aB	807	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
10	aB	819	CLA	C4C-C3C-C2C	-2.29	103.57	106.89
10	cB	806	CLA	O1D-CGD-CBD	-2.29	119.73	124.48
10	bA	843	CLA	CHB-C4A-NA	2.29	127.68	124.51
10	bA	812	CLA	CMC-C2C-C1C	2.29	128.52	125.03
10	bA	835	CLA	CMB-C2B-C3B	2.29	129.10	124.80
10	aB	809	CLA	CHD-C4C-NC	2.29	127.81	124.20
10	bB	821	CLA	CMC-C2C-C1C	2.29	128.52	125.03
10	cA	820	CLA	C4-C3-C5	2.29	119.23	115.29
10	aB	824	CLA	CBC-CAC-C3C	-2.29	106.08	112.43
10	aA	810	CLA	C4-C3-C5	2.29	119.23	115.29
16	cB	848	LMG	C40-C39-C38	-2.29	102.62	114.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	836	CLA	OBD-CAD-C3D	-2.29	123.99	128.04
10	bB	833	CLA	CHB-C4A-NA	2.29	127.67	124.51
10	bB	828	CLA	CMB-C2B-C3B	2.29	129.09	124.80
10	bB	819	CLA	C4C-C3C-C2C	-2.29	103.58	106.89
10	aB	802	CLA	CHD-C4C-NC	2.29	127.81	124.20
13	aI	102	BCR	C3-C4-C5	-2.29	110.01	113.99
10	cB	828	CLA	CMB-C2B-C3B	2.29	129.09	124.80
10	aB	809	CLA	C11-C12-C13	-2.29	108.64	115.77
10	cA	835	CLA	CMB-C2B-C3B	2.28	129.09	124.80
13	cM	101	BCR	C20-C21-C22	-2.28	124.05	127.31
10	bB	820	CLA	CMB-C2B-C3B	2.28	129.08	124.80
10	aB	803	CLA	C4-C3-C5	2.28	119.22	115.29
10	aA	831	CLA	C4-C3-C5	2.28	119.22	115.29
10	cB	811	CLA	CHA-C1A-NA	-2.28	121.17	126.40
10	cB	817	CLA	CBC-CAC-C3C	-2.28	106.09	112.43
10	cA	805	CLA	CAC-C3C-C4C	2.28	127.80	124.82
10	bB	802	CLA	CHD-C4C-NC	2.28	127.80	124.20
10	cA	802	CLA	O2D-CGD-O1D	-2.28	119.32	123.83
10	bB	817	CLA	CBC-CAC-C3C	-2.28	106.09	112.43
10	bB	809	CLA	C11-C12-C13	-2.28	108.65	115.77
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	bA	842	CLA	C4-C3-C5	2.28	119.21	115.29
10	cB	802	CLA	CHD-C4C-NC	2.28	127.80	124.20
10	cA	842	CLA	C4-C3-C5	2.28	119.21	115.29
10	cB	839	CLA	CHB-C4A-NA	2.28	127.66	124.51
10	bA	809	CLA	CHB-C4A-NA	2.28	127.66	124.51
10	cA	821	CLA	CBC-CAC-C3C	-2.28	106.10	112.43
10	bA	810	CLA	C4-C3-C5	2.28	119.21	115.29
10	bB	804	CLA	C4-C3-C2	-2.28	117.76	123.68
10	bA	817	CLA	O2D-CGD-O1D	-2.28	119.33	123.83
10	cA	810	CLA	C1-O2A-CGA	2.28	122.77	116.54
10	cA	813	CLA	CBC-CAC-C3C	-2.28	106.11	112.43
10	bB	810	CLA	C1-C2-C3	-2.28	122.11	126.04
10	cA	807	CLA	CBC-CAC-C3C	-2.28	106.11	112.43
10	cB	833	CLA	CHB-C4A-NA	2.28	127.66	124.51
10	aA	836	CLA	OBD-CAD-C3D	-2.28	124.01	128.04
10	cA	810	CLA	C4-C3-C5	2.28	119.21	115.29
10	aB	828	CLA	CMB-C2B-C3B	2.28	129.07	124.80
10	bA	831	CLA	C4-C3-C5	2.27	119.20	115.29
10	aB	817	CLA	CBC-CAC-C3C	-2.27	106.11	112.43
10	aB	820	CLA	CMB-C2B-C3B	2.27	129.07	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bA	825	CLA	CHB-C4A-NA	2.27	127.66	124.51
10	aA	821	CLA	CBC-CAC-C3C	-2.27	106.11	112.43
10	cB	824	CLA	CBC-CAC-C3C	-2.27	106.12	112.43
10	aB	828	CLA	C4-C3-C5	2.27	119.20	115.29
13	bB	845	BCR	C33-C5-C6	-2.27	121.98	124.51
10	bB	824	CLA	CBC-CAC-C3C	-2.27	106.12	112.43
10	aA	817	CLA	O2D-CGD-O1D	-2.27	119.34	123.83
10	bA	823	CLA	C4-C3-C5	2.27	119.20	115.29
10	aA	823	CLA	C4-C3-C5	2.27	119.20	115.29
10	aB	839	CLA	CHB-C4A-NA	2.27	127.65	124.51
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	817	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
10	cB	820	CLA	CMB-C2B-C3B	2.27	129.06	124.80
10	aA	820	CLA	C4-C3-C5	2.27	119.20	115.29
10	bA	826	CLA	CMC-C2C-C1C	2.27	128.48	125.03
10	bA	836	CLA	OBD-CAD-C3D	-2.27	124.02	128.04
10	aA	842	CLA	C4-C3-C5	2.27	119.19	115.29
10	bB	809	CLA	CHD-C4C-NC	2.27	127.78	124.20
10	aA	812	CLA	CMC-C2C-C1C	2.27	128.48	125.03
10	bB	829	CLA	CMC-C2C-C1C	2.27	128.48	125.03
10	cB	829	CLA	CMC-C2C-C1C	2.27	128.48	125.03
10	aB	823	CLA	C4-C3-C5	2.27	119.19	115.29
10	cB	823	CLA	C4-C3-C5	2.27	119.19	115.29
13	cB	843	BCR	C7-C8-C9	-2.27	122.81	126.21
10	bA	821	CLA	CBC-CAC-C3C	-2.27	106.14	112.43
10	cB	817	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
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	cB	818	CLA	CBC-CAC-C3C	-2.26	106.14	112.43
10	cL	202	CLA	CHD-C4C-NC	2.26	127.77	124.20
10	aB	809	CLA	C6-C7-C8	-2.26	108.71	115.77
10	aB	829	CLA	CMC-C2C-C1C	2.26	128.47	125.03
10	bL	204	CLA	CHB-C4A-NA	2.26	127.64	124.51
10	bB	813	CLA	CHB-C4A-NA	2.26	127.64	124.51
10	cA	839	CLA	CED-O2D-CGD	2.26	121.11	115.95
10	bB	817	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
10	aB	810	CLA	C1-C2-C3	-2.26	122.13	126.04
10	aA	813	CLA	CBC-CAC-C3C	-2.26	106.16	112.43
10	cB	809	CLA	C11-C12-C13	-2.26	108.72	115.77
10	bB	809	CLA	CHB-C4A-NA	2.26	127.64	124.51
10	bA	830	CLA	CBC-CAC-C3C	-2.26	106.16	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	aB	845	BCR	C15-C16-C17	-2.26	118.76	123.51
10	aB	838	CLA	CBA-CAA-C2A	2.25	120.56	113.85
10	aA	825	CLA	CHB-C4A-NA	2.25	127.63	124.51
13	aB	843	BCR	C7-C8-C9	-2.25	122.83	126.21
10	bB	823	CLA	C4-C3-C5	2.25	119.17	115.29
10	bA	839	CLA	CED-O2D-CGD	2.25	121.10	115.95
10	aA	830	CLA	CBC-CAC-C3C	-2.25	106.17	112.43
13	bI	101	BCR	C27-C26-C25	2.25	126.02	122.74
10	bA	813	CLA	CBC-CAC-C3C	-2.25	106.18	112.43
13	bB	845	BCR	C15-C16-C17	-2.25	118.78	123.51
14	cA	852	LHG	C20-C19-C18	-2.25	102.81	114.44
10	bB	811	CLA	CHA-C1A-NA	-2.25	121.24	126.40
10	aL	202	CLA	CHD-C4C-NC	2.25	127.75	124.20
10	cA	830	CLA	CBC-CAC-C3C	-2.25	106.19	112.43
10	cB	813	CLA	CHB-C4A-NA	2.25	127.62	124.51
10	bA	826	CLA	CHB-C4A-NA	2.25	127.62	124.51
10	aA	840	CLA	CMC-C2C-C1C	2.25	128.45	125.03
10	bB	807	CLA	C1-C2-C3	-2.25	122.15	126.04
14	bA	852	LHG	C20-C19-C18	-2.25	102.83	114.44
14	aA	852	LHG	C20-C19-C18	-2.25	102.83	114.44
10	aB	813	CLA	CHB-C4A-NA	2.25	127.62	124.51
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	818	CLA	CBC-CAC-C3C	-2.25	106.19	112.43
10	bA	802	CLA	CMB-C2B-C3B	2.25	129.01	124.80
10	cA	823	CLA	C4-C3-C5	2.25	119.16	115.29
10	bL	203	CLA	C4-C3-C5	2.25	119.16	115.29
10	aA	833	CLA	CMB-C2B-C3B	2.25	129.01	124.80
10	cB	838	CLA	CBA-CAA-C2A	2.25	120.53	113.85
10	bB	809	CLA	C6-C7-C8	-2.25	108.77	115.77
10	bA	815	CLA	CMB-C2B-C3B	2.24	129.01	124.80
13	cB	845	BCR	C15-C16-C17	-2.24	118.79	123.51
10	aA	839	CLA	CED-O2D-CGD	2.24	121.07	115.95
10	bA	820	CLA	C4-C3-C5	2.24	119.15	115.29
10	cA	834	CLA	CMA-C3A-C2A	-2.24	104.75	113.78
10	cB	809	CLA	CHB-C4A-NA	2.24	127.61	124.51
10	cA	831	CLA	CHB-C4A-NA	2.24	127.61	124.51
10	cA	815	CLA	CMB-C2B-C3B	2.24	129.00	124.80
10	bA	833	CLA	CMB-C2B-C3B	2.24	129.00	124.80
10	cB	820	CLA	CBC-CAC-C3C	-2.24	106.21	112.43
10	cB	832	CLA	CBC-CAC-C3C	-2.24	106.21	112.43
13	aI	101	BCR	C27-C26-C25	2.24	126.00	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	809	CLA	C6-C7-C8	-2.24	108.79	115.77
10	bB	838	CLA	CBA-CAA-C2A	2.24	120.51	113.85
10	aA	834	CLA	CMA-C3A-C2A	-2.24	104.76	113.78
14	aA	852	LHG	O8-C23-C24	2.24	119.11	111.93
10	bA	834	CLA	CMA-C3A-C2A	-2.24	104.76	113.78
10	bA	831	CLA	CBC-CAC-C3C	-2.24	106.22	112.43
10	aB	833	CLA	O2A-CGA-CBA	2.24	119.11	111.93
10	aB	801	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
10	bA	819	CLA	O1D-CGD-CBD	-2.24	119.85	124.48
14	cA	852	LHG	O8-C23-C24	2.24	119.11	111.93
16	cB	848	LMG	C38-C37-C36	-2.24	102.89	114.44
10	cA	854	CLA	C4-C3-C5	2.24	119.14	115.29
10	cB	824	CLA	CHB-C4A-NA	2.24	127.60	124.51
10	cA	831	CLA	CBC-CAC-C3C	-2.24	106.22	112.43
10	aB	837	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
10	aB	820	CLA	CBC-CAC-C3C	-2.23	106.22	112.43
10	cA	812	CLA	O1D-CGD-CBD	-2.23	119.85	124.48
10	aL	205	CLA	CHB-C4A-NA	2.23	127.60	124.51
10	aL	204	CLA	CHB-C4A-NA	2.23	127.60	124.51
10	cB	807	CLA	C1-C2-C3	-2.23	122.18	126.04
10	bA	840	CLA	CMC-C2C-C1C	2.23	128.43	125.03
10	bB	832	CLA	CBC-CAC-C3C	-2.23	106.23	112.43
10	cB	801	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
10	cA	833	CLA	CMB-C2B-C3B	2.23	128.99	124.80
10	aB	832	CLA	CBC-CAC-C3C	-2.23	106.23	112.43
10	cL	205	CLA	CHB-C4A-NA	2.23	127.60	124.51
10	aA	831	CLA	CBC-CAC-C3C	-2.23	106.23	112.43
10	cA	840	CLA	CMC-C2C-C1C	2.23	128.43	125.03
10	bA	815	CLA	O2A-CGA-CBA	2.23	119.09	111.93
10	bB	838	CLA	CBC-CAC-C3C	-2.23	106.24	112.43
10	bA	854	CLA	C4-C3-C5	2.23	119.13	115.29
10	bB	820	CLA	CBC-CAC-C3C	-2.23	106.24	112.43
10	bB	818	CLA	CBC-CAC-C3C	-2.23	106.24	112.43
10	bA	819	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
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
10	bB	830	CLA	C4-C3-C5	2.23	119.12	115.29
10	cB	833	CLA	O2A-CGA-CBA	2.23	119.08	111.93
10	aA	815	CLA	O2A-CGA-CBA	2.23	119.08	111.93
14	bA	852	LHG	O8-C23-C24	2.23	119.08	111.93
13	cB	845	BCR	C33-C5-C6	-2.23	122.03	124.51
10	bL	202	CLA	CHD-C4C-NC	2.23	127.71	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	812	CLA	O1D-CGD-CBD	-2.23	119.87	124.48
13	bB	843	BCR	C7-C8-C9	-2.23	122.87	126.21
10	cA	815	CLA	O2A-CGA-CBA	2.23	119.08	111.93
10	bB	813	CLA	CAC-C3C-C4C	2.23	127.73	124.82
10	bB	827	CLA	O2A-CGA-O1A	-2.23	117.87	123.56
10	bB	820	CLA	C1-C2-C3	-2.23	122.19	126.04
16	aB	848	LMG	C38-C37-C36	-2.23	102.94	114.44
16	aB	848	LMG	O2-C2-C1	-2.23	104.64	110.06
10	aA	824	CLA	CHA-C1A-NA	-2.23	121.30	126.40
10	aA	815	CLA	CMB-C2B-C3B	2.22	128.97	124.80
10	aA	819	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
10	bB	833	CLA	O2A-CGA-CBA	2.22	119.07	111.93
13	cB	845	BCR	C40-C30-C25	2.22	113.90	110.30
16	bB	848	LMG	C38-C37-C36	-2.22	102.95	114.44
10	bB	818	CLA	C4-C3-C5	2.22	119.12	115.29
16	aB	848	LMG	O1-C1-C2	-2.22	104.72	108.26
16	cB	848	LMG	O1-C1-C2	-2.22	104.72	108.26
10	bA	831	CLA	CHB-C4A-NA	2.22	127.58	124.51
10	bB	837	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
10	aA	802	CLA	CMB-C2B-C3B	2.22	128.97	124.80
10	bA	812	CLA	O1D-CGD-CBD	-2.22	119.88	124.48
10	aB	827	CLA	O2A-CGA-O1A	-2.22	117.89	123.56
10	aA	826	CLA	CHB-C4A-NA	2.22	127.58	124.51
13	aB	845	BCR	C40-C30-C25	2.22	113.90	110.30
10	bB	801	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
10	bB	841	CLA	O2D-CGD-O1D	-2.22	119.45	123.83
10	cB	821	CLA	CMB-C2B-C3B	2.22	128.96	124.80
10	cB	818	CLA	C4-C3-C5	2.22	119.11	115.29
10	aA	854	CLA	C4-C3-C5	2.22	119.11	115.29
10	cA	819	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
16	bB	848	LMG	O1-C1-C2	-2.22	104.73	108.26
10	cA	802	CLA	CMB-C2B-C3B	2.22	128.96	124.80
10	cA	816	CLA	C1-C2-C3	-2.22	122.21	126.04
10	bA	804	CLA	CMC-C2C-C1C	2.22	128.41	125.03
10	aB	838	CLA	CBC-CAC-C3C	-2.22	106.27	112.43
10	bA	804	CLA	CMB-C2B-C3B	2.22	128.96	124.80
10	aA	819	CLA	O1D-CGD-CBD	-2.22	119.88	124.48
10	cA	838	CLA	CHA-C1A-NA	-2.22	121.32	126.40
10	aA	804	CLA	CMC-C2C-C1C	2.22	128.41	125.03
13	bA	847	BCR	C24-C23-C22	-2.22	122.88	126.21
13	cI	102	BCR	C27-C26-C25	2.22	125.97	122.74
10	bA	816	CLA	C1-C2-C3	-2.22	122.21	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
16	cB	848	LMG	O2-C2-C1	-2.21	104.66	110.06
13	cB	849	BCR	C31-C1-C6	2.21	113.89	110.30
10	aB	818	CLA	C4-C3-C5	2.21	119.10	115.29
10	bB	835	CLA	CHA-C1A-NA	-2.21	121.33	126.40
10	aA	825	CLA	OBD-CAD-C3D	-2.21	124.12	128.04
10	aA	842	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
10	bA	842	CLA	CED-O2D-CGD	2.21	121.00	115.95
10	cB	835	CLA	CHA-C1A-NA	-2.21	121.33	126.40
10	cB	827	CLA	O2A-CGA-O1A	-2.21	117.91	123.56
10	aB	813	CLA	CAC-C3C-C4C	2.21	127.71	124.82
13	aA	847	BCR	C24-C23-C22	-2.21	122.89	126.21
10	aB	807	CLA	C1-C2-C3	-2.21	122.22	126.04
13	bB	845	BCR	C40-C30-C25	2.21	113.88	110.30
10	cA	827	CLA	O1D-CGD-CBD	-2.21	119.90	124.48
13	bL	206	BCR	C15-C16-C17	-2.21	118.86	123.51
10	bA	827	CLA	O1D-CGD-CBD	-2.21	119.90	124.48
10	cB	838	CLA	CBC-CAC-C3C	-2.21	106.30	112.43
10	aB	824	CLA	CHB-C4A-NA	2.21	127.57	124.51
13	aB	845	BCR	C38-C26-C27	-2.21	109.44	113.57
10	cA	804	CLA	CMB-C2B-C3B	2.21	128.94	124.80
10	bB	821	CLA	CMB-C2B-C3B	2.21	128.94	124.80
10	aA	838	CLA	CHA-C1A-NA	-2.21	121.34	126.40
10	cB	830	CLA	C4-C3-C5	2.21	119.09	115.29
10	aB	830	CLA	C4-C3-C5	2.21	119.09	115.29
10	cA	842	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
10	bB	814	CLA	CHD-C4C-NC	2.21	127.68	124.20
10	aB	814	CLA	CHD-C4C-NC	2.21	127.68	124.20
10	cA	818	CLA	CAC-C3C-C4C	2.21	127.70	124.82
10	cA	819	CLA	O1D-CGD-CBD	-2.21	119.91	124.48
10	aL	203	CLA	C4-C3-C5	2.21	119.08	115.29
13	cA	847	BCR	C24-C23-C22	-2.21	122.90	126.21
10	cA	832	CLA	CMA-C3A-C4A	-2.20	105.85	111.77
16	bB	848	LMG	O2-C2-C1	-2.20	104.69	110.06
10	cA	842	CLA	CED-O2D-CGD	2.20	120.98	115.95
10	aB	835	CLA	CHA-C1A-NA	-2.20	121.35	126.40
13	cB	849	BCR	C2-C1-C6	2.20	113.89	110.48
13	aB	849	BCR	C31-C1-C6	2.20	113.87	110.30
10	bL	205	CLA	CMC-C2C-C1C	2.20	128.38	125.03
10	cL	203	CLA	C4-C3-C5	2.20	119.08	115.29
10	cB	807	CLA	CMC-C2C-C1C	2.20	128.38	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	836	CLA	CHB-C4A-NA	2.20	127.56	124.51
10	cB	813	CLA	CAC-C3C-C4C	2.20	127.69	124.82
10	aB	830	CLA	CBC-CAC-C3C	-2.20	106.32	112.43
13	cL	206	BCR	C15-C16-C17	-2.20	118.89	123.51
10	bA	838	CLA	CHA-C1A-NA	-2.20	121.36	126.40
10	aA	804	CLA	CMB-C2B-C3B	2.20	128.92	124.80
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	842	CLA	CED-O2D-CGD	2.20	120.97	115.95
10	aA	827	CLA	O1D-CGD-CBD	-2.20	119.93	124.48
10	aA	829	CLA	CHD-C4C-NC	2.20	127.66	124.20
10	cB	806	CLA	C4-C3-C5	2.20	119.07	115.29
11	bA	844	PQN	C2M-C2-C3	-2.20	119.83	124.21
10	bB	816	CLA	CMC-C2C-C1C	2.20	128.37	125.03
13	bA	850	BCR	C24-C23-C22	-2.20	122.91	126.21
10	cB	823	CLA	O2D-CGD-O1D	-2.20	119.50	123.83
10	bA	826	CLA	CAC-C3C-C4C	2.19	127.69	124.82
10	bB	826	CLA	CBC-CAC-C3C	-2.19	106.34	112.43
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
13	bB	845	BCR	C38-C26-C27	-2.19	109.47	113.57
10	aA	826	CLA	CAC-C3C-C4C	2.19	127.69	124.82
10	aA	838	CLA	C5-C3-C4	2.19	119.52	114.59
10	aB	836	CLA	CHB-C4A-NA	2.19	127.54	124.51
10	aB	826	CLA	CBC-CAC-C3C	-2.19	106.34	112.43
10	cB	830	CLA	CBC-CAC-C3C	-2.19	106.34	112.43
10	aB	832	CLA	O2A-CGA-CBA	2.19	118.97	111.93
10	aB	821	CLA	CMB-C2B-C3B	2.19	128.91	124.80
10	aA	842	CLA	O2A-CGA-CBA	2.19	118.97	111.93
13	aL	206	BCR	C15-C16-C17	-2.19	118.90	123.51
10	bB	835	CLA	CBC-CAC-C3C	-2.19	106.35	112.43
10	aA	835	CLA	CHB-C4A-NA	2.19	127.54	124.51
10	aA	854	CLA	C1-C2-C3	-2.19	122.25	126.04
10	aB	806	CLA	C4-C3-C5	2.19	119.06	115.29
10	bB	821	CLA	O2A-CGA-CBA	2.19	118.96	111.93
10	cA	804	CLA	CMC-C2C-C1C	2.19	128.36	125.03
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
13	bB	849	BCR	C2-C1-C6	2.19	113.87	110.48
10	cB	821	CLA	O2A-CGA-CBA	2.19	118.96	111.93
10	aB	821	CLA	O2A-CGA-CBA	2.19	118.96	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aL	205	CLA	CMC-C2C-C1C	2.19	128.36	125.03
13	cB	845	BCR	C38-C26-C27	-2.19	109.48	113.57
10	bA	809	CLA	CMB-C2B-C3B	2.19	128.90	124.80
10	aA	811	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
10	cA	826	CLA	CAC-C3C-C4C	2.19	127.68	124.82
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	aA	834	CLA	CMC-C2C-C1C	2.19	128.36	125.03
10	bB	832	CLA	O2A-CGA-CBA	2.19	118.95	111.93
13	aA	850	BCR	C24-C23-C22	-2.19	122.93	126.21
10	aB	835	CLA	CBC-CAC-C3C	-2.19	106.36	112.43
10	cB	826	CLA	CBC-CAC-C3C	-2.19	106.36	112.43
10	cA	826	CLA	CHB-C4A-NA	2.19	127.53	124.51
10	bA	835	CLA	O2A-CGA-CBA	2.19	118.95	111.93
10	bB	823	CLA	O2D-CGD-O1D	-2.18	119.52	123.83
10	bB	806	CLA	C4-C3-C5	2.18	119.05	115.29
13	bA	846	BCR	C33-C5-C6	-2.18	122.08	124.51
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
10	cA	829	CLA	CHD-C4C-NC	2.18	127.64	124.20
10	aA	805	CLA	O2A-CGA-O1A	-2.18	117.98	123.56
10	cA	834	CLA	CMC-C2C-C1C	2.18	128.35	125.03
10	cA	825	CLA	OBD-CAD-C3D	-2.18	124.17	128.04
10	cA	805	CLA	O1D-CGD-CBD	-2.18	119.96	124.48
10	bB	830	CLA	CBC-CAC-C3C	-2.18	106.37	112.43
10	bA	842	CLA	O2A-CGA-CBA	2.18	118.94	111.93
10	cB	802	CLA	C1-C2-C3	-2.18	122.27	126.04
13	cA	850	BCR	C24-C23-C22	-2.18	122.93	126.21
10	bA	838	CLA	C5-C3-C4	2.18	119.49	114.59
10	bA	834	CLA	CMC-C2C-C1C	2.18	128.35	125.03
10	cB	841	CLA	O2D-CGD-O1D	-2.18	119.52	123.83
10	aB	816	CLA	CMC-C2C-C1C	2.18	128.35	125.03
10	cA	842	CLA	O2A-CGA-CBA	2.18	118.93	111.93
10	aA	837	CLA	C1-O2A-CGA	2.18	122.50	116.54
10	cB	835	CLA	CBC-CAC-C3C	-2.18	106.38	112.43
10	aB	840	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
10	aA	835	CLA	O2A-CGA-CBA	2.18	118.92	111.93
10	cL	205	CLA	CMC-C2C-C1C	2.18	128.34	125.03
11	aA	844	PQN	C2M-C2-C3	-2.18	119.87	124.21
10	cB	832	CLA	O2A-CGA-CBA	2.18	118.92	111.93
10	cB	834	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
10	bB	840	CLA	CAA-C2A-C3A	-2.18	106.82	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	839	CLA	CMB-C2B-C3B	2.18	128.88	124.80
10	cA	835	CLA	O2A-CGA-CBA	2.18	118.92	111.93
10	aB	839	CLA	CMB-C2B-C3B	2.18	128.88	124.80
10	aA	826	CLA	O2A-CGA-O1A	-2.18	118.00	123.56
13	aA	848	BCR	C35-C13-C14	-2.18	119.88	122.92
10	aB	841	CLA	O2D-CGD-O1D	-2.18	119.53	123.83
10	cB	839	CLA	CMB-C2B-C3B	2.18	128.88	124.80
10	bA	811	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
10	bA	825	CLA	OBD-CAD-C3D	-2.18	124.19	128.04
10	aB	818	CLA	CMC-C2C-C1C	2.18	128.34	125.03
16	aB	848	LMG	C42-C41-C40	-2.17	103.20	114.44
10	bA	805	CLA	O1D-CGD-CBD	-2.17	119.97	124.48
10	cA	837	CLA	C1-O2A-CGA	2.17	122.48	116.54
10	aA	837	CLA	C4-C3-C5	2.17	119.03	115.29
10	cA	826	CLA	O2A-CGA-O1A	-2.17	118.01	123.56
16	bB	848	LMG	C42-C41-C40	-2.17	103.21	114.44
10	cA	811	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
13	cA	848	BCR	C35-C13-C14	-2.17	119.88	122.92
10	cA	804	CLA	O2A-CGA-CBA	2.17	118.91	111.93
10	aB	802	CLA	O2A-CGA-CBA	2.17	118.91	111.93
16	cB	848	LMG	C42-C41-C40	-2.17	103.22	114.44
13	cA	849	BCR	C24-C23-C22	-2.17	122.95	126.21
10	cA	809	CLA	CMB-C2B-C3B	2.17	128.87	124.80
11	cA	844	PQN	C2M-C2-C3	-2.17	119.88	124.21
10	bA	837	CLA	C1-O2A-CGA	2.17	122.48	116.54
13	aB	849	BCR	C2-C1-C6	2.17	113.84	110.48
10	bA	804	CLA	O2A-CGA-CBA	2.17	118.90	111.93
10	cA	838	CLA	C5-C3-C4	2.17	119.47	114.59
10	aA	809	CLA	CMB-C2B-C3B	2.17	128.87	124.80
10	aB	823	CLA	O2D-CGD-O1D	-2.17	119.55	123.83
13	bB	849	BCR	C31-C1-C6	2.17	113.81	110.30
13	aA	847	BCR	C29-C30-C25	2.17	113.84	110.48
10	cB	816	CLA	CMC-C2C-C1C	2.17	128.33	125.03
10	bA	837	CLA	C4-C3-C5	2.17	119.02	115.29
10	cB	820	CLA	C1-C2-C3	-2.17	122.29	126.04
10	bA	818	CLA	CAC-C3C-C4C	2.17	127.65	124.82
10	aA	818	CLA	CAC-C3C-C4C	2.17	127.65	124.82
13	bA	849	BCR	C33-C5-C6	-2.17	122.10	124.51
10	cB	840	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
10	bA	805	CLA	O2A-CGA-O1A	-2.16	118.03	123.56
10	bB	810	CLA	C4-C3-C5	2.16	119.02	115.29
10	aA	805	CLA	O1D-CGD-CBD	-2.16	120.00	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bA	847	BCR	C29-C30-C25	2.16	113.83	110.48
10	aB	801	CLA	C1-C2-C3	-2.16	122.30	126.04
10	aB	835	CLA	CMC-C2C-C1C	2.16	128.32	125.03
10	aB	802	CLA	C1-C2-C3	-2.16	122.30	126.04
10	cA	805	CLA	O2A-CGA-O1A	-2.16	118.03	123.56
10	bB	802	CLA	C1-C2-C3	-2.16	122.30	126.04
10	bB	802	CLA	O2A-CGA-CBA	2.16	118.87	111.93
10	bA	826	CLA	O2A-CGA-O1A	-2.16	118.04	123.56
13	cA	847	BCR	C29-C30-C25	2.16	113.83	110.48
10	aA	834	CLA	CED-O2D-CGD	2.16	120.89	115.95
10	cB	802	CLA	O2A-CGA-CBA	2.16	118.86	111.93
10	aA	809	CLA	CMC-C2C-C1C	2.16	128.32	125.03
10	aB	807	CLA	CMC-C2C-C1C	2.16	128.32	125.03
10	cA	830	CLA	CMB-C2B-C3B	2.16	128.85	124.80
10	aB	810	CLA	C4-C3-C5	2.16	119.00	115.29
10	aB	805	CLA	C1-C2-C3	-2.16	122.31	126.04
10	aA	804	CLA	O2A-CGA-CBA	2.16	118.86	111.93
10	cB	801	CLA	C1-C2-C3	-2.16	122.31	126.04
10	cB	835	CLA	CMC-C2C-C1C	2.16	128.31	125.03
10	bA	820	CLA	CMC-C2C-C1C	2.16	128.31	125.03
13	bA	848	BCR	C35-C13-C14	-2.16	119.90	122.92
9	cA	801	CL0	O2A-CGA-O1A	-2.16	118.05	123.56
10	cA	829	CLA	CHB-C4A-NA	2.16	127.49	124.51
10	bB	807	CLA	CMC-C2C-C1C	2.15	128.31	125.03
9	bA	801	CL0	O2A-CGA-O1A	-2.15	118.06	123.56
13	cA	849	BCR	C33-C5-C6	-2.15	122.11	124.51
13	aA	849	BCR	C24-C23-C22	-2.15	122.98	126.21
10	aA	828	CLA	CHA-C1A-NA	-2.15	121.47	126.40
10	cB	810	CLA	C4-C3-C5	2.15	118.99	115.29
10	cA	837	CLA	C4-C3-C5	2.15	118.99	115.29
10	cA	820	CLA	CMC-C2C-C1C	2.15	128.30	125.03
10	aA	830	CLA	CMB-C2B-C3B	2.15	128.83	124.80
10	bA	829	CLA	O1D-CGD-CBD	-2.15	120.03	124.48
10	bA	830	CLA	CMB-C2B-C3B	2.15	128.83	124.80
10	bB	835	CLA	CMC-C2C-C1C	2.15	128.30	125.03
10	bA	827	CLA	C1-O2A-CGA	2.15	122.41	116.54
10	aA	820	CLA	CMC-C2C-C1C	2.15	128.30	125.03
10	bA	809	CLA	CMC-C2C-C1C	2.15	128.30	125.03
13	cA	846	BCR	C33-C5-C6	-2.15	122.12	124.51
10	cB	818	CLA	CMC-C2C-C1C	2.15	128.30	125.03
10	aB	841	CLA	CMC-C2C-C1C	2.15	128.30	125.03
10	aB	833	CLA	CBC-CAC-C3C	-2.15	106.47	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
10	bB	824	CLA	O2D-CGD-O1D	-2.15	119.59	123.83
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
10	cA	834	CLA	CED-O2D-CGD	2.15	120.85	115.95
10	aA	829	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
10	aA	834	CLA	O2D-CGD-O1D	-2.14	119.60	123.83
10	aB	837	CLA	O1D-CGD-CBD	-2.14	120.04	124.48
9	aA	801	CL0	O2A-CGA-O1A	-2.14	118.08	123.56
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	aA	834	CLA	O2A-CGA-O1A	-2.14	118.08	123.56
10	bA	829	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
10	cB	836	CLA	CHB-C4A-NA	2.14	127.48	124.51
10	cA	834	CLA	O2A-CGA-O1A	-2.14	118.08	123.56
10	cA	834	CLA	O2D-CGD-O1D	-2.14	119.60	123.83
13	aA	849	BCR	C33-C5-C6	-2.14	122.12	124.51
10	bB	819	CLA	O2A-CGA-CBA	2.14	118.81	111.93
10	cA	809	CLA	CMC-C2C-C1C	2.14	128.29	125.03
10	bA	825	CLA	O2A-CGA-CBA	2.14	118.81	111.93
10	bB	818	CLA	CMC-C2C-C1C	2.14	128.29	125.03
10	aB	824	CLA	O2D-CGD-O1D	-2.14	119.60	123.83
10	cA	820	CLA	O2D-CGD-O1D	-2.14	119.60	123.83
13	cM	101	BCR	C7-C8-C9	-2.14	122.99	126.21
10	cA	828	CLA	CHA-C1A-NA	-2.14	121.50	126.40
10	aA	820	CLA	O2D-CGD-O1D	-2.14	119.61	123.83
14	cA	852	LHG	O8-C23-O10	-2.14	118.09	123.56
10	bA	834	CLA	CED-O2D-CGD	2.14	120.83	115.95
10	bA	834	CLA	O2A-CGA-O1A	-2.14	118.10	123.56
10	cB	833	CLA	CBC-CAC-C3C	-2.14	106.50	112.43
10	cA	854	CLA	CHB-C4A-NA	2.14	127.47	124.51
10	aA	817	CLA	CBA-CAA-C2A	2.14	120.21	113.85
10	cB	824	CLA	O2D-CGD-O1D	-2.14	119.61	123.83
10	cB	841	CLA	CMC-C2C-C1C	2.14	128.28	125.03
10	cA	825	CLA	O2A-CGA-CBA	2.14	118.79	111.93
10	cB	810	CLA	CMC-C2C-C1C	2.14	128.28	125.03
10	cA	836	CLA	CHA-C1A-NA	-2.14	121.51	126.40
10	cA	813	CLA	O2D-CGD-O1D	-2.13	119.61	123.83
10	bA	854	CLA	C1-C2-C3	-2.13	122.35	126.04
13	cB	847	BCR	C15-C14-C13	-2.13	124.26	127.31
13	bA	849	BCR	C24-C23-C22	-2.13	123.01	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	822	CLA	CBC-CAC-C3C	-2.13	106.50	112.43
10	bA	822	CLA	CBC-CAC-C3C	-2.13	106.51	112.43
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	bB	804	CLA	O1D-CGD-CBD	-2.13	120.06	124.48
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
13	aM	101	BCR	C24-C23-C22	-2.13	123.01	126.21
10	aB	819	CLA	O2A-CGA-CBA	2.13	118.77	111.93
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
15	bA	853	LMT	C1'-C2'-C3'	2.13	114.43	109.98
10	cA	829	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
10	bA	820	CLA	O2D-CGD-O1D	-2.13	119.62	123.83
15	aA	853	LMT	C1'-C2'-C3'	2.13	114.43	109.98
10	aA	827	CLA	C1-O2A-CGA	2.13	122.36	116.54
10	aA	829	CLA	O1D-CGD-CBD	-2.13	120.07	124.48
10	bB	833	CLA	CBC-CAC-C3C	-2.13	106.52	112.43
10	aB	839	CLA	CBC-CAC-C3C	-2.13	106.52	112.43
10	bA	829	CLA	CHB-C4A-NA	2.13	127.45	124.51
10	aA	816	CLA	CBC-CAC-C3C	-2.13	106.52	112.43
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	aA	825	CLA	O2A-CGA-CBA	2.13	118.76	111.93
10	bB	841	CLA	CMC-C2C-C1C	2.13	128.27	125.03
10	bA	812	CLA	O2A-CGA-CBA	2.13	118.76	111.93
10	cA	816	CLA	CBC-CAC-C3C	-2.13	106.53	112.43
10	aA	812	CLA	O2A-CGA-CBA	2.13	118.76	111.93
10	cB	837	CLA	O1D-CGD-CBD	-2.13	120.07	124.48
10	cA	827	CLA	C1-O2A-CGA	2.13	122.35	116.54
10	cA	823	CLA	CBA-CAA-C2A	2.13	120.18	113.85
10	cA	835	CLA	CMC-C2C-C1C	2.13	128.26	125.03
10	aA	829	CLA	CHB-C4A-NA	2.12	127.45	124.51
10	cB	819	CLA	O2A-CGA-CBA	2.12	118.75	111.93
10	aB	837	CLA	CHA-C1A-NA	-2.12	121.53	126.40
10	bA	834	CLA	O2D-CGD-O1D	-2.12	119.64	123.83
14	aA	852	LHG	O8-C23-O10	-2.12	118.14	123.56
10	cA	817	CLA	CBA-CAA-C2A	2.12	120.17	113.85
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aA	828	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
10	aA	822	CLA	CBC-CAC-C3C	-2.12	106.54	112.43
10	bB	810	CLA	CMC-C2C-C1C	2.12	128.26	125.03
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	aB	804	CLA	O1D-CGD-CBD	-2.12	120.08	124.48
10	bA	810	CLA	CMC-C2C-C1C	2.12	128.26	125.03
13	bB	847	BCR	C15-C14-C13	-2.12	124.28	127.31
13	bM	101	BCR	C7-C8-C9	-2.12	123.03	126.21
10	aA	819	CLA	CMC-C2C-C1C	2.12	128.26	125.03
10	bA	816	CLA	CBC-CAC-C3C	-2.12	106.54	112.43
10	cA	829	CLA	O1D-CGD-CBD	-2.12	120.09	124.48
10	aA	813	CLA	O2D-CGD-O1D	-2.12	119.65	123.83
10	cB	839	CLA	CBC-CAC-C3C	-2.12	106.55	112.43
10	aB	822	CLA	CBC-CAC-C3C	-2.12	106.55	112.43
10	bA	817	CLA	CBA-CAA-C2A	2.12	120.16	113.85
10	bA	836	CLA	CHA-C1A-NA	-2.12	121.55	126.40
14	bA	852	LHG	O8-C23-O10	-2.12	118.15	123.56
10	aA	835	CLA	CMC-C2C-C1C	2.12	128.25	125.03
10	bA	813	CLA	O2D-CGD-O1D	-2.12	119.65	123.83
10	bB	815	CLA	C4-C3-C5	2.12	118.93	115.29
10	cB	804	CLA	CHB-C4A-NA	2.12	127.44	124.51
10	cB	804	CLA	O1D-CGD-CBD	-2.12	120.09	124.48
10	aA	821	CLA	CHB-C4A-NA	2.12	127.44	124.51
10	bA	823	CLA	CBA-CAA-C2A	2.12	120.15	113.85
10	aB	823	CLA	CHA-C1A-NA	-2.12	121.55	126.40
10	aA	823	CLA	CBA-CAA-C2A	2.12	120.15	113.85
10	bB	839	CLA	CBC-CAC-C3C	-2.12	106.56	112.43
10	cA	818	CLA	CHB-C4A-NA	2.11	127.44	124.51
10	cB	831	CLA	CED-O2D-CGD	2.11	120.78	115.95
15	cA	853	LMT	C1'-C2'-C3'	2.11	114.40	109.98
10	bB	801	CLA	O2A-CGA-O1A	-2.11	118.16	123.56
10	cA	821	CLA	CHB-C4A-NA	2.11	127.43	124.51
10	bB	831	CLA	CED-O2D-CGD	2.11	120.78	115.95
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
10	cA	812	CLA	O2A-CGA-CBA	2.11	118.71	111.93
10	aB	813	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
10	bA	835	CLA	CMC-C2C-C1C	2.11	128.24	125.03
10	bB	821	CLA	CBC-CAC-C3C	-2.11	106.57	112.43
10	bB	808	CLA	OBD-CAD-C3D	-2.11	124.30	128.04
10	cB	815	CLA	CMC-C2C-C1C	2.11	128.24	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bL	204	CLA	CMB-C2B-C3B	2.11	128.76	124.80
10	cB	811	CLA	CHD-C4C-NC	2.11	127.53	124.20
10	bB	837	CLA	O1D-CGD-CBD	-2.11	120.11	124.48
10	aB	811	CLA	CHD-C4C-NC	2.11	127.53	124.20
10	bB	822	CLA	CBC-CAC-C3C	-2.11	106.58	112.43
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	aB	810	CLA	CMC-C2C-C1C	2.11	128.24	125.03
10	aB	831	CLA	CED-O2D-CGD	2.11	120.76	115.95
10	bB	823	CLA	CMC-C2C-C1C	2.11	128.24	125.03
10	cB	813	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
13	cM	101	BCR	C24-C23-C22	-2.11	123.05	126.21
13	cM	101	BCR	C15-C14-C13	-2.10	124.31	127.31
10	bB	823	CLA	CHA-C1A-NA	-2.10	121.58	126.40
10	aB	801	CLA	O2A-CGA-O1A	-2.10	118.18	123.56
10	bA	821	CLA	O1D-CGD-CBD	-2.10	120.12	124.48
10	aB	815	CLA	C4-C3-C5	2.10	118.91	115.29
10	cB	825	CLA	CGD-CBD-CAD	-2.10	103.92	110.73
10	aB	815	CLA	CMC-C2C-C1C	2.10	128.23	125.03
10	bB	823	CLA	CBC-CAC-C3C	-2.10	106.59	112.43
10	aB	808	CLA	OBD-CAD-C3D	-2.10	124.31	128.04
10	cB	821	CLA	CBC-CAC-C3C	-2.10	106.59	112.43
10	cA	833	CLA	CAC-C3C-C4C	2.10	127.57	124.82
10	cB	831	CLA	CBC-CAC-C3C	-2.10	106.59	112.43
10	cB	812	CLA	CHB-C4A-NA	2.10	127.42	124.51
10	aL	204	CLA	CMB-C2B-C3B	2.10	128.74	124.80
10	cB	826	CLA	C1-O2A-CGA	2.10	122.29	116.54
13	bM	101	BCR	C24-C23-C22	-2.10	123.06	126.21
10	bB	831	CLA	CBC-CAC-C3C	-2.10	106.60	112.43
10	bB	812	CLA	CHB-C4A-NA	2.10	127.42	124.51
10	aA	821	CLA	O1D-CGD-CBD	-2.10	120.13	124.48
10	aB	821	CLA	CBC-CAC-C3C	-2.10	106.60	112.43
10	cB	808	CLA	OBD-CAD-C3D	-2.10	124.32	128.04
10	aA	833	CLA	CAC-C3C-C4C	2.10	127.56	124.82
10	cB	815	CLA	C4-C3-C5	2.10	118.90	115.29
10	bA	811	CLA	CMC-C2C-C1C	2.10	128.23	125.03
10	bB	813	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
10	aB	823	CLA	CBC-CAC-C3C	-2.10	106.60	112.43
10	bA	828	CLA	CHB-C4A-NA	2.10	127.41	124.51
10	aB	826	CLA	C1-O2A-CGA	2.10	122.28	116.54
10	aA	804	CLA	C6-C7-C8	-2.10	109.22	115.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	830	CLA	O2A-CGA-O1A	-2.10	118.20	123.56
14	aA	852	LHG	C18-C17-C16	-2.10	103.60	114.44
10	bA	804	CLA	C6-C7-C8	-2.10	109.22	115.77
10	cA	810	CLA	CMC-C2C-C1C	2.10	128.22	125.03
10	aB	830	CLA	O2A-CGA-O1A	-2.10	118.20	123.56
10	cB	801	CLA	O2A-CGA-O1A	-2.10	118.20	123.56
14	cA	852	LHG	C18-C17-C16	-2.10	103.61	114.44
10	cA	804	CLA	C6-C7-C8	-2.10	109.23	115.77
10	bB	826	CLA	C1-O2A-CGA	2.10	122.27	116.54
13	aA	846	BCR	C33-C5-C6	-2.10	122.17	124.51
10	cB	822	CLA	CBC-CAC-C3C	-2.10	106.61	112.43
10	aB	831	CLA	CBC-CAC-C3C	-2.10	106.61	112.43
10	cA	811	CLA	CMC-C2C-C1C	2.09	128.22	125.03
10	cA	819	CLA	CMC-C2C-C1C	2.09	128.22	125.03
10	aB	841	CLA	C4-C3-C5	2.09	118.89	115.29
10	aA	810	CLA	CMC-C2C-C1C	2.09	128.22	125.03
10	bB	815	CLA	CMC-C2C-C1C	2.09	128.22	125.03
14	bA	852	LHG	C18-C17-C16	-2.09	103.64	114.44
10	cA	810	CLA	CHA-C1A-NA	-2.09	121.61	126.40
10	cB	830	CLA	O2A-CGA-O1A	-2.09	118.22	123.56
10	cB	823	CLA	CBC-CAC-C3C	-2.09	106.62	112.43
10	bA	833	CLA	CAC-C3C-C4C	2.09	127.55	124.82
10	aB	825	CLA	CGD-CBD-CAD	-2.09	103.96	110.73
10	aA	854	CLA	CHB-C4A-NA	2.09	127.40	124.51
10	aA	828	CLA	CBC-CAC-C3C	-2.09	106.63	112.43
10	bA	820	CLA	O2A-CGA-O1A	-2.09	118.22	123.56
10	cA	821	CLA	O1D-CGD-CBD	-2.09	120.15	124.48
10	cB	814	CLA	CHA-C1A-NA	-2.09	121.62	126.40
10	aA	816	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
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
10	bA	803	CLA	CAA-C2A-C3A	-2.09	107.07	112.78
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	cB	837	CLA	C4-C3-C5	2.08	118.87	115.29
13	aM	101	BCR	C7-C8-C9	-2.08	123.08	126.21
10	aA	811	CLA	CMC-C2C-C1C	2.08	128.20	125.03
10	cB	819	CLA	CAA-C2A-C1A	-2.08	105.15	111.97
10	bB	830	CLA	CHB-C4A-NA	2.08	127.39	124.51
10	bB	831	CLA	O2D-CGD-O1D	-2.08	119.72	123.83
10	aA	832	CLA	C4-C3-C5	2.08	118.87	115.29
10	bB	809	CLA	C11-C10-C8	-2.08	109.28	115.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cB	806	CLA	C1-O2A-CGA	2.08	122.23	116.54
10	aB	811	CLA	CMB-C2B-C3B	2.08	128.70	124.80
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	cA	816	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
10	bB	841	CLA	C4-C3-C5	2.08	118.87	115.29
10	aB	837	CLA	C4-C3-C5	2.08	118.87	115.29
10	bA	819	CLA	CMC-C2C-C1C	2.08	128.19	125.03
10	bB	814	CLA	CHA-C1A-NA	-2.08	121.64	126.40
10	cB	823	CLA	CMC-C2C-C1C	2.08	128.19	125.03
13	cI	102	BCR	C15-C16-C17	-2.08	119.15	123.51
10	aB	805	CLA	CED-O2D-CGD	2.08	120.69	115.95
10	bB	825	CLA	CGD-CBD-CAD	-2.07	104.01	110.73
10	cA	832	CLA	C4-C3-C5	2.07	118.86	115.29
13	cA	848	BCR	C1-C6-C5	-2.07	119.69	122.59
10	aB	823	CLA	CMC-C2C-C1C	2.07	128.19	125.03
10	aA	807	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
10	cB	809	CLA	C11-C10-C8	-2.07	109.30	115.77
10	bA	814	CLA	O1D-CGD-CBD	-2.07	120.18	124.48
10	cA	828	CLA	CBC-CAC-C3C	-2.07	106.67	112.43
10	aB	819	CLA	CAA-C2A-C1A	-2.07	105.18	111.97
10	cB	841	CLA	C4-C3-C5	2.07	118.86	115.29
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	bA	805	CLA	CBC-CAC-C3C	-2.07	106.68	112.43
10	aA	837	CLA	CHB-C4A-NA	2.07	127.38	124.51
10	aA	805	CLA	CBC-CAC-C3C	-2.07	106.68	112.43
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	cA	820	CLA	O2A-CGA-O1A	-2.07	118.27	123.56
10	cL	204	CLA	CMB-C2B-C3B	2.07	128.69	124.80
10	aB	809	CLA	C11-C10-C8	-2.07	109.31	115.77
10	bB	811	CLA	CMB-C2B-C3B	2.07	128.68	124.80
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	cB	836	CLA	CMC-C2C-C1C	2.07	128.18	125.03
14	cA	852	LHG	C27-C26-C25	-2.07	103.75	114.44
14	bA	852	LHG	C27-C26-C25	-2.07	103.75	114.44
10	aA	842	CLA	C1-O2A-CGA	2.07	122.20	116.54
10	aB	812	CLA	CHB-C4A-NA	2.07	127.37	124.51
10	aA	836	CLA	CHB-C4A-NA	2.07	127.37	124.51
10	bA	802	CLA	CMC-C2C-C1C	2.07	128.18	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bM	101	BCR	C16-C15-C14	-2.07	119.16	123.51
14	aA	852	LHG	C27-C26-C25	-2.07	103.76	114.44
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	bA	836	CLA	CHB-C4A-NA	2.07	127.37	124.51
10	bA	828	CLA	CBC-CAC-C3C	-2.07	106.69	112.43
10	aA	810	CLA	C1-C2-C3	-2.06	122.47	126.04
10	aA	820	CLA	O2A-CGA-O1A	-2.06	118.29	123.56
10	bB	821	CLA	O1D-CGD-CBD	-2.06	120.20	124.48
13	aI	101	BCR	C15-C16-C17	-2.06	119.17	123.51
10	aA	806	CLA	O2A-CGA-O1A	-2.06	118.29	123.56
10	bA	810	CLA	CHA-C1A-NA	-2.06	121.67	126.40
10	aA	817	CLA	O2A-CGA-O1A	-2.06	118.29	123.56
10	bA	837	CLA	CHB-C4A-NA	2.06	127.36	124.51
10	bB	837	CLA	C4-C3-C5	2.06	118.84	115.29
10	aB	837	CLA	CBA-CAA-C2A	-2.06	107.72	113.85
10	aA	828	CLA	C4-C3-C5	2.06	118.84	115.29
10	bA	832	CLA	C4-C3-C5	2.06	118.84	115.29
10	cA	805	CLA	CBC-CAC-C3C	-2.06	106.70	112.43
10	cB	821	CLA	O1D-CGD-CBD	-2.06	120.21	124.48
10	bB	826	CLA	O1D-CGD-CBD	-2.06	120.21	124.48
10	bB	805	CLA	CED-O2D-CGD	2.06	120.66	115.95
10	bL	203	CLA	CHB-C4A-NA	2.06	127.36	124.51
10	aB	806	CLA	C1-O2A-CGA	2.06	122.17	116.54
10	aA	840	CLA	CHB-C4A-NA	2.06	127.36	124.51
13	bA	848	BCR	C1-C6-C5	-2.06	119.71	122.59
10	cA	817	CLA	O2A-CGA-O1A	-2.06	118.30	123.56
10	bB	837	CLA	CBA-CAA-C2A	-2.06	107.73	113.85
10	aB	825	CLA	C1-C2-C3	-2.06	122.48	126.04
10	cB	811	CLA	CMB-C2B-C3B	2.06	128.66	124.80
10	cA	826	CLA	CMB-C2B-C3B	2.06	128.66	124.80
10	cA	803	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
10	cA	828	CLA	C4-C3-C5	2.06	118.83	115.29
10	bA	826	CLA	CMB-C2B-C3B	2.06	128.66	124.80
10	bA	842	CLA	C1-O2A-CGA	2.06	122.16	116.54
10	aB	831	CLA	O2D-CGD-O1D	-2.06	119.77	123.83
10	cB	831	CLA	O2D-CGD-O1D	-2.06	119.77	123.83
13	cB	849	BCR	C1-C6-C5	-2.06	119.72	122.59
10	bB	806	CLA	C1-O2A-CGA	2.06	122.16	116.54
10	aB	830	CLA	CHB-C4A-NA	2.06	127.35	124.51
10	bB	833	CLA	CHC-C1C-NC	2.05	127.32	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	826	CLA	O2A-CGA-O1A	-2.05	118.31	123.56
10	cB	805	CLA	CED-O2D-CGD	2.05	120.64	115.95
10	aA	826	CLA	CMB-C2B-C3B	2.05	128.65	124.80
10	bB	825	CLA	C1-C2-C3	-2.05	122.49	126.04
13	aM	101	BCR	C15-C14-C13	-2.05	124.38	127.31
10	bA	817	CLA	O2A-CGA-O1A	-2.05	118.32	123.56
10	cB	826	CLA	O2A-CGA-O1A	-2.05	118.32	123.56
10	bA	807	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
13	bI	101	BCR	C15-C16-C17	-2.05	119.20	123.51
10	cB	810	CLA	O1D-CGD-CBD	-2.05	120.23	124.48
10	cA	814	CLA	O1D-CGD-CBD	-2.05	120.23	124.48
10	cA	837	CLA	O2A-CGA-CBA	2.05	118.51	111.93
10	bA	806	CLA	O2A-CGA-O1A	-2.05	118.32	123.56
13	bB	849	BCR	C1-C6-C5	-2.05	119.72	122.59
13	cM	101	BCR	C16-C15-C14	-2.05	119.20	123.51
10	cB	825	CLA	C1-C2-C3	-2.05	122.50	126.04
10	bA	810	CLA	C1-C2-C3	-2.05	122.50	126.04
10	aB	807	CLA	CBA-CAA-C2A	2.05	119.95	113.85
10	cB	826	CLA	O1D-CGD-CBD	-2.05	120.23	124.48
10	cB	837	CLA	CBA-CAA-C2A	-2.05	107.76	113.85
10	cA	806	CLA	O2A-CGA-O1A	-2.05	118.33	123.56
10	cL	204	CLA	C4-C3-C5	2.05	118.81	115.29
10	cB	833	CLA	C1-C2-C3	-2.05	122.50	126.04
15	aA	853	LMT	C3'-C4'-C5'	-2.05	106.21	110.92
10	cA	842	CLA	C1-O2A-CGA	2.05	122.14	116.54
13	cL	206	BCR	C2-C1-C6	2.05	113.65	110.48
10	cA	802	CLA	CMC-C2C-C1C	2.05	128.15	125.03
9	aA	801	CL0	C4A-NA-C1A	-2.05	105.79	106.71
10	bB	814	CLA	O2A-CGA-O1A	-2.05	118.33	123.56
13	bA	846	BCR	C1-C6-C5	-2.05	119.73	122.59
10	aA	809	CLA	O2D-CGD-O1D	-2.05	119.79	123.83
10	aB	826	CLA	O2A-CGA-O1A	-2.05	118.33	123.56
10	aA	802	CLA	CMC-C2C-C1C	2.04	128.14	125.03
13	bM	101	BCR	C37-C22-C21	-2.04	120.06	122.92
10	cL	202	CLA	O2A-CGA-O1A	-2.04	118.34	123.56
10	aB	826	CLA	O1D-CGD-CBD	-2.04	120.24	124.48
10	aA	837	CLA	O2A-CGA-CBA	2.04	118.49	111.93
10	cB	820	CLA	O2A-CGA-O1A	-2.04	118.34	123.56
10	cA	809	CLA	O2D-CGD-O1D	-2.04	119.80	123.83
13	bL	206	BCR	C15-C14-C13	-2.04	124.40	127.31
10	bL	202	CLA	O2A-CGA-O1A	-2.04	118.34	123.56
13	aA	848	BCR	C1-C6-C5	-2.04	119.74	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	aB	843	BCR	C33-C5-C6	-2.04	122.24	124.51
10	bB	836	CLA	CMC-C2C-C1C	2.04	128.14	125.03
10	aB	836	CLA	CED-O2D-CGD	2.04	120.61	115.95
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
13	aA	850	BCR	C2-C1-C6	2.04	113.64	110.48
10	bL	204	CLA	C4-C3-C5	2.04	118.80	115.29
10	bA	828	CLA	C4-C3-C5	2.04	118.80	115.29
10	bB	830	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
13	aB	849	BCR	C1-C6-C5	-2.04	119.74	122.59
10	bL	202	CLA	CHB-C4A-NA	2.04	127.33	124.51
10	aB	820	CLA	O2A-CGA-O1A	-2.04	118.35	123.56
10	aB	836	CLA	CMC-C2C-C1C	2.04	128.13	125.03
10	aB	806	CLA	CHA-C1A-NA	-2.04	121.73	126.40
10	bB	807	CLA	CBA-CAA-C2A	2.04	119.91	113.85
10	aB	833	CLA	CHC-C1C-NC	2.04	127.29	124.20
10	bA	809	CLA	O2D-CGD-O1D	-2.04	119.81	123.83
10	cA	837	CLA	CHB-C4A-NA	2.04	127.33	124.51
10	bA	838	CLA	CMB-C2B-C3B	2.04	128.62	124.80
10	cB	807	CLA	C11-C10-C8	-2.04	109.42	115.77
10	bB	828	CLA	CHB-C4A-NA	2.04	127.33	124.51
10	aL	202	CLA	O2A-CGA-O1A	-2.04	118.36	123.56
10	cB	807	CLA	CBA-CAA-C2A	2.03	119.91	113.85
13	aL	206	BCR	C15-C14-C13	-2.03	124.41	127.31
13	bL	206	BCR	C2-C1-C6	2.03	113.63	110.48
10	cB	814	CLA	O2A-CGA-O1A	-2.03	118.36	123.56
10	aA	827	CLA	CBC-CAC-C3C	-2.03	106.78	112.43
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	aB	821	CLA	O1D-CGD-CBD	-2.03	120.27	124.48
10	cA	856	CLA	O2D-CGD-O1D	-2.03	119.81	123.83
10	aA	838	CLA	CMB-C2B-C3B	2.03	128.61	124.80
10	aB	814	CLA	O2A-CGA-O1A	-2.03	118.37	123.56
13	aL	206	BCR	C11-C10-C9	-2.03	124.41	127.31
10	bB	817	CLA	C1-C2-C3	-2.03	122.53	126.04
10	aA	814	CLA	O1D-CGD-CBD	-2.03	120.27	124.48
10	bA	827	CLA	CBC-CAC-C3C	-2.03	106.79	112.43
15	bA	853	LMT	C3'-C4'-C5'	-2.03	106.24	110.92
13	cA	850	BCR	C2-C1-C6	2.03	113.63	110.48
10	cA	838	CLA	CMB-C2B-C3B	2.03	128.61	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bB	806	CLA	CHA-C1A-NA	-2.03	121.75	126.40
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	aB	832	CLA	CHA-C1A-NA	-2.03	121.75	126.40
10	cB	836	CLA	CED-O2D-CGD	2.03	120.58	115.95
10	bB	836	CLA	CED-O2D-CGD	2.03	120.58	115.95
13	aL	206	BCR	C2-C1-C6	2.03	113.62	110.48
10	bB	810	CLA	O1D-CGD-CBD	-2.03	120.28	124.48
10	bB	834	CLA	O2D-CGD-O1D	-2.03	119.83	123.83
13	aM	101	BCR	C16-C15-C14	-2.03	119.25	123.51
10	cB	806	CLA	CHA-C1A-NA	-2.03	121.75	126.40
15	cA	853	LMT	C3'-C4'-C5'	-2.03	106.25	110.92
10	aB	807	CLA	C11-C10-C8	-2.03	109.44	115.77
10	cB	832	CLA	C1-O2A-CGA	2.03	122.08	116.54
10	cA	843	CLA	CBC-CAC-C3C	-2.03	106.80	112.43
10	bA	837	CLA	O2A-CGA-CBA	2.03	118.44	111.93
10	aA	843	CLA	CBC-CAC-C3C	-2.03	106.80	112.43
10	aB	816	CLA	CHA-C1A-NA	-2.03	121.76	126.40
10	aB	834	CLA	O2D-CGD-O1D	-2.03	119.83	123.83
10	bB	820	CLA	O2A-CGA-O1A	-2.03	118.39	123.56
10	cB	833	CLA	CHC-C1C-NC	2.03	127.28	124.20
10	aB	808	CLA	CHA-C1A-NA	-2.03	121.76	126.40
10	cB	808	CLA	CHA-C1A-NA	-2.02	121.76	126.40
10	aB	840	CLA	CED-O2D-CGD	2.02	120.57	115.95
10	bB	807	CLA	C11-C10-C8	-2.02	109.46	115.77
13	cM	101	BCR	C10-C11-C12	-2.02	117.22	123.31
10	cB	827	CLA	CHA-C1A-NA	-2.02	121.77	126.40
13	cA	851	BCR	C32-C1-C6	2.02	113.58	110.30
10	cL	203	CLA	CHB-C4A-NA	2.02	127.31	124.51
13	bA	851	BCR	C32-C1-C6	2.02	113.57	110.30
10	aA	856	CLA	O2D-CGD-O1D	-2.02	119.84	123.83
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	cL	206	BCR	C15-C14-C13	-2.02	124.43	127.31
10	bB	832	CLA	C1-O2A-CGA	2.02	122.06	116.54
13	bB	843	BCR	C33-C5-C6	-2.02	122.26	124.51
13	bL	206	BCR	C11-C10-C9	-2.02	124.43	127.31
13	cL	206	BCR	C1-C6-C5	-2.02	119.77	122.59
13	bA	850	BCR	C2-C1-C6	2.02	113.61	110.48
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aL	202	CLA	CHB-C4A-NA	2.02	127.30	124.51
10	cA	832	CLA	CMA-C3A-C2A	-2.02	105.66	113.78
10	aA	832	CLA	CMA-C3A-C2A	-2.01	105.66	113.78
13	cB	843	BCR	C33-C5-C6	-2.01	122.27	124.51
13	bA	846	BCR	C20-C21-C22	-2.01	124.44	127.31
10	bA	838	CLA	CBC-CAC-C3C	-2.01	106.84	112.43
10	cB	829	CLA	CBA-CAA-C2A	2.01	119.84	113.85
13	aM	101	BCR	C10-C11-C12	-2.01	117.25	123.31
13	aA	851	BCR	C32-C1-C6	2.01	113.56	110.30
10	aB	829	CLA	CBA-CAA-C2A	2.01	119.84	113.85
10	bB	832	CLA	CHA-C1A-NA	-2.01	121.79	126.40
10	bA	832	CLA	CMA-C3A-C2A	-2.01	105.67	113.78
10	aB	828	CLA	CHB-C4A-NA	2.01	127.29	124.51
10	cB	840	CLA	CED-O2D-CGD	2.01	120.54	115.95
13	bL	206	BCR	C1-C6-C5	-2.01	119.78	122.59
10	aA	838	CLA	CBC-CAC-C3C	-2.01	106.85	112.43
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	856	CLA	O2D-CGD-O1D	-2.01	119.86	123.83
10	aA	803	CLA	CBC-CAC-C3C	-2.01	106.85	112.43
10	bA	803	CLA	CBC-CAC-C3C	-2.01	106.85	112.43
13	cA	846	BCR	C1-C6-C5	-2.01	119.78	122.59
10	bA	837	CLA	C1-C2-C3	-2.01	122.57	126.04
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	bA	811	CLA	CBC-CAC-C3C	-2.01	106.85	112.43
10	aB	810	CLA	O1D-CGD-CBD	-2.01	120.32	124.48
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	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	832	CLA	C1-O2A-CGA	2.01	122.03	116.54
10	cA	811	CLA	CBC-CAC-C3C	-2.01	106.86	112.43
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	cB	834	CLA	O2D-CGD-O1D	-2.01	119.87	123.83
13	bM	101	BCR	C10-C11-C12	-2.01	117.27	123.31
10	cA	838	CLA	CBC-CAC-C3C	-2.00	106.86	112.43
10	cL	202	CLA	CHB-C4A-NA	2.00	127.28	124.51
10	bB	840	CLA	CED-O2D-CGD	2.00	120.53	115.95
10	aL	204	CLA	C4-C3-C5	2.00	118.74	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	803	CLA	CBC-CAC-C3C	-2.00	106.86	112.43
13	bI	102	BCR	C7-C8-C9	-2.00	123.20	126.21
10	cB	819	CLA	CHA-C1A-NA	-2.00	121.81	126.40
10	cA	827	CLA	CBC-CAC-C3C	-2.00	106.87	112.43
10	bA	843	CLA	CBC-CAC-C3C	-2.00	106.87	112.43
10	cB	808	CLA	C4-C3-C5	2.00	118.74	115.29
10	cB	816	CLA	CHA-C1A-NA	-2.00	121.81	126.40
10	cB	810	CLA	CMB-C2B-C3B	2.00	128.56	124.80
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	aA	840	CLA	O1D-CGD-CBD	-2.00	120.33	124.48
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	bB	829	CLA	CBA-CAA-C2A	2.00	119.81	113.85
10	aA	811	CLA	CBC-CAC-C3C	-2.00	106.87	112.43
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

All (738) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	cA	818	CLA	NC
10	cA	818	CLA	ND
10	bB	822	CLA	NC
10	bB	822	CLA	NA
10	bB	806	CLA	NC
10	bB	806	CLA	ND
10	bB	806	CLA	NA
10	aB	809	CLA	ND
10	aB	809	CLA	NA
10	aA	833	CLA	NC
10	aA	833	CLA	ND
10	aA	833	CLA	NA
10	bB	834	CLA	NC
10	bB	834	CLA	ND
10	bB	834	CLA	NA
10	aA	802	CLA	ND
10	aA	802	CLA	NA
10	aB	812	CLA	NC
10	aB	812	CLA	ND
10	aB	812	CLA	NA

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Mol	Chain	Res	Type	Atom
10	bB	837	CLA	NA
10	bB	837	CLA	NC
10	bB	837	CLA	ND
10	aA	825	CLA	NC
10	aA	825	CLA	ND
10	aA	825	CLA	NA
10	bB	821	CLA	NC
10	bB	821	CLA	ND
10	bB	821	CLA	NA
10	bA	821	CLA	NC
10	bA	821	CLA	ND
10	bA	821	CLA	NA
10	cB	822	CLA	NC
10	cB	822	CLA	NA
10	bB	824	CLA	NC
10	bB	824	CLA	ND
10	bB	824	CLA	NA
10	bA	817	CLA	NC
10	bA	817	CLA	NA
10	cA	841	CLA	NC
10	cA	841	CLA	ND
10	cA	841	CLA	NA
10	cB	825	CLA	NA
10	cB	825	CLA	NC
10	cB	825	CLA	ND
10	bA	808	CLA	NC
10	bA	808	CLA	ND
10	bA	808	CLA	NA
10	cA	823	CLA	NC
10	cA	823	CLA	ND
10	cA	823	CLA	NA
10	cB	841	CLA	NC
10	cB	841	CLA	ND
10	cB	841	CLA	NA
10	bB	811	CLA	ND
10	bB	811	CLA	NA
10	cB	819	CLA	NC
10	cB	819	CLA	ND
10	cB	819	CLA	NA
10	aB	829	CLA	NC
10	aB	829	CLA	ND
10	aB	829	CLA	NA

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Mol	Chain	Res	Type	Atom
10	bB	823	CLA	NC
10	bB	823	CLA	ND
10	bB	823	CLA	NA
10	aB	820	CLA	NC
10	aB	820	CLA	ND
10	aB	820	CLA	NA
10	aA	803	CLA	NC
10	aA	803	CLA	ND
10	aA	803	CLA	NA
10	bB	802	CLA	NC
10	bB	802	CLA	ND
10	bB	802	CLA	NA
10	cB	839	CLA	NC
10	cB	839	CLA	ND
10	cB	839	CLA	NA
10	bB	801	CLA	ND
10	aB	816	CLA	NC
10	aB	816	CLA	ND
10	aB	816	CLA	NA
10	cA	828	CLA	NC
10	cA	828	CLA	ND
10	cA	828	CLA	NA
10	aA	807	CLA	NC
10	aA	807	CLA	ND
10	aA	807	CLA	NA
10	aB	832	CLA	NC
10	aB	832	CLA	ND
10	aB	832	CLA	NA
10	cB	809	CLA	ND
10	cB	809	CLA	NA
10	cA	816	CLA	NC
10	cA	816	CLA	NA
10	cA	830	CLA	NC
10	cA	830	CLA	ND
10	cA	830	CLA	NA
10	cB	813	CLA	NC
10	cB	813	CLA	NA
10	bA	805	CLA	NC
10	bA	805	CLA	ND
10	bA	805	CLA	NA
10	aA	812	CLA	NA
10	aA	812	CLA	NC

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Mol	Chain	Res	Type	Atom
10	aA	812	CLA	ND
10	aB	840	CLA	NC
10	aB	840	CLA	ND
10	aB	840	CLA	NA
10	aA	805	CLA	NC
10	aA	805	CLA	ND
10	aA	805	CLA	NA
10	cA	840	CLA	NC
10	cA	840	CLA	ND
10	cA	840	CLA	NA
10	bB	839	CLA	NC
10	bB	839	CLA	ND
10	bB	839	CLA	NA
10	aB	806	CLA	NC
10	aB	806	CLA	ND
10	aB	806	CLA	NA
10	aA	827	CLA	NC
10	aA	827	CLA	ND
10	cB	818	CLA	NC
10	cB	818	CLA	ND
10	cB	818	CLA	NA
10	cB	801	CLA	ND
10	cA	856	CLA	NC
10	cA	856	CLA	ND
10	cA	856	CLA	NA
10	cB	836	CLA	ND
10	cB	836	CLA	NA
10	cA	807	CLA	NC
10	cA	807	CLA	ND
10	cA	807	CLA	NA
10	bA	822	CLA	NC
10	bA	822	CLA	ND
10	bA	823	CLA	NC
10	bA	823	CLA	ND
10	bA	823	CLA	NA
10	cB	821	CLA	NC
10	cB	821	CLA	ND
10	cB	821	CLA	NA
10	cB	833	CLA	NC
10	cB	833	CLA	ND
10	cB	833	CLA	NA
10	aA	834	CLA	NC

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Mol	Chain	Res	Type	Atom
10	aA	834	CLA	ND
10	aA	834	CLA	NA
10	cB	830	CLA	NC
10	cB	830	CLA	ND
10	cB	830	CLA	NA
10	cB	835	CLA	NC
10	cB	835	CLA	ND
10	cB	835	CLA	NA
10	aB	808	CLA	NC
10	aB	808	CLA	ND
10	aB	808	CLA	NA
10	aB	821	CLA	NC
10	aB	821	CLA	ND
10	aB	821	CLA	NA
10	bA	807	CLA	NC
10	bA	807	CLA	ND
10	bA	807	CLA	NA
10	cB	804	CLA	ND
10	aB	836	CLA	ND
10	aB	836	CLA	NA
10	bA	827	CLA	NC
10	bA	827	CLA	ND
10	aB	835	CLA	NC
10	aB	835	CLA	ND
10	aB	835	CLA	NA
10	aA	839	CLA	NC
10	aA	839	CLA	ND
10	cA	827	CLA	NC
10	cA	827	CLA	ND
10	cA	805	CLA	NC
10	cA	805	CLA	ND
10	cA	805	CLA	NA
10	aA	841	CLA	NC
10	aA	841	CLA	ND
10	aA	841	CLA	NA
10	aA	829	CLA	NC
10	aA	829	CLA	ND
10	aA	829	CLA	NA
10	bB	819	CLA	NC
10	bB	819	CLA	ND
10	bB	819	CLA	NA
10	bA	835	CLA	NC

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Mol	Chain	Res	Type	Atom
10	bA	835	CLA	ND
10	bA	835	CLA	NA
10	aB	801	CLA	ND
10	aA	804	CLA	NC
10	aA	804	CLA	ND
10	aA	804	CLA	NA
10	cA	831	CLA	NC
10	cA	831	CLA	ND
10	cA	831	CLA	NA
9	cA	801	CL0	NC
9	cA	801	CL0	ND
9	cA	801	CL0	NA
10	bA	810	CLA	NC
10	bA	810	CLA	ND
10	bA	810	CLA	NA
10	aB	824	CLA	NC
10	aB	824	CLA	ND
10	aB	824	CLA	NA
10	aA	808	CLA	NC
10	aA	808	CLA	ND
10	aA	808	CLA	NA
10	cA	814	CLA	NC
10	cA	814	CLA	ND
10	cA	814	CLA	NA
10	cL	204	CLA	NC
10	cL	204	CLA	ND
10	cL	204	CLA	NA
10	cB	806	CLA	NC
10	cB	806	CLA	ND
10	cB	806	CLA	NA
10	cA	822	CLA	NC
10	cA	822	CLA	ND
10	aA	832	CLA	NC
10	aA	832	CLA	ND
10	aA	832	CLA	NA
10	aA	817	CLA	NC
10	aA	817	CLA	NA
10	cA	835	CLA	NC
10	cA	835	CLA	ND
10	cA	835	CLA	NA
10	bA	837	CLA	NC
10	bA	837	CLA	ND

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Mol	Chain	Res	Type	Atom
10	bA	837	CLA	NA
10	bA	818	CLA	NC
10	bA	818	CLA	ND
10	cA	806	CLA	NC
10	cA	806	CLA	ND
10	cA	806	CLA	NA
10	bB	814	CLA	NA
10	bB	814	CLA	NC
10	bB	814	CLA	ND
10	bB	831	CLA	NC
10	bB	831	CLA	ND
10	bB	831	CLA	NA
10	cB	810	CLA	NC
10	cB	810	CLA	ND
10	bA	842	CLA	NC
10	bA	842	CLA	ND
10	bA	842	CLA	NA
10	aA	820	CLA	NC
10	aA	820	CLA	ND
10	aA	820	CLA	NA
10	aB	818	CLA	NC
10	aB	818	CLA	ND
10	aB	818	CLA	NA
10	aL	202	CLA	NC
10	aL	202	CLA	ND
10	aL	202	CLA	NA
10	cB	834	CLA	NC
10	cB	834	CLA	ND
10	cB	834	CLA	NA
10	bB	807	CLA	NC
10	bB	807	CLA	ND
10	bB	807	CLA	NA
10	bB	808	CLA	NC
10	bB	808	CLA	ND
10	bB	808	CLA	NA
10	cB	823	CLA	NC
10	cB	823	CLA	ND
10	cB	823	CLA	NA
10	cB	820	CLA	NC
10	cB	820	CLA	ND
10	cB	820	CLA	NA
10	bB	828	CLA	ND

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Mol	Chain	Res	Type	Atom
10	cA	813	CLA	NC
10	cA	813	CLA	ND
10	cA	813	CLA	NA
10	bA	820	CLA	NC
10	bA	820	CLA	ND
10	bA	820	CLA	NA
10	bA	811	CLA	NC
10	bA	811	CLA	ND
10	bA	811	CLA	NA
10	cA	824	CLA	NA
10	cA	824	CLA	NC
10	cA	824	CLA	ND
10	cA	836	CLA	NC
10	cA	836	CLA	ND
10	cA	836	CLA	NA
10	bA	804	CLA	NC
10	bA	804	CLA	ND
10	bA	804	CLA	NA
10	aB	823	CLA	NC
10	aB	823	CLA	ND
10	aB	823	CLA	NA
10	cB	807	CLA	NC
10	cB	807	CLA	ND
10	cB	807	CLA	NA
10	aA	814	CLA	NC
10	aA	814	CLA	ND
10	aA	814	CLA	NA
10	aA	806	CLA	NC
10	aA	806	CLA	ND
10	aA	806	CLA	NA
10	bA	824	CLA	NA
10	bA	824	CLA	NC
10	bA	824	CLA	ND
10	aB	803	CLA	NC
10	aB	803	CLA	ND
10	bB	833	CLA	NC
10	bB	833	CLA	ND
10	bB	833	CLA	NA
10	aA	816	CLA	NC
10	aA	816	CLA	NA
10	bA	838	CLA	NC
10	bA	838	CLA	ND

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Mol	Chain	Res	Type	Atom
10	bA	838	CLA	NA
10	bB	820	CLA	NC
10	bB	820	CLA	ND
10	bB	820	CLA	NA
10	aA	811	CLA	NC
10	aA	811	CLA	ND
10	aA	811	CLA	NA
10	aB	827	CLA	NC
10	aB	827	CLA	ND
10	aB	827	CLA	NA
10	cA	825	CLA	NC
10	cA	825	CLA	ND
10	cA	825	CLA	NA
10	aB	810	CLA	NC
10	aB	810	CLA	ND
10	bL	204	CLA	NC
10	bL	204	CLA	ND
10	bL	204	CLA	NA
10	cA	834	CLA	NC
10	cA	834	CLA	ND
10	cA	834	CLA	NA
10	cA	833	CLA	NC
10	cA	833	CLA	ND
10	cA	833	CLA	NA
10	bB	840	CLA	NC
10	bB	840	CLA	ND
10	bB	840	CLA	NA
10	aA	813	CLA	NC
10	aA	813	CLA	ND
10	aA	813	CLA	NA
10	bA	806	CLA	NC
10	bA	806	CLA	ND
10	bA	806	CLA	NA
10	bB	836	CLA	ND
10	bB	836	CLA	NA
10	aL	203	CLA	NC
10	aL	203	CLA	NA
10	bB	825	CLA	NA
10	bB	825	CLA	NC
10	bB	825	CLA	ND
10	cA	804	CLA	NC
10	cA	804	CLA	ND

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Mol	Chain	Res	Type	Atom
10	cA	804	CLA	NA
10	aA	854	CLA	NC
10	aA	854	CLA	NA
10	aB	841	CLA	NC
10	aB	841	CLA	ND
10	aB	841	CLA	NA
10	bA	803	CLA	NC
10	bA	803	CLA	ND
10	bA	803	CLA	NA
10	cB	808	CLA	NC
10	cB	808	CLA	ND
10	cB	808	CLA	NA
10	aB	811	CLA	ND
10	aB	811	CLA	NA
10	bA	814	CLA	NC
10	bA	814	CLA	ND
10	bA	814	CLA	NA
10	bA	813	CLA	NC
10	bA	813	CLA	ND
10	bA	813	CLA	NA
10	aB	819	CLA	NC
10	aB	819	CLA	ND
10	aB	819	CLA	NA
10	aA	828	CLA	NC
10	aA	828	CLA	ND
10	aA	828	CLA	NA
10	bB	809	CLA	ND
10	bB	809	CLA	NA
10	cB	812	CLA	NC
10	cB	812	CLA	ND
10	cB	812	CLA	NA
10	cA	812	CLA	NA
10	cA	812	CLA	NC
10	cA	812	CLA	ND
10	cB	837	CLA	NA
10	cB	837	CLA	NC
10	cB	837	CLA	ND
10	cA	811	CLA	NC
10	cA	811	CLA	ND
10	cA	811	CLA	NA
10	cB	827	CLA	NC
10	cB	827	CLA	ND

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Mol	Chain	Res	Type	Atom
10	cB	827	CLA	NA
10	cA	842	CLA	NC
10	cA	842	CLA	ND
10	cA	842	CLA	NA
10	bB	827	CLA	NC
10	bB	827	CLA	ND
10	bB	827	CLA	NA
10	aA	843	CLA	NC
10	aA	843	CLA	ND
10	aA	843	CLA	NA
10	bB	829	CLA	NC
10	bB	829	CLA	ND
10	bB	829	CLA	NA
10	aA	821	CLA	NC
10	aA	821	CLA	ND
10	aA	821	CLA	NA
10	aB	813	CLA	NC
10	aB	813	CLA	NA
10	aA	823	CLA	NC
10	aA	823	CLA	ND
10	aA	823	CLA	NA
10	cA	815	CLA	NC
10	cA	815	CLA	ND
10	cA	815	CLA	NA
10	aA	840	CLA	NC
10	aA	840	CLA	ND
10	aA	840	CLA	NA
10	cB	832	CLA	NC
10	cB	832	CLA	ND
10	cB	832	CLA	NA
10	cA	819	CLA	NC
10	cA	819	CLA	ND
10	cA	819	CLA	NA
10	cA	837	CLA	NC
10	cA	837	CLA	ND
10	cA	837	CLA	NA
10	aB	834	CLA	NC
10	aB	834	CLA	ND
10	aB	834	CLA	NA
10	cB	838	CLA	NC
10	cB	838	CLA	ND
10	cB	838	CLA	NA

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Mol	Chain	Res	Type	Atom
10	aB	826	CLA	NC
10	aB	826	CLA	ND
10	aB	826	CLA	NA
10	bA	819	CLA	NC
10	bA	819	CLA	ND
10	bA	819	CLA	NA
10	bA	830	CLA	NC
10	bA	830	CLA	ND
10	bA	830	CLA	NA
10	aB	825	CLA	NA
10	aB	825	CLA	NC
10	aB	825	CLA	ND
10	cB	826	CLA	NC
10	cB	826	CLA	ND
10	cB	826	CLA	NA
10	cB	829	CLA	NC
10	cB	829	CLA	ND
10	cB	829	CLA	NA
10	bA	828	CLA	NC
10	bA	828	CLA	ND
10	bA	828	CLA	NA
10	bL	202	CLA	NC
10	bL	202	CLA	ND
10	bL	202	CLA	NA
10	cB	814	CLA	NA
10	cB	814	CLA	NC
10	cB	814	CLA	ND
10	bB	816	CLA	NC
10	bB	816	CLA	ND
10	bB	816	CLA	NA
10	aA	810	CLA	NC
10	aA	810	CLA	ND
10	aA	810	CLA	NA
10	cA	854	CLA	NC
10	cA	854	CLA	NA
10	bA	833	CLA	NC
10	bA	833	CLA	ND
10	bA	833	CLA	NA
10	bB	826	CLA	NC
10	bB	826	CLA	ND
10	bB	826	CLA	NA
10	bB	805	CLA	ND

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Mol	Chain	Res	Type	Atom
10	bB	805	CLA	NA
10	aA	819	CLA	NC
10	aA	819	CLA	ND
10	aA	819	CLA	NA
10	bA	856	CLA	NC
10	bA	856	CLA	ND
10	bA	856	CLA	NA
10	bA	832	CLA	NC
10	bA	832	CLA	ND
10	bA	832	CLA	NA
10	aB	839	CLA	NC
10	aB	839	CLA	ND
10	aB	839	CLA	NA
10	aA	838	CLA	NC
10	aA	838	CLA	ND
10	aA	838	CLA	NA
10	cL	205	CLA	NC
10	cL	205	CLA	NA
10	aA	818	CLA	NC
10	aA	818	CLA	ND
10	cA	808	CLA	NC
10	cA	808	CLA	ND
10	cA	808	CLA	NA
10	bB	818	CLA	NC
10	bB	818	CLA	ND
10	bB	818	CLA	NA
10	aA	815	CLA	NC
10	aA	815	CLA	ND
10	aA	815	CLA	NA
10	cB	811	CLA	ND
10	cB	811	CLA	NA
10	aL	205	CLA	NC
10	aL	205	CLA	NA
10	cB	817	CLA	NC
10	cB	817	CLA	ND
10	cB	817	CLA	NA
10	cB	828	CLA	ND
10	aA	837	CLA	NC
10	aA	837	CLA	ND
10	aA	837	CLA	NA
10	aB	805	CLA	ND
10	aB	805	CLA	NA

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Mol	Chain	Res	Type	Atom
10	aA	822	CLA	NC
10	aA	822	CLA	ND
10	aA	824	CLA	NA
10	aA	824	CLA	NC
10	aA	824	CLA	ND
10	aB	804	CLA	ND
10	bA	831	CLA	NC
10	bA	831	CLA	ND
10	bA	831	CLA	NA
9	bA	801	CL0	NC
9	bA	801	CL0	ND
9	bA	801	CL0	NA
10	aA	809	CLA	NC
10	aA	809	CLA	ND
10	aA	809	CLA	NA
10	bA	854	CLA	NC
10	bA	854	CLA	NA
10	cA	829	CLA	NC
10	cA	829	CLA	ND
10	cA	829	CLA	NA
10	cB	803	CLA	NC
10	cB	803	CLA	ND
10	bA	841	CLA	NC
10	bA	841	CLA	ND
10	bA	841	CLA	NA
10	bB	841	CLA	NC
10	bB	841	CLA	ND
10	bB	841	CLA	NA
10	aA	856	CLA	NC
10	aA	856	CLA	ND
10	aA	856	CLA	NA
10	aA	826	CLA	NC
10	aA	826	CLA	ND
10	aA	826	CLA	NA
10	bA	829	CLA	NC
10	bA	829	CLA	ND
10	bA	829	CLA	NA
10	cA	821	CLA	NC
10	cA	821	CLA	ND
10	cA	821	CLA	NA
10	bA	840	CLA	NC
10	bA	840	CLA	ND

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Mol	Chain	Res	Type	Atom
10	bA	840	CLA	NA
10	cB	815	CLA	NC
10	cB	815	CLA	ND
10	cB	815	CLA	NA
10	cA	838	CLA	NC
10	cA	838	CLA	ND
10	cA	838	CLA	NA
10	bB	817	CLA	NC
10	bB	817	CLA	ND
10	bB	817	CLA	NA
10	aA	836	CLA	NC
10	aA	836	CLA	ND
10	aA	836	CLA	NA
10	aB	831	CLA	NC
10	aB	831	CLA	ND
10	aB	831	CLA	NA
10	bL	203	CLA	NC
10	bL	203	CLA	NA
10	bB	832	CLA	NC
10	bB	832	CLA	ND
10	bB	832	CLA	NA
10	aB	807	CLA	NC
10	aB	807	CLA	ND
10	aB	807	CLA	NA
10	bL	205	CLA	NC
10	bL	205	CLA	NA
10	bB	803	CLA	NC
10	bB	803	CLA	ND
10	cB	805	CLA	ND
10	cB	805	CLA	NA
10	bA	836	CLA	NC
10	bA	836	CLA	ND
10	bA	836	CLA	NA
10	bA	816	CLA	NC
10	bA	816	CLA	NA
10	cL	202	CLA	NC
10	cL	202	CLA	ND
10	cL	202	CLA	NA
10	bB	804	CLA	ND
10	bB	813	CLA	NC
10	bB	813	CLA	NA
10	bA	825	CLA	NC

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Mol	Chain	Res	Type	Atom
10	bA	825	CLA	ND
10	bA	825	CLA	NA
10	aA	830	CLA	NC
10	aA	830	CLA	ND
10	aA	830	CLA	NA
10	cA	802	CLA	ND
10	cA	802	CLA	NA
10	aB	815	CLA	NC
10	aB	815	CLA	ND
10	aB	815	CLA	NA
10	cA	832	CLA	NC
10	cA	832	CLA	ND
10	cA	832	CLA	NA
10	bA	843	CLA	NC
10	bA	843	CLA	ND
10	bA	843	CLA	NA
10	cA	817	CLA	NC
10	cA	817	CLA	NA
10	aL	204	CLA	NC
10	aL	204	CLA	ND
10	aL	204	CLA	NA
10	bB	830	CLA	NC
10	bB	830	CLA	ND
10	bB	830	CLA	NA
10	cB	802	CLA	NC
10	cB	802	CLA	ND
10	cB	802	CLA	NA
10	aB	802	CLA	NC
10	aB	802	CLA	ND
10	aB	802	CLA	NA
10	bA	802	CLA	ND
10	bA	802	CLA	NA
10	bA	839	CLA	NC
10	bA	839	CLA	ND
10	cA	839	CLA	NC
10	cA	839	CLA	ND
10	bB	838	CLA	NC
10	bB	838	CLA	ND
10	bB	838	CLA	NA
10	bA	809	CLA	NC
10	bA	809	CLA	ND
10	bA	809	CLA	NA

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Mol	Chain	Res	Type	Atom
10	aB	817	CLA	NC
10	aB	817	CLA	ND
10	aB	817	CLA	NA
10	bB	835	CLA	NC
10	bB	835	CLA	ND
10	bB	835	CLA	NA
10	cA	803	CLA	NC
10	cA	803	CLA	ND
10	cA	803	CLA	NA
10	cA	809	CLA	NC
10	cA	809	CLA	ND
10	cA	809	CLA	NA
10	cA	820	CLA	NC
10	cA	820	CLA	ND
10	cA	820	CLA	NA
10	bB	810	CLA	NC
10	bB	810	CLA	ND
10	aA	842	CLA	NC
10	aA	842	CLA	ND
10	aA	842	CLA	NA
10	cB	816	CLA	NC
10	cB	816	CLA	ND
10	cB	816	CLA	NA
10	cL	203	CLA	NC
10	cL	203	CLA	NA
10	aB	838	CLA	NC
10	aB	838	CLA	ND
10	aB	838	CLA	NA
10	aB	822	CLA	NC
10	aB	822	CLA	NA
10	cB	824	CLA	NC
10	cB	824	CLA	ND
10	cB	824	CLA	NA
10	aA	835	CLA	NC
10	aA	835	CLA	ND
10	aA	835	CLA	NA
10	cB	831	CLA	NC
10	cB	831	CLA	ND
10	cB	831	CLA	NA
10	aB	837	CLA	NA
10	aB	837	CLA	NC
10	aB	837	CLA	ND

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Mol	Chain	Res	Type	Atom
9	aA	801	CL0	NC
9	aA	801	CL0	ND
9	aA	801	CL0	NA
10	bA	826	CLA	NC
10	bA	826	CLA	ND
10	bA	826	CLA	NA
10	aB	830	CLA	NC
10	aB	830	CLA	ND
10	aB	830	CLA	NA
10	aA	831	CLA	NC
10	aA	831	CLA	ND
10	aA	831	CLA	NA
10	cB	840	CLA	NC
10	cB	840	CLA	ND
10	cB	840	CLA	NA
10	aB	814	CLA	NA
10	aB	814	CLA	NC
10	aB	814	CLA	ND
10	bA	812	CLA	NA
10	bA	812	CLA	NC
10	bA	812	CLA	ND
10	bB	812	CLA	NC
10	bB	812	CLA	ND
10	bB	812	CLA	NA
10	bA	834	CLA	NC
10	bA	834	CLA	ND
10	bA	834	CLA	NA
10	aB	828	CLA	ND
10	bB	815	CLA	NC
10	bB	815	CLA	ND
10	bB	815	CLA	NA
10	cA	826	CLA	NC
10	cA	826	CLA	ND
10	cA	826	CLA	NA
10	bA	815	CLA	NC
10	bA	815	CLA	ND
10	bA	815	CLA	NA
10	cA	810	CLA	NC
10	cA	810	CLA	ND
10	cA	810	CLA	NA
10	aB	833	CLA	NC
10	aB	833	CLA	ND

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Mol	Chain	Res	Type	Atom
10	aB	833	CLA	NA
10	cA	843	CLA	NC
10	cA	843	CLA	ND
10	cA	843	CLA	NA

All (3024) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	cA	818	CLA	C1A-C2A-CAA-CBA
10	cA	818	CLA	CHA-CBD-CGD-O1D
10	cA	818	CLA	CHA-CBD-CGD-O2D
15	cA	853	LMT	C2'-C1'-O1'-C1
15	cA	853	LMT	O5'-C1'-O1'-C1
10	bB	822	CLA	C2A-CAA-CBA-CGA
10	bB	822	CLA	CHA-CBD-CGD-O1D
10	bB	822	CLA	CHA-CBD-CGD-O2D
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
10	bB	806	CLA	C1A-C2A-CAA-CBA
10	bB	806	CLA	C3A-C2A-CAA-CBA
13	cB	846	BCR	C1-C6-C7-C8
13	cB	846	BCR	C7-C8-C9-C34
13	cB	846	BCR	C10-C11-C12-C13
10	aA	825	CLA	C2-C3-C5-C6
10	aA	825	CLA	C4-C3-C5-C6
10	bA	821	CLA	CHA-CBD-CGD-O1D
10	bA	821	CLA	CHA-CBD-CGD-O2D
10	cB	822	CLA	C2A-CAA-CBA-CGA
10	cB	822	CLA	CHA-CBD-CGD-O1D
10	cB	822	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	cA	841	CLA	C2-C3-C5-C6
10	cB	825	CLA	C1A-C2A-CAA-CBA
10	cB	825	CLA	C3A-C2A-CAA-CBA
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

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Mol	Chain	Res	Type	Atoms
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
10	bB	811	CLA	C3A-C2A-CAA-CBA
10	bB	811	CLA	C2-C3-C5-C6
10	bB	811	CLA	C4-C3-C5-C6
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
10	cB	819	CLA	C1A-C2A-CAA-CBA
10	cB	819	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
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	cA	851	BCR	C7-C8-C9-C34
13	cA	851	BCR	C18-C19-C20-C21
13	cA	851	BCR	C37-C22-C23-C24
10	aA	807	CLA	C3A-C2A-CAA-CBA
10	aA	807	CLA	CHA-CBD-CGD-O2D
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
10	cA	816	CLA	CHA-CBD-CGD-O1D
10	cA	816	CLA	CHA-CBD-CGD-O2D
10	cA	830	CLA	C2A-CAA-CBA-CGA
10	bA	805	CLA	C1A-C2A-CAA-CBA
13	cL	207	BCR	C23-C24-C25-C30
10	aA	805	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
13	aB	844	BCR	C1-C6-C7-C8
13	aB	844	BCR	C16-C17-C18-C36
13	aB	844	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
10	aB	806	CLA	C1A-C2A-CAA-CBA
10	aB	806	CLA	C3A-C2A-CAA-CBA
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
10	aA	827	CLA	C1A-C2A-CAA-CBA
10	cA	856	CLA	CBD-CGD-O2D-CED
13	aA	851	BCR	C7-C8-C9-C34
13	aA	851	BCR	C18-C19-C20-C21
13	aA	851	BCR	C37-C22-C23-C24
10	cA	807	CLA	C3A-C2A-CAA-CBA
10	cA	807	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	cB	833	CLA	C2-C3-C5-C6
10	cB	833	CLA	C4-C3-C5-C6
13	bB	849	BCR	C12-C13-C14-C15
13	bB	849	BCR	C35-C13-C14-C15
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	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
15	bA	853	LMT	C2'-C1'-O1'-C1
15	bA	853	LMT	O5'-C1'-O1'-C1
10	cB	835	CLA	CBD-CGD-O2D-CED
10	bA	807	CLA	C3A-C2A-CAA-CBA
10	bA	807	CLA	CHA-CBD-CGD-O2D
10	cB	804	CLA	C1A-C2A-CAA-CBA
10	cB	804	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
10	bA	827	CLA	C1A-C2A-CAA-CBA
10	aB	835	CLA	CBD-CGD-O2D-CED
10	cA	827	CLA	C1A-C2A-CAA-CBA
10	cA	805	CLA	C1A-C2A-CAA-CBA
10	aA	841	CLA	C2-C3-C5-C6
10	aA	829	CLA	CHA-CBD-CGD-O1D
10	aA	829	CLA	CHA-CBD-CGD-O2D
10	bB	819	CLA	C1A-C2A-CAA-CBA
10	bB	819	CLA	C3A-C2A-CAA-CBA
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	cA	831	CLA	C2-C3-C5-C6
10	cA	831	CLA	C4-C3-C5-C6
10	bA	810	CLA	C1A-C2A-CAA-CBA
10	bA	810	CLA	C3A-C2A-CAA-CBA
10	bA	810	CLA	CHA-CBD-CGD-O1D
14	aA	855	LHG	C3-O3-P-O5
10	cL	204	CLA	C1A-C2A-CAA-CBA
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
10	cB	806	CLA	C1A-C2A-CAA-CBA
10	cB	806	CLA	C3A-C2A-CAA-CBA
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	aA	817	CLA	C3A-C2A-CAA-CBA
10	aA	817	CLA	C2-C3-C5-C6
10	aA	817	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	bA	818	CLA	C1A-C2A-CAA-CBA
10	bA	818	CLA	CHA-CBD-CGD-O1D
10	bA	818	CLA	CHA-CBD-CGD-O2D
10	cA	806	CLA	C2-C3-C5-C6
10	cA	806	CLA	C4-C3-C5-C6
10	bB	814	CLA	C1A-C2A-CAA-CBA
10	bB	814	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	bA	851	BCR	C7-C8-C9-C34
13	bA	851	BCR	C18-C19-C20-C21
13	bA	851	BCR	C37-C22-C23-C24
10	bB	831	CLA	C2A-CAA-CBA-CGA
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	846	BCR	C1-C6-C7-C8
13	bB	846	BCR	C7-C8-C9-C34
13	bB	846	BCR	C10-C11-C12-C13
10	bB	807	CLA	C1A-C2A-CAA-CBA
10	bB	807	CLA	C3A-C2A-CAA-CBA
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
10	bB	828	CLA	C1A-C2A-CAA-CBA
10	bB	828	CLA	C3A-C2A-CAA-CBA
13	bA	847	BCR	C20-C21-C22-C37
13	bA	847	BCR	C21-C22-C23-C24
13	bA	847	BCR	C37-C22-C23-C24
10	cA	836	CLA	C2-C3-C5-C6
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
10	cB	807	CLA	C1A-C2A-CAA-CBA
10	cB	807	CLA	C3A-C2A-CAA-CBA
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
10	aA	806	CLA	C2-C3-C5-C6
10	aA	806	CLA	C4-C3-C5-C6
10	aB	803	CLA	CHA-CBD-CGD-O1D
10	aB	803	CLA	CHA-CBD-CGD-O2D
10	bB	833	CLA	C2-C3-C5-C6
10	bB	833	CLA	C4-C3-C5-C6
13	cA	850	BCR	C1-C6-C7-C8
13	cA	850	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
13	cA	850	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
10	aA	816	CLA	CHA-CBD-CGD-O1D
10	aA	816	CLA	CHA-CBD-CGD-O2D
10	aA	816	CLA	C4-C3-C5-C6
13	bL	207	BCR	C23-C24-C25-C30
10	bA	838	CLA	C1A-C2A-CAA-CBA
13	bL	206	BCR	C7-C8-C9-C10
13	bL	206	BCR	C7-C8-C9-C34
13	bL	206	BCR	C23-C24-C25-C26
10	cA	825	CLA	C2-C3-C5-C6
10	cA	825	CLA	C4-C3-C5-C6
14	cA	852	LHG	C1-C2-C3-O3
14	cA	852	LHG	C3-O3-P-O4
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
10	bL	204	CLA	C1A-C2A-CAA-CBA
10	bA	806	CLA	C2-C3-C5-C6
10	bA	806	CLA	C4-C3-C5-C6
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	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
10	bB	825	CLA	C1A-C2A-CAA-CBA
10	bB	825	CLA	C3A-C2A-CAA-CBA
10	aA	854	CLA	C3-C5-C6-C7
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	aL	206	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
13	aL	206	BCR	C7-C8-C9-C34
13	aL	206	BCR	C23-C24-C25-C26
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	819	CLA	C1A-C2A-CAA-CBA
10	aB	819	CLA	C3A-C2A-CAA-CBA
14	bA	855	LHG	C3-O3-P-O5
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	aA	821	CLA	CHA-CBD-CGD-O1D
10	aA	821	CLA	CHA-CBD-CGD-O2D
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	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
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	aM	101	BCR	C7-C8-C9-C34
13	aM	101	BCR	C20-C21-C22-C37
13	aM	101	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
10	aB	826	CLA	CHA-CBD-CGD-O1D
10	aB	826	CLA	CHA-CBD-CGD-O2D
13	aB	846	BCR	C1-C6-C7-C8
13	aB	846	BCR	C7-C8-C9-C34
13	aB	846	BCR	C10-C11-C12-C13
10	bA	830	CLA	C2A-CAA-CBA-CGA
10	aB	825	CLA	C1A-C2A-CAA-CBA
10	aB	825	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
10	cB	826	CLA	CHA-CBD-CGD-O1D
10	cB	826	CLA	CHA-CBD-CGD-O2D
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
13	cL	206	BCR	C7-C8-C9-C10
13	cL	206	BCR	C7-C8-C9-C34
13	cL	206	BCR	C23-C24-C25-C26
10	cB	814	CLA	C1A-C2A-CAA-CBA
10	cB	814	CLA	C3A-C2A-CAA-CBA
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	850	BCR	C1-C6-C7-C8
13	aA	850	BCR	C21-C22-C23-C24
13	aA	850	BCR	C37-C22-C23-C24
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	cA	854	CLA	C3-C5-C6-C7
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	bM	101	BCR	C7-C8-C9-C34
13	bM	101	BCR	C20-C21-C22-C37
13	bM	101	BCR	C37-C22-C23-C24
10	bB	826	CLA	CHA-CBD-CGD-O1D
10	bB	826	CLA	CHA-CBD-CGD-O2D
14	aA	852	LHG	C1-C2-C3-O3
14	aA	852	LHG	C3-O3-P-O4
10	bA	856	CLA	CBD-CGD-O2D-CED
10	aA	838	CLA	C1A-C2A-CAA-CBA
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	cB	811	CLA	C3A-C2A-CAA-CBA
10	cB	811	CLA	C2-C3-C5-C6
10	cB	811	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
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
10	cB	828	CLA	C1A-C2A-CAA-CBA
10	cB	828	CLA	C3A-C2A-CAA-CBA
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
15	aA	853	LMT	C2'-C1'-O1'-C1
15	aA	853	LMT	O5'-C1'-O1'-C1
10	aB	804	CLA	C1A-C2A-CAA-CBA
10	aB	804	CLA	C3A-C2A-CAA-CBA
10	bA	831	CLA	C2-C3-C5-C6
10	bA	831	CLA	C4-C3-C5-C6
10	aA	809	CLA	CHA-CBD-CGD-O1D
10	aA	809	CLA	CHA-CBD-CGD-O2D
10	bA	854	CLA	C3-C5-C6-C7
14	cA	855	LHG	C3-O3-P-O5
10	cA	829	CLA	CHA-CBD-CGD-O1D
10	cA	829	CLA	CHA-CBD-CGD-O2D
10	cB	803	CLA	CHA-CBD-CGD-O1D
10	cB	803	CLA	CHA-CBD-CGD-O2D
10	bA	841	CLA	C2-C3-C5-C6
10	aA	856	CLA	CBD-CGD-O2D-CED
10	bA	829	CLA	CHA-CBD-CGD-O1D
10	bA	829	CLA	CHA-CBD-CGD-O2D
10	cA	821	CLA	CHA-CBD-CGD-O1D
10	cA	821	CLA	CHA-CBD-CGD-O2D
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	cA	838	CLA	C1A-C2A-CAA-CBA
10	aA	836	CLA	C2-C3-C5-C6
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

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Mol	Chain	Res	Type	Atoms
10	aB	831	CLA	C2A-CAA-CBA-CGA
10	aB	807	CLA	C1A-C2A-CAA-CBA
10	aB	807	CLA	C3A-C2A-CAA-CBA
10	bB	803	CLA	CHA-CBD-CGD-O1D
10	bB	803	CLA	CHA-CBD-CGD-O2D
10	bA	836	CLA	C2-C3-C5-C6
10	bA	816	CLA	CHA-CBD-CGD-O1D
10	bA	816	CLA	CHA-CBD-CGD-O2D
10	bB	804	CLA	C1A-C2A-CAA-CBA
10	bB	804	CLA	C3A-C2A-CAA-CBA
10	bA	825	CLA	C2-C3-C5-C6
10	bA	825	CLA	C4-C3-C5-C6
13	cA	847	BCR	C20-C21-C22-C37
13	cA	847	BCR	C21-C22-C23-C24
13	cA	847	BCR	C37-C22-C23-C24
10	aA	830	CLA	C2A-CAA-CBA-CGA
10	cA	817	CLA	C3A-C2A-CAA-CBA
10	cA	817	CLA	C2-C3-C5-C6
10	cA	817	CLA	C4-C3-C5-C6
13	bA	850	BCR	C1-C6-C7-C8
13	bA	850	BCR	C21-C22-C23-C24
13	bA	850	BCR	C37-C22-C23-C24
10	aL	204	CLA	C1A-C2A-CAA-CBA
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
10	bA	809	CLA	CHA-CBD-CGD-O1D
10	bA	809	CLA	CHA-CBD-CGD-O2D
10	bB	835	CLA	CBD-CGD-O2D-CED
10	cA	809	CLA	CHA-CBD-CGD-O1D
10	cA	809	CLA	CHA-CBD-CGD-O2D
10	aB	822	CLA	C2A-CAA-CBA-CGA
10	aB	822	CLA	CHA-CBD-CGD-O1D
10	aB	822	CLA	CHA-CBD-CGD-O2D
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	cB	831	CLA	C2A-CAA-CBA-CGA
13	bB	843	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
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	aA	849	BCR	C18-C19-C20-C21
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	cM	101	BCR	C7-C8-C9-C34
13	cM	101	BCR	C20-C21-C22-C37
13	cM	101	BCR	C37-C22-C23-C24
13	aL	207	BCR	C23-C24-C25-C30
10	aA	831	CLA	C2-C3-C5-C6
10	aA	831	CLA	C4-C3-C5-C6
10	aB	814	CLA	C1A-C2A-CAA-CBA
10	aB	814	CLA	C3A-C2A-CAA-CBA
10	aB	828	CLA	C1A-C2A-CAA-CBA
10	aB	828	CLA	C3A-C2A-CAA-CBA
10	cA	810	CLA	C1A-C2A-CAA-CBA
10	cA	810	CLA	C3A-C2A-CAA-CBA
10	cA	810	CLA	CHA-CBD-CGD-O1D
14	bA	852	LHG	C1-C2-C3-O3
14	bA	852	LHG	C3-O3-P-O4
10	aB	833	CLA	C2-C3-C5-C6
10	aB	833	CLA	C4-C3-C5-C6
10	cB	835	CLA	O1D-CGD-O2D-CED
10	aB	835	CLA	O1D-CGD-O2D-CED
10	bB	835	CLA	O1D-CGD-O2D-CED
10	aA	833	CLA	CBD-CGD-O2D-CED
10	bB	824	CLA	CBD-CGD-O2D-CED
10	aA	839	CLA	CBD-CGD-O2D-CED
10	aB	824	CLA	CBD-CGD-O2D-CED
10	aA	820	CLA	CBD-CGD-O2D-CED
10	bA	820	CLA	CBD-CGD-O2D-CED
10	bA	838	CLA	CBD-CGD-O2D-CED
10	cA	833	CLA	CBD-CGD-O2D-CED
10	bA	833	CLA	CBD-CGD-O2D-CED
10	aA	838	CLA	CBD-CGD-O2D-CED
10	cA	838	CLA	CBD-CGD-O2D-CED
10	bA	839	CLA	CBD-CGD-O2D-CED
10	cA	839	CLA	CBD-CGD-O2D-CED
10	cA	820	CLA	CBD-CGD-O2D-CED
10	cB	824	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
10	bA	822	CLA	O1A-CGA-O2A-C1
10	cA	822	CLA	O1A-CGA-O2A-C1
14	cA	852	LHG	O10-C23-O8-C6
14	aA	852	LHG	O10-C23-O8-C6
10	aA	822	CLA	O1A-CGA-O2A-C1
14	bA	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	cB	841	CLA	CBD-CGD-O2D-CED
10	aA	807	CLA	CBD-CGD-O2D-CED
10	cA	807	CLA	CBD-CGD-O2D-CED
10	bA	807	CLA	CBD-CGD-O2D-CED
10	bB	828	CLA	CBD-CGD-O2D-CED
10	aB	841	CLA	CBD-CGD-O2D-CED
10	cB	817	CLA	CBD-CGD-O2D-CED
10	cB	828	CLA	CBD-CGD-O2D-CED
10	bB	841	CLA	CBD-CGD-O2D-CED
10	bB	817	CLA	CBD-CGD-O2D-CED
10	aB	817	CLA	CBD-CGD-O2D-CED
10	aB	828	CLA	CBD-CGD-O2D-CED
10	bB	806	CLA	O1A-CGA-O2A-C1
10	aB	806	CLA	O1A-CGA-O2A-C1
14	aA	855	LHG	O10-C23-O8-C6
10	cB	806	CLA	O1A-CGA-O2A-C1
10	aA	820	CLA	O1A-CGA-O2A-C1
10	bA	820	CLA	O1A-CGA-O2A-C1
14	bA	855	LHG	O10-C23-O8-C6
10	aB	826	CLA	O1A-CGA-O2A-C1
10	cB	826	CLA	O1A-CGA-O2A-C1
10	bB	826	CLA	O1A-CGA-O2A-C1
14	cA	855	LHG	O10-C23-O8-C6
10	cA	820	CLA	O1A-CGA-O2A-C1
10	cA	816	CLA	CBD-CGD-O2D-CED
10	aA	816	CLA	CBD-CGD-O2D-CED
10	bA	816	CLA	CBD-CGD-O2D-CED
10	cA	856	CLA	O1D-CGD-O2D-CED
10	bA	856	CLA	O1D-CGD-O2D-CED
10	aA	856	CLA	O1D-CGD-O2D-CED
10	bA	817	CLA	C3-C5-C6-C7
10	cB	819	CLA	C3-C5-C6-C7
10	cB	804	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
10	aA	839	CLA	C3-C5-C6-C7
10	bB	819	CLA	C3-C5-C6-C7
10	bA	835	CLA	C3-C5-C6-C7
10	cA	831	CLA	C3-C5-C6-C7
10	aA	817	CLA	C3-C5-C6-C7
10	cA	835	CLA	C3-C5-C6-C7
10	bA	837	CLA	C3-C5-C6-C7
10	bA	811	CLA	C3-C5-C6-C7
10	aA	811	CLA	C3-C5-C6-C7
10	aB	819	CLA	C3-C5-C6-C7
10	cA	811	CLA	C3-C5-C6-C7
10	cA	837	CLA	C3-C5-C6-C7
10	aA	837	CLA	C3-C5-C6-C7
10	aB	804	CLA	C3-C5-C6-C7
10	bA	831	CLA	C3-C5-C6-C7
10	bB	804	CLA	C3-C5-C6-C7
10	cA	817	CLA	C3-C5-C6-C7
10	bA	839	CLA	C3-C5-C6-C7
10	cA	839	CLA	C3-C5-C6-C7
10	aA	835	CLA	C3-C5-C6-C7
10	aA	831	CLA	C3-C5-C6-C7
10	bB	806	CLA	CBA-CGA-O2A-C1
10	aB	806	CLA	CBA-CGA-O2A-C1
10	bA	822	CLA	CBA-CGA-O2A-C1
10	cB	806	CLA	CBA-CGA-O2A-C1
10	cA	822	CLA	CBA-CGA-O2A-C1
10	aA	822	CLA	CBA-CGA-O2A-C1
10	cA	818	CLA	CBD-CGD-O2D-CED
10	bA	822	CLA	CBD-CGD-O2D-CED
10	cA	822	CLA	CBD-CGD-O2D-CED
10	bA	818	CLA	CBD-CGD-O2D-CED
10	bB	831	CLA	CBD-CGD-O2D-CED
10	aA	818	CLA	CBD-CGD-O2D-CED
10	aA	822	CLA	CBD-CGD-O2D-CED
10	aB	831	CLA	CBD-CGD-O2D-CED
10	cB	831	CLA	CBD-CGD-O2D-CED
10	bB	811	CLA	C2A-CAA-CBA-CGA
10	bB	823	CLA	C2A-CAA-CBA-CGA
10	cA	828	CLA	C2A-CAA-CBA-CGA
10	aB	840	CLA	C2A-CAA-CBA-CGA
10	cB	823	CLA	C2A-CAA-CBA-CGA
10	bA	811	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
10	aB	823	CLA	C2A-CAA-CBA-CGA
10	aA	811	CLA	C2A-CAA-CBA-CGA
10	bB	840	CLA	C2A-CAA-CBA-CGA
10	aB	811	CLA	C2A-CAA-CBA-CGA
10	aA	828	CLA	C2A-CAA-CBA-CGA
10	cA	811	CLA	C2A-CAA-CBA-CGA
10	bA	828	CLA	C2A-CAA-CBA-CGA
10	cB	811	CLA	C2A-CAA-CBA-CGA
10	cB	840	CLA	C2A-CAA-CBA-CGA
10	cB	833	CLA	CBD-CGD-O2D-CED
10	bB	833	CLA	CBD-CGD-O2D-CED
10	aB	833	CLA	CBD-CGD-O2D-CED
10	bB	806	CLA	C4-C3-C5-C6
10	cA	841	CLA	C4-C3-C5-C6
10	bB	823	CLA	C4-C3-C5-C6
10	cA	816	CLA	C4-C3-C5-C6
10	aB	806	CLA	C4-C3-C5-C6
10	aA	841	CLA	C4-C3-C5-C6
10	cB	806	CLA	C4-C3-C5-C6
10	cB	823	CLA	C4-C3-C5-C6
10	aB	823	CLA	C4-C3-C5-C6
10	bA	841	CLA	C4-C3-C5-C6
10	bA	816	CLA	C4-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	aB	823	CLA	C2-C3-C5-C6
10	aA	816	CLA	C2-C3-C5-C6
10	bA	816	CLA	C2-C3-C5-C6
10	bA	805	CLA	C3-C5-C6-C7
10	aA	805	CLA	C3-C5-C6-C7
11	cA	844	PQN	C13-C15-C16-C17
10	cA	805	CLA	C3-C5-C6-C7
11	aA	844	PQN	C13-C15-C16-C17
10	cB	817	CLA	C3-C5-C6-C7
10	bB	817	CLA	C3-C5-C6-C7
11	bA	844	PQN	C13-C15-C16-C17
10	aB	817	CLA	C3-C5-C6-C7
10	cA	823	CLA	CBA-CGA-O2A-C1
10	cA	830	CLA	CBA-CGA-O2A-C1
10	bA	823	CLA	CBA-CGA-O2A-C1
10	cB	830	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	cB	804	CLA	CBA-CGA-O2A-C1
10	aA	820	CLA	CBA-CGA-O2A-C1
10	bA	820	CLA	CBA-CGA-O2A-C1
14	cA	852	LHG	C24-C23-O8-C6
10	aA	823	CLA	CBA-CGA-O2A-C1
10	aB	826	CLA	CBA-CGA-O2A-C1
10	bA	830	CLA	CBA-CGA-O2A-C1
10	cB	826	CLA	CBA-CGA-O2A-C1
10	bB	826	CLA	CBA-CGA-O2A-C1
14	aA	852	LHG	C24-C23-O8-C6
10	aB	804	CLA	CBA-CGA-O2A-C1
10	bB	804	CLA	CBA-CGA-O2A-C1
10	aA	830	CLA	CBA-CGA-O2A-C1
10	bB	830	CLA	CBA-CGA-O2A-C1
10	cA	820	CLA	CBA-CGA-O2A-C1
10	aB	830	CLA	CBA-CGA-O2A-C1
14	bA	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	bB	822	CLA	CBD-CGD-O2D-CED
10	cB	822	CLA	CBD-CGD-O2D-CED
10	bB	802	CLA	CBD-CGD-O2D-CED
10	cB	802	CLA	CBD-CGD-O2D-CED
10	aB	802	CLA	CBD-CGD-O2D-CED
10	aB	822	CLA	CBD-CGD-O2D-CED
10	bB	824	CLA	C2A-CAA-CBA-CGA
10	aB	824	CLA	C2A-CAA-CBA-CGA
10	cB	824	CLA	C2A-CAA-CBA-CGA
10	cB	804	CLA	O1A-CGA-O2A-C1
10	aB	804	CLA	O1A-CGA-O2A-C1
10	bB	804	CLA	O1A-CGA-O2A-C1
13	aB	849	BCR	C15-C16-C17-C18
13	bB	849	BCR	C15-C16-C17-C18
13	cB	849	BCR	C15-C16-C17-C18
13	aA	848	BCR	C9-C10-C11-C12
13	cA	848	BCR	C9-C10-C11-C12
13	bA	848	BCR	C9-C10-C11-C12
10	bB	806	CLA	CBD-CGD-O2D-CED
10	aB	806	CLA	CBD-CGD-O2D-CED
10	cB	806	CLA	CBD-CGD-O2D-CED
10	aA	820	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
10	bA	820	CLA	O1D-CGD-O2D-CED
10	cA	820	CLA	O1D-CGD-O2D-CED
10	bB	823	CLA	C3-C5-C6-C7
10	bB	802	CLA	C3-C5-C6-C7
10	bB	801	CLA	C3-C5-C6-C7
10	cB	801	CLA	C3-C5-C6-C7
10	aB	808	CLA	C3-C5-C6-C7
10	aB	801	CLA	C3-C5-C6-C7
10	aL	202	CLA	C3-C5-C6-C7
10	bB	808	CLA	C3-C5-C6-C7
10	cB	823	CLA	C3-C5-C6-C7
10	aB	823	CLA	C3-C5-C6-C7
10	cB	808	CLA	C3-C5-C6-C7
10	bL	202	CLA	C3-C5-C6-C7
10	cB	815	CLA	C3-C5-C6-C7
10	cL	202	CLA	C3-C5-C6-C7
10	aB	815	CLA	C3-C5-C6-C7
10	cB	802	CLA	C3-C5-C6-C7
10	aB	802	CLA	C3-C5-C6-C7
10	bB	815	CLA	C3-C5-C6-C7
15	cA	853	LMT	O5B-C5B-C6B-O6B
15	bA	853	LMT	O5B-C5B-C6B-O6B
15	aA	853	LMT	O5B-C5B-C6B-O6B
10	cB	830	CLA	O1A-CGA-O2A-C1
10	bB	830	CLA	O1A-CGA-O2A-C1
10	aB	830	CLA	O1A-CGA-O2A-C1
10	bA	810	CLA	CBA-CGA-O2A-C1
10	bA	842	CLA	CBA-CGA-O2A-C1
10	cA	842	CLA	CBA-CGA-O2A-C1
10	aA	810	CLA	CBA-CGA-O2A-C1
10	aA	842	CLA	CBA-CGA-O2A-C1
10	cA	810	CLA	CBA-CGA-O2A-C1
14	cA	852	LHG	O2-C2-C3-O3
14	aA	852	LHG	O2-C2-C3-O3
14	bA	852	LHG	O2-C2-C3-O3
10	bA	838	CLA	O1D-CGD-O2D-CED
10	aA	838	CLA	O1D-CGD-O2D-CED
10	cA	838	CLA	O1D-CGD-O2D-CED
10	aB	810	CLA	CBD-CGD-O2D-CED
10	cA	830	CLA	O1A-CGA-O2A-C1
10	aA	830	CLA	O1A-CGA-O2A-C1
14	cA	852	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
14	aA	852	LHG	C2-C3-O3-P
14	bA	852	LHG	C2-C3-O3-P
10	cB	810	CLA	CBD-CGD-O2D-CED
10	bB	810	CLA	CBD-CGD-O2D-CED
10	cA	823	CLA	O1A-CGA-O2A-C1
10	bA	823	CLA	O1A-CGA-O2A-C1
10	aA	823	CLA	O1A-CGA-O2A-C1
10	bA	830	CLA	O1A-CGA-O2A-C1
10	aA	827	CLA	C4-C3-C5-C6
10	bA	827	CLA	C4-C3-C5-C6
10	cA	827	CLA	C4-C3-C5-C6
10	cA	819	CLA	C4-C3-C5-C6
10	bA	819	CLA	C4-C3-C5-C6
10	aA	819	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
10	bA	810	CLA	O1A-CGA-O2A-C1
10	bA	842	CLA	O1A-CGA-O2A-C1
10	cA	842	CLA	O1A-CGA-O2A-C1
10	aA	810	CLA	O1A-CGA-O2A-C1
10	aA	842	CLA	O1A-CGA-O2A-C1
10	cA	810	CLA	O1A-CGA-O2A-C1
10	bB	824	CLA	O1D-CGD-O2D-CED
10	aB	824	CLA	O1D-CGD-O2D-CED
10	cB	824	CLA	O1D-CGD-O2D-CED
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	cB	839	CLA	CBD-CGD-O2D-CED
10	bB	839	CLA	CBD-CGD-O2D-CED
10	aB	839	CLA	CBD-CGD-O2D-CED
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	aA	827	CLA	O1A-CGA-O2A-C1
10	bA	827	CLA	O1A-CGA-O2A-C1
10	cA	827	CLA	O1A-CGA-O2A-C1
10	aA	833	CLA	O1D-CGD-O2D-CED
10	cA	833	CLA	O1D-CGD-O2D-CED
10	bA	833	CLA	O1D-CGD-O2D-CED
10	aB	841	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
10	bA	810	CLA	C8-C10-C11-C12
10	aA	820	CLA	C15-C16-C17-C18
10	bA	820	CLA	C15-C16-C17-C18
10	aA	810	CLA	C8-C10-C11-C12
10	cA	820	CLA	C15-C16-C17-C18
10	cA	810	CLA	C8-C10-C11-C12
10	bB	823	CLA	CBA-CGA-O2A-C1
10	aB	832	CLA	CBA-CGA-O2A-C1
10	bA	805	CLA	CBA-CGA-O2A-C1
10	aA	805	CLA	CBA-CGA-O2A-C1
10	cA	805	CLA	CBA-CGA-O2A-C1
10	cB	823	CLA	CBA-CGA-O2A-C1
10	aB	823	CLA	CBA-CGA-O2A-C1
10	cA	815	CLA	CBA-CGA-O2A-C1
10	cB	832	CLA	CBA-CGA-O2A-C1
10	cA	819	CLA	CBA-CGA-O2A-C1
10	bA	819	CLA	CBA-CGA-O2A-C1
10	aA	819	CLA	CBA-CGA-O2A-C1
10	aA	826	CLA	CBA-CGA-O2A-C1
10	bB	832	CLA	CBA-CGA-O2A-C1
10	bA	826	CLA	CBA-CGA-O2A-C1
10	cA	826	CLA	CBA-CGA-O2A-C1
10	aA	812	CLA	C10-C11-C12-C13
10	cA	812	CLA	C10-C11-C12-C13
10	cL	205	CLA	C10-C11-C12-C13
10	aL	205	CLA	C10-C11-C12-C13
10	bL	205	CLA	C10-C11-C12-C13
10	bA	812	CLA	C10-C11-C12-C13
10	cB	841	CLA	O1D-CGD-O2D-CED
10	bB	841	CLA	O1D-CGD-O2D-CED
16	bB	848	LMG	O6-C5-C6-O5
16	cB	848	LMG	O6-C5-C6-O5
10	cA	832	CLA	CBD-CGD-O2D-CED
10	aB	826	CLA	C3-C5-C6-C7
10	cB	826	CLA	C3-C5-C6-C7
10	bB	826	CLA	C3-C5-C6-C7
10	cA	818	CLA	C11-C12-C13-C14
10	cB	819	CLA	C11-C10-C8-C9
10	bB	819	CLA	C11-C10-C8-C9
10	bA	818	CLA	C11-C12-C13-C14
10	bB	828	CLA	C11-C10-C8-C9
10	aB	819	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
10	aA	818	CLA	C11-C12-C13-C14
10	cB	828	CLA	C11-C10-C8-C9
10	aB	828	CLA	C11-C10-C8-C9
16	aB	848	LMG	O6-C5-C6-O5
10	aA	812	CLA	C8-C10-C11-C12
10	cB	804	CLA	C5-C6-C7-C8
10	cB	810	CLA	C5-C6-C7-C8
10	aB	827	CLA	C13-C15-C16-C17
10	aB	810	CLA	C5-C6-C7-C8
10	cA	812	CLA	C8-C10-C11-C12
10	cB	827	CLA	C13-C15-C16-C17
10	bB	827	CLA	C13-C15-C16-C17
10	cB	838	CLA	C5-C6-C7-C8
10	cB	838	CLA	C8-C10-C11-C12
10	aB	804	CLA	C5-C6-C7-C8
10	bB	804	CLA	C5-C6-C7-C8
10	bB	838	CLA	C5-C6-C7-C8
10	bB	838	CLA	C8-C10-C11-C12
10	aB	838	CLA	C5-C6-C7-C8
10	aB	838	CLA	C8-C10-C11-C12
13	aB	843	BCR	C37-C22-C23-C24
13	bB	845	BCR	C11-C12-C13-C35
13	cB	845	BCR	C11-C12-C13-C35
13	cA	849	BCR	C7-C8-C9-C34
13	cA	849	BCR	C37-C22-C23-C24
13	cL	207	BCR	C36-C18-C19-C20
13	aB	844	BCR	C37-C22-C23-C24
13	bA	849	BCR	C7-C8-C9-C34
13	bA	849	BCR	C37-C22-C23-C24
13	aB	845	BCR	C11-C12-C13-C35
13	cA	850	BCR	C7-C8-C9-C34
13	bL	207	BCR	C36-C18-C19-C20
13	bL	206	BCR	C37-C22-C23-C24
13	aL	206	BCR	C37-C22-C23-C24
13	cL	206	BCR	C37-C22-C23-C24
13	aA	848	BCR	C37-C22-C23-C24
13	aA	850	BCR	C7-C8-C9-C34
13	cA	848	BCR	C37-C22-C23-C24
13	cB	843	BCR	C37-C22-C23-C24
13	bA	850	BCR	C7-C8-C9-C34
13	bA	848	BCR	C37-C22-C23-C24
13	bB	843	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
13	aA	849	BCR	C7-C8-C9-C34
13	aA	849	BCR	C37-C22-C23-C24
13	aL	207	BCR	C36-C18-C19-C20
10	cA	816	CLA	C2A-CAA-CBA-CGA
10	aA	816	CLA	C2A-CAA-CBA-CGA
10	bA	816	CLA	C2A-CAA-CBA-CGA
10	bB	823	CLA	O1A-CGA-O2A-C1
10	cA	805	CLA	O1A-CGA-O2A-C1
10	cB	823	CLA	O1A-CGA-O2A-C1
10	aB	823	CLA	O1A-CGA-O2A-C1
10	bA	826	CLA	O1A-CGA-O2A-C1
13	bL	206	BCR	C21-C22-C23-C24
13	aL	206	BCR	C21-C22-C23-C24
13	cL	206	BCR	C21-C22-C23-C24
13	aA	848	BCR	C7-C8-C9-C10
13	cA	848	BCR	C7-C8-C9-C10
13	bA	848	BCR	C7-C8-C9-C10
10	aA	815	CLA	CBA-CGA-O2A-C1
10	bA	815	CLA	CBA-CGA-O2A-C1
10	aA	832	CLA	CBD-CGD-O2D-CED
10	bA	832	CLA	CBD-CGD-O2D-CED
10	bB	806	CLA	C2-C3-C5-C6
10	aB	806	CLA	C2-C3-C5-C6
10	cB	806	CLA	C2-C3-C5-C6
10	bB	837	CLA	C8-C10-C11-C12
10	cA	823	CLA	C5-C6-C7-C8
10	bB	802	CLA	C15-C16-C17-C18
10	bB	801	CLA	C10-C11-C12-C13
10	cB	801	CLA	C10-C11-C12-C13
10	bA	823	CLA	C5-C6-C7-C8
10	aA	829	CLA	C13-C15-C16-C17
10	aB	801	CLA	C10-C11-C12-C13
10	cA	831	CLA	C10-C11-C12-C13
10	cL	204	CLA	C8-C10-C11-C12
10	bL	204	CLA	C8-C10-C11-C12
10	cB	837	CLA	C8-C10-C11-C12
10	aA	823	CLA	C5-C6-C7-C8
10	cB	838	CLA	C10-C11-C12-C13
10	bA	831	CLA	C10-C11-C12-C13
10	cA	829	CLA	C13-C15-C16-C17
10	bA	829	CLA	C13-C15-C16-C17
10	aL	204	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
10	cB	802	CLA	C15-C16-C17-C18
10	aB	802	CLA	C15-C16-C17-C18
10	bB	838	CLA	C10-C11-C12-C13
10	bB	810	CLA	C5-C6-C7-C8
10	aB	838	CLA	C10-C11-C12-C13
10	aB	837	CLA	C8-C10-C11-C12
10	aA	831	CLA	C10-C11-C12-C13
10	bA	812	CLA	C8-C10-C11-C12
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	aB	832	CLA	O1A-CGA-O2A-C1
10	bA	805	CLA	O1A-CGA-O2A-C1
10	aA	805	CLA	O1A-CGA-O2A-C1
10	cB	832	CLA	O1A-CGA-O2A-C1
10	cA	819	CLA	O1A-CGA-O2A-C1
10	bA	819	CLA	O1A-CGA-O2A-C1
10	aA	819	CLA	O1A-CGA-O2A-C1
10	aA	826	CLA	O1A-CGA-O2A-C1
10	bB	832	CLA	O1A-CGA-O2A-C1
10	cA	826	CLA	O1A-CGA-O2A-C1
10	bB	828	CLA	O1D-CGD-O2D-CED
10	cA	818	CLA	C13-C15-C16-C17
10	bA	818	CLA	C13-C15-C16-C17
10	bB	828	CLA	C13-C15-C16-C17
10	aA	818	CLA	C13-C15-C16-C17
10	cB	817	CLA	C5-C6-C7-C8
10	cB	828	CLA	C13-C15-C16-C17
10	bB	817	CLA	C5-C6-C7-C8
10	aB	817	CLA	C5-C6-C7-C8
10	aB	828	CLA	C13-C15-C16-C17
10	cB	828	CLA	O1D-CGD-O2D-CED
10	aB	828	CLA	O1D-CGD-O2D-CED
10	aA	827	CLA	C8-C10-C11-C12
10	cB	830	CLA	C13-C15-C16-C17
10	bA	827	CLA	C8-C10-C11-C12
10	cA	827	CLA	C8-C10-C11-C12
10	bB	830	CLA	C13-C15-C16-C17
10	aB	830	CLA	C13-C15-C16-C17
10	cB	817	CLA	O1D-CGD-O2D-CED
10	bB	817	CLA	O1D-CGD-O2D-CED
10	aB	817	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
10	bB	837	CLA	C5-C6-C7-C8
10	cA	841	CLA	C5-C6-C7-C8
10	aB	832	CLA	C15-C16-C17-C18
10	aA	841	CLA	C5-C6-C7-C8
10	cB	837	CLA	C5-C6-C7-C8
10	cB	832	CLA	C15-C16-C17-C18
10	bA	841	CLA	C5-C6-C7-C8
10	bB	832	CLA	C15-C16-C17-C18
10	aB	837	CLA	C5-C6-C7-C8
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	aB	820	CLA	CBD-CGD-O2D-CED
10	cB	820	CLA	CBD-CGD-O2D-CED
10	bB	820	CLA	CBD-CGD-O2D-CED
10	bB	805	CLA	C8-C10-C11-C12
10	aB	805	CLA	C8-C10-C11-C12
10	aA	826	CLA	C5-C6-C7-C8
10	cB	805	CLA	C8-C10-C11-C12
10	bA	826	CLA	C5-C6-C7-C8
10	cA	826	CLA	C5-C6-C7-C8
10	cA	819	CLA	C2-C1-O2A-CGA
10	bA	819	CLA	C2-C1-O2A-CGA
10	aA	819	CLA	C2-C1-O2A-CGA
15	cA	853	LMT	C4B-C5B-C6B-O6B
15	bA	853	LMT	C4B-C5B-C6B-O6B
15	aA	853	LMT	C4B-C5B-C6B-O6B
10	cB	818	CLA	C11-C10-C8-C7
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	cA	804	CLA	C11-C10-C8-C7
10	bB	818	CLA	C11-C10-C8-C7
10	cB	819	CLA	C5-C6-C7-C8
10	aB	832	CLA	C8-C10-C11-C12
10	bB	819	CLA	C5-C6-C7-C8
10	bA	835	CLA	C15-C16-C17-C18
10	bB	814	CLA	C13-C15-C16-C17
10	aB	819	CLA	C5-C6-C7-C8
10	cB	832	CLA	C8-C10-C11-C12
10	cB	814	CLA	C13-C15-C16-C17
10	bB	832	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
10	aB	814	CLA	C13-C15-C16-C17
10	aA	807	CLA	O1D-CGD-O2D-CED
10	cA	807	CLA	O1D-CGD-O2D-CED
10	bA	807	CLA	O1D-CGD-O2D-CED
10	cB	825	CLA	C2A-CAA-CBA-CGA
10	bB	825	CLA	C2A-CAA-CBA-CGA
10	aB	825	CLA	C2A-CAA-CBA-CGA
10	cA	819	CLA	C3-C5-C6-C7
10	bA	819	CLA	C3-C5-C6-C7
10	aA	819	CLA	C3-C5-C6-C7
13	aB	843	BCR	C19-C20-C21-C22
13	aM	101	BCR	C19-C20-C21-C22
13	bM	101	BCR	C19-C20-C21-C22
13	cB	843	BCR	C19-C20-C21-C22
13	bB	843	BCR	C19-C20-C21-C22
13	cM	101	BCR	C19-C20-C21-C22
10	cA	835	CLA	C15-C16-C17-C18
10	aA	835	CLA	C15-C16-C17-C18
10	cA	815	CLA	O1A-CGA-O2A-C1
10	aA	815	CLA	O1A-CGA-O2A-C1
10	bA	815	CLA	O1A-CGA-O2A-C1
10	aA	804	CLA	C4-C3-C5-C6
10	bA	804	CLA	C4-C3-C5-C6
10	cA	804	CLA	C4-C3-C5-C6
10	cA	824	CLA	C2-C3-C5-C6
10	bA	824	CLA	C2-C3-C5-C6
10	aA	824	CLA	C2-C3-C5-C6
10	aA	812	CLA	C5-C6-C7-C8
10	aA	827	CLA	C13-C15-C16-C17
10	bA	827	CLA	C13-C15-C16-C17
10	cA	827	CLA	C13-C15-C16-C17
10	bA	842	CLA	C15-C16-C17-C18
10	aL	203	CLA	C10-C11-C12-C13
10	cA	812	CLA	C5-C6-C7-C8
10	cA	842	CLA	C15-C16-C17-C18
10	cL	205	CLA	C5-C6-C7-C8
10	aL	205	CLA	C5-C6-C7-C8
10	bA	841	CLA	C15-C16-C17-C18
10	bL	203	CLA	C10-C11-C12-C13
10	bL	205	CLA	C5-C6-C7-C8
10	aA	842	CLA	C15-C16-C17-C18
10	cL	203	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
10	bA	812	CLA	C5-C6-C7-C8
13	bA	846	BCR	C10-C11-C12-C13
13	bA	846	BCR	C18-C19-C20-C21
13	cA	846	BCR	C10-C11-C12-C13
13	cA	846	BCR	C18-C19-C20-C21
13	aA	846	BCR	C10-C11-C12-C13
13	aA	846	BCR	C18-C19-C20-C21
13	aM	101	BCR	C18-C19-C20-C21
13	aA	848	BCR	C18-C19-C20-C21
13	bM	101	BCR	C18-C19-C20-C21
13	cA	848	BCR	C18-C19-C20-C21
13	bA	848	BCR	C18-C19-C20-C21
13	cM	101	BCR	C18-C19-C20-C21
10	cA	818	CLA	C10-C11-C12-C13
10	cA	841	CLA	C15-C16-C17-C18
10	aA	812	CLA	C13-C15-C16-C17
10	aA	841	CLA	C15-C16-C17-C18
10	bA	818	CLA	C10-C11-C12-C13
10	bA	842	CLA	C8-C10-C11-C12
10	cA	812	CLA	C13-C15-C16-C17
10	cA	842	CLA	C8-C10-C11-C12
11	aA	844	PQN	C18-C20-C21-C22
10	bB	805	CLA	C13-C15-C16-C17
10	aA	818	CLA	C10-C11-C12-C13
10	cB	811	CLA	C5-C6-C7-C8
10	aB	805	CLA	C13-C15-C16-C17
10	cB	805	CLA	C13-C15-C16-C17
11	bA	844	PQN	C18-C20-C21-C22
10	aA	842	CLA	C8-C10-C11-C12
10	bA	812	CLA	C13-C15-C16-C17
10	cA	816	CLA	O1D-CGD-O2D-CED
10	aA	816	CLA	O1D-CGD-O2D-CED
10	bA	816	CLA	O1D-CGD-O2D-CED
10	aA	825	CLA	CBD-CGD-O2D-CED
10	cA	825	CLA	CBD-CGD-O2D-CED
10	bA	825	CLA	CBD-CGD-O2D-CED
14	aA	855	LHG	C4-O6-P-O3
14	cA	852	LHG	C3-O3-P-O6
14	bA	855	LHG	C4-O6-P-O3
14	aA	852	LHG	C3-O3-P-O6
14	cA	855	LHG	C4-O6-P-O3
14	bA	852	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
10	bB	811	CLA	C5-C6-C7-C8
11	cA	844	PQN	C18-C20-C21-C22
10	bA	837	CLA	C15-C16-C17-C18
10	bB	807	CLA	C10-C11-C12-C13
10	cA	824	CLA	C5-C6-C7-C8
10	cB	807	CLA	C10-C11-C12-C13
10	bA	824	CLA	C5-C6-C7-C8
10	aB	827	CLA	C15-C16-C17-C18
10	aB	811	CLA	C5-C6-C7-C8
10	cB	827	CLA	C15-C16-C17-C18
10	bB	827	CLA	C15-C16-C17-C18
10	cA	837	CLA	C15-C16-C17-C18
10	aA	837	CLA	C15-C16-C17-C18
10	aA	824	CLA	C5-C6-C7-C8
10	aB	807	CLA	C10-C11-C12-C13
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	bB	802	CLA	C13-C15-C16-C17
10	cB	802	CLA	C13-C15-C16-C17
10	aB	802	CLA	C13-C15-C16-C17
10	cA	823	CLA	C3-C5-C6-C7
10	bA	823	CLA	C3-C5-C6-C7
10	aA	823	CLA	C3-C5-C6-C7
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	cA	834	CLA	CBA-CGA-O2A-C1
10	bB	801	CLA	C2A-CAA-CBA-CGA
10	cB	801	CLA	C2A-CAA-CBA-CGA
10	aB	801	CLA	C2A-CAA-CBA-CGA
10	bA	818	CLA	O1D-CGD-O2D-CED
10	aA	829	CLA	C4-C3-C5-C6
10	bA	835	CLA	C4-C3-C5-C6
10	cA	835	CLA	C4-C3-C5-C6
10	cA	824	CLA	C4-C3-C5-C6
10	bA	824	CLA	C4-C3-C5-C6
10	aA	824	CLA	C4-C3-C5-C6
10	cA	829	CLA	C4-C3-C5-C6
10	bA	829	CLA	C4-C3-C5-C6
10	aA	835	CLA	C4-C3-C5-C6
10	aA	807	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
10	cA	807	CLA	C2A-CAA-CBA-CGA
10	bA	807	CLA	C2A-CAA-CBA-CGA
10	aA	804	CLA	C2-C3-C5-C6
10	bA	804	CLA	C2-C3-C5-C6
10	cA	804	CLA	C2-C3-C5-C6
10	cA	819	CLA	C2-C3-C5-C6
10	bA	819	CLA	C2-C3-C5-C6
10	aA	819	CLA	C2-C3-C5-C6
10	cA	818	CLA	O1D-CGD-O2D-CED
10	aA	818	CLA	O1D-CGD-O2D-CED
13	aB	843	BCR	C20-C21-C22-C37
13	cB	846	BCR	C20-C21-C22-C37
13	aB	847	BCR	C35-C13-C14-C15
13	aB	847	BCR	C20-C21-C22-C37
13	cB	844	BCR	C20-C21-C22-C37
13	cA	851	BCR	C20-C21-C22-C37
13	cB	847	BCR	C35-C13-C14-C15
13	cB	847	BCR	C20-C21-C22-C37
13	aB	844	BCR	C20-C21-C22-C37
13	aA	851	BCR	C20-C21-C22-C37
13	bA	851	BCR	C20-C21-C22-C37
13	bB	844	BCR	C20-C21-C22-C37
13	bB	846	BCR	C20-C21-C22-C37
13	cA	850	BCR	C20-C21-C22-C37
13	aB	846	BCR	C20-C21-C22-C37
13	aA	848	BCR	C20-C21-C22-C37
13	aA	850	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
13	cB	843	BCR	C20-C21-C22-C37
13	bA	850	BCR	C20-C21-C22-C37
13	bA	848	BCR	C20-C21-C22-C37
13	bB	843	BCR	C20-C21-C22-C37
10	cB	833	CLA	CBA-CGA-O2A-C1
10	aA	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	aB	814	CLA	CBA-CGA-O2A-C1
10	bA	834	CLA	CBA-CGA-O2A-C1
10	aB	833	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	cA	853	LMT	C2-C3-C4-C5
10	aB	826	CLA	C10-C11-C12-C13
10	cB	826	CLA	C10-C11-C12-C13
10	bB	826	CLA	C10-C11-C12-C13
15	bA	853	LMT	C2-C3-C4-C5
15	aA	853	LMT	C2-C3-C4-C5
10	bB	831	CLA	O1D-CGD-O2D-CED
10	aB	831	CLA	O1D-CGD-O2D-CED
10	aA	812	CLA	C3-C5-C6-C7
10	cA	812	CLA	C3-C5-C6-C7
10	bA	812	CLA	C3-C5-C6-C7
10	cB	831	CLA	O1D-CGD-O2D-CED
10	aA	825	CLA	C6-C7-C8-C9
11	cA	844	PQN	C26-C27-C28-C29
10	cA	825	CLA	C6-C7-C8-C9
11	aA	844	PQN	C26-C27-C28-C29
10	bA	825	CLA	C6-C7-C8-C9
11	bA	844	PQN	C26-C27-C28-C29
14	cA	852	LHG	C9-C10-C11-C12
14	aA	852	LHG	C9-C10-C11-C12
14	bA	852	LHG	C9-C10-C11-C12
13	aB	843	BCR	C20-C21-C22-C23
13	cB	844	BCR	C16-C17-C18-C19
13	cA	851	BCR	C11-C10-C9-C8
13	aB	844	BCR	C16-C17-C18-C19
13	aB	849	BCR	C16-C17-C18-C19
13	aA	851	BCR	C11-C10-C9-C8
13	bB	849	BCR	C16-C17-C18-C19
13	bA	851	BCR	C11-C10-C9-C8
13	bB	844	BCR	C16-C17-C18-C19
13	cB	849	BCR	C16-C17-C18-C19
13	bA	847	BCR	C20-C21-C22-C23
13	bA	846	BCR	C20-C21-C22-C23
13	aI	102	BCR	C11-C10-C9-C8
13	bI	102	BCR	C11-C10-C9-C8
13	cA	846	BCR	C20-C21-C22-C23
13	aA	846	BCR	C20-C21-C22-C23
13	aM	101	BCR	C20-C21-C22-C23
13	cI	103	BCR	C11-C10-C9-C8
13	aA	848	BCR	C11-C10-C9-C8
13	aA	847	BCR	C20-C21-C22-C23
13	bM	101	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
13	cA	848	BCR	C11-C10-C9-C8
13	cB	843	BCR	C20-C21-C22-C23
13	cA	847	BCR	C20-C21-C22-C23
13	bA	848	BCR	C11-C10-C9-C8
13	bB	843	BCR	C20-C21-C22-C23
13	cM	101	BCR	C20-C21-C22-C23
10	cB	841	CLA	CBA-CGA-O2A-C1
10	aB	841	CLA	CBA-CGA-O2A-C1
10	bB	841	CLA	CBA-CGA-O2A-C1
10	aA	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
10	bA	834	CLA	C5-C6-C7-C8
16	cB	848	LMG	C21-C22-C23-C24
14	bA	852	LHG	C28-C29-C30-C31
10	cA	818	CLA	C3-C5-C6-C7
10	aA	834	CLA	C3-C5-C6-C7
10	bA	818	CLA	C3-C5-C6-C7
10	cA	834	CLA	C3-C5-C6-C7
10	aA	818	CLA	C3-C5-C6-C7
10	bA	834	CLA	C3-C5-C6-C7
15	cA	853	LMT	C3-C4-C5-C6
15	bA	853	LMT	C3-C4-C5-C6
14	cA	852	LHG	C28-C29-C30-C31
14	cA	852	LHG	C30-C31-C32-C33
14	aA	852	LHG	C28-C29-C30-C31
14	aA	852	LHG	C30-C31-C32-C33
15	aA	853	LMT	C3-C4-C5-C6
14	bA	852	LHG	C30-C31-C32-C33
10	aB	833	CLA	O1D-CGD-O2D-CED
10	aA	827	CLA	C14-C13-C15-C16
10	bA	827	CLA	C14-C13-C15-C16
10	cA	827	CLA	C14-C13-C15-C16
10	cA	831	CLA	C14-C13-C15-C16
10	bA	831	CLA	C14-C13-C15-C16
10	aA	831	CLA	C14-C13-C15-C16
13	aB	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
13	bB	844	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
14	bA	855	LHG	O1-C1-C2-C3
13	bB	847	BCR	C7-C8-C9-C34
14	cA	855	LHG	O1-C1-C2-C3
10	bB	811	CLA	C16-C17-C18-C20
10	cB	811	CLA	C16-C17-C18-C20
13	aB	847	BCR	C7-C8-C9-C10
13	cA	849	BCR	C21-C22-C23-C24
13	cB	847	BCR	C7-C8-C9-C10
13	aB	849	BCR	C21-C22-C23-C24
13	bB	849	BCR	C21-C22-C23-C24
13	bA	849	BCR	C21-C22-C23-C24
13	cB	849	BCR	C21-C22-C23-C24
13	bB	847	BCR	C7-C8-C9-C10
13	aA	849	BCR	C21-C22-C23-C24
10	bA	811	CLA	C5-C6-C7-C8
10	cA	811	CLA	C5-C6-C7-C8
10	bB	837	CLA	CBD-CGD-O2D-CED
10	cB	837	CLA	CBD-CGD-O2D-CED
10	aB	837	CLA	CBD-CGD-O2D-CED
10	aB	832	CLA	C4-C3-C5-C6
10	cB	832	CLA	C4-C3-C5-C6
10	bB	832	CLA	C4-C3-C5-C6
10	cB	833	CLA	O1D-CGD-O2D-CED
10	bB	833	CLA	O1D-CGD-O2D-CED
10	aB	832	CLA	C2-C3-C5-C6
10	bA	835	CLA	C2-C3-C5-C6
10	aA	832	CLA	C2-C3-C5-C6
10	cA	835	CLA	C2-C3-C5-C6
10	cB	832	CLA	C2-C3-C5-C6
10	bA	832	CLA	C2-C3-C5-C6
10	bB	832	CLA	C2-C3-C5-C6
10	cA	832	CLA	C2-C3-C5-C6
10	aA	835	CLA	C2-C3-C5-C6
10	aA	811	CLA	C5-C6-C7-C8
10	cB	815	CLA	C5-C6-C7-C8
10	aB	815	CLA	C5-C6-C7-C8
10	bB	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	825	CLA	C6-C7-C8-C10
10	bB	811	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
10	aB	827	CLA	C16-C17-C18-C19
10	cA	825	CLA	C6-C7-C8-C10
10	aB	811	CLA	C16-C17-C18-C19
10	aB	811	CLA	C16-C17-C18-C20
10	cB	827	CLA	C16-C17-C18-C19
10	bB	827	CLA	C16-C17-C18-C19
10	cB	811	CLA	C16-C17-C18-C19
10	bA	825	CLA	C6-C7-C8-C10
10	cB	813	CLA	C2A-CAA-CBA-CGA
10	aB	813	CLA	C2A-CAA-CBA-CGA
10	bB	813	CLA	C2A-CAA-CBA-CGA
10	aA	802	CLA	C3A-C2A-CAA-CBA
10	bB	801	CLA	C3A-C2A-CAA-CBA
10	aA	812	CLA	C3A-C2A-CAA-CBA
10	cA	840	CLA	C3A-C2A-CAA-CBA
10	aA	827	CLA	C3A-C2A-CAA-CBA
10	cB	801	CLA	C3A-C2A-CAA-CBA
10	bA	827	CLA	C3A-C2A-CAA-CBA
10	cA	827	CLA	C3A-C2A-CAA-CBA
10	bA	835	CLA	C3A-C2A-CAA-CBA
10	aB	801	CLA	C3A-C2A-CAA-CBA
10	cA	835	CLA	C3A-C2A-CAA-CBA
10	cA	836	CLA	C3A-C2A-CAA-CBA
10	cA	812	CLA	C3A-C2A-CAA-CBA
10	aA	840	CLA	C3A-C2A-CAA-CBA
10	bA	840	CLA	C3A-C2A-CAA-CBA
10	aA	836	CLA	C3A-C2A-CAA-CBA
10	bA	836	CLA	C3A-C2A-CAA-CBA
10	cA	802	CLA	C3A-C2A-CAA-CBA
10	bA	802	CLA	C3A-C2A-CAA-CBA
10	aA	835	CLA	C3A-C2A-CAA-CBA
10	bA	812	CLA	C3A-C2A-CAA-CBA
14	cA	852	LHG	C15-C16-C17-C18
14	bA	852	LHG	C15-C16-C17-C18
14	aA	852	LHG	C15-C16-C17-C18
11	cA	844	PQN	C26-C27-C28-C30
11	aA	844	PQN	C26-C27-C28-C30
11	bA	844	PQN	C26-C27-C28-C30
10	bB	811	CLA	C8-C10-C11-C12
10	aB	811	CLA	C8-C10-C11-C12
16	aB	848	LMG	C40-C41-C42-C43
10	cB	811	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
16	bB	848	LMG	C40-C41-C42-C43
16	cB	848	LMG	C40-C41-C42-C43
10	bB	830	CLA	CBD-CGD-O2D-CED
10	aB	830	CLA	CBD-CGD-O2D-CED
10	bB	806	CLA	C3-C5-C6-C7
10	aB	806	CLA	C3-C5-C6-C7
10	cB	806	CLA	C3-C5-C6-C7
10	aB	822	CLA	O1D-CGD-O2D-CED
10	bA	838	CLA	C2A-CAA-CBA-CGA
10	aA	838	CLA	C2A-CAA-CBA-CGA
10	cA	838	CLA	C2A-CAA-CBA-CGA
14	aA	855	LHG	O1-C1-C2-O2
14	bA	855	LHG	O1-C1-C2-O2
14	cA	855	LHG	O1-C1-C2-O2
10	cB	822	CLA	O1D-CGD-O2D-CED
10	cB	830	CLA	CBD-CGD-O2D-CED
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	cA	828	CLA	C5-C6-C7-C8
10	aA	804	CLA	C15-C16-C17-C18
10	bA	804	CLA	C15-C16-C17-C18
14	cA	852	LHG	C24-C25-C26-C27
10	cA	804	CLA	C15-C16-C17-C18
14	aA	852	LHG	C24-C25-C26-C27
14	bA	852	LHG	C24-C25-C26-C27
10	aA	833	CLA	C2-C3-C5-C6
10	cA	833	CLA	C2-C3-C5-C6
10	bA	833	CLA	C2-C3-C5-C6
10	bB	822	CLA	O1D-CGD-O2D-CED
14	cA	852	LHG	C32-C33-C34-C35
14	aA	852	LHG	C32-C33-C34-C35
14	bA	852	LHG	C32-C33-C34-C35
10	aA	834	CLA	O1A-CGA-O2A-C1
10	cA	834	CLA	O1A-CGA-O2A-C1
10	bA	834	CLA	O1A-CGA-O2A-C1
10	aB	829	CLA	C5-C6-C7-C8
10	aA	828	CLA	C5-C6-C7-C8
10	bB	829	CLA	C5-C6-C7-C8
10	cB	829	CLA	C5-C6-C7-C8
10	bA	828	CLA	C5-C6-C7-C8
16	aB	848	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
16	bB	848	LMG	C35-C36-C37-C38
16	cB	848	LMG	C35-C36-C37-C38
13	aB	843	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	bB	845	BCR	C1-C6-C7-C8
13	bB	845	BCR	C5-C6-C7-C8
13	cB	845	BCR	C1-C6-C7-C8
13	cB	845	BCR	C5-C6-C7-C8
13	cB	844	BCR	C5-C6-C7-C8
13	cA	851	BCR	C23-C24-C25-C26
13	cA	851	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	cL	207	BCR	C23-C24-C25-C26
13	aB	844	BCR	C5-C6-C7-C8
13	aA	851	BCR	C23-C24-C25-C26
13	aA	851	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	aB	845	BCR	C1-C6-C7-C8
13	aB	845	BCR	C5-C6-C7-C8
13	bA	851	BCR	C23-C24-C25-C26
13	bA	851	BCR	C23-C24-C25-C30
13	bB	844	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	bA	847	BCR	C23-C24-C25-C26
13	bA	847	BCR	C23-C24-C25-C30
13	bI	101	BCR	C1-C6-C7-C8
13	bI	101	BCR	C5-C6-C7-C8
13	cI	102	BCR	C1-C6-C7-C8
13	cI	102	BCR	C5-C6-C7-C8
13	cA	850	BCR	C5-C6-C7-C8
13	cA	850	BCR	C23-C24-C25-C30
13	bA	846	BCR	C5-C6-C7-C8
13	bL	207	BCR	C23-C24-C25-C26
13	bL	206	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
13	aI	101	BCR	C1-C6-C7-C8
13	aI	101	BCR	C5-C6-C7-C8
13	aI	102	BCR	C23-C24-C25-C26
13	bI	102	BCR	C23-C24-C25-C26
13	cA	846	BCR	C5-C6-C7-C8
13	aL	206	BCR	C23-C24-C25-C30
13	aA	846	BCR	C5-C6-C7-C8
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	cI	103	BCR	C23-C24-C25-C26
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	cL	206	BCR	C23-C24-C25-C30
13	aA	850	BCR	C5-C6-C7-C8
13	aA	850	BCR	C23-C24-C25-C30
13	aA	847	BCR	C23-C24-C25-C26
13	aA	847	BCR	C23-C24-C25-C30
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	cB	843	BCR	C5-C6-C7-C8
13	cA	847	BCR	C23-C24-C25-C26
13	cA	847	BCR	C23-C24-C25-C30
13	bA	850	BCR	C5-C6-C7-C8
13	bA	850	BCR	C23-C24-C25-C30
13	bB	843	BCR	C5-C6-C7-C8
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	cM	101	BCR	C5-C6-C7-C8
13	cM	101	BCR	C23-C24-C25-C26
13	cM	101	BCR	C23-C24-C25-C30
13	aL	207	BCR	C23-C24-C25-C26
10	cB	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	aB	814	CLA	O1A-CGA-O2A-C1
10	aB	833	CLA	O1A-CGA-O2A-C1
10	cA	818	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	bA	818	CLA	CBA-CGA-O2A-C1
10	aA	818	CLA	CBA-CGA-O2A-C1
10	bB	828	CLA	C2-C1-O2A-CGA
10	cA	824	CLA	C2-C1-O2A-CGA
10	bA	824	CLA	C2-C1-O2A-CGA
10	cB	828	CLA	C2-C1-O2A-CGA
10	aA	824	CLA	C2-C1-O2A-CGA
10	aB	828	CLA	C2-C1-O2A-CGA
10	bB	802	CLA	C10-C11-C12-C13
10	cB	802	CLA	C10-C11-C12-C13
10	aB	802	CLA	C10-C11-C12-C13
10	cB	810	CLA	C3-C5-C6-C7
10	aB	810	CLA	C3-C5-C6-C7
10	bB	810	CLA	C3-C5-C6-C7
10	aA	827	CLA	C12-C13-C15-C16
10	bA	827	CLA	C12-C13-C15-C16
10	cA	827	CLA	C12-C13-C15-C16
10	aA	820	CLA	C11-C12-C13-C15
10	bA	820	CLA	C11-C12-C13-C15
10	cL	205	CLA	C11-C12-C13-C15
10	aL	205	CLA	C11-C12-C13-C15
10	bL	205	CLA	C11-C12-C13-C15
10	cA	820	CLA	C11-C12-C13-C15
10	cB	841	CLA	O1A-CGA-O2A-C1
10	cB	819	CLA	O1A-CGA-O2A-C1
10	bB	819	CLA	O1A-CGA-O2A-C1
10	aL	202	CLA	O1A-CGA-O2A-C1
10	aB	841	CLA	O1A-CGA-O2A-C1
10	aB	819	CLA	O1A-CGA-O2A-C1
10	bL	202	CLA	O1A-CGA-O2A-C1
10	bB	841	CLA	O1A-CGA-O2A-C1
10	cL	202	CLA	O1A-CGA-O2A-C1
16	aB	848	LMG	C36-C37-C38-C39
16	bB	848	LMG	C36-C37-C38-C39
16	cB	848	LMG	C36-C37-C38-C39
10	cA	816	CLA	CBA-CGA-O2A-C1
10	aA	829	CLA	CBA-CGA-O2A-C1
10	aL	202	CLA	CBA-CGA-O2A-C1
10	bB	807	CLA	CBA-CGA-O2A-C1
10	bA	811	CLA	CBA-CGA-O2A-C1
10	cB	807	CLA	CBA-CGA-O2A-C1
10	aA	816	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	aA	811	CLA	CBA-CGA-O2A-C1
10	cA	811	CLA	CBA-CGA-O2A-C1
10	bL	202	CLA	CBA-CGA-O2A-C1
10	cA	829	CLA	CBA-CGA-O2A-C1
10	bA	829	CLA	CBA-CGA-O2A-C1
10	cB	815	CLA	CBA-CGA-O2A-C1
10	aB	807	CLA	CBA-CGA-O2A-C1
10	bA	816	CLA	CBA-CGA-O2A-C1
10	cL	202	CLA	CBA-CGA-O2A-C1
10	aB	815	CLA	CBA-CGA-O2A-C1
10	bB	815	CLA	CBA-CGA-O2A-C1
10	cB	818	CLA	C10-C11-C12-C13
10	aB	818	CLA	C10-C11-C12-C13
14	cA	852	LHG	C12-C13-C14-C15
10	aL	203	CLA	C13-C15-C16-C17
14	aA	852	LHG	C12-C13-C14-C15
10	bB	818	CLA	C10-C11-C12-C13
10	bL	203	CLA	C13-C15-C16-C17
10	cL	203	CLA	C13-C15-C16-C17
14	bA	852	LHG	C12-C13-C14-C15
10	bA	817	CLA	C2A-CAA-CBA-CGA
10	cA	823	CLA	C2A-CAA-CBA-CGA
10	bA	823	CLA	C2A-CAA-CBA-CGA
10	aA	817	CLA	C2A-CAA-CBA-CGA
10	cA	836	CLA	C2A-CAA-CBA-CGA
10	aL	203	CLA	C2A-CAA-CBA-CGA
10	aA	823	CLA	C2A-CAA-CBA-CGA
10	aA	836	CLA	C2A-CAA-CBA-CGA
10	bL	203	CLA	C2A-CAA-CBA-CGA
10	bA	836	CLA	C2A-CAA-CBA-CGA
10	cA	817	CLA	C2A-CAA-CBA-CGA
10	cL	203	CLA	C2A-CAA-CBA-CGA
10	bA	822	CLA	O1D-CGD-O2D-CED
10	cA	822	CLA	O1D-CGD-O2D-CED
10	aA	822	CLA	O1D-CGD-O2D-CED
11	cA	844	PQN	C15-C16-C17-C18
11	aA	844	PQN	C15-C16-C17-C18
11	bA	844	PQN	C15-C16-C17-C18
10	aB	809	CLA	C4-C3-C5-C6
10	aA	833	CLA	C4-C3-C5-C6
10	cB	809	CLA	C4-C3-C5-C6
10	aA	839	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	cA	833	CLA	C4-C3-C5-C6
10	bB	809	CLA	C4-C3-C5-C6
10	bA	833	CLA	C4-C3-C5-C6
10	cB	817	CLA	C4-C3-C5-C6
10	bB	817	CLA	C4-C3-C5-C6
10	bA	839	CLA	C4-C3-C5-C6
10	cA	839	CLA	C4-C3-C5-C6
10	aB	817	CLA	C4-C3-C5-C6
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	cL	205	CLA	CBA-CGA-O2A-C1
10	aL	205	CLA	CBA-CGA-O2A-C1
10	bL	205	CLA	CBA-CGA-O2A-C1
10	aA	820	CLA	C10-C11-C12-C13
10	bA	820	CLA	C10-C11-C12-C13
10	cA	820	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	bB	801	CLA	C6-C7-C8-C9
10	cB	801	CLA	C6-C7-C8-C9
10	aB	801	CLA	C6-C7-C8-C9
10	bA	810	CLA	C6-C7-C8-C9
10	aA	820	CLA	C11-C12-C13-C14
10	bA	820	CLA	C11-C12-C13-C14
10	aA	810	CLA	C6-C7-C8-C9
10	cA	820	CLA	C11-C12-C13-C14
10	cA	810	CLA	C6-C7-C8-C9
10	aA	802	CLA	C1A-C2A-CAA-CBA
10	aB	812	CLA	C1A-C2A-CAA-CBA
10	bA	817	CLA	C1A-C2A-CAA-CBA
10	cB	841	CLA	C1A-C2A-CAA-CBA
10	bB	811	CLA	C1A-C2A-CAA-CBA
10	cB	839	CLA	C1A-C2A-CAA-CBA
10	aA	807	CLA	C1A-C2A-CAA-CBA
10	aA	812	CLA	C1A-C2A-CAA-CBA
10	cA	840	CLA	C1A-C2A-CAA-CBA
10	bB	839	CLA	C1A-C2A-CAA-CBA
10	cA	807	CLA	C1A-C2A-CAA-CBA
10	aA	834	CLA	C1A-C2A-CAA-CBA
10	bA	807	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
10	cA	831	CLA	C1A-C2A-CAA-CBA
10	aA	817	CLA	C1A-C2A-CAA-CBA
10	cA	836	CLA	C1A-C2A-CAA-CBA
10	cA	834	CLA	C1A-C2A-CAA-CBA
10	aL	203	CLA	C1A-C2A-CAA-CBA
10	aB	841	CLA	C1A-C2A-CAA-CBA
10	aB	811	CLA	C1A-C2A-CAA-CBA
10	cB	812	CLA	C1A-C2A-CAA-CBA
10	cA	812	CLA	C1A-C2A-CAA-CBA
10	aA	840	CLA	C1A-C2A-CAA-CBA
10	aB	839	CLA	C1A-C2A-CAA-CBA
10	cB	811	CLA	C1A-C2A-CAA-CBA
10	bA	831	CLA	C1A-C2A-CAA-CBA
10	bB	841	CLA	C1A-C2A-CAA-CBA
10	bA	840	CLA	C1A-C2A-CAA-CBA
10	aA	836	CLA	C1A-C2A-CAA-CBA
10	bL	203	CLA	C1A-C2A-CAA-CBA
10	bA	836	CLA	C1A-C2A-CAA-CBA
10	cA	802	CLA	C1A-C2A-CAA-CBA
10	cA	817	CLA	C1A-C2A-CAA-CBA
10	bA	802	CLA	C1A-C2A-CAA-CBA
10	cL	203	CLA	C1A-C2A-CAA-CBA
10	aA	831	CLA	C1A-C2A-CAA-CBA
10	bA	812	CLA	C1A-C2A-CAA-CBA
10	bB	812	CLA	C1A-C2A-CAA-CBA
10	bA	834	CLA	C1A-C2A-CAA-CBA
10	bA	842	CLA	C10-C11-C12-C13
10	cA	842	CLA	C10-C11-C12-C13
10	aA	842	CLA	C10-C11-C12-C13
13	aB	849	BCR	C7-C8-C9-C34
13	bB	849	BCR	C7-C8-C9-C34
13	cB	849	BCR	C7-C8-C9-C34
13	cA	850	BCR	C11-C12-C13-C35
13	aA	850	BCR	C11-C12-C13-C35
13	bA	850	BCR	C11-C12-C13-C35
10	cL	204	CLA	C2A-CAA-CBA-CGA
10	bL	204	CLA	C2A-CAA-CBA-CGA
10	aL	204	CLA	C2A-CAA-CBA-CGA
10	cA	818	CLA	O1A-CGA-O2A-C1
10	bA	818	CLA	O1A-CGA-O2A-C1
10	bB	807	CLA	O1A-CGA-O2A-C1
10	cB	807	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	aA	818	CLA	O1A-CGA-O2A-C1
10	cB	815	CLA	O1A-CGA-O2A-C1
10	aB	807	CLA	O1A-CGA-O2A-C1
10	aB	815	CLA	O1A-CGA-O2A-C1
10	bB	815	CLA	O1A-CGA-O2A-C1
13	bI	101	BCR	C21-C22-C23-C24
13	cI	102	BCR	C21-C22-C23-C24
16	aB	848	LMG	C17-C18-C19-C20
16	bB	848	LMG	C17-C18-C19-C20
16	cB	848	LMG	C17-C18-C19-C20
15	cA	853	LMT	C1-C2-C3-C4
15	bA	853	LMT	C1-C2-C3-C4
15	aA	853	LMT	C1-C2-C3-C4
16	aB	848	LMG	C15-C16-C17-C18
16	bB	848	LMG	C15-C16-C17-C18
16	cB	848	LMG	C15-C16-C17-C18
10	aB	808	CLA	C4-C3-C5-C6
10	bB	808	CLA	C4-C3-C5-C6
10	cB	808	CLA	C4-C3-C5-C6
10	cL	205	CLA	C4-C3-C5-C6
10	aL	205	CLA	C4-C3-C5-C6
10	bL	205	CLA	C4-C3-C5-C6
10	aB	809	CLA	C2-C3-C5-C6
10	cB	809	CLA	C2-C3-C5-C6
10	aB	808	CLA	C2-C3-C5-C6
10	aA	839	CLA	C2-C3-C5-C6
10	aA	829	CLA	C2-C3-C5-C6
10	bB	808	CLA	C2-C3-C5-C6
10	cB	808	CLA	C2-C3-C5-C6
10	bB	809	CLA	C2-C3-C5-C6
10	cL	205	CLA	C2-C3-C5-C6
10	aL	205	CLA	C2-C3-C5-C6
10	cB	817	CLA	C2-C3-C5-C6
10	cA	829	CLA	C2-C3-C5-C6
10	bA	829	CLA	C2-C3-C5-C6
10	bB	817	CLA	C2-C3-C5-C6
10	bL	205	CLA	C2-C3-C5-C6
10	bA	839	CLA	C2-C3-C5-C6
10	cA	839	CLA	C2-C3-C5-C6
10	aB	817	CLA	C2-C3-C5-C6
10	aB	826	CLA	C16-C17-C18-C20
10	bB	826	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
10	aB	820	CLA	C13-C15-C16-C17
10	bB	820	CLA	C13-C15-C16-C17
10	bB	814	CLA	C10-C11-C12-C13
10	cB	820	CLA	C13-C15-C16-C17
10	cB	814	CLA	C10-C11-C12-C13
10	aB	814	CLA	C10-C11-C12-C13
10	cB	826	CLA	C16-C17-C18-C20
10	cA	816	CLA	O1A-CGA-O2A-C1
10	aA	829	CLA	O1A-CGA-O2A-C1
10	aA	816	CLA	O1A-CGA-O2A-C1
10	cA	829	CLA	O1A-CGA-O2A-C1
10	bA	829	CLA	O1A-CGA-O2A-C1
10	bA	816	CLA	O1A-CGA-O2A-C1
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	bB	811	CLA	C13-C15-C16-C17
10	aB	811	CLA	C13-C15-C16-C17
10	cB	811	CLA	C13-C15-C16-C17
10	bA	842	CLA	C4-C3-C5-C6
10	cA	842	CLA	C4-C3-C5-C6
10	aA	842	CLA	C4-C3-C5-C6
10	bA	811	CLA	O1A-CGA-O2A-C1
10	aA	811	CLA	O1A-CGA-O2A-C1
10	cA	811	CLA	O1A-CGA-O2A-C1
10	cL	205	CLA	O1A-CGA-O2A-C1
10	aL	205	CLA	O1A-CGA-O2A-C1
10	bL	205	CLA	O1A-CGA-O2A-C1
15	cA	853	LMT	C9-C10-C11-C12
15	bA	853	LMT	C9-C10-C11-C12
15	aA	853	LMT	C9-C10-C11-C12
13	bB	845	BCR	C20-C21-C22-C37
13	cB	845	BCR	C20-C21-C22-C37
13	cA	851	BCR	C16-C17-C18-C36
13	aA	851	BCR	C16-C17-C18-C36
13	aB	845	BCR	C20-C21-C22-C37
13	bA	851	BCR	C16-C17-C18-C36
10	aA	812	CLA	C15-C16-C17-C18
10	cL	204	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
10	bL	204	CLA	C10-C11-C12-C13
10	cA	812	CLA	C15-C16-C17-C18
10	aL	204	CLA	C10-C11-C12-C13
10	bA	812	CLA	C15-C16-C17-C18
10	cB	802	CLA	O1D-CGD-O2D-CED
10	aB	802	CLA	O1D-CGD-O2D-CED
14	aA	855	LHG	C10-C11-C12-C13
14	bA	855	LHG	C10-C11-C12-C13
14	cA	855	LHG	C10-C11-C12-C13
10	bB	802	CLA	O1D-CGD-O2D-CED
10	bB	814	CLA	C5-C6-C7-C8
10	cB	814	CLA	C5-C6-C7-C8
10	aB	814	CLA	C5-C6-C7-C8
10	cB	839	CLA	O1D-CGD-O2D-CED
10	bB	839	CLA	O1D-CGD-O2D-CED
10	aB	808	CLA	CBA-CGA-O2A-C1
10	cA	831	CLA	CBA-CGA-O2A-C1
10	bB	808	CLA	CBA-CGA-O2A-C1
10	cB	808	CLA	CBA-CGA-O2A-C1
10	bA	831	CLA	CBA-CGA-O2A-C1
10	aA	831	CLA	CBA-CGA-O2A-C1
10	bB	828	CLA	C8-C10-C11-C12
16	aB	848	LMG	C23-C24-C25-C26
10	cB	828	CLA	C8-C10-C11-C12
16	bB	848	LMG	C34-C35-C36-C37
10	aB	828	CLA	C8-C10-C11-C12
10	aB	839	CLA	O1D-CGD-O2D-CED
16	aB	848	LMG	C34-C35-C36-C37
16	bB	848	LMG	C23-C24-C25-C26
16	cB	848	LMG	C23-C24-C25-C26
16	cB	848	LMG	C34-C35-C36-C37
10	aB	806	CLA	O1D-CGD-O2D-CED
10	bB	806	CLA	O1D-CGD-O2D-CED
10	cB	806	CLA	O1D-CGD-O2D-CED
10	aA	854	CLA	CBA-CGA-O2A-C1
10	cA	854	CLA	CBA-CGA-O2A-C1
10	bA	854	CLA	CBA-CGA-O2A-C1
10	bB	811	CLA	O1A-CGA-O2A-C1
10	aB	811	CLA	O1A-CGA-O2A-C1
10	cB	811	CLA	O1A-CGA-O2A-C1
10	aA	827	CLA	C2-C1-O2A-CGA
10	cB	804	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
10	bA	827	CLA	C2-C1-O2A-CGA
10	cA	827	CLA	C2-C1-O2A-CGA
9	cA	801	CL0	C2-C1-O2A-CGA
10	aB	804	CLA	C2-C1-O2A-CGA
9	bA	801	CL0	C2-C1-O2A-CGA
10	bB	804	CLA	C2-C1-O2A-CGA
9	aA	801	CL0	C2-C1-O2A-CGA
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	aA	833	CLA	C12-C13-C15-C16
10	bB	801	CLA	C6-C7-C8-C10
10	bA	805	CLA	C12-C13-C15-C16
10	aA	805	CLA	C12-C13-C15-C16
10	cB	801	CLA	C6-C7-C8-C10
10	cB	830	CLA	C6-C7-C8-C10
10	cA	805	CLA	C12-C13-C15-C16
10	aA	829	CLA	C12-C13-C15-C16
10	aB	801	CLA	C6-C7-C8-C10
10	bA	810	CLA	C6-C7-C8-C10
10	bB	808	CLA	C11-C12-C13-C15
10	cA	833	CLA	C12-C13-C15-C16
10	cB	808	CLA	C11-C12-C13-C15
10	aA	810	CLA	C6-C7-C8-C10
10	bA	833	CLA	C12-C13-C15-C16
10	cA	829	CLA	C12-C13-C15-C16
10	bA	829	CLA	C12-C13-C15-C16
10	bB	830	CLA	C6-C7-C8-C10
10	aB	830	CLA	C6-C7-C8-C10
10	cA	810	CLA	C6-C7-C8-C10
10	aB	808	CLA	O1A-CGA-O2A-C1
10	bB	808	CLA	O1A-CGA-O2A-C1
10	cB	808	CLA	O1A-CGA-O2A-C1
16	bB	848	LMG	C16-C17-C18-C19
16	aB	848	LMG	C16-C17-C18-C19
16	cB	848	LMG	C16-C17-C18-C19
10	cB	830	CLA	C6-C7-C8-C9
10	aB	808	CLA	C11-C10-C8-C9
10	aB	808	CLA	C11-C12-C13-C14
10	aA	829	CLA	C14-C13-C15-C16
10	bA	842	CLA	C11-C10-C8-C9
10	bB	808	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
10	bB	808	CLA	C11-C12-C13-C14
10	cB	808	CLA	C11-C10-C8-C9
10	cB	808	CLA	C11-C12-C13-C14
10	cA	842	CLA	C11-C10-C8-C9
10	cA	819	CLA	C6-C7-C8-C9
10	bA	819	CLA	C6-C7-C8-C9
10	bB	805	CLA	C11-C12-C13-C14
10	aA	819	CLA	C6-C7-C8-C9
10	aB	805	CLA	C11-C12-C13-C14
10	cA	829	CLA	C14-C13-C15-C16
10	bA	829	CLA	C14-C13-C15-C16
10	cB	805	CLA	C11-C12-C13-C14
10	bB	830	CLA	C6-C7-C8-C9
10	aA	842	CLA	C11-C10-C8-C9
10	aB	830	CLA	C6-C7-C8-C9
10	cA	831	CLA	C13-C15-C16-C17
10	bA	831	CLA	C13-C15-C16-C17
10	aA	831	CLA	C13-C15-C16-C17
13	bA	847	BCR	C7-C8-C9-C34
13	aA	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
13	cM	101	BCR	C21-C22-C23-C24
10	aA	825	CLA	CBA-CGA-O2A-C1
10	cB	819	CLA	CBA-CGA-O2A-C1
10	bB	819	CLA	CBA-CGA-O2A-C1
10	cA	825	CLA	CBA-CGA-O2A-C1
10	aB	819	CLA	CBA-CGA-O2A-C1
10	bA	825	CLA	CBA-CGA-O2A-C1
10	aA	828	CLA	C15-C16-C17-C18
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	cA	828	CLA	C15-C16-C17-C18
10	bA	828	CLA	C15-C16-C17-C18
10	bB	811	CLA	CBA-CGA-O2A-C1
10	cA	836	CLA	CBA-CGA-O2A-C1
10	aB	811	CLA	CBA-CGA-O2A-C1
10	cB	811	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	aA	836	CLA	CBA-CGA-O2A-C1
10	bA	836	CLA	CBA-CGA-O2A-C1
10	aB	810	CLA	O1D-CGD-O2D-CED
10	cB	810	CLA	O1D-CGD-O2D-CED
10	cL	204	CLA	C5-C6-C7-C8
14	cA	852	LHG	C16-C17-C18-C19
10	bL	204	CLA	C5-C6-C7-C8
14	aA	852	LHG	C16-C17-C18-C19
10	aL	204	CLA	C5-C6-C7-C8
14	bA	852	LHG	C16-C17-C18-C19
10	bB	821	CLA	CBA-CGA-O2A-C1
10	cB	821	CLA	CBA-CGA-O2A-C1
10	aB	820	CLA	C3-C5-C6-C7
10	cB	820	CLA	C3-C5-C6-C7
10	bB	820	CLA	C3-C5-C6-C7
10	bB	818	CLA	CAA-CBA-CGA-O2A
10	bB	822	CLA	C3A-C2A-CAA-CBA
10	cB	822	CLA	C3A-C2A-CAA-CBA
10	bA	805	CLA	C3A-C2A-CAA-CBA
10	aA	805	CLA	C3A-C2A-CAA-CBA
10	cA	805	CLA	C3A-C2A-CAA-CBA
10	cL	204	CLA	C3A-C2A-CAA-CBA
10	bL	204	CLA	C3A-C2A-CAA-CBA
10	aL	204	CLA	C3A-C2A-CAA-CBA
10	aB	822	CLA	C3A-C2A-CAA-CBA
10	aB	821	CLA	CBA-CGA-O2A-C1
14	cA	852	LHG	C29-C30-C31-C32
14	aA	852	LHG	C29-C30-C31-C32
14	bA	852	LHG	C29-C30-C31-C32
10	aB	820	CLA	C4-C3-C5-C6
10	cB	820	CLA	C4-C3-C5-C6
10	bB	820	CLA	C4-C3-C5-C6
14	cA	855	LHG	C11-C10-C9-C8
10	bA	842	CLA	C2-C3-C5-C6
10	cA	842	CLA	C2-C3-C5-C6
10	aA	842	CLA	C2-C3-C5-C6
13	aB	849	BCR	C13-C14-C15-C16
13	bB	849	BCR	C13-C14-C15-C16
13	cB	849	BCR	C13-C14-C15-C16
14	aA	855	LHG	C11-C10-C9-C8
14	bA	855	LHG	C11-C10-C9-C8
10	cB	818	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
10	aB	818	CLA	CAA-CBA-CGA-O2A
15	cA	853	LMT	O1'-C1-C2-C3
15	bA	853	LMT	O1'-C1-C2-C3
15	aA	853	LMT	O1'-C1-C2-C3
10	bA	817	CLA	CBA-CGA-O2A-C1
10	aA	817	CLA	CBA-CGA-O2A-C1
10	cA	824	CLA	CBA-CGA-O2A-C1
10	bA	824	CLA	CBA-CGA-O2A-C1
10	aA	824	CLA	CBA-CGA-O2A-C1
10	cA	817	CLA	CBA-CGA-O2A-C1
10	aA	825	CLA	O1D-CGD-O2D-CED
10	cA	825	CLA	O1D-CGD-O2D-CED
10	bA	825	CLA	O1D-CGD-O2D-CED
14	cA	852	LHG	C11-C10-C9-C8
14	aA	852	LHG	C11-C10-C9-C8
14	bA	852	LHG	C11-C10-C9-C8
10	aA	854	CLA	O1A-CGA-O2A-C1
10	cA	854	CLA	O1A-CGA-O2A-C1
10	bA	831	CLA	O1A-CGA-O2A-C1
10	bA	854	CLA	O1A-CGA-O2A-C1
10	aA	831	CLA	O1A-CGA-O2A-C1
10	aA	825	CLA	O1A-CGA-O2A-C1
10	cA	831	CLA	O1A-CGA-O2A-C1
10	cA	825	CLA	O1A-CGA-O2A-C1
10	bA	825	CLA	O1A-CGA-O2A-C1
10	aB	809	CLA	C15-C16-C17-C18
10	cB	809	CLA	C15-C16-C17-C18
10	bB	809	CLA	C15-C16-C17-C18
10	cA	823	CLA	C4-C3-C5-C6
10	bA	823	CLA	C4-C3-C5-C6
10	aB	827	CLA	C4-C3-C5-C6
10	cB	827	CLA	C4-C3-C5-C6
10	bB	827	CLA	C4-C3-C5-C6
10	aA	823	CLA	C4-C3-C5-C6
10	cB	838	CLA	C4-C3-C5-C6
10	bB	838	CLA	C4-C3-C5-C6
10	aB	838	CLA	C4-C3-C5-C6
10	cA	831	CLA	C8-C10-C11-C12
10	bA	831	CLA	C8-C10-C11-C12
10	aA	831	CLA	C8-C10-C11-C12
13	aB	843	BCR	C23-C24-C25-C30
13	aB	847	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	aB	847	BCR	C23-C24-C25-C26
13	aB	847	BCR	C23-C24-C25-C30
10	aA	833	CLA	C14-C13-C15-C16
10	cA	841	CLA	C6-C7-C8-C9
13	cB	844	BCR	C23-C24-C25-C26
13	cB	844	BCR	C23-C24-C25-C30
13	cA	851	BCR	C5-C6-C7-C8
13	cA	849	BCR	C23-C24-C25-C26
13	cL	207	BCR	C5-C6-C7-C8
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	aB	844	BCR	C23-C24-C25-C26
13	aB	844	BCR	C23-C24-C25-C30
13	aB	849	BCR	C23-C24-C25-C26
13	aA	851	BCR	C5-C6-C7-C8
13	bB	849	BCR	C23-C24-C25-C26
13	bA	849	BCR	C23-C24-C25-C26
10	aA	841	CLA	C6-C7-C8-C9
13	bA	851	BCR	C5-C6-C7-C8
10	bA	842	CLA	C14-C13-C15-C16
13	bB	844	BCR	C23-C24-C25-C26
13	bB	844	BCR	C23-C24-C25-C30
10	aA	820	CLA	C14-C13-C15-C16
13	cB	849	BCR	C23-C24-C25-C26
10	bA	820	CLA	C14-C13-C15-C16
13	bA	847	BCR	C1-C6-C7-C8
13	cA	850	BCR	C23-C24-C25-C26
13	bA	846	BCR	C23-C24-C25-C26
13	bA	846	BCR	C23-C24-C25-C30
13	bL	207	BCR	C5-C6-C7-C8
13	bL	206	BCR	C5-C6-C7-C8
10	cA	833	CLA	C14-C13-C15-C16
13	cA	846	BCR	C23-C24-C25-C26
13	cA	846	BCR	C23-C24-C25-C30
13	aL	206	BCR	C5-C6-C7-C8
10	cA	842	CLA	C14-C13-C15-C16
13	aA	846	BCR	C23-C24-C25-C26
13	aA	846	BCR	C23-C24-C25-C30
13	aM	101	BCR	C1-C6-C7-C8
13	cL	206	BCR	C5-C6-C7-C8
13	aA	850	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
13	aA	847	BCR	C1-C6-C7-C8
10	bA	833	CLA	C14-C13-C15-C16
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	bM	101	BCR	C1-C6-C7-C8
10	bB	805	CLA	C11-C10-C8-C9
10	aB	805	CLA	C11-C10-C8-C9
10	bA	841	CLA	C6-C7-C8-C9
13	cB	843	BCR	C23-C24-C25-C30
10	cB	805	CLA	C11-C10-C8-C9
13	cA	847	BCR	C1-C6-C7-C8
13	bA	850	BCR	C23-C24-C25-C26
10	cA	820	CLA	C14-C13-C15-C16
10	aA	842	CLA	C14-C13-C15-C16
13	bB	843	BCR	C23-C24-C25-C30
13	aA	849	BCR	C23-C24-C25-C26
13	cM	101	BCR	C1-C6-C7-C8
13	aL	207	BCR	C5-C6-C7-C8
10	aB	826	CLA	C16-C17-C18-C19
10	bB	826	CLA	C16-C17-C18-C19
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	aL	203	CLA	C3-C5-C6-C7
10	cB	833	CLA	CAA-CBA-CGA-O2A
10	bB	833	CLA	CAA-CBA-CGA-O2A
10	aB	833	CLA	CAA-CBA-CGA-O2A
13	cA	851	BCR	C7-C8-C9-C10
13	aA	851	BCR	C7-C8-C9-C10
13	bA	851	BCR	C7-C8-C9-C10
10	aB	832	CLA	C2-C1-O2A-CGA
10	cB	832	CLA	C2-C1-O2A-CGA
10	bB	832	CLA	C2-C1-O2A-CGA
10	bA	822	CLA	C4-C3-C5-C6
10	cA	822	CLA	C4-C3-C5-C6
10	aA	822	CLA	C4-C3-C5-C6
10	bL	203	CLA	C3-C5-C6-C7
10	cL	203	CLA	C3-C5-C6-C7
10	aB	827	CLA	C16-C17-C18-C20
10	cB	827	CLA	C16-C17-C18-C20
10	bB	827	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
10	cB	826	CLA	C16-C17-C18-C19
10	cB	841	CLA	C11-C12-C13-C15
10	cB	819	CLA	C11-C10-C8-C7
10	aB	832	CLA	C6-C7-C8-C10
10	aB	808	CLA	C11-C10-C8-C7
10	aB	808	CLA	C11-C12-C13-C15
10	bB	819	CLA	C11-C10-C8-C7
10	cL	204	CLA	C6-C7-C8-C10
10	bA	842	CLA	C12-C13-C15-C16
10	aA	820	CLA	C12-C13-C15-C16
10	bB	808	CLA	C11-C10-C8-C7
10	bA	820	CLA	C12-C13-C15-C16
10	bL	204	CLA	C6-C7-C8-C10
10	aB	841	CLA	C11-C12-C13-C15
10	cB	808	CLA	C11-C10-C8-C7
10	aB	819	CLA	C11-C10-C8-C7
10	cA	842	CLA	C12-C13-C15-C16
10	cB	832	CLA	C6-C7-C8-C10
10	cA	819	CLA	C6-C7-C8-C10
10	bA	819	CLA	C6-C7-C8-C10
10	bB	805	CLA	C11-C12-C13-C15
10	aA	819	CLA	C6-C7-C8-C10
10	aB	805	CLA	C11-C12-C13-C15
10	bB	841	CLA	C11-C12-C13-C15
10	bB	832	CLA	C6-C7-C8-C10
10	cB	805	CLA	C11-C12-C13-C15
10	aL	204	CLA	C6-C7-C8-C10
10	cA	820	CLA	C12-C13-C15-C16
10	aA	842	CLA	C12-C13-C15-C16
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	bA	817	CLA	O1A-CGA-O2A-C1
10	aA	817	CLA	O1A-CGA-O2A-C1
10	cA	817	CLA	O1A-CGA-O2A-C1
13	cB	844	BCR	C35-C13-C14-C15
13	cL	207	BCR	C16-C17-C18-C36
13	aB	844	BCR	C35-C13-C14-C15
13	bB	844	BCR	C35-C13-C14-C15
13	bL	207	BCR	C16-C17-C18-C36
13	aM	101	BCR	C16-C17-C18-C36
13	aA	848	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
13	bM	101	BCR	C16-C17-C18-C36
13	cA	848	BCR	C35-C13-C14-C15
13	bA	848	BCR	C35-C13-C14-C15
13	cM	101	BCR	C16-C17-C18-C36
13	aL	207	BCR	C16-C17-C18-C36
10	cB	815	CLA	C2A-CAA-CBA-CGA
10	aB	815	CLA	C2A-CAA-CBA-CGA
10	bB	815	CLA	C2A-CAA-CBA-CGA
14	cA	852	LHG	O9-C7-O7-C5
14	aA	852	LHG	O9-C7-O7-C5
14	bA	852	LHG	O9-C7-O7-C5
10	cA	856	CLA	CBA-CGA-O2A-C1
10	bA	856	CLA	CBA-CGA-O2A-C1
10	aA	856	CLA	CBA-CGA-O2A-C1
10	bB	823	CLA	CAD-CBD-CGD-O2D
10	aB	832	CLA	CAD-CBD-CGD-O2D
10	bA	805	CLA	CAD-CBD-CGD-O2D
10	aA	805	CLA	CAD-CBD-CGD-O2D
10	bA	822	CLA	CAD-CBD-CGD-O2D
10	cB	830	CLA	CAD-CBD-CGD-O2D
10	cB	835	CLA	CAD-CBD-CGD-O2D
10	aB	835	CLA	CAD-CBD-CGD-O2D
10	cA	805	CLA	CAD-CBD-CGD-O2D
10	cA	822	CLA	CAD-CBD-CGD-O2D
10	aL	202	CLA	CAD-CBD-CGD-O2D
10	cB	823	CLA	CAD-CBD-CGD-O2D
10	aB	823	CLA	CAD-CBD-CGD-O2D
10	cB	832	CLA	CAD-CBD-CGD-O2D
10	bL	202	CLA	CAD-CBD-CGD-O2D
10	cB	817	CLA	CAD-CBD-CGD-O2D
10	aA	822	CLA	CAD-CBD-CGD-O2D
10	bB	817	CLA	CAD-CBD-CGD-O2D
10	bB	832	CLA	CAD-CBD-CGD-O2D
10	cL	202	CLA	CAD-CBD-CGD-O2D
10	bB	830	CLA	CAD-CBD-CGD-O2D
10	aB	817	CLA	CAD-CBD-CGD-O2D
10	bB	835	CLA	CAD-CBD-CGD-O2D
10	aB	830	CLA	CAD-CBD-CGD-O2D
10	cA	816	CLA	C3-C5-C6-C7
10	aA	816	CLA	C3-C5-C6-C7
10	bA	816	CLA	C3-C5-C6-C7
10	cB	838	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	bB	838	CLA	C2-C3-C5-C6
10	aB	838	CLA	C2-C3-C5-C6
14	cA	852	LHG	C4-C5-C6-O8
14	aA	852	LHG	C4-C5-C6-O8
14	bA	852	LHG	C4-C5-C6-O8
10	aA	804	CLA	C8-C10-C11-C12
10	cA	804	CLA	C8-C10-C11-C12
16	aB	848	LMG	C19-C20-C21-C22
16	bB	848	LMG	C19-C20-C21-C22
16	cB	848	LMG	C19-C20-C21-C22
13	aI	102	BCR	C20-C21-C22-C23
13	bI	102	BCR	C20-C21-C22-C23
13	cI	103	BCR	C20-C21-C22-C23
10	bB	806	CLA	C6-C7-C8-C9
10	bA	804	CLA	C8-C10-C11-C12
11	bA	844	PQN	C25-C26-C27-C28
10	bA	837	CLA	O1A-CGA-O2A-C1
10	cA	836	CLA	O1A-CGA-O2A-C1
10	cA	837	CLA	O1A-CGA-O2A-C1
10	aA	837	CLA	O1A-CGA-O2A-C1
10	aA	836	CLA	O1A-CGA-O2A-C1
10	bA	836	CLA	O1A-CGA-O2A-C1
10	aB	806	CLA	C6-C7-C8-C9
10	cB	806	CLA	C6-C7-C8-C9
11	cA	844	PQN	C25-C26-C27-C28
10	bA	842	CLA	C13-C15-C16-C17
10	cA	842	CLA	C13-C15-C16-C17
11	aA	844	PQN	C25-C26-C27-C28
10	aA	842	CLA	C13-C15-C16-C17
14	cA	852	LHG	O7-C5-C6-O8
14	aA	852	LHG	O7-C5-C6-O8
14	bA	852	LHG	O7-C5-C6-O8
10	aA	823	CLA	C13-C15-C16-C17
10	bB	837	CLA	CBA-CGA-O2A-C1
10	cB	837	CLA	CBA-CGA-O2A-C1
10	aB	837	CLA	CBA-CGA-O2A-C1
10	bB	830	CLA	O1D-CGD-O2D-CED
10	aB	830	CLA	O1D-CGD-O2D-CED
10	bB	821	CLA	O1A-CGA-O2A-C1
10	cB	821	CLA	O1A-CGA-O2A-C1
10	aB	821	CLA	O1A-CGA-O2A-C1
10	cA	824	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	bA	824	CLA	O1A-CGA-O2A-C1
10	bA	823	CLA	C13-C15-C16-C17
10	aA	802	CLA	CHA-CBD-CGD-O1D
10	aA	802	CLA	CHA-CBD-CGD-O2D
10	cB	825	CLA	CHA-CBD-CGD-O1D
10	cB	825	CLA	CHA-CBD-CGD-O2D
10	aA	803	CLA	CHA-CBD-CGD-O1D
10	aA	807	CLA	CHA-CBD-CGD-O1D
10	cA	807	CLA	CHA-CBD-CGD-O1D
10	bA	807	CLA	CHA-CBD-CGD-O1D
10	cB	804	CLA	CHA-CBD-CGD-O1D
10	cB	804	CLA	CHA-CBD-CGD-O2D
10	aA	804	CLA	CHA-CBD-CGD-O1D
10	aA	804	CLA	CHA-CBD-CGD-O2D
10	bA	810	CLA	CHA-CBD-CGD-O2D
10	cA	814	CLA	CHA-CBD-CGD-O1D
10	cA	814	CLA	CHA-CBD-CGD-O2D
10	cB	810	CLA	CHA-CBD-CGD-O1D
10	cB	810	CLA	CHA-CBD-CGD-O2D
10	bB	807	CLA	CHA-CBD-CGD-O1D
10	bB	807	CLA	CHA-CBD-CGD-O2D
10	bA	804	CLA	CHA-CBD-CGD-O1D
10	bA	804	CLA	CHA-CBD-CGD-O2D
10	cB	807	CLA	CHA-CBD-CGD-O1D
10	cB	807	CLA	CHA-CBD-CGD-O2D
10	aA	814	CLA	CHA-CBD-CGD-O1D
10	aA	814	CLA	CHA-CBD-CGD-O2D
10	aB	810	CLA	CHA-CBD-CGD-O1D
10	aB	810	CLA	CHA-CBD-CGD-O2D
10	bB	825	CLA	CHA-CBD-CGD-O1D
10	bB	825	CLA	CHA-CBD-CGD-O2D
10	cA	804	CLA	CHA-CBD-CGD-O1D
10	cA	804	CLA	CHA-CBD-CGD-O2D
10	aA	854	CLA	CHA-CBD-CGD-O1D
10	aA	854	CLA	CHA-CBD-CGD-O2D
10	bA	803	CLA	CHA-CBD-CGD-O1D
10	bA	814	CLA	CHA-CBD-CGD-O1D
10	bA	814	CLA	CHA-CBD-CGD-O2D
10	aB	825	CLA	CHA-CBD-CGD-O1D
10	aB	825	CLA	CHA-CBD-CGD-O2D
10	aA	810	CLA	CHA-CBD-CGD-O2D
10	cA	854	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
10	cA	854	CLA	CHA-CBD-CGD-O2D
10	aB	804	CLA	CHA-CBD-CGD-O1D
10	aB	804	CLA	CHA-CBD-CGD-O2D
10	bA	854	CLA	CHA-CBD-CGD-O1D
10	bA	854	CLA	CHA-CBD-CGD-O2D
10	aB	807	CLA	CHA-CBD-CGD-O1D
10	aB	807	CLA	CHA-CBD-CGD-O2D
10	bB	804	CLA	CHA-CBD-CGD-O1D
10	bB	804	CLA	CHA-CBD-CGD-O2D
10	cA	802	CLA	CHA-CBD-CGD-O1D
10	cA	802	CLA	CHA-CBD-CGD-O2D
10	bA	802	CLA	CHA-CBD-CGD-O1D
10	bA	802	CLA	CHA-CBD-CGD-O2D
10	cA	803	CLA	CHA-CBD-CGD-O1D
10	bB	810	CLA	CHA-CBD-CGD-O1D
10	bB	810	CLA	CHA-CBD-CGD-O2D
10	cA	810	CLA	CHA-CBD-CGD-O2D
10	cB	830	CLA	O1D-CGD-O2D-CED
10	cB	820	CLA	O1D-CGD-O2D-CED
14	cA	852	LHG	C26-C27-C28-C29
14	aA	852	LHG	C26-C27-C28-C29
14	bA	852	LHG	C26-C27-C28-C29
9	cA	801	CL0	C16-C17-C18-C20
9	bA	801	CL0	C16-C17-C18-C20
9	aA	801	CL0	C16-C17-C18-C20
10	cA	823	CLA	C13-C15-C16-C17
10	cB	833	CLA	C3-C5-C6-C7
10	bA	810	CLA	C3-C5-C6-C7
10	bB	833	CLA	C3-C5-C6-C7
10	aA	810	CLA	C3-C5-C6-C7
10	cA	810	CLA	C3-C5-C6-C7
10	aB	833	CLA	C3-C5-C6-C7
10	aA	824	CLA	O1A-CGA-O2A-C1
13	bA	846	BCR	C22-C23-C24-C25
13	cA	846	BCR	C22-C23-C24-C25
13	aA	846	BCR	C22-C23-C24-C25
10	aB	820	CLA	O1D-CGD-O2D-CED
10	bB	820	CLA	O1D-CGD-O2D-CED
10	aB	832	CLA	C11-C12-C13-C14
10	cB	833	CLA	C11-C10-C8-C9
10	cB	804	CLA	C6-C7-C8-C9
10	bB	833	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
10	aB	827	CLA	C14-C13-C15-C16
10	cB	827	CLA	C14-C13-C15-C16
10	bB	827	CLA	C14-C13-C15-C16
10	cB	832	CLA	C11-C12-C13-C14
10	aB	804	CLA	C6-C7-C8-C9
10	bB	832	CLA	C11-C12-C13-C14
10	bB	804	CLA	C6-C7-C8-C9
10	aB	833	CLA	C11-C10-C8-C9
10	bA	808	CLA	C1A-C2A-CAA-CBA
10	cA	856	CLA	C1A-C2A-CAA-CBA
10	aA	808	CLA	C1A-C2A-CAA-CBA
10	cA	806	CLA	C1A-C2A-CAA-CBA
10	aA	806	CLA	C1A-C2A-CAA-CBA
10	bA	806	CLA	C1A-C2A-CAA-CBA
10	cA	815	CLA	C1A-C2A-CAA-CBA
10	bA	856	CLA	C1A-C2A-CAA-CBA
10	cA	808	CLA	C1A-C2A-CAA-CBA
10	aA	815	CLA	C1A-C2A-CAA-CBA
10	aA	856	CLA	C1A-C2A-CAA-CBA
10	bA	815	CLA	C1A-C2A-CAA-CBA
10	cA	827	CLA	C5-C6-C7-C8
14	cA	852	LHG	C17-C18-C19-C20
14	aA	852	LHG	C17-C18-C19-C20
14	bA	852	LHG	C17-C18-C19-C20
14	aA	852	LHG	C7-C8-C9-C10
14	bA	852	LHG	C7-C8-C9-C10
10	aA	802	CLA	C2A-CAA-CBA-CGA
10	cA	802	CLA	C2A-CAA-CBA-CGA
10	bA	802	CLA	C2A-CAA-CBA-CGA
10	cA	856	CLA	O1A-CGA-O2A-C1
10	bA	856	CLA	O1A-CGA-O2A-C1
10	aA	856	CLA	O1A-CGA-O2A-C1
13	aB	849	BCR	C7-C8-C9-C10
13	bB	849	BCR	C7-C8-C9-C10
13	cB	849	BCR	C7-C8-C9-C10
14	cA	852	LHG	C7-C8-C9-C10
10	cB	818	CLA	C11-C12-C13-C14
10	bA	827	CLA	C5-C6-C7-C8
10	aB	818	CLA	C11-C12-C13-C14
10	bB	818	CLA	C11-C12-C13-C14
14	aA	855	LHG	C4-O6-P-O5
14	bA	855	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
14	cA	855	LHG	C4-O6-P-O5
10	aA	827	CLA	C5-C6-C7-C8
10	cL	203	CLA	CBA-CGA-O2A-C1
10	cB	804	CLA	C4-C3-C5-C6
10	bB	807	CLA	C4-C3-C5-C6
10	cB	807	CLA	C4-C3-C5-C6
10	cB	815	CLA	C4-C3-C5-C6
10	aB	807	CLA	C4-C3-C5-C6
10	aB	815	CLA	C4-C3-C5-C6
10	bB	815	CLA	C4-C3-C5-C6
14	cA	852	LHG	O6-C4-C5-C6
14	aA	852	LHG	O6-C4-C5-C6
14	bA	852	LHG	O6-C4-C5-C6
10	aA	803	CLA	CAD-CBD-CGD-O1D
10	aA	812	CLA	CAD-CBD-CGD-O1D
10	cB	804	CLA	CAD-CBD-CGD-O1D
10	aA	804	CLA	CAD-CBD-CGD-O1D
10	bB	807	CLA	CAD-CBD-CGD-O1D
10	bA	804	CLA	CAD-CBD-CGD-O1D
10	cB	807	CLA	CAD-CBD-CGD-O1D
10	cA	804	CLA	CAD-CBD-CGD-O1D
10	aA	854	CLA	CAD-CBD-CGD-O1D
10	bA	803	CLA	CAD-CBD-CGD-O1D
10	cA	812	CLA	CAD-CBD-CGD-O1D
10	cB	814	CLA	CAD-CBD-CGD-O1D
10	cA	854	CLA	CAD-CBD-CGD-O1D
10	aB	804	CLA	CAD-CBD-CGD-O1D
10	bA	854	CLA	CAD-CBD-CGD-O1D
10	aB	807	CLA	CAD-CBD-CGD-O1D
10	bB	804	CLA	CAD-CBD-CGD-O1D
10	cA	803	CLA	CAD-CBD-CGD-O1D
10	bA	812	CLA	CAD-CBD-CGD-O1D
10	aB	805	CLA	C2C-C3C-CAC-CBC
10	aL	203	CLA	CBA-CGA-O2A-C1
10	bL	203	CLA	CBA-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
10	aB	837	CLA	O1A-CGA-O2A-C1
10	bB	805	CLA	C2C-C3C-CAC-CBC
10	cB	805	CLA	C2C-C3C-CAC-CBC
10	bA	821	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
10	aA	821	CLA	C2A-CAA-CBA-CGA
10	cA	821	CLA	C2A-CAA-CBA-CGA
10	cB	841	CLA	C2-C1-O2A-CGA
10	aA	829	CLA	C2-C1-O2A-CGA
10	bB	807	CLA	C2-C1-O2A-CGA
10	cA	836	CLA	C2-C1-O2A-CGA
10	cB	807	CLA	C2-C1-O2A-CGA
10	aB	841	CLA	C2-C1-O2A-CGA
10	cA	829	CLA	C2-C1-O2A-CGA
10	bB	841	CLA	C2-C1-O2A-CGA
10	bA	829	CLA	C2-C1-O2A-CGA
10	aA	836	CLA	C2-C1-O2A-CGA
10	aB	807	CLA	C2-C1-O2A-CGA
10	bA	836	CLA	C2-C1-O2A-CGA
10	aB	820	CLA	O1A-CGA-O2A-C1
10	bB	820	CLA	O1A-CGA-O2A-C1
10	aB	826	CLA	C15-C16-C17-C18
10	cB	826	CLA	C15-C16-C17-C18
10	bB	826	CLA	C15-C16-C17-C18
10	cB	841	CLA	C11-C10-C8-C7
10	aB	829	CLA	C6-C7-C8-C10
10	aB	832	CLA	C11-C12-C13-C15
10	aA	812	CLA	C11-C12-C13-C15
10	cB	833	CLA	C11-C10-C8-C7
10	aA	829	CLA	C11-C12-C13-C15
10	bA	842	CLA	C11-C10-C8-C7
10	cA	824	CLA	C11-C12-C13-C15
10	bA	824	CLA	C11-C12-C13-C15
10	bB	833	CLA	C11-C10-C8-C7
10	aB	827	CLA	C12-C13-C15-C16
10	aB	841	CLA	C11-C10-C8-C7
10	cA	812	CLA	C11-C12-C13-C15
10	cB	827	CLA	C12-C13-C15-C16
10	cA	842	CLA	C11-C10-C8-C7
10	bB	827	CLA	C12-C13-C15-C16
10	bB	829	CLA	C6-C7-C8-C10
10	cB	832	CLA	C11-C12-C13-C15
10	cB	838	CLA	C12-C13-C15-C16
10	cB	829	CLA	C6-C7-C8-C10
10	bB	805	CLA	C11-C10-C8-C7
10	cL	205	CLA	C6-C7-C8-C10
10	aL	205	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
10	aB	805	CLA	C11-C10-C8-C7
10	aA	824	CLA	C11-C12-C13-C15
10	cA	829	CLA	C11-C12-C13-C15
10	bB	841	CLA	C11-C10-C8-C7
10	bA	829	CLA	C11-C12-C13-C15
10	bB	832	CLA	C11-C12-C13-C15
10	bL	205	CLA	C6-C7-C8-C10
10	cB	805	CLA	C11-C10-C8-C7
10	bB	838	CLA	C12-C13-C15-C16
10	aA	842	CLA	C11-C10-C8-C7
10	aB	838	CLA	C12-C13-C15-C16
10	bA	812	CLA	C11-C12-C13-C15
10	aB	833	CLA	C11-C10-C8-C7
14	cA	852	LHG	O6-C4-C5-O7
14	aA	852	LHG	O6-C4-C5-O7
14	bA	852	LHG	O6-C4-C5-O7
9	cA	801	CL0	C15-C16-C17-C18
9	bA	801	CL0	C15-C16-C17-C18
9	aA	801	CL0	C15-C16-C17-C18
10	aB	804	CLA	C4-C3-C5-C6
10	bB	804	CLA	C4-C3-C5-C6
10	cA	823	CLA	C2-C3-C5-C6
10	aB	820	CLA	C2-C3-C5-C6
10	bA	823	CLA	C2-C3-C5-C6
10	bB	807	CLA	C2-C3-C5-C6
10	cB	807	CLA	C2-C3-C5-C6
10	aA	823	CLA	C2-C3-C5-C6
10	aB	807	CLA	C2-C3-C5-C6
10	aB	820	CLA	CBA-CGA-O2A-C1
10	bB	820	CLA	CBA-CGA-O2A-C1
10	aA	825	CLA	C5-C6-C7-C8
10	cA	825	CLA	C5-C6-C7-C8
10	bA	825	CLA	C5-C6-C7-C8
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	cB	820	CLA	CBA-CGA-O2A-C1
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	cA	827	CLA	C10-C11-C12-C13
10	aA	827	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
10	bA	827	CLA	C10-C11-C12-C13
10	cB	837	CLA	O1D-CGD-O2D-CED
10	cB	841	CLA	C11-C12-C13-C14
10	aB	832	CLA	C6-C7-C8-C9
10	aA	805	CLA	C14-C13-C15-C16
10	cB	818	CLA	C11-C10-C8-C9
10	cA	805	CLA	C14-C13-C15-C16
10	aA	804	CLA	C11-C10-C8-C9
10	cL	204	CLA	C6-C7-C8-C9
10	aB	818	CLA	C11-C10-C8-C9
10	bA	804	CLA	C11-C10-C8-C9
10	bL	204	CLA	C6-C7-C8-C9
10	cA	804	CLA	C11-C10-C8-C9
10	aB	841	CLA	C11-C12-C13-C14
10	cB	832	CLA	C6-C7-C8-C9
10	bB	818	CLA	C11-C10-C8-C9
10	bB	841	CLA	C11-C12-C13-C14
10	bB	832	CLA	C6-C7-C8-C9
10	aL	204	CLA	C6-C7-C8-C9
10	bB	837	CLA	O1D-CGD-O2D-CED
10	aB	837	CLA	O1D-CGD-O2D-CED
10	bB	802	CLA	C2A-CAA-CBA-CGA
10	aA	827	CLA	C2A-CAA-CBA-CGA
10	bA	827	CLA	C2A-CAA-CBA-CGA
10	cA	827	CLA	C2A-CAA-CBA-CGA
10	bA	842	CLA	C2A-CAA-CBA-CGA
10	cA	842	CLA	C2A-CAA-CBA-CGA
10	cB	802	CLA	C2A-CAA-CBA-CGA
10	aB	802	CLA	C2A-CAA-CBA-CGA
10	aA	842	CLA	C2A-CAA-CBA-CGA
10	cB	817	CLA	CAA-CBA-CGA-O2A
10	bB	817	CLA	CAA-CBA-CGA-O2A
10	aB	817	CLA	CAA-CBA-CGA-O2A
10	aB	840	CLA	C16-C17-C18-C20
10	bB	814	CLA	C4-C3-C5-C6
10	cB	814	CLA	C4-C3-C5-C6
10	aB	814	CLA	C4-C3-C5-C6
10	cB	820	CLA	C2-C3-C5-C6
10	bB	820	CLA	C2-C3-C5-C6
10	bB	840	CLA	C16-C17-C18-C20
10	cB	840	CLA	C16-C17-C18-C20
10	cA	841	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
10	aA	841	CLA	C2A-CAA-CBA-CGA
10	bA	841	CLA	C2A-CAA-CBA-CGA
13	aB	843	BCR	C23-C24-C25-C26
13	aB	847	BCR	C1-C6-C7-C8
13	cB	847	BCR	C1-C6-C7-C8
13	aB	849	BCR	C5-C6-C7-C8
13	aB	849	BCR	C23-C24-C25-C30
13	bB	849	BCR	C5-C6-C7-C8
13	bB	849	BCR	C23-C24-C25-C30
13	cB	849	BCR	C5-C6-C7-C8
13	cB	849	BCR	C23-C24-C25-C30
13	bA	847	BCR	C5-C6-C7-C8
13	aA	847	BCR	C5-C6-C7-C8
13	bB	847	BCR	C1-C6-C7-C8
13	cB	843	BCR	C23-C24-C25-C26
13	cA	847	BCR	C5-C6-C7-C8
13	bB	843	BCR	C23-C24-C25-C26
14	cA	852	LHG	C10-C11-C12-C13
14	aA	852	LHG	C10-C11-C12-C13
14	bA	852	LHG	C10-C11-C12-C13
14	aA	852	LHG	C14-C15-C16-C17
14	bA	852	LHG	C14-C15-C16-C17
14	aA	855	LHG	C3-O3-P-O6
14	bA	855	LHG	C3-O3-P-O6
14	cA	855	LHG	C3-O3-P-O6
14	cA	852	LHG	C14-C15-C16-C17
10	aB	827	CLA	C2-C3-C5-C6
10	bA	821	CLA	C1-C2-C3-C4
10	cA	856	CLA	C1-C2-C3-C4
10	aA	821	CLA	C1-C2-C3-C4
10	bA	856	CLA	C1-C2-C3-C4
10	aA	856	CLA	C1-C2-C3-C4
10	cA	821	CLA	C1-C2-C3-C4
10	cA	841	CLA	C2-C1-O2A-CGA
10	bB	811	CLA	C2-C1-O2A-CGA
10	cA	828	CLA	C2-C1-O2A-CGA
10	cB	818	CLA	C2-C1-O2A-CGA
10	aA	841	CLA	C2-C1-O2A-CGA
10	aB	818	CLA	C2-C1-O2A-CGA
10	aB	811	CLA	C2-C1-O2A-CGA
10	aA	828	CLA	C2-C1-O2A-CGA
10	bA	828	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
10	bB	818	CLA	C2-C1-O2A-CGA
10	cB	811	CLA	C2-C1-O2A-CGA
10	bA	841	CLA	C2-C1-O2A-CGA
10	aA	841	CLA	C10-C11-C12-C13
10	aB	830	CLA	C10-C11-C12-C13
10	bB	805	CLA	C2A-CAA-CBA-CGA
10	aB	805	CLA	C2A-CAA-CBA-CGA
10	cB	805	CLA	C2A-CAA-CBA-CGA
10	cA	841	CLA	C10-C11-C12-C13
10	cB	830	CLA	C10-C11-C12-C13
10	bA	841	CLA	C10-C11-C12-C13
10	cB	836	CLA	C2A-CAA-CBA-CGA
10	aB	836	CLA	C2A-CAA-CBA-CGA
10	bB	828	CLA	C12-C13-C15-C16
10	bB	836	CLA	C2A-CAA-CBA-CGA
10	cB	828	CLA	C12-C13-C15-C16
10	aB	828	CLA	C12-C13-C15-C16
10	bB	830	CLA	C10-C11-C12-C13
10	bB	823	CLA	C6-C7-C8-C10
10	cB	823	CLA	C6-C7-C8-C10
10	aB	823	CLA	C6-C7-C8-C10
10	bB	837	CLA	C4-C3-C5-C6
10	bA	811	CLA	C4-C3-C5-C6
10	aA	811	CLA	C4-C3-C5-C6
10	cA	811	CLA	C4-C3-C5-C6
10	aB	837	CLA	C4-C3-C5-C6
10	cB	841	CLA	C11-C10-C8-C9
10	aB	829	CLA	C6-C7-C8-C9
10	bA	805	CLA	C14-C13-C15-C16
10	aA	829	CLA	C11-C12-C13-C14
10	bB	814	CLA	C11-C12-C13-C14
10	cA	824	CLA	C11-C12-C13-C14
10	bA	824	CLA	C11-C12-C13-C14
10	aB	841	CLA	C11-C10-C8-C9
10	bB	829	CLA	C6-C7-C8-C9
10	cB	829	CLA	C6-C7-C8-C9
10	cB	814	CLA	C11-C12-C13-C14
10	cL	205	CLA	C6-C7-C8-C9
10	aL	205	CLA	C6-C7-C8-C9
10	aA	824	CLA	C11-C12-C13-C14
10	cA	829	CLA	C11-C12-C13-C14
10	bB	841	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
10	aA	826	CLA	C6-C7-C8-C9
10	bA	829	CLA	C11-C12-C13-C14
10	bL	205	CLA	C6-C7-C8-C9
10	bA	826	CLA	C6-C7-C8-C9
10	aB	814	CLA	C11-C12-C13-C14
10	cA	826	CLA	C6-C7-C8-C9
10	cB	827	CLA	C2-C3-C5-C6
10	bB	827	CLA	C2-C3-C5-C6
10	bA	837	CLA	C8-C10-C11-C12
10	cA	837	CLA	C8-C10-C11-C12
10	aL	202	CLA	CBD-CGD-O2D-CED
10	bL	202	CLA	CBD-CGD-O2D-CED
10	aA	837	CLA	C8-C10-C11-C12
10	cL	202	CLA	CBD-CGD-O2D-CED
10	aB	803	CLA	C8-C10-C11-C12
10	bB	803	CLA	C8-C10-C11-C12
10	bA	817	CLA	CAA-CBA-CGA-O2A
10	aA	817	CLA	CAA-CBA-CGA-O2A
10	cA	817	CLA	CAA-CBA-CGA-O2A
10	cB	803	CLA	C8-C10-C11-C12
10	bA	837	CLA	CBA-CGA-O2A-C1
10	cA	837	CLA	CBA-CGA-O2A-C1
10	aA	837	CLA	CBA-CGA-O2A-C1
10	cB	837	CLA	C4-C3-C5-C6
10	cB	815	CLA	C2-C3-C5-C6
10	aB	815	CLA	C2-C3-C5-C6
10	bB	815	CLA	C2-C3-C5-C6
10	bB	807	CLA	CAA-CBA-CGA-O2A
10	cB	807	CLA	CAA-CBA-CGA-O2A
10	aB	820	CLA	C15-C16-C17-C18
10	cB	820	CLA	C15-C16-C17-C18
10	cB	818	CLA	O1A-CGA-O2A-C1
10	aB	818	CLA	O1A-CGA-O2A-C1
10	aB	807	CLA	CAA-CBA-CGA-O2A
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	bB	820	CLA	C15-C16-C17-C18
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	aA	832	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	bA	828	CLA	CAA-CBA-CGA-O2A
10	aA	833	CLA	C2A-CAA-CBA-CGA
10	cA	833	CLA	C2A-CAA-CBA-CGA
10	bA	833	CLA	C2A-CAA-CBA-CGA
13	bB	845	BCR	C11-C10-C9-C34
13	cB	845	BCR	C11-C10-C9-C34
13	cA	851	BCR	C11-C10-C9-C34
13	cL	207	BCR	C20-C21-C22-C37
13	aB	849	BCR	C16-C17-C18-C36
13	aA	851	BCR	C11-C10-C9-C34
13	bB	849	BCR	C16-C17-C18-C36
13	aB	845	BCR	C11-C10-C9-C34
13	bA	851	BCR	C11-C10-C9-C34
13	cB	849	BCR	C16-C17-C18-C36
13	bA	846	BCR	C20-C21-C22-C37
13	bL	207	BCR	C20-C21-C22-C37
13	aI	102	BCR	C20-C21-C22-C37
13	bI	102	BCR	C20-C21-C22-C37
13	cA	846	BCR	C20-C21-C22-C37
13	aA	846	BCR	C20-C21-C22-C37
13	cI	103	BCR	C20-C21-C22-C37
13	aL	207	BCR	C20-C21-C22-C37
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	cA	828	CLA	CAA-CBA-CGA-O2A
10	aA	828	CLA	CAA-CBA-CGA-O2A
10	cB	818	CLA	CBA-CGA-O2A-C1
10	aB	818	CLA	CBA-CGA-O2A-C1
10	aA	812	CLA	C11-C10-C8-C9
10	cA	812	CLA	C11-C10-C8-C9
10	bA	812	CLA	C11-C10-C8-C9
10	cA	838	CLA	O1A-CGA-O2A-C1
10	bB	823	CLA	C2-C1-O2A-CGA
10	cB	823	CLA	C2-C1-O2A-CGA
10	bA	811	CLA	C2-C1-O2A-CGA
10	aB	823	CLA	C2-C1-O2A-CGA
10	aA	811	CLA	C2-C1-O2A-CGA
10	cA	811	CLA	C2-C1-O2A-CGA
10	bB	822	CLA	C1A-C2A-CAA-CBA
10	cB	822	CLA	C1A-C2A-CAA-CBA
10	aB	820	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
10	bB	801	CLA	C1A-C2A-CAA-CBA
10	cA	830	CLA	C1A-C2A-CAA-CBA
10	cB	813	CLA	C1A-C2A-CAA-CBA
10	cB	801	CLA	C1A-C2A-CAA-CBA
10	aB	801	CLA	C1A-C2A-CAA-CBA
10	cB	820	CLA	C1A-C2A-CAA-CBA
10	bB	820	CLA	C1A-C2A-CAA-CBA
10	aB	813	CLA	C1A-C2A-CAA-CBA
10	bA	830	CLA	C1A-C2A-CAA-CBA
10	bB	813	CLA	C1A-C2A-CAA-CBA
10	aA	830	CLA	C1A-C2A-CAA-CBA
10	aB	822	CLA	C1A-C2A-CAA-CBA
10	bB	818	CLA	CBA-CGA-O2A-C1
10	aA	820	CLA	C8-C10-C11-C12
10	bA	820	CLA	C8-C10-C11-C12
10	bA	811	CLA	C2-C3-C5-C6
10	cA	811	CLA	C2-C3-C5-C6
10	aA	838	CLA	O1A-CGA-O2A-C1
11	cB	842	PQN	C26-C27-C28-C29
11	bB	842	PQN	C26-C27-C28-C29
11	aB	842	PQN	C26-C27-C28-C29
10	cA	820	CLA	C8-C10-C11-C12
10	bB	802	CLA	C12-C13-C15-C16
10	bA	835	CLA	C12-C13-C15-C16
9	cA	801	CL0	C12-C13-C15-C16
10	cA	835	CLA	C12-C13-C15-C16
9	bA	801	CL0	C12-C13-C15-C16
10	cB	802	CLA	C12-C13-C15-C16
10	aB	802	CLA	C12-C13-C15-C16
10	aA	835	CLA	C12-C13-C15-C16
9	aA	801	CL0	C12-C13-C15-C16
10	bA	838	CLA	O1A-CGA-O2A-C1
10	bB	837	CLA	C2-C3-C5-C6
10	bB	814	CLA	C2-C3-C5-C6
10	aA	811	CLA	C2-C3-C5-C6
10	cB	837	CLA	C2-C3-C5-C6
10	cB	814	CLA	C2-C3-C5-C6
10	aB	837	CLA	C2-C3-C5-C6
10	aB	814	CLA	C2-C3-C5-C6
10	bA	832	CLA	CBA-CGA-O2A-C1
13	bB	845	BCR	C11-C10-C9-C8
13	bB	845	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
13	cB	845	BCR	C11-C10-C9-C8
13	cB	845	BCR	C20-C21-C22-C23
13	cA	851	BCR	C16-C17-C18-C19
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
10	cA	819	CLA	C5-C6-C7-C8
10	aA	819	CLA	C5-C6-C7-C8
10	bA	819	CLA	C5-C6-C7-C8
10	aB	811	CLA	C3-C5-C6-C7
10	cB	811	CLA	C3-C5-C6-C7
13	aB	847	BCR	C9-C10-C11-C12
13	cB	847	BCR	C9-C10-C11-C12
13	bB	847	BCR	C9-C10-C11-C12
10	aB	820	CLA	C10-C11-C12-C13
10	cB	820	CLA	C10-C11-C12-C13
10	bB	820	CLA	C10-C11-C12-C13
10	cB	808	CLA	C10-C11-C12-C13
10	aB	808	CLA	C10-C11-C12-C13
10	bB	808	CLA	C10-C11-C12-C13
10	bB	811	CLA	C3-C5-C6-C7
10	aA	832	CLA	CBA-CGA-O2A-C1
10	cA	832	CLA	CBA-CGA-O2A-C1
10	cB	819	CLA	C4-C3-C5-C6
10	bB	819	CLA	C4-C3-C5-C6
10	aA	820	CLA	C4-C3-C5-C6
10	bA	820	CLA	C4-C3-C5-C6
10	aB	819	CLA	C4-C3-C5-C6
10	cA	820	CLA	C4-C3-C5-C6
10	cB	832	CLA	C2A-CAA-CBA-CGA
10	cB	818	CLA	C8-C10-C11-C12
10	aB	818	CLA	C8-C10-C11-C12
10	bB	818	CLA	C8-C10-C11-C12
10	bB	837	CLA	C11-C12-C13-C15
10	cB	837	CLA	C11-C12-C13-C15
10	aB	837	CLA	C11-C12-C13-C15
13	cA	851	BCR	C1-C6-C7-C8
13	cL	207	BCR	C1-C6-C7-C8
13	aB	849	BCR	C1-C6-C7-C8
13	aA	851	BCR	C1-C6-C7-C8
13	bB	849	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
10	cA	831	CLA	C11-C10-C8-C9
13	bA	851	BCR	C1-C6-C7-C8
13	cB	849	BCR	C1-C6-C7-C8
13	bI	101	BCR	C23-C24-C25-C30
13	cI	102	BCR	C23-C24-C25-C30
13	bL	207	BCR	C1-C6-C7-C8
13	bL	206	BCR	C1-C6-C7-C8
13	aI	101	BCR	C23-C24-C25-C30
13	aL	206	BCR	C1-C6-C7-C8
10	cA	812	CLA	C11-C12-C13-C14
13	cL	206	BCR	C1-C6-C7-C8
13	aA	848	BCR	C23-C24-C25-C26
13	aA	848	BCR	C23-C24-C25-C30
13	cA	848	BCR	C23-C24-C25-C26
13	cA	848	BCR	C23-C24-C25-C30
10	bA	831	CLA	C11-C10-C8-C9
13	bA	848	BCR	C23-C24-C25-C26
13	bA	848	BCR	C23-C24-C25-C30
13	aL	207	BCR	C1-C6-C7-C8
10	aA	831	CLA	C11-C10-C8-C9
10	bA	812	CLA	C11-C12-C13-C14
10	cA	805	CLA	C15-C16-C17-C18
13	cA	849	BCR	C19-C20-C21-C22
13	bA	849	BCR	C19-C20-C21-C22
13	aA	849	BCR	C19-C20-C21-C22
16	aB	848	LMG	C20-C21-C22-C23
16	cB	848	LMG	C20-C21-C22-C23
10	bA	805	CLA	C15-C16-C17-C18
10	aA	805	CLA	C15-C16-C17-C18
16	bB	848	LMG	C20-C21-C22-C23
10	aB	826	CLA	C4-C3-C5-C6
10	cB	826	CLA	C4-C3-C5-C6
10	bB	826	CLA	C4-C3-C5-C6
10	bB	832	CLA	C2A-CAA-CBA-CGA
13	cB	846	BCR	C7-C8-C9-C10
13	aB	847	BCR	C21-C22-C23-C24
13	cB	847	BCR	C21-C22-C23-C24
13	bB	846	BCR	C7-C8-C9-C10
13	aB	846	BCR	C7-C8-C9-C10
13	bB	847	BCR	C21-C22-C23-C24
10	bB	833	CLA	C10-C11-C12-C13
10	aB	833	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
10	cB	833	CLA	C10-C11-C12-C13
10	aA	812	CLA	C11-C10-C8-C7
10	cA	812	CLA	C11-C10-C8-C7
10	bA	812	CLA	C11-C10-C8-C7
10	aA	820	CLA	C2-C3-C5-C6
10	bA	820	CLA	C2-C3-C5-C6
10	aB	826	CLA	C2-C3-C5-C6
10	cB	826	CLA	C2-C3-C5-C6
10	bB	826	CLA	C2-C3-C5-C6
10	cA	820	CLA	C2-C3-C5-C6
10	aB	832	CLA	C2A-CAA-CBA-CGA
10	aL	205	CLA	C8-C10-C11-C12
10	bL	205	CLA	C8-C10-C11-C12
10	cB	832	CLA	CBD-CGD-O2D-CED
10	bB	832	CLA	CBD-CGD-O2D-CED
10	cA	854	CLA	C4C-C3C-CAC-CBC
10	bA	854	CLA	C4C-C3C-CAC-CBC
10	aA	854	CLA	C4C-C3C-CAC-CBC
10	bB	814	CLA	CAA-CBA-CGA-O2A
10	cB	814	CLA	CAA-CBA-CGA-O2A
16	aB	848	LMG	O7-C10-C11-C12
16	bB	848	LMG	O7-C10-C11-C12
10	aB	814	CLA	CAA-CBA-CGA-O2A
16	cB	848	LMG	O7-C10-C11-C12
10	cL	205	CLA	C8-C10-C11-C12
10	cB	818	CLA	CAA-CBA-CGA-O1A
10	aB	818	CLA	CAA-CBA-CGA-O1A
10	bB	818	CLA	CAA-CBA-CGA-O1A
10	cA	841	CLA	CAA-CBA-CGA-O2A
10	aA	841	CLA	CAA-CBA-CGA-O2A
10	cB	823	CLA	CAA-CBA-CGA-O2A
10	aB	823	CLA	CAA-CBA-CGA-O2A
10	bB	825	CLA	CAA-CBA-CGA-O2A
10	aB	825	CLA	CAA-CBA-CGA-O2A
10	bA	841	CLA	CAA-CBA-CGA-O2A
10	bB	823	CLA	C6-C7-C8-C9
10	cB	823	CLA	C6-C7-C8-C9
10	aB	832	CLA	CBD-CGD-O2D-CED
10	cB	810	CLA	C4-C3-C5-C6
10	aB	810	CLA	C4-C3-C5-C6
10	bB	810	CLA	C4-C3-C5-C6
10	cB	825	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
10	bB	823	CLA	CAA-CBA-CGA-O2A
10	aL	202	CLA	CAA-CBA-CGA-O2A
10	bL	202	CLA	CAA-CBA-CGA-O2A
10	cL	202	CLA	CAA-CBA-CGA-O2A
10	bB	819	CLA	C2-C3-C5-C6
10	bB	829	CLA	CBA-CGA-O2A-C1
10	cB	829	CLA	CBA-CGA-O2A-C1
10	aA	838	CLA	CBA-CGA-O2A-C1
11	cB	842	PQN	C26-C27-C28-C30
10	aB	823	CLA	C6-C7-C8-C9
11	bB	842	PQN	C26-C27-C28-C30
11	aB	842	PQN	C26-C27-C28-C30
14	cA	852	LHG	O7-C7-C8-C9
14	aA	852	LHG	O7-C7-C8-C9
14	bA	852	LHG	O7-C7-C8-C9
10	cB	817	CLA	C3A-C2A-CAA-CBA
10	bB	817	CLA	C3A-C2A-CAA-CBA
10	aB	817	CLA	C3A-C2A-CAA-CBA
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	cA	828	CLA	C10-C11-C12-C13
10	aA	828	CLA	C10-C11-C12-C13
10	bA	828	CLA	C10-C11-C12-C13
10	aA	812	CLA	C11-C12-C13-C14
10	cB	838	CLA	C14-C13-C15-C16
10	bB	838	CLA	C14-C13-C15-C16
10	aB	838	CLA	C14-C13-C15-C16
10	bB	821	CLA	CAD-CBD-CGD-O2D
10	bA	808	CLA	CAD-CBD-CGD-O2D
10	cB	821	CLA	CAD-CBD-CGD-O2D
10	aB	821	CLA	CAD-CBD-CGD-O2D
10	aA	808	CLA	CAD-CBD-CGD-O2D
10	cA	813	CLA	CAD-CBD-CGD-O2D
10	aA	813	CLA	CAD-CBD-CGD-O2D
10	bA	813	CLA	CAD-CBD-CGD-O2D
10	cA	808	CLA	CAD-CBD-CGD-O2D
10	bB	811	CLA	CAA-CBA-CGA-O2A
10	aB	811	CLA	CAA-CBA-CGA-O2A
10	cA	819	CLA	CAA-CBA-CGA-O2A
10	bA	819	CLA	CAA-CBA-CGA-O2A
10	aA	819	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
10	cB	811	CLA	CAA-CBA-CGA-O2A
10	cA	818	CLA	C4-C3-C5-C6
10	bB	802	CLA	C4-C3-C5-C6
10	bA	818	CLA	C4-C3-C5-C6
10	aL	203	CLA	C4-C3-C5-C6
10	aA	818	CLA	C4-C3-C5-C6
10	bL	203	CLA	C4-C3-C5-C6
10	cB	802	CLA	C4-C3-C5-C6
10	aB	802	CLA	C4-C3-C5-C6
10	cL	203	CLA	C4-C3-C5-C6
10	bA	804	CLA	C13-C15-C16-C17
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	823	CLA	O2A-C1-C2-C3
10	bA	831	CLA	O2A-C1-C2-C3
10	aA	831	CLA	O2A-C1-C2-C3
10	cB	819	CLA	C2-C3-C5-C6
10	aL	203	CLA	C2-C3-C5-C6
10	aB	819	CLA	C2-C3-C5-C6
10	bL	203	CLA	C2-C3-C5-C6
10	cL	203	CLA	C2-C3-C5-C6
10	cB	829	CLA	O1A-CGA-O2A-C1
13	cA	849	BCR	C7-C8-C9-C10
13	bA	849	BCR	C7-C8-C9-C10
13	bA	846	BCR	C17-C18-C19-C20
13	cA	846	BCR	C17-C18-C19-C20
13	aA	846	BCR	C17-C18-C19-C20
13	aM	101	BCR	C7-C8-C9-C10
13	bM	101	BCR	C7-C8-C9-C10
13	aA	849	BCR	C7-C8-C9-C10
13	cM	101	BCR	C7-C8-C9-C10
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	aB	829	CLA	O1A-CGA-O2A-C1
10	bB	829	CLA	O1A-CGA-O2A-C1
10	cB	838	CLA	O1A-CGA-O2A-C1
10	bB	838	CLA	O1A-CGA-O2A-C1
10	aB	838	CLA	O1A-CGA-O2A-C1
10	bB	803	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
10	aB	803	CLA	C15-C16-C17-C18
10	bA	833	CLA	C13-C15-C16-C17
10	aA	834	CLA	C4-C3-C5-C6
10	cA	834	CLA	C4-C3-C5-C6
10	aA	826	CLA	C4-C3-C5-C6
10	bA	826	CLA	C4-C3-C5-C6
10	bA	834	CLA	C4-C3-C5-C6
10	cA	826	CLA	C4-C3-C5-C6
10	cB	817	CLA	C2A-CAA-CBA-CGA
10	bB	817	CLA	C2A-CAA-CBA-CGA
10	aB	817	CLA	C2A-CAA-CBA-CGA
10	aA	833	CLA	C13-C15-C16-C17
10	cA	833	CLA	C13-C15-C16-C17
10	bB	802	CLA	C2-C3-C5-C6
10	cB	804	CLA	C2-C3-C5-C6
10	aB	804	CLA	C2-C3-C5-C6
10	bB	804	CLA	C2-C3-C5-C6
10	cB	802	CLA	C2-C3-C5-C6
10	aB	802	CLA	C2-C3-C5-C6
14	aA	852	LHG	C35-C36-C37-C38
14	bA	852	LHG	C35-C36-C37-C38
14	cA	852	LHG	C35-C36-C37-C38
10	bB	828	CLA	C10-C11-C12-C13
10	cB	828	CLA	C10-C11-C12-C13
10	aB	828	CLA	C10-C11-C12-C13
14	aA	855	LHG	O7-C7-C8-C9
14	bA	855	LHG	O7-C7-C8-C9
14	cA	855	LHG	O7-C7-C8-C9
9	cA	801	CL0	C3-C5-C6-C7
10	bB	806	CLA	CHA-CBD-CGD-O2D
10	aA	833	CLA	CHA-CBD-CGD-O1D
10	aA	833	CLA	CHA-CBD-CGD-O2D
10	aB	829	CLA	CHA-CBD-CGD-O1D
10	aB	829	CLA	CHA-CBD-CGD-O2D
10	aA	803	CLA	CHA-CBD-CGD-O2D
10	aB	816	CLA	CHA-CBD-CGD-O1D
10	aB	816	CLA	CHA-CBD-CGD-O2D
10	aA	812	CLA	CHA-CBD-CGD-O1D
10	aB	806	CLA	CHA-CBD-CGD-O2D
10	cB	833	CLA	CHA-CBD-CGD-O1D
10	cB	833	CLA	CHA-CBD-CGD-O2D
10	cB	806	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
10	bB	831	CLA	CHA-CBD-CGD-O2D
10	cA	824	CLA	CHA-CBD-CGD-O1D
10	cA	824	CLA	CHA-CBD-CGD-O2D
10	bA	824	CLA	CHA-CBD-CGD-O1D
10	bA	824	CLA	CHA-CBD-CGD-O2D
10	bB	833	CLA	CHA-CBD-CGD-O1D
10	bB	833	CLA	CHA-CBD-CGD-O2D
10	cA	833	CLA	CHA-CBD-CGD-O1D
10	cA	833	CLA	CHA-CBD-CGD-O2D
10	bA	803	CLA	CHA-CBD-CGD-O2D
10	cA	812	CLA	CHA-CBD-CGD-O1D
10	bB	829	CLA	CHA-CBD-CGD-O1D
10	bB	829	CLA	CHA-CBD-CGD-O2D
10	cB	829	CLA	CHA-CBD-CGD-O1D
10	cB	829	CLA	CHA-CBD-CGD-O2D
10	bB	816	CLA	CHA-CBD-CGD-O1D
10	bB	816	CLA	CHA-CBD-CGD-O2D
10	bA	833	CLA	CHA-CBD-CGD-O1D
10	bA	833	CLA	CHA-CBD-CGD-O2D
10	aA	824	CLA	CHA-CBD-CGD-O1D
10	aA	824	CLA	CHA-CBD-CGD-O2D
10	aB	831	CLA	CHA-CBD-CGD-O2D
10	cA	803	CLA	CHA-CBD-CGD-O2D
10	cB	816	CLA	CHA-CBD-CGD-O1D
10	cB	816	CLA	CHA-CBD-CGD-O2D
10	cB	831	CLA	CHA-CBD-CGD-O2D
10	bA	812	CLA	CHA-CBD-CGD-O1D
10	aB	833	CLA	CHA-CBD-CGD-O1D
10	aB	833	CLA	CHA-CBD-CGD-O2D
14	aA	852	LHG	O8-C23-C24-C25
14	bA	852	LHG	O8-C23-C24-C25
10	aA	826	CLA	C10-C11-C12-C13
10	bA	826	CLA	C10-C11-C12-C13
10	cA	826	CLA	C10-C11-C12-C13
9	aA	801	CL0	C3-C5-C6-C7
10	bA	835	CLA	CAA-CBA-CGA-O2A
10	bA	837	CLA	CAA-CBA-CGA-O2A
14	cA	852	LHG	O8-C23-C24-C25
10	cA	837	CLA	CAA-CBA-CGA-O2A
10	aA	837	CLA	CAA-CBA-CGA-O2A
10	aB	809	CLA	C6-C7-C8-C9
10	bB	802	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
10	cB	809	CLA	C6-C7-C8-C9
10	cB	818	CLA	C6-C7-C8-C9
10	bA	835	CLA	C14-C13-C15-C16
10	cA	835	CLA	C14-C13-C15-C16
10	aB	818	CLA	C6-C7-C8-C9
10	bB	828	CLA	C14-C13-C15-C16
10	bB	809	CLA	C6-C7-C8-C9
10	bB	818	CLA	C6-C7-C8-C9
10	cB	828	CLA	C14-C13-C15-C16
10	cB	802	CLA	C14-C13-C15-C16
10	aB	802	CLA	C14-C13-C15-C16
10	aA	835	CLA	C14-C13-C15-C16
10	aB	828	CLA	C14-C13-C15-C16
10	bB	837	CLA	C11-C12-C13-C14
10	cB	837	CLA	C11-C12-C13-C14
10	aB	837	CLA	C11-C12-C13-C14
10	cA	835	CLA	CAA-CBA-CGA-O2A
10	aA	835	CLA	CAA-CBA-CGA-O2A
10	cA	824	CLA	C1A-C2A-CAA-CBA
10	bA	824	CLA	C1A-C2A-CAA-CBA
10	aA	824	CLA	C1A-C2A-CAA-CBA
10	bA	839	CLA	C5-C6-C7-C8
10	cA	839	CLA	C5-C6-C7-C8
10	aL	202	CLA	CAA-CBA-CGA-O1A
10	bB	833	CLA	CAA-CBA-CGA-O1A
10	bL	202	CLA	CAA-CBA-CGA-O1A
10	cL	202	CLA	CAA-CBA-CGA-O1A
10	aA	839	CLA	C5-C6-C7-C8
9	bA	801	CL0	C3-C5-C6-C7
10	cB	804	CLA	C2A-CAA-CBA-CGA
10	aB	804	CLA	C2A-CAA-CBA-CGA
10	bB	804	CLA	C2A-CAA-CBA-CGA
10	cA	841	CLA	CAA-CBA-CGA-O1A
10	aA	841	CLA	CAA-CBA-CGA-O1A
10	aB	811	CLA	CAA-CBA-CGA-O1A
10	cB	811	CLA	CAA-CBA-CGA-O1A
10	bA	841	CLA	CAA-CBA-CGA-O1A
10	aA	854	CLA	C2C-C3C-CAC-CBC
10	bB	811	CLA	CAA-CBA-CGA-O1A
10	bB	823	CLA	CAA-CBA-CGA-O1A
10	cB	833	CLA	CAA-CBA-CGA-O1A
10	cB	823	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
10	aB	823	CLA	CAA-CBA-CGA-O1A
10	aB	833	CLA	CAA-CBA-CGA-O1A
10	aA	841	CLA	C16-C17-C18-C20
10	cA	854	CLA	C2C-C3C-CAC-CBC
10	bA	854	CLA	C2C-C3C-CAC-CBC
10	aA	819	CLA	CAA-CBA-CGA-O1A
10	cA	841	CLA	C16-C17-C18-C20
10	bA	841	CLA	C16-C17-C18-C20
10	cA	819	CLA	CAA-CBA-CGA-O1A
10	bA	819	CLA	CAA-CBA-CGA-O1A
13	bB	845	BCR	C23-C24-C25-C26
13	cB	845	BCR	C23-C24-C25-C26
13	aB	845	BCR	C23-C24-C25-C26
13	aA	848	BCR	C5-C6-C7-C8
13	cA	848	BCR	C5-C6-C7-C8
13	bA	848	BCR	C5-C6-C7-C8
10	bB	805	CLA	C10-C11-C12-C13
10	aB	805	CLA	C10-C11-C12-C13
10	cB	805	CLA	C10-C11-C12-C13
10	bB	814	CLA	CAA-CBA-CGA-O1A
10	aB	814	CLA	CAA-CBA-CGA-O1A
10	cA	830	CLA	CAD-CBD-CGD-O1D
9	cA	801	CL0	CAD-CBD-CGD-O1D
10	bB	814	CLA	CAD-CBD-CGD-O1D
10	aB	827	CLA	CAD-CBD-CGD-O1D
10	cB	827	CLA	CAD-CBD-CGD-O1D
10	bB	827	CLA	CAD-CBD-CGD-O1D
10	bA	830	CLA	CAD-CBD-CGD-O1D
9	bA	801	CL0	CAD-CBD-CGD-O1D
10	aA	830	CLA	CAD-CBD-CGD-O1D
9	aA	801	CL0	CAD-CBD-CGD-O1D
10	aB	814	CLA	CAD-CBD-CGD-O1D
16	bB	848	LMG	C14-C15-C16-C17
10	cB	814	CLA	CAA-CBA-CGA-O1A
10	bL	203	CLA	C8-C10-C11-C12
16	aB	848	LMG	C14-C15-C16-C17
16	cB	848	LMG	C14-C15-C16-C17
10	bA	838	CLA	CAA-CBA-CGA-O2A
10	cB	808	CLA	CAA-CBA-CGA-O2A
10	aA	838	CLA	CAA-CBA-CGA-O2A
10	cA	838	CLA	CAA-CBA-CGA-O2A
10	cB	839	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
10	bB	839	CLA	C2-C1-O2A-CGA
10	aB	839	CLA	C2-C1-O2A-CGA
10	cA	856	CLA	O2A-C1-C2-C3
10	bA	856	CLA	O2A-C1-C2-C3
10	aA	856	CLA	O2A-C1-C2-C3
10	bB	825	CLA	CAA-CBA-CGA-O1A
10	aB	825	CLA	CAA-CBA-CGA-O1A
10	bB	811	CLA	CBD-CGD-O2D-CED
10	aB	811	CLA	CBD-CGD-O2D-CED
10	cB	811	CLA	CBD-CGD-O2D-CED
10	bB	814	CLA	C15-C16-C17-C18
10	cB	814	CLA	C15-C16-C17-C18
10	cL	203	CLA	C8-C10-C11-C12
10	aB	814	CLA	C15-C16-C17-C18
10	aA	834	CLA	CAA-CBA-CGA-O2A
10	aB	808	CLA	CAA-CBA-CGA-O2A
10	bB	808	CLA	CAA-CBA-CGA-O2A
10	cA	834	CLA	CAA-CBA-CGA-O2A
10	bA	834	CLA	CAA-CBA-CGA-O2A
10	bA	842	CLA	C2-C1-O2A-CGA
10	aB	803	CLA	C2-C1-O2A-CGA
10	cA	842	CLA	C2-C1-O2A-CGA
10	cB	803	CLA	C2-C1-O2A-CGA
10	bB	803	CLA	C2-C1-O2A-CGA
10	aA	842	CLA	C2-C1-O2A-CGA
10	cB	825	CLA	CAA-CBA-CGA-O1A
10	aA	834	CLA	CAA-CBA-CGA-O1A
14	cA	852	LHG	O9-C7-C8-C9
10	cA	834	CLA	CAA-CBA-CGA-O1A
14	aA	852	LHG	O9-C7-C8-C9
10	bA	834	CLA	CAA-CBA-CGA-O1A
14	bA	852	LHG	O9-C7-C8-C9
10	bB	802	CLA	CBA-CGA-O2A-C1
10	cB	802	CLA	CBA-CGA-O2A-C1
10	aB	802	CLA	CBA-CGA-O2A-C1
10	aL	203	CLA	C8-C10-C11-C12
10	cB	810	CLA	C2-C3-C5-C6
10	aB	810	CLA	C2-C3-C5-C6
10	bB	810	CLA	C2-C3-C5-C6
10	bB	821	CLA	CAA-CBA-CGA-O2A
10	aB	821	CLA	CAA-CBA-CGA-O2A
10	aA	812	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
11	cA	844	PQN	C24-C23-C25-C26
10	aL	203	CLA	C11-C10-C8-C9
10	cA	812	CLA	C6-C7-C8-C9
11	aA	844	PQN	C24-C23-C25-C26
10	bL	203	CLA	C11-C10-C8-C9
11	bA	844	PQN	C24-C23-C25-C26
10	cL	203	CLA	C11-C10-C8-C9
10	bA	812	CLA	C6-C7-C8-C9
10	cB	821	CLA	CAA-CBA-CGA-O2A
10	cA	818	CLA	C11-C12-C13-C15
10	aB	809	CLA	C6-C7-C8-C10
10	cB	809	CLA	C6-C7-C8-C10
10	aA	827	CLA	C6-C7-C8-C10
11	cA	844	PQN	C22-C23-C25-C26
10	bA	827	CLA	C6-C7-C8-C10
10	cA	827	CLA	C6-C7-C8-C10
10	cA	831	CLA	C11-C10-C8-C7
10	bA	818	CLA	C11-C12-C13-C15
10	bB	809	CLA	C6-C7-C8-C10
11	aA	844	PQN	C22-C23-C25-C26
10	aA	818	CLA	C11-C12-C13-C15
10	bA	831	CLA	C11-C10-C8-C7
11	bA	844	PQN	C22-C23-C25-C26
10	aA	831	CLA	C11-C10-C8-C7
10	bA	837	CLA	CAA-CBA-CGA-O1A
10	bA	838	CLA	CAA-CBA-CGA-O1A
10	cA	837	CLA	CAA-CBA-CGA-O1A
10	aA	838	CLA	CAA-CBA-CGA-O1A
10	aA	837	CLA	CAA-CBA-CGA-O1A
10	cA	838	CLA	CAA-CBA-CGA-O1A
10	cB	839	CLA	CAA-CBA-CGA-O2A
10	bB	839	CLA	CAA-CBA-CGA-O2A
10	bB	805	CLA	CAA-CBA-CGA-O2A
10	aB	839	CLA	CAA-CBA-CGA-O2A
10	aB	805	CLA	CAA-CBA-CGA-O2A
10	bA	838	CLA	C3A-C2A-CAA-CBA
10	aA	838	CLA	C3A-C2A-CAA-CBA
10	cA	838	CLA	C3A-C2A-CAA-CBA
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	aB	809	CLA	CAA-CBA-CGA-O2A

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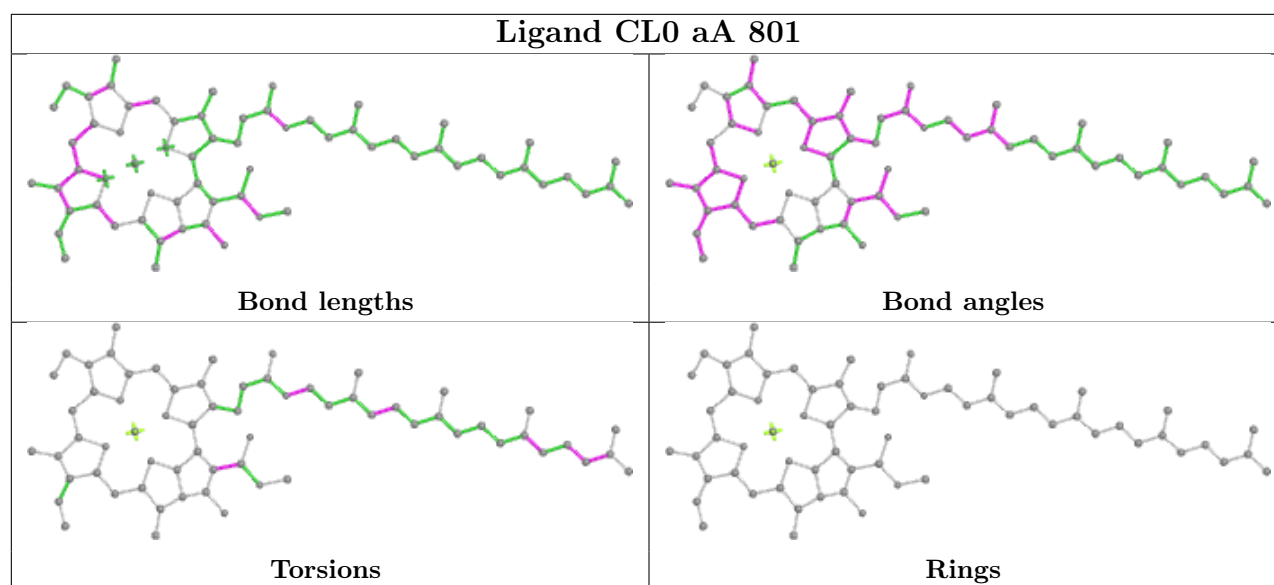
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Mol	Chain	Res	Type	Atoms
10	cB	809	CLA	CAA-CBA-CGA-O2A
10	bB	809	CLA	CAA-CBA-CGA-O2A
10	cB	838	CLA	CAA-CBA-CGA-O2A
10	cB	805	CLA	CAA-CBA-CGA-O2A
10	bB	838	CLA	CAA-CBA-CGA-O2A
10	aB	838	CLA	CAA-CBA-CGA-O2A
10	cB	821	CLA	CAA-CBA-CGA-O1A
10	aB	821	CLA	CAA-CBA-CGA-O1A

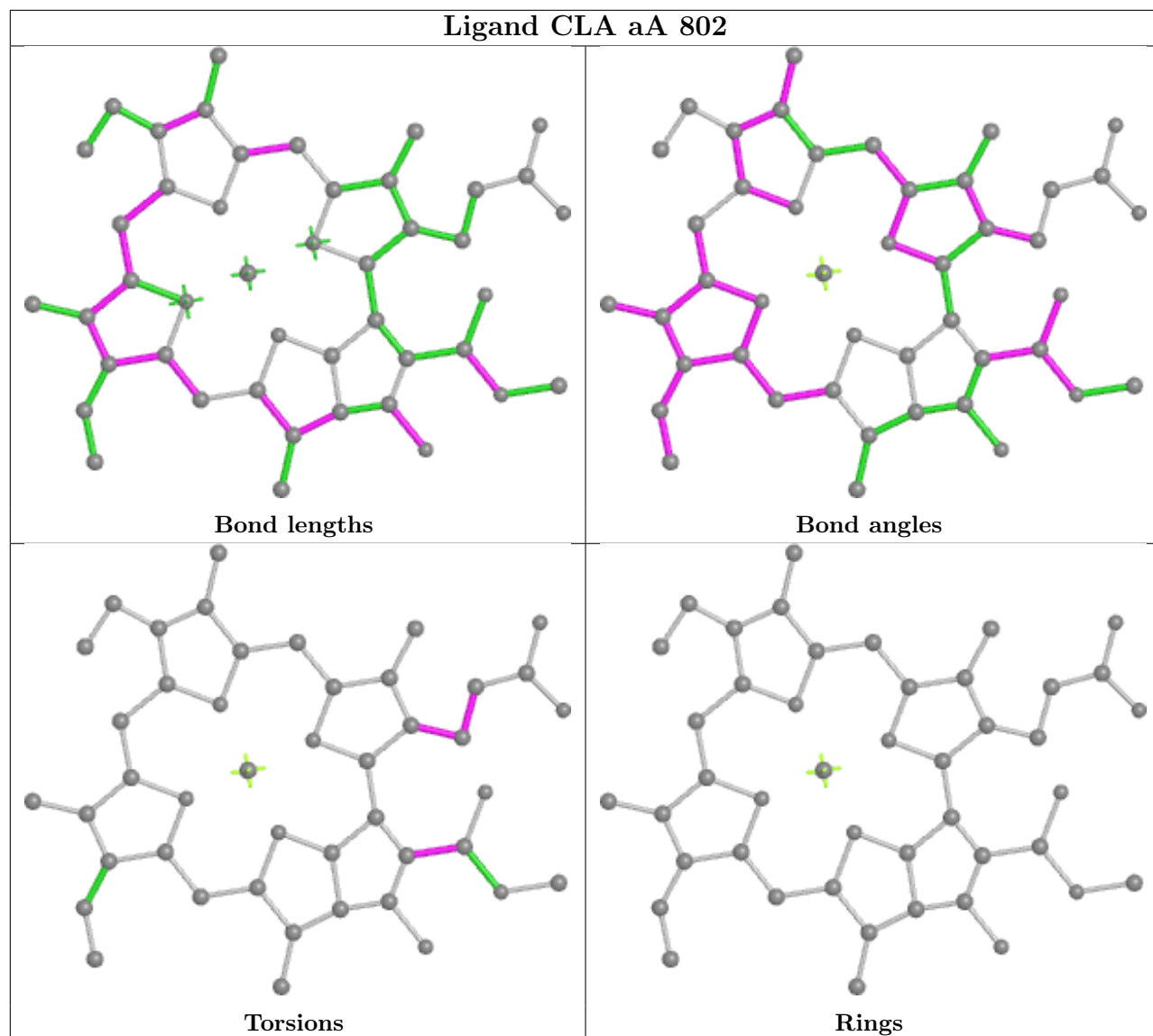
There are no ring outliers.

No monomer is involved in short contacts.

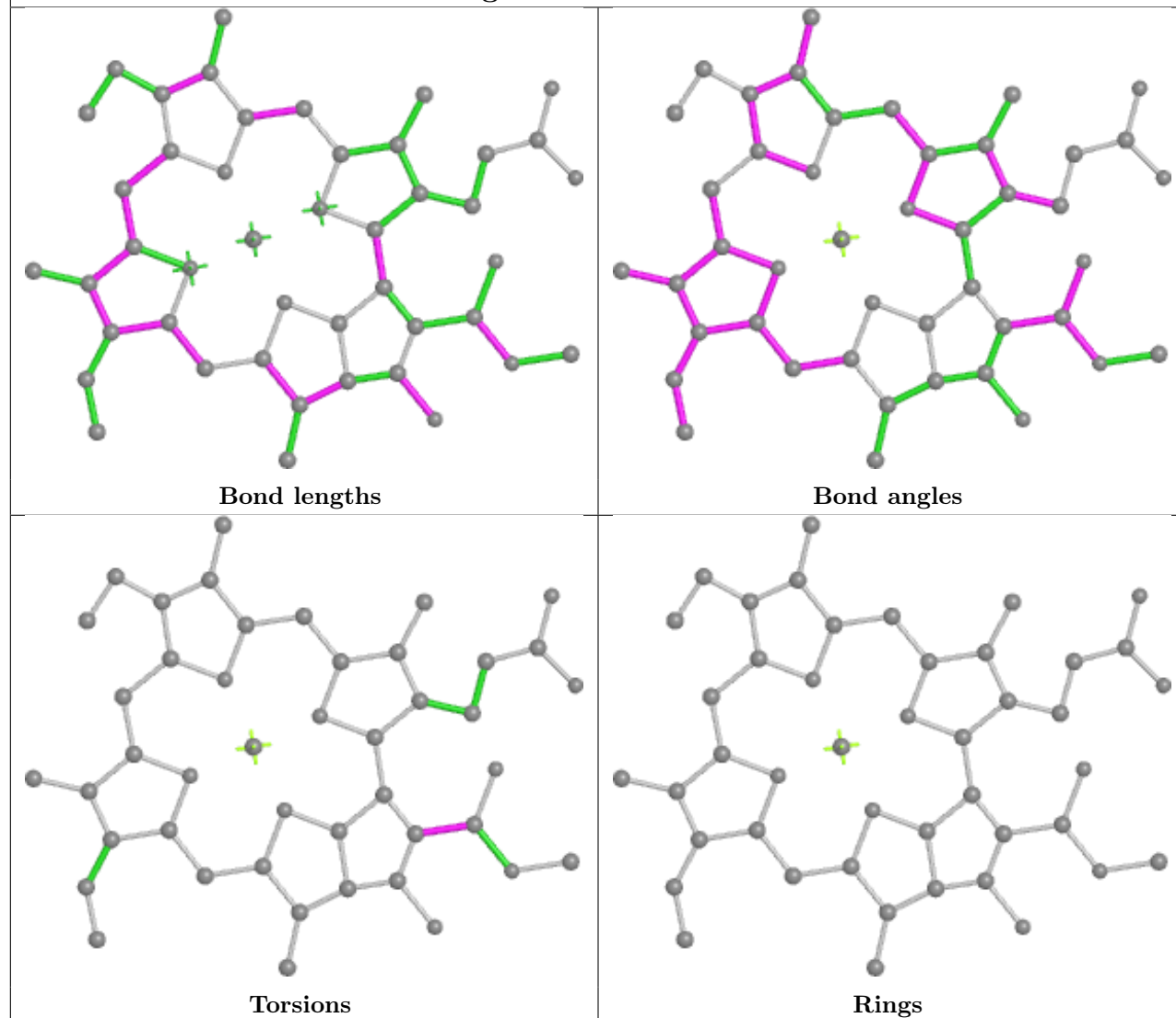
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



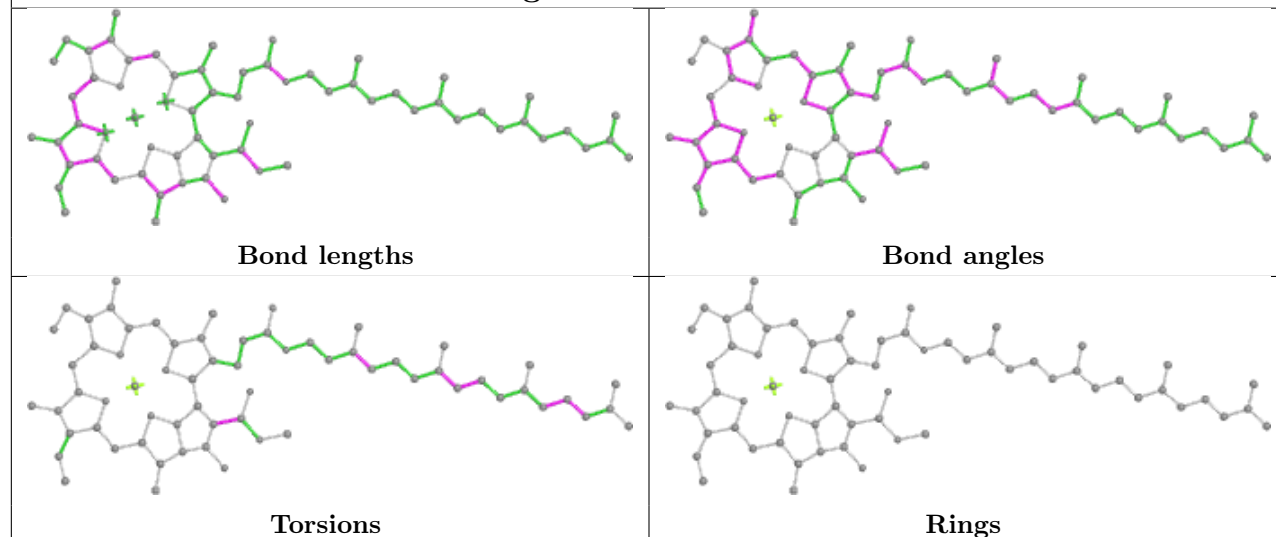
## Ligand CLA aA 802



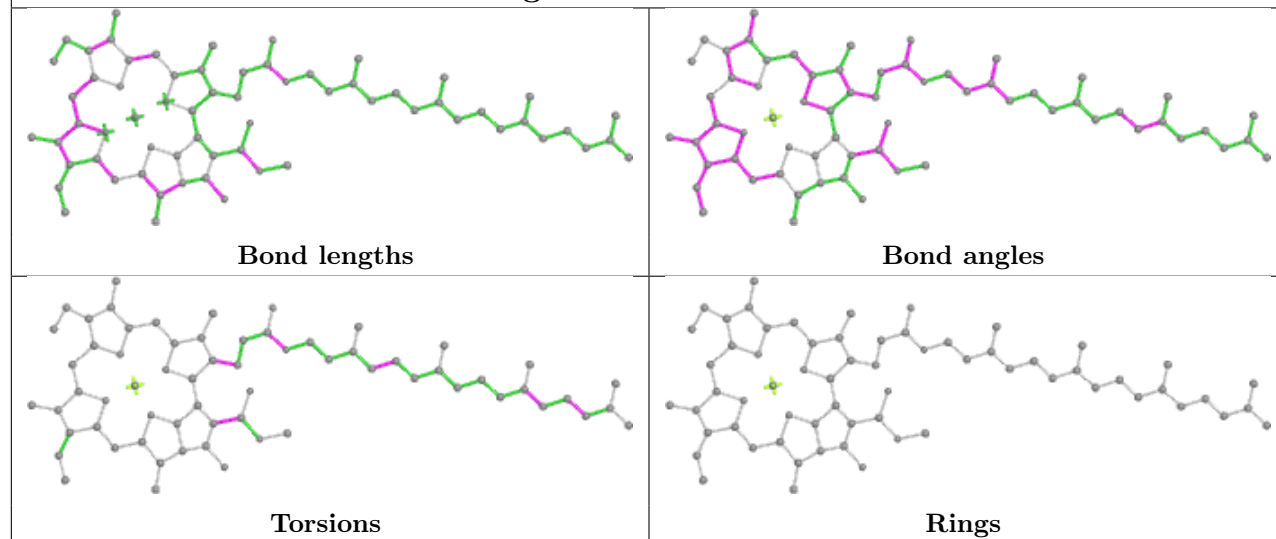
## Ligand CLA aA 803



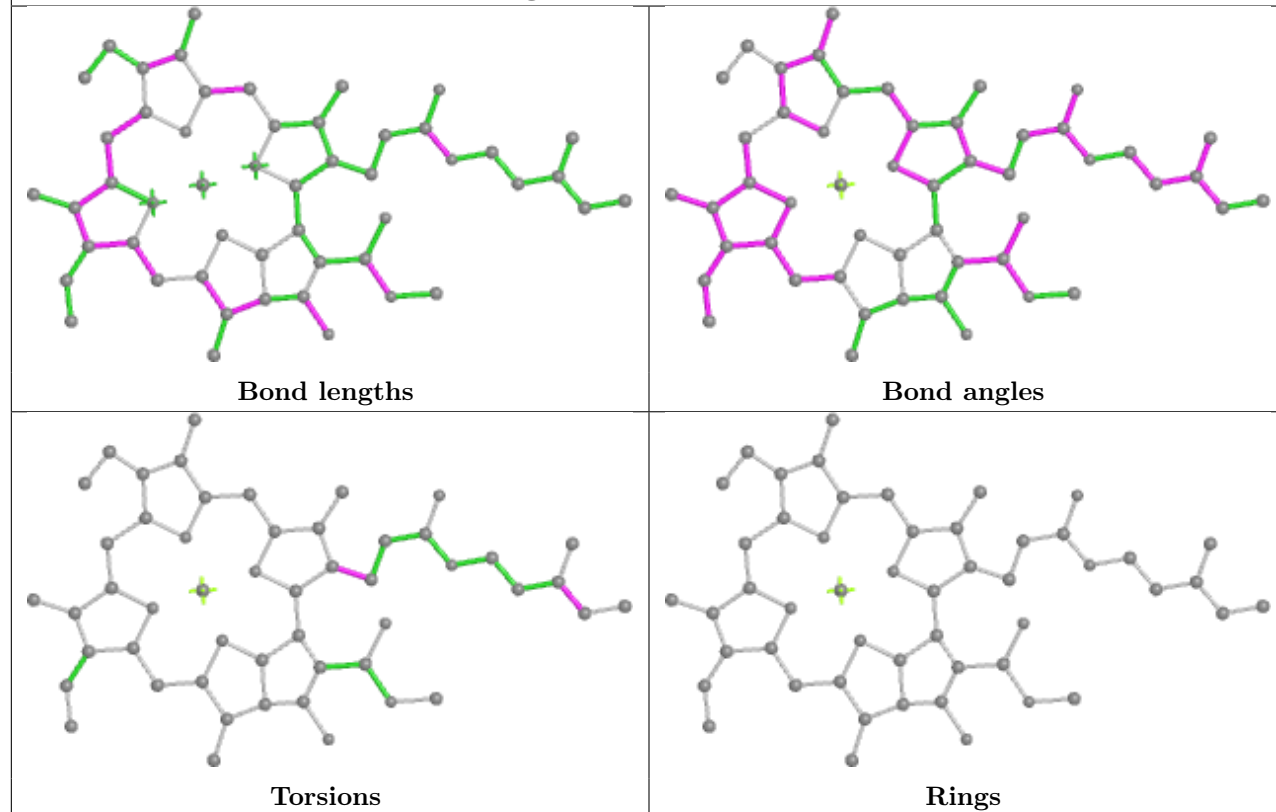
## Ligand CLA aA 804



## Ligand CLA aA 805

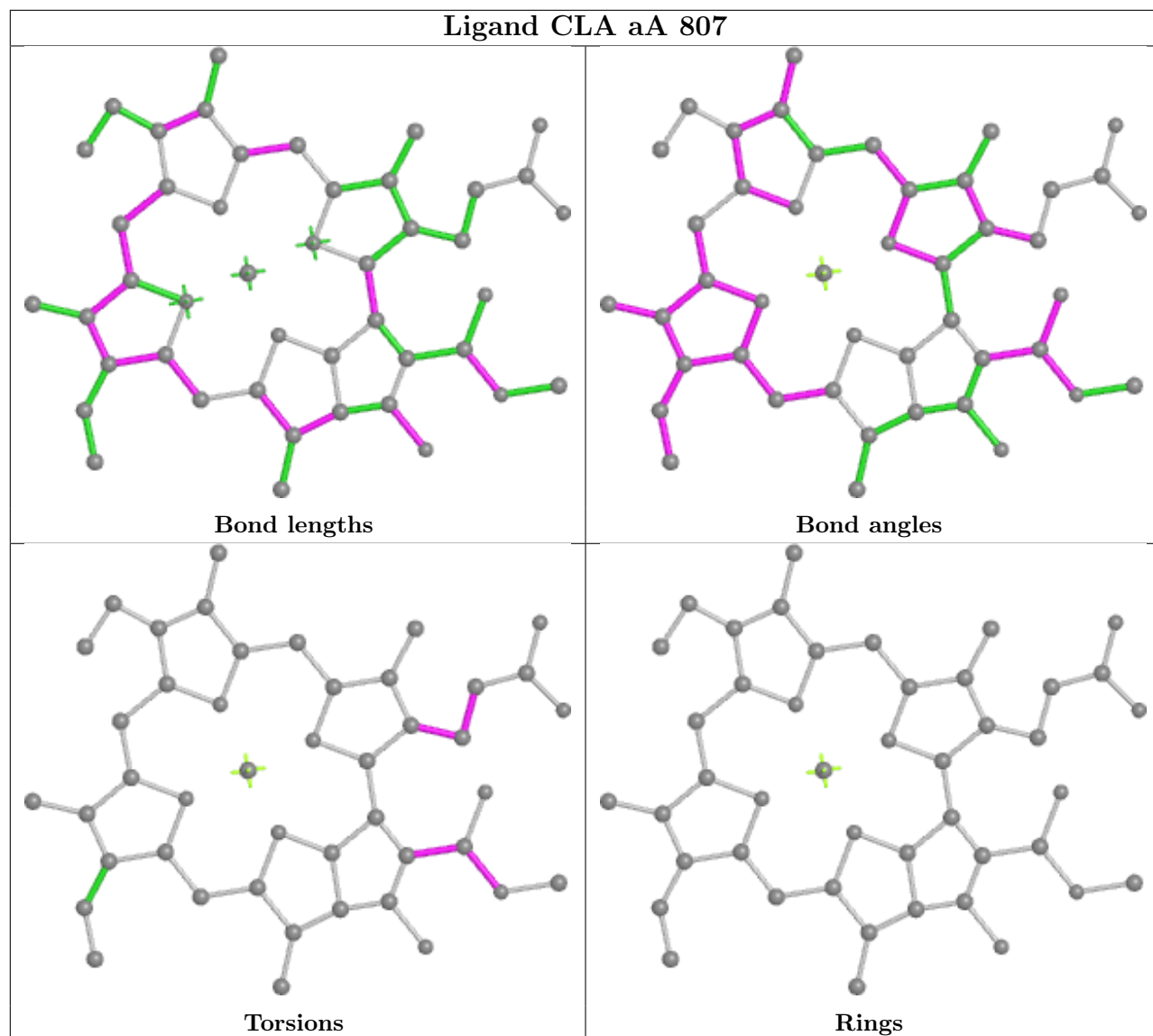


## Ligand CLA aA 806

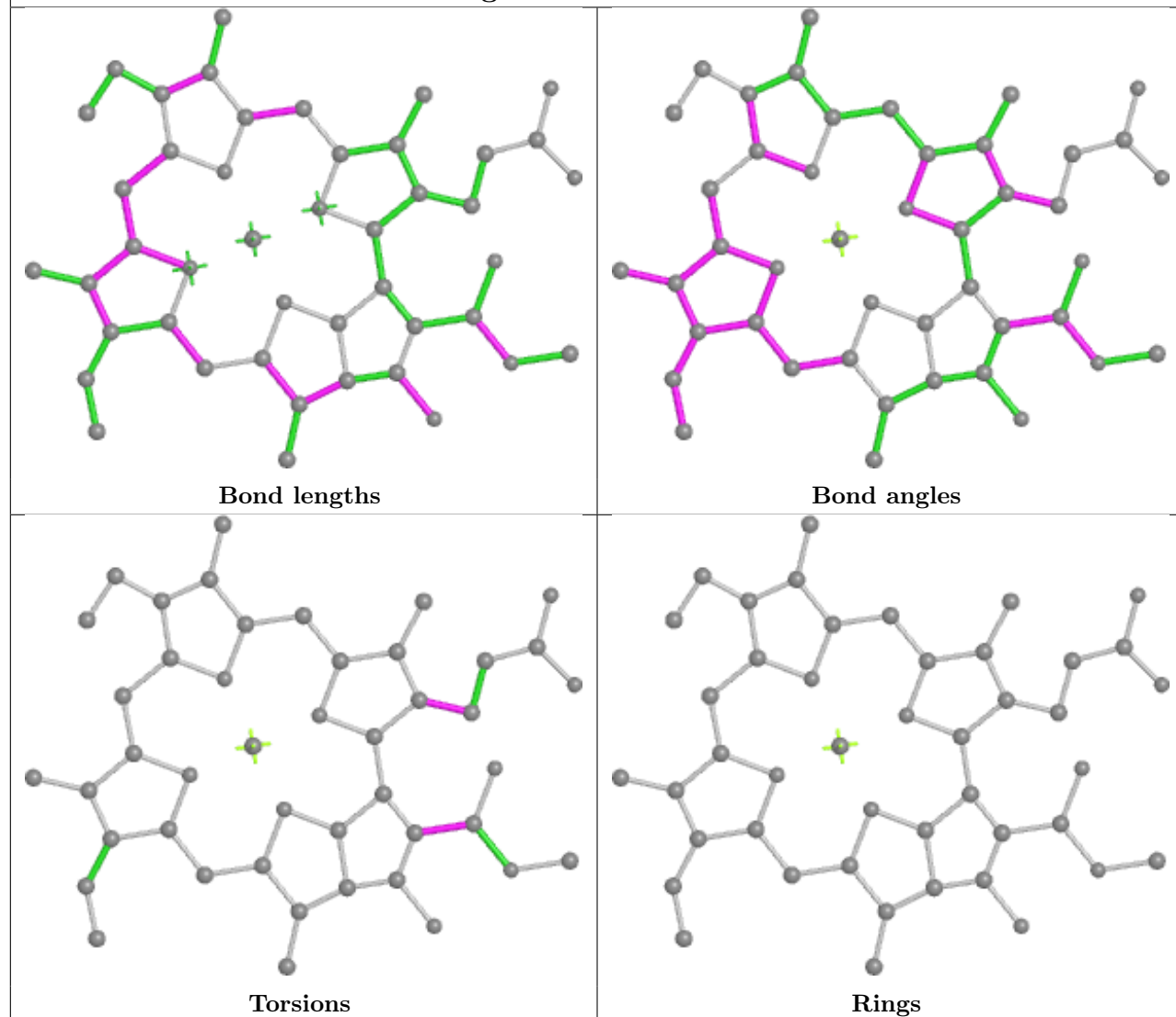




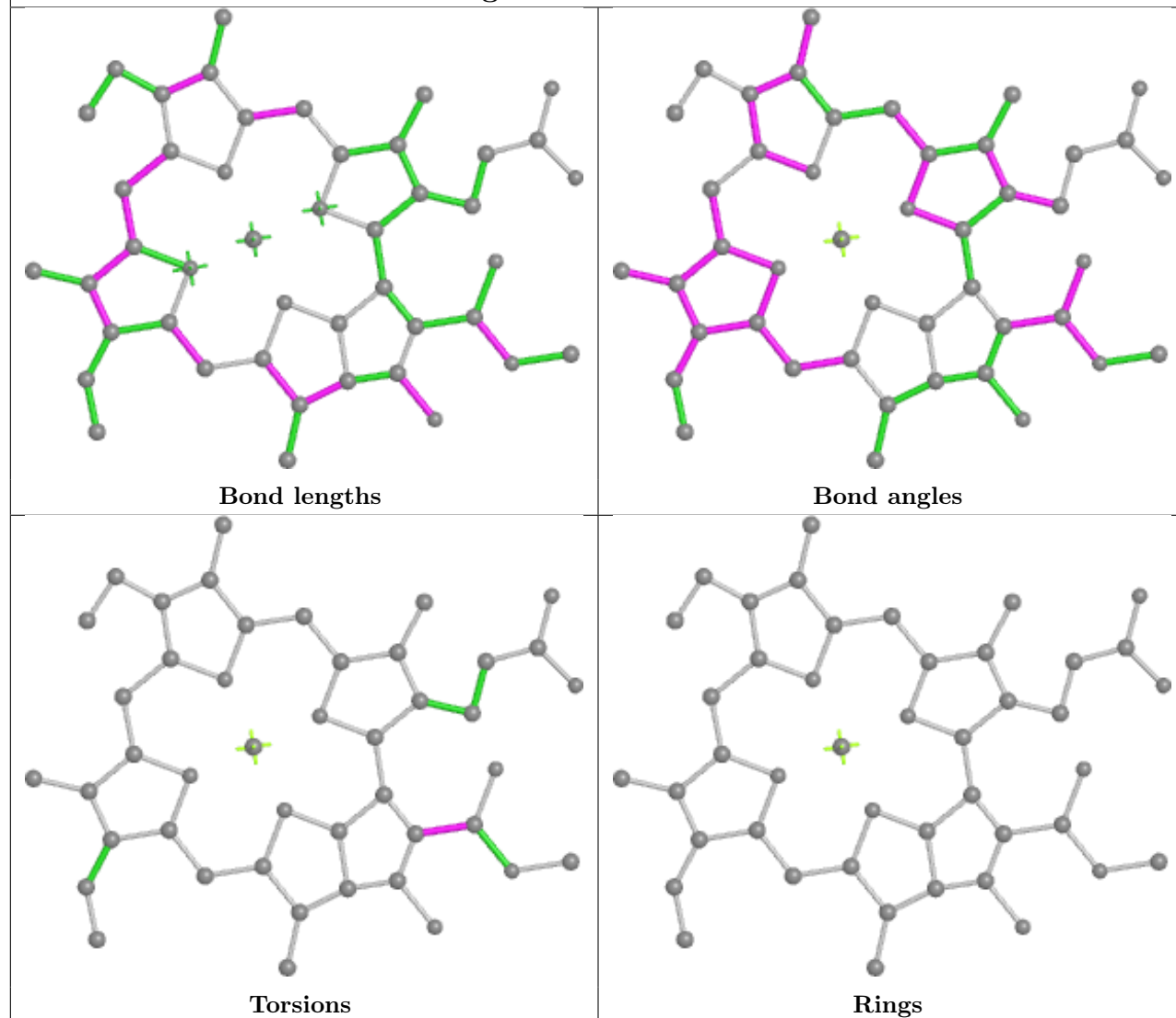
## Ligand CLA aA 807



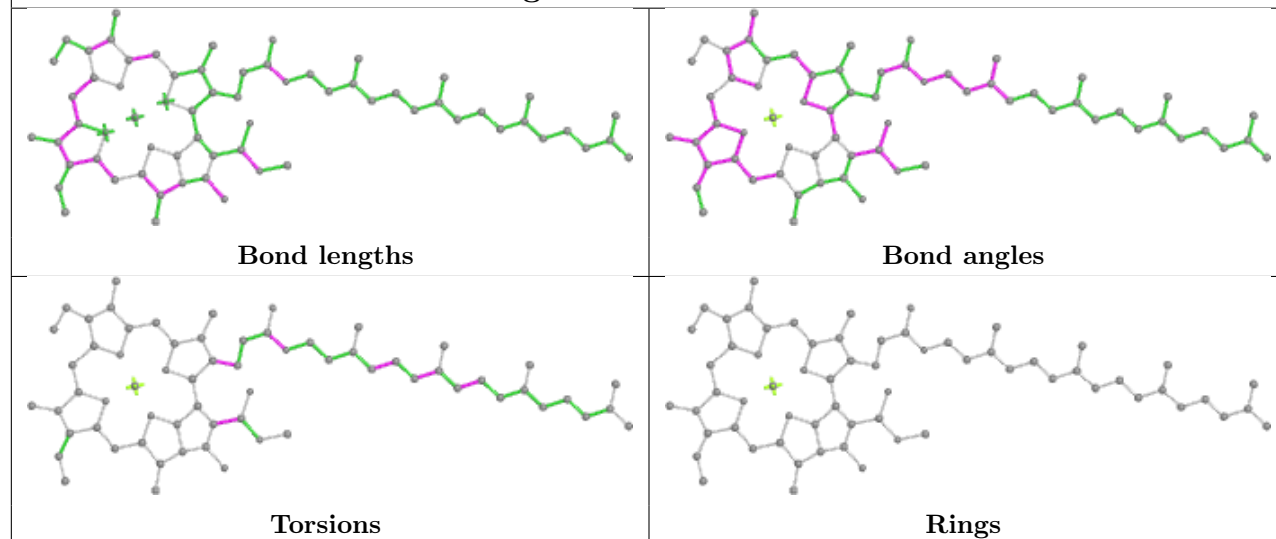
## Ligand CLA aA 808

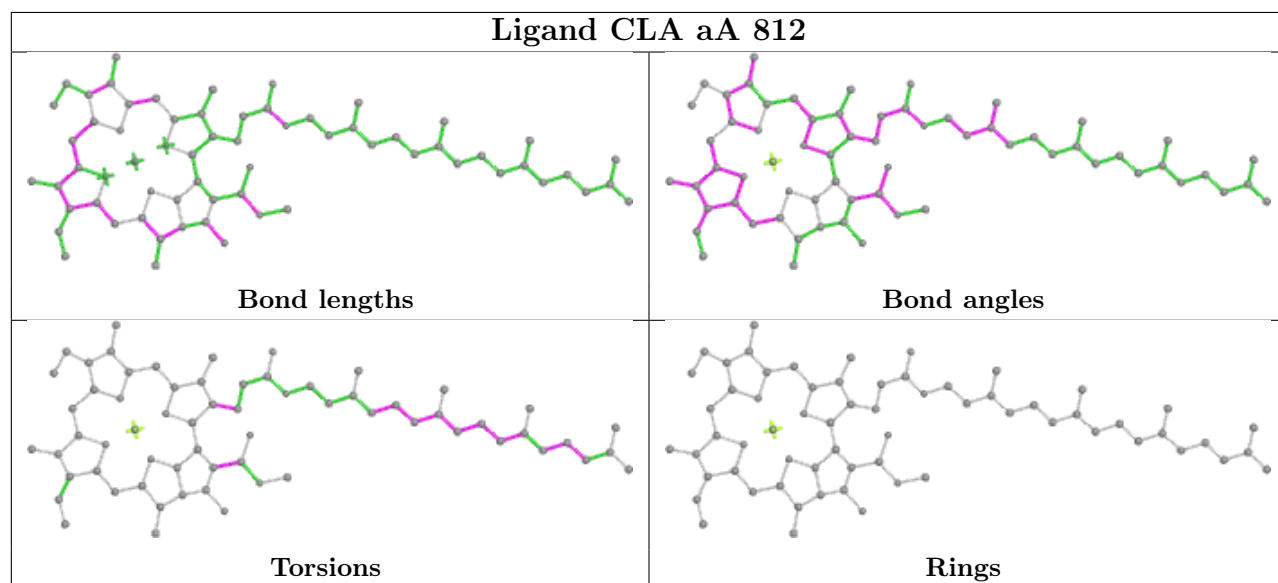
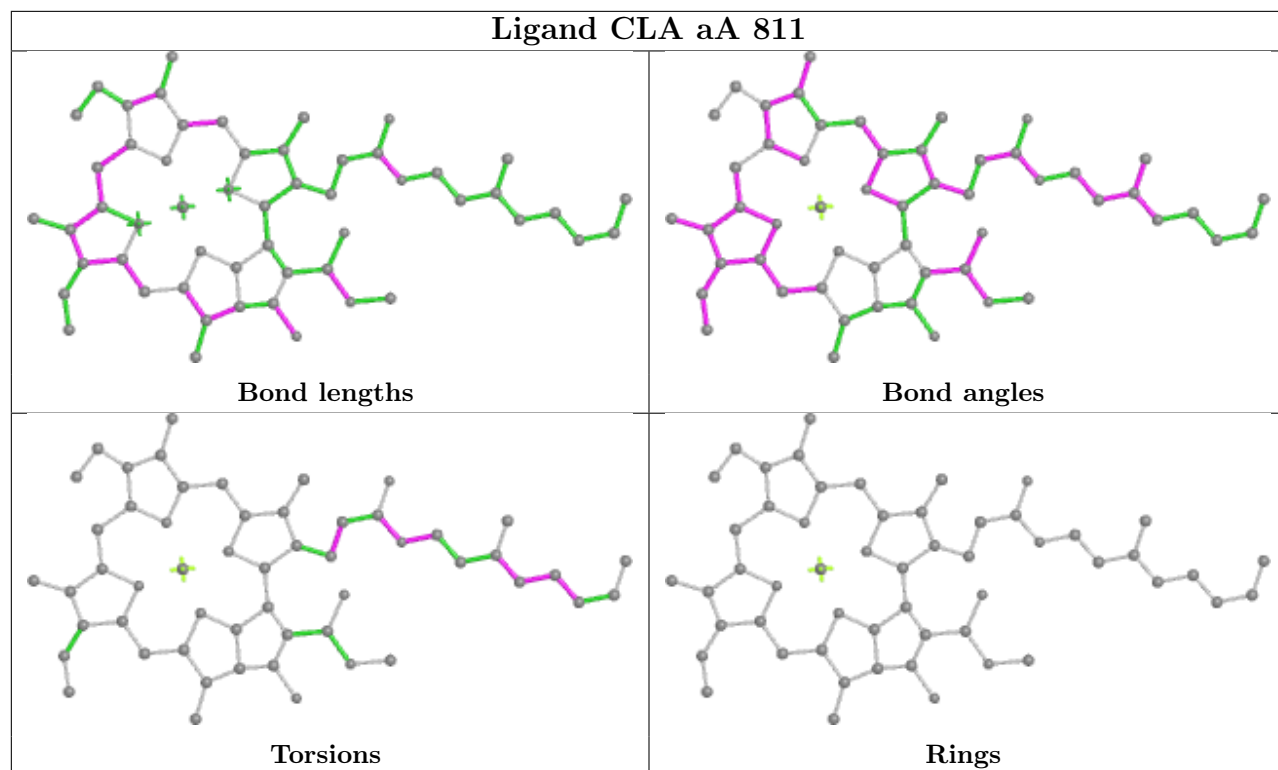


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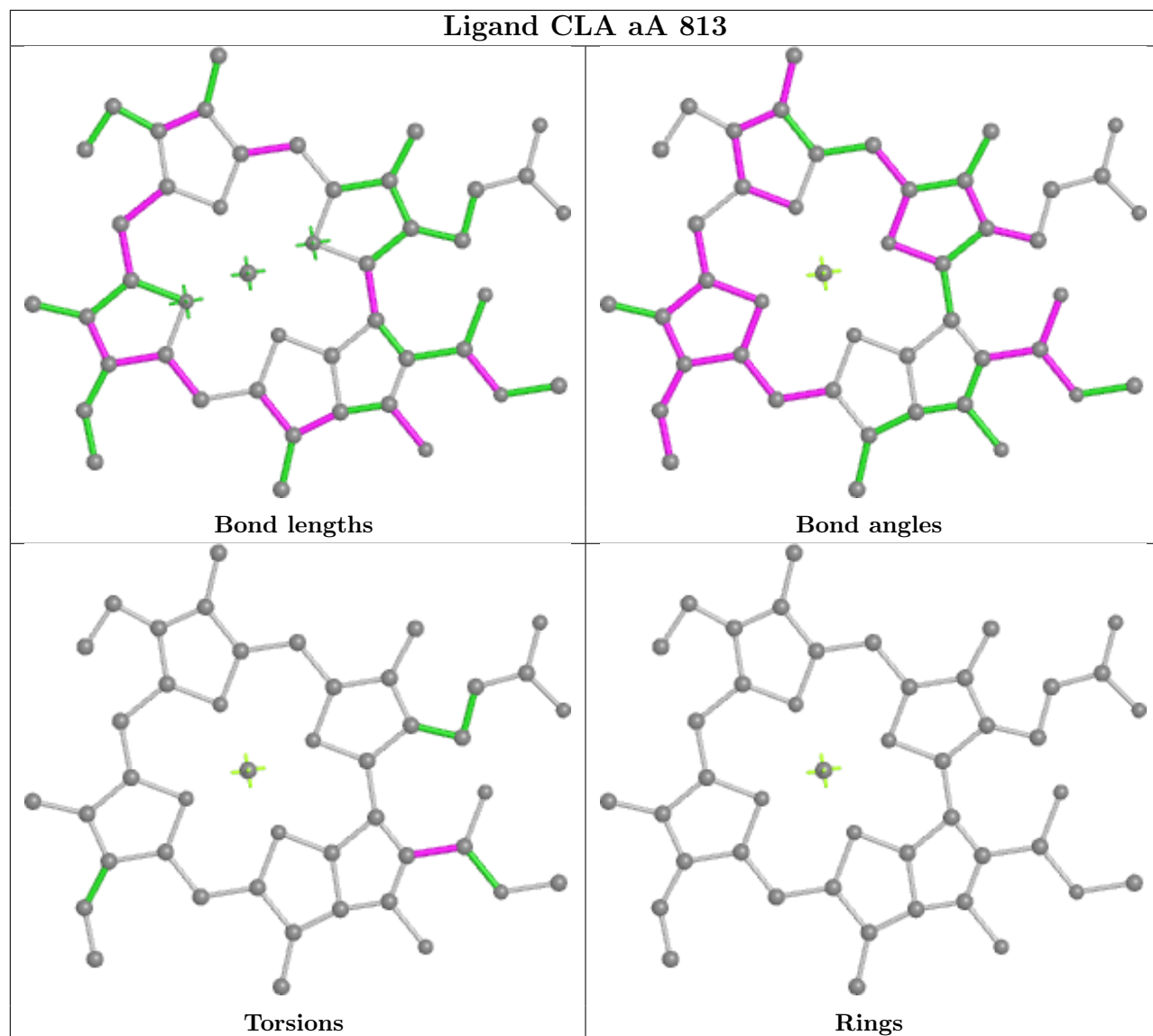


## Ligand CLA aA 810

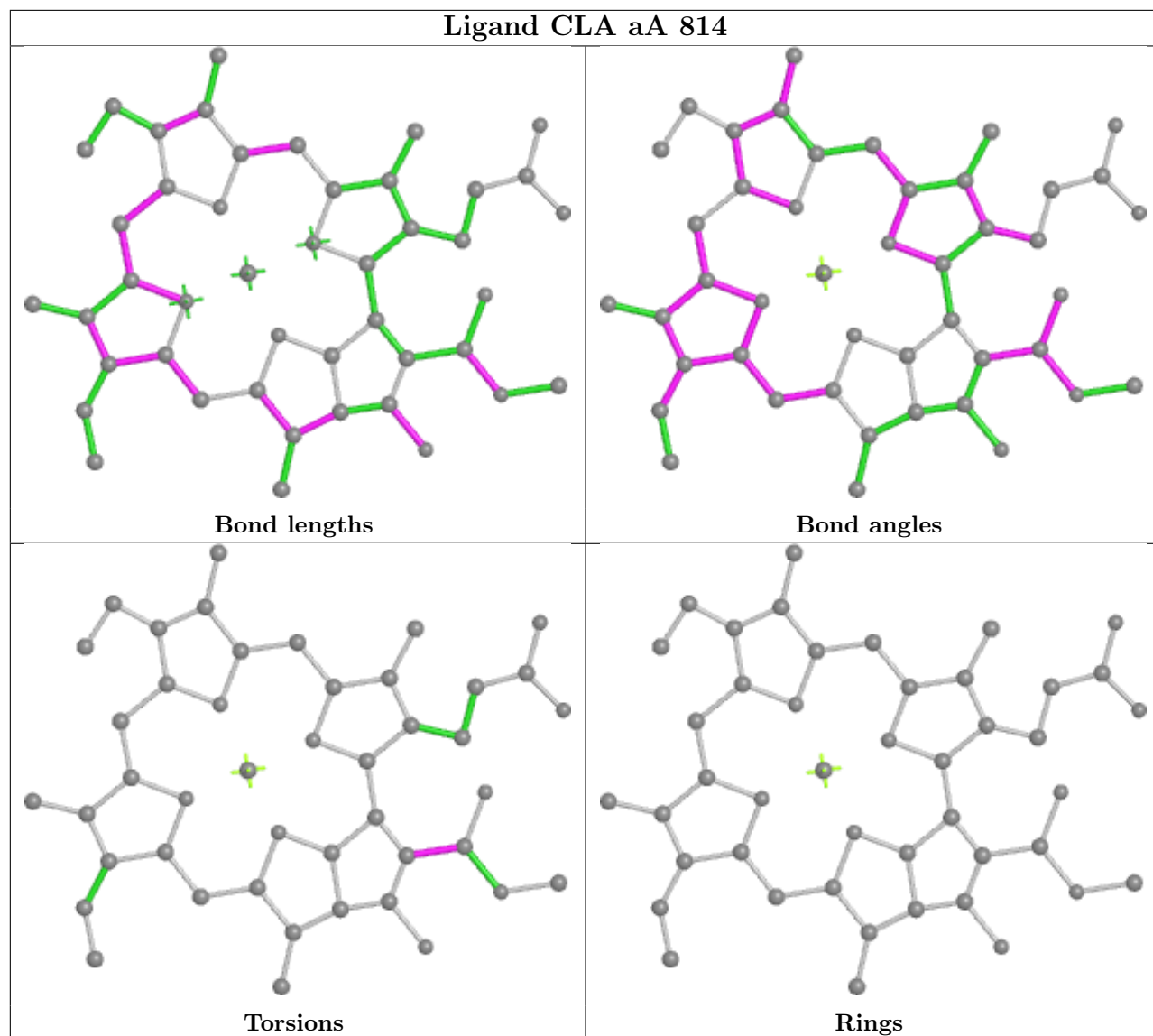




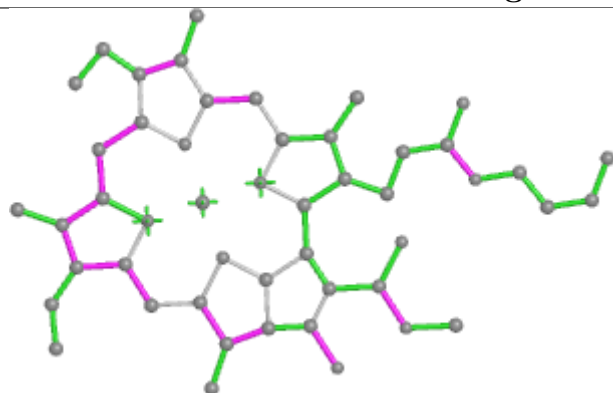
## Ligand CLA aA 813



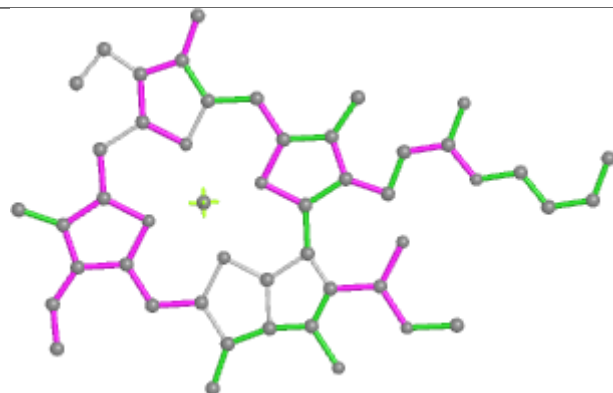
## Ligand CLA aA 814



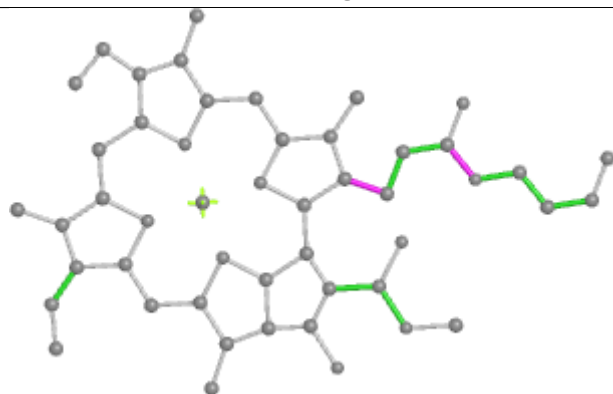
## Ligand CLA aA 815



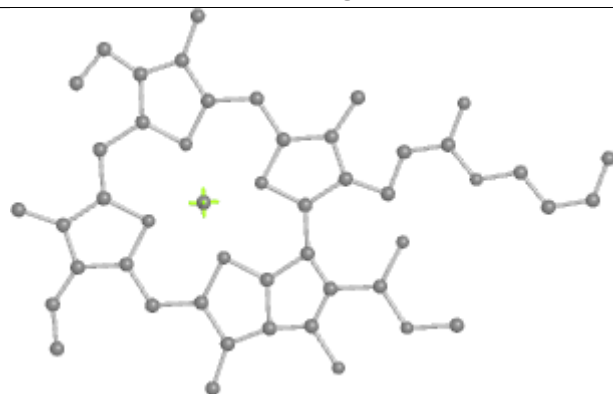
Bond lengths



Bond angles

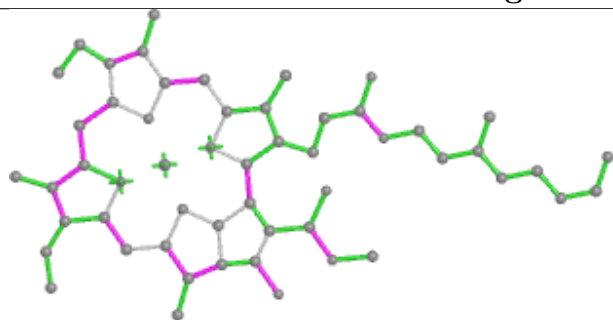


Torsions

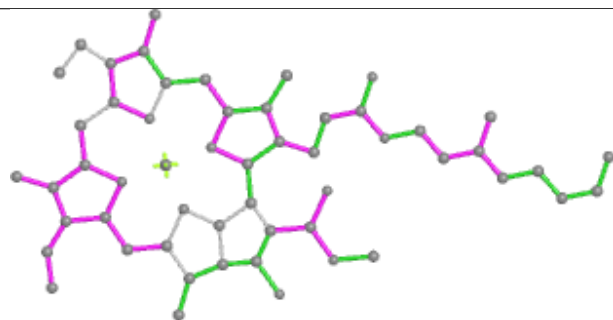


Rings

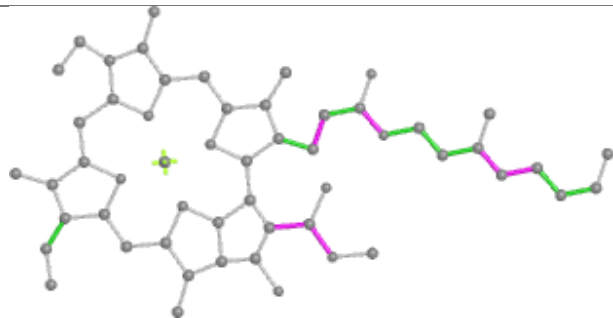
## Ligand CLA aA 816



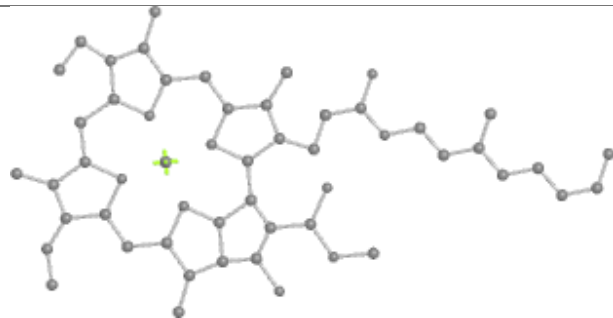
Bond lengths



Bond angles

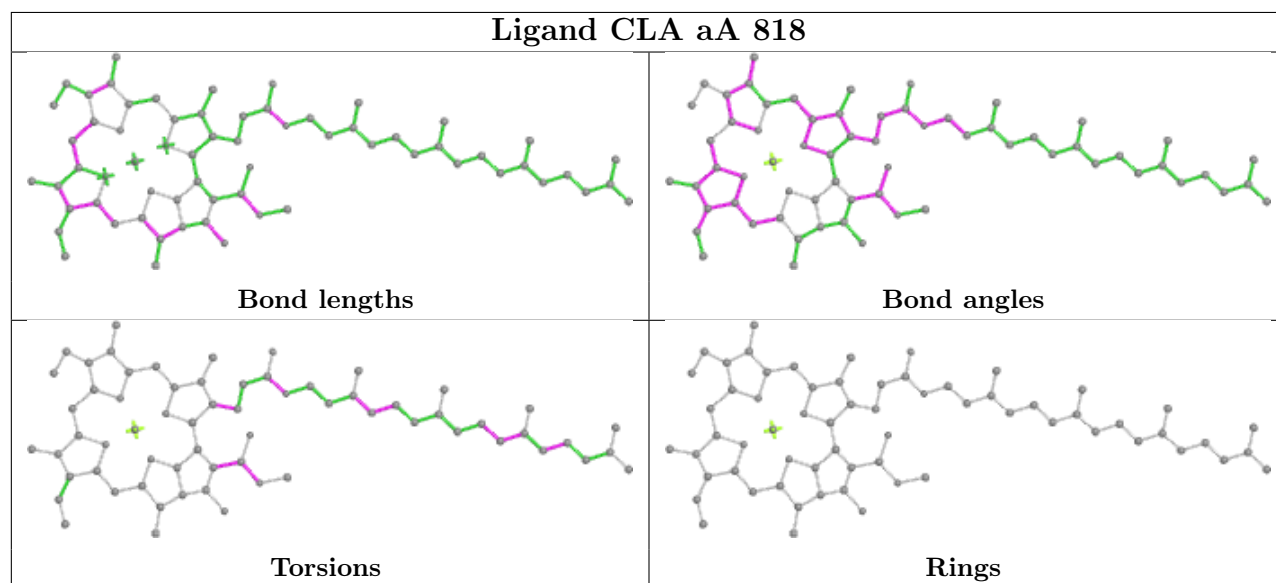
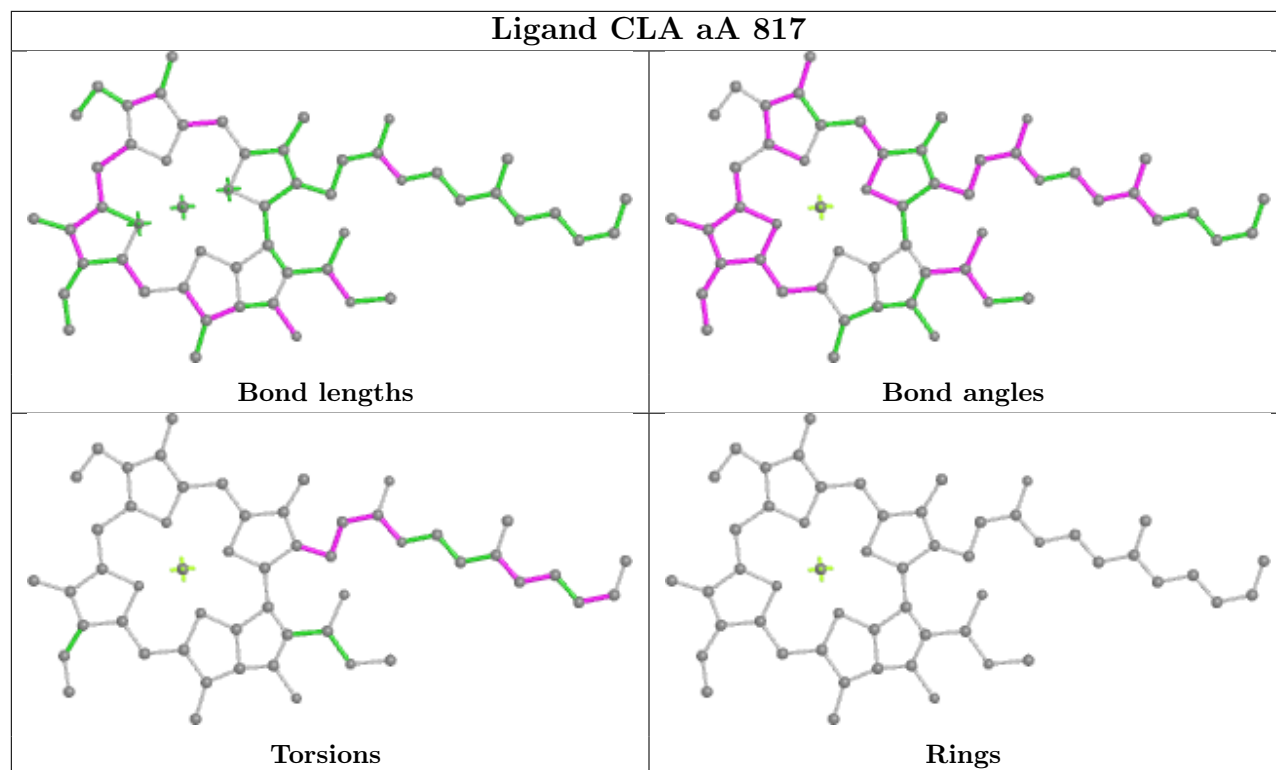


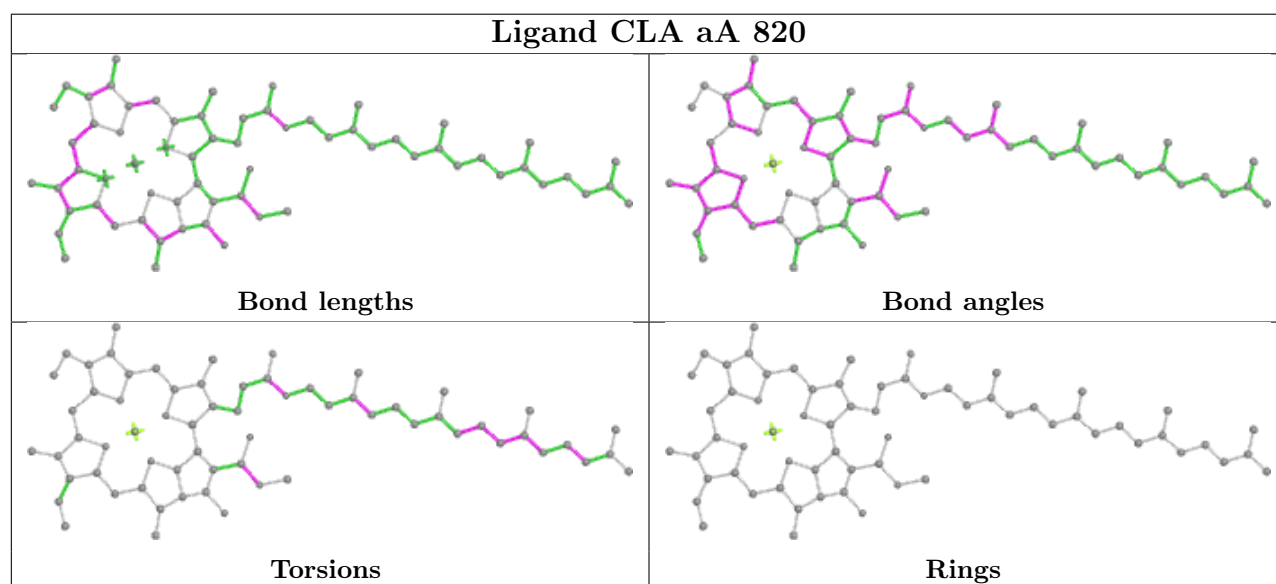
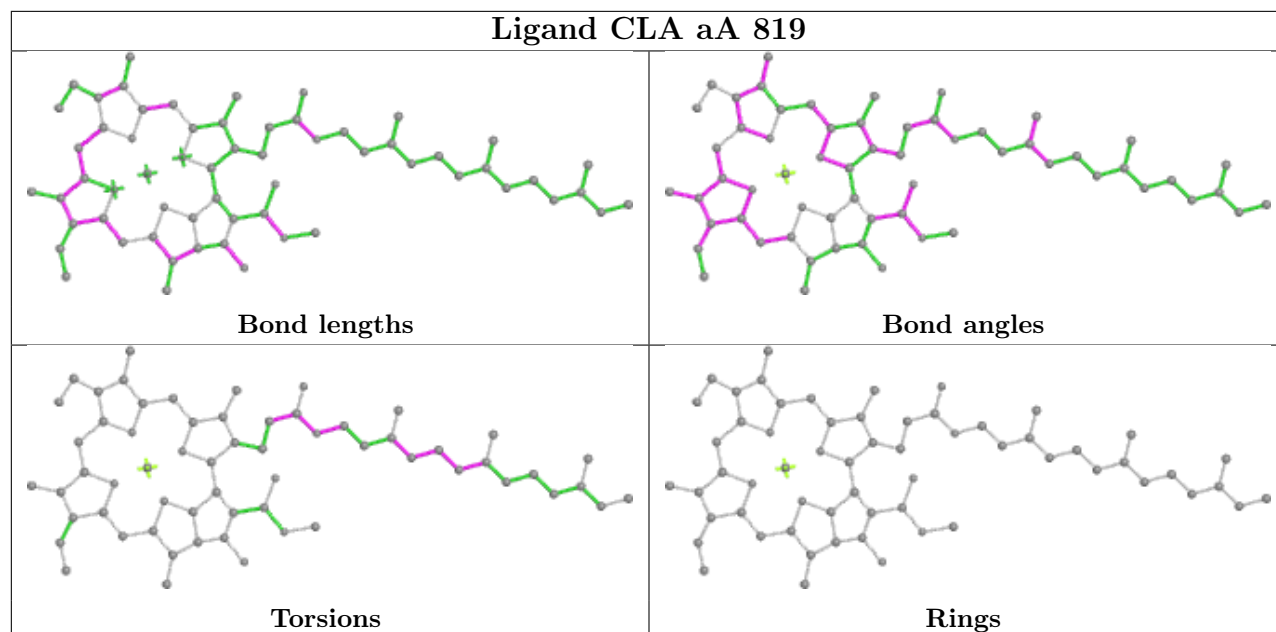
Torsions

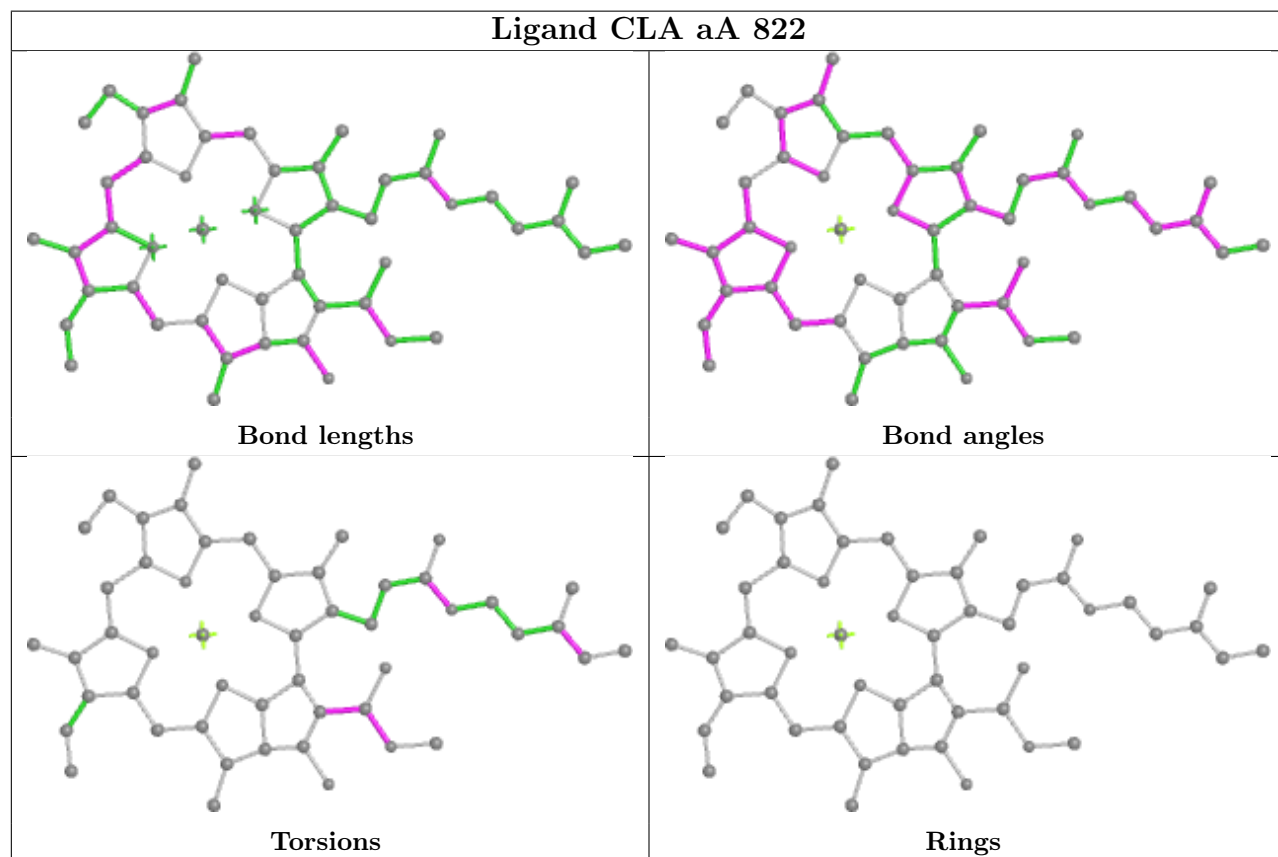
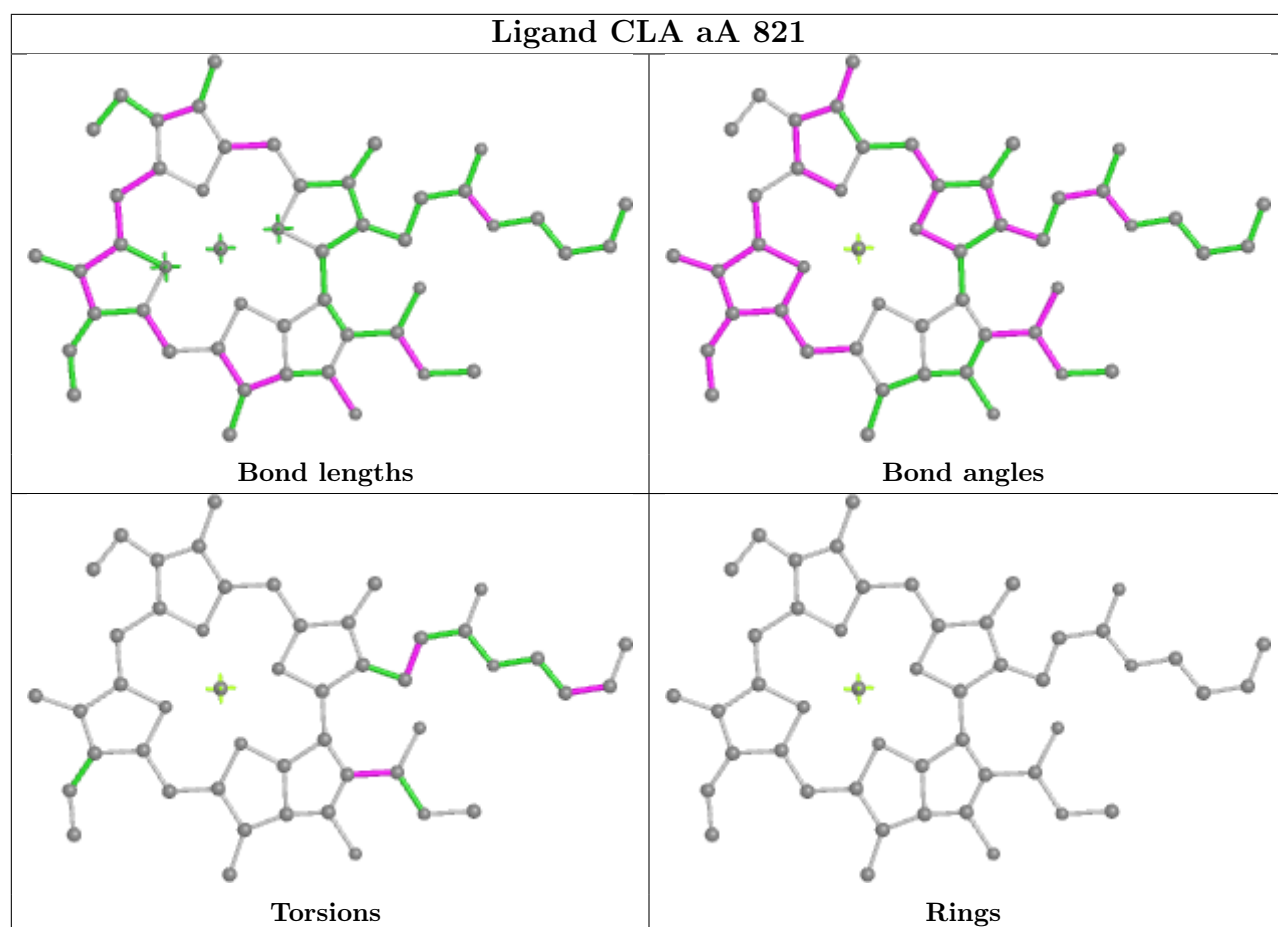


Rings

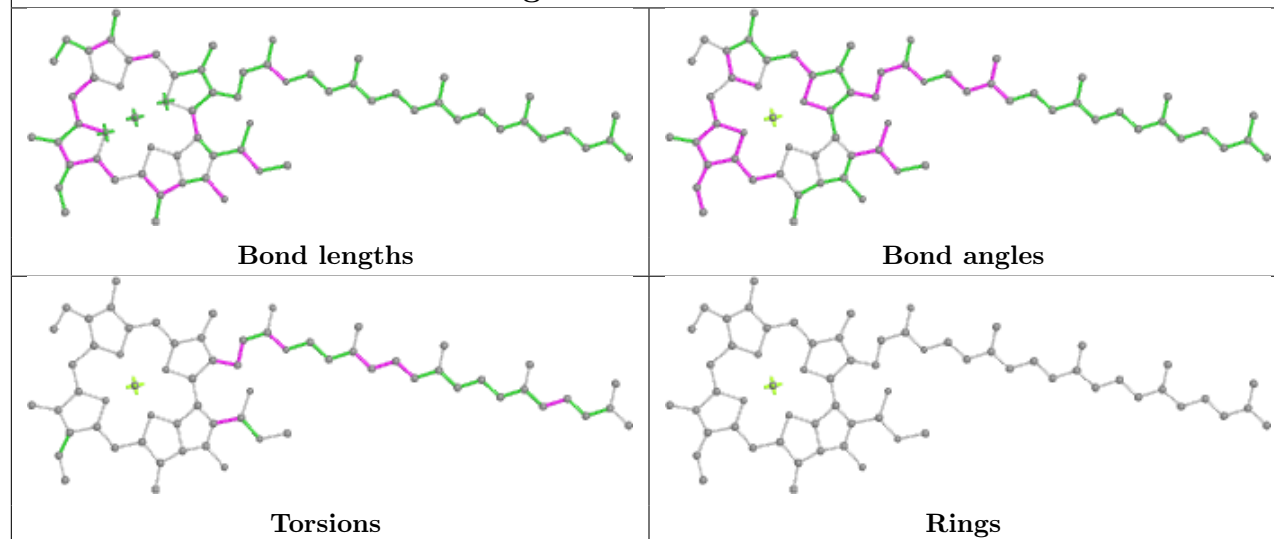




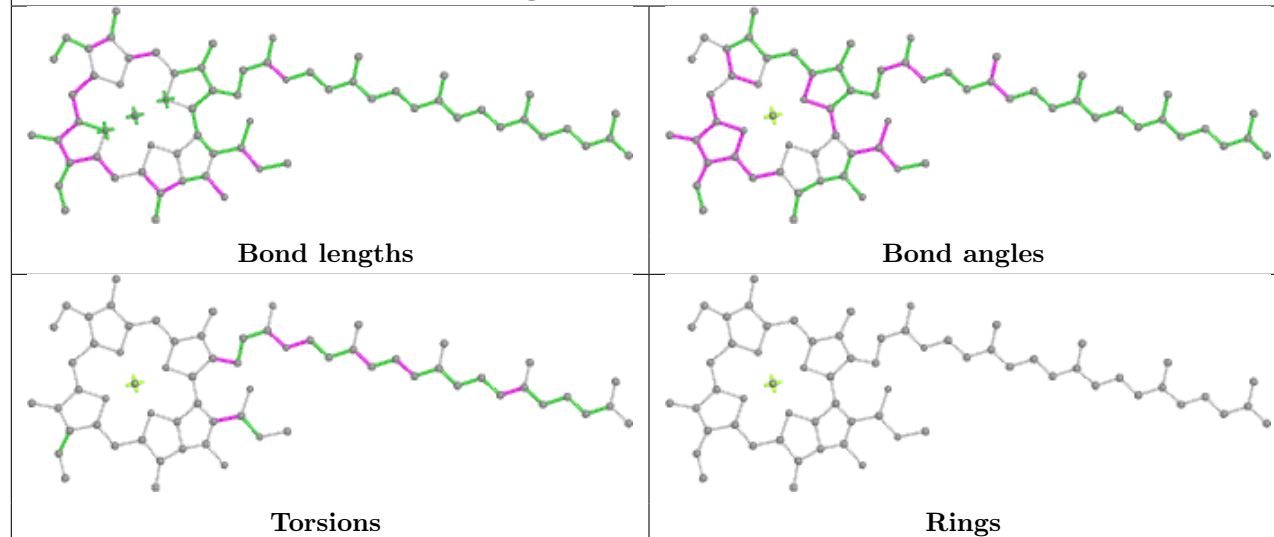


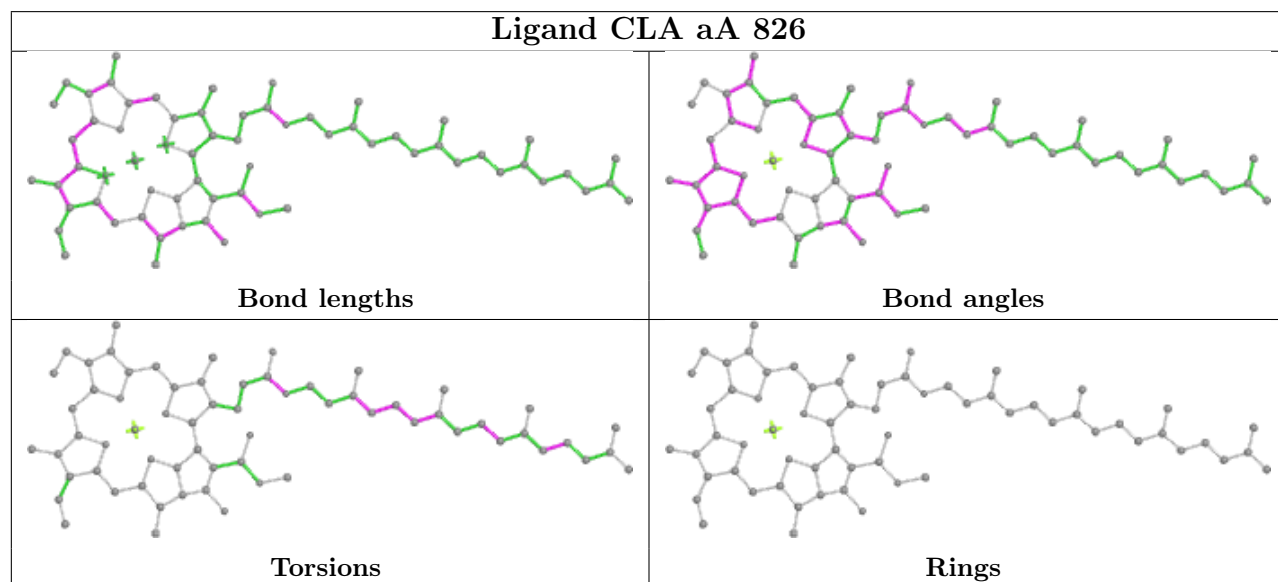
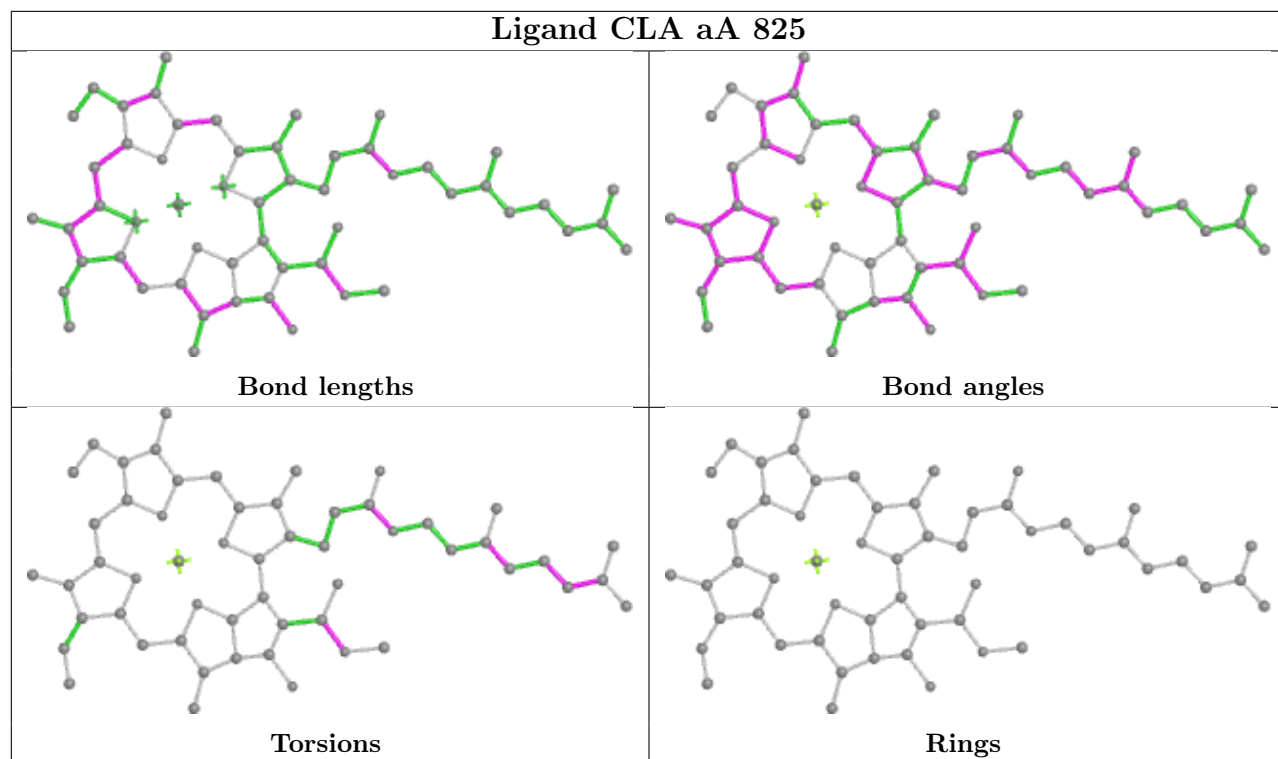


## Ligand CLA aA 823

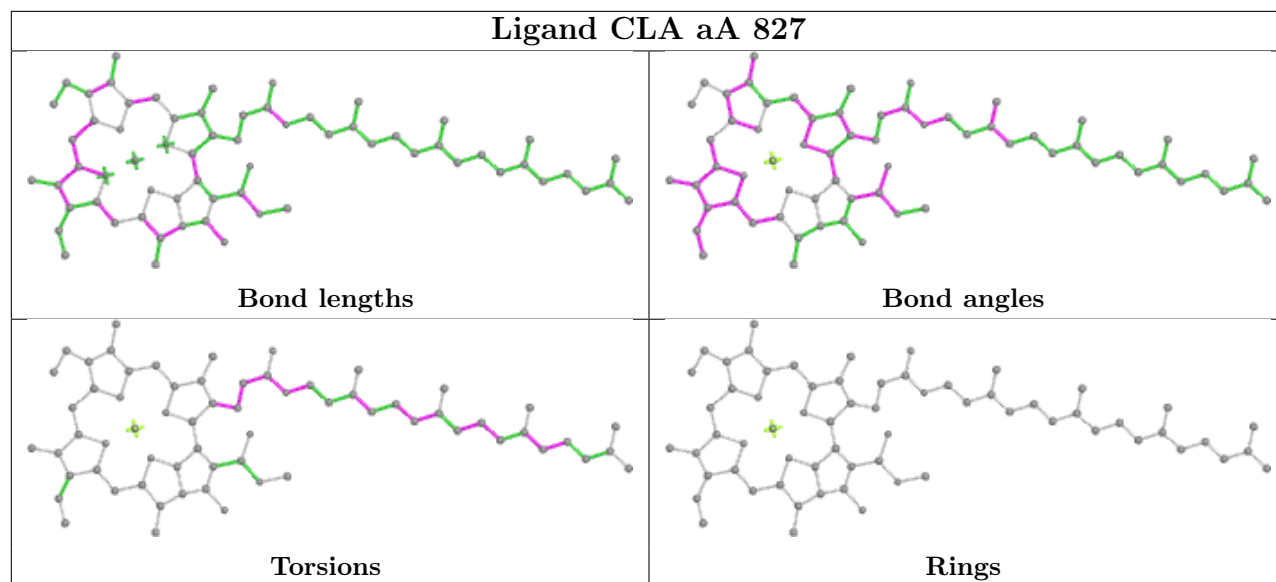


## Ligand CLA aA 824

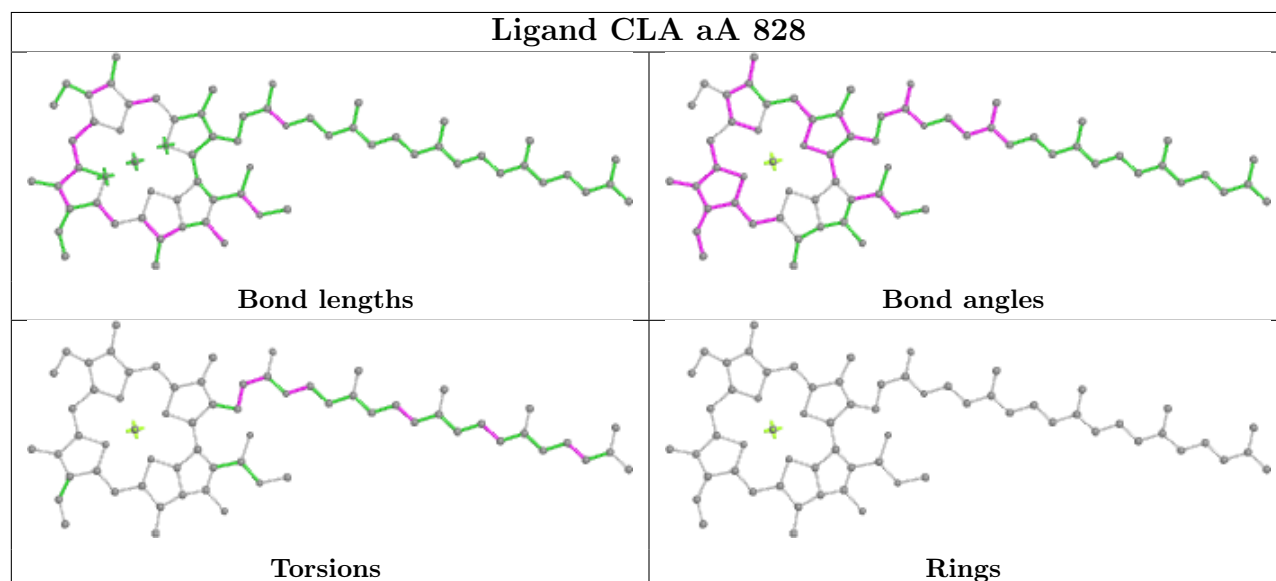




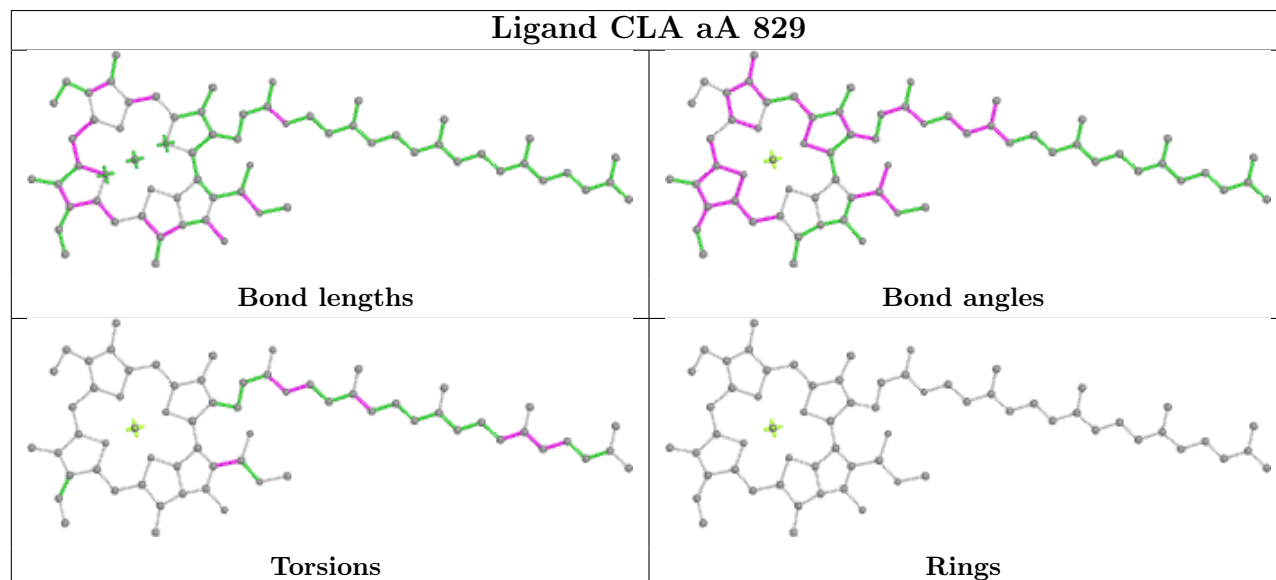
## Ligand CLA aA 827

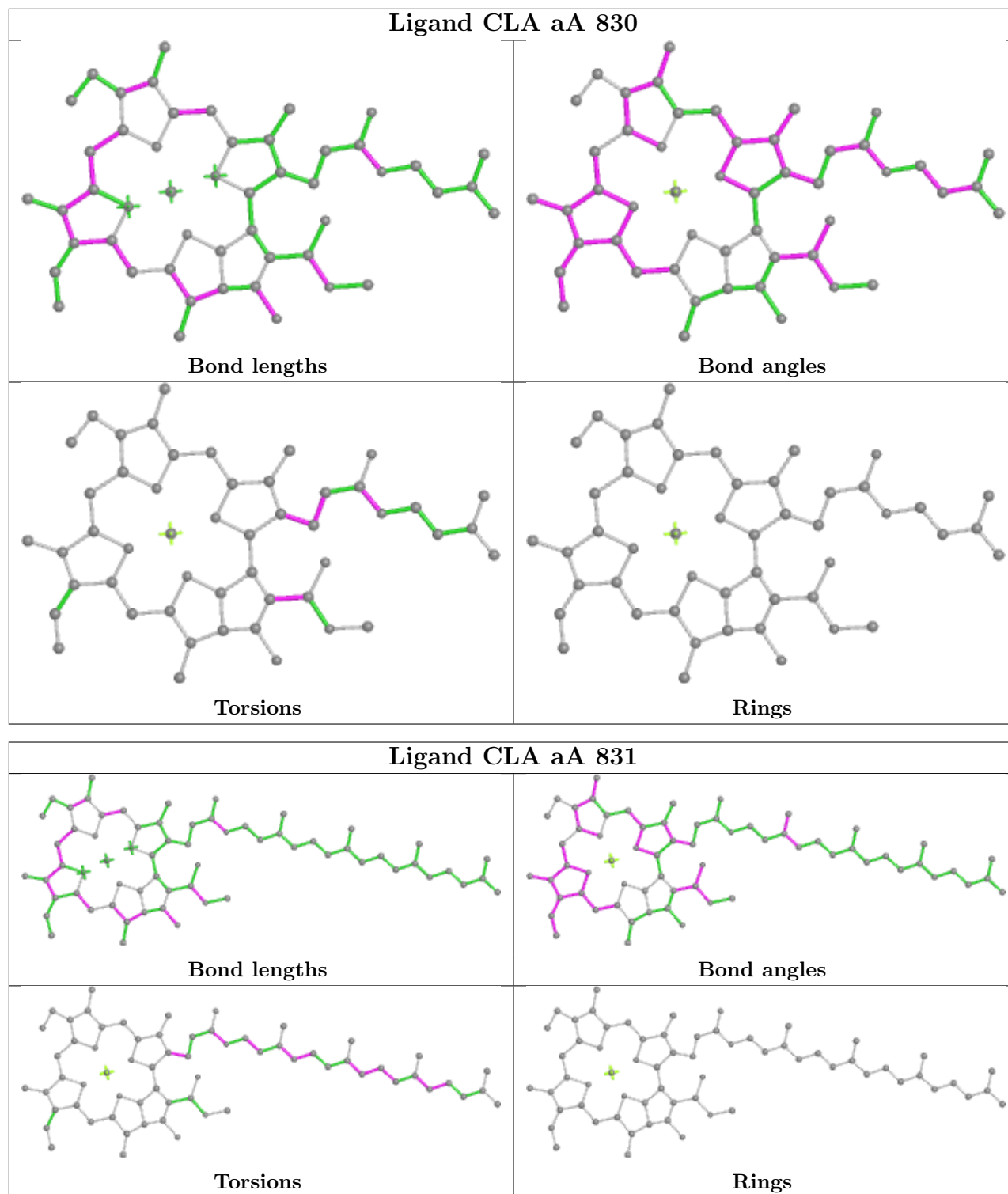


## Ligand CLA aA 828



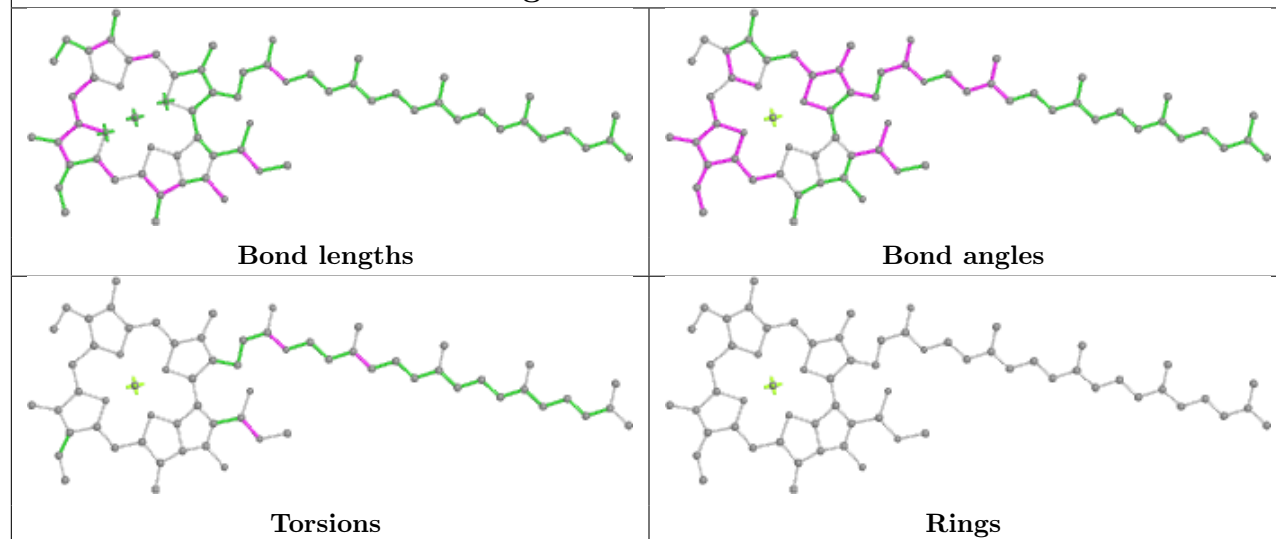
## Ligand CLA aA 829



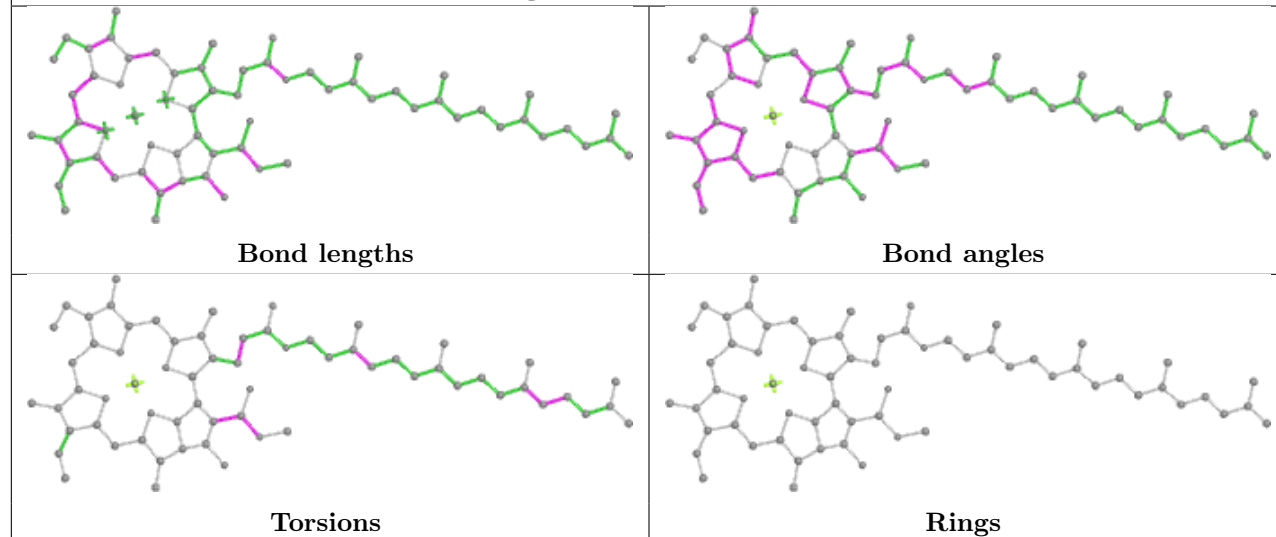


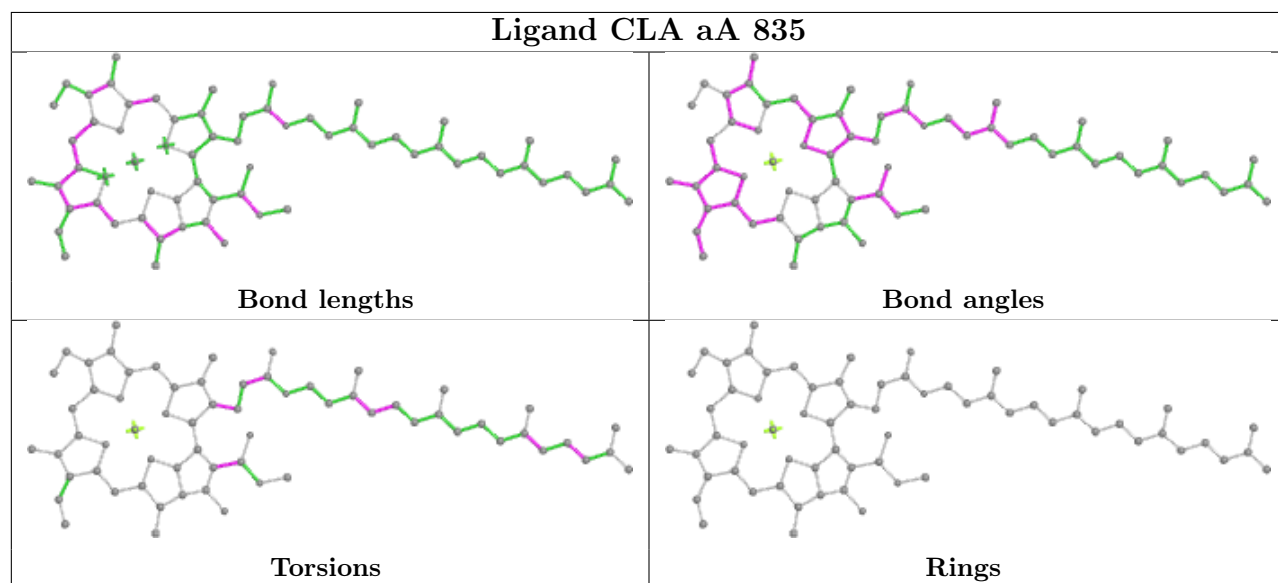
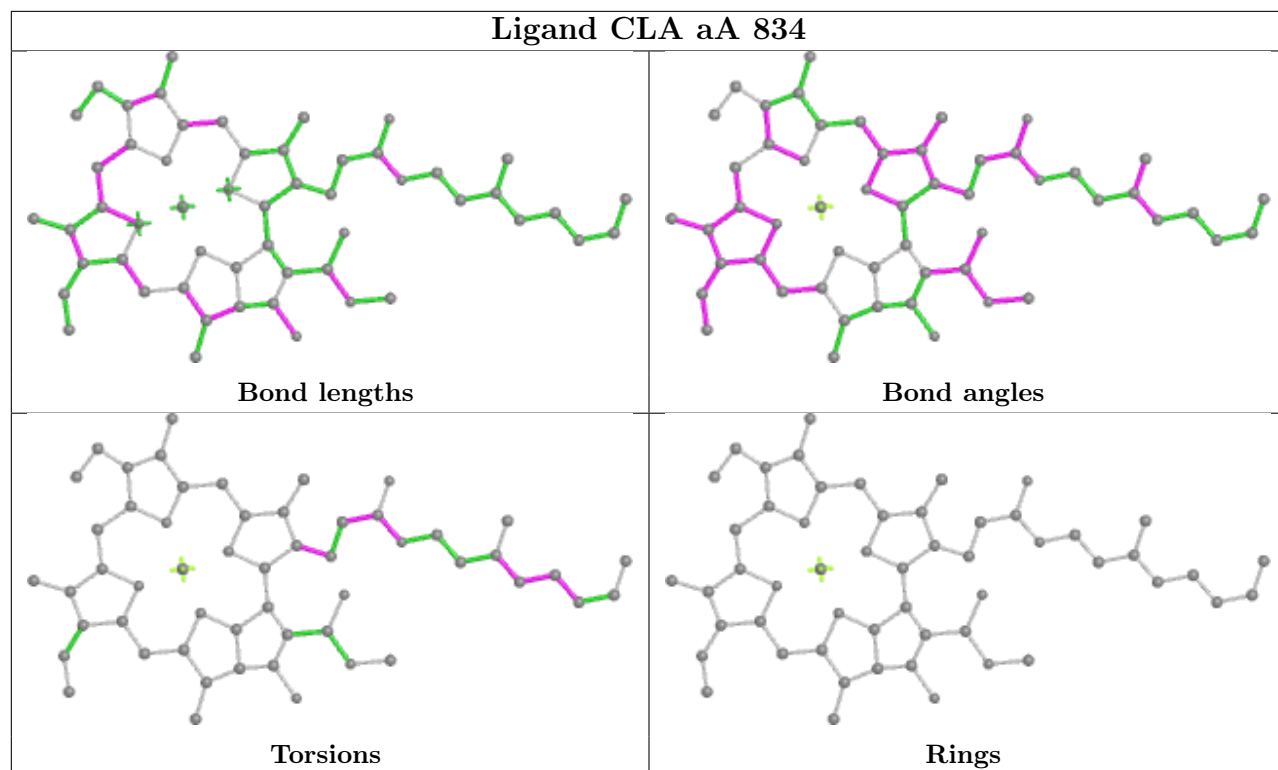


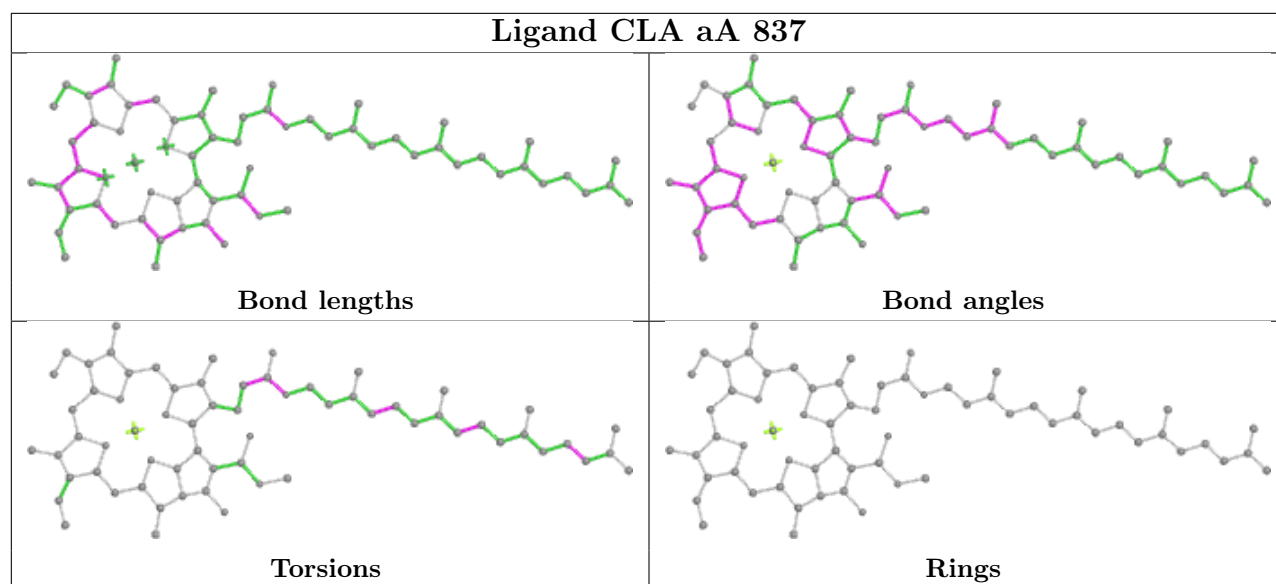
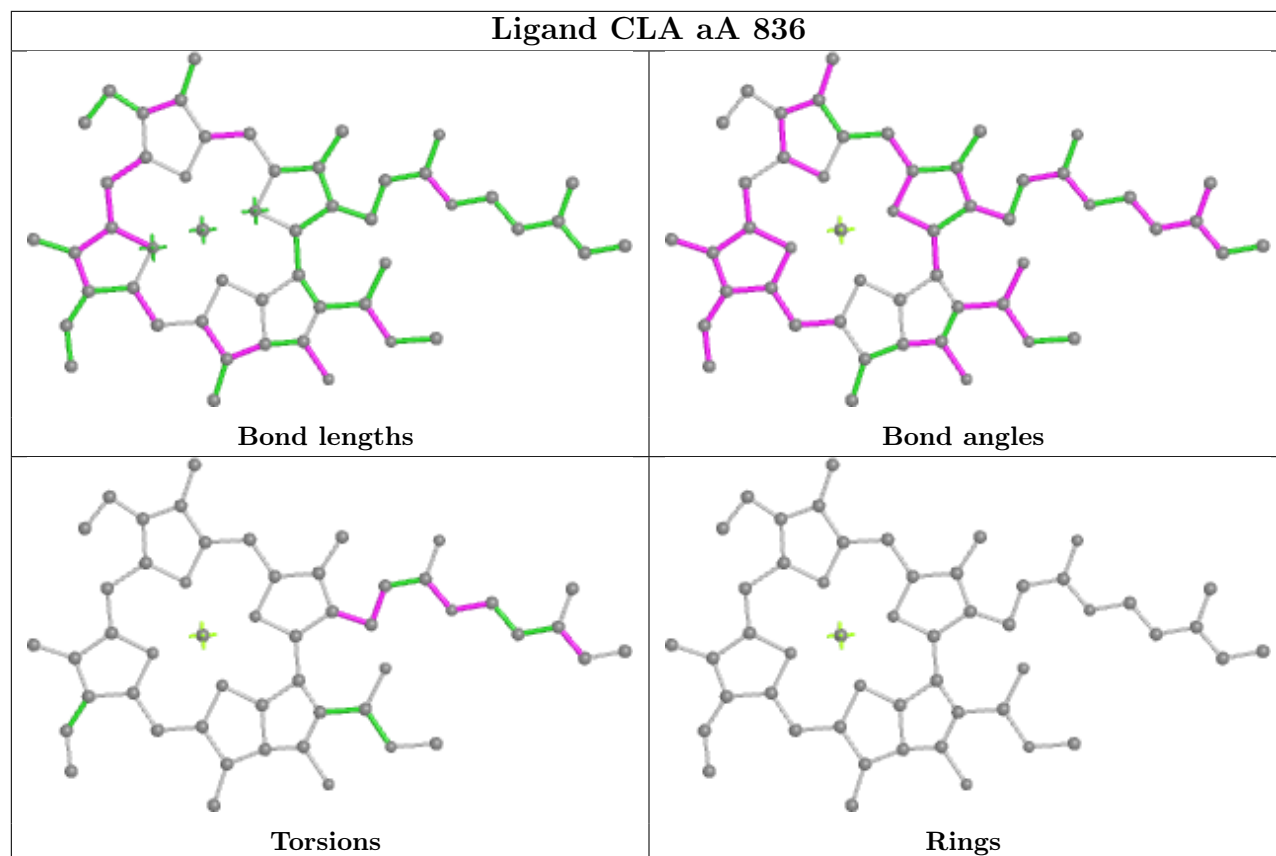
## Ligand CLA aA 832

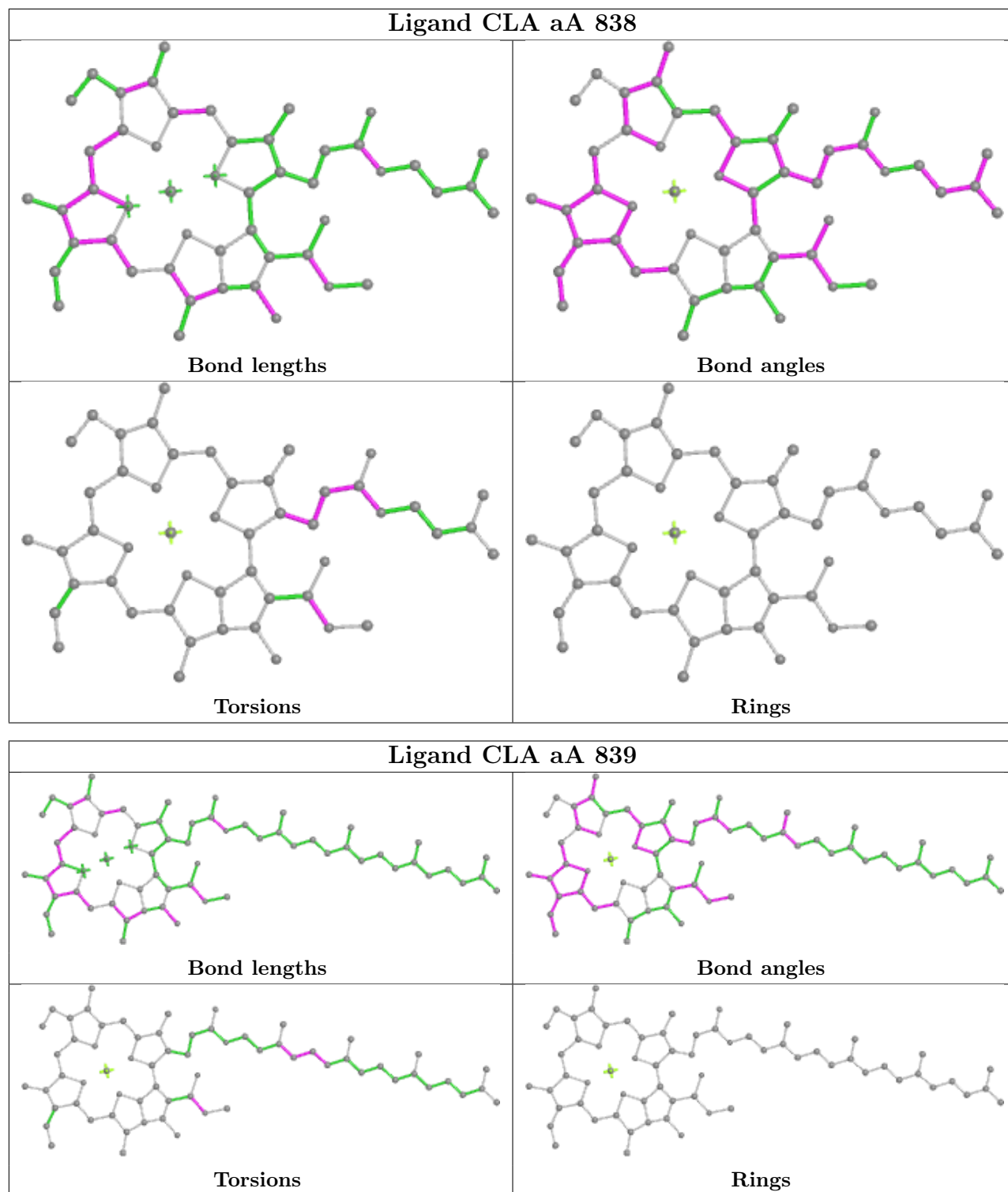


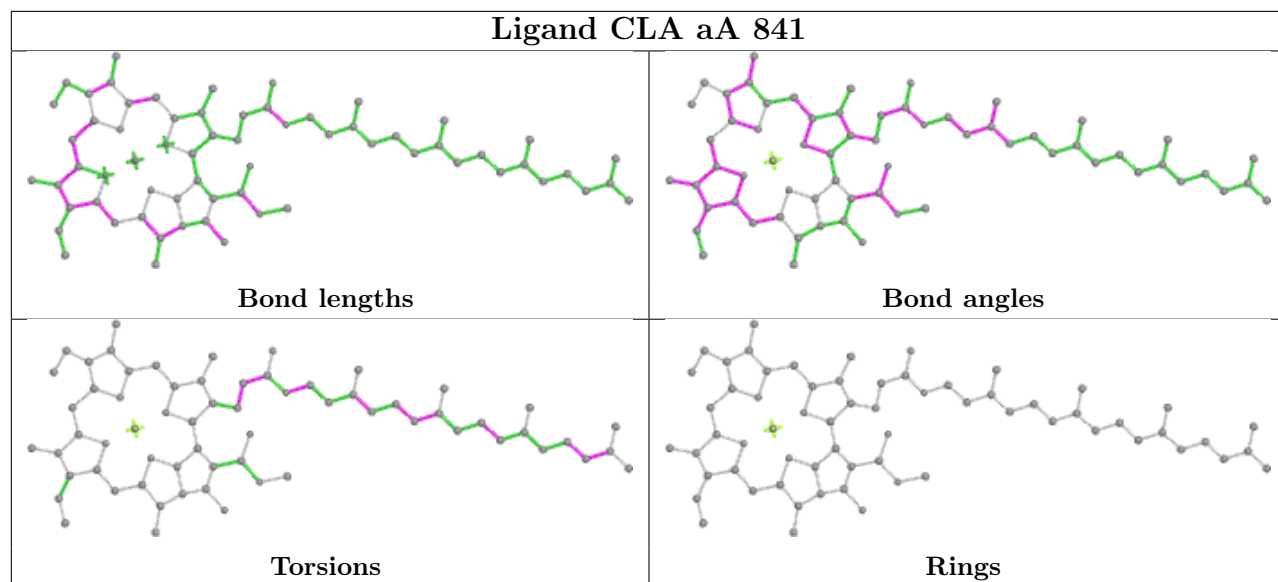
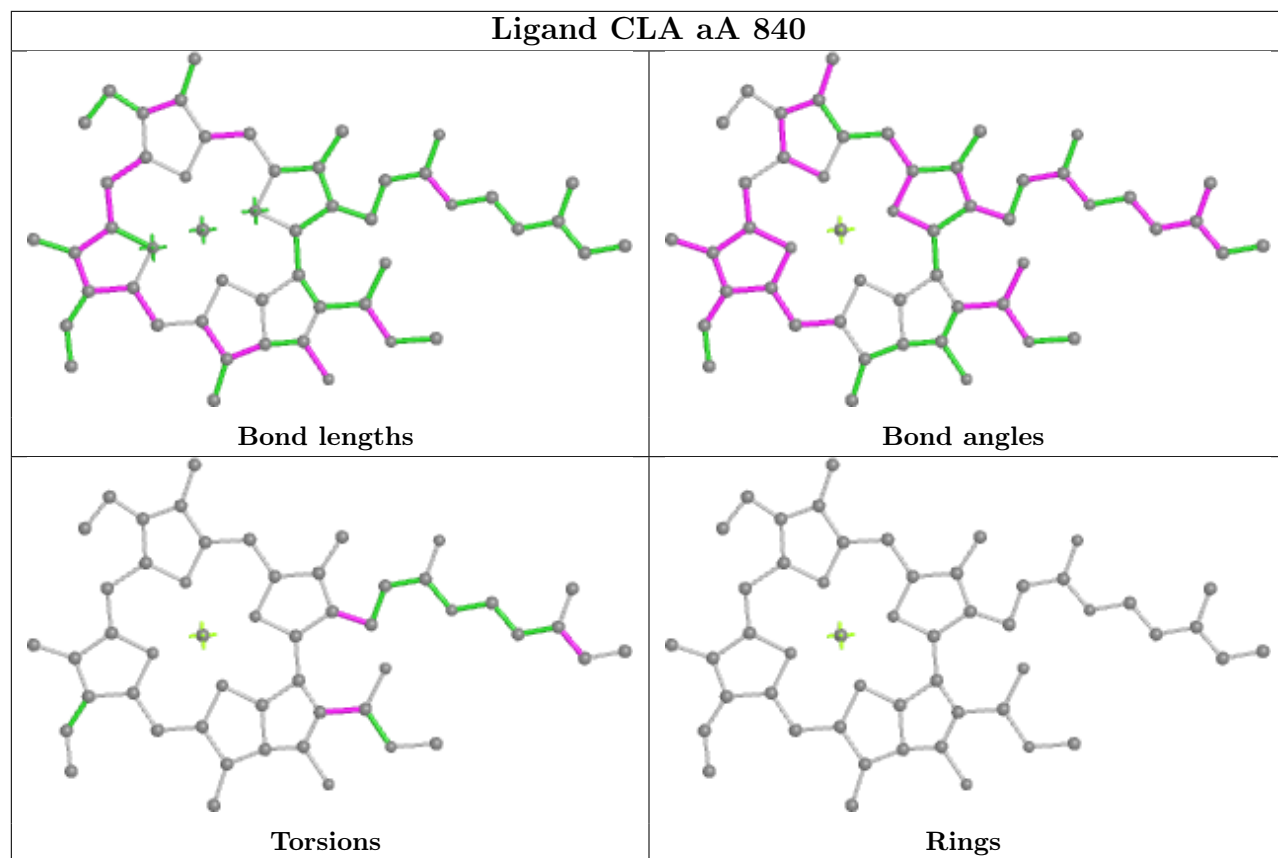
## Ligand CLA aA 833

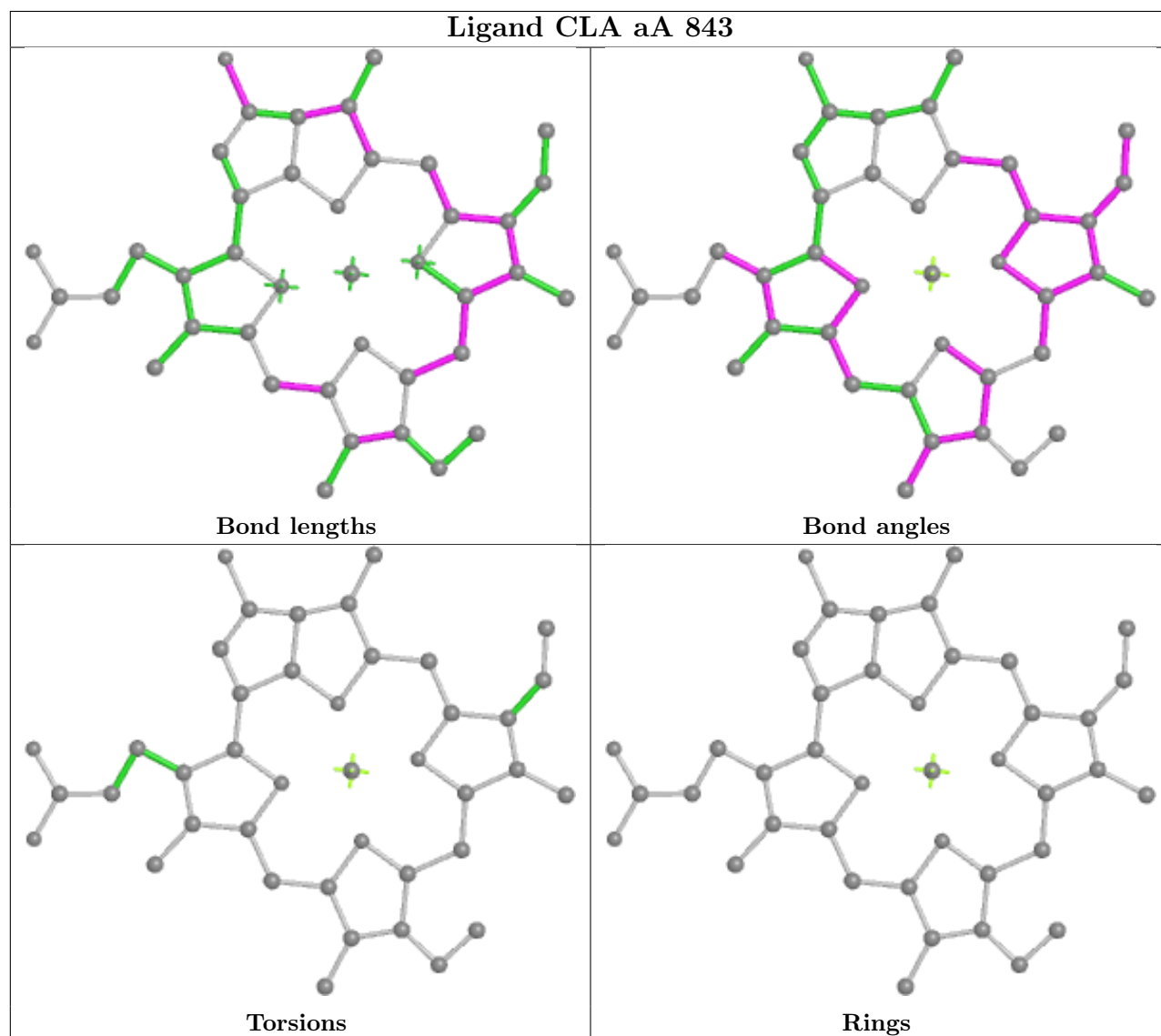
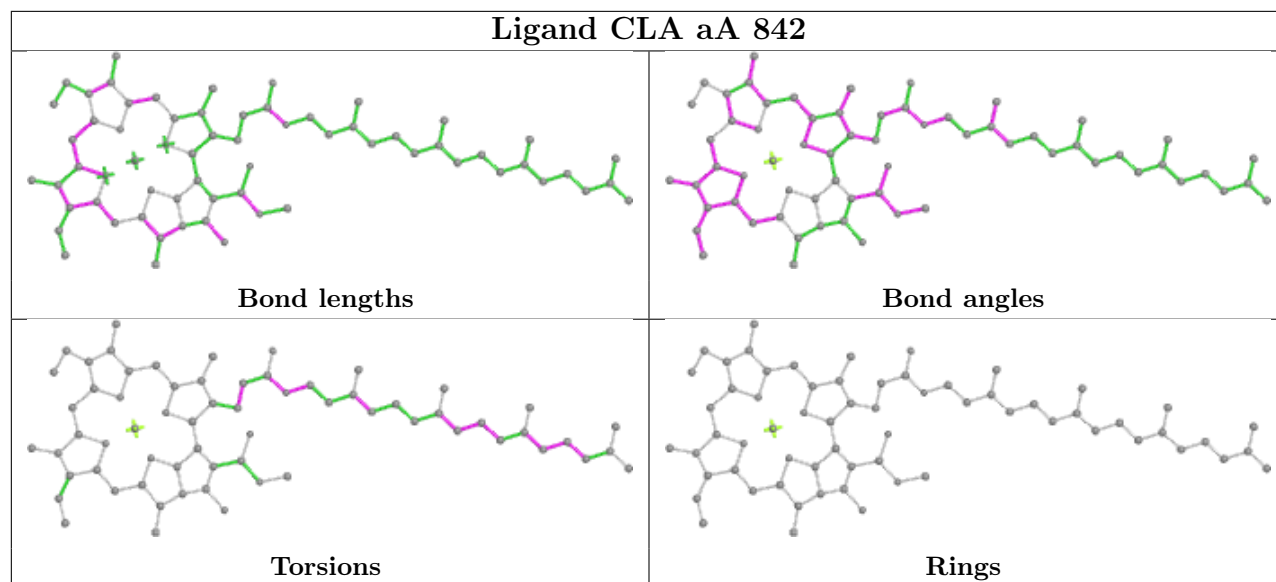


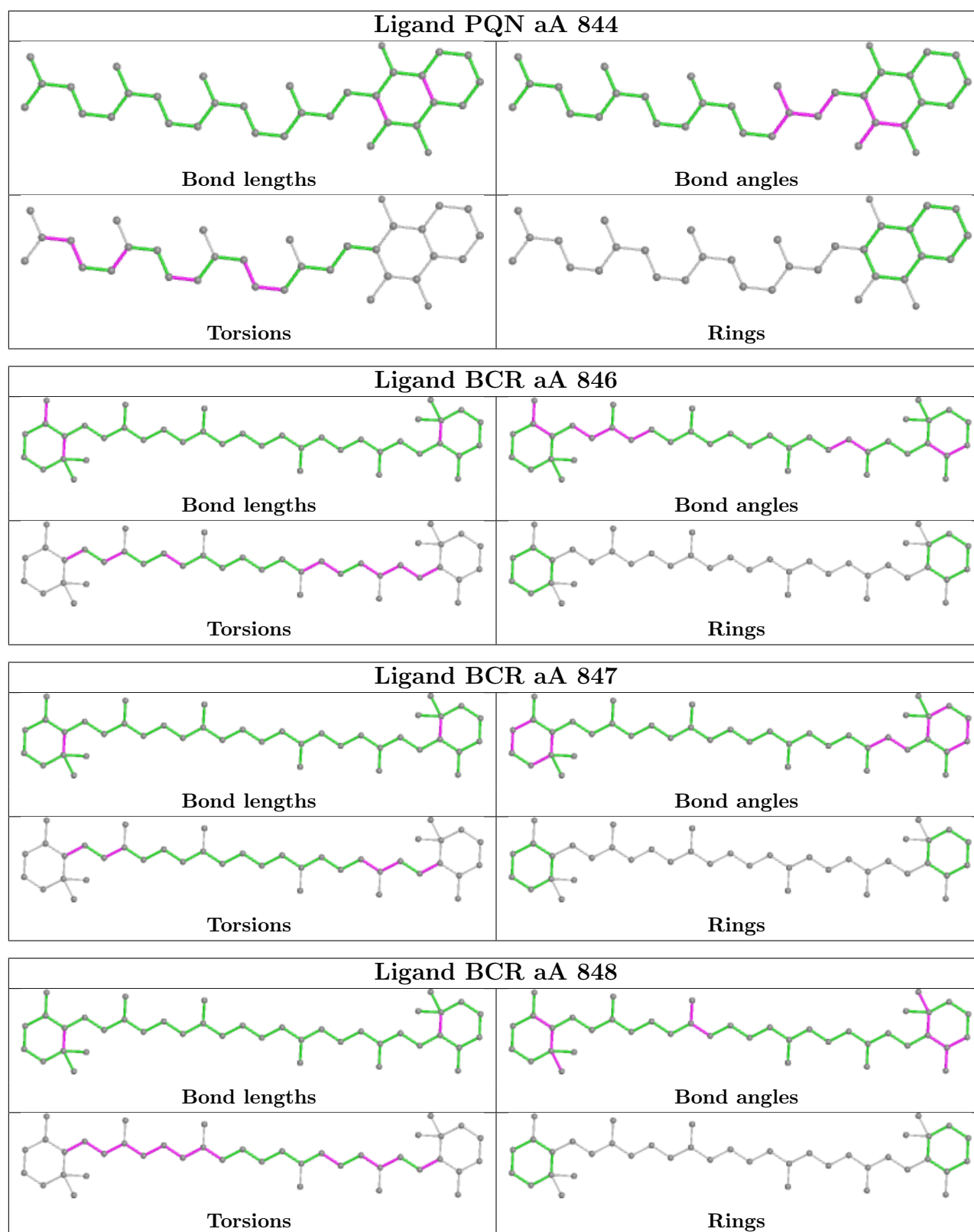




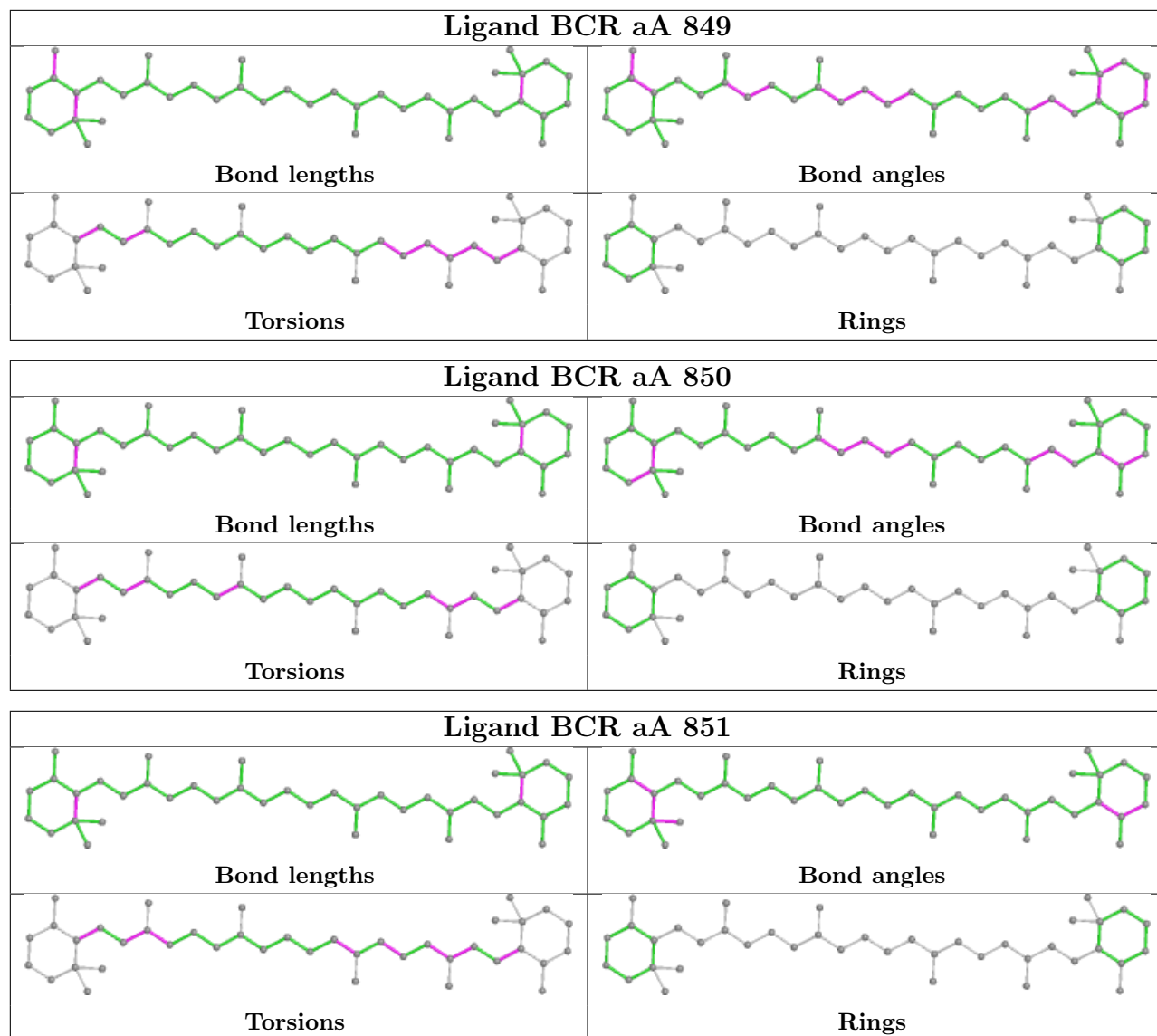


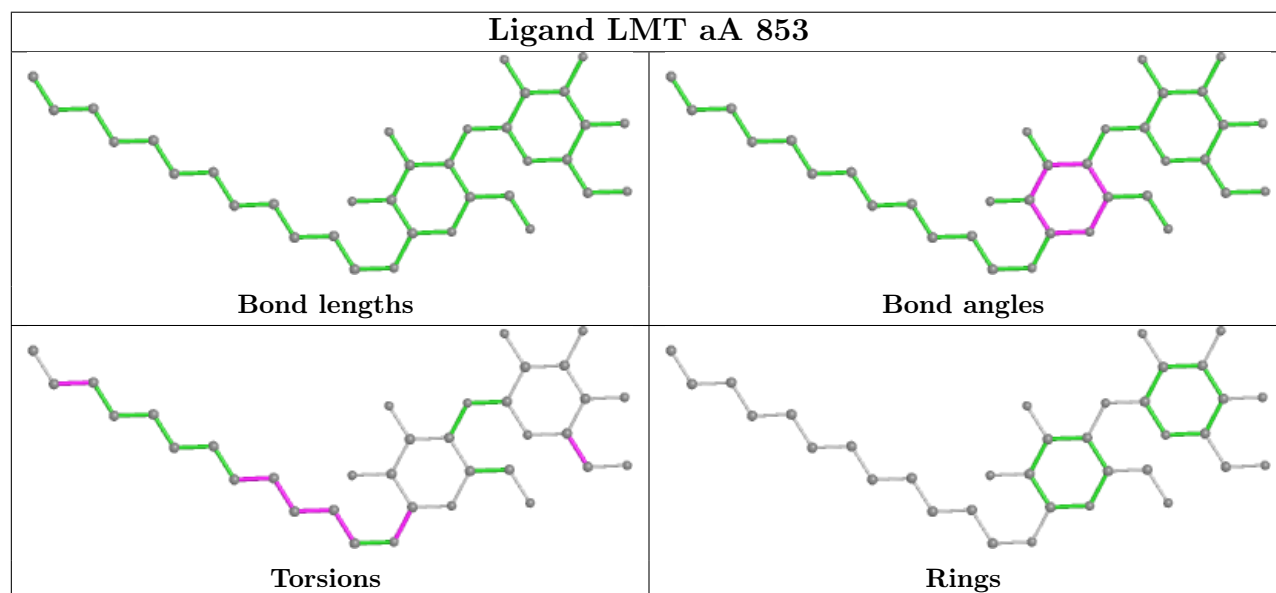
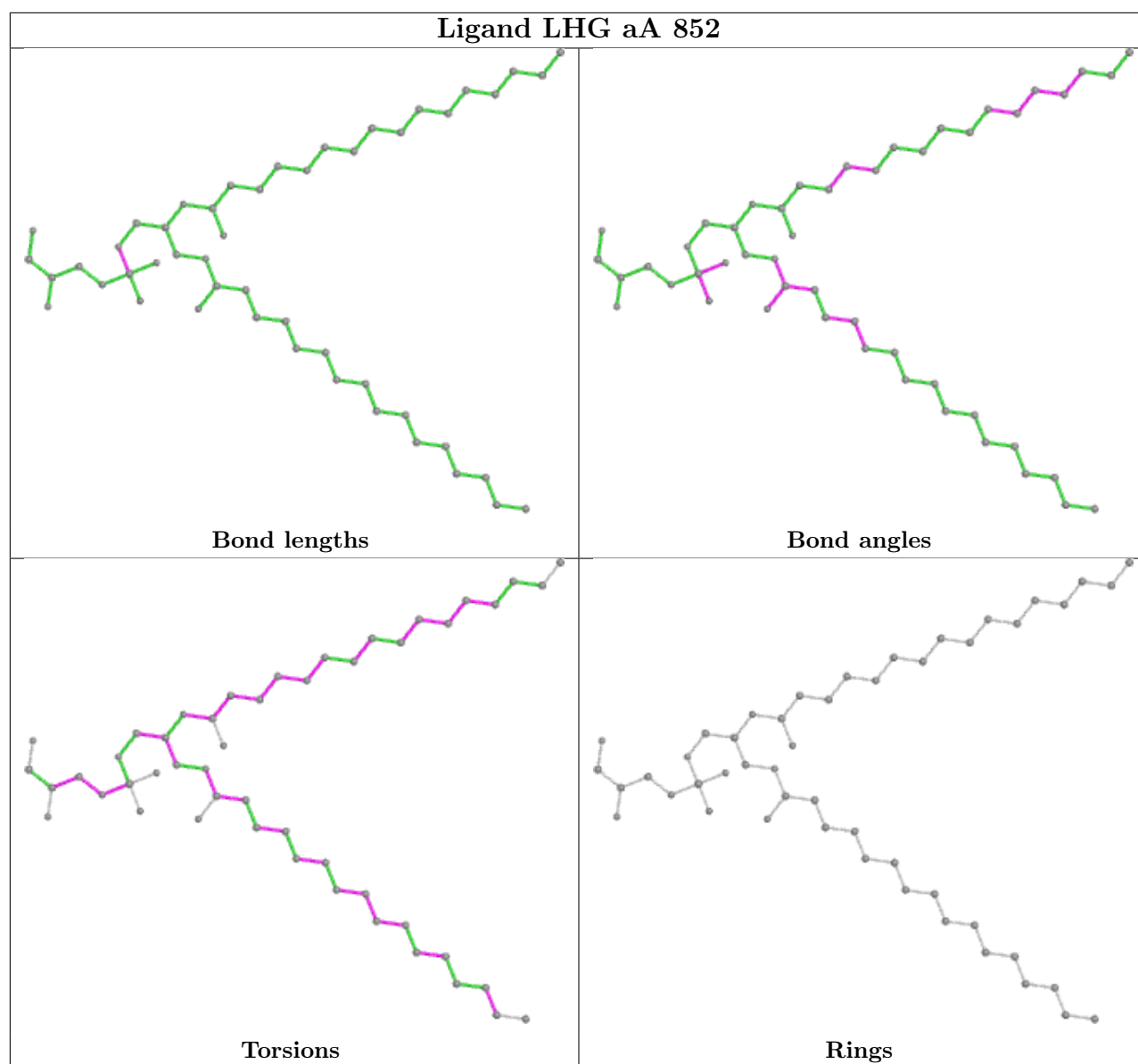


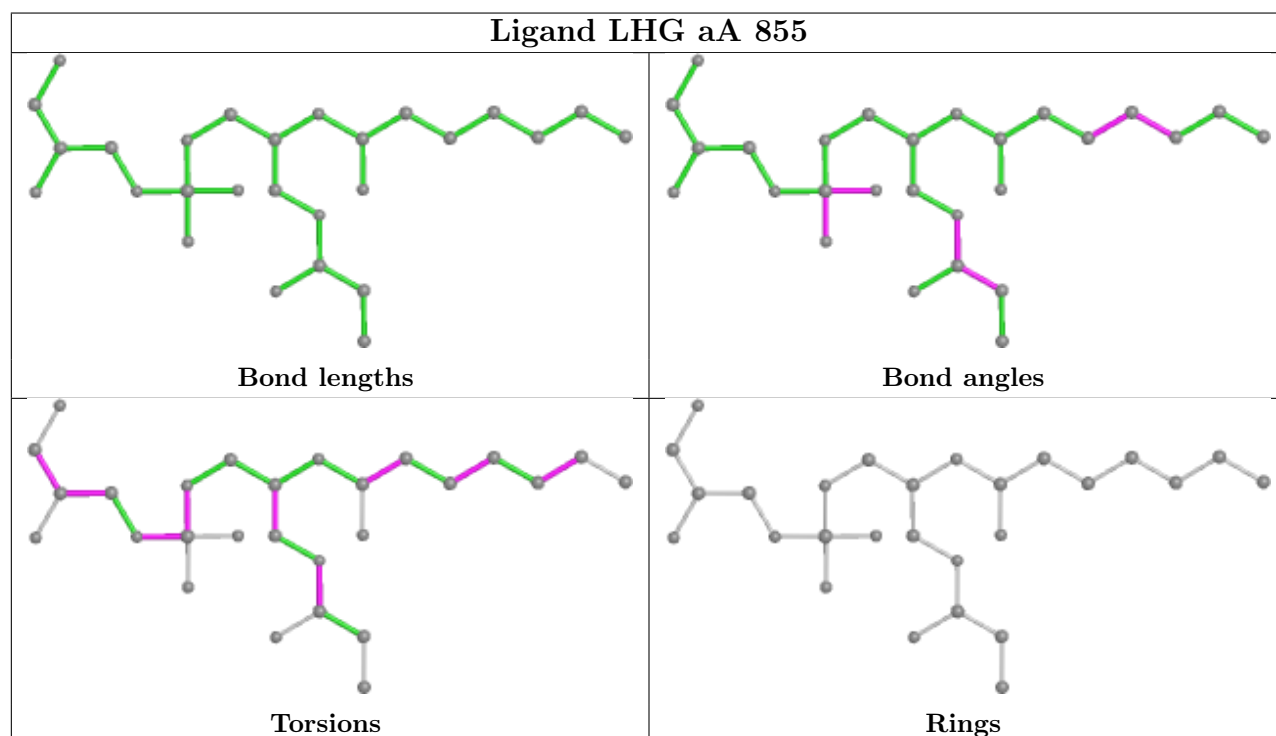
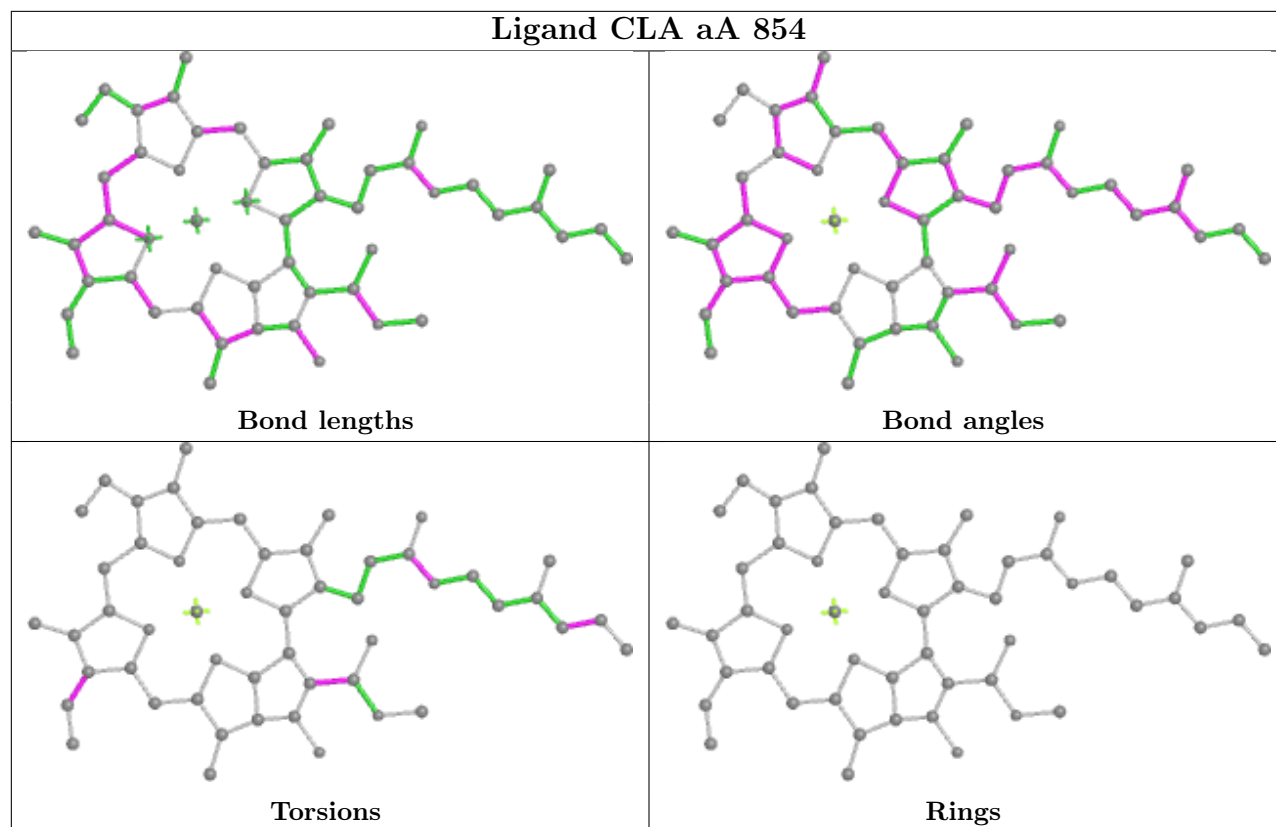


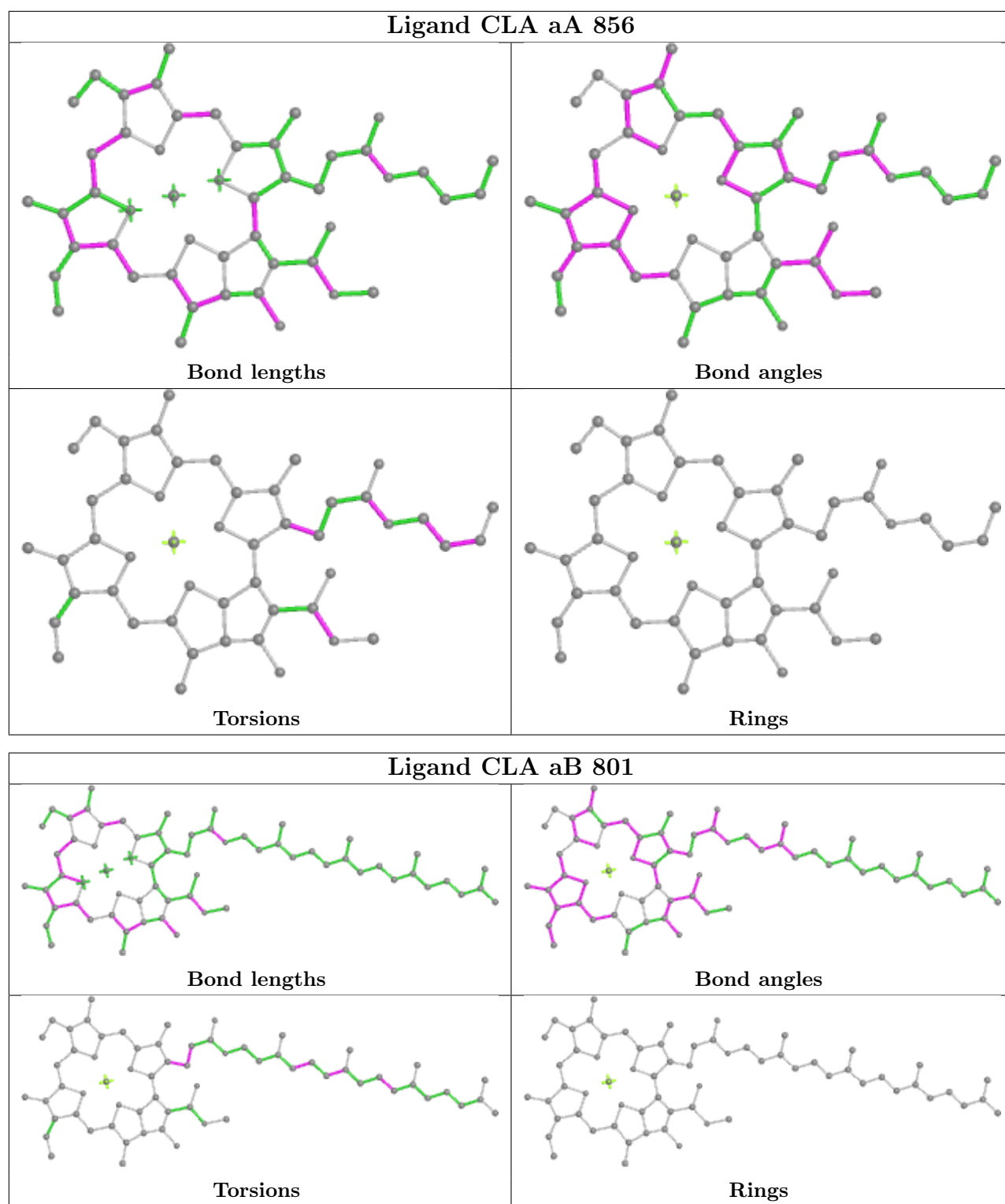




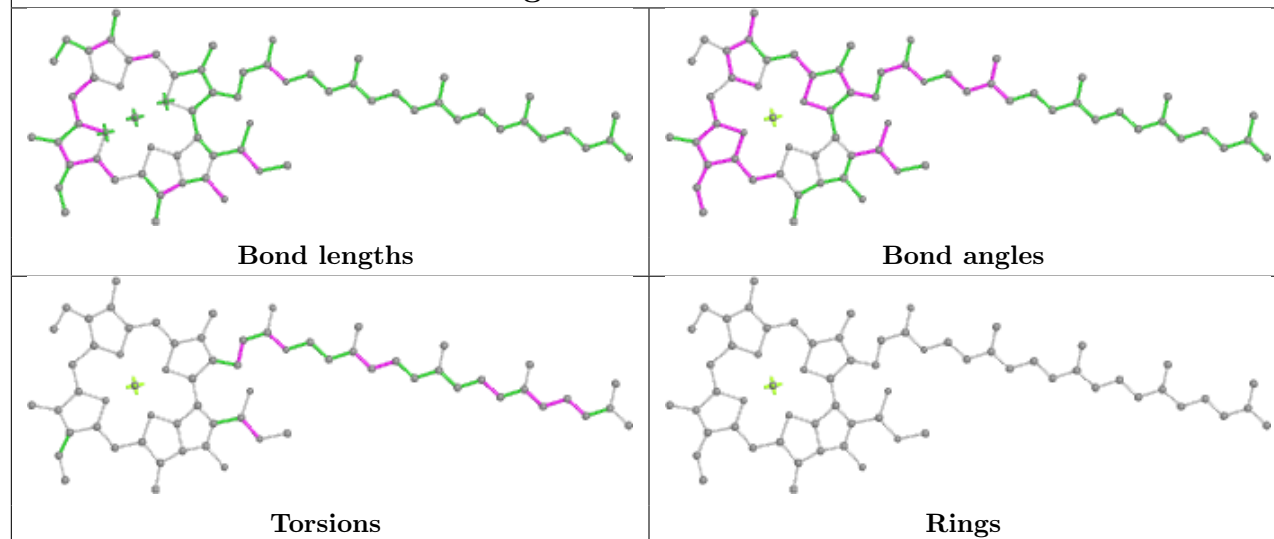




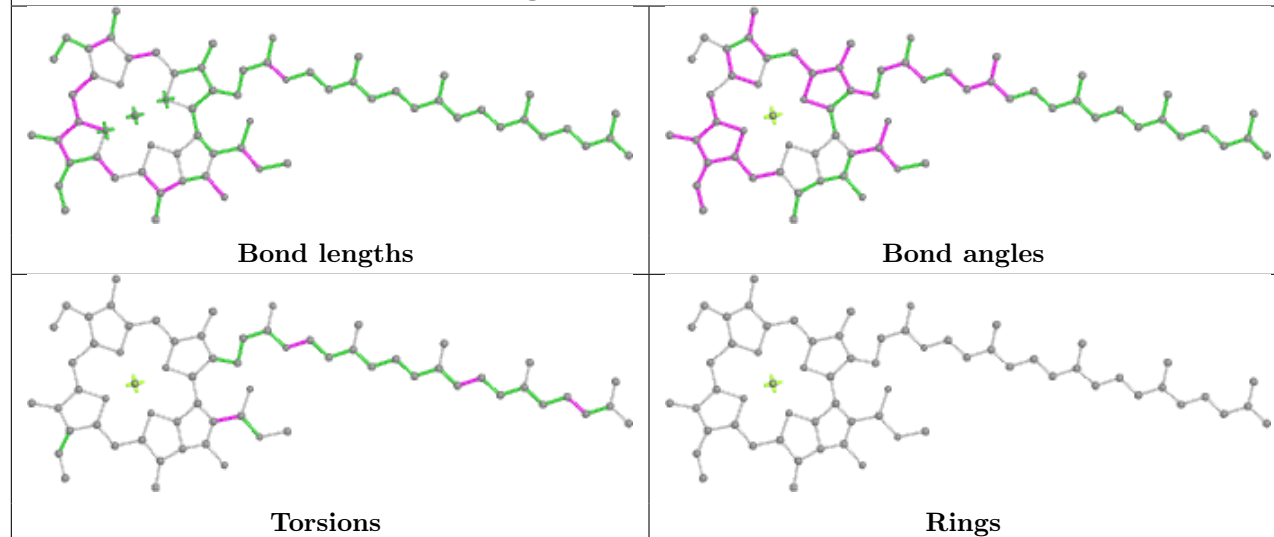


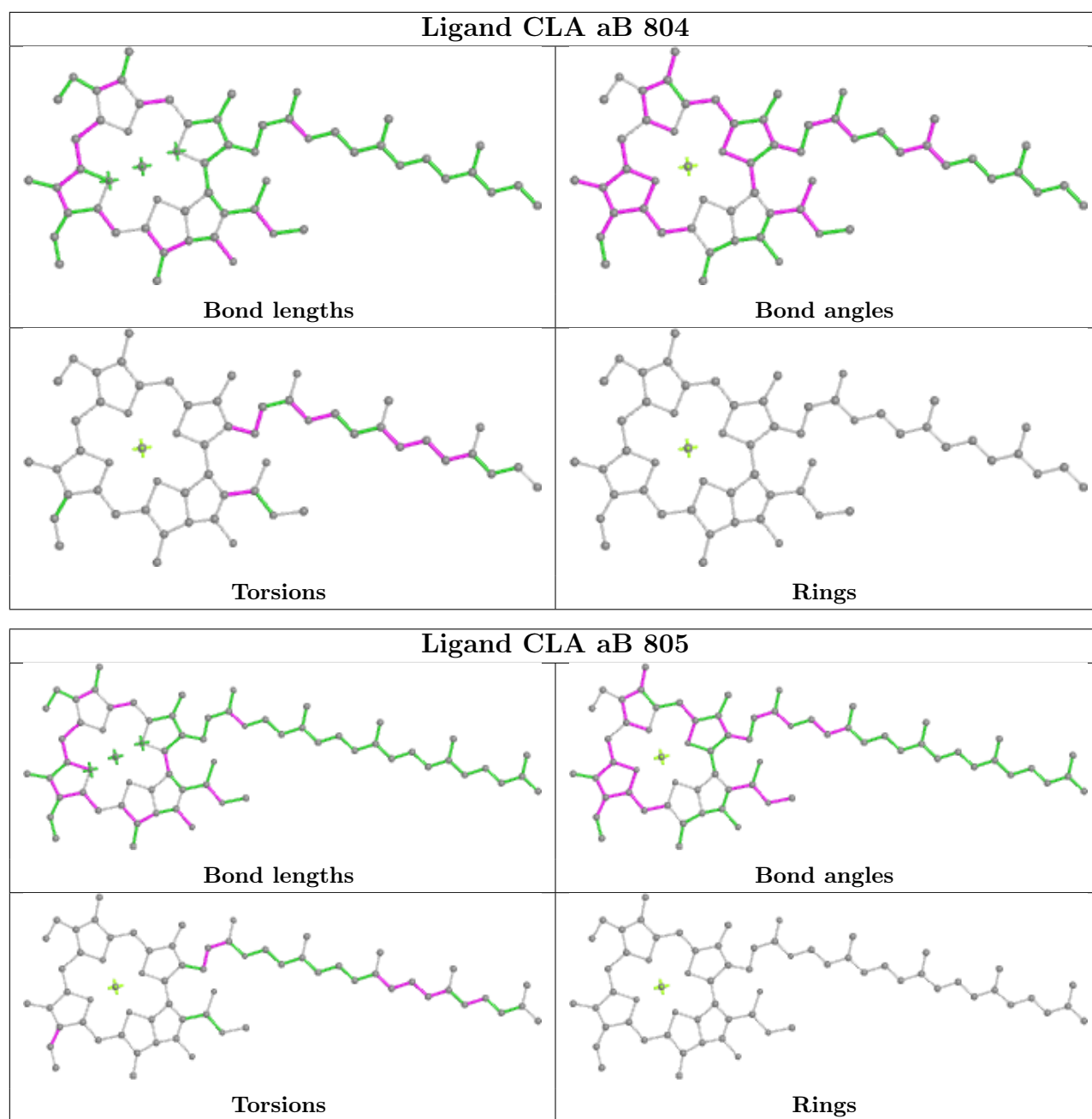


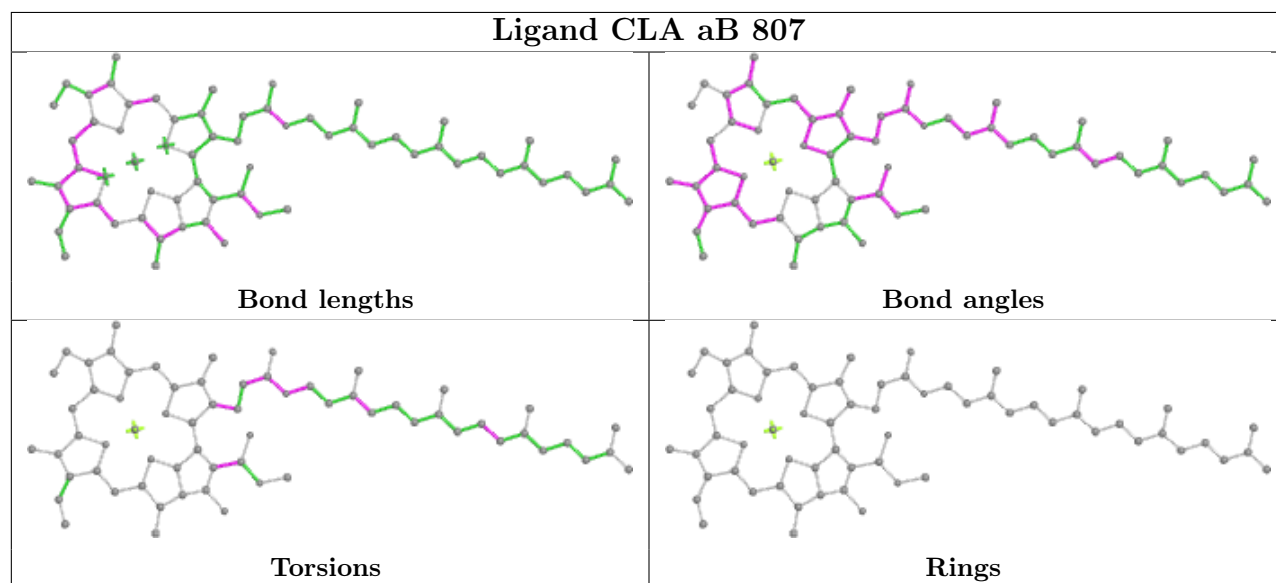
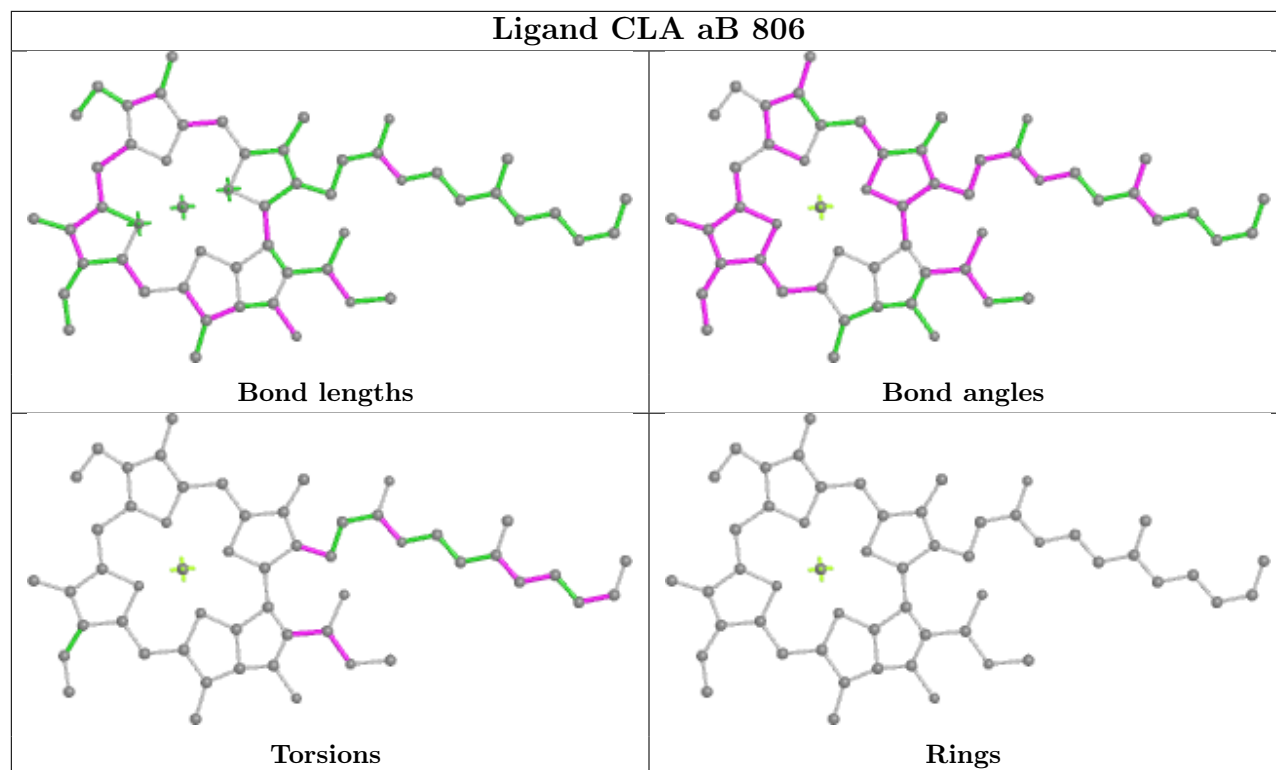
## Ligand CLA aB 802



## Ligand CLA aB 803

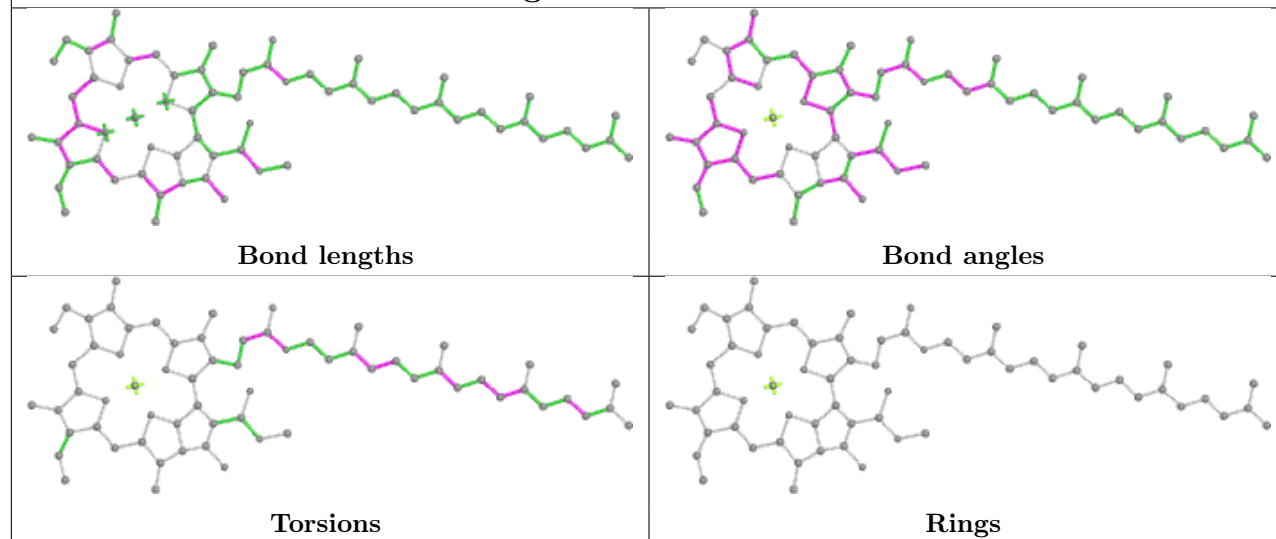




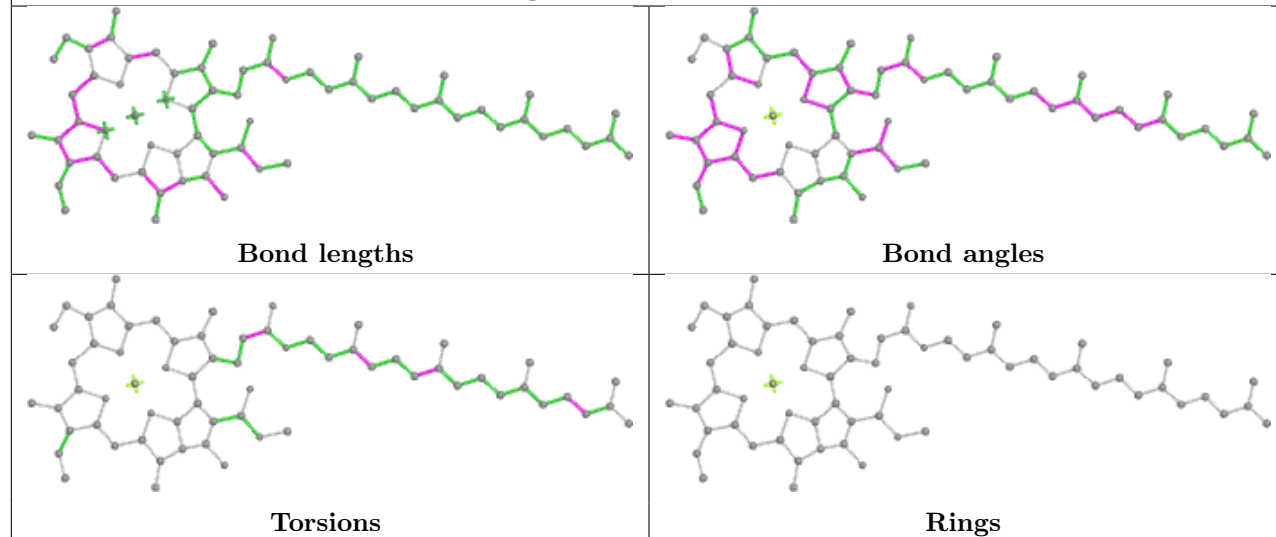


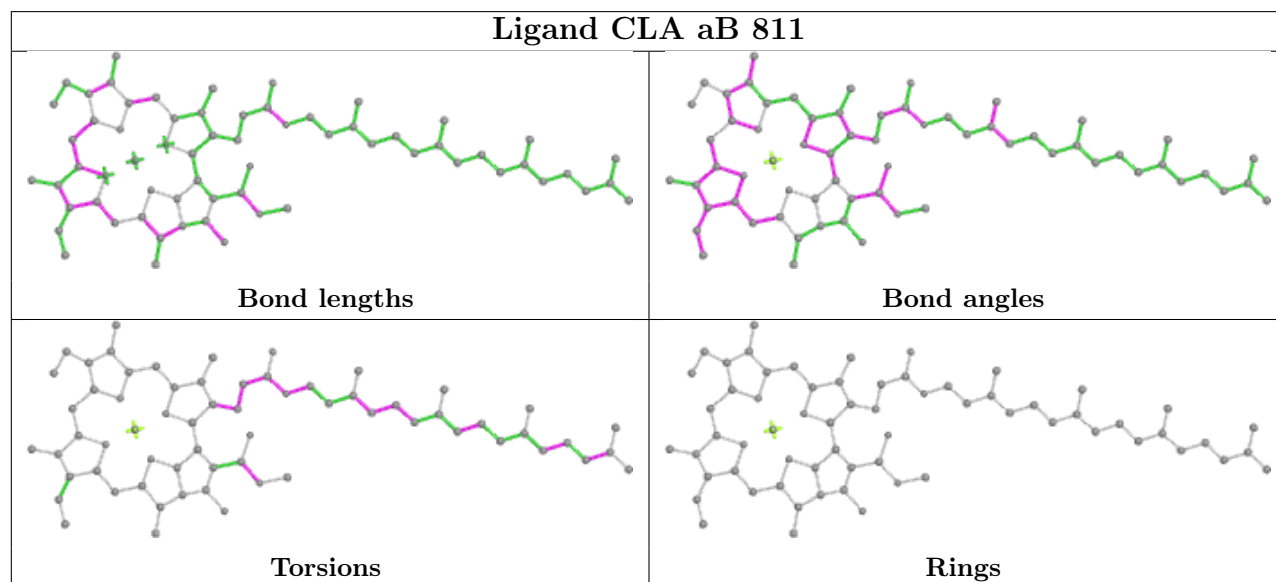
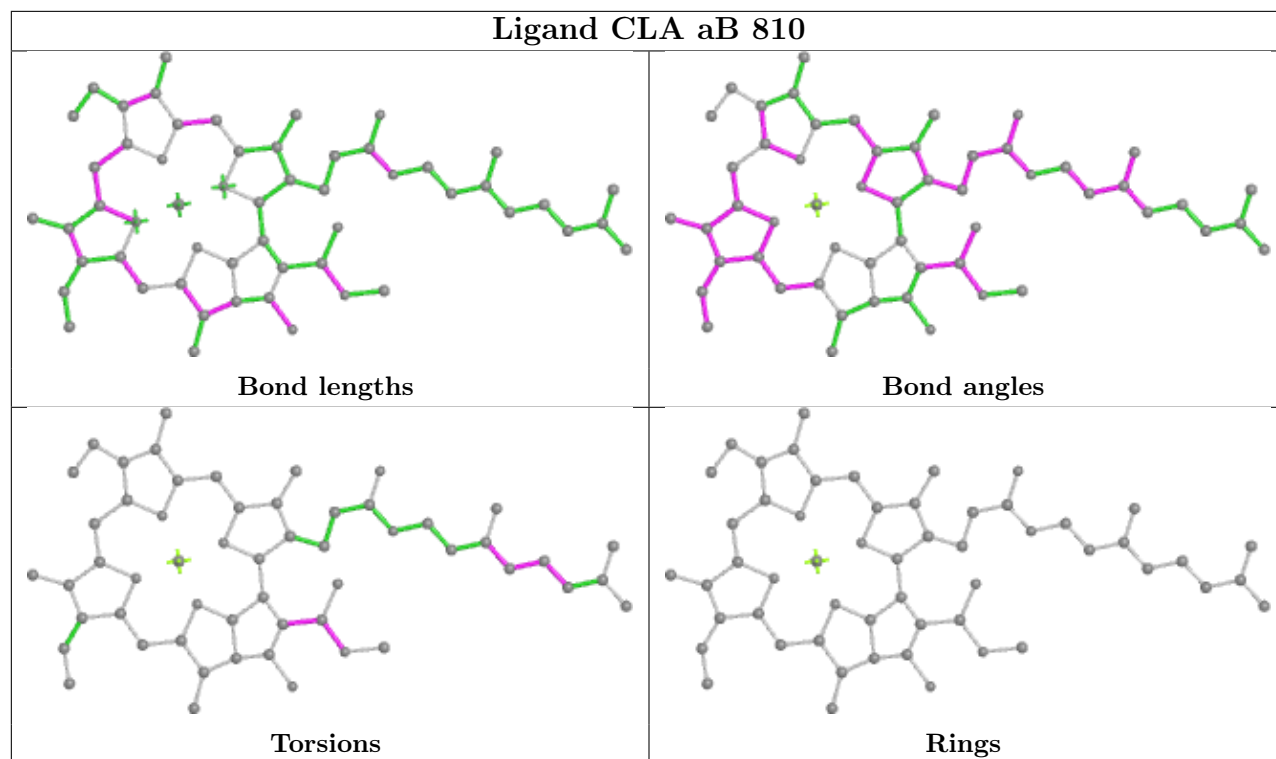


## Ligand CLA aB 808

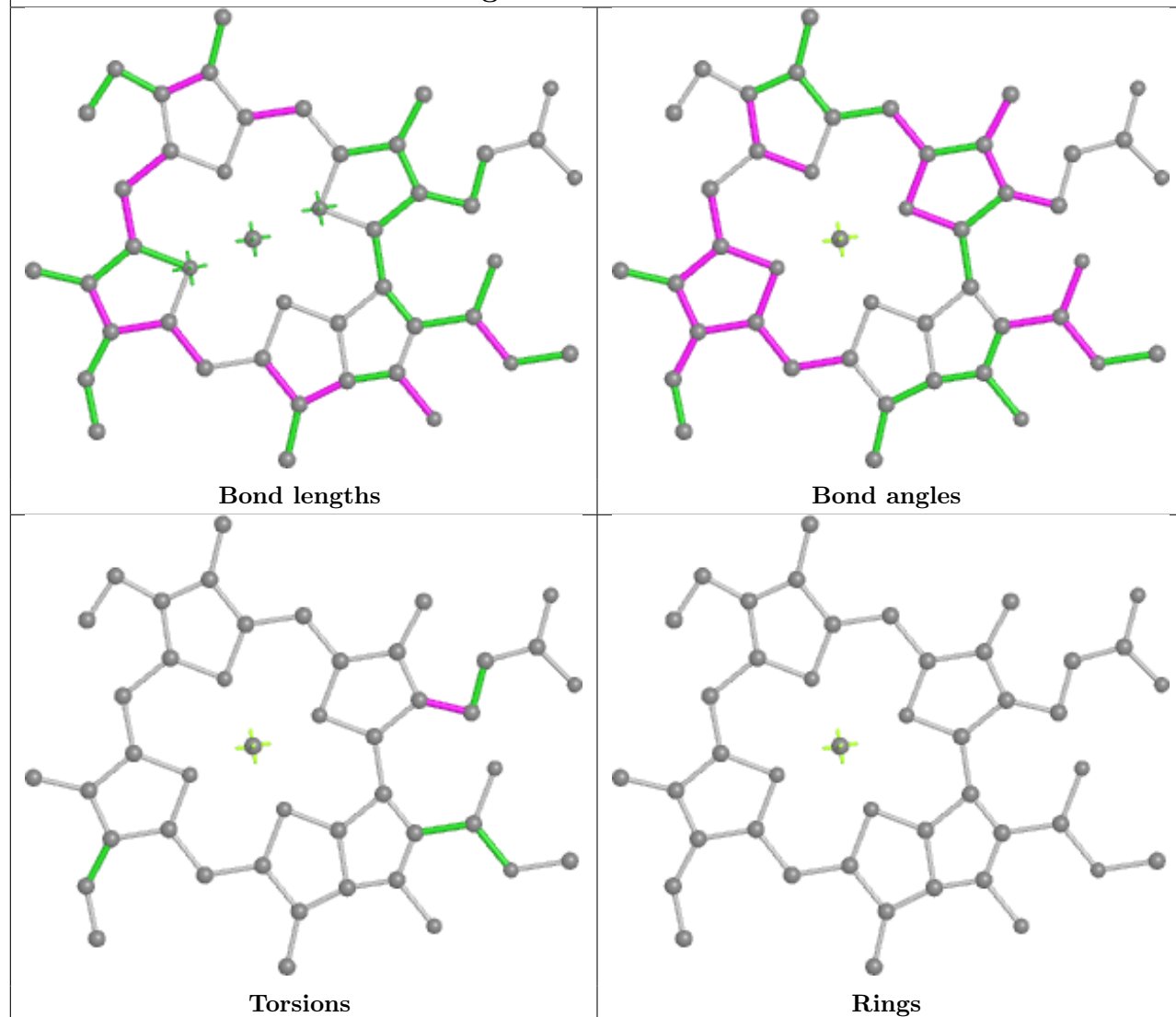


## Ligand CLA aB 809

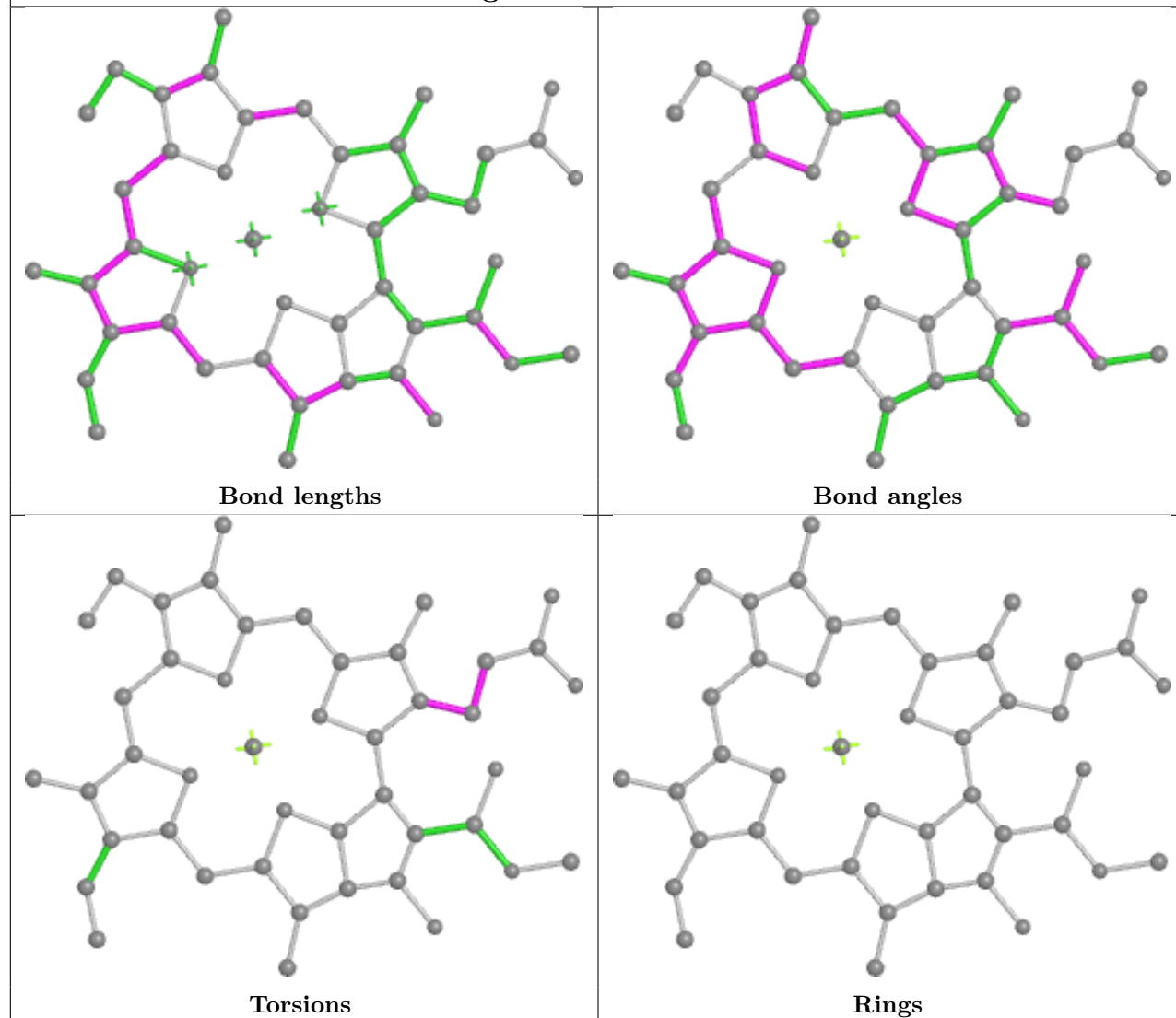




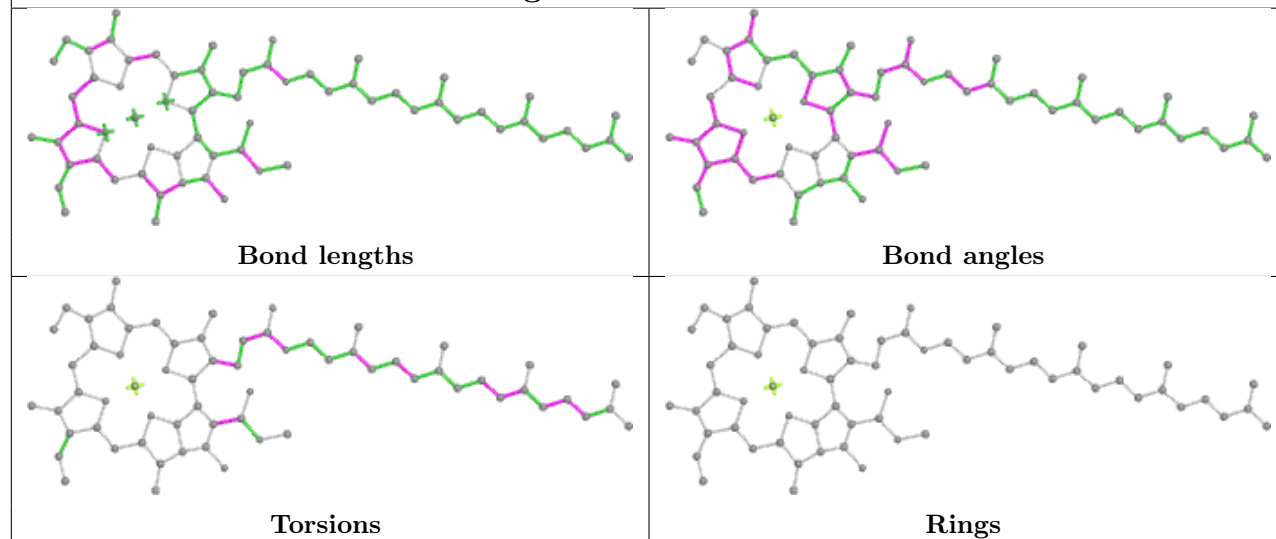
## Ligand CLA aB 812

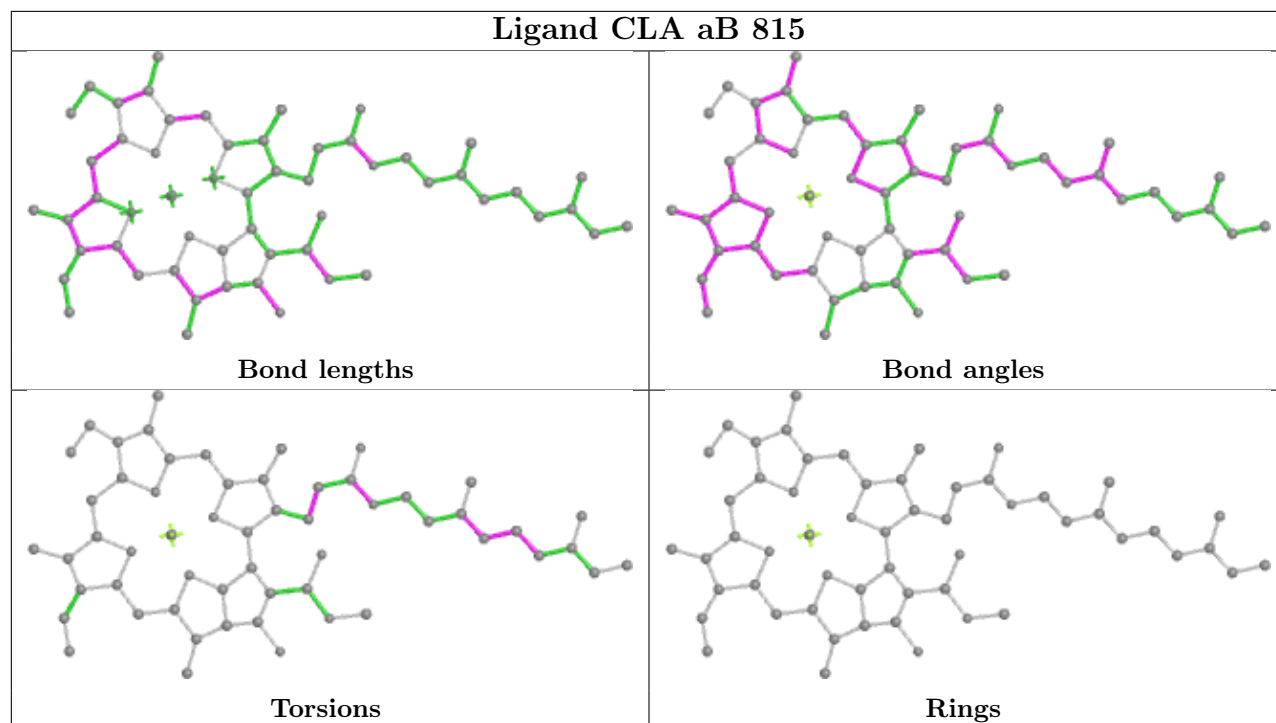


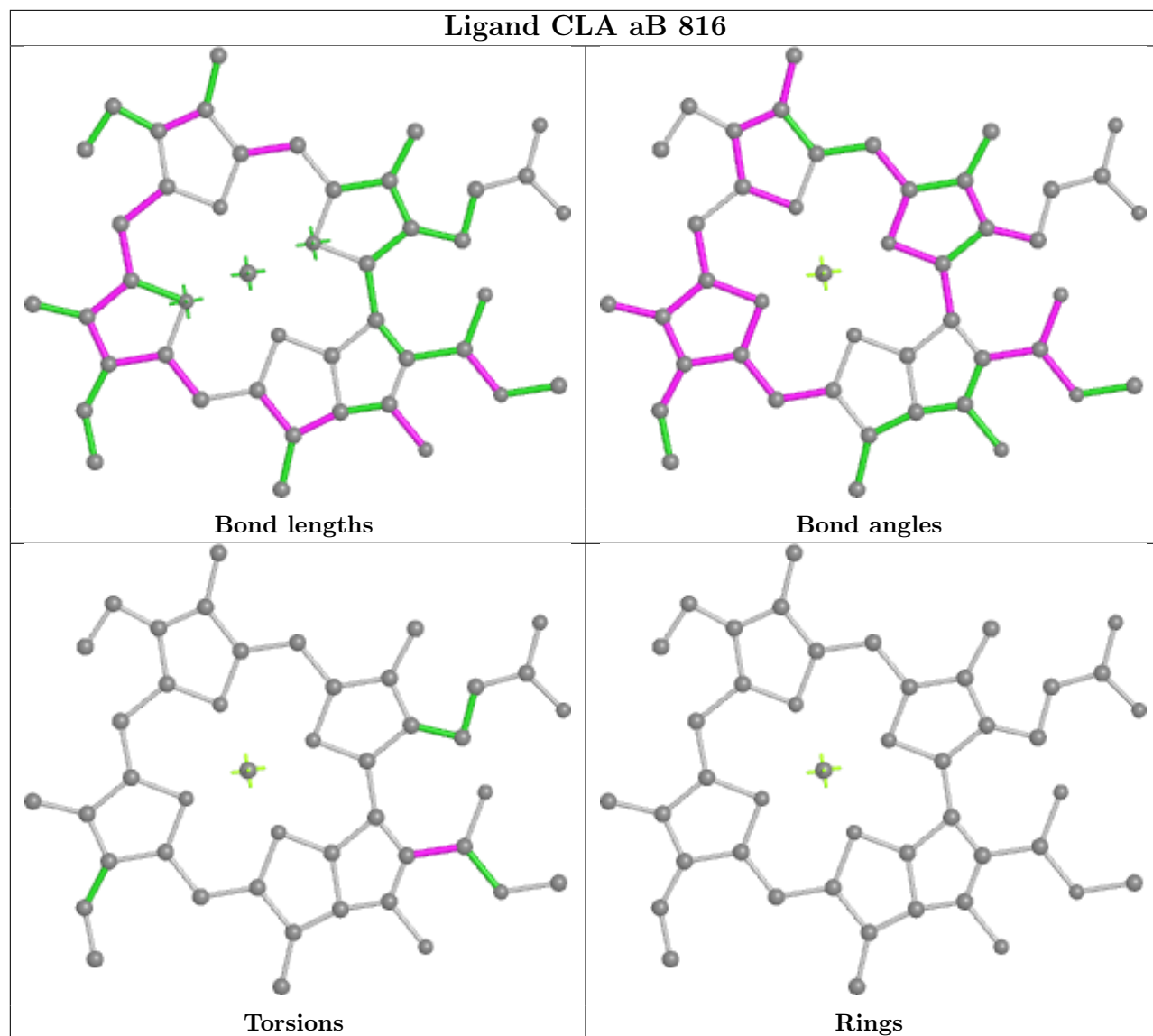
## Ligand CLA aB 813

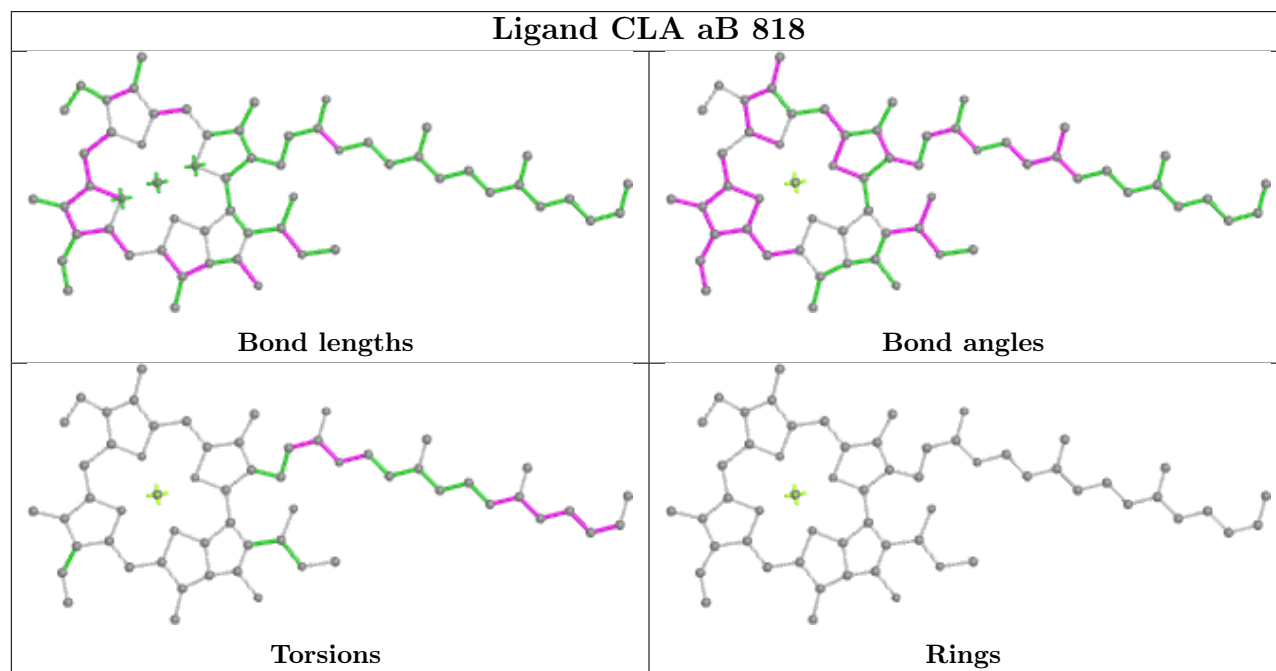
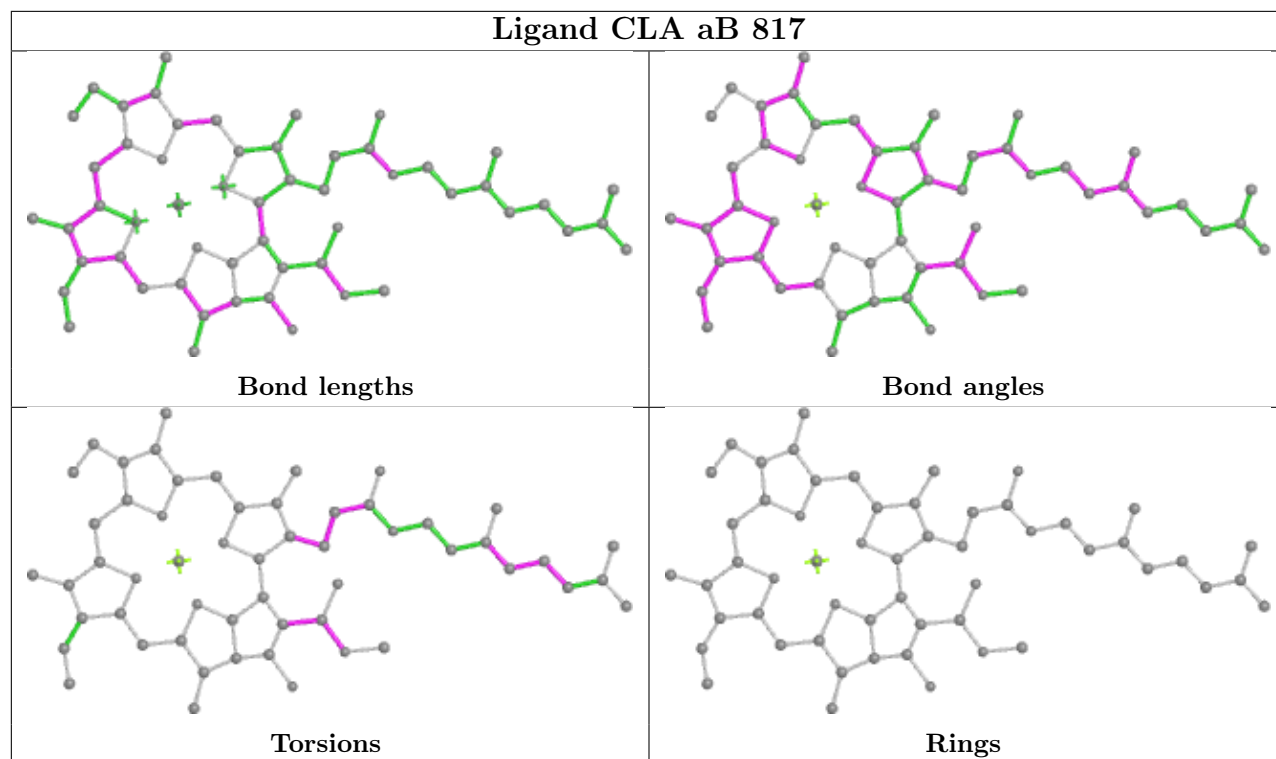


## Ligand CLA aB 814



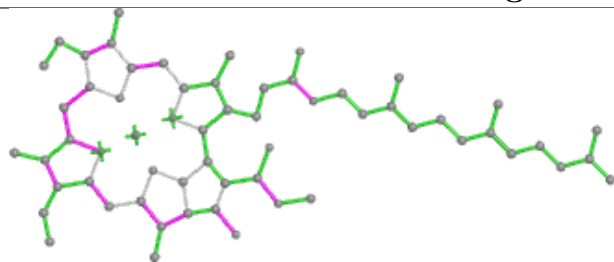




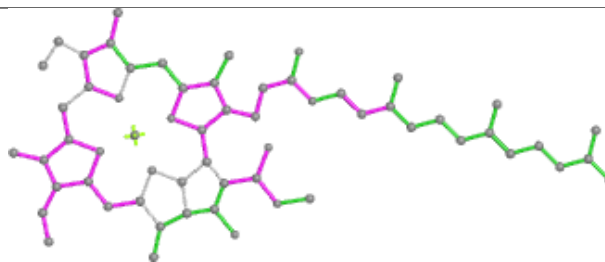




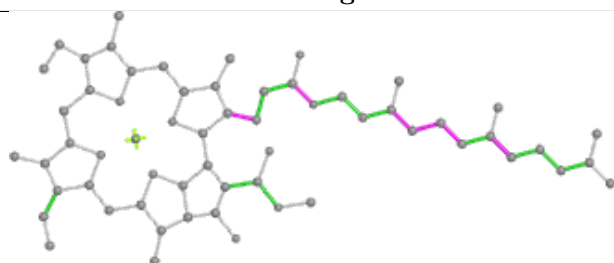
## Ligand CLA aB 819



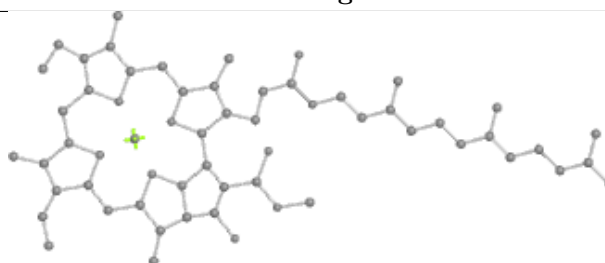
Bond lengths



Bond angles

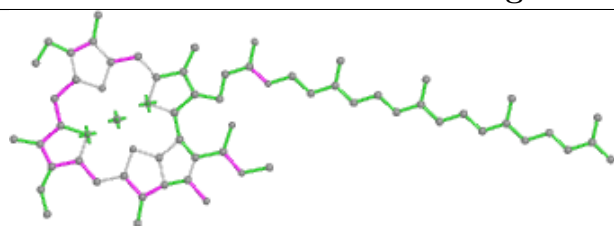


Torsions

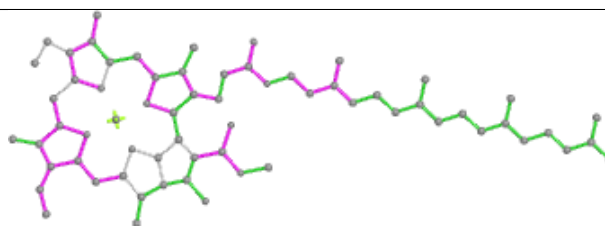


Rings

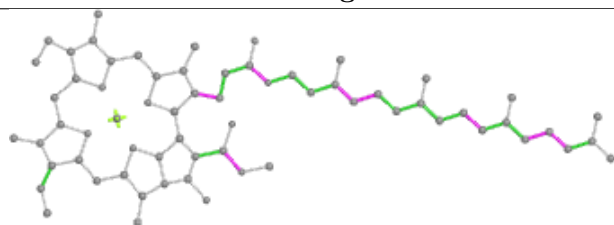
## Ligand CLA aB 820



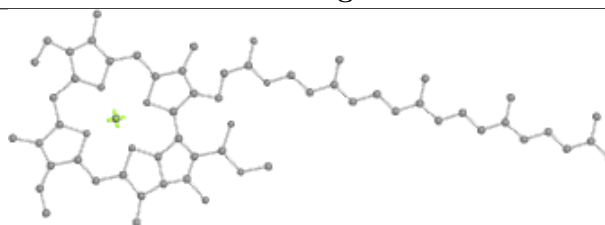
Bond lengths



Bond angles

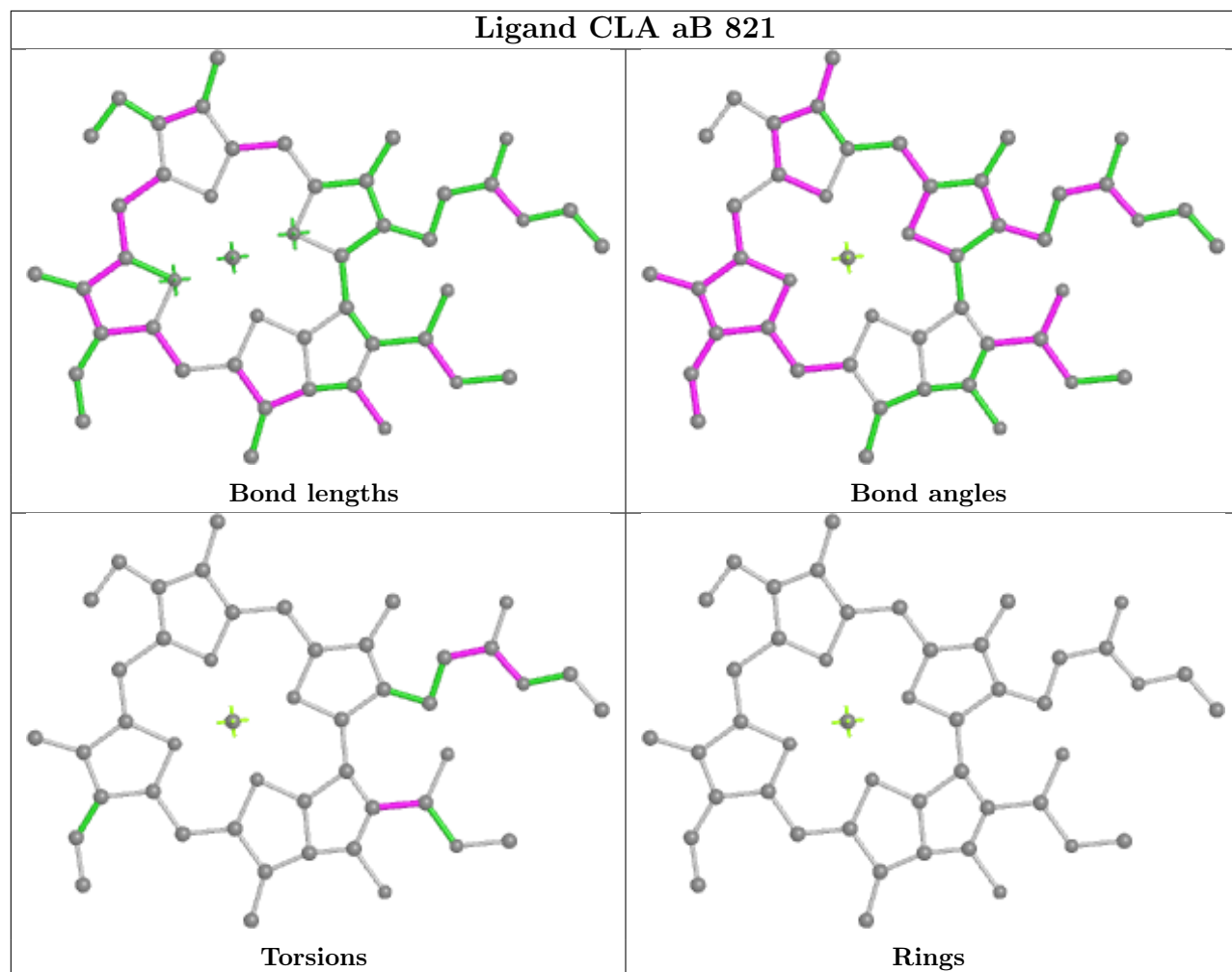


Torsions

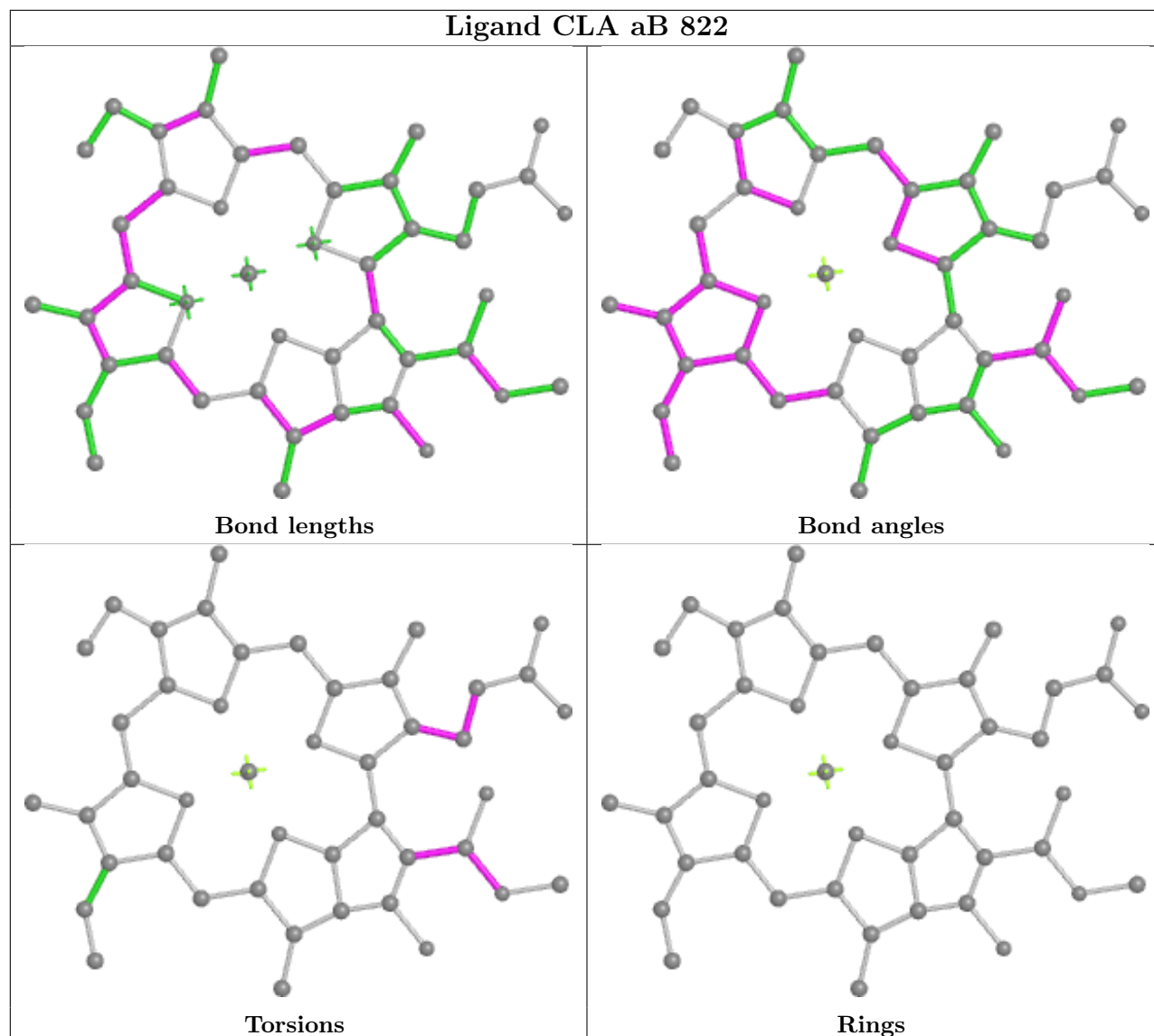


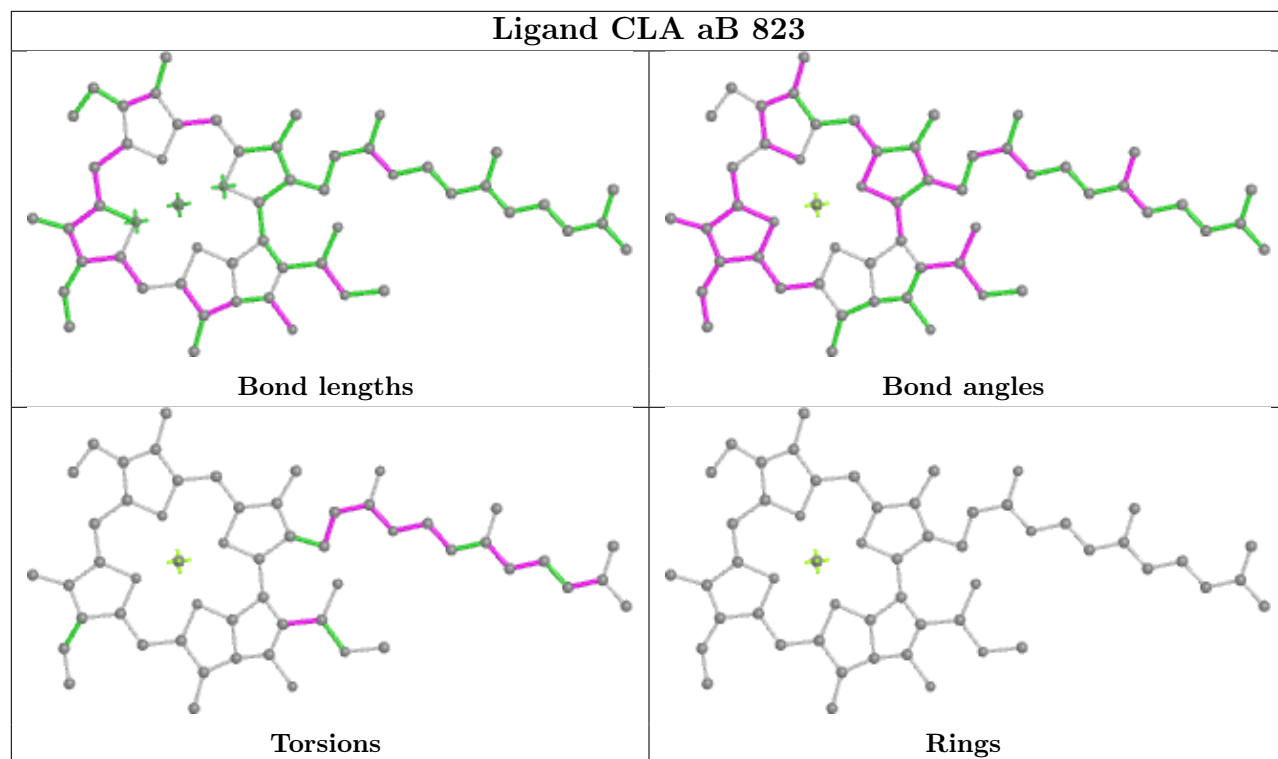
Rings

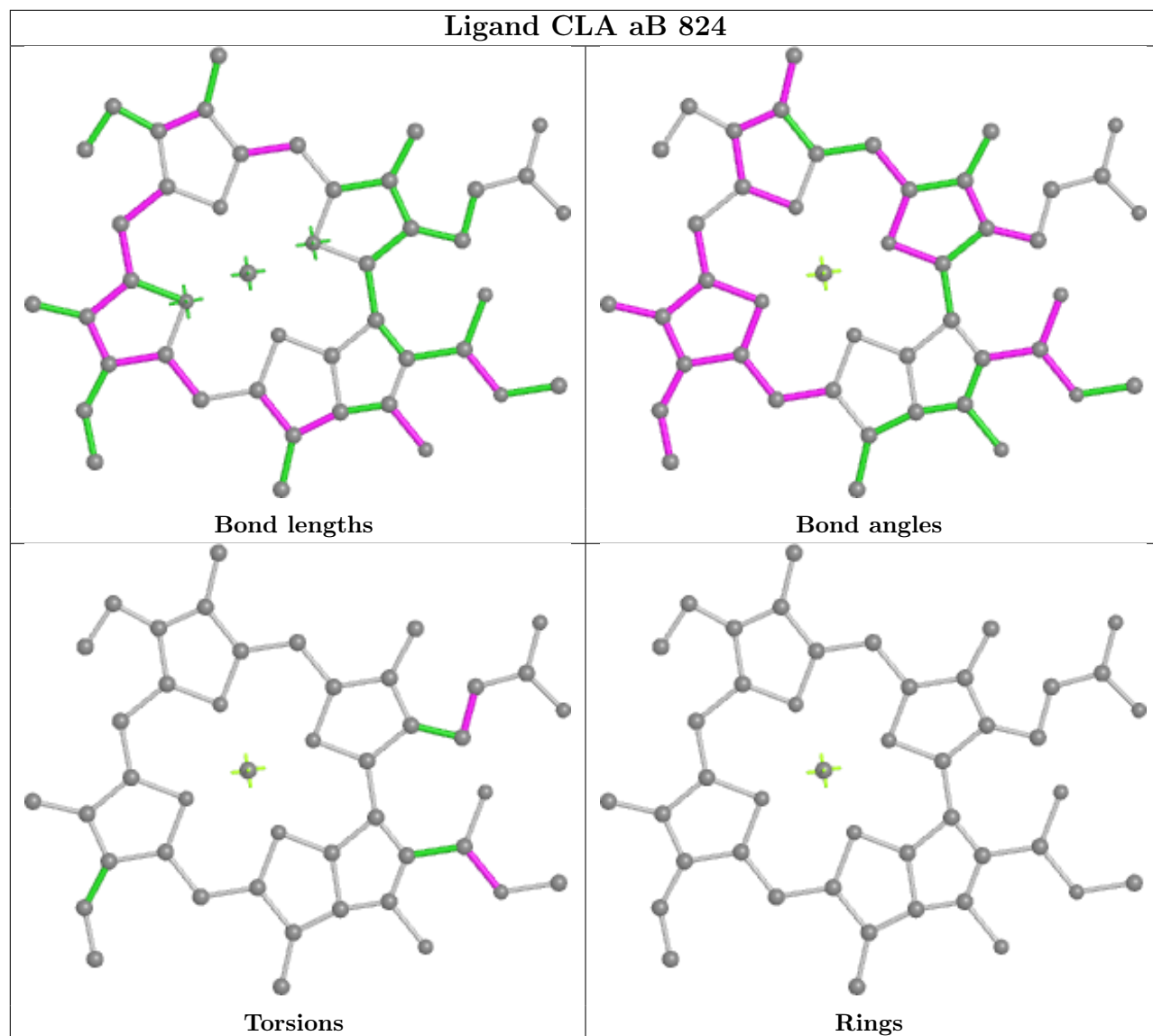
## Ligand CLA aB 821

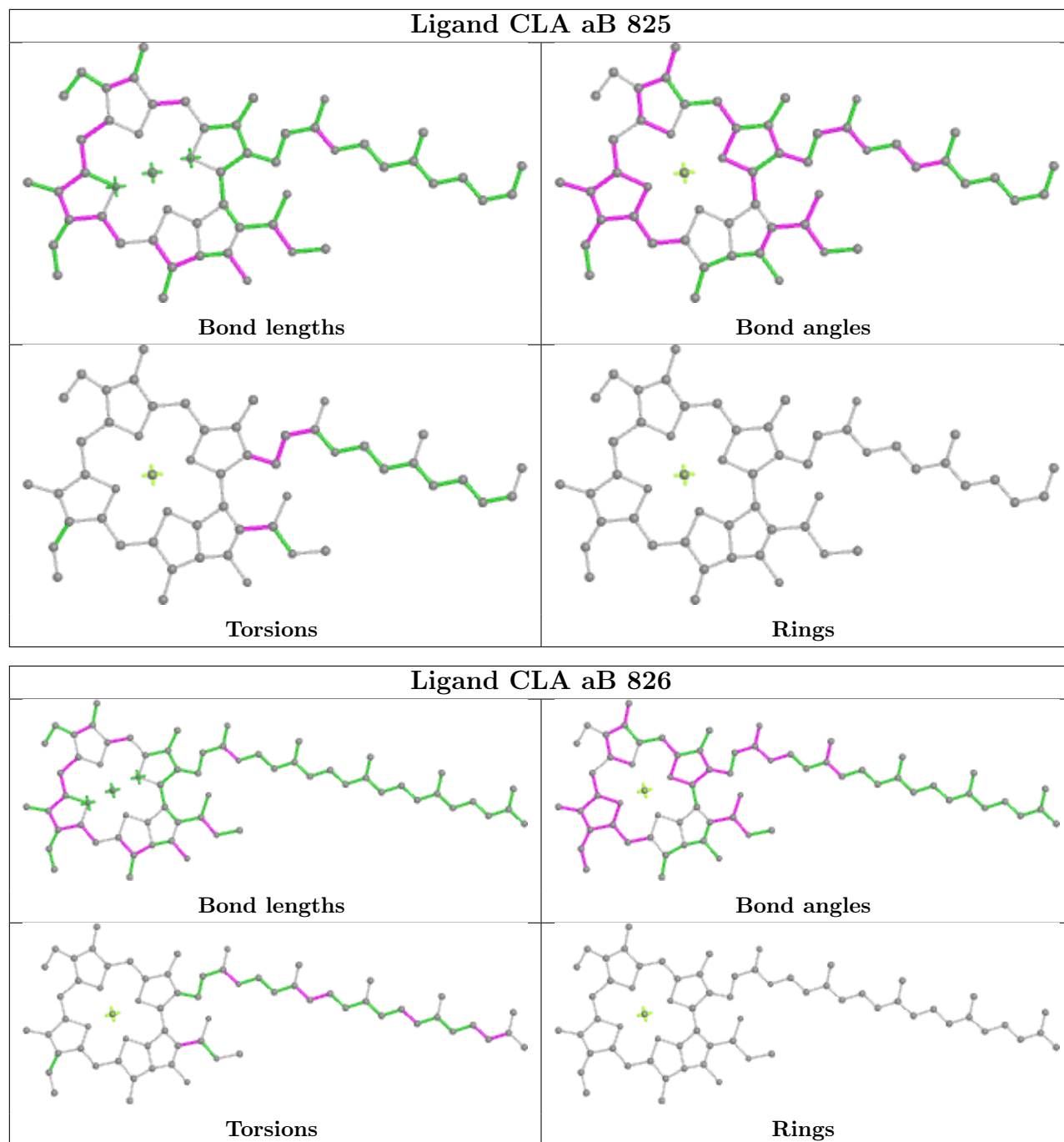


## Ligand CLA aB 822

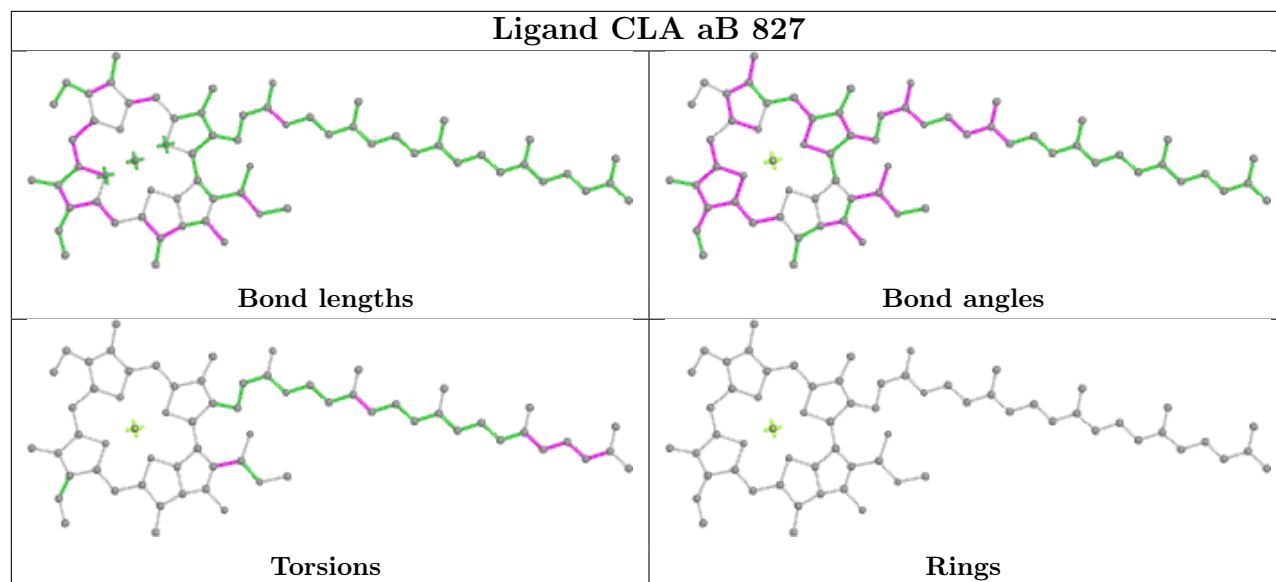




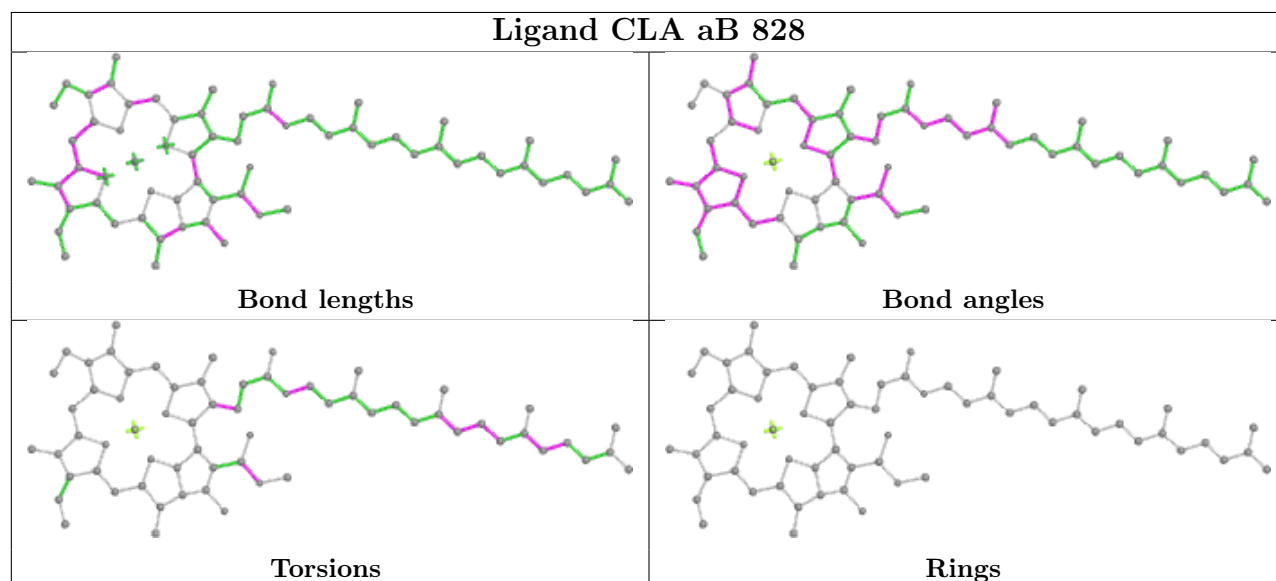




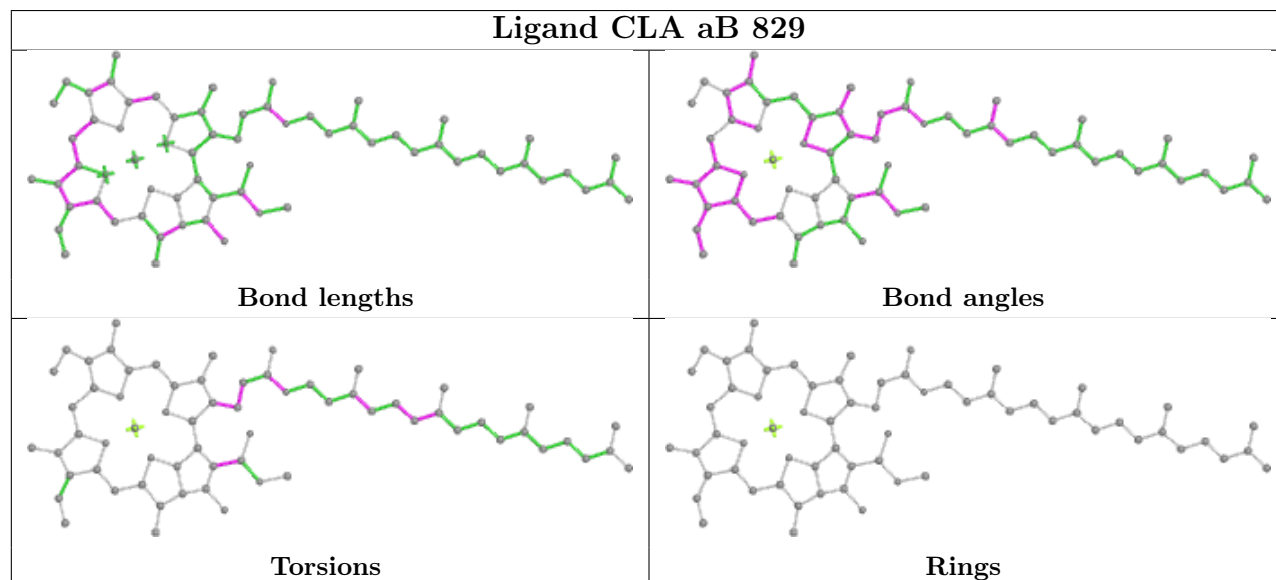
## Ligand CLA aB 827



## Ligand CLA aB 828

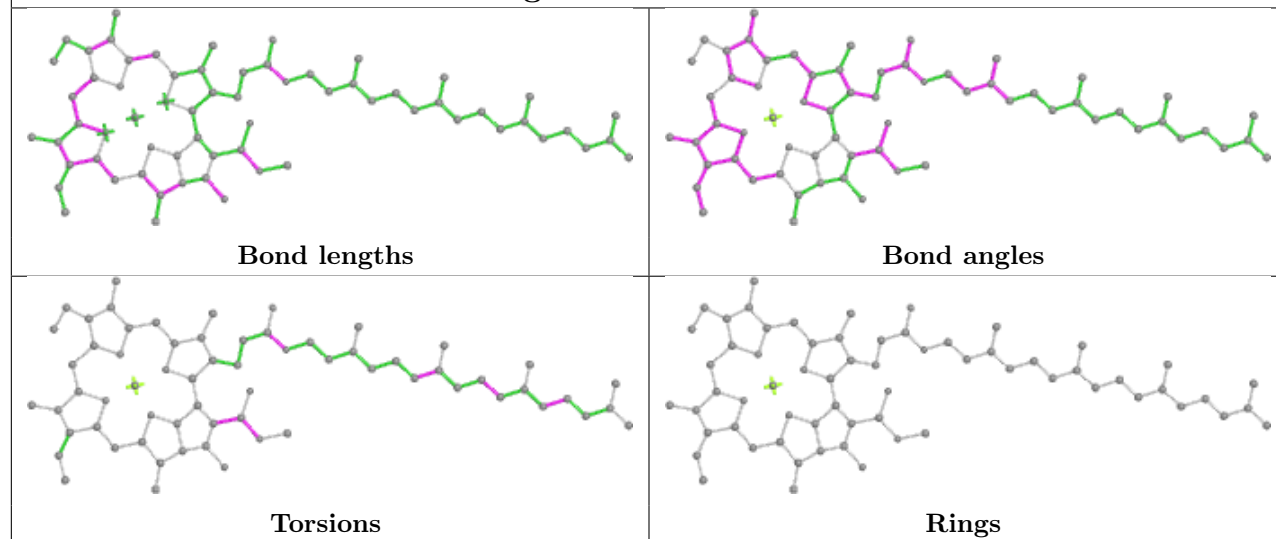


## Ligand CLA aB 829

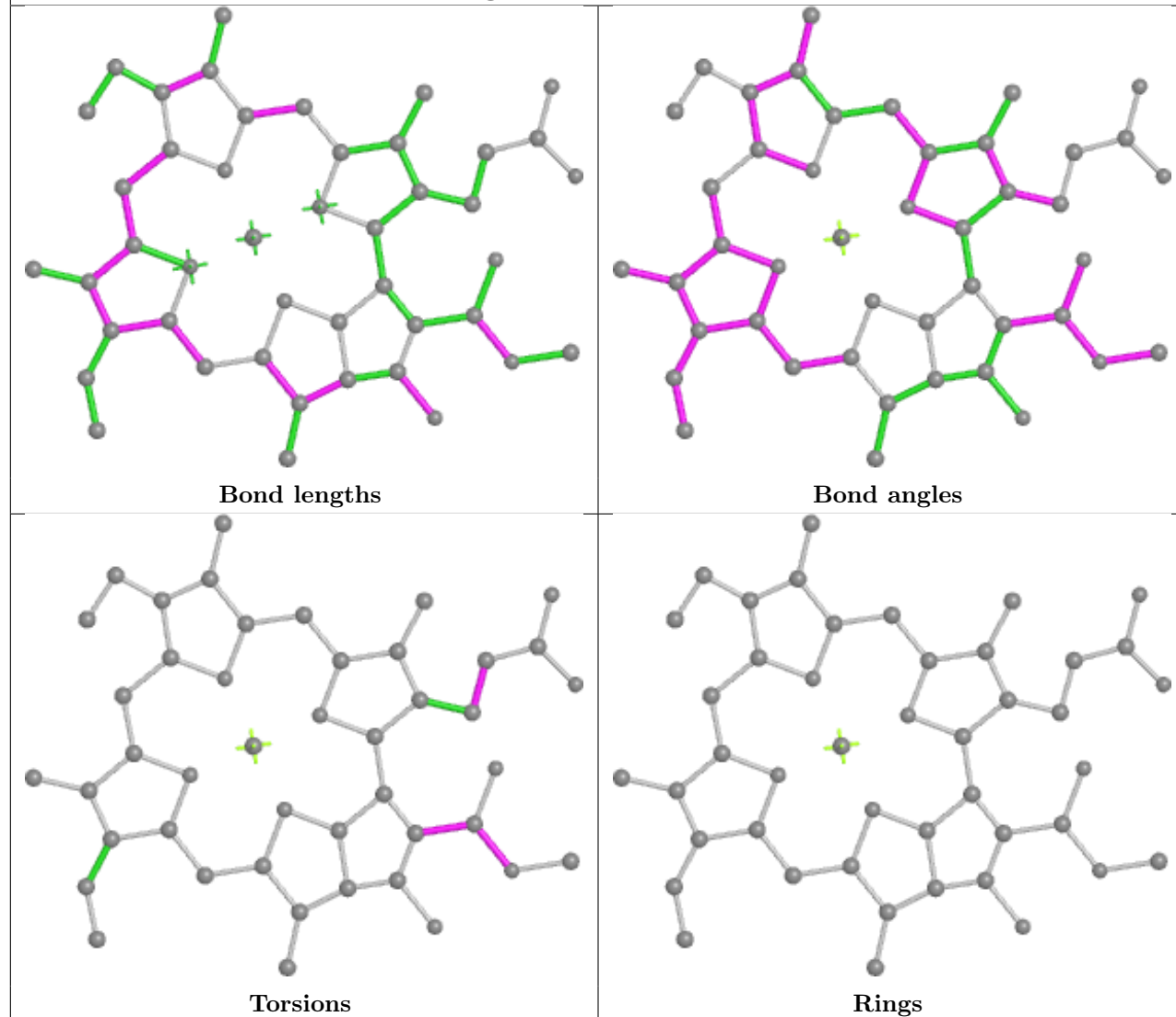




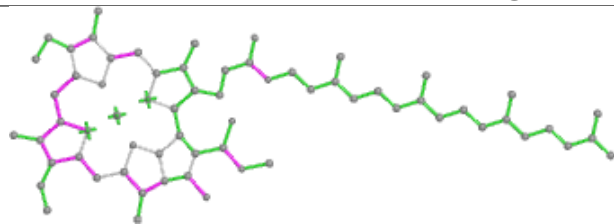
## Ligand CLA aB 830



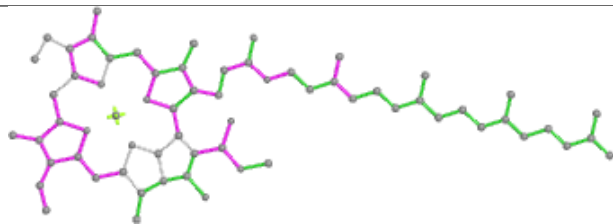
## Ligand CLA aB 831



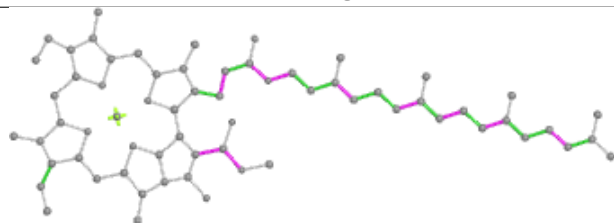
## Ligand CLA aB 832



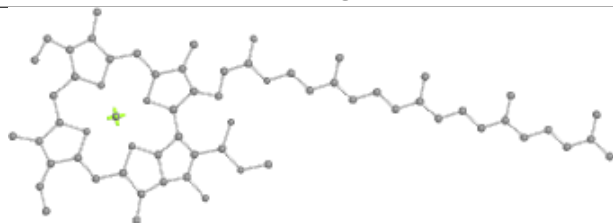
Bond lengths



Bond angles

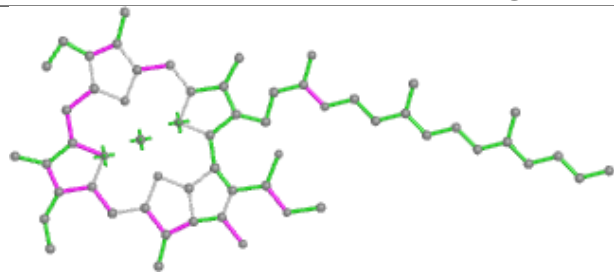


Torsions

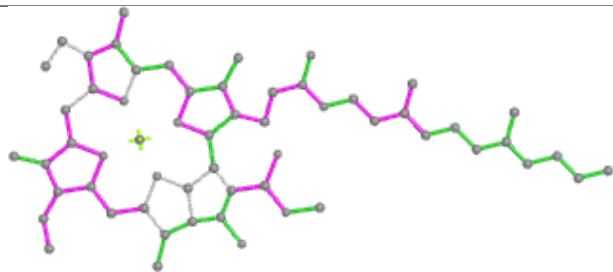


Rings

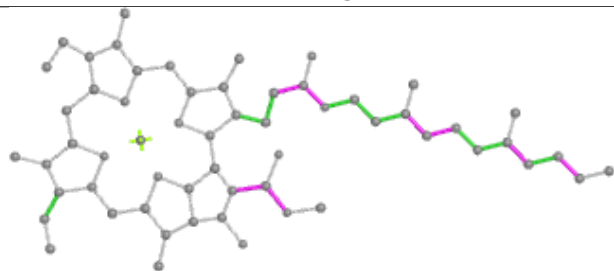
## Ligand CLA aB 833



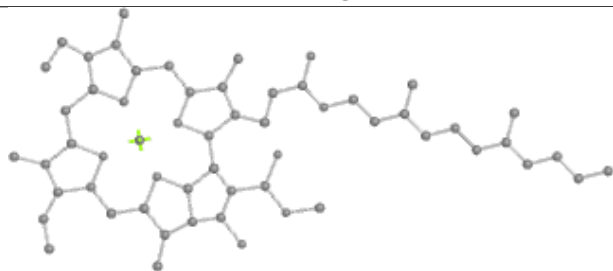
Bond lengths



Bond angles

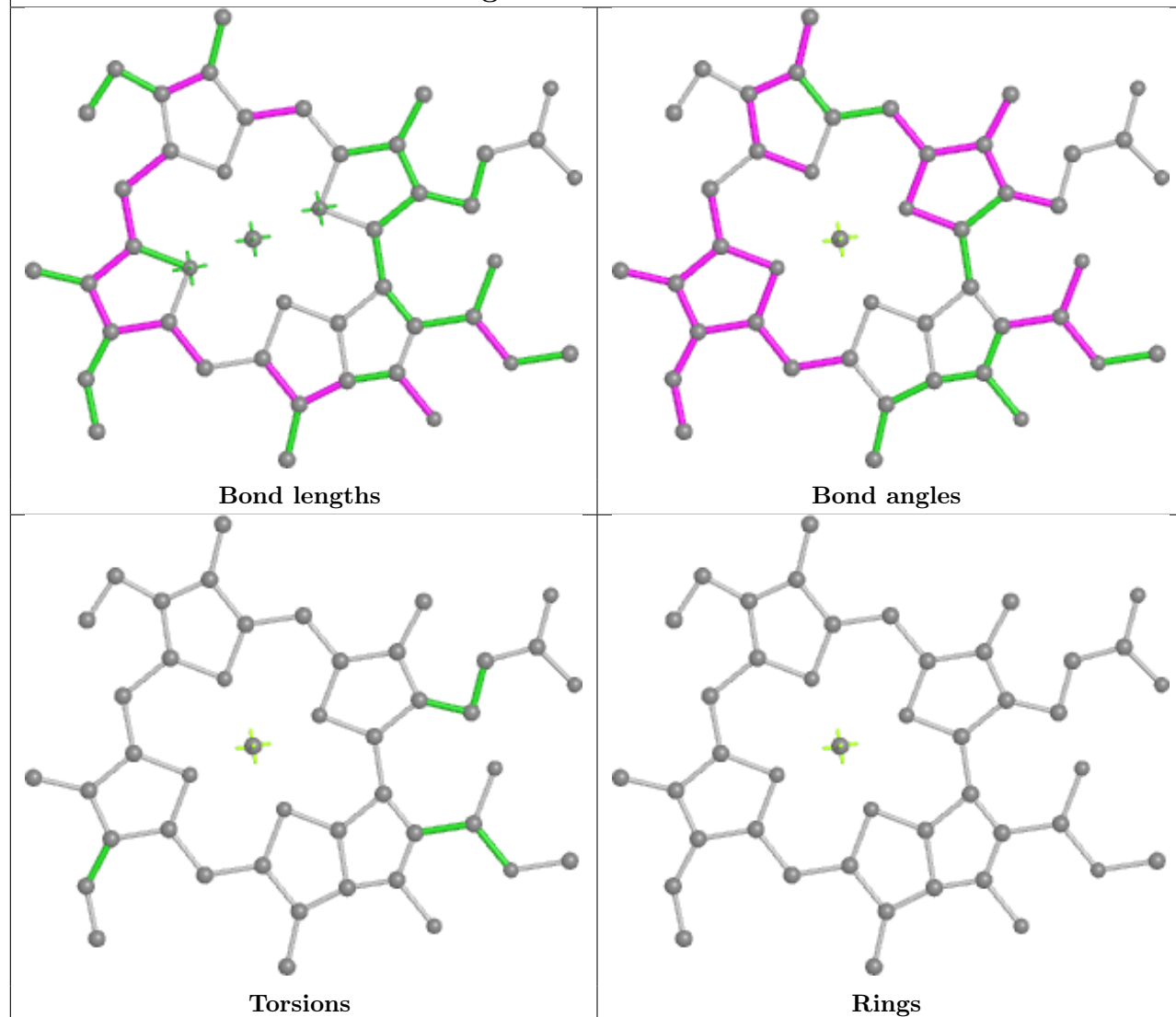


Torsions

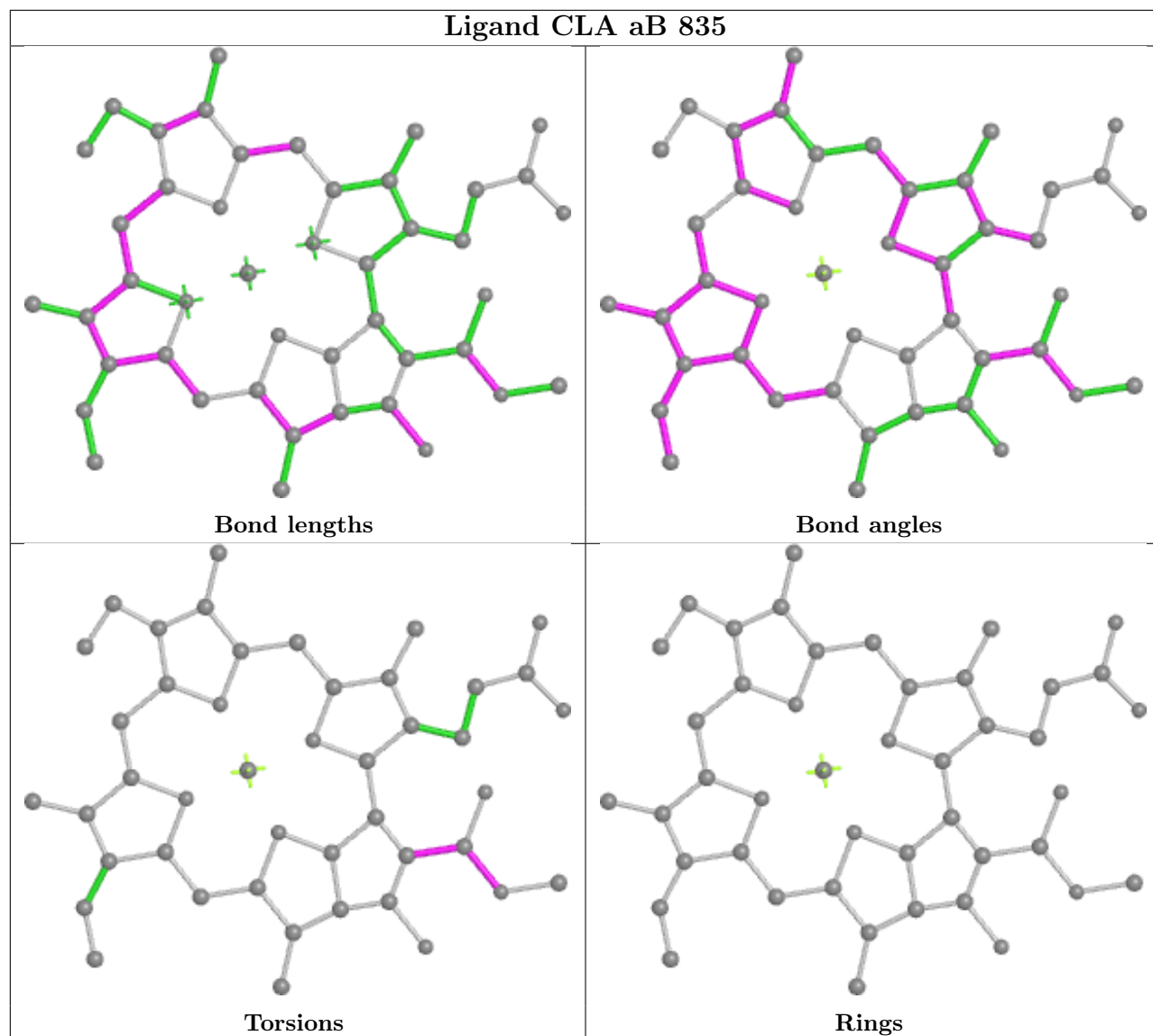


Rings

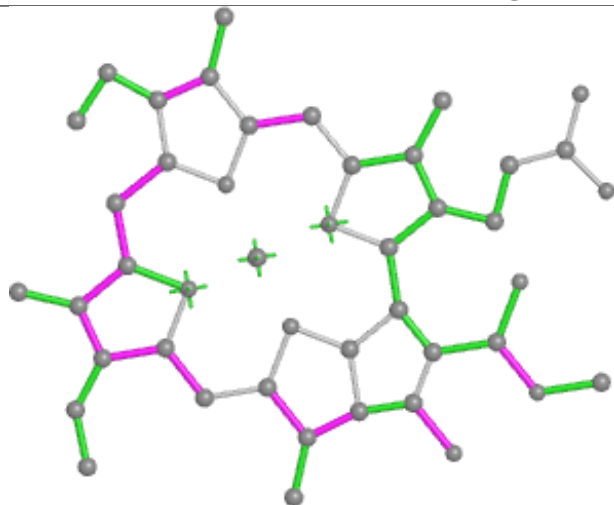
## Ligand CLA aB 834



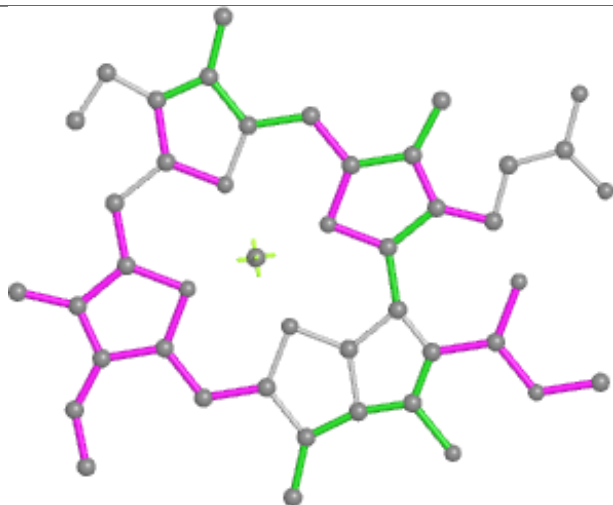
## Ligand CLA aB 835



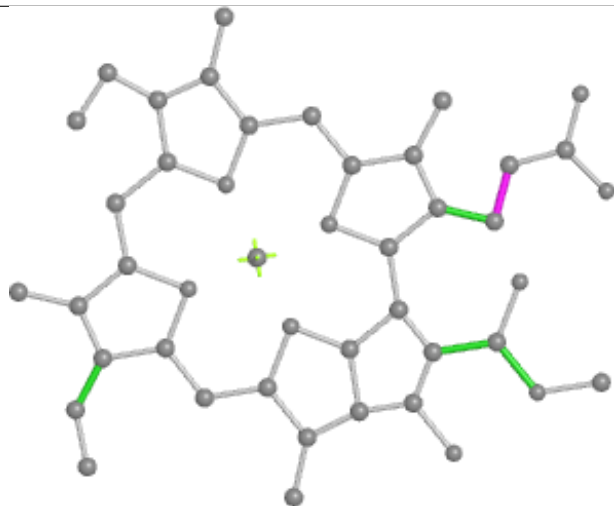
## Ligand CLA aB 836



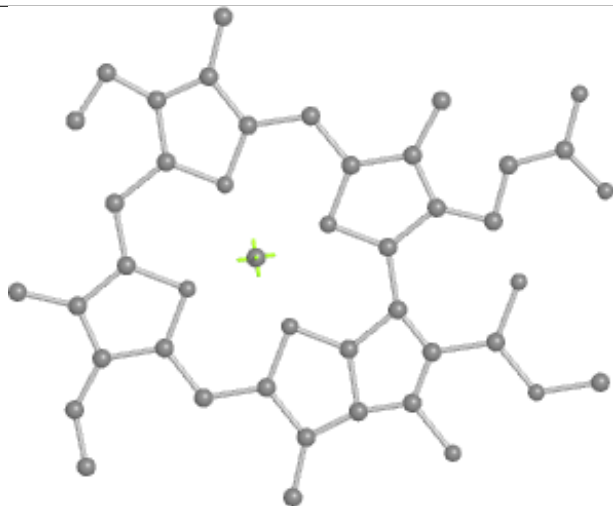
Bond lengths



Bond angles

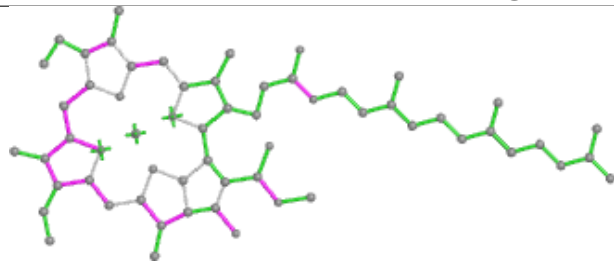


Torsions

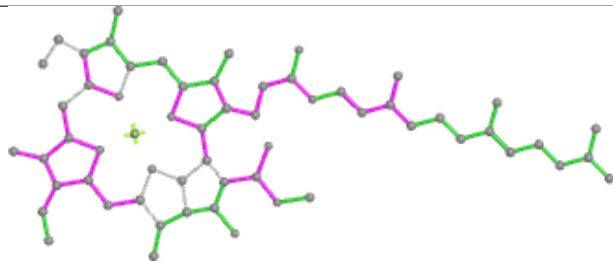


Rings

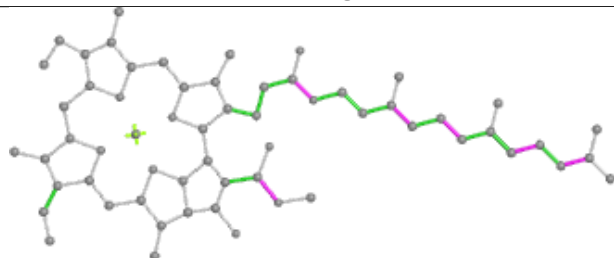
## Ligand CLA aB 837



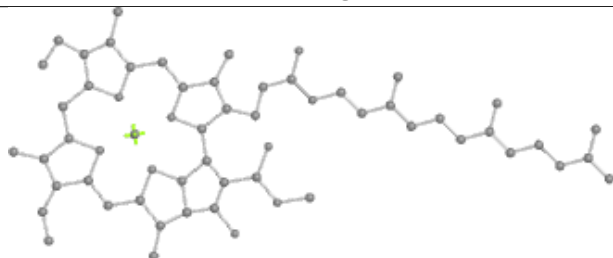
Bond lengths



Bond angles

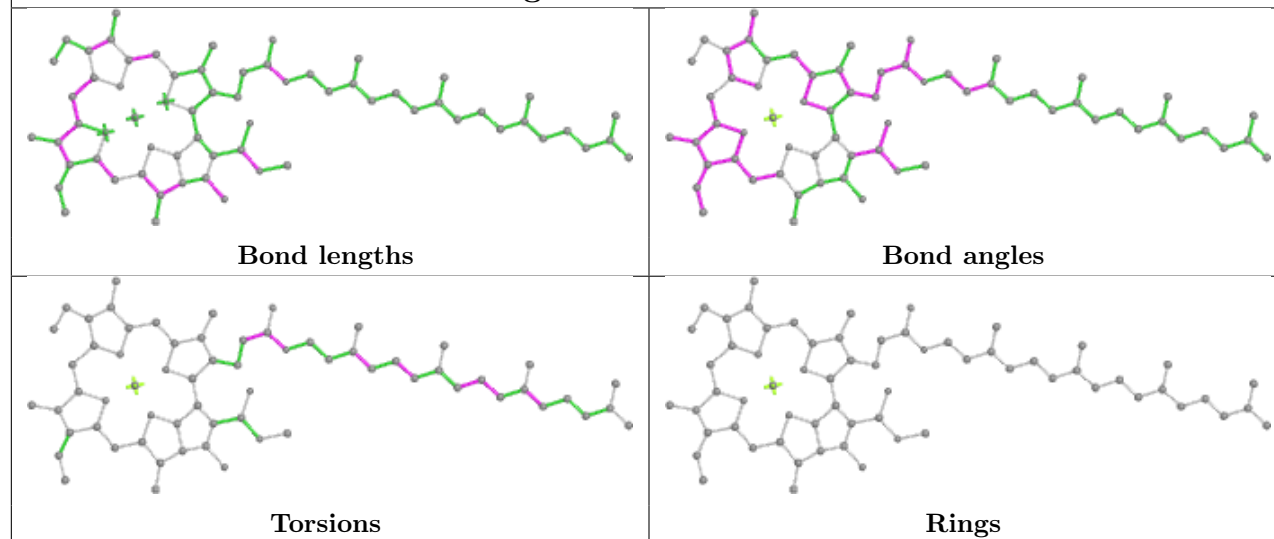


Torsions

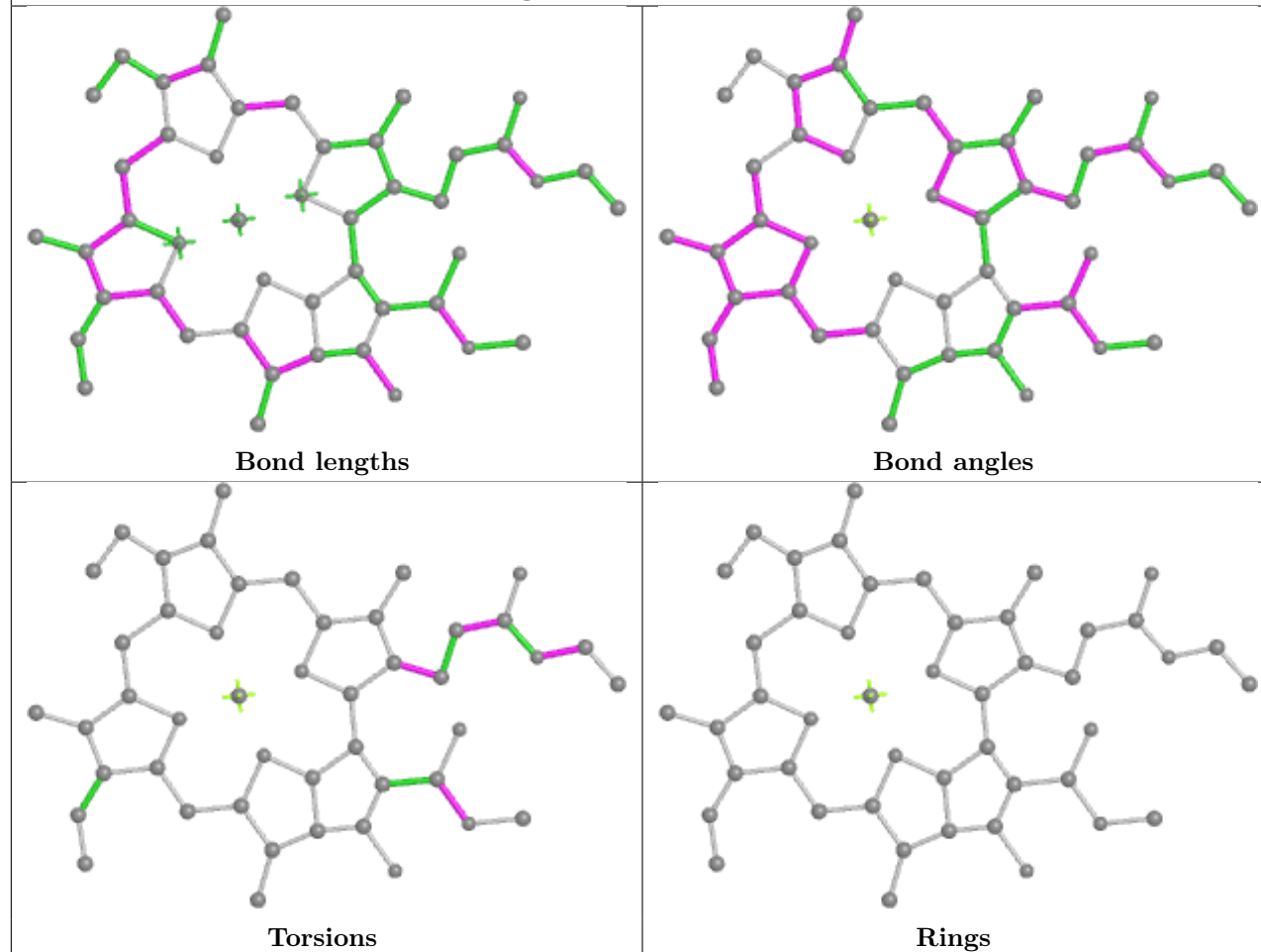


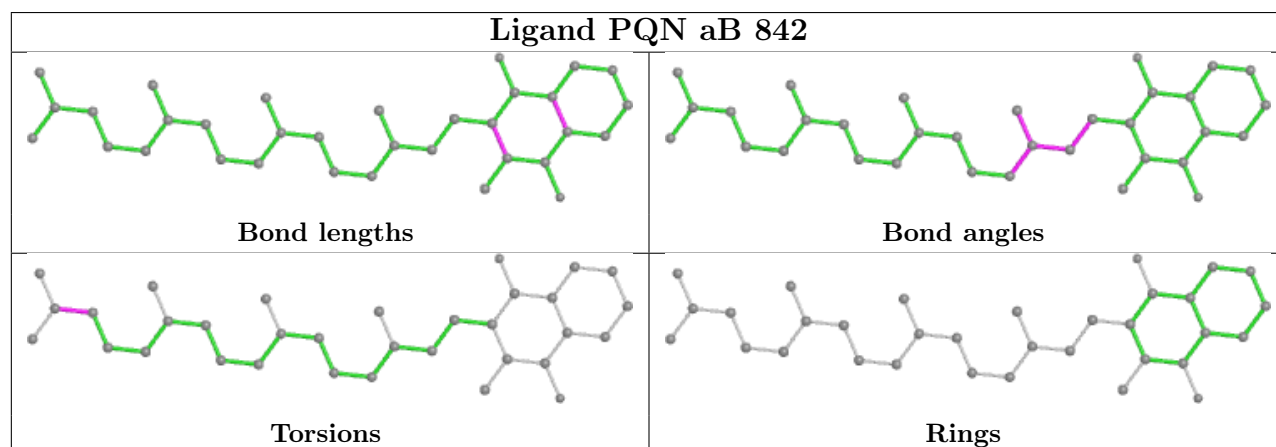
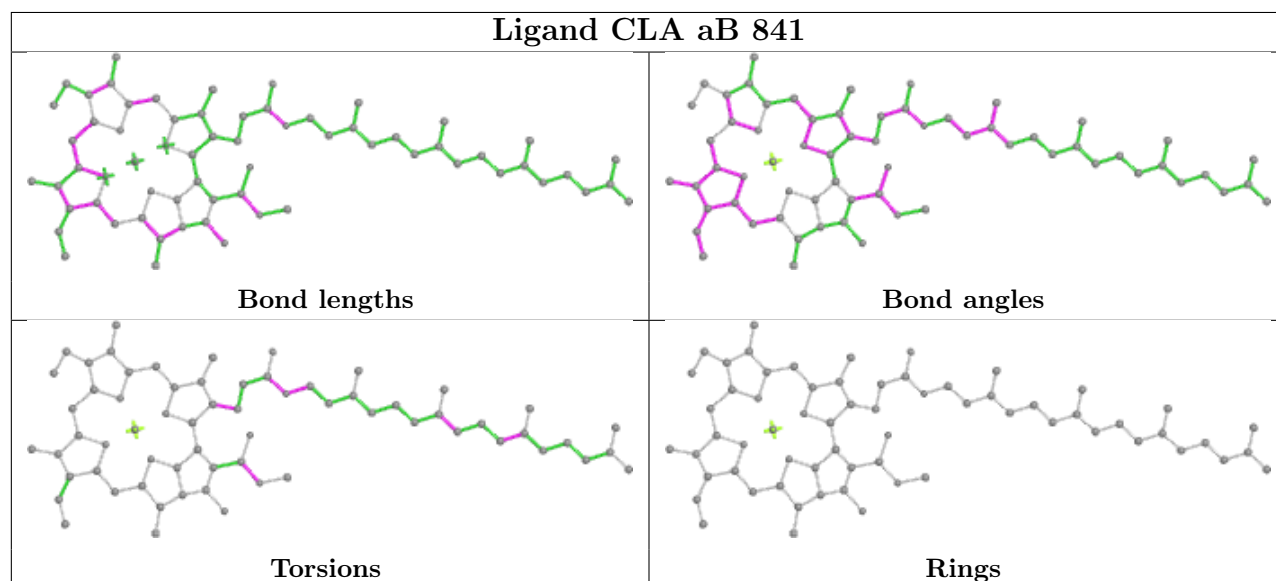
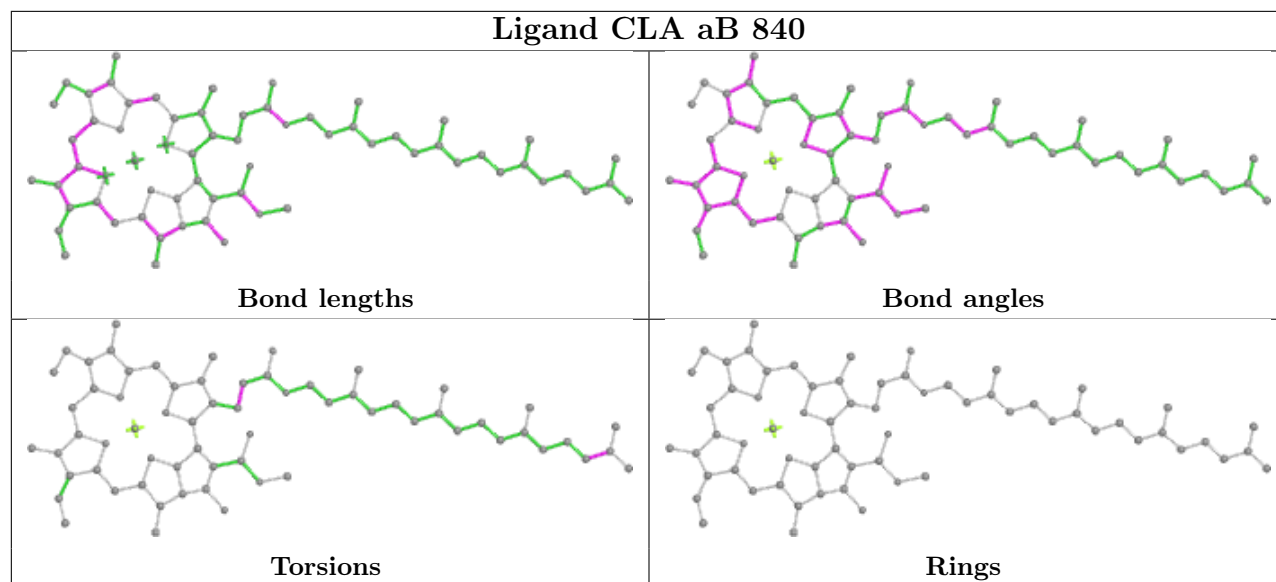
Rings

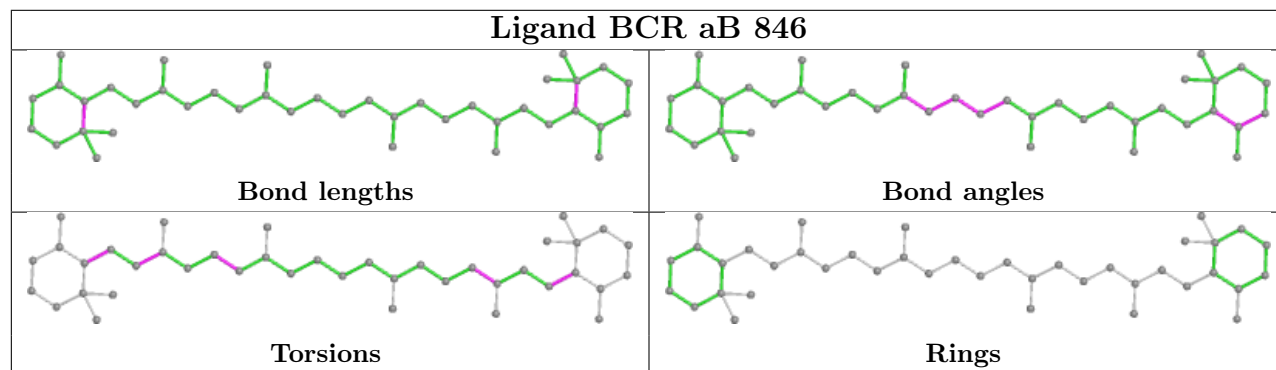
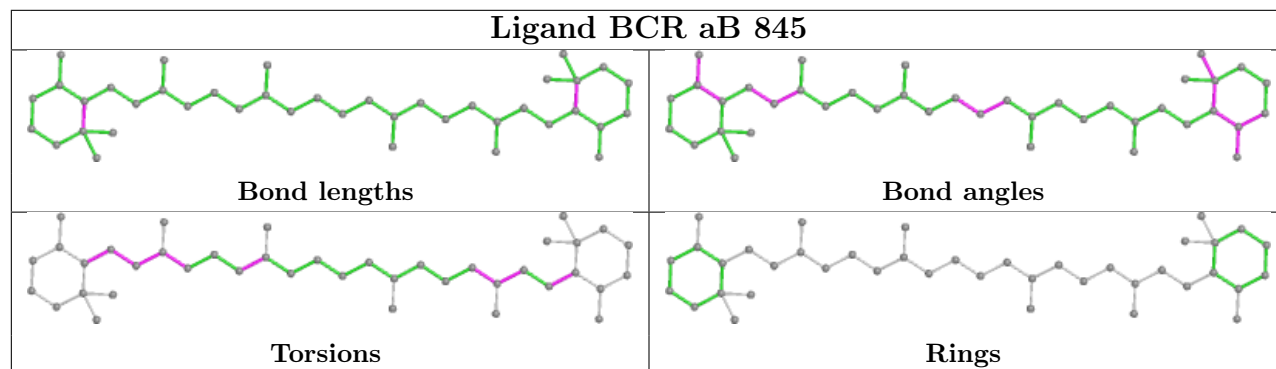
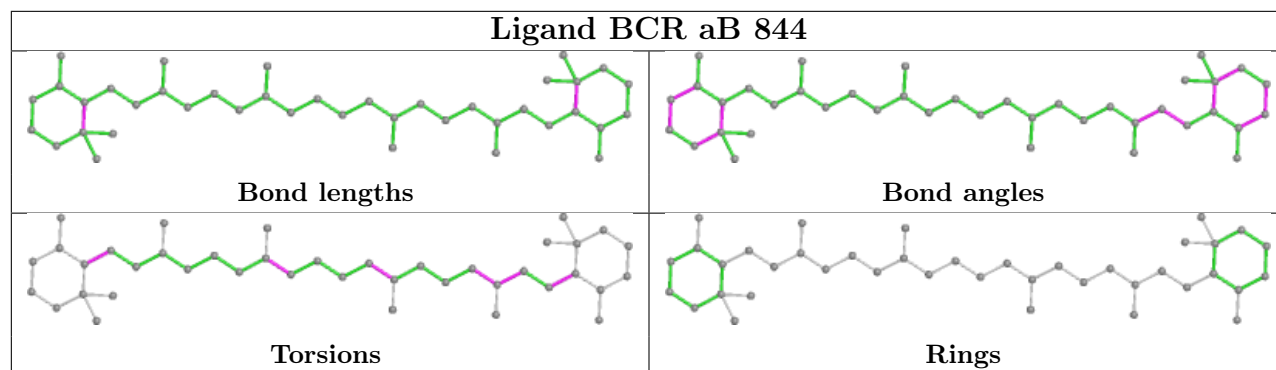
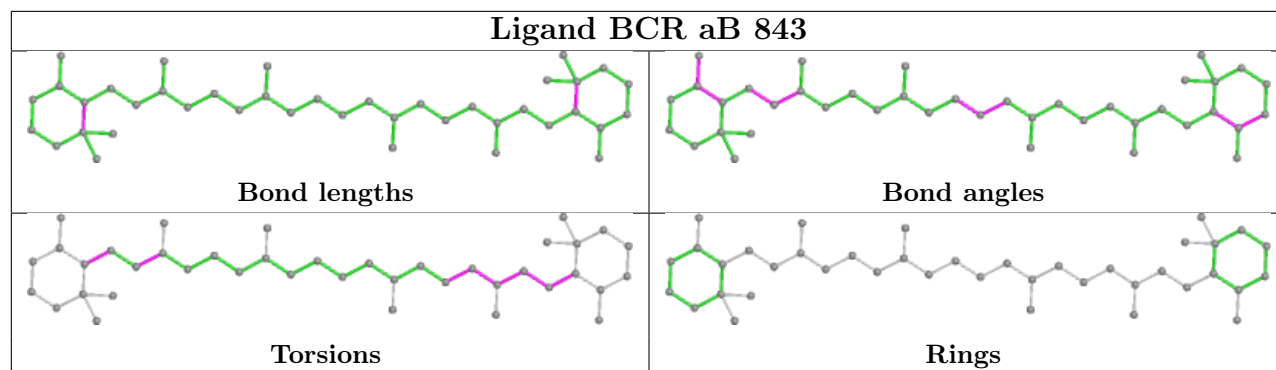
## Ligand CLA aB 838



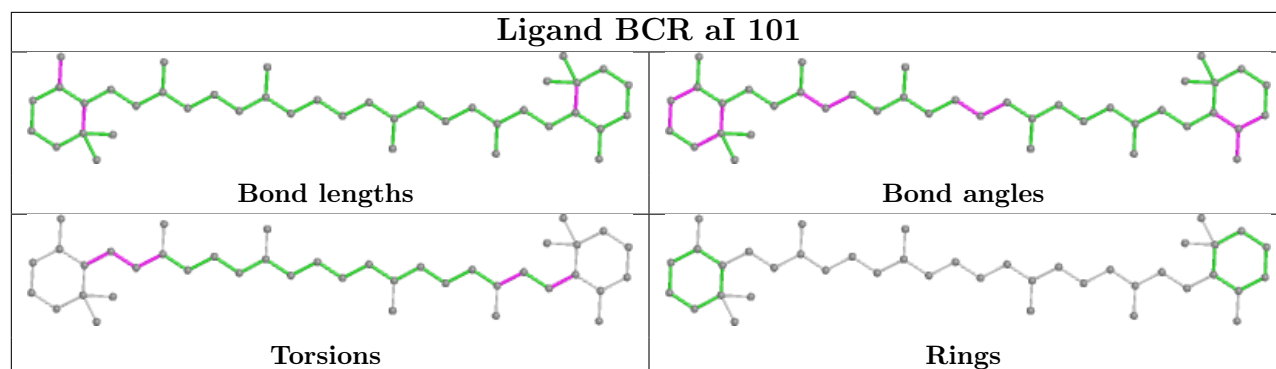
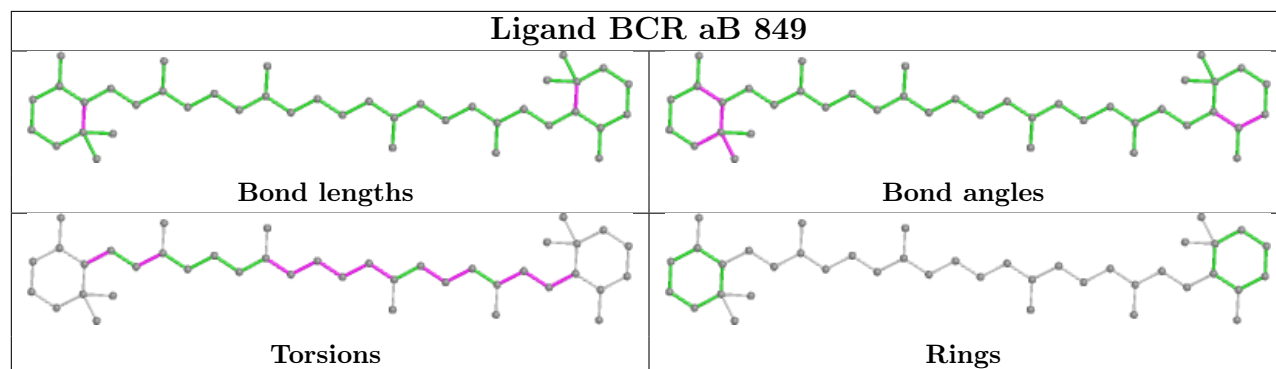
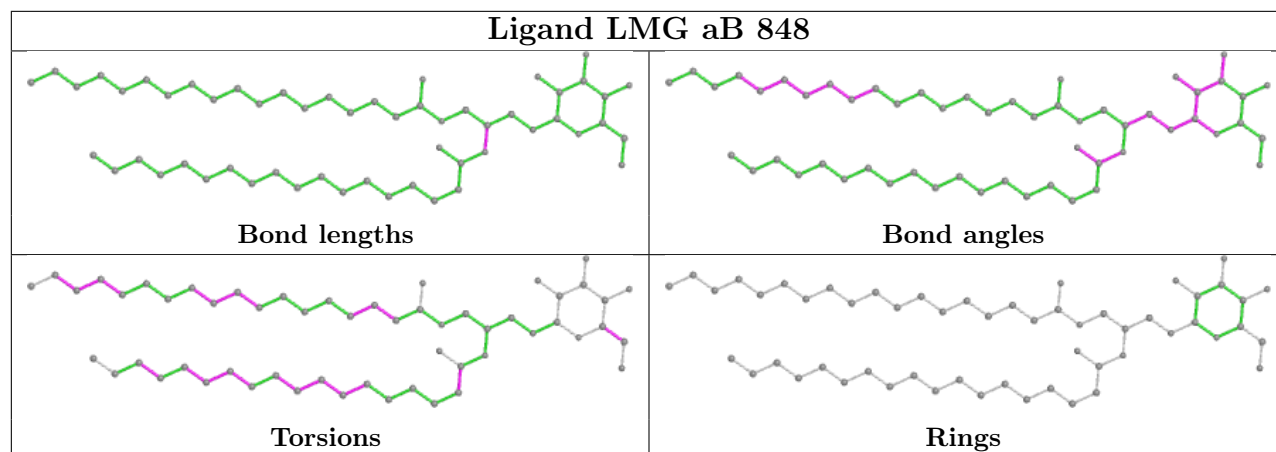
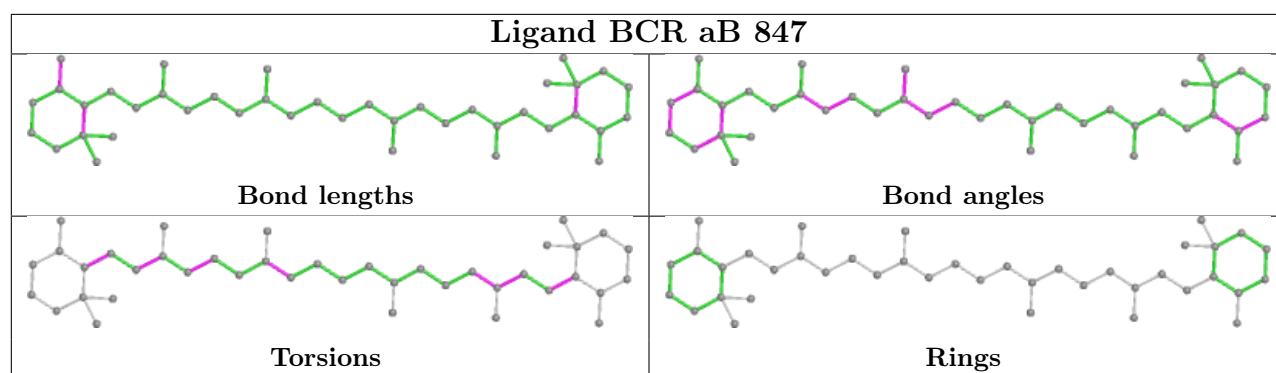
## Ligand CLA aB 839

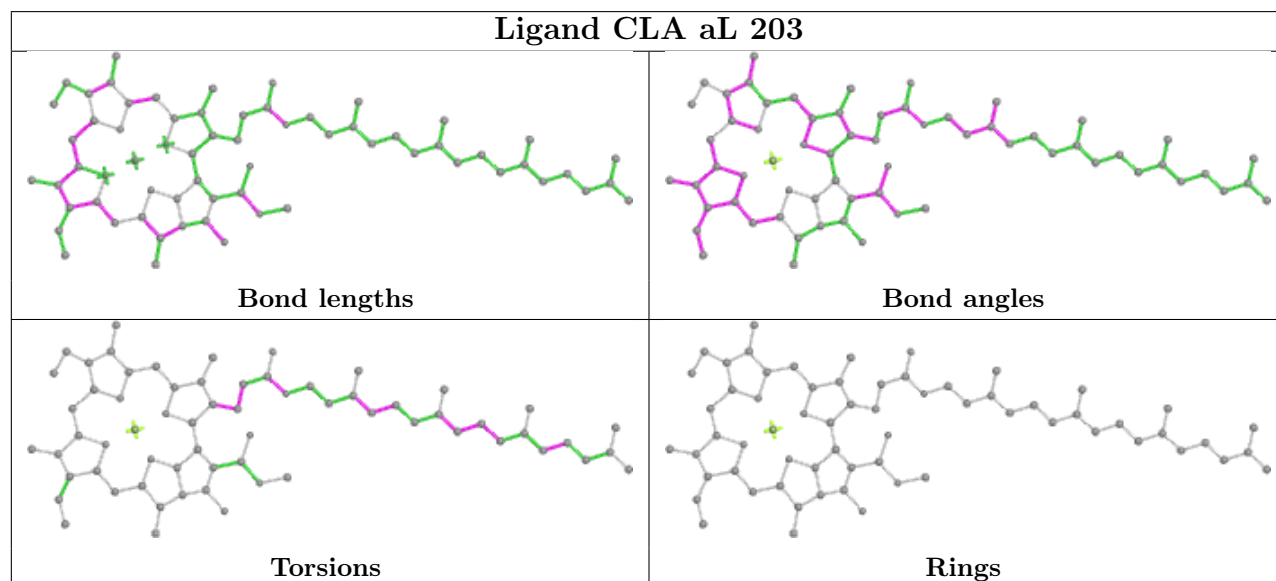
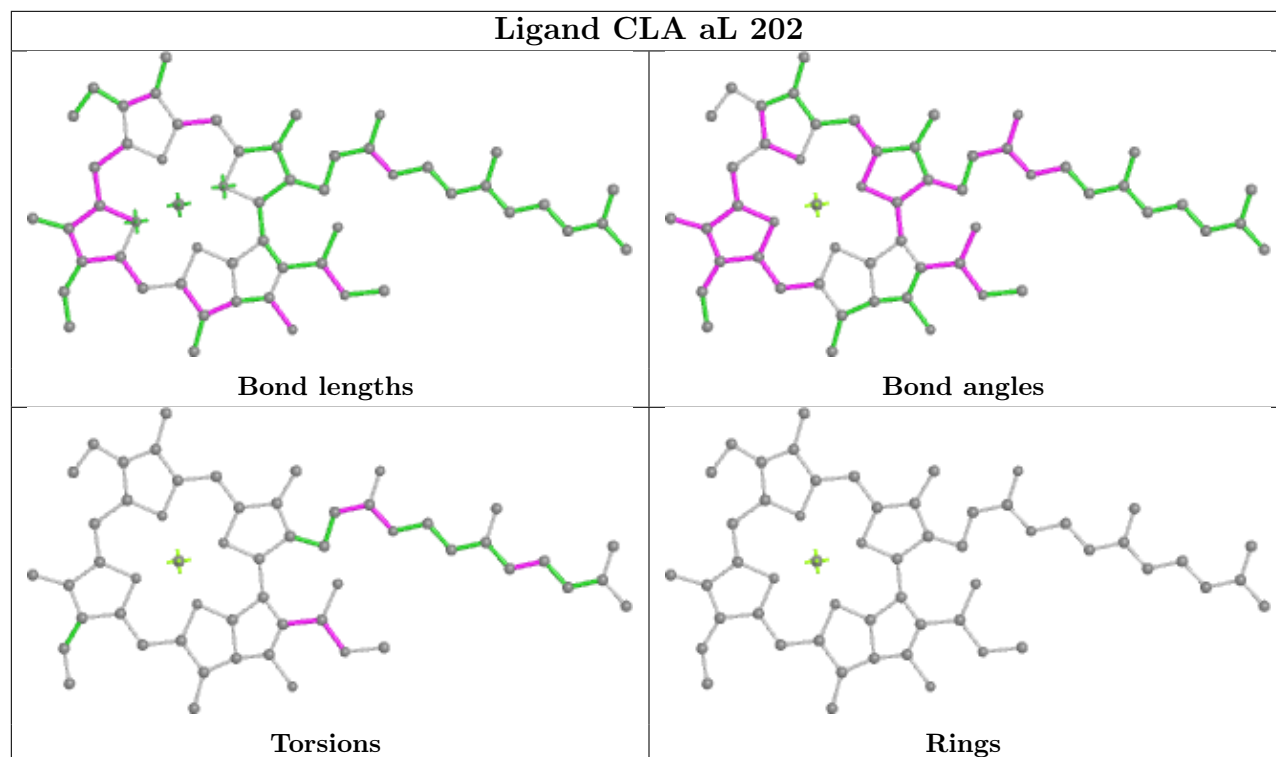
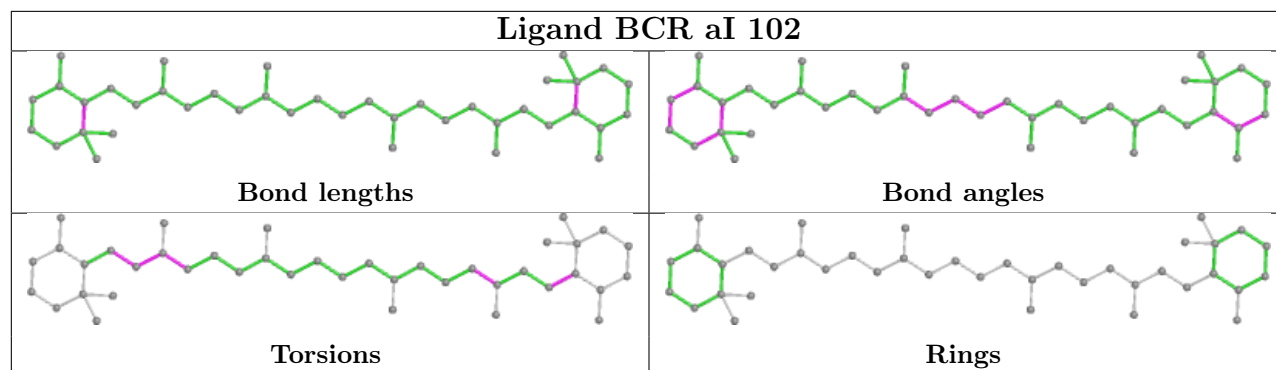


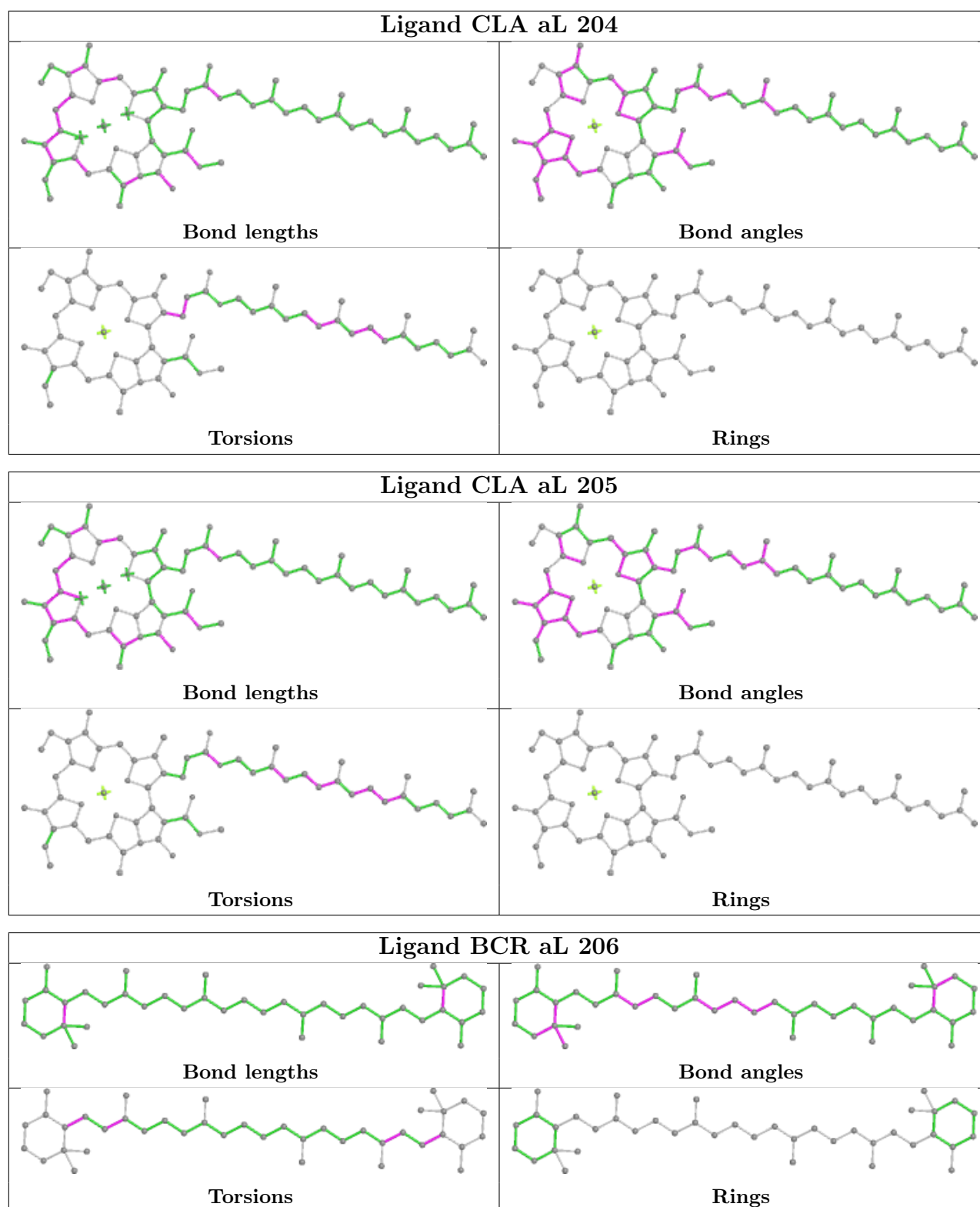


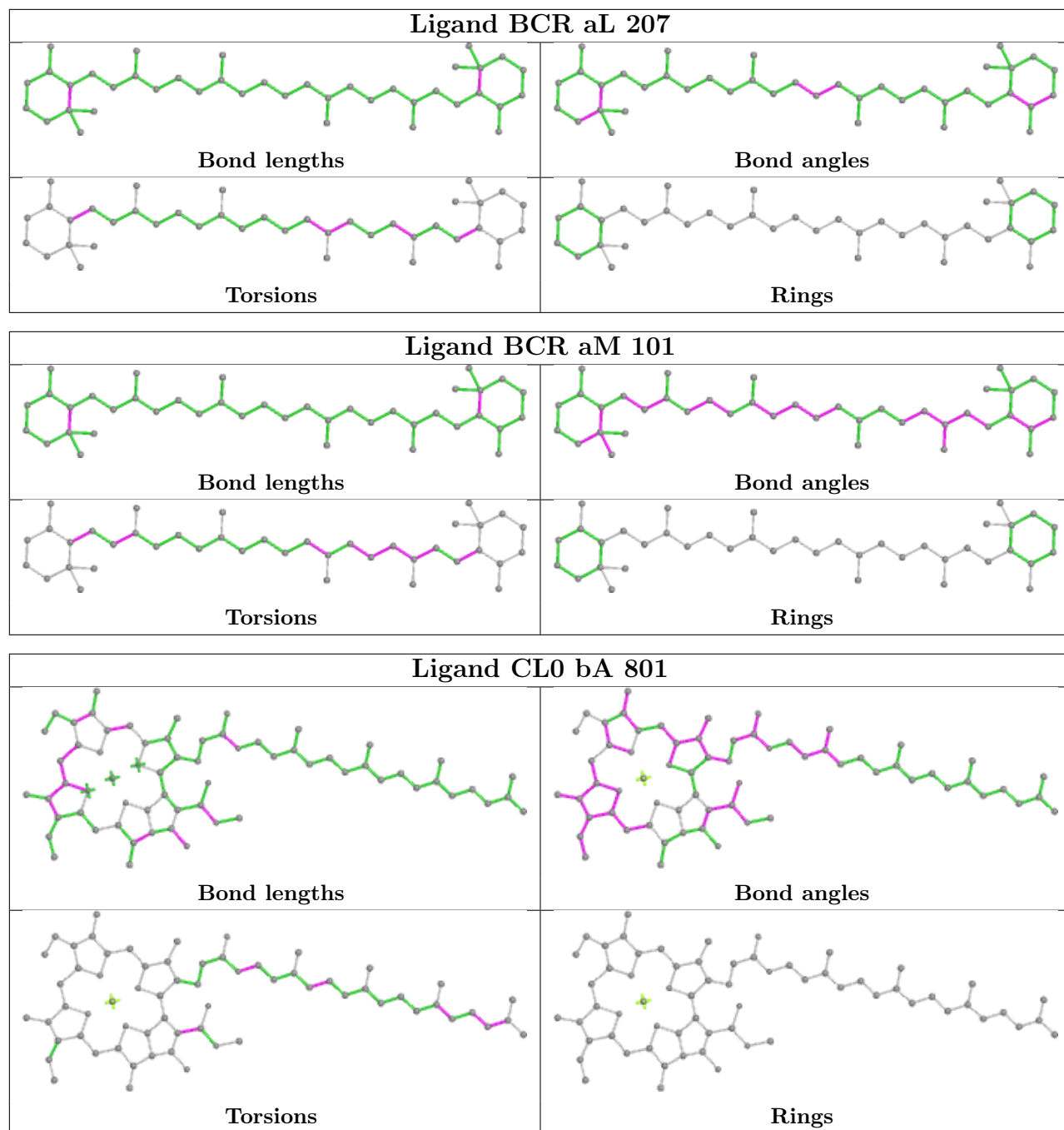




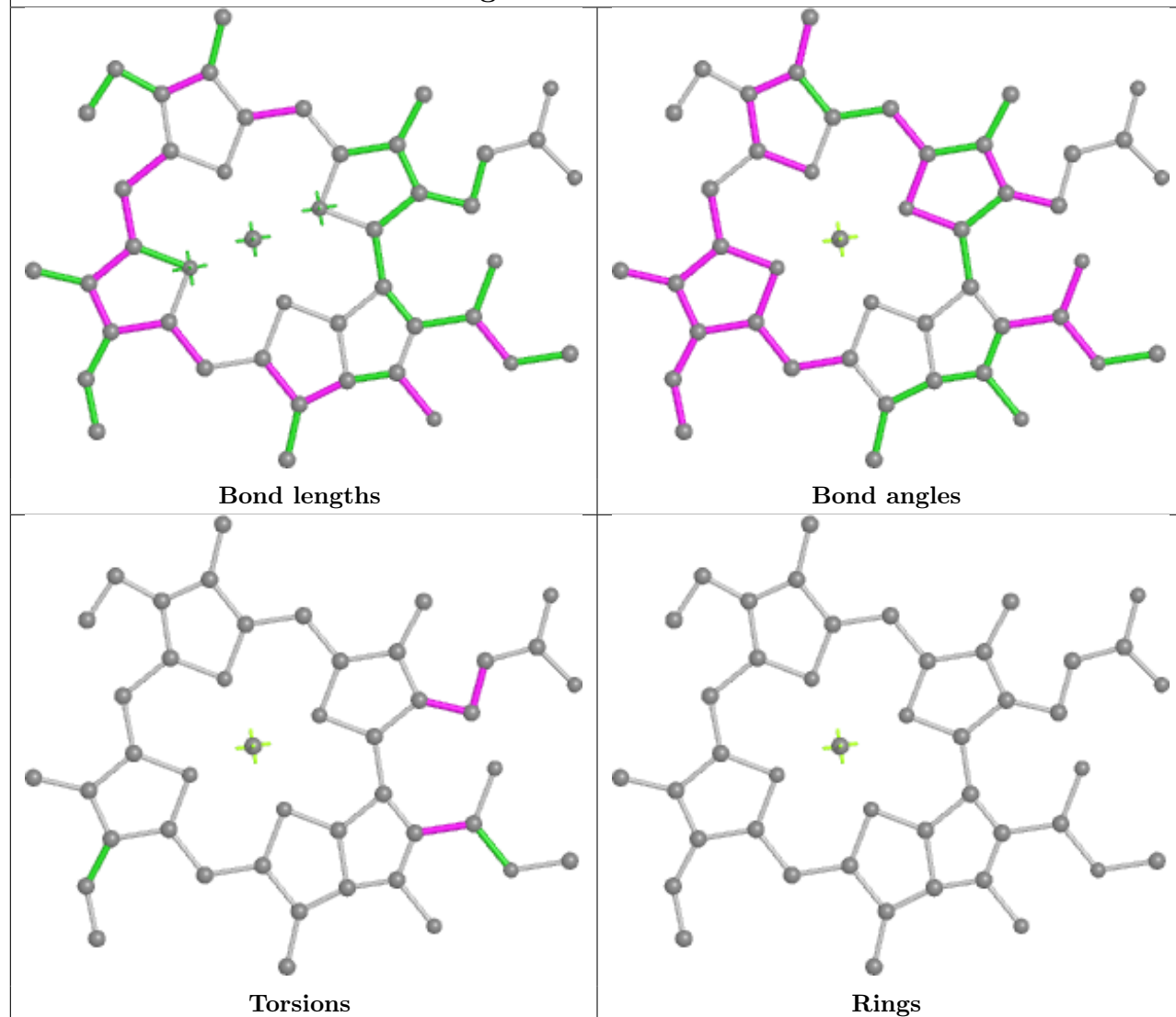




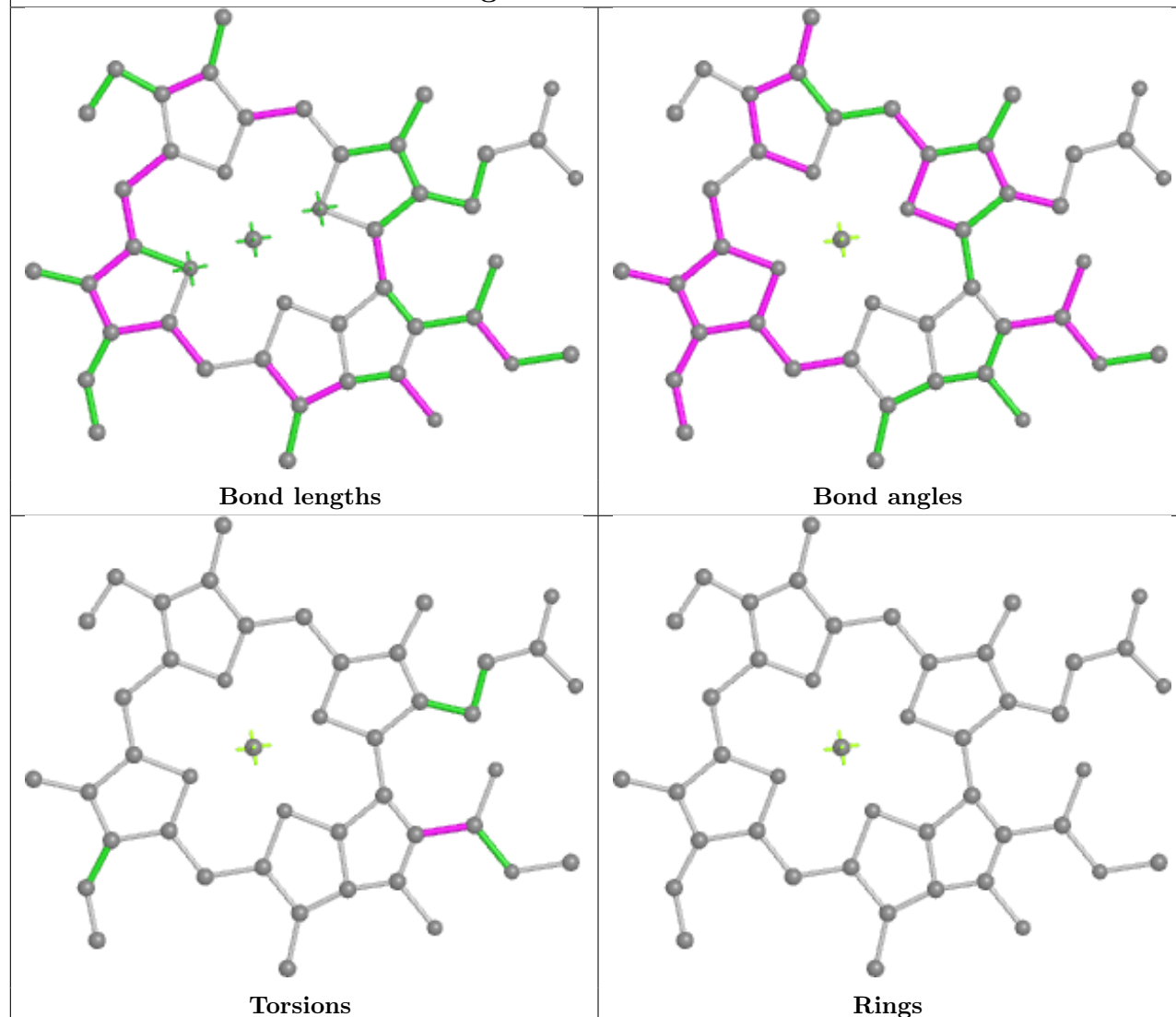




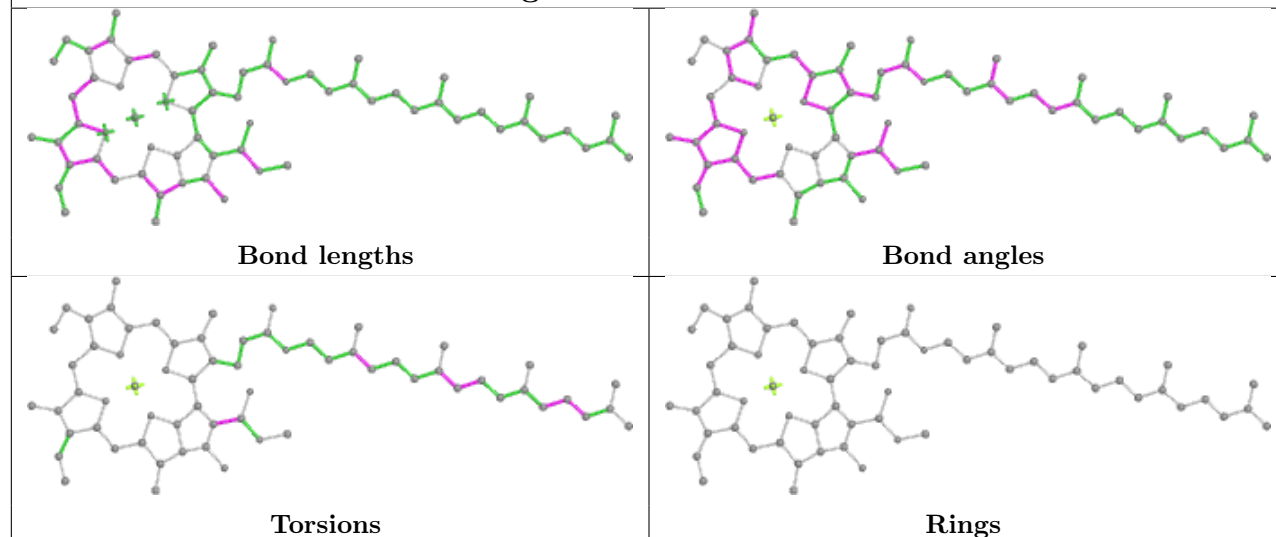
## Ligand CLA bA 802



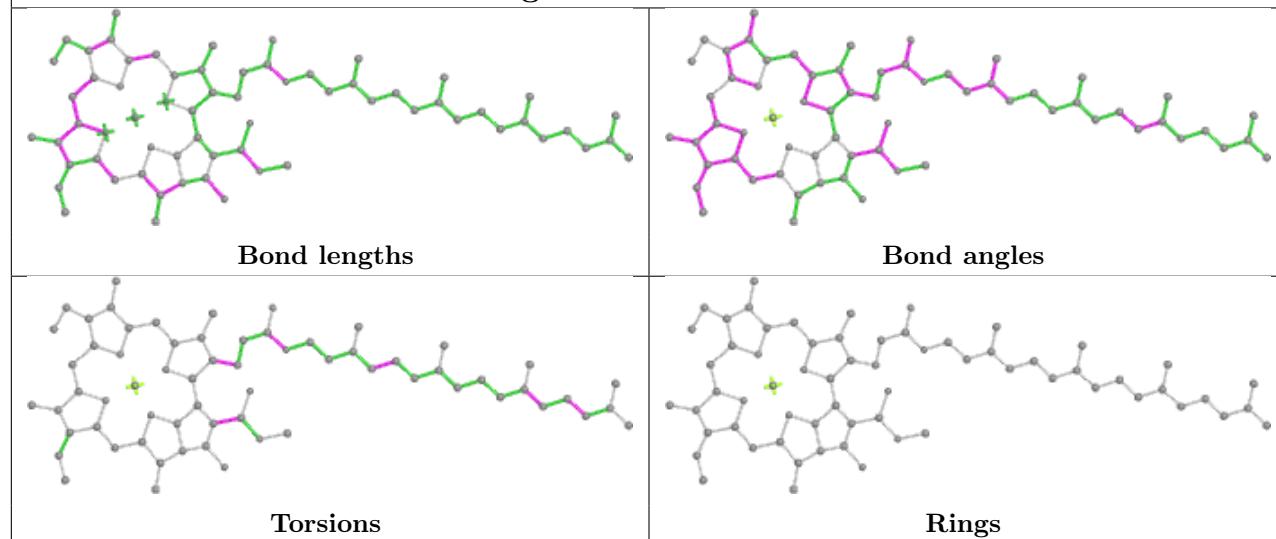
## Ligand CLA bA 803



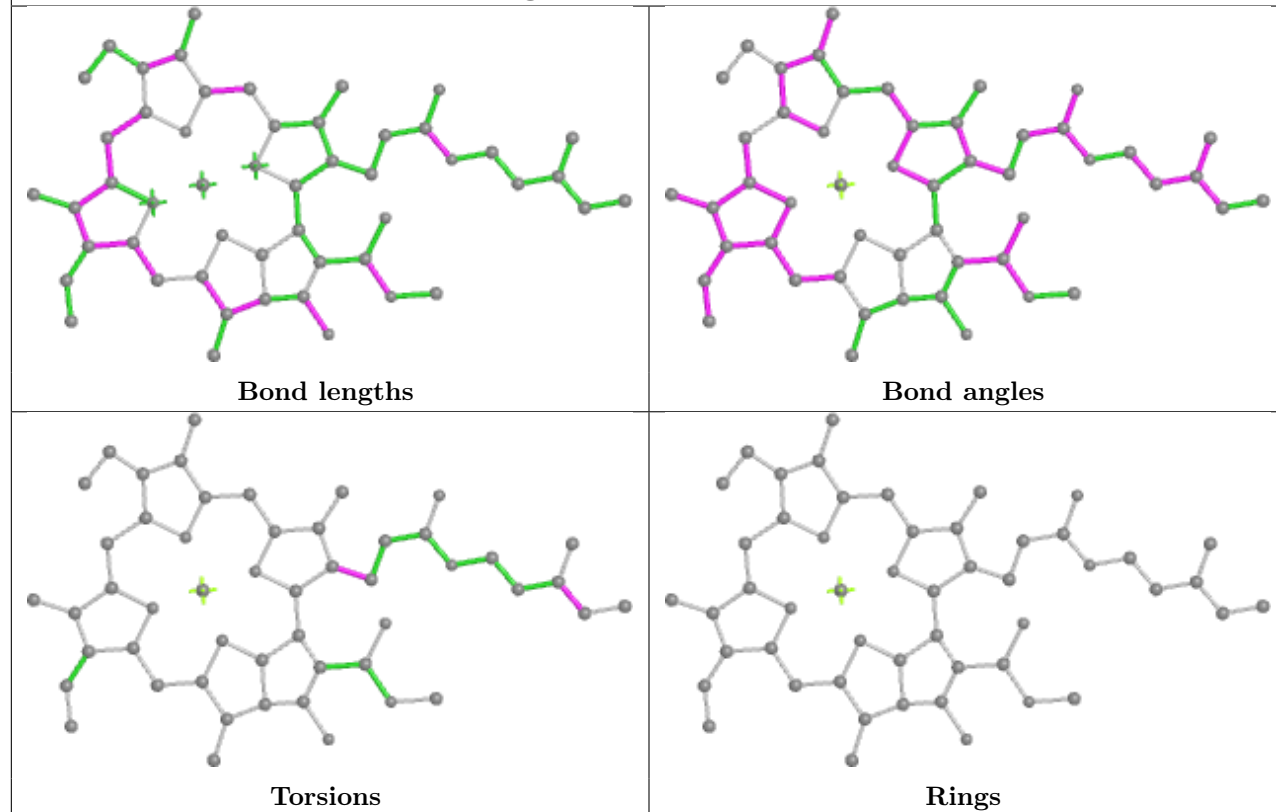
## Ligand CLA bA 804



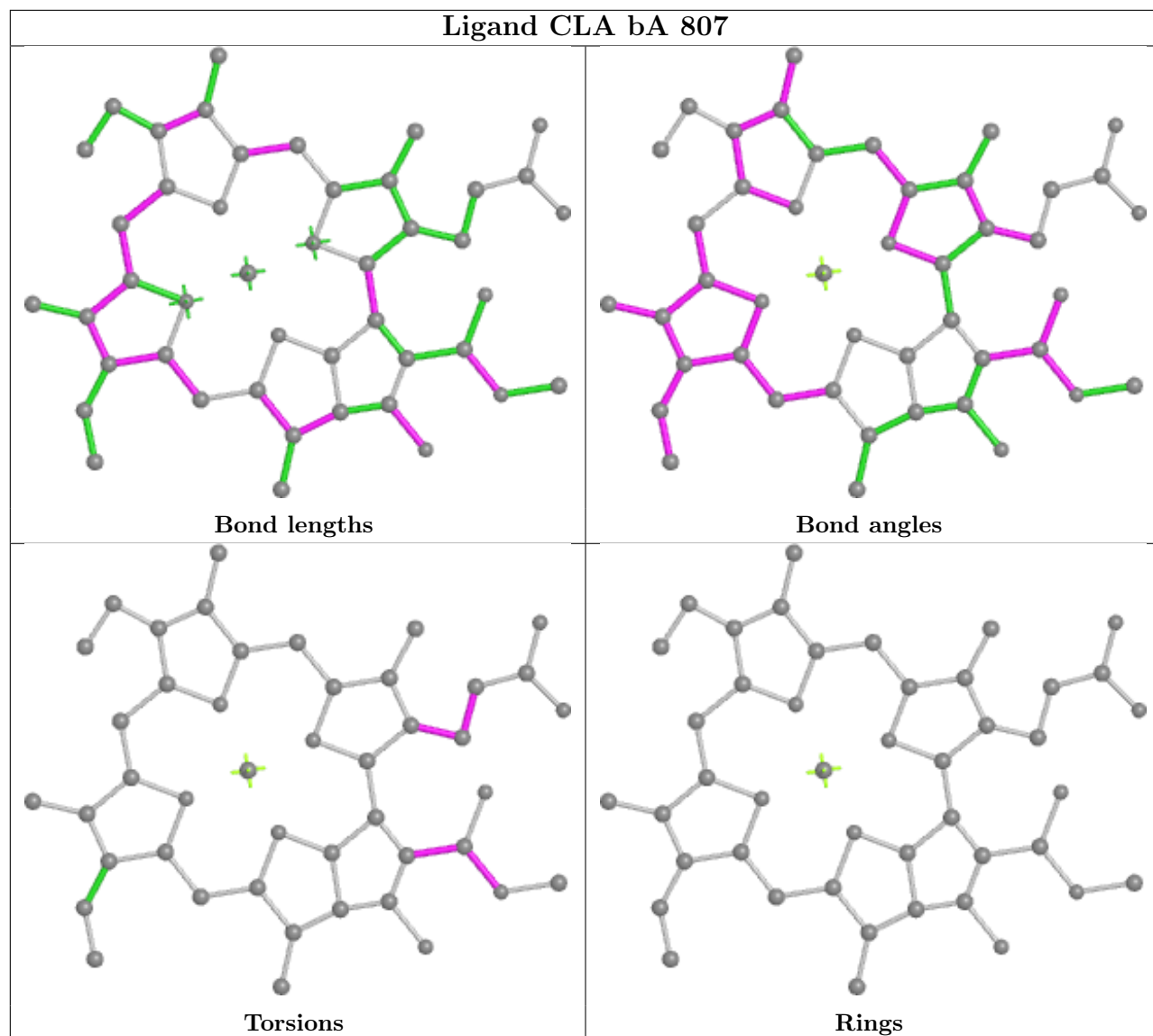
## Ligand CLA bA 805



## Ligand CLA bA 806

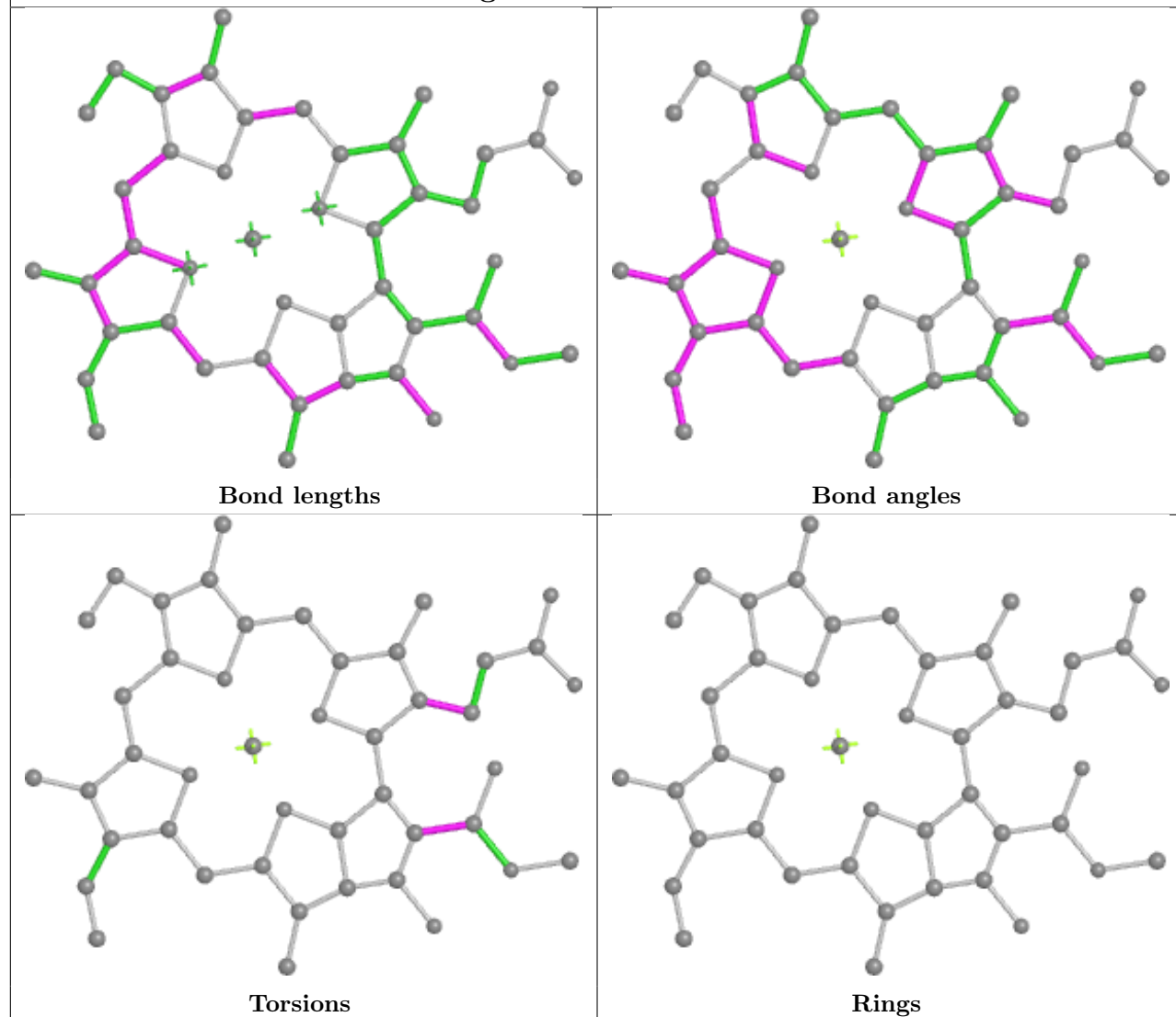


## Ligand CLA bA 807

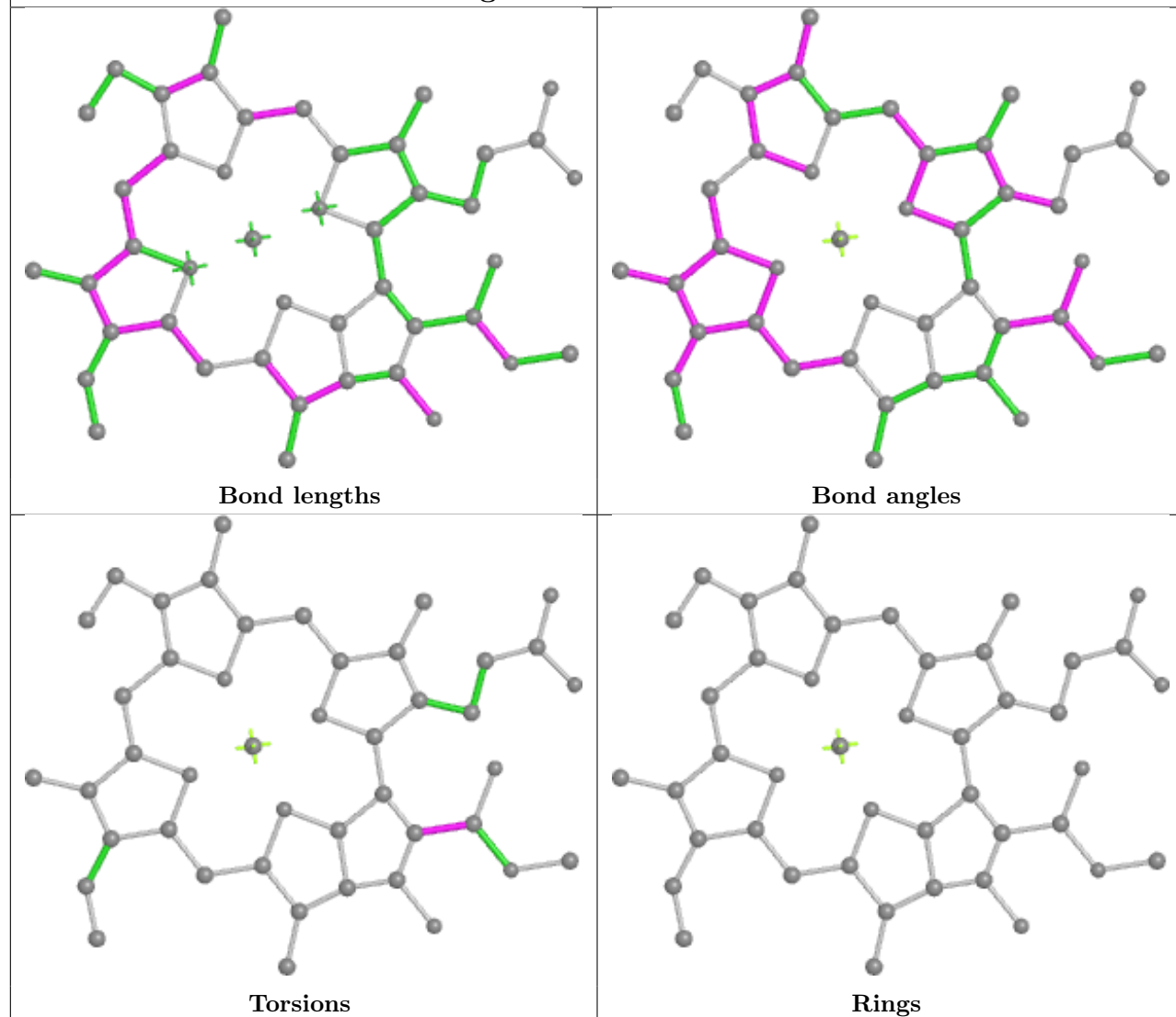




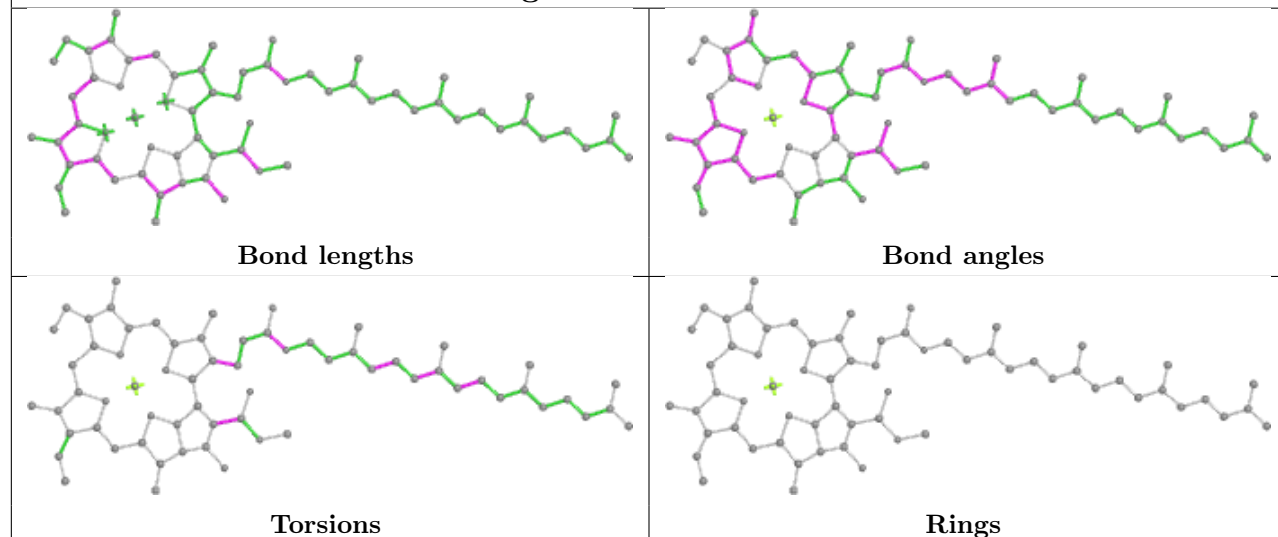
## Ligand CLA bA 808

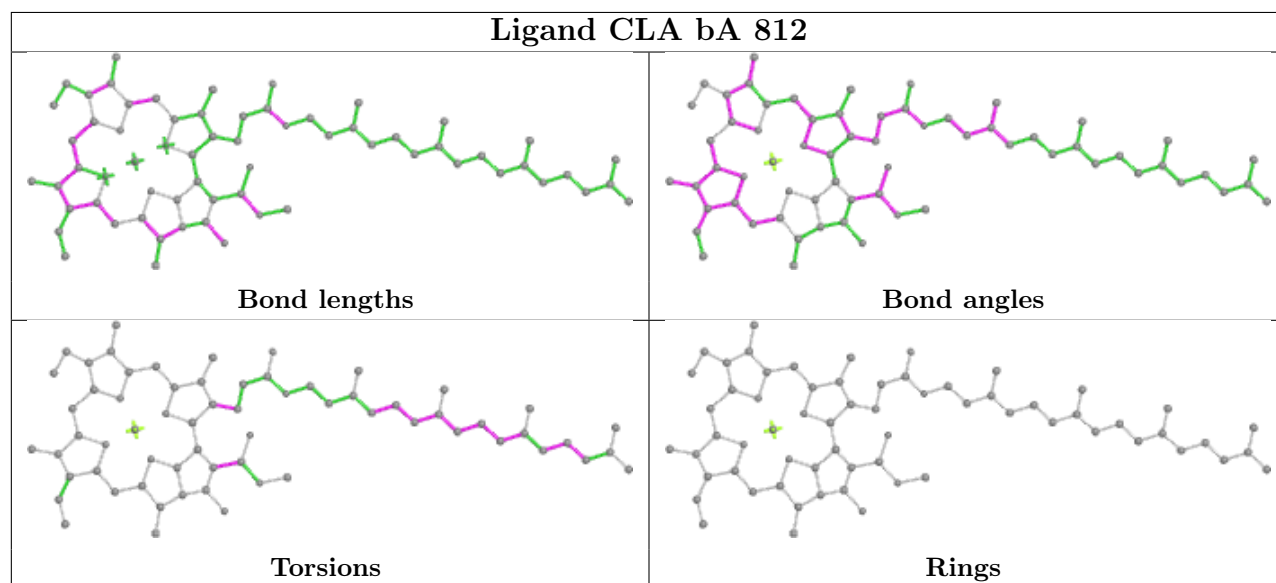
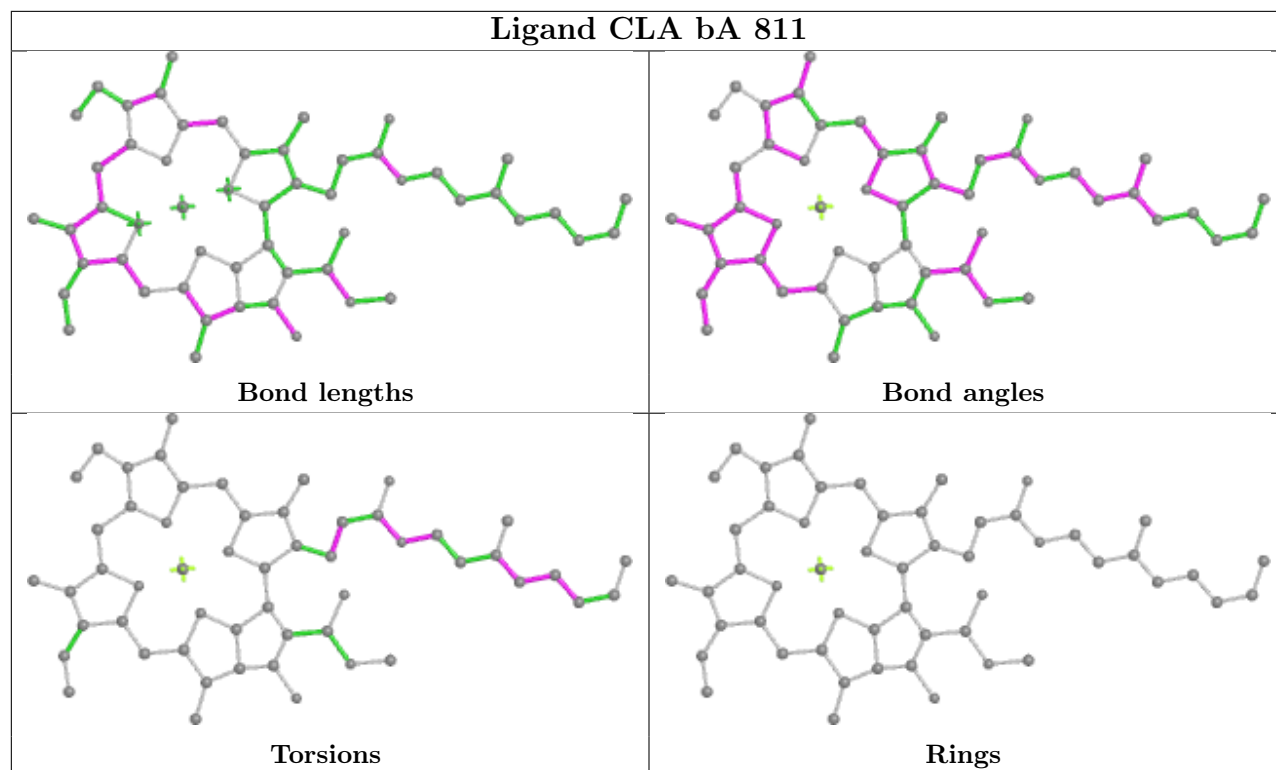


## Ligand CLA bA 809

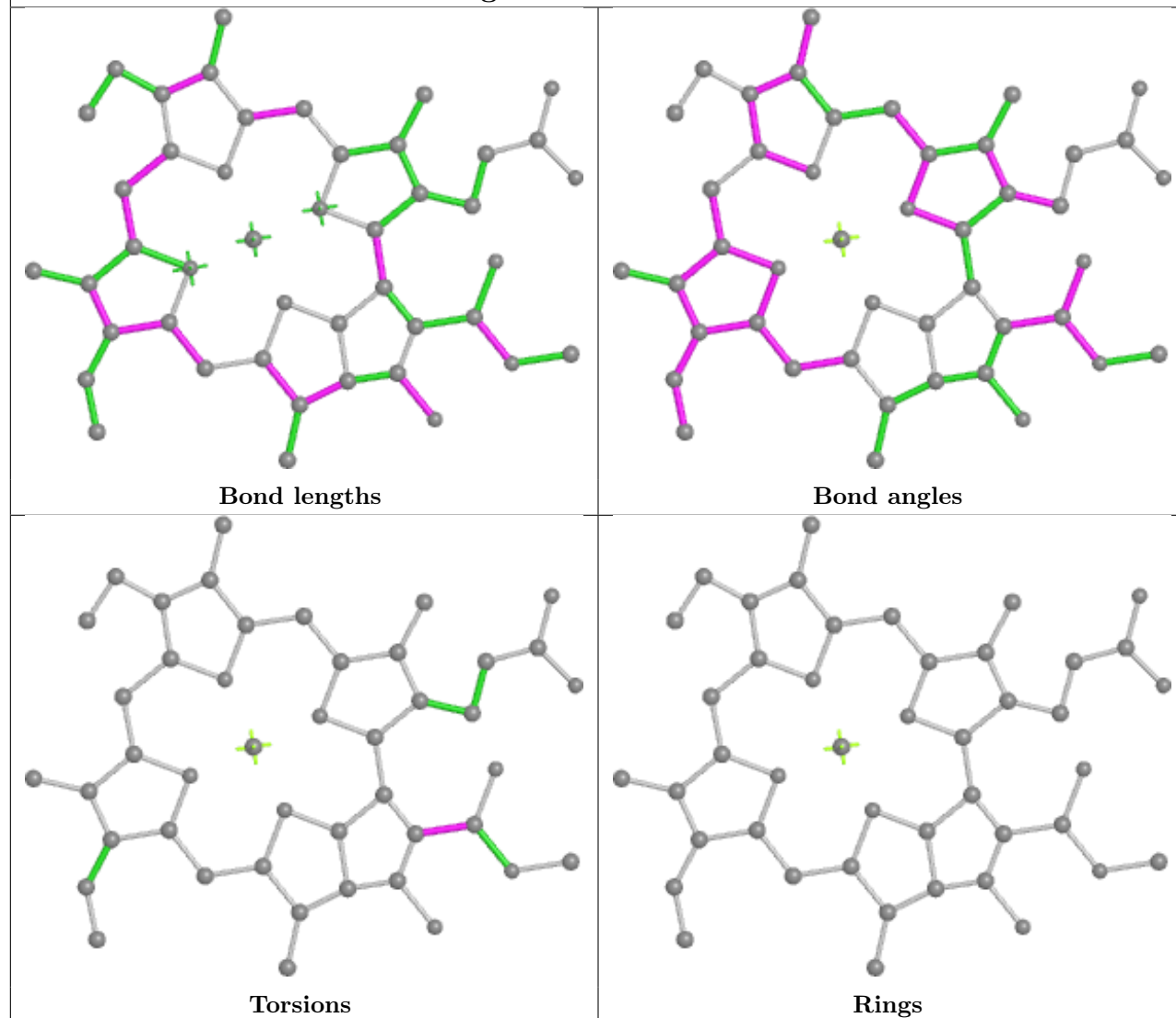


## Ligand CLA bA 810

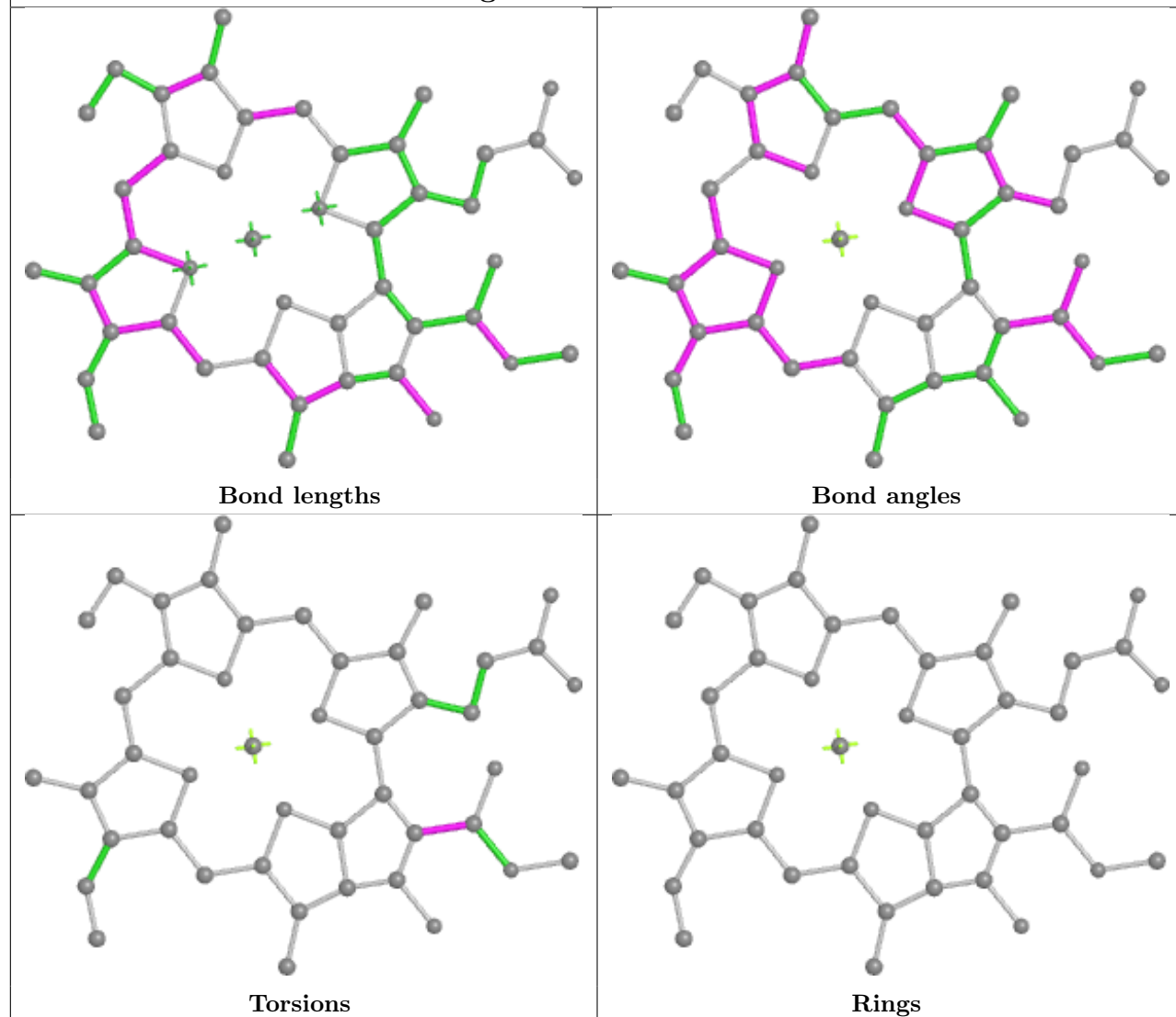




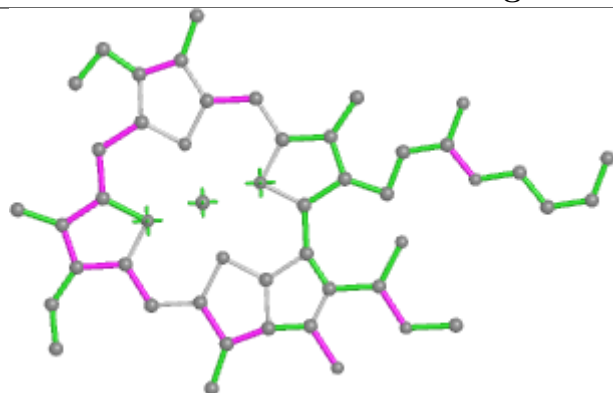
## Ligand CLA bA 813



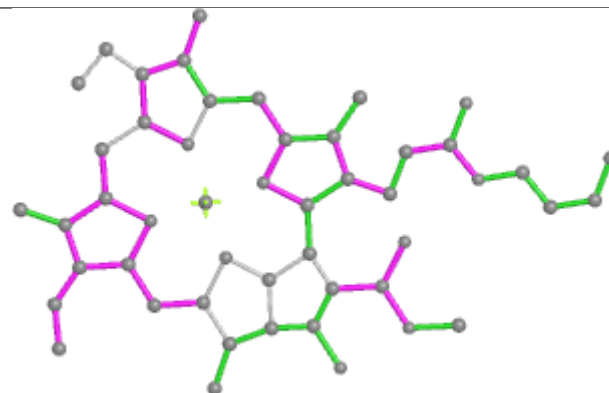
## Ligand CLA bA 814



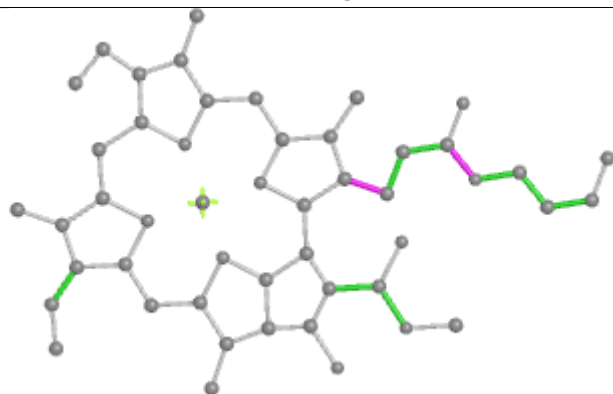
## Ligand CLA bA 815



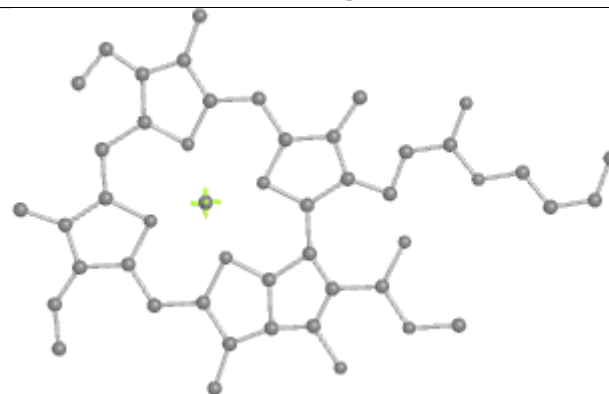
Bond lengths



Bond angles

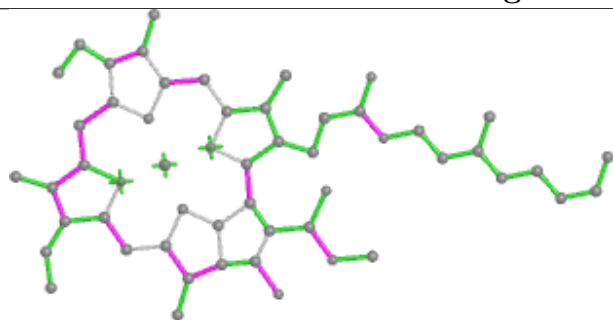


Torsions

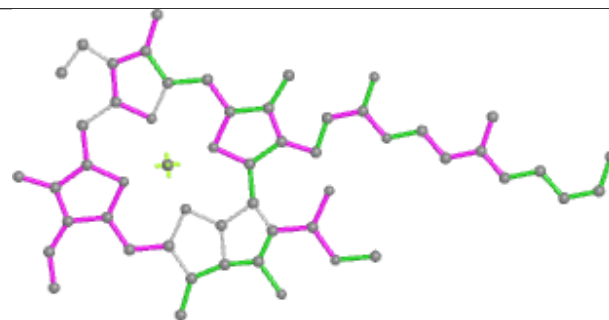


Rings

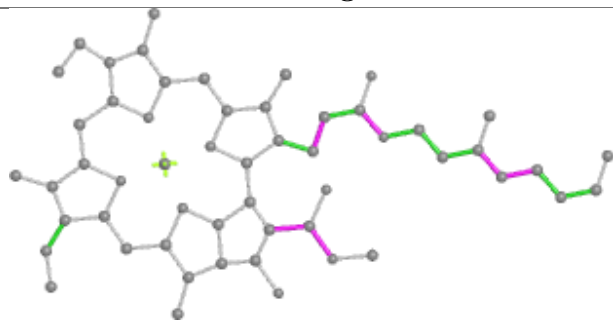
## Ligand CLA bA 816



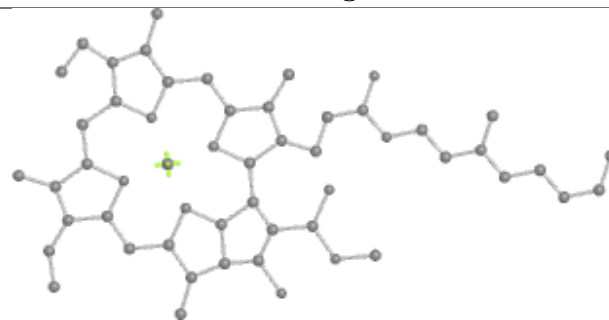
Bond lengths



Bond angles

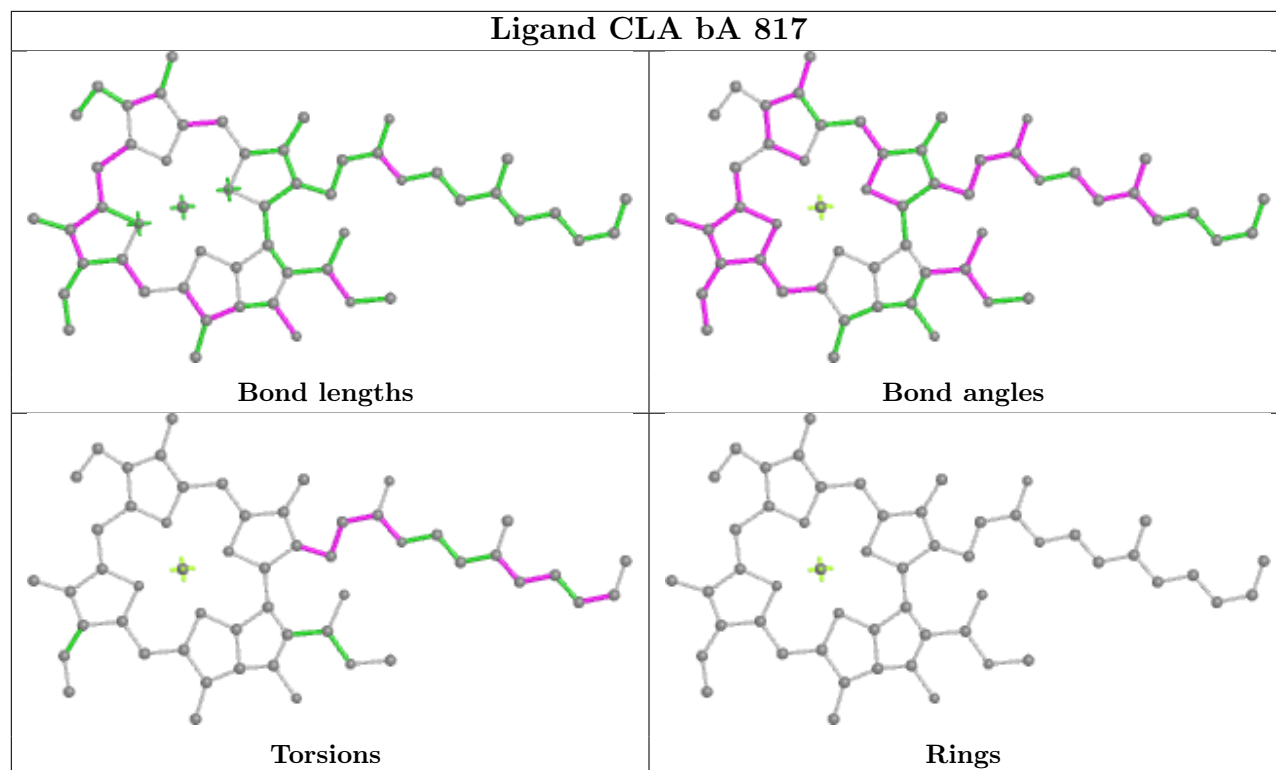


Torsions

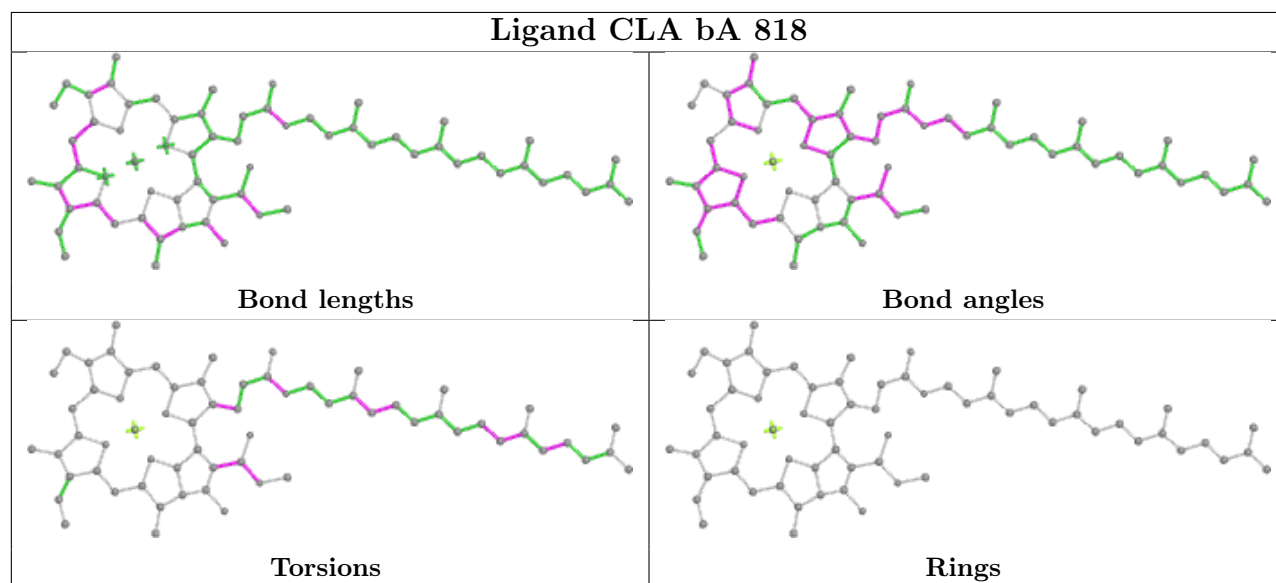


Rings

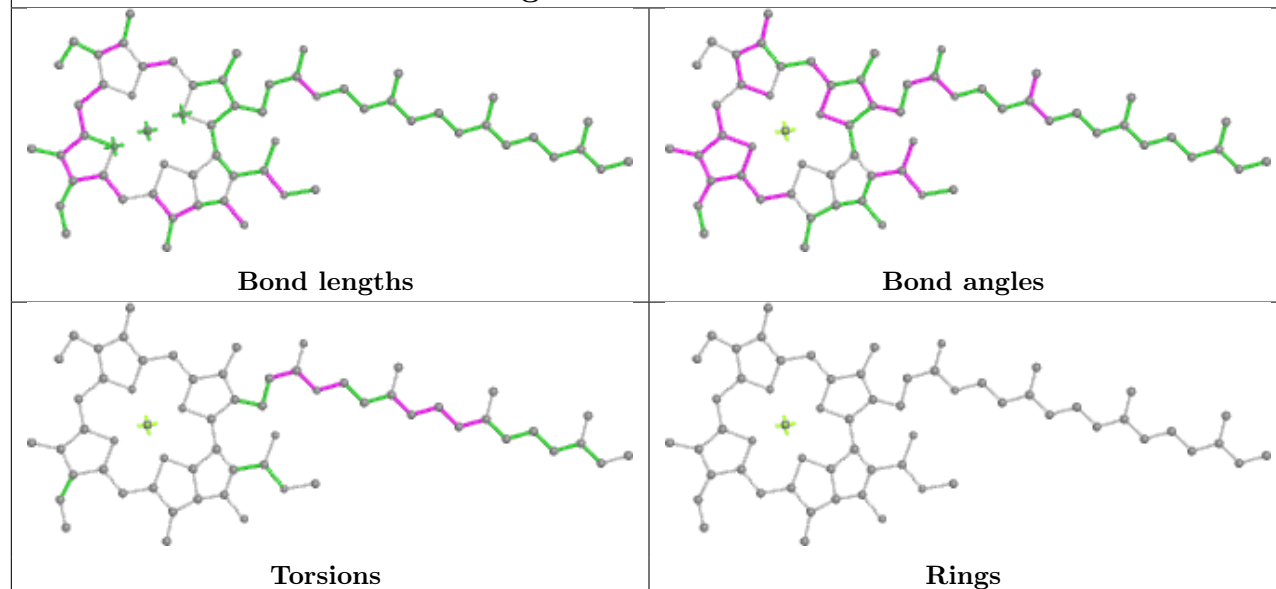
## Ligand CLA bA 817



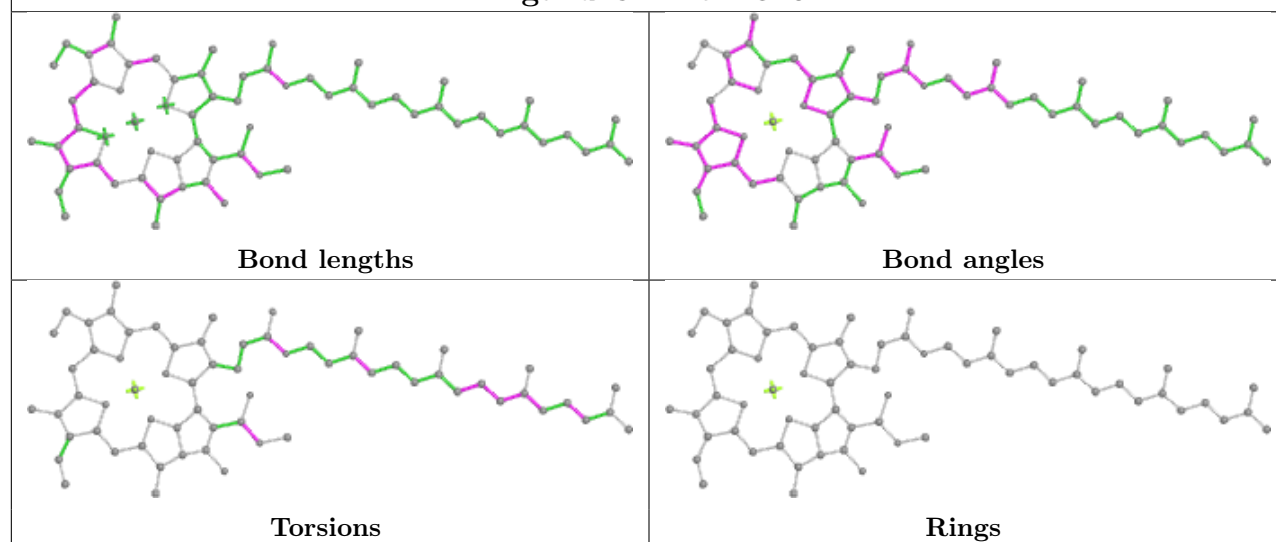
## Ligand CLA bA 818



## Ligand CLA bA 819

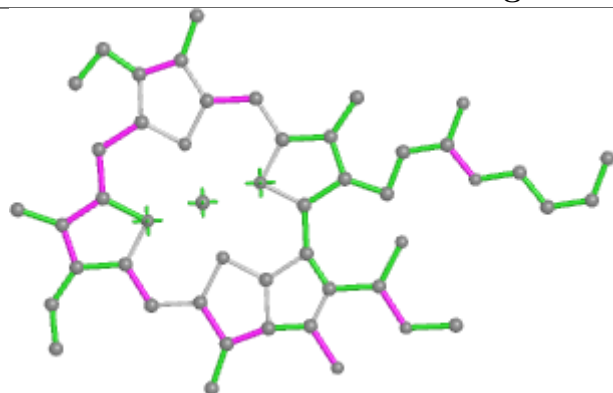


## Ligand CLA bA 820

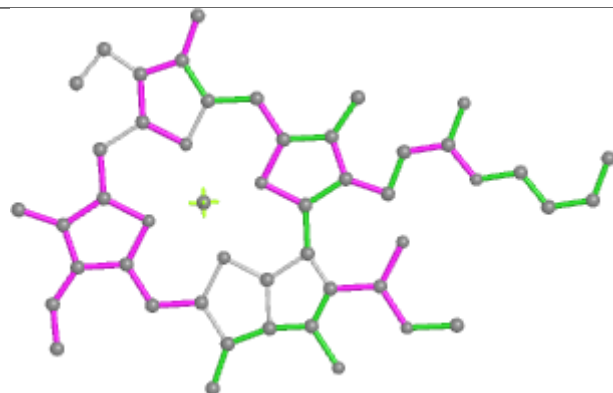




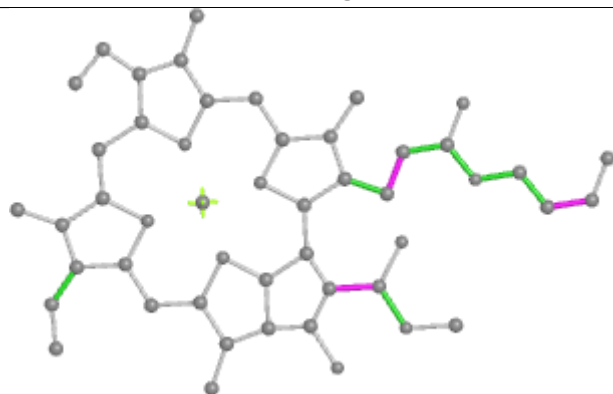
## Ligand CLA bA 821



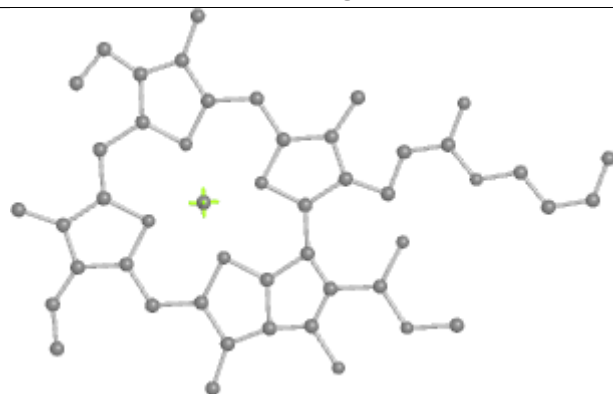
Bond lengths



Bond angles

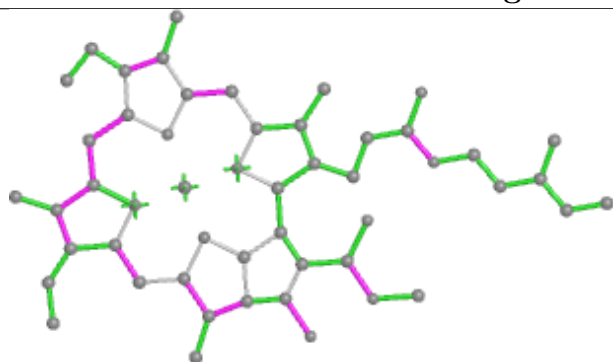


Torsions

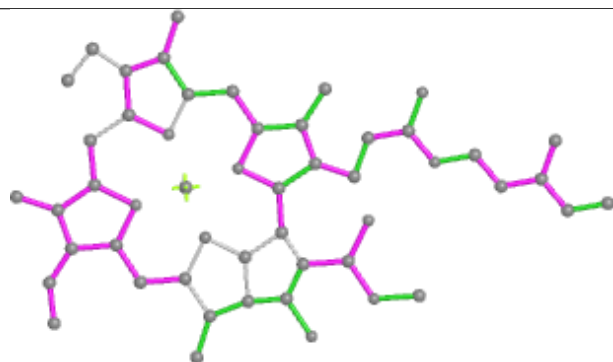


Rings

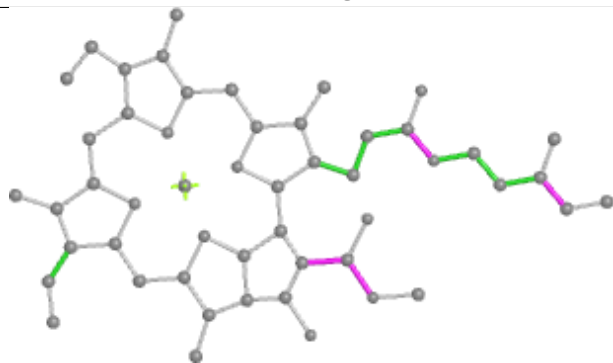
## Ligand CLA bA 822



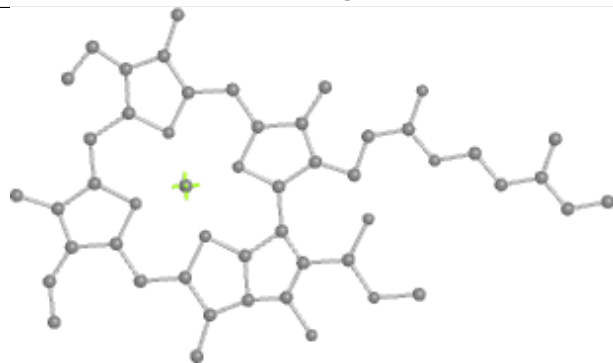
Bond lengths



Bond angles

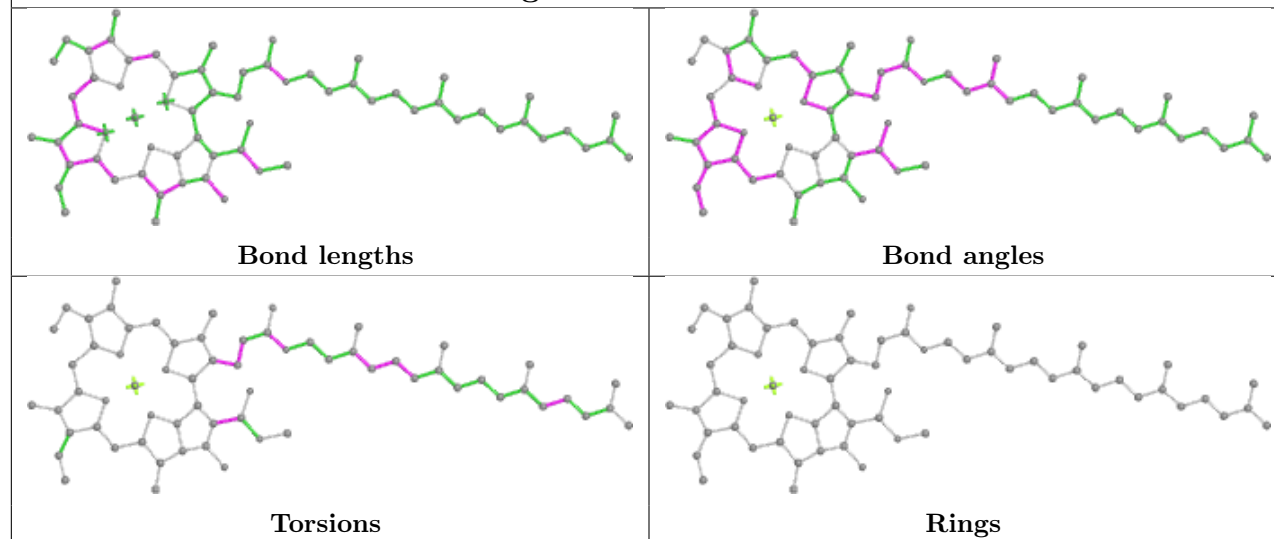


Torsions

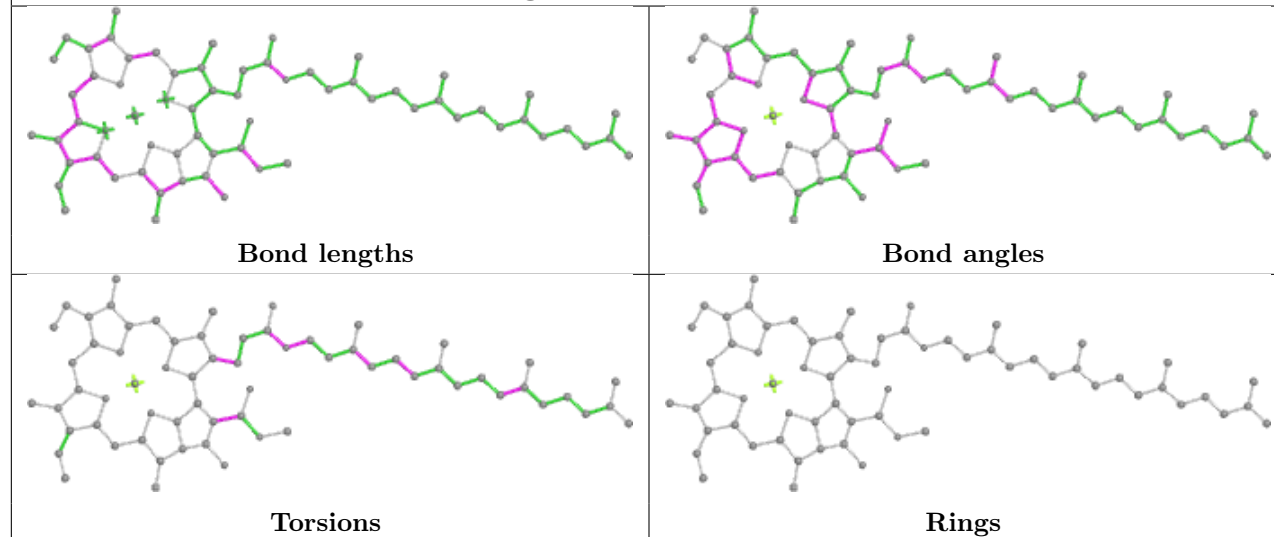


Rings

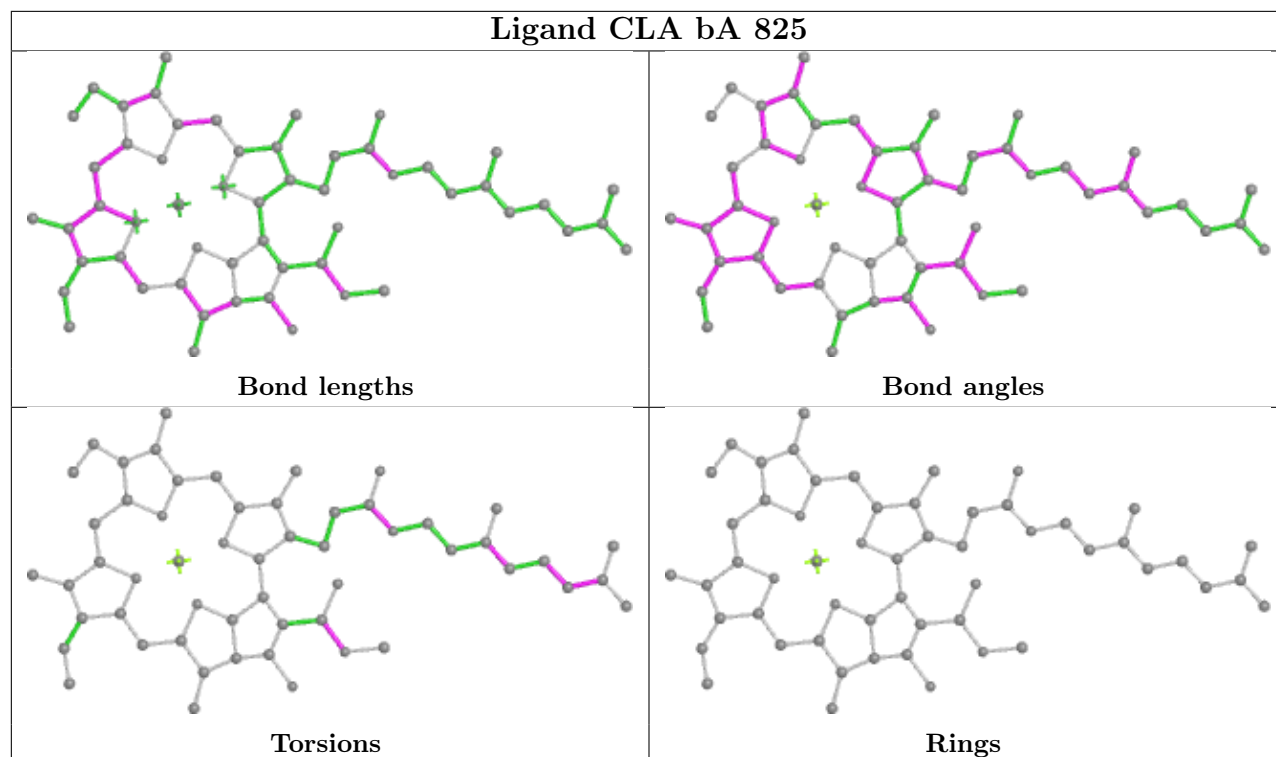
## Ligand CLA bA 823



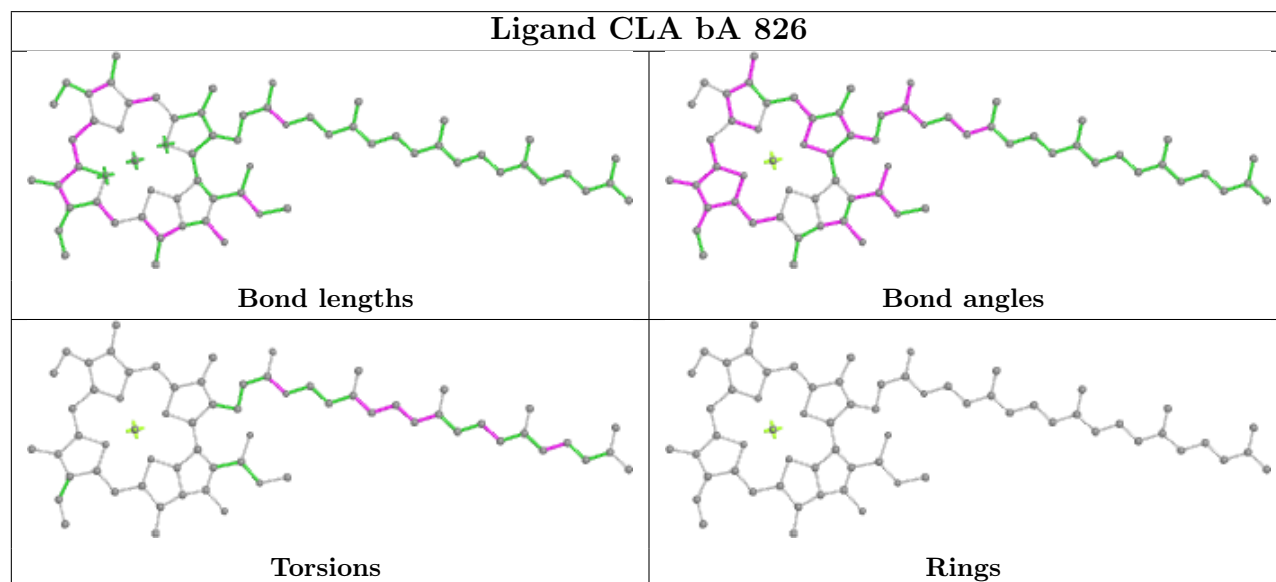
## Ligand CLA bA 824



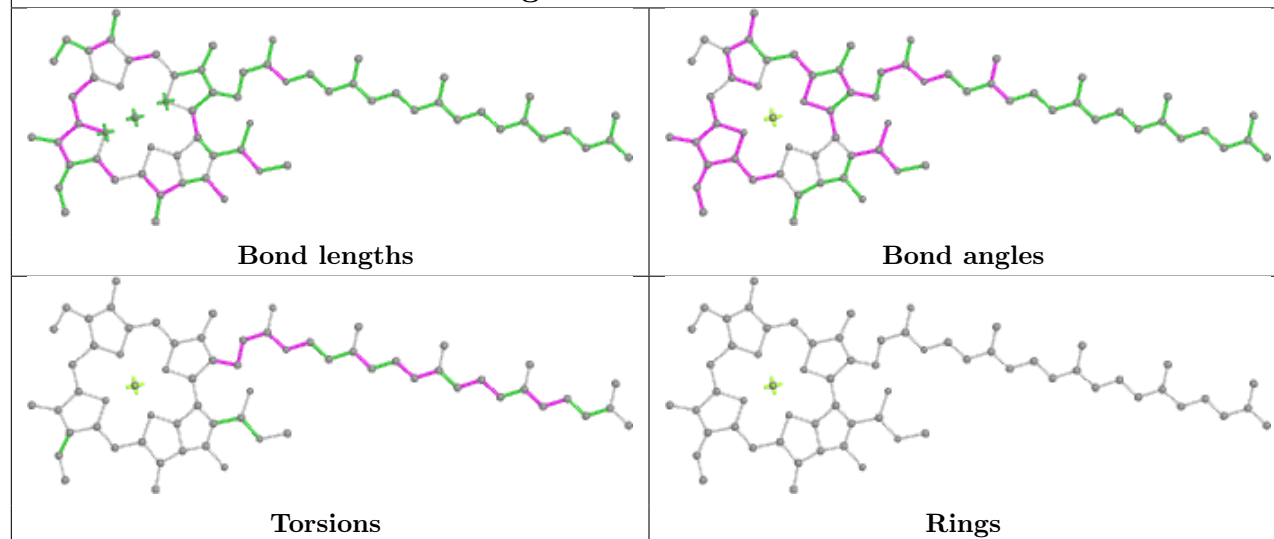
## Ligand CLA bA 825



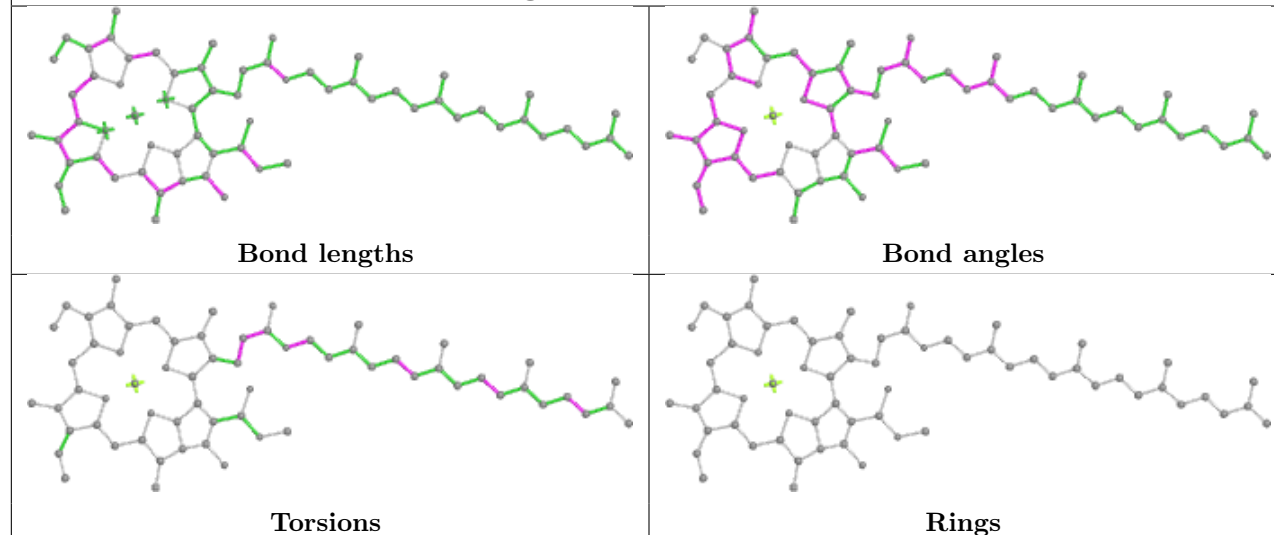
## Ligand CLA bA 826



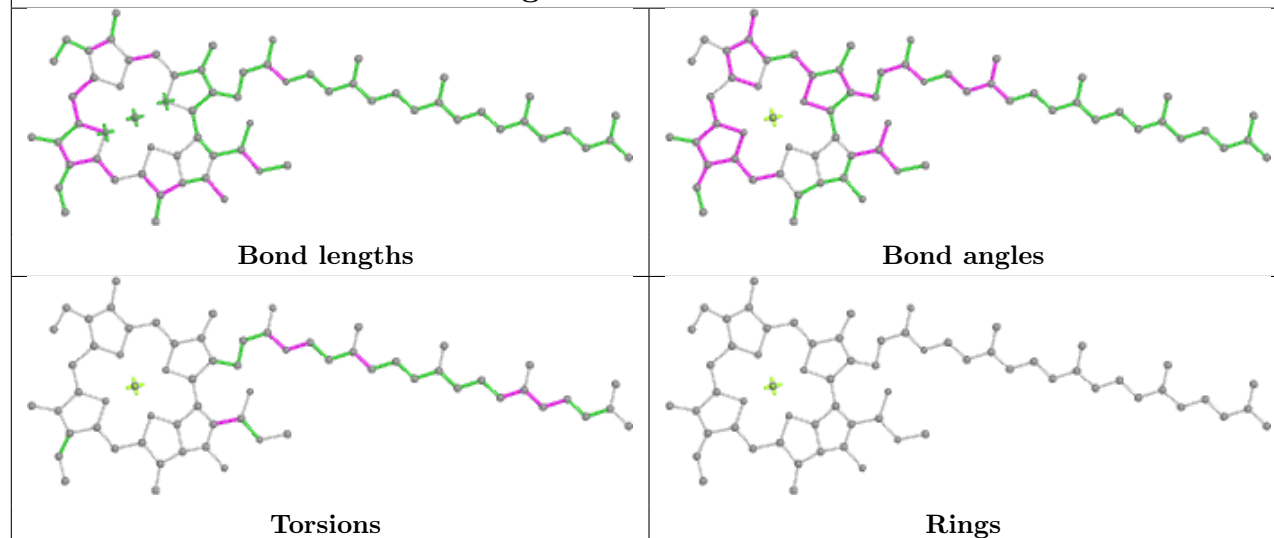
## Ligand CLA ba 827



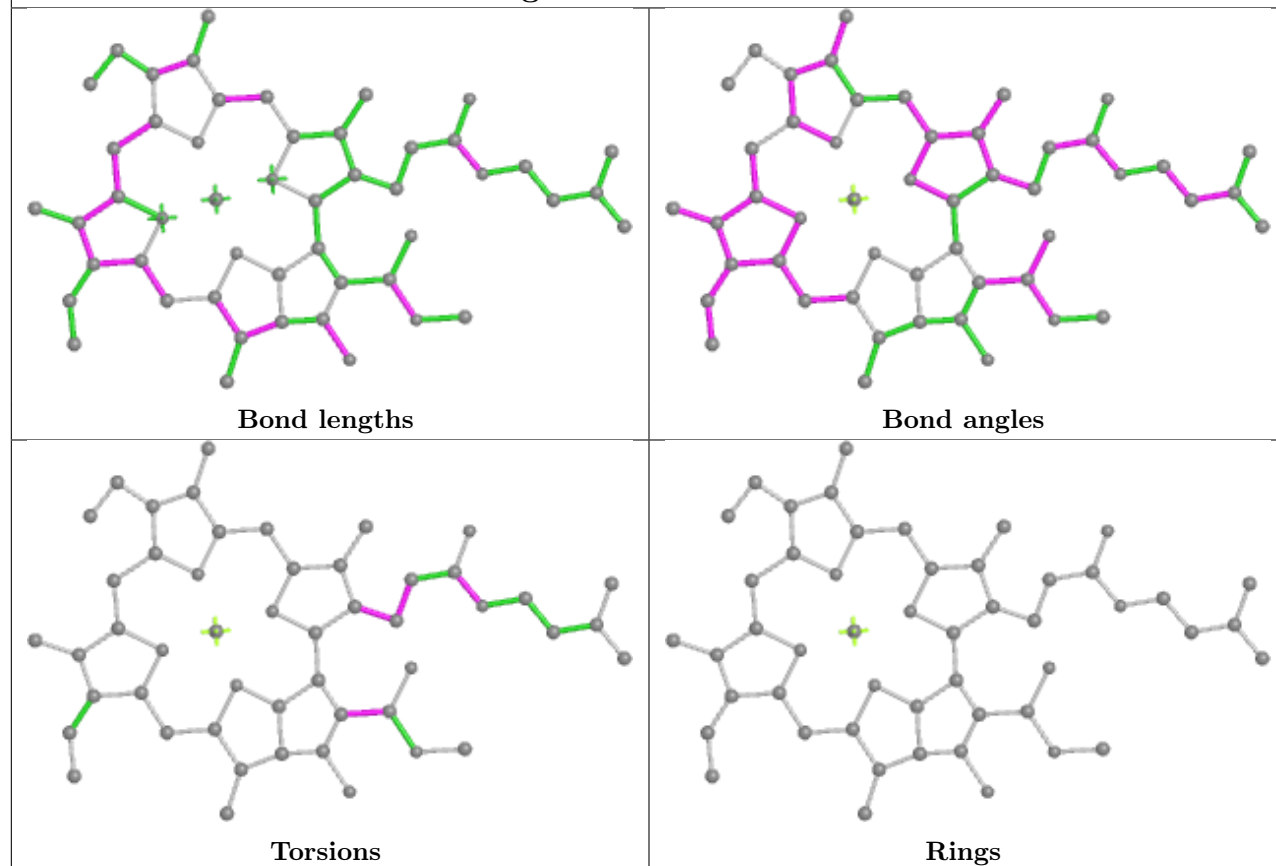
## Ligand CLA ba 828



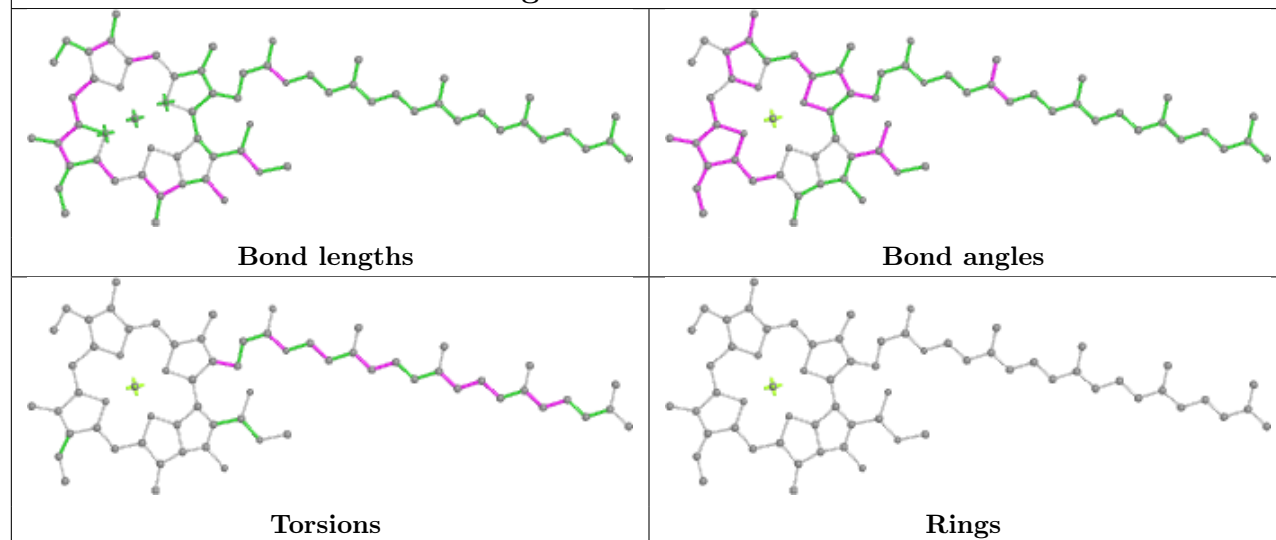
## Ligand CLA ba 829



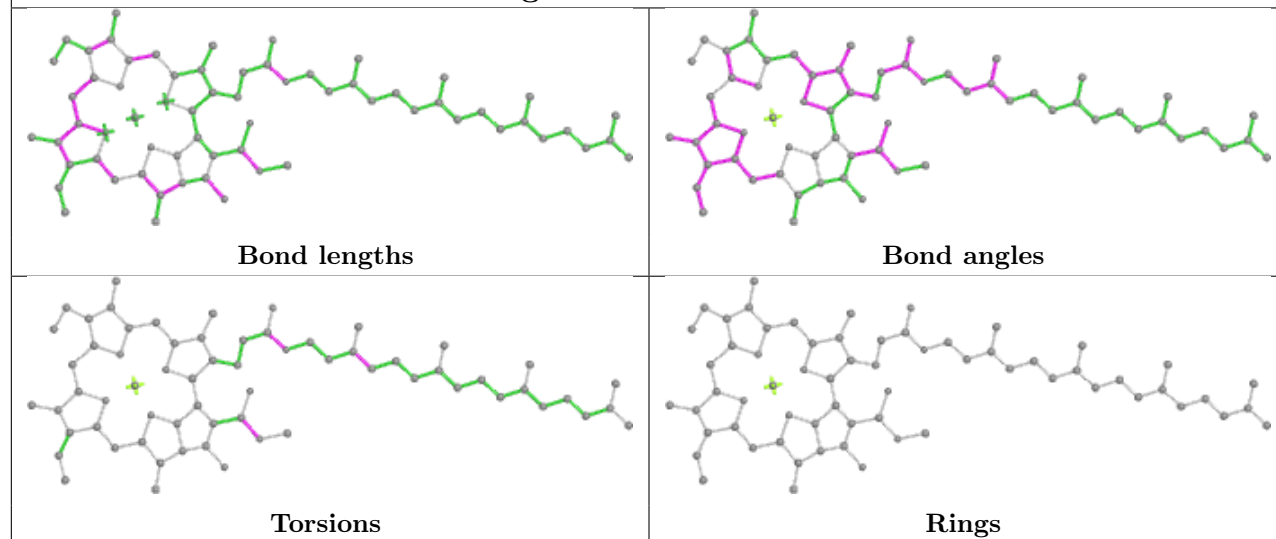
## Ligand CLA bA 830



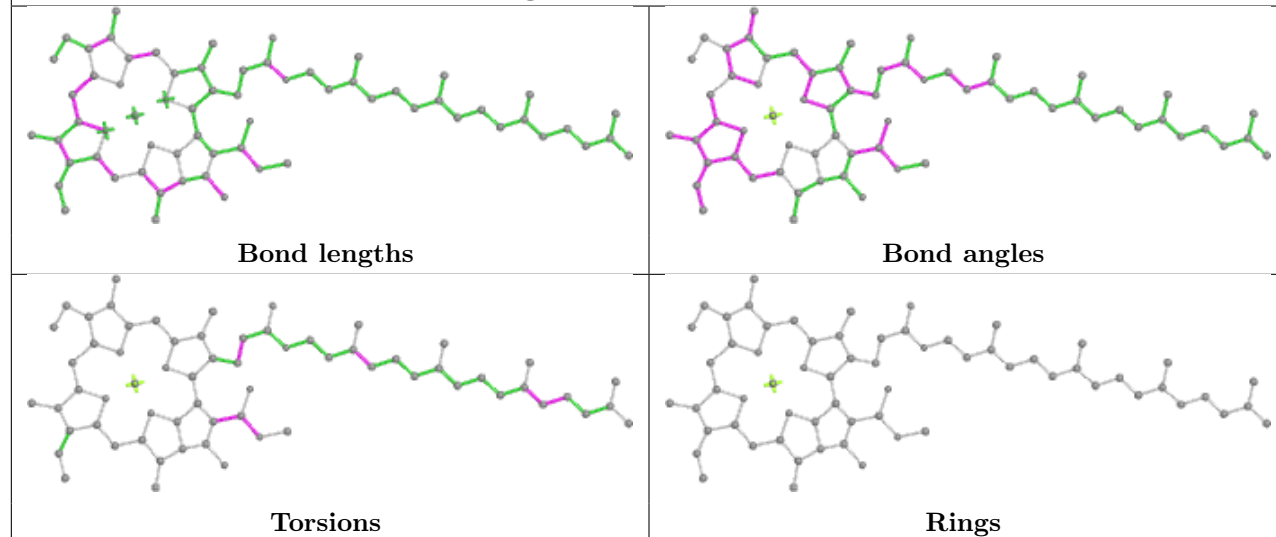
## Ligand CLA bA 831



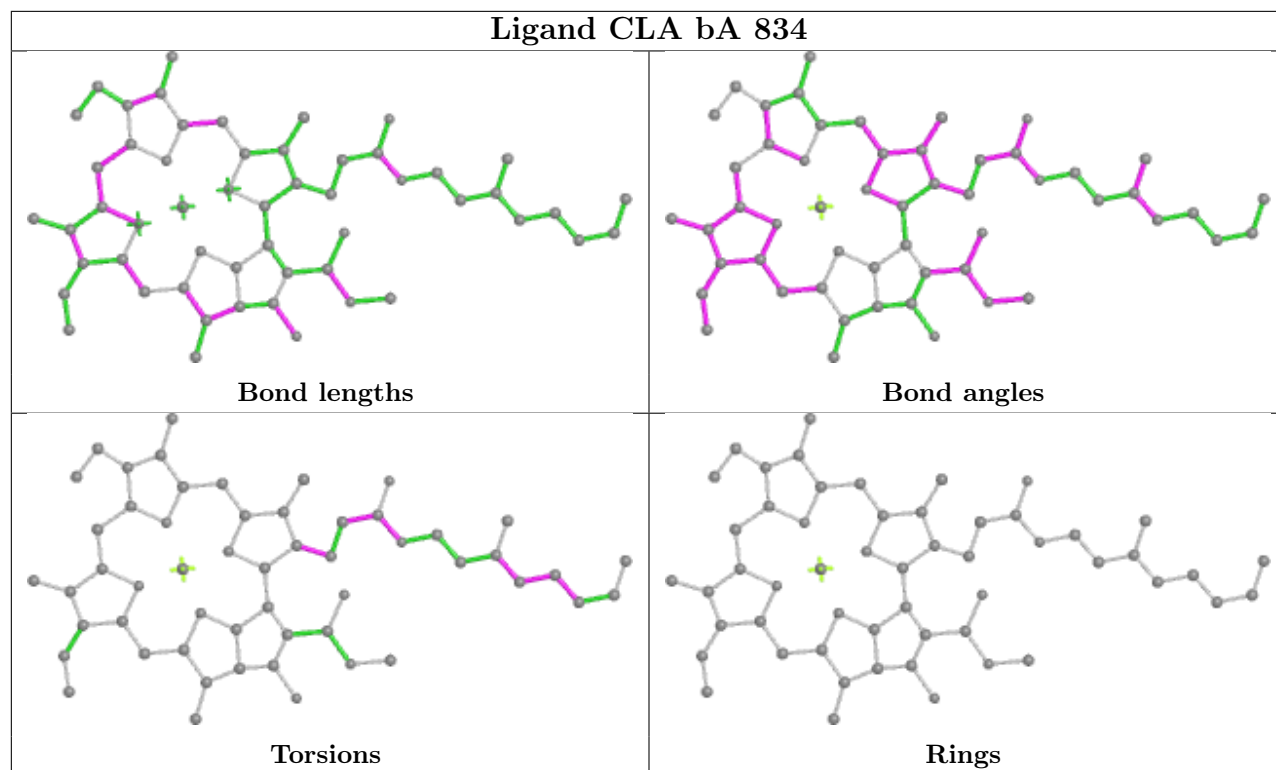
## Ligand CLA bA 832



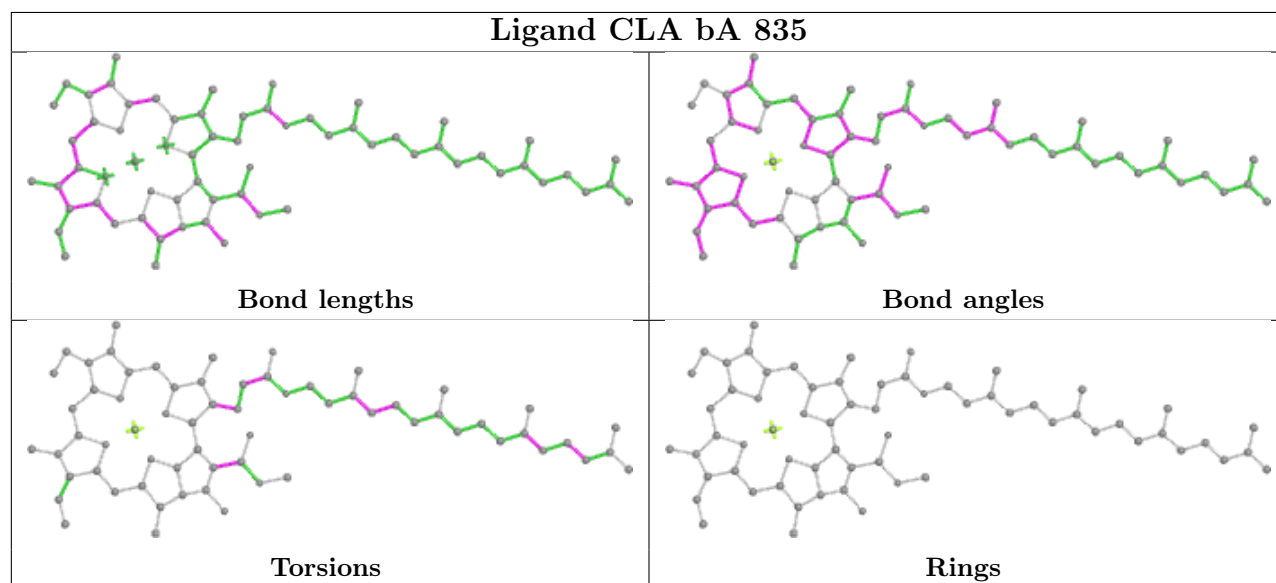
## Ligand CLA bA 833

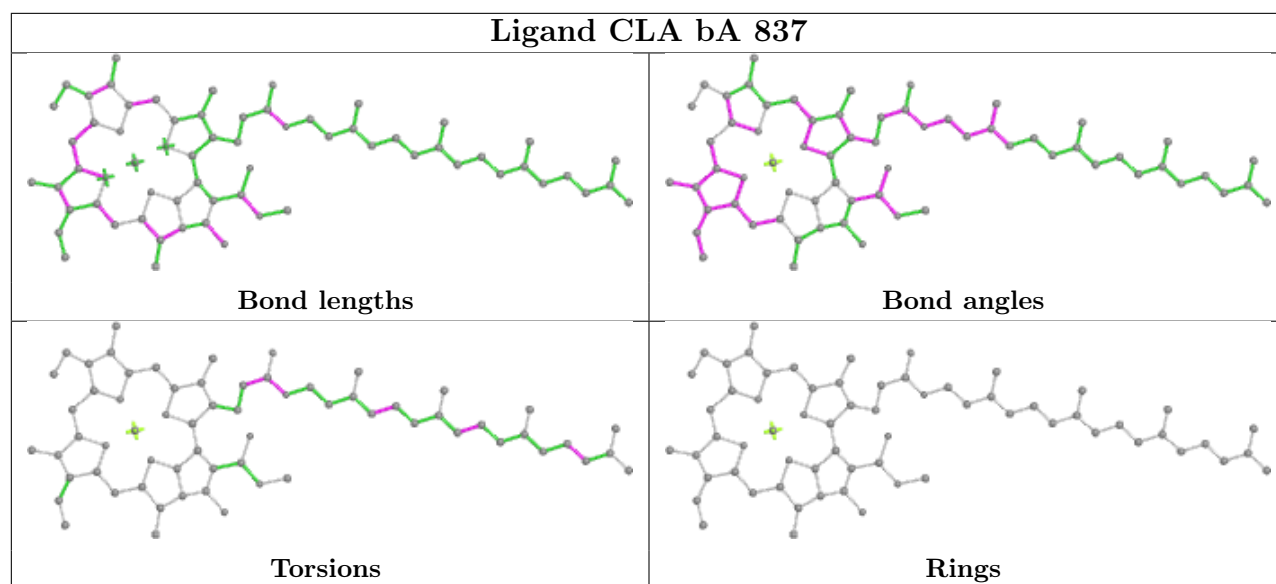
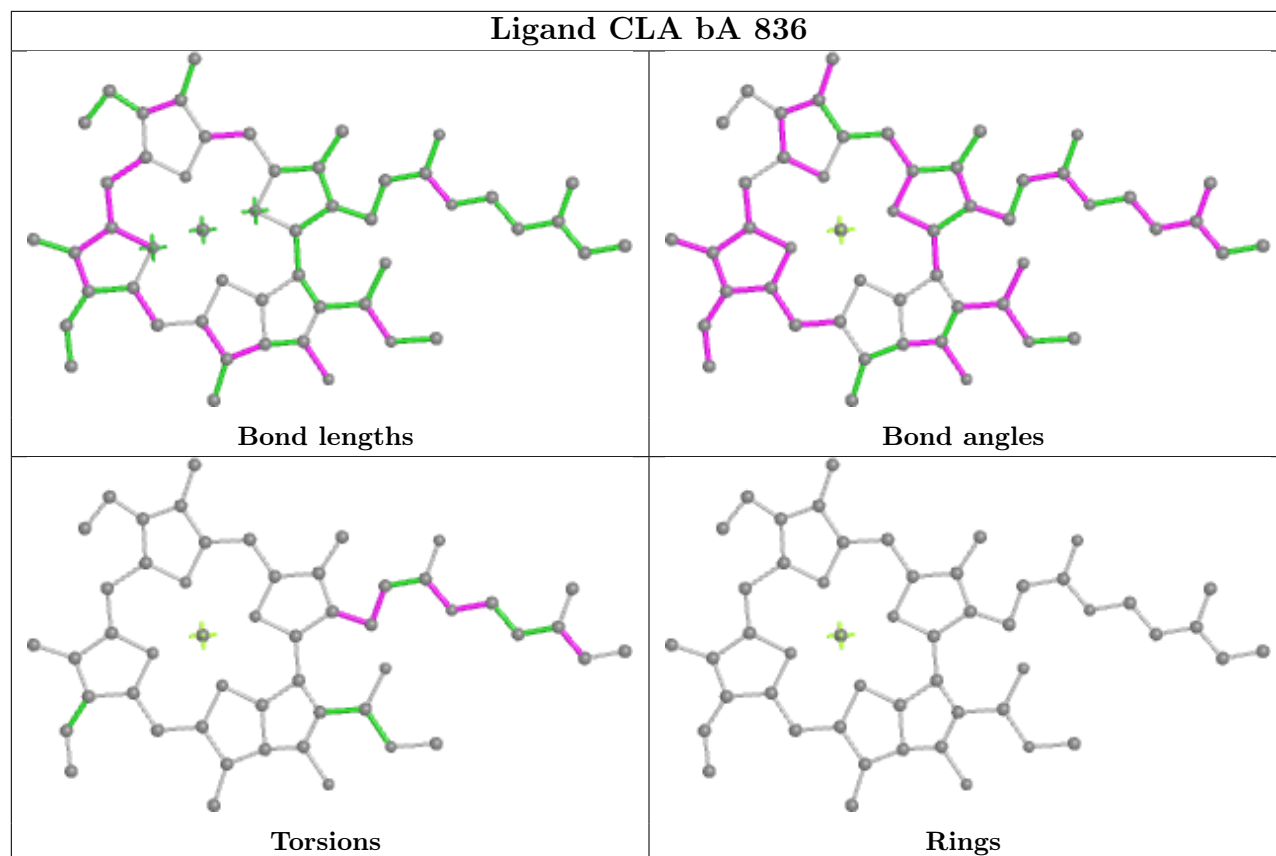


## Ligand CLA bA 834



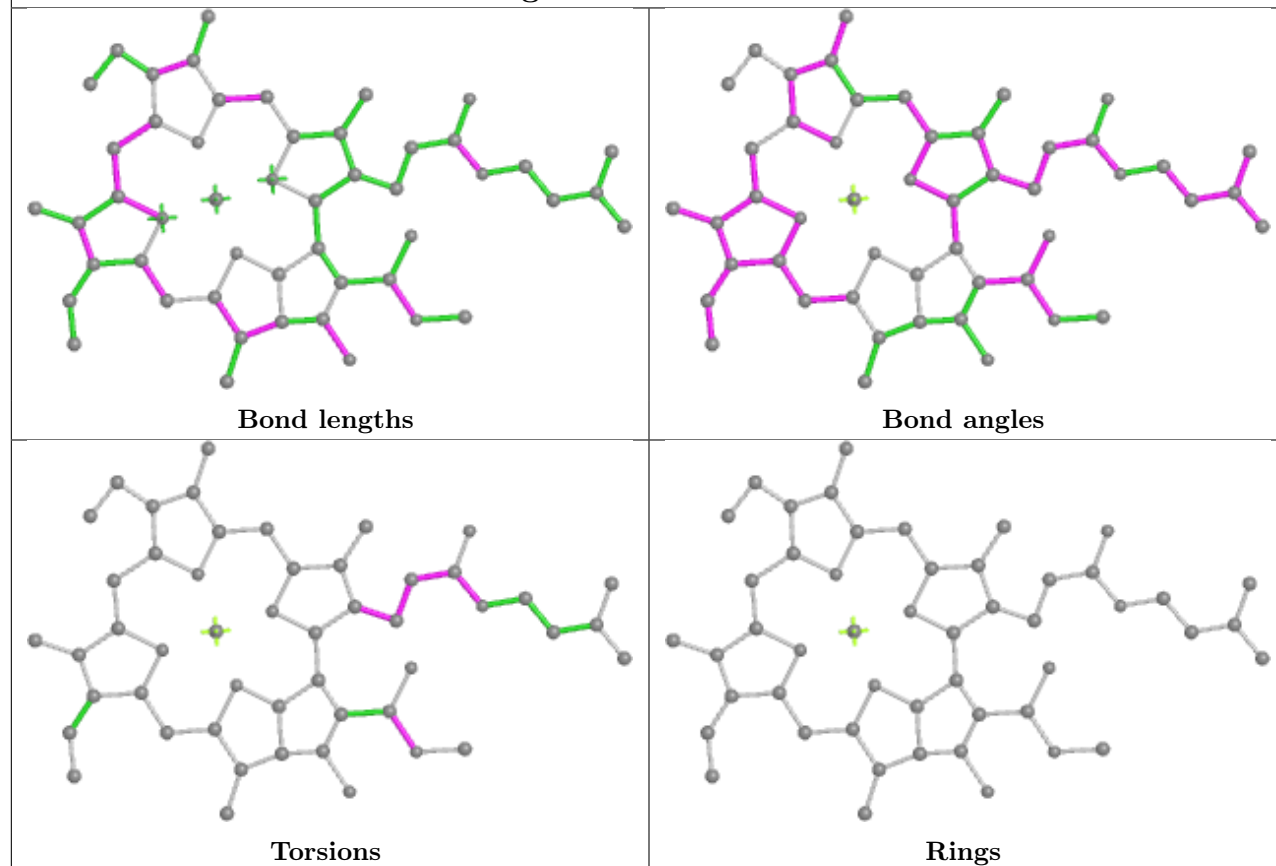
## Ligand CLA bA 835



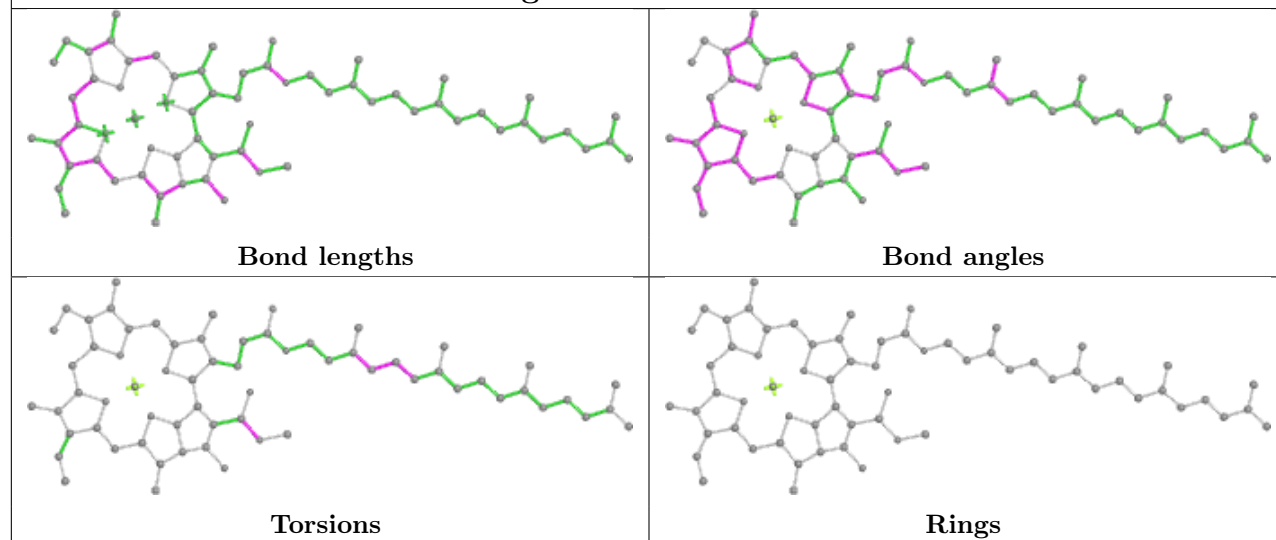


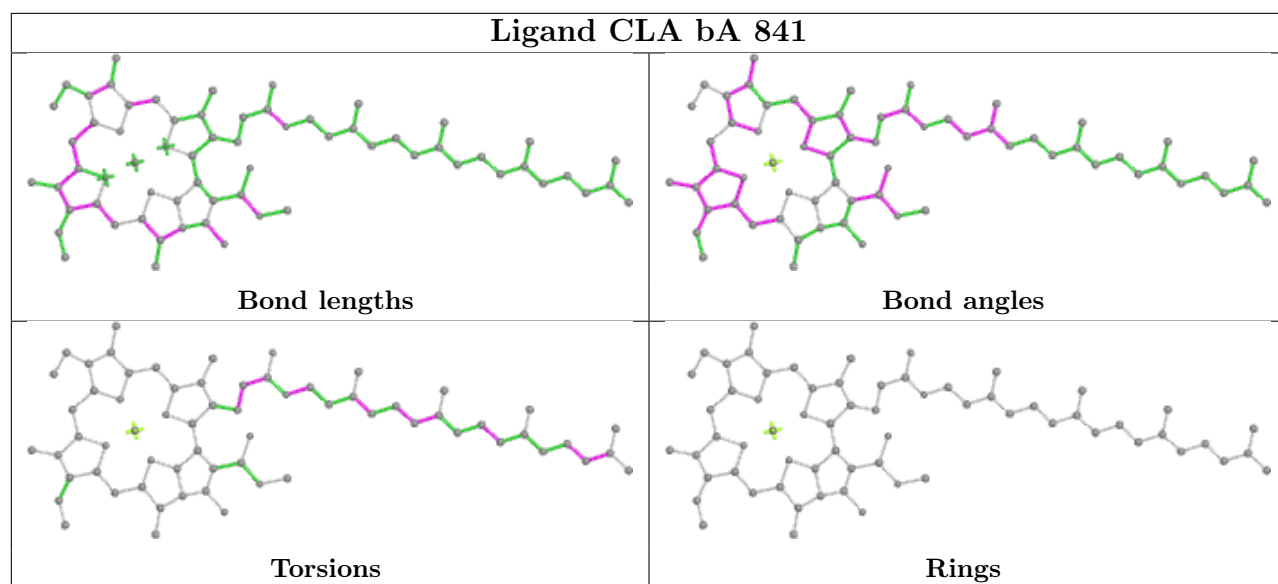
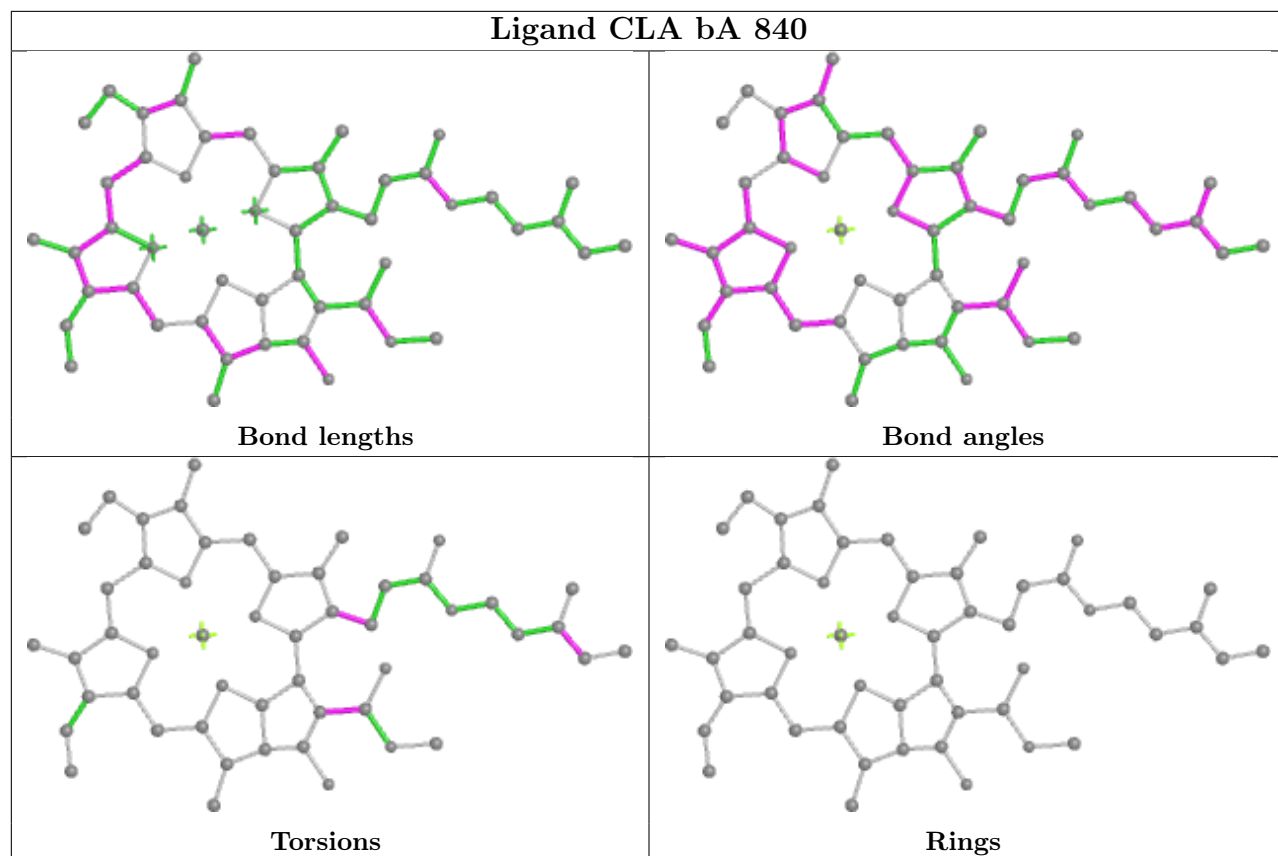


## Ligand CLA bA 838

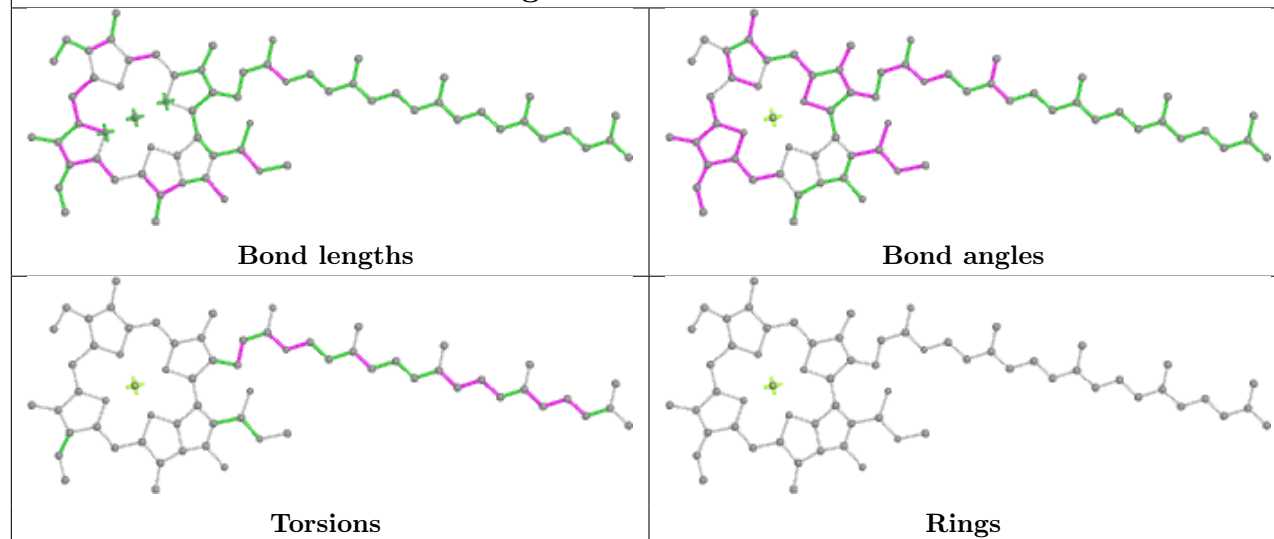


## Ligand CLA bA 839

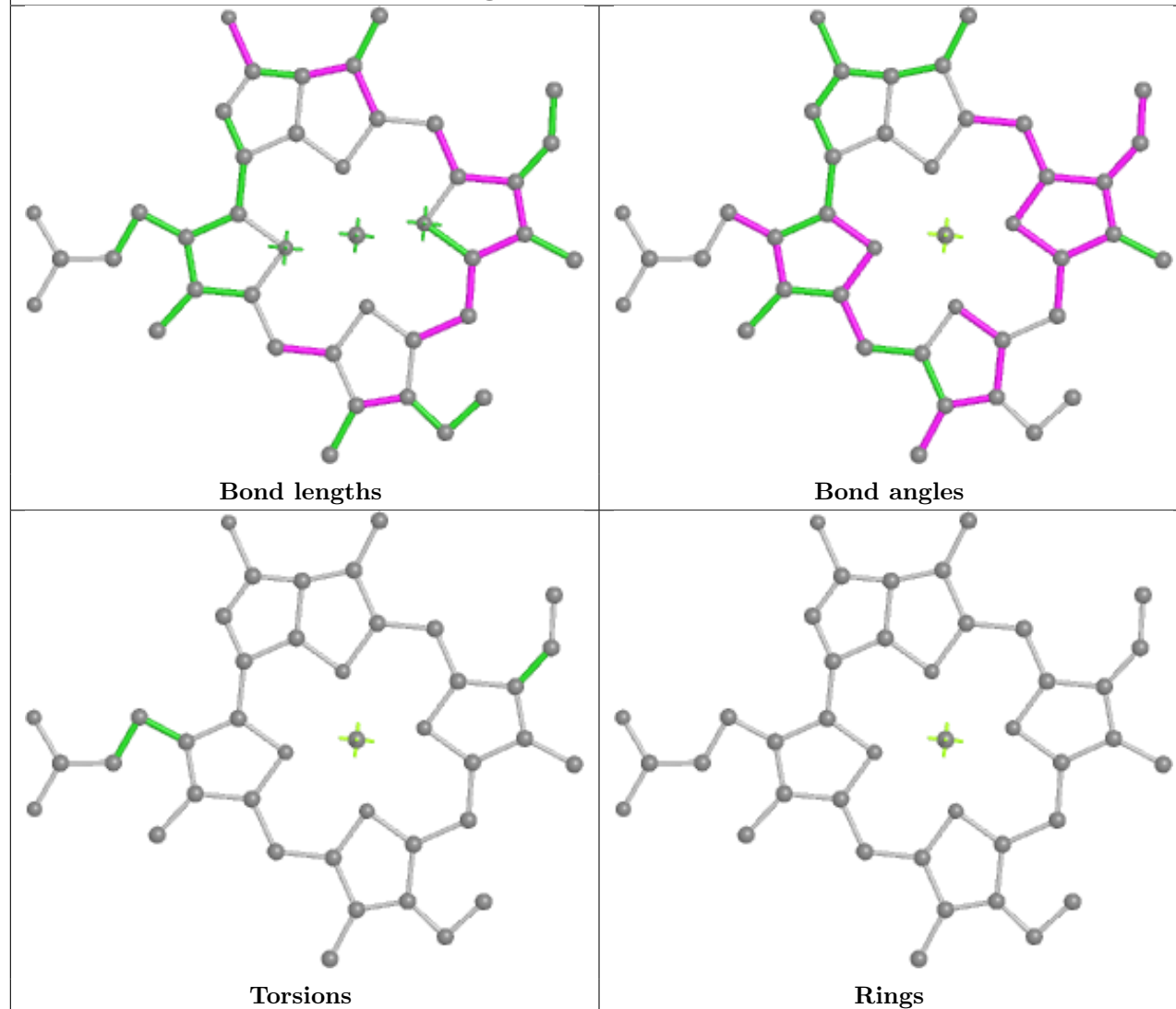


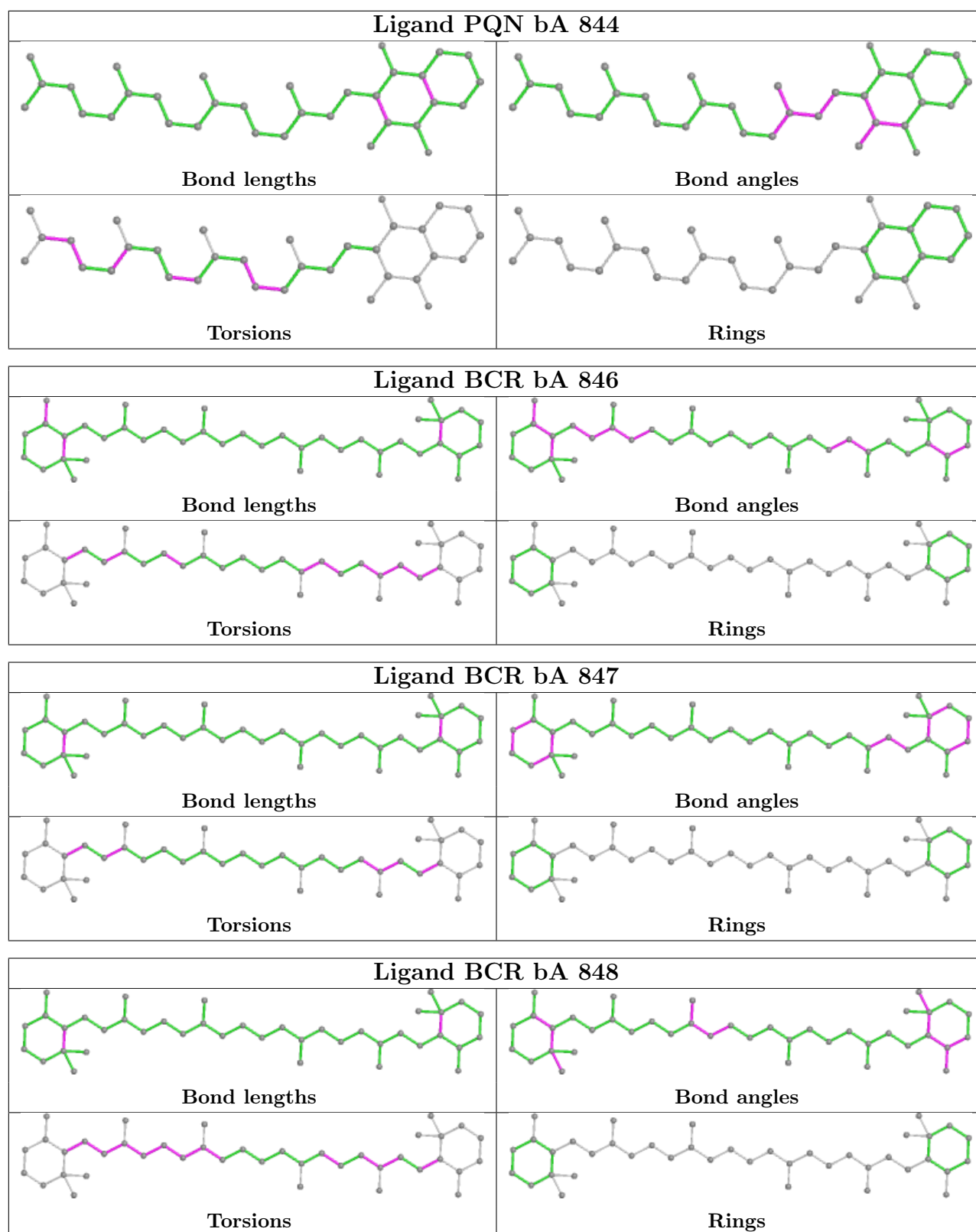


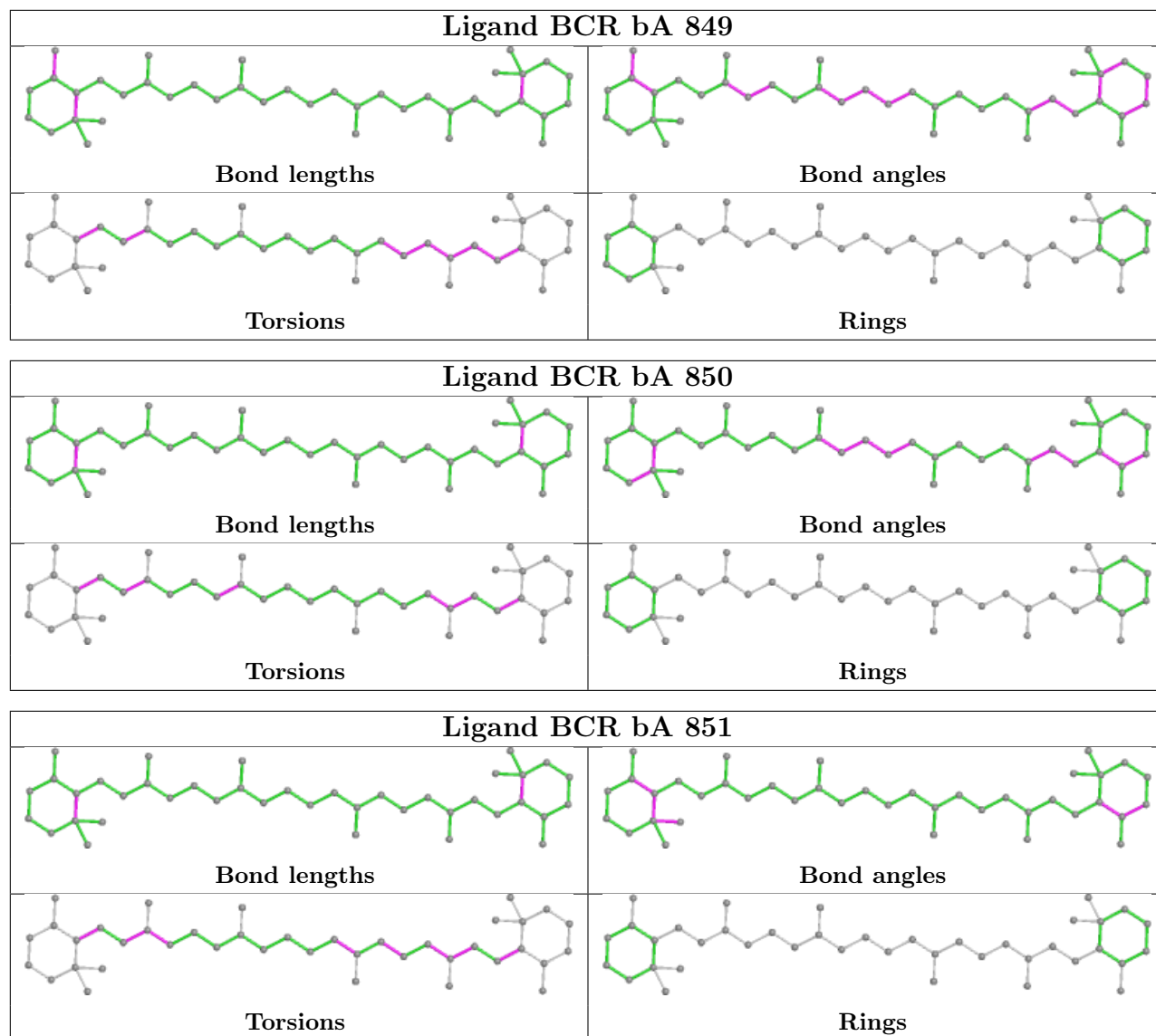
## Ligand CLA bA 842

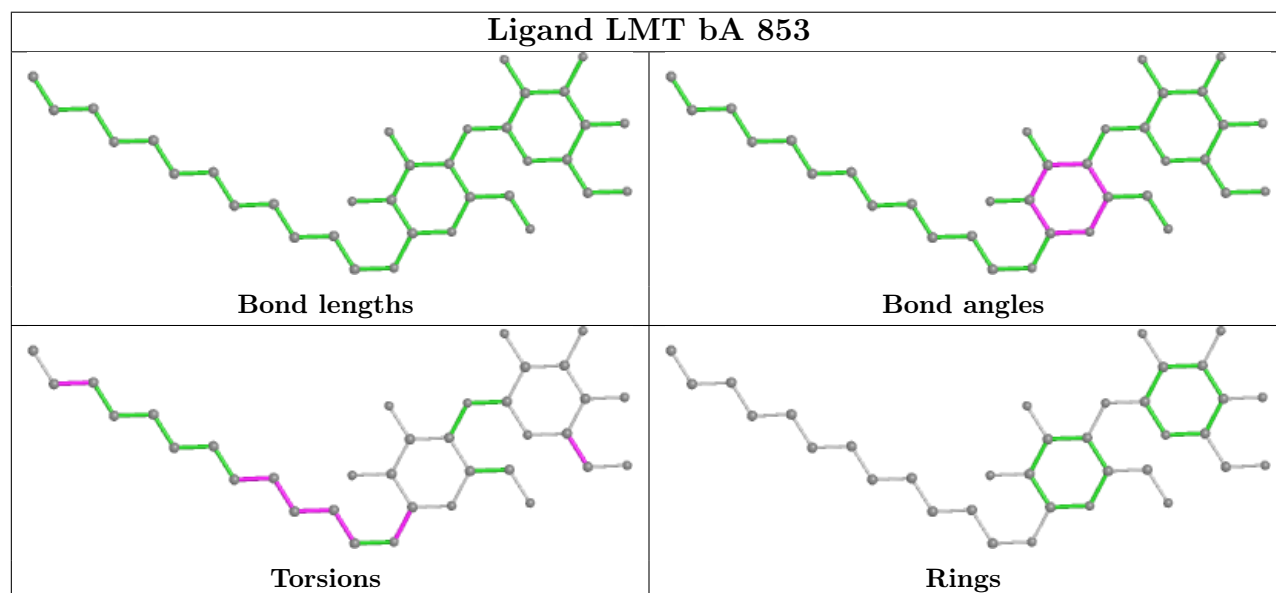
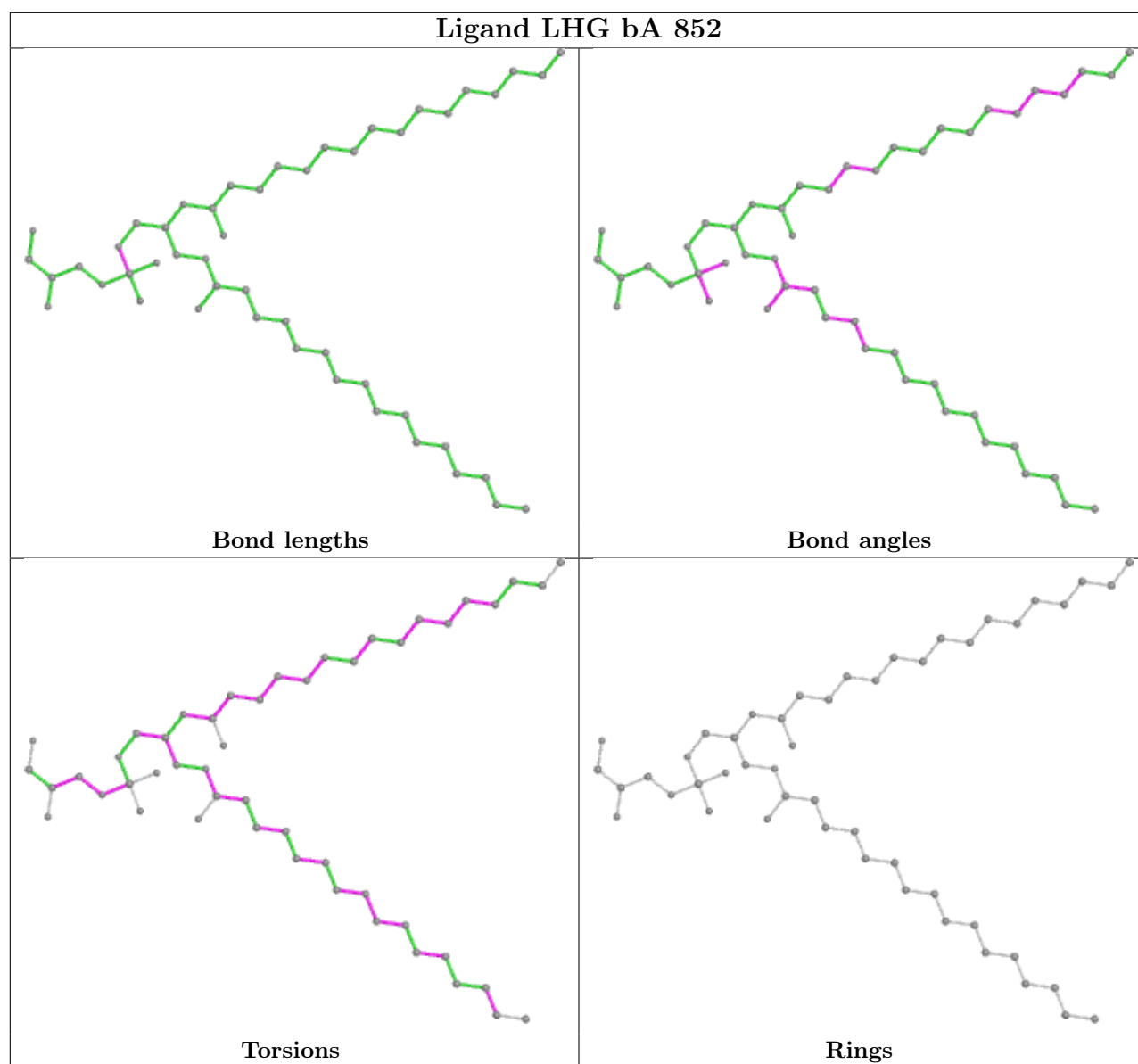


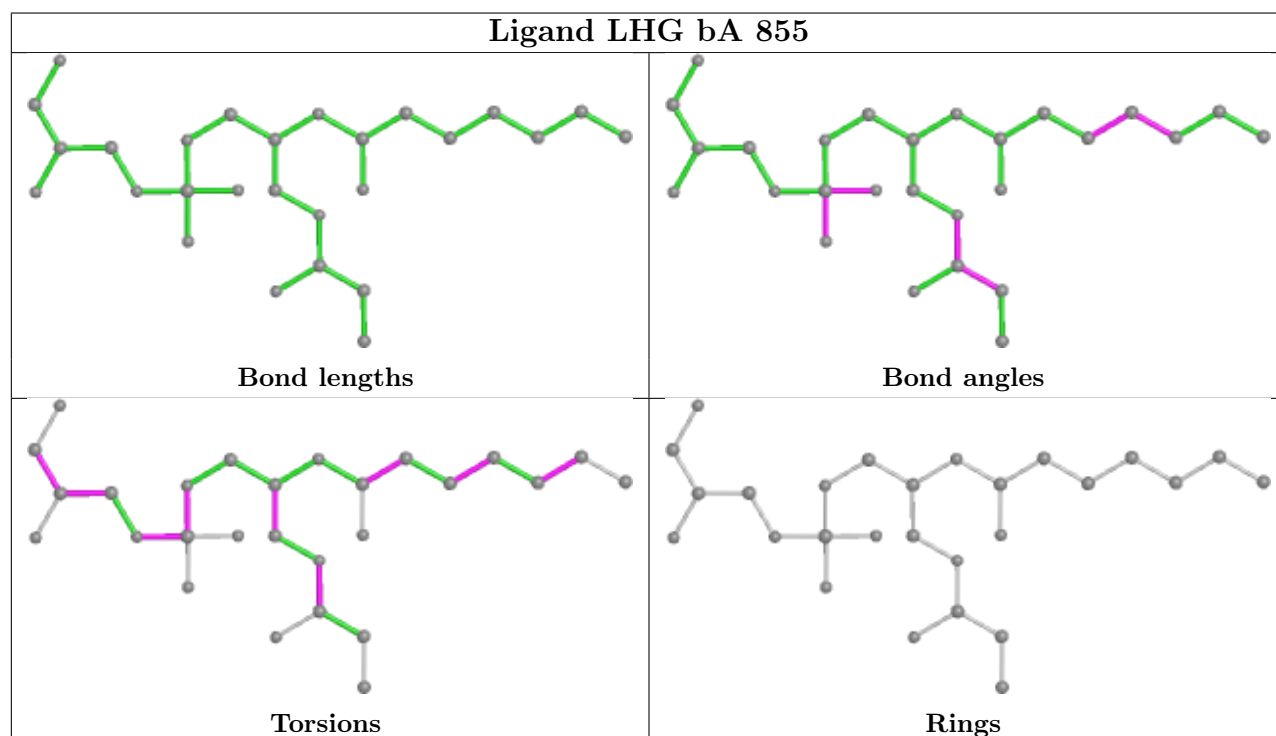
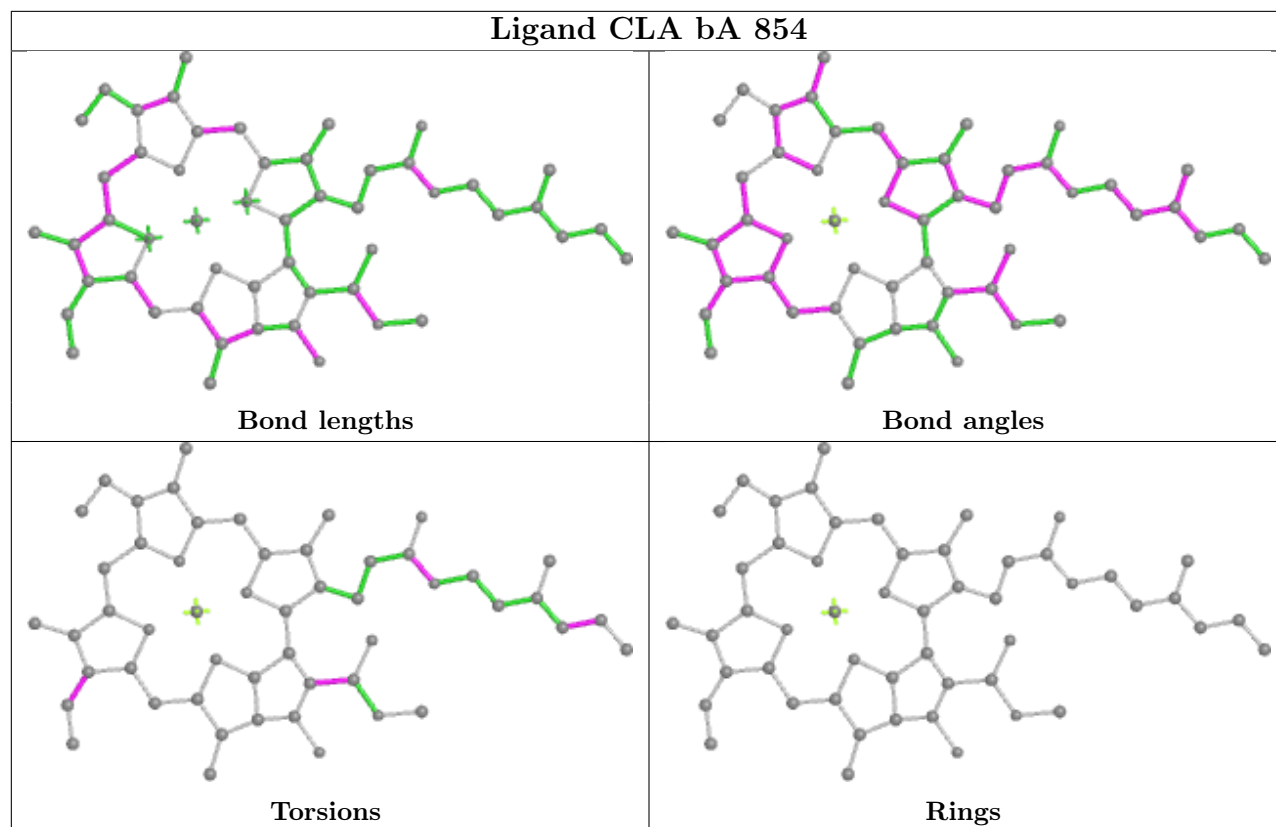
## Ligand CLA bA 843



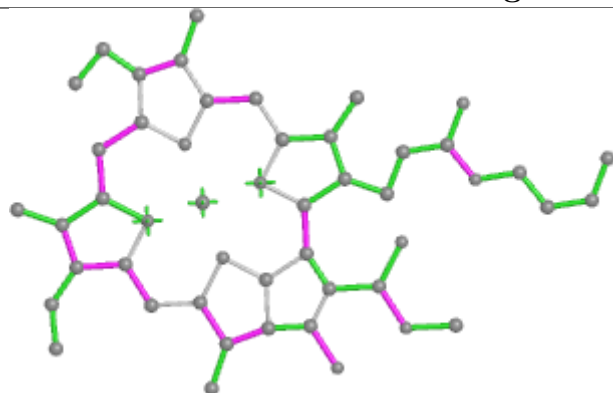




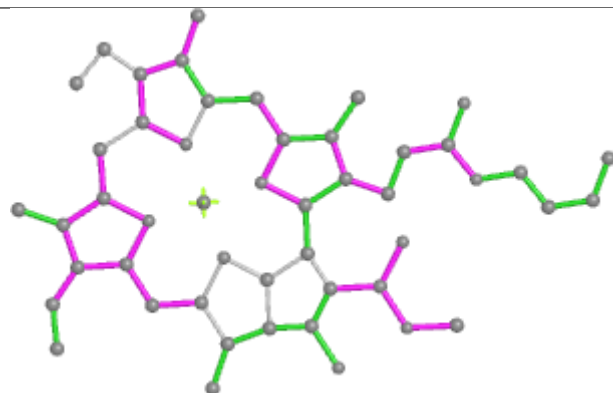




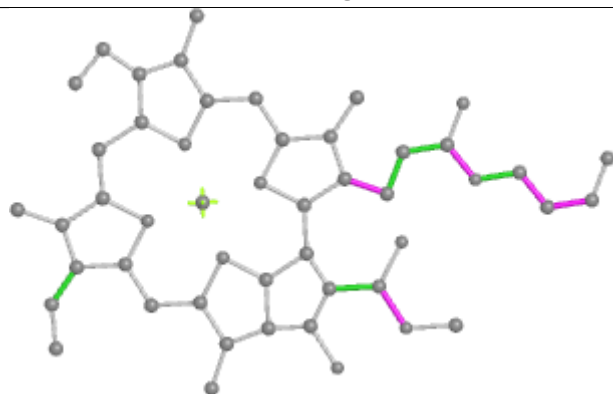
## Ligand CLA bA 856



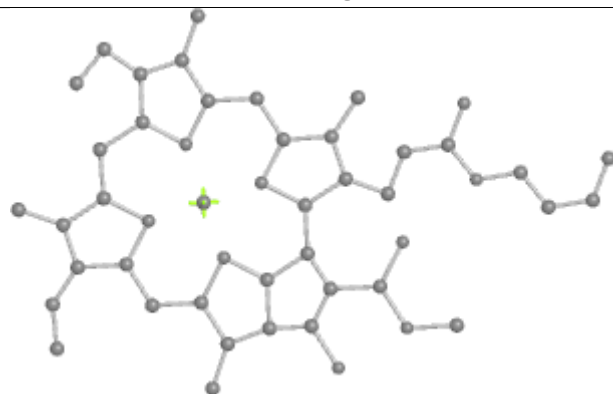
Bond lengths



Bond angles

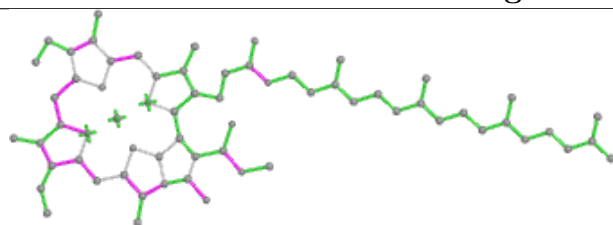


Torsions

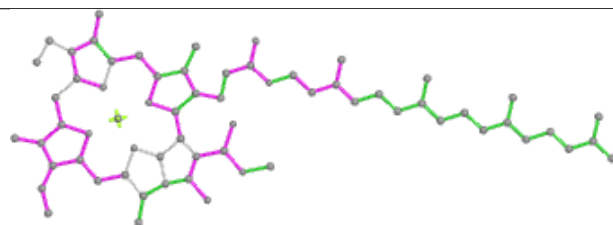


Rings

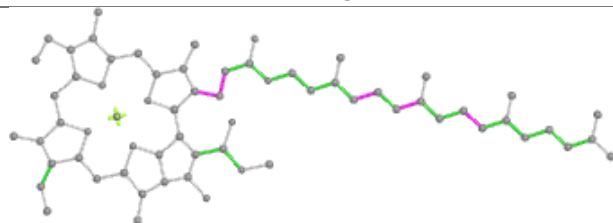
## Ligand CLA bB 801



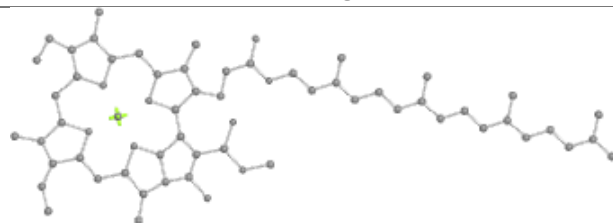
Bond lengths



Bond angles



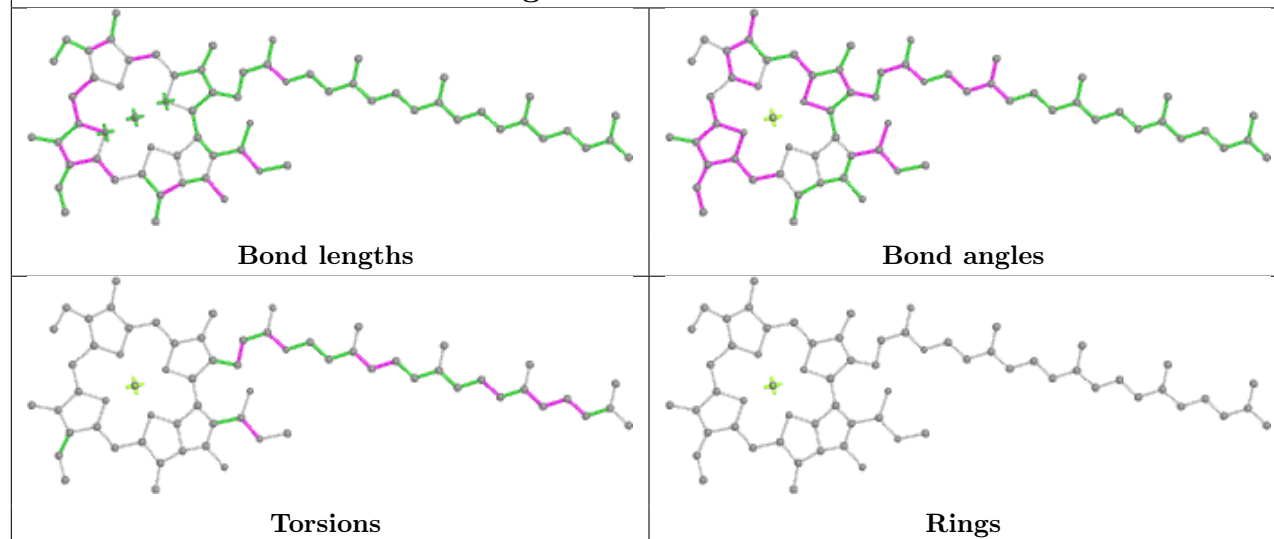
Torsions



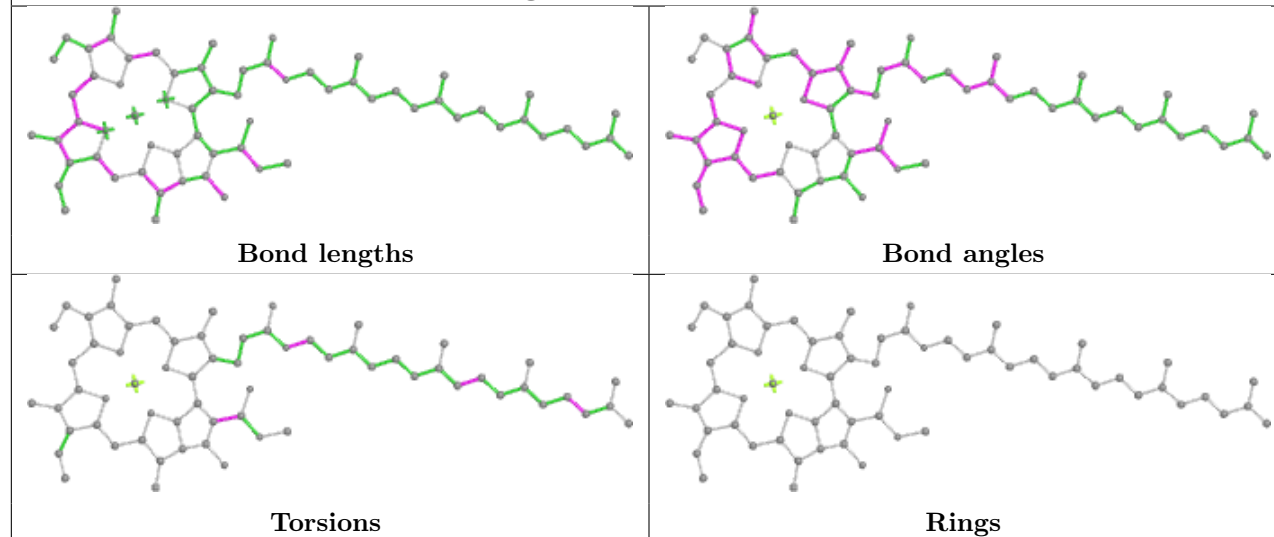
Rings



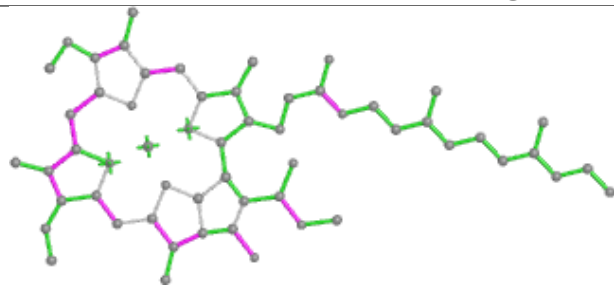
## Ligand CLA bB 802



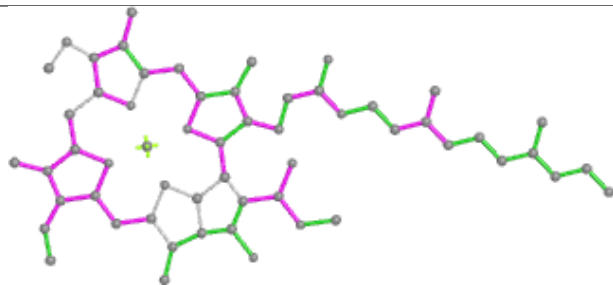
## Ligand CLA bB 803



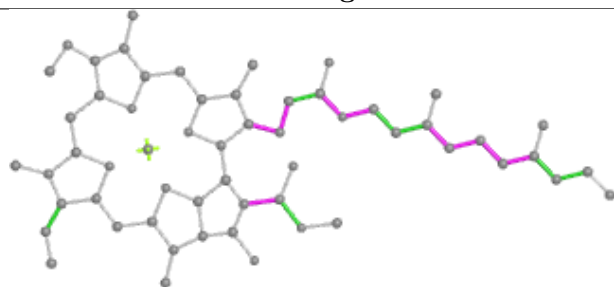
## Ligand CLA bB 804



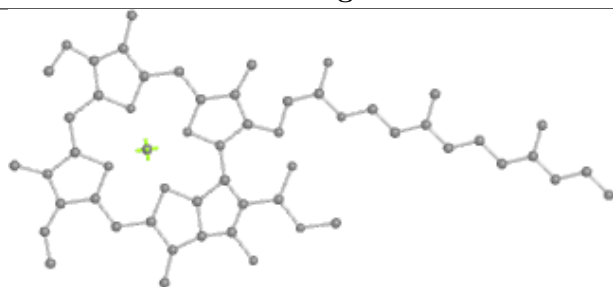
Bond lengths



Bond angles

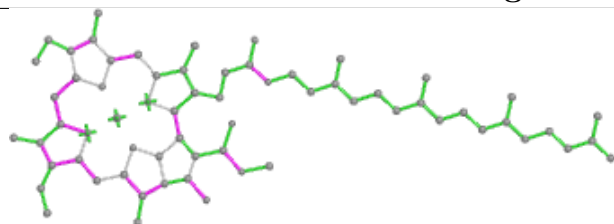


Torsions

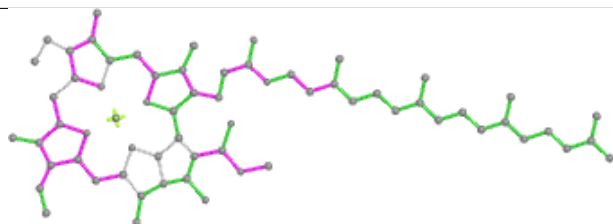


Rings

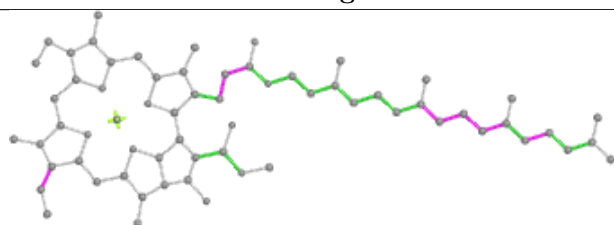
## Ligand CLA bB 805



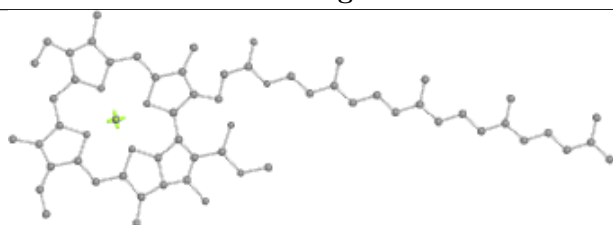
Bond lengths



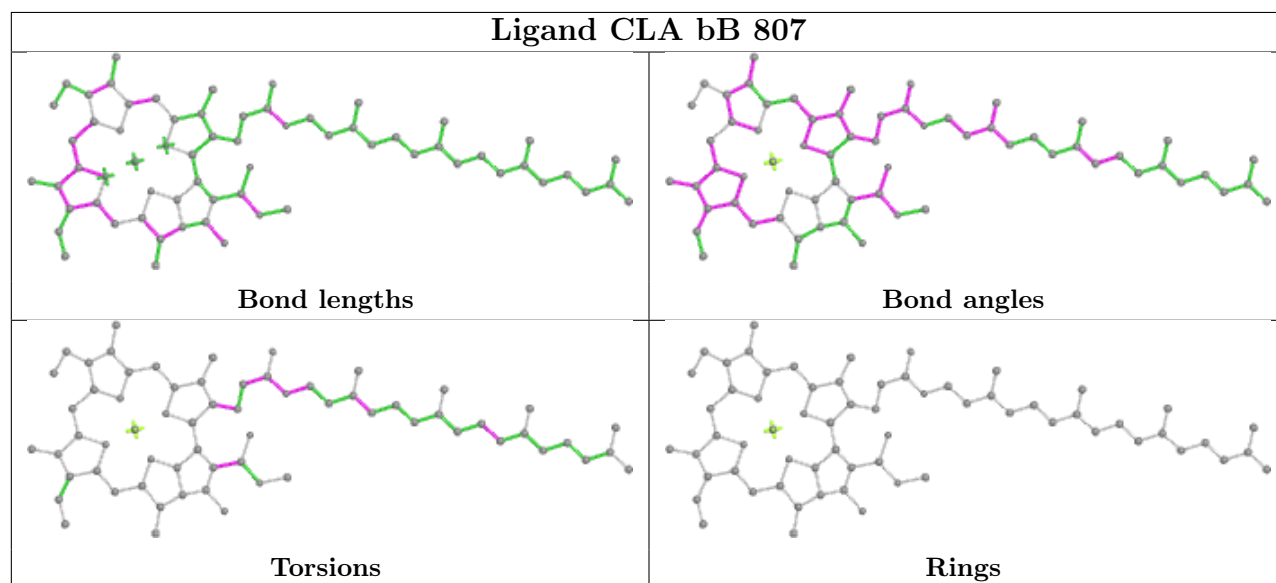
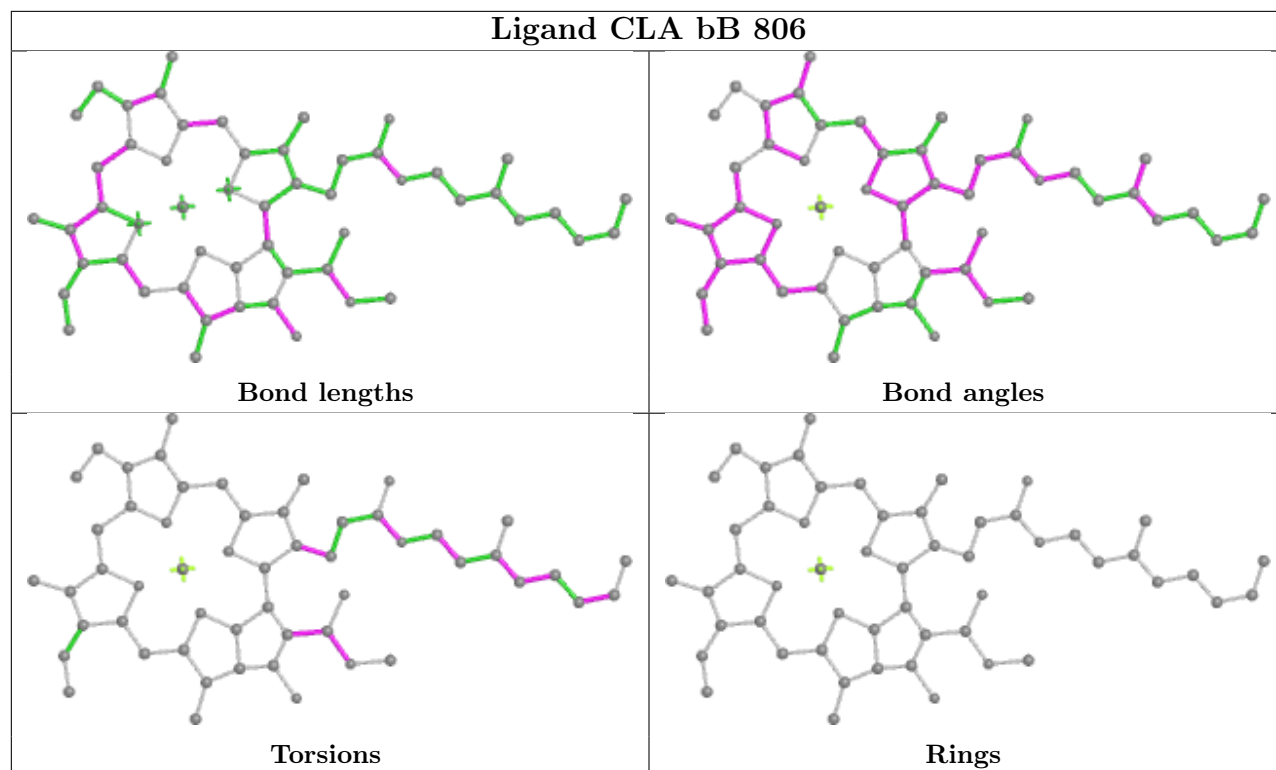
Bond angles



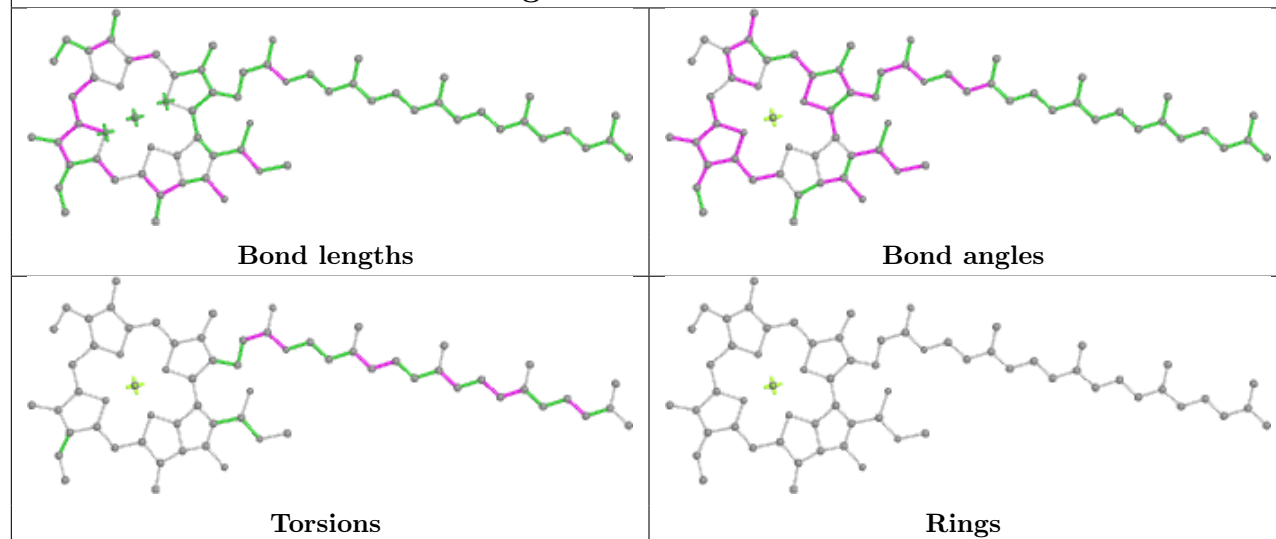
Torsions



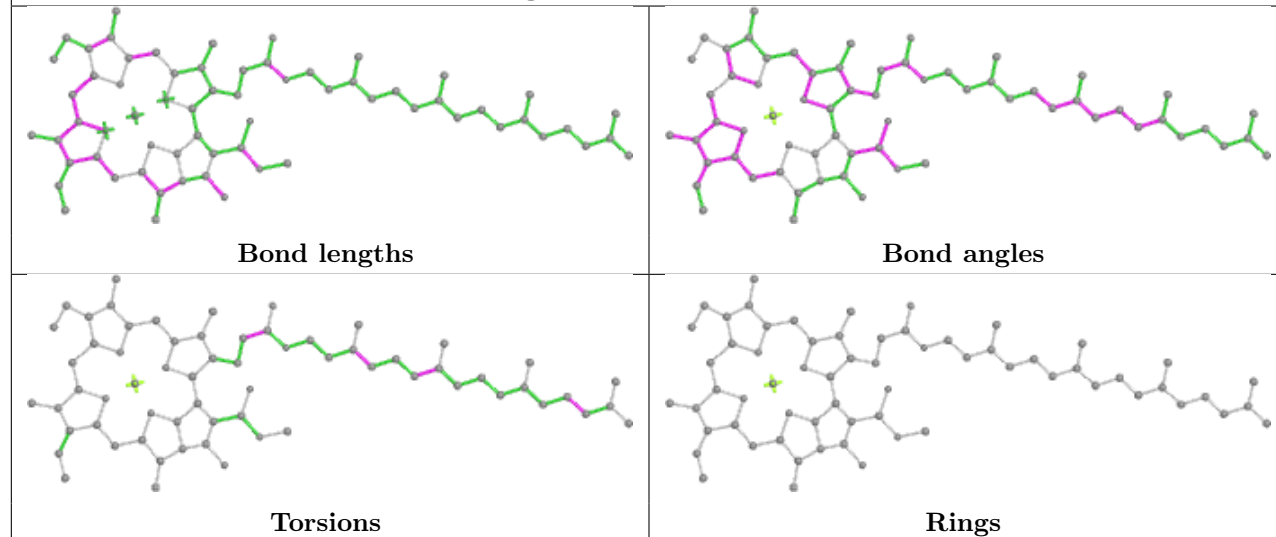
Rings

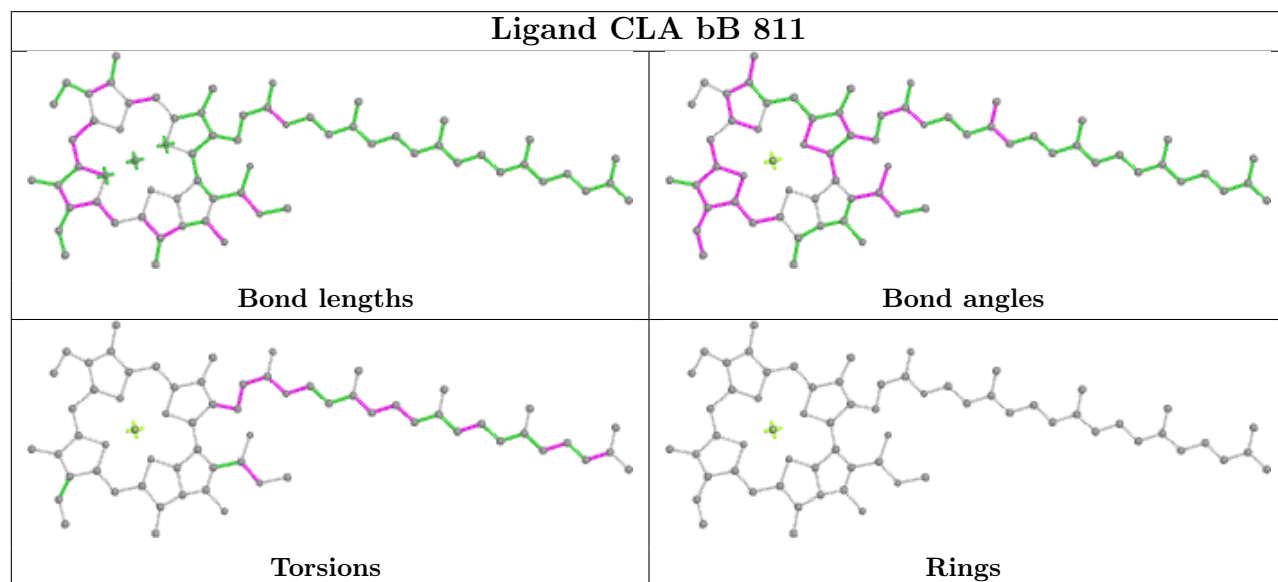
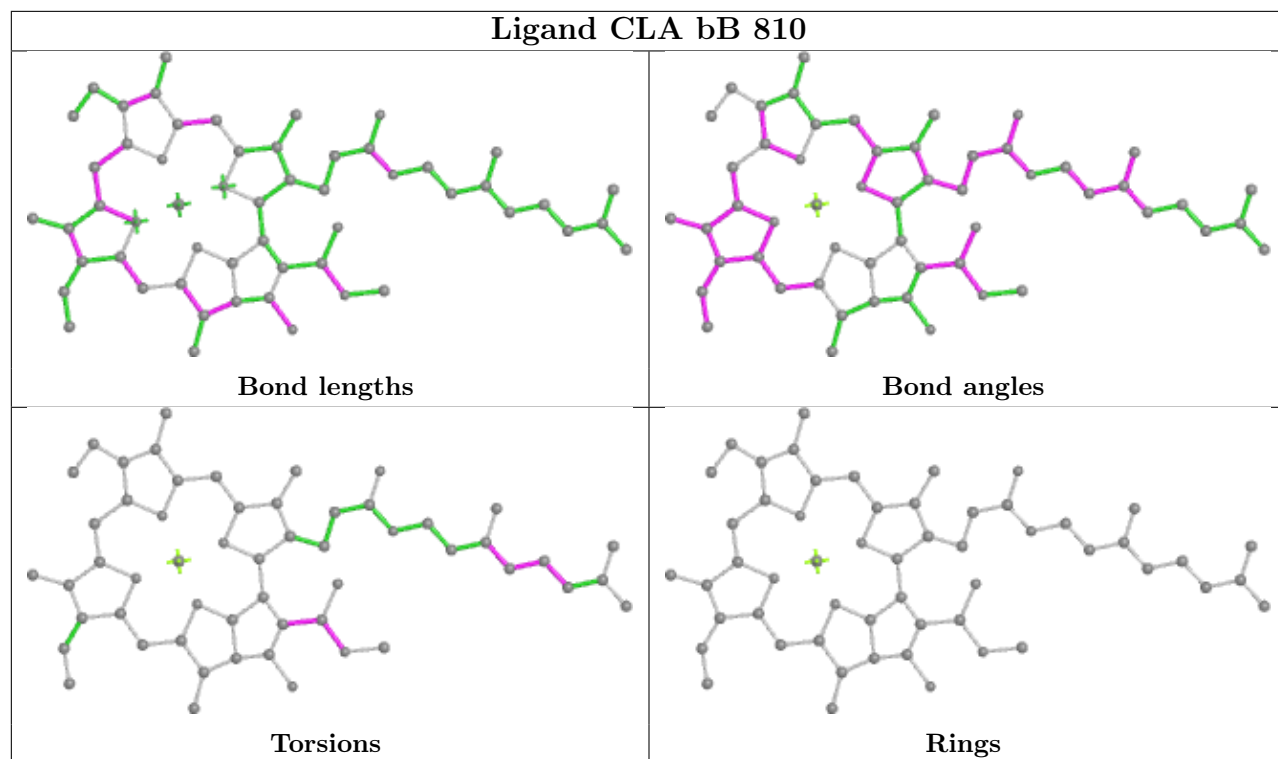


## Ligand CLA bB 808

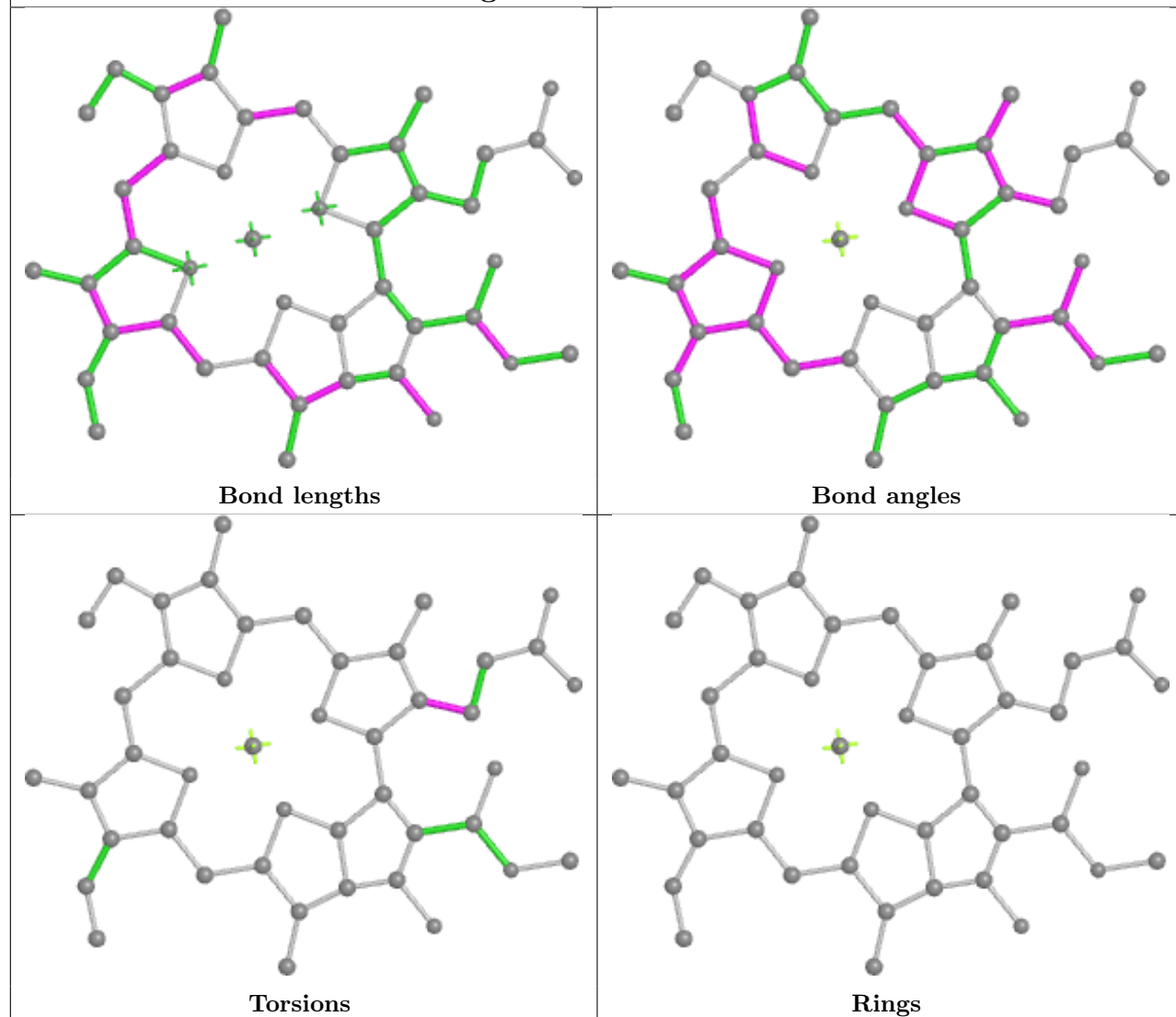


## Ligand CLA bB 809

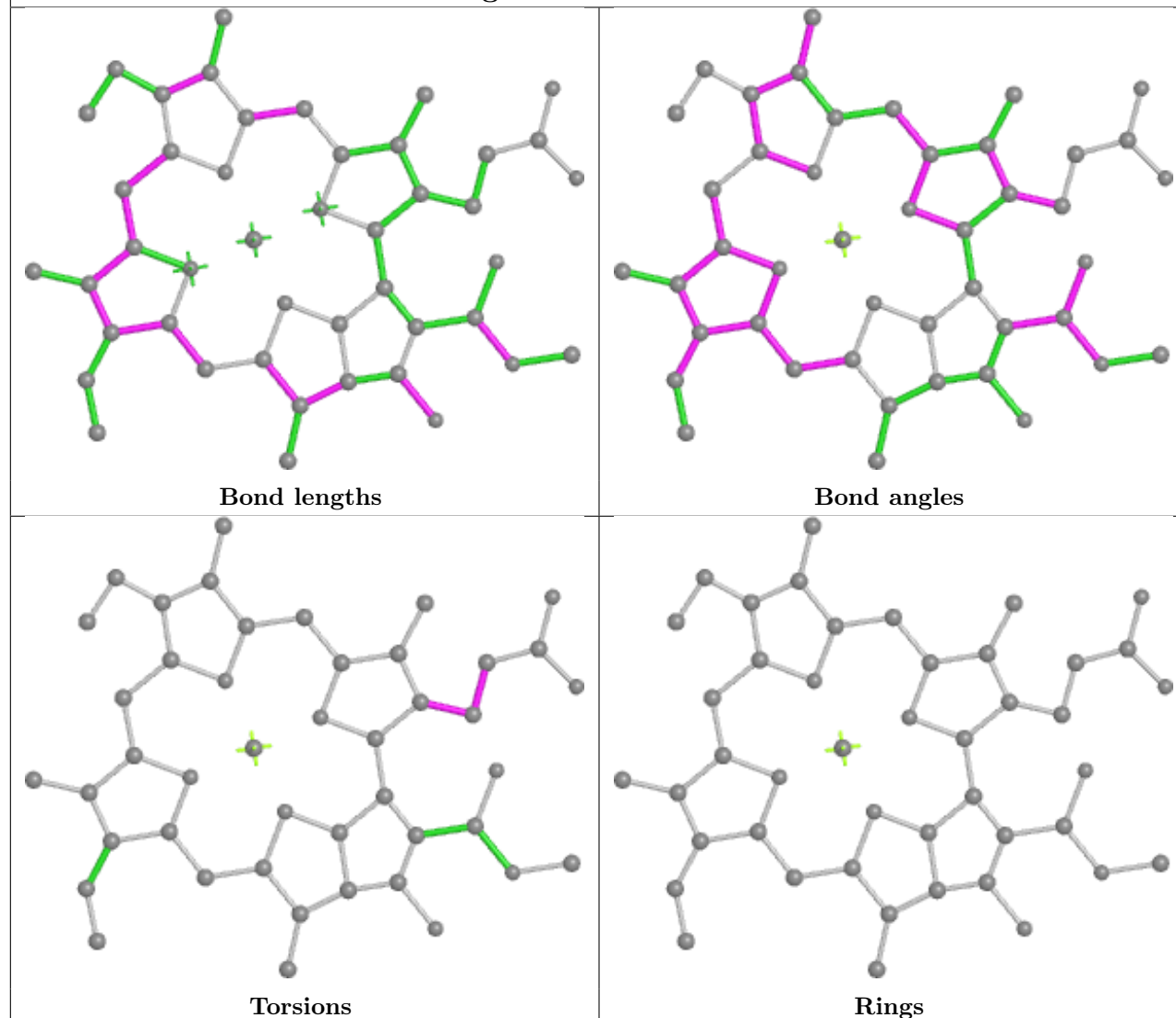




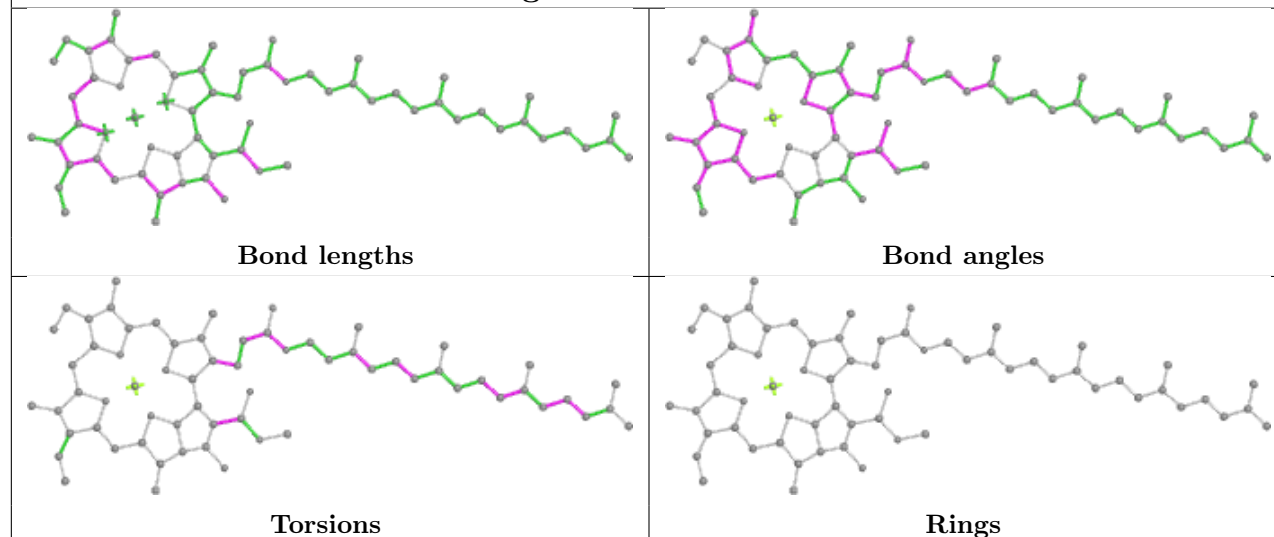
## Ligand CLA bB 812

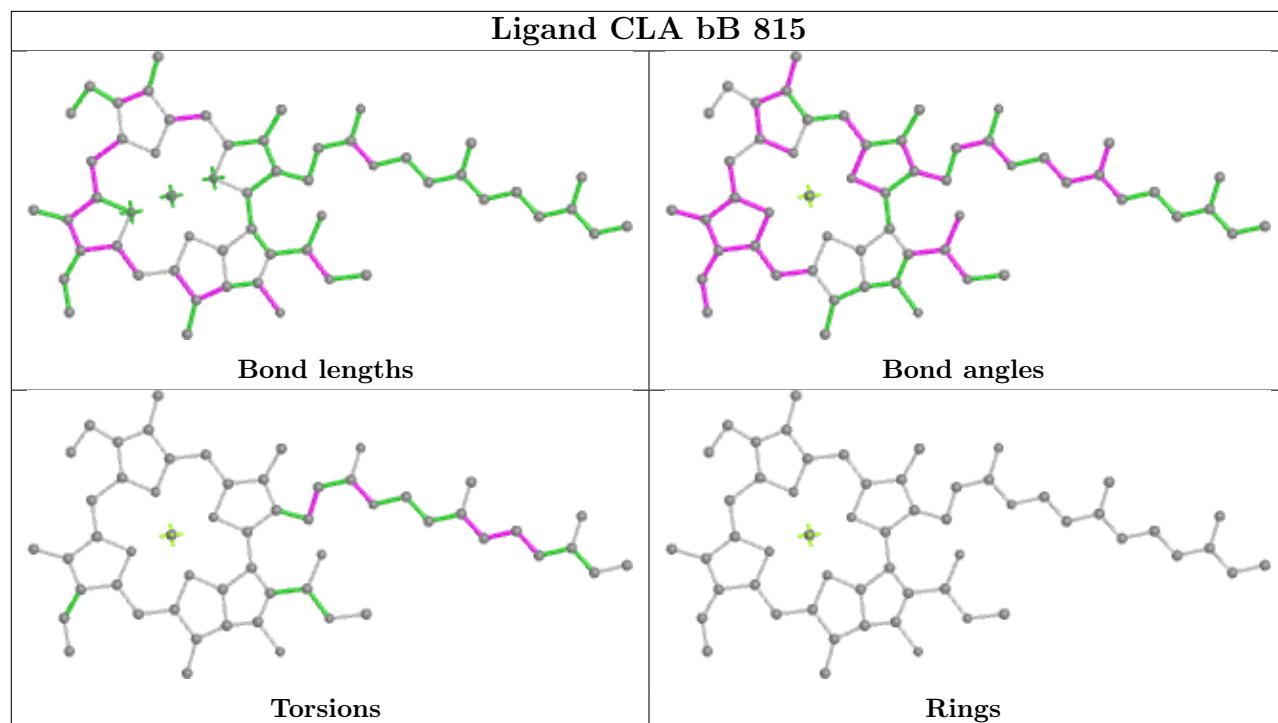


## Ligand CLA bB 813



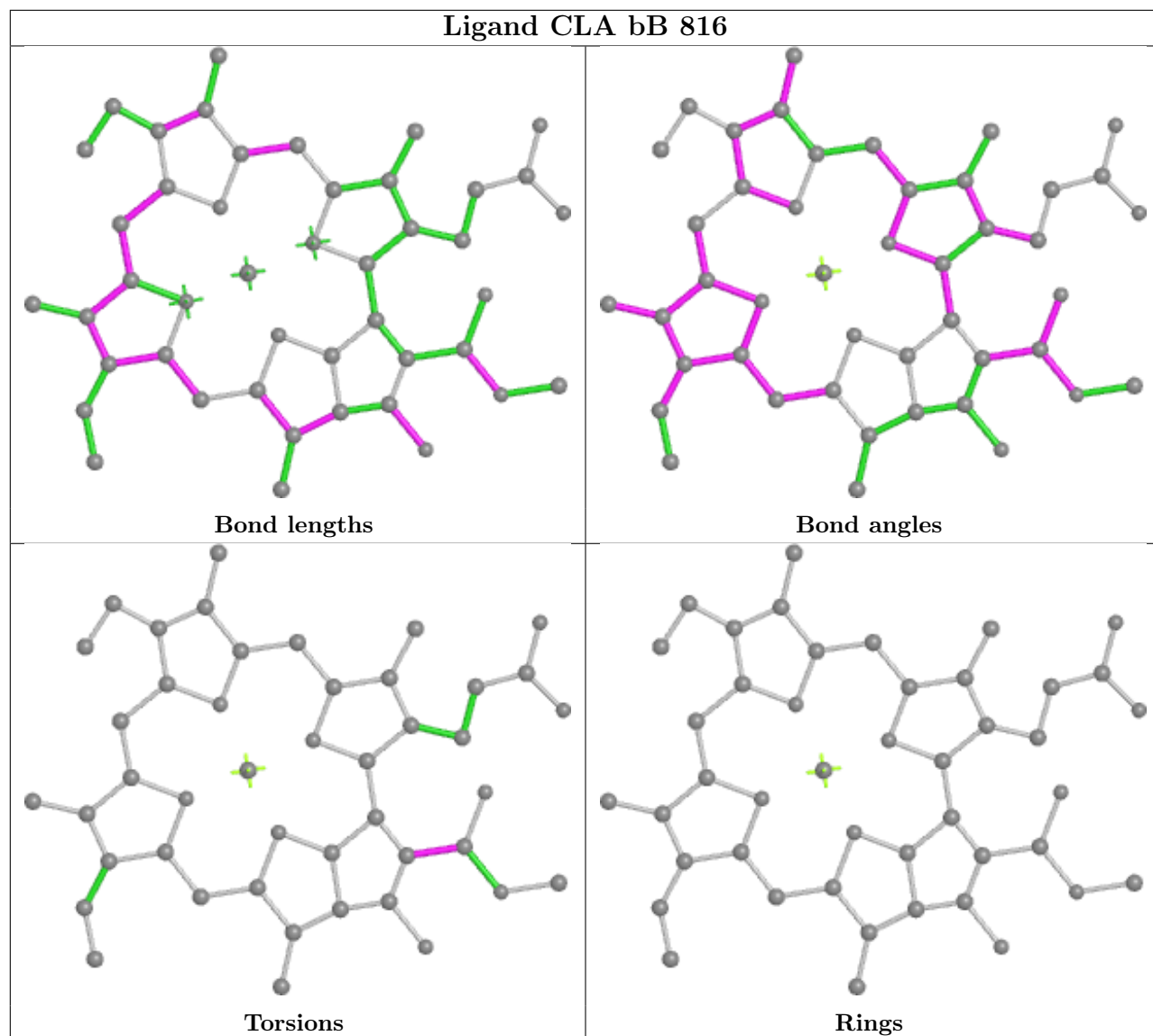
## Ligand CLA bB 814

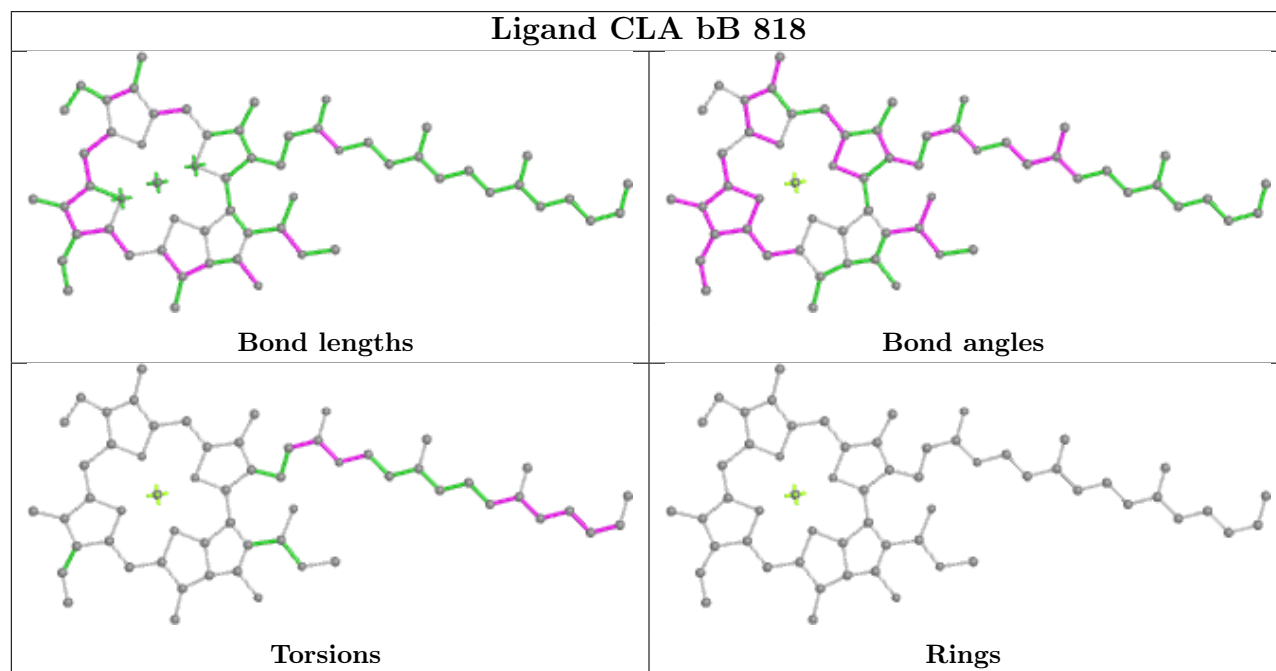
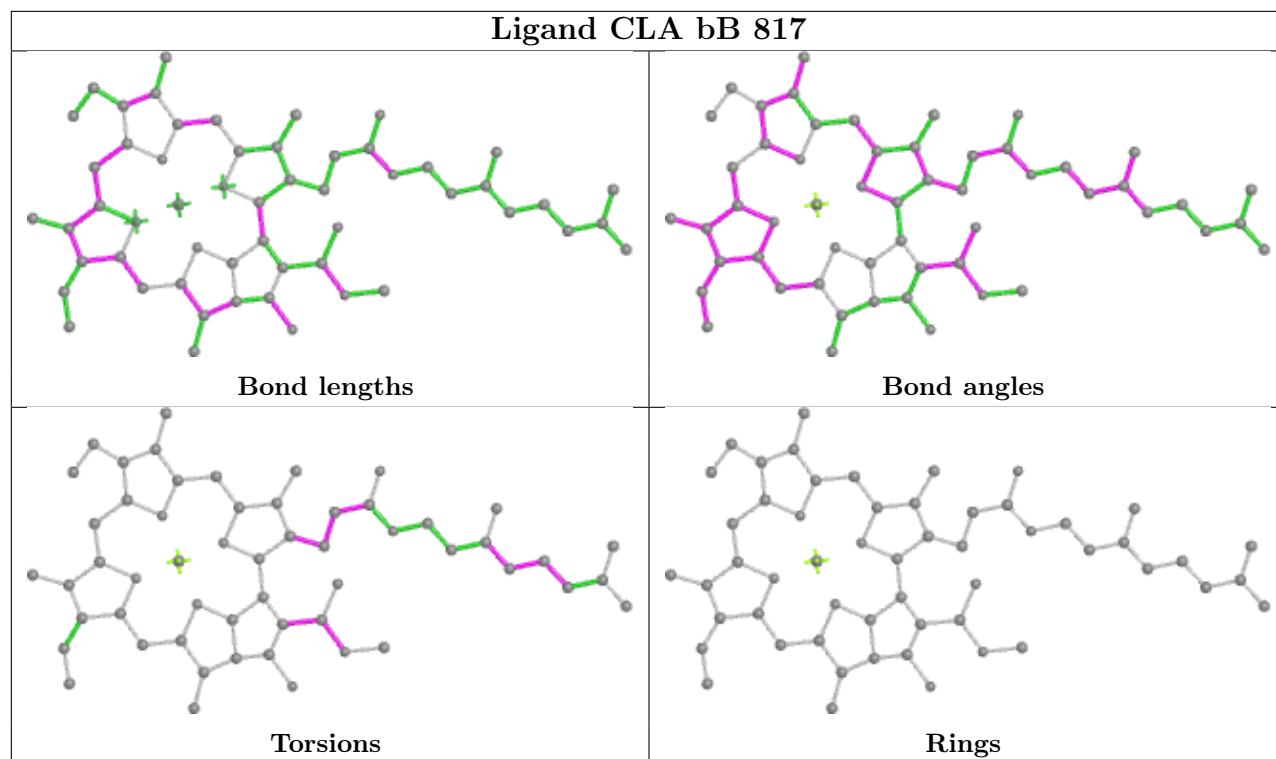




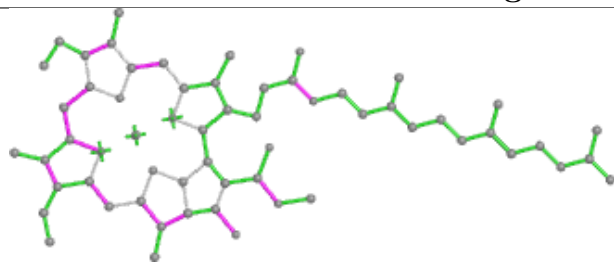


## Ligand CLA bB 816

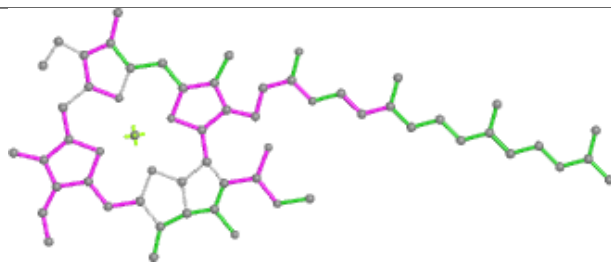




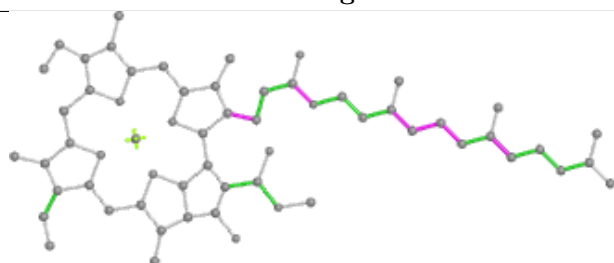
## Ligand CLA bB 819



Bond lengths



Bond angles

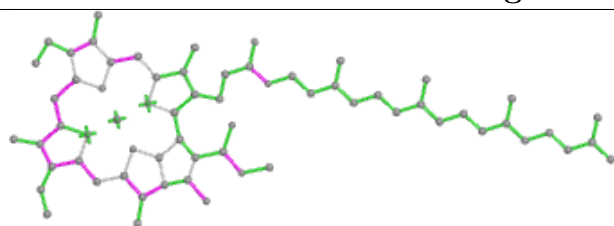


Torsions

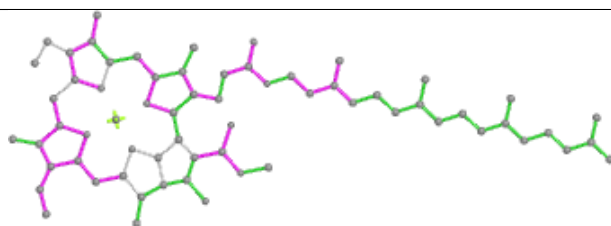


Rings

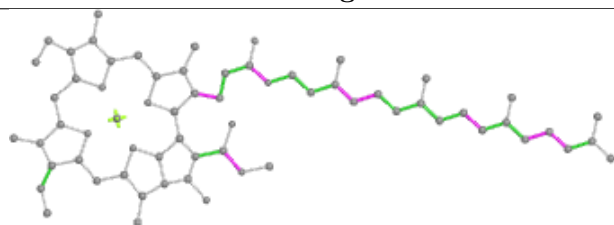
## Ligand CLA bB 820



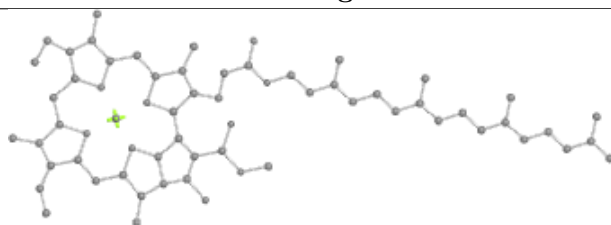
Bond lengths



Bond angles

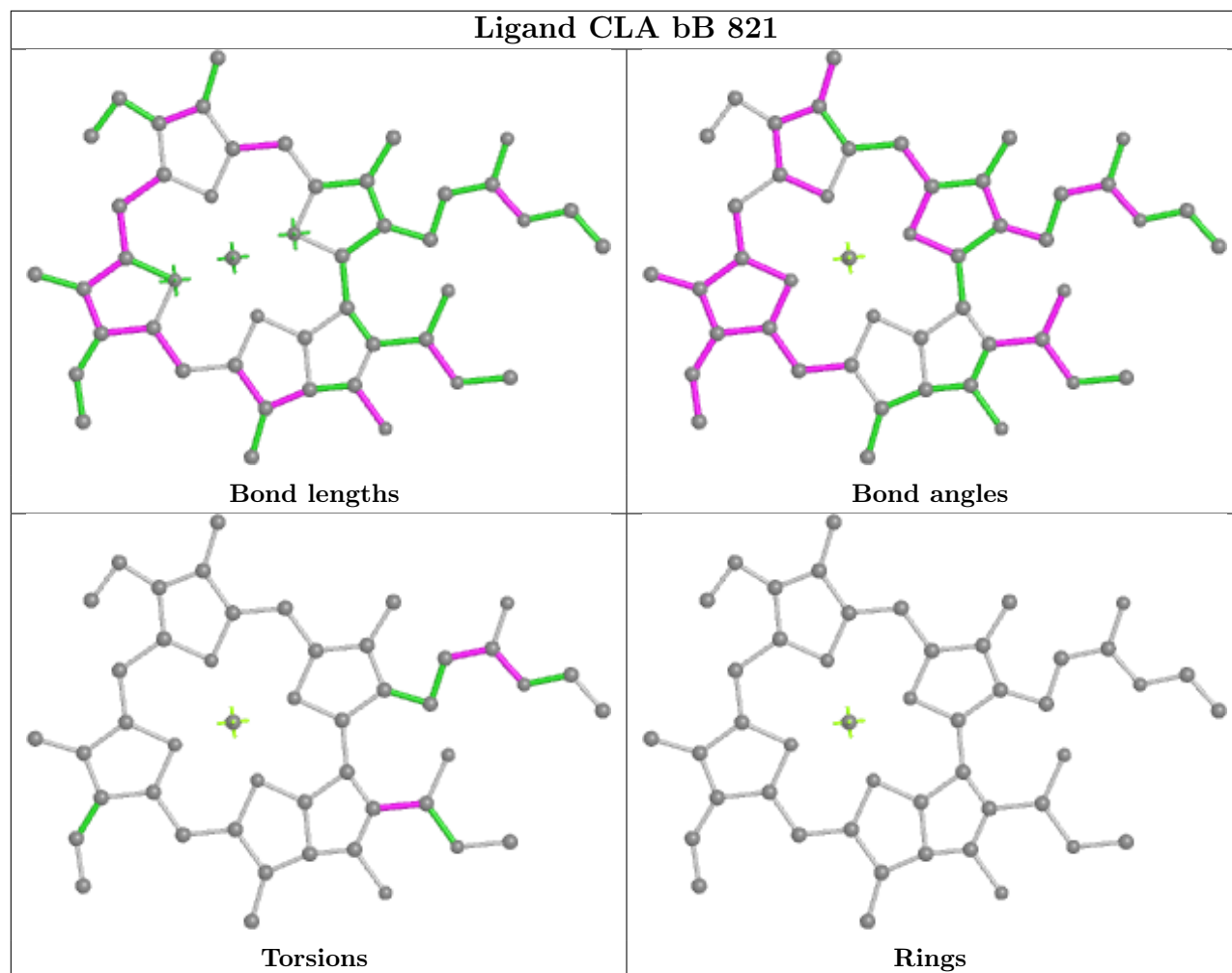


Torsions

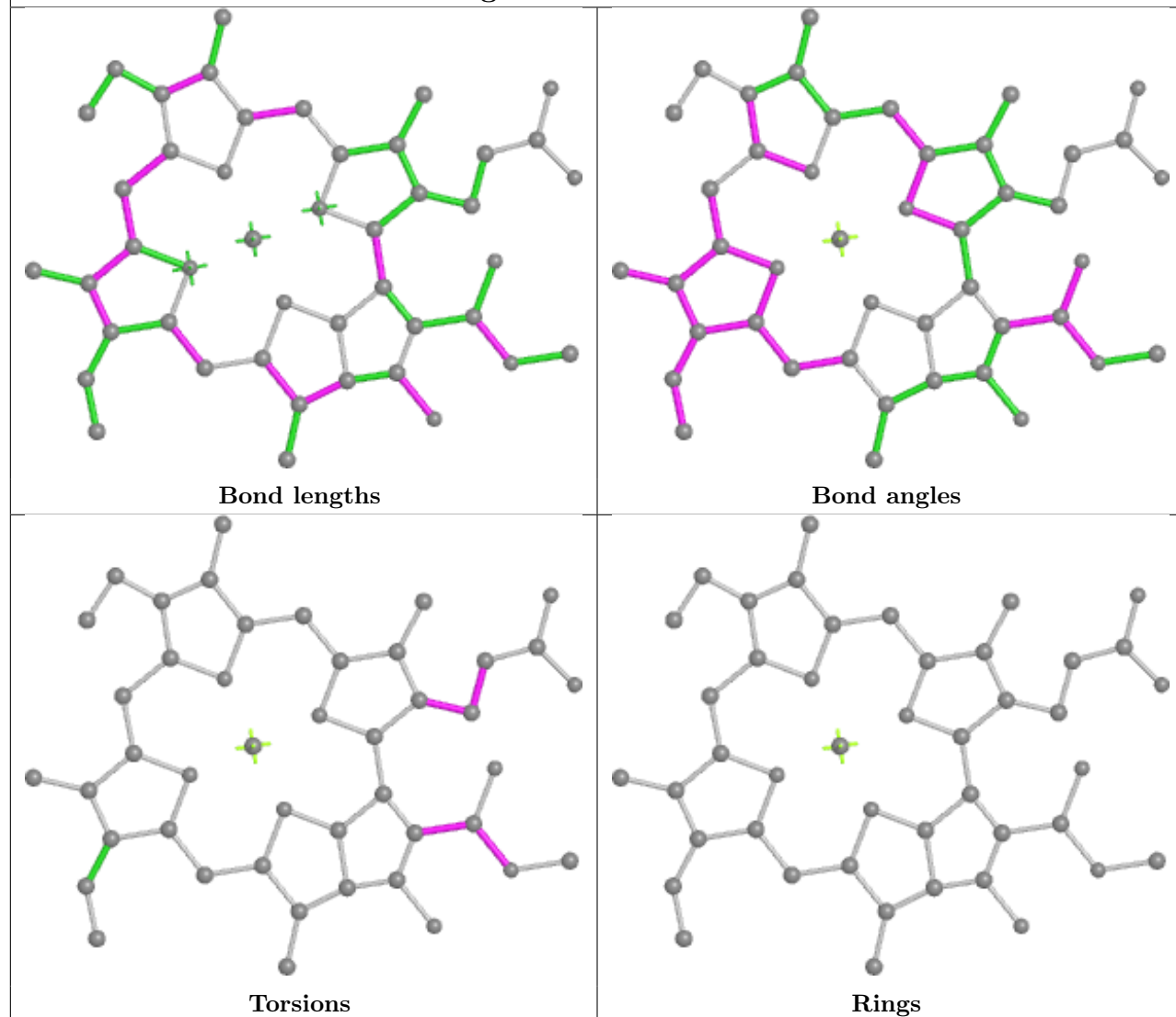


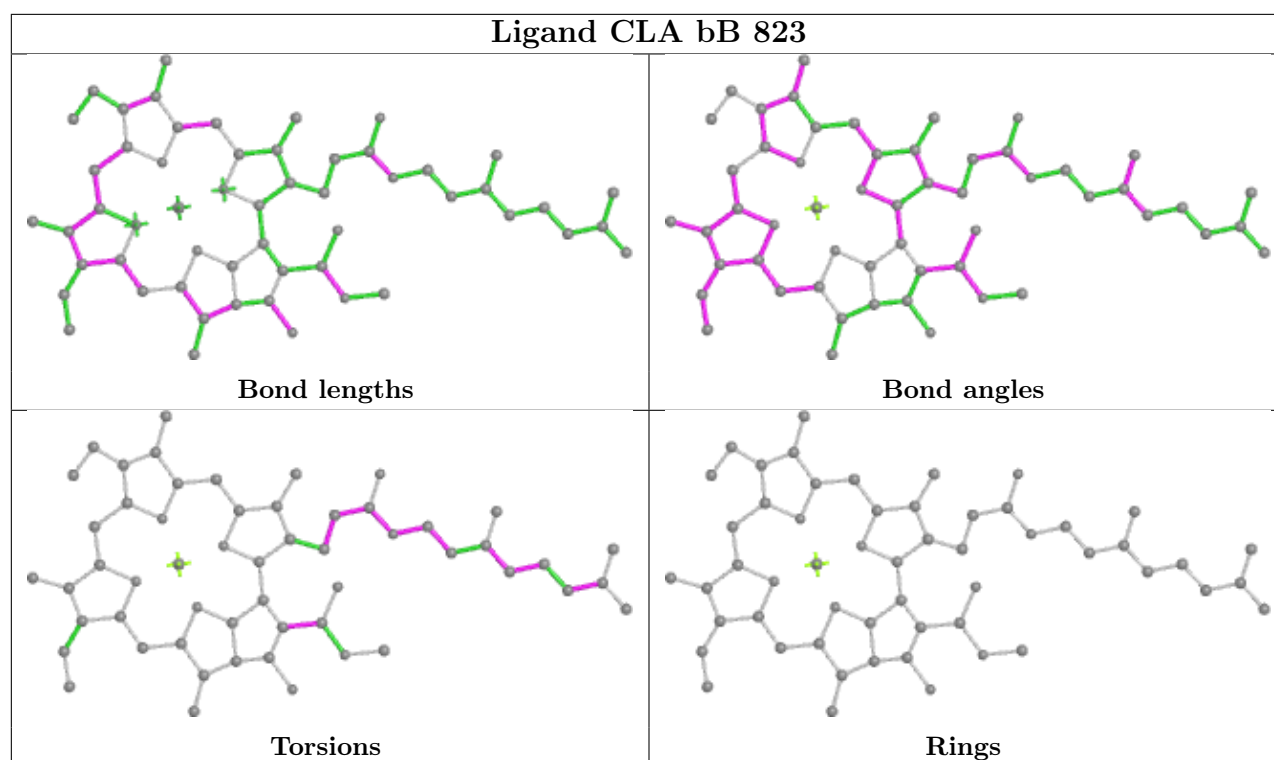
Rings

## Ligand CLA bB 821

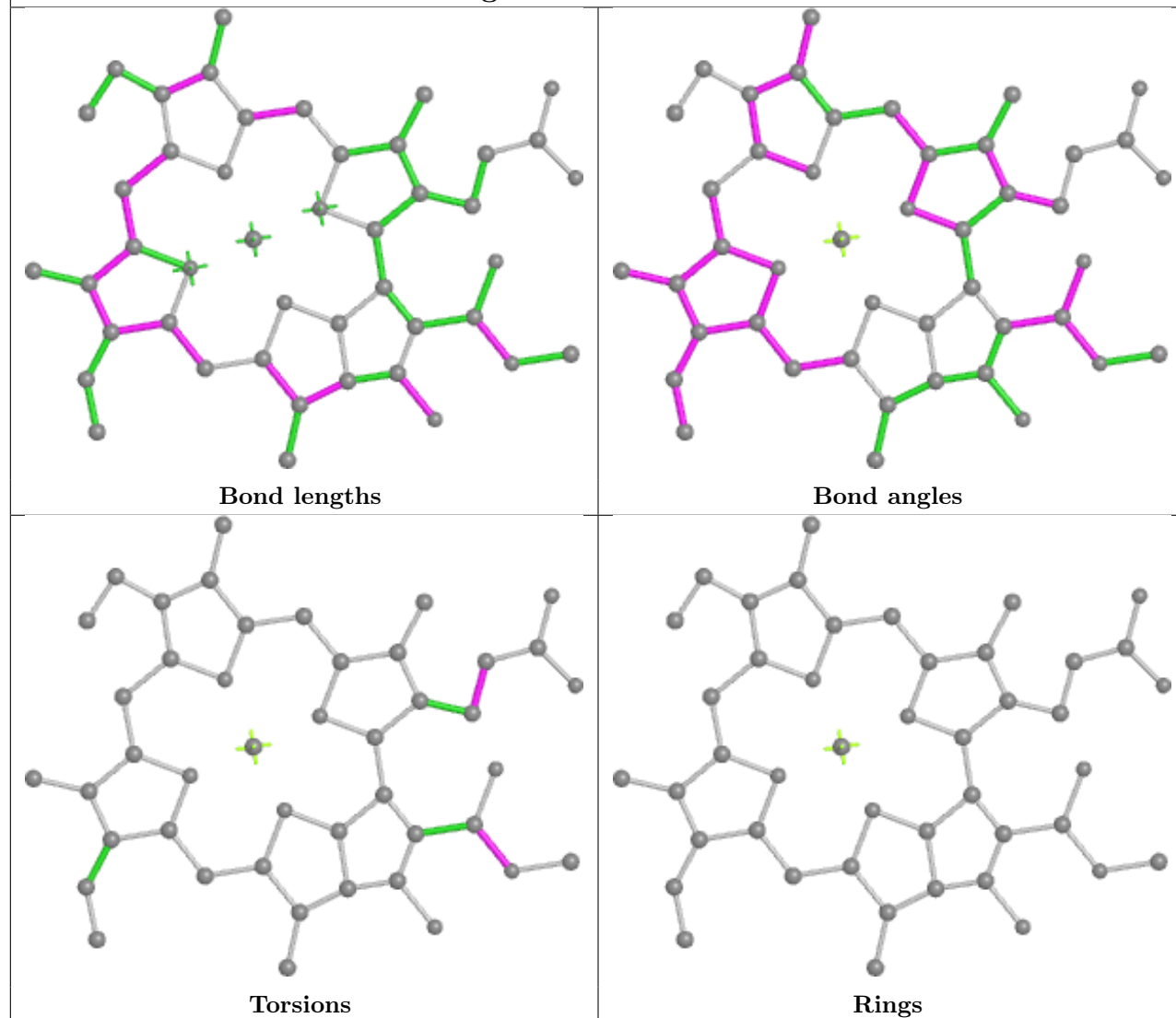


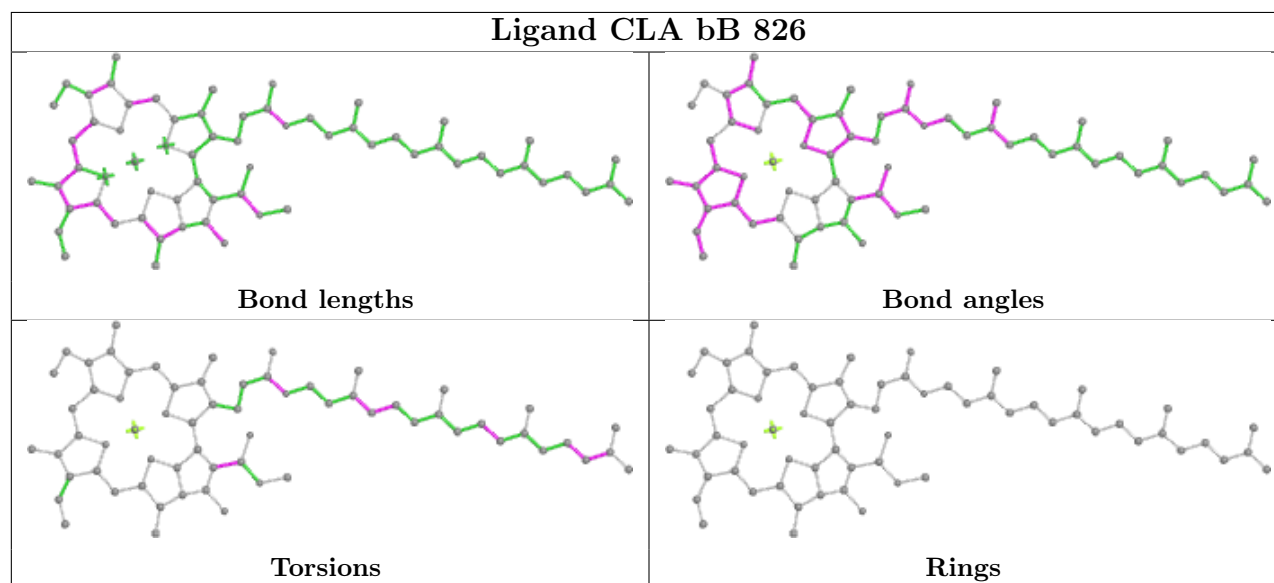
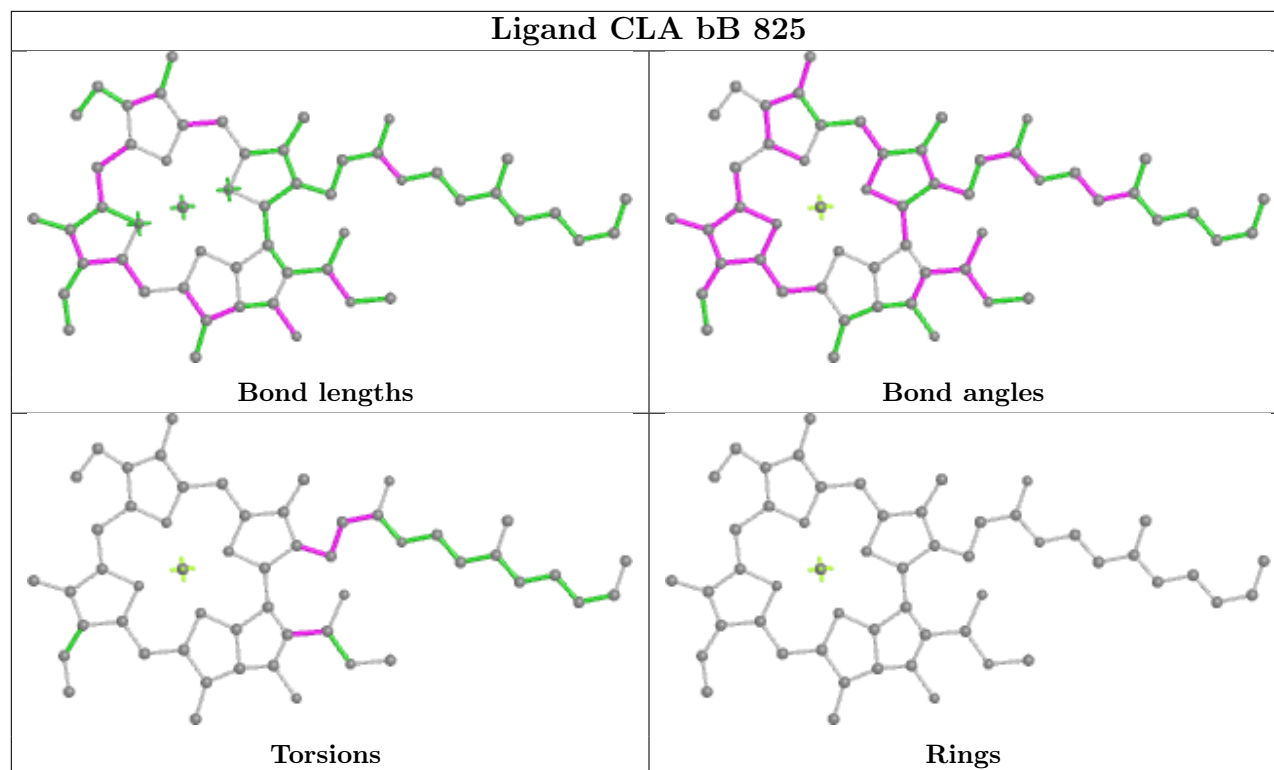
## Ligand CLA bB 822





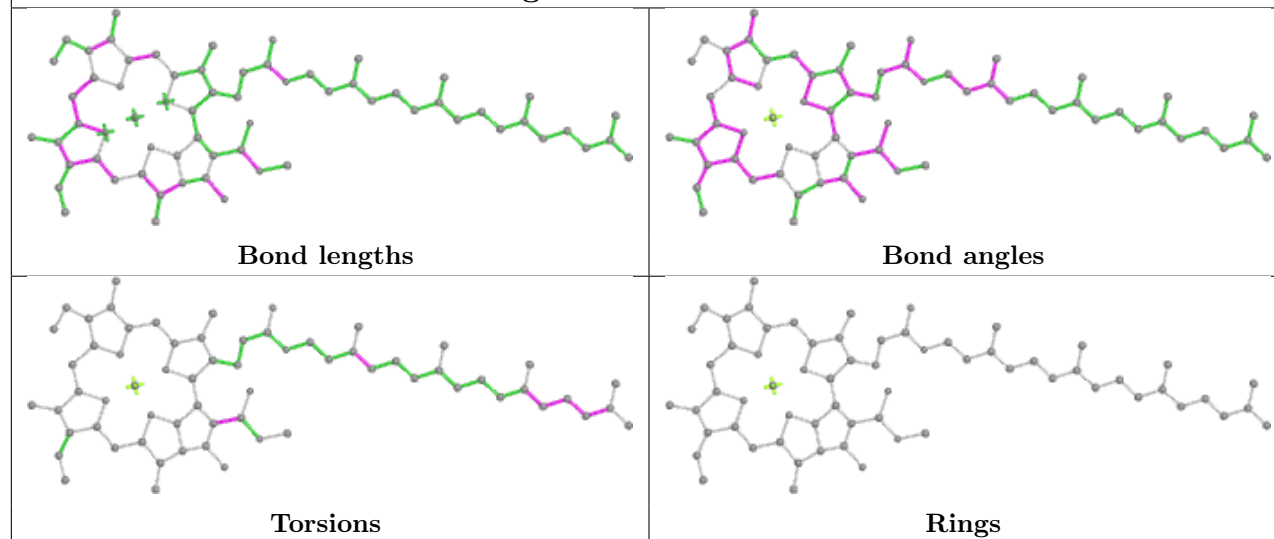
## Ligand CLA bB 824



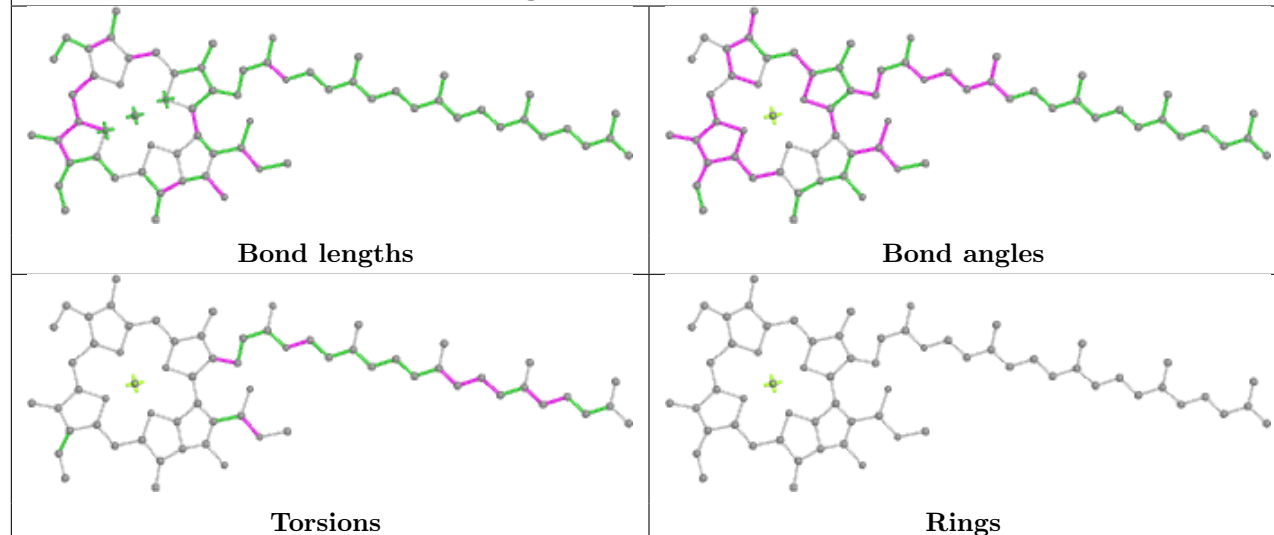




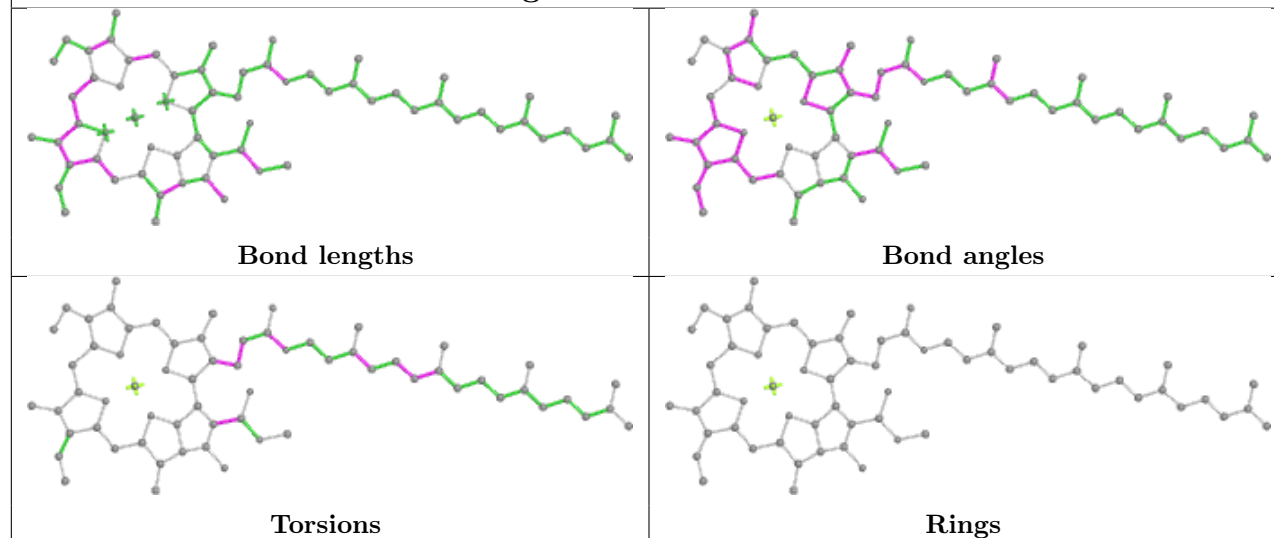
## Ligand CLA bB 827



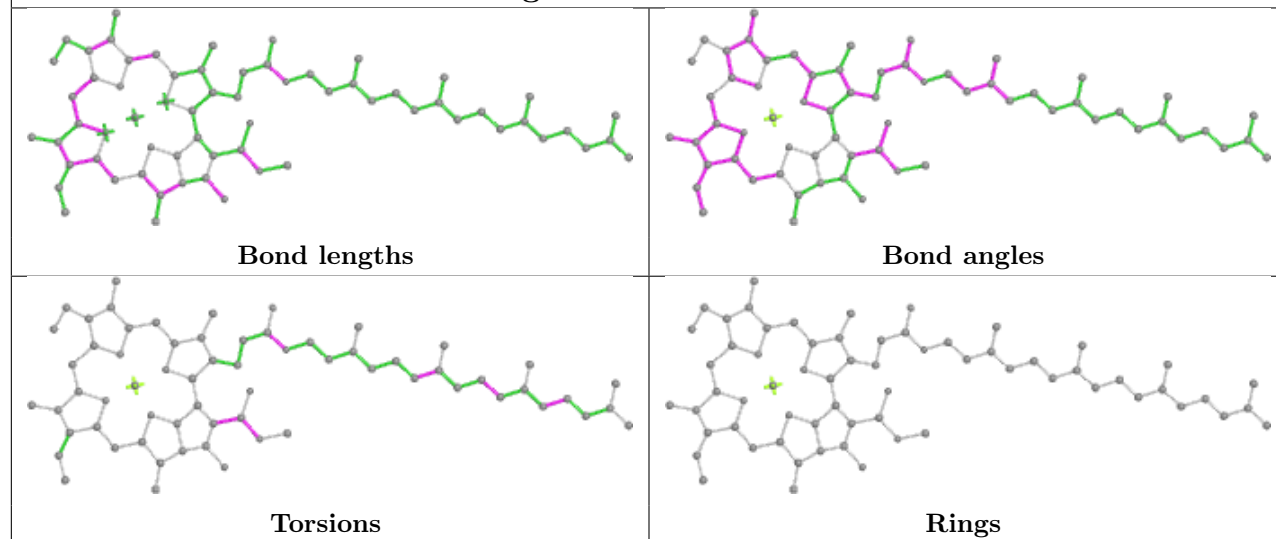
## Ligand CLA bB 828



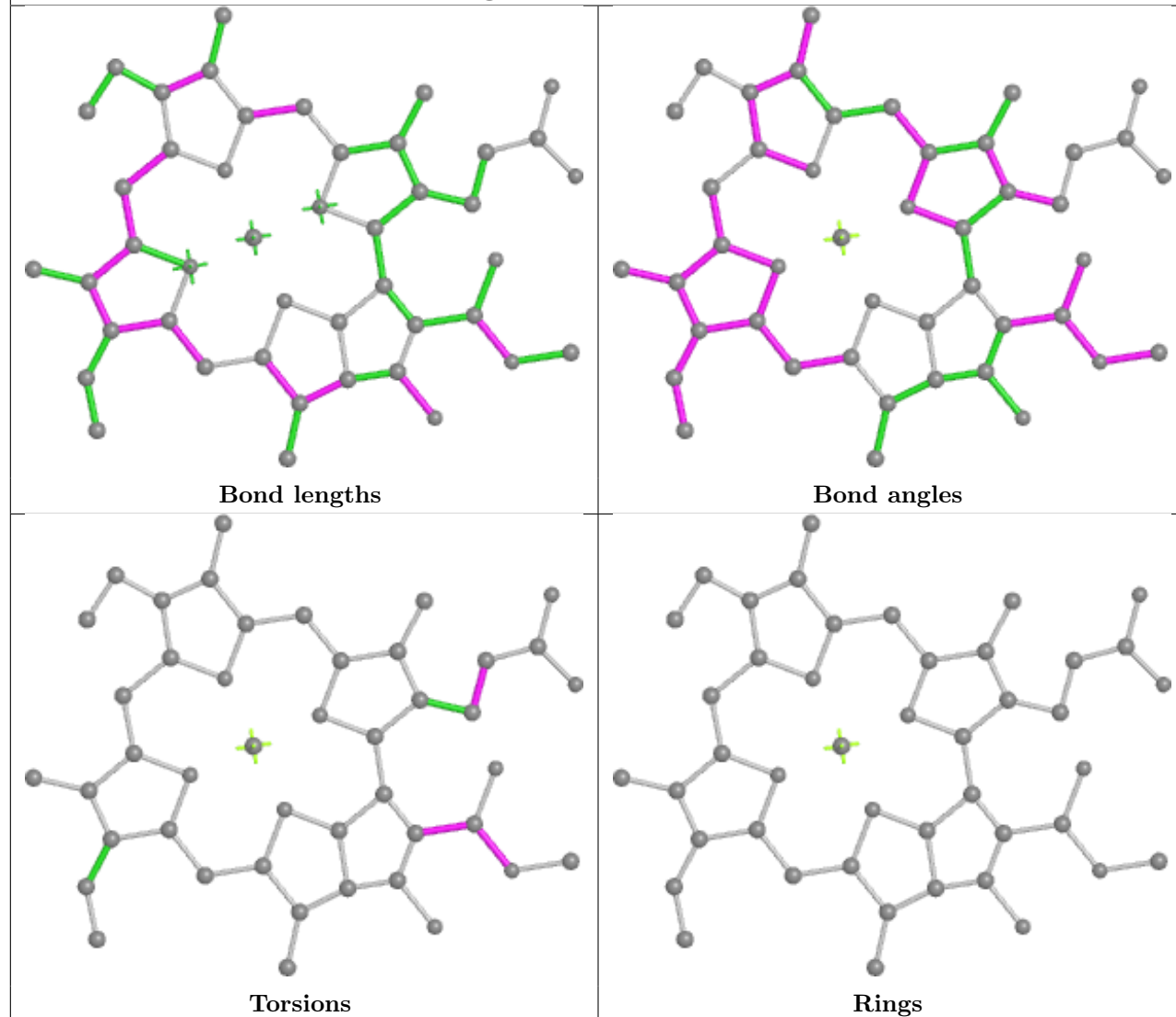
## Ligand CLA bB 829



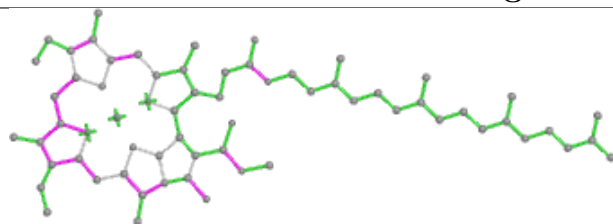
## Ligand CLA bB 830



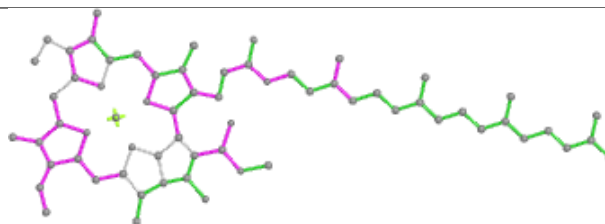
## Ligand CLA bB 831



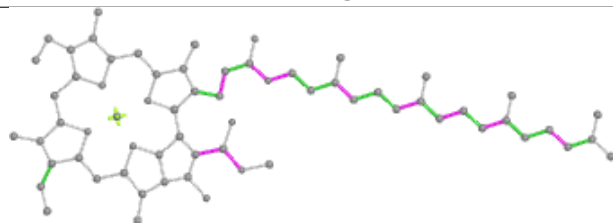
## Ligand CLA bB 832



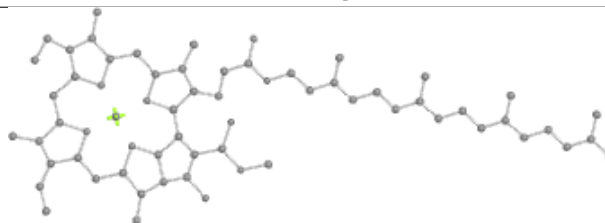
Bond lengths



Bond angles

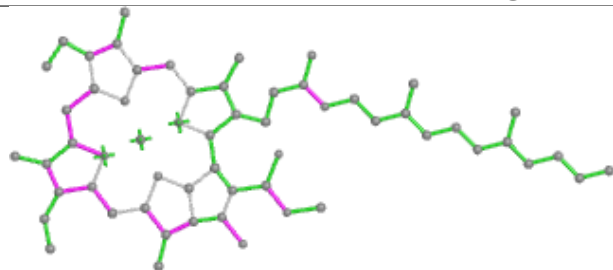


Torsions

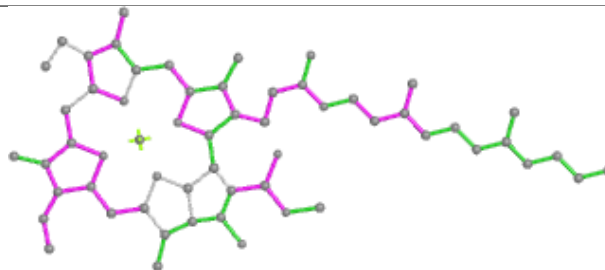


Rings

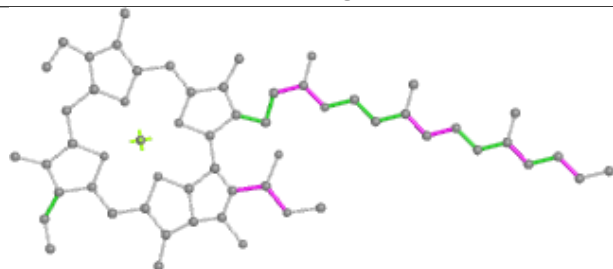
## Ligand CLA bB 833



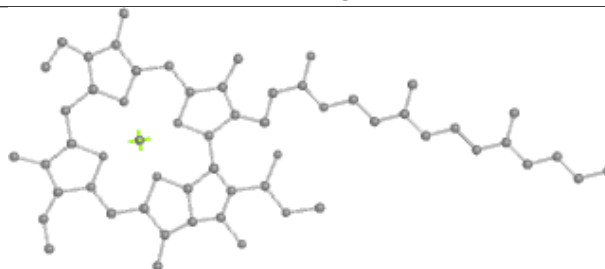
Bond lengths



Bond angles

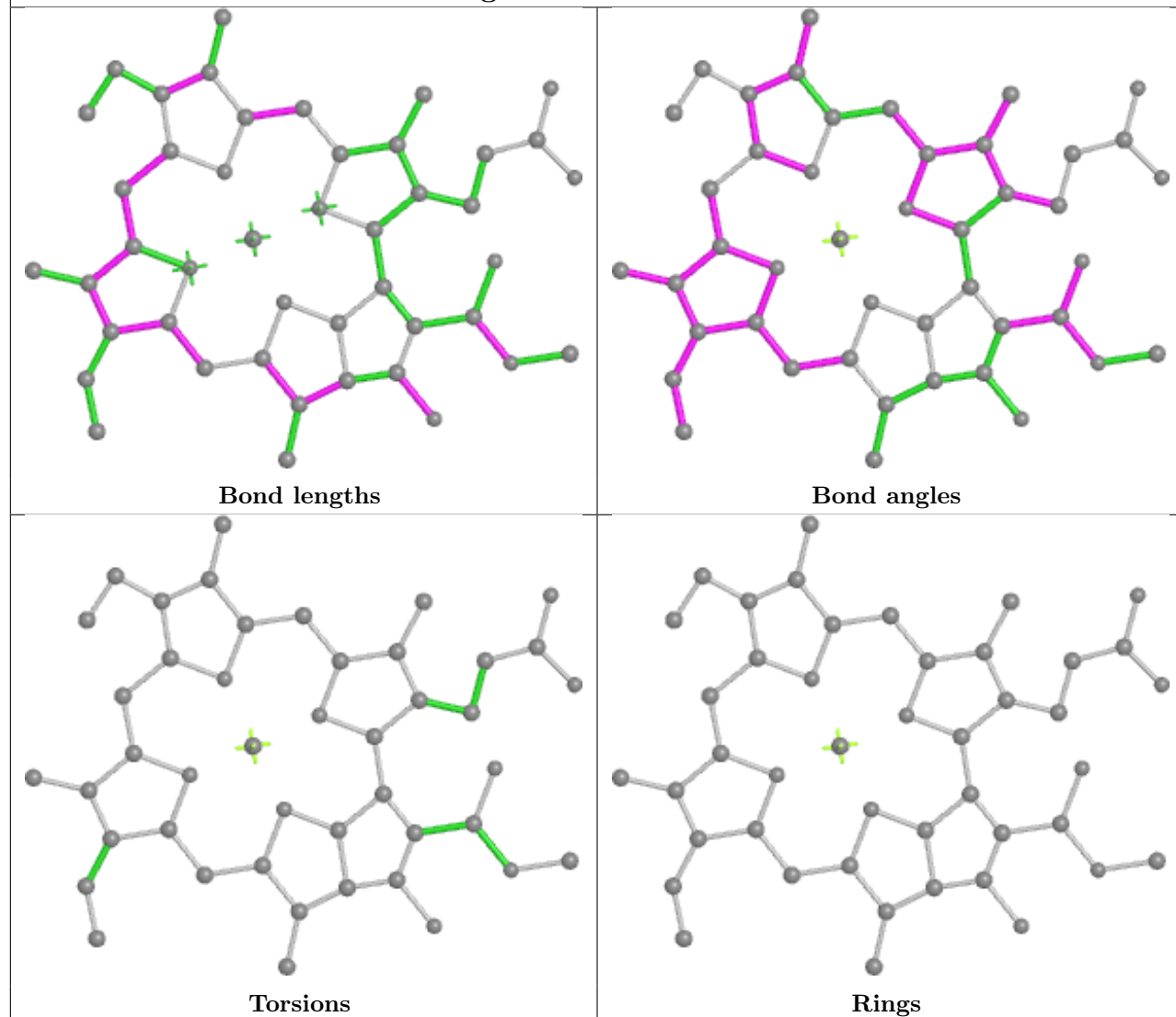


Torsions

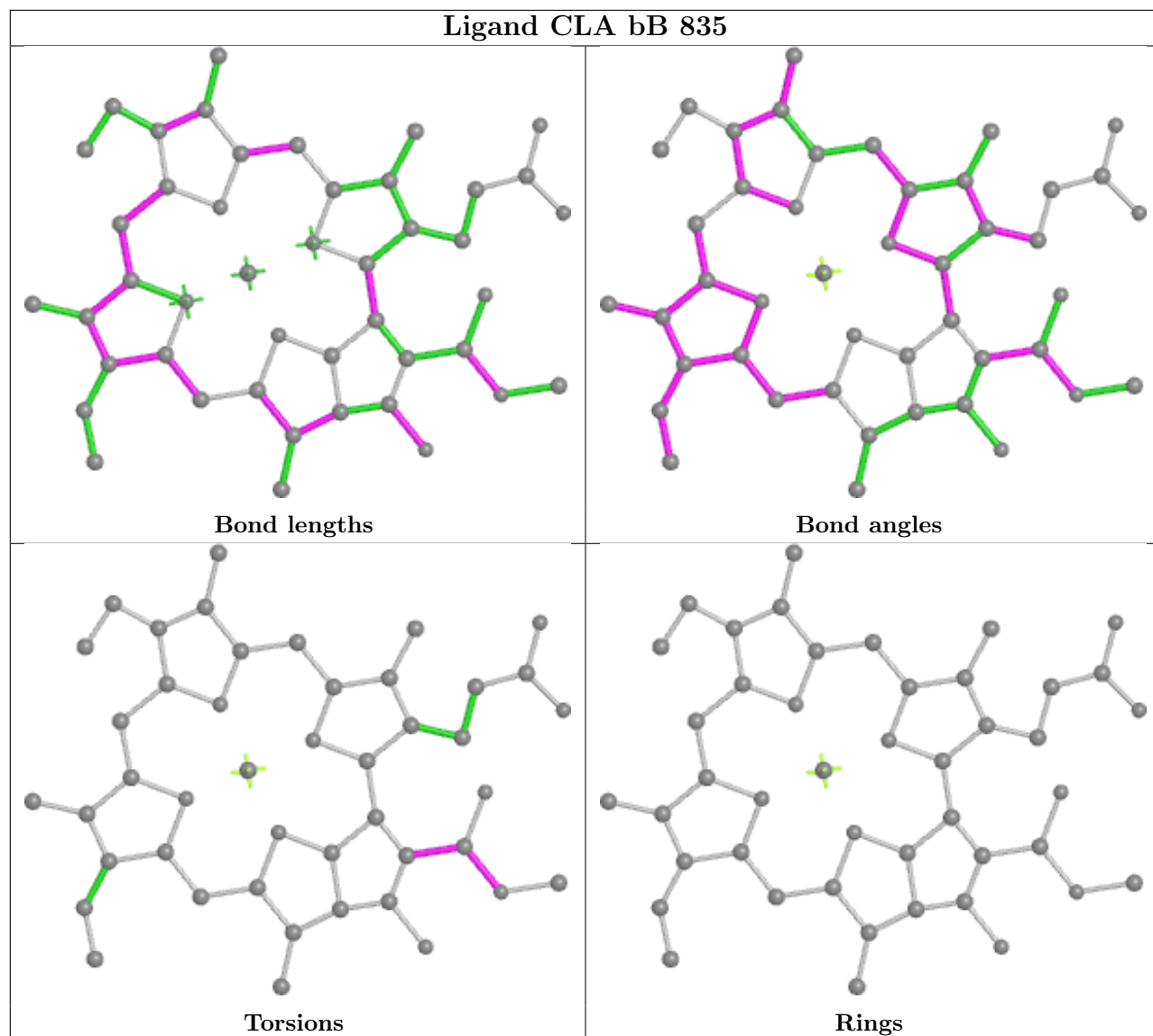


Rings

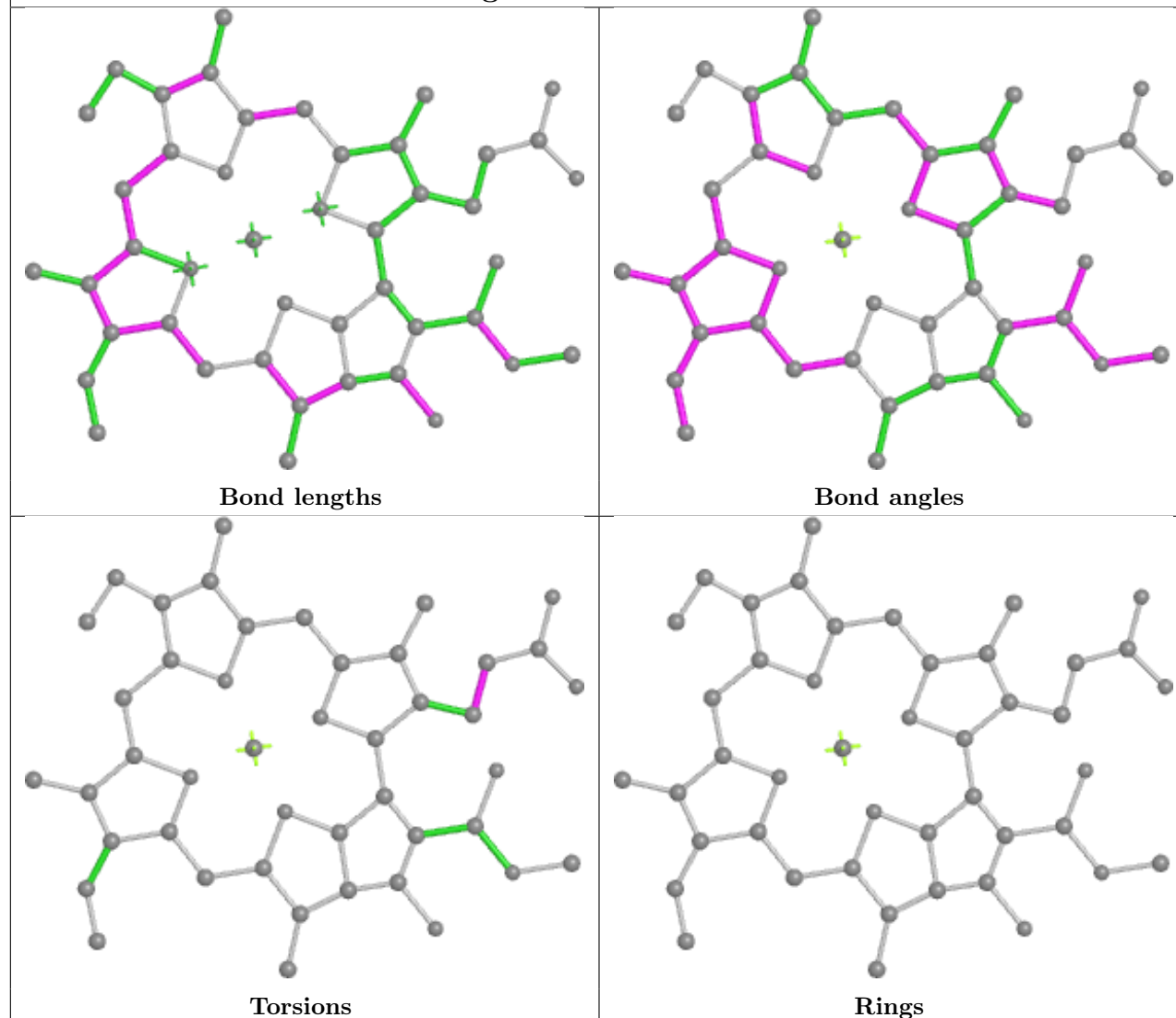
## Ligand CLA bB 834



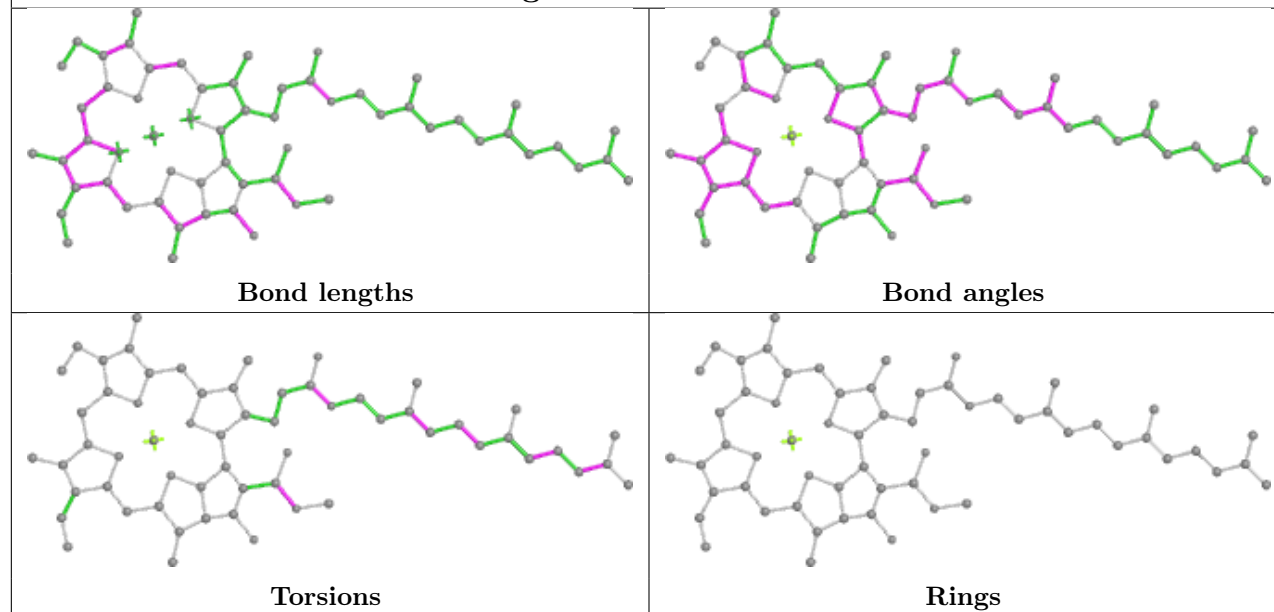
## Ligand CLA bB 835



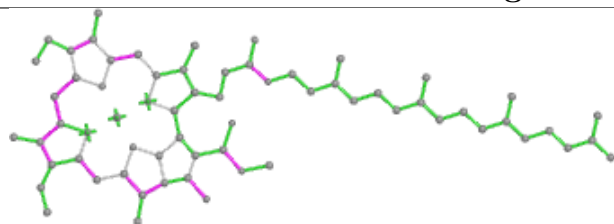
## Ligand CLA bB 836



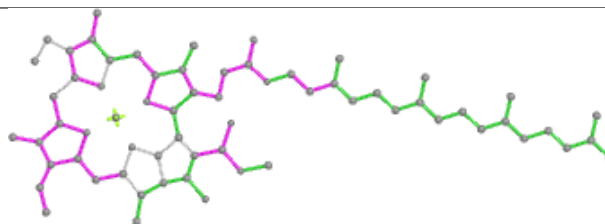
## Ligand CLA bB 837



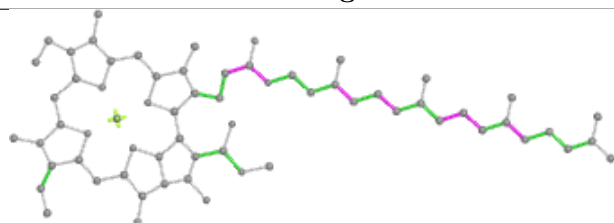
## Ligand CLA bB 838



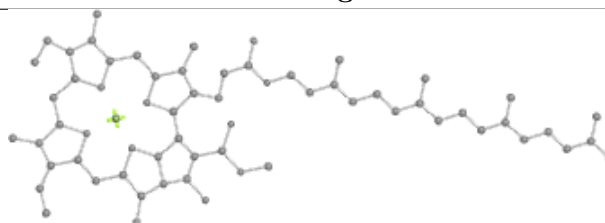
Bond lengths



Bond angles

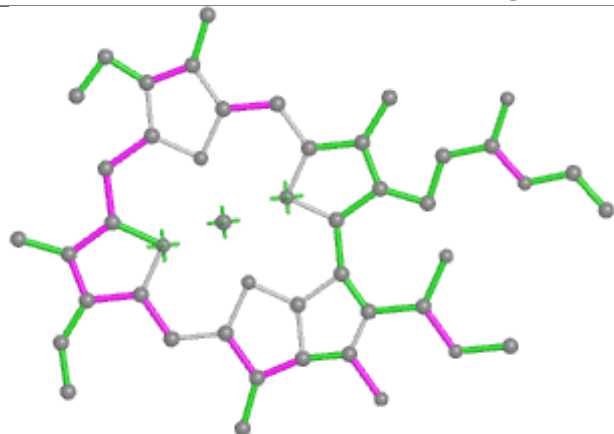


Torsions

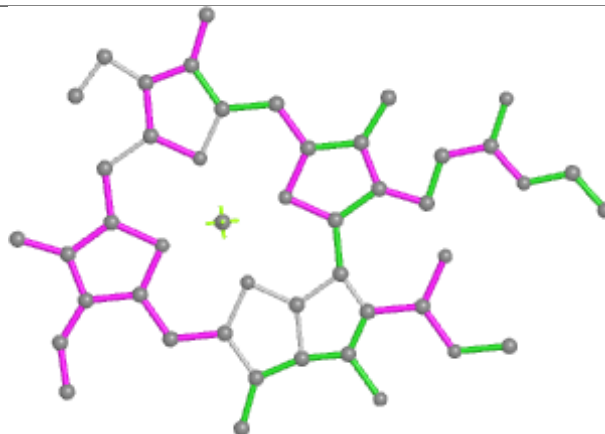


Rings

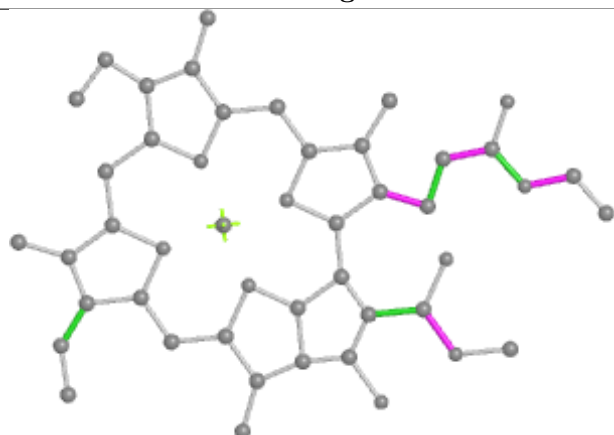
## Ligand CLA bB 839



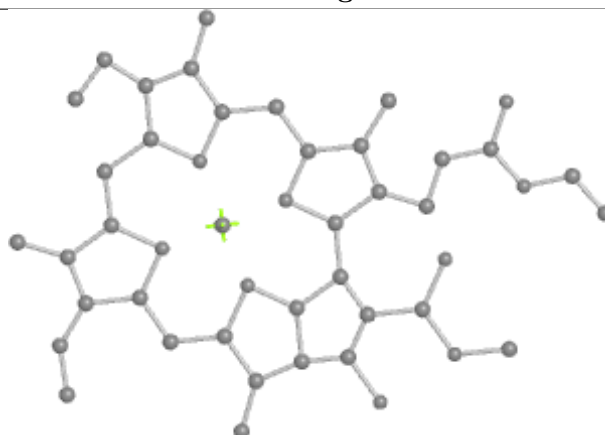
Bond lengths



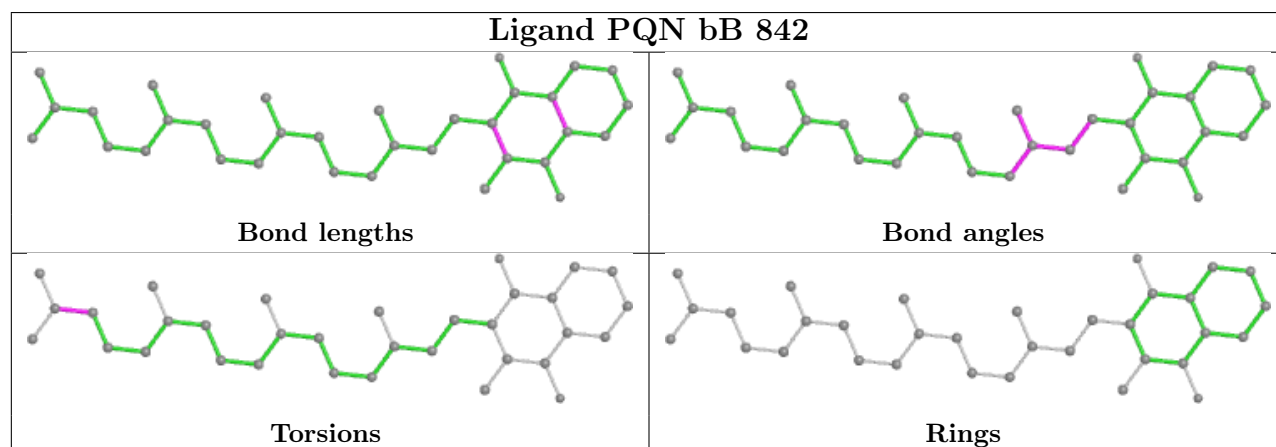
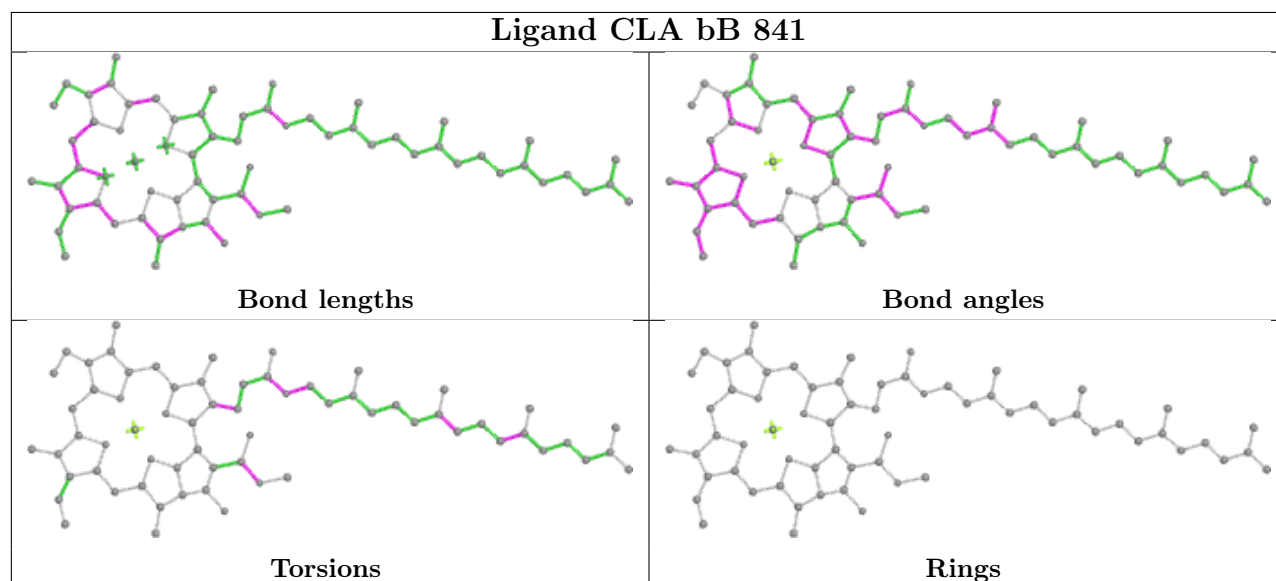
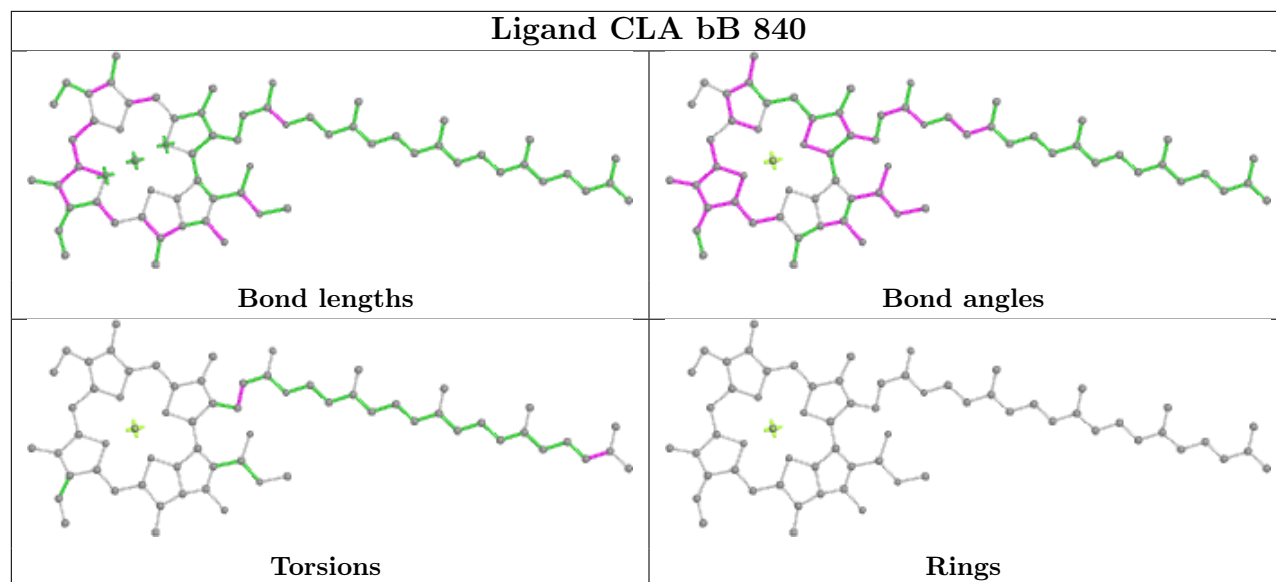
Bond angles



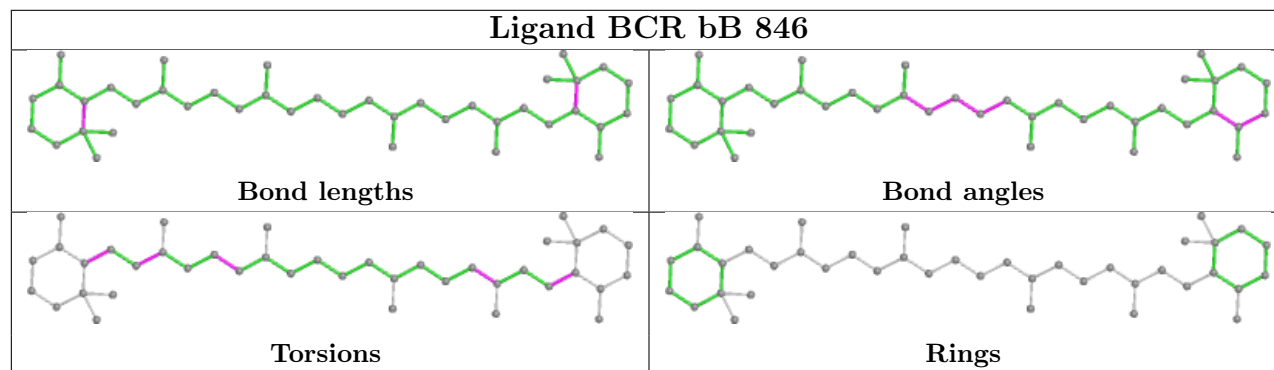
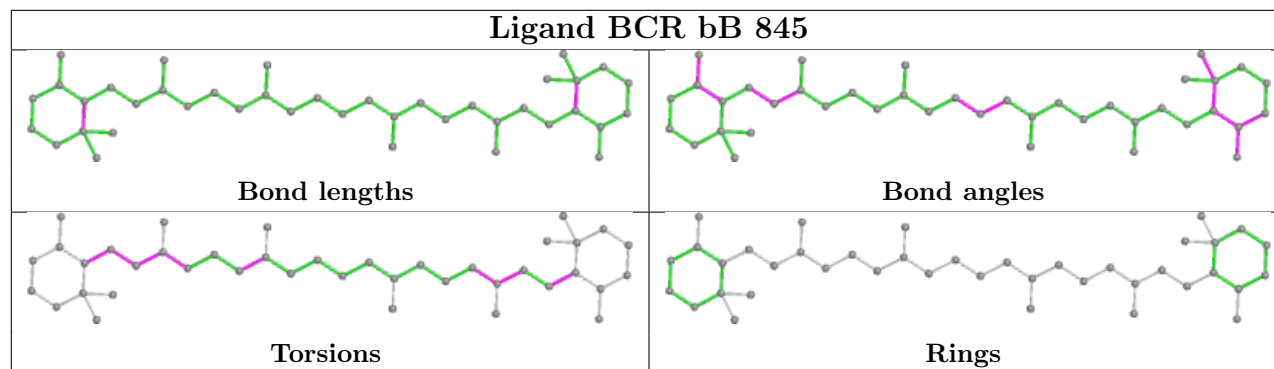
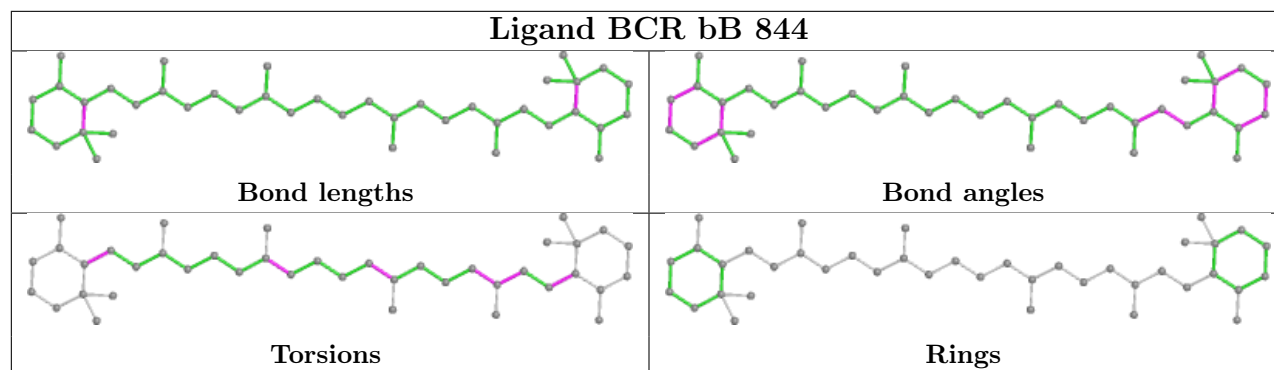
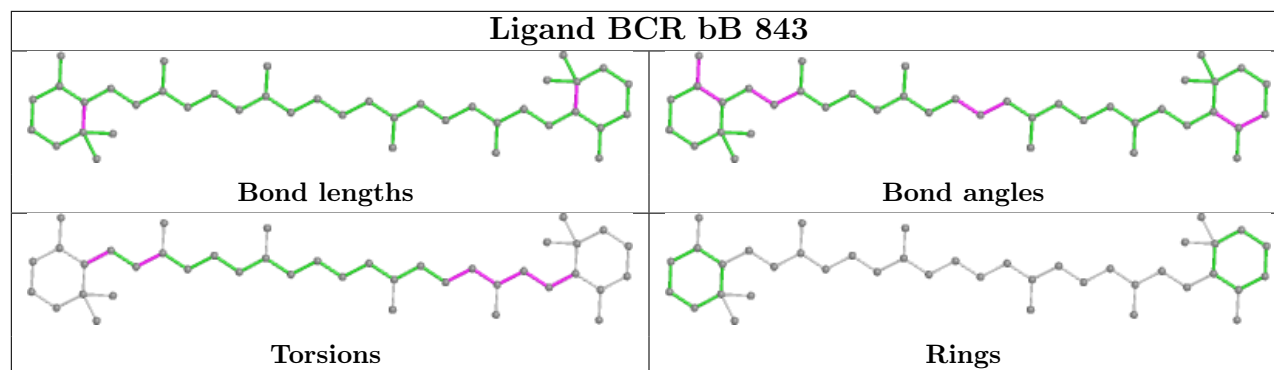
Torsions

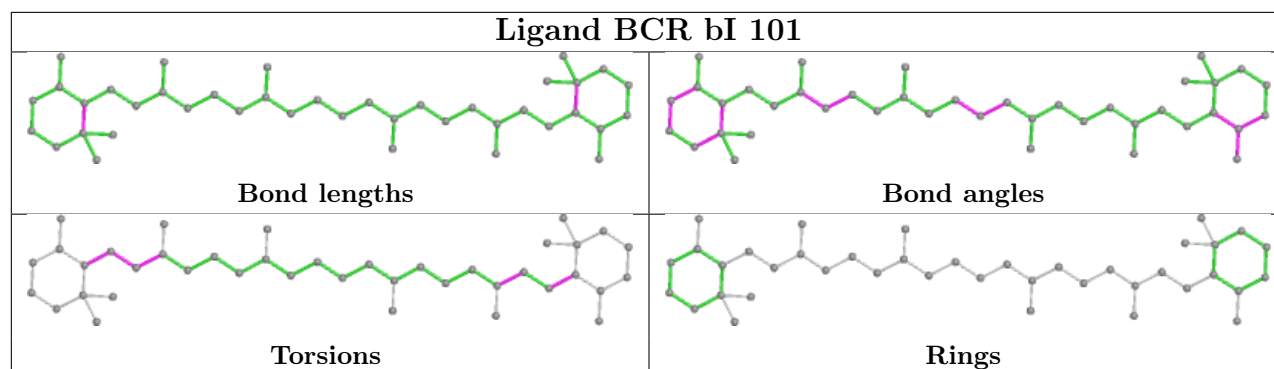
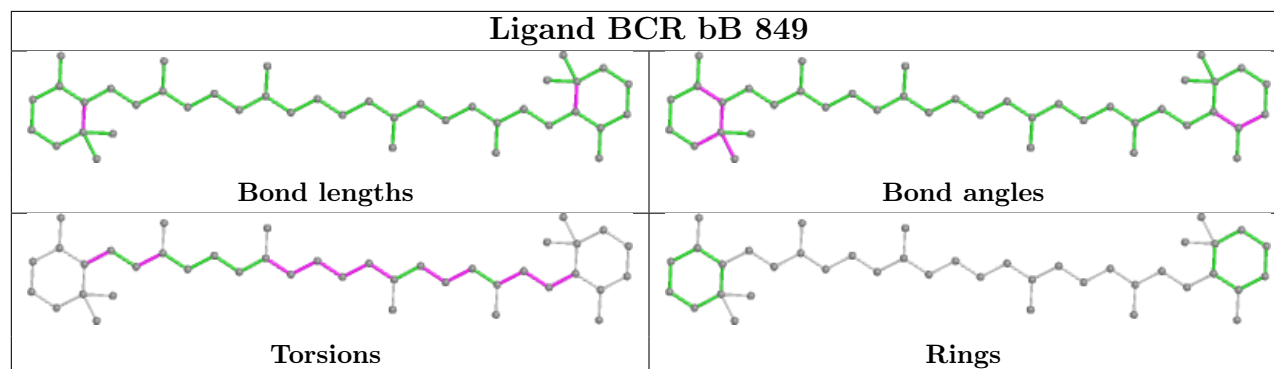
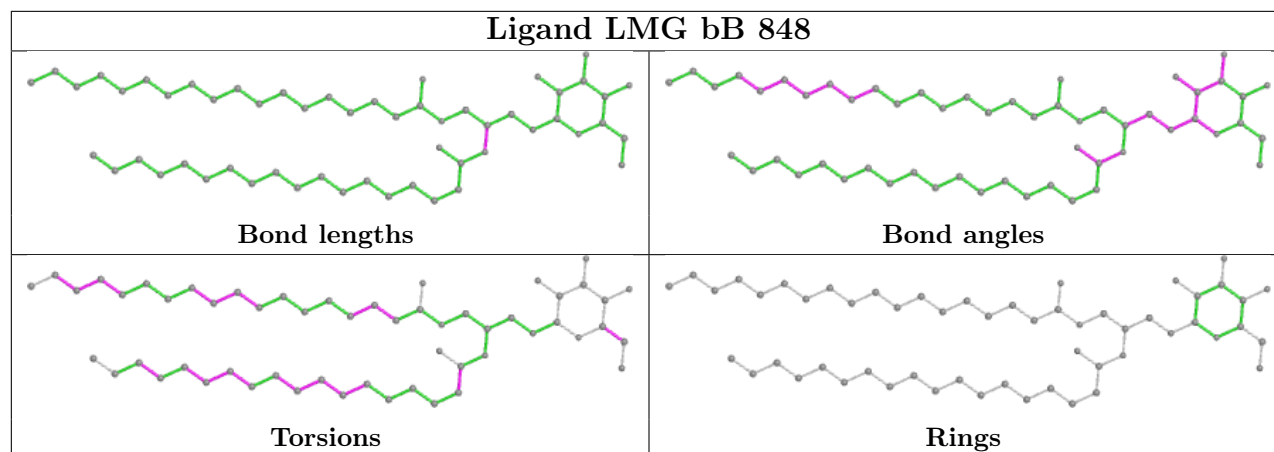
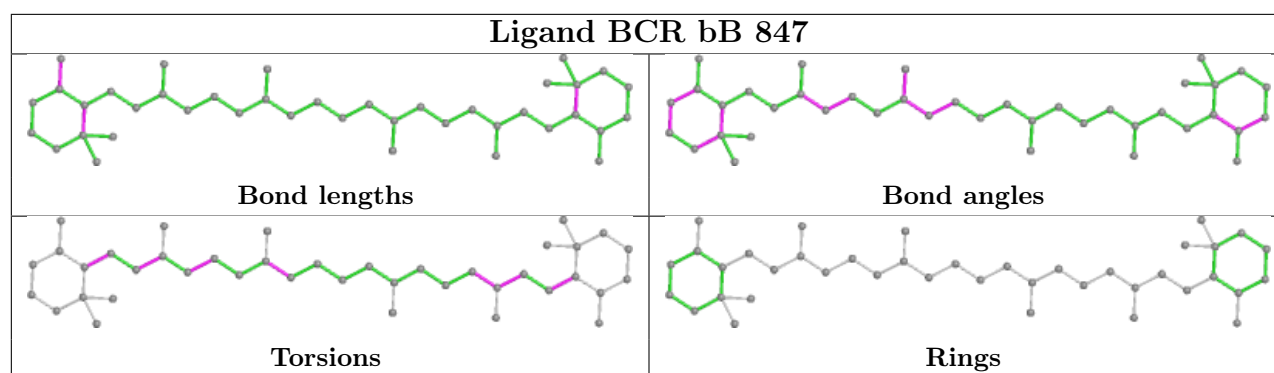


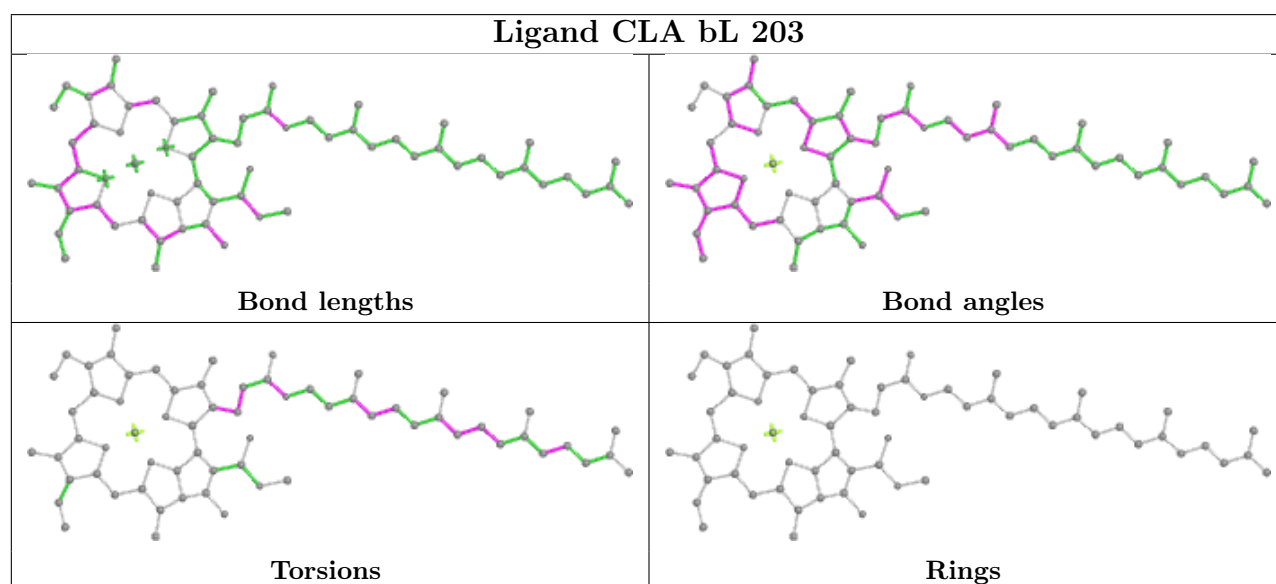
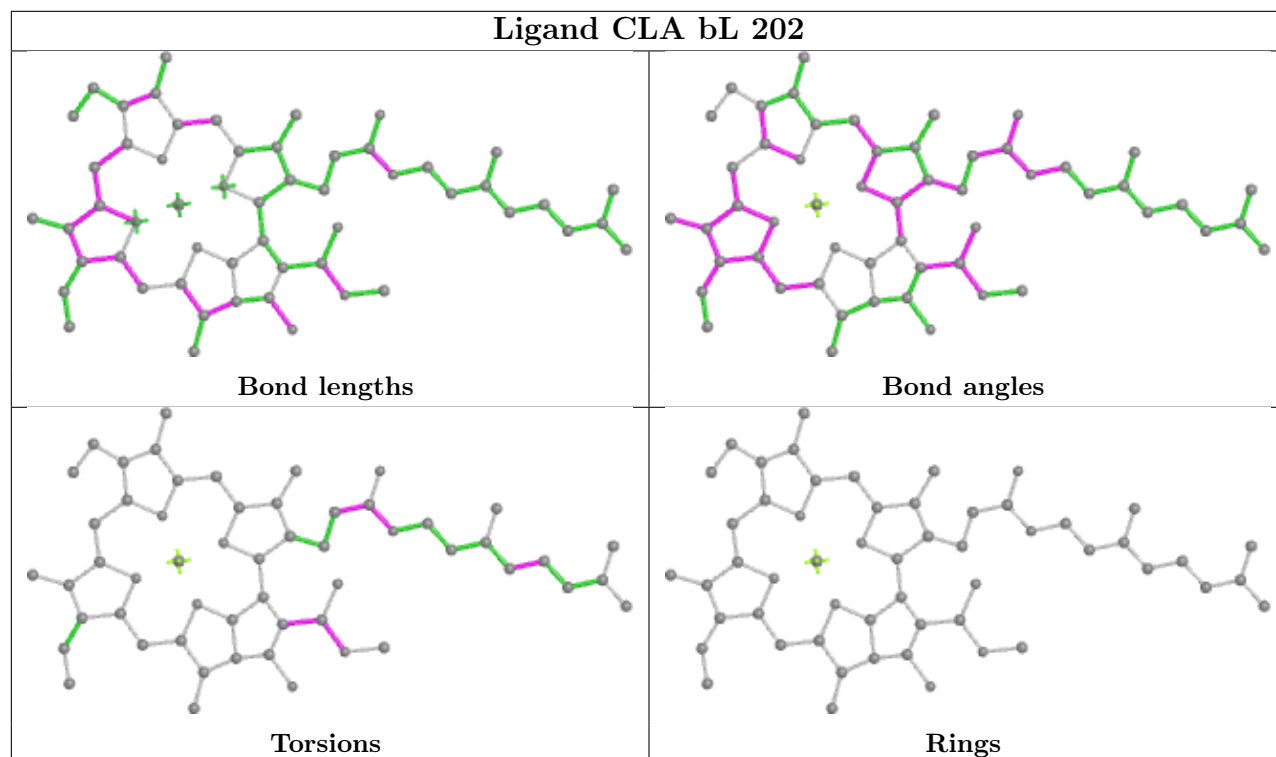
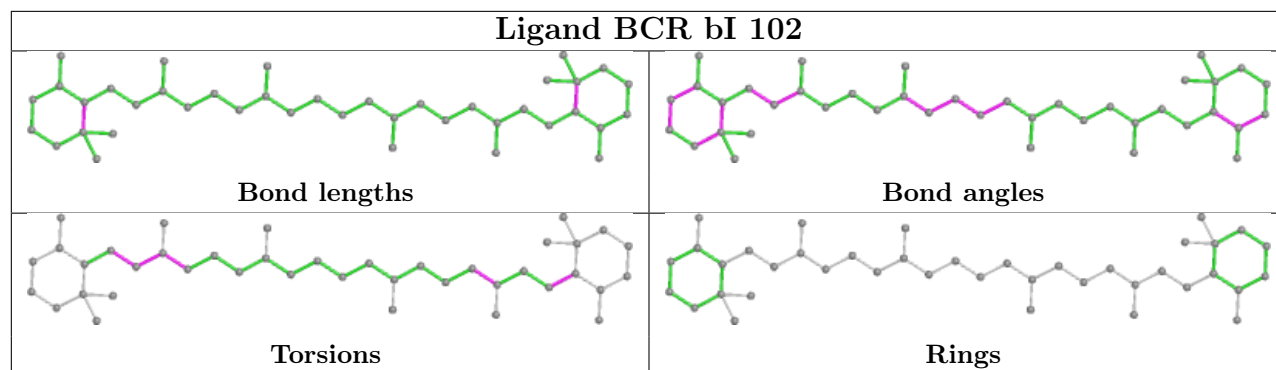
Rings

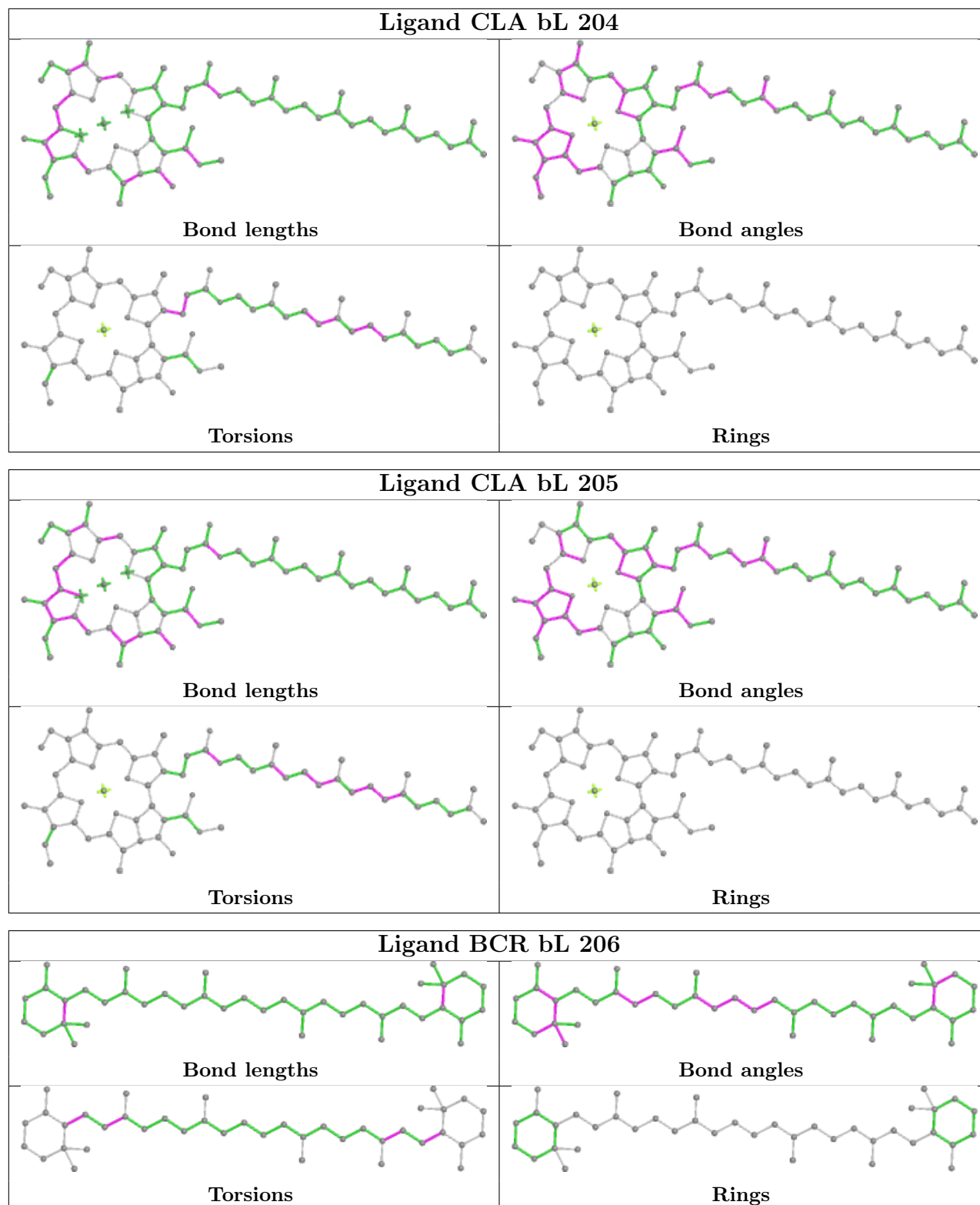


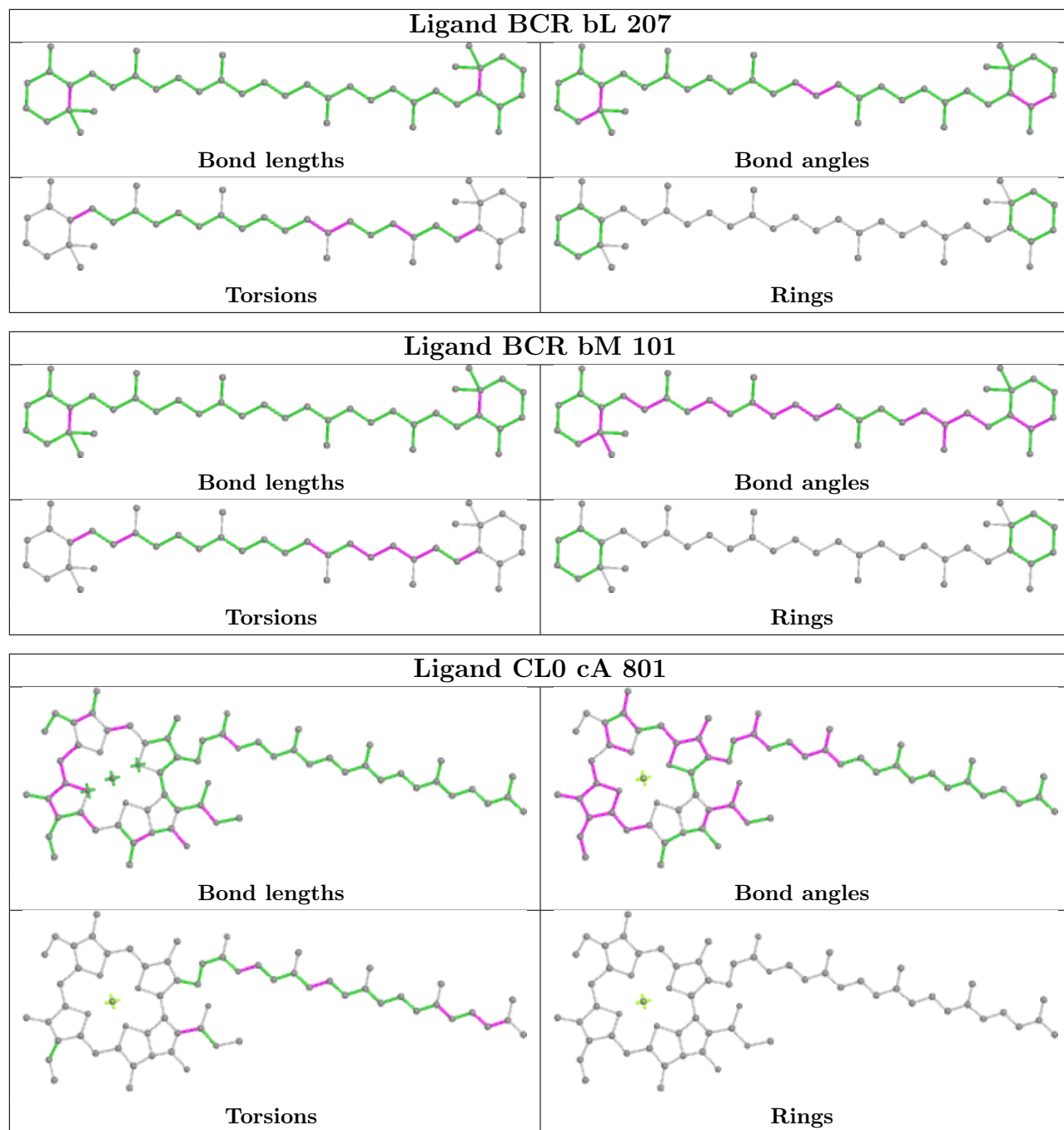




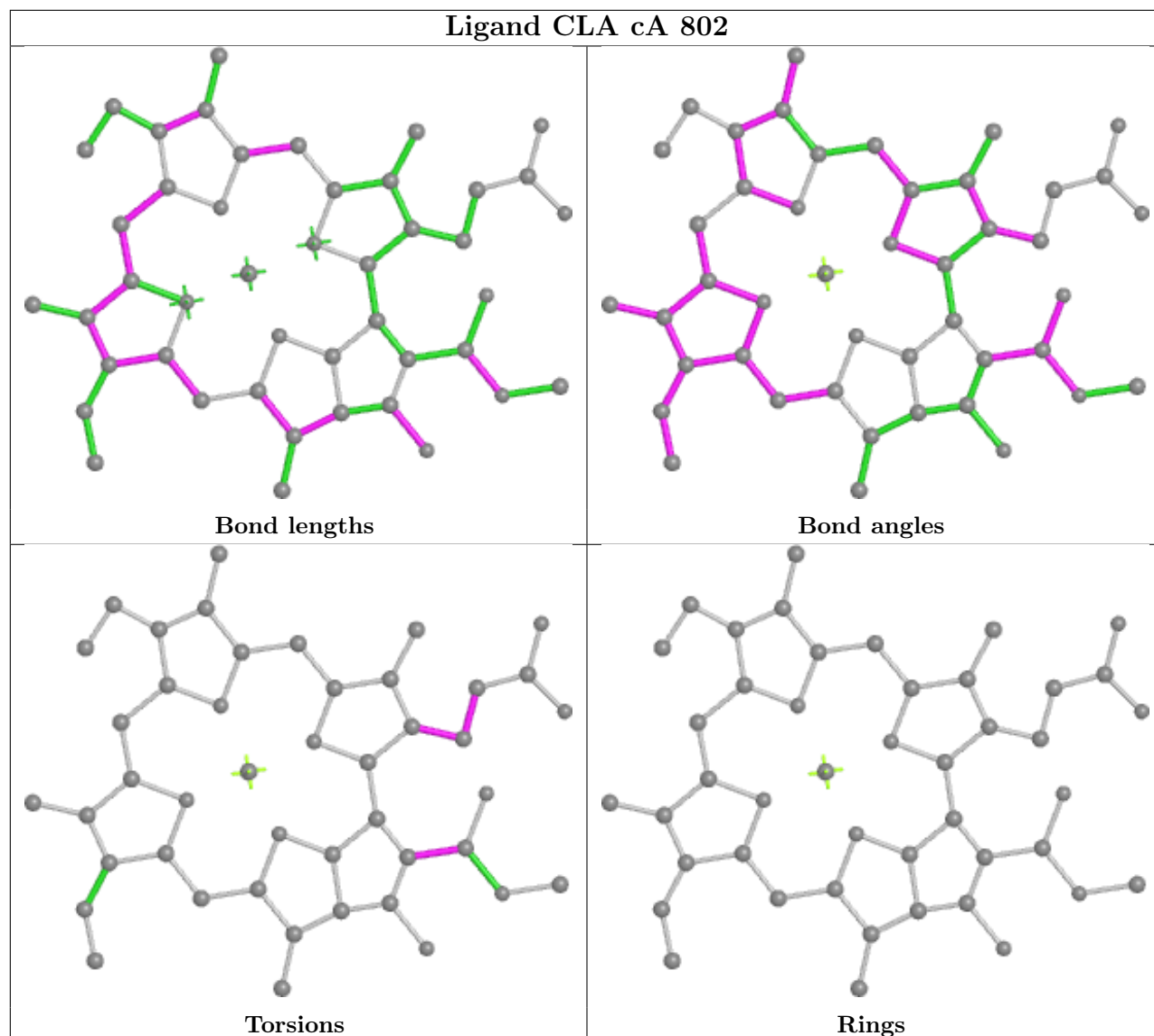


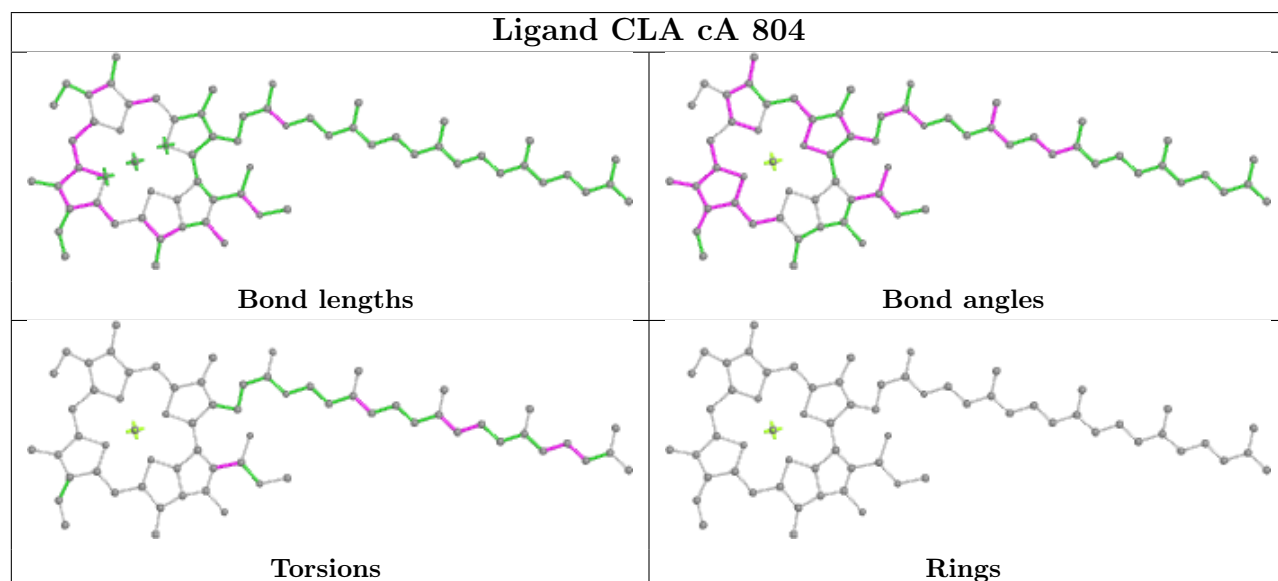
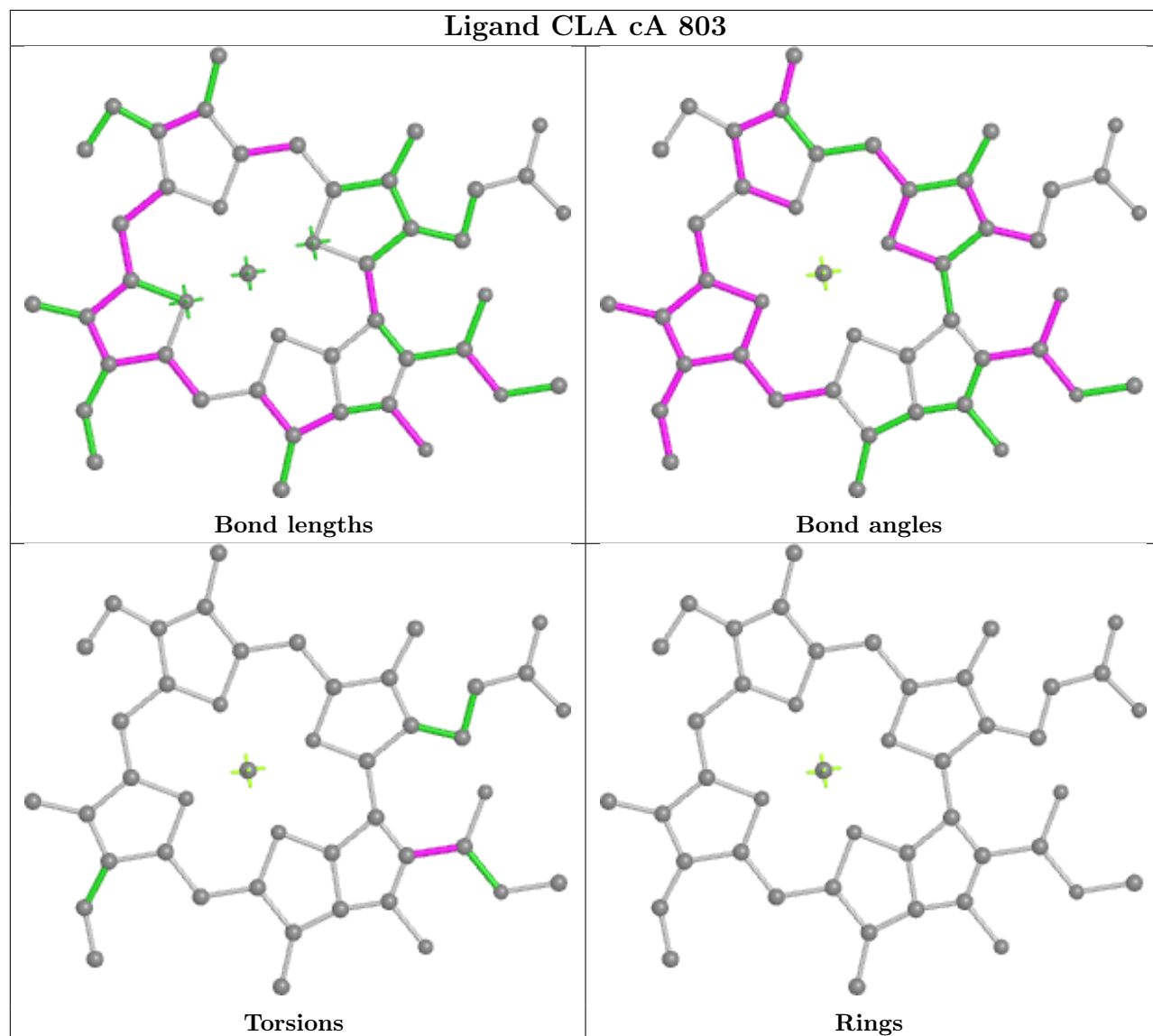




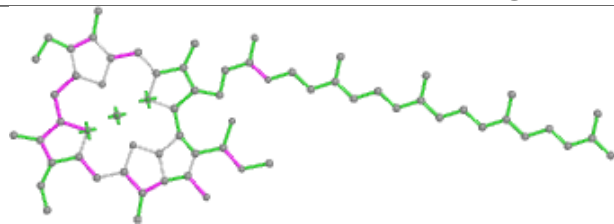


## Ligand CLA cA 802

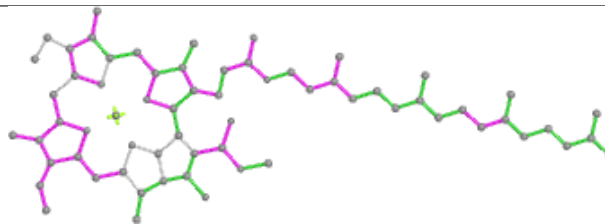




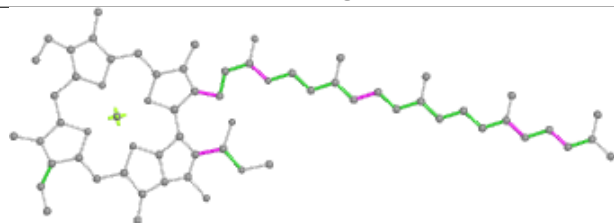
## Ligand CLA cA 805



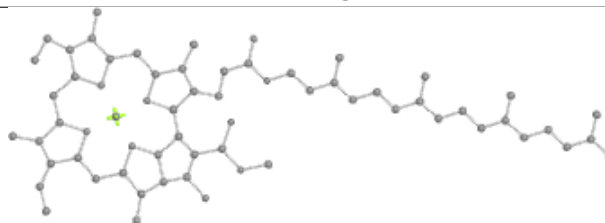
Bond lengths



Bond angles

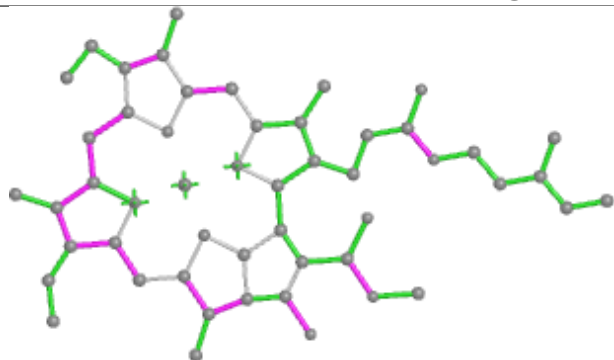


Torsions

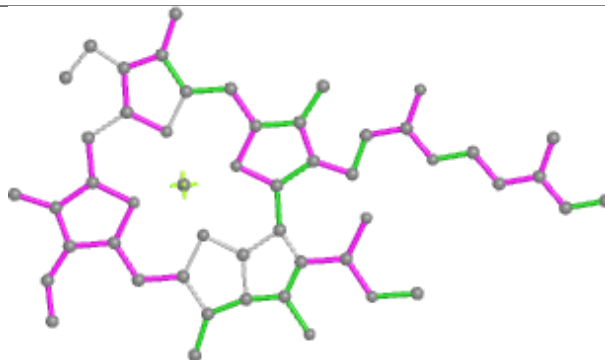


Rings

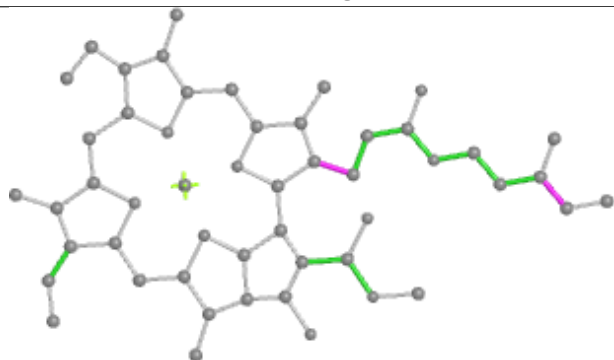
## Ligand CLA cA 806



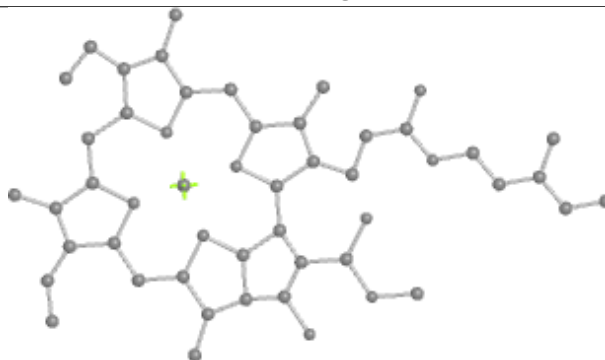
Bond lengths



Bond angles

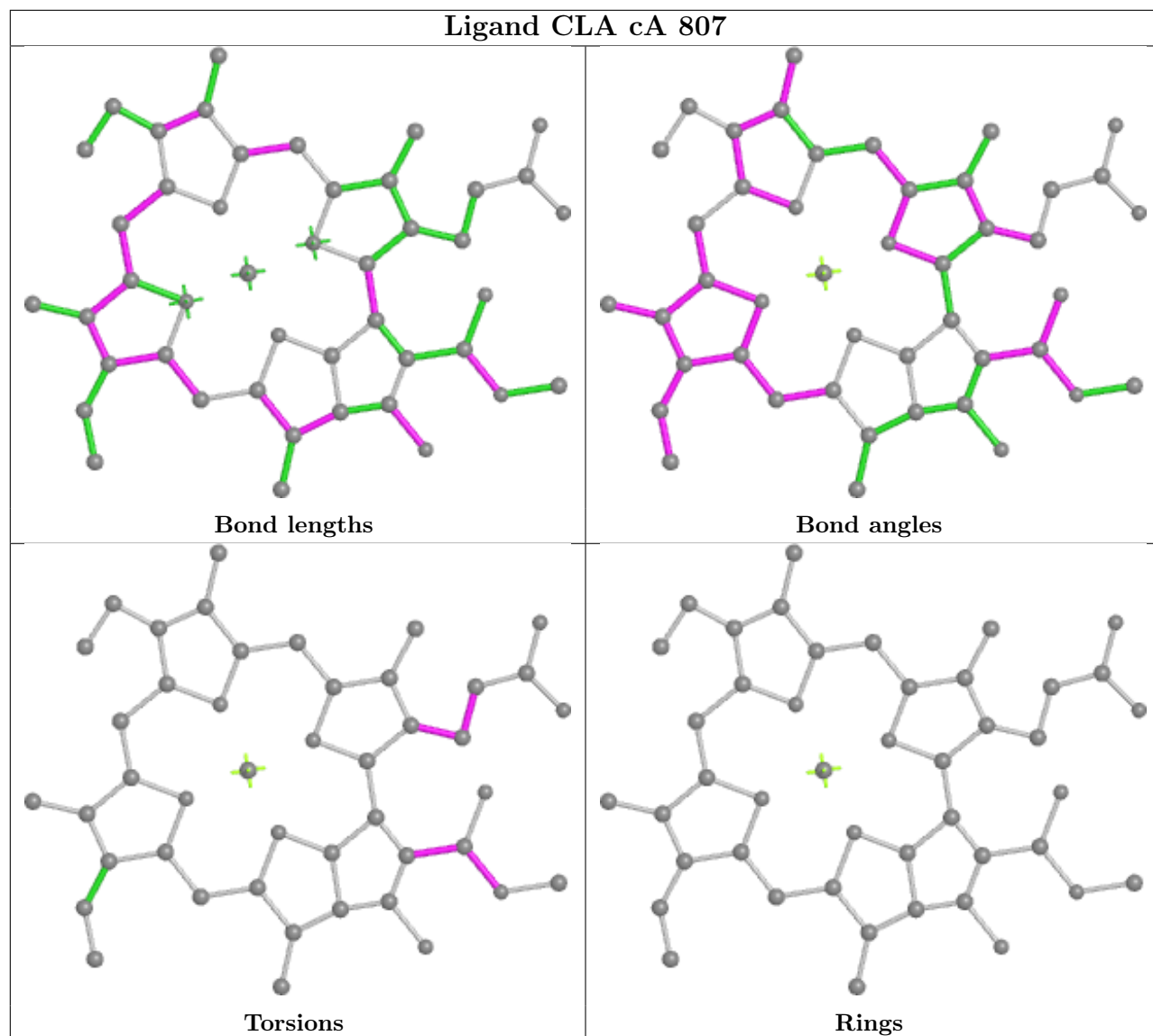


Torsions

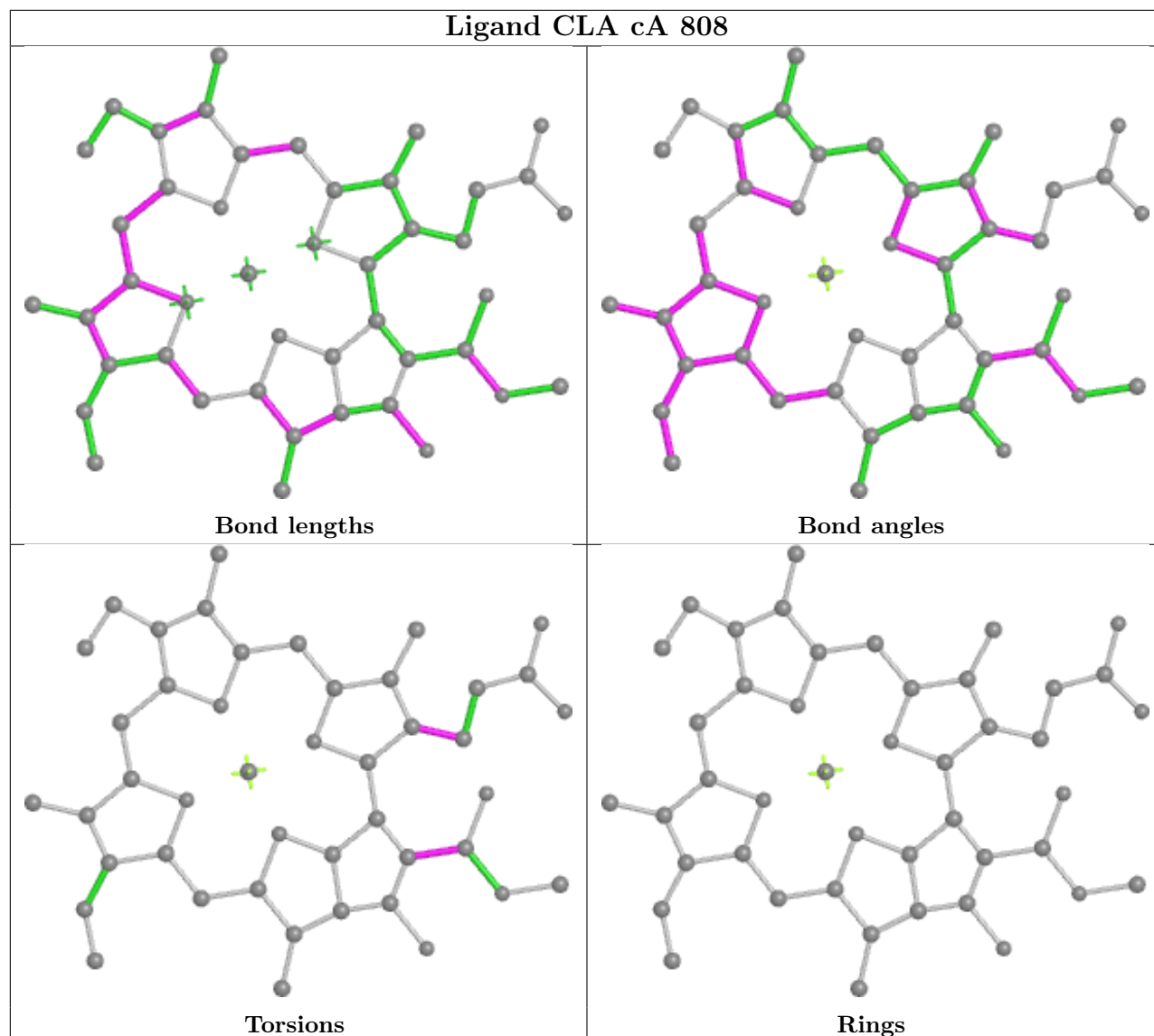


Rings

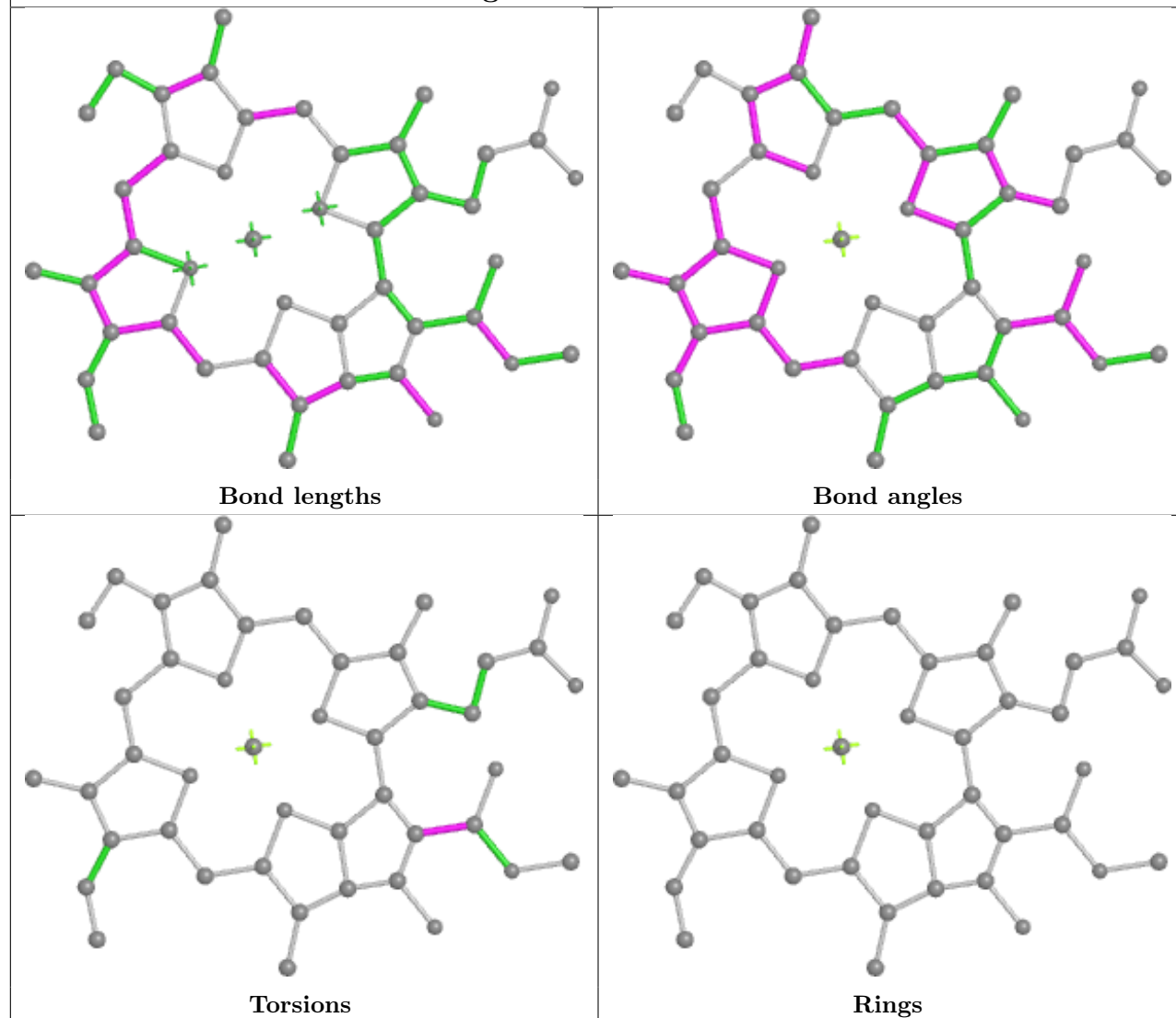




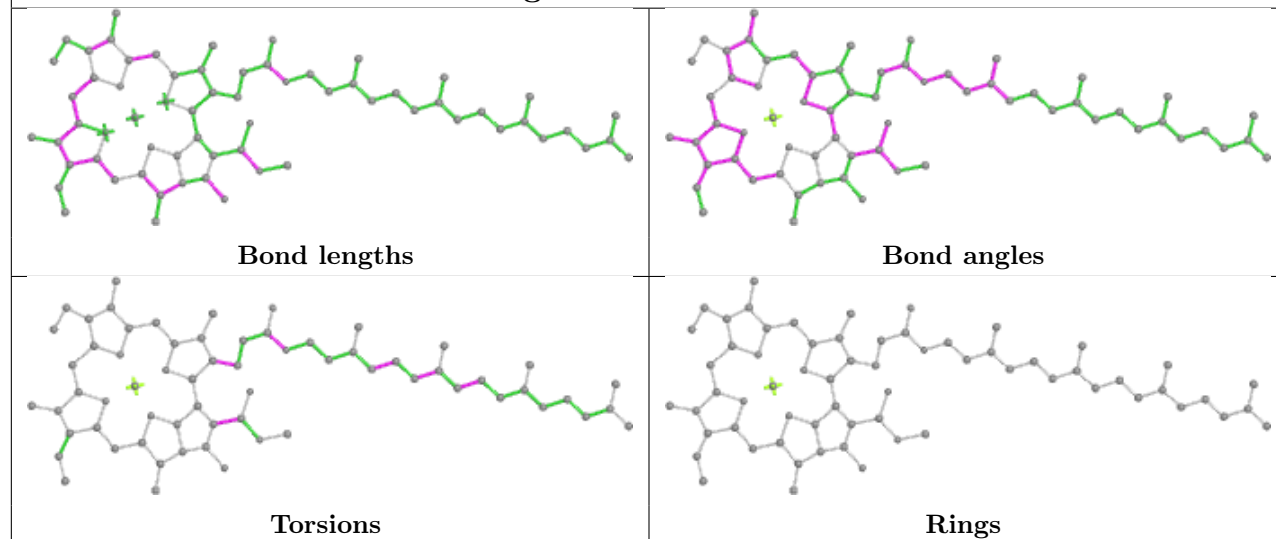
## Ligand CLA cA 808

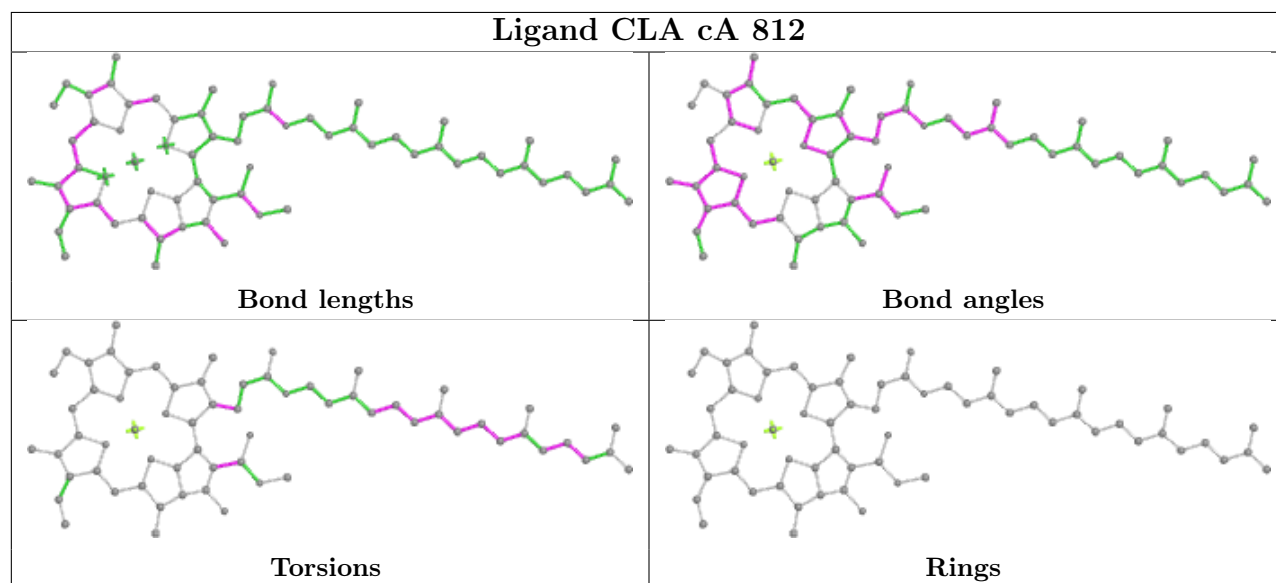
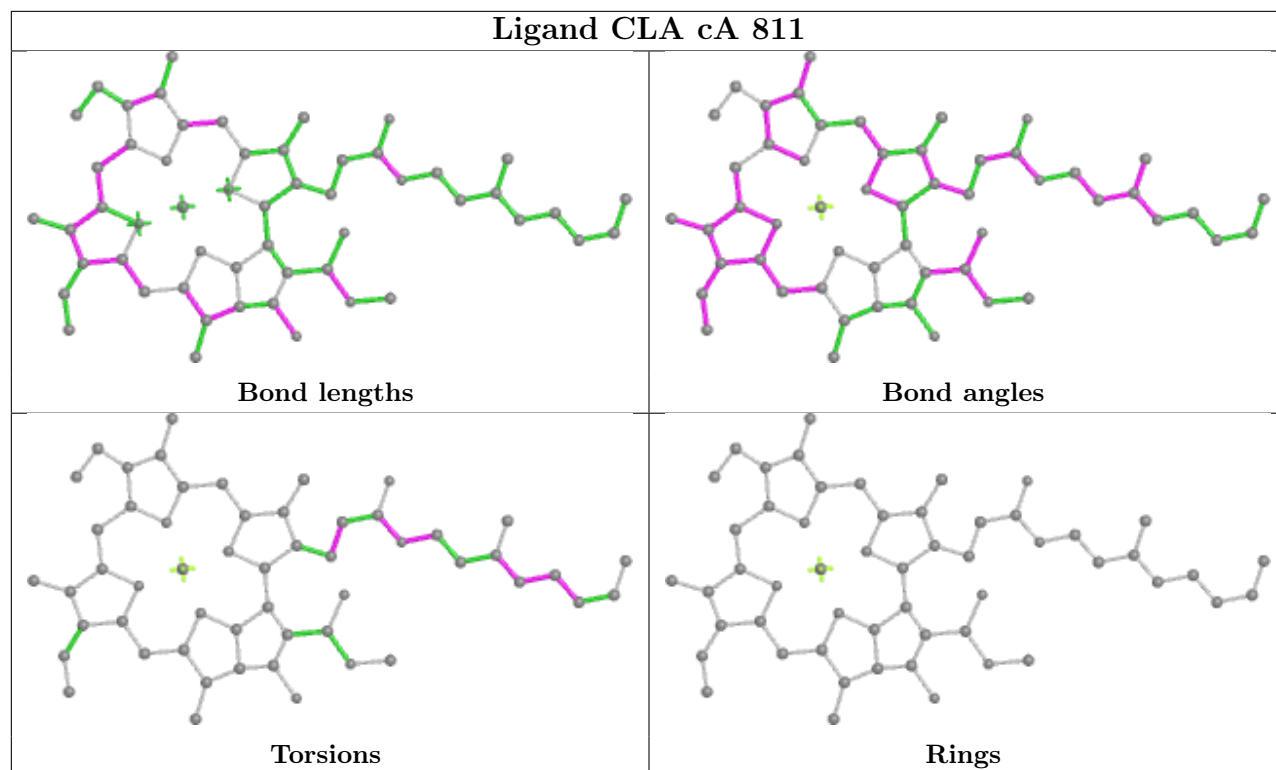


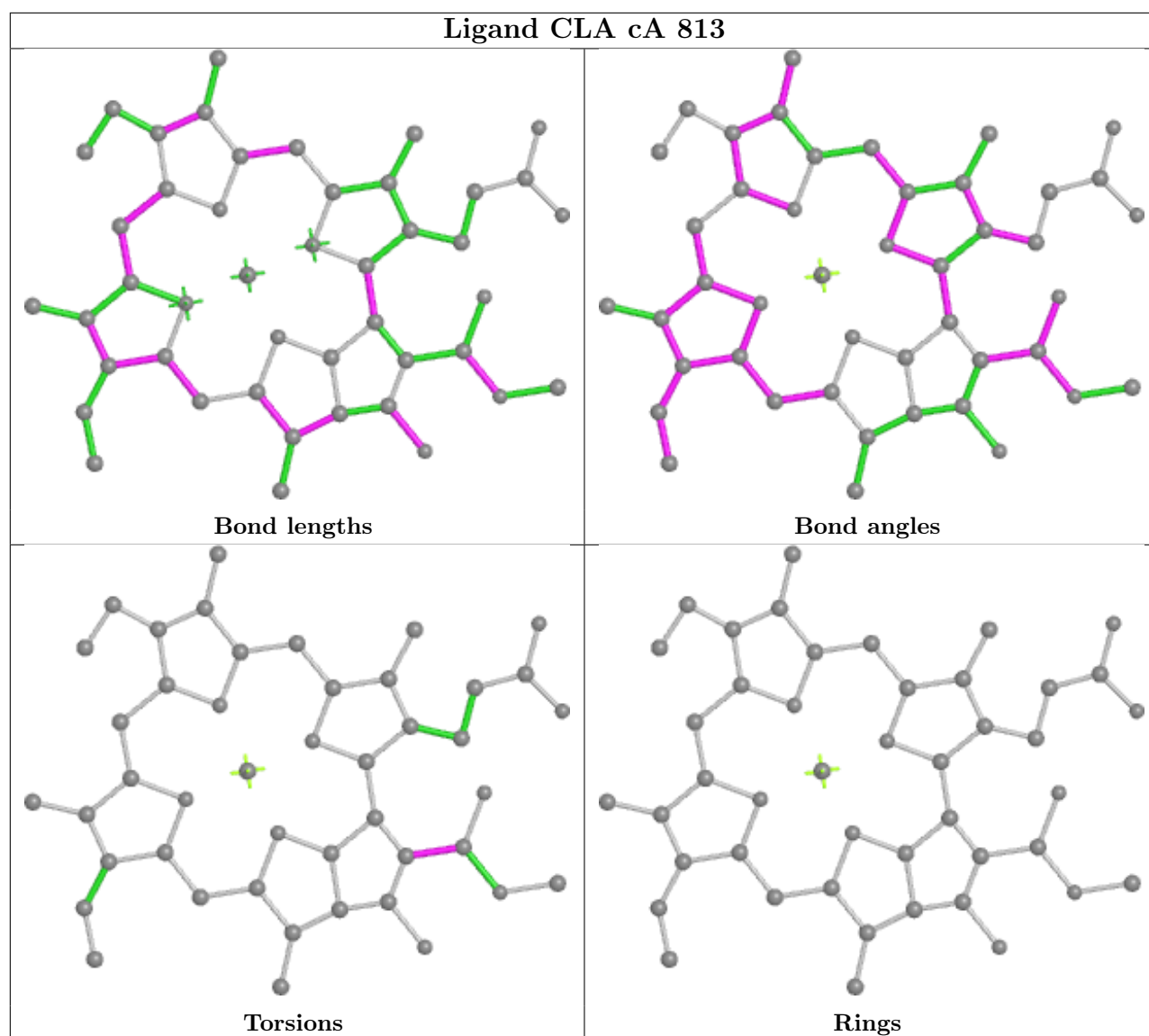
## Ligand CLA cA 809

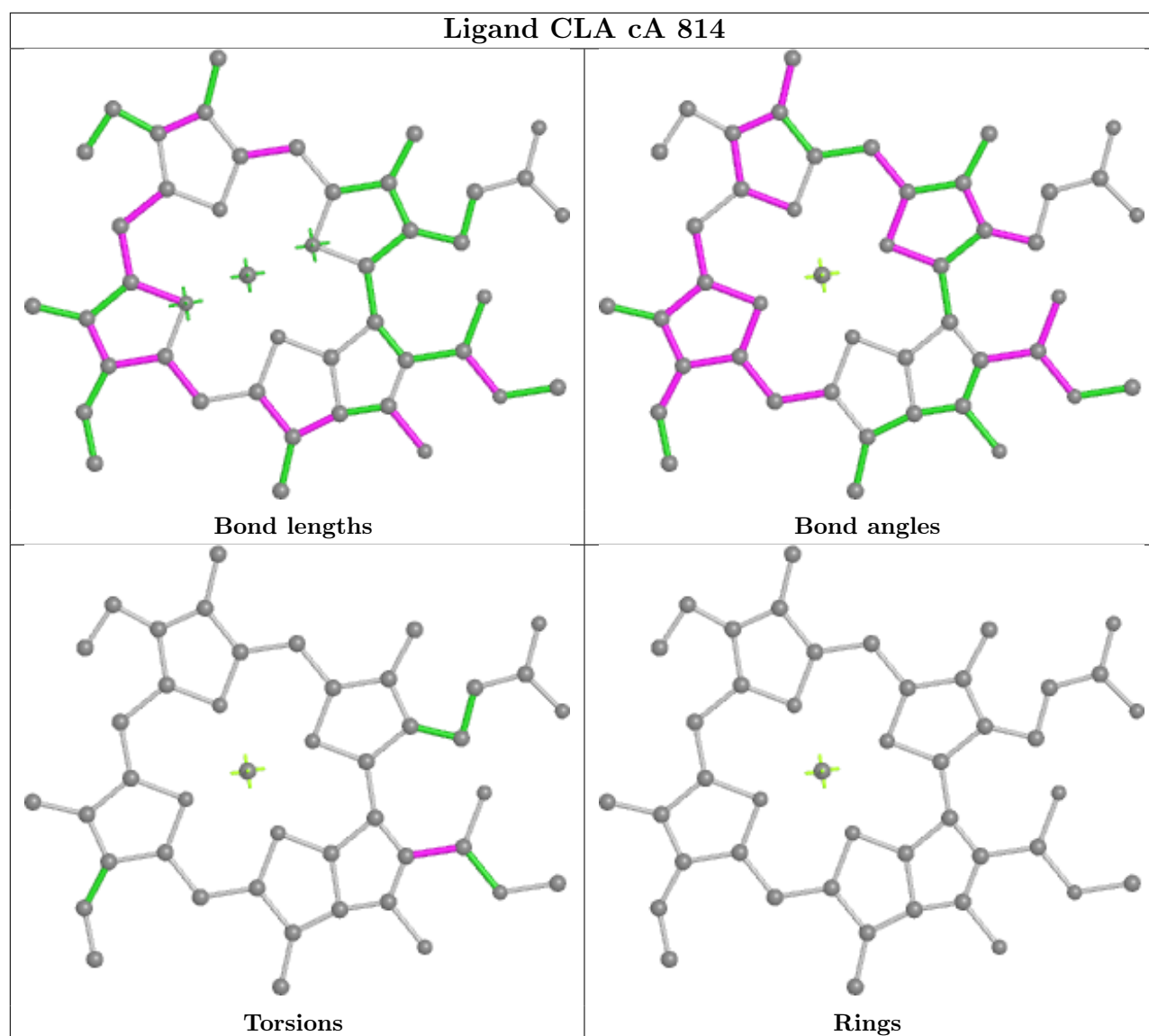


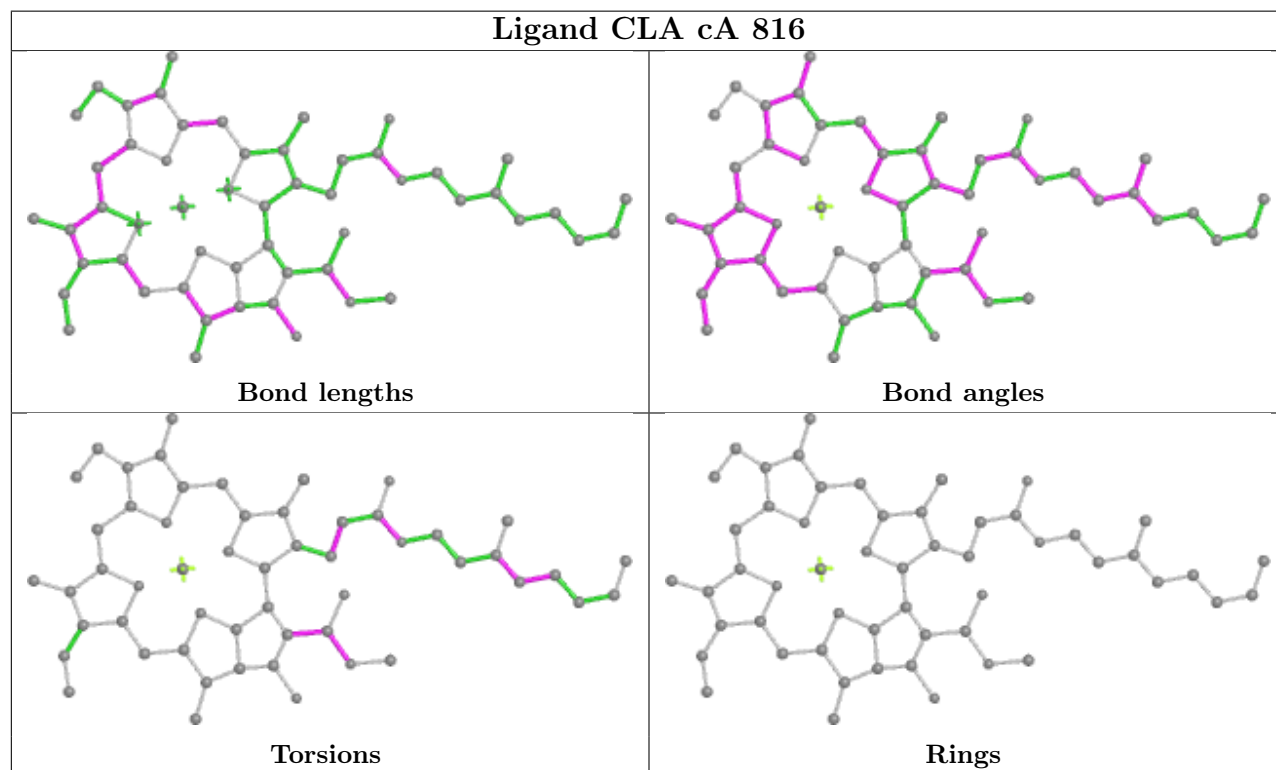
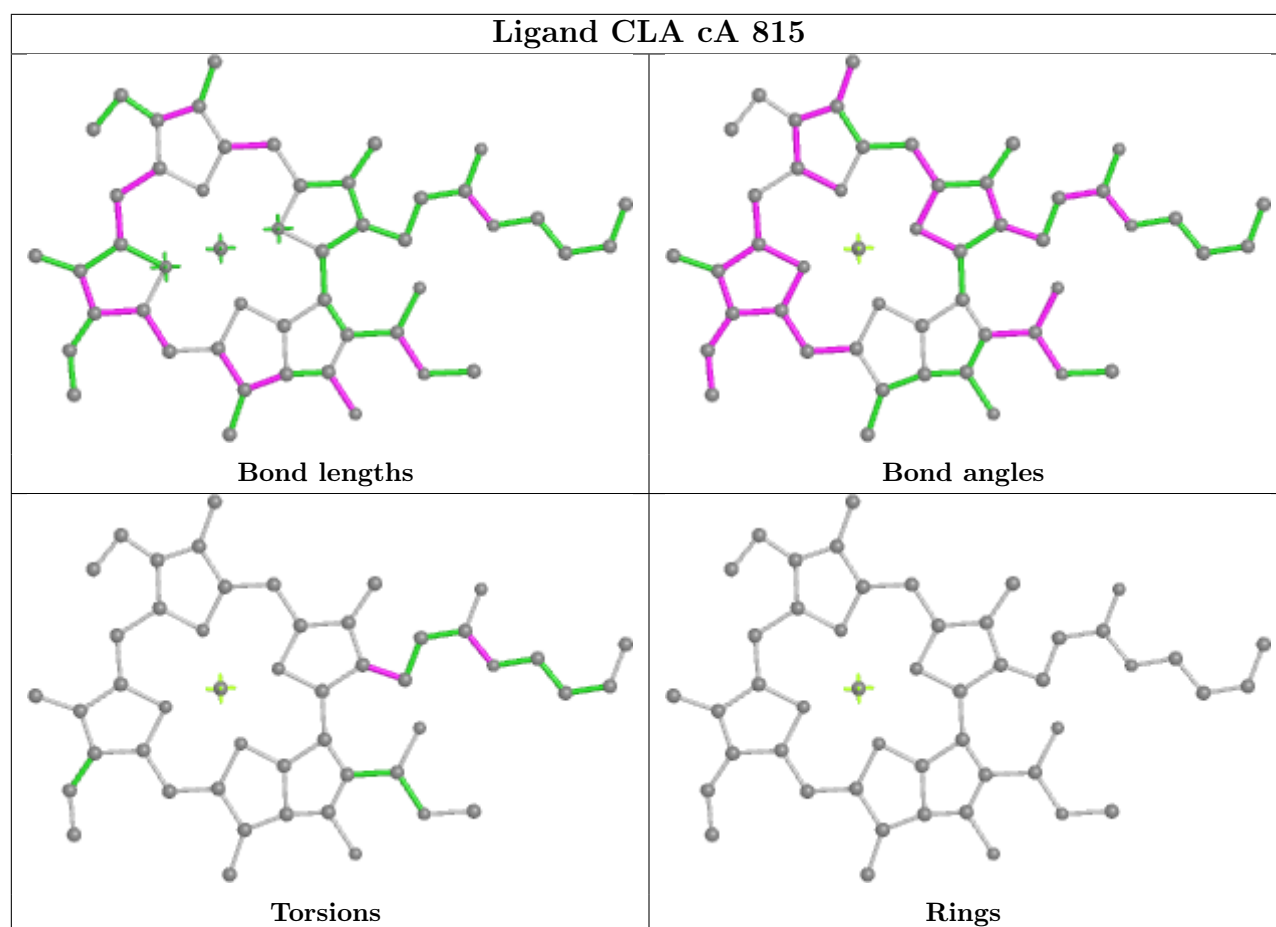
## Ligand CLA cA 810

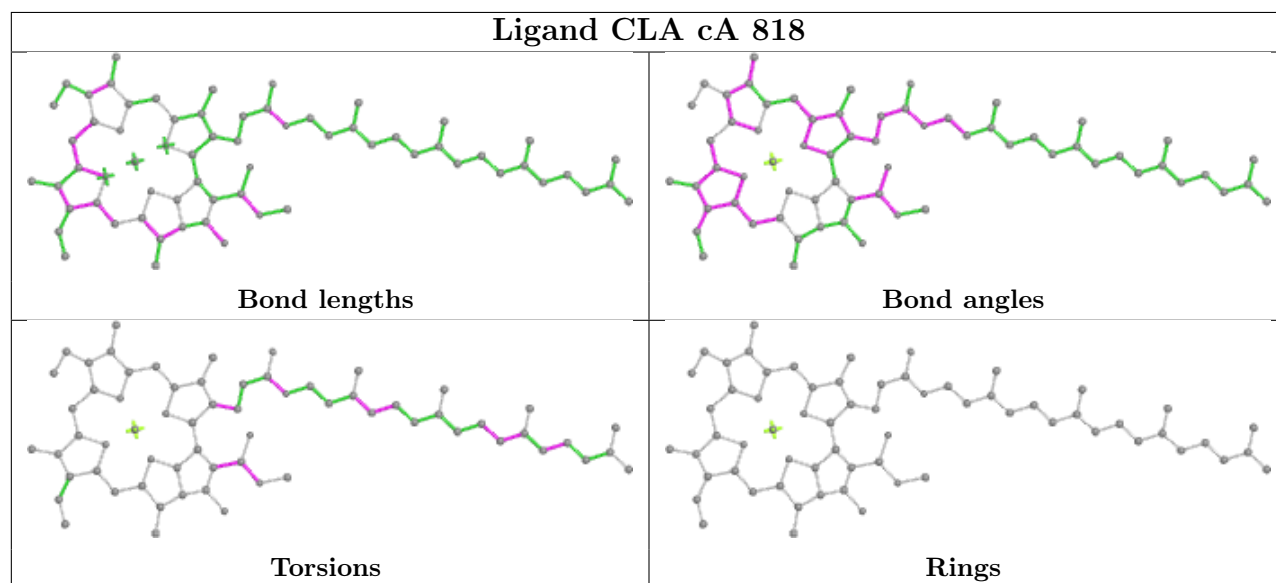
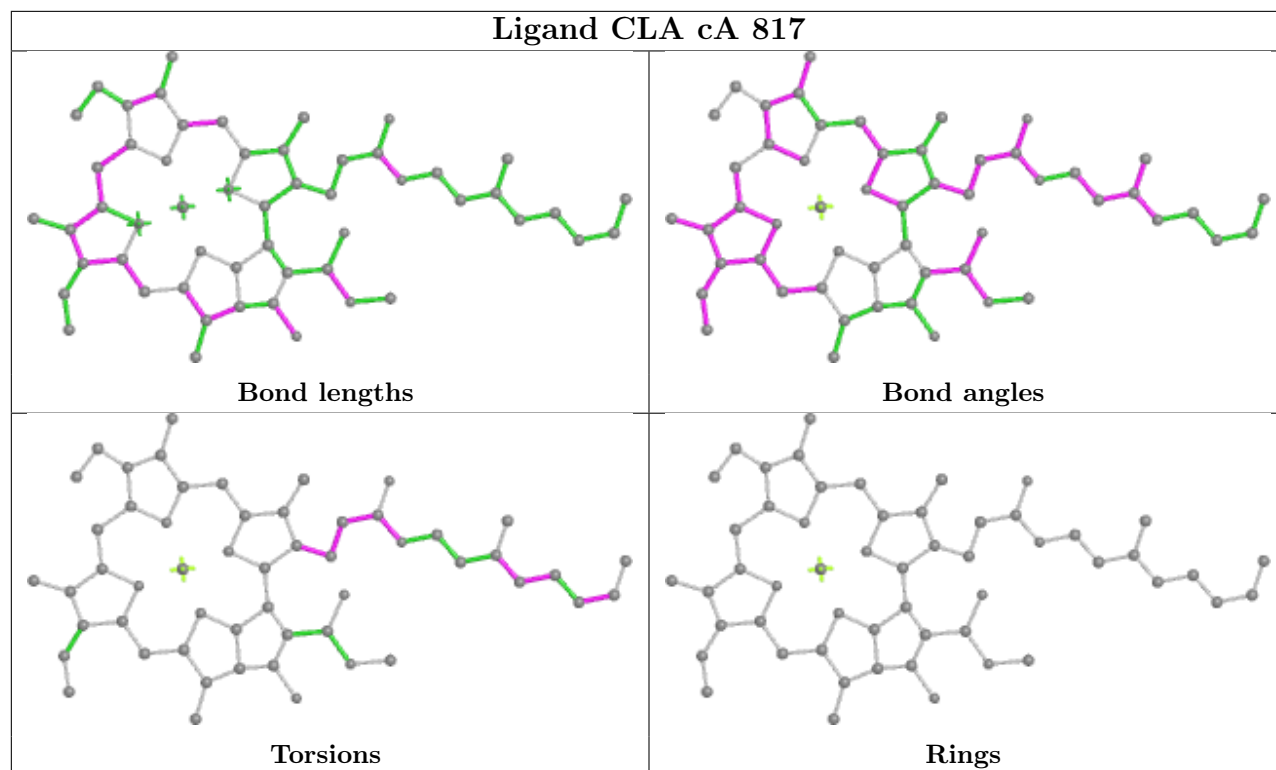




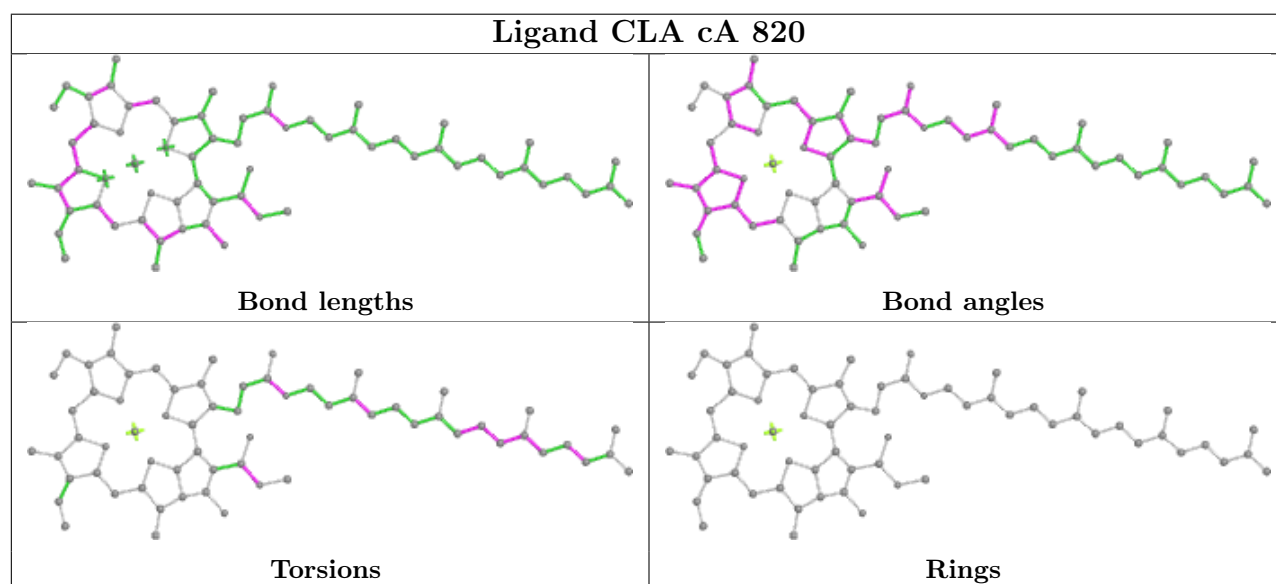
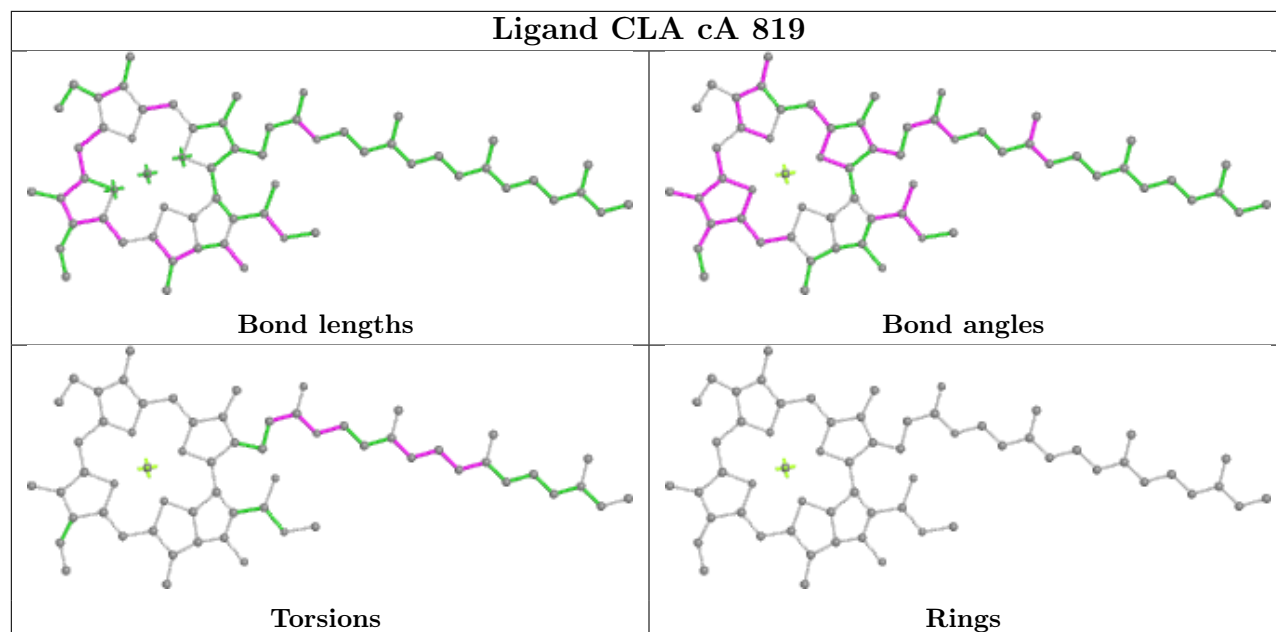




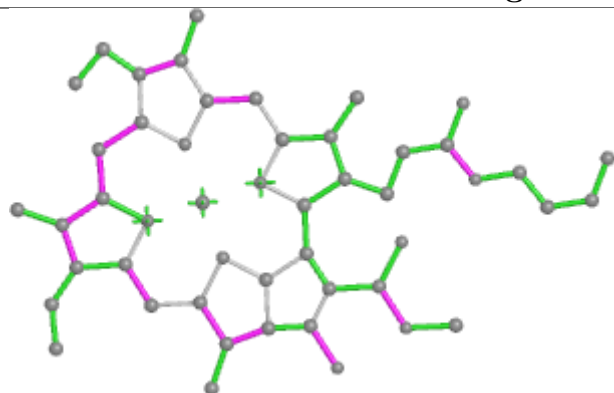




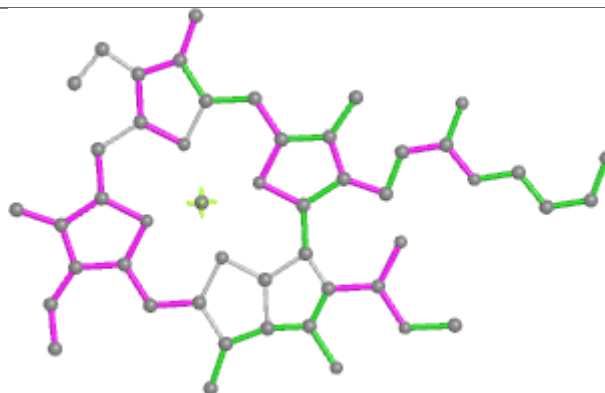




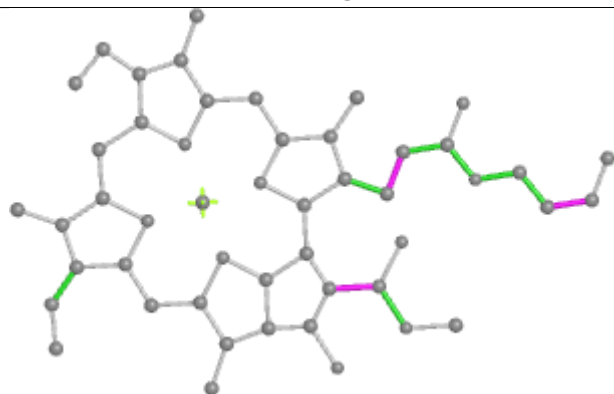
## Ligand CLA cA 821



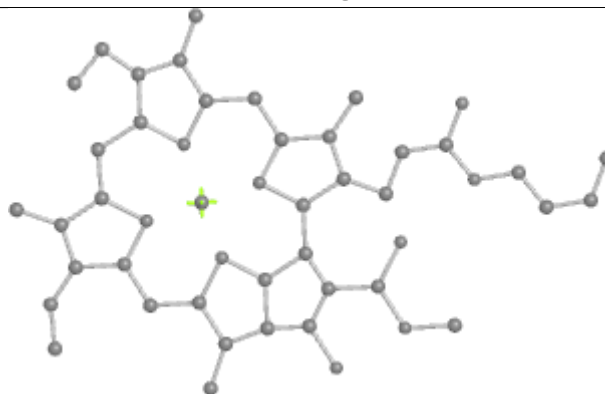
Bond lengths



Bond angles

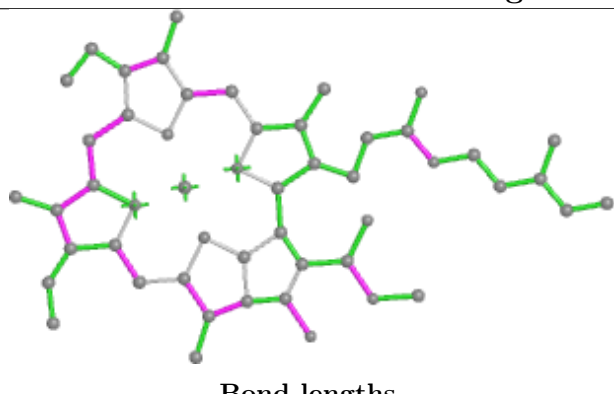


Torsions

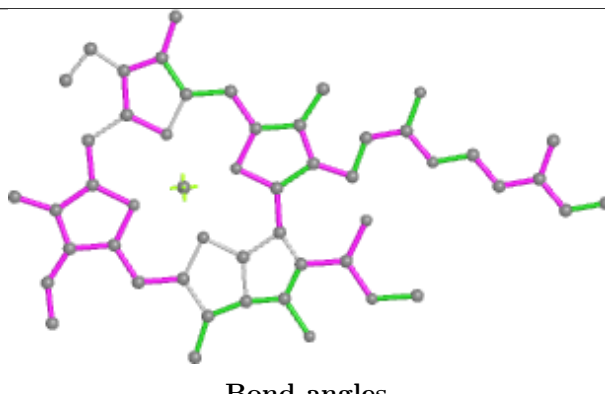


Rings

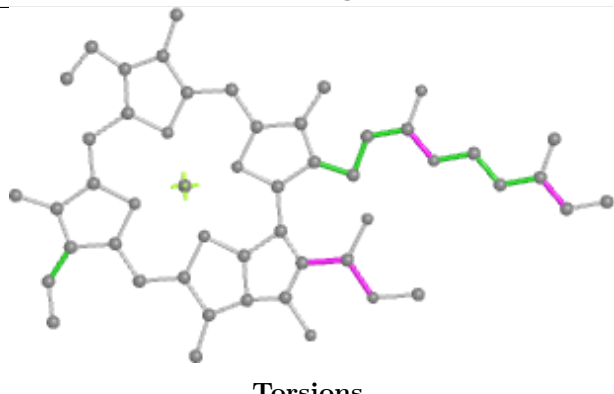
## Ligand CLA cA 822



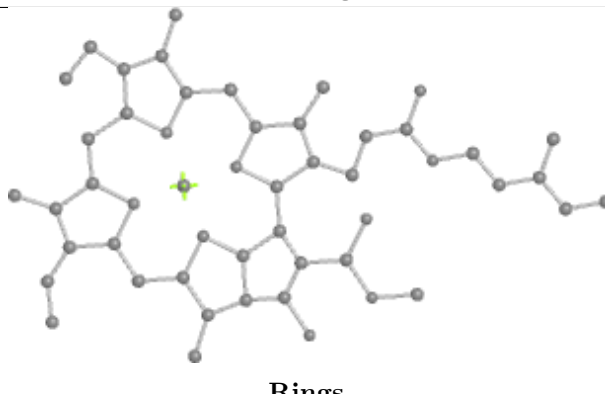
Bond lengths



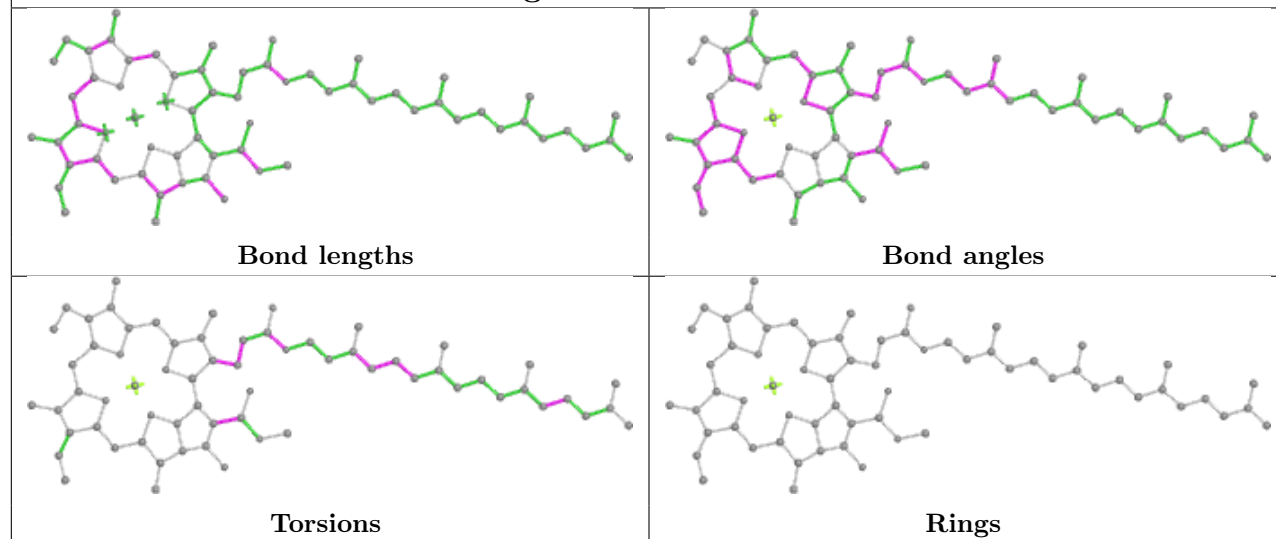
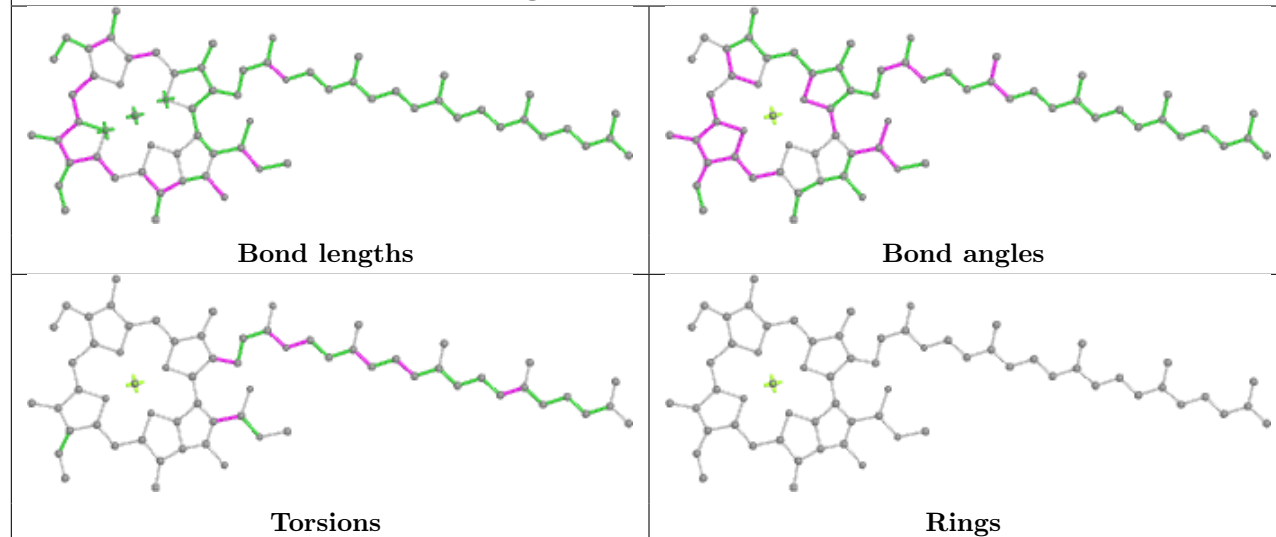
Bond angles

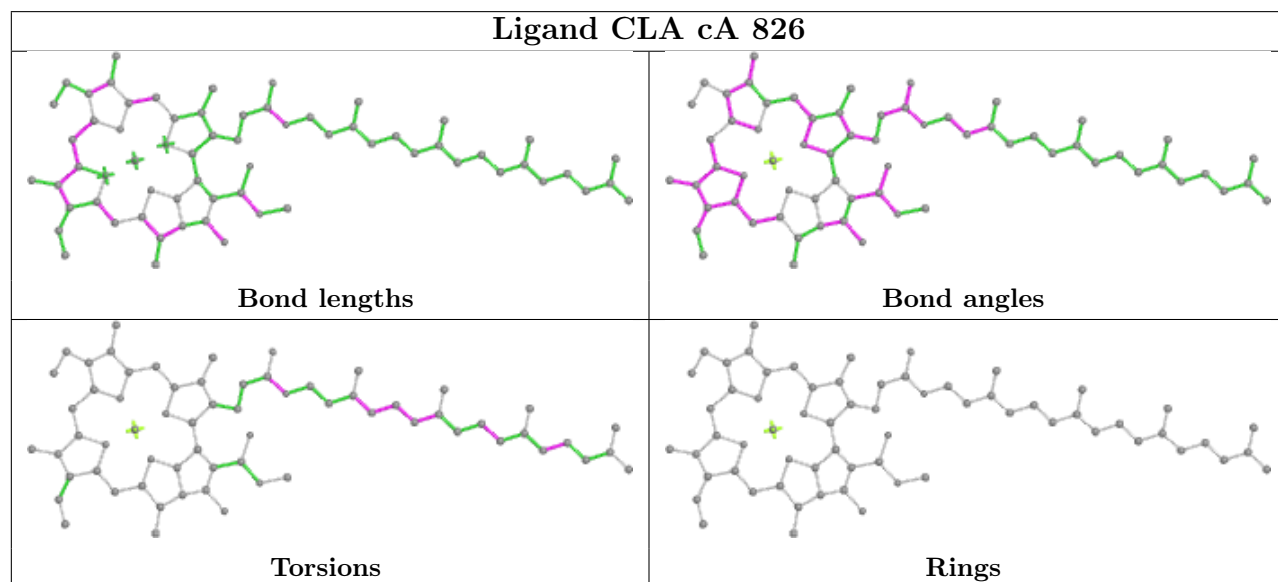
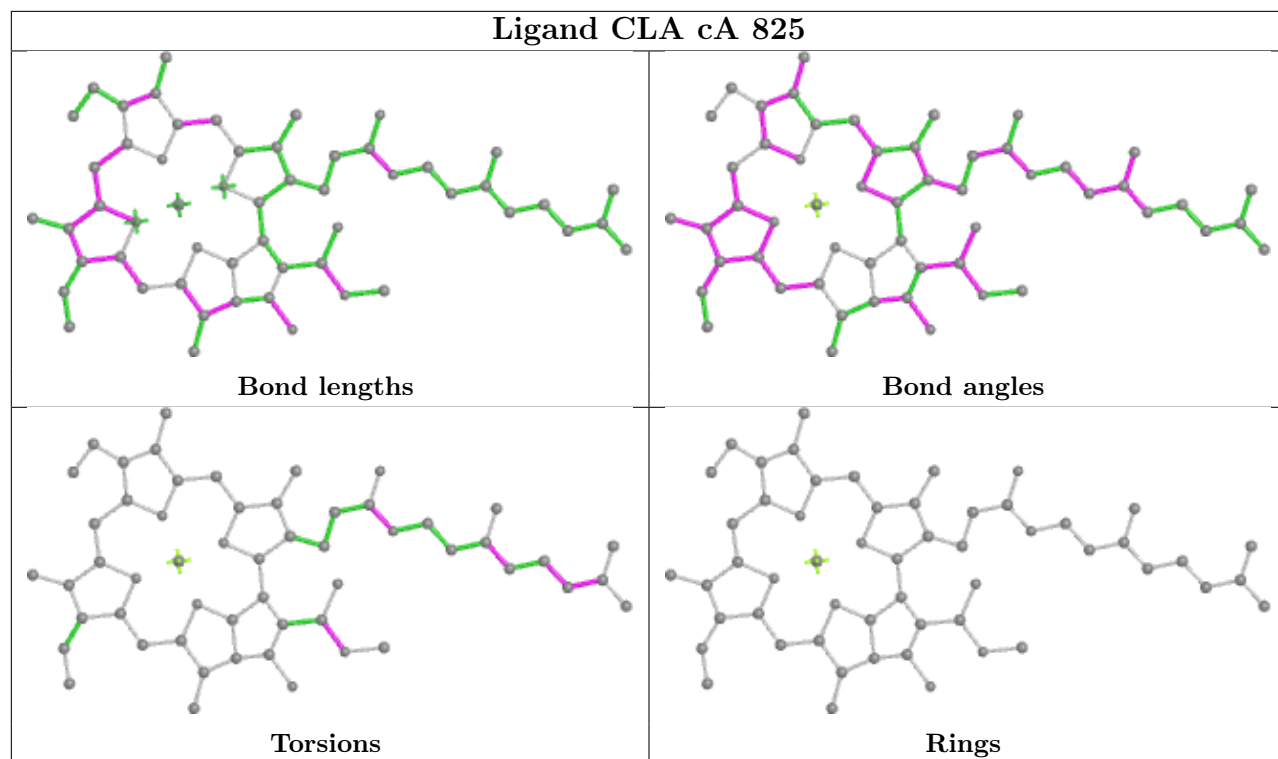


Torsions

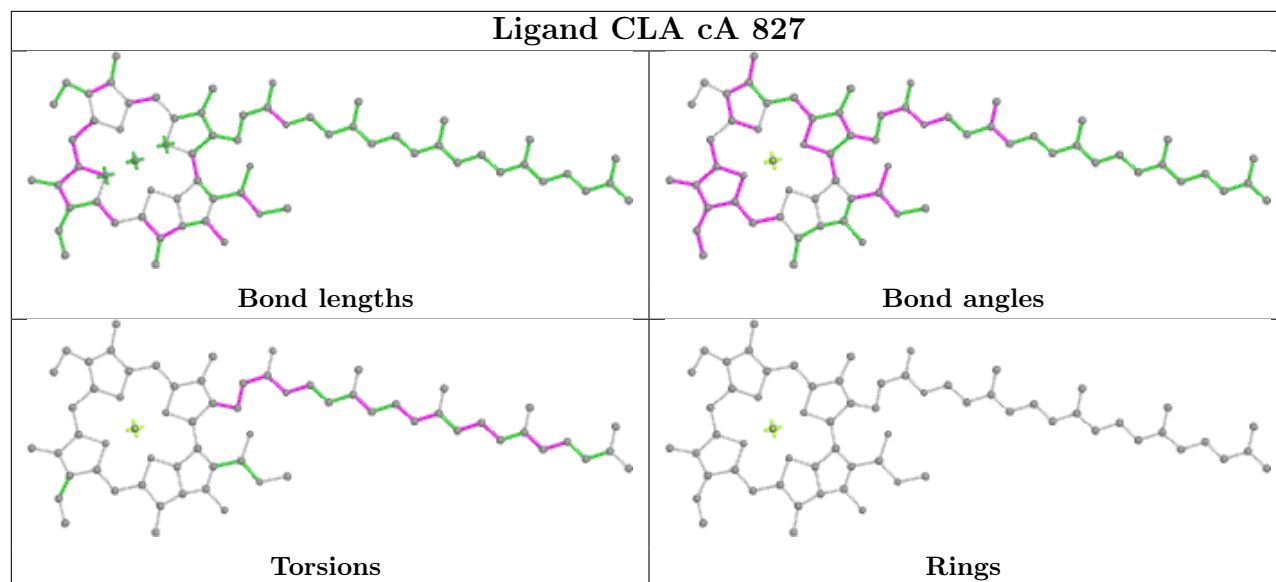


Rings

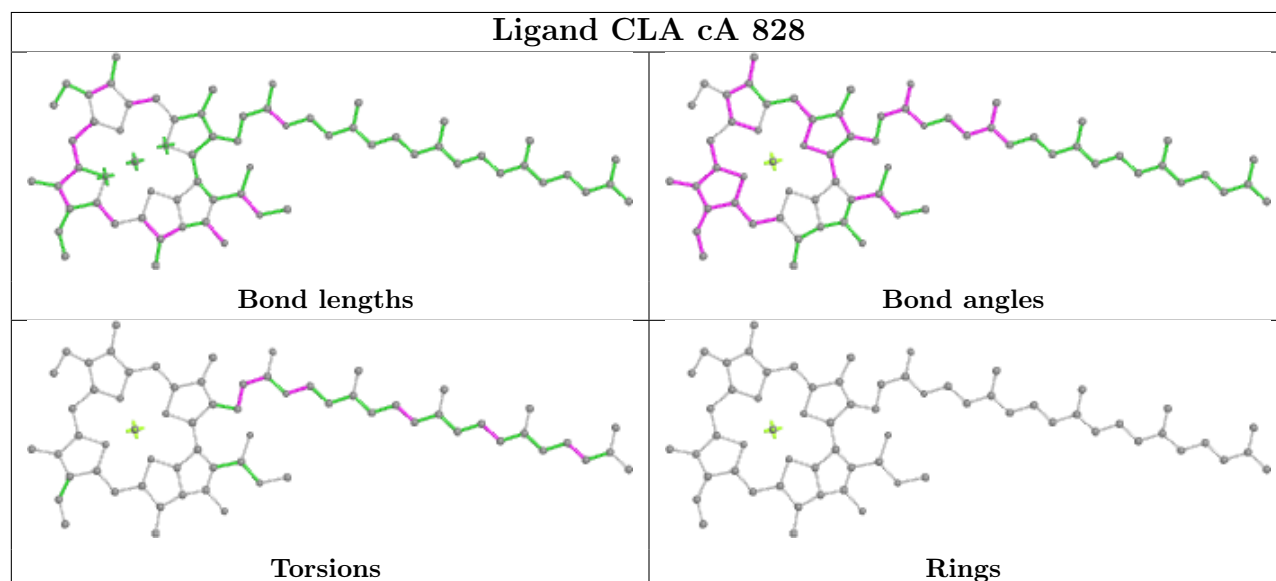
**Ligand CLA cA 823****Ligand CLA cA 824**



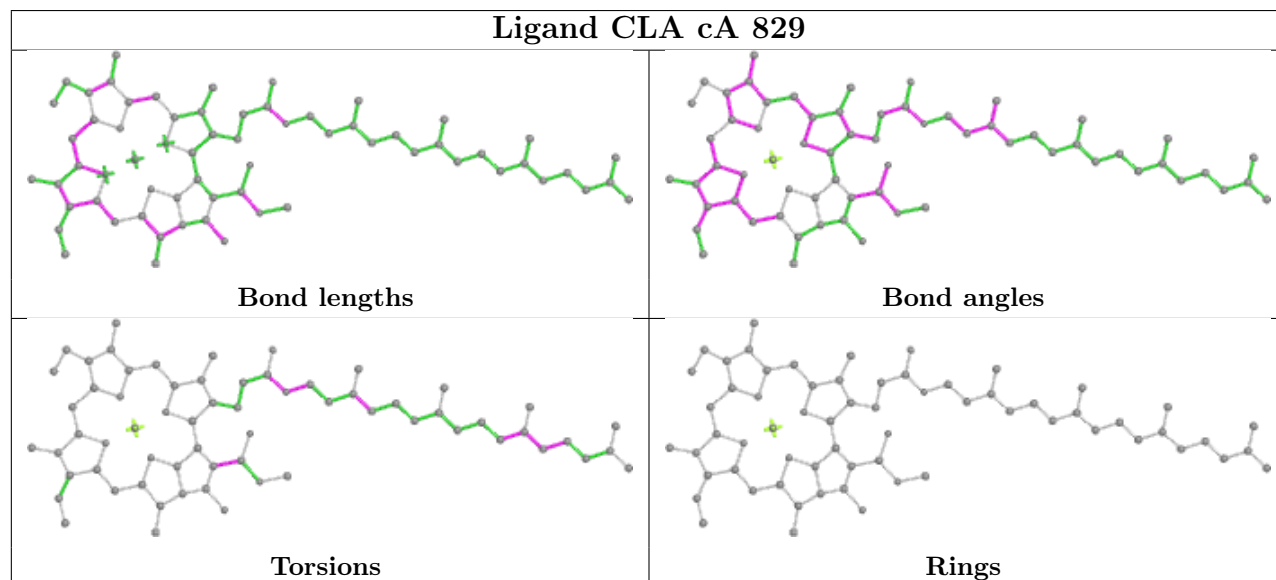
## Ligand CLA cA 827

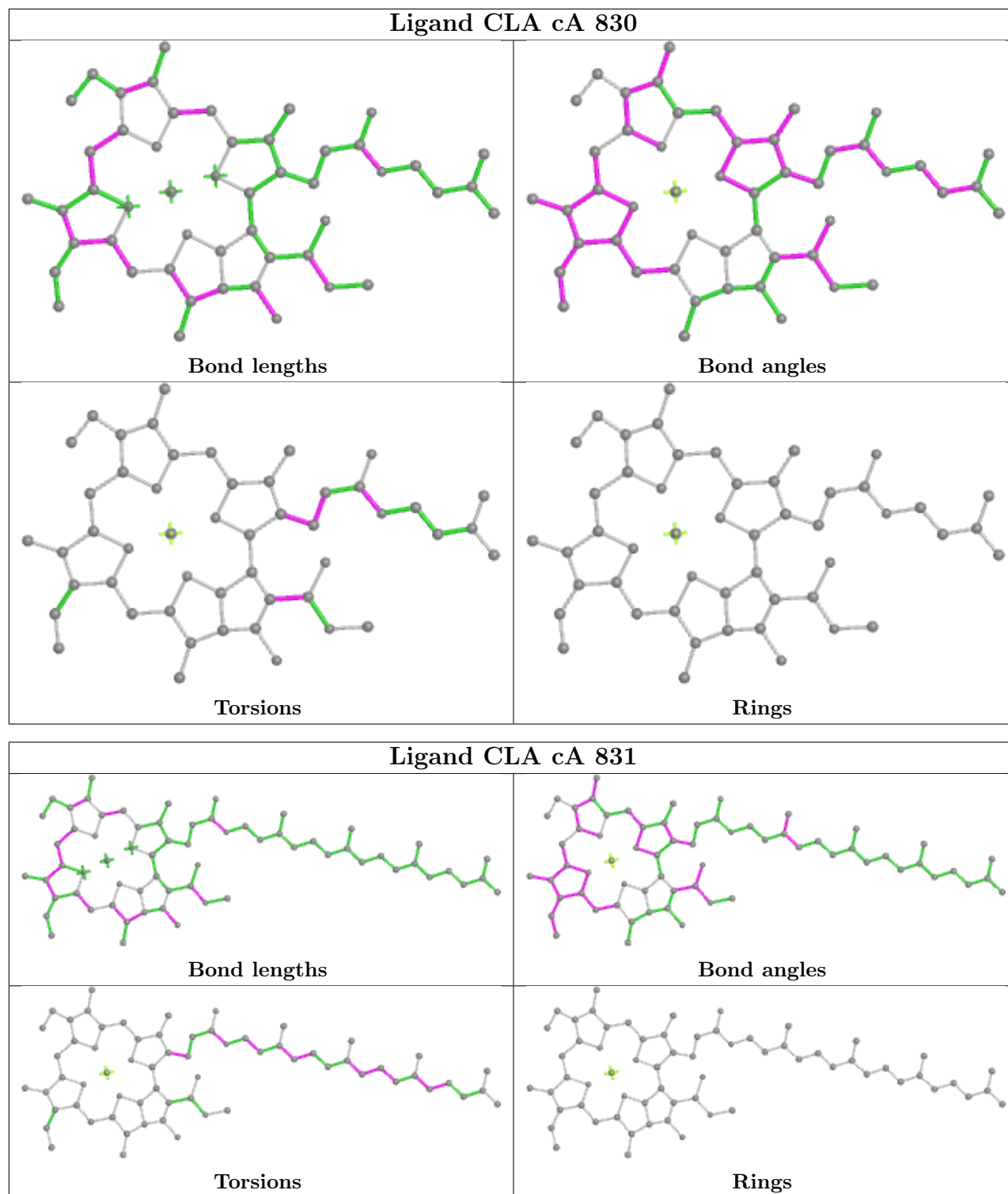


## Ligand CLA cA 828

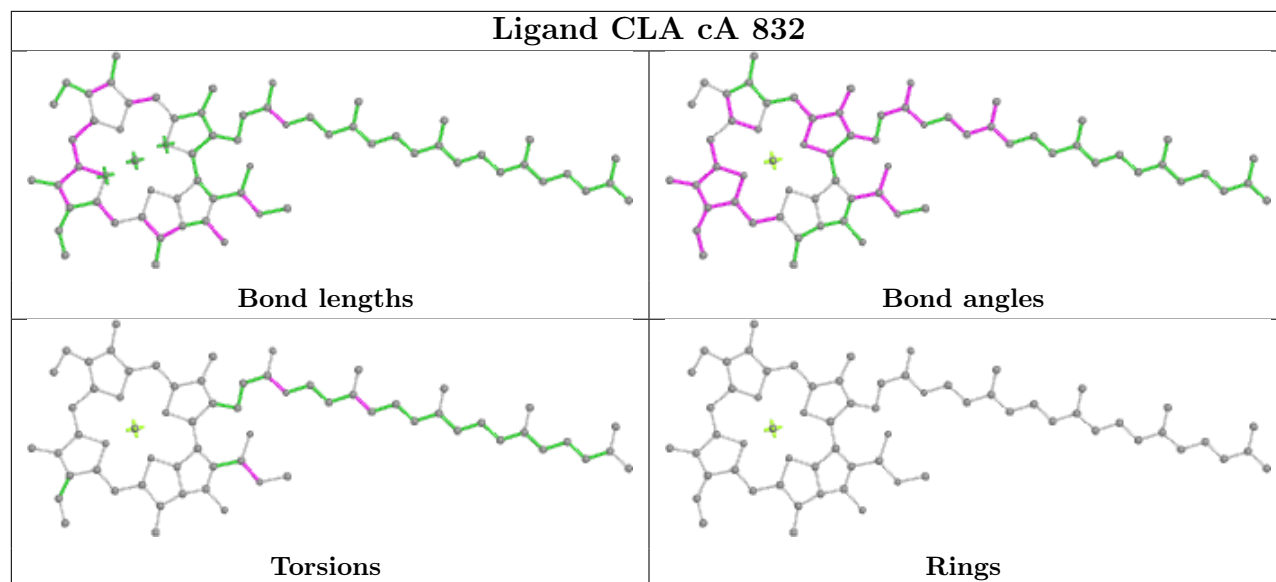


## Ligand CLA cA 829

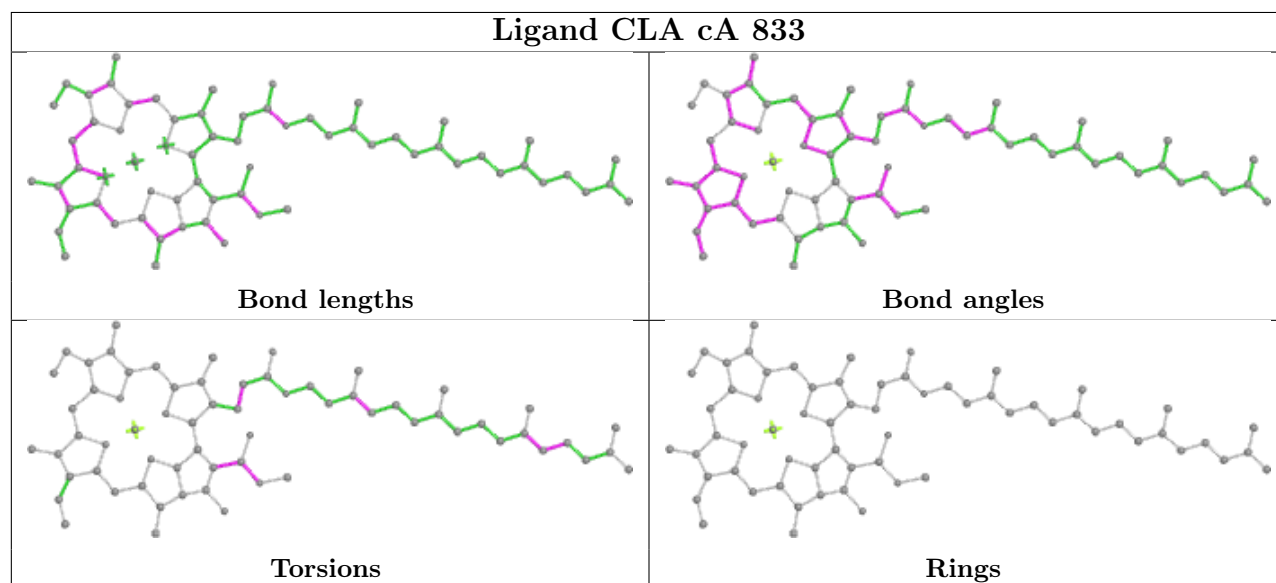


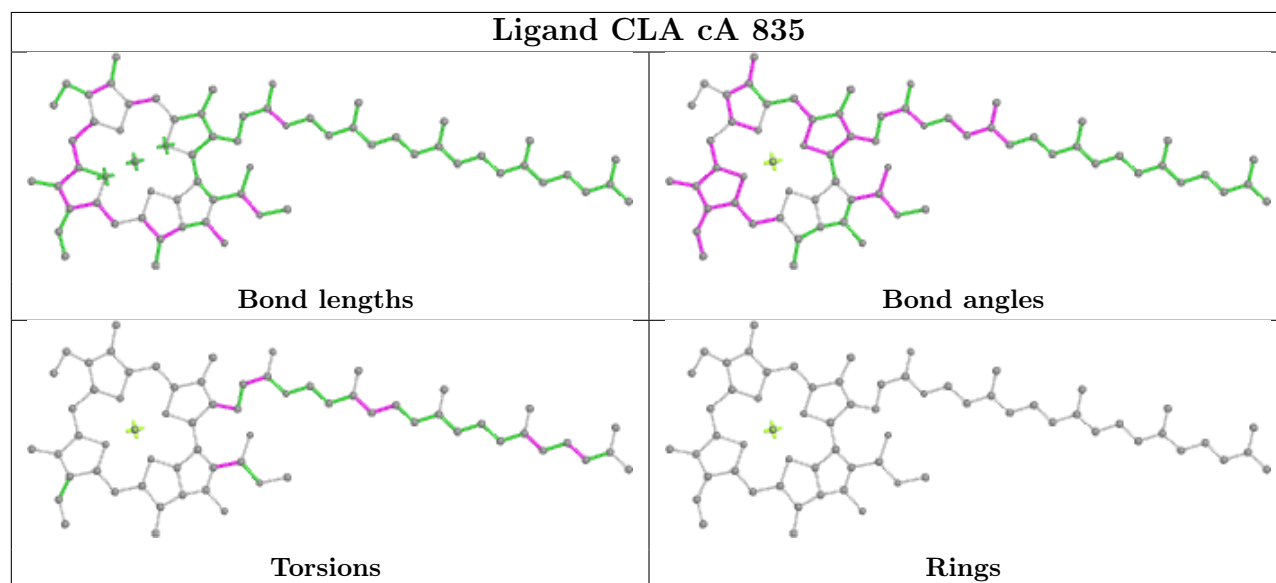
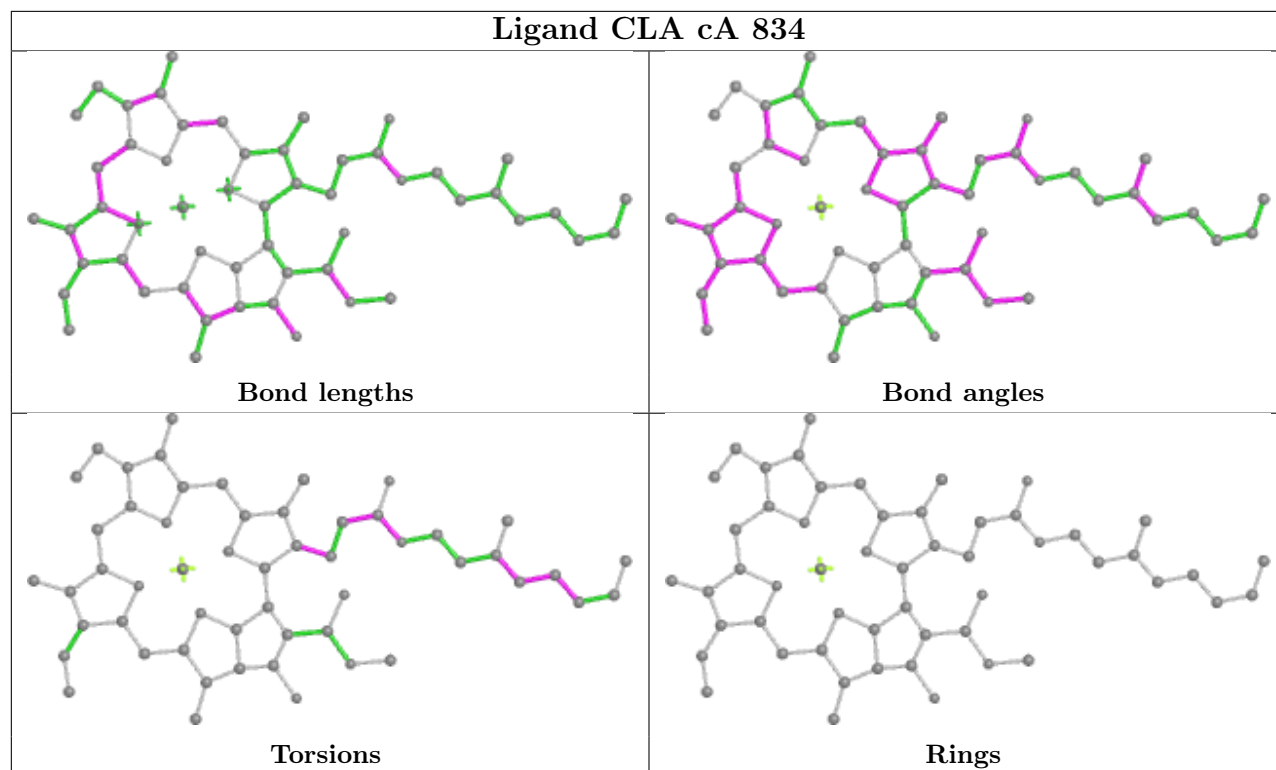


## Ligand CLA cA 832

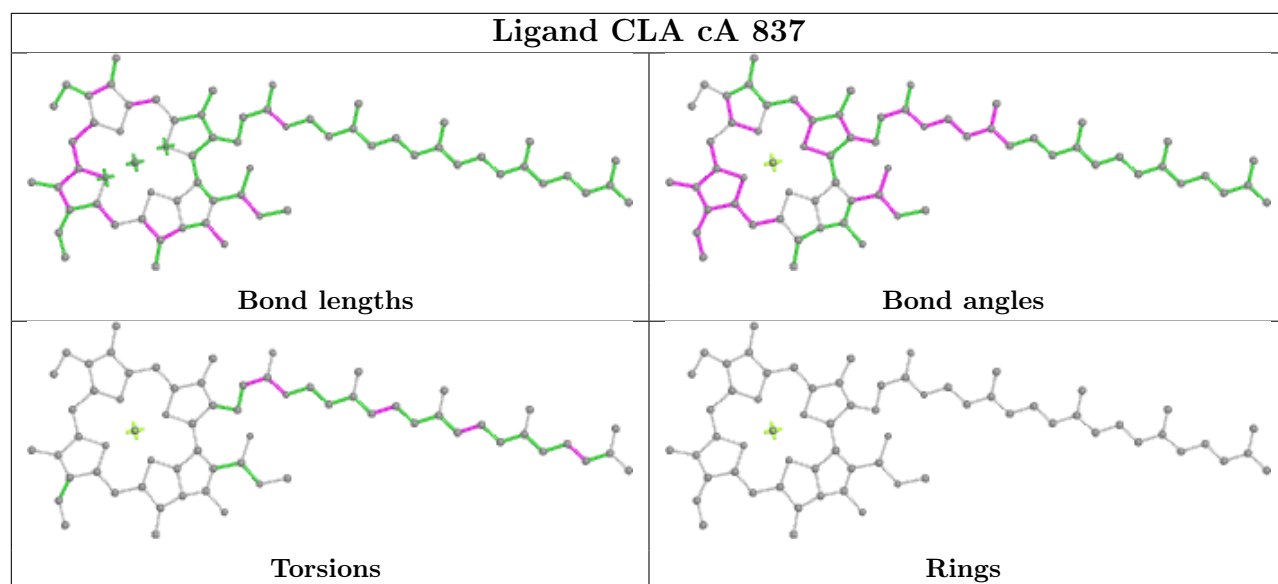
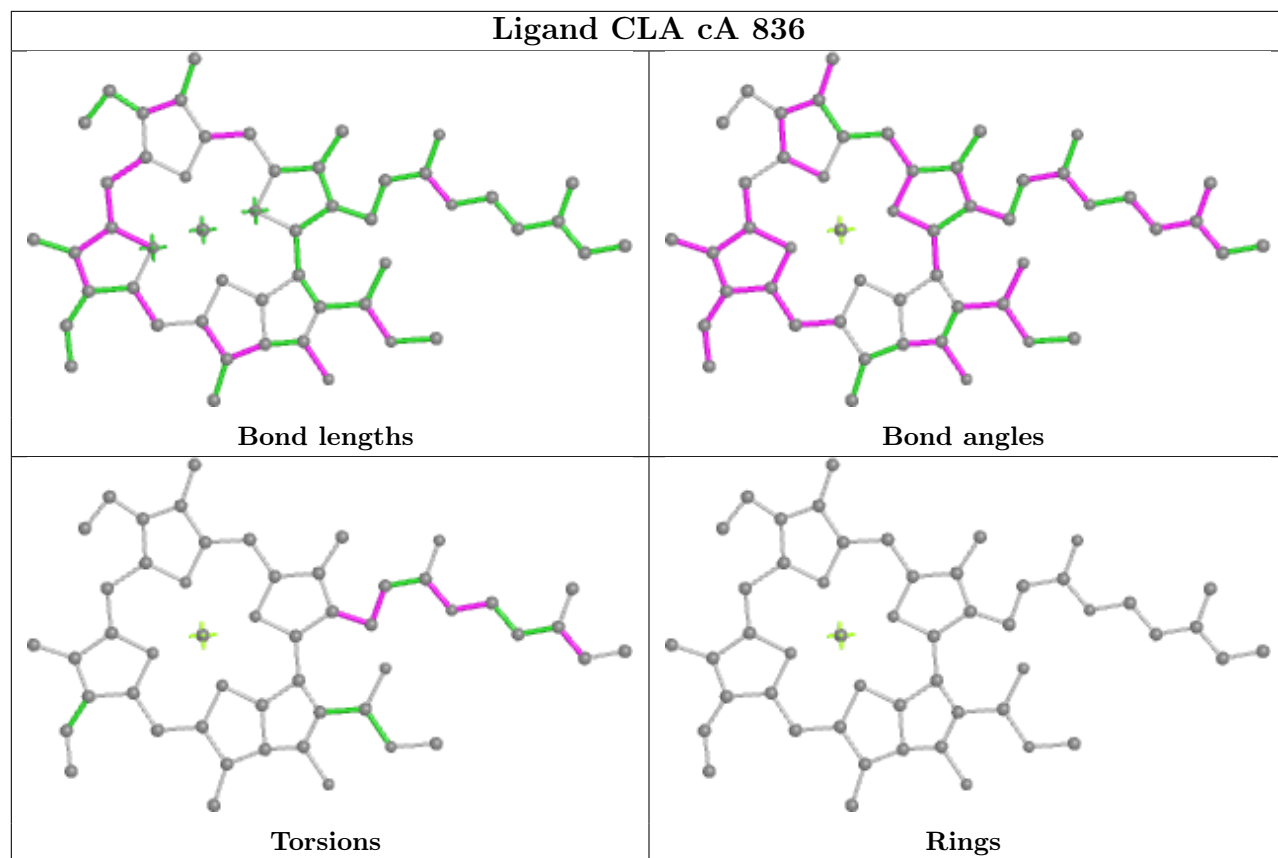


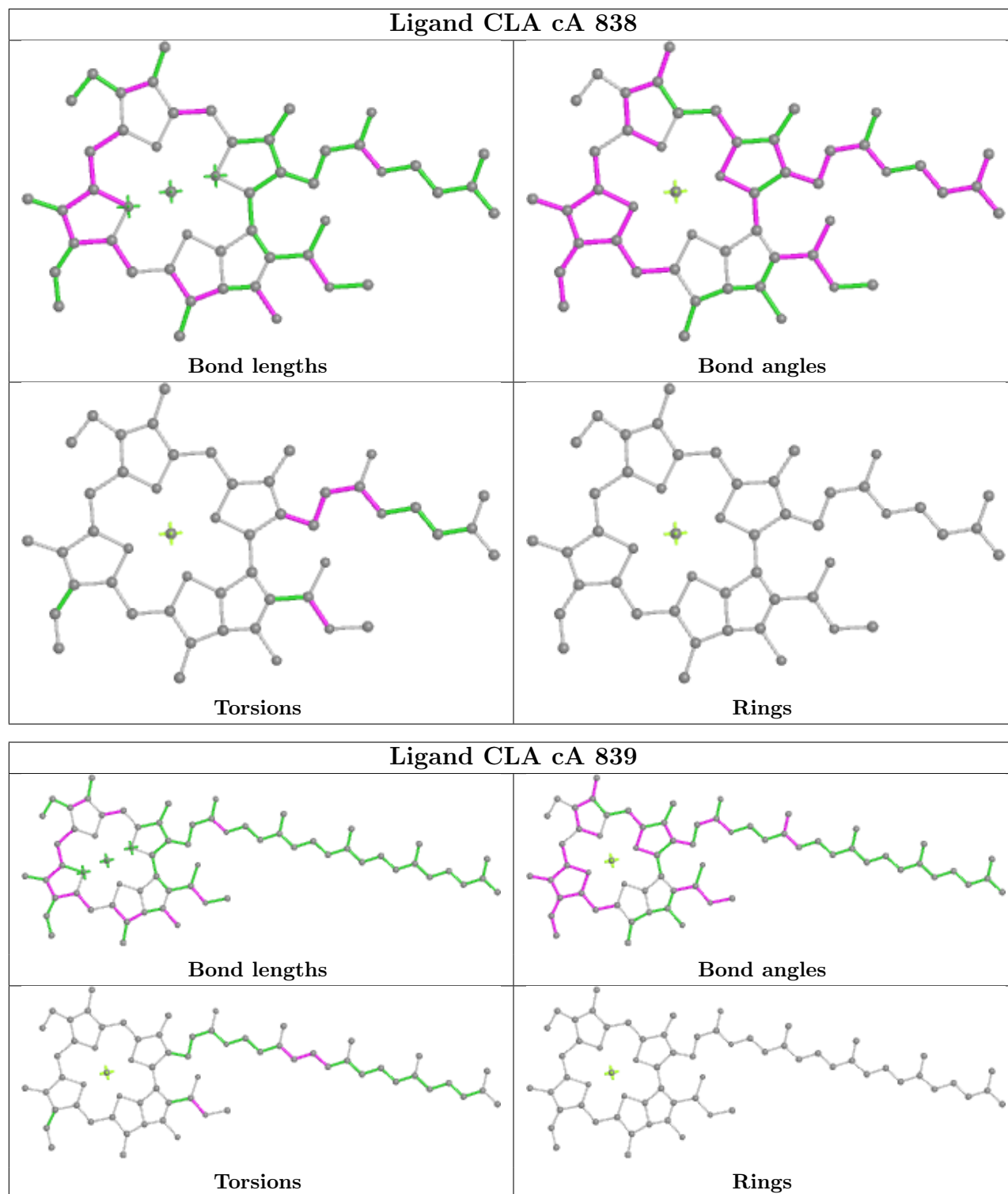
## Ligand CLA cA 833

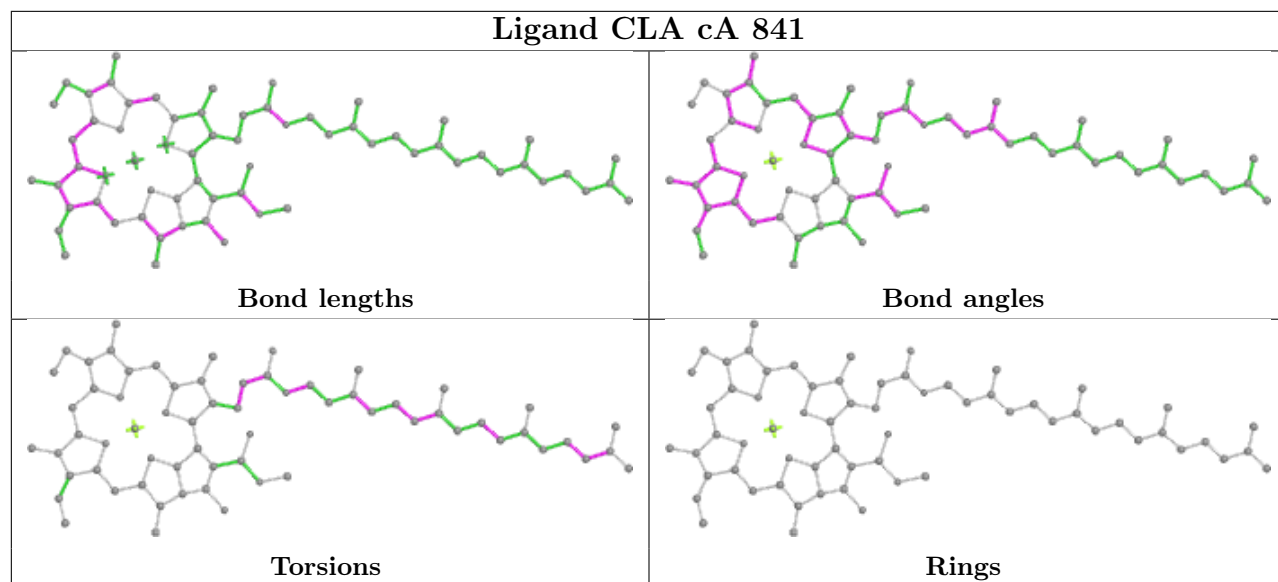
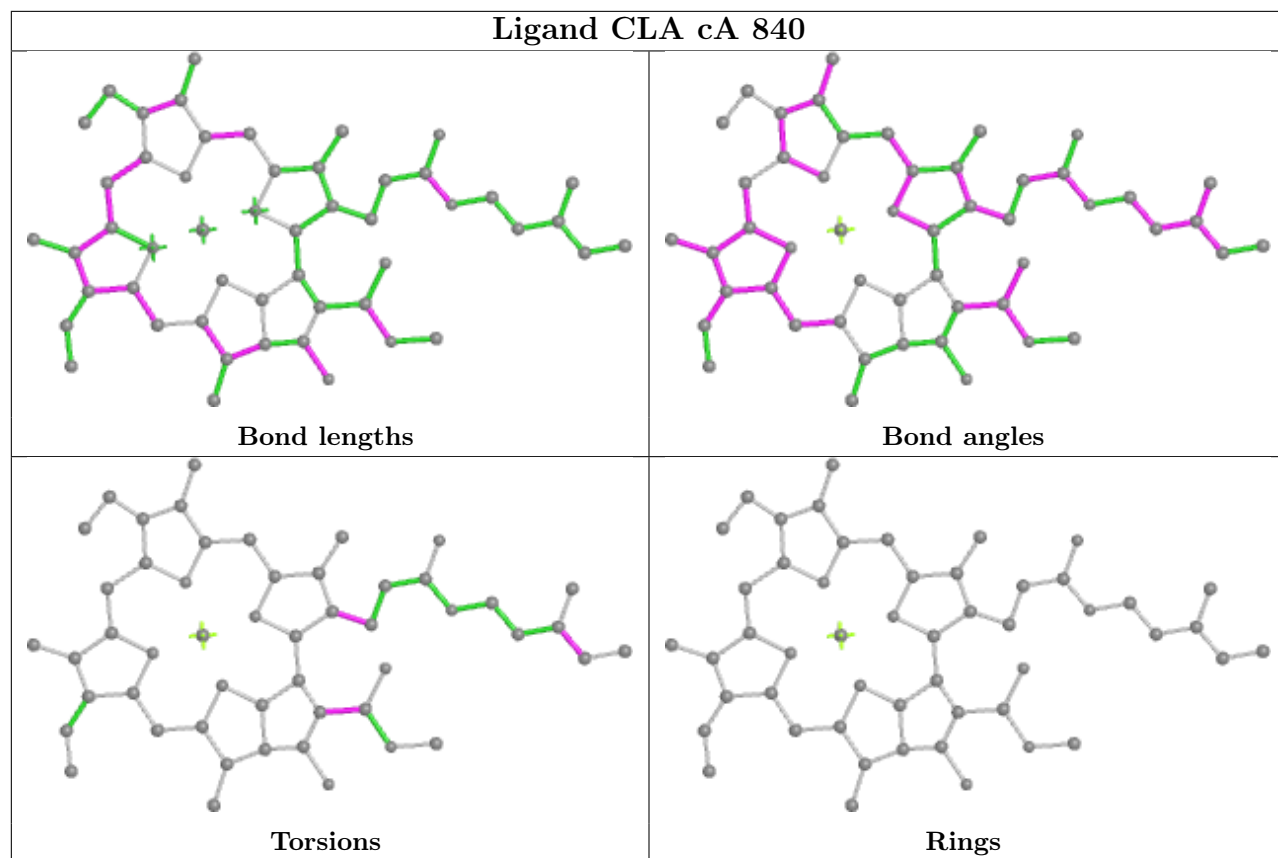


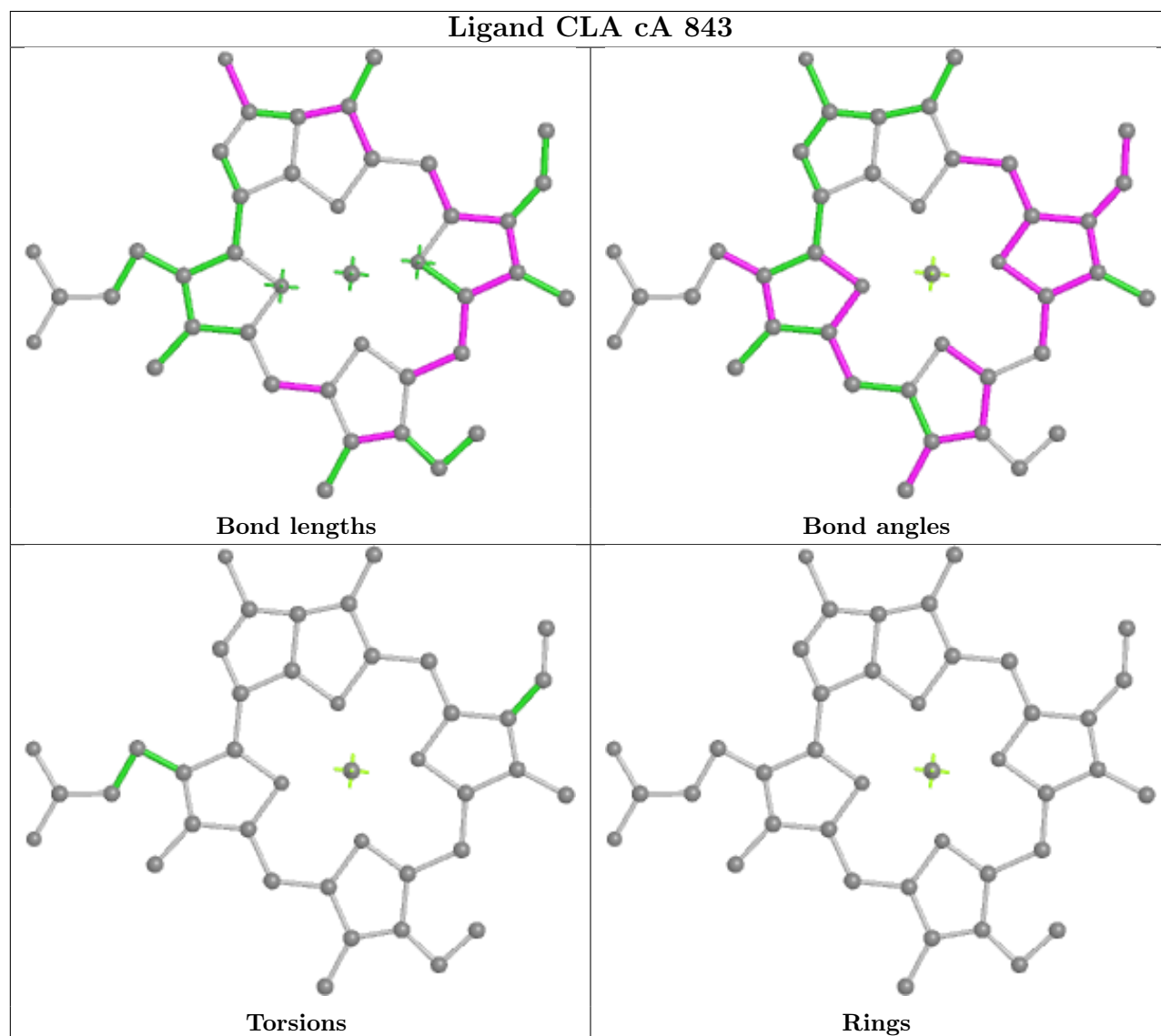
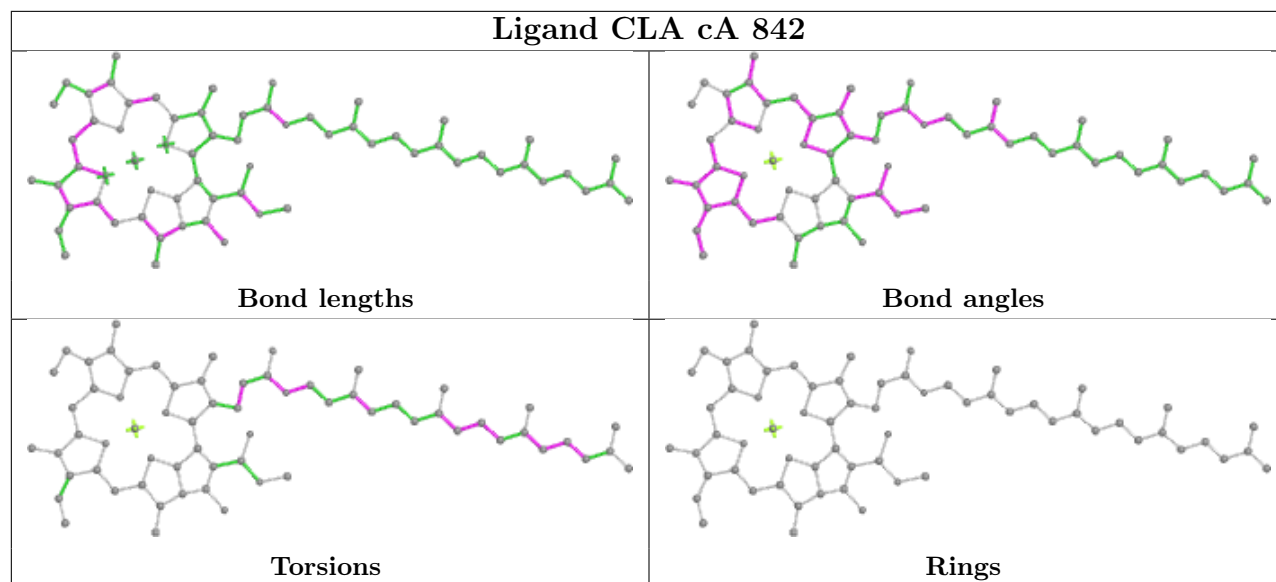


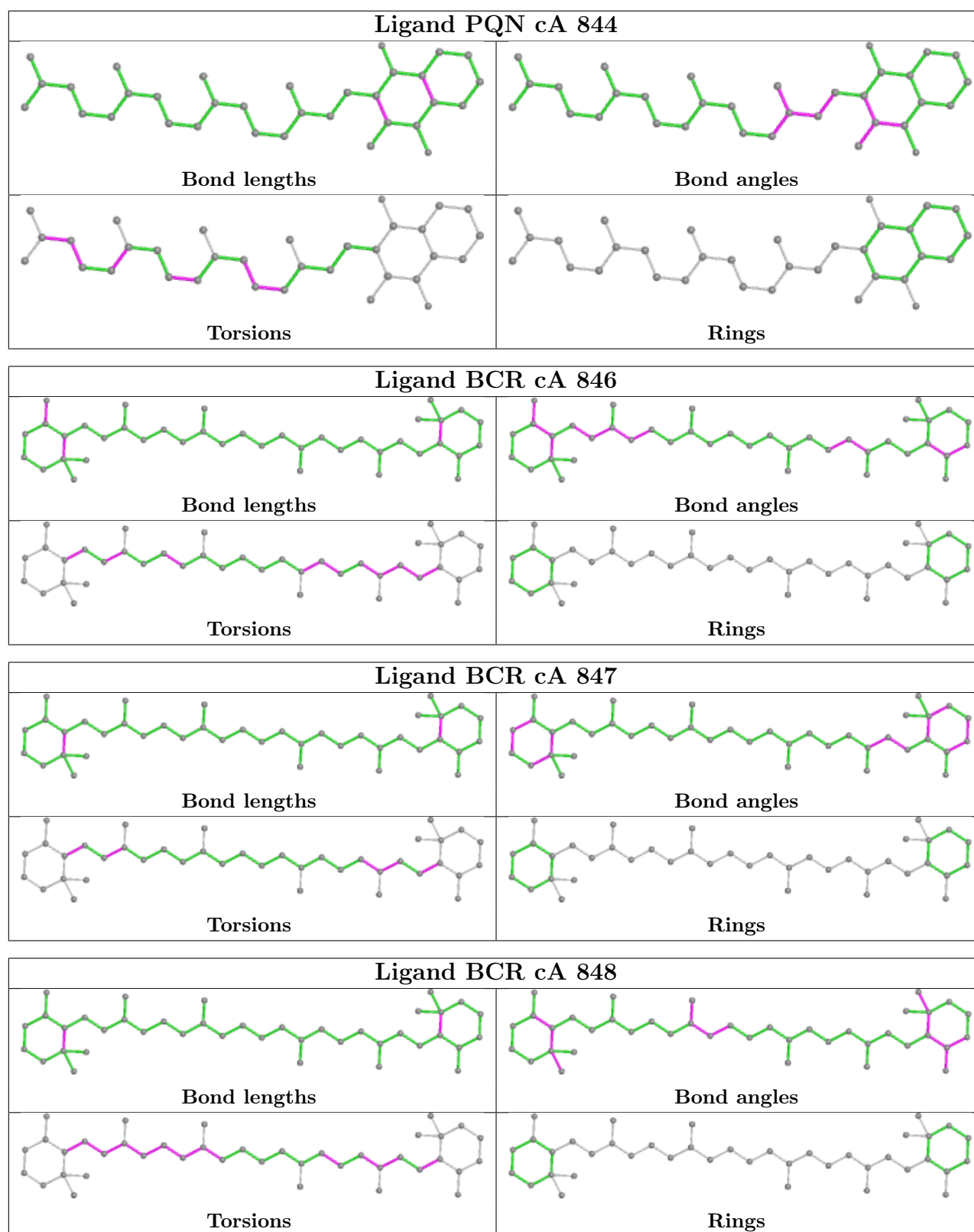


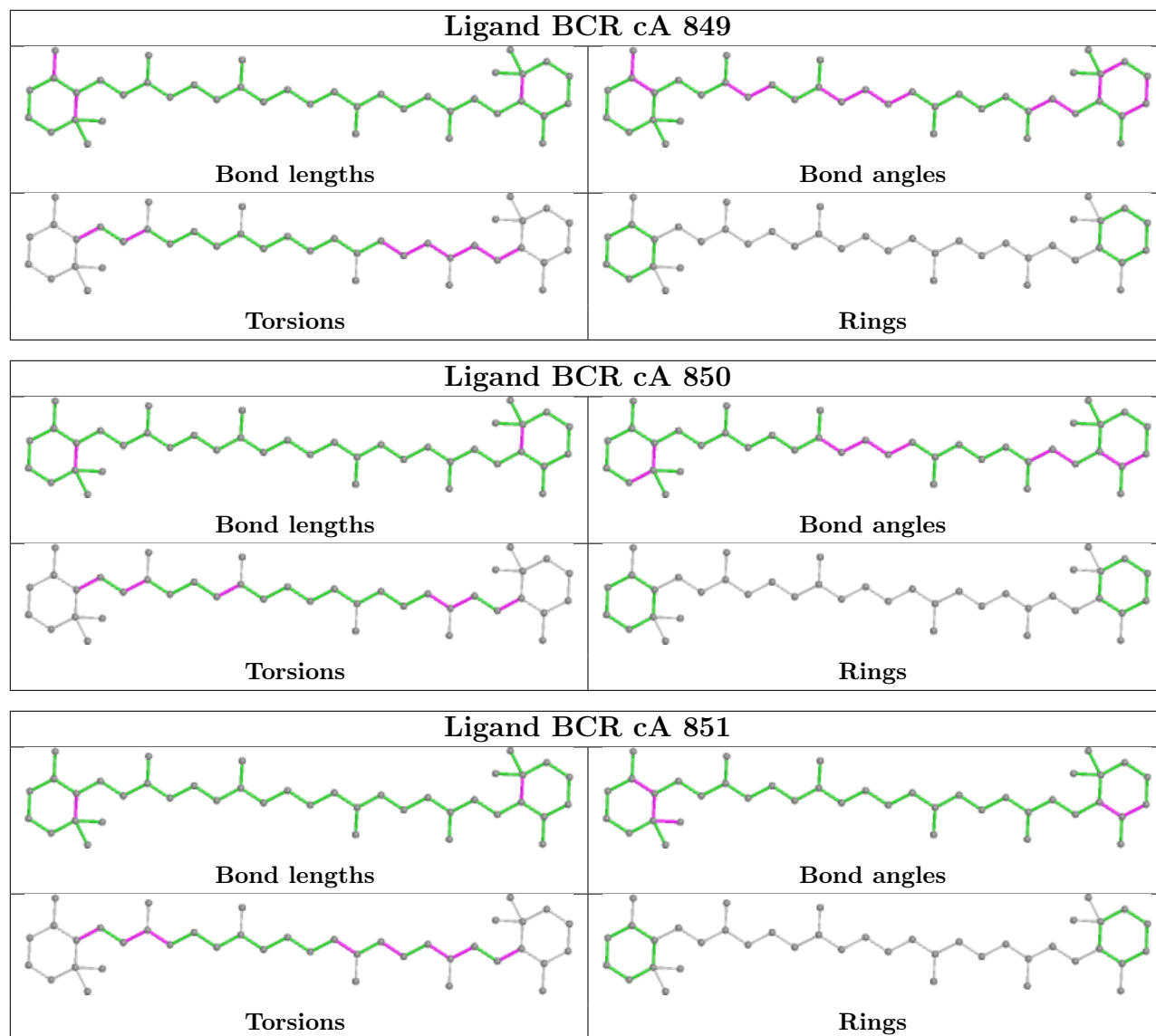


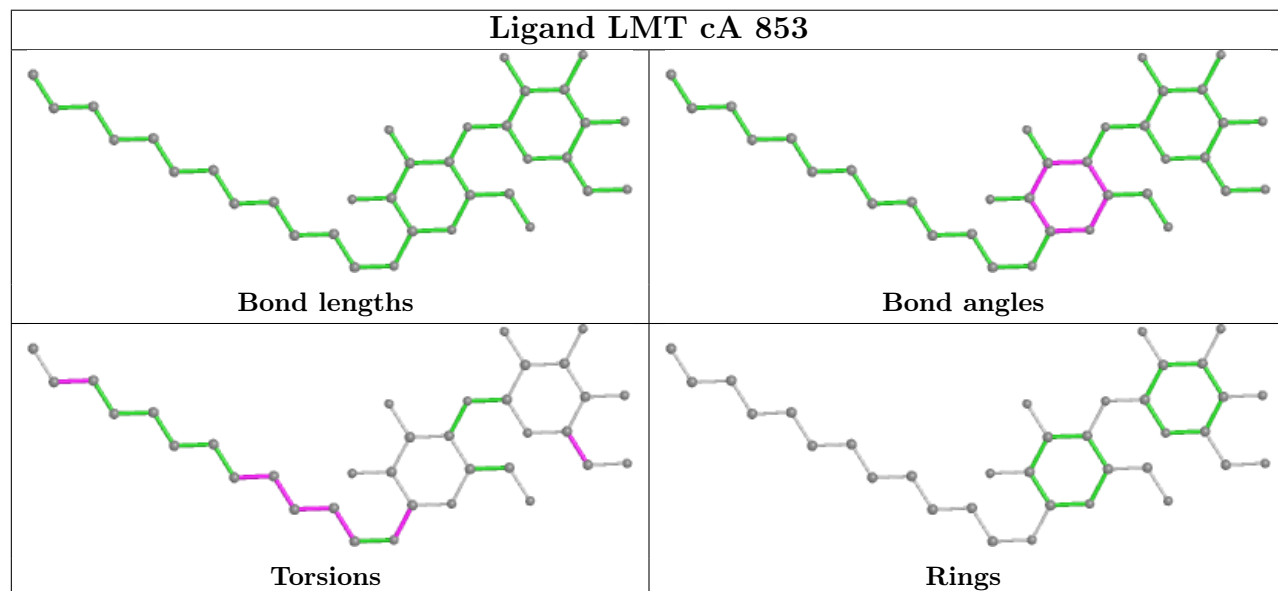
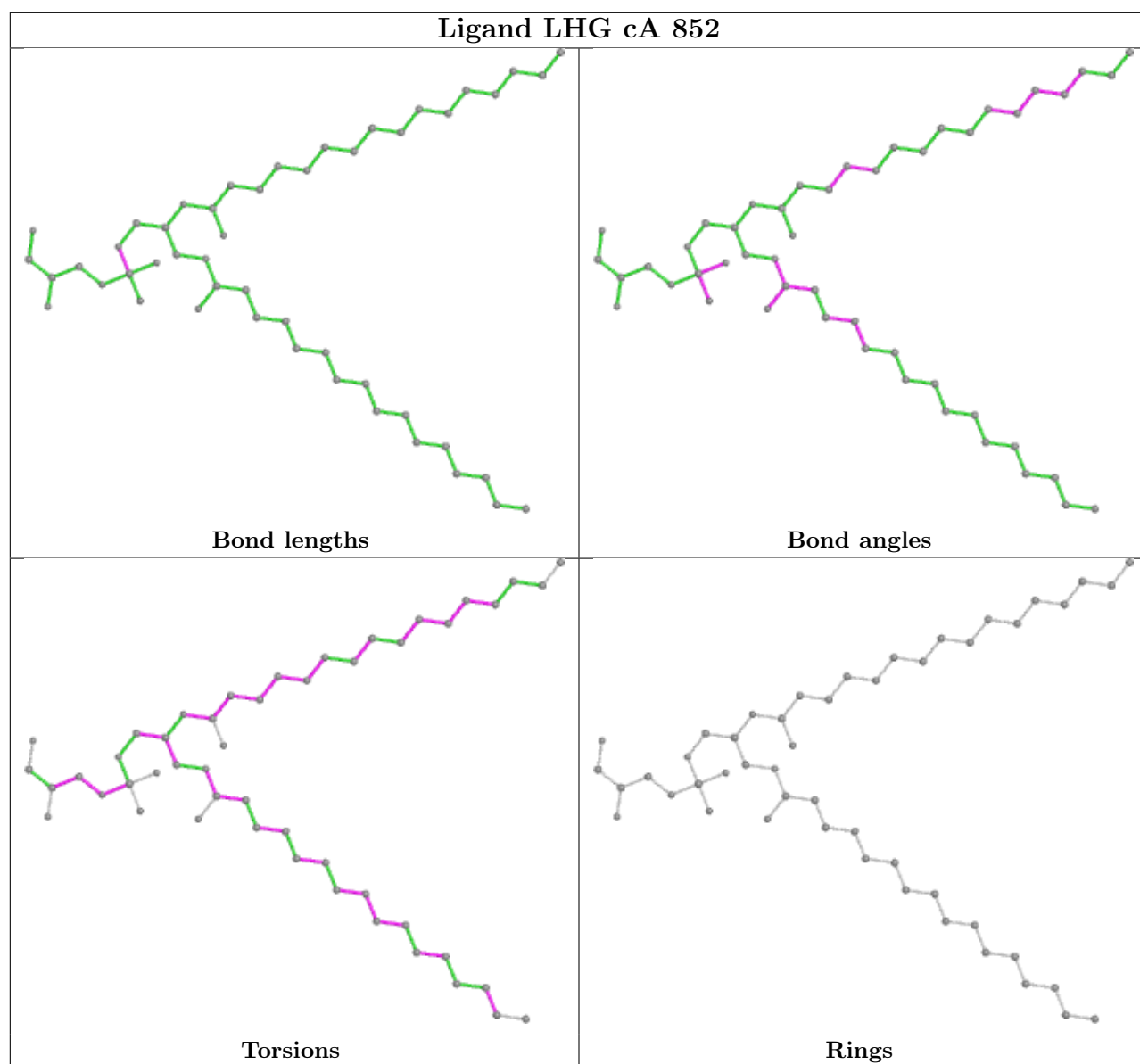


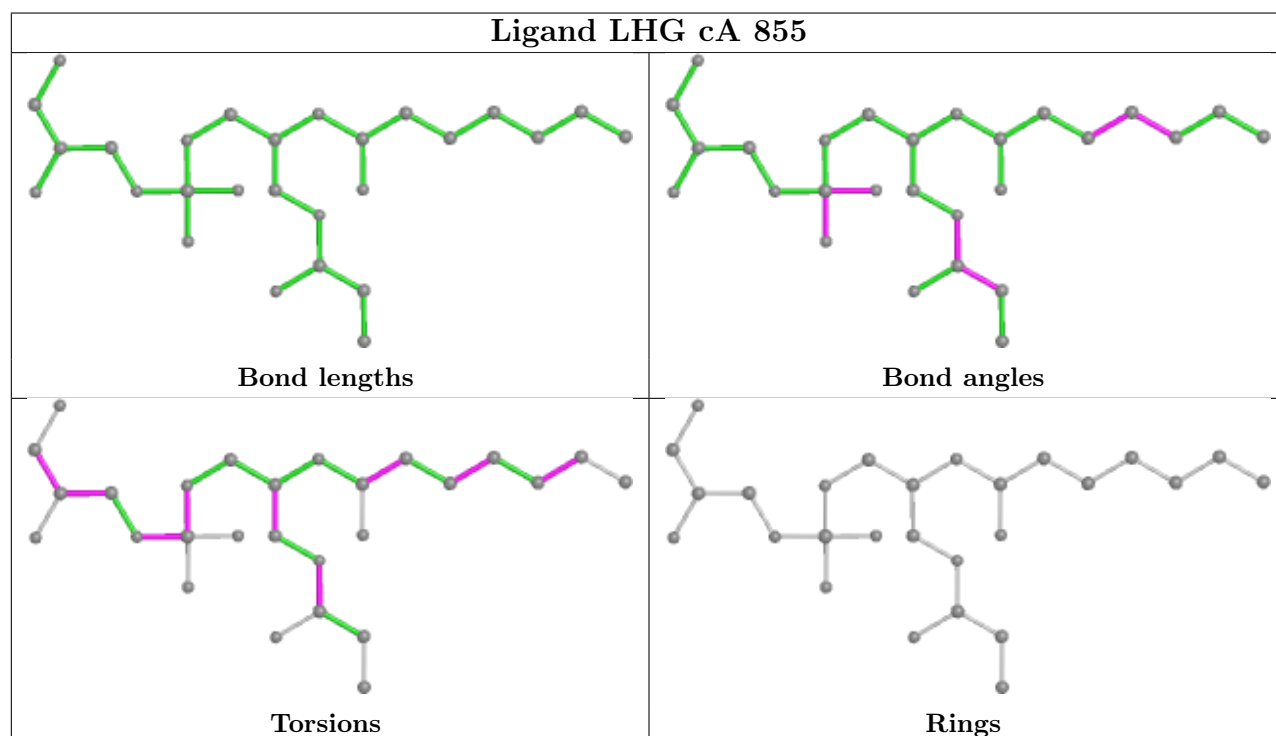
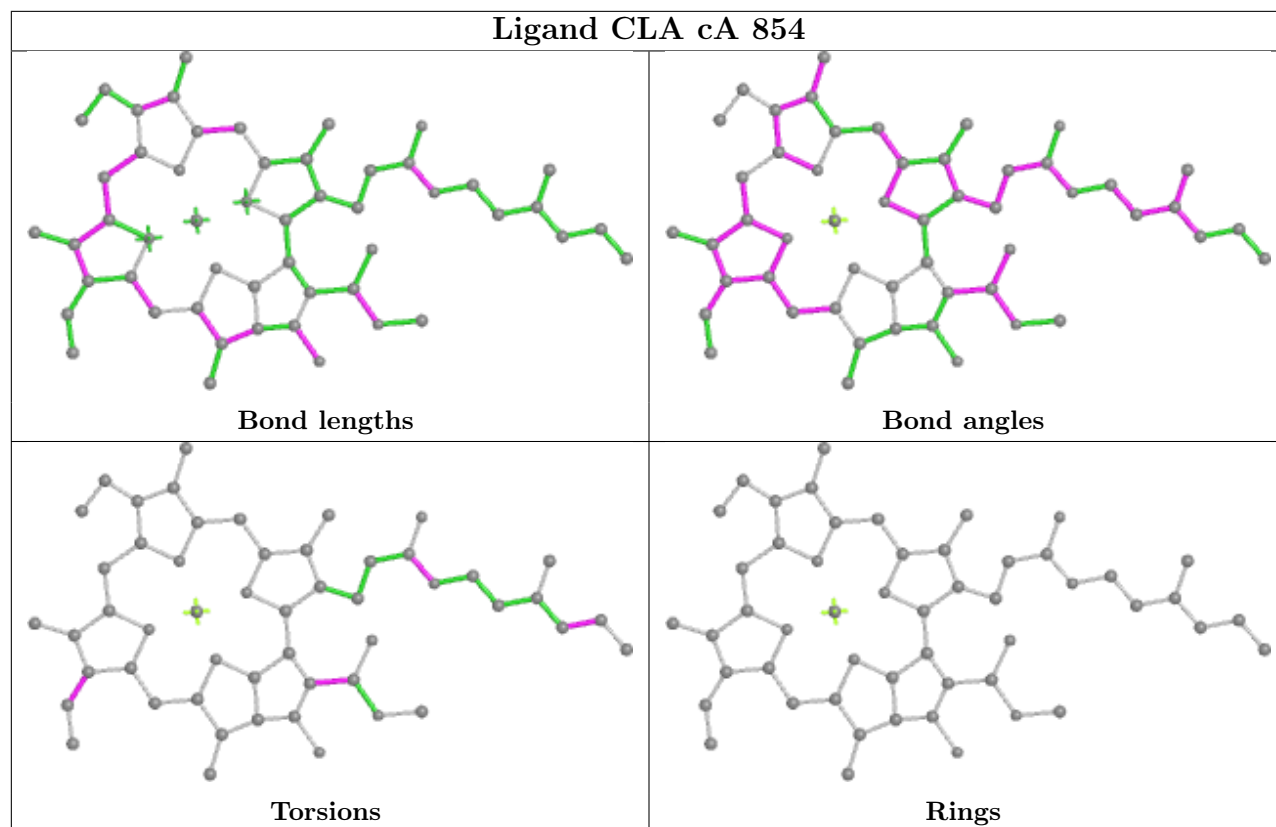




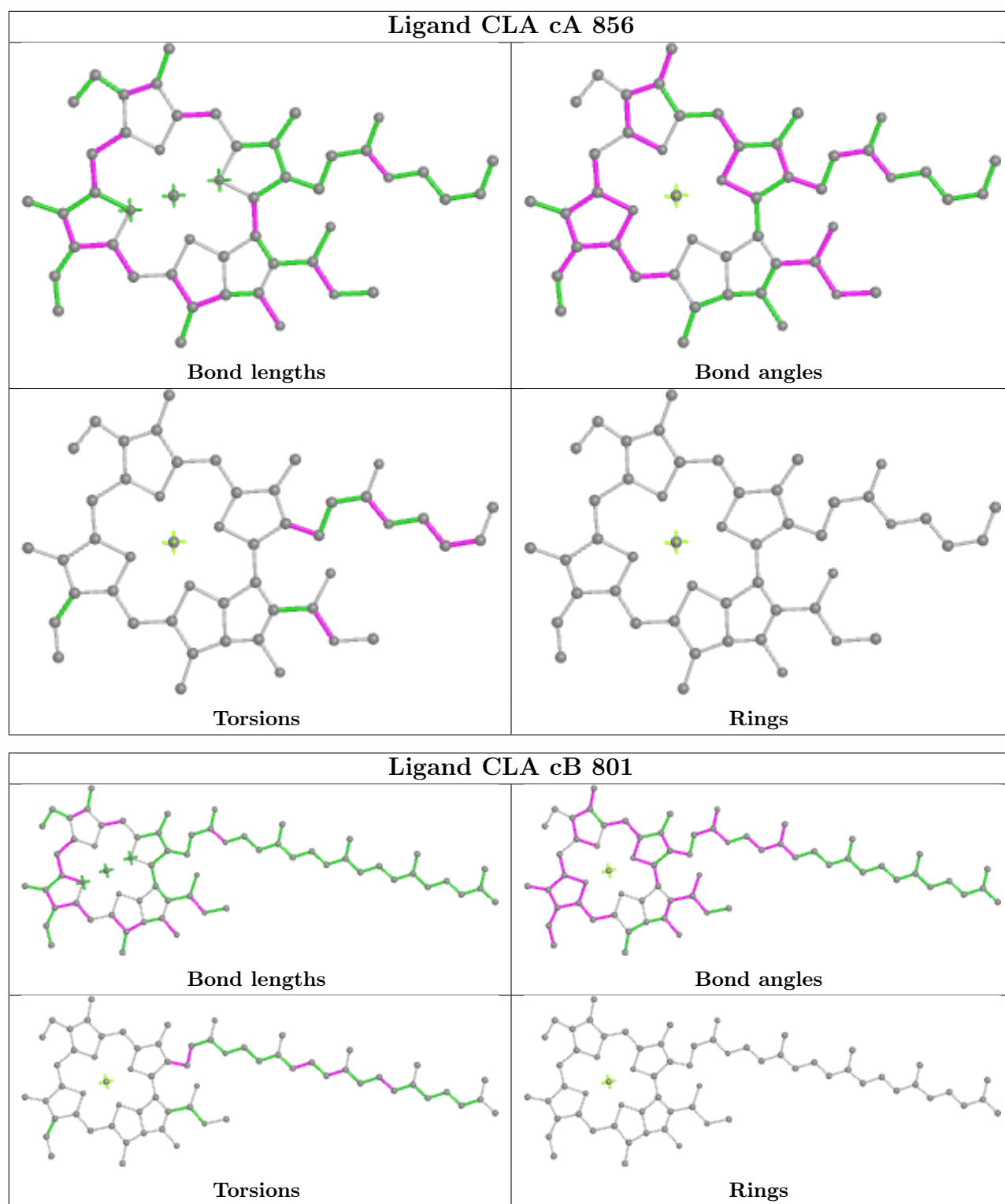


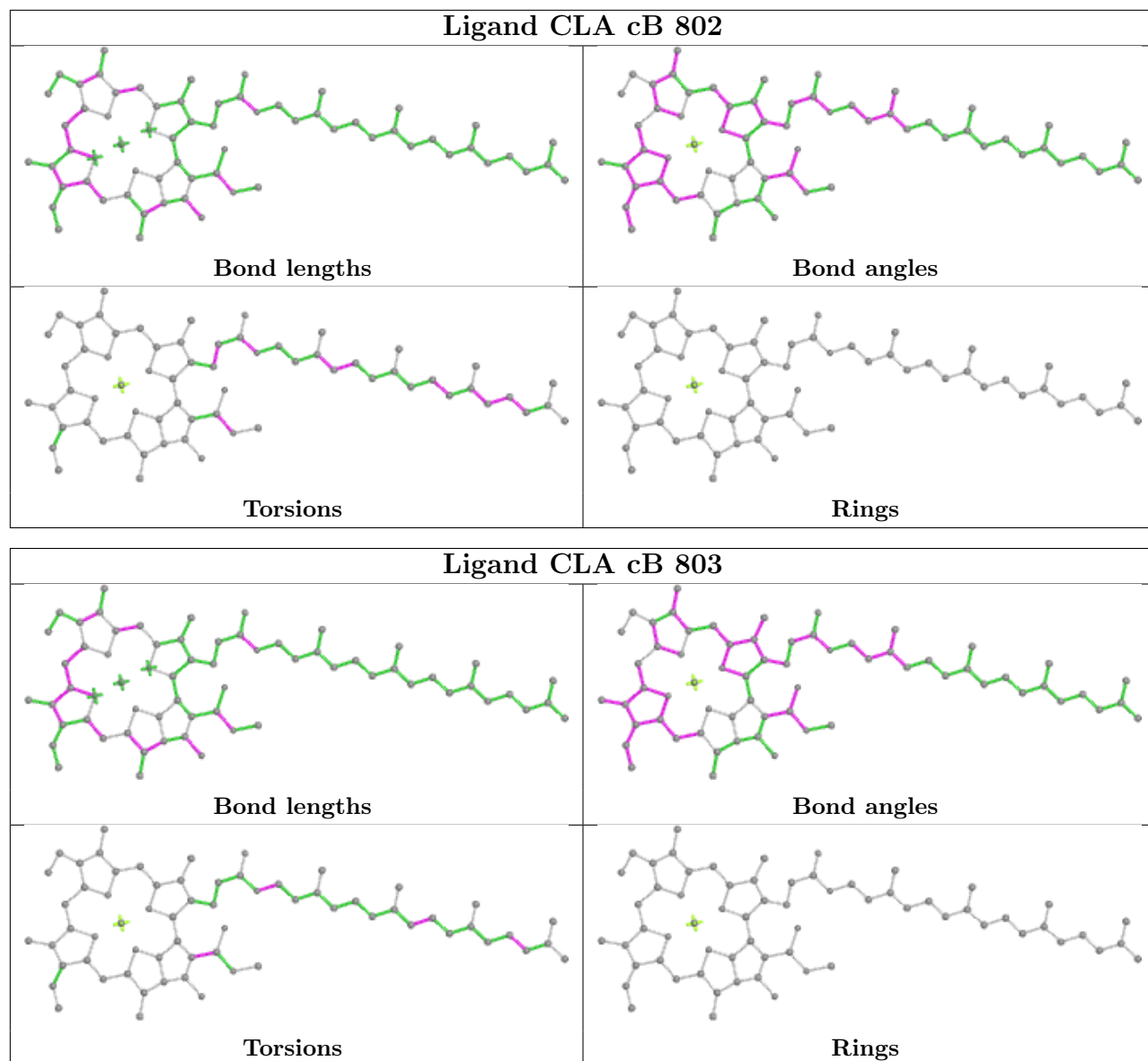


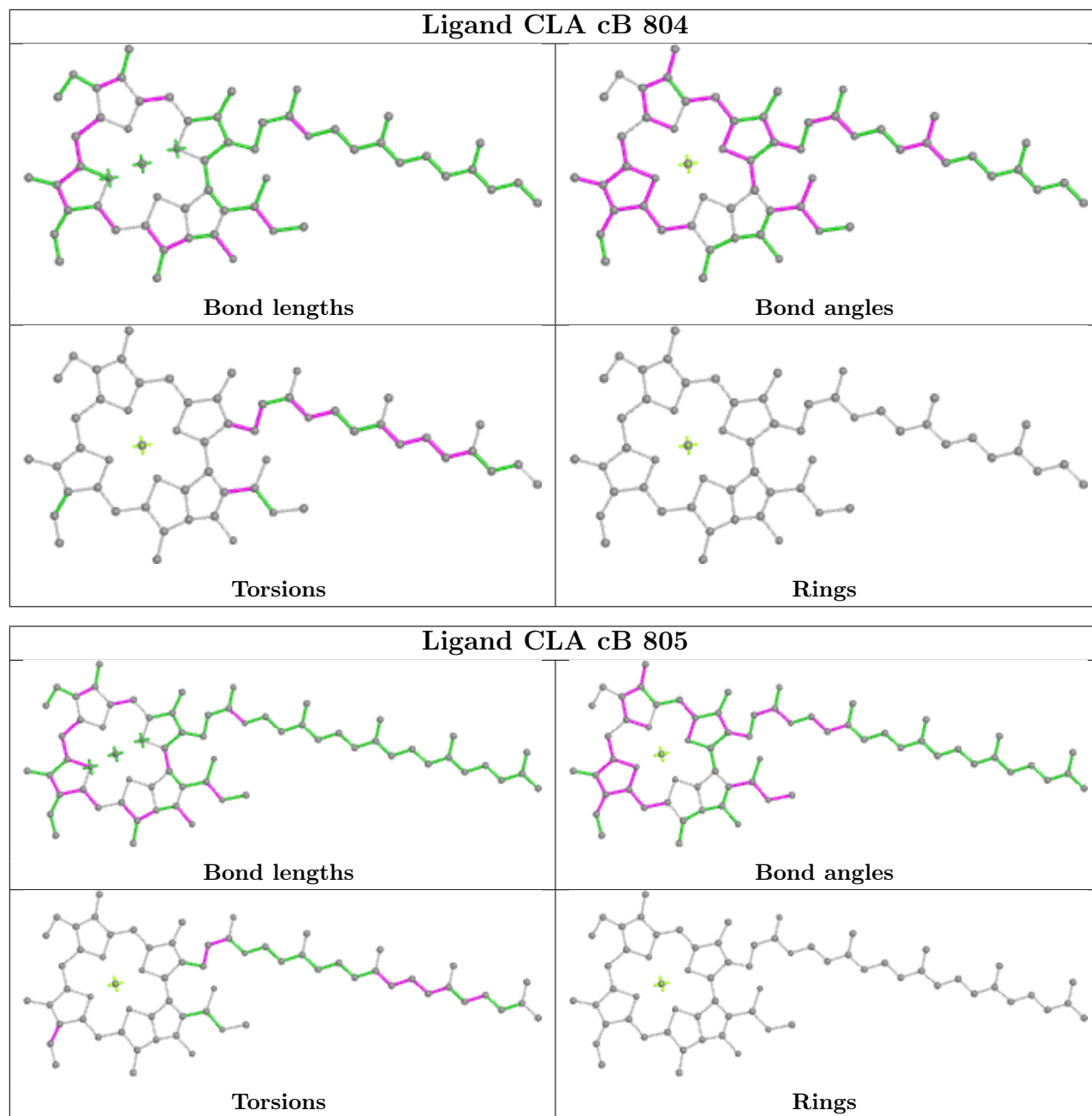


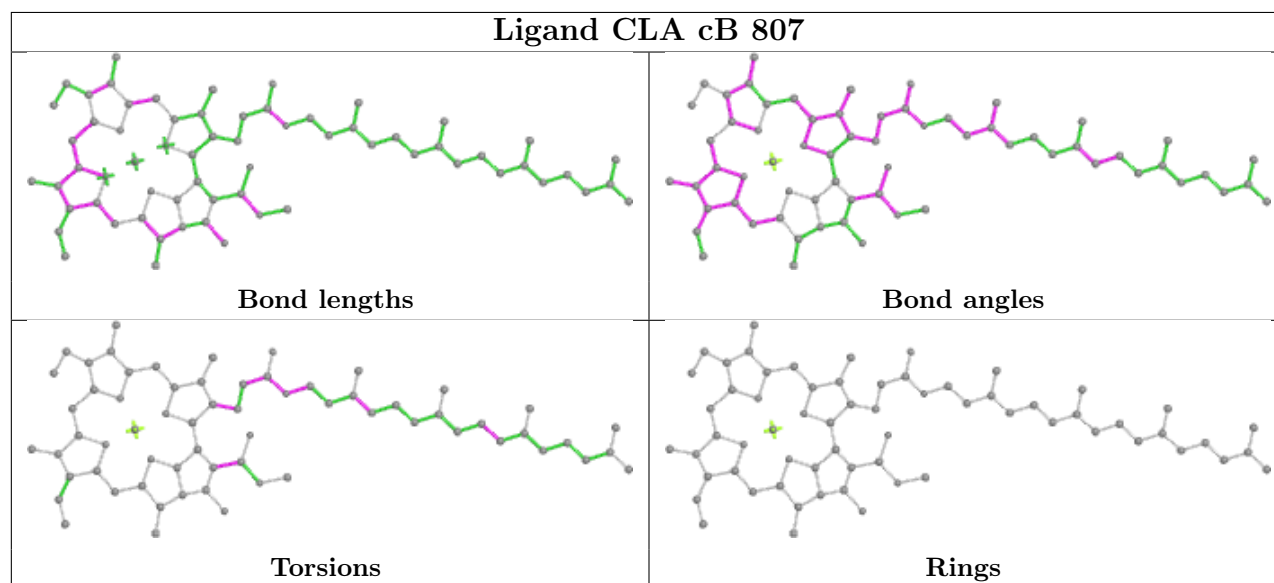
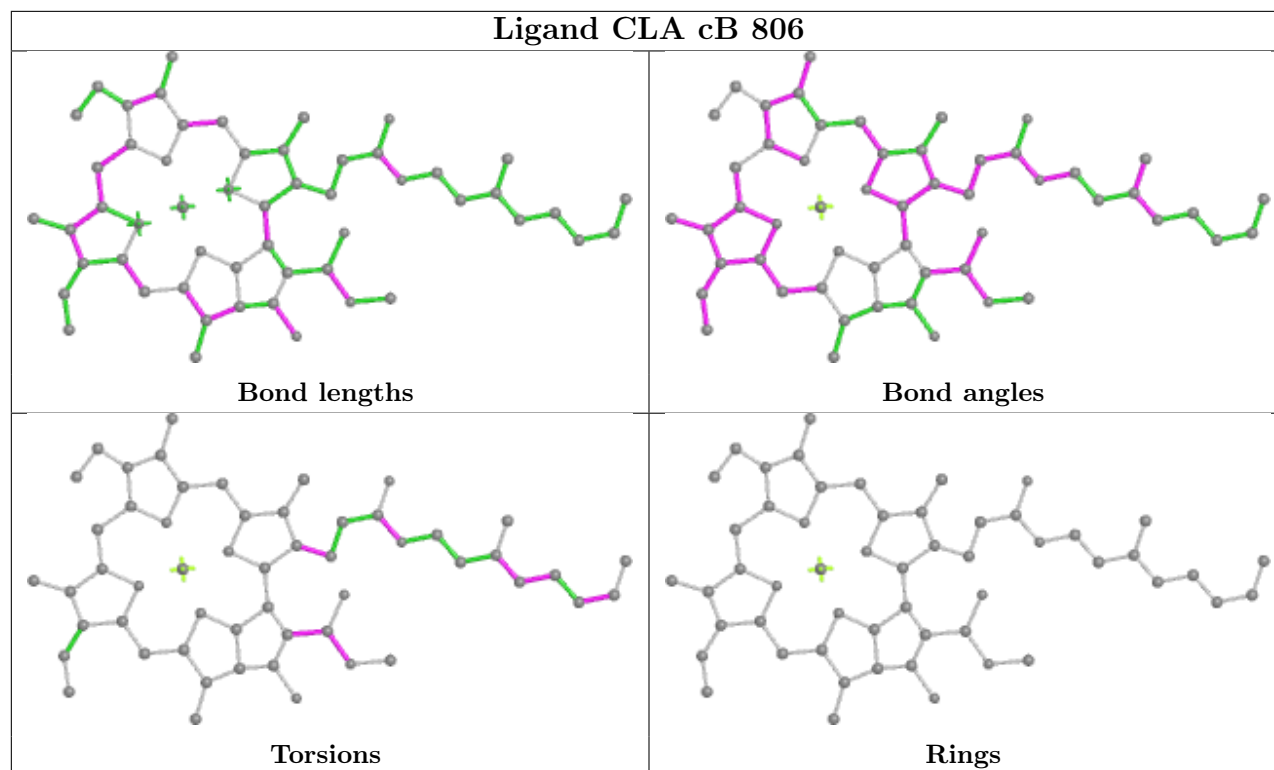




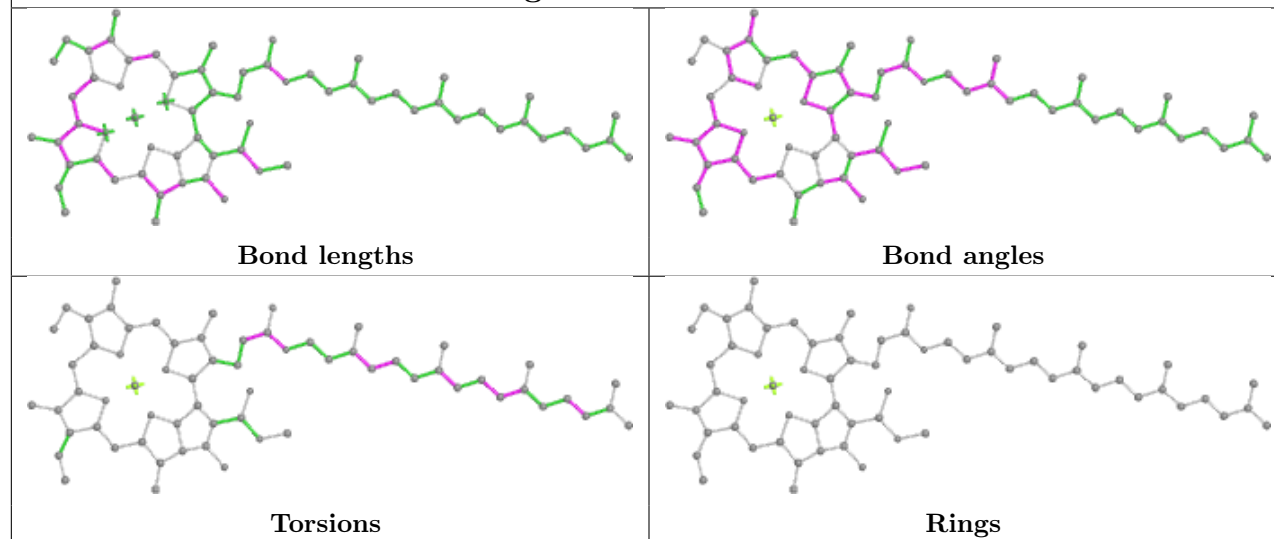




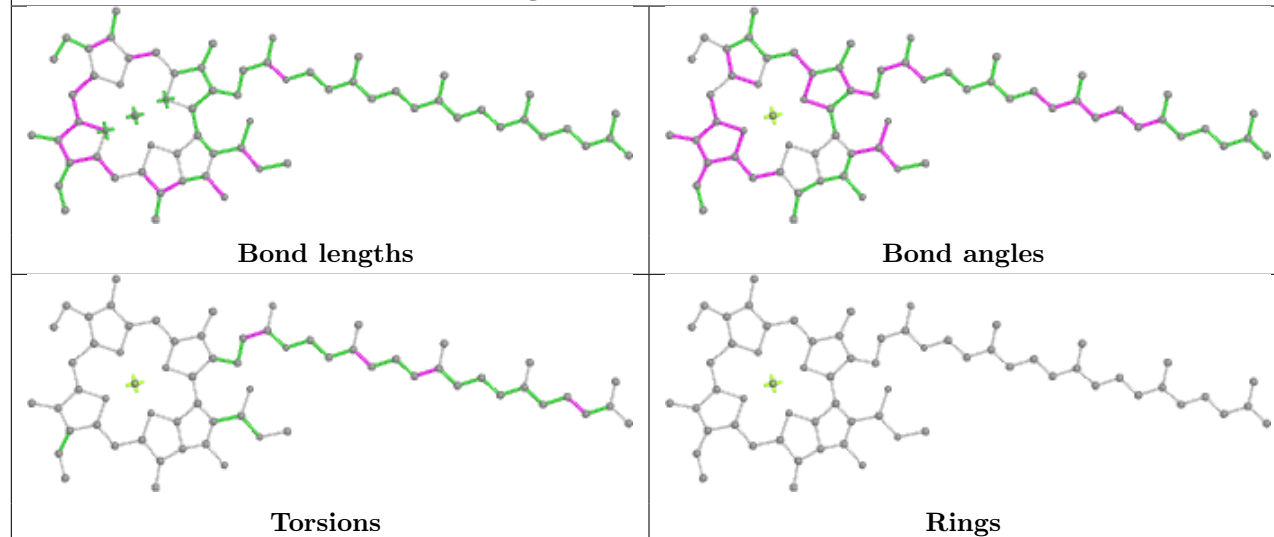


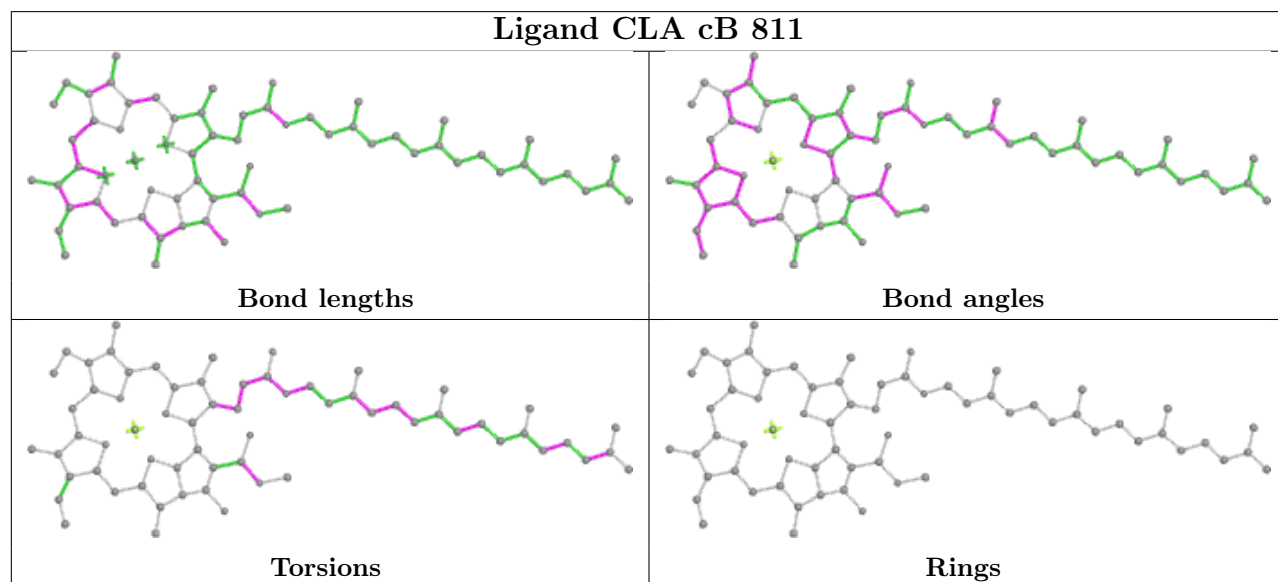
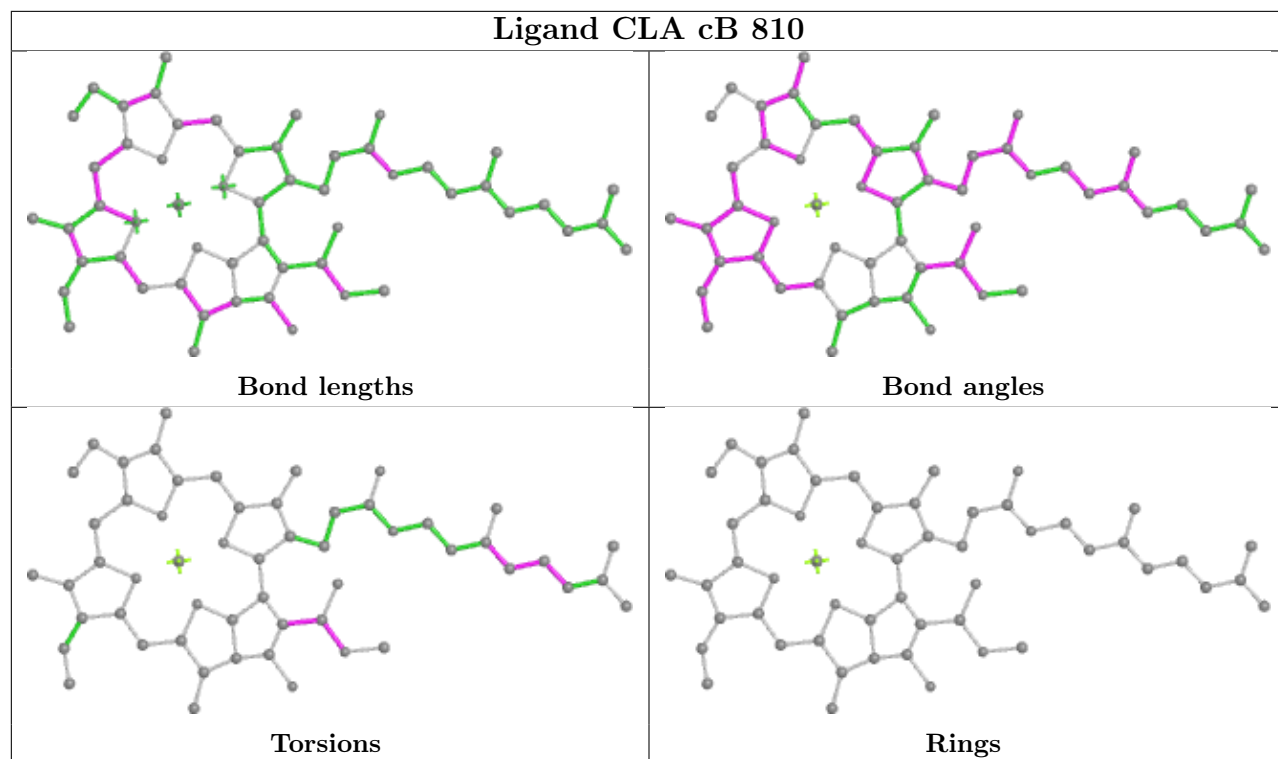


## Ligand CLA cB 808

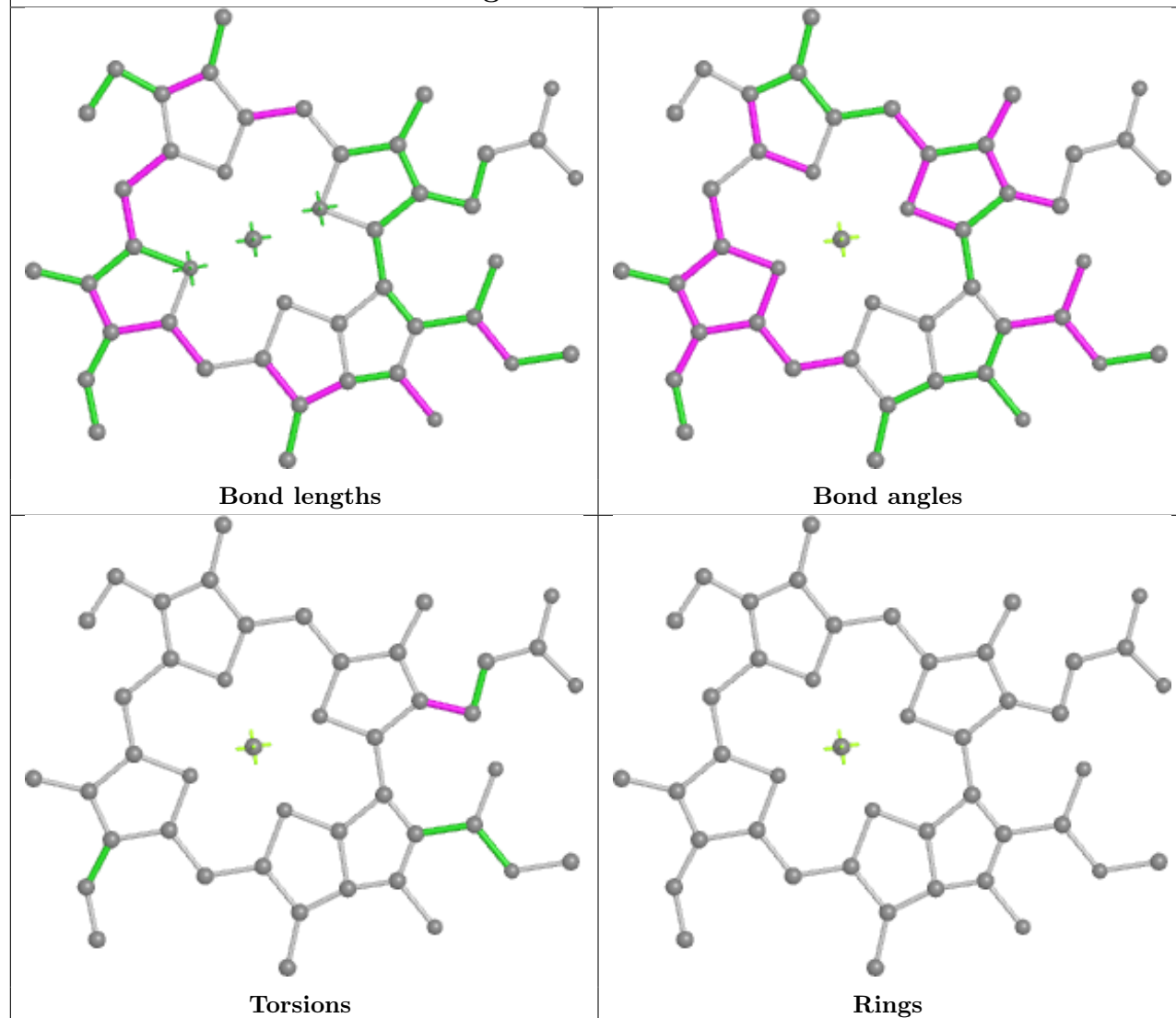


## Ligand CLA cB 809

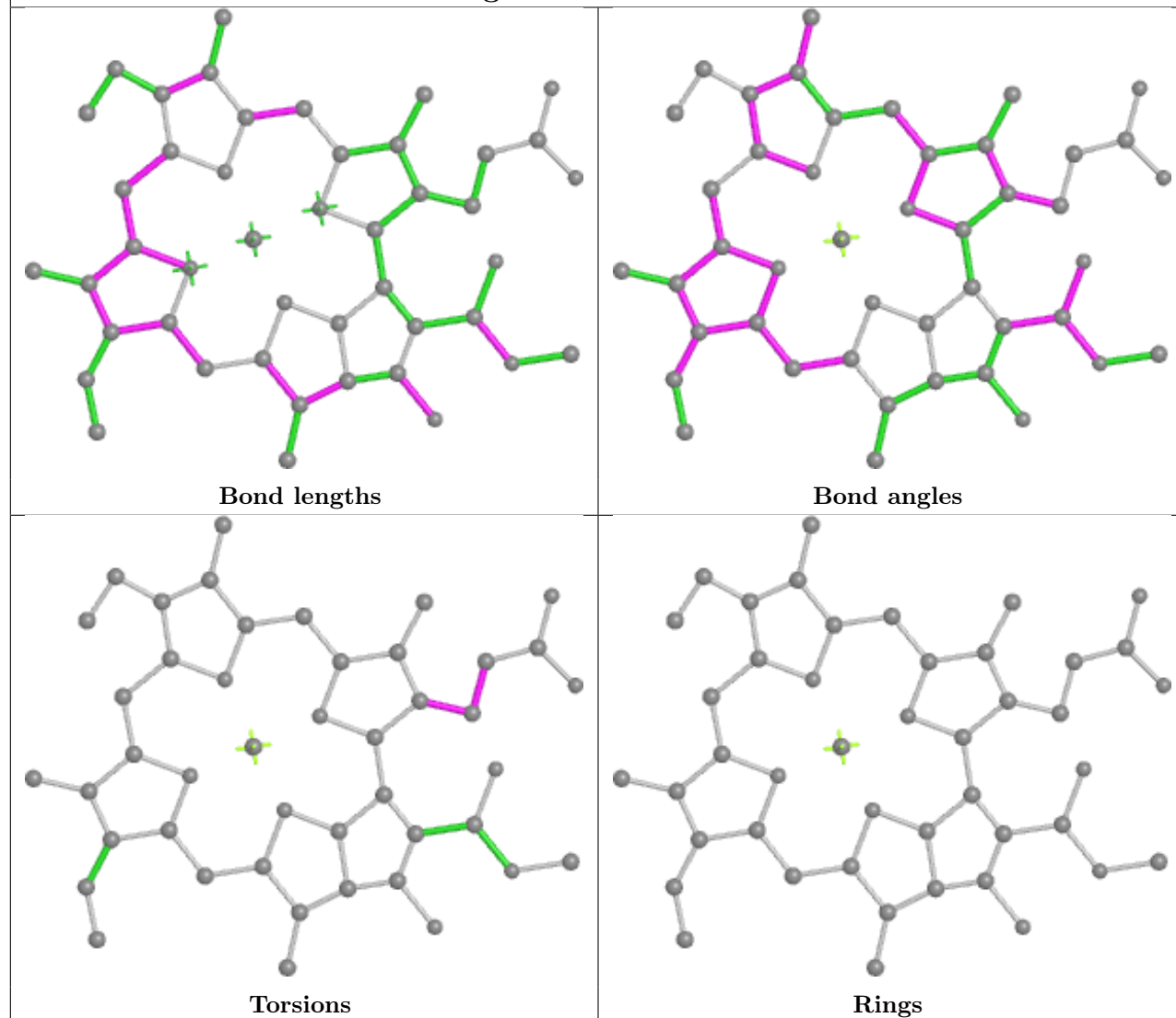




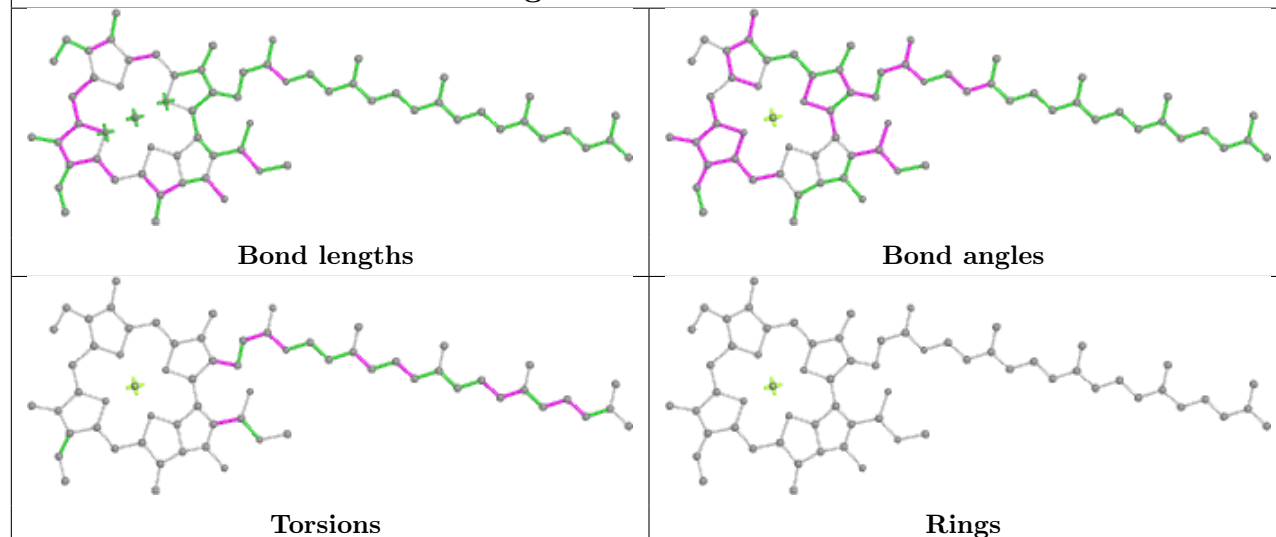
## Ligand CLA cB 812



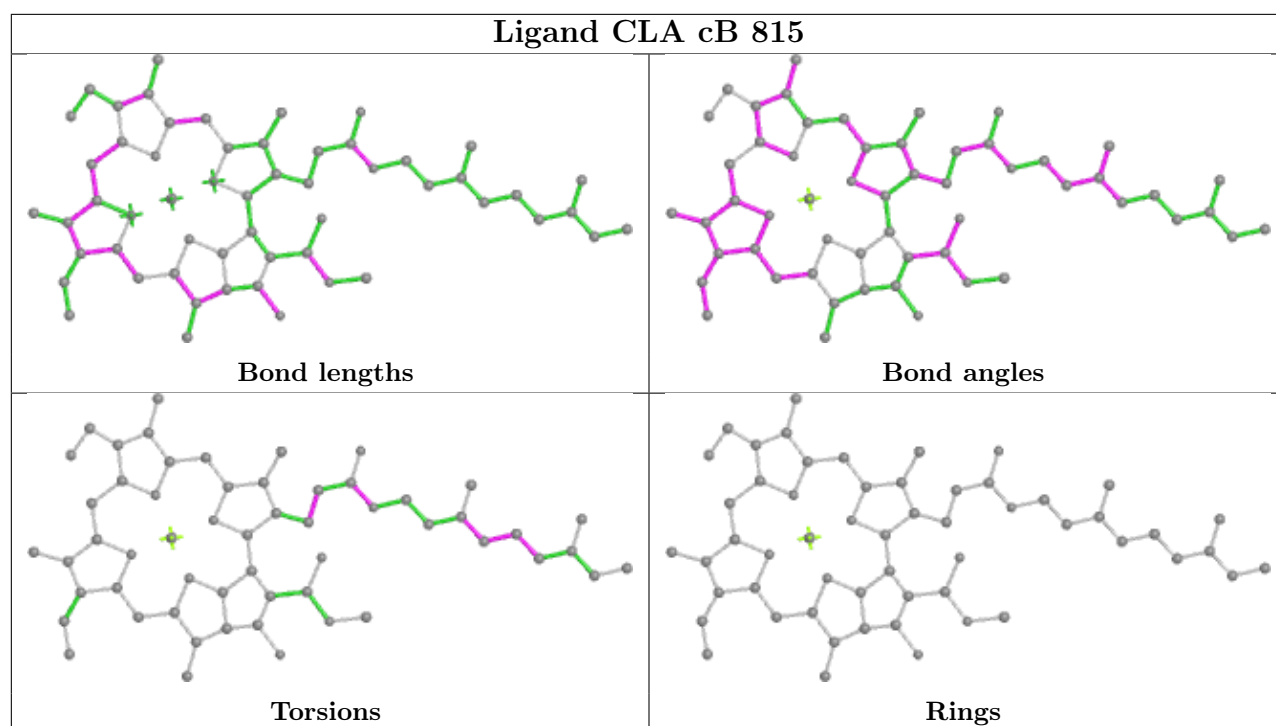
## Ligand CLA cB 813

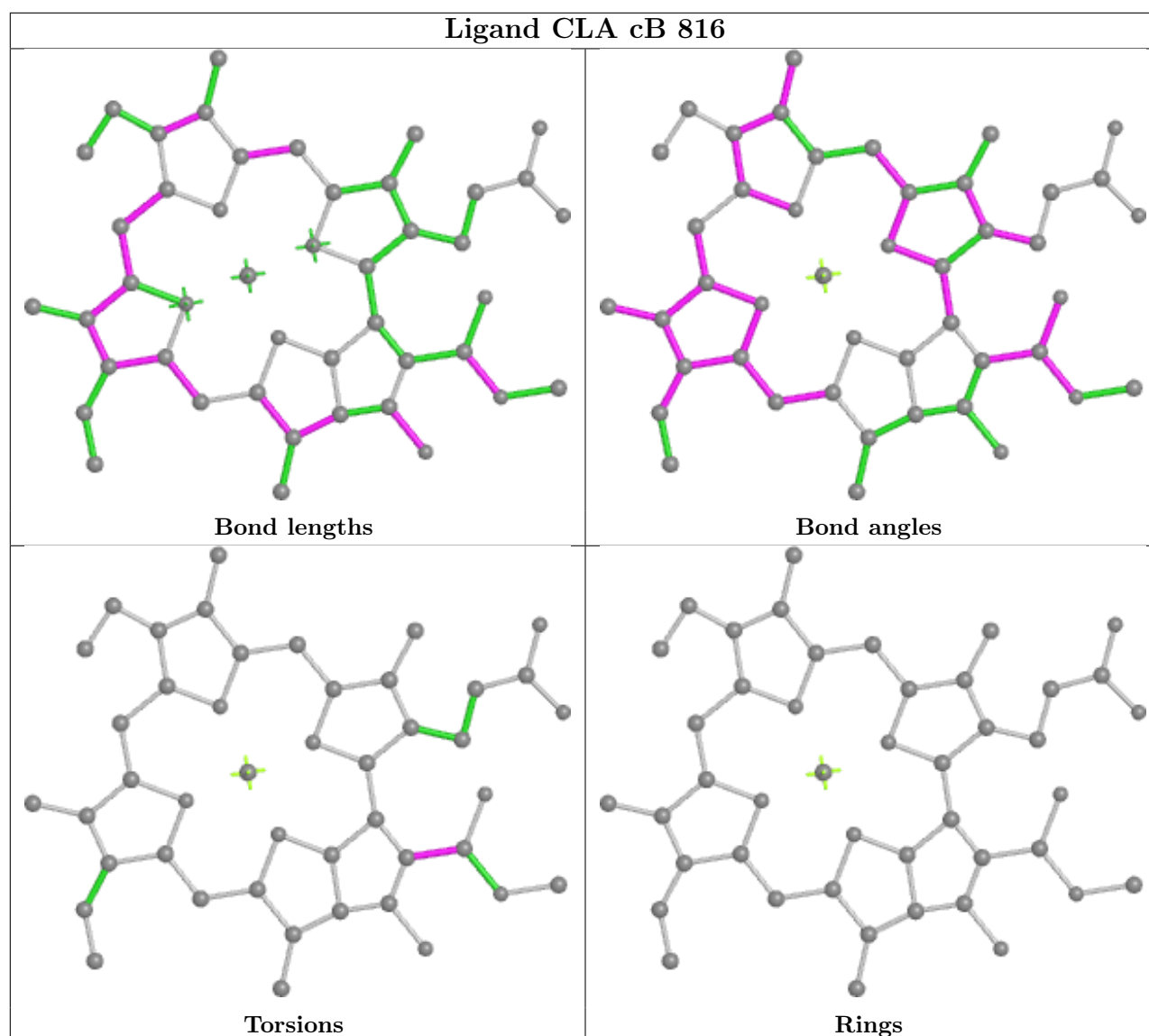


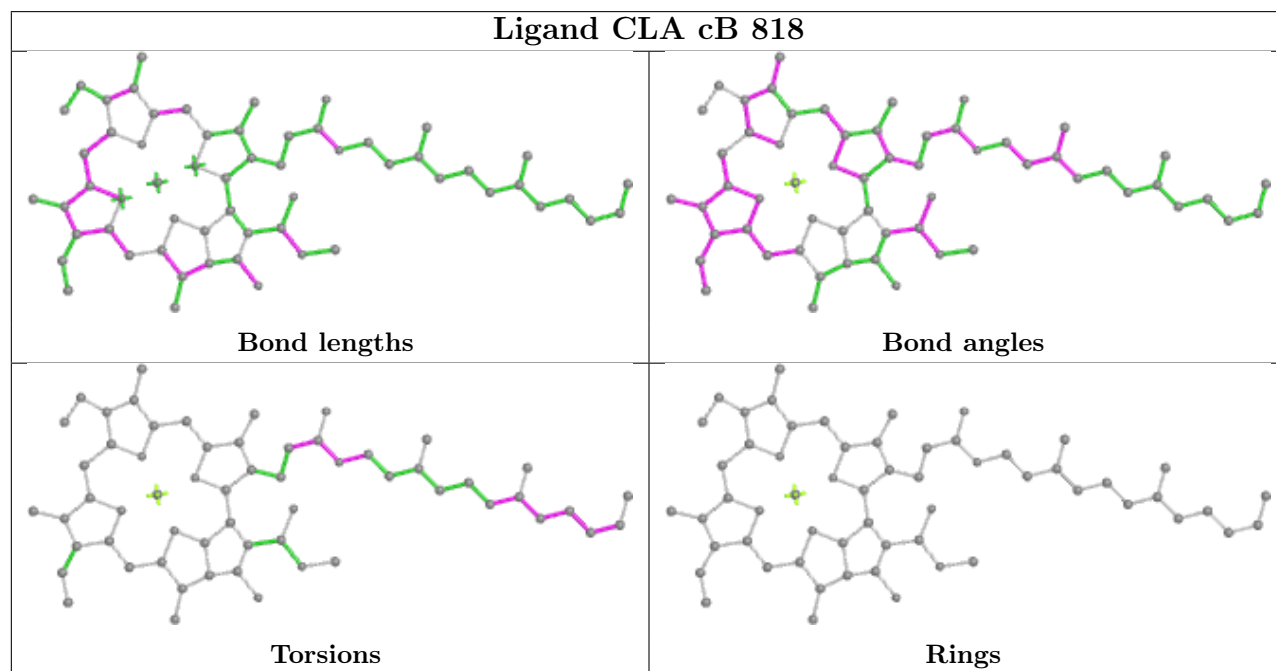
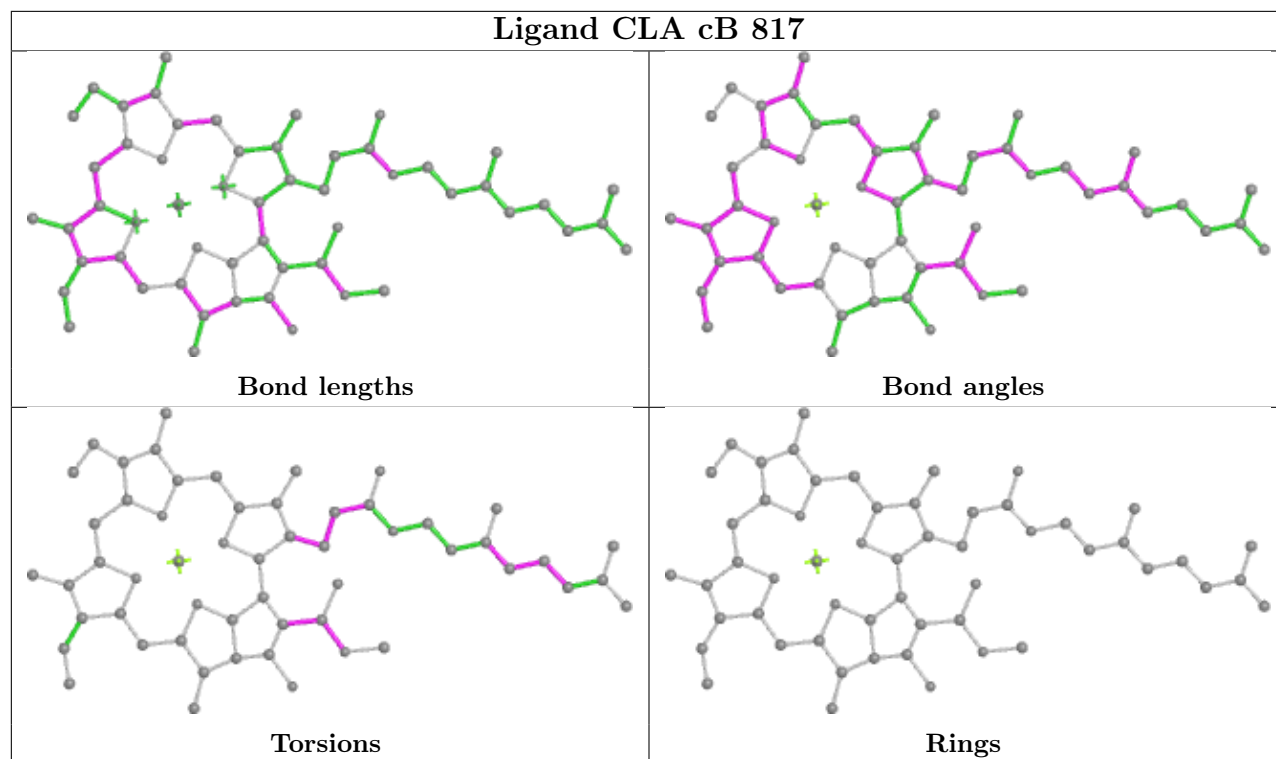
## Ligand CLA cB 814

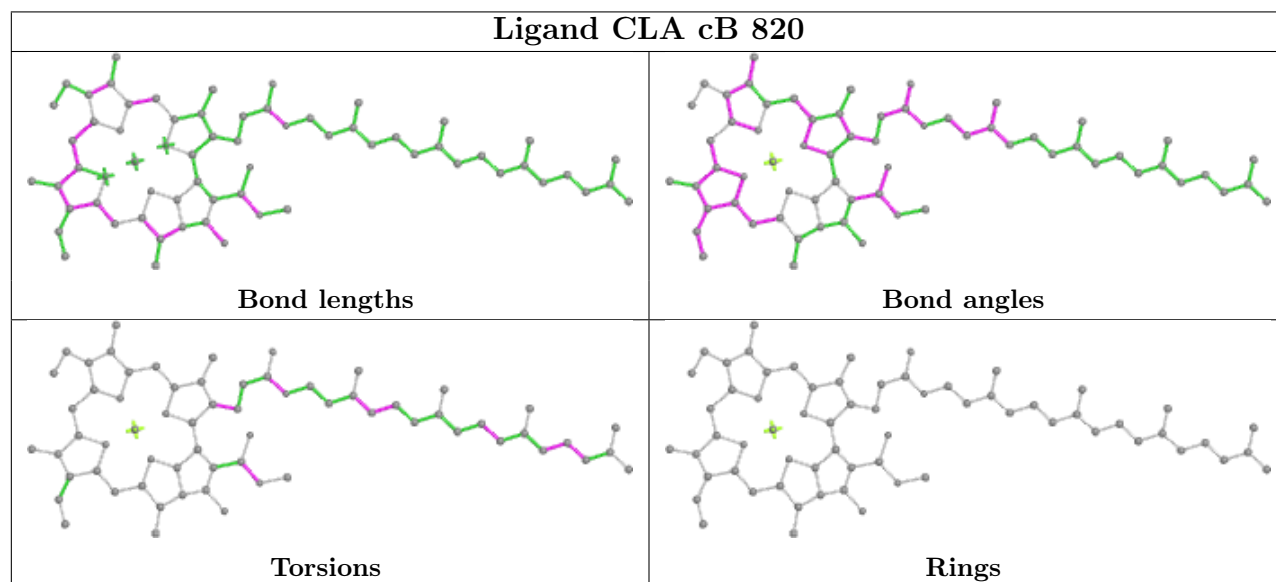
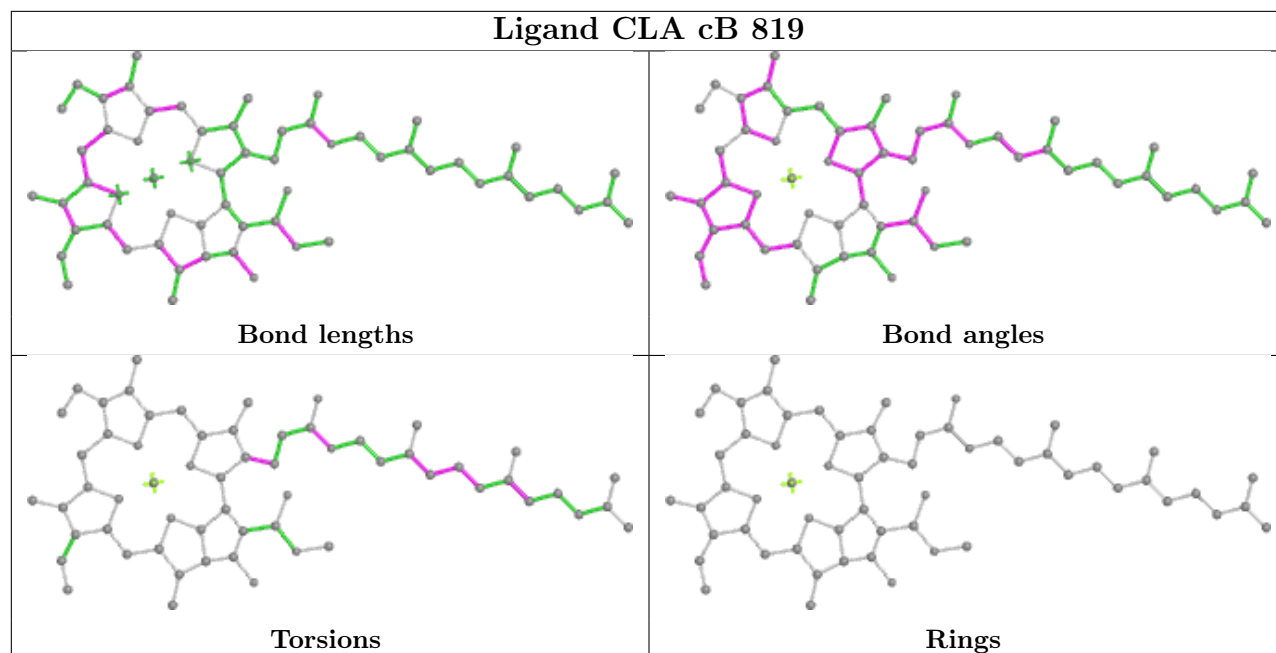


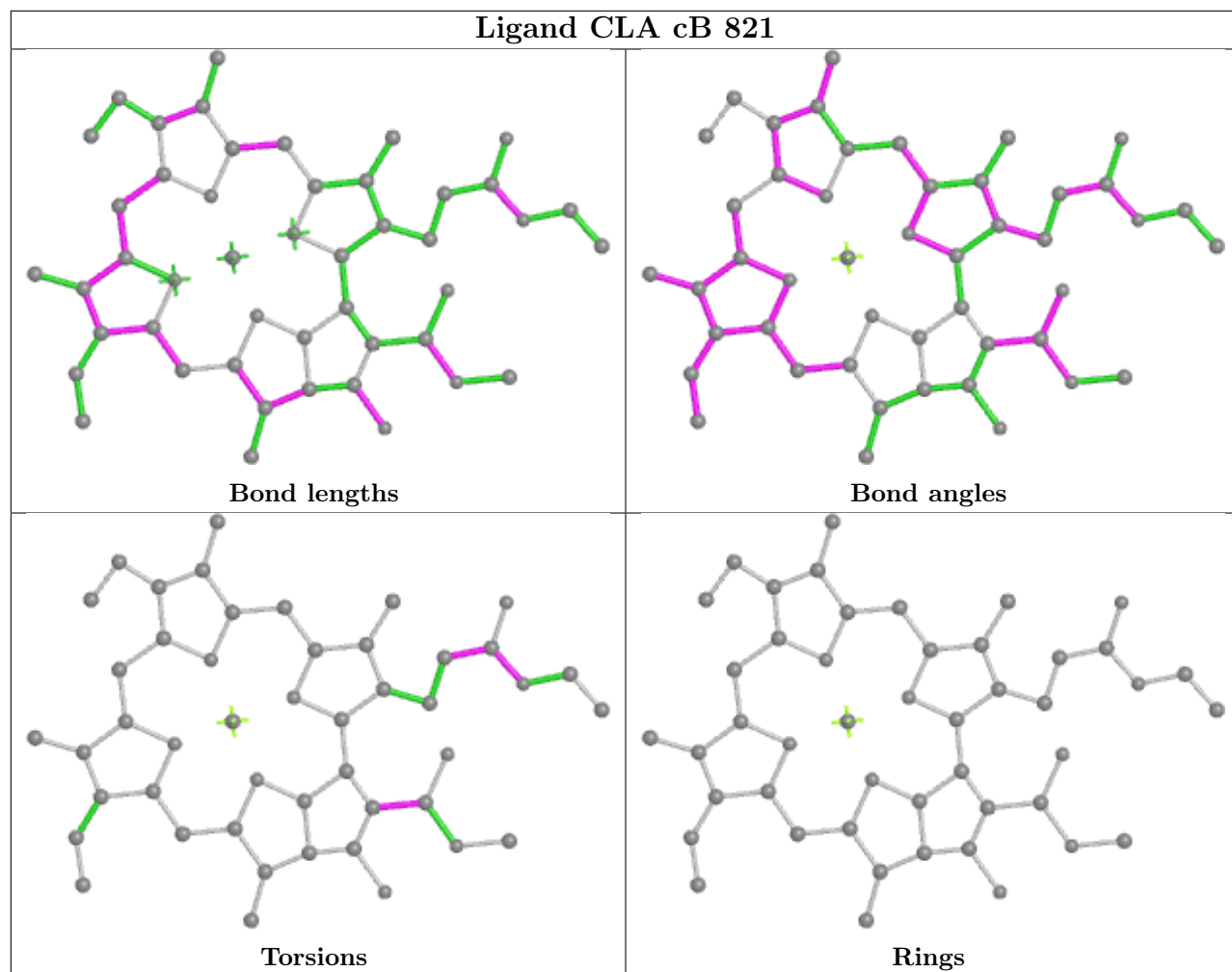


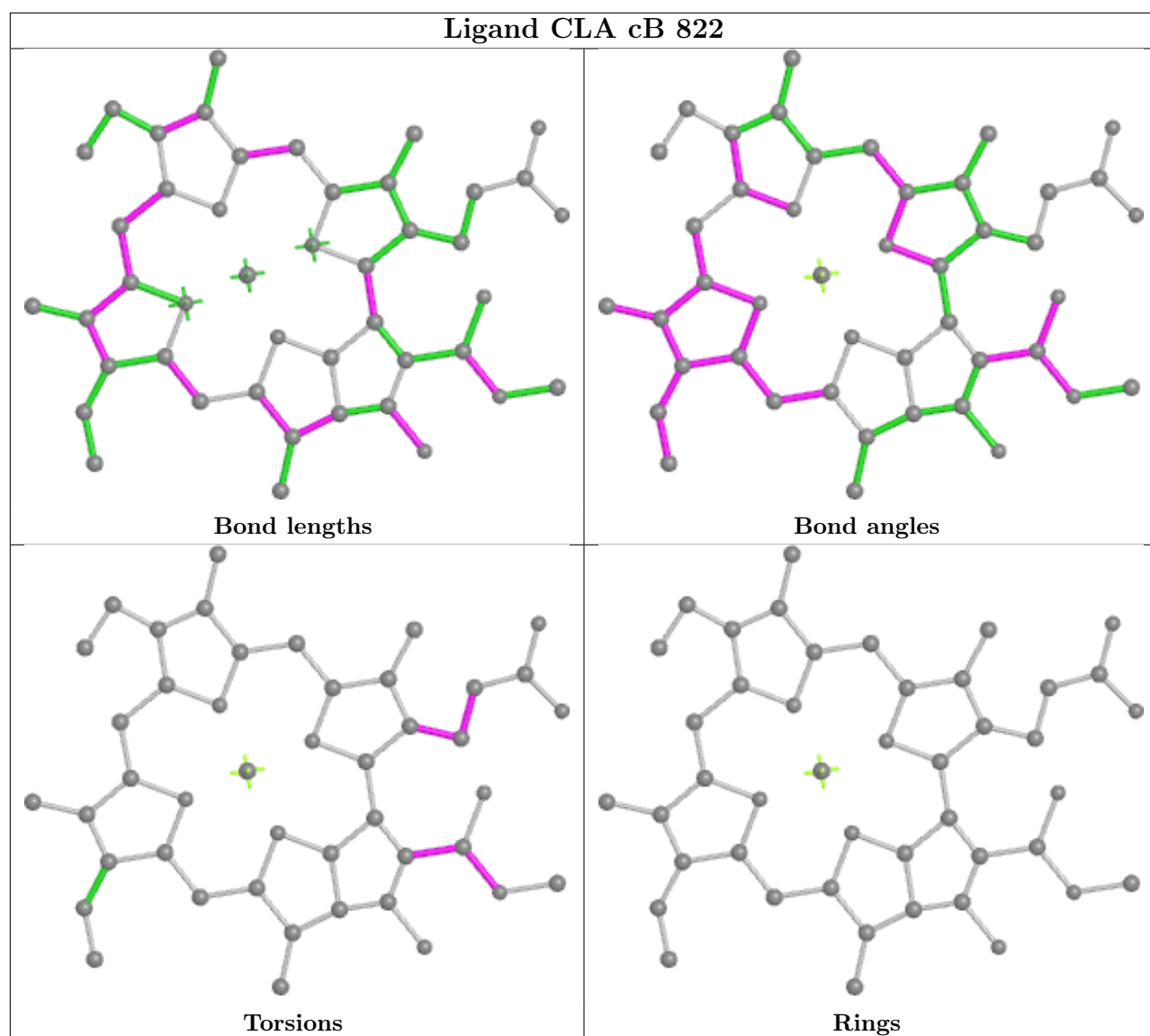


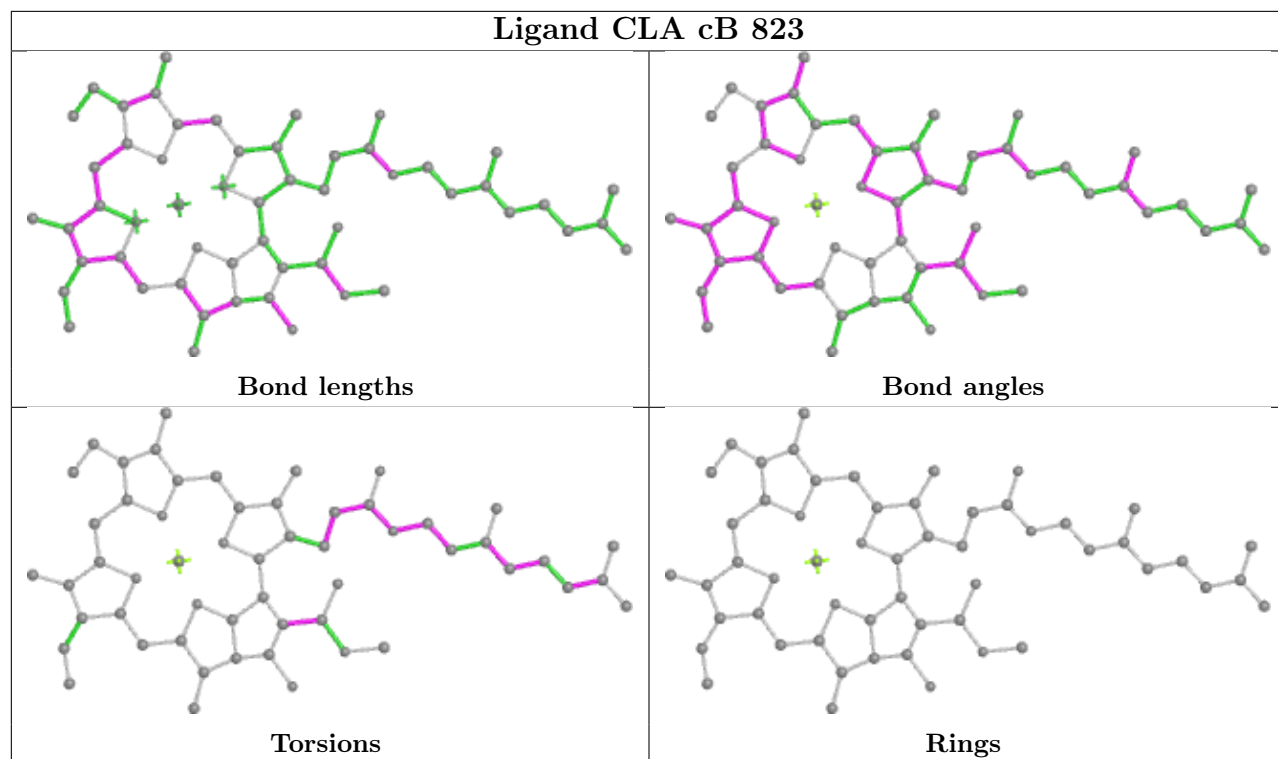


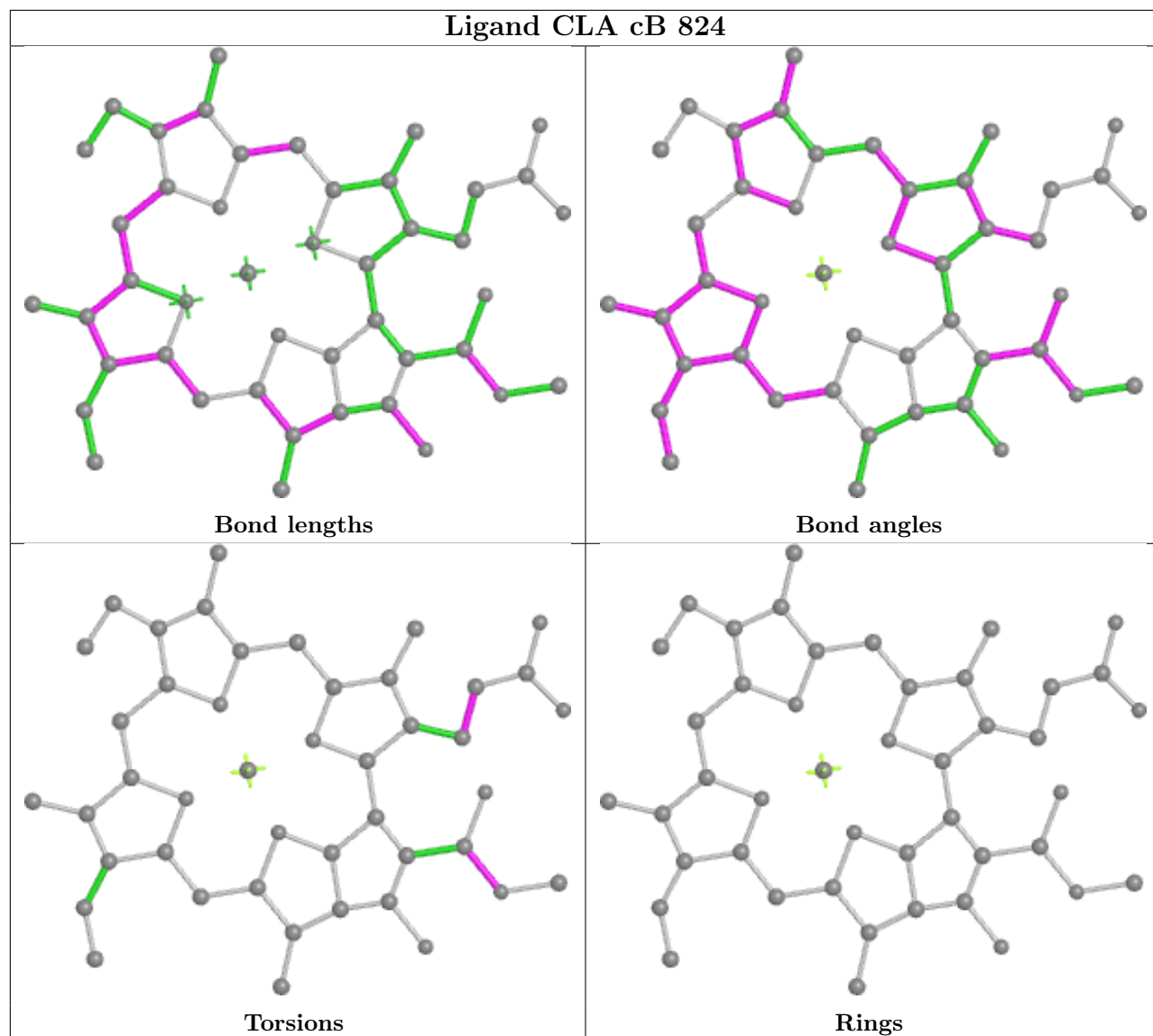




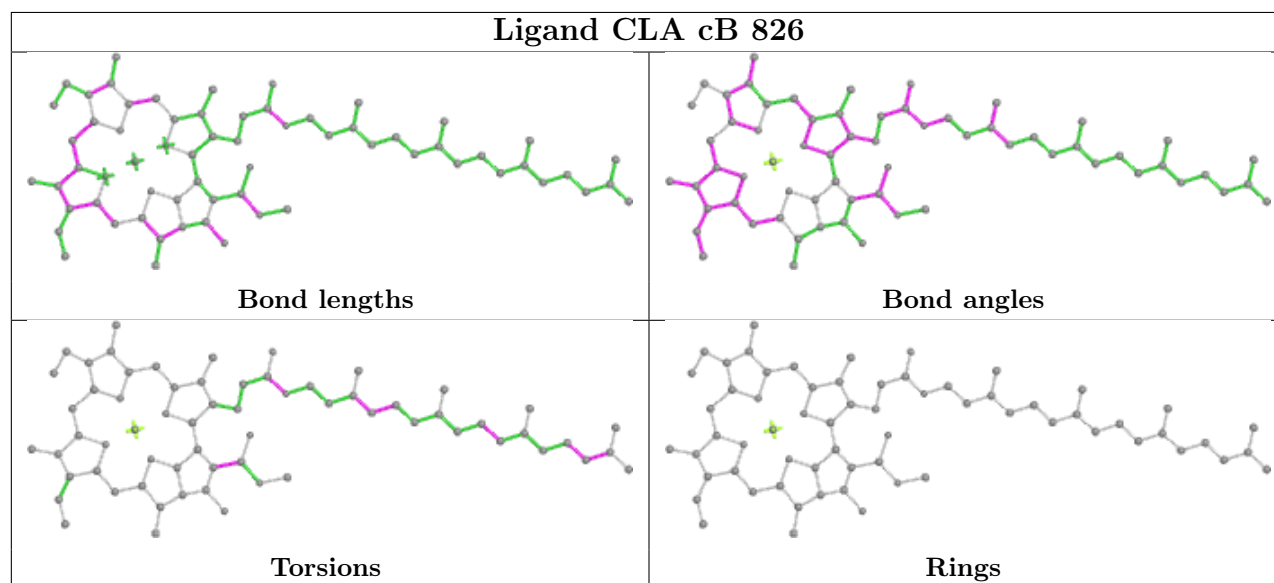
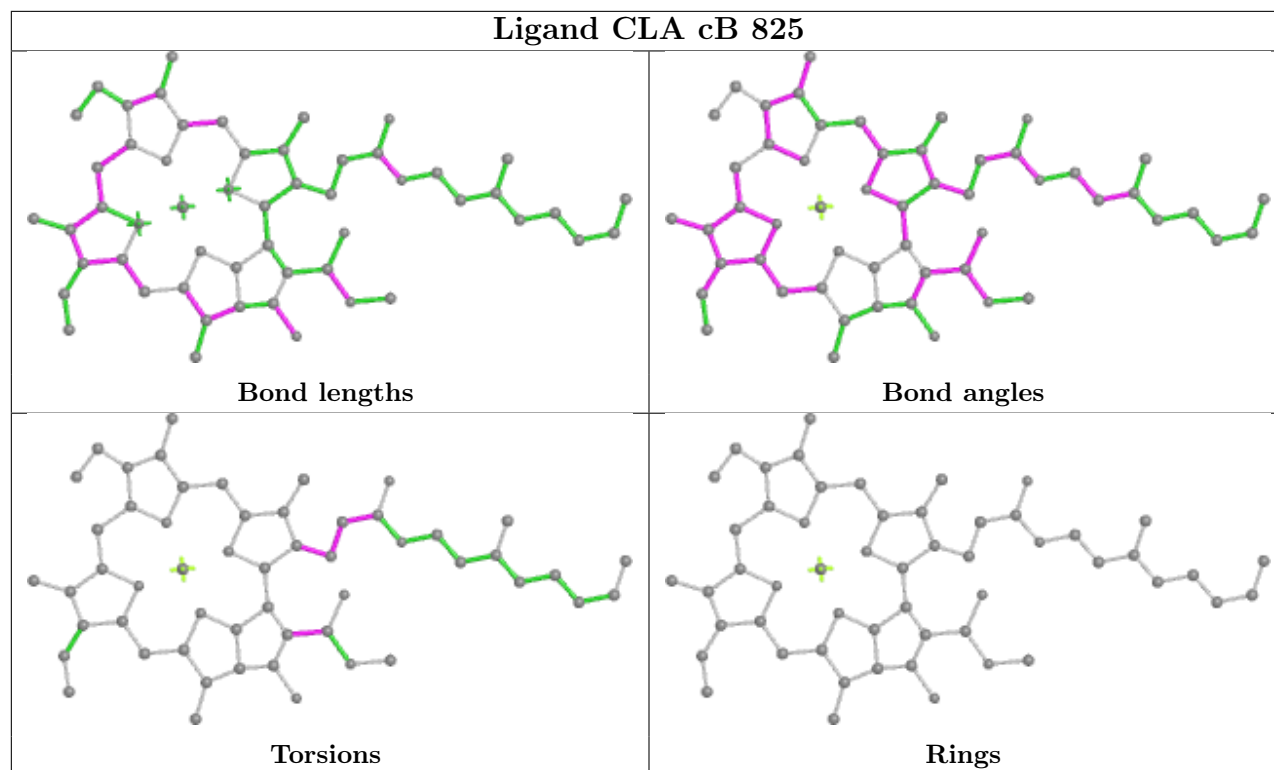


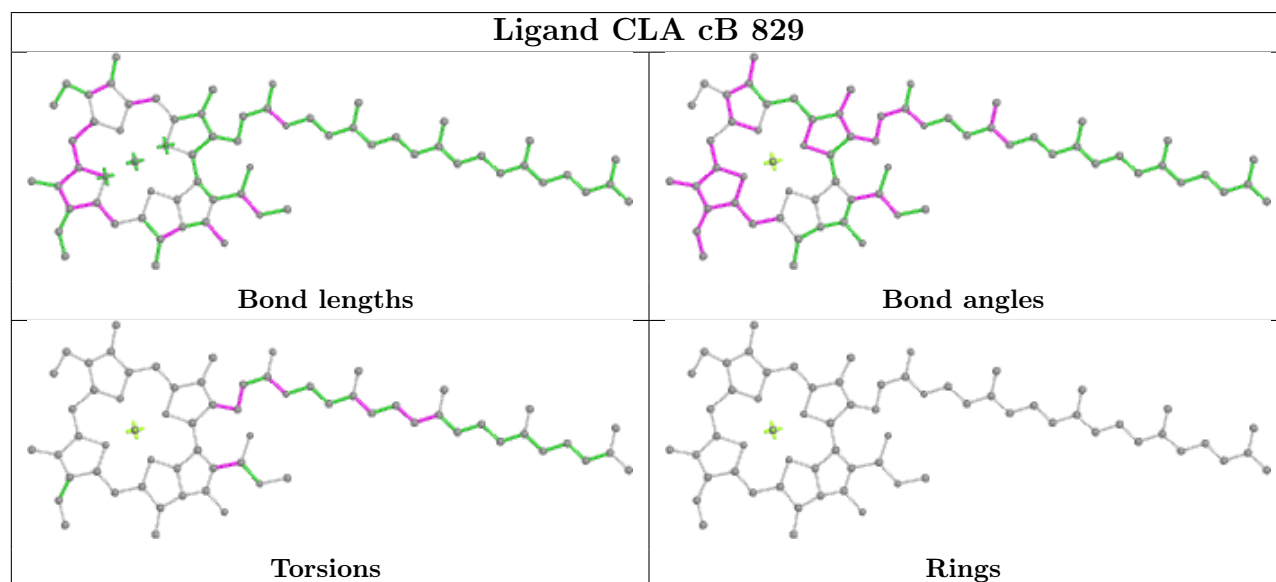
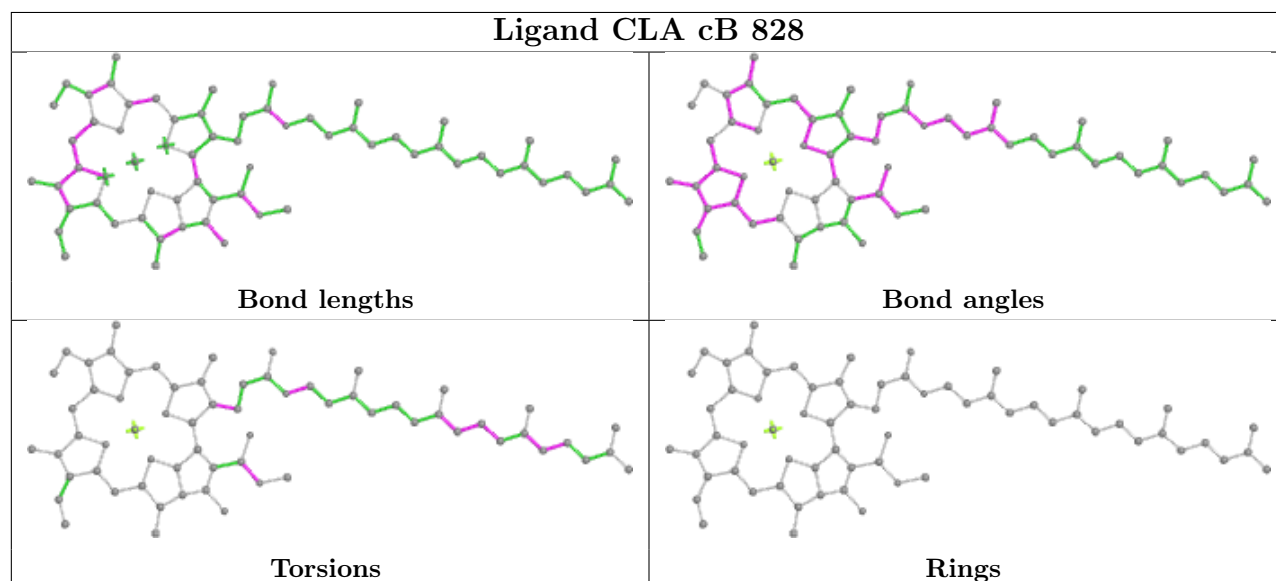
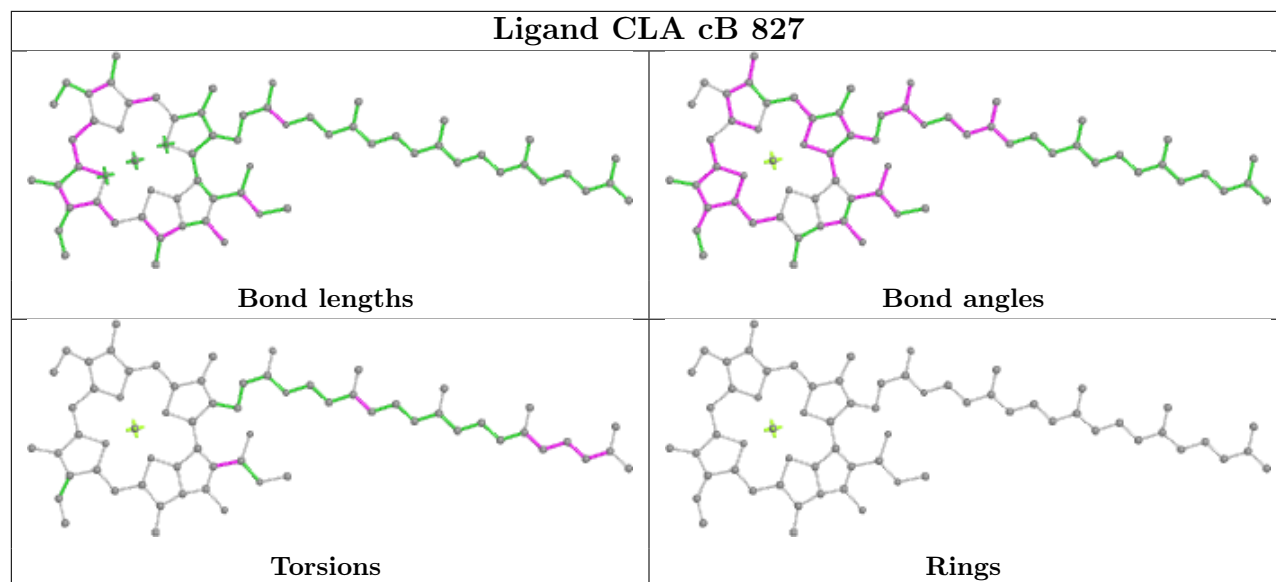


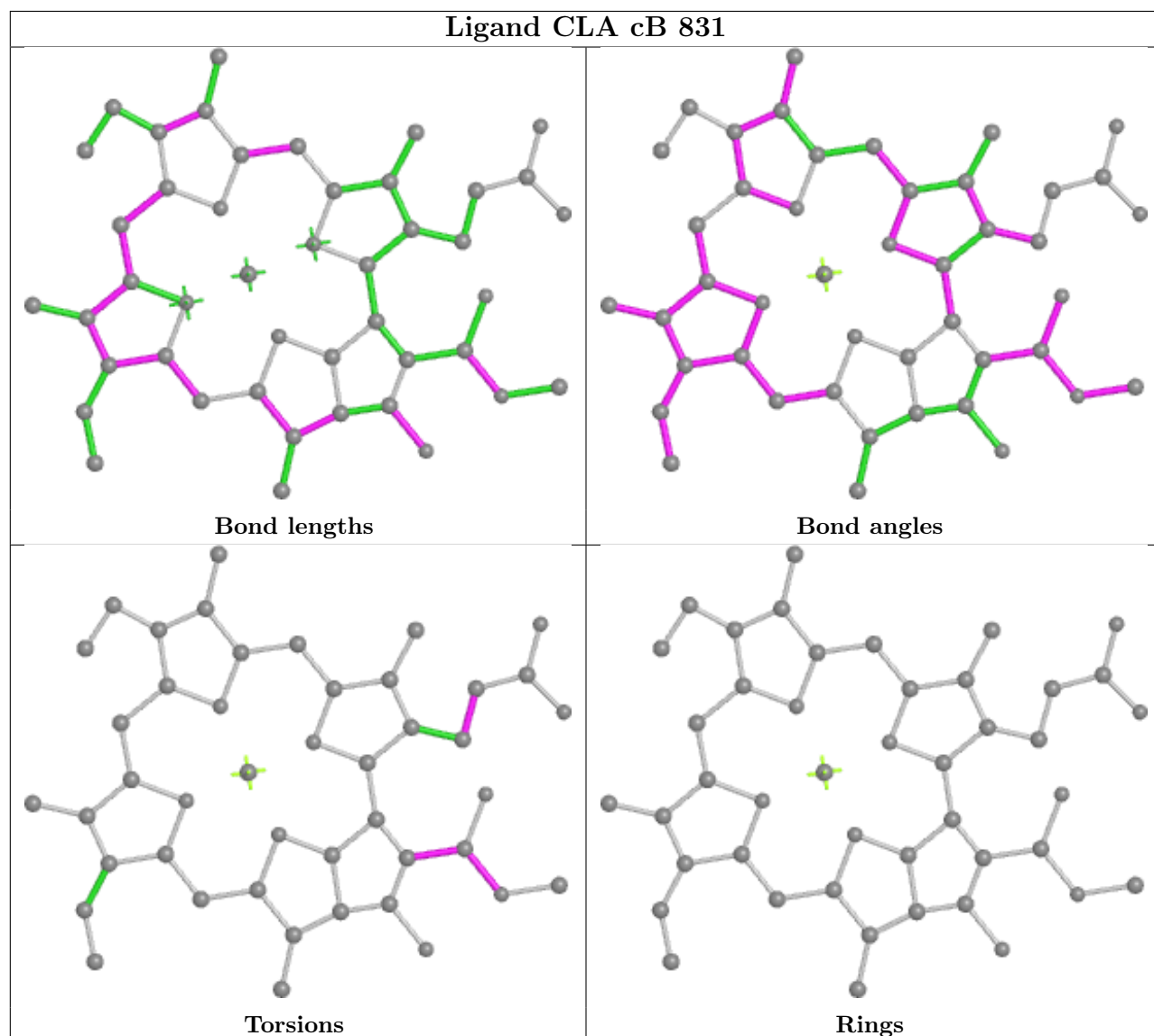
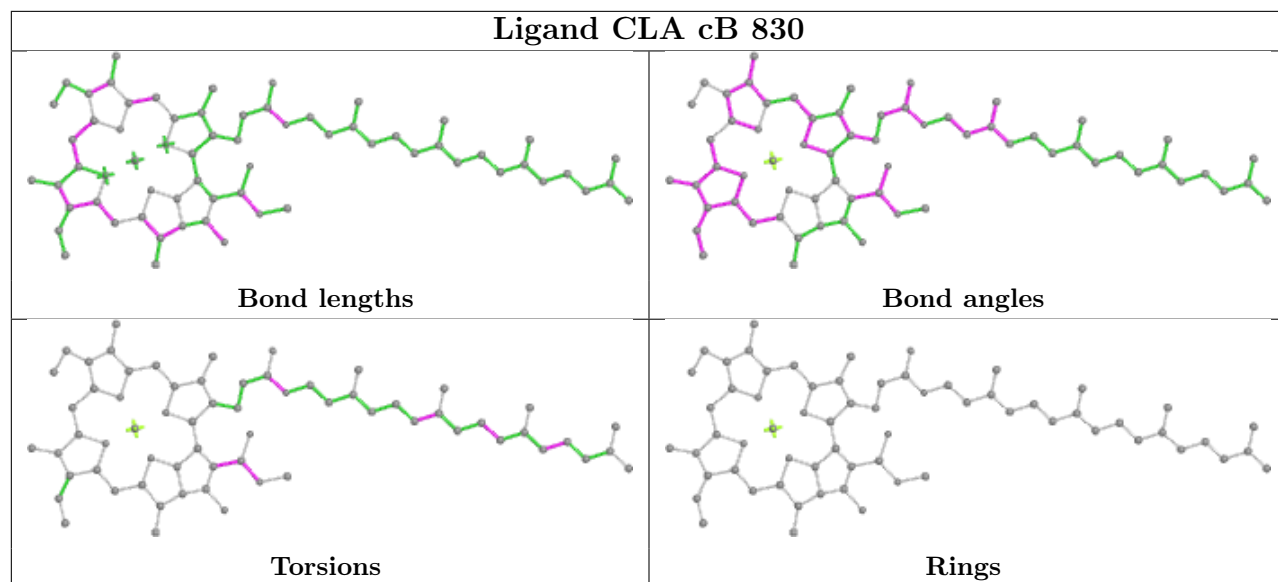




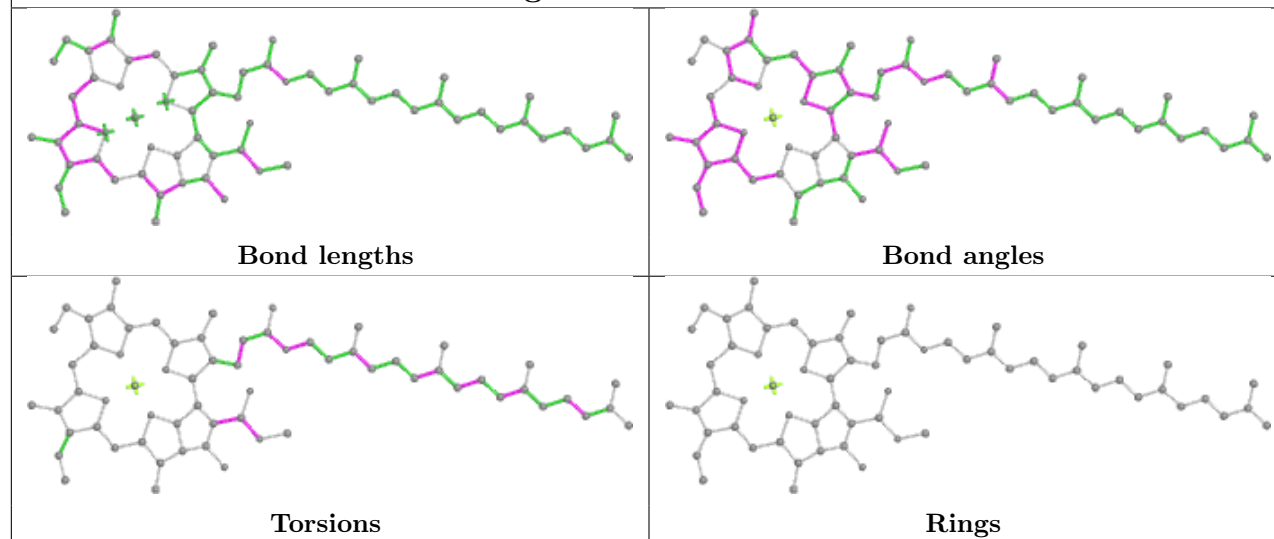




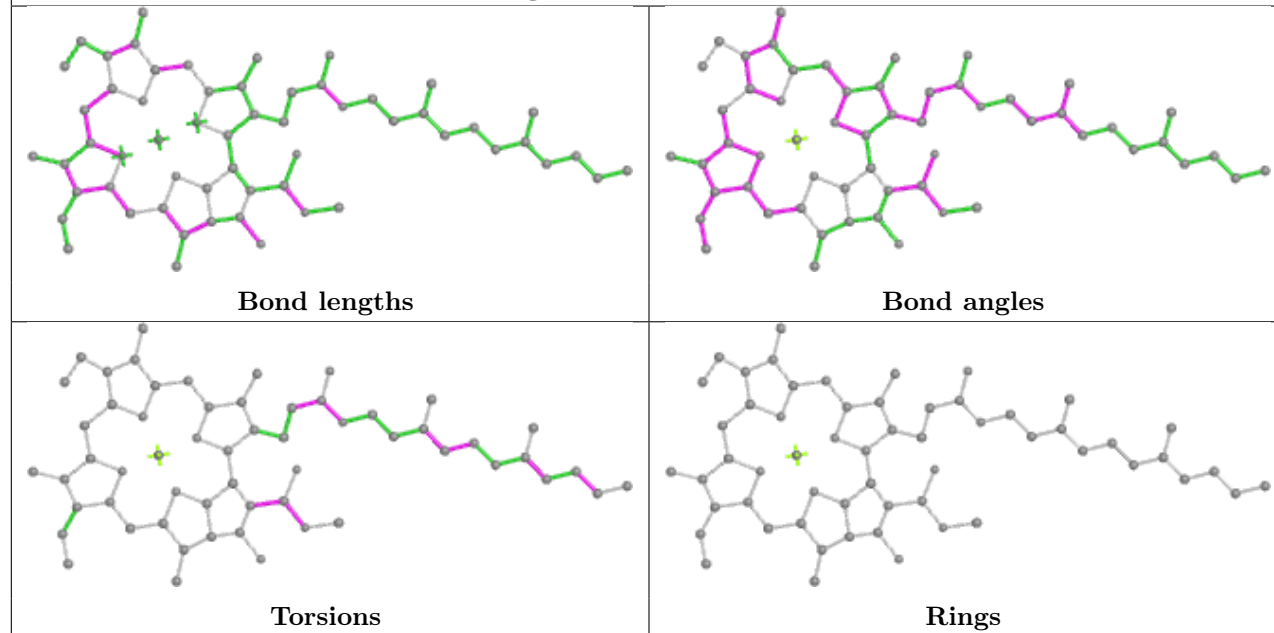


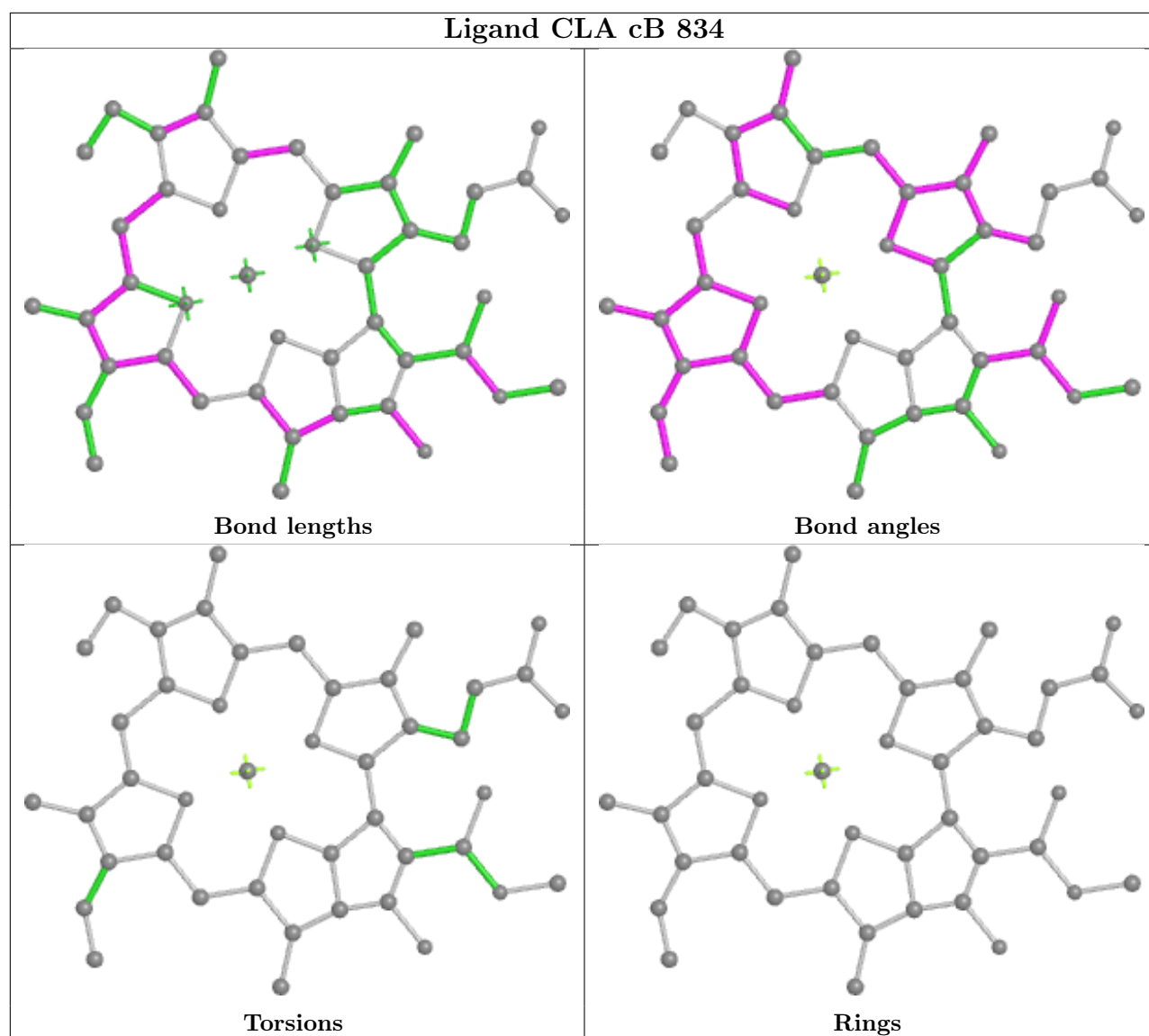


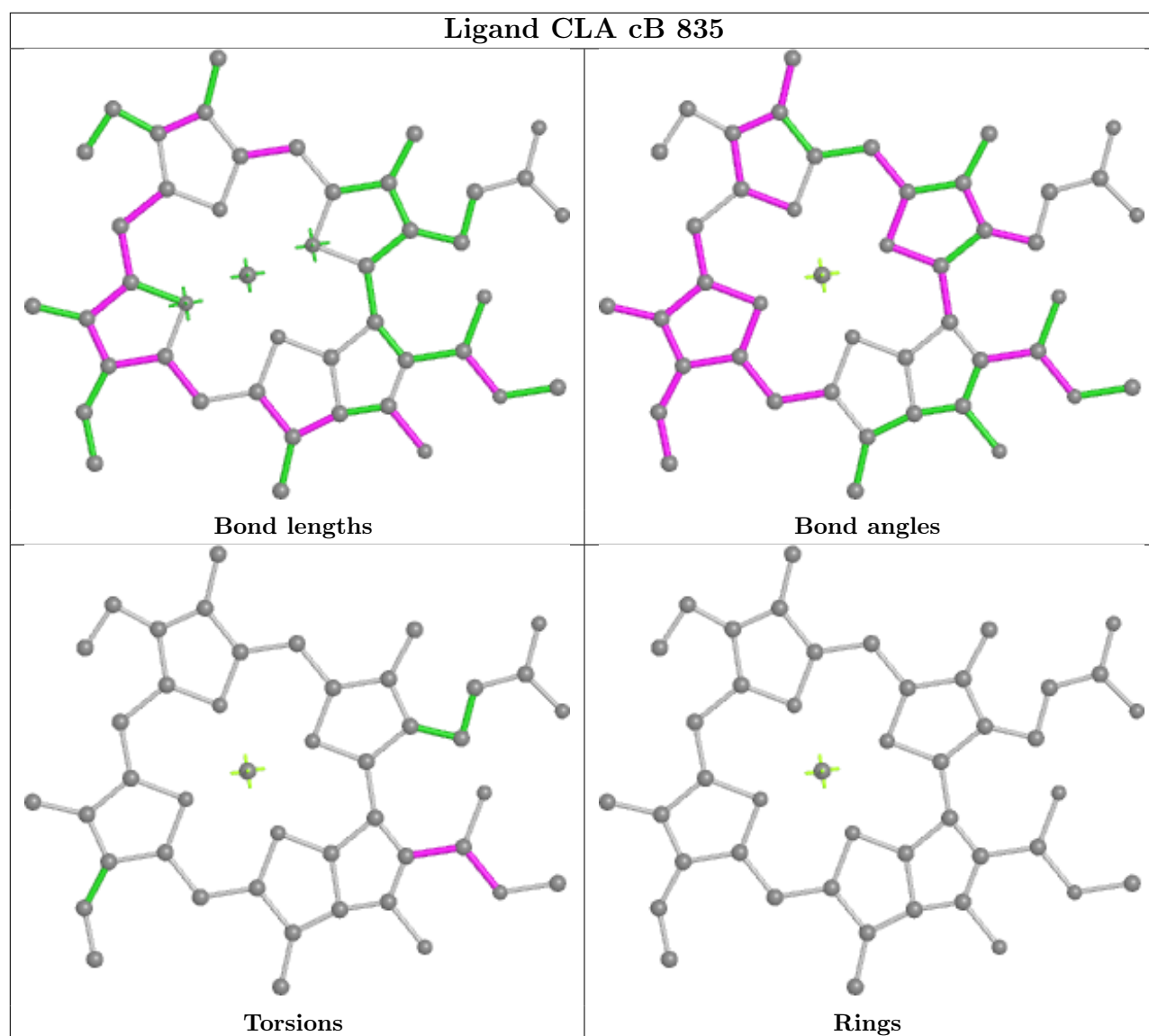
## Ligand CLA cB 832



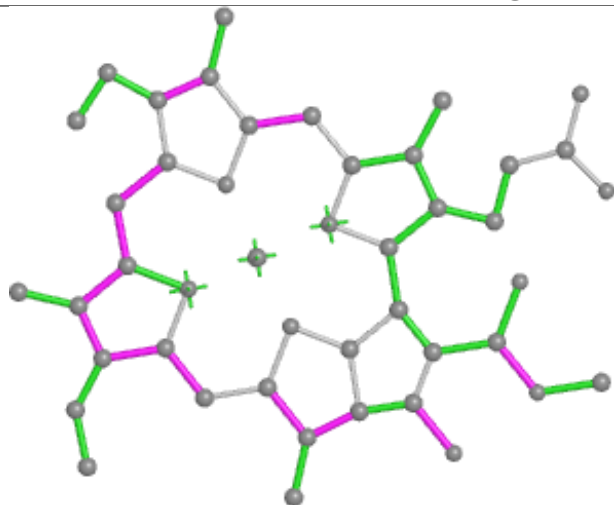
## Ligand CLA cB 833



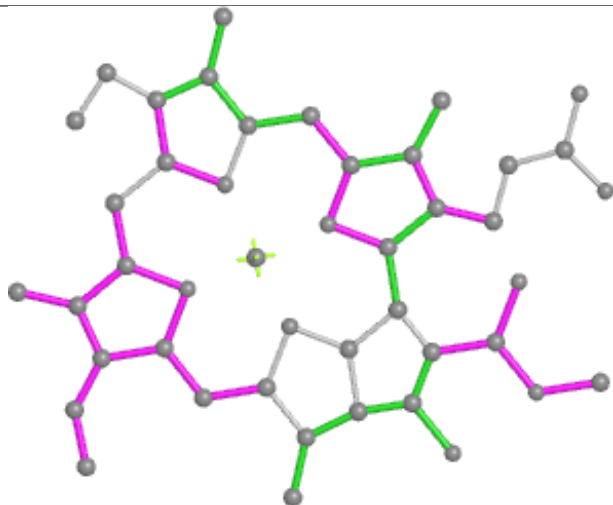




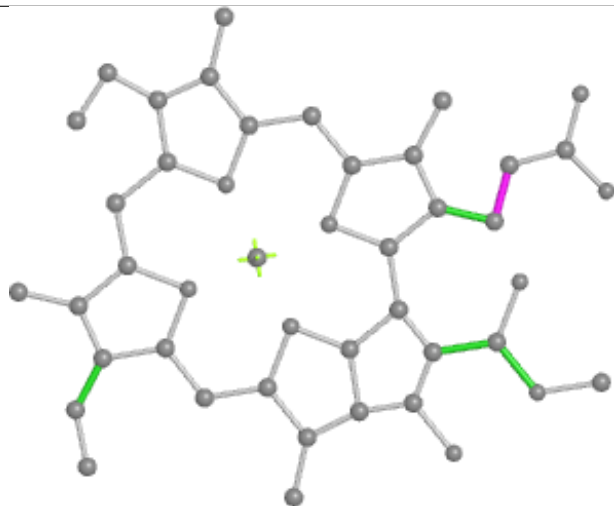
## Ligand CLA cB 836



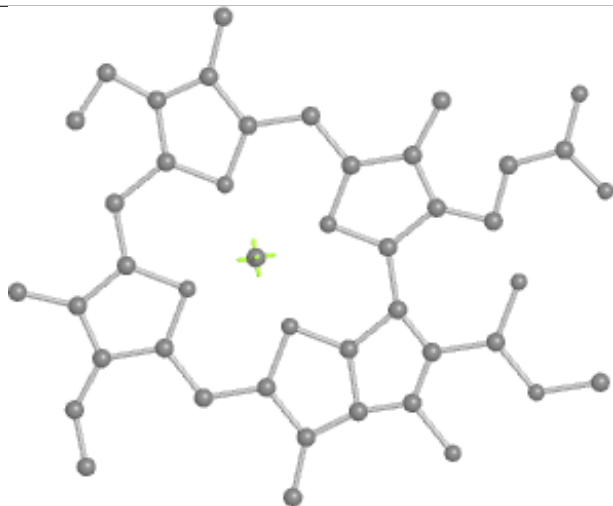
Bond lengths



Bond angles

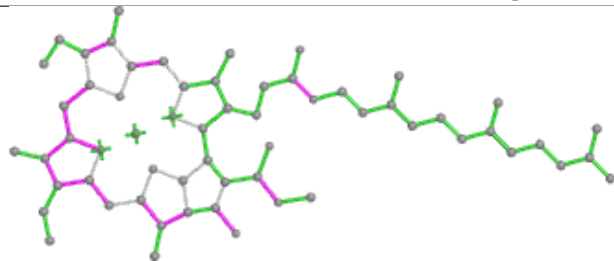


Torsions

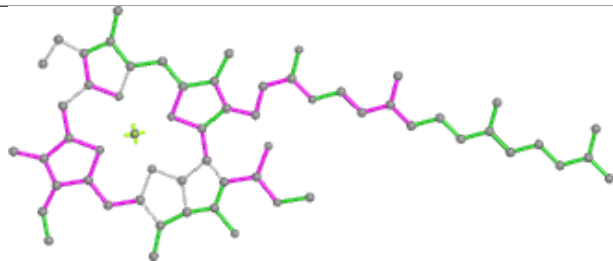


Rings

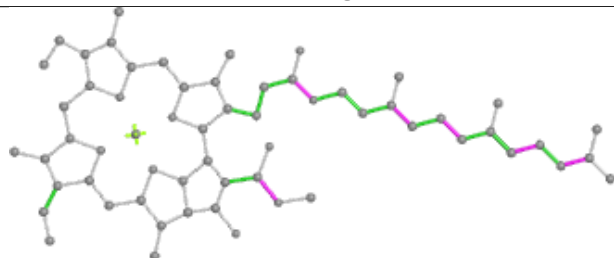
## Ligand CLA cB 837



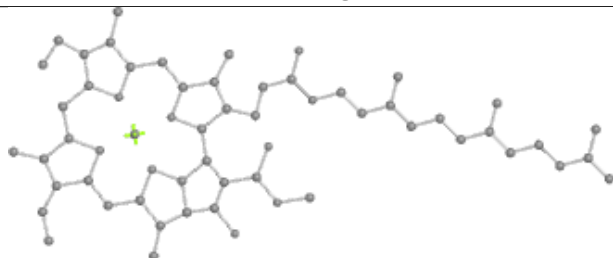
Bond lengths



Bond angles

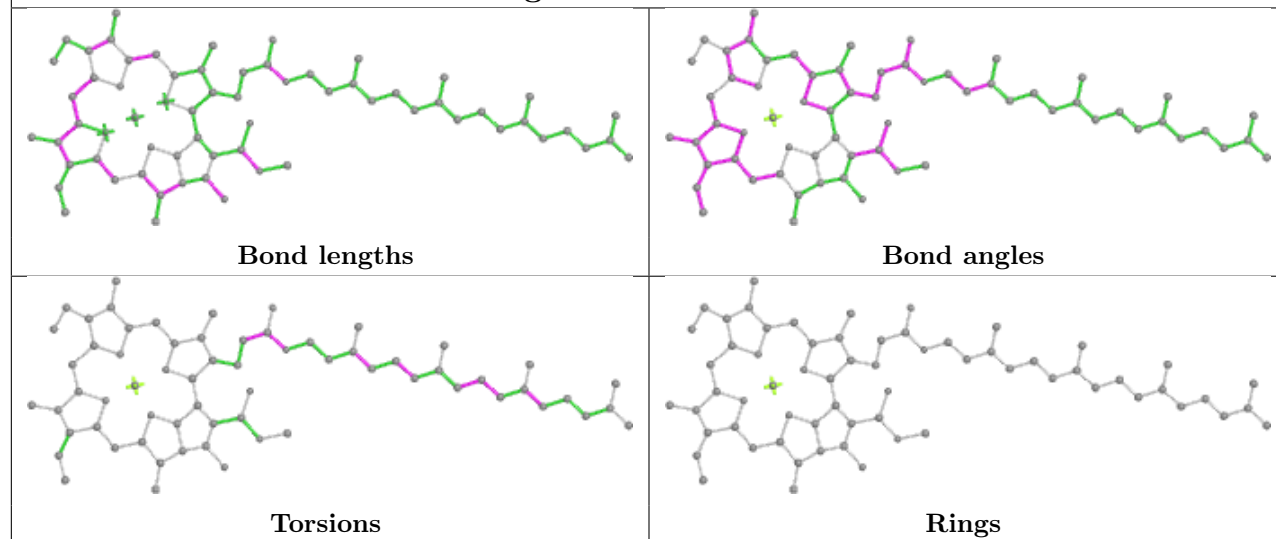


Torsions

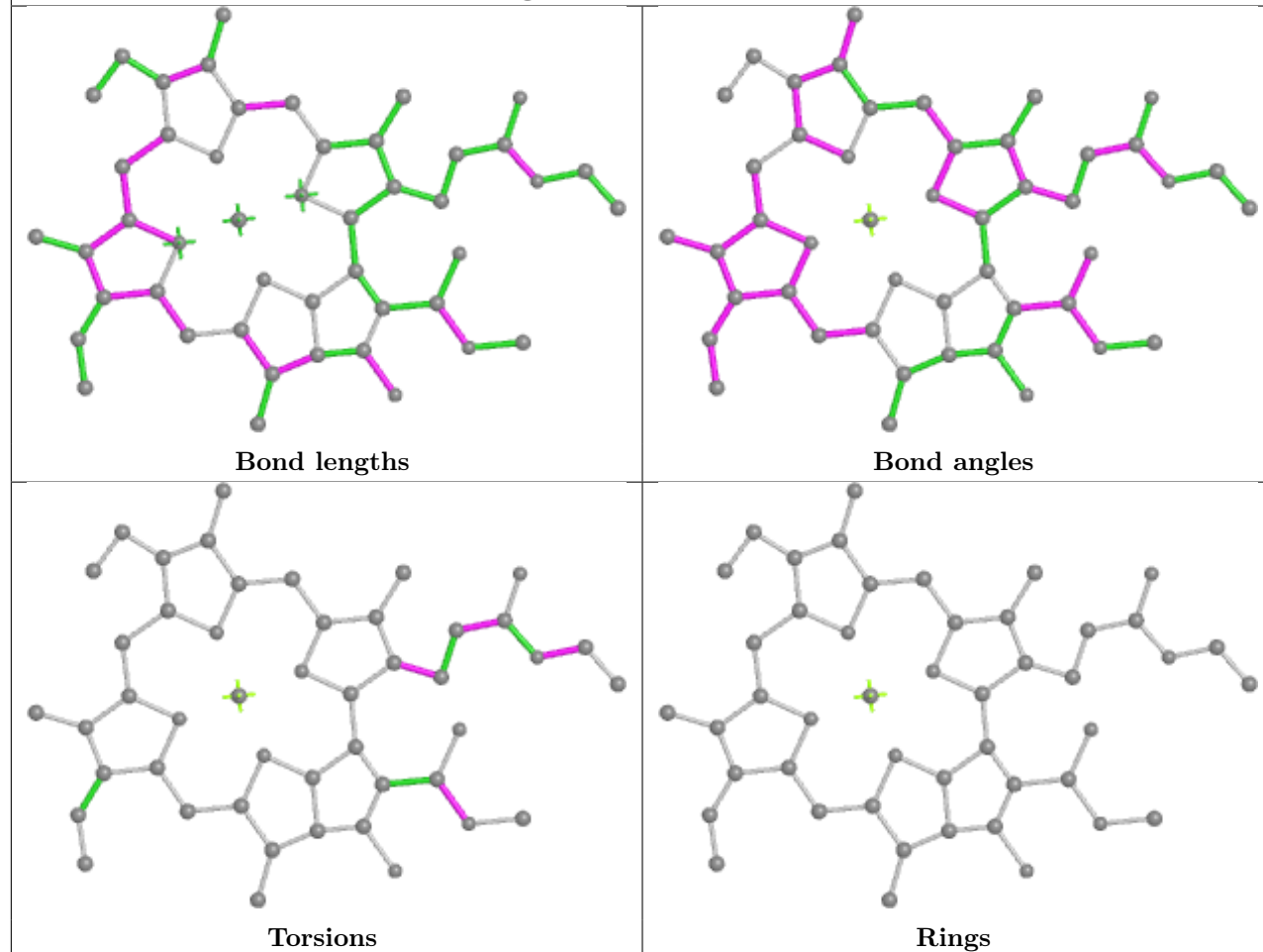


Rings

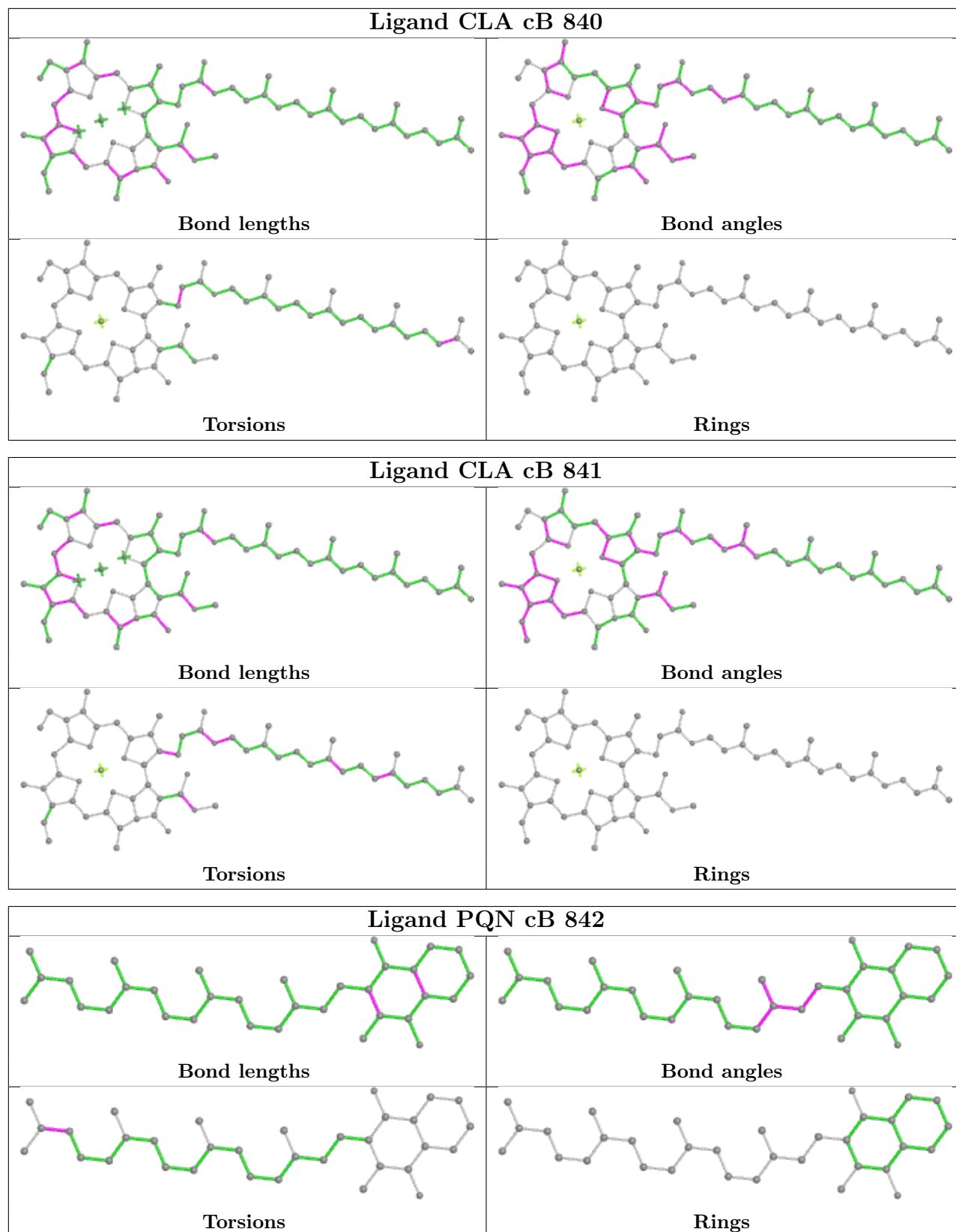
## Ligand CLA cB 838

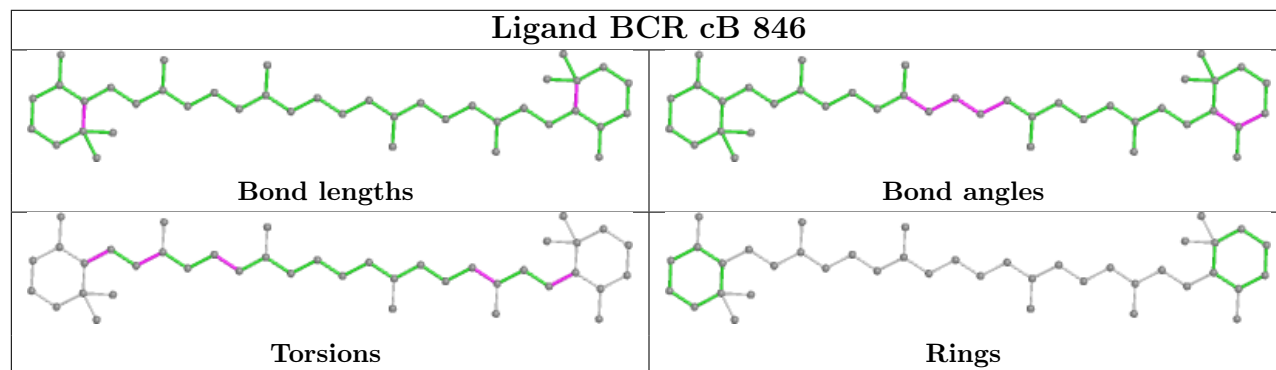
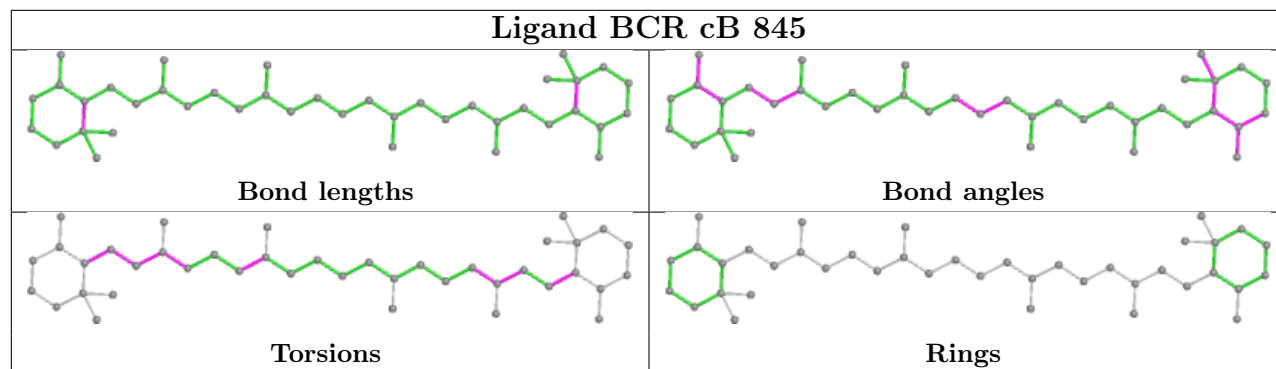
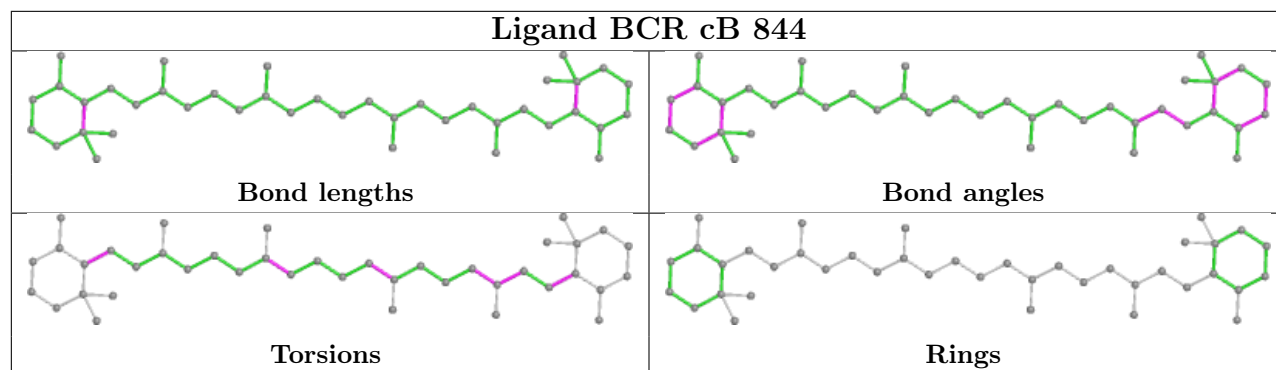
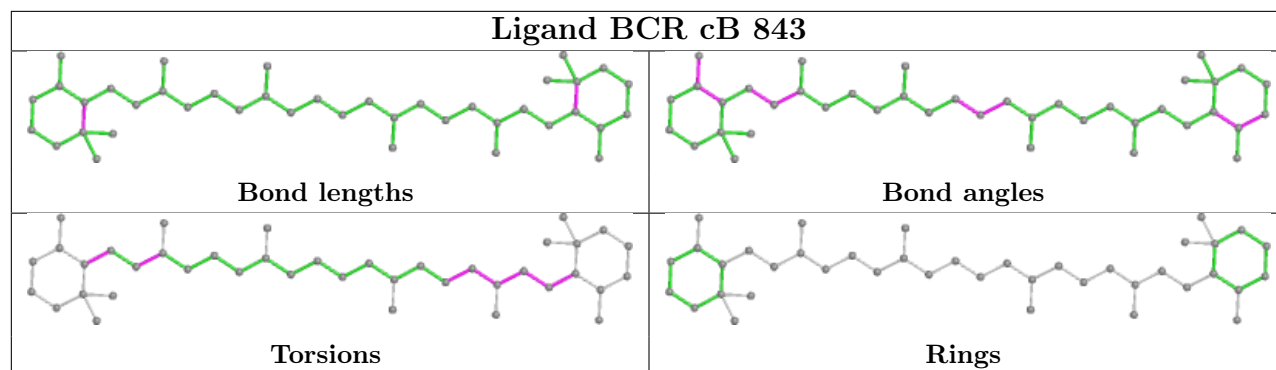


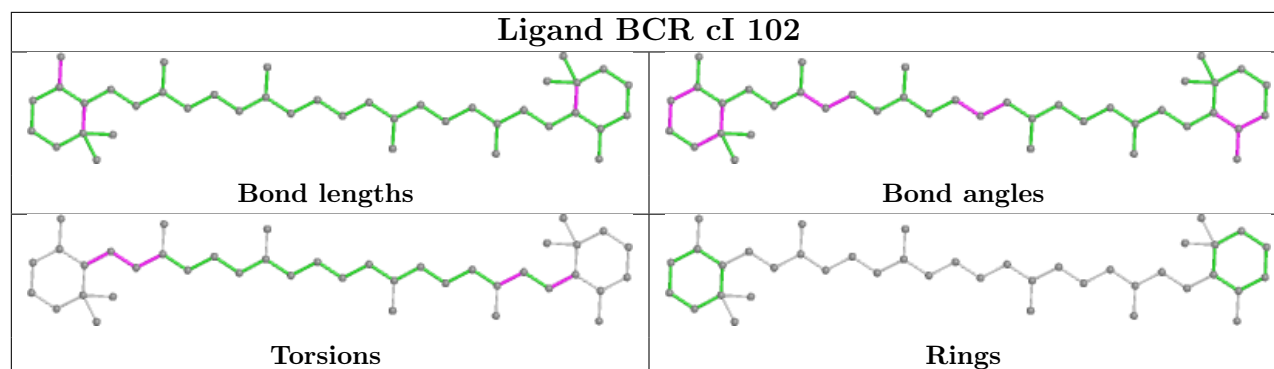
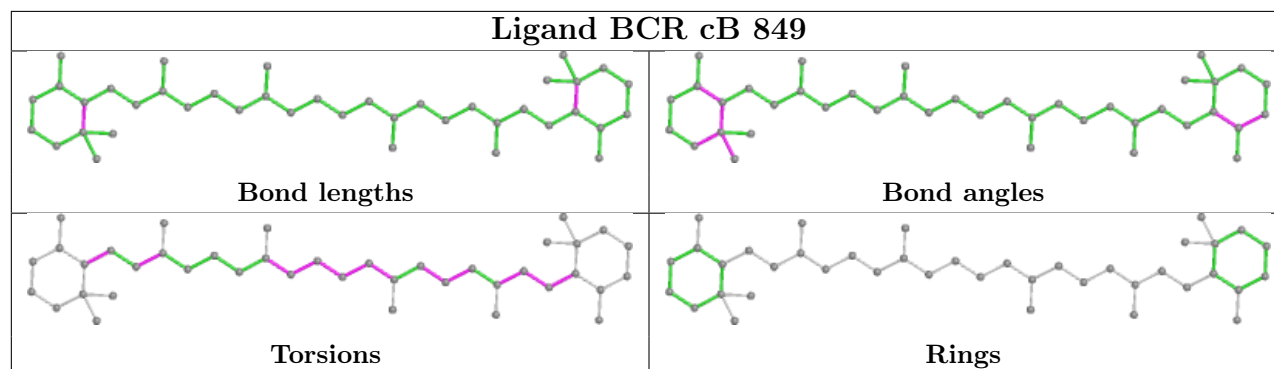
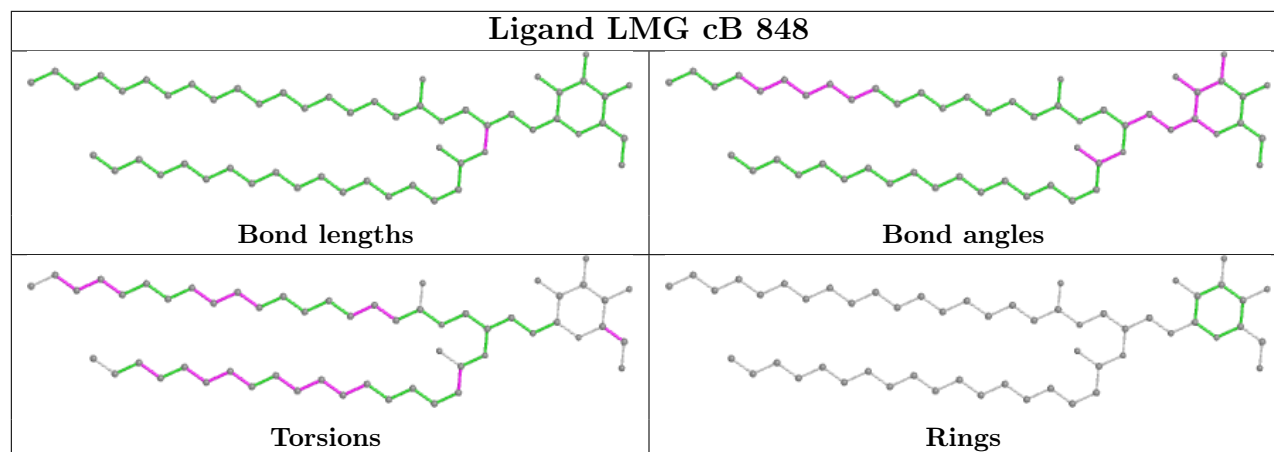
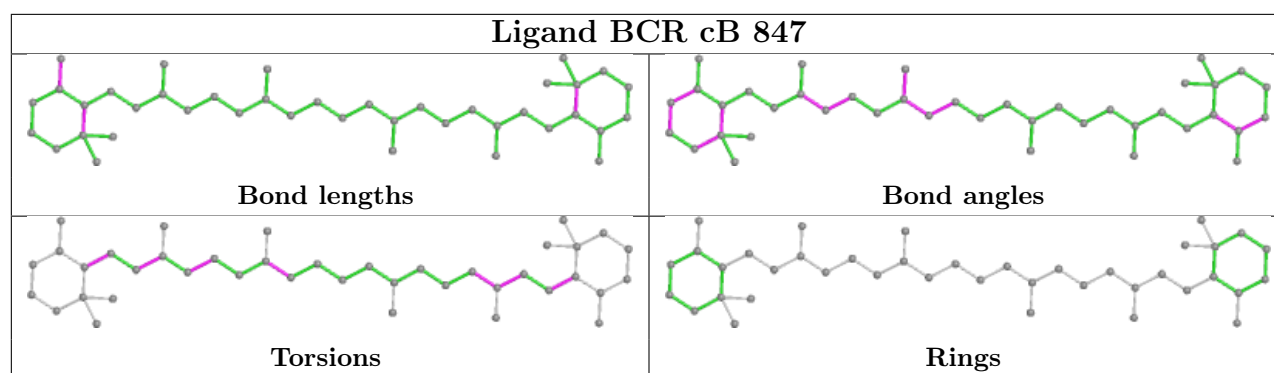
## Ligand CLA cB 839

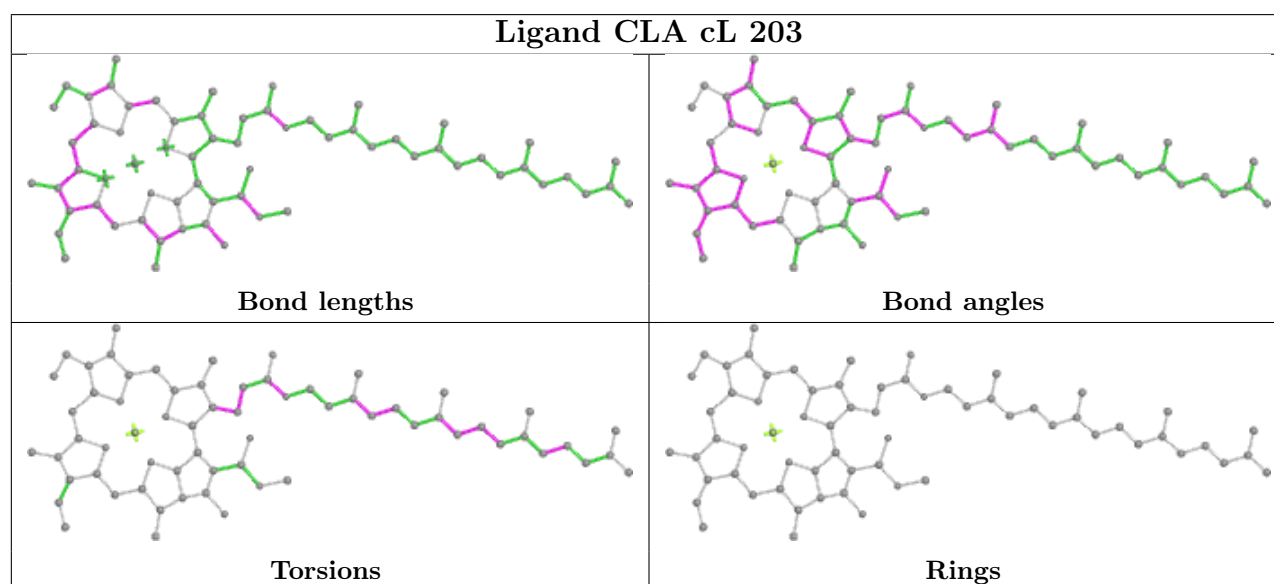
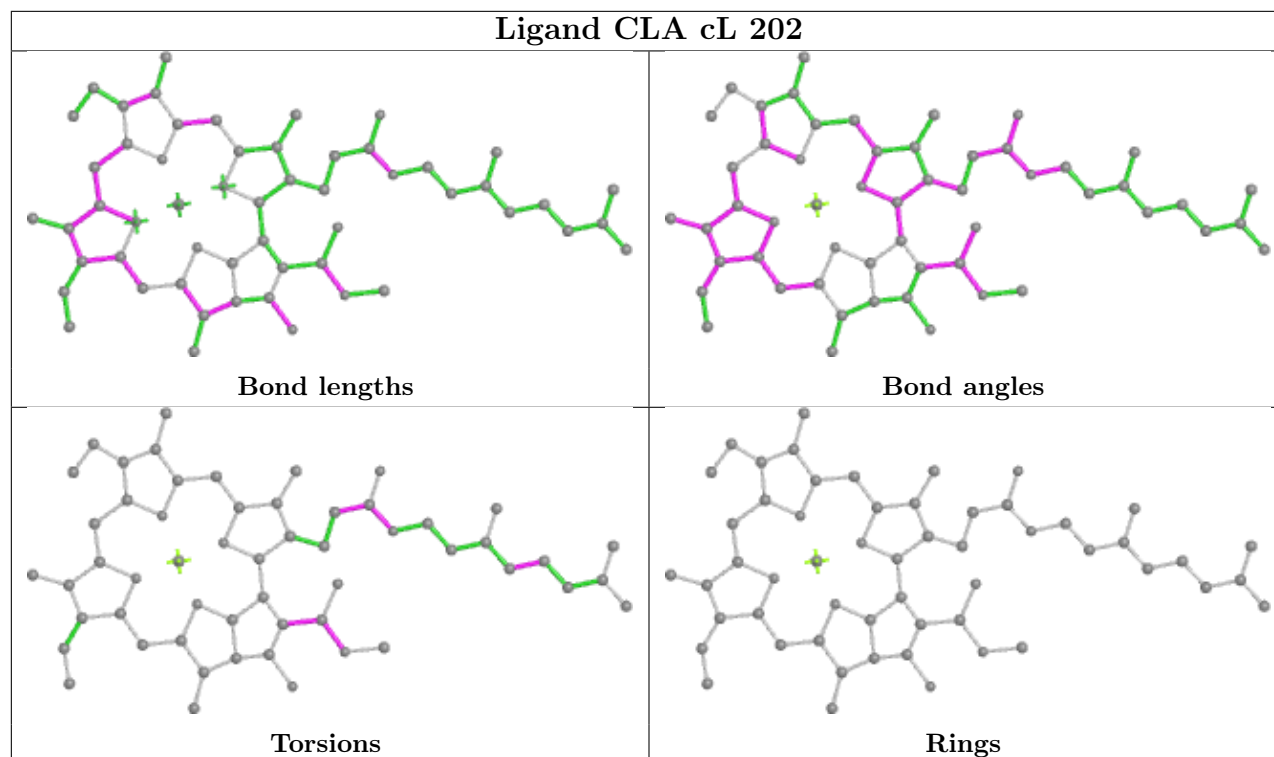
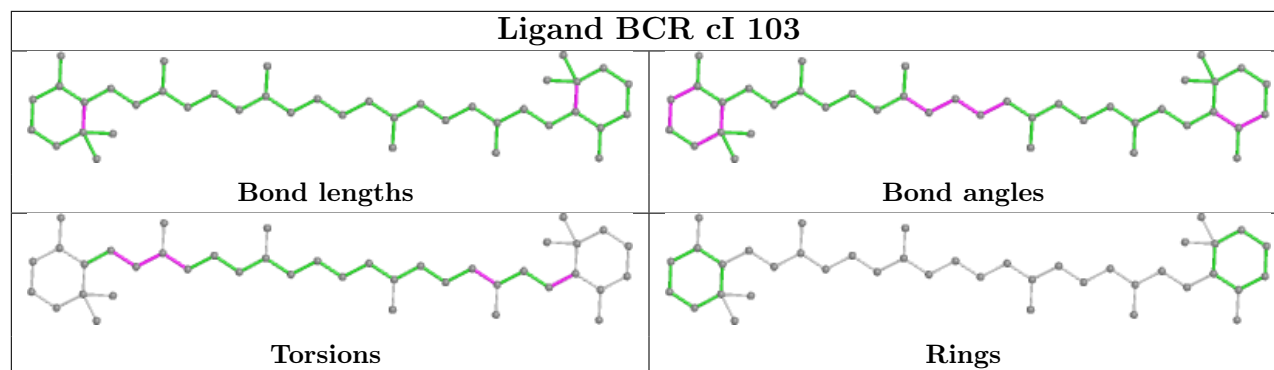


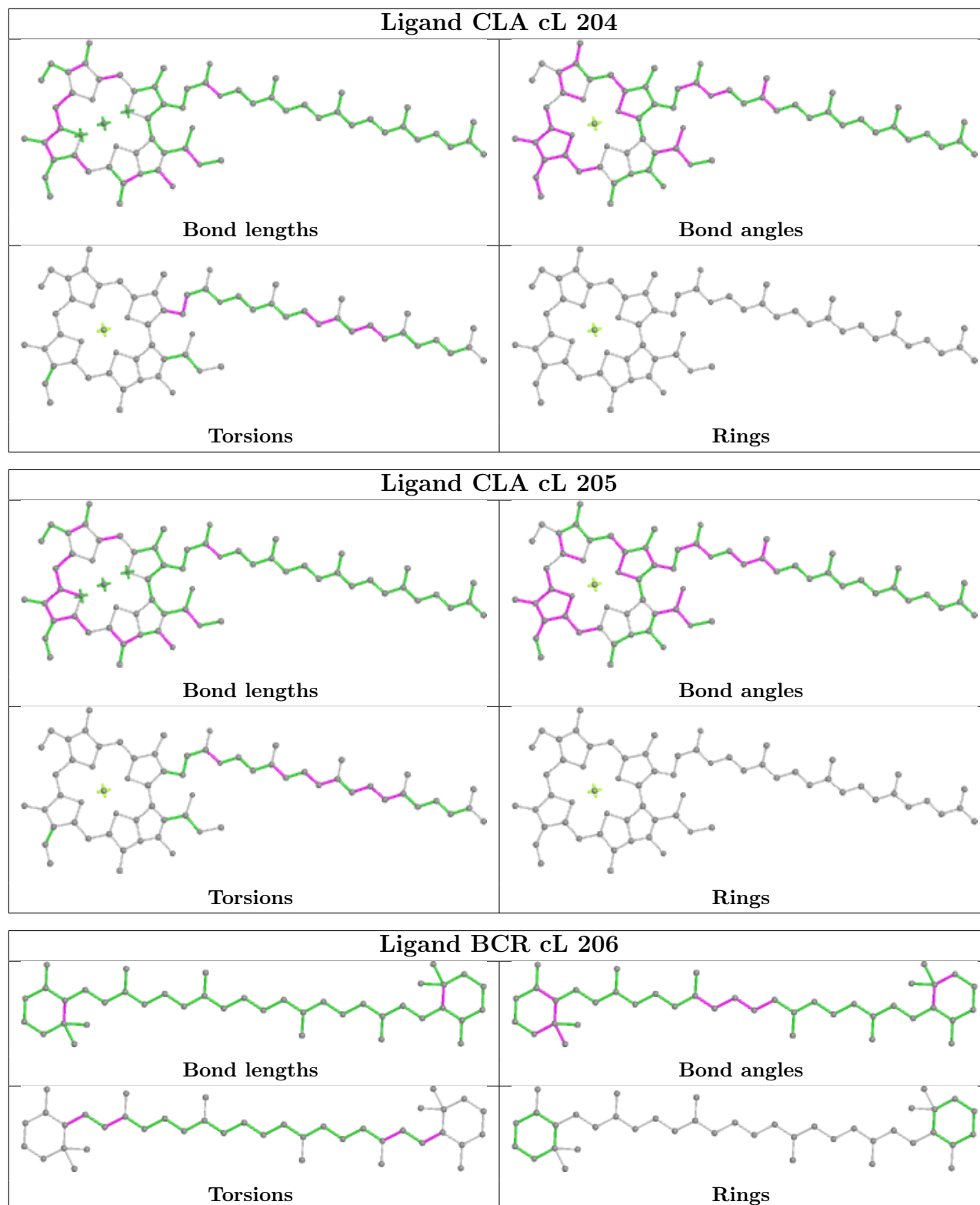


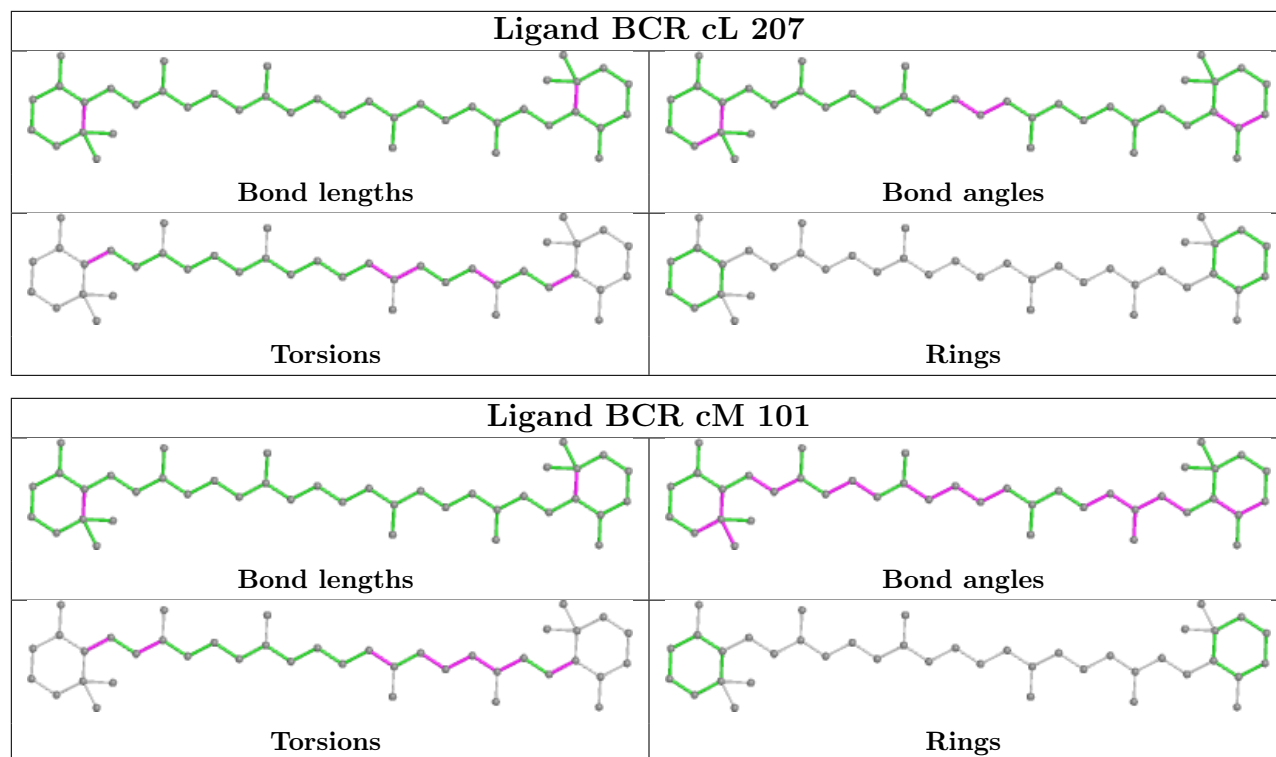












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.