



Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 03:40 PM EDT

PDB ID : 8VU3 / pdb_00008vu3
EMDB ID : EMD-43525
Title : Cryo-EM structure of cyanobacterial PSI with bound platinum nanoparticles
Authors : Gisriel, C.J.; Malavath, T.; Brudvig, G.W.; Utschig, L.M.
Deposited on : 2024-01-28
Resolution : 2.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

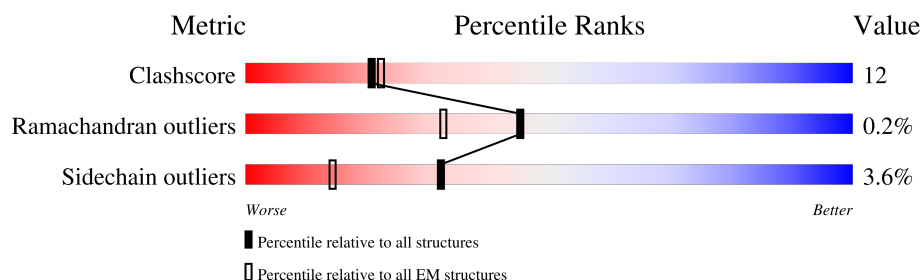
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

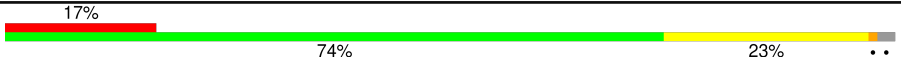



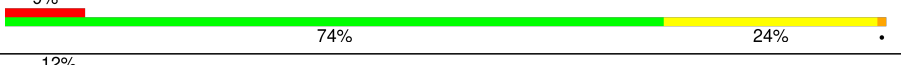

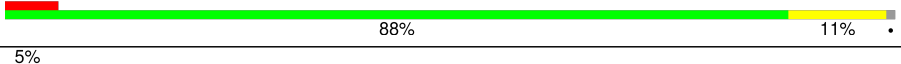

The reported resolution of this entry is 2.27 Å.

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	755	
1	G	755	
1	a	755	
2	B	741	
2	H	741	
2	b	741	
3	C	81	
3	N	81	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	81	
4	D	139	
4	O	139	
4	d	139	
5	E	75	
5	P	75	
5	e	75	
6	F	164	
6	Q	164	
6	f	164	
7	I	40	
7	R	40	
7	i	40	
8	J	43	
8	S	43	
8	j	43	
9	K	83	
9	T	83	
9	k	83	
10	L	155	
10	U	155	
10	l	155	
11	M	31	
11	V	31	
11	m	31	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
12	W	36	<div> <div>61%</div> <div>58%</div> <div>17%</div> <div>25%</div> </div>
12	X	36	<div> <div>64%</div> <div>58%</div> <div>17%</div> <div>25%</div> </div>
12	x	36	<div> <div>64%</div> <div>61%</div> <div>14%</div> <div>25%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL0	A	801	X	-	-	-
13	CL0	G	801	X	-	-	-
13	CL0	a	801	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	844	X	-	-	-
14	CLA	A	845	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	802	X	-	-	-
14	CLA	B	803	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	823	X	-	-	-
14	CLA	B	824	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	F	1301	X	-	-	-
14	CLA	F	1303	X	-	-	-
14	CLA	G	802	X	-	-	-
14	CLA	G	803	X	-	-	-
14	CLA	G	804	X	-	-	-
14	CLA	G	805	X	-	-	-
14	CLA	G	806	X	-	-	-
14	CLA	G	807	X	-	-	-
14	CLA	G	808	X	-	-	-
14	CLA	G	809	X	-	-	-
14	CLA	G	810	X	-	-	-
14	CLA	G	811	X	-	-	-
14	CLA	G	812	X	-	-	-
14	CLA	G	813	X	-	-	-
14	CLA	G	814	X	-	-	-
14	CLA	G	815	X	-	-	-
14	CLA	G	816	X	-	-	-
14	CLA	G	817	X	-	-	-
14	CLA	G	818	X	-	-	-
14	CLA	G	819	X	-	-	-
14	CLA	G	820	X	-	-	-
14	CLA	G	821	X	-	-	-
14	CLA	G	822	X	-	-	-
14	CLA	G	823	X	-	-	-
14	CLA	G	824	X	-	-	-
14	CLA	G	825	X	-	-	-
14	CLA	G	826	X	-	-	-
14	CLA	G	827	X	-	-	-
14	CLA	G	828	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	G	829	X	-	-	-
14	CLA	G	830	X	-	-	-
14	CLA	G	831	X	-	-	-
14	CLA	G	832	X	-	-	-
14	CLA	G	833	X	-	-	-
14	CLA	G	834	X	-	-	-
14	CLA	G	835	X	-	-	-
14	CLA	G	836	X	-	-	-
14	CLA	G	837	X	-	-	-
14	CLA	G	838	X	-	-	-
14	CLA	G	839	X	-	-	-
14	CLA	G	840	X	-	-	-
14	CLA	G	841	X	-	-	-
14	CLA	G	842	X	-	-	-
14	CLA	G	843	X	-	-	-
14	CLA	G	844	X	-	-	-
14	CLA	G	845	X	-	-	-
14	CLA	H	801	X	-	-	-
14	CLA	H	802	X	-	-	-
14	CLA	H	803	X	-	-	-
14	CLA	H	804	X	-	-	-
14	CLA	H	805	X	-	-	-
14	CLA	H	806	X	-	-	-
14	CLA	H	807	X	-	-	-
14	CLA	H	808	X	-	-	-
14	CLA	H	809	X	-	-	-
14	CLA	H	810	X	-	-	-
14	CLA	H	811	X	-	-	-
14	CLA	H	812	X	-	-	-
14	CLA	H	813	X	-	-	-
14	CLA	H	814	X	-	-	-
14	CLA	H	815	X	-	-	-
14	CLA	H	816	X	-	-	-
14	CLA	H	817	X	-	-	-
14	CLA	H	818	X	-	-	-
14	CLA	H	819	X	-	-	-
14	CLA	H	820	X	-	-	-
14	CLA	H	821	X	-	-	-
14	CLA	H	822	X	-	-	-
14	CLA	H	823	X	-	-	-
14	CLA	H	824	X	-	-	-
14	CLA	H	825	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	H	826	X	-	-	-
14	CLA	H	827	X	-	-	-
14	CLA	H	828	X	-	-	-
14	CLA	H	829	X	-	-	-
14	CLA	H	830	X	-	-	-
14	CLA	H	831	X	-	-	-
14	CLA	H	832	X	-	-	-
14	CLA	H	833	X	-	-	-
14	CLA	H	834	X	-	-	-
14	CLA	H	835	X	-	-	-
14	CLA	H	836	X	-	-	-
14	CLA	H	837	X	-	-	-
14	CLA	H	838	X	-	-	-
14	CLA	H	839	X	-	-	-
14	CLA	H	840	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	102	X	-	-	-
14	CLA	L	201	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	L	206	X	-	-	-
14	CLA	M	1601	X	-	-	-
14	CLA	Q	201	X	-	-	-
14	CLA	Q	203	X	-	-	-
14	CLA	S	101	X	-	-	-
14	CLA	S	102	X	-	-	-
14	CLA	T	1401	X	-	-	-
14	CLA	U	201	X	-	-	-
14	CLA	U	204	X	-	-	-
14	CLA	U	205	X	-	-	-
14	CLA	U	206	X	-	-	-
14	CLA	V	1601	X	-	-	-
14	CLA	W	1701	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	a	802	X	-	-	-
14	CLA	a	803	X	-	-	-
14	CLA	a	804	X	-	-	-
14	CLA	a	805	X	-	-	-
14	CLA	a	806	X	-	-	-
14	CLA	a	807	X	-	-	-
14	CLA	a	808	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	809	X	-	-	-
14	CLA	a	810	X	-	-	-
14	CLA	a	811	X	-	-	-
14	CLA	a	812	X	-	-	-
14	CLA	a	813	X	-	-	-
14	CLA	a	814	X	-	-	-
14	CLA	a	815	X	-	-	-
14	CLA	a	816	X	-	-	-
14	CLA	a	817	X	-	-	-
14	CLA	a	818	X	-	-	-
14	CLA	a	819	X	-	-	-
14	CLA	a	820	X	-	-	-
14	CLA	a	821	X	-	-	-
14	CLA	a	822	X	-	-	-
14	CLA	a	823	X	-	-	-
14	CLA	a	824	X	-	-	-
14	CLA	a	825	X	-	-	-
14	CLA	a	826	X	-	-	-
14	CLA	a	827	X	-	-	-
14	CLA	a	828	X	-	-	-
14	CLA	a	829	X	-	-	-
14	CLA	a	830	X	-	-	-
14	CLA	a	831	X	-	-	-
14	CLA	a	832	X	-	-	-
14	CLA	a	833	X	-	-	-
14	CLA	a	834	X	-	-	-
14	CLA	a	835	X	-	-	-
14	CLA	a	836	X	-	-	-
14	CLA	a	837	X	-	-	-
14	CLA	a	838	X	-	-	-
14	CLA	a	839	X	-	-	-
14	CLA	a	840	X	-	-	-
14	CLA	a	841	X	-	-	-
14	CLA	a	842	X	-	-	-
14	CLA	a	843	X	-	-	-
14	CLA	a	844	X	-	-	-
14	CLA	a	855	X	-	-	-
14	CLA	b	801	X	-	-	-
14	CLA	b	802	X	-	-	-
14	CLA	b	803	X	-	-	-
14	CLA	b	804	X	-	-	-
14	CLA	b	805	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	806	X	-	-	-
14	CLA	b	807	X	-	-	-
14	CLA	b	808	X	-	-	-
14	CLA	b	809	X	-	-	-
14	CLA	b	810	X	-	-	-
14	CLA	b	811	X	-	-	-
14	CLA	b	812	X	-	-	-
14	CLA	b	813	X	-	-	-
14	CLA	b	814	X	-	-	-
14	CLA	b	815	X	-	-	-
14	CLA	b	816	X	-	-	-
14	CLA	b	817	X	-	-	-
14	CLA	b	818	X	-	-	-
14	CLA	b	819	X	-	-	-
14	CLA	b	820	X	-	-	-
14	CLA	b	821	X	-	-	-
14	CLA	b	822	X	-	-	-
14	CLA	b	823	X	-	-	-
14	CLA	b	824	X	-	-	-
14	CLA	b	825	X	-	-	-
14	CLA	b	826	X	-	-	-
14	CLA	b	827	X	-	-	-
14	CLA	b	828	X	-	-	-
14	CLA	b	829	X	-	-	-
14	CLA	b	830	X	-	-	-
14	CLA	b	831	X	-	-	-
14	CLA	b	832	X	-	-	-
14	CLA	b	833	X	-	-	-
14	CLA	b	834	X	-	-	-
14	CLA	b	835	X	-	-	-
14	CLA	b	836	X	-	-	-
14	CLA	b	837	X	-	-	-
14	CLA	b	838	X	-	-	-
14	CLA	b	839	X	-	-	-
14	CLA	b	840	X	-	-	-
14	CLA	f	202	X	-	-	-
14	CLA	i	101	X	-	-	-
14	CLA	j	101	X	-	-	-
14	CLA	j	102	X	-	-	-
14	CLA	k	1401	X	-	-	-
14	CLA	l	202	X	-	-	-
14	CLA	l	205	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	l	206	X	-	-	-
14	CLA	l	207	X	-	-	-
14	CLA	m	1601	X	-	-	-
14	CLA	x	1701	X	-	-	-

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 71694 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	740	Total	C	N	O	S	0	0
			5777	3791	987	976	23		
1	G	740	Total	C	N	O	S	0	0
			5777	3791	987	976	23		
1	a	740	Total	C	N	O	S	0	0
			5777	3791	987	976	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	739	Total	C	N	O	S	0	0
			5892	3876	988	1008	20		
2	H	739	Total	C	N	O	S	0	0
			5892	3876	988	1008	20		
2	b	739	Total	C	N	O	S	0	0
			5892	3876	988	1008	20		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1076	683	187	203	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	138	Total	C	N	O	S	0	0
			1076	683	187	203	3		
4	d	138	Total	C	N	O	S	0	0
			1076	683	187	203	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	69	Total	C	N	O		0	0
			534	337	92	105			
5	P	69	Total	C	N	O		0	0
			534	337	92	105			
5	e	69	Total	C	N	O		0	0
			534	337	92	105			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	53	GLY	SER	conflict	UNP A0A2D2Q1I4
P	53	GLY	SER	conflict	UNP A0A2D2Q1I4
e	53	GLY	SER	conflict	UNP A0A2D2Q1I4

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1064	679	184	197	4		
6	Q	141	Total	C	N	O	S	0	0
			1064	679	184	197	4		
6	f	141	Total	C	N	O	S	0	0
			1064	679	184	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	39	Total	C	N	O	S	0	0
			308	213	42	48	5		
7	R	39	Total	C	N	O	S	0	0
			308	213	42	48	5		
7	i	39	Total	C	N	O	S	0	0
			308	213	42	48	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	43	Total	C	N	O	S	0	0
			351	237	54	58	2		
8	S	43	Total	C	N	O	S	0	0
			351	237	54	58	2		
8	j	43	Total	C	N	O	S	0	0
			351	237	54	58	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	63	Total	C	N	O	0	0
			307	181	63	63		
9	T	63	Total	C	N	O	0	0
			307	181	63	63		
9	k	63	Total	C	N	O	0	0
			307	181	63	63		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	152	Total	C	N	O	S	0	0
			1125	737	181	203	4		
10	U	152	Total	C	N	O	S	0	0
			1125	737	181	203	4		
10	l	152	Total	C	N	O	S	0	0
			1125	737	181	203	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			240	161	36	42	1		
11	V	31	Total	C	N	O	S	0	0
			240	161	36	42	1		
11	m	31	Total	C	N	O	S	0	0
			240	161	36	42	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	27	ALA	THR	conflict	UNP A0A3B7MIX8

Continued on next page...

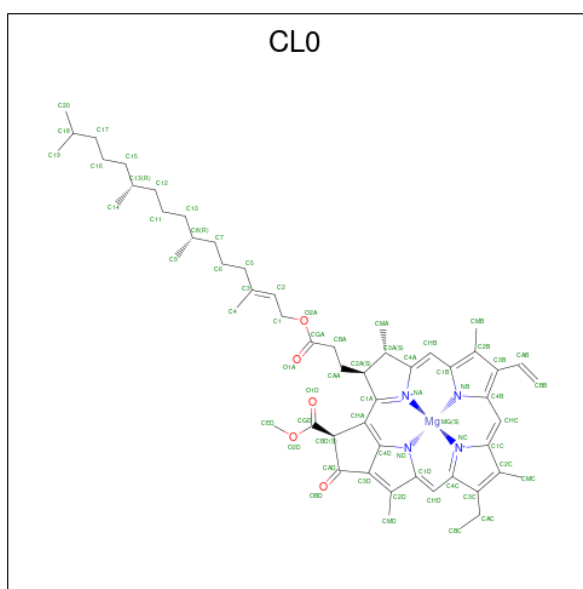
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
V	27	ALA	THR	conflict	UNP A0A3B7MIX8
m	27	ALA	THR	conflict	UNP A0A3B7MIX8

- Molecule 12 is a protein called Phosphorylase.

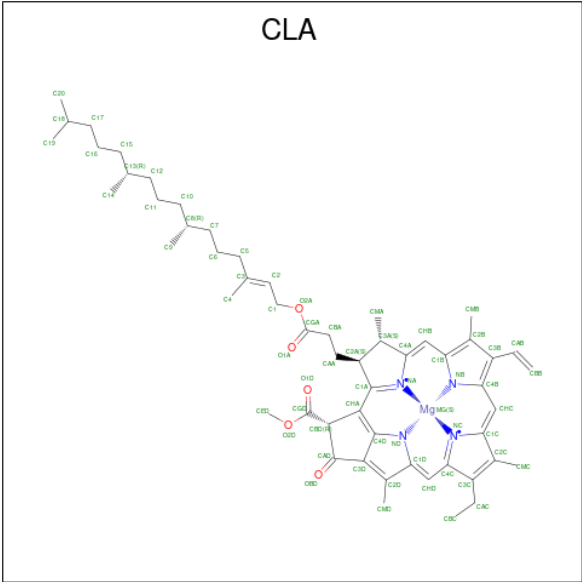
Mol	Chain	Residues	Atoms				AltConf	Trace
12	W	27	Total	C	N	O	0	0
			228	162	32	34		
12	X	27	Total	C	N	O	0	0
			228	162	32	34		
12	x	27	Total	C	N	O	0	0
			228	162	32	34		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	F	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 50	C 40	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	S	1	Total 37	C 31	Mg 1	N 4	O 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	U	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

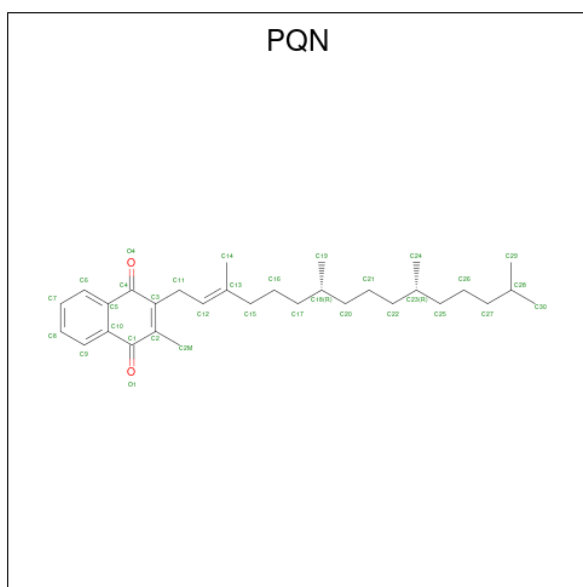
Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

Continued on next page...

Continued from previous page...

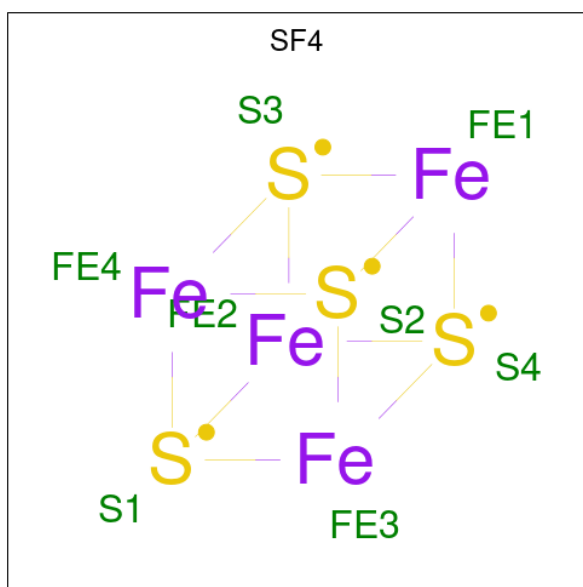
Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	m	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	x	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



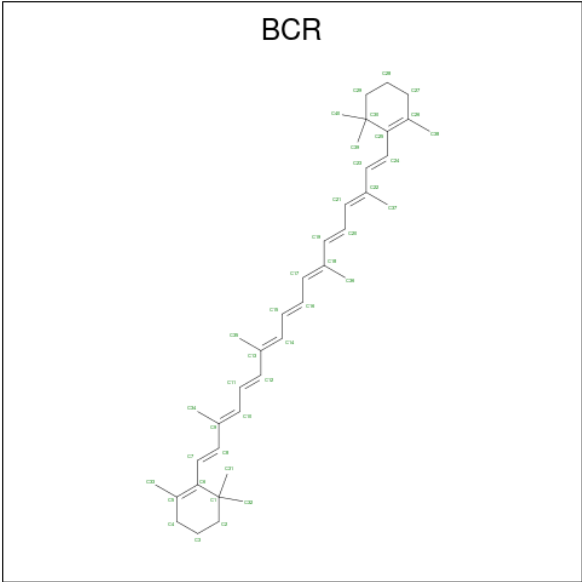
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	
15	B	1	Total	C	O	0
			33	31	2	
15	G	1	Total	C	O	0
			33	31	2	
15	H	1	Total	C	O	0
			33	31	2	
15	a	1	Total	C	O	0
			33	31	2	
15	b	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			25	25	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
17	F	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	H	1	Total C 40 40	0
17	H	1	Total C 40 40	0
17	H	1	Total C 40 40	0
17	H	1	Total C 25 25	0
17	H	1	Total C 40 40	0
17	H	1	Total C 40 40	0
17	H	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

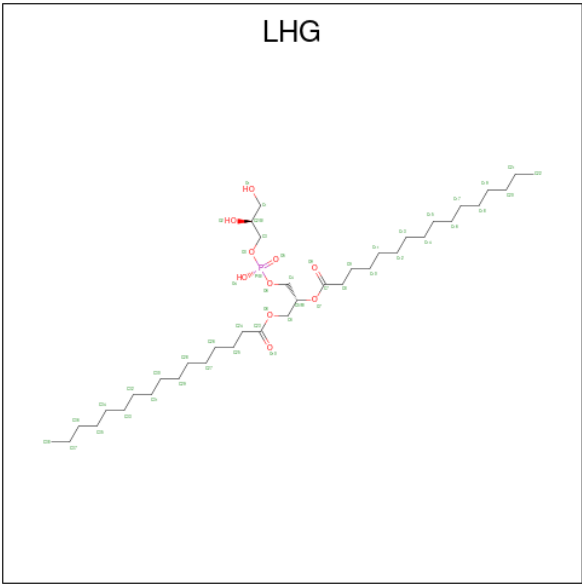
Mol	Chain	Residues	Atoms	AltConf
17	Q	1	Total C 40 40	0
17	Q	1	Total C 40 40	0
17	R	1	Total C 40 40	0
17	R	1	Total C 40 40	0
17	R	1	Total C 40 40	0
17	S	1	Total C 40 40	0
17	S	1	Total C 40 40	0
17	U	1	Total C 40 40	0
17	V	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 25 25	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

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

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



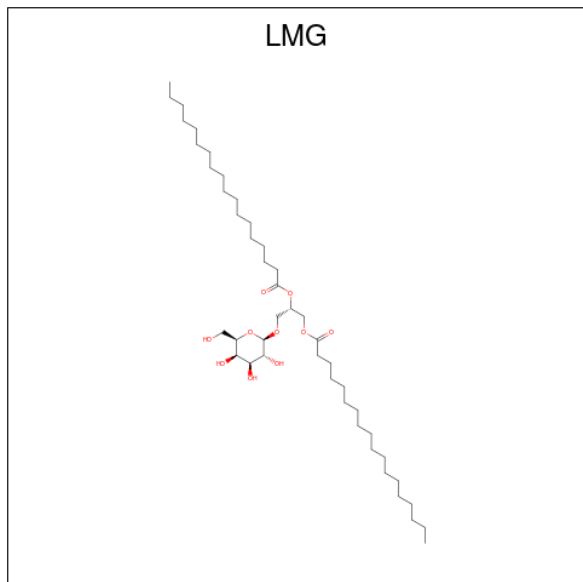
Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			49	38	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			27	16	10	1	
18	G	1	Total	C	O	P	0
			49	38	10	1	
18	G	1	Total	C	O	P	0
			27	16	10	1	
18	a	1	Total	C	O	P	0
			49	38	10	1	
18	a	1	Total	C	O	P	0
			27	16	10	1	

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total	C	O	0
			49	39	10	
19	H	1	Total	C	O	0
			49	39	10	
19	b	1	Total	C	O	0
			49	39	10	

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
20	L	1	Total	Ca	0
			1	1	

Continued on next page...

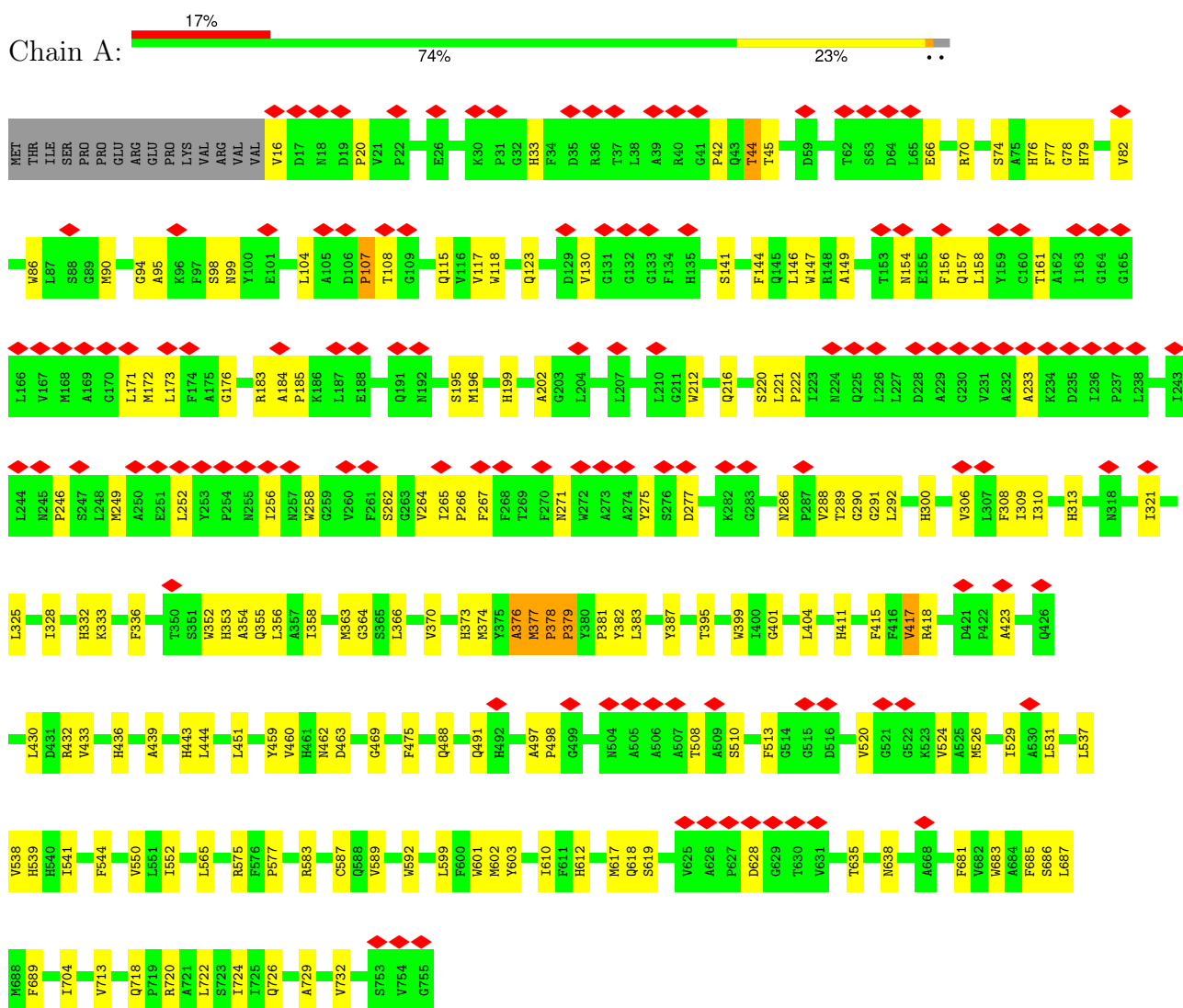
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
20	U	1	Total 1	Ca 1	0
20	1	1	Total 1	Ca 1	0

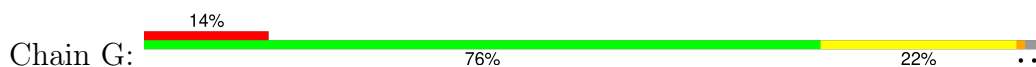
3 Residue-property plots

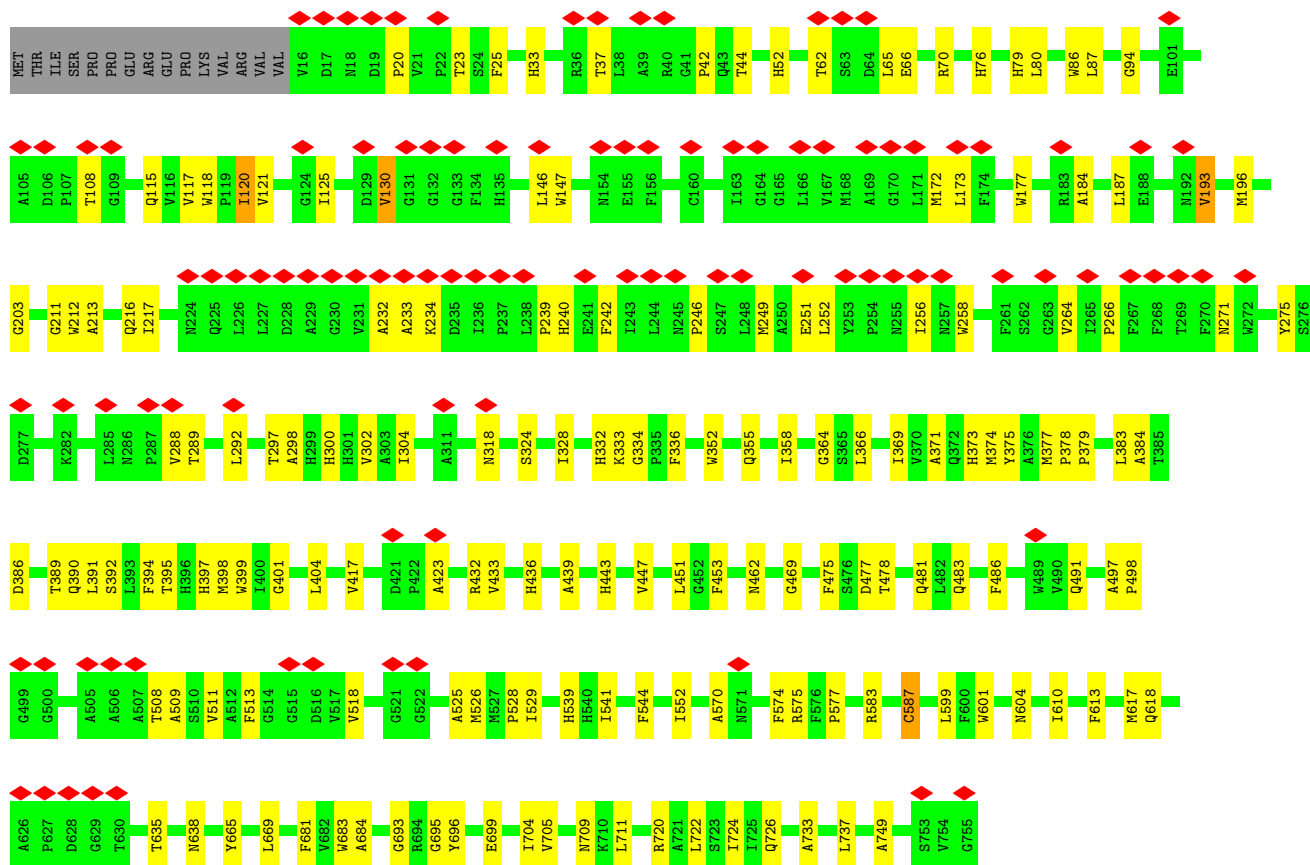
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

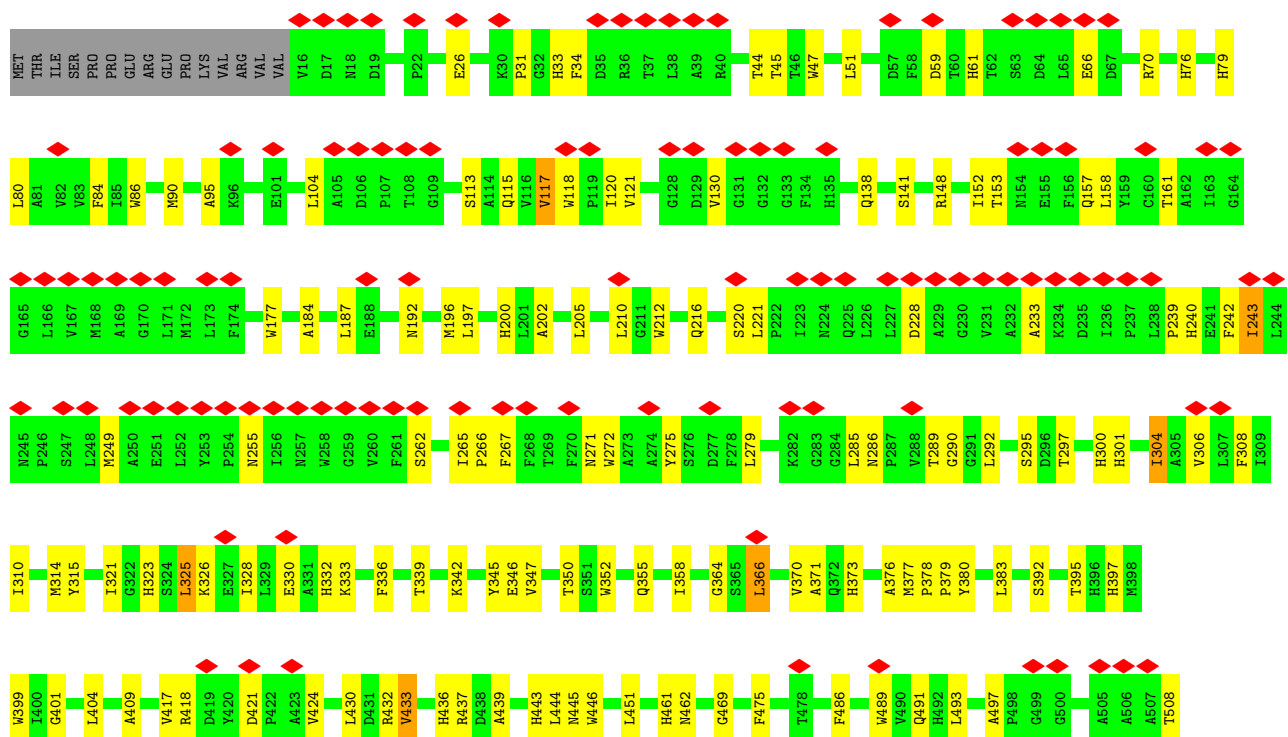


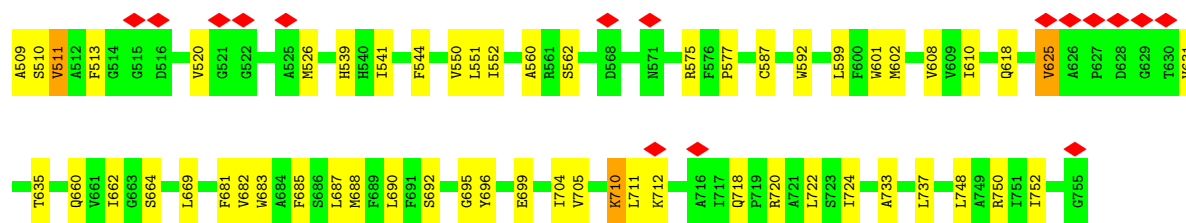
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



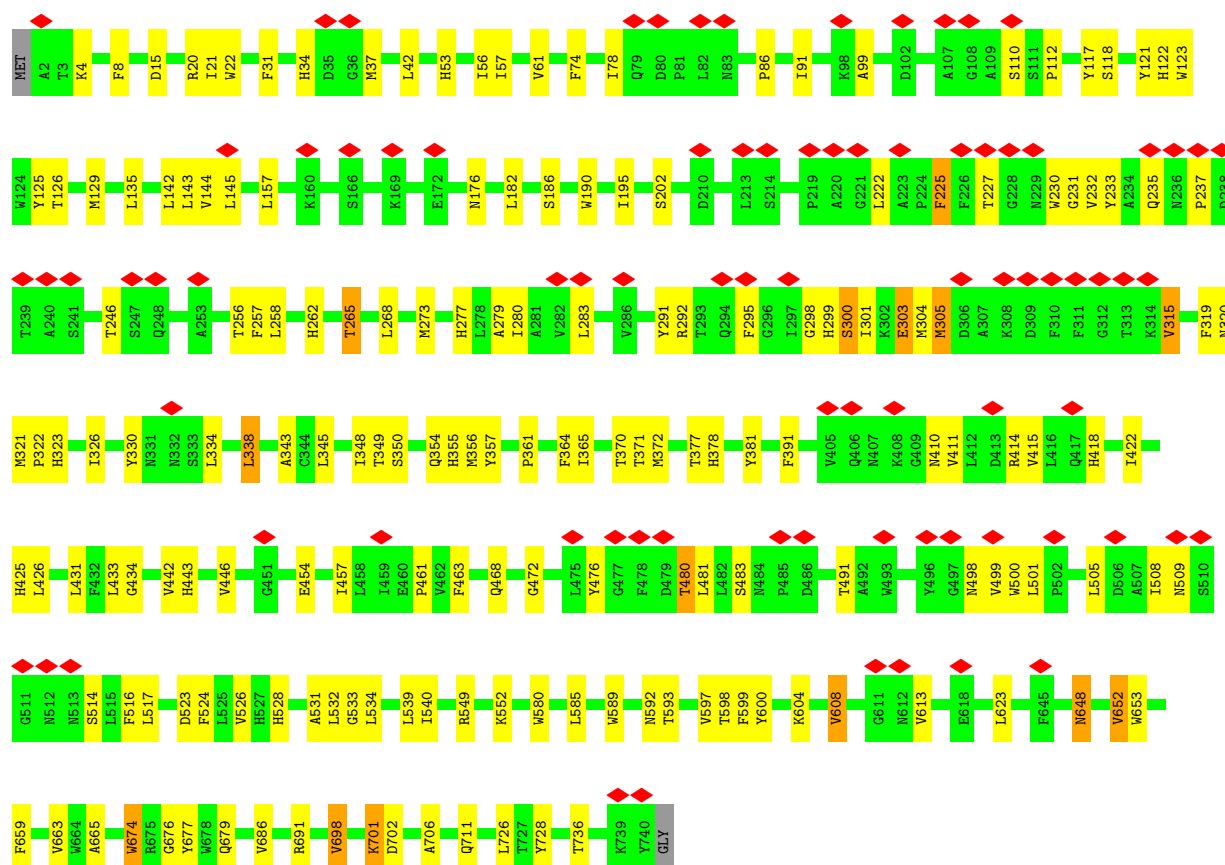
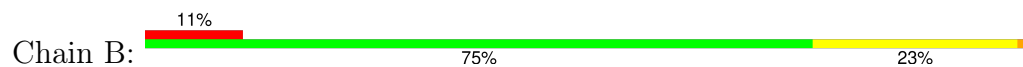


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

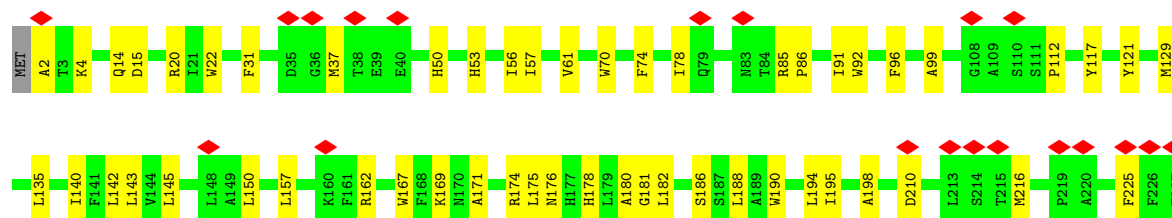


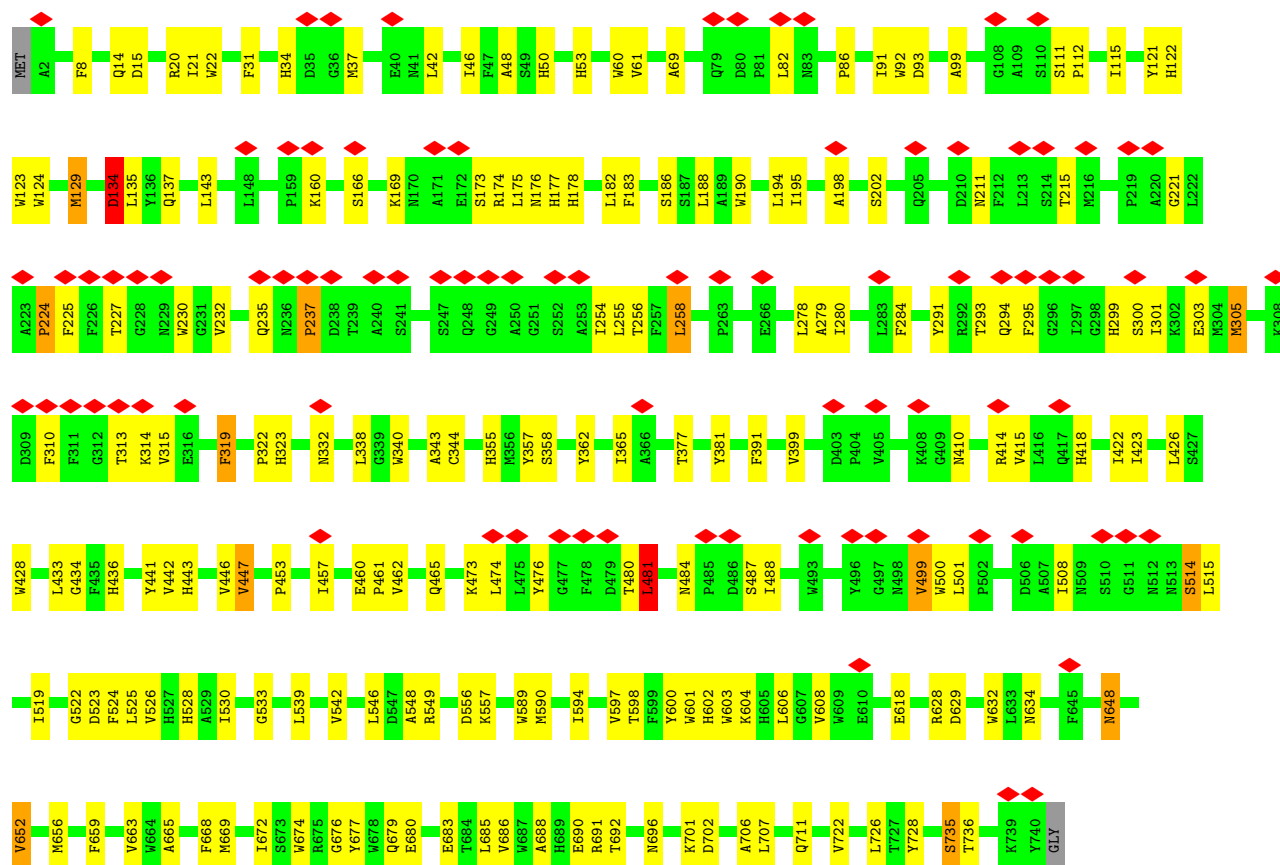
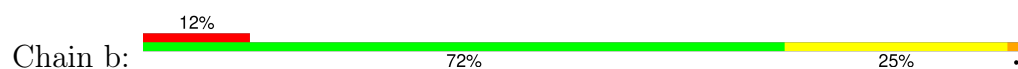
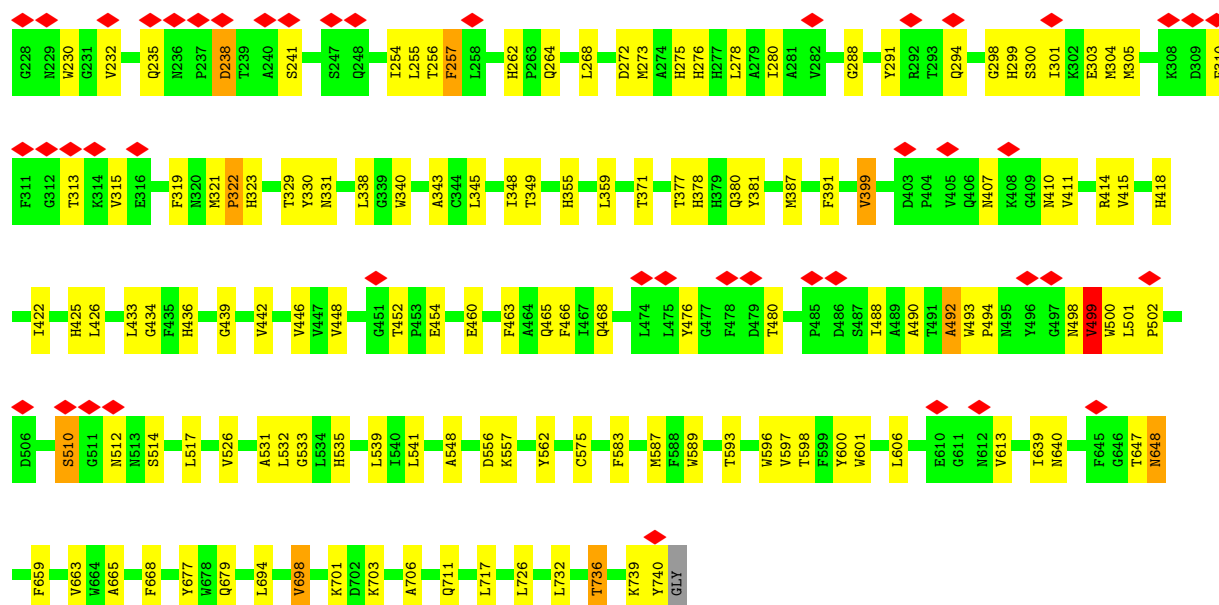


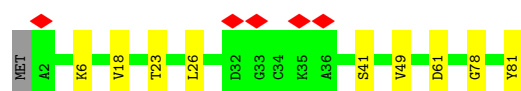
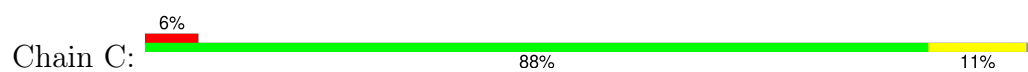
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



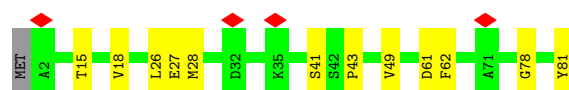
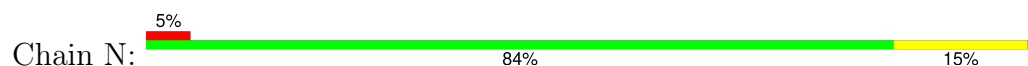
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



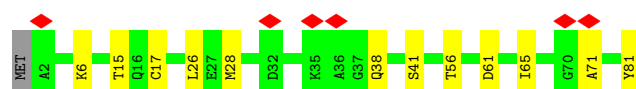
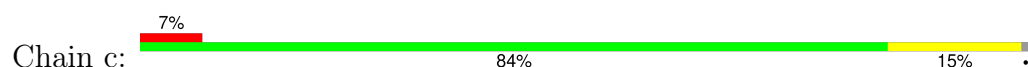




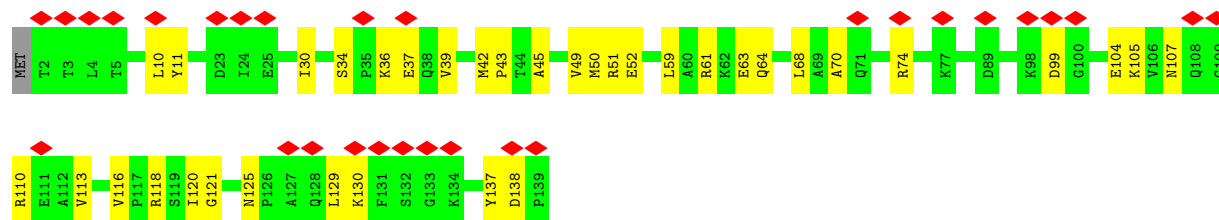
- Molecule 3: Photosystem I iron-sulfur center



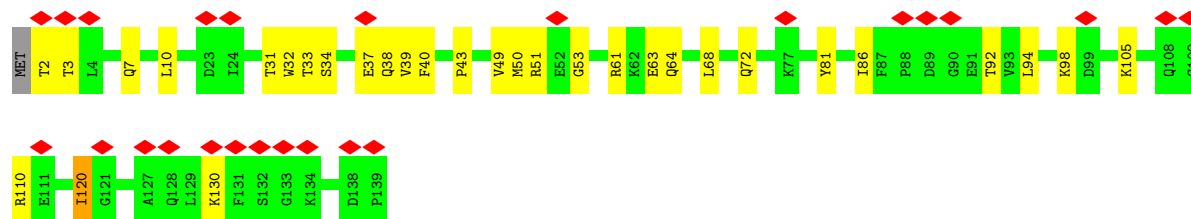
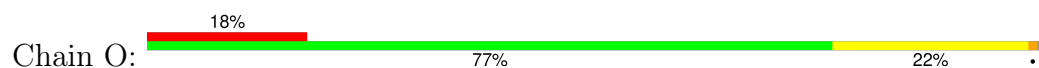
- Molecule 3: Photosystem I iron-sulfur center



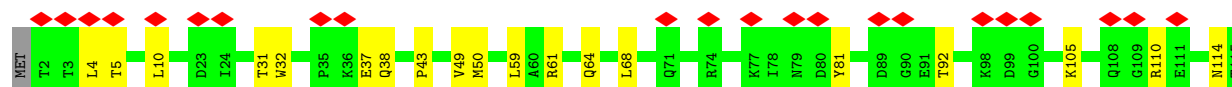
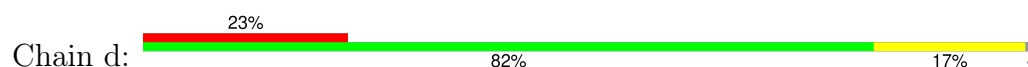
- Molecule 4: Photosystem I reaction center subunit II

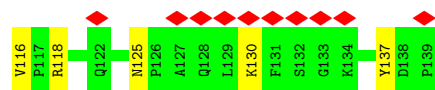


- Molecule 4: Photosystem I reaction center subunit II

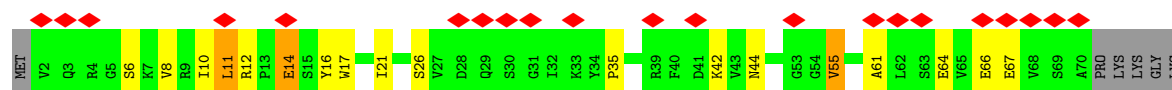


- Molecule 4: Photosystem I reaction center subunit II

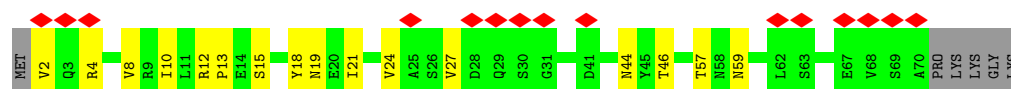




• Molecule 5: Photosystem I reaction center subunit IV



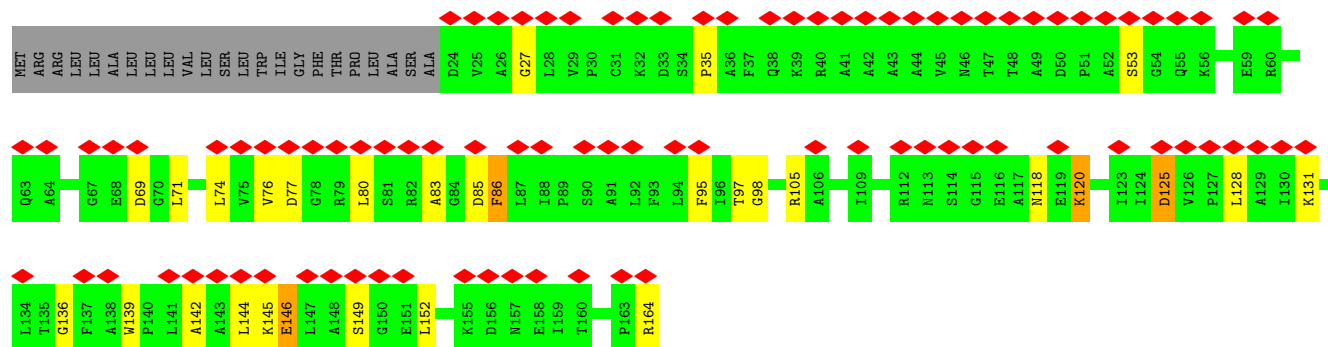
• Molecule 5: Photosystem I reaction center subunit IV



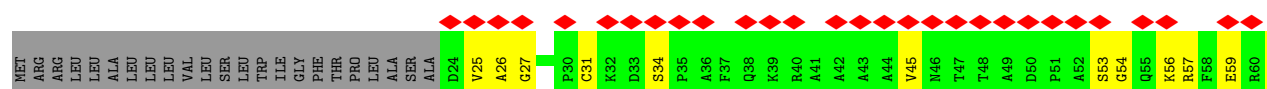
• Molecule 5: Photosystem I reaction center subunit IV

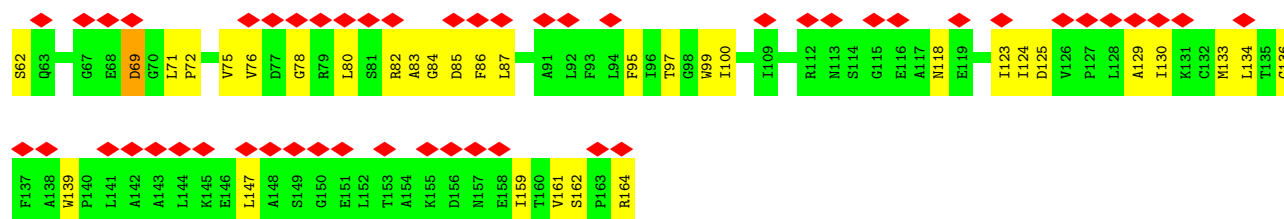


• Molecule 6: Photosystem I reaction center subunit III

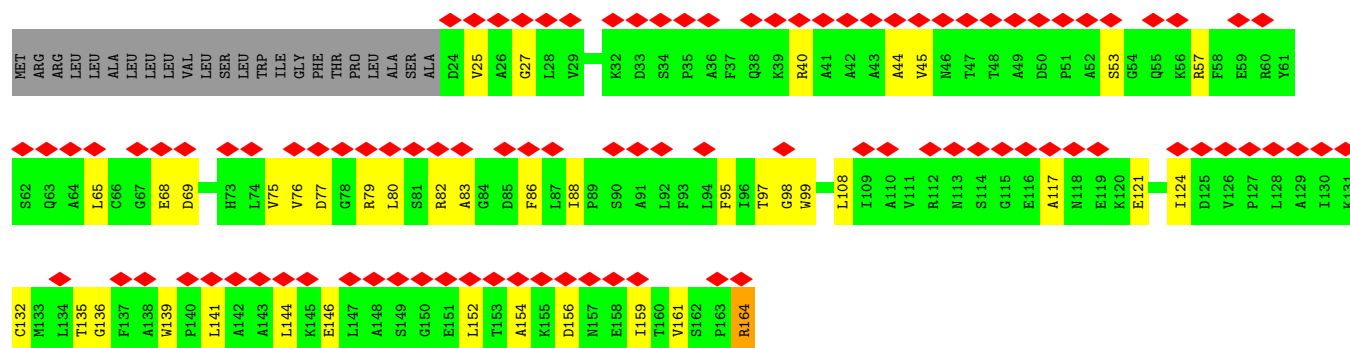


• Molecule 6: Photosystem I reaction center subunit III





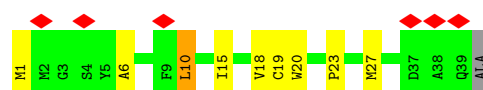
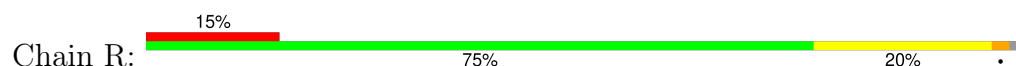
• Molecule 6: Photosystem I reaction center subunit III



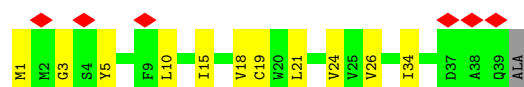
• Molecule 7: Photosystem I reaction center subunit VIII



• Molecule 7: Photosystem I reaction center subunit VIII

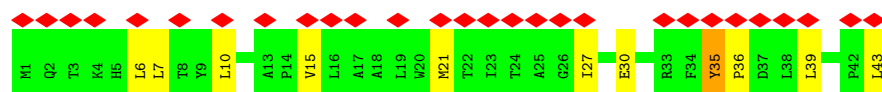


• Molecule 7: Photosystem I reaction center subunit VIII

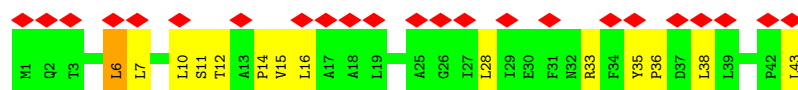


• Molecule 8: Photosystem I reaction center subunit IX

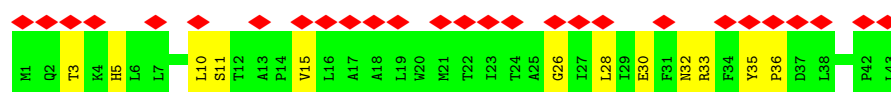
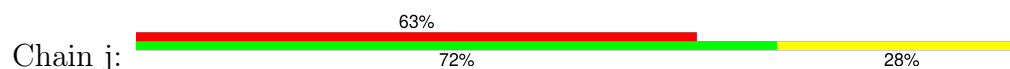




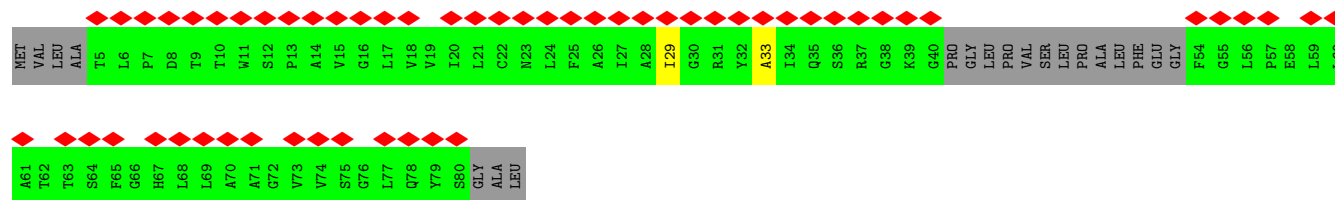
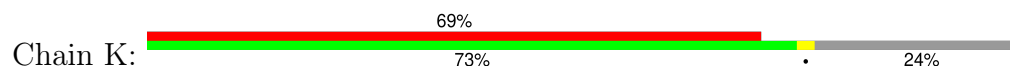
• Molecule 8: Photosystem I reaction center subunit IX



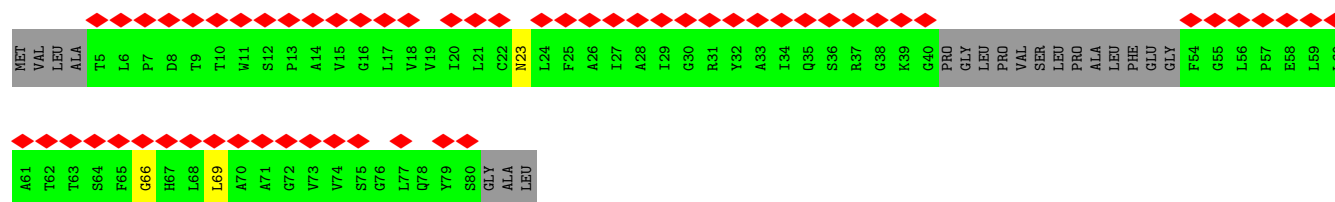
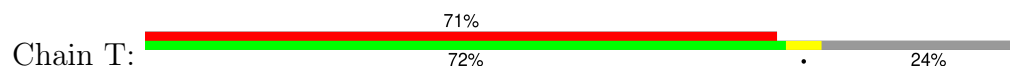
• Molecule 8: Photosystem I reaction center subunit IX



• Molecule 9: Photosystem I reaction center subunit Psak

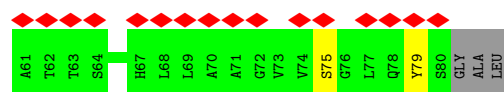


• Molecule 9: Photosystem I reaction center subunit Psak

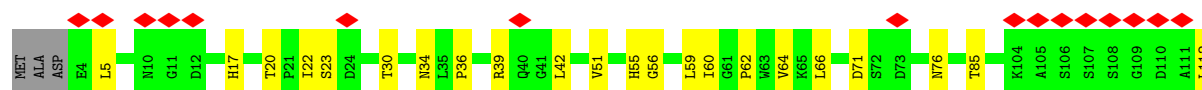
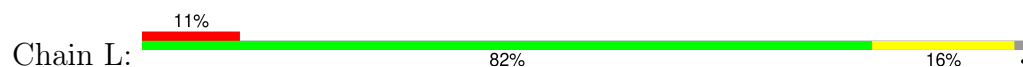


• Molecule 9: Photosystem I reaction center subunit Psak

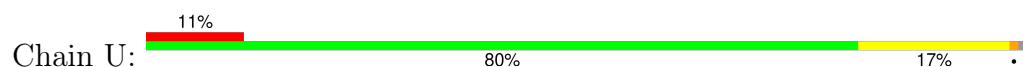




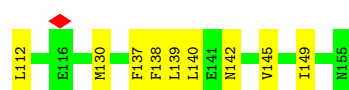
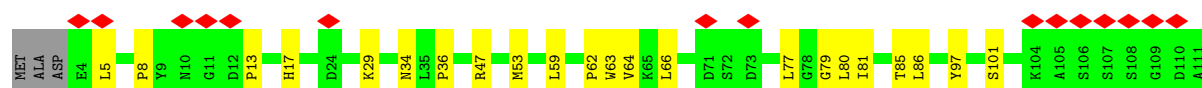
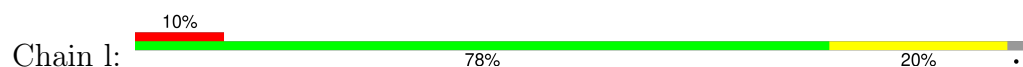
- Molecule 10: Photosystem I reaction center subunit XI



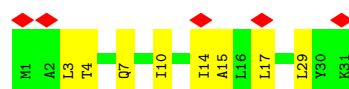
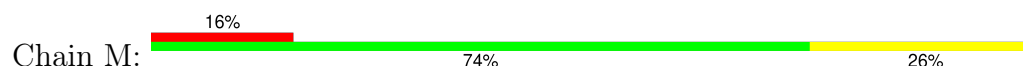
- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XI

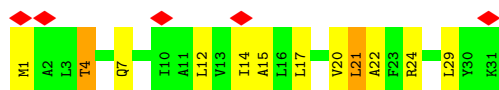


- Molecule 11: Photosystem I reaction center subunit XII

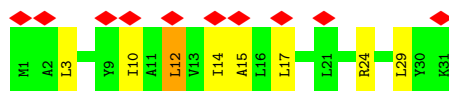
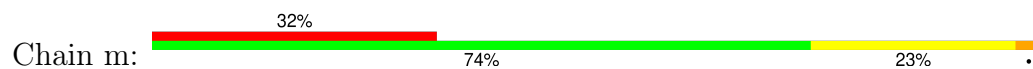


- Molecule 11: Photosystem I reaction center subunit XII





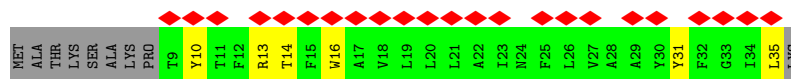
- Molecule 11: Photosystem I reaction center subunit XII



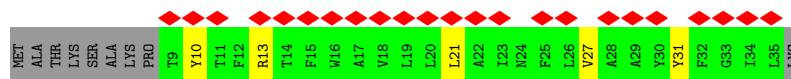
- Molecule 12: Phosphorylase



- Molecule 12: Phosphorylase



- Molecule 12: Phosphorylase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	189655	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00404	Depositor
Map size (Å)	297.0, 297.0, 297.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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, CA, BCR, CL0, PQN, SF4, LMG, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	4/5978 (0.1%)	0.83	11/8158 (0.1%)
1	G	0.30	0/5978	0.63	6/8158 (0.1%)
1	a	0.31	0/5978	0.64	2/8158 (0.0%)
2	B	0.31	0/6110	0.65	2/8350 (0.0%)
2	H	0.40	2/6110 (0.0%)	0.70	9/8350 (0.1%)
2	b	0.49	6/6110 (0.1%)	0.83	20/8350 (0.2%)
3	C	0.24	0/608	0.51	0/824
3	N	0.23	0/608	0.54	0/824
3	c	0.21	0/608	0.54	0/824
4	D	0.27	0/1101	0.64	0/1492
4	O	0.29	0/1101	0.64	0/1492
4	d	0.27	0/1101	0.64	0/1492
5	E	0.22	0/544	0.63	0/737
5	P	0.28	0/544	0.61	0/737
5	e	0.69	2/544 (0.4%)	1.50	3/737 (0.4%)
6	F	0.30	0/1086	0.84	4/1474 (0.3%)
6	Q	0.32	0/1086	0.79	2/1474 (0.1%)
6	f	0.29	0/1086	0.73	0/1474
7	I	0.31	0/319	0.74	0/436
7	R	0.30	0/319	0.67	0/436
7	i	0.31	0/319	0.69	0/436
8	J	0.40	0/362	0.85	0/494
8	S	0.31	0/362	0.79	0/494
8	j	0.33	0/362	0.81	0/494
9	K	0.23	0/305	0.83	0/419
9	T	0.22	0/305	0.84	0/419
9	k	0.22	0/305	0.82	0/419
10	L	0.29	0/1153	0.55	0/1562
10	U	0.29	0/1153	0.56	0/1562
10	l	0.27	0/1153	0.53	0/1562
11	M	0.32	0/243	0.53	0/330
11	V	0.34	0/243	0.52	0/330

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	m	0.36	0/243	0.54	0/330
12	W	0.24	0/236	0.55	0/323
12	X	0.23	0/236	0.61	0/323
12	x	0.23	0/236	0.59	0/323
All	All	0.37	14/54135 (0.0%)	0.71	59/73797 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
4	D	0	1
4	O	0	1
4	d	0	1
6	F	0	1
All	All	0	6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	224	PRO	CG-CD	-22.05	0.75	1.50
1	A	379	PRO	CB-CG	19.23	2.45	1.49
1	A	379	PRO	CG-CD	-18.55	0.87	1.50
2	H	502	PRO	CG-CD	-16.15	0.95	1.50
5	e	13	PRO	N-CA	9.72	1.59	1.47
2	b	237	PRO	CG-CD	-9.69	1.17	1.50
5	e	13	PRO	CB-CG	-8.50	1.07	1.49
2	b	224	PRO	N-CA	7.75	1.57	1.47
2	H	501	LEU	C-N	7.28	1.42	1.34
2	b	237	PRO	CB-CG	-6.99	1.14	1.49
2	b	481	LEU	CG-CD2	-6.58	1.30	1.52
2	b	453	PRO	CG-CD	-6.53	1.28	1.50
1	A	379	PRO	N-CA	-6.47	1.39	1.47
1	A	379	PRO	N-CD	6.34	1.56	1.47

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	PRO	CB-CG-CD	-33.15	0.01	106.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	224	PRO	N-CD-CG	-23.99	67.21	103.20
5	e	13	PRO	N-CD-CG	-23.22	68.37	103.20
5	e	13	PRO	CB-CG-CD	23.05	179.88	106.10
5	e	13	PRO	CA-CB-CG	-18.14	70.04	104.50
2	b	224	PRO	CA-CB-CG	-18.08	70.15	104.50
2	H	502	PRO	N-CD-CG	-17.18	77.44	103.20
2	b	237	PRO	N-CD-CG	-16.71	78.13	103.20
1	A	379	PRO	CA-N-CD	-16.56	88.82	112.00
1	A	107	PRO	CA-N-CD	-13.95	92.47	112.00
2	b	237	PRO	CA-CB-CG	-13.81	78.27	104.50
1	A	379	PRO	N-CA-CB	-12.45	90.18	103.25
2	b	453	PRO	N-CD-CG	-10.46	87.52	103.20
2	H	502	PRO	CA-CB-CG	-10.44	84.67	104.50
1	G	498	PRO	N-CD-CG	-10.08	88.08	103.20
1	A	379	PRO	CA-CB-CG	-10.05	85.41	104.50
2	b	224	PRO	CA-N-CD	-9.63	98.52	112.00
2	b	453	PRO	CA-N-CD	-8.61	99.95	112.00
2	b	224	PRO	CB-CG-CD	8.33	132.75	106.10
1	A	378	PRO	C-N-CD	8.28	158.96	125.00
2	b	237	PRO	CA-N-CD	-7.91	100.92	112.00
6	F	35	PRO	N-CD-CG	-7.66	91.70	103.20
1	G	498	PRO	CA-N-CD	-7.56	101.42	112.00
2	b	129	MET	CG-SD-CE	-7.25	84.94	100.90
1	a	130	VAL	N-CA-C	-7.22	104.97	113.42
2	b	237	PRO	CB-CG-CD	7.10	128.81	106.10
2	H	257	PHE	N-CA-C	-6.91	102.15	110.44
6	F	125	ASP	CA-C-N	6.78	124.51	120.24
6	F	125	ASP	C-N-CA	6.78	124.51	120.24
2	H	322	PRO	N-CD-CG	-6.71	93.14	103.20
2	H	492	ALA	CA-C-N	6.69	132.12	121.62
2	H	492	ALA	C-N-CA	6.69	132.12	121.62
1	A	90	MET	CG-SD-CE	-6.49	86.63	100.90
6	Q	125	ASP	CA-C-N	6.25	125.33	120.33
6	Q	125	ASP	C-N-CA	6.25	125.33	120.33
2	b	224	PRO	N-CA-CB	-6.15	96.80	103.25
1	A	378	PRO	CA-C-N	-6.11	112.20	119.84
1	A	378	PRO	C-N-CA	-6.11	112.20	119.84
2	H	502	PRO	CA-N-CD	-6.02	103.58	112.00
2	B	305	MET	CB-CG-SD	5.95	130.55	112.70
2	H	512	ASN	N-CA-C	-5.93	104.90	114.09
1	A	264	VAL	CA-C-N	5.83	123.91	120.24
1	A	264	VAL	C-N-CA	5.83	123.91	120.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	35	PRO	CA-CB-CG	-5.63	93.80	104.50
2	B	280	ILE	CB-CG1-CD1	5.62	125.61	113.80
1	G	264	VAL	CA-C-N	5.54	123.73	120.24
1	G	264	VAL	C-N-CA	5.54	123.73	120.24
2	b	129	MET	CB-CA-C	5.51	118.53	110.26
1	a	243	ILE	N-CA-C	-5.45	108.19	113.53
2	b	134	ASP	CB-CG-OD2	-5.45	105.87	118.40
1	G	130	VAL	N-CA-C	-5.44	107.97	113.47
2	b	453	PRO	CA-CB-CG	-5.18	94.66	104.50
2	b	314	LYS	CA-C-N	5.08	131.12	121.97
2	b	314	LYS	C-N-CA	5.08	131.12	121.97
2	H	322	PRO	CA-N-CD	-5.08	104.89	112.00
1	G	498	PRO	CA-CB-CG	-5.07	94.87	104.50
2	b	221	GLY	CA-C-N	5.04	131.16	121.54
2	b	221	GLY	C-N-CA	5.04	131.16	121.54
2	b	129	MET	N-CA-CB	-5.01	102.00	109.71

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	ALA	Peptide
2	B	674	TRP	Peptide
4	D	130	LYS	Peptide
6	F	86	PHE	Peptide
4	O	130	LYS	Peptide
4	d	130	LYS	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	A	5777	0	5627	151	0
1	G	5777	0	5627	130	0
1	a	5777	0	5627	156	0
2	B	5892	0	5646	143	0
2	H	5892	0	5646	145	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	5892	0	5646	156	0
3	C	598	0	577	9	0
3	N	598	0	577	11	0
3	c	598	0	577	11	0
4	D	1076	0	1083	23	0
4	O	1076	0	1083	19	0
4	d	1076	0	1083	13	0
5	E	534	0	519	12	0
5	P	534	0	519	9	0
5	e	534	0	519	11	0
6	F	1064	0	1072	19	0
6	Q	1064	0	1072	29	0
6	f	1064	0	1072	28	0
7	I	308	0	314	7	0
7	R	308	0	314	10	0
7	i	308	0	314	8	0
8	J	351	0	364	6	0
8	S	351	0	364	10	0
8	j	351	0	364	8	0
9	K	307	0	150	1	0
9	T	307	0	150	2	0
9	k	307	0	150	3	0
10	L	1125	0	1129	18	0
10	U	1125	0	1129	20	0
10	l	1125	0	1129	25	0
11	M	240	0	264	5	0
11	V	240	0	264	8	0
11	m	240	0	264	5	0
12	W	228	0	230	3	0
12	X	228	0	230	3	0
12	x	228	0	230	5	0
13	A	65	0	72	3	0
13	G	65	0	72	6	0
13	a	65	0	72	5	0
14	A	2455	0	2328	126	0
14	B	2239	0	2141	133	0
14	F	82	0	57	1	0
14	G	2451	0	2327	109	0
14	H	2239	0	2137	127	0
14	J	45	0	32	1	0
14	K	86	0	61	0	0
14	L	255	0	274	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	M	45	0	32	1	0
14	Q	90	0	65	3	0
14	S	82	0	56	0	0
14	T	45	0	32	1	0
14	U	255	0	273	17	0
14	V	45	0	32	1	0
14	W	45	0	32	1	0
14	X	45	0	32	1	0
14	a	2431	0	2281	125	0
14	b	2239	0	2137	142	0
14	f	45	0	32	2	0
14	i	65	0	72	7	0
14	j	82	0	56	2	0
14	k	45	0	32	0	0
14	l	255	0	274	17	0
14	m	45	0	32	3	0
14	x	45	0	32	1	0
15	A	33	0	46	7	0
15	B	33	0	46	4	0
15	G	33	0	46	6	0
15	H	33	0	46	3	0
15	a	33	0	46	4	0
15	b	33	0	46	4	0
16	A	8	0	0	0	0
16	C	16	0	0	0	0
16	G	8	0	0	1	0
16	N	16	0	0	0	0
16	a	8	0	0	0	0
16	c	16	0	0	1	0
17	A	240	0	293	20	0
17	B	305	0	372	28	0
17	F	40	0	49	3	0
17	G	240	0	294	15	0
17	H	265	0	322	25	0
17	I	80	0	98	9	0
17	J	80	0	97	7	0
17	L	80	0	98	6	0
17	M	40	0	49	2	0
17	Q	80	0	98	7	0
17	R	120	0	147	10	0
17	S	80	0	97	12	0
17	U	40	0	49	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	V	40	0	49	3	0
17	a	240	0	293	22	0
17	b	265	0	323	26	0
17	f	80	0	98	10	0
17	i	40	0	49	6	0
17	j	80	0	98	11	0
17	l	120	0	147	6	0
17	m	40	0	49	4	0
18	A	76	0	98	6	0
18	G	76	0	98	6	0
18	a	76	0	98	1	0
19	B	49	0	71	3	0
19	H	49	0	71	2	0
19	b	49	0	71	2	0
20	L	1	0	0	0	0
20	U	1	0	0	0	0
20	l	1	0	0	0	0
All	All	71694	0	69952	1676	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1676) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:PRO:CG	1:A:379:PRO:N	1.92	1.32
1:A:379:PRO:CD	1:A:379:PRO:HG2	1.65	1.14
1:A:379:PRO:CD	1:A:379:PRO:HG3	1.65	1.13
1:A:379:PRO:CG	1:A:379:PRO:HD2	1.53	1.00
1:A:379:PRO:CG	1:A:379:PRO:HD3	1.53	1.00
2:H:182:LEU:O	2:H:186:SER:HB2	1.62	1.00
1:A:379:PRO:CG	1:A:379:PRO:CB	2.45	0.94
1:A:399:TRP:HD1	14:A:829:CLA:HAB	1.36	0.89
14:a:840:CLA:H111	14:a:840:CLA:HAB	1.54	0.88
1:A:379:PRO:CG	1:A:379:PRO:CD	0.87	0.87
1:A:722:LEU:HB3	1:A:726:GLN:HG2	1.58	0.85
1:A:399:TRP:CD1	14:A:829:CLA:HAB	2.11	0.85
2:b:182:LEU:O	2:b:186:SER:HB2	1.78	0.84
1:G:399:TRP:CD1	14:G:829:CLA:HAB	2.15	0.81
1:a:399:TRP:CD1	14:a:828:CLA:HAB	2.16	0.81
14:A:845:CLA:HAA2	14:m:1601:CLA:HAA2	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:829:CLA:HBB2	14:b:838:CLA:HBB2	1.66	0.77
7:i:15:ILE:O	7:i:19:CYS:HB2	1.85	0.76
10:U:34:ASN:HB3	14:U:204:CLA:HAC1	1.66	0.76
2:b:305:MET:HG3	2:b:323:HIS:HB3	1.68	0.75
14:A:841:CLA:HAB	14:A:841:CLA:H111	1.67	0.75
1:G:722:LEU:HB3	1:G:726:GLN:HG2	1.67	0.74
14:G:841:CLA:H111	14:G:841:CLA:HAB	1.68	0.74
14:A:828:CLA:HED1	14:A:836:CLA:HAB	1.70	0.73
2:B:182:LEU:O	2:B:186:SER:HB2	1.89	0.73
6:F:146:GLU:HB3	6:F:152:LEU:HB2	1.70	0.73
1:A:377:MET:HE1	14:A:828:CLA:HHC	1.71	0.72
14:G:845:CLA:HAA2	14:M:1601:CLA:HAA2	1.71	0.72
1:A:86:TRP:HA	14:A:808:CLA:HBB2	1.72	0.71
14:H:829:CLA:HBB2	14:H:838:CLA:HBB2	1.70	0.71
14:A:845:CLA:HED1	10:L:5:LEU:HD11	1.72	0.70
1:A:355:GLN:HG3	14:A:826:CLA:H152	1.73	0.70
2:b:481:LEU:HD23	14:b:834:CLA:HBC2	1.74	0.70
2:b:129:MET:HE2	2:b:135:LEU:HD23	1.72	0.70
2:B:303:GLU:OE2	2:B:303:GLU:N	2.24	0.70
1:G:583:ARG:HG2	3:N:78:GLY:HA3	1.73	0.70
1:A:583:ARG:HG2	3:C:78:GLY:HA3	1.74	0.69
2:B:305:MET:HE3	2:B:323:HIS:HB3	1.75	0.69
7:R:19:CYS:HB3	14:U:201:CLA:HAB	1.74	0.69
14:B:806:CLA:H143	14:B:827:CLA:HBB2	1.75	0.69
2:b:319:PHE:HD2	14:b:822:CLA:HMA3	1.57	0.69
1:G:462:ASN:HD21	1:G:475:PHE:H	1.40	0.69
1:G:737:LEU:HD11	17:G:853:BCR:HC8	1.75	0.69
8:j:28:LEU:O	8:j:32:ASN:ND2	2.26	0.69
2:H:268:LEU:HB2	2:H:273:MET:HE3	1.75	0.68
1:G:70:ARG:HG2	1:G:184:ALA:HB1	1.73	0.68
2:b:31:PHE:HB3	2:b:37:MET:HE2	1.76	0.68
1:A:70:ARG:HG2	1:A:184:ALA:HB1	1.75	0.68
2:H:268:LEU:HD22	14:H:816:CLA:HBA1	1.74	0.68
2:B:305:MET:HE2	2:B:326:ILE:HB	1.74	0.68
2:B:299:HIS:HD1	2:B:304:MET:HE2	1.58	0.68
10:U:62:PRO:O	10:U:66:LEU:HB2	1.93	0.68
1:A:333:LYS:H	14:A:845:CLA:HBC3	1.59	0.67
14:B:828:CLA:H2	19:B:849:LMG:H312	1.76	0.67
2:b:422:ILE:HA	14:b:829:CLA:HBB1	1.74	0.67
1:G:120:ILE:HB	17:S:104:BCR:H322	1.74	0.67
1:G:292:LEU:HB2	1:G:379:PRO:HA	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:254:ILE:HG13	2:H:255:LEU:HD13	1.75	0.67
2:b:701:LYS:HB2	14:b:839:CLA:HED3	1.77	0.67
2:B:268:LEU:HB2	2:B:273:MET:HE3	1.75	0.67
2:B:4:LYS:HD3	7:I:38:ALA:HB3	1.75	0.67
2:B:422:ILE:HA	14:B:829:CLA:HBB1	1.77	0.67
1:a:333:LYS:H	14:a:844:CLA:HBC3	1.60	0.67
14:b:806:CLA:H2	14:b:806:CLA:HAA2	1.75	0.67
3:c:61:ASP:HB2	5:e:44:ASN:HD21	1.58	0.67
4:D:104:GLU:HG2	4:D:105:LYS:HE2	1.76	0.66
2:b:358:SER:HA	2:b:514:SER:HB2	1.77	0.66
2:H:422:ILE:HA	14:H:829:CLA:HBB1	1.76	0.66
17:a:852:BCR:H362	14:a:855:CLA:H42	1.78	0.66
2:b:129:MET:HE1	2:b:134:ASP:HB2	1.78	0.66
14:B:808:CLA:HAB	14:B:809:CLA:HAA2	1.77	0.66
6:Q:61:TYR:HD1	6:Q:72:PRO:HG2	1.61	0.66
14:b:813:CLA:HMA2	17:b:844:BCR:H282	1.77	0.66
2:H:257:PHE:CE2	2:H:500:TRP:HB3	2.31	0.66
1:a:242:PHE:HB3	1:a:249:MET:HE1	1.77	0.66
14:b:807:CLA:H162	14:b:827:CLA:HBB2	1.76	0.66
14:a:809:CLA:H11	17:j:103:BCR:H19C	1.78	0.65
2:H:348:ILE:HD13	14:H:823:CLA:H43	1.78	0.65
4:D:61:ARG:HB2	4:D:64:GLN:HG3	1.77	0.65
1:G:86:TRP:HZ3	17:G:850:BCR:H401	1.60	0.65
14:H:807:CLA:HHB	14:H:808:CLA:HMB3	1.78	0.65
1:a:439:ALA:O	1:a:443:HIS:ND1	2.27	0.65
14:b:829:CLA:HBC1	17:b:845:BCR:H23C	1.79	0.65
14:B:805:CLA:H2	14:B:805:CLA:HAA2	1.77	0.65
14:G:829:CLA:H93	17:S:103:BCR:H361	1.77	0.65
1:A:601:TRP:CH2	14:A:803:CLA:HAB	2.32	0.65
2:b:381:TYR:CD2	14:b:826:CLA:HAB	2.32	0.64
1:G:601:TRP:CH2	14:G:803:CLA:HAB	2.32	0.64
2:b:443:HIS:CD2	2:b:457:ILE:HG13	2.32	0.64
1:G:417:VAL:HG11	1:G:574:PHE:HB2	1.79	0.64
1:a:285:LEU:HD11	1:a:378:PRO:HD2	1.78	0.64
14:a:804:CLA:H2	14:a:811:CLA:H92	1.79	0.64
1:a:462:ASN:HD21	1:a:475:PHE:H	1.44	0.64
2:b:124:TRP:O	2:b:129:MET:HB2	1.98	0.64
11:M:4:THR:H	11:M:7:GLN:HE21	1.46	0.64
14:H:839:CLA:H13	17:R:101:BCR:H372	1.79	0.64
1:a:355:GLN:HG3	14:a:825:CLA:H152	1.79	0.64
14:B:829:CLA:HBB2	14:B:838:CLA:HBB2	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:162:SER:O	6:Q:164:ARG:NH1	2.31	0.63
14:a:855:CLA:HAB	2:b:589:TRP:CH2	2.33	0.63
2:H:181:GLY:HA3	14:H:812:CLA:HBB1	1.81	0.63
4:D:10:LEU:HB2	4:D:49:VAL:HB	1.80	0.63
14:G:804:CLA:HBB1	17:S:104:BCR:H271	1.80	0.63
2:b:176:ASN:HD21	2:b:291:TYR:H	1.44	0.63
1:A:328:ILE:O	1:A:332:HIS:ND1	2.32	0.63
14:b:837:CLA:HBC2	17:b:849:BCR:HC7	1.80	0.63
1:G:491:GLN:HG2	1:G:513:PHE:HA	1.80	0.63
2:H:225:PHE:HD2	2:H:230:TRP:NE1	1.97	0.63
2:H:701:LYS:HB2	14:H:839:CLA:HED3	1.79	0.63
1:a:243:ILE:HD11	14:a:816:CLA:HBC2	1.79	0.63
1:A:76:HIS:ND1	14:A:814:CLA:OBD	2.31	0.63
10:L:34:ASN:HB3	14:L:204:CLA:HAC1	1.79	0.63
1:G:86:TRP:HA	14:G:808:CLA:HBB2	1.81	0.62
2:b:93:ASP:H	7:i:1:MET:HE3	1.64	0.62
2:B:426:LEU:HD13	2:B:539:LEU:HA	1.79	0.62
2:B:472:GLY:O	2:B:509:ASN:ND2	2.31	0.62
1:a:373:HIS:ND1	14:a:818:CLA:OBD	2.32	0.62
2:B:370:THR:HG23	2:B:736:THR:HB	1.81	0.62
2:B:268:LEU:HD22	14:B:816:CLA:HBA1	1.82	0.62
4:D:37:GLU:HA	4:D:50:MET:O	2.00	0.62
10:U:77:LEU:HD13	10:l:145:VAL:HG21	1.80	0.62
14:a:821:CLA:HBA1	14:a:827:CLA:H91	1.82	0.62
4:d:61:ARG:HB2	4:d:64:GLN:HG3	1.81	0.62
1:A:462:ASN:HD21	1:A:475:PHE:H	1.48	0.62
6:F:136:GLY:O	6:F:139:TRP:HB3	2.00	0.62
2:H:262:HIS:HD2	2:H:264:GLN:H	1.46	0.62
2:B:129:MET:HE3	2:B:135:LEU:HD23	1.82	0.61
17:A:853:BCR:H362	14:B:801:CLA:H42	1.82	0.61
14:G:843:CLA:HAB	2:H:698:VAL:HG21	1.82	0.61
14:b:839:CLA:H13	17:i:102:BCR:H372	1.80	0.61
14:b:802:CLA:H203	10:l:59:LEU:HD21	1.82	0.61
6:f:76:VAL:HG12	6:f:86:PHE:HB2	1.82	0.61
1:A:256:ILE:HG22	1:A:258:TRP:H	1.65	0.61
1:A:86:TRP:HZ3	17:A:850:BCR:H401	1.65	0.61
2:B:53:HIS:ND1	14:B:805:CLA:O1A	2.33	0.61
14:G:822:CLA:HMB2	14:G:826:CLA:HED2	1.81	0.61
17:G:853:BCR:H362	14:H:801:CLA:H42	1.83	0.61
2:b:648:ASN:N	2:b:648:ASN:OD1	2.34	0.61
4:O:32:TRP:NE1	4:O:50:MET:SD	2.67	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:6:LYS:HD3	4:d:114:ASN:HB3	1.83	0.61
11:V:4:THR:H	11:V:7:GLN:HE21	1.48	0.61
14:a:803:CLA:HBB2	14:a:811:CLA:H111	1.82	0.61
4:d:10:LEU:HB2	4:d:49:VAL:HB	1.82	0.61
3:C:41:SER:HG	4:D:113:VAL:H	1.47	0.61
1:A:379:PRO:N	1:A:379:PRO:HG2	1.92	0.60
14:a:824:CLA:HAC1	17:a:850:BCR:HC8	1.82	0.60
1:G:378:PRO:HG2	1:G:384:ALA:HB2	1.83	0.60
14:b:804:CLA:H142	17:i:102:BCR:H271	1.83	0.60
2:B:176:ASN:HD21	2:B:291:TYR:H	1.49	0.60
14:B:840:CLA:HAC2	17:B:848:BCR:H23C	1.84	0.60
14:B:839:CLA:H13	17:I:101:BCR:H372	1.84	0.60
1:G:52:HIS:HB2	18:G:854:LHG:H102	1.82	0.60
1:G:709:ASN:HB3	6:Q:159:ILE:HG13	1.84	0.60
4:O:38:GLN:HG3	4:O:50:MET:HE3	1.83	0.60
10:l:34:ASN:HB3	14:l:205:CLA:HAC1	1.83	0.60
1:A:42:PRO:HD2	6:F:118:ASN:HB3	1.84	0.60
1:A:325:LEU:HD23	14:A:822:CLA:HED3	1.83	0.60
1:A:373:HIS:ND1	14:A:819:CLA:OBD	2.33	0.60
6:F:74:LEU:HG	6:F:85:ASP:HB3	1.84	0.60
6:f:124:ILE:O	8:j:11:SER:OG	2.20	0.60
2:B:381:TYR:CD2	14:B:826:CLA:HAB	2.36	0.60
2:B:726:LEU:HD11	14:B:828:CLA:H203	1.83	0.60
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.83	0.60
5:P:12:ARG:NH2	5:P:59:ASN:O	2.35	0.60
1:a:262:SER:HA	1:a:265:ILE:HD12	1.84	0.60
1:a:486:PHE:HB3	14:a:837:CLA:H2	1.84	0.59
2:b:53:HIS:ND1	14:b:806:CLA:O1A	2.35	0.59
5:P:8:VAL:O	5:P:21:ILE:HA	2.02	0.59
1:a:118:TRP:CZ3	17:j:104:BCR:HC8	2.36	0.59
4:O:61:ARG:NH2	4:O:63:GLU:OE1	2.35	0.59
4:D:43:PRO:HD3	4:D:68:LEU:HD13	1.85	0.59
7:R:15:ILE:O	7:R:19:CYS:HB2	2.02	0.59
1:A:376:ALA:HA	1:A:526:MET:HE3	1.84	0.59
1:A:541:ILE:HD12	13:A:801:CL0:H63	1.84	0.59
17:A:848:BCR:H332	17:A:849:BCR:H23C	1.85	0.59
1:G:333:LYS:H	14:G:845:CLA:HBC3	1.67	0.59
2:B:648:ASN:N	2:B:648:ASN:OD1	2.34	0.58
14:B:829:CLA:HBC1	17:B:845:BCR:H23C	1.84	0.58
14:H:827:CLA:H111	17:H:844:BCR:H372	1.84	0.58
14:a:833:CLA:HAB	14:a:834:CLA:HHB	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:a:845:PQN:H172	17:f:201:BCR:H382	1.84	0.58
11:m:24:ARG:HH12	14:m:1601:CLA:HED3	1.68	0.58
14:G:805:CLA:H2	14:G:812:CLA:H92	1.86	0.58
1:A:439:ALA:O	1:A:443:HIS:ND1	2.27	0.58
1:a:352:TRP:HB3	14:a:805:CLA:HAC1	1.86	0.58
2:b:21:ILE:HG12	7:i:34:ILE:HD12	1.85	0.58
2:b:50:HIS:HE1	14:b:806:CLA:H161	1.69	0.58
2:b:176:ASN:HB3	14:b:819:CLA:HMD2	1.85	0.58
4:D:107:ASN:HD22	4:D:110:ARG:HG3	1.66	0.58
2:H:411:VAL:HA	2:H:414:ARG:HD2	1.83	0.58
2:b:426:LEU:HD13	2:b:539:LEU:HA	1.85	0.58
1:a:601:TRP:CH2	14:a:802:CLA:HAB	2.38	0.58
14:i:101:CLA:HBC2	11:m:12:LEU:HD13	1.85	0.58
10:l:85:THR:HG23	17:l:203:BCR:H333	1.85	0.58
1:G:334:GLY:HA3	18:G:855:LHG:HC32	1.84	0.58
1:G:529:ILE:HD13	1:G:617:MET:HE1	1.84	0.58
1:A:352:TRP:HB3	14:A:806:CLA:HAC1	1.85	0.58
14:b:804:CLA:H143	17:b:847:BCR:H362	1.86	0.57
14:B:821:CLA:HBB2	12:X:16:TRP:HZ2	1.70	0.57
14:B:822:CLA:HBA2	17:B:845:BCR:H14C	1.85	0.57
4:D:70:ALA:HA	4:D:74:ARG:HD3	1.86	0.57
6:f:141:LEU:HA	6:f:144:LEU:HD12	1.86	0.57
2:H:433:LEU:HD11	14:H:837:CLA:HMB2	1.86	0.57
1:a:76:HIS:ND1	14:a:813:CLA:OBD	2.35	0.57
2:B:728:TYR:HB2	14:B:802:CLA:HED3	1.86	0.57
14:H:840:CLA:HAC2	17:H:847:BCR:H23C	1.87	0.57
1:a:699:GLU:OE2	2:b:557:LYS:NZ	2.36	0.57
14:H:811:CLA:HAB	14:H:819:CLA:C4C	2.35	0.57
6:Q:59:GLU:O	6:Q:62:SER:OG	2.22	0.57
2:b:728:TYR:HB2	14:b:803:CLA:HED3	1.85	0.57
5:e:44:ASN:HB3	5:e:46:THR:H	1.68	0.57
14:A:843:CLA:HAC1	15:A:846:PQN:H171	1.84	0.57
3:C:26:LEU:HA	3:C:41:SER:O	2.04	0.57
14:H:806:CLA:H143	14:H:827:CLA:HBB2	1.87	0.57
1:A:115:GLN:NE2	14:A:810:CLA:OBD	2.36	0.57
1:G:377:MET:HE3	14:G:828:CLA:HMC3	1.86	0.57
2:H:355:HIS:ND1	14:H:816:CLA:OBD	2.37	0.57
14:H:831:CLA:HBB2	17:Q:202:BCR:HC41	1.87	0.57
1:a:737:LEU:HD11	17:a:852:BCR:HC8	1.87	0.57
2:b:481:LEU:H	2:b:481:LEU:HD12	1.69	0.57
3:c:15:THR:HG22	3:c:28:MET:HE2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:LEU:HD23	11:M:14:ILE:HG22	1.86	0.57
1:G:251:GLU:HG2	1:G:252:LEU:HD22	1.87	0.57
14:H:813:CLA:HMA2	17:H:844:BCR:H282	1.85	0.57
1:a:451:LEU:HB3	1:a:544:PHE:HB2	1.86	0.57
8:S:28:LEU:HD13	17:S:103:BCR:HC7	1.87	0.56
2:b:123:TRP:HD1	2:b:362:TYR:CE1	2.22	0.56
1:G:246:PRO:HA	1:G:249:MET:HG2	1.86	0.56
15:G:846:PQN:H172	17:Q:202:BCR:H382	1.87	0.56
6:Q:76:VAL:HG12	6:Q:86:PHE:HB2	1.87	0.56
1:A:289:THR:HG23	1:A:291:GLY:H	1.69	0.56
2:H:15:ASP:HB3	2:H:20:ARG:HB2	1.87	0.56
14:L:201:CLA:HED2	14:L:201:CLA:H12	1.86	0.56
3:c:6:LYS:HG3	4:d:137:TYR:HB2	1.87	0.56
1:G:439:ALA:O	1:G:443:HIS:ND1	2.31	0.56
2:H:442:VAL:HG13	14:H:801:CLA:H52	1.87	0.56
1:a:308:PHE:HZ	14:a:819:CLA:H112	1.70	0.56
2:B:315:VAL:HA	2:B:320:ASN:HD22	1.69	0.56
2:B:355:HIS:ND1	14:B:816:CLA:OBD	2.38	0.56
2:B:523:ASP:OD2	2:B:604:LYS:NZ	2.37	0.56
10:U:60:ILE:HG22	10:U:83:GLY:HA3	1.87	0.56
1:a:462:ASN:ND2	1:a:475:PHE:H	2.04	0.56
2:b:665:ALA:C	14:b:804:CLA:HAB	2.30	0.56
1:G:373:HIS:ND1	14:G:819:CLA:OBD	2.38	0.56
2:H:381:TYR:CD2	14:H:826:CLA:HAB	2.40	0.56
14:a:844:CLA:HED1	10:l:5:LEU:HD11	1.87	0.56
14:b:822:CLA:HBA2	17:b:845:BCR:H14C	1.86	0.56
1:G:352:TRP:HB3	14:G:806:CLA:HAC1	1.87	0.56
4:O:10:LEU:HB2	4:O:49:VAL:HB	1.88	0.56
14:a:814:CLA:HBA2	17:a:848:BCR:H342	1.88	0.56
1:A:118:TRP:CZ3	17:J:103:BCR:HC8	2.40	0.56
10:U:24:ASP:O	10:U:29:LYS:NZ	2.38	0.56
14:B:803:CLA:H111	17:B:848:BCR:H362	1.88	0.56
14:a:828:CLA:H93	17:j:103:BCR:H361	1.88	0.56
1:A:377:MET:SD	1:A:510:SER:HB2	2.46	0.56
2:B:21:ILE:HG12	7:I:34:ILE:HD12	1.87	0.56
4:O:37:GLU:HA	4:O:50:MET:O	2.06	0.56
14:b:832:CLA:H12	17:f:201:BCR:HC32	1.87	0.56
14:H:822:CLA:HAB	14:H:829:CLA:HMD1	1.87	0.55
14:a:806:CLA:H202	14:a:808:CLA:H41	1.87	0.55
14:a:833:CLA:H91	14:b:840:CLA:H93	1.88	0.55
10:l:97:TYR:O	10:l:101:SER:HB2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:665:ALA:C	14:B:803:CLA:HAB	2.30	0.55
1:a:718:GLN:HE22	5:e:43:VAL:H	1.54	0.55
2:B:433:LEU:HD11	14:B:837:CLA:HMB2	1.88	0.55
1:G:462:ASN:ND2	1:G:475:PHE:H	2.04	0.55
2:H:446:VAL:HG21	14:H:832:CLA:HAC2	1.88	0.55
1:a:433:VAL:HG11	14:a:821:CLA:H192	1.87	0.55
1:A:583:ARG:HG3	3:C:49:VAL:HB	1.88	0.55
1:G:404:LEU:HD21	14:G:807:CLA:H142	1.89	0.55
14:G:843:CLA:H192	10:U:59:LEU:HD21	1.89	0.55
14:H:834:CLA:NC	14:H:835:CLA:HAB	2.22	0.55
14:a:827:CLA:HED1	14:a:835:CLA:HAB	1.86	0.55
10:l:138:PHE:O	10:l:142:ASN:ND2	2.40	0.55
1:G:599:LEU:HD21	14:G:831:CLA:HBC1	1.88	0.55
2:B:176:ASN:HB3	14:B:819:CLA:HMD2	1.89	0.55
14:b:808:CLA:HAB	14:b:809:CLA:HAA2	1.87	0.55
1:A:16:VAL:HG12	1:A:183:ARG:HG2	1.89	0.55
1:A:149:ALA:HB2	1:A:381:PRO:HD2	1.88	0.55
2:H:665:ALA:C	14:H:803:CLA:HAB	2.32	0.55
15:b:841:PQN:H142	17:b:847:BCR:H271	1.87	0.55
2:B:61:VAL:HG21	14:B:827:CLA:H42	1.88	0.55
14:B:809:CLA:H72	14:B:826:CLA:H193	1.89	0.55
1:G:486:PHE:HB3	14:G:838:CLA:H2	1.88	0.55
1:A:183:ARG:NH1	1:A:183:ARG:HB2	2.22	0.55
14:B:809:CLA:H92	17:B:848:BCR:H341	1.89	0.55
1:G:256:ILE:HG22	1:G:258:TRP:H	1.72	0.55
14:G:842:CLA:HAC1	15:G:846:PQN:H171	1.88	0.55
2:b:169:LYS:HE2	2:b:332:ASN:HA	1.89	0.55
2:B:143:LEU:HD21	11:M:15:ALA:HB2	1.89	0.54
2:B:533:GLY:HA2	2:B:589:TRP:HZ3	1.72	0.54
1:A:246:PRO:HA	1:A:249:MET:HG2	1.90	0.54
10:L:22:ILE:HG12	14:m:1601:CLA:HMD1	1.89	0.54
2:b:15:ASP:HB3	2:b:20:ARG:HB2	1.88	0.54
2:b:726:LEU:HD11	14:b:828:CLA:H203	1.88	0.54
14:A:804:CLA:H2	14:A:804:CLA:HED2	1.89	0.54
1:a:90:MET:HE1	14:a:808:CLA:HAA2	1.90	0.54
1:A:117:VAL:HA	14:A:810:CLA:HED3	1.89	0.54
1:A:462:ASN:ND2	1:A:475:PHE:H	2.05	0.54
14:A:832:CLA:HBB2	14:A:840:CLA:HMC1	1.90	0.54
2:H:514:SER:HA	2:H:517:LEU:HD21	1.89	0.54
2:H:703:LYS:NZ	3:N:81:TYR:O	2.40	0.54
1:a:95:ALA:HB2	1:a:158:LEU:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:366:LEU:HD22	14:a:827:CLA:H41	1.89	0.54
2:b:301:ILE:HG21	14:b:823:CLA:HAC1	1.89	0.54
2:H:426:LEU:HD13	2:H:539:LEU:HA	1.89	0.54
2:B:122:HIS:O	2:B:126:THR:OG1	2.25	0.54
1:G:355:GLN:HG3	14:G:826:CLA:H152	1.90	0.54
14:G:807:CLA:H201	18:G:854:LHG:H221	1.90	0.54
4:O:105:LYS:O	4:O:110:ARG:NH1	2.41	0.54
1:a:718:GLN:HE22	5:e:43:VAL:HG22	1.72	0.54
1:A:286:ASN:HB3	1:A:289:THR:HG22	1.88	0.54
2:B:701:LYS:HB2	14:B:839:CLA:HED3	1.88	0.54
14:B:807:CLA:H111	17:I:101:BCR:HC21	1.89	0.54
1:G:118:TRP:HB3	17:S:104:BCR:HC21	1.89	0.54
1:A:430:LEU:HD13	14:A:825:CLA:HBC1	1.90	0.54
6:F:76:VAL:HG12	6:F:86:PHE:HB2	1.88	0.54
14:H:807:CLA:H12	7:R:18:VAL:HG21	1.89	0.54
1:a:152:ILE:HG12	14:a:814:CLA:HED3	1.89	0.54
2:b:433:LEU:HD11	14:b:837:CLA:HMB2	1.90	0.54
1:A:33:HIS:NE2	14:A:812:CLA:O1A	2.40	0.54
2:H:230:TRP:HB3	14:H:815:CLA:H3A	1.89	0.54
2:H:606:LEU:HD22	2:H:739:LYS:HZ1	1.73	0.54
1:a:358:ILE:HG12	17:a:850:BCR:HC7	1.90	0.54
2:b:462:VAL:HG11	6:f:75:VAL:HG13	1.89	0.54
3:N:26:LEU:HA	3:N:41:SER:O	2.07	0.54
1:a:722:LEU:HD21	15:a:845:PQN:H151	1.89	0.54
1:a:328:ILE:O	1:a:332:HIS:ND1	2.30	0.53
6:Q:78:GLY:HA2	6:Q:87:LEU:HD21	1.91	0.53
14:A:843:CLA:HBA1	18:A:854:LHG:H181	1.89	0.53
1:G:711:LEU:HD13	17:Q:204:BCR:H321	1.90	0.53
1:A:292:LEU:HD12	1:A:379:PRO:HB3	1.90	0.53
14:A:832:CLA:HMA2	10:L:20:THR:HG21	1.91	0.53
2:B:446:VAL:HG21	14:B:832:CLA:HAC2	1.89	0.53
2:B:701:LYS:HZ1	7:I:37:ASP:HB2	1.73	0.53
2:H:439:GLY:HA3	14:H:832:CLA:HAB	1.91	0.53
7:I:23:PRO:O	7:I:27:MET:HG3	2.09	0.53
3:N:61:ASP:OD1	5:P:15:SER:HA	2.08	0.53
1:a:271:ASN:HD22	9:k:10:THR:HA	1.74	0.53
1:A:262:SER:HA	1:A:265:ILE:HD12	1.89	0.53
2:H:460:GLU:OE1	2:H:465:GLN:NE2	2.35	0.53
2:b:722:VAL:HG22	19:b:848:LMG:H441	1.90	0.53
1:A:95:ALA:HB2	1:A:158:LEU:HB2	1.91	0.53
1:A:488:GLN:NE2	1:A:531:LEU:O	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:822:CLA:H61	17:A:851:BCR:H352	1.89	0.53
2:B:480:THR:HG22	2:B:481:LEU:HD12	1.89	0.53
14:H:832:CLA:HBA2	17:S:103:BCR:HC42	1.89	0.53
8:S:14:PRO:HB2	17:S:104:BCR:H292	1.90	0.53
2:b:178:HIS:ND1	14:b:823:CLA:O1D	2.37	0.53
2:b:340:TRP:HE1	14:b:823:CLA:C2B	2.22	0.53
2:H:589:TRP:CH2	14:H:801:CLA:HAB	2.44	0.53
1:a:575:ARG:NH1	14:a:830:CLA:O1D	2.42	0.53
2:b:61:VAL:HG11	14:b:827:CLA:H42	1.89	0.53
14:b:831:CLA:H121	17:f:203:BCR:HC8	1.91	0.53
14:A:809:CLA:H71	14:A:831:CLA:H151	1.89	0.53
14:A:815:CLA:HBA2	17:A:849:BCR:H342	1.91	0.53
5:E:10:ILE:HG22	5:E:12:ARG:H	1.74	0.53
10:l:53:MET:HE1	14:l:205:CLA:HED2	1.91	0.53
2:H:2:ALA:HB2	2:H:14:GLN:HG3	1.91	0.53
2:b:549:ARG:HH22	4:d:125:ASN:HD21	1.57	0.53
2:b:677:TYR:OH	14:b:804:CLA:OBD	2.26	0.53
14:A:820:CLA:H2	14:A:830:CLA:H92	1.91	0.53
14:G:816:CLA:HBB2	17:G:849:BCR:H363	1.90	0.53
14:G:841:CLA:HAA2	14:H:830:CLA:HMB2	1.89	0.53
2:H:319:PHE:CD2	14:H:821:CLA:HAB	2.44	0.53
2:H:343:ALA:HB2	17:H:846:BCR:H372	1.91	0.53
8:S:7:LEU:O	8:S:11:SER:OG	2.22	0.53
1:a:377:MET:HG3	1:a:510:SER:HB2	1.91	0.53
2:b:188:LEU:HD21	17:b:842:BCR:HC7	1.90	0.53
2:B:461:PRO:HG3	2:B:524:PHE:HB2	1.90	0.52
1:G:328:ILE:O	1:G:332:HIS:ND1	2.42	0.52
4:O:86:ILE:HG13	4:O:92:THR:HG23	1.91	0.52
1:a:395:THR:HB	14:a:828:CLA:HMB2	1.91	0.52
1:a:444:LEU:HD21	1:a:550:VAL:HG12	1.91	0.52
10:l:62:PRO:HA	14:l:207:CLA:HMB2	1.90	0.52
14:A:804:CLA:HBB1	17:J:103:BCR:H271	1.91	0.52
2:H:143:LEU:HD21	11:V:15:ALA:HB2	1.90	0.52
2:H:294:GLN:HG2	14:H:811:CLA:HMA2	1.91	0.52
1:a:669:LEU:HD21	1:a:752:ILE:HG21	1.91	0.52
14:a:840:CLA:H102	14:b:831:CLA:H43	1.91	0.52
14:i:101:CLA:H13	17:i:102:BCR:H323	1.91	0.52
10:l:36:PRO:HG3	14:l:206:CLA:HED2	1.91	0.52
2:B:343:ALA:HB2	17:B:846:BCR:H372	1.91	0.52
6:F:80:LEU:HA	6:F:83:ALA:HB2	1.91	0.52
14:G:843:CLA:H91	17:R:103:BCR:H392	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:HIS:ND1	14:H:823:CLA:O1D	2.34	0.52
2:H:257:PHE:CD2	2:H:500:TRP:HB3	2.44	0.52
4:O:34:SER:OG	4:O:51:ARG:O	2.27	0.52
2:b:446:VAL:HG21	14:b:832:CLA:HAC2	1.91	0.52
1:a:200:HIS:HB3	14:a:825:CLA:HED3	1.90	0.52
1:a:239:PRO:HA	1:a:242:PHE:HD1	1.74	0.52
2:H:176:ASN:ND2	2:H:291:TYR:O	2.42	0.52
2:b:182:LEU:HD21	14:b:812:CLA:H12	1.91	0.52
5:e:12:ARG:NH2	5:e:59:ASN:O	2.42	0.52
2:B:231:GLY:HA2	14:B:815:CLA:HAA2	1.92	0.52
17:L:207:BCR:H14C	14:l:202:CLA:H192	1.91	0.52
14:a:842:CLA:HAC1	15:a:845:PQN:H171	1.91	0.52
1:A:601:TRP:HH2	14:A:803:CLA:HAB	1.74	0.52
14:H:803:CLA:H111	17:H:847:BCR:H362	1.92	0.52
6:Q:123:ILE:HG12	8:S:12:THR:HG22	1.91	0.52
2:b:473:LYS:HG2	2:b:508:ILE:HG23	1.92	0.52
14:b:808:CLA:HMB2	14:i:101:CLA:H3A	1.90	0.52
1:A:378:PRO:HB3	1:A:383:LEU:HD23	1.92	0.52
1:A:722:LEU:HB3	1:A:726:GLN:CG	2.37	0.52
1:G:433:VAL:HA	1:G:436:HIS:CE1	2.45	0.52
14:V:1601:CLA:HAA2	14:a:844:CLA:HAA2	1.91	0.52
1:a:66:GLU:HG3	1:a:187:LEU:HB2	1.91	0.52
14:b:831:CLA:HBB2	17:f:201:BCR:HC41	1.90	0.52
2:H:129:MET:HE3	2:H:135:LEU:HD23	1.90	0.52
10:L:143:PHE:CD1	14:L:206:CLA:H12	2.44	0.52
6:f:136:GLY:O	6:f:139:TRP:HB3	2.10	0.52
1:A:444:LEU:HD21	1:A:550:VAL:HG12	1.91	0.52
2:H:61:VAL:HG21	14:H:827:CLA:H42	1.90	0.52
2:b:322:PRO:HB2	2:b:410:ASN:HA	1.92	0.52
6:f:132:CYS:O	6:f:135:THR:OG1	2.28	0.52
2:B:319:PHE:CD2	14:B:821:CLA:HAB	2.45	0.51
14:B:813:CLA:HMA2	17:B:844:BCR:H282	1.92	0.51
1:G:125:ILE:HD11	6:Q:45:VAL:HG11	1.92	0.51
1:G:451:LEU:HB3	1:G:544:PHE:HB2	1.91	0.51
14:G:836:CLA:HBB2	14:G:838:CLA:HBA1	1.92	0.51
2:H:301:ILE:HG21	14:H:823:CLA:HMC1	1.91	0.51
10:L:36:PRO:HG3	14:L:205:CLA:HED2	1.91	0.51
7:R:27:MET:HG2	17:R:103:BCR:C11	2.40	0.51
1:A:212:TRP:O	1:A:216:GLN:N	2.44	0.51
14:A:825:CLA:HBB1	18:A:855:LHG:HC42	1.93	0.51
5:E:11:LEU:HD21	5:E:66:GLU:HG3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:587:CYS:HB3	16:G:847:SF4:S4	2.49	0.51
14:L:201:CLA:HHC	14:L:201:CLA:HBB1	1.91	0.51
1:a:491:GLN:HG2	1:a:513:PHE:HA	1.92	0.51
14:A:805:CLA:H2	14:A:812:CLA:H92	1.93	0.51
15:A:846:PQN:H172	17:B:847:BCR:H382	1.92	0.51
4:D:34:SER:OG	4:D:51:ARG:O	2.28	0.51
8:J:6:LEU:HG	8:J:10:LEU:HD23	1.92	0.51
10:U:71:ASP:OD2	10:U:71:ASP:N	2.34	0.51
14:a:838:CLA:H101	14:l:206:CLA:H191	1.91	0.51
2:b:278:LEU:HD11	14:b:814:CLA:HAC1	1.91	0.51
14:A:802:CLA:HBA1	2:B:431:LEU:HD12	1.92	0.51
14:A:825:CLA:HMA3	14:A:845:CLA:HAB	1.93	0.51
2:B:348:ILE:HD13	14:B:823:CLA:H43	1.93	0.51
14:H:804:CLA:HMA3	11:V:29:LEU:HD13	1.91	0.51
2:b:129:MET:CE	2:b:134:ASP:HB2	2.40	0.51
14:B:807:CLA:H3A	14:B:808:CLA:HMB2	1.93	0.51
1:G:318:ASN:HD22	14:G:813:CLA:HMA2	1.75	0.51
2:H:157:LEU:O	2:H:162:ARG:NH1	2.43	0.51
1:a:84:PHE:HZ	14:a:813:CLA:H52	1.74	0.51
1:A:451:LEU:HB3	1:A:544:PHE:HB2	1.92	0.51
2:B:338:LEU:HD11	14:B:828:CLA:HBB1	1.93	0.51
2:H:583:PHE:HZ	19:H:848:LMG:H341	1.75	0.51
14:a:833:CLA:H203	14:b:839:CLA:HMA3	1.93	0.51
2:H:493:TRP:CE3	2:H:494:PRO:HD3	2.45	0.51
1:a:177:TRP:CD1	14:a:811:CLA:HBB1	2.45	0.51
2:b:143:LEU:HD11	11:m:15:ALA:HB2	1.92	0.51
2:b:194:LEU:HA	2:b:198:ALA:HB3	1.93	0.51
2:b:676:GLY:O	2:b:680:GLU:HG3	2.11	0.51
1:A:395:THR:HG23	1:A:610:ILE:HG21	1.92	0.51
14:A:827:CLA:H12	14:A:839:CLA:HBA1	1.92	0.51
3:C:61:ASP:HB2	5:E:44:ASN:HD21	1.75	0.51
5:E:35:PRO:HD2	5:E:61:ALA:HA	1.93	0.51
1:G:23:THR:HG21	1:G:177:TRP:HE1	1.75	0.51
1:G:539:HIS:CG	14:G:839:CLA:HED2	2.45	0.51
14:H:806:CLA:H162	14:H:827:CLA:HBB2	1.93	0.51
3:N:15:THR:HG22	3:N:28:MET:HG3	1.93	0.51
1:A:575:ARG:NH2	18:A:854:LHG:O2	2.44	0.51
14:A:820:CLA:H92	14:A:830:CLA:H91	1.93	0.51
14:A:829:CLA:O1D	14:A:830:CLA:HHB	2.11	0.51
1:a:599:LEU:HD21	14:a:830:CLA:HBC1	1.93	0.51
5:e:11:LEU:HD11	5:e:66:GLU:HG2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:GLN:HG2	1:A:513:PHE:HA	1.93	0.51
14:A:831:CLA:H18	14:A:843:CLA:HBA2	1.93	0.51
14:B:837:CLA:HBC2	17:B:850:BCR:HC7	1.92	0.51
5:E:12:ARG:HB2	5:E:64:GLU:HG2	1.93	0.51
2:H:291:TYR:HA	2:H:299:HIS:H	1.75	0.51
14:H:809:CLA:H92	17:H:847:BCR:H341	1.93	0.51
1:a:710:LYS:NZ	6:f:156:ASP:OD1	2.39	0.51
2:b:414:ARG:O	2:b:418:HIS:ND1	2.40	0.51
1:A:157:GLN:NE2	14:A:815:CLA:O1D	2.37	0.50
2:B:190:TRP:NE1	14:B:817:CLA:O1D	2.35	0.50
14:B:831:CLA:H102	17:F:1302:BCR:H312	1.93	0.50
14:a:821:CLA:H161	17:a:850:BCR:H332	1.92	0.50
14:b:802:CLA:HHD	17:b:847:BCR:H383	1.93	0.50
2:H:255:LEU:HD11	14:H:814:CLA:HBC1	1.93	0.50
2:H:436:HIS:HB2	17:H:849:BCR:HC32	1.93	0.50
2:b:190:TRP:NE1	14:b:817:CLA:O1D	2.38	0.50
14:A:822:CLA:HMB2	14:A:826:CLA:HED2	1.93	0.50
2:B:322:PRO:HB2	2:B:410:ASN:HA	1.92	0.50
2:B:468:GLN:HG2	2:B:516:PHE:HB3	1.92	0.50
1:G:722:LEU:HD21	15:G:846:PQN:H151	1.93	0.50
2:H:256:THR:OG1	2:H:272:ASP:OD1	2.30	0.50
2:b:526:VAL:HG11	2:b:600:TYR:HB2	1.93	0.50
4:d:32:TRP:NE1	4:d:50:MET:SD	2.77	0.50
6:f:40:ARG:NH2	6:f:69:ASP:O	2.34	0.50
8:j:10:LEU:HA	8:j:15:VAL:HG11	1.93	0.50
1:A:352:TRP:CH2	14:A:826:CLA:H143	2.47	0.50
2:B:61:VAL:HB	2:B:142:LEU:HD13	1.93	0.50
1:G:511:VAL:HG12	1:G:528:PRO:HD3	1.94	0.50
2:H:176:ASN:HB3	14:H:819:CLA:HMD2	1.94	0.50
2:b:441:TYR:CE1	2:b:525:LEU:HB3	2.46	0.50
2:B:357:TYR:O	2:B:514:SER:OG	2.30	0.50
14:B:805:CLA:H101	14:B:812:CLA:HBA1	1.93	0.50
1:a:216:GLN:HA	1:a:220:SER:HB2	1.94	0.50
14:b:805:CLA:HBC1	19:b:848:LMG:H181	1.94	0.50
2:B:237:PRO:HB3	2:B:256:THR:HG21	1.94	0.50
1:G:391:LEU:HA	1:G:613:PHE:HE2	1.77	0.50
2:H:329:THR:OG1	2:H:407:ASN:ND2	2.42	0.50
10:U:62:PRO:HA	14:U:206:CLA:HMB2	1.94	0.50
1:A:377:MET:HE3	14:A:819:CLA:HBD	1.94	0.50
1:A:704:ILE:HD13	14:A:841:CLA:HMD2	1.92	0.50
4:D:121:GLY:N	5:E:14:GLU:OE2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:822:CLA:H143	14:G:825:CLA:H91	1.94	0.50
14:G:822:CLA:HMD3	14:G:824:CLA:HHD	1.93	0.50
2:H:468:GLN:NE2	2:H:476:TYR:OH	2.45	0.50
4:O:40:PHE:HB2	4:O:72:GLN:HE21	1.76	0.50
2:B:391:PHE:CZ	14:B:824:CLA:HAB	2.47	0.50
2:B:517:LEU:HD22	2:B:608:VAL:HG21	1.93	0.50
14:B:803:CLA:H143	17:B:848:BCR:H362	1.94	0.50
1:G:80:LEU:HD11	14:G:814:CLA:HBA2	1.93	0.50
14:G:827:CLA:HAB	17:G:852:BCR:C8	2.42	0.50
2:H:85:ARG:HH21	2:H:740:TYR:HE2	1.60	0.50
6:Q:31:CYS:HB2	6:Q:62:SER:HA	1.94	0.50
1:a:117:VAL:HA	14:a:809:CLA:HED3	1.93	0.50
2:b:91:ILE:HB	2:b:112:PRO:HB2	1.94	0.50
14:b:806:CLA:H152	14:b:812:CLA:CAD	2.42	0.50
1:G:266:PRO:HA	1:G:271:ASN:HB3	1.93	0.50
2:H:414:ARG:O	2:H:418:HIS:ND1	2.44	0.50
2:b:355:HIS:ND1	14:b:816:CLA:OBD	2.45	0.50
14:b:840:CLA:HAC2	17:b:847:BCR:H23C	1.94	0.50
14:A:844:CLA:HAB	2:B:698:VAL:HG21	1.94	0.49
1:G:681:PHE:CG	17:G:853:BCR:H363	2.47	0.49
6:Q:161:VAL:HG21	6:Q:164:ARG:HH22	1.77	0.49
1:a:376:ALA:HA	1:a:526:MET:HE3	1.94	0.49
14:a:840:CLA:H12	14:b:831:CLA:HAA1	1.95	0.49
1:A:256:ILE:HB	1:A:258:TRP:CE2	2.47	0.49
1:A:718:GLN:OE1	5:E:16:TYR:OH	2.29	0.49
14:B:806:CLA:H162	14:B:827:CLA:HBB2	1.94	0.49
2:H:330:TYR:HH	2:H:340:TRP:CD1	2.30	0.49
2:H:526:VAL:HG11	2:H:600:TYR:HB2	1.94	0.49
1:a:437:ARG:NH1	1:a:562:SER:O	2.45	0.49
2:b:480:THR:O	2:b:484:ASN:N	2.44	0.49
2:b:528:HIS:HD2	17:b:849:BCR:HC22	1.77	0.49
14:B:839:CLA:HBB2	15:B:841:PQN:H141	1.94	0.49
2:H:74:PHE:O	2:H:78:ILE:HG12	2.12	0.49
1:a:243:ILE:HA	14:a:815:CLA:HED3	1.93	0.49
14:b:809:CLA:H92	17:b:847:BCR:H341	1.93	0.49
1:G:239:PRO:HA	1:G:242:PHE:HD1	1.77	0.49
6:Q:95:PHE:HA	6:Q:139:TRP:HE1	1.77	0.49
1:a:192:ASN:HD22	14:a:812:CLA:HED3	1.75	0.49
1:a:432:ARG:O	1:a:436:HIS:ND1	2.40	0.49
2:B:442:VAL:HG13	14:B:801:CLA:H52	1.94	0.49
1:G:172:MET:HE1	14:G:814:CLA:H92	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:822:CLA:HED2	14:G:825:CLA:HED2	1.93	0.49
1:a:221:LEU:HD11	1:a:295:SER:HA	1.94	0.49
1:a:272:TRP:HA	1:a:275:TYR:HD2	1.78	0.49
1:a:688:MET:O	1:a:692:SER:OG	2.25	0.49
3:C:6:LYS:HG3	4:D:137:TYR:HB2	1.94	0.49
14:H:803:CLA:H143	17:H:847:BCR:H362	1.95	0.49
1:a:469:GLY:HA3	2:b:99:ALA:HB3	1.94	0.49
14:b:832:CLA:HBA2	17:j:103:BCR:HC42	1.94	0.49
2:B:298:GLY:HA2	14:B:820:CLA:HMD2	1.95	0.49
2:B:528:HIS:HD2	17:B:850:BCR:HC22	1.78	0.49
6:F:77:ASP:OD2	12:X:31:TYR:OH	2.26	0.49
14:G:829:CLA:H11	17:G:853:BCR:H312	1.94	0.49
6:Q:129:ALA:O	6:Q:133:MET:HG2	2.13	0.49
12:X:10:TYR:O	12:X:14:THR:OG1	2.25	0.49
2:B:391:PHE:HZ	14:B:824:CLA:HAB	1.77	0.49
1:G:583:ARG:HG3	3:N:49:VAL:HB	1.95	0.49
6:Q:80:LEU:HA	6:Q:83:ALA:HB2	1.93	0.49
1:a:377:MET:HE2	14:a:827:CLA:HMC2	1.94	0.49
2:b:556:ASP:OD1	2:b:556:ASP:N	2.45	0.49
2:b:691:ARG:HE	10:l:17:HIS:HB2	1.78	0.49
1:A:266:PRO:HB2	1:A:275:TYR:CZ	2.48	0.49
1:A:366:LEU:HD21	14:A:820:CLA:H71	1.93	0.49
2:H:91:ILE:HB	2:H:112:PRO:HB2	1.94	0.49
1:a:216:GLN:NE2	1:a:297:THR:OG1	2.40	0.49
1:a:346:GLU:O	1:a:350:THR:OG1	2.17	0.49
2:b:319:PHE:CD2	14:b:822:CLA:HMA3	2.43	0.49
2:b:343:ALA:HB2	17:b:846:BCR:H372	1.95	0.49
2:B:117:TYR:HA	2:B:371:THR:HG22	1.94	0.49
1:G:203:GLY:HA2	14:G:821:CLA:HBC1	1.95	0.49
14:G:815:CLA:C4C	14:G:817:CLA:HAB	2.43	0.49
2:H:499:VAL:HG11	14:H:815:CLA:HED2	1.95	0.49
14:L:206:CLA:H141	7:i:21:LEU:HB2	1.95	0.49
3:N:62:PHE:HB3	4:O:120:ILE:HG21	1.94	0.49
1:a:687:LEU:HB2	14:b:801:CLA:HMC2	1.95	0.49
1:G:336:PHE:O	1:G:432:ARG:NH2	2.43	0.48
14:G:832:CLA:HMA2	10:U:20:THR:HG21	1.94	0.48
2:H:310:PHE:O	2:H:313:THR:OG1	2.31	0.48
2:H:391:PHE:CZ	14:H:824:CLA:HAB	2.48	0.48
9:T:23:ASN:HA	9:T:66:GLY:HA3	1.94	0.48
14:a:833:CLA:H41	14:b:802:CLA:HBC2	1.95	0.48
2:b:668:PHE:HB3	14:b:804:CLA:HMC2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:36:PRO:O	10:l:47:ARG:NH1	2.42	0.48
1:A:395:THR:HB	14:A:829:CLA:HMB2	1.95	0.48
2:B:129:MET:HG2	14:B:813:CLA:HED3	1.95	0.48
2:B:425:HIS:HB2	14:B:829:CLA:HBB2	1.95	0.48
15:B:841:PQN:H142	17:B:848:BCR:H271	1.95	0.48
14:U:201:CLA:HBA1	10:l:149:ILE:HG23	1.94	0.48
14:a:821:CLA:H2	17:a:850:BCR:H352	1.94	0.48
2:B:262:HIS:CD2	2:B:265:THR:H	2.31	0.48
2:B:589:TRP:CH2	14:B:801:CLA:HAB	2.47	0.48
5:E:44:ASN:HD22	5:E:55:VAL:HG22	1.77	0.48
1:G:552:ILE:HG12	14:H:803:CLA:HMD3	1.95	0.48
2:H:276:HIS:HB2	14:H:816:CLA:C1B	2.43	0.48
1:a:80:LEU:HD11	14:a:813:CLA:HBA2	1.94	0.48
1:a:141:SER:HB3	14:a:828:CLA:HAA2	1.95	0.48
1:a:681:PHE:CG	17:a:852:BCR:H363	2.48	0.48
2:b:14:GLN:NE2	3:c:71:ALA:HB1	2.28	0.48
8:j:30:GLU:OE1	8:j:33:ARG:NH1	2.40	0.48
1:A:196:MET:HE1	14:A:826:CLA:H142	1.95	0.48
1:A:222:PRO:HG3	1:A:249:MET:HE1	1.95	0.48
14:A:827:CLA:H8	17:A:852:BCR:H392	1.95	0.48
1:G:196:MET:HB2	14:G:814:CLA:HBC2	1.95	0.48
14:G:822:CLA:HBC3	14:G:828:CLA:H18	1.94	0.48
14:H:839:CLA:H122	14:H:840:CLA:H142	1.95	0.48
10:L:39:ARG:HB3	10:L:42:LEU:HD13	1.94	0.48
1:a:300:HIS:HE2	14:a:819:CLA:C1B	2.27	0.48
2:B:592:ASN:HB2	14:B:801:CLA:HBC2	1.95	0.48
1:G:711:LEU:HD11	17:Q:204:BCR:H342	1.96	0.48
14:H:803:CLA:H142	17:R:101:BCR:H271	1.95	0.48
14:H:817:CLA:HMD2	14:H:827:CLA:H71	1.95	0.48
1:G:212:TRP:NE1	1:G:216:GLN:OE1	2.47	0.48
1:G:417:VAL:HG23	1:G:570:ALA:HA	1.95	0.48
2:H:380:GLN:HE21	2:H:597:VAL:HG11	1.78	0.48
4:O:61:ARG:HB2	4:O:64:GLN:HG3	1.95	0.48
7:R:23:PRO:O	7:R:27:MET:HB2	2.14	0.48
14:a:828:CLA:H11	17:a:852:BCR:H312	1.95	0.48
14:b:840:CLA:HAC1	15:b:841:PQN:H161	1.96	0.48
2:B:623:LEU:HD21	14:B:802:CLA:H162	1.94	0.48
14:G:835:CLA:H152	17:R:102:BCR:H372	1.95	0.48
4:O:94:LEU:O	4:O:98:LYS:NZ	2.43	0.48
14:a:803:CLA:HBB1	17:j:104:BCR:H271	1.95	0.48
3:c:28:MET:HE3	3:c:38:GLN:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:VAL:HA	1:A:436:HIS:CE1	2.48	0.48
14:A:827:CLA:HAB	17:A:852:BCR:C8	2.44	0.48
14:B:814:CLA:HBB1	17:B:842:BCR:H333	1.96	0.48
1:G:604:ASN:HD21	13:G:801:CL0:H68	1.78	0.48
14:G:825:CLA:HAB	14:G:832:CLA:HMD1	1.96	0.48
6:Q:54:GLY:HA2	6:Q:57:ARG:NH1	2.29	0.48
2:b:300:SER:HB3	2:b:303:GLU:HB2	1.95	0.48
2:b:391:PHE:CZ	14:b:824:CLA:HAB	2.48	0.48
14:A:829:CLA:H93	17:J:102:BCR:H361	1.94	0.48
14:B:829:CLA:H3A	14:B:829:CLA:HBA2	1.48	0.48
14:B:838:CLA:HBC2	14:X:1701:CLA:HBC3	1.95	0.48
2:H:22:TRP:CG	2:H:711:GLN:HE22	2.31	0.48
2:H:677:TYR:OH	14:H:803:CLA:OBD	2.28	0.48
1:a:249:MET:N	1:a:249:MET:SD	2.87	0.48
1:a:539:HIS:CG	14:a:838:CLA:HED2	2.48	0.48
2:b:230:TRP:HB3	14:b:815:CLA:H3A	1.94	0.48
2:b:293:THR:OG1	2:b:294:GLN:N	2.47	0.48
2:b:500:TRP:HH2	14:b:834:CLA:H2A	1.79	0.48
2:b:679:GLN:O	2:b:683:GLU:HG3	2.14	0.48
14:A:813:CLA:CHD	14:A:814:CLA:HAB	2.44	0.48
2:B:498:ASN:O	2:B:500:TRP:N	2.42	0.48
14:B:836:CLA:H2	14:B:836:CLA:H62	1.58	0.48
1:G:44:THR:HB	1:G:720:ARG:HG3	1.94	0.48
1:G:477:ASP:OD1	1:G:483:GLN:NE2	2.46	0.48
14:G:809:CLA:H112	14:G:831:CLA:H203	1.94	0.48
14:L:205:CLA:HMA1	14:L:206:CLA:HBC1	1.95	0.48
1:a:306:VAL:HG21	14:a:817:CLA:HBB2	1.95	0.48
1:G:575:ARG:NH1	14:G:831:CLA:O1D	2.47	0.47
2:H:359:LEU:HD13	14:H:816:CLA:HAA2	1.96	0.47
2:H:668:PHE:HB3	14:H:803:CLA:HMC2	1.96	0.47
1:a:695:GLY:O	1:a:699:GLU:HG3	2.13	0.47
2:b:526:VAL:O	2:b:530:ILE:HG13	2.14	0.47
10:l:63:TRP:HH2	10:l:86:LEU:HD22	1.78	0.47
14:A:844:CLA:H41	14:A:844:CLA:H62	1.52	0.47
14:A:844:CLA:HHD	17:B:848:BCR:H383	1.96	0.47
2:B:377:THR:HB	14:B:826:CLA:HMB2	1.96	0.47
14:B:801:CLA:H61	14:B:801:CLA:H41	1.44	0.47
14:B:832:CLA:H41	14:B:832:CLA:H61	1.63	0.47
1:G:601:TRP:HH2	14:G:803:CLA:HAB	1.77	0.47
2:H:391:PHE:HZ	14:H:824:CLA:HAB	1.78	0.47
1:a:682:VAL:HG11	1:a:737:LEU:HD23	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:ILE:HG13	17:V:1602:BCR:H343	1.97	0.47
2:H:190:TRP:NE1	14:H:817:CLA:O1D	2.40	0.47
1:a:696:TYR:CE1	14:b:801:CLA:HMD1	2.48	0.47
14:b:817:CLA:H41	14:b:817:CLA:H62	1.59	0.47
4:d:37:GLU:HA	4:d:50:MET:O	2.13	0.47
14:A:802:CLA:HMD3	2:B:540:ILE:HG12	1.95	0.47
14:B:806:CLA:HHB	14:B:828:CLA:HAB	1.97	0.47
2:H:407:ASN:HD22	2:H:410:ASN:HD21	1.63	0.47
2:H:454:GLU:HA	6:Q:71:LEU:HD22	1.96	0.47
7:I:15:ILE:O	7:I:19:CYS:HB2	2.14	0.47
3:N:61:ASP:HB2	5:P:44:ASN:HD21	1.79	0.47
1:a:395:THR:HG23	1:a:610:ILE:HG21	1.95	0.47
14:a:836:CLA:H3A	14:a:836:CLA:HBA2	1.65	0.47
15:a:845:PQN:H161	15:a:845:PQN:H141	1.69	0.47
6:f:77:ASP:OD2	12:x:31:TYR:OH	2.31	0.47
1:A:687:LEU:HB2	14:A:802:CLA:HMC2	1.95	0.47
14:B:834:CLA:NC	14:B:835:CLA:HAB	2.30	0.47
17:F:1302:BCR:H371	17:F:1302:BCR:H24C	1.69	0.47
14:H:816:CLA:H3A	14:H:816:CLA:HBA2	1.47	0.47
8:J:35:TYR:HA	8:J:36:PRO:HD3	1.75	0.47
1:a:44:THR:HB	1:a:720:ARG:HG3	1.96	0.47
1:a:120:ILE:HD13	17:j:104:BCR:H322	1.96	0.47
1:a:712:LYS:HD3	6:f:154:ALA:HB2	1.96	0.47
1:a:748:LEU:HD23	1:a:748:LEU:HA	1.71	0.47
2:b:522:GLY:O	2:b:526:VAL:HG23	2.15	0.47
1:A:195:SER:O	1:A:199:HIS:ND1	2.44	0.47
1:A:366:LEU:HD21	14:A:820:CLA:H52	1.97	0.47
1:A:370:VAL:O	1:A:374:MET:HG3	2.15	0.47
14:A:819:CLA:HBA2	14:A:819:CLA:H3A	1.63	0.47
1:G:42:PRO:O	6:Q:118:ASN:ND2	2.41	0.47
2:H:31:PHE:HB3	2:H:37:MET:HE3	1.96	0.47
1:a:733:ALA:HA	18:a:853:LHG:H341	1.97	0.47
14:a:831:CLA:HMC1	14:a:839:CLA:HAB	1.96	0.47
1:A:94:GLY:O	1:A:98:SER:OG	2.33	0.47
14:A:809:CLA:HAB	17:J:102:BCR:H363	1.97	0.47
14:A:826:CLA:H18	14:A:826:CLA:H151	1.65	0.47
2:B:330:TYR:HB3	14:B:823:CLA:HBC3	1.97	0.47
2:B:443:HIS:CD2	2:B:457:ILE:HG13	2.49	0.47
14:B:822:CLA:HBA2	14:B:822:CLA:H3A	1.70	0.47
17:B:844:BCR:H351	17:B:844:BCR:H15C	1.66	0.47
6:F:95:PHE:HA	6:F:139:TRP:HE1	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:145:LYS:O	6:F:149:SER:N	2.46	0.47
1:G:79:HIS:CE1	14:G:806:CLA:HMA2	2.49	0.47
1:G:469:GLY:HA3	2:H:99:ALA:HB3	1.97	0.47
14:G:831:CLA:H18	14:G:842:CLA:H3A	1.97	0.47
14:G:843:CLA:HHD	17:H:847:BCR:H383	1.96	0.47
14:H:839:CLA:H18	17:R:101:BCR:H362	1.96	0.47
17:M:1602:BCR:H351	17:M:1602:BCR:H15C	1.77	0.47
1:a:461:HIS:HD2	1:a:462:ASN:HD22	1.63	0.47
1:a:511:VAL:HB	1:a:526:MET:HG3	1.96	0.47
14:a:842:CLA:H202	17:a:852:BCR:H292	1.97	0.47
2:b:284:PHE:CE1	14:b:818:CLA:HAB	2.49	0.47
14:b:827:CLA:H3A	14:b:827:CLA:HBA2	1.54	0.47
6:f:95:PHE:HA	6:f:139:TRP:HE1	1.78	0.47
14:A:802:CLA:HMD1	2:B:585:LEU:HB3	1.97	0.47
14:A:807:CLA:H151	14:A:830:CLA:HBB2	1.97	0.47
2:B:501:LEU:HD12	2:B:501:LEU:HA	1.77	0.47
2:B:593:THR:O	2:B:597:VAL:HG13	2.15	0.47
1:G:33:HIS:NE2	14:G:812:CLA:O1A	2.47	0.47
2:H:305:MET:HE2	2:H:323:HIS:HB3	1.97	0.47
17:H:845:BCR:H24C	17:H:845:BCR:H371	1.44	0.47
17:U:202:BCR:H24C	17:U:202:BCR:H371	1.72	0.47
1:a:120:ILE:HG23	1:a:121:VAL:HG22	1.96	0.47
14:b:831:CLA:O1A	6:f:97:THR:OG1	2.33	0.47
1:A:722:LEU:HD21	15:A:846:PQN:H151	1.96	0.47
14:G:833:CLA:H61	14:G:833:CLA:H41	1.59	0.47
2:H:194:LEU:HA	2:H:198:ALA:HB3	1.97	0.47
2:H:589:TRP:HH2	14:H:801:CLA:HAB	1.79	0.47
14:H:840:CLA:HBA2	15:H:841:PQN:H241	1.96	0.47
10:L:62:PRO:HA	14:L:206:CLA:HMB2	1.96	0.47
1:a:417:VAL:HG23	1:a:560:ALA:HB1	1.97	0.47
1:a:577:PRO:HB3	1:a:724:ILE:HB	1.96	0.47
14:b:804:CLA:H111	17:b:847:BCR:H362	1.97	0.47
6:f:45:VAL:O	6:f:57:ARG:NH2	2.48	0.47
2:B:356:MET:HE1	14:B:827:CLA:CAD	2.45	0.47
14:B:803:CLA:H142	17:I:101:BCR:H271	1.96	0.47
2:H:117:TYR:HA	2:H:371:THR:HG22	1.98	0.47
9:K:29:ILE:O	9:K:33:ALA:N	2.48	0.47
10:L:51:VAL:O	10:L:55:HIS:ND1	2.45	0.47
6:Q:61:TYR:CD1	6:Q:72:PRO:HG2	2.46	0.47
1:a:202:ALA:HB1	14:a:820:CLA:HBC3	1.97	0.47
1:a:326:LYS:O	1:a:330:GLU:HG2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:660:GLN:O	1:a:664:SER:OG	2.33	0.47
14:i:101:CLA:HBB1	14:i:101:CLA:H111	1.97	0.47
1:A:77:PHE:HD1	1:A:176:GLY:HA2	1.79	0.46
14:A:833:CLA:H72	14:L:205:CLA:H102	1.97	0.46
14:A:837:CLA:H3A	14:A:837:CLA:HBA2	1.61	0.46
14:B:834:CLA:C4C	14:B:835:CLA:HAB	2.45	0.46
14:B:840:CLA:HBA1	17:B:848:BCR:H352	1.97	0.46
14:H:817:CLA:H62	14:H:817:CLA:H41	1.60	0.46
17:H:843:BCR:H351	17:H:843:BCR:H15C	1.80	0.46
6:Q:136:GLY:O	6:Q:139:TRP:HB3	2.15	0.46
14:a:830:CLA:H18	14:a:842:CLA:H3A	1.96	0.46
2:b:526:VAL:HG13	14:b:803:CLA:H141	1.98	0.46
14:b:831:CLA:H62	14:b:831:CLA:H2	1.67	0.46
14:b:836:CLA:H2	14:b:836:CLA:H62	1.60	0.46
17:b:846:BCR:H15C	17:b:846:BCR:H351	1.70	0.46
3:c:17:CYS:HB3	16:c:102:SF4:S4	2.54	0.46
6:f:99:TRP:CD1	6:f:136:GLY:HA3	2.50	0.46
2:H:377:THR:HG23	2:H:598:THR:HG21	1.96	0.46
8:S:10:LEU:HD13	8:S:15:VAL:HG11	1.96	0.46
1:a:33:HIS:NE2	14:a:811:CLA:O1A	2.47	0.46
1:a:228:ASP:OD2	1:a:286:ASN:ND2	2.48	0.46
1:a:552:ILE:HG12	14:b:804:CLA:HMD3	1.96	0.46
14:a:855:CLA:H72	2:b:442:VAL:HG13	1.97	0.46
2:b:310:PHE:HD1	14:b:821:CLA:HBA2	1.80	0.46
14:b:816:CLA:H41	14:b:833:CLA:HAA2	1.97	0.46
14:l:205:CLA:C1B	14:l:206:CLA:HED1	2.45	0.46
2:B:230:TRP:HB3	14:B:815:CLA:H3A	1.97	0.46
1:G:336:PHE:HB2	18:G:855:LHG:HC41	1.98	0.46
14:G:809:CLA:HAB	17:S:103:BCR:H363	1.97	0.46
14:G:827:CLA:H8	17:G:852:BCR:H392	1.96	0.46
14:b:812:CLA:H172	17:b:843:BCR:H271	1.96	0.46
14:b:834:CLA:NC	14:b:835:CLA:HAB	2.30	0.46
17:b:847:BCR:H351	17:b:847:BCR:H15C	1.65	0.46
2:B:549:ARG:HH22	4:D:125:ASN:ND2	2.13	0.46
1:G:399:TRP:HD1	14:G:829:CLA:HAB	1.76	0.46
1:G:696:TYR:CE1	14:G:802:CLA:HMD1	2.50	0.46
2:H:171:ALA:HA	14:H:823:CLA:HMD3	1.96	0.46
2:H:322:PRO:HB2	2:H:410:ASN:HA	1.97	0.46
2:H:490:ALA:O	2:H:498:ASN:ND2	2.49	0.46
2:H:640:ASN:O	2:H:648:ASN:ND2	2.49	0.46
2:b:37:MET:HE3	2:b:42:LEU:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:232:VAL:HA	2:b:235:GLN:HG2	1.97	0.46
2:b:237:PRO:HB3	2:b:258:LEU:HD21	1.96	0.46
9:k:75:SER:O	9:k:79:TYR:CB	2.64	0.46
12:x:10:TYR:HA	12:x:13:ARG:HE	1.81	0.46
1:A:141:SER:HB3	14:A:829:CLA:HAA2	1.96	0.46
1:A:364:GLY:HA2	1:A:401:GLY:HA2	1.98	0.46
2:B:300:SER:HB3	2:B:303:GLU:CD	2.41	0.46
2:B:457:ILE:HG12	8:J:39:LEU:CD2	2.45	0.46
4:D:118:ARG:NH2	4:D:138:ASP:O	2.38	0.46
15:H:841:PQN:H142	17:H:847:BCR:H271	1.97	0.46
1:a:86:TRP:HZ3	17:a:849:BCR:H401	1.79	0.46
14:a:827:CLA:CED	14:a:835:CLA:HAB	2.45	0.46
14:a:842:CLA:H41	14:a:842:CLA:H62	1.65	0.46
2:b:344:CYS:HB3	14:b:823:CLA:H42	1.96	0.46
1:G:541:ILE:HD12	13:G:801:CL0:H63	1.97	0.46
14:G:819:CLA:HBA2	14:G:819:CLA:H3A	1.58	0.46
2:H:92:TRP:N	14:H:809:CLA:O1D	2.49	0.46
2:H:96:PHE:HB2	7:R:1:MET:HE1	1.98	0.46
5:P:10:ILE:HG22	5:P:12:ARG:H	1.81	0.46
6:Q:124:ILE:HD12	8:S:16:LEU:HD12	1.96	0.46
14:a:826:CLA:H51	14:a:837:CLA:H43	1.98	0.46
2:b:53:HIS:CE1	14:b:806:CLA:HMA2	2.51	0.46
2:b:602:HIS:NE2	2:b:736:THR:OG1	2.43	0.46
12:x:10:TYR:HA	12:x:13:ARG:HH21	1.80	0.46
14:A:809:CLA:H202	18:A:854:LHG:H182	1.98	0.46
14:B:827:CLA:H3A	14:B:827:CLA:HBA2	1.58	0.46
17:G:852:BCR:H15C	17:G:852:BCR:H351	1.74	0.46
2:b:428:TRP:NE1	14:b:831:CLA:OBD	2.48	0.46
2:b:488:ILE:HG13	14:b:834:CLA:HBC1	1.98	0.46
1:A:321:ILE:HG13	14:A:823:CLA:HMD3	1.97	0.46
14:A:806:CLA:HED2	14:A:831:CLA:HBB2	1.97	0.46
2:B:74:PHE:O	2:B:78:ILE:HG12	2.16	0.46
14:G:829:CLA:O1D	14:G:830:CLA:HBB	2.16	0.46
14:G:831:CLA:H162	14:G:842:CLA:HMA3	1.97	0.46
2:H:188:LEU:HD11	17:H:842:BCR:HC7	1.98	0.46
17:H:842:BCR:H15C	17:H:842:BCR:H351	1.57	0.46
10:L:30:THR:O	10:L:34:ASN:ND2	2.40	0.46
14:L:205:CLA:H93	14:L:205:CLA:H61	1.81	0.46
1:a:104:LEU:HD21	1:a:148:ARG:HB2	1.98	0.46
1:a:541:ILE:HG21	13:a:801:CL0:H60	1.97	0.46
2:b:391:PHE:HZ	14:b:824:CLA:HAB	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:811:CLA:HAB	14:b:819:CLA:C4C	2.46	0.46
17:l:203:BCR:H351	17:l:203:BCR:H15C	1.74	0.46
14:B:803:CLA:H122	17:I:101:BCR:H281	1.96	0.46
14:B:805:CLA:HBA1	14:B:805:CLA:H3A	1.76	0.46
1:G:695:GLY:O	1:G:699:GLU:HG3	2.16	0.46
14:G:828:CLA:HED1	14:G:836:CLA:HAB	1.98	0.46
2:H:143:LEU:HD23	11:V:14:ILE:HG22	1.97	0.46
2:H:216:MET:HB3	2:H:216:MET:HE2	1.62	0.46
10:U:21:PRO:HA	10:U:25:SER:HB2	1.97	0.46
1:a:267:PHE:N	1:a:275:TYR:OH	2.49	0.46
14:a:827:CLA:HBB1	14:a:835:CLA:HAA2	1.98	0.46
2:b:549:ARG:HH22	4:d:125:ASN:ND2	2.14	0.46
17:b:844:BCR:H351	17:b:844:BCR:H15C	1.74	0.46
17:B:848:BCR:H15C	17:B:848:BCR:H351	1.69	0.46
4:D:129:LEU:HD12	4:D:129:LEU:HA	1.49	0.46
5:E:17:TRP:NE1	5:E:42:LYS:O	2.37	0.46
13:G:801:CL0:H12	14:H:801:CLA:CAD	2.46	0.46
17:H:846:BCR:H15C	17:H:846:BCR:H351	1.62	0.46
17:R:102:BCR:H351	17:R:102:BCR:H15C	1.70	0.46
1:a:445:ASN:ND2	2:b:685:LEU:HD21	2.31	0.46
2:b:399:VAL:HG23	2:b:548:ALA:HB1	1.98	0.46
17:i:102:BCR:H15C	17:i:102:BCR:H351	1.74	0.46
17:i:102:BCR:H24C	17:i:102:BCR:H371	1.70	0.46
14:A:810:CLA:H91	17:J:103:BCR:H373	1.98	0.45
2:B:292:ARG:N	2:B:299:HIS:O	2.30	0.45
2:B:295:PHE:CE2	14:B:811:CLA:HMA3	2.50	0.45
2:B:301:ILE:HG21	14:B:823:CLA:HMC1	1.98	0.45
1:G:193:VAL:HG11	14:G:826:CLA:HAC2	1.98	0.45
1:G:266:PRO:HB2	1:G:275:TYR:CZ	2.51	0.45
1:G:392:SER:HA	14:G:829:CLA:HMB3	1.97	0.45
14:H:827:CLA:H3A	14:H:827:CLA:HBA2	1.58	0.45
1:a:196:MET:HE3	14:a:825:CLA:H142	1.97	0.45
1:a:216:GLN:OE1	1:a:301:HIS:ND1	2.44	0.45
13:a:801:CL0:H12	14:a:855:CLA:CAD	2.45	0.45
2:b:50:HIS:ND1	14:b:812:CLA:OBD	2.43	0.45
2:b:460:GLU:OE1	2:b:465:GLN:NE2	2.39	0.45
6:f:161:VAL:HG21	6:f:164:ARG:HH22	1.82	0.45
5:E:8:VAL:HG12	5:E:67:GLU:HA	1.98	0.45
1:G:618:GLN:HB3	1:G:635:THR:HG23	1.98	0.45
2:H:587:MET:HG3	2:H:717:LEU:HD21	1.98	0.45
14:H:803:CLA:H111	14:H:803:CLA:H143	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:834:CLA:C4C	14:H:835:CLA:HAB	2.46	0.45
2:b:48:ALA:HB3	11:m:29:LEU:HD21	1.98	0.45
2:b:319:PHE:HA	14:b:821:CLA:CAB	2.47	0.45
14:b:801:CLA:H193	14:b:801:CLA:H161	1.81	0.45
14:A:807:CLA:H93	14:A:807:CLA:H192	1.99	0.45
14:B:817:CLA:H41	14:B:817:CLA:H62	1.64	0.45
1:G:66:GLU:OE2	1:G:187:LEU:N	2.50	0.45
1:G:508:THR:OG1	1:G:509:ALA:N	2.49	0.45
14:H:805:CLA:H101	14:H:812:CLA:HBA1	1.98	0.45
14:H:832:CLA:H61	14:H:832:CLA:H41	1.61	0.45
6:Q:82:ARG:NH2	6:Q:85:ASP:OD1	2.48	0.45
1:a:377:MET:HG2	1:a:509:ALA:O	2.15	0.45
1:a:409:ALA:HA	17:a:851:BCR:HC41	1.98	0.45
1:a:444:LEU:HG	1:a:551:LEU:HB2	1.99	0.45
14:b:807:CLA:H143	14:b:827:CLA:HBB2	1.97	0.45
14:b:818:CLA:H62	14:b:818:CLA:H41	1.62	0.45
17:A:852:BCR:H351	17:A:852:BCR:H15C	1.76	0.45
2:B:463:PHE:HB3	14:B:836:CLA:H42	1.97	0.45
14:B:830:CLA:H3A	14:B:830:CLA:HBA2	1.56	0.45
1:G:115:GLN:NE2	14:G:810:CLA:OBD	2.45	0.45
1:G:373:HIS:HB3	14:G:819:CLA:HED2	1.98	0.45
1:G:432:ARG:O	1:G:436:HIS:ND1	2.41	0.45
1:G:683:TRP:CD2	13:G:801:CL0:H5	2.51	0.45
14:G:842:CLA:H62	14:G:842:CLA:H41	1.61	0.45
14:H:833:CLA:CHD	14:H:834:CLA:HAB	2.47	0.45
1:a:446:TRP:HH2	14:a:838:CLA:H141	1.82	0.45
1:A:277:ASP:OD1	1:A:277:ASP:N	2.44	0.45
1:A:618:GLN:HB3	1:A:635:THR:HG23	1.99	0.45
1:A:638:ASN:OD1	1:A:638:ASN:N	2.50	0.45
6:F:128:LEU:HD12	6:F:131:LYS:HE3	1.97	0.45
1:G:358:ILE:HG12	17:G:851:BCR:HC7	1.99	0.45
14:G:843:CLA:HMC2	14:H:839:CLA:H11	1.98	0.45
2:H:476:TYR:HB3	6:Q:26:ALA:HA	1.98	0.45
2:H:476:TYR:O	6:Q:27:GLY:N	2.50	0.45
10:L:62:PRO:O	10:L:66:LEU:HB2	2.16	0.45
1:a:364:GLY:HA2	1:a:401:GLY:HA2	1.98	0.45
8:j:26:GLY:C	14:j:101:CLA:HAB	2.41	0.45
1:A:149:ALA:HB1	14:A:820:CLA:HED2	1.99	0.45
1:A:300:HIS:HE2	14:A:820:CLA:C1B	2.29	0.45
1:A:358:ILE:HG12	17:A:851:BCR:HC7	1.99	0.45
14:A:842:CLA:HHC	14:A:842:CLA:HBB1	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:533:GLY:HA2	2:B:589:TRP:CZ3	2.52	0.45
14:B:816:CLA:HBA2	14:B:816:CLA:H3A	1.59	0.45
1:G:453:PHE:HE1	14:H:803:CLA:H102	1.81	0.45
1:a:34:PHE:HB2	1:a:61:HIS:CE1	2.50	0.45
1:a:210:LEU:HD23	17:a:848:BCR:H361	1.99	0.45
1:a:336:PHE:O	1:a:432:ARG:NH2	2.50	0.45
14:a:825:CLA:H151	14:a:825:CLA:H18	1.77	0.45
2:b:134:ASP:O	2:b:137:GLN:HG3	2.16	0.45
2:b:195:ILE:HD13	2:b:254:ILE:HD12	1.99	0.45
14:b:825:CLA:HBA1	14:b:825:CLA:H3A	1.71	0.45
14:b:834:CLA:C4C	14:b:835:CLA:HAB	2.46	0.45
14:b:840:CLA:HBA2	15:b:841:PQN:H241	1.99	0.45
17:l:201:BCR:H15C	17:l:201:BCR:H351	1.67	0.45
14:A:815:CLA:HMB3	17:A:850:BCR:H362	1.98	0.45
2:B:305:MET:HE1	2:B:323:HIS:HD2	1.82	0.45
2:B:319:PHE:CD2	14:B:822:CLA:HMA3	2.52	0.45
14:F:1301:CLA:HMC1	8:J:21:MET:HE1	1.99	0.45
17:G:849:BCR:H351	17:G:849:BCR:H15C	1.82	0.45
14:H:812:CLA:H2	14:H:812:CLA:H62	1.72	0.45
14:H:838:CLA:HBC2	14:W:1701:CLA:HBC3	1.99	0.45
5:P:44:ASN:HB3	5:P:46:THR:H	1.82	0.45
1:a:205:LEU:HD11	14:a:829:CLA:H192	1.99	0.45
1:a:323:HIS:HA	14:a:822:CLA:HED1	1.99	0.45
1:a:339:THR:HB	1:a:342:LYS:HE3	1.97	0.45
1:a:421:ASP:OD1	1:a:424:VAL:N	2.46	0.45
14:a:833:CLA:H112	14:a:833:CLA:H152	1.73	0.45
14:a:840:CLA:HAA2	14:b:830:CLA:HMB2	1.99	0.45
2:b:484:ASN:HB3	2:b:487:SER:HB3	1.99	0.45
14:b:826:CLA:O1D	14:b:827:CLA:HHB	2.16	0.45
14:b:829:CLA:HBB2	14:b:838:CLA:CBB	2.43	0.45
14:b:830:CLA:HAC2	17:f:203:BCR:H362	1.98	0.45
6:f:44:ALA:HB1	6:f:57:ARG:HH21	1.81	0.45
17:m:1602:BCR:H351	17:m:1602:BCR:H15C	1.74	0.45
1:A:44:THR:HB	1:A:720:ARG:HG3	1.98	0.45
14:A:829:CLA:H62	14:A:829:CLA:H41	1.72	0.45
2:B:531:ALA:HA	14:B:838:CLA:HED3	1.98	0.45
2:B:652:VAL:HG23	2:B:653:TRP:CD1	2.52	0.45
14:B:831:CLA:HBB2	17:B:847:BCR:HC41	1.99	0.45
1:G:298:ALA:O	1:G:302:VAL:HG23	2.17	0.45
1:G:366:LEU:HD21	14:G:820:CLA:H93	1.97	0.45
1:G:395:THR:HG23	1:G:610:ILE:HG21	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:829:CLA:H41	14:G:829:CLA:H62	1.57	0.45
17:G:848:BCR:H15C	17:G:848:BCR:H351	1.60	0.45
14:L:204:CLA:HBA2	14:L:204:CLA:H3A	1.61	0.45
6:Q:99:TRP:CD1	6:Q:136:GLY:HA3	2.51	0.45
14:a:833:CLA:H102	14:a:833:CLA:H62	1.80	0.45
14:a:842:CLA:H111	14:b:801:CLA:H143	1.99	0.45
2:b:291:TYR:HA	2:b:299:HIS:H	1.81	0.45
2:b:533:GLY:HA2	2:b:589:TRP:HZ3	1.81	0.45
2:b:594:ILE:HA	2:b:597:VAL:HG12	1.99	0.45
1:A:70:ARG:NE	1:A:185:PRO:O	2.45	0.45
14:A:803:CLA:H72	2:B:659:PHE:HD1	1.82	0.45
2:B:415:VAL:HA	2:B:418:HIS:CE1	2.52	0.45
14:B:812:CLA:H141	14:B:812:CLA:H162	1.82	0.45
1:G:292:LEU:HD21	14:G:819:CLA:H2A	1.99	0.45
1:G:379:PRO:HG2	14:G:820:CLA:HBA2	1.97	0.45
14:H:829:CLA:H3A	14:H:829:CLA:HBA2	1.47	0.45
14:H:837:CLA:H61	17:Q:204:BCR:H372	1.98	0.45
14:a:832:CLA:H41	14:a:832:CLA:H61	1.61	0.45
1:A:308:PHE:HZ	14:A:820:CLA:H112	1.82	0.45
2:H:466:PHE:CD2	12:W:31:TYR:HD1	2.35	0.45
2:H:492:ALA:HA	14:H:834:CLA:HMD2	1.99	0.45
14:L:201:CLA:H161	14:U:206:CLA:H91	1.98	0.45
17:Q:202:BCR:H331	14:Q:203:CLA:HMB3	1.98	0.45
14:a:836:CLA:HHC	14:a:836:CLA:HBB1	1.98	0.45
2:b:122:HIS:HB2	2:b:365:ILE:HD12	1.98	0.45
2:b:422:ILE:HG21	17:b:845:BCR:H282	1.98	0.45
5:e:61:ALA:HB3	5:e:64:GLU:HG3	1.99	0.45
14:l:206:CLA:H111	14:l:206:CLA:H152	1.66	0.45
14:A:825:CLA:H43	17:A:851:BCR:H19C	1.99	0.44
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.97	0.44
17:B:847:BCR:H24C	17:B:847:BCR:H371	1.79	0.44
2:H:601:TRP:CD1	14:H:836:CLA:HBC2	2.52	0.44
2:H:726:LEU:HD11	14:H:828:CLA:H203	1.98	0.44
10:U:80:LEU:HD23	10:l:138:PHE:CZ	2.52	0.44
10:U:131:GLY:O	10:U:135:VAL:HG12	2.17	0.44
14:b:809:CLA:H192	7:i:26:VAL:HG11	1.99	0.44
14:b:838:CLA:HBC2	14:x:1701:CLA:HBC3	1.99	0.44
4:d:116:VAL:HG12	4:d:118:ARG:HG2	1.99	0.44
14:B:817:CLA:HMD2	14:B:827:CLA:H71	2.00	0.44
1:G:366:LEU:HD11	14:G:820:CLA:H93	1.98	0.44
2:H:345:LEU:O	2:H:349:THR:OG1	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:19:ASN:ND2	6:Q:159:ILE:O	2.46	0.44
14:a:828:CLA:O1D	14:a:829:CLA:HHB	2.16	0.44
14:i:101:CLA:H52	17:m:1602:BCR:H362	1.99	0.44
14:A:811:CLA:H3A	14:A:811:CLA:HBA2	1.59	0.44
14:B:819:CLA:H3A	14:B:819:CLA:HBA2	1.57	0.44
14:B:832:CLA:HBA2	17:J:102:BCR:HC41	2.00	0.44
15:H:841:PQN:H28	19:H:848:LMG:H192	1.99	0.44
4:O:105:LYS:HB2	4:O:105:LYS:HE2	1.67	0.44
14:U:204:CLA:H3A	14:U:204:CLA:HBA2	1.54	0.44
1:a:212:TRP:NE1	14:a:819:CLA:O1D	2.35	0.44
1:a:704:ILE:HD13	14:a:840:CLA:HMD2	1.99	0.44
14:b:806:CLA:HBA1	14:b:806:CLA:H3A	1.79	0.44
14:b:809:CLA:CMA	14:l:202:CLA:HAB	2.46	0.44
14:b:831:CLA:CAB	17:f:201:BCR:H323	2.47	0.44
6:f:65:LEU:H	6:f:82:ARG:HH12	1.65	0.44
14:A:834:CLA:H41	14:A:844:CLA:HBC2	1.99	0.44
1:G:364:GLY:HA2	1:G:401:GLY:HA2	2.00	0.44
1:G:375:TYR:HA	1:G:390:GLN:HE22	1.81	0.44
1:G:423:ALA:HA	4:O:39:VAL:HG11	2.00	0.44
17:G:850:BCR:H24C	17:G:850:BCR:H371	1.78	0.44
14:H:808:CLA:H122	14:H:826:CLA:H122	1.99	0.44
10:U:146:VAL:O	10:U:150:MET:HG2	2.17	0.44
1:a:31:PRO:HB2	1:a:47:TRP:HH2	1.82	0.44
1:a:710:LYS:HG2	14:b:830:CLA:HMA1	1.99	0.44
17:a:849:BCR:H24C	17:a:849:BCR:H371	1.73	0.44
2:b:659:PHE:O	2:b:663:VAL:HG23	2.17	0.44
14:b:802:CLA:HBB1	14:b:802:CLA:H71	1.98	0.44
4:d:43:PRO:HD3	4:d:68:LEU:HD12	1.99	0.44
1:A:216:GLN:HA	1:A:220:SER:HB2	2.00	0.44
1:G:94:GLY:HA3	1:G:147:TRP:CH2	2.53	0.44
1:G:378:PRO:HA	1:G:379:PRO:HD3	1.88	0.44
1:G:699:GLU:OE2	2:H:557:LYS:NZ	2.41	0.44
1:a:380:TYR:CE1	14:a:819:CLA:HAA2	2.52	0.44
14:a:840:CLA:H43	14:b:831:CLA:HAA2	2.00	0.44
17:a:850:BCR:H15C	17:a:850:BCR:H351	1.75	0.44
2:b:174:ARG:HB3	14:b:823:CLA:HMD1	1.98	0.44
2:b:305:MET:HE2	2:b:305:MET:HB2	1.74	0.44
4:d:38:GLN:HB2	4:d:50:MET:HE3	2.00	0.44
6:f:65:LEU:N	6:f:82:ARG:HH12	2.16	0.44
1:A:156:PHE:HZ	14:A:817:CLA:HAA2	1.83	0.44
1:A:292:LEU:HD12	1:A:379:PRO:CB	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ILE:O	1:A:313:HIS:ND1	2.50	0.44
1:A:681:PHE:CG	17:A:853:BCR:H363	2.52	0.44
17:B:847:BCR:HC22	17:B:850:BCR:H363	1.99	0.44
14:H:806:CLA:H72	14:H:806:CLA:H111	1.42	0.44
17:V:1602:BCR:H15C	17:V:1602:BCR:H351	1.80	0.44
1:a:683:TRP:HZ3	14:a:855:CLA:HMD3	1.83	0.44
5:e:44:ASN:HB2	5:e:55:VAL:H	1.82	0.44
2:B:257:PHE:CE2	2:B:500:TRP:HB3	2.53	0.44
2:B:377:THR:HG23	2:B:598:THR:HG21	1.99	0.44
14:B:824:CLA:HBD	14:B:836:CLA:HMB2	2.00	0.44
14:G:829:CLA:H3A	14:G:829:CLA:HBA2	1.70	0.44
14:G:842:CLA:H192	14:Q:203:CLA:HBB1	2.00	0.44
2:H:232:VAL:HA	2:H:235:GLN:HG2	1.99	0.44
14:H:837:CLA:HBC2	17:H:849:BCR:HC7	2.00	0.44
1:a:79:HIS:CE1	14:a:805:CLA:HMA2	2.53	0.44
1:a:711:LEU:HD13	17:f:203:BCR:H321	1.99	0.44
14:a:813:CLA:H8	14:a:813:CLA:H122	1.75	0.44
14:a:818:CLA:HBA2	14:a:818:CLA:H3A	1.65	0.44
2:b:69:ALA:HB2	2:b:135:LEU:HB2	2.00	0.44
2:b:377:THR:HB	14:b:826:CLA:HMB1	1.99	0.44
2:B:526:VAL:HG11	2:B:600:TYR:HB2	1.99	0.44
1:G:120:ILE:HG13	1:G:121:VAL:HG22	1.98	0.44
2:H:268:LEU:HD21	2:H:359:LEU:HD22	2.00	0.44
2:H:304:MET:HG3	14:H:821:CLA:HED2	2.00	0.44
2:H:399:VAL:HG23	2:H:548:ALA:HB1	2.00	0.44
14:H:826:CLA:O1D	14:H:827:CLA:HHB	2.17	0.44
14:H:833:CLA:C4C	14:H:834:CLA:HAB	2.48	0.44
14:a:826:CLA:H93	14:a:826:CLA:H62	1.80	0.44
2:b:86:PRO:HB3	2:b:121:TYR:CG	2.53	0.44
14:b:808:CLA:H121	14:b:826:CLA:H171	1.99	0.44
1:A:173:LEU:HD11	14:A:810:CLA:H201	1.99	0.44
1:A:399:TRP:CH2	1:A:603:TYR:HA	2.52	0.44
14:A:829:CLA:HBA2	14:A:829:CLA:H3A	1.59	0.44
17:A:851:BCR:H351	17:A:851:BCR:H15C	1.67	0.44
2:B:414:ARG:O	2:B:418:HIS:ND1	2.39	0.44
2:B:528:HIS:CD2	17:B:850:BCR:HC22	2.53	0.44
14:B:839:CLA:H111	14:B:839:CLA:H72	1.60	0.44
17:B:846:BCR:H24C	17:B:846:BCR:H371	1.77	0.44
1:G:76:HIS:ND1	14:G:814:CLA:OBD	2.49	0.44
2:H:174:ARG:HB3	14:H:823:CLA:HMD1	2.00	0.44
2:H:679:GLN:NE2	2:H:706:ALA:H	2.15	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:2:THR:OG1	4:O:3:THR:N	2.44	0.44
7:R:19:CYS:CB	14:U:201:CLA:HAB	2.45	0.44
1:a:601:TRP:HH2	14:a:802:CLA:HAB	1.80	0.44
1:a:625:VAL:HG13	1:a:631:VAL:HG22	2.00	0.44
1:a:660:GLN:HG3	1:a:750:ARG:HA	2.00	0.44
2:b:8:PHE:HB2	2:b:34:HIS:CG	2.53	0.44
2:b:686:VAL:HG11	3:c:81:TYR:CG	2.52	0.44
14:b:809:CLA:HMA2	14:l:202:CLA:HAB	2.00	0.44
17:b:845:BCR:H24C	17:b:845:BCR:H371	1.79	0.44
6:f:80:LEU:HA	6:f:83:ALA:HB2	2.00	0.44
9:k:29:ILE:O	9:k:33:ALA:N	2.50	0.44
1:A:154:ASN:ND2	1:A:157:GLN:OE1	2.51	0.43
1:A:306:VAL:HG13	17:A:848:BCR:H352	2.00	0.43
14:A:802:CLA:H102	14:A:843:CLA:HMC2	2.00	0.43
17:A:853:BCR:H371	17:A:853:BCR:H24C	1.62	0.43
14:B:828:CLA:H92	14:B:828:CLA:H61	1.83	0.43
4:D:11:TYR:OH	4:D:45:ALA:O	2.30	0.43
5:E:12:ARG:HD3	5:E:64:GLU:OE1	2.18	0.43
6:F:98:GLY:HA3	6:F:139:TRP:CZ2	2.53	0.43
1:G:232:ALA:O	1:G:234:LYS:N	2.50	0.43
14:H:805:CLA:HAA2	14:H:805:CLA:H2	2.00	0.43
17:L:207:BCR:H15C	17:L:207:BCR:H351	1.66	0.43
17:Q:204:BCR:H24C	17:Q:204:BCR:H371	1.66	0.43
11:V:24:ARG:HD2	11:V:24:ARG:HA	1.72	0.43
14:b:822:CLA:HAB	14:b:829:CLA:HMD2	2.00	0.43
15:b:841:PQN:H212	15:b:841:PQN:H172	1.74	0.43
10:l:62:PRO:O	10:l:66:LEU:HB2	2.18	0.43
2:B:86:PRO:HB3	2:B:121:TYR:CG	2.53	0.43
2:B:232:VAL:HA	2:B:235:GLN:HG2	2.00	0.43
2:B:434:GLY:HA2	2:B:532:LEU:HD22	1.99	0.43
14:B:826:CLA:O1D	14:B:827:CLA:HHB	2.18	0.43
14:H:829:CLA:HBC1	17:H:845:BCR:H23C	2.00	0.43
14:U:206:CLA:H2	14:U:206:CLA:H61	1.79	0.43
1:a:618:GLN:HB3	1:a:635:THR:HG23	2.00	0.43
14:a:842:CLA:H162	14:a:842:CLA:H141	1.82	0.43
14:b:814:CLA:H3A	14:b:814:CLA:HBA2	1.73	0.43
14:l:205:CLA:HBA2	14:l:205:CLA:H3A	1.58	0.43
1:A:20:PRO:HG2	1:A:184:ALA:HB3	2.00	0.43
1:A:117:VAL:HB	1:A:123:GLN:HE21	1.84	0.43
1:A:539:HIS:CG	14:A:839:CLA:HED2	2.52	0.43
1:A:713:VAL:HG23	6:F:105:ARG:HG3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:809:CLA:H3A	14:A:809:CLA:HBA2	1.51	0.43
14:A:836:CLA:CBB	14:A:838:CLA:HBA1	2.48	0.43
17:A:850:BCR:H24C	17:A:850:BCR:H371	1.66	0.43
2:B:677:TYR:OH	14:B:803:CLA:OBD	2.25	0.43
14:B:812:CLA:H193	14:B:812:CLA:H161	1.79	0.43
14:B:831:CLA:H152	14:B:831:CLA:H112	1.60	0.43
14:G:828:CLA:H202	14:G:828:CLA:H162	1.82	0.43
2:H:86:PRO:HB3	2:H:121:TYR:CG	2.53	0.43
2:H:425:HIS:HB2	14:H:829:CLA:HBB2	1.99	0.43
14:U:206:CLA:H3A	14:U:206:CLA:HBA1	1.65	0.43
1:a:321:ILE:HD11	14:a:820:CLA:H2A	1.99	0.43
14:a:814:CLA:HMB3	17:a:849:BCR:H362	1.99	0.43
17:a:851:BCR:H351	17:a:851:BCR:H15C	1.75	0.43
2:b:211:ASN:ND2	2:b:215:THR:OG1	2.49	0.43
14:b:839:CLA:H18	17:i:102:BCR:H362	1.99	0.43
6:f:79:ARG:O	6:f:82:ARG:N	2.49	0.43
14:l:206:CLA:HMA1	14:l:207:CLA:HBC1	2.00	0.43
1:A:266:PRO:HA	1:A:271:ASN:HB3	2.00	0.43
1:A:336:PHE:O	1:A:432:ARG:NH2	2.50	0.43
2:B:361:PRO:HG3	14:B:817:CLA:HBA1	2.00	0.43
4:D:42:MET:HE1	4:D:59:LEU:HD21	1.99	0.43
1:G:288:VAL:HG13	1:G:289:THR:HG23	2.00	0.43
14:G:802:CLA:H102	14:G:842:CLA:HMC1	1.99	0.43
14:G:802:CLA:H193	14:G:802:CLA:H161	1.85	0.43
14:G:825:CLA:HHC	14:G:832:CLA:HMD1	2.00	0.43
15:G:846:PQN:H141	15:G:846:PQN:H161	1.80	0.43
2:H:510:SER:O	2:H:510:SER:OG	2.30	0.43
14:H:827:CLA:H112	17:H:843:BCR:H19C	1.99	0.43
10:L:64:VAL:HG22	10:L:76:ASN:HA	1.99	0.43
3:N:27:GLU:OE1	3:N:43:PRO:HG3	2.18	0.43
10:U:6:VAL:HG22	10:U:20:THR:HG22	2.00	0.43
10:U:51:VAL:O	10:U:55:HIS:ND1	2.45	0.43
1:a:26:GLU:HG2	8:j:5:HIS:CD2	2.53	0.43
1:a:587:CYS:HB2	2:b:674:TRP:HB3	1.99	0.43
14:a:826:CLA:HAB	17:a:851:BCR:C8	2.48	0.43
17:a:852:BCR:H371	17:a:852:BCR:H24C	1.80	0.43
2:b:183:PHE:HE2	14:b:823:CLA:H2	1.84	0.43
17:j:103:BCR:H351	17:j:103:BCR:H15C	1.80	0.43
17:l:208:BCR:H15C	17:l:208:BCR:H351	1.75	0.43
1:A:202:ALA:HB1	14:A:821:CLA:HBC3	2.00	0.43
1:A:599:LEU:HD21	14:A:831:CLA:HBC1	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:825:CLA:H92	14:A:825:CLA:H62	1.84	0.43
14:B:831:CLA:H2	14:B:831:CLA:H62	1.56	0.43
1:G:617:MET:HE3	14:G:838:CLA:HBC1	2.00	0.43
2:H:50:HIS:HE1	14:H:805:CLA:H161	1.83	0.43
14:H:807:CLA:HBC2	11:V:12:LEU:HD23	2.00	0.43
14:H:825:CLA:H61	14:H:825:CLA:H101	1.75	0.43
17:H:847:BCR:H351	17:H:847:BCR:H15C	1.75	0.43
17:H:849:BCR:H392	8:S:38:LEU:HD21	2.00	0.43
2:b:173:SER:O	2:b:177:HIS:HD2	2.01	0.43
14:b:824:CLA:HBA2	14:b:824:CLA:H3A	1.80	0.43
14:A:843:CLA:HBA2	14:A:843:CLA:H3A	1.70	0.43
14:B:818:CLA:H102	14:B:818:CLA:H61	1.76	0.43
2:H:275:HIS:HB3	14:H:816:CLA:HMB2	2.00	0.43
2:H:278:LEU:HG	14:H:815:CLA:HAB	2.01	0.43
14:H:801:CLA:HMB3	14:H:802:CLA:H201	2.01	0.43
14:H:805:CLA:HBA1	14:H:805:CLA:H3A	1.73	0.43
17:H:844:BCR:H15C	17:H:844:BCR:H351	1.79	0.43
1:a:685:PHE:HZ	14:a:842:CLA:HBC2	1.83	0.43
1:a:690:LEU:HB3	2:b:672:ILE:HG12	2.00	0.43
1:A:161:THR:HG23	14:A:815:CLA:HBA1	1.99	0.43
2:B:145:LEU:HD23	2:B:145:LEU:HA	1.91	0.43
2:B:225:PHE:HB3	2:B:233:TYR:HE2	1.83	0.43
14:G:807:CLA:H193	14:G:807:CLA:H161	1.84	0.43
14:G:829:CLA:H51	14:G:829:CLA:H8	1.77	0.43
14:G:841:CLA:HAC1	15:G:846:PQN:H221	1.99	0.43
2:H:70:TRP:NE1	7:R:6:ALA:O	2.39	0.43
2:H:225:PHE:CD2	2:H:230:TRP:NE1	2.83	0.43
2:H:694:LEU:HB2	17:R:102:BCR:H282	2.00	0.43
14:H:826:CLA:H72	14:H:826:CLA:H111	1.79	0.43
6:Q:147:LEU:HD23	6:Q:147:LEU:HA	1.81	0.43
17:R:101:BCR:H371	17:R:101:BCR:H24C	1.76	0.43
1:a:113:SER:HB2	1:a:138:GLN:HA	2.00	0.43
14:a:828:CLA:H41	14:a:828:CLA:H62	1.55	0.43
14:b:837:CLA:HMA3	14:b:838:CLA:HED2	2.01	0.43
14:A:825:CLA:HAC1	17:A:851:BCR:HC8	2.01	0.43
14:A:832:CLA:HAB	14:A:840:CLA:HBB2	2.00	0.43
14:A:841:CLA:HBC1	15:A:846:PQN:H193	2.01	0.43
15:A:846:PQN:H111	17:B:847:BCR:H393	2.00	0.43
2:B:22:TRP:CG	2:B:711:GLN:HE22	2.37	0.43
14:B:827:CLA:H202	14:B:827:CLA:H161	1.86	0.43
1:G:371:ALA:HB2	1:G:397:HIS:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:377:MET:SD	14:G:819:CLA:HBD	2.58	0.43
14:G:805:CLA:HBA1	14:G:805:CLA:H3A	1.88	0.43
2:H:53:HIS:CE1	14:H:805:CLA:HMA2	2.53	0.43
1:a:70:ARG:HG2	1:a:184:ALA:HB1	1.99	0.43
1:a:153:THR:H	1:a:157:GLN:HE22	1.65	0.43
1:a:196:MET:HB2	14:a:813:CLA:HBC2	2.00	0.43
2:b:294:GLN:NE2	14:b:811:CLA:HAA2	2.33	0.43
2:b:597:VAL:CG2	14:b:836:CLA:HAB	2.49	0.43
2:b:679:GLN:NE2	2:b:706:ALA:H	2.16	0.43
17:b:843:BCR:H351	17:b:843:BCR:H15C	1.80	0.43
1:A:66:GLU:O	1:A:70:ARG:HD2	2.18	0.43
1:A:79:HIS:CE1	14:A:806:CLA:HMA2	2.53	0.43
1:A:118:TRP:O	1:A:123:GLN:NE2	2.51	0.43
14:B:826:CLA:HBA2	14:B:826:CLA:H3A	1.81	0.43
1:G:526:MET:HE3	1:G:526:MET:HB3	1.89	0.43
14:G:810:CLA:H91	17:S:104:BCR:H373	2.00	0.43
2:H:562:TYR:HE2	14:H:828:CLA:HMD1	1.82	0.43
17:J:102:BCR:H15C	17:J:102:BCR:H351	1.82	0.43
17:L:207:BCR:H371	17:L:207:BCR:H24C	1.82	0.43
17:R:101:BCR:H351	17:R:101:BCR:H15C	1.74	0.43
11:V:21:LEU:HD12	11:V:21:LEU:HA	1.85	0.43
14:a:828:CLA:H93	14:a:828:CLA:H111	1.86	0.43
14:b:817:CLA:H142	14:b:825:CLA:HBA1	2.01	0.43
14:b:831:CLA:H102	17:f:203:BCR:H312	2.00	0.43
6:f:82:ARG:HA	6:f:82:ARG:HD3	1.81	0.43
7:i:3:GLY:HA3	7:i:5:TYR:CE2	2.53	0.43
1:A:172:MET:HE1	14:A:814:CLA:H92	2.00	0.43
1:A:469:GLY:HA3	2:B:99:ALA:HB3	2.01	0.43
1:A:552:ILE:HG12	14:B:803:CLA:HMD3	2.01	0.43
2:B:597:VAL:HG11	14:B:836:CLA:HBB2	2.01	0.43
2:B:679:GLN:NE2	2:B:706:ALA:H	2.16	0.43
14:B:804:CLA:HMA3	11:M:29:LEU:HD13	2.01	0.43
14:B:826:CLA:H152	14:B:828:CLA:H151	2.01	0.43
14:B:837:CLA:HMA3	14:B:838:CLA:HED2	2.01	0.43
14:B:839:CLA:H141	14:B:839:CLA:H162	1.74	0.43
14:G:805:CLA:H91	17:S:104:BCR:H272	2.01	0.43
14:G:826:CLA:H111	14:G:826:CLA:H143	1.74	0.43
14:G:831:CLA:H62	14:G:831:CLA:H41	1.75	0.43
14:H:806:CLA:H41	14:H:806:CLA:H61	1.53	0.43
14:H:826:CLA:H143	14:H:826:CLA:H162	1.90	0.43
6:Q:56:LYS:HA	6:Q:59:GLU:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:255:ASN:N	1:a:255:ASN:OD1	2.51	0.43
14:a:806:CLA:H72	14:a:806:CLA:H111	1.82	0.43
2:b:436:HIS:HB2	17:b:849:BCR:HC32	2.01	0.43
14:b:803:CLA:H41	14:b:803:CLA:H62	1.73	0.43
14:b:831:CLA:H152	14:b:831:CLA:H112	1.57	0.43
4:d:31:THR:O	4:d:81:TYR:HA	2.19	0.43
1:A:459:TYR:CE2	1:A:537:LEU:HB3	2.54	0.42
1:A:683:TRP:CE3	13:A:801:CL0:H6	2.54	0.42
14:A:829:CLA:H193	14:A:829:CLA:H161	1.86	0.42
6:F:69:ASP:OD1	6:F:69:ASP:N	2.52	0.42
6:F:144:LEU:HD12	6:F:144:LEU:HA	1.90	0.42
1:G:394:PHE:CZ	1:G:398:MET:HE3	2.54	0.42
14:G:828:CLA:CED	14:G:836:CLA:HAB	2.49	0.42
2:H:225:PHE:HD2	2:H:230:TRP:HE1	1.67	0.42
2:H:531:ALA:O	2:H:535:HIS:ND1	2.48	0.42
14:H:807:CLA:H52	17:V:1602:BCR:H362	2.01	0.42
4:O:31:THR:O	4:O:81:TYR:HA	2.18	0.42
9:T:69:LEU:HA	14:T:1401:CLA:HBC2	2.01	0.42
14:b:822:CLA:HMD3	14:b:823:CLA:HHC	2.01	0.42
4:d:105:LYS:O	4:d:110:ARG:NH1	2.52	0.42
1:A:99:ASN:N	1:A:99:ASN:OD1	2.52	0.42
1:A:417:VAL:HG12	1:A:418:ARG:HG3	2.00	0.42
14:B:826:CLA:H143	14:B:826:CLA:H162	1.81	0.42
14:B:832:CLA:H2A	14:B:832:CLA:HED2	2.00	0.42
4:D:36:LYS:HA	4:D:52:GLU:OE1	2.19	0.42
1:G:173:LEU:HD23	1:G:173:LEU:HA	1.90	0.42
14:G:829:CLA:H93	14:G:829:CLA:H111	1.86	0.42
2:H:556:ASP:OD1	2:H:556:ASP:N	2.51	0.42
14:H:802:CLA:H102	14:H:802:CLA:H62	1.74	0.42
3:N:18:VAL:HG22	3:N:26:LEU:HB2	2.01	0.42
17:U:202:BCR:H15C	17:U:202:BCR:H351	1.76	0.42
14:a:828:CLA:H193	14:a:828:CLA:H161	1.87	0.42
2:b:22:TRP:CG	2:b:711:GLN:HE22	2.37	0.42
14:b:817:CLA:H3A	14:b:817:CLA:HBA2	1.66	0.42
14:b:839:CLA:H192	7:i:24:VAL:HG23	2.01	0.42
1:A:491:GLN:NE2	1:A:529:ILE:O	2.50	0.42
1:A:592:TRP:CD1	14:A:831:CLA:HMD1	2.54	0.42
2:B:476:TYR:O	6:F:27:GLY:N	2.51	0.42
14:B:821:CLA:HBA2	14:B:821:CLA:H3A	1.81	0.42
1:G:297:THR:HG21	14:G:820:CLA:HED1	2.00	0.42
14:H:816:CLA:C2D	14:H:825:CLA:HMB2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:204:CLA:C1B	14:L:205:CLA:HED1	2.49	0.42
14:L:205:CLA:H111	14:L:205:CLA:H152	1.90	0.42
14:L:206:CLA:HBA1	14:L:206:CLA:H3A	1.74	0.42
4:O:33:THR:HA	4:O:53:GLY:O	2.19	0.42
2:b:319:PHE:CG	14:b:821:CLA:HAB	2.55	0.42
2:b:415:VAL:HA	2:b:418:HIS:CE1	2.55	0.42
2:b:501:LEU:HD12	2:b:501:LEU:HA	1.86	0.42
2:b:508:ILE:HG12	2:b:515:LEU:HD23	2.00	0.42
14:b:806:CLA:H142	14:b:806:CLA:H111	1.83	0.42
10:l:80:LEU:HD22	10:l:137:PHE:CG	2.54	0.42
15:A:846:PQN:H161	15:A:846:PQN:H141	1.77	0.42
2:B:283:LEU:HD22	14:B:818:CLA:HMC3	2.01	0.42
5:P:13:PRO:HA	5:P:18:TYR:CD1	2.54	0.42
14:U:206:CLA:H92	14:U:206:CLA:H62	1.76	0.42
12:W:35:LEU:HD12	12:W:35:LEU:HA	1.91	0.42
14:a:808:CLA:H91	14:a:811:CLA:H191	2.00	0.42
2:b:60:TRP:NE1	14:b:826:CLA:OBD	2.53	0.42
2:b:434:GLY:HA3	14:b:801:CLA:O2A	2.19	0.42
6:f:117:ALA:O	6:f:121:GLU:HG3	2.20	0.42
8:j:35:TYR:HA	8:j:36:PRO:HD3	1.84	0.42
10:l:139:LEU:HB3	14:l:207:CLA:H41	2.01	0.42
17:m:1602:BCR:H24C	17:m:1602:BCR:H371	1.84	0.42
1:A:587:CYS:HB2	2:B:674:TRP:HB3	2.02	0.42
2:B:319:PHE:HA	14:B:821:CLA:HAB	2.00	0.42
2:B:549:ARG:NH1	6:F:164:ARG:OXT	2.41	0.42
1:G:433:VAL:HG21	14:G:822:CLA:H192	2.01	0.42
1:G:583:ARG:NH1	4:O:63:GLU:OE2	2.52	0.42
1:G:733:ALA:HA	18:G:854:LHG:H341	2.02	0.42
10:L:113:LYS:HA	10:L:113:LYS:HD2	1.86	0.42
14:U:201:CLA:H2	10:l:149:ILE:HG21	2.02	0.42
1:a:118:TRP:HB3	17:j:104:BCR:HC21	2.01	0.42
1:a:292:LEU:HB2	1:a:379:PRO:HA	2.01	0.42
17:j:104:BCR:H371	17:j:104:BCR:H24C	1.71	0.42
1:A:363:MET:HE1	14:A:826:CLA:H12	2.01	0.42
17:A:849:BCR:H351	17:A:849:BCR:H15C	1.86	0.42
2:B:354:GLN:HE22	14:B:836:CLA:C4B	2.33	0.42
14:B:822:CLA:HAB	14:B:829:CLA:HMD1	2.01	0.42
6:F:142:ALA:HA	6:F:145:LYS:HG3	2.01	0.42
1:G:66:GLU:O	1:G:70:ARG:HD2	2.19	0.42
1:G:669:LEU:HD13	1:G:749:ALA:HA	2.01	0.42
14:G:802:CLA:H191	14:G:809:CLA:H193	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:805:CLA:H93	14:G:812:CLA:H41	2.02	0.42
2:H:145:LEU:HD23	2:H:145:LEU:HA	1.89	0.42
2:H:321:MET:HB2	2:H:323:HIS:HE1	1.84	0.42
14:H:828:CLA:H143	14:H:828:CLA:H111	1.86	0.42
17:H:846:BCR:H402	17:H:846:BCR:H282	1.77	0.42
1:a:80:LEU:HD12	14:a:813:CLA:HED3	2.00	0.42
14:b:836:CLA:H52	12:x:27:VAL:HG11	2.01	0.42
17:b:846:BCR:H24C	17:b:846:BCR:H371	1.81	0.42
1:A:308:PHE:CE1	14:A:822:CLA:HAB	2.55	0.42
1:A:685:PHE:HZ	14:A:843:CLA:HBC2	1.84	0.42
1:A:689:PHE:HZ	14:A:843:CLA:HBC3	1.83	0.42
2:B:125:TYR:HE2	2:B:364:PHE:HE2	1.67	0.42
2:B:190:TRP:HD1	2:B:277:HIS:CD2	2.37	0.42
14:B:812:CLA:H62	14:B:812:CLA:H2	1.72	0.42
2:H:150:LEU:HD13	11:V:22:ALA:N	2.35	0.42
2:H:593:THR:O	2:H:597:VAL:HG23	2.19	0.42
14:H:825:CLA:C4B	14:H:833:CLA:HMA3	2.50	0.42
17:I:102:BCR:H351	17:I:102:BCR:H15C	1.70	0.42
1:a:148:ARG:NH2	1:a:228:ASP:OD1	2.53	0.42
1:a:325:LEU:HB2	1:a:345:TYR:HE1	1.84	0.42
2:b:129:MET:HE2	2:b:135:LEU:CD2	2.45	0.42
14:l:206:CLA:HAC2	17:l:208:BCR:H382	2.00	0.42
1:A:589:VAL:HG13	2:B:676:GLY:HA3	2.02	0.42
14:A:812:CLA:H193	14:A:812:CLA:H161	1.86	0.42
14:A:827:CLA:H93	14:A:827:CLA:H62	1.86	0.42
2:B:182:LEU:HD13	14:B:812:CLA:HHB	2.00	0.42
2:B:334:LEU:HD23	2:B:334:LEU:HA	1.83	0.42
2:B:663:VAL:HG22	14:B:840:CLA:HMB3	2.01	0.42
14:G:834:CLA:H41	14:G:843:CLA:HBC2	2.02	0.42
2:H:463:PHE:HB3	14:H:836:CLA:H42	2.01	0.42
4:O:43:PRO:HD3	4:O:68:LEU:HD12	2.02	0.42
1:a:196:MET:HE1	14:a:813:CLA:HMD2	2.01	0.42
1:a:577:PRO:HD2	5:e:48:PHE:HE2	1.83	0.42
2:b:652:VAL:HG11	14:b:808:CLA:HAC1	2.01	0.42
3:c:61:ASP:N	5:e:58:ASN:OD1	2.47	0.42
6:f:108:LEU:HA	6:f:108:LEU:HD23	1.71	0.42
1:A:267:PHE:N	1:A:275:TYR:OH	2.53	0.42
2:B:57:ILE:O	2:B:61:VAL:HG23	2.19	0.42
2:B:454:GLU:HA	6:F:71:LEU:HD22	2.02	0.42
14:B:825:CLA:HBA1	14:B:825:CLA:H3A	1.70	0.42
1:G:693:GLY:HA3	2:H:575:CYS:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:846:PQN:H243	15:G:846:PQN:H211	1.85	0.42
14:H:827:CLA:H202	14:H:827:CLA:H161	1.84	0.42
11:M:10:ILE:HD13	11:M:10:ILE:HA	1.87	0.42
10:U:20:THR:O	10:U:24:ASP:N	2.53	0.42
14:a:802:CLA:H142	14:a:802:CLA:H111	1.78	0.42
14:a:842:CLA:H3A	14:a:842:CLA:HBA2	1.74	0.42
14:a:842:CLA:H201	17:j:103:BCR:C10	2.50	0.42
2:b:195:ILE:HD11	2:b:255:LEU:HD21	2.02	0.42
14:b:801:CLA:H8	14:b:801:CLA:H122	1.66	0.42
14:b:816:CLA:C2D	14:b:825:CLA:HMB2	2.50	0.42
11:m:10:ILE:O	11:m:14:ILE:HG12	2.20	0.42
12:x:21:LEU:HD12	12:x:21:LEU:HA	1.88	0.42
14:A:802:CLA:H151	14:A:843:CLA:HAB	2.00	0.42
1:G:369:ILE:HG21	14:G:820:CLA:H191	2.01	0.42
1:G:665:TYR:HD2	2:H:448:VAL:HG12	1.85	0.42
14:G:809:CLA:H3A	14:G:809:CLA:HBA2	1.52	0.42
2:H:169:LYS:HA	2:H:331:ASN:HD21	1.84	0.42
2:H:180:ALA:HB2	2:H:288:GLY:HA3	2.02	0.42
2:H:533:GLY:HA2	2:H:589:TRP:HZ3	1.85	0.42
14:H:839:CLA:H111	14:H:839:CLA:H72	1.54	0.42
17:I:101:BCR:H15C	17:I:101:BCR:H351	1.79	0.42
5:P:2:VAL:HG21	5:P:24:VAL:HG21	2.02	0.42
6:Q:100:ILE:HG12	14:Q:203:CLA:C1D	2.49	0.42
7:R:20:TRP:HE1	14:U:201:CLA:C2B	2.33	0.42
2:b:115:ILE:O	14:b:808:CLA:HMD2	2.20	0.42
2:b:423:ILE:HD11	2:b:546:LEU:HB2	2.00	0.42
2:b:696:ASN:HD22	2:b:696:ASN:HA	1.59	0.42
6:f:69:ASP:OD1	6:f:69:ASP:N	2.52	0.42
10:l:29:LYS:HB2	10:l:29:LYS:HE2	1.78	0.42
1:A:184:ALA:HA	1:A:185:PRO:HD3	1.91	0.41
1:A:565:LEU:O	4:D:61:ARG:NH1	2.45	0.41
14:A:820:CLA:HAB	14:A:820:CLA:H8	2.01	0.41
2:B:53:HIS:CE1	14:B:805:CLA:HMA2	2.54	0.41
2:B:321:MET:HB2	2:B:323:HIS:HE1	1.84	0.41
14:B:813:CLA:HMB1	17:B:844:BCR:H23C	2.02	0.41
14:B:840:CLA:HBA2	15:B:841:PQN:H241	2.02	0.41
1:G:304:ILE:HD13	1:G:304:ILE:HA	1.82	0.41
14:H:817:CLA:H93	14:H:817:CLA:H61	1.89	0.41
14:H:821:CLA:HBA2	14:H:821:CLA:H3A	1.79	0.41
1:a:430:LEU:HD13	14:a:824:CLA:HBC1	2.00	0.41
14:a:833:CLA:HBA1	14:a:833:CLA:H3A	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:842:CLA:H91	14:a:842:CLA:H112	1.81	0.41
2:b:480:THR:HB	2:b:481:LEU:HD12	2.02	0.41
1:A:404:LEU:HD21	14:A:807:CLA:H142	2.00	0.41
1:A:726:GLN:HA	18:A:854:LHG:HC5	2.01	0.41
14:B:804:CLA:HBC1	19:B:849:LMG:H181	2.02	0.41
14:B:840:CLA:H91	14:B:840:CLA:H112	1.90	0.41
17:B:845:BCR:H15C	17:B:845:BCR:H351	1.66	0.41
3:C:18:VAL:HG22	3:C:26:LEU:HB2	2.02	0.41
1:G:211:GLY:HA2	14:G:816:CLA:HBB2	2.02	0.41
17:G:851:BCR:H15C	17:G:851:BCR:H351	1.78	0.41
2:H:61:VAL:HB	2:H:142:LEU:HD13	2.02	0.41
2:H:422:ILE:HA	14:H:829:CLA:CBB	2.48	0.41
1:a:710:LYS:HD3	14:b:830:CLA:HAA2	2.01	0.41
2:b:182:LEU:HD13	14:b:812:CLA:HHB	2.01	0.41
1:A:498:PRO:HG3	1:A:508:THR:HB	2.02	0.41
14:A:820:CLA:H143	14:A:828:CLA:H72	2.01	0.41
2:B:279:ALA:HA	14:B:815:CLA:HMC2	2.01	0.41
2:B:378:HIS:HB2	14:B:826:CLA:C1B	2.50	0.41
14:B:830:CLA:HAC2	17:F:1302:BCR:H362	2.01	0.41
17:B:847:BCR:H15C	17:B:847:BCR:H351	1.90	0.41
14:G:802:CLA:H151	14:G:842:CLA:HAB	2.03	0.41
14:G:816:CLA:C1B	17:G:848:BCR:HC42	2.50	0.41
14:G:829:CLA:H193	14:G:829:CLA:H161	1.88	0.41
14:G:836:CLA:CBB	14:G:838:CLA:HBA1	2.50	0.41
14:H:829:CLA:CBB	14:H:838:CLA:HBB2	2.47	0.41
17:L:202:BCR:H351	17:L:202:BCR:H15C	1.74	0.41
17:U:202:BCR:H341	14:U:206:CLA:HAC1	2.01	0.41
1:a:489:TRP:O	1:a:493:LEU:HG	2.20	0.41
14:a:810:CLA:HBA2	14:a:810:CLA:H3A	1.54	0.41
14:a:838:CLA:H61	14:a:838:CLA:H92	1.88	0.41
2:b:92:TRP:N	14:b:809:CLA:O1D	2.46	0.41
14:b:802:CLA:H91	17:l:208:BCR:H392	2.01	0.41
17:b:842:BCR:H351	17:b:842:BCR:H15C	1.72	0.41
6:f:88:ILE:HG23	14:j:102:CLA:HBB1	2.01	0.41
1:A:212:TRP:NE1	14:A:820:CLA:O1D	2.33	0.41
1:A:387:TYR:OH	1:A:524:VAL:O	2.33	0.41
1:A:423:ALA:HA	4:D:39:VAL:HG11	2.02	0.41
1:A:683:TRP:HZ3	14:B:801:CLA:HMD3	1.84	0.41
2:B:8:PHE:HB2	2:B:34:HIS:CG	2.56	0.41
2:B:56:ILE:HD11	17:M:1602:BCR:HC7	2.01	0.41
2:B:123:TRP:CH2	17:B:844:BCR:H292	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:580:TRP:NE1	19:B:849:LMG:O10	2.52	0.41
2:B:585:LEU:HD23	2:B:585:LEU:HA	1.88	0.41
1:G:711:LEU:HD23	1:G:711:LEU:HA	1.88	0.41
14:G:811:CLA:H3A	14:G:811:CLA:HBA2	1.65	0.41
2:H:195:ILE:HD12	2:H:254:ILE:HB	2.02	0.41
14:H:820:CLA:HBA2	17:H:842:BCR:H282	2.02	0.41
10:U:80:LEU:HD22	10:U:137:PHE:CD2	2.56	0.41
10:U:84:ILE:HG13	10:U:130:MET:SD	2.60	0.41
14:U:205:CLA:H111	14:U:205:CLA:H152	1.86	0.41
12:W:21:LEU:HD12	12:W:21:LEU:HA	1.93	0.41
1:a:602:MET:HE3	1:a:602:MET:HB3	1.82	0.41
1:a:683:TRP:CE3	13:a:801:CL0:H6	2.55	0.41
14:a:834:CLA:HBA2	14:l:202:CLA:OBD	2.21	0.41
17:a:850:BCR:H371	17:a:850:BCR:H24C	1.78	0.41
2:b:377:THR:HG23	2:b:598:THR:HG21	2.02	0.41
2:b:443:HIS:O	2:b:447:VAL:HB	2.20	0.41
2:b:688:ALA:O	2:b:692:THR:OG1	2.37	0.41
6:f:146:GLU:HB2	6:f:152:LEU:HB2	2.02	0.41
14:f:202:CLA:HMB1	8:j:28:LEU:HD21	2.03	0.41
14:i:101:CLA:H121	17:m:1602:BCR:C11	2.50	0.41
1:A:354:ALA:HB2	1:A:415:PHE:CD1	2.55	0.41
1:A:460:VAL:HA	1:A:463:ASP:OD2	2.20	0.41
13:A:801:CL0:H49	13:A:801:CL0:H41	1.85	0.41
14:A:802:CLA:H201	14:A:831:CLA:H201	2.03	0.41
14:A:822:CLA:HBC3	14:A:828:CLA:H18	2.02	0.41
14:B:817:CLA:H93	14:B:817:CLA:H61	1.86	0.41
14:B:832:CLA:H43	17:B:847:BCR:HC32	2.01	0.41
1:G:638:ASN:OD1	1:G:638:ASN:N	2.54	0.41
1:G:684:ALA:C	14:G:802:CLA:HAB	2.46	0.41
14:G:812:CLA:H193	14:G:812:CLA:H161	1.90	0.41
14:G:842:CLA:HBA1	18:G:854:LHG:H181	2.02	0.41
2:H:238:ASP:OD1	2:H:238:ASP:N	2.53	0.41
2:H:732:LEU:O	2:H:736:THR:OG1	2.31	0.41
14:H:801:CLA:H61	14:H:801:CLA:H41	1.45	0.41
8:J:30:GLU:HG3	14:J:101:CLA:C4B	2.50	0.41
1:a:314:MET:HE2	1:a:314:MET:HB3	1.93	0.41
14:a:828:CLA:H51	14:a:828:CLA:H8	1.82	0.41
14:a:855:CLA:H41	14:a:855:CLA:H61	1.46	0.41
2:b:295:PHE:CE1	14:b:811:CLA:HMA3	2.56	0.41
14:b:807:CLA:H111	14:b:807:CLA:H72	1.62	0.41
17:b:845:BCR:H351	17:b:845:BCR:H15C	1.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:8:PRO:HB3	10:l:13:PRO:HA	2.03	0.41
10:l:77:LEU:O	10:l:81:ILE:HG12	2.21	0.41
1:A:98:SER:HB2	1:A:144:PHE:HZ	1.85	0.41
1:A:729:ALA:HA	1:A:732:VAL:HG12	2.03	0.41
2:B:426:LEU:HG	14:B:838:CLA:CBB	2.51	0.41
2:B:691:ARG:HD2	10:L:17:HIS:CD2	2.55	0.41
14:B:813:CLA:H62	14:B:813:CLA:H2	1.91	0.41
14:B:839:CLA:H18	17:I:101:BCR:H362	2.01	0.41
4:D:30:ILE:HG21	4:D:68:LEU:HD23	2.02	0.41
1:G:20:PRO:HG2	1:G:184:ALA:HB3	2.03	0.41
1:G:300:HIS:HE2	14:G:820:CLA:C1B	2.33	0.41
1:G:577:PRO:HB3	1:G:724:ILE:HB	2.01	0.41
10:L:56:GLY:HA2	10:L:59:LEU:HD12	2.02	0.41
14:U:201:CLA:H112	14:U:201:CLA:H152	1.80	0.41
1:a:86:TRP:HA	14:a:807:CLA:HBB2	2.02	0.41
1:a:266:PRO:HB2	1:a:275:TYR:CZ	2.55	0.41
1:a:306:VAL:O	1:a:310:ILE:HG13	2.20	0.41
1:a:370:VAL:HG21	14:a:829:CLA:HHD	2.03	0.41
2:b:441:TYR:CZ	2:b:525:LEU:HB3	2.55	0.41
14:b:826:CLA:HBA2	14:b:826:CLA:H3A	1.82	0.41
10:l:64:VAL:HG23	10:l:79:GLY:HA3	2.01	0.41
1:A:290:GLY:N	1:A:520:VAL:HG21	2.36	0.41
14:A:810:CLA:H92	14:A:810:CLA:H62	1.80	0.41
14:A:837:CLA:HHC	14:A:837:CLA:HBB1	2.02	0.41
2:B:534:LEU:HD23	2:B:593:THR:HG21	2.03	0.41
2:B:686:VAL:HG11	3:C:81:TYR:CG	2.56	0.41
14:B:801:CLA:HED2	14:B:802:CLA:H71	2.02	0.41
5:E:8:VAL:O	5:E:21:ILE:HA	2.21	0.41
2:H:167:TRP:CE2	14:H:812:CLA:HAC2	2.56	0.41
2:H:659:PHE:O	2:H:663:VAL:HG23	2.21	0.41
7:I:30:LEU:HD23	7:I:30:LEU:HA	1.93	0.41
1:a:66:GLU:HA	1:a:187:LEU:HD13	2.02	0.41
2:b:46:ILE:HD12	14:b:806:CLA:C2C	2.49	0.41
17:b:847:BCR:H24C	17:b:847:BCR:H371	1.75	0.41
17:f:203:BCR:H371	17:f:203:BCR:H24C	1.75	0.41
1:A:94:GLY:HA3	1:A:147:TRP:CH2	2.56	0.41
1:A:171:LEU:HD12	1:A:171:LEU:HA	1.96	0.41
1:A:602:MET:HG2	14:A:827:CLA:HBC1	2.02	0.41
14:A:803:CLA:H142	14:A:803:CLA:H111	1.88	0.41
14:A:814:CLA:HBD	14:A:826:CLA:H52	2.03	0.41
14:A:841:CLA:HAA2	14:B:830:CLA:HMB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:THR:HG22	4:D:63:GLU:HB2	2.02	0.41
1:G:118:TRP:CE2	17:S:104:BCR:HC41	2.56	0.41
2:H:411:VAL:O	2:H:415:VAL:HG23	2.20	0.41
14:H:817:CLA:H3A	14:H:817:CLA:HBA2	1.70	0.41
6:Q:84:GLY:H	8:S:43:LEU:HD22	1.86	0.41
14:a:808:CLA:HBB2	14:a:828:CLA:H193	2.02	0.41
2:b:279:ALA:HB1	14:b:815:CLA:HBC2	2.03	0.41
2:b:357:TYR:HB2	2:b:601:TRP:HZ2	1.86	0.41
14:b:807:CLA:H72	14:b:807:CLA:H151	2.01	0.41
14:i:101:CLA:H202	14:i:101:CLA:H162	1.92	0.41
14:l:206:CLA:H202	14:l:206:CLA:H162	1.82	0.41
14:l:207:CLA:H143	14:l:207:CLA:H111	1.84	0.41
1:A:78:GLY:O	1:A:82:VAL:HG13	2.20	0.41
1:A:353:HIS:HD2	1:A:411:HIS:ND1	2.19	0.41
14:A:810:CLA:H93	14:A:810:CLA:H111	1.85	0.41
14:A:834:CLA:HBB1	14:A:835:CLA:H2	2.02	0.41
14:A:843:CLA:H91	14:A:843:CLA:H112	1.84	0.41
18:A:854:LHG:H161	18:A:854:LHG:H132	1.93	0.41
2:B:279:ALA:HB1	14:B:815:CLA:HBC2	2.03	0.41
2:B:505:LEU:HA	2:B:508:ILE:HG22	2.03	0.41
14:B:806:CLA:H72	14:B:806:CLA:H111	1.49	0.41
4:D:116:VAL:HG12	4:D:118:ARG:HG2	2.03	0.41
1:G:25:PHE:CD1	8:S:6:LEU:HG	2.56	0.41
1:G:374:MET:HE1	14:G:830:CLA:O1D	2.20	0.41
14:G:831:CLA:H18	14:G:842:CLA:HBA2	2.02	0.41
2:H:175:LEU:HD23	2:H:175:LEU:HA	1.94	0.41
2:H:391:PHE:HB3	2:H:541:LEU:HB3	2.02	0.41
2:H:434:GLY:HA2	2:H:532:LEU:HD22	2.03	0.41
14:H:806:CLA:C2B	14:H:806:CLA:H141	2.51	0.41
14:H:812:CLA:H172	17:H:843:BCR:H271	2.03	0.41
14:H:829:CLA:HMB1	14:H:830:CLA:C3D	2.51	0.41
8:J:10:LEU:HD12	8:J:15:VAL:HG11	2.03	0.41
7:R:10:LEU:HD12	7:R:10:LEU:HA	1.90	0.41
14:U:204:CLA:H2	14:U:204:CLA:H61	1.82	0.41
1:a:59:ASP:OD1	1:a:418:ARG:NH1	2.54	0.41
1:a:115:GLN:NE2	14:a:809:CLA:OBD	2.45	0.41
14:a:813:CLA:HBD	14:a:825:CLA:H52	2.03	0.41
14:a:828:CLA:H151	14:a:855:CLA:H18	2.03	0.41
14:a:830:CLA:H122	14:a:830:CLA:H162	1.86	0.41
14:a:832:CLA:HBC2	14:a:839:CLA:HMC2	2.02	0.41
14:a:840:CLA:H91	14:a:840:CLA:H112	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:851:BCR:HC32	17:a:851:BCR:H312	1.89	0.41
2:b:224:PRO:HB3	2:b:232:VAL:HB	2.02	0.41
2:b:461:PRO:HG3	2:b:524:PHE:HB2	2.02	0.41
2:b:523:ASP:OD2	2:b:604:LYS:HE2	2.21	0.41
2:b:606:LEU:HD23	2:b:606:LEU:HA	1.92	0.41
2:b:634:ASN:HB3	2:b:735:SER:HB2	2.02	0.41
1:A:529:ILE:HD13	1:A:617:MET:HE1	2.01	0.41
14:A:843:CLA:H62	14:A:843:CLA:H41	1.67	0.41
17:A:853:BCR:H15C	17:A:853:BCR:H351	1.82	0.41
1:G:518:VAL:HB	1:G:525:ALA:HB3	2.03	0.41
14:G:841:CLA:H91	14:G:841:CLA:H112	1.93	0.41
2:H:387:MET:HE1	17:H:846:BCR:H361	2.03	0.41
2:H:531:ALA:HA	14:H:838:CLA:HED3	2.02	0.41
14:H:812:CLA:H142	14:H:812:CLA:H112	1.77	0.41
10:L:112:LEU:HD23	10:L:112:LEU:HA	1.90	0.41
17:S:103:BCR:H351	17:S:103:BCR:H15C	1.69	0.41
10:U:36:PRO:HG3	14:U:205:CLA:HED2	2.03	0.41
1:a:161:THR:HG22	17:a:848:BCR:HC32	2.03	0.41
14:a:808:CLA:HBA2	14:a:808:CLA:H3A	1.56	0.41
2:b:603:TRP:HZ2	2:b:629:ASP:HB2	1.86	0.41
2:b:690:GLU:C	2:b:696:ASN:HD21	2.28	0.41
14:b:808:CLA:HAB	14:b:809:CLA:CAA	2.50	0.41
14:b:832:CLA:H2A	14:b:832:CLA:HED2	2.03	0.41
14:b:832:CLA:H61	14:b:832:CLA:H41	1.68	0.41
3:c:56:THR:HG21	5:e:48:PHE:HD1	1.86	0.41
17:f:201:BCR:C11	14:f:202:CLA:HAB	2.51	0.41
7:i:10:LEU:HD23	7:i:10:LEU:HA	1.92	0.41
14:A:827:CLA:HAB	17:A:852:BCR:H311	2.01	0.40
2:B:411:VAL:O	2:B:415:VAL:HG23	2.22	0.40
15:B:841:PQN:H292	17:I:102:BCR:HC7	2.03	0.40
1:G:541:ILE:HG21	13:G:801:CL0:H60	2.02	0.40
14:H:807:CLA:H2	14:H:807:CLA:H62	1.77	0.40
7:I:29:LEU:HA	7:I:29:LEU:HD23	1.88	0.40
10:L:131:GLY:C	17:L:207:BCR:H23C	2.45	0.40
1:a:290:GLY:N	1:a:520:VAL:HG21	2.36	0.40
1:a:575:ARG:HG3	1:a:592:TRP:CD1	2.56	0.40
2:b:476:TYR:O	6:f:27:GLY:N	2.55	0.40
14:b:816:CLA:H93	14:b:816:CLA:H61	1.84	0.40
1:A:292:LEU:HB2	1:A:379:PRO:HA	2.03	0.40
14:A:835:CLA:HBA2	14:L:201:CLA:OBD	2.21	0.40
2:B:31:PHE:HB3	2:B:37:MET:HE3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:TRP:HH2	14:B:834:CLA:H2A	1.86	0.40
6:F:120:LYS:NZ	6:F:125:ASP:OD1	2.50	0.40
1:G:213:ALA:O	1:G:217:ILE:HG12	2.21	0.40
1:G:386:ASP:OD1	1:G:389:THR:OG1	2.29	0.40
13:G:801:CL0:H10	13:G:801:CL0:H72	1.81	0.40
14:G:841:CLA:H92	14:G:841:CLA:H61	1.95	0.40
10:L:143:PHE:HD1	14:L:206:CLA:H12	1.86	0.40
6:Q:69:ASP:OD1	6:Q:71:LEU:HB2	2.20	0.40
2:b:707:LEU:HD22	2:b:711:GLN:NE2	2.37	0.40
10:l:64:VAL:HG11	10:l:140:LEU:HD13	2.04	0.40
1:A:107:PRO:HB3	1:A:382:TYR:CD1	2.57	0.40
1:A:356:LEU:HD11	14:A:831:CLA:HBB1	2.03	0.40
1:A:538:VAL:HG21	1:A:612:HIS:CD2	2.56	0.40
1:A:577:PRO:HB3	1:A:724:ILE:HB	2.03	0.40
14:A:810:CLA:H151	14:A:812:CLA:H13	2.03	0.40
2:B:237:PRO:HB2	2:B:258:LEU:HD11	2.02	0.40
2:B:365:ILE:HG12	2:B:372:MET:HE3	2.04	0.40
2:B:599:PHE:HE2	14:B:802:CLA:H62	1.86	0.40
14:B:802:CLA:H3A	14:B:802:CLA:HBA2	1.85	0.40
14:B:828:CLA:H143	14:B:828:CLA:H111	1.88	0.40
14:G:845:CLA:HED1	10:U:5:LEU:HD11	2.03	0.40
2:H:4:LYS:HE2	2:H:4:LYS:HB2	1.73	0.40
2:H:57:ILE:O	2:H:61:VAL:HG23	2.21	0.40
2:H:298:GLY:HA2	14:H:820:CLA:HMD2	2.04	0.40
2:H:596:TRP:CG	14:H:802:CLA:H152	2.57	0.40
17:I:101:BCR:H371	17:I:101:BCR:H24C	1.70	0.40
1:a:662:ILE:HD12	2:b:628:ARG:HG3	2.02	0.40
13:a:801:CL0:H21	2:b:632:TRP:HD1	1.86	0.40
14:b:803:CLA:H62	14:b:803:CLA:H102	1.61	0.40
6:f:98:GLY:HA3	6:f:139:TRP:CE2	2.56	0.40
1:A:306:VAL:O	1:A:310:ILE:HG13	2.22	0.40
15:A:846:PQN:H243	15:A:846:PQN:H211	1.96	0.40
2:B:345:LEU:O	2:B:349:THR:OG1	2.30	0.40
2:B:659:PHE:O	2:B:663:VAL:HG23	2.21	0.40
1:G:481:GLN:HE21	1:G:481:GLN:HB3	1.74	0.40
2:H:305:MET:HE3	14:H:822:CLA:O1D	2.22	0.40
2:H:378:HIS:HB2	14:H:826:CLA:C1B	2.52	0.40
14:H:805:CLA:H142	14:H:805:CLA:H111	1.85	0.40
1:a:304:ILE:HD13	1:a:304:ILE:HA	1.82	0.40
1:a:371:ALA:HB2	1:a:397:HIS:HB2	2.02	0.40
1:a:608:VAL:HG21	13:a:801:CL0:H64	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:824:CLA:HAB	14:a:831:CLA:HMD2	2.04	0.40
14:a:826:CLA:H91	14:a:826:CLA:H111	1.77	0.40
2:b:20:ARG:NH2	2:b:702:ASP:OD1	2.54	0.40
2:b:656:MET:HE3	2:b:656:MET:HB2	1.87	0.40
14:b:824:CLA:CHB	14:b:838:CLA:HAA2	2.51	0.40
17:b:847:BCR:H342	17:b:847:BCR:HC7	1.93	0.40
14:A:829:CLA:H62	14:A:829:CLA:H101	1.80	0.40
2:B:74:PHE:CG	2:B:135:LEU:HD11	2.57	0.40
4:D:99:ASP:OD1	4:D:99:ASP:N	2.53	0.40
2:H:303:GLU:N	2:H:303:GLU:OE2	2.55	0.40
2:H:425:HIS:HB2	14:H:829:CLA:CBB	2.52	0.40
17:L:207:BCR:H393	10:l:130:MET:HB3	2.03	0.40
3:N:61:ASP:HA	3:N:62:PHE:HA	1.94	0.40
8:S:35:TYR:HA	8:S:36:PRO:HD3	1.85	0.40
1:a:86:TRP:O	1:a:90:MET:HG2	2.22	0.40
1:a:197:LEU:HB3	1:a:315:TYR:CE2	2.56	0.40
2:b:174:ARG:HB2	14:b:812:CLA:HBC2	2.04	0.40
2:b:175:LEU:HD12	2:b:175:LEU:HA	1.82	0.40
3:c:26:LEU:HA	3:c:41:SER:O	2.21	0.40
17:j:104:BCR:H351	17:j:104:BCR:H15C	1.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	738/755 (98%)	707 (96%)	29 (4%)	2 (0%)	37	45
1	G	738/755 (98%)	708 (96%)	28 (4%)	2 (0%)	37	45
1	a	738/755 (98%)	704 (95%)	32 (4%)	2 (0%)	37	45
2	B	737/741 (100%)	701 (95%)	34 (5%)	2 (0%)	37	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	737/741 (100%)	699 (95%)	36 (5%)	2 (0%)	37	45
2	b	737/741 (100%)	698 (95%)	37 (5%)	2 (0%)	37	45
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	N	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	c	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
4	D	136/139 (98%)	123 (90%)	13 (10%)	0	100	100
4	O	136/139 (98%)	123 (90%)	13 (10%)	0	100	100
4	d	136/139 (98%)	124 (91%)	12 (9%)	0	100	100
5	E	67/75 (89%)	65 (97%)	2 (3%)	0	100	100
5	P	67/75 (89%)	64 (96%)	3 (4%)	0	100	100
5	e	67/75 (89%)	63 (94%)	4 (6%)	0	100	100
6	F	139/164 (85%)	126 (91%)	12 (9%)	1 (1%)	19	22
6	Q	139/164 (85%)	125 (90%)	13 (9%)	1 (1%)	19	22
6	f	139/164 (85%)	124 (89%)	14 (10%)	1 (1%)	19	22
7	I	37/40 (92%)	33 (89%)	4 (11%)	0	100	100
7	R	37/40 (92%)	35 (95%)	2 (5%)	0	100	100
7	i	37/40 (92%)	37 (100%)	0	0	100	100
8	J	41/43 (95%)	35 (85%)	6 (15%)	0	100	100
8	S	41/43 (95%)	35 (85%)	6 (15%)	0	100	100
8	j	41/43 (95%)	35 (85%)	6 (15%)	0	100	100
9	K	59/83 (71%)	54 (92%)	5 (8%)	0	100	100
9	T	59/83 (71%)	55 (93%)	4 (7%)	0	100	100
9	k	59/83 (71%)	54 (92%)	5 (8%)	0	100	100
10	L	150/155 (97%)	146 (97%)	4 (3%)	0	100	100
10	U	150/155 (97%)	144 (96%)	6 (4%)	0	100	100
10	l	150/155 (97%)	145 (97%)	5 (3%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	V	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
12	W	25/36 (69%)	24 (96%)	1 (4%)	0	100	100
12	X	25/36 (69%)	24 (96%)	1 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	x	25/36 (69%)	24 (96%)	1 (4%)	0	100	100
All	All	6708/7029 (95%)	6344 (95%)	349 (5%)	15 (0%)	45	53

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	ALA
2	B	315	VAL
1	G	233	ALA
1	G	497	ALA
2	H	315	VAL
1	a	497	ALA
2	b	315	VAL
1	A	233	ALA
2	B	499	VAL
6	Q	53	SER
2	b	499	VAL
6	F	53	SER
1	a	233	ALA
2	H	499	VAL
6	f	53	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	588/603 (98%)	573 (97%)	15 (3%)	41	56
1	G	588/603 (98%)	570 (97%)	18 (3%)	35	49
1	a	588/603 (98%)	569 (97%)	19 (3%)	34	47
2	B	599/600 (100%)	572 (96%)	27 (4%)	23	32
2	H	599/600 (100%)	580 (97%)	19 (3%)	34	47
2	b	599/600 (100%)	570 (95%)	29 (5%)	21	29
3	C	67/68 (98%)	67 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	67/68 (98%)	67 (100%)	0	100	100
3	c	67/68 (98%)	66 (98%)	1 (2%)	60	74
4	D	115/116 (99%)	114 (99%)	1 (1%)	75	86
4	O	115/116 (99%)	113 (98%)	2 (2%)	56	70
4	d	115/116 (99%)	111 (96%)	4 (4%)	31	43
5	E	58/63 (92%)	53 (91%)	5 (9%)	8	10
5	P	58/63 (92%)	55 (95%)	3 (5%)	19	26
5	e	58/63 (92%)	56 (97%)	2 (3%)	32	45
6	F	109/128 (85%)	106 (97%)	3 (3%)	38	52
6	Q	109/128 (85%)	102 (94%)	7 (6%)	14	18
6	f	109/128 (85%)	105 (96%)	4 (4%)	29	41
7	I	33/33 (100%)	32 (97%)	1 (3%)	36	50
7	R	33/33 (100%)	32 (97%)	1 (3%)	36	50
7	i	33/33 (100%)	32 (97%)	1 (3%)	36	50
8	J	38/38 (100%)	34 (90%)	4 (10%)	5	5
8	S	38/38 (100%)	36 (95%)	2 (5%)	19	25
8	j	38/38 (100%)	37 (97%)	1 (3%)	41	56
10	L	115/117 (98%)	111 (96%)	4 (4%)	31	43
10	U	115/117 (98%)	111 (96%)	4 (4%)	31	43
10	l	115/117 (98%)	114 (99%)	1 (1%)	75	86
11	M	25/25 (100%)	23 (92%)	2 (8%)	10	11
11	V	25/25 (100%)	20 (80%)	5 (20%)	1	1
11	m	25/25 (100%)	22 (88%)	3 (12%)	4	4
12	W	22/29 (76%)	19 (86%)	3 (14%)	3	2
12	X	22/29 (76%)	20 (91%)	2 (9%)	7	8
12	x	22/29 (76%)	22 (100%)	0	100	100
All	All	5307/5460 (97%)	5114 (96%)	193 (4%)	32	42

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	45	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	74	SER
1	A	104	LEU
1	A	108	THR
1	A	130	VAL
1	A	146	LEU
1	A	221	LEU
1	A	252	LEU
1	A	288	VAL
1	A	377	MET
1	A	417	VAL
1	A	619	SER
1	A	628	ASP
1	A	686	SER
2	B	42	LEU
2	B	110	SER
2	B	118	SER
2	B	144	VAL
2	B	157	LEU
2	B	195	ILE
2	B	202	SER
2	B	222	LEU
2	B	225	PHE
2	B	227	THR
2	B	246	THR
2	B	265	THR
2	B	300	SER
2	B	303	GLU
2	B	338	LEU
2	B	350	SER
2	B	480	THR
2	B	483	SER
2	B	491	THR
2	B	552	LYS
2	B	608	VAL
2	B	613	VAL
2	B	648	ASN
2	B	652	VAL
2	B	698	VAL
2	B	701	LYS
2	B	702	ASP
4	D	120	ILE
5	E	6	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	11	LEU
5	E	14	GLU
5	E	26	SER
5	E	55	VAL
6	F	97	THR
6	F	120	LYS
6	F	146	GLU
1	G	37	THR
1	G	62	THR
1	G	65	LEU
1	G	87	LEU
1	G	108	THR
1	G	117	VAL
1	G	120	ILE
1	G	130	VAL
1	G	146	LEU
1	G	193	VAL
1	G	240	HIS
1	G	324	SER
1	G	383	LEU
1	G	447	VAL
1	G	478	THR
1	G	587	CYS
1	G	704	ILE
1	G	705	VAL
2	H	140	ILE
2	H	210	ASP
2	H	238	ASP
2	H	241	SER
2	H	280	ILE
2	H	300	SER
2	H	338	LEU
2	H	399	VAL
2	H	452	THR
2	H	480	THR
2	H	488	ILE
2	H	499	VAL
2	H	510	SER
2	H	613	VAL
2	H	639	ILE
2	H	647	THR
2	H	648	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	698	VAL
2	H	736	THR
7	I	8	SER
8	J	7	LEU
8	J	27	ILE
8	J	35	TYR
8	J	43	LEU
10	L	23	SER
10	L	60	ILE
10	L	71	ASP
10	L	85	THR
11	M	3	LEU
11	M	17	LEU
4	O	7	GLN
4	O	120	ILE
5	P	4	ARG
5	P	27	VAL
5	P	57	THR
6	Q	25	VAL
6	Q	34	SER
6	Q	69	ASP
6	Q	75	VAL
6	Q	97	THR
6	Q	130	ILE
6	Q	134	LEU
7	R	10	LEU
8	S	6	LEU
8	S	33	ARG
10	U	5	LEU
10	U	19	SER
10	U	42	LEU
10	U	71	ASP
11	V	1	MET
11	V	4	THR
11	V	17	LEU
11	V	20	VAL
11	V	21	LEU
12	W	18	VAL
12	W	19	LEU
12	W	26	LEU
12	X	13	ARG
12	X	35	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	45	THR
1	a	51	LEU
1	a	117	VAL
1	a	240	HIS
1	a	279	LEU
1	a	289	THR
1	a	304	ILE
1	a	325	LEU
1	a	347	VAL
1	a	366	LEU
1	a	383	LEU
1	a	392	SER
1	a	404	LEU
1	a	433	VAL
1	a	508	THR
1	a	511	VAL
1	a	625	VAL
1	a	705	VAL
1	a	710	LYS
2	b	82	LEU
2	b	111	SER
2	b	134	ASP
2	b	160	LYS
2	b	166	SER
2	b	202	SER
2	b	225	PHE
2	b	227	THR
2	b	256	THR
2	b	258	LEU
2	b	280	ILE
2	b	305	MET
2	b	313	THR
2	b	319	PHE
2	b	338	LEU
2	b	447	VAL
2	b	474	LEU
2	b	481	LEU
2	b	499	VAL
2	b	514	SER
2	b	519	ILE
2	b	542	VAL
2	b	590	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	608	VAL
2	b	618	GLU
2	b	648	ASN
2	b	652	VAL
2	b	669	MET
2	b	735	SER
3	c	65	ILE
4	d	4	LEU
4	d	5	THR
4	d	59	LEU
4	d	92	THR
5	e	51	SER
5	e	63	SER
6	f	25	VAL
6	f	68	GLU
6	f	159	ILE
6	f	164	ARG
7	i	18	VAL
8	j	3	THR
10	l	112	LEU
11	m	3	LEU
11	m	12	LEU
11	m	17	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	43	GLN
1	A	79	HIS
1	A	123	GLN
1	A	192	ASN
1	A	224	ASN
1	A	301	HIS
1	A	318	ASN
1	A	353	HIS
1	A	372	GLN
1	A	462	ASN
1	A	481	GLN
1	A	542	HIS
1	A	571	ASN
1	A	647	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	14	GLN
2	B	41	ASN
2	B	79	GLN
2	B	176	ASN
2	B	205	GLN
2	B	262	HIS
2	B	320	ASN
2	B	324	GLN
2	B	354	GLN
2	B	367	GLN
2	B	369	HIS
2	B	407	ASN
2	B	592	ASN
2	B	615	GLN
2	B	640	ASN
2	B	679	GLN
4	D	64	GLN
4	D	72	GLN
4	D	107	ASN
4	D	125	ASN
4	D	128	GLN
5	E	19	ASN
5	E	44	ASN
6	F	63	GLN
1	G	79	HIS
1	G	154	ASN
1	G	225	GLN
1	G	318	ASN
1	G	353	HIS
1	G	359	ASN
1	G	390	GLN
1	G	445	ASN
1	G	462	ASN
1	G	481	GLN
1	G	492	HIS
1	G	542	HIS
1	G	647	ASN
1	G	718	GLN
2	H	10	GLN
2	H	83	ASN
2	H	95	GLN
2	H	137	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	262	HIS
2	H	289	HIS
2	H	341	HIS
2	H	354	GLN
2	H	369	HIS
2	H	407	ASN
2	H	417	GLN
2	H	468	GLN
2	H	634	ASN
2	H	679	GLN
2	H	689	HIS
8	J	5	HIS
8	J	32	ASN
11	M	7	GLN
4	O	72	GLN
4	O	107	ASN
8	S	2	GLN
10	U	10	ASN
10	U	17	HIS
10	U	103	GLN
11	V	7	GLN
12	W	24	ASN
1	a	43	GLN
1	a	79	HIS
1	a	115	GLN
1	a	157	GLN
1	a	192	ASN
1	a	200	HIS
1	a	225	GLN
1	a	271	ASN
1	a	318	ASN
1	a	353	HIS
1	a	359	ASN
1	a	426	GLN
1	a	462	ASN
1	a	481	GLN
1	a	542	HIS
1	a	571	ASN
1	a	647	ASN
1	a	660	GLN
1	a	718	GLN
2	b	41	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	79	GLN
2	b	95	GLN
2	b	176	ASN
2	b	177	HIS
2	b	229	ASN
2	b	235	GLN
2	b	262	HIS
2	b	289	HIS
2	b	294	GLN
2	b	337	GLN
2	b	354	GLN
2	b	407	ASN
2	b	498	ASN
2	b	617	ASN
2	b	679	GLN
2	b	696	ASN
2	b	711	GLN
4	d	107	ASN
4	d	114	ASN
5	e	19	ASN
5	e	44	ASN
6	f	63	GLN
6	f	113	ASN
8	j	5	HIS
10	l	10	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 381 ligands modelled in this entry, 3 are monoatomic - leaving 378 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$
17	BCR	S	104	-	41,41,41	2.72	6 (14%)	56,56,56	6.88	20 (35%)
14	CLA	a	812	-	48,58,73	2.65	21 (43%)	56,95,113	2.77	22 (39%)
14	CLA	b	810	-	43,53,73	2.72	19 (44%)	50,89,113	2.83	21 (42%)
14	CLA	U	204	10	58,68,73	2.39	20 (34%)	68,107,113	2.61	21 (30%)
14	CLA	B	823	2	48,58,73	2.62	18 (37%)	56,95,113	2.72	22 (39%)
14	CLA	b	804	-	63,73,73	2.24	20 (31%)	74,113,113	2.49	26 (35%)
17	BCR	b	847	-	41,41,41	2.67	6 (14%)	56,56,56	6.78	18 (32%)
14	CLA	j	101	-	43,53,73	2.67	20 (46%)	50,89,113	2.95	24 (48%)
14	CLA	a	822	-	43,53,73	2.66	18 (41%)	50,89,113	2.85	20 (40%)
14	CLA	H	817	-	58,68,73	2.37	21 (36%)	68,107,113	2.57	25 (36%)
17	BCR	B	842	-	41,41,41	2.67	6 (14%)	56,56,56	6.60	18 (32%)
14	CLA	b	821	-	53,63,73	2.51	21 (39%)	62,101,113	2.66	27 (43%)
14	CLA	A	820	-	63,73,73	2.30	21 (33%)	74,113,113	2.44	28 (37%)
14	CLA	A	807	-	63,73,73	2.26	19 (30%)	74,113,113	2.50	24 (32%)
17	BCR	b	846	-	41,41,41	2.69	6 (14%)	56,56,56	6.59	23 (41%)
19	LMG	H	848	-	49,49,55	1.40	6 (12%)	57,57,63	1.05	3 (5%)
14	CLA	X	1701	12	43,53,73	2.65	20 (46%)	50,89,113	2.83	20 (40%)
14	CLA	G	844	-	39,49,73	2.62	17 (43%)	46,83,113	2.86	22 (47%)
14	CLA	G	820	-	63,73,73	2.32	21 (33%)	74,113,113	2.57	27 (36%)
14	CLA	H	840	-	63,73,73	2.22	20 (31%)	74,113,113	2.59	25 (33%)
14	CLA	U	201	2	63,73,73	2.26	21 (33%)	74,113,113	2.62	28 (37%)
15	PQN	B	841	-	34,34,34	1.59	2 (5%)	43,45,45	1.15	5 (11%)
14	CLA	b	817	-	58,68,73	2.36	20 (34%)	68,107,113	2.57	23 (33%)
17	BCR	B	846	-	41,41,41	2.73	6 (14%)	56,56,56	6.59	24 (42%)
14	CLA	H	832	-	53,63,73	2.53	22 (41%)	62,101,113	2.77	24 (38%)
14	CLA	H	828	-	63,73,73	2.32	20 (31%)	74,113,113	2.53	26 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	H	830	-	43,53,73	2.67	20 (46%)	50,89,113	2.80	22 (44%)
14	CLA	Q	203	-	43,53,73	2.66	18 (41%)	50,89,113	2.60	19 (38%)
18	LHG	A	855	14	26,26,48	1.26	2 (7%)	29,32,54	1.19	2 (6%)
14	CLA	b	818	-	63,73,73	2.33	20 (31%)	74,113,113	2.49	25 (33%)
14	CLA	a	825	-	63,73,73	2.35	20 (31%)	74,113,113	2.31	27 (36%)
14	CLA	m	1601	-	43,53,73	2.66	20 (46%)	50,89,113	2.92	23 (46%)
14	CLA	b	807	-	63,73,73	2.27	19 (30%)	74,113,113	2.50	23 (31%)
14	CLA	a	827	-	63,73,73	2.23	19 (30%)	74,113,113	2.71	27 (36%)
14	CLA	H	808	-	63,73,73	2.26	18 (28%)	74,113,113	2.49	24 (32%)
14	CLA	B	839	-	63,73,73	2.27	20 (31%)	74,113,113	2.40	24 (32%)
14	CLA	A	837	1	43,53,73	2.67	19 (44%)	50,89,113	2.78	21 (42%)
17	BCR	R	102	-	41,41,41	2.75	6 (14%)	56,56,56	6.53	25 (44%)
14	CLA	b	824	-	43,53,73	2.69	19 (44%)	50,89,113	2.74	19 (38%)
14	CLA	G	810	1	63,73,73	2.29	19 (30%)	74,113,113	2.48	25 (33%)
14	CLA	H	818	-	63,73,73	2.27	21 (33%)	74,113,113	2.50	24 (32%)
14	CLA	a	802	-	63,73,73	2.26	18 (28%)	74,113,113	2.35	24 (32%)
14	CLA	G	813	-	48,58,73	2.63	20 (41%)	56,95,113	2.76	24 (42%)
14	CLA	b	806	-	63,73,73	2.30	20 (31%)	74,113,113	2.56	28 (37%)
14	CLA	j	102	-	35,45,73	2.80	18 (51%)	42,78,113	2.85	19 (45%)
14	CLA	B	806	-	63,73,73	2.24	19 (30%)	74,113,113	2.54	24 (32%)
14	CLA	G	837	1	43,53,73	2.66	20 (46%)	50,89,113	2.87	21 (42%)
14	CLA	b	836	-	58,68,73	2.43	20 (34%)	68,107,113	2.50	24 (35%)
14	CLA	A	804	-	53,63,73	2.49	20 (37%)	62,101,113	2.71	25 (40%)
14	CLA	b	829	-	43,53,73	2.57	18 (41%)	50,89,113	2.97	24 (48%)
14	CLA	a	833	-	63,73,73	2.29	20 (31%)	74,113,113	2.43	22 (29%)
15	PQN	A	846	-	34,34,34	1.63	2 (5%)	43,45,45	1.27	5 (11%)
14	CLA	a	834	-	63,73,73	2.27	19 (30%)	74,113,113	2.44	22 (29%)
14	CLA	L	205	-	63,73,73	2.28	19 (30%)	74,113,113	2.54	25 (33%)
14	CLA	F	1303	-	35,45,73	2.77	18 (51%)	42,78,113	2.84	18 (42%)
14	CLA	H	833	-	43,53,73	2.66	19 (44%)	50,89,113	2.76	21 (42%)
14	CLA	G	804	-	53,63,73	2.50	20 (37%)	62,101,113	2.72	26 (41%)
18	LHG	a	853	-	48,48,48	0.91	2 (4%)	51,54,54	1.12	3 (5%)
14	CLA	G	841	-	63,73,73	2.29	21 (33%)	74,113,113	2.49	25 (33%)
14	CLA	B	834	-	43,53,73	2.64	19 (44%)	50,89,113	2.78	20 (40%)
17	BCR	M	1602	-	41,41,41	2.57	6 (14%)	56,56,56	6.73	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	a	849	-	41,41,41	2.70	6 (14%)	56,56,56	6.56	23 (41%)
14	CLA	G	827	-	58,68,73	2.39	20 (34%)	68,107,113	2.58	26 (38%)
17	BCR	b	844	-	41,41,41	2.61	6 (14%)	56,56,56	6.63	22 (39%)
14	CLA	B	815	-	43,53,73	2.68	18 (41%)	50,89,113	2.88	21 (42%)
14	CLA	G	821	-	48,58,73	2.61	19 (39%)	56,95,113	2.94	26 (46%)
14	CLA	A	805	14	53,63,73	2.50	21 (39%)	62,101,113	2.81	26 (41%)
14	CLA	b	815	-	43,53,73	2.63	19 (44%)	50,89,113	2.84	21 (42%)
14	CLA	a	809	-	63,73,73	2.29	18 (28%)	74,113,113	2.47	26 (35%)
14	CLA	B	831	-	63,73,73	2.31	20 (31%)	74,113,113	2.51	25 (33%)
14	CLA	G	809	1	63,73,73	2.27	20 (31%)	74,113,113	2.57	27 (36%)
14	CLA	G	843	-	63,73,73	2.26	19 (30%)	74,113,113	2.37	24 (32%)
14	CLA	b	805	-	52,62,73	2.55	21 (40%)	60,99,113	2.80	24 (40%)
14	CLA	a	855	-	63,73,73	2.30	19 (30%)	74,113,113	2.40	25 (33%)
14	CLA	a	838	-	63,73,73	2.28	20 (31%)	74,113,113	2.49	27 (36%)
14	CLA	a	824	-	53,63,73	2.50	20 (37%)	62,101,113	2.68	24 (38%)
14	CLA	A	839	-	63,73,73	2.25	21 (33%)	74,113,113	2.51	28 (37%)
17	BCR	B	847	-	41,41,41	2.69	6 (14%)	56,56,56	6.65	24 (42%)
17	BCR	V	1602	-	41,41,41	2.58	6 (14%)	56,56,56	6.72	20 (35%)
14	CLA	B	804	-	52,62,73	2.54	21 (40%)	60,99,113	2.81	24 (40%)
14	CLA	H	822	-	43,53,73	2.61	17 (39%)	50,89,113	2.83	21 (42%)
19	LMG	b	848	-	49,49,55	1.40	6 (12%)	57,57,63	1.06	4 (7%)
14	CLA	A	810	1	63,73,73	2.28	19 (30%)	74,113,113	2.48	25 (33%)
14	CLA	G	822	-	63,73,73	2.29	20 (31%)	74,113,113	2.42	26 (35%)
14	CLA	a	810	-	43,53,73	2.69	19 (44%)	50,89,113	2.77	21 (42%)
14	CLA	A	816	-	43,53,73	2.68	20 (46%)	50,89,113	2.84	21 (42%)
14	CLA	a	826	-	58,68,73	2.33	19 (32%)	68,107,113	2.70	25 (36%)
14	CLA	S	101	8	43,53,73	2.67	20 (46%)	50,89,113	2.82	22 (44%)
17	BCR	G	851	-	41,41,41	2.73	6 (14%)	56,56,56	6.71	22 (39%)
14	CLA	G	803	-	63,73,73	2.25	17 (26%)	74,113,113	2.35	25 (33%)
17	BCR	a	851	-	41,41,41	2.67	6 (14%)	56,56,56	6.61	22 (39%)
14	CLA	a	807	-	43,53,73	2.66	19 (44%)	50,89,113	2.81	21 (42%)
14	CLA	A	823	-	43,53,73	2.67	19 (44%)	50,89,113	2.91	20 (40%)
14	CLA	A	825	-	53,63,73	2.48	20 (37%)	62,101,113	2.71	24 (38%)
14	CLA	A	841	-	63,73,73	2.33	20 (31%)	74,113,113	2.51	23 (31%)
14	CLA	H	823	2	48,58,73	2.62	18 (37%)	56,95,113	2.68	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	H	825	-	63,73,73	2.27	19 (30%)	74,113,113	2.53	26 (35%)
14	CLA	b	839	-	63,73,73	2.26	20 (31%)	74,113,113	2.48	26 (35%)
14	CLA	a	811	14	63,73,73	2.26	21 (33%)	74,113,113	2.54	22 (29%)
14	CLA	G	840	-	43,53,73	2.62	19 (44%)	50,89,113	2.78	19 (38%)
14	CLA	B	818	-	63,73,73	2.28	21 (33%)	74,113,113	2.49	24 (32%)
14	CLA	B	835	-	43,53,73	2.66	19 (44%)	50,89,113	2.83	21 (42%)
14	CLA	G	807	-	63,73,73	2.27	19 (30%)	74,113,113	2.53	23 (31%)
16	SF4	a	846	2,1	0,12,12	-	-	-	-	-
14	CLA	a	823	-	43,53,73	2.65	19 (44%)	50,89,113	2.89	21 (42%)
17	BCR	G	853	-	41,41,41	2.69	6 (14%)	56,56,56	6.81	25 (44%)
14	CLA	A	815	-	43,53,73	2.65	20 (46%)	50,89,113	2.90	22 (44%)
14	CLA	T	1401	-	43,53,73	2.69	20 (46%)	50,89,113	2.74	23 (46%)
14	CLA	G	811	-	43,53,73	2.66	20 (46%)	50,89,113	2.98	22 (44%)
15	PQN	a	845	-	34,34,34	1.61	2 (5%)	43,45,45	1.26	5 (11%)
14	CLA	A	835	-	63,73,73	2.24	18 (28%)	74,113,113	2.42	21 (28%)
14	CLA	M	1601	-	43,53,73	2.64	19 (44%)	50,89,113	2.91	20 (40%)
14	CLA	H	805	-	63,73,73	2.29	18 (28%)	74,113,113	2.51	25 (33%)
15	PQN	G	846	-	34,34,34	1.59	2 (5%)	43,45,45	1.19	4 (9%)
14	CLA	H	804	-	52,62,73	2.56	21 (40%)	60,99,113	2.76	25 (41%)
14	CLA	a	816	-	43,53,73	2.65	20 (46%)	50,89,113	2.78	21 (42%)
17	BCR	a	847	-	41,41,41	2.66	6 (14%)	56,56,56	6.63	19 (33%)
14	CLA	G	802	-	63,73,73	2.23	18 (28%)	74,113,113	2.52	23 (31%)
15	PQN	H	841	-	34,34,34	1.59	2 (5%)	43,45,45	1.11	3 (6%)
14	CLA	B	830	-	43,53,73	2.68	19 (44%)	50,89,113	2.82	24 (48%)
14	CLA	a	832	-	53,63,73	2.55	20 (37%)	62,101,113	2.68	25 (40%)
17	BCR	R	103	-	41,41,41	2.60	6 (14%)	56,56,56	6.59	20 (35%)
14	CLA	A	824	-	43,53,73	2.68	19 (44%)	50,89,113	2.87	21 (42%)
14	CLA	F	1301	-	43,53,73	2.67	18 (41%)	50,89,113	2.66	21 (42%)
14	CLA	H	802	-	63,73,73	2.26	18 (28%)	74,113,113	2.44	25 (33%)
14	CLA	B	816	-	53,63,73	2.50	20 (37%)	62,101,113	2.68	27 (43%)
14	CLA	b	823	2	48,58,73	2.59	18 (37%)	56,95,113	2.66	23 (41%)
14	CLA	B	813	-	53,63,73	2.50	19 (35%)	62,101,113	2.71	22 (35%)
14	CLA	l	202	2	63,73,73	2.25	19 (30%)	74,113,113	2.69	31 (41%)
14	CLA	A	812	14	63,73,73	2.26	21 (33%)	74,113,113	2.52	24 (32%)
17	BCR	L	207	-	41,41,41	2.73	6 (14%)	56,56,56	6.38	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	B	844	-	41,41,41	2.64	6 (14%)	56,56,56	6.53	22 (39%)
14	CLA	a	839	-	43,53,73	2.63	19 (44%)	50,89,113	2.78	22 (44%)
14	CLA	A	829	-	63,73,73	2.28	18 (28%)	74,113,113	2.40	24 (32%)
17	BCR	G	850	-	41,41,41	2.79	6 (14%)	56,56,56	6.63	26 (46%)
14	CLA	B	828	-	63,73,73	2.28	19 (30%)	74,113,113	2.49	25 (33%)
14	CLA	H	835	-	43,53,73	2.65	19 (44%)	50,89,113	3.17	24 (48%)
14	CLA	U	206	-	63,73,73	2.30	20 (31%)	74,113,113	2.44	23 (31%)
14	CLA	G	839	-	63,73,73	2.28	20 (31%)	74,113,113	2.43	27 (36%)
14	CLA	b	838	-	43,53,73	2.60	19 (44%)	50,89,113	2.92	21 (42%)
14	CLA	G	829	-	63,73,73	2.30	19 (30%)	74,113,113	2.45	25 (33%)
14	CLA	B	829	-	43,53,73	2.57	18 (41%)	50,89,113	2.97	23 (46%)
14	CLA	A	834	-	63,73,73	2.29	20 (31%)	74,113,113	2.42	23 (31%)
17	BCR	A	851	-	41,41,41	2.76	6 (14%)	56,56,56	6.72	26 (46%)
17	BCR	l	208	-	41,41,41	2.65	6 (14%)	56,56,56	6.63	20 (35%)
14	CLA	G	838	-	48,58,73	2.63	20 (41%)	56,95,113	2.82	25 (44%)
17	BCR	b	849	-	41,41,41	2.61	6 (14%)	56,56,56	6.61	18 (32%)
14	CLA	H	836	-	58,68,73	2.41	20 (34%)	68,107,113	2.59	24 (35%)
17	BCR	H	842	-	41,41,41	2.66	6 (14%)	56,56,56	6.57	18 (32%)
14	CLA	G	825	-	53,63,73	2.52	21 (39%)	62,101,113	2.60	23 (37%)
14	CLA	B	821	-	53,63,73	2.50	22 (41%)	62,101,113	2.58	24 (38%)
14	CLA	H	806	-	63,73,73	2.25	19 (30%)	74,113,113	2.52	25 (33%)
14	CLA	l	205	10	58,68,73	2.39	20 (34%)	68,107,113	2.55	24 (35%)
14	CLA	a	814	-	43,53,73	2.68	20 (46%)	50,89,113	2.96	22 (44%)
14	CLA	G	836	-	43,53,73	2.62	19 (44%)	50,89,113	2.70	20 (40%)
14	CLA	A	813	-	48,58,73	2.63	19 (39%)	56,95,113	2.68	22 (39%)
14	CLA	H	827	-	63,73,73	2.30	19 (30%)	74,113,113	2.28	22 (29%)
14	CLA	H	813	-	53,63,73	2.53	19 (35%)	62,101,113	2.63	25 (40%)
14	CLA	b	820	-	43,53,73	2.59	19 (44%)	50,89,113	2.91	20 (40%)
16	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	H	810	-	43,53,73	2.73	20 (46%)	50,89,113	2.86	22 (44%)
14	CLA	b	835	-	43,53,73	2.67	20 (46%)	50,89,113	2.76	21 (42%)
14	CLA	A	811	-	43,53,73	2.67	18 (41%)	50,89,113	2.96	22 (44%)
14	CLA	G	826	-	63,73,73	2.29	20 (31%)	74,113,113	2.42	28 (37%)
14	CLA	H	811	-	43,53,73	2.68	19 (44%)	50,89,113	2.71	18 (36%)
17	BCR	J	103	-	41,41,41	2.62	6 (14%)	56,56,56	6.99	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	G	828	-	63,73,73	2.26	20 (31%)	74,113,113	2.52	23 (31%)
14	CLA	A	838	-	48,58,73	2.64	21 (43%)	56,95,113	2.82	23 (41%)
14	CLA	a	842	-	63,73,73	2.30	20 (31%)	74,113,113	2.54	23 (31%)
17	BCR	b	843	-	41,41,41	2.66	7 (17%)	56,56,56	6.72	22 (39%)
16	SF4	A	847	2,1	0,12,12	-	-	-	-	-
14	CLA	b	813	-	53,63,73	2.50	19 (35%)	62,101,113	2.68	24 (38%)
16	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	a	815	-	43,53,73	2.69	20 (46%)	50,89,113	2.83	20 (40%)
14	CLA	B	802	-	63,73,73	2.25	18 (28%)	74,113,113	2.50	25 (33%)
14	CLA	a	821	-	63,73,73	2.32	20 (31%)	74,113,113	2.33	24 (32%)
14	CLA	H	829	-	43,53,73	2.57	18 (41%)	50,89,113	2.81	22 (44%)
14	CLA	W	1701	12	43,53,73	2.65	20 (46%)	50,89,113	2.83	21 (42%)
17	BCR	G	848	-	41,41,41	2.66	6 (14%)	56,56,56	6.58	20 (35%)
14	CLA	B	840	-	63,73,73	2.24	19 (30%)	74,113,113	2.60	24 (32%)
14	CLA	A	803	-	63,73,73	2.26	17 (26%)	74,113,113	2.36	24 (32%)
14	CLA	B	825	-	63,73,73	2.29	19 (30%)	74,113,113	2.50	25 (33%)
14	CLA	A	826	-	63,73,73	2.31	20 (31%)	74,113,113	2.48	28 (37%)
14	CLA	b	831	-	63,73,73	2.33	21 (33%)	74,113,113	2.49	26 (35%)
14	CLA	G	815	-	43,53,73	2.67	19 (44%)	50,89,113	2.89	21 (42%)
17	BCR	f	203	-	41,41,41	2.64	6 (14%)	56,56,56	6.28	23 (41%)
15	PQN	b	841	-	34,34,34	1.59	2 (5%)	43,45,45	1.13	5 (11%)
17	BCR	A	850	-	41,41,41	2.67	6 (14%)	56,56,56	6.52	23 (41%)
17	BCR	B	843	-	41,41,41	2.68	7 (17%)	56,56,56	6.66	23 (41%)
17	BCR	j	103	-	41,41,41	2.66	6 (14%)	56,56,56	6.63	23 (41%)
14	CLA	a	844	18	43,53,73	2.68	19 (44%)	50,89,113	3.08	24 (48%)
17	BCR	H	847	-	41,41,41	2.66	6 (14%)	56,56,56	6.82	17 (30%)
14	CLA	a	837	-	48,58,73	2.66	19 (39%)	56,95,113	2.83	26 (46%)
14	CLA	G	833	-	53,63,73	2.54	20 (37%)	62,101,113	2.67	24 (38%)
14	CLA	a	835	-	43,53,73	2.62	18 (41%)	50,89,113	2.67	19 (38%)
17	BCR	I	101	-	41,41,41	2.71	7 (17%)	56,56,56	6.73	19 (33%)
14	CLA	b	834	-	43,53,73	2.65	19 (44%)	50,89,113	3.05	20 (40%)
14	CLA	B	820	-	43,53,73	2.67	19 (44%)	50,89,113	2.94	19 (38%)
14	CLA	a	804	14	53,63,73	2.52	20 (37%)	62,101,113	2.78	25 (40%)
14	CLA	a	806	-	63,73,73	2.25	19 (30%)	74,113,113	2.53	23 (31%)
17	BCR	F	1302	-	41,41,41	2.59	6 (14%)	56,56,56	6.17	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	H	820	-	43,53,73	2.65	19 (44%)	50,89,113	2.88	19 (38%)
14	CLA	H	839	-	63,73,73	2.27	19 (30%)	74,113,113	2.42	23 (31%)
14	CLA	G	814	-	58,68,73	2.41	21 (36%)	68,107,113	2.51	27 (39%)
14	CLA	A	832	-	48,58,73	2.61	18 (37%)	56,95,113	2.70	23 (41%)
14	CLA	a	828	-	63,73,73	2.29	19 (30%)	74,113,113	2.40	25 (33%)
17	BCR	l	203	-	41,41,41	2.76	6 (14%)	56,56,56	6.44	22 (39%)
14	CLA	b	826	-	63,73,73	2.31	20 (31%)	74,113,113	2.41	21 (28%)
14	CLA	A	827	-	58,68,73	2.34	18 (31%)	68,107,113	2.63	25 (36%)
17	BCR	a	850	-	41,41,41	2.76	6 (14%)	56,56,56	6.79	22 (39%)
14	CLA	V	1601	-	43,53,73	2.66	19 (44%)	50,89,113	2.91	23 (46%)
14	CLA	G	806	-	43,53,73	2.61	18 (41%)	50,89,113	2.85	20 (40%)
14	CLA	G	845	18	43,53,73	2.61	19 (44%)	50,89,113	3.14	25 (50%)
17	BCR	B	850	-	41,41,41	2.60	6 (14%)	56,56,56	6.57	17 (30%)
14	CLA	G	832	-	48,58,73	2.60	19 (39%)	56,95,113	2.70	24 (42%)
14	CLA	b	833	-	43,53,73	2.66	19 (44%)	50,89,113	2.82	20 (40%)
14	CLA	A	809	1	63,73,73	2.21	20 (31%)	74,113,113	2.64	27 (36%)
14	CLA	a	817	-	43,53,73	2.63	18 (41%)	50,89,113	2.74	21 (42%)
14	CLA	B	832	-	53,63,73	2.47	21 (39%)	62,101,113	2.66	24 (38%)
14	CLA	H	834	-	43,53,73	2.63	19 (44%)	50,89,113	2.79	19 (38%)
14	CLA	b	814	-	43,53,73	2.67	19 (44%)	50,89,113	2.96	22 (44%)
14	CLA	A	843	-	63,73,73	2.29	18 (28%)	74,113,113	2.41	23 (31%)
14	CLA	a	843	-	39,49,73	2.63	17 (43%)	46,83,113	2.86	22 (47%)
14	CLA	A	828	-	63,73,73	2.21	20 (31%)	74,113,113	2.58	27 (36%)
14	CLA	G	818	-	43,53,73	2.65	18 (41%)	50,89,113	2.84	20 (40%)
14	CLA	K	102	-	43,53,73	2.67	19 (44%)	50,89,113	2.79	21 (42%)
14	CLA	B	826	-	63,73,73	2.29	18 (28%)	74,113,113	2.46	25 (33%)
16	SF4	c	102	3	0,12,12	-	-	-	-	-
17	BCR	S	103	-	41,41,41	2.72	6 (14%)	56,56,56	6.53	23 (41%)
17	BCR	H	843	-	41,41,41	2.66	6 (14%)	56,56,56	6.65	21 (37%)
14	CLA	S	102	-	35,45,73	2.82	19 (54%)	42,78,113	2.85	17 (40%)
14	CLA	K	101	-	39,49,73	2.62	17 (43%)	46,83,113	2.78	22 (47%)
14	CLA	A	817	-	43,53,73	2.65	20 (46%)	50,89,113	2.76	20 (40%)
14	CLA	f	202	-	43,53,73	2.69	20 (46%)	50,89,113	2.73	23 (46%)
18	LHG	G	855	14	26,26,48	1.26	2 (7%)	29,32,54	1.26	2 (6%)
17	BCR	A	848	-	41,41,41	2.61	6 (14%)	56,56,56	6.68	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	844	-	63,73,73	2.25	19 (30%)	74,113,113	2.42	25 (33%)
14	CLA	b	816	-	53,63,73	2.52	20 (37%)	62,101,113	2.68	26 (41%)
14	CLA	b	809	2	63,73,73	2.24	18 (28%)	74,113,113	2.50	26 (35%)
14	CLA	B	838	-	43,53,73	2.60	19 (44%)	50,89,113	2.83	20 (40%)
14	CLA	H	815	-	43,53,73	2.64	18 (41%)	50,89,113	2.83	20 (40%)
14	CLA	G	819	-	48,58,73	2.63	21 (43%)	56,95,113	2.81	25 (44%)
14	CLA	L	204	10	58,68,73	2.37	20 (34%)	68,107,113	2.60	25 (36%)
14	CLA	b	803	-	63,73,73	2.27	18 (28%)	74,113,113	2.45	25 (33%)
17	BCR	L	202	-	41,41,41	2.73	6 (14%)	56,56,56	6.49	19 (33%)
14	CLA	i	101	-	63,73,73	2.28	20 (31%)	74,113,113	2.48	24 (32%)
17	BCR	G	849	-	41,41,41	2.69	6 (14%)	56,56,56	6.81	25 (44%)
14	CLA	a	836	1	43,53,73	2.65	19 (44%)	50,89,113	2.76	20 (40%)
14	CLA	b	840	-	63,73,73	2.25	20 (31%)	74,113,113	2.60	26 (35%)
14	CLA	a	829	-	63,73,73	2.32	20 (31%)	74,113,113	2.39	26 (35%)
17	BCR	l	201	-	41,41,41	2.75	6 (14%)	56,56,56	6.32	22 (39%)
17	BCR	A	852	-	41,41,41	2.68	6 (14%)	56,56,56	6.67	20 (35%)
14	CLA	A	821	-	48,58,73	2.62	20 (41%)	56,95,113	2.84	24 (42%)
17	BCR	a	852	-	41,41,41	2.67	6 (14%)	56,56,56	6.67	21 (37%)
17	BCR	B	848	-	41,41,41	2.67	6 (14%)	56,56,56	6.83	22 (39%)
14	CLA	H	838	-	43,53,73	2.60	19 (44%)	50,89,113	2.90	23 (46%)
14	CLA	b	825	-	63,73,73	2.32	20 (31%)	74,113,113	2.51	25 (33%)
14	CLA	B	836	-	58,68,73	2.40	19 (32%)	68,107,113	2.54	22 (32%)
14	CLA	G	805	14	53,63,73	2.50	20 (37%)	62,101,113	2.79	26 (41%)
14	CLA	l	206	-	63,73,73	2.25	18 (28%)	74,113,113	2.57	23 (31%)
14	CLA	H	809	2	63,73,73	2.27	19 (30%)	74,113,113	2.42	28 (37%)
14	CLA	G	824	-	43,53,73	2.64	19 (44%)	50,89,113	2.83	20 (40%)
14	CLA	B	810	-	43,53,73	2.73	19 (44%)	50,89,113	2.80	21 (42%)
14	CLA	H	824	-	43,53,73	2.67	19 (44%)	50,89,113	2.78	21 (42%)
14	CLA	b	828	-	63,73,73	2.29	19 (30%)	74,113,113	2.50	24 (32%)
14	CLA	B	811	-	43,53,73	2.65	19 (44%)	50,89,113	2.80	21 (42%)
14	CLA	b	830	-	43,53,73	2.66	20 (46%)	50,89,113	2.86	21 (42%)
18	LHG	a	854	14	26,26,48	1.27	2 (7%)	29,32,54	1.38	5 (17%)
14	CLA	A	806	-	43,53,73	2.66	18 (41%)	50,89,113	2.86	22 (44%)
17	BCR	A	853	-	41,41,41	2.67	6 (14%)	56,56,56	6.92	20 (35%)
14	CLA	A	822	-	63,73,73	2.29	20 (31%)	74,113,113	2.41	28 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	837	-	58,68,73	2.37	19 (32%)	68,107,113	2.59	24 (35%)
14	CLA	B	833	-	43,53,73	2.65	19 (44%)	50,89,113	2.74	20 (40%)
14	CLA	A	818	-	43,53,73	2.60	18 (41%)	50,89,113	2.75	20 (40%)
14	CLA	H	826	-	63,73,73	2.27	19 (30%)	74,113,113	2.46	22 (29%)
18	LHG	G	854	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
14	CLA	G	808	-	43,53,73	2.66	19 (44%)	50,89,113	2.82	21 (42%)
14	CLA	a	803	-	53,63,73	2.50	18 (33%)	62,101,113	2.72	23 (37%)
13	CL0	A	801	-	63,73,73	2.28	19 (30%)	74,113,113	2.39	23 (31%)
14	CLA	A	840	-	43,53,73	2.64	19 (44%)	50,89,113	2.75	22 (44%)
16	SF4	N	102	3	0,12,12	-	-	-	-	-
17	BCR	Q	202	-	41,41,41	2.69	6 (14%)	56,56,56	6.64	19 (33%)
17	BCR	R	101	-	41,41,41	2.70	6 (14%)	56,56,56	6.74	18 (32%)
13	CL0	a	801	-	63,73,73	2.27	18 (28%)	74,113,113	2.41	25 (33%)
14	CLA	B	809	2	63,73,73	2.25	19 (30%)	74,113,113	2.47	26 (35%)
16	SF4	N	101	3	0,12,12	-	-	-	-	-
17	BCR	j	104	-	41,41,41	2.63	7 (17%)	56,56,56	6.73	21 (37%)
17	BCR	J	102	-	41,41,41	2.74	6 (14%)	56,56,56	6.53	22 (39%)
14	CLA	J	101	-	43,53,73	2.67	20 (46%)	50,89,113	2.89	26 (52%)
14	CLA	a	819	-	63,73,73	2.30	20 (31%)	74,113,113	2.52	26 (35%)
14	CLA	A	808	-	43,53,73	2.66	19 (44%)	50,89,113	2.83	23 (46%)
14	CLA	A	831	-	63,73,73	2.27	19 (30%)	74,113,113	2.39	22 (29%)
14	CLA	a	831	-	48,58,73	2.62	19 (39%)	56,95,113	2.70	23 (41%)
14	CLA	G	812	14	63,73,73	2.27	20 (31%)	74,113,113	2.60	25 (33%)
14	CLA	H	812	-	63,73,73	2.26	20 (31%)	74,113,113	2.54	28 (37%)
19	LMG	B	849	-	49,49,55	1.38	6 (12%)	57,57,63	1.08	4 (7%)
14	CLA	G	816	-	43,53,73	2.67	20 (46%)	50,89,113	2.84	23 (46%)
14	CLA	Q	201	-	43,53,73	2.62	17 (39%)	50,89,113	2.78	19 (38%)
14	CLA	H	807	-	63,73,73	2.25	20 (31%)	74,113,113	2.49	24 (32%)
17	BCR	b	842	-	41,41,41	2.63	6 (14%)	56,56,56	6.56	18 (32%)
14	CLA	B	822	-	43,53,73	2.62	17 (39%)	50,89,113	2.72	20 (40%)
17	BCR	H	844	-	41,41,41	2.63	6 (14%)	56,56,56	6.47	21 (37%)
14	CLA	G	823	-	43,53,73	2.67	18 (41%)	50,89,113	2.87	20 (40%)
14	CLA	a	820	-	48,58,73	2.60	20 (41%)	56,95,113	2.91	27 (48%)
14	CLA	U	205	-	63,73,73	2.29	19 (30%)	74,113,113	2.54	24 (32%)
14	CLA	b	819	-	43,53,73	2.64	19 (44%)	50,89,113	2.88	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	841	-	43,53,73	2.61	17 (39%)	50,89,113	2.79	20 (40%)
14	CLA	b	832	-	53,63,73	2.48	21 (39%)	62,101,113	2.73	24 (38%)
17	BCR	m	1602	-	41,41,41	2.60	6 (14%)	56,56,56	6.73	20 (35%)
14	CLA	H	801	-	63,73,73	2.27	19 (30%)	74,113,113	2.47	28 (37%)
14	CLA	b	808	-	63,73,73	2.24	18 (28%)	74,113,113	2.55	24 (32%)
14	CLA	L	206	-	63,73,73	2.31	20 (31%)	74,113,113	2.48	25 (33%)
17	BCR	a	848	-	41,41,41	2.68	6 (14%)	56,56,56	6.74	26 (46%)
14	CLA	G	830	-	63,73,73	2.26	19 (30%)	74,113,113	2.45	23 (31%)
18	LHG	A	854	-	48,48,48	0.93	2 (4%)	51,54,54	1.16	4 (7%)
14	CLA	b	811	-	43,53,73	2.67	20 (46%)	50,89,113	2.85	21 (42%)
17	BCR	b	845	-	25,25,41	2.15	2 (8%)	33,33,56	7.38	15 (45%)
17	BCR	G	852	-	41,41,41	2.71	6 (14%)	56,56,56	6.77	21 (37%)
17	BCR	i	102	-	41,41,41	2.70	6 (14%)	56,56,56	6.73	21 (37%)
14	CLA	b	801	-	63,73,73	2.24	18 (28%)	74,113,113	2.50	27 (36%)
14	CLA	B	808	-	63,73,73	2.30	19 (30%)	74,113,113	2.39	25 (33%)
14	CLA	A	814	-	58,68,73	2.40	20 (34%)	68,107,113	2.56	26 (38%)
14	CLA	B	837	-	58,68,73	2.33	19 (32%)	68,107,113	2.69	25 (36%)
17	BCR	B	845	-	25,25,41	2.14	2 (8%)	33,33,56	7.43	16 (48%)
14	CLA	A	830	-	63,73,73	2.29	19 (30%)	74,113,113	2.42	24 (32%)
14	CLA	x	1701	12	43,53,73	2.66	19 (44%)	50,89,113	2.77	21 (42%)
14	CLA	A	819	-	48,58,73	2.63	21 (43%)	56,95,113	2.85	22 (39%)
14	CLA	a	830	-	63,73,73	2.27	19 (30%)	74,113,113	2.44	25 (33%)
14	CLA	H	819	-	43,53,73	2.68	21 (48%)	50,89,113	2.84	20 (40%)
17	BCR	U	202	-	41,41,41	2.75	6 (14%)	56,56,56	6.58	24 (42%)
14	CLA	B	801	-	63,73,73	2.26	20 (31%)	74,113,113	2.46	26 (35%)
17	BCR	H	849	-	41,41,41	2.60	6 (14%)	56,56,56	6.41	19 (33%)
14	CLA	G	831	-	63,73,73	2.28	19 (30%)	74,113,113	2.42	24 (32%)
14	CLA	A	802	-	63,73,73	2.27	18 (28%)	74,113,113	2.47	27 (36%)
14	CLA	H	816	-	53,63,73	2.52	19 (35%)	62,101,113	2.71	26 (41%)
14	CLA	G	817	-	43,53,73	2.63	20 (46%)	50,89,113	2.76	20 (40%)
17	BCR	I	102	-	41,41,41	2.59	6 (14%)	56,56,56	6.64	20 (35%)
14	CLA	H	803	-	63,73,73	2.23	20 (31%)	74,113,113	2.56	25 (33%)
14	CLA	a	818	-	48,58,73	2.61	20 (41%)	56,95,113	2.81	23 (41%)
14	CLA	A	842	-	43,53,73	2.61	18 (41%)	50,89,113	2.71	19 (38%)
16	SF4	c	101	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	805	-	63,73,73	2.31	20 (31%)	74,113,113	2.49	27 (36%)
14	CLA	G	842	-	63,73,73	2.30	20 (31%)	74,113,113	2.52	26 (35%)
14	CLA	b	812	-	63,73,73	2.28	21 (33%)	74,113,113	2.54	29 (39%)
14	CLA	l	207	-	63,73,73	2.29	20 (31%)	74,113,113	2.45	27 (36%)
13	CL0	G	801	-	63,73,73	2.30	19 (30%)	74,113,113	2.45	25 (33%)
14	CLA	a	840	-	63,73,73	2.32	20 (31%)	74,113,113	2.47	29 (39%)
17	BCR	H	845	-	25,25,41	2.18	2 (8%)	33,33,56	7.45	20 (60%)
14	CLA	B	803	-	63,73,73	2.24	20 (31%)	74,113,113	2.47	24 (32%)
14	CLA	G	834	-	63,73,73	2.31	20 (31%)	74,113,113	2.43	22 (29%)
16	SF4	G	847	2,1	0,12,12	-	-	-	-	-
14	CLA	H	814	-	43,53,73	2.60	19 (44%)	50,89,113	2.98	21 (42%)
14	CLA	A	836	-	43,53,73	2.60	18 (41%)	50,89,113	2.73	18 (36%)
14	CLA	b	822	-	43,53,73	2.68	20 (46%)	50,89,113	2.73	20 (40%)
14	CLA	A	833	-	53,63,73	2.57	20 (37%)	62,101,113	2.66	25 (40%)
17	BCR	A	849	-	41,41,41	2.68	6 (14%)	56,56,56	6.87	27 (48%)
14	CLA	B	817	-	58,68,73	2.36	20 (34%)	68,107,113	2.58	24 (35%)
14	CLA	L	201	2	63,73,73	2.25	19 (30%)	74,113,113	2.65	27 (36%)
14	CLA	B	824	-	43,53,73	2.68	18 (41%)	50,89,113	2.73	19 (38%)
14	CLA	a	805	-	43,53,73	2.62	18 (41%)	50,89,113	2.84	20 (40%)
14	CLA	b	802	-	63,73,73	2.24	19 (30%)	74,113,113	2.42	22 (29%)
14	CLA	H	831	-	63,73,73	2.34	21 (33%)	74,113,113	2.57	27 (36%)
17	BCR	f	201	-	41,41,41	2.77	6 (14%)	56,56,56	6.57	20 (35%)
14	CLA	a	808	1	63,73,73	2.24	20 (31%)	74,113,113	2.58	26 (35%)
14	CLA	H	837	-	58,68,73	2.40	20 (34%)	68,107,113	2.60	23 (33%)
14	CLA	B	814	-	43,53,73	2.62	18 (41%)	50,89,113	2.89	21 (42%)
14	CLA	B	819	-	43,53,73	2.65	19 (44%)	50,89,113	2.78	20 (40%)
14	CLA	A	845	18	43,53,73	2.65	19 (44%)	50,89,113	3.05	24 (48%)
14	CLA	a	813	-	58,68,73	2.36	20 (34%)	68,107,113	2.56	24 (35%)
14	CLA	k	1401	-	43,53,73	2.68	19 (44%)	50,89,113	2.76	20 (40%)
14	CLA	G	835	-	63,73,73	2.27	19 (30%)	74,113,113	2.50	22 (29%)
14	CLA	b	827	-	63,73,73	2.28	19 (30%)	74,113,113	2.37	22 (29%)
14	CLA	H	821	-	53,63,73	2.52	20 (37%)	62,101,113	2.63	23 (37%)
14	CLA	B	812	-	63,73,73	2.29	19 (30%)	74,113,113	2.55	26 (35%)
14	CLA	B	827	-	63,73,73	2.32	19 (30%)	74,113,113	2.23	24 (32%)
17	BCR	H	846	-	41,41,41	2.73	7 (17%)	56,56,56	6.61	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	Q	204	-	41,41,41	2.60	6 (14%)	56,56,56	6.59	22 (39%)
14	CLA	B	807	-	63,73,73	2.27	20 (31%)	74,113,113	2.48	24 (32%)

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
17	BCR	S	104	-	-	12/29/63/63	0/2/2/2
14	CLA	a	812	-	1/1/12/20	3/19/97/115	-
14	CLA	b	810	-	1/1/11/20	3/13/91/115	-
14	CLA	U	204	10	1/1/14/20	13/31/109/115	-
14	CLA	B	823	2	1/1/12/20	8/19/97/115	-
14	CLA	b	804	-	1/1/15/20	16/37/115/115	-
17	BCR	b	847	-	-	9/29/63/63	0/2/2/2
14	CLA	j	101	-	1/1/11/20	6/13/91/115	-
14	CLA	a	822	-	1/1/11/20	6/13/91/115	-
14	CLA	H	817	-	1/1/14/20	13/31/109/115	-
17	BCR	B	842	-	-	11/29/63/63	0/2/2/2
14	CLA	b	821	-	1/1/13/20	10/25/103/115	-
14	CLA	A	820	-	1/1/15/20	13/37/115/115	-
14	CLA	A	807	-	1/1/15/20	18/37/115/115	-
17	BCR	b	846	-	-	6/29/63/63	0/2/2/2
19	LMG	H	848	-	-	9/44/64/70	0/1/1/1
14	CLA	X	1701	12	1/1/11/20	6/13/91/115	-
14	CLA	G	844	-	1/1/9/20	3/7/81/115	-
14	CLA	G	820	-	1/1/15/20	17/37/115/115	-
14	CLA	H	840	-	1/1/15/20	11/37/115/115	-
14	CLA	U	201	2	1/1/15/20	10/37/115/115	-
15	PQN	B	841	-	-	4/23/43/43	0/2/2/2
14	CLA	b	817	-	1/1/14/20	14/31/109/115	-
17	BCR	B	846	-	-	9/29/63/63	0/2/2/2
14	CLA	H	832	-	1/1/13/20	10/25/103/115	-
14	CLA	H	828	-	1/1/15/20	9/37/115/115	-
14	CLA	H	830	-	1/1/11/20	7/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Q	203	-	1/1/11/20	4/13/91/115	-
18	LHG	A	855	14	-	16/31/31/53	-
14	CLA	b	818	-	1/1/15/20	13/37/115/115	-
14	CLA	a	825	-	1/1/15/20	17/37/115/115	-
14	CLA	m	1601	-	1/1/11/20	7/13/91/115	-
14	CLA	b	807	-	1/1/15/20	18/37/115/115	-
14	CLA	a	827	-	1/1/15/20	17/37/115/115	-
14	CLA	H	808	-	1/1/15/20	15/37/115/115	-
14	CLA	B	839	-	1/1/15/20	14/37/115/115	-
14	CLA	A	837	1	1/1/11/20	5/13/91/115	-
17	BCR	R	102	-	-	10/29/63/63	0/2/2/2
14	CLA	b	824	-	1/1/11/20	4/13/91/115	-
14	CLA	G	810	1	1/1/15/20	11/37/115/115	-
14	CLA	H	818	-	1/1/15/20	11/37/115/115	-
14	CLA	a	802	-	1/1/15/20	14/37/115/115	-
14	CLA	G	813	-	1/1/12/20	4/19/97/115	-
14	CLA	b	806	-	1/1/15/20	14/37/115/115	-
14	CLA	j	102	-	1/1/8/20	0/2/76/115	-
14	CLA	B	806	-	1/1/15/20	20/37/115/115	-
14	CLA	G	837	1	1/1/11/20	5/13/91/115	-
14	CLA	b	836	-	1/1/14/20	12/31/109/115	-
14	CLA	A	804	-	1/1/13/20	12/25/103/115	-
14	CLA	b	829	-	1/1/11/20	6/13/91/115	-
14	CLA	a	833	-	1/1/15/20	7/37/115/115	-
15	PQN	A	846	-	-	9/23/43/43	0/2/2/2
14	CLA	a	834	-	1/1/15/20	11/37/115/115	-
14	CLA	L	205	-	1/1/15/20	12/37/115/115	-
14	CLA	F	1303	-	1/1/8/20	0/2/76/115	-
14	CLA	H	833	-	1/1/11/20	4/13/91/115	-
14	CLA	G	804	-	1/1/13/20	11/25/103/115	-
18	LHG	a	853	-	-	26/53/53/53	-
14	CLA	G	841	-	1/1/15/20	11/37/115/115	-
14	CLA	B	834	-	1/1/11/20	7/13/91/115	-
17	BCR	M	1602	-	-	10/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	a	849	-	-	11/29/63/63	0/2/2/2
14	CLA	G	827	-	1/1/14/20	7/31/109/115	-
17	BCR	b	844	-	-	10/29/63/63	0/2/2/2
14	CLA	B	815	-	1/1/11/20	4/13/91/115	-
14	CLA	G	821	-	1/1/12/20	9/19/97/115	-
14	CLA	A	805	14	1/1/13/20	12/25/103/115	-
14	CLA	b	815	-	1/1/11/20	3/13/91/115	-
14	CLA	a	809	-	1/1/15/20	14/37/115/115	-
14	CLA	B	831	-	1/1/15/20	18/37/115/115	-
14	CLA	G	809	1	1/1/15/20	17/37/115/115	-
14	CLA	G	843	-	1/1/15/20	15/37/115/115	-
14	CLA	b	805	-	1/1/12/20	8/24/102/115	-
14	CLA	a	855	-	1/1/15/20	15/37/115/115	-
14	CLA	a	838	-	1/1/15/20	9/37/115/115	-
14	CLA	a	824	-	1/1/13/20	8/25/103/115	-
14	CLA	A	839	-	1/1/15/20	10/37/115/115	-
17	BCR	B	847	-	-	9/29/63/63	0/2/2/2
17	BCR	V	1602	-	-	11/29/63/63	0/2/2/2
14	CLA	B	804	-	1/1/12/20	7/24/102/115	-
14	CLA	H	822	-	1/1/11/20	2/13/91/115	-
19	LMG	b	848	-	-	13/44/64/70	0/1/1/1
14	CLA	A	810	1	1/1/15/20	12/37/115/115	-
14	CLA	G	822	-	1/1/15/20	13/37/115/115	-
14	CLA	a	810	-	1/1/11/20	5/13/91/115	-
14	CLA	A	816	-	1/1/11/20	5/13/91/115	-
14	CLA	a	826	-	1/1/14/20	9/31/109/115	-
14	CLA	S	101	8	1/1/11/20	6/13/91/115	-
17	BCR	G	851	-	-	9/29/63/63	0/2/2/2
14	CLA	G	803	-	1/1/15/20	14/37/115/115	-
17	BCR	a	851	-	-	6/29/63/63	0/2/2/2
14	CLA	a	807	-	1/1/11/20	5/13/91/115	-
14	CLA	A	823	-	1/1/11/20	6/13/91/115	-
14	CLA	A	825	-	1/1/13/20	6/25/103/115	-
14	CLA	A	841	-	1/1/15/20	10/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	823	2	1/1/12/20	6/19/97/115	-
14	CLA	H	825	-	1/1/15/20	10/37/115/115	-
14	CLA	b	839	-	1/1/15/20	15/37/115/115	-
14	CLA	a	811	14	1/1/15/20	13/37/115/115	-
14	CLA	G	840	-	1/1/11/20	3/13/91/115	-
14	CLA	B	818	-	1/1/15/20	8/37/115/115	-
14	CLA	B	835	-	1/1/11/20	6/13/91/115	-
14	CLA	G	807	-	1/1/15/20	18/37/115/115	-
16	SF4	a	846	2,1	-	-	0/6/5/5
14	CLA	a	823	-	1/1/11/20	4/13/91/115	-
17	BCR	G	853	-	-	13/29/63/63	0/2/2/2
14	CLA	A	815	-	1/1/11/20	4/13/91/115	-
14	CLA	T	1401	-	1/1/11/20	6/13/91/115	-
14	CLA	G	811	-	1/1/11/20	6/13/91/115	-
15	PQN	a	845	-	-	8/23/43/43	0/2/2/2
14	CLA	A	835	-	1/1/15/20	12/37/115/115	-
14	CLA	M	1601	-	1/1/11/20	9/13/91/115	-
14	CLA	H	805	-	1/1/15/20	17/37/115/115	-
15	PQN	G	846	-	-	9/23/43/43	0/2/2/2
14	CLA	H	804	-	1/1/12/20	8/24/102/115	-
14	CLA	a	816	-	1/1/11/20	3/13/91/115	-
17	BCR	a	847	-	-	10/29/63/63	0/2/2/2
14	CLA	G	802	-	1/1/15/20	12/37/115/115	-
15	PQN	H	841	-	-	5/23/43/43	0/2/2/2
14	CLA	B	830	-	1/1/11/20	7/13/91/115	-
14	CLA	a	832	-	1/1/13/20	11/25/103/115	-
17	BCR	R	103	-	-	8/29/63/63	0/2/2/2
14	CLA	A	824	-	1/1/11/20	4/13/91/115	-
14	CLA	F	1301	-	1/1/11/20	4/13/91/115	-
14	CLA	H	802	-	1/1/15/20	15/37/115/115	-
14	CLA	B	816	-	1/1/13/20	8/25/103/115	-
14	CLA	b	823	2	1/1/12/20	7/19/97/115	-
14	CLA	B	813	-	1/1/13/20	8/25/103/115	-
14	CLA	l	202	2	1/1/15/20	7/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	812	14	1/1/15/20	14/37/115/115	-
17	BCR	L	207	-	-	5/29/63/63	0/2/2/2
17	BCR	B	844	-	-	9/29/63/63	0/2/2/2
14	CLA	a	839	-	1/1/11/20	3/13/91/115	-
14	CLA	A	829	-	1/1/15/20	17/37/115/115	-
17	BCR	G	850	-	-	13/29/63/63	0/2/2/2
14	CLA	B	828	-	1/1/15/20	8/37/115/115	-
14	CLA	H	835	-	1/1/11/20	6/13/91/115	-
14	CLA	U	206	-	1/1/15/20	16/37/115/115	-
14	CLA	G	839	-	1/1/15/20	12/37/115/115	-
14	CLA	b	838	-	1/1/11/20	5/13/91/115	-
14	CLA	G	829	-	1/1/15/20	17/37/115/115	-
14	CLA	B	829	-	1/1/11/20	7/13/91/115	-
14	CLA	A	834	-	1/1/15/20	15/37/115/115	-
17	BCR	A	851	-	-	11/29/63/63	0/2/2/2
17	BCR	l	208	-	-	8/29/63/63	0/2/2/2
14	CLA	G	838	-	1/1/12/20	5/19/97/115	-
17	BCR	b	849	-	-	9/29/63/63	0/2/2/2
14	CLA	H	836	-	1/1/14/20	16/31/109/115	-
17	BCR	H	842	-	-	12/29/63/63	0/2/2/2
14	CLA	G	825	-	1/1/13/20	6/25/103/115	-
14	CLA	B	821	-	1/1/13/20	9/25/103/115	-
14	CLA	H	806	-	1/1/15/20	19/37/115/115	-
14	CLA	l	205	10	1/1/14/20	10/31/109/115	-
14	CLA	a	814	-	1/1/11/20	5/13/91/115	-
14	CLA	G	836	-	1/1/11/20	5/13/91/115	-
14	CLA	A	813	-	1/1/12/20	4/19/97/115	-
14	CLA	H	827	-	1/1/15/20	12/37/115/115	-
14	CLA	H	813	-	1/1/13/20	9/25/103/115	-
14	CLA	b	820	-	1/1/11/20	4/13/91/115	-
16	SF4	C	101	3	-	-	0/6/5/5
14	CLA	H	810	-	1/1/11/20	3/13/91/115	-
14	CLA	b	835	-	1/1/11/20	6/13/91/115	-
14	CLA	A	811	-	1/1/11/20	5/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	826	-	1/1/15/20	16/37/115/115	-
14	CLA	H	811	-	1/1/11/20	4/13/91/115	-
17	BCR	J	103	-	-	12/29/63/63	0/2/2/2
14	CLA	G	828	-	1/1/15/20	17/37/115/115	-
14	CLA	A	838	-	1/1/12/20	6/19/97/115	-
14	CLA	a	842	-	1/1/15/20	16/37/115/115	-
17	BCR	b	843	-	-	6/29/63/63	0/2/2/2
16	SF4	A	847	2,1	-	-	0/6/5/5
14	CLA	b	813	-	1/1/13/20	8/25/103/115	-
16	SF4	C	102	3	-	-	0/6/5/5
14	CLA	a	815	-	1/1/11/20	7/13/91/115	-
14	CLA	B	802	-	1/1/15/20	11/37/115/115	-
14	CLA	a	821	-	1/1/15/20	12/37/115/115	-
14	CLA	H	829	-	1/1/11/20	7/13/91/115	-
14	CLA	W	1701	12	1/1/11/20	5/13/91/115	-
17	BCR	G	848	-	-	11/29/63/63	0/2/2/2
14	CLA	B	840	-	1/1/15/20	11/37/115/115	-
14	CLA	A	803	-	1/1/15/20	15/37/115/115	-
14	CLA	B	825	-	1/1/15/20	12/37/115/115	-
14	CLA	A	826	-	1/1/15/20	18/37/115/115	-
14	CLA	b	831	-	1/1/15/20	20/37/115/115	-
14	CLA	G	815	-	1/1/11/20	2/13/91/115	-
17	BCR	f	203	-	-	8/29/63/63	0/2/2/2
15	PQN	b	841	-	-	9/23/43/43	0/2/2/2
17	BCR	A	850	-	-	11/29/63/63	0/2/2/2
17	BCR	B	843	-	-	6/29/63/63	0/2/2/2
17	BCR	j	103	-	-	9/29/63/63	0/2/2/2
14	CLA	a	844	18	1/1/11/20	8/13/91/115	-
17	BCR	H	847	-	-	11/29/63/63	0/2/2/2
14	CLA	a	837	-	1/1/12/20	6/19/97/115	-
14	CLA	G	833	-	1/1/13/20	11/25/103/115	-
14	CLA	a	835	-	1/1/11/20	5/13/91/115	-
17	BCR	I	101	-	-	7/29/63/63	0/2/2/2
14	CLA	b	834	-	1/1/11/20	7/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	820	-	1/1/11/20	6/13/91/115	-
14	CLA	a	804	14	1/1/13/20	12/25/103/115	-
14	CLA	a	806	-	1/1/15/20	17/37/115/115	-
17	BCR	F	1302	-	-	10/29/63/63	0/2/2/2
14	CLA	H	820	-	1/1/11/20	6/13/91/115	-
14	CLA	H	839	-	1/1/15/20	18/37/115/115	-
14	CLA	G	814	-	1/1/14/20	16/31/109/115	-
14	CLA	A	832	-	1/1/12/20	5/19/97/115	-
14	CLA	a	828	-	1/1/15/20	18/37/115/115	-
17	BCR	l	203	-	-	13/29/63/63	0/2/2/2
14	CLA	b	826	-	1/1/15/20	17/37/115/115	-
14	CLA	A	827	-	1/1/14/20	10/31/109/115	-
17	BCR	a	850	-	-	13/29/63/63	0/2/2/2
14	CLA	V	1601	-	1/1/11/20	9/13/91/115	-
14	CLA	G	806	-	1/1/11/20	6/13/91/115	-
14	CLA	G	845	18	1/1/11/20	8/13/91/115	-
17	BCR	B	850	-	-	11/29/63/63	0/2/2/2
14	CLA	G	832	-	1/1/12/20	5/19/97/115	-
14	CLA	b	833	-	1/1/11/20	6/13/91/115	-
14	CLA	A	809	1	1/1/15/20	18/37/115/115	-
14	CLA	a	817	-	1/1/11/20	3/13/91/115	-
14	CLA	B	832	-	1/1/13/20	9/25/103/115	-
14	CLA	H	834	-	1/1/11/20	6/13/91/115	-
14	CLA	b	814	-	1/1/11/20	9/13/91/115	-
14	CLA	A	843	-	1/1/15/20	19/37/115/115	-
14	CLA	a	843	-	1/1/9/20	3/7/81/115	-
14	CLA	A	828	-	1/1/15/20	13/37/115/115	-
14	CLA	G	818	-	1/1/11/20	4/13/91/115	-
14	CLA	K	102	-	1/1/11/20	7/13/91/115	-
14	CLA	B	826	-	1/1/15/20	18/37/115/115	-
16	SF4	c	102	3	-	-	0/6/5/5
17	BCR	S	103	-	-	14/29/63/63	0/2/2/2
17	BCR	H	843	-	-	6/29/63/63	0/2/2/2
14	CLA	S	102	-	1/1/8/20	0/2/76/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	K	101	-	1/1/9/20	4/7/81/115	-
14	CLA	A	817	-	1/1/11/20	4/13/91/115	-
14	CLA	f	202	-	1/1/11/20	2/13/91/115	-
18	LHG	G	855	14	-	14/31/31/53	-
17	BCR	A	848	-	-	13/29/63/63	0/2/2/2
14	CLA	A	844	-	1/1/15/20	19/37/115/115	-
14	CLA	b	816	-	1/1/13/20	7/25/103/115	-
14	CLA	b	809	2	1/1/15/20	18/37/115/115	-
14	CLA	B	838	-	1/1/11/20	5/13/91/115	-
14	CLA	H	815	-	1/1/11/20	5/13/91/115	-
14	CLA	G	819	-	1/1/12/20	8/19/97/115	-
14	CLA	L	204	10	1/1/14/20	13/31/109/115	-
14	CLA	b	803	-	1/1/15/20	13/37/115/115	-
17	BCR	L	202	-	-	10/29/63/63	0/2/2/2
14	CLA	i	101	-	1/1/15/20	5/37/115/115	-
17	BCR	G	849	-	-	11/29/63/63	0/2/2/2
14	CLA	a	836	1	1/1/11/20	4/13/91/115	-
14	CLA	b	840	-	1/1/15/20	17/37/115/115	-
14	CLA	a	829	-	1/1/15/20	16/37/115/115	-
17	BCR	l	201	-	-	4/29/63/63	0/2/2/2
17	BCR	A	852	-	-	7/29/63/63	0/2/2/2
14	CLA	A	821	-	1/1/12/20	7/19/97/115	-
17	BCR	a	852	-	-	11/29/63/63	0/2/2/2
17	BCR	B	848	-	-	11/29/63/63	0/2/2/2
14	CLA	H	838	-	1/1/11/20	5/13/91/115	-
14	CLA	b	825	-	1/1/15/20	9/37/115/115	-
14	CLA	B	836	-	1/1/14/20	12/31/109/115	-
14	CLA	G	805	14	1/1/13/20	8/25/103/115	-
14	CLA	l	206	-	1/1/15/20	10/37/115/115	-
14	CLA	H	809	2	1/1/15/20	11/37/115/115	-
14	CLA	G	824	-	1/1/11/20	5/13/91/115	-
14	CLA	B	810	-	1/1/11/20	3/13/91/115	-
14	CLA	H	824	-	1/1/11/20	4/13/91/115	-
14	CLA	b	828	-	1/1/15/20	9/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	811	-	1/1/11/20	4/13/91/115	-
14	CLA	b	830	-	1/1/11/20	7/13/91/115	-
18	LHG	a	854	14	-	19/31/31/53	-
14	CLA	A	806	-	1/1/11/20	6/13/91/115	-
17	BCR	A	853	-	-	16/29/63/63	0/2/2/2
14	CLA	A	822	-	1/1/15/20	8/37/115/115	-
14	CLA	b	837	-	1/1/14/20	9/31/109/115	-
14	CLA	B	833	-	1/1/11/20	5/13/91/115	-
14	CLA	A	818	-	1/1/11/20	4/13/91/115	-
14	CLA	H	826	-	1/1/15/20	13/37/115/115	-
18	LHG	G	854	-	-	28/53/53/53	-
14	CLA	G	808	-	1/1/11/20	4/13/91/115	-
14	CLA	a	803	-	1/1/13/20	11/25/103/115	-
13	CL0	A	801	-	3/3/20/25	9/37/135/135	-
14	CLA	A	840	-	1/1/11/20	3/13/91/115	-
17	BCR	Q	202	-	-	9/29/63/63	0/2/2/2
16	SF4	N	102	3	-	-	0/6/5/5
17	BCR	R	101	-	-	6/29/63/63	0/2/2/2
13	CL0	a	801	-	3/3/20/25	4/37/135/135	-
14	CLA	B	809	2	1/1/15/20	11/37/115/115	-
16	SF4	N	101	3	-	-	0/6/5/5
17	BCR	j	104	-	-	9/29/63/63	0/2/2/2
17	BCR	J	102	-	-	13/29/63/63	0/2/2/2
14	CLA	J	101	-	1/1/11/20	4/13/91/115	-
14	CLA	a	819	-	1/1/15/20	15/37/115/115	-
14	CLA	A	808	-	1/1/11/20	4/13/91/115	-
14	CLA	A	831	-	1/1/15/20	13/37/115/115	-
14	CLA	a	831	-	1/1/12/20	3/19/97/115	-
14	CLA	G	812	14	1/1/15/20	13/37/115/115	-
14	CLA	H	812	-	1/1/15/20	17/37/115/115	-
19	LMG	B	849	-	-	13/44/64/70	0/1/1/1
14	CLA	G	816	-	1/1/11/20	5/13/91/115	-
14	CLA	Q	201	-	1/1/11/20	6/13/91/115	-
14	CLA	H	807	-	1/1/15/20	7/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	b	842	-	-	12/29/63/63	0/2/2/2
14	CLA	B	822	-	1/1/11/20	4/13/91/115	-
17	BCR	H	844	-	-	10/29/63/63	0/2/2/2
14	CLA	G	823	-	1/1/11/20	5/13/91/115	-
14	CLA	a	820	-	1/1/12/20	9/19/97/115	-
14	CLA	U	205	-	1/1/15/20	11/37/115/115	-
14	CLA	b	819	-	1/1/11/20	7/13/91/115	-
14	CLA	a	841	-	1/1/11/20	6/13/91/115	-
14	CLA	b	832	-	1/1/13/20	12/25/103/115	-
17	BCR	m	1602	-	-	13/29/63/63	0/2/2/2
14	CLA	H	801	-	1/1/15/20	20/37/115/115	-
14	CLA	b	808	-	1/1/15/20	11/37/115/115	-
14	CLA	L	206	-	1/1/15/20	13/37/115/115	-
17	BCR	a	848	-	-	14/29/63/63	0/2/2/2
14	CLA	G	830	-	1/1/15/20	18/37/115/115	-
18	LHG	A	854	-	-	32/53/53/53	-
14	CLA	b	811	-	1/1/11/20	1/13/91/115	-
17	BCR	b	845	-	-	1/18/35/63	0/1/1/2
17	BCR	G	852	-	-	7/29/63/63	0/2/2/2
17	BCR	i	102	-	-	6/29/63/63	0/2/2/2
14	CLA	b	801	-	1/1/15/20	13/37/115/115	-
14	CLA	B	808	-	1/1/15/20	13/37/115/115	-
14	CLA	A	814	-	1/1/14/20	17/31/109/115	-
14	CLA	B	837	-	1/1/14/20	9/31/109/115	-
17	BCR	B	845	-	-	0/18/35/63	0/1/1/2
14	CLA	A	830	-	1/1/15/20	15/37/115/115	-
14	CLA	x	1701	12	1/1/11/20	5/13/91/115	-
14	CLA	A	819	-	1/1/12/20	8/19/97/115	-
14	CLA	a	830	-	1/1/15/20	13/37/115/115	-
14	CLA	H	819	-	1/1/11/20	6/13/91/115	-
17	BCR	U	202	-	-	8/29/63/63	0/2/2/2
14	CLA	B	801	-	1/1/15/20	14/37/115/115	-
17	BCR	H	849	-	-	12/29/63/63	0/2/2/2
14	CLA	G	831	-	1/1/15/20	13/37/115/115	-
14	CLA	A	802	-	1/1/15/20	17/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	816	-	1/1/13/20	10/25/103/115	-
14	CLA	G	817	-	1/1/11/20	3/13/91/115	-
17	BCR	I	102	-	-	8/29/63/63	0/2/2/2
14	CLA	H	803	-	1/1/15/20	11/37/115/115	-
14	CLA	a	818	-	1/1/12/20	9/19/97/115	-
14	CLA	A	842	-	1/1/11/20	4/13/91/115	-
16	SF4	c	101	3	-	-	0/6/5/5
14	CLA	B	805	-	1/1/15/20	14/37/115/115	-
14	CLA	G	842	-	1/1/15/20	18/37/115/115	-
14	CLA	b	812	-	1/1/15/20	22/37/115/115	-
14	CLA	l	207	-	1/1/15/20	15/37/115/115	-
13	CL0	G	801	-	3/3/20/25	6/37/135/135	-
14	CLA	a	840	-	1/1/15/20	8/37/115/115	-
17	BCR	H	845	-	-	0/18/35/63	0/1/1/2
14	CLA	B	803	-	1/1/15/20	11/37/115/115	-
14	CLA	G	834	-	1/1/15/20	13/37/115/115	-
16	SF4	G	847	2,1	-	-	0/6/5/5
14	CLA	H	814	-	1/1/11/20	9/13/91/115	-
14	CLA	A	836	-	1/1/11/20	5/13/91/115	-
14	CLA	b	822	-	1/1/11/20	4/13/91/115	-
14	CLA	A	833	-	1/1/13/20	11/25/103/115	-
17	BCR	A	849	-	-	14/29/63/63	0/2/2/2
14	CLA	B	817	-	1/1/14/20	16/31/109/115	-
14	CLA	L	201	2	1/1/15/20	13/37/115/115	-
14	CLA	B	824	-	1/1/11/20	4/13/91/115	-
14	CLA	a	805	-	1/1/11/20	6/13/91/115	-
14	CLA	b	802	-	1/1/15/20	19/37/115/115	-
14	CLA	H	831	-	1/1/15/20	15/37/115/115	-
17	BCR	f	201	-	-	7/29/63/63	0/2/2/2
14	CLA	a	808	1	1/1/15/20	17/37/115/115	-
14	CLA	H	837	-	1/1/14/20	12/31/109/115	-
14	CLA	B	814	-	1/1/11/20	7/13/91/115	-
14	CLA	B	819	-	1/1/11/20	6/13/91/115	-
14	CLA	A	845	18	1/1/11/20	6/13/91/115	-
14	CLA	a	813	-	1/1/14/20	10/31/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	k	1401	-	1/1/11/20	7/13/91/115	-
14	CLA	G	835	-	1/1/15/20	14/37/115/115	-
14	CLA	b	827	-	1/1/15/20	13/37/115/115	-
14	CLA	H	821	-	1/1/13/20	10/25/103/115	-
14	CLA	B	812	-	1/1/15/20	22/37/115/115	-
14	CLA	B	827	-	1/1/15/20	12/37/115/115	-
17	BCR	H	846	-	-	7/29/63/63	0/2/2/2
17	BCR	Q	204	-	-	5/29/63/63	0/2/2/2
14	CLA	B	807	-	1/1/15/20	6/37/115/115	-

All (5995) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	850	BCR	C8-C9	-9.07	1.26	1.46
17	l	203	BCR	C8-C9	-8.85	1.27	1.46
17	U	202	BCR	C8-C9	-8.81	1.27	1.46
17	a	850	BCR	C8-C9	-8.74	1.27	1.46
17	R	102	BCR	C8-C9	-8.69	1.27	1.46
17	S	103	BCR	C8-C9	-8.69	1.27	1.46
17	J	102	BCR	C8-C9	-8.69	1.27	1.46
17	G	853	BCR	C8-C9	-8.67	1.27	1.46
17	f	201	BCR	C8-C9	-8.66	1.27	1.46
17	l	201	BCR	C8-C9	-8.66	1.27	1.46
17	A	851	BCR	C8-C9	-8.62	1.27	1.46
17	A	853	BCR	C8-C9	-8.61	1.27	1.46
17	S	104	BCR	C8-C9	-8.60	1.27	1.46
17	L	202	BCR	C8-C9	-8.57	1.27	1.46
17	G	851	BCR	C8-C9	-8.56	1.27	1.46
17	L	207	BCR	C8-C9	-8.56	1.27	1.46
17	G	852	BCR	C8-C9	-8.52	1.27	1.46
17	G	849	BCR	C8-C9	-8.52	1.27	1.46
17	A	850	BCR	C8-C9	-8.50	1.27	1.46
17	B	842	BCR	C8-C9	-8.50	1.27	1.46
17	a	852	BCR	C8-C9	-8.49	1.27	1.46
17	G	848	BCR	C8-C9	-8.49	1.27	1.46
17	H	842	BCR	C8-C9	-8.48	1.27	1.46
17	b	846	BCR	C8-C9	-8.48	1.27	1.46
17	a	849	BCR	C8-C9	-8.46	1.27	1.46
17	a	848	BCR	C8-C9	-8.44	1.27	1.46
17	a	847	BCR	C8-C9	-8.44	1.27	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	j	104	BCR	C8-C9	-8.43	1.27	1.46
17	f	203	BCR	C8-C9	-8.41	1.27	1.46
17	B	847	BCR	C8-C9	-8.41	1.27	1.46
17	B	846	BCR	C8-C9	-8.41	1.28	1.46
17	R	101	BCR	C8-C9	-8.39	1.28	1.46
17	H	846	BCR	C8-C9	-8.38	1.28	1.46
17	a	850	BCR	C11-C10	-8.38	1.17	1.43
17	I	101	BCR	C8-C9	-8.37	1.28	1.46
17	Q	202	BCR	C8-C9	-8.37	1.28	1.46
17	b	842	BCR	C8-C9	-8.37	1.28	1.46
17	l	208	BCR	C8-C9	-8.36	1.28	1.46
17	A	849	BCR	C8-C9	-8.35	1.28	1.46
17	B	846	BCR	C11-C10	-8.33	1.17	1.43
17	i	102	BCR	C8-C9	-8.32	1.28	1.46
17	j	103	BCR	C8-C9	-8.32	1.28	1.46
17	f	201	BCR	C11-C10	-8.31	1.17	1.43
17	B	848	BCR	C8-C9	-8.30	1.28	1.46
17	a	851	BCR	C8-C9	-8.29	1.28	1.46
17	A	851	BCR	C11-C10	-8.29	1.17	1.43
17	G	851	BCR	C11-C10	-8.29	1.17	1.43
17	H	847	BCR	C8-C9	-8.29	1.28	1.46
17	J	103	BCR	C8-C9	-8.29	1.28	1.46
17	A	848	BCR	C8-C9	-8.28	1.28	1.46
17	B	843	BCR	C8-C9	-8.25	1.28	1.46
17	J	102	BCR	C11-C10	-8.25	1.17	1.43
17	m	1602	BCR	C8-C9	-8.25	1.28	1.46
17	S	103	BCR	C11-C10	-8.25	1.17	1.43
17	A	852	BCR	C8-C9	-8.25	1.28	1.46
17	l	203	BCR	C11-C10	-8.25	1.17	1.43
17	S	104	BCR	C11-C10	-8.24	1.17	1.43
17	F	1302	BCR	C8-C9	-8.24	1.28	1.46
17	R	102	BCR	C11-C10	-8.23	1.17	1.43
17	H	846	BCR	C11-C10	-8.23	1.17	1.43
17	H	843	BCR	C8-C9	-8.23	1.28	1.46
17	L	207	BCR	C11-C10	-8.23	1.17	1.43
17	G	850	BCR	C11-C10	-8.22	1.17	1.43
17	V	1602	BCR	C8-C9	-8.21	1.28	1.46
17	b	846	BCR	C11-C10	-8.21	1.17	1.43
17	G	852	BCR	C11-C10	-8.20	1.17	1.43
17	U	202	BCR	C11-C10	-8.19	1.17	1.43
17	L	202	BCR	C11-C10	-8.19	1.17	1.43
17	B	850	BCR	C8-C9	-8.18	1.28	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	I	102	BCR	C8-C9	-8.18	1.28	1.46
17	G	849	BCR	C11-C10	-8.16	1.17	1.43
17	B	844	BCR	C8-C9	-8.16	1.28	1.46
17	b	849	BCR	C8-C9	-8.15	1.28	1.46
17	i	102	BCR	C11-C10	-8.15	1.17	1.43
17	R	103	BCR	C8-C9	-8.15	1.28	1.46
17	H	844	BCR	C8-C9	-8.15	1.28	1.46
17	Q	202	BCR	C11-C10	-8.15	1.17	1.43
17	l	201	BCR	C11-C10	-8.14	1.17	1.43
17	a	848	BCR	C11-C10	-8.14	1.18	1.43
17	B	847	BCR	C11-C10	-8.13	1.18	1.43
17	a	851	BCR	C11-C10	-8.13	1.18	1.43
17	H	849	BCR	C8-C9	-8.12	1.28	1.46
17	b	843	BCR	C8-C9	-8.12	1.28	1.46
17	Q	204	BCR	C8-C9	-8.12	1.28	1.46
17	B	843	BCR	C11-C10	-8.11	1.18	1.43
17	R	101	BCR	C11-C10	-8.11	1.18	1.43
17	G	848	BCR	C11-C10	-8.11	1.18	1.43
17	H	847	BCR	C11-C10	-8.11	1.18	1.43
17	A	852	BCR	C11-C10	-8.10	1.18	1.43
17	A	849	BCR	C11-C10	-8.10	1.18	1.43
17	B	842	BCR	C11-C10	-8.10	1.18	1.43
17	a	847	BCR	C11-C10	-8.09	1.18	1.43
17	I	101	BCR	C11-C10	-8.07	1.18	1.43
17	b	847	BCR	C8-C9	-8.07	1.28	1.46
17	H	843	BCR	C11-C10	-8.07	1.18	1.43
17	H	842	BCR	C11-C10	-8.07	1.18	1.43
17	G	853	BCR	C11-C10	-8.04	1.18	1.43
17	a	849	BCR	C11-C10	-8.04	1.18	1.43
17	b	847	BCR	C11-C10	-8.04	1.18	1.43
17	j	103	BCR	C11-C10	-8.04	1.18	1.43
17	A	850	BCR	C11-C10	-8.03	1.18	1.43
17	B	848	BCR	C11-C10	-8.02	1.18	1.43
17	B	844	BCR	C11-C10	-8.01	1.18	1.43
17	b	843	BCR	C11-C10	-8.00	1.18	1.43
17	M	1602	BCR	C8-C9	-7.99	1.28	1.46
17	l	208	BCR	C11-C10	-7.99	1.18	1.43
17	H	844	BCR	C11-C10	-7.99	1.18	1.43
17	b	842	BCR	C11-C10	-7.99	1.18	1.43
17	H	849	BCR	C11-C10	-7.98	1.18	1.43
17	a	852	BCR	C11-C10	-7.98	1.18	1.43
17	m	1602	BCR	C11-C10	-7.97	1.18	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	853	BCR	C11-C10	-7.96	1.18	1.43
17	b	844	BCR	C8-C9	-7.95	1.28	1.46
17	A	848	BCR	C11-C10	-7.93	1.18	1.43
17	B	850	BCR	C11-C10	-7.91	1.18	1.43
17	b	849	BCR	C11-C10	-7.91	1.18	1.43
17	b	844	BCR	C11-C10	-7.89	1.18	1.43
17	f	203	BCR	C11-C10	-7.89	1.18	1.43
17	R	103	BCR	C11-C10	-7.88	1.18	1.43
17	I	102	BCR	C11-C10	-7.88	1.18	1.43
17	J	103	BCR	C11-C10	-7.87	1.18	1.43
17	V	1602	BCR	C11-C10	-7.87	1.18	1.43
17	Q	204	BCR	C11-C10	-7.87	1.18	1.43
17	M	1602	BCR	C11-C10	-7.86	1.18	1.43
17	j	104	BCR	C11-C10	-7.85	1.18	1.43
17	G	850	BCR	C20-C21	-7.82	1.18	1.43
17	a	852	BCR	C20-C21	-7.77	1.19	1.43
14	b	836	CLA	MG-NA	7.76	2.24	2.06
17	F	1302	BCR	C11-C10	-7.76	1.19	1.43
15	A	846	PQN	C3-C2	7.73	1.49	1.35
17	a	849	BCR	C20-C21	-7.71	1.19	1.43
17	A	853	BCR	C20-C21	-7.71	1.19	1.43
17	l	201	BCR	C20-C21	-7.71	1.19	1.43
15	H	841	PQN	C3-C2	7.70	1.49	1.35
17	I	101	BCR	C20-C21	-7.70	1.19	1.43
14	G	816	CLA	MG-NA	7.69	2.24	2.06
14	f	202	CLA	MG-NA	7.68	2.24	2.06
14	b	834	CLA	MG-NA	7.67	2.24	2.06
14	A	833	CLA	MG-NA	7.67	2.24	2.06
14	a	843	CLA	MG-NA	7.67	2.24	2.06
14	T	1401	CLA	MG-NA	7.66	2.24	2.06
14	S	101	CLA	MG-NA	7.66	2.24	2.06
17	U	202	BCR	C20-C21	-7.66	1.19	1.43
17	R	101	BCR	C20-C21	-7.66	1.19	1.43
14	x	1701	CLA	MG-NA	7.65	2.24	2.06
15	a	845	PQN	C3-C2	7.65	1.48	1.35
14	W	1701	CLA	MG-NA	7.64	2.24	2.06
14	X	1701	CLA	MG-NA	7.64	2.24	2.06
17	G	853	BCR	C20-C21	-7.63	1.19	1.43
17	A	849	BCR	C20-C21	-7.63	1.19	1.43
14	H	819	CLA	MG-NA	7.63	2.24	2.06
14	a	837	CLA	MG-NA	7.62	2.24	2.06
17	b	847	BCR	C20-C21	-7.62	1.19	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	f	201	BCR	C20-C21	-7.62	1.19	1.43
17	f	201	BCR	C16-C17	-7.62	1.19	1.43
14	b	825	CLA	MG-NA	7.62	2.24	2.06
14	H	827	CLA	MG-NA	7.62	2.24	2.06
15	b	841	PQN	C3-C2	7.62	1.48	1.35
14	G	828	CLA	MG-NA	7.61	2.24	2.06
17	R	102	BCR	C16-C17	-7.61	1.19	1.43
17	l	203	BCR	C20-C21	-7.61	1.19	1.43
17	A	851	BCR	C20-C21	-7.61	1.19	1.43
17	H	846	BCR	C20-C21	-7.61	1.19	1.43
17	A	851	BCR	C16-C17	-7.60	1.19	1.43
17	G	850	BCR	C16-C17	-7.60	1.19	1.43
17	L	207	BCR	C20-C21	-7.60	1.19	1.43
17	G	851	BCR	C16-C17	-7.60	1.19	1.43
17	i	102	BCR	C20-C21	-7.60	1.19	1.43
15	B	841	PQN	C3-C2	7.60	1.48	1.35
14	G	833	CLA	MG-NA	7.60	2.24	2.06
14	a	829	CLA	MG-NA	7.60	2.24	2.06
14	A	821	CLA	MG-NA	7.59	2.24	2.06
17	l	201	BCR	C16-C17	-7.58	1.19	1.43
14	B	820	CLA	MG-NA	7.58	2.24	2.06
14	B	835	CLA	MG-NA	7.58	2.24	2.06
14	a	838	CLA	MG-NA	7.58	2.24	2.06
14	b	835	CLA	MG-NA	7.58	2.24	2.06
14	H	832	CLA	MG-NA	7.57	2.24	2.06
17	R	102	BCR	C20-C21	-7.57	1.19	1.43
14	b	819	CLA	MG-NA	7.57	2.24	2.06
14	B	811	CLA	MG-NA	7.57	2.24	2.06
14	b	814	CLA	MG-NA	7.57	2.24	2.06
17	L	202	BCR	C20-C21	-7.57	1.19	1.43
14	G	844	CLA	MG-NA	7.57	2.24	2.06
14	J	101	CLA	MG-NA	7.57	2.24	2.06
14	j	102	CLA	MG-NA	7.56	2.24	2.06
14	K	101	CLA	MG-NA	7.56	2.24	2.06
14	B	821	CLA	MG-NA	7.56	2.24	2.06
17	l	203	BCR	C16-C17	-7.56	1.19	1.43
14	G	821	CLA	MG-NA	7.56	2.24	2.06
14	H	821	CLA	MG-NA	7.56	2.24	2.06
14	S	102	CLA	MG-NA	7.56	2.24	2.06
14	B	827	CLA	MG-NA	7.55	2.24	2.06
14	B	834	CLA	MG-NA	7.55	2.24	2.06
17	a	849	BCR	C16-C17	-7.55	1.19	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	837	CLA	MG-NA	7.55	2.24	2.06
14	a	823	CLA	MG-NA	7.55	2.24	2.06
17	Q	202	BCR	C20-C21	-7.54	1.19	1.43
17	a	850	BCR	C16-C17	-7.54	1.19	1.43
14	a	815	CLA	MG-NA	7.54	2.24	2.06
14	K	102	CLA	MG-NA	7.54	2.24	2.06
17	B	847	BCR	C20-C21	-7.54	1.19	1.43
14	b	821	CLA	MG-NA	7.54	2.24	2.06
14	A	819	CLA	MG-NA	7.54	2.24	2.06
14	H	830	CLA	MG-NA	7.54	2.24	2.06
14	a	814	CLA	MG-NA	7.53	2.24	2.06
14	G	825	CLA	MG-NA	7.53	2.24	2.06
14	a	825	CLA	MG-NA	7.53	2.24	2.06
14	b	811	CLA	MG-NA	7.53	2.24	2.06
14	H	836	CLA	MG-NA	7.53	2.24	2.06
14	A	824	CLA	MG-NA	7.53	2.24	2.06
14	a	827	CLA	MG-NA	7.53	2.24	2.06
14	A	826	CLA	MG-NA	7.52	2.24	2.06
17	J	102	BCR	C16-C17	-7.52	1.19	1.43
15	G	846	PQN	C3-C2	7.52	1.48	1.35
14	B	830	CLA	MG-NA	7.52	2.24	2.06
17	L	202	BCR	C16-C17	-7.52	1.19	1.43
14	Q	203	CLA	MG-NA	7.52	2.24	2.06
14	j	101	CLA	MG-NA	7.52	2.24	2.06
14	A	804	CLA	MG-NA	7.51	2.24	2.06
17	G	852	BCR	C20-C21	-7.51	1.19	1.43
14	b	832	CLA	MG-NA	7.51	2.24	2.06
14	B	819	CLA	MG-NA	7.51	2.24	2.06
14	B	825	CLA	MG-NA	7.51	2.24	2.06
17	H	846	BCR	C16-C17	-7.51	1.19	1.43
14	A	823	CLA	MG-NA	7.51	2.24	2.06
14	a	839	CLA	MG-NA	7.51	2.24	2.06
17	l	208	BCR	C20-C21	-7.51	1.19	1.43
14	G	837	CLA	MG-NA	7.50	2.24	2.06
14	H	834	CLA	MG-NA	7.50	2.24	2.06
17	S	103	BCR	C16-C17	-7.50	1.19	1.43
17	B	846	BCR	C16-C17	-7.50	1.19	1.43
17	B	846	BCR	C20-C21	-7.50	1.19	1.43
17	a	850	BCR	C20-C21	-7.50	1.19	1.43
14	k	1401	CLA	MG-NA	7.50	2.24	2.06
17	B	848	BCR	C20-C21	-7.50	1.19	1.43
14	A	843	CLA	MG-NA	7.50	2.24	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	803	CLA	MG-NA	7.50	2.24	2.06
14	A	830	CLA	MG-NA	7.50	2.24	2.06
14	V	1601	CLA	MG-NA	7.50	2.24	2.06
17	G	851	BCR	C20-C21	-7.50	1.19	1.43
14	G	829	CLA	MG-NA	7.50	2.24	2.06
17	U	202	BCR	C16-C17	-7.50	1.19	1.43
14	B	832	CLA	MG-NA	7.50	2.24	2.06
14	a	832	CLA	MG-NA	7.50	2.24	2.06
14	a	818	CLA	MG-NA	7.50	2.24	2.06
14	a	828	CLA	MG-NA	7.49	2.24	2.06
14	G	838	CLA	MG-NA	7.49	2.24	2.06
14	b	831	CLA	MG-NA	7.49	2.24	2.06
14	A	816	CLA	MG-NA	7.49	2.24	2.06
17	Q	202	BCR	C16-C17	-7.49	1.20	1.43
14	A	832	CLA	MG-NA	7.49	2.24	2.06
14	G	826	CLA	MG-NA	7.49	2.24	2.06
17	b	843	BCR	C20-C21	-7.49	1.20	1.43
17	b	844	BCR	C20-C21	-7.49	1.20	1.43
17	A	850	BCR	C20-C21	-7.48	1.20	1.43
14	G	824	CLA	MG-NA	7.48	2.24	2.06
14	G	832	CLA	MG-NA	7.48	2.24	2.06
17	H	842	BCR	C20-C21	-7.48	1.20	1.43
17	G	849	BCR	C16-C17	-7.48	1.20	1.43
14	a	831	CLA	MG-NA	7.48	2.24	2.06
14	H	811	CLA	MG-NA	7.47	2.24	2.06
14	G	842	CLA	MG-NA	7.47	2.24	2.06
14	G	819	CLA	MG-NA	7.47	2.24	2.06
14	b	830	CLA	MG-NA	7.47	2.24	2.06
17	I	101	BCR	C16-C17	-7.46	1.20	1.43
14	G	840	CLA	MG-NA	7.46	2.24	2.06
14	b	826	CLA	MG-NA	7.46	2.24	2.06
14	L	206	CLA	MG-NA	7.46	2.24	2.06
14	A	840	CLA	MG-NA	7.46	2.24	2.06
14	G	834	CLA	MG-NA	7.46	2.24	2.06
14	H	816	CLA	MG-NA	7.46	2.24	2.06
14	H	820	CLA	MG-NA	7.46	2.24	2.06
14	a	824	CLA	MG-NA	7.46	2.24	2.06
14	H	831	CLA	MG-NA	7.46	2.24	2.06
17	L	207	BCR	C16-C17	-7.46	1.20	1.43
17	G	852	BCR	C16-C17	-7.45	1.20	1.43
14	A	810	CLA	MG-NA	7.45	2.24	2.06
17	A	852	BCR	C16-C17	-7.45	1.20	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	822	CLA	MG-NA	7.45	2.24	2.06
14	m	1601	CLA	MG-NA	7.45	2.24	2.06
14	G	814	CLA	MG-NA	7.45	2.24	2.06
14	b	816	CLA	MG-NA	7.45	2.24	2.06
17	B	847	BCR	C16-C17	-7.45	1.20	1.43
17	H	843	BCR	C20-C21	-7.45	1.20	1.43
17	j	103	BCR	C20-C21	-7.45	1.20	1.43
14	G	808	CLA	MG-NA	7.45	2.24	2.06
14	G	804	CLA	MG-NA	7.45	2.24	2.06
14	B	836	CLA	MG-NA	7.44	2.24	2.06
14	F	1301	CLA	MG-NA	7.44	2.24	2.06
14	a	812	CLA	MG-NA	7.44	2.24	2.06
14	B	814	CLA	MG-NA	7.44	2.24	2.06
14	G	839	CLA	MG-NA	7.44	2.23	2.06
14	G	805	CLA	MG-NA	7.44	2.23	2.06
14	G	811	CLA	MG-NA	7.44	2.23	2.06
14	G	843	CLA	MG-NA	7.44	2.23	2.06
14	M	1601	CLA	MG-NA	7.44	2.23	2.06
14	a	820	CLA	MG-NA	7.44	2.23	2.06
14	a	855	CLA	MG-NA	7.44	2.23	2.06
14	a	821	CLA	MG-NA	7.44	2.23	2.06
14	A	834	CLA	MG-NA	7.43	2.23	2.06
14	a	833	CLA	MG-NA	7.43	2.23	2.06
14	F	1303	CLA	MG-NA	7.43	2.23	2.06
14	A	815	CLA	MG-NA	7.43	2.23	2.06
17	A	852	BCR	C20-C21	-7.43	1.20	1.43
14	B	801	CLA	MG-NA	7.43	2.23	2.06
14	a	842	CLA	MG-NA	7.43	2.23	2.06
17	H	847	BCR	C20-C21	-7.43	1.20	1.43
14	H	818	CLA	MG-NA	7.43	2.23	2.06
14	A	838	CLA	MG-NA	7.43	2.23	2.06
14	a	804	CLA	MG-NA	7.42	2.23	2.06
14	Q	201	CLA	MG-NA	7.42	2.23	2.06
14	A	803	CLA	MG-NA	7.42	2.23	2.06
14	G	813	CLA	MG-NA	7.42	2.23	2.06
17	a	851	BCR	C20-C21	-7.41	1.20	1.43
17	S	104	BCR	C16-C17	-7.41	1.20	1.43
14	G	815	CLA	MG-NA	7.41	2.23	2.06
17	B	842	BCR	C20-C21	-7.41	1.20	1.43
17	j	103	BCR	C16-C17	-7.40	1.20	1.43
14	B	810	CLA	MG-NA	7.40	2.23	2.06
17	B	843	BCR	C20-C21	-7.40	1.20	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	823	CLA	MG-NA	7.40	2.23	2.06
14	U	201	CLA	MG-NA	7.40	2.23	2.06
17	a	848	BCR	C20-C21	-7.40	1.20	1.43
14	H	825	CLA	MG-NA	7.40	2.23	2.06
17	B	844	BCR	C20-C21	-7.40	1.20	1.43
14	H	810	CLA	MG-NA	7.40	2.23	2.06
14	H	801	CLA	MG-NA	7.39	2.23	2.06
17	i	102	BCR	C16-C17	-7.39	1.20	1.43
14	a	809	CLA	MG-NA	7.39	2.23	2.06
14	L	201	CLA	MG-NA	7.39	2.23	2.06
14	a	810	CLA	MG-NA	7.39	2.23	2.06
14	G	830	CLA	MG-NA	7.39	2.23	2.06
14	B	818	CLA	MG-NA	7.39	2.23	2.06
17	J	102	BCR	C20-C21	-7.39	1.20	1.43
14	A	820	CLA	MG-NA	7.39	2.23	2.06
14	A	839	CLA	MG-NA	7.39	2.23	2.06
17	a	848	BCR	C16-C17	-7.39	1.20	1.43
14	A	805	CLA	MG-NA	7.39	2.23	2.06
14	B	815	CLA	MG-NA	7.39	2.23	2.06
14	A	814	CLA	MG-NA	7.39	2.23	2.06
14	b	810	CLA	MG-NA	7.39	2.23	2.06
14	B	831	CLA	MG-NA	7.38	2.23	2.06
14	b	827	CLA	MG-NA	7.38	2.23	2.06
17	B	843	BCR	C16-C17	-7.38	1.20	1.43
17	B	844	BCR	C16-C17	-7.38	1.20	1.43
14	A	828	CLA	MG-NA	7.38	2.23	2.06
17	b	846	BCR	C20-C21	-7.38	1.20	1.43
14	b	815	CLA	MG-NA	7.38	2.23	2.06
17	G	849	BCR	C20-C21	-7.38	1.20	1.43
14	A	817	CLA	MG-NA	7.38	2.23	2.06
14	H	835	CLA	MG-NA	7.38	2.23	2.06
14	G	818	CLA	MG-NA	7.38	2.23	2.06
14	A	813	CLA	MG-NA	7.38	2.23	2.06
17	b	846	BCR	C16-C17	-7.38	1.20	1.43
17	H	845	BCR	C20-C21	-7.38	1.20	1.43
14	A	829	CLA	MG-NA	7.38	2.23	2.06
14	H	817	CLA	MG-NA	7.37	2.23	2.06
14	b	838	CLA	MG-NA	7.37	2.23	2.06
14	A	836	CLA	MG-NA	7.37	2.23	2.06
17	f	203	BCR	C20-C21	-7.37	1.20	1.43
17	S	104	BCR	C20-C21	-7.37	1.20	1.43
14	A	811	CLA	MG-NA	7.37	2.23	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	824	CLA	MG-NA	7.37	2.23	2.06
14	a	813	CLA	MG-NA	7.37	2.23	2.06
14	b	820	CLA	MG-NA	7.36	2.23	2.06
14	a	841	CLA	MG-NA	7.36	2.23	2.06
14	H	809	CLA	MG-NA	7.36	2.23	2.06
14	B	804	CLA	MG-NA	7.36	2.23	2.06
17	H	844	BCR	C20-C21	-7.36	1.20	1.43
17	J	103	BCR	C20-C21	-7.36	1.20	1.43
14	A	812	CLA	MG-NA	7.36	2.23	2.06
17	A	849	BCR	C16-C17	-7.36	1.20	1.43
17	Q	204	BCR	C20-C21	-7.36	1.20	1.43
17	H	844	BCR	C16-C17	-7.35	1.20	1.43
14	G	820	CLA	MG-NA	7.35	2.23	2.06
14	B	839	CLA	MG-NA	7.35	2.23	2.06
14	H	814	CLA	MG-NA	7.35	2.23	2.06
17	B	848	BCR	C16-C17	-7.35	1.20	1.43
17	R	101	BCR	C16-C17	-7.35	1.20	1.43
14	B	826	CLA	MG-NA	7.35	2.23	2.06
14	A	808	CLA	MG-NA	7.35	2.23	2.06
14	b	824	CLA	MG-NA	7.34	2.23	2.06
17	B	842	BCR	C16-C17	-7.34	1.20	1.43
14	b	822	CLA	MG-NA	7.34	2.23	2.06
14	G	836	CLA	MG-NA	7.34	2.23	2.06
14	l	205	CLA	MG-NA	7.34	2.23	2.06
17	a	851	BCR	C16-C17	-7.34	1.20	1.43
14	A	842	CLA	MG-NA	7.34	2.23	2.06
14	H	838	CLA	MG-NA	7.34	2.23	2.06
14	i	101	CLA	MG-NA	7.34	2.23	2.06
14	A	825	CLA	MG-NA	7.34	2.23	2.06
14	a	836	CLA	MG-NA	7.34	2.23	2.06
14	G	810	CLA	MG-NA	7.33	2.23	2.06
17	b	843	BCR	C16-C17	-7.33	1.20	1.43
17	A	850	BCR	C16-C17	-7.33	1.20	1.43
14	H	829	CLA	MG-NA	7.33	2.23	2.06
17	l	208	BCR	C16-C17	-7.33	1.20	1.43
14	A	844	CLA	MG-NA	7.33	2.23	2.06
14	B	838	CLA	MG-NA	7.33	2.23	2.06
14	H	804	CLA	MG-NA	7.33	2.23	2.06
17	b	845	BCR	C20-C21	-7.33	1.20	1.43
14	a	816	CLA	MG-NA	7.32	2.23	2.06
14	B	808	CLA	MG-NA	7.32	2.23	2.06
14	U	204	CLA	MG-NA	7.32	2.23	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	837	CLA	MG-NA	7.32	2.23	2.06
14	H	823	CLA	MG-NA	7.32	2.23	2.06
14	a	844	CLA	MG-NA	7.32	2.23	2.06
17	b	847	BCR	C16-C17	-7.32	1.20	1.43
17	R	103	BCR	C20-C21	-7.32	1.20	1.43
17	G	848	BCR	C20-C21	-7.32	1.20	1.43
17	f	203	BCR	C16-C17	-7.31	1.20	1.43
14	a	811	CLA	MG-NA	7.31	2.23	2.06
14	G	803	CLA	MG-NA	7.31	2.23	2.06
14	B	805	CLA	MG-NA	7.31	2.23	2.06
14	H	822	CLA	MG-NA	7.31	2.23	2.06
17	b	844	BCR	C16-C17	-7.30	1.20	1.43
17	S	103	BCR	C20-C21	-7.30	1.20	1.43
14	b	837	CLA	MG-NA	7.30	2.23	2.06
14	A	841	CLA	MG-NA	7.30	2.23	2.06
17	H	842	BCR	C16-C17	-7.30	1.20	1.43
14	G	817	CLA	MG-NA	7.30	2.23	2.06
14	l	202	CLA	MG-NA	7.30	2.23	2.06
14	a	840	CLA	MG-NA	7.30	2.23	2.06
17	H	843	BCR	C16-C17	-7.29	1.20	1.43
17	a	847	BCR	C20-C21	-7.29	1.20	1.43
14	B	823	CLA	MG-NA	7.29	2.23	2.06
17	I	102	BCR	C20-C21	-7.29	1.20	1.43
14	a	802	CLA	MG-NA	7.29	2.23	2.06
14	U	206	CLA	MG-NA	7.29	2.23	2.06
14	B	822	CLA	MG-NA	7.29	2.23	2.06
14	b	818	CLA	MG-NA	7.29	2.23	2.06
17	b	842	BCR	C20-C21	-7.29	1.20	1.43
17	a	847	BCR	C16-C17	-7.29	1.20	1.43
14	b	805	CLA	MG-NA	7.29	2.23	2.06
17	m	1602	BCR	C20-C21	-7.29	1.20	1.43
17	M	1602	BCR	C20-C21	-7.28	1.20	1.43
14	B	812	CLA	MG-NA	7.28	2.23	2.06
14	B	809	CLA	MG-NA	7.28	2.23	2.06
14	B	840	CLA	MG-NA	7.28	2.23	2.06
14	H	828	CLA	MG-NA	7.28	2.23	2.06
14	L	204	CLA	MG-NA	7.28	2.23	2.06
17	b	849	BCR	C20-C21	-7.28	1.20	1.43
14	G	809	CLA	MG-NA	7.28	2.23	2.06
14	B	807	CLA	MG-NA	7.27	2.23	2.06
14	b	812	CLA	MG-NA	7.27	2.23	2.06
17	j	104	BCR	C16-C17	-7.27	1.20	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	802	CLA	MG-NA	7.27	2.23	2.06
14	B	816	CLA	MG-NA	7.27	2.23	2.06
14	H	826	CLA	MG-NA	7.27	2.23	2.06
17	V	1602	BCR	C20-C21	-7.27	1.20	1.43
17	H	847	BCR	C16-C17	-7.27	1.20	1.43
14	G	812	CLA	MG-NA	7.27	2.23	2.06
14	H	815	CLA	MG-NA	7.26	2.23	2.06
17	Q	204	BCR	C16-C17	-7.26	1.20	1.43
14	B	824	CLA	MG-NA	7.26	2.23	2.06
17	A	848	BCR	C20-C21	-7.26	1.20	1.43
17	b	842	BCR	C16-C17	-7.26	1.20	1.43
17	H	845	BCR	C16-C17	-7.26	1.20	1.43
14	b	817	CLA	MG-NA	7.25	2.23	2.06
14	b	809	CLA	MG-NA	7.25	2.23	2.06
14	G	822	CLA	MG-NA	7.25	2.23	2.06
17	B	845	BCR	C20-C21	-7.25	1.20	1.43
14	a	807	CLA	MG-NA	7.25	2.23	2.06
14	A	822	CLA	MG-NA	7.24	2.23	2.06
14	H	813	CLA	MG-NA	7.24	2.23	2.06
17	G	853	BCR	C16-C17	-7.24	1.20	1.43
17	J	103	BCR	C16-C17	-7.24	1.20	1.43
17	b	845	BCR	C16-C17	-7.24	1.20	1.43
17	j	104	BCR	C20-C21	-7.23	1.20	1.43
17	H	849	BCR	C20-C21	-7.23	1.20	1.43
14	G	827	CLA	MG-NA	7.23	2.23	2.06
14	H	808	CLA	MG-NA	7.23	2.23	2.06
17	G	848	BCR	C16-C17	-7.23	1.20	1.43
13	G	801	CL0	MG-NA	7.23	2.23	2.06
14	a	819	CLA	MG-NA	7.23	2.23	2.06
14	G	841	CLA	MG-NA	7.22	2.23	2.06
14	a	835	CLA	MG-NA	7.22	2.23	2.06
14	b	840	CLA	MG-NA	7.22	2.23	2.06
14	b	829	CLA	MG-NA	7.21	2.23	2.06
14	b	823	CLA	MG-NA	7.21	2.23	2.06
14	B	806	CLA	MG-NA	7.21	2.23	2.06
14	a	817	CLA	MG-NA	7.21	2.23	2.06
14	A	845	CLA	MG-NA	7.20	2.23	2.06
17	B	850	BCR	C20-C21	-7.20	1.20	1.43
14	B	833	CLA	MG-NA	7.20	2.23	2.06
14	b	839	CLA	MG-NA	7.20	2.23	2.06
17	A	853	BCR	C16-C17	-7.20	1.20	1.43
14	H	812	CLA	MG-NA	7.20	2.23	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	1602	BCR	C16-C17	-7.20	1.20	1.43
14	H	839	CLA	MG-NA	7.20	2.23	2.06
13	A	801	CL0	MG-NA	7.20	2.23	2.06
14	H	840	CLA	MG-NA	7.19	2.23	2.06
17	M	1602	BCR	C16-C17	-7.19	1.20	1.43
14	a	834	CLA	MG-NA	7.19	2.23	2.06
17	a	852	BCR	C16-C17	-7.19	1.20	1.43
14	B	829	CLA	MG-NA	7.18	2.23	2.06
14	U	205	CLA	MG-NA	7.18	2.23	2.06
14	l	207	CLA	MG-NA	7.18	2.23	2.06
17	F	1302	BCR	C16-C17	-7.18	1.20	1.43
17	F	1302	BCR	C20-C21	-7.17	1.20	1.43
17	B	845	BCR	C16-C17	-7.17	1.20	1.43
14	G	835	CLA	MG-NA	7.17	2.23	2.06
14	H	833	CLA	MG-NA	7.17	2.23	2.06
14	H	807	CLA	MG-NA	7.17	2.23	2.06
17	R	103	BCR	C16-C17	-7.16	1.21	1.43
14	A	831	CLA	MG-NA	7.16	2.23	2.06
17	A	848	BCR	C16-C17	-7.16	1.21	1.43
14	b	807	CLA	MG-NA	7.16	2.23	2.06
14	G	831	CLA	MG-NA	7.16	2.23	2.06
17	m	1602	BCR	C16-C17	-7.15	1.21	1.43
14	A	818	CLA	MG-NA	7.15	2.23	2.06
14	H	805	CLA	MG-NA	7.13	2.23	2.06
14	b	828	CLA	MG-NA	7.13	2.23	2.06
14	A	802	CLA	MG-NA	7.12	2.23	2.06
14	B	828	CLA	MG-NA	7.12	2.23	2.06
14	b	806	CLA	MG-NA	7.12	2.23	2.06
14	H	806	CLA	MG-NA	7.12	2.23	2.06
14	b	833	CLA	MG-NA	7.12	2.23	2.06
14	a	806	CLA	MG-NA	7.12	2.23	2.06
14	L	205	CLA	MG-NA	7.11	2.23	2.06
14	b	813	CLA	MG-NA	7.11	2.23	2.06
17	I	102	BCR	C16-C17	-7.10	1.21	1.43
14	b	808	CLA	MG-NA	7.10	2.23	2.06
14	B	817	CLA	MG-NA	7.08	2.23	2.06
14	G	807	CLA	MG-NA	7.08	2.23	2.06
14	a	830	CLA	MG-NA	7.08	2.23	2.06
14	A	827	CLA	MG-NA	7.07	2.23	2.06
14	B	837	CLA	MG-NA	7.07	2.23	2.06
14	A	806	CLA	MG-NA	7.07	2.23	2.06
17	H	849	BCR	C16-C17	-7.07	1.21	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	845	CLA	MG-NA	7.05	2.23	2.06
14	B	813	CLA	MG-NA	7.04	2.23	2.06
14	b	804	CLA	MG-NA	7.04	2.23	2.06
14	A	807	CLA	MG-NA	7.03	2.23	2.06
14	H	802	CLA	MG-NA	7.02	2.22	2.06
14	a	826	CLA	MG-NA	7.01	2.22	2.06
14	B	803	CLA	MG-NA	7.01	2.22	2.06
14	b	803	CLA	MG-NA	7.01	2.22	2.06
14	a	808	CLA	MG-NA	7.01	2.22	2.06
14	A	835	CLA	MG-NA	7.01	2.22	2.06
14	b	801	CLA	MG-NA	7.00	2.22	2.06
14	B	802	CLA	MG-NA	7.00	2.22	2.06
14	l	206	CLA	MG-NA	7.00	2.22	2.06
17	b	849	BCR	C16-C17	-7.00	1.21	1.43
13	a	801	CL0	MG-NA	6.98	2.22	2.06
17	B	850	BCR	C16-C17	-6.97	1.21	1.43
14	a	805	CLA	MG-NA	6.97	2.22	2.06
14	G	802	CLA	MG-NA	6.96	2.22	2.06
14	G	806	CLA	MG-NA	6.83	2.22	2.06
14	A	809	CLA	MG-NA	6.78	2.22	2.06
14	H	803	CLA	MG-NA	6.75	2.22	2.06
14	G	828	CLA	CHC-C1C	5.79	1.48	1.34
14	H	801	CLA	CHC-C1C	5.72	1.48	1.34
14	H	816	CLA	CHC-C1C	5.69	1.48	1.34
14	B	816	CLA	CHC-C1C	5.68	1.48	1.34
14	A	818	CLA	CHC-C1C	5.66	1.48	1.34
14	H	832	CLA	O2A-C1	5.65	1.61	1.46
14	A	828	CLA	CHC-C1C	5.65	1.48	1.34
14	b	824	CLA	CHC-C1C	5.65	1.48	1.34
14	H	831	CLA	CHC-C1C	5.64	1.48	1.34
14	G	819	CLA	CHC-C1C	5.61	1.48	1.34
14	B	824	CLA	CHC-C1C	5.60	1.48	1.34
14	b	808	CLA	O2A-C1	5.59	1.61	1.46
14	A	819	CLA	CHC-C1C	5.58	1.48	1.34
14	H	808	CLA	O2A-C1	5.58	1.61	1.46
14	b	816	CLA	CHC-C1C	5.57	1.48	1.34
14	b	833	CLA	CHC-C1C	5.57	1.48	1.34
14	b	831	CLA	O2A-C1	5.57	1.61	1.46
14	b	835	CLA	CHC-C1C	5.56	1.48	1.34
14	a	818	CLA	CHC-C1C	5.56	1.48	1.34
14	a	817	CLA	CHC-C1C	5.56	1.48	1.34
14	L	201	CLA	O2A-C1	5.56	1.61	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	813	CLA	C3B-C2B	5.55	1.47	1.40
14	H	810	CLA	C3B-C2B	5.55	1.47	1.40
14	A	811	CLA	O2D-CGD	5.55	1.46	1.33
14	a	855	CLA	CHC-C1C	5.54	1.48	1.34
14	S	102	CLA	CHC-C1C	5.54	1.48	1.34
14	B	820	CLA	C3B-C2B	5.54	1.47	1.40
14	H	811	CLA	CHC-C1C	5.54	1.48	1.34
14	T	1401	CLA	CHC-C1C	5.54	1.48	1.34
14	a	842	CLA	O2A-C1	5.53	1.61	1.46
14	B	801	CLA	CHC-C1C	5.53	1.48	1.34
14	G	805	CLA	CHC-C1C	5.53	1.48	1.34
14	G	827	CLA	CHC-C1C	5.53	1.48	1.34
14	H	831	CLA	C3B-C2B	5.52	1.47	1.40
14	B	831	CLA	O2A-C1	5.52	1.61	1.46
14	H	839	CLA	CHC-C1C	5.52	1.48	1.34
14	a	804	CLA	CHC-C1C	5.52	1.48	1.34
14	B	812	CLA	C3B-C2B	5.52	1.47	1.40
14	U	204	CLA	CHC-C1C	5.52	1.48	1.34
14	b	805	CLA	O2A-C1	5.51	1.61	1.46
14	A	823	CLA	C3B-C2B	5.51	1.47	1.40
14	a	808	CLA	CHC-C1C	5.51	1.48	1.34
14	A	843	CLA	O2A-C1	5.51	1.61	1.46
14	b	827	CLA	O2A-C1	5.51	1.61	1.46
14	b	818	CLA	CHC-C1C	5.51	1.48	1.34
14	a	821	CLA	CHC-C1C	5.51	1.48	1.34
14	G	842	CLA	O2A-C1	5.51	1.61	1.46
14	G	809	CLA	CHC-C1C	5.50	1.48	1.34
14	G	812	CLA	O2A-C1	5.50	1.60	1.46
14	H	827	CLA	O2A-C1	5.50	1.60	1.46
14	a	819	CLA	O2A-C1	5.50	1.60	1.46
14	B	839	CLA	CHC-C1C	5.49	1.48	1.34
14	a	827	CLA	CHC-C1C	5.49	1.48	1.34
14	a	855	CLA	O2A-C1	5.49	1.60	1.46
14	a	828	CLA	CHC-C1C	5.48	1.48	1.34
14	b	831	CLA	CHC-C1C	5.48	1.48	1.34
14	b	811	CLA	CHC-C1C	5.48	1.48	1.34
14	A	802	CLA	CHC-C1C	5.48	1.48	1.34
14	H	831	CLA	O2A-C1	5.48	1.60	1.46
14	H	840	CLA	O2A-C1	5.48	1.60	1.46
14	B	804	CLA	O2A-C1	5.48	1.60	1.46
14	H	801	CLA	O2A-C1	5.47	1.60	1.46
14	Q	203	CLA	CHC-C1C	5.47	1.48	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	801	CLA	CHC-C1C	5.47	1.48	1.34
14	A	814	CLA	O2A-C1	5.47	1.60	1.46
14	b	826	CLA	O2A-C1	5.47	1.60	1.46
14	G	804	CLA	CHC-C1C	5.47	1.48	1.34
14	A	816	CLA	C3B-C2B	5.47	1.47	1.40
14	b	810	CLA	CHC-C1C	5.47	1.48	1.34
14	a	832	CLA	C3B-C2B	5.47	1.47	1.40
14	B	808	CLA	O2A-C1	5.47	1.60	1.46
14	A	806	CLA	CHC-C1C	5.47	1.48	1.34
14	a	820	CLA	O2A-C1	5.46	1.60	1.46
14	b	840	CLA	O2A-C1	5.46	1.60	1.46
14	B	801	CLA	O2A-C1	5.46	1.60	1.46
14	H	823	CLA	O2A-C1	5.46	1.60	1.46
14	a	812	CLA	CHC-C1C	5.46	1.48	1.34
14	B	803	CLA	O2A-C1	5.45	1.60	1.46
14	G	802	CLA	O2A-C1	5.45	1.60	1.46
14	G	814	CLA	CHC-C1C	5.45	1.48	1.34
14	B	813	CLA	C3B-C2B	5.45	1.47	1.40
14	a	824	CLA	C3B-C2B	5.45	1.47	1.40
14	G	826	CLA	O2A-C1	5.45	1.60	1.46
14	b	804	CLA	CHC-C1C	5.45	1.48	1.34
14	G	835	CLA	O2A-C1	5.45	1.60	1.46
14	a	837	CLA	C3B-C2B	5.45	1.47	1.40
14	B	810	CLA	C3B-C2B	5.44	1.47	1.40
14	a	844	CLA	CHC-C1C	5.44	1.48	1.34
14	A	808	CLA	CHC-C1C	5.44	1.48	1.34
14	A	833	CLA	CHC-C1C	5.44	1.48	1.34
14	H	815	CLA	CHC-C1C	5.44	1.48	1.34
14	A	805	CLA	CHC-C1C	5.44	1.48	1.34
14	G	833	CLA	C3B-C2B	5.44	1.47	1.40
14	A	838	CLA	O2A-C1	5.44	1.60	1.46
14	B	823	CLA	C3B-C2B	5.44	1.47	1.40
14	B	833	CLA	CHC-C1C	5.44	1.48	1.34
14	H	813	CLA	C3B-C2B	5.43	1.47	1.40
14	b	833	CLA	C3B-C2B	5.43	1.47	1.40
14	B	804	CLA	CHC-C1C	5.43	1.47	1.34
14	H	804	CLA	CHC-C1C	5.43	1.47	1.34
14	H	813	CLA	CHC-C1C	5.43	1.47	1.34
14	H	810	CLA	CHC-C1C	5.43	1.47	1.34
14	a	809	CLA	CHC-C1C	5.43	1.47	1.34
14	H	804	CLA	O2A-C1	5.42	1.60	1.46
14	a	840	CLA	CHC-C1C	5.42	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	817	CLA	CHC-C1C	5.42	1.47	1.34
14	A	812	CLA	O2A-C1	5.42	1.60	1.46
14	A	803	CLA	CHC-C1C	5.42	1.47	1.34
14	L	205	CLA	CHC-C1C	5.42	1.47	1.34
14	G	821	CLA	O2A-C1	5.42	1.60	1.46
14	B	823	CLA	O2A-C1	5.42	1.60	1.46
14	G	803	CLA	CHC-C1C	5.42	1.47	1.34
14	B	826	CLA	O2A-C1	5.42	1.60	1.46
14	B	827	CLA	O2A-C1	5.42	1.60	1.46
14	U	201	CLA	O2A-C1	5.42	1.60	1.46
14	b	825	CLA	O2A-C1	5.42	1.60	1.46
14	H	818	CLA	CHC-C1C	5.41	1.47	1.34
14	a	826	CLA	CHC-C1C	5.41	1.47	1.34
14	a	803	CLA	CHC-C1C	5.41	1.47	1.34
14	a	825	CLA	C3B-C2B	5.41	1.47	1.40
14	b	806	CLA	O2A-C1	5.41	1.60	1.46
14	A	804	CLA	CHC-C1C	5.41	1.47	1.34
14	G	822	CLA	CHC-C1C	5.41	1.47	1.34
14	A	843	CLA	CHC-C1C	5.41	1.47	1.34
14	B	818	CLA	CHC-C1C	5.41	1.47	1.34
14	H	837	CLA	CHC-C1C	5.41	1.47	1.34
14	B	810	CLA	CHC-C1C	5.41	1.47	1.34
14	b	805	CLA	CHC-C1C	5.41	1.47	1.34
14	b	814	CLA	C3B-C2B	5.41	1.47	1.40
14	A	824	CLA	CHC-C1C	5.40	1.47	1.34
14	a	825	CLA	CHC-C1C	5.40	1.47	1.34
14	U	206	CLA	C3B-C2B	5.40	1.47	1.40
14	G	813	CLA	O2A-C1	5.40	1.60	1.46
14	G	833	CLA	CHC-C1C	5.40	1.47	1.34
14	H	805	CLA	CHC-C1C	5.40	1.47	1.34
14	A	832	CLA	O2A-C1	5.40	1.60	1.46
14	m	1601	CLA	O2D-CGD	5.40	1.46	1.33
14	H	825	CLA	O2A-C1	5.40	1.60	1.46
14	U	205	CLA	CHC-C1C	5.40	1.47	1.34
14	U	204	CLA	O2A-C1	5.40	1.60	1.46
14	A	825	CLA	C3B-C2B	5.40	1.47	1.40
14	a	828	CLA	O2A-C1	5.40	1.60	1.46
14	G	823	CLA	C3B-C2B	5.39	1.47	1.40
14	G	808	CLA	CHC-C1C	5.39	1.47	1.34
14	f	202	CLA	CHC-C1C	5.39	1.47	1.34
14	A	838	CLA	C3B-C2B	5.39	1.47	1.40
14	a	837	CLA	O2A-C1	5.39	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	k	1401	CLA	CHC-C1C	5.39	1.47	1.34
14	G	842	CLA	CHC-C1C	5.39	1.47	1.34
14	b	822	CLA	CHC-C1C	5.39	1.47	1.34
14	b	819	CLA	CHC-C1C	5.38	1.47	1.34
14	B	804	CLA	C3B-C2B	5.38	1.47	1.40
14	B	813	CLA	O2A-C1	5.38	1.60	1.46
14	H	821	CLA	CHC-C1C	5.38	1.47	1.34
14	a	837	CLA	CHC-C1C	5.38	1.47	1.34
14	a	809	CLA	O2A-C1	5.38	1.60	1.46
14	H	833	CLA	CHC-C1C	5.38	1.47	1.34
14	a	836	CLA	CHC-C1C	5.38	1.47	1.34
14	G	810	CLA	O2A-C1	5.38	1.60	1.46
14	H	813	CLA	O2A-C1	5.38	1.60	1.46
14	a	831	CLA	CHC-C1C	5.38	1.47	1.34
14	b	810	CLA	C3B-C2B	5.38	1.47	1.40
14	H	819	CLA	CHC-C1C	5.38	1.47	1.34
14	b	815	CLA	CHC-C1C	5.37	1.47	1.34
14	A	806	CLA	C3B-C2B	5.37	1.47	1.40
14	H	824	CLA	CHC-C1C	5.37	1.47	1.34
14	H	830	CLA	CHC-C1C	5.37	1.47	1.34
14	B	822	CLA	CHC-C1C	5.37	1.47	1.34
14	B	831	CLA	CHC-C1C	5.37	1.47	1.34
14	B	815	CLA	CHC-C1C	5.37	1.47	1.34
14	a	807	CLA	CHC-C1C	5.37	1.47	1.34
14	b	837	CLA	CHC-C1C	5.37	1.47	1.34
14	L	205	CLA	O2A-C1	5.37	1.60	1.46
14	b	823	CLA	O2A-C1	5.37	1.60	1.46
14	B	809	CLA	O2A-C1	5.37	1.60	1.46
14	l	206	CLA	O2A-C1	5.37	1.60	1.46
14	G	831	CLA	O2A-C1	5.37	1.60	1.46
14	A	842	CLA	CHC-C1C	5.37	1.47	1.34
14	B	840	CLA	O2A-C1	5.36	1.60	1.46
14	A	840	CLA	CHC-C1C	5.36	1.47	1.34
14	L	206	CLA	CHC-C1C	5.36	1.47	1.34
14	a	813	CLA	CHC-C1C	5.36	1.47	1.34
14	A	834	CLA	CHC-C1C	5.36	1.47	1.34
14	b	825	CLA	CHC-C1C	5.36	1.47	1.34
14	A	807	CLA	O2A-C1	5.36	1.60	1.46
14	B	817	CLA	O2A-C1	5.36	1.60	1.46
14	b	839	CLA	CHC-C1C	5.36	1.47	1.34
14	a	811	CLA	O2A-C1	5.36	1.60	1.46
14	A	833	CLA	C3B-C2B	5.36	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	823	CLA	C3B-C2B	5.36	1.47	1.40
14	A	841	CLA	CHC-C1C	5.36	1.47	1.34
14	x	1701	CLA	CHC-C1C	5.36	1.47	1.34
14	B	812	CLA	O2A-C1	5.36	1.60	1.46
14	b	836	CLA	O2A-C1	5.36	1.60	1.46
14	B	813	CLA	CHC-C1C	5.36	1.47	1.34
14	F	1303	CLA	CHC-C1C	5.36	1.47	1.34
14	H	825	CLA	C3B-C2B	5.36	1.47	1.40
14	l	205	CLA	CHC-C1C	5.36	1.47	1.34
14	A	827	CLA	CHC-C1C	5.36	1.47	1.34
14	L	206	CLA	C3B-C2B	5.36	1.47	1.40
14	a	802	CLA	CHC-C1C	5.36	1.47	1.34
14	G	845	CLA	CHC-C1C	5.35	1.47	1.34
14	H	805	CLA	C3B-C2B	5.35	1.47	1.40
14	W	1701	CLA	CHC-C1C	5.35	1.47	1.34
14	B	803	CLA	CHC-C1C	5.35	1.47	1.34
14	b	837	CLA	O2A-C1	5.35	1.60	1.46
14	b	813	CLA	CHC-C1C	5.35	1.47	1.34
14	b	822	CLA	C3B-C2B	5.35	1.47	1.40
14	b	802	CLA	O2A-C1	5.35	1.60	1.46
14	S	101	CLA	CHC-C1C	5.35	1.47	1.34
14	A	822	CLA	CHC-C1C	5.35	1.47	1.34
14	H	822	CLA	CHC-C1C	5.35	1.47	1.34
14	A	810	CLA	O2A-C1	5.35	1.60	1.46
14	U	205	CLA	O2A-C1	5.35	1.60	1.46
14	a	822	CLA	CHC-C1C	5.35	1.47	1.34
14	K	102	CLA	CHC-C1C	5.34	1.47	1.34
14	B	819	CLA	CHC-C1C	5.34	1.47	1.34
14	G	832	CLA	O2A-C1	5.34	1.60	1.46
14	G	834	CLA	CHC-C1C	5.34	1.47	1.34
14	G	807	CLA	O2A-C1	5.34	1.60	1.46
14	a	840	CLA	O2A-C1	5.34	1.60	1.46
14	A	841	CLA	C3B-C2B	5.34	1.47	1.40
14	B	825	CLA	CHC-C1C	5.34	1.47	1.34
14	A	841	CLA	O2A-C1	5.34	1.60	1.46
14	G	838	CLA	C3B-C2B	5.34	1.47	1.40
14	A	825	CLA	O2A-C1	5.34	1.60	1.46
14	b	807	CLA	CHC-C1C	5.33	1.47	1.34
14	B	816	CLA	C3B-C2B	5.33	1.47	1.40
14	a	812	CLA	O2A-C1	5.33	1.60	1.46
14	b	817	CLA	O2A-C1	5.33	1.60	1.46
14	a	844	CLA	C3B-C2B	5.33	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	j	102	CLA	CHC-C1C	5.33	1.47	1.34
14	K	101	CLA	CHC-C1C	5.33	1.47	1.34
14	A	813	CLA	O2A-C1	5.33	1.60	1.46
14	H	816	CLA	C3B-C2B	5.33	1.47	1.40
14	A	813	CLA	CHC-C1C	5.33	1.47	1.34
14	a	804	CLA	O2A-C1	5.33	1.60	1.46
14	b	821	CLA	O2A-C1	5.33	1.60	1.46
14	B	821	CLA	CHC-C1C	5.33	1.47	1.34
14	a	805	CLA	CHC-C1C	5.33	1.47	1.34
14	B	823	CLA	CHC-C1C	5.32	1.47	1.34
14	a	813	CLA	O2A-C1	5.32	1.60	1.46
14	a	825	CLA	O2A-C1	5.32	1.60	1.46
14	A	821	CLA	CHC-C1C	5.32	1.47	1.34
14	l	205	CLA	O2A-C1	5.32	1.60	1.46
14	a	803	CLA	O2A-C1	5.32	1.60	1.46
14	b	832	CLA	O2A-C1	5.32	1.60	1.46
14	B	811	CLA	CHC-C1C	5.32	1.47	1.34
14	G	825	CLA	CHC-C1C	5.32	1.47	1.34
14	a	816	CLA	CHC-C1C	5.32	1.47	1.34
14	a	804	CLA	C3B-C2B	5.32	1.47	1.40
14	G	836	CLA	CHC-C1C	5.32	1.47	1.34
14	G	823	CLA	CHC-C1C	5.32	1.47	1.34
14	A	829	CLA	CHC-C1C	5.32	1.47	1.34
14	a	815	CLA	C3B-C2B	5.31	1.47	1.40
14	Q	201	CLA	CHC-C1C	5.31	1.47	1.34
14	M	1601	CLA	O2D-CGD	5.31	1.46	1.33
14	a	832	CLA	CHC-C1C	5.31	1.47	1.34
14	b	816	CLA	O2A-C1	5.31	1.60	1.46
14	b	816	CLA	C3B-C2B	5.31	1.47	1.40
14	a	806	CLA	O2A-C1	5.31	1.60	1.46
14	G	825	CLA	O2A-C1	5.31	1.60	1.46
14	M	1601	CLA	CHC-C1C	5.31	1.47	1.34
14	A	804	CLA	O2A-C1	5.31	1.60	1.46
14	G	841	CLA	O2A-C1	5.31	1.60	1.46
14	A	826	CLA	O2A-C1	5.31	1.60	1.46
14	A	817	CLA	CHC-C1C	5.31	1.47	1.34
14	B	835	CLA	CHC-C1C	5.31	1.47	1.34
14	H	803	CLA	O2A-C1	5.31	1.60	1.46
14	a	824	CLA	O2A-C1	5.31	1.60	1.46
14	A	823	CLA	CHC-C1C	5.31	1.47	1.34
14	G	809	CLA	O2A-C1	5.31	1.60	1.46
14	G	813	CLA	CHC-C1C	5.31	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	838	CLA	CHC-C1C	5.31	1.47	1.34
14	G	818	CLA	CHC-C1C	5.31	1.47	1.34
14	L	204	CLA	CHC-C1C	5.30	1.47	1.34
14	b	830	CLA	CHC-C1C	5.30	1.47	1.34
14	H	806	CLA	CHC-C1C	5.30	1.47	1.34
14	A	829	CLA	O2A-C1	5.30	1.60	1.46
14	A	845	CLA	C3B-C2B	5.30	1.47	1.40
14	H	825	CLA	CHC-C1C	5.30	1.47	1.34
14	B	820	CLA	CHC-C1C	5.30	1.47	1.34
14	A	821	CLA	O2A-C1	5.30	1.60	1.46
14	B	805	CLA	O2A-C1	5.30	1.60	1.46
14	G	829	CLA	O2A-C1	5.30	1.60	1.46
14	a	842	CLA	CHC-C1C	5.30	1.47	1.34
14	A	802	CLA	O2A-C1	5.30	1.60	1.46
14	G	828	CLA	O2A-C1	5.30	1.60	1.46
14	H	836	CLA	O2A-C1	5.30	1.60	1.46
14	G	829	CLA	CHC-C1C	5.30	1.47	1.34
14	G	814	CLA	O2A-C1	5.30	1.60	1.46
14	X	1701	CLA	CHC-C1C	5.29	1.47	1.34
14	F	1301	CLA	CHC-C1C	5.29	1.47	1.34
14	H	816	CLA	O2A-C1	5.29	1.60	1.46
14	G	839	CLA	O2A-C1	5.29	1.60	1.46
14	b	839	CLA	O2A-C1	5.29	1.60	1.46
14	H	804	CLA	C3B-C2B	5.29	1.47	1.40
14	H	839	CLA	O2A-C1	5.29	1.60	1.46
14	H	809	CLA	O2A-C1	5.29	1.60	1.46
14	B	837	CLA	O2A-C1	5.29	1.60	1.46
14	b	825	CLA	C3B-C2B	5.29	1.47	1.40
14	A	805	CLA	O2A-C1	5.29	1.60	1.46
14	L	204	CLA	O2A-C1	5.29	1.60	1.46
14	B	836	CLA	O2A-C1	5.29	1.60	1.46
14	a	819	CLA	CHC-C1C	5.29	1.47	1.34
14	G	820	CLA	O2A-C1	5.29	1.60	1.46
14	a	806	CLA	CHC-C1C	5.29	1.47	1.34
14	b	814	CLA	CHC-C1C	5.29	1.47	1.34
14	l	202	CLA	O2A-C1	5.29	1.60	1.46
14	a	834	CLA	CHC-C1C	5.28	1.47	1.34
14	b	836	CLA	CHC-C1C	5.28	1.47	1.34
14	G	838	CLA	O2A-C1	5.28	1.60	1.46
14	a	831	CLA	O2A-C1	5.28	1.60	1.46
14	J	101	CLA	CHC-C1C	5.28	1.47	1.34
14	a	840	CLA	O2D-CGD	5.28	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	844	CLA	CHC-C1C	5.28	1.47	1.34
14	G	838	CLA	CHC-C1C	5.28	1.47	1.34
14	b	813	CLA	O2A-C1	5.28	1.60	1.46
14	a	814	CLA	CHC-C1C	5.28	1.47	1.34
14	H	805	CLA	O2A-C1	5.28	1.60	1.46
14	V	1601	CLA	O2D-CGD	5.28	1.46	1.33
14	G	821	CLA	CHC-C1C	5.28	1.47	1.34
14	G	827	CLA	O2A-C1	5.28	1.60	1.46
14	H	837	CLA	O2A-C1	5.27	1.60	1.46
14	A	814	CLA	CHC-C1C	5.27	1.47	1.34
14	l	207	CLA	CHC-C1C	5.27	1.47	1.34
14	A	835	CLA	O2A-C1	5.27	1.60	1.46
14	B	825	CLA	O2A-C1	5.27	1.60	1.46
14	G	843	CLA	O2A-C1	5.27	1.60	1.46
14	A	828	CLA	O2A-C1	5.27	1.60	1.46
14	H	807	CLA	O2A-C1	5.27	1.60	1.46
14	H	826	CLA	O2A-C1	5.27	1.60	1.46
14	b	804	CLA	O2A-C1	5.27	1.60	1.46
14	a	823	CLA	CHC-C1C	5.26	1.47	1.34
14	A	845	CLA	CHC-C1C	5.26	1.47	1.34
14	A	832	CLA	CHC-C1C	5.26	1.47	1.34
14	A	831	CLA	O2A-C1	5.26	1.60	1.46
14	A	826	CLA	CHC-C1C	5.26	1.47	1.34
14	B	830	CLA	CHC-C1C	5.26	1.47	1.34
14	B	834	CLA	CHC-C1C	5.26	1.47	1.34
14	G	811	CLA	CHC-C1C	5.26	1.47	1.34
14	G	837	CLA	CHC-C1C	5.26	1.47	1.34
14	B	805	CLA	CHC-C1C	5.26	1.47	1.34
14	a	832	CLA	O2A-C1	5.26	1.60	1.46
14	G	841	CLA	CHC-C1C	5.25	1.47	1.34
14	a	835	CLA	CHC-C1C	5.25	1.47	1.34
14	b	809	CLA	O2A-C1	5.25	1.60	1.46
14	B	827	CLA	CHC-C1C	5.25	1.47	1.34
14	G	810	CLA	CHC-C1C	5.25	1.47	1.34
14	B	815	CLA	C3B-C2B	5.25	1.47	1.40
14	a	805	CLA	C3B-C2B	5.25	1.47	1.40
14	A	808	CLA	O2D-CGD	5.25	1.46	1.33
14	a	822	CLA	C3B-C2B	5.25	1.47	1.40
14	j	101	CLA	CHC-C1C	5.25	1.47	1.34
14	H	828	CLA	O2A-C1	5.25	1.60	1.46
14	B	802	CLA	CHC-C1C	5.25	1.47	1.34
14	b	821	CLA	O2D-CGD	5.25	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	832	CLA	CHC-C1C	5.25	1.47	1.34
14	A	841	CLA	O2D-CGD	5.25	1.46	1.33
14	B	821	CLA	O2A-C1	5.25	1.60	1.46
14	B	816	CLA	O2A-C1	5.24	1.60	1.46
14	B	832	CLA	CHC-C1C	5.24	1.47	1.34
14	B	837	CLA	CHC-C1C	5.24	1.47	1.34
14	a	820	CLA	CHC-C1C	5.24	1.47	1.34
14	G	804	CLA	O2A-C1	5.24	1.60	1.46
14	G	824	CLA	CHC-C1C	5.24	1.47	1.34
14	U	206	CLA	CHC-C1C	5.24	1.47	1.34
13	G	801	CL0	O2A-C1	5.24	1.60	1.46
14	A	809	CLA	CHC-C1C	5.24	1.47	1.34
14	a	815	CLA	CHC-C1C	5.24	1.47	1.34
14	B	832	CLA	O2A-C1	5.24	1.60	1.46
14	A	844	CLA	O2A-C1	5.23	1.60	1.46
14	A	839	CLA	O2A-C1	5.23	1.60	1.46
14	H	820	CLA	CHC-C1C	5.23	1.47	1.34
14	A	837	CLA	CHC-C1C	5.23	1.47	1.34
14	G	807	CLA	CHC-C1C	5.23	1.47	1.34
14	b	812	CLA	C3B-C2B	5.23	1.47	1.40
14	H	803	CLA	CHC-C1C	5.23	1.47	1.34
14	G	839	CLA	CHC-C1C	5.23	1.47	1.34
14	A	807	CLA	CHC-C1C	5.23	1.47	1.34
14	G	830	CLA	O2A-C1	5.22	1.60	1.46
14	G	805	CLA	O2A-C1	5.22	1.60	1.46
14	l	206	CLA	CHC-C1C	5.22	1.47	1.34
14	H	808	CLA	CHC-C1C	5.22	1.47	1.34
14	G	806	CLA	C3B-C2B	5.22	1.47	1.40
14	G	833	CLA	O2A-C1	5.22	1.60	1.46
14	a	839	CLA	CHC-C1C	5.22	1.47	1.34
14	H	836	CLA	C3B-C2B	5.22	1.47	1.40
14	G	835	CLA	CHC-C1C	5.22	1.47	1.34
14	G	834	CLA	O2A-C1	5.22	1.60	1.46
14	G	840	CLA	CHC-C1C	5.22	1.47	1.34
14	a	843	CLA	CHC-C1C	5.22	1.47	1.34
14	l	207	CLA	C3B-C2B	5.21	1.47	1.40
14	B	828	CLA	O2A-C1	5.21	1.60	1.46
14	a	830	CLA	O2A-C1	5.21	1.60	1.46
14	A	820	CLA	CHC-C1C	5.21	1.47	1.34
14	G	816	CLA	CHC-C1C	5.21	1.47	1.34
14	L	204	CLA	O2D-CGD	5.21	1.46	1.33
14	H	836	CLA	CHC-C1C	5.21	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	802	CLA	O2A-C1	5.21	1.60	1.46
14	G	810	CLA	C3B-C2B	5.21	1.47	1.40
13	a	801	CL0	O2A-C1	5.21	1.60	1.46
14	b	801	CLA	O2A-C1	5.21	1.60	1.46
14	B	806	CLA	CHC-C1C	5.21	1.47	1.34
14	b	801	CLA	C3B-C2B	5.21	1.47	1.40
14	B	839	CLA	O2A-C1	5.20	1.60	1.46
14	a	824	CLA	CHC-C1C	5.20	1.47	1.34
14	H	806	CLA	O2A-C1	5.20	1.60	1.46
14	a	810	CLA	CHC-C1C	5.20	1.47	1.34
14	H	821	CLA	O2D-CGD	5.20	1.46	1.33
14	a	833	CLA	CHC-C1C	5.20	1.47	1.34
14	A	805	CLA	C3B-C2B	5.20	1.47	1.40
14	A	836	CLA	CHC-C1C	5.20	1.47	1.34
14	B	822	CLA	C3B-C2B	5.20	1.47	1.40
14	b	807	CLA	O2A-C1	5.20	1.60	1.46
14	H	821	CLA	O2A-C1	5.20	1.60	1.46
14	G	815	CLA	CHC-C1C	5.20	1.47	1.34
14	a	814	CLA	C3B-C2B	5.20	1.47	1.40
14	b	831	CLA	C3B-C2B	5.20	1.47	1.40
14	F	1301	CLA	O2D-CGD	5.19	1.46	1.33
14	G	806	CLA	CHC-C1C	5.19	1.47	1.34
14	G	841	CLA	O2D-CGD	5.19	1.46	1.33
14	G	819	CLA	O2A-C1	5.19	1.60	1.46
14	A	835	CLA	CHC-C1C	5.19	1.47	1.34
14	b	826	CLA	CHC-C1C	5.19	1.47	1.34
14	A	830	CLA	O2A-C1	5.19	1.60	1.46
14	b	828	CLA	O2A-C1	5.19	1.60	1.46
14	B	806	CLA	O2A-C1	5.19	1.60	1.46
14	B	838	CLA	CHC-C1C	5.19	1.47	1.34
14	a	821	CLA	O2A-C1	5.19	1.60	1.46
14	H	812	CLA	O2A-C1	5.19	1.60	1.46
14	a	829	CLA	O2A-C1	5.18	1.60	1.46
14	b	818	CLA	O2A-C1	5.18	1.60	1.46
13	A	801	CL0	O2A-C1	5.18	1.60	1.46
14	a	838	CLA	CHC-C1C	5.18	1.47	1.34
14	A	810	CLA	CHC-C1C	5.18	1.47	1.34
14	A	811	CLA	CHC-C1C	5.18	1.47	1.34
14	a	810	CLA	O2D-CGD	5.18	1.46	1.33
14	B	826	CLA	CHC-C1C	5.18	1.47	1.34
14	G	825	CLA	C3B-C2B	5.18	1.47	1.40
14	A	809	CLA	O2A-C1	5.18	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	818	CLA	O2A-C1	5.18	1.60	1.46
14	H	827	CLA	O2D-CGD	5.18	1.46	1.33
14	k	1401	CLA	O2D-CGD	5.17	1.45	1.33
14	a	834	CLA	O2A-C1	5.17	1.60	1.46
14	H	823	CLA	C3B-C2B	5.17	1.47	1.40
14	G	822	CLA	O2A-C1	5.17	1.60	1.46
14	T	1401	CLA	O2D-CGD	5.17	1.45	1.33
14	i	101	CLA	O2A-C1	5.17	1.60	1.46
14	b	832	CLA	O2D-CGD	5.17	1.45	1.33
14	i	101	CLA	CHC-C1C	5.17	1.47	1.34
14	a	818	CLA	O2A-C1	5.17	1.60	1.46
14	A	810	CLA	C3B-C2B	5.17	1.47	1.40
14	H	823	CLA	CHC-C1C	5.16	1.47	1.34
14	b	812	CLA	O2A-C1	5.16	1.60	1.46
14	G	822	CLA	O2D-CGD	5.16	1.45	1.33
14	b	834	CLA	O2D-CGD	5.16	1.45	1.33
14	b	803	CLA	CHC-C1C	5.16	1.47	1.34
14	A	833	CLA	O2A-C1	5.16	1.60	1.46
14	G	833	CLA	O2D-CGD	5.16	1.45	1.33
14	B	805	CLA	C3B-C2B	5.16	1.47	1.40
14	G	820	CLA	CHC-C1C	5.16	1.47	1.34
14	a	835	CLA	O2D-CGD	5.16	1.45	1.33
14	G	811	CLA	O2D-CGD	5.16	1.45	1.33
14	a	838	CLA	O2A-C1	5.16	1.60	1.46
14	A	802	CLA	C3B-C2B	5.16	1.47	1.40
14	A	816	CLA	CHC-C1C	5.16	1.47	1.34
14	m	1601	CLA	CHC-C1C	5.16	1.47	1.34
14	A	823	CLA	O2D-CGD	5.16	1.45	1.33
14	A	827	CLA	O2A-C1	5.16	1.60	1.46
14	a	829	CLA	CHC-C1C	5.16	1.47	1.34
14	B	816	CLA	O2D-CGD	5.15	1.45	1.33
14	H	832	CLA	O2D-CGD	5.15	1.45	1.33
14	b	818	CLA	O2D-CGD	5.15	1.45	1.33
14	A	822	CLA	O2A-C1	5.15	1.60	1.46
14	a	841	CLA	CHC-C1C	5.15	1.47	1.34
14	b	806	CLA	CHC-C1C	5.15	1.47	1.34
14	b	821	CLA	CHC-C1C	5.15	1.47	1.34
14	U	206	CLA	O2A-C1	5.15	1.60	1.46
14	f	202	CLA	O2D-CGD	5.15	1.45	1.33
14	b	826	CLA	O2D-CGD	5.15	1.45	1.33
14	L	206	CLA	O2A-C1	5.15	1.60	1.46
14	b	830	CLA	O2D-CGD	5.15	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	S	102	CLA	C3B-C2B	5.15	1.47	1.40
14	A	819	CLA	O2A-C1	5.15	1.60	1.46
14	B	815	CLA	O2D-CGD	5.15	1.45	1.33
14	B	807	CLA	O2A-C1	5.15	1.60	1.46
14	a	829	CLA	O2D-CGD	5.15	1.45	1.33
14	V	1601	CLA	CHC-C1C	5.15	1.47	1.34
14	H	820	CLA	O2D-CGD	5.15	1.45	1.33
14	b	836	CLA	C3B-C2B	5.15	1.47	1.40
13	a	801	CL0	CHC-C1C	5.14	1.47	1.34
14	b	807	CLA	O2D-CGD	5.14	1.45	1.33
14	A	836	CLA	O2D-CGD	5.14	1.45	1.33
14	H	817	CLA	O2A-C1	5.14	1.60	1.46
14	G	832	CLA	CHC-C1C	5.14	1.47	1.34
14	b	810	CLA	O2D-CGD	5.14	1.45	1.33
14	B	812	CLA	CHC-C1C	5.14	1.47	1.34
14	A	812	CLA	O2D-CGD	5.14	1.45	1.33
14	b	802	CLA	O2D-CGD	5.14	1.45	1.33
14	a	833	CLA	O2A-C1	5.13	1.59	1.46
14	b	805	CLA	C3B-C2B	5.13	1.47	1.40
14	a	809	CLA	C3B-C2B	5.13	1.47	1.40
14	B	830	CLA	O2D-CGD	5.13	1.45	1.33
14	b	803	CLA	O2A-C1	5.13	1.59	1.46
14	H	810	CLA	O2D-CGD	5.13	1.45	1.33
14	B	827	CLA	O2D-CGD	5.13	1.45	1.33
14	B	821	CLA	O2D-CGD	5.13	1.45	1.33
14	a	822	CLA	O2D-CGD	5.13	1.45	1.33
14	b	803	CLA	O2D-CGD	5.13	1.45	1.33
14	B	831	CLA	C3B-C2B	5.13	1.47	1.40
14	A	833	CLA	O2D-CGD	5.12	1.45	1.33
14	b	812	CLA	CHC-C1C	5.12	1.47	1.34
14	a	811	CLA	CHC-C1C	5.12	1.47	1.34
14	A	817	CLA	O2D-CGD	5.12	1.45	1.33
14	l	202	CLA	O2D-CGD	5.12	1.45	1.33
14	B	830	CLA	C3B-C2B	5.12	1.47	1.40
14	Q	203	CLA	O2D-CGD	5.12	1.45	1.33
14	H	827	CLA	CHC-C1C	5.12	1.47	1.34
14	A	803	CLA	O2A-C1	5.12	1.59	1.46
14	G	818	CLA	O2D-CGD	5.12	1.45	1.33
14	b	823	CLA	CHC-C1C	5.12	1.47	1.34
14	G	812	CLA	O2D-CGD	5.12	1.45	1.33
14	H	834	CLA	O2D-CGD	5.12	1.45	1.33
14	G	807	CLA	C3B-C2B	5.12	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	844	CLA	O2D-CGD	5.12	1.45	1.33
14	A	820	CLA	O2A-C1	5.12	1.59	1.46
14	b	816	CLA	O2D-CGD	5.12	1.45	1.33
14	B	836	CLA	C3B-C2B	5.12	1.47	1.40
14	H	806	CLA	O2D-CGD	5.11	1.45	1.33
14	A	825	CLA	CHC-C1C	5.11	1.47	1.34
14	H	830	CLA	O2D-CGD	5.11	1.45	1.33
14	b	820	CLA	CHC-C1C	5.11	1.47	1.34
14	H	802	CLA	O2D-CGD	5.11	1.45	1.33
14	B	826	CLA	O2D-CGD	5.11	1.45	1.33
14	a	808	CLA	O2A-C1	5.11	1.59	1.46
14	K	102	CLA	O2D-CGD	5.11	1.45	1.33
14	b	817	CLA	O2D-CGD	5.11	1.45	1.33
14	A	834	CLA	O2A-C1	5.11	1.59	1.46
14	A	839	CLA	CHC-C1C	5.10	1.47	1.34
14	B	837	CLA	O2D-CGD	5.10	1.45	1.33
14	B	832	CLA	O2D-CGD	5.10	1.45	1.33
14	B	807	CLA	O2D-CGD	5.10	1.45	1.33
14	B	834	CLA	O2D-CGD	5.10	1.45	1.33
14	G	843	CLA	O2D-CGD	5.10	1.45	1.33
14	G	802	CLA	CHC-C1C	5.10	1.47	1.34
14	A	822	CLA	O2D-CGD	5.10	1.45	1.33
14	H	826	CLA	O2D-CGD	5.10	1.45	1.33
14	G	830	CLA	CHC-C1C	5.10	1.47	1.34
14	a	818	CLA	O2D-CGD	5.09	1.45	1.33
14	H	802	CLA	O2A-C1	5.09	1.59	1.46
14	b	838	CLA	CHC-C1C	5.09	1.47	1.34
14	G	803	CLA	O2A-C1	5.09	1.59	1.46
14	B	825	CLA	C3B-C2B	5.09	1.47	1.40
14	G	823	CLA	O2D-CGD	5.09	1.45	1.33
13	A	801	CL0	CHC-C1C	5.09	1.47	1.34
14	S	101	CLA	O2D-CGD	5.08	1.45	1.33
14	a	803	CLA	O2D-CGD	5.08	1.45	1.33
14	A	824	CLA	O2D-CGD	5.08	1.45	1.33
14	a	826	CLA	O2A-C1	5.08	1.59	1.46
14	H	821	CLA	C3B-C2B	5.08	1.47	1.40
14	A	826	CLA	O2D-CGD	5.08	1.45	1.33
14	A	818	CLA	O2D-CGD	5.08	1.45	1.33
14	a	807	CLA	O2D-CGD	5.08	1.45	1.33
14	B	810	CLA	O2D-CGD	5.08	1.45	1.33
14	G	820	CLA	O2D-CGD	5.08	1.45	1.33
14	a	832	CLA	O2D-CGD	5.08	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	815	CLA	CHC-C1C	5.07	1.47	1.34
14	i	101	CLA	O2D-CGD	5.07	1.45	1.33
14	A	812	CLA	CHC-C1C	5.07	1.47	1.34
14	b	830	CLA	C3B-C2B	5.07	1.47	1.40
14	G	829	CLA	O2D-CGD	5.07	1.45	1.33
14	B	807	CLA	CHC-C1C	5.07	1.47	1.34
14	G	816	CLA	O2D-CGD	5.07	1.45	1.33
14	H	814	CLA	CHC-C1C	5.07	1.47	1.34
14	H	805	CLA	O2D-CGD	5.07	1.45	1.33
14	b	835	CLA	O2D-CGD	5.06	1.45	1.33
14	G	815	CLA	O2D-CGD	5.06	1.45	1.33
14	B	802	CLA	O2A-C1	5.06	1.59	1.46
14	l	207	CLA	O2A-C1	5.06	1.59	1.46
14	G	808	CLA	O2D-CGD	5.06	1.45	1.33
14	H	828	CLA	CHC-C1C	5.06	1.47	1.34
14	A	842	CLA	O2D-CGD	5.06	1.45	1.33
14	H	817	CLA	O2D-CGD	5.06	1.45	1.33
14	a	808	CLA	O2D-CGD	5.06	1.45	1.33
14	B	840	CLA	O2D-CGD	5.06	1.45	1.33
14	a	819	CLA	O2D-CGD	5.06	1.45	1.33
14	a	831	CLA	O2D-CGD	5.06	1.45	1.33
14	b	840	CLA	O2D-CGD	5.06	1.45	1.33
14	B	814	CLA	CHC-C1C	5.06	1.47	1.34
14	G	805	CLA	C3B-C2B	5.06	1.47	1.40
14	G	815	CLA	C3B-C2B	5.06	1.47	1.40
14	G	824	CLA	O2D-CGD	5.06	1.45	1.33
14	b	824	CLA	C3B-C2B	5.06	1.47	1.40
14	a	817	CLA	O2D-CGD	5.05	1.45	1.33
14	A	811	CLA	C3B-C2B	5.05	1.47	1.40
14	A	807	CLA	O2D-CGD	5.05	1.45	1.33
14	H	807	CLA	CHC-C1C	5.05	1.47	1.34
14	H	834	CLA	CHC-C1C	5.05	1.47	1.34
14	b	806	CLA	C3B-C2B	5.05	1.47	1.40
14	A	810	CLA	O2D-CGD	5.05	1.45	1.33
14	G	813	CLA	O2D-CGD	5.05	1.45	1.33
14	b	820	CLA	O2D-CGD	5.05	1.45	1.33
14	B	806	CLA	O2D-CGD	5.05	1.45	1.33
13	A	801	CL0	O2D-CGD	5.05	1.45	1.33
14	G	836	CLA	O2D-CGD	5.05	1.45	1.33
14	H	816	CLA	O2D-CGD	5.05	1.45	1.33
14	B	835	CLA	O2D-CGD	5.05	1.45	1.33
14	b	829	CLA	O2D-CGD	5.05	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	818	CLA	C3B-C2B	5.05	1.47	1.40
14	H	804	CLA	O2D-CGD	5.05	1.45	1.33
14	j	101	CLA	O2D-CGD	5.05	1.45	1.33
14	b	837	CLA	O2D-CGD	5.05	1.45	1.33
14	A	816	CLA	O2D-CGD	5.04	1.45	1.33
14	b	815	CLA	O2D-CGD	5.04	1.45	1.33
14	b	827	CLA	CHC-C1C	5.04	1.47	1.34
14	H	826	CLA	CHC-C1C	5.04	1.47	1.34
14	B	802	CLA	O2D-CGD	5.04	1.45	1.33
14	J	101	CLA	O2D-CGD	5.04	1.45	1.33
14	G	810	CLA	O2D-CGD	5.04	1.45	1.33
14	G	817	CLA	O2D-CGD	5.04	1.45	1.33
14	a	837	CLA	O2D-CGD	5.04	1.45	1.33
14	G	841	CLA	C3B-C2B	5.04	1.47	1.40
14	B	836	CLA	CHC-C1C	5.04	1.47	1.34
13	G	801	CL0	O2D-CGD	5.04	1.45	1.33
14	b	825	CLA	O2D-CGD	5.04	1.45	1.33
13	a	801	CL0	O2D-CGD	5.03	1.45	1.33
14	U	206	CLA	O2D-CGD	5.03	1.45	1.33
14	a	806	CLA	O2D-CGD	5.03	1.45	1.33
14	a	812	CLA	O2D-CGD	5.03	1.45	1.33
14	G	826	CLA	CHC-C1C	5.03	1.47	1.34
14	H	807	CLA	O2D-CGD	5.03	1.45	1.33
14	b	808	CLA	CHC-C1C	5.03	1.46	1.34
14	H	833	CLA	C3B-C2B	5.03	1.47	1.40
14	H	815	CLA	O2D-CGD	5.03	1.45	1.33
14	A	804	CLA	O2D-CGD	5.03	1.45	1.33
14	H	812	CLA	CHC-C1C	5.03	1.46	1.34
14	B	823	CLA	O2D-CGD	5.03	1.45	1.33
14	G	837	CLA	O2D-CGD	5.02	1.45	1.33
14	B	817	CLA	O2D-CGD	5.02	1.45	1.33
14	a	809	CLA	O2D-CGD	5.02	1.45	1.33
14	G	842	CLA	O2D-CGD	5.02	1.45	1.33
14	B	819	CLA	O2D-CGD	5.02	1.45	1.33
14	U	204	CLA	C3B-C2B	5.02	1.47	1.40
14	G	819	CLA	O2D-CGD	5.02	1.45	1.33
14	G	809	CLA	O2D-CGD	5.02	1.45	1.33
14	B	820	CLA	O2D-CGD	5.02	1.45	1.33
14	A	820	CLA	O2D-CGD	5.02	1.45	1.33
14	a	824	CLA	O2D-CGD	5.02	1.45	1.33
14	H	840	CLA	O2D-CGD	5.02	1.45	1.33
14	G	804	CLA	O2D-CGD	5.01	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	828	CLA	O2D-CGD	5.01	1.45	1.33
14	H	832	CLA	CHC-C1C	5.01	1.46	1.34
14	a	821	CLA	O2D-CGD	5.01	1.45	1.33
14	H	817	CLA	CHC-C1C	5.01	1.46	1.34
14	H	824	CLA	O2D-CGD	5.01	1.45	1.33
14	a	836	CLA	O2D-CGD	5.01	1.45	1.33
15	A	846	PQN	C10-C5	5.01	1.48	1.40
14	B	824	CLA	C3B-C2B	5.01	1.47	1.40
14	A	813	CLA	O2D-CGD	5.01	1.45	1.33
14	a	816	CLA	O2D-CGD	5.01	1.45	1.33
13	G	801	CL0	CHC-C1C	5.01	1.46	1.34
14	a	823	CLA	O2D-CGD	5.01	1.45	1.33
14	L	201	CLA	O2D-CGD	5.00	1.45	1.33
14	B	828	CLA	CHC-C1C	5.00	1.46	1.34
14	H	835	CLA	CHC-C1C	5.00	1.46	1.34
14	a	842	CLA	O2D-CGD	5.00	1.45	1.33
14	A	845	CLA	C3C-C2C	5.00	1.47	1.36
14	b	818	CLA	C3B-C2B	5.00	1.47	1.40
14	a	834	CLA	O2D-CGD	5.00	1.45	1.33
14	B	824	CLA	O2D-CGD	5.00	1.45	1.33
14	b	819	CLA	O2D-CGD	5.00	1.45	1.33
14	G	826	CLA	O2D-CGD	4.99	1.45	1.33
14	l	205	CLA	C3B-C2B	4.99	1.47	1.40
14	b	805	CLA	O2D-CGD	4.99	1.45	1.33
14	A	809	CLA	O2D-CGD	4.99	1.45	1.33
14	B	804	CLA	O2D-CGD	4.99	1.45	1.33
14	a	844	CLA	C3C-C2C	4.99	1.47	1.36
14	B	825	CLA	O2D-CGD	4.99	1.45	1.33
14	a	802	CLA	O2D-CGD	4.99	1.45	1.33
14	B	805	CLA	O2D-CGD	4.99	1.45	1.33
14	B	812	CLA	O2D-CGD	4.99	1.45	1.33
14	H	815	CLA	C3B-C2B	4.98	1.47	1.40
14	L	201	CLA	CHC-C1C	4.98	1.46	1.34
14	H	823	CLA	O2D-CGD	4.98	1.45	1.33
14	B	808	CLA	CHC-C1C	4.98	1.46	1.34
14	a	827	CLA	O2D-CGD	4.98	1.45	1.33
14	H	835	CLA	O2D-CGD	4.98	1.45	1.33
14	B	829	CLA	O2D-CGD	4.98	1.45	1.33
14	U	201	CLA	CHC-C1C	4.98	1.46	1.34
14	H	802	CLA	CHC-C1C	4.98	1.46	1.34
14	L	206	CLA	O2D-CGD	4.98	1.45	1.33
14	a	811	CLA	O2D-CGD	4.98	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	809	CLA	O2D-CGD	4.97	1.45	1.33
14	H	833	CLA	O2D-CGD	4.97	1.45	1.33
14	H	837	CLA	O2D-CGD	4.97	1.45	1.33
15	a	845	PQN	C10-C5	4.97	1.48	1.40
14	G	831	CLA	CHC-C1C	4.97	1.46	1.34
14	A	815	CLA	O2D-CGD	4.97	1.45	1.33
14	H	829	CLA	O2D-CGD	4.97	1.45	1.33
14	a	815	CLA	O2D-CGD	4.97	1.45	1.33
14	G	838	CLA	O2D-CGD	4.97	1.45	1.33
14	U	205	CLA	C3B-C2B	4.97	1.47	1.40
14	B	818	CLA	O2A-C1	4.97	1.59	1.46
14	a	829	CLA	C3B-C2B	4.97	1.47	1.40
14	G	807	CLA	O2D-CGD	4.97	1.45	1.33
14	G	825	CLA	O2D-CGD	4.97	1.45	1.33
14	G	845	CLA	C3B-C2B	4.97	1.47	1.40
14	b	813	CLA	O2D-CGD	4.96	1.45	1.33
14	U	201	CLA	O2D-CGD	4.96	1.45	1.33
14	b	824	CLA	O2D-CGD	4.96	1.45	1.33
14	b	828	CLA	CHC-C1C	4.96	1.46	1.34
14	G	814	CLA	O2D-CGD	4.96	1.45	1.33
14	G	835	CLA	O2D-CGD	4.96	1.45	1.33
14	A	830	CLA	O2D-CGD	4.96	1.45	1.33
14	H	825	CLA	O2D-CGD	4.96	1.45	1.33
14	a	841	CLA	O2D-CGD	4.96	1.45	1.33
14	A	840	CLA	O2D-CGD	4.96	1.45	1.33
14	l	205	CLA	O2D-CGD	4.96	1.45	1.33
14	A	821	CLA	O2D-CGD	4.96	1.45	1.33
14	B	836	CLA	O2D-CGD	4.96	1.45	1.33
14	H	812	CLA	C3B-C2B	4.96	1.47	1.40
14	b	823	CLA	O2D-CGD	4.95	1.45	1.33
14	G	818	CLA	C3B-C2B	4.95	1.47	1.40
14	B	808	CLA	O2D-CGD	4.95	1.45	1.33
15	G	846	PQN	C10-C5	4.95	1.48	1.40
14	b	806	CLA	O2D-CGD	4.95	1.45	1.33
14	B	828	CLA	O2D-CGD	4.95	1.45	1.33
14	G	812	CLA	CHC-C1C	4.95	1.46	1.34
14	A	806	CLA	O2D-CGD	4.95	1.45	1.33
14	U	204	CLA	O2D-CGD	4.95	1.45	1.33
14	A	825	CLA	O2D-CGD	4.95	1.45	1.33
14	A	819	CLA	O2D-CGD	4.94	1.45	1.33
14	A	837	CLA	O2D-CGD	4.94	1.45	1.33
14	H	822	CLA	C3B-C2B	4.94	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	832	CLA	O2D-CGD	4.94	1.45	1.33
14	G	821	CLA	O2D-CGD	4.94	1.45	1.33
14	G	826	CLA	C3B-C2B	4.94	1.47	1.40
14	H	812	CLA	O2D-CGD	4.94	1.45	1.33
14	G	834	CLA	O2D-CGD	4.94	1.45	1.33
14	a	825	CLA	O2D-CGD	4.93	1.45	1.33
14	B	814	CLA	O2D-CGD	4.93	1.45	1.33
14	a	827	CLA	C3B-C2B	4.93	1.47	1.40
14	a	805	CLA	O2D-CGD	4.93	1.45	1.33
14	b	836	CLA	O2D-CGD	4.93	1.45	1.33
14	A	838	CLA	O2D-CGD	4.93	1.45	1.33
14	U	205	CLA	O2D-CGD	4.93	1.45	1.33
14	A	802	CLA	O2D-CGD	4.93	1.45	1.33
14	b	827	CLA	O2D-CGD	4.93	1.45	1.33
14	H	819	CLA	O2D-CGD	4.92	1.45	1.33
14	a	814	CLA	O2D-CGD	4.92	1.45	1.33
14	Q	201	CLA	O2D-CGD	4.91	1.45	1.33
14	a	839	CLA	O2D-CGD	4.91	1.45	1.33
14	G	828	CLA	O2D-CGD	4.91	1.45	1.33
14	b	839	CLA	O2D-CGD	4.91	1.45	1.33
14	H	839	CLA	O2D-CGD	4.91	1.45	1.33
14	G	802	CLA	O2D-CGD	4.91	1.45	1.33
14	a	830	CLA	CHC-C1C	4.91	1.46	1.34
14	A	843	CLA	O2D-CGD	4.91	1.45	1.33
14	b	834	CLA	CHC-C1C	4.91	1.46	1.34
14	G	831	CLA	O2D-CGD	4.90	1.45	1.33
14	a	827	CLA	O2A-C1	4.90	1.59	1.46
14	B	817	CLA	CHC-C1C	4.90	1.46	1.34
14	a	804	CLA	O2D-CGD	4.90	1.45	1.33
14	X	1701	CLA	C3B-C2B	4.90	1.47	1.40
14	A	834	CLA	O2D-CGD	4.90	1.45	1.33
14	b	828	CLA	O2D-CGD	4.90	1.45	1.33
14	A	827	CLA	O2D-CGD	4.89	1.45	1.33
14	a	844	CLA	O2D-CGD	4.89	1.45	1.33
14	a	834	CLA	C3B-C2B	4.89	1.47	1.40
14	G	840	CLA	O2D-CGD	4.89	1.45	1.33
14	G	830	CLA	O2D-CGD	4.89	1.45	1.33
14	G	845	CLA	C3C-C2C	4.89	1.47	1.36
14	A	803	CLA	O2D-CGD	4.89	1.45	1.33
14	l	207	CLA	O2D-CGD	4.88	1.45	1.33
14	a	840	CLA	C3B-C2B	4.88	1.47	1.40
14	H	838	CLA	CHC-C1C	4.88	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	808	CLA	O2D-CGD	4.88	1.45	1.33
14	b	801	CLA	O2D-CGD	4.88	1.45	1.33
14	G	828	CLA	C3B-C2B	4.88	1.47	1.40
14	l	206	CLA	C3B-C2B	4.88	1.47	1.40
14	H	811	CLA	O2D-CGD	4.88	1.45	1.33
14	H	820	CLA	C3B-C2B	4.87	1.47	1.40
14	G	803	CLA	O2D-CGD	4.87	1.45	1.33
14	a	830	CLA	O2D-CGD	4.87	1.45	1.33
14	A	826	CLA	C3B-C2B	4.87	1.47	1.40
14	A	830	CLA	CHC-C1C	4.87	1.46	1.34
14	a	820	CLA	O2D-CGD	4.87	1.45	1.33
14	A	828	CLA	C3B-C2B	4.87	1.47	1.40
14	b	809	CLA	O2D-CGD	4.87	1.45	1.33
14	L	205	CLA	C3B-C2B	4.86	1.47	1.40
14	b	802	CLA	CHC-C1C	4.86	1.46	1.34
14	G	832	CLA	O2D-CGD	4.86	1.45	1.33
14	j	102	CLA	C3B-C2B	4.86	1.47	1.40
14	a	833	CLA	O2D-CGD	4.86	1.45	1.33
14	B	833	CLA	C3B-C2B	4.86	1.47	1.40
14	H	837	CLA	C3B-C2B	4.86	1.47	1.40
14	B	813	CLA	O2D-CGD	4.86	1.45	1.33
14	A	815	CLA	C3B-C2B	4.86	1.47	1.40
14	G	820	CLA	C3B-C2B	4.86	1.47	1.40
14	A	835	CLA	O2D-CGD	4.86	1.45	1.33
14	b	811	CLA	O2D-CGD	4.86	1.45	1.33
14	H	808	CLA	O2D-CGD	4.86	1.45	1.33
14	b	817	CLA	CHC-C1C	4.85	1.46	1.34
14	B	839	CLA	O2D-CGD	4.85	1.45	1.33
14	G	845	CLA	O2D-CGD	4.85	1.45	1.33
14	b	814	CLA	O2D-CGD	4.85	1.45	1.33
14	b	812	CLA	O2D-CGD	4.85	1.45	1.33
14	H	838	CLA	O2D-CGD	4.85	1.45	1.33
14	A	807	CLA	C3B-C2B	4.85	1.46	1.40
14	B	809	CLA	O2D-CGD	4.85	1.45	1.33
14	b	833	CLA	O2D-CGD	4.83	1.45	1.33
14	a	855	CLA	O2D-CGD	4.83	1.45	1.33
14	H	817	CLA	C3B-C2B	4.83	1.46	1.40
14	L	204	CLA	C3B-C2B	4.83	1.46	1.40
14	G	827	CLA	O2D-CGD	4.83	1.45	1.33
14	a	810	CLA	CHD-C1D	4.83	1.47	1.38
14	b	818	CLA	CHD-C1D	4.83	1.47	1.38
14	H	830	CLA	C3B-C2B	4.82	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	826	CLA	C3B-C2B	4.82	1.46	1.40
14	A	831	CLA	CHC-C1C	4.82	1.46	1.34
14	b	821	CLA	C3B-C2B	4.82	1.46	1.40
14	H	828	CLA	C3D-C4D	-4.82	1.33	1.44
14	A	828	CLA	O2D-CGD	4.82	1.45	1.33
17	a	850	BCR	C10-C9	-4.82	1.24	1.35
14	B	822	CLA	O2D-CGD	4.82	1.45	1.33
14	H	836	CLA	O2D-CGD	4.82	1.45	1.33
14	G	843	CLA	CHC-C1C	4.81	1.46	1.34
14	b	831	CLA	O2D-CGD	4.81	1.45	1.33
14	a	821	CLA	C3B-C2B	4.81	1.46	1.40
14	A	805	CLA	O2D-CGD	4.80	1.45	1.33
14	a	838	CLA	O2D-CGD	4.80	1.45	1.33
14	l	202	CLA	C3B-C2B	4.80	1.46	1.40
17	B	846	BCR	C10-C9	-4.80	1.24	1.35
14	G	814	CLA	C3B-C2B	4.80	1.46	1.40
14	b	803	CLA	C3B-C2B	4.80	1.46	1.40
13	G	801	CL0	C3B-C2B	4.80	1.46	1.40
14	K	101	CLA	CHD-C1D	4.80	1.47	1.38
14	B	811	CLA	O2D-CGD	4.80	1.45	1.33
14	a	843	CLA	CHD-C1D	4.80	1.47	1.38
14	G	839	CLA	O2D-CGD	4.79	1.45	1.33
14	L	205	CLA	O2D-CGD	4.79	1.45	1.33
14	G	805	CLA	O2D-CGD	4.79	1.45	1.33
14	H	802	CLA	C3B-C2B	4.79	1.46	1.40
14	B	817	CLA	C3B-C2B	4.79	1.46	1.40
14	B	801	CLA	O2D-CGD	4.78	1.45	1.33
17	A	851	BCR	C10-C9	-4.78	1.24	1.35
14	A	831	CLA	O2D-CGD	4.78	1.45	1.33
14	G	830	CLA	C3B-C2B	4.77	1.46	1.40
14	l	202	CLA	CHC-C1C	4.77	1.46	1.34
14	G	806	CLA	O2D-CGD	4.77	1.45	1.33
14	B	834	CLA	C3C-C2C	4.77	1.47	1.36
14	H	829	CLA	CHC-C1C	4.77	1.46	1.34
14	G	802	CLA	C3B-C2B	4.77	1.46	1.40
14	b	822	CLA	O2D-CGD	4.77	1.44	1.33
13	a	801	CL0	C3B-C2B	4.76	1.46	1.40
14	B	831	CLA	O2D-CGD	4.76	1.44	1.33
14	b	815	CLA	C3B-C2B	4.76	1.46	1.40
15	B	841	PQN	C10-C5	4.76	1.48	1.40
14	G	827	CLA	C3B-C2B	4.76	1.46	1.40
14	a	828	CLA	C3B-C2B	4.76	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	822	CLA	C3B-C2B	4.75	1.46	1.40
14	A	824	CLA	CHD-C1D	4.75	1.47	1.38
14	B	838	CLA	O2D-CGD	4.75	1.44	1.33
14	H	814	CLA	O2D-CGD	4.75	1.44	1.33
14	a	827	CLA	C3D-C4D	-4.75	1.33	1.44
14	G	816	CLA	C3B-C2B	4.75	1.46	1.40
14	H	801	CLA	O2D-CGD	4.74	1.44	1.33
14	B	803	CLA	O2D-CGD	4.74	1.44	1.33
14	H	803	CLA	O2D-CGD	4.74	1.44	1.33
14	a	821	CLA	CHD-C1D	4.74	1.47	1.38
14	b	825	CLA	C3C-C2C	4.74	1.47	1.36
14	B	808	CLA	C3D-C4D	-4.74	1.33	1.44
14	b	838	CLA	O2D-CGD	4.74	1.44	1.33
14	A	844	CLA	CHC-C1C	4.74	1.46	1.34
14	l	206	CLA	O2D-CGD	4.73	1.44	1.33
14	A	829	CLA	O2D-CGD	4.73	1.44	1.33
14	b	828	CLA	C3D-C4D	-4.73	1.33	1.44
14	T	1401	CLA	C3B-C2B	4.73	1.46	1.40
14	a	813	CLA	O2D-CGD	4.73	1.44	1.33
17	J	102	BCR	C10-C9	-4.73	1.24	1.35
14	H	813	CLA	O2D-CGD	4.73	1.44	1.33
14	W	1701	CLA	O2D-CGD	4.73	1.44	1.33
14	F	1301	CLA	C3C-C2C	4.72	1.47	1.36
14	A	837	CLA	CHD-C1D	4.72	1.47	1.38
14	B	825	CLA	C3C-C2C	4.72	1.47	1.36
14	A	845	CLA	O2D-CGD	4.72	1.44	1.33
14	a	826	CLA	O2D-CGD	4.72	1.44	1.33
14	a	807	CLA	CHD-C1D	4.72	1.47	1.38
14	A	839	CLA	O2D-CGD	4.71	1.44	1.33
14	G	812	CLA	CHD-C1D	4.71	1.47	1.38
15	b	841	PQN	C10-C5	4.71	1.48	1.40
14	a	830	CLA	C3C-C2C	4.71	1.46	1.36
14	B	840	CLA	CHC-C1C	4.71	1.46	1.34
14	b	807	CLA	C3B-C2B	4.71	1.46	1.40
14	X	1701	CLA	O2D-CGD	4.71	1.44	1.33
14	a	819	CLA	C3B-C2B	4.71	1.46	1.40
14	A	820	CLA	C3B-C2B	4.70	1.46	1.40
14	B	810	CLA	CHD-C1D	4.70	1.47	1.38
17	S	104	BCR	C10-C9	-4.70	1.24	1.35
14	H	831	CLA	O2D-CGD	4.70	1.44	1.33
14	G	815	CLA	CHD-C1D	4.70	1.47	1.38
17	f	201	BCR	C10-C9	-4.70	1.24	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	812	CLA	C3B-C2B	4.70	1.46	1.40
14	B	806	CLA	C3B-C2B	4.69	1.46	1.40
14	a	840	CLA	CHD-C1D	4.69	1.47	1.38
14	H	824	CLA	C3B-C2B	4.69	1.46	1.40
14	H	840	CLA	CHC-C1C	4.69	1.46	1.34
14	b	828	CLA	CHD-C1D	4.68	1.47	1.38
14	j	101	CLA	CHD-C1D	4.68	1.47	1.38
14	a	810	CLA	C3B-C2B	4.68	1.46	1.40
14	H	822	CLA	O2D-CGD	4.68	1.44	1.33
14	F	1303	CLA	C3B-C2B	4.68	1.46	1.40
14	A	822	CLA	C3B-C2B	4.68	1.46	1.40
17	l	203	BCR	C10-C9	-4.68	1.25	1.35
14	a	833	CLA	C3B-C2B	4.68	1.46	1.40
17	R	102	BCR	C10-C9	-4.68	1.25	1.35
14	H	828	CLA	CHD-C1D	4.67	1.47	1.38
14	B	833	CLA	O2D-CGD	4.67	1.44	1.33
14	B	802	CLA	C3B-C2B	4.67	1.46	1.40
14	G	844	CLA	CHD-C1D	4.67	1.47	1.38
14	B	828	CLA	C3D-C4D	-4.67	1.33	1.44
14	A	812	CLA	CHD-C1D	4.67	1.47	1.38
14	B	829	CLA	CHC-C1C	4.67	1.46	1.34
14	A	814	CLA	C3B-C2B	4.66	1.46	1.40
14	A	817	CLA	CHD-C1D	4.66	1.47	1.38
14	b	818	CLA	C3C-C2C	4.66	1.46	1.36
14	G	803	CLA	C3D-C4D	-4.66	1.33	1.44
14	b	809	CLA	CHC-C1C	4.66	1.46	1.34
14	a	836	CLA	CHD-C1D	4.66	1.47	1.38
14	A	843	CLA	C3B-C2B	4.65	1.46	1.40
14	H	814	CLA	C3B-C2B	4.65	1.46	1.40
14	G	831	CLA	C3C-C2C	4.65	1.46	1.36
14	k	1401	CLA	C3B-C2B	4.65	1.46	1.40
14	H	809	CLA	CHC-C1C	4.65	1.46	1.34
14	b	834	CLA	C3C-C2C	4.65	1.46	1.36
14	A	804	CLA	C3B-C2B	4.64	1.46	1.40
14	a	841	CLA	C3B-C2B	4.64	1.46	1.40
14	a	807	CLA	C3B-C2B	4.64	1.46	1.40
14	x	1701	CLA	C3B-C2B	4.64	1.46	1.40
14	G	834	CLA	C3B-C2B	4.64	1.46	1.40
14	H	832	CLA	CHD-C1D	4.64	1.47	1.38
14	B	837	CLA	C3B-C2B	4.64	1.46	1.40
14	H	833	CLA	CHD-C1D	4.64	1.47	1.38
14	H	819	CLA	C3B-C2B	4.64	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	840	CLA	CHC-C1C	4.64	1.46	1.34
14	B	818	CLA	O2D-CGD	4.64	1.44	1.33
14	G	811	CLA	C3B-C2B	4.64	1.46	1.40
14	G	820	CLA	CHD-C1D	4.63	1.47	1.38
14	H	831	CLA	C3C-C2C	4.63	1.46	1.36
14	B	826	CLA	C3B-C2B	4.63	1.46	1.40
14	H	837	CLA	C3D-C4D	-4.63	1.33	1.44
14	A	828	CLA	C3D-C4D	-4.63	1.33	1.44
17	a	848	BCR	C10-C9	-4.63	1.25	1.35
17	S	103	BCR	C10-C9	-4.63	1.25	1.35
14	H	828	CLA	C3B-C2B	4.63	1.46	1.40
14	f	202	CLA	C3B-C2B	4.63	1.46	1.40
14	G	821	CLA	C3B-C2B	4.62	1.46	1.40
14	A	815	CLA	CHD-C1D	4.62	1.47	1.38
14	b	829	CLA	CHC-C1C	4.62	1.45	1.34
14	G	835	CLA	C3B-C2B	4.62	1.46	1.40
14	G	842	CLA	C3B-C2B	4.62	1.46	1.40
14	G	829	CLA	C3B-C2B	4.62	1.46	1.40
14	U	204	CLA	C3C-C2C	4.62	1.46	1.36
14	a	823	CLA	C3C-C2C	4.62	1.46	1.36
14	B	810	CLA	C3C-C2C	4.62	1.46	1.36
14	a	803	CLA	C3B-C2B	4.61	1.46	1.40
14	H	828	CLA	C3C-C2C	4.61	1.46	1.36
14	b	806	CLA	C3D-C4D	-4.61	1.33	1.44
14	G	837	CLA	CHD-C1D	4.61	1.47	1.38
14	b	819	CLA	C3B-C2B	4.61	1.46	1.40
14	K	102	CLA	C3B-C2B	4.61	1.46	1.40
14	j	102	CLA	CHD-C1D	4.61	1.47	1.38
14	B	814	CLA	C3B-C2B	4.61	1.46	1.40
17	L	202	BCR	C10-C9	-4.60	1.25	1.35
14	L	205	CLA	C3C-C2C	4.60	1.46	1.36
17	l	201	BCR	C10-C9	-4.60	1.25	1.35
14	H	837	CLA	CHD-C1D	4.60	1.47	1.38
14	a	813	CLA	C3B-C2B	4.60	1.46	1.40
14	H	805	CLA	C3D-C4D	-4.60	1.33	1.44
14	G	813	CLA	CHD-C1D	4.60	1.47	1.38
14	a	833	CLA	CHD-C1D	4.60	1.47	1.38
14	A	831	CLA	C3C-C2C	4.60	1.46	1.36
14	j	101	CLA	C3B-C2B	4.60	1.46	1.40
14	F	1303	CLA	CHD-C1D	4.60	1.47	1.38
14	a	815	CLA	CHD-C1D	4.60	1.47	1.38
14	H	830	CLA	C3C-C2C	4.60	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	808	CLA	CHD-C1D	4.59	1.47	1.38
14	B	835	CLA	CHD-C1D	4.59	1.47	1.38
14	G	813	CLA	C3B-C2B	4.59	1.46	1.40
14	G	816	CLA	CHD-C1D	4.59	1.47	1.38
14	B	830	CLA	CHD-C1D	4.59	1.47	1.38
14	b	811	CLA	CHD-C1D	4.59	1.47	1.38
14	a	838	CLA	C3B-C2B	4.59	1.46	1.40
14	G	844	CLA	C3B-C2B	4.59	1.46	1.40
14	B	805	CLA	C3C-C2C	4.59	1.46	1.36
14	A	821	CLA	C3B-C2B	4.59	1.46	1.40
17	U	202	BCR	C10-C9	-4.59	1.25	1.35
14	G	831	CLA	C3B-C2B	4.58	1.46	1.40
14	b	840	CLA	C3C-C2C	4.58	1.46	1.36
17	G	851	BCR	C10-C9	-4.58	1.25	1.35
14	b	804	CLA	O2D-CGD	4.58	1.44	1.33
14	a	842	CLA	C3C-C2C	4.58	1.46	1.36
14	S	101	CLA	CHD-C1D	4.58	1.47	1.38
14	B	809	CLA	CHC-C1C	4.58	1.45	1.34
14	H	824	CLA	CHD-C1D	4.58	1.47	1.38
14	k	1401	CLA	C3C-C2C	4.58	1.46	1.36
14	W	1701	CLA	C3B-C2B	4.58	1.46	1.40
14	B	811	CLA	C3B-C2B	4.58	1.46	1.40
14	b	804	CLA	C3B-C2B	4.58	1.46	1.40
14	a	802	CLA	C3D-C4D	-4.57	1.33	1.44
14	U	205	CLA	C3C-C2C	4.57	1.46	1.36
14	b	810	CLA	CHD-C1D	4.57	1.47	1.38
15	H	841	PQN	C10-C5	4.57	1.48	1.40
14	B	828	CLA	CHD-C1D	4.57	1.47	1.38
14	A	813	CLA	C3B-C2B	4.57	1.46	1.40
14	B	819	CLA	C3B-C2B	4.57	1.46	1.40
14	a	815	CLA	C3C-C2C	4.57	1.46	1.36
14	a	843	CLA	C3B-C2B	4.56	1.46	1.40
14	a	817	CLA	CHD-C1D	4.56	1.47	1.38
14	G	827	CLA	C3C-C2C	4.56	1.46	1.36
14	G	804	CLA	C3B-C2B	4.56	1.46	1.40
14	A	822	CLA	C3C-C2C	4.56	1.46	1.36
14	A	834	CLA	C3B-C2B	4.56	1.46	1.40
14	x	1701	CLA	O2D-CGD	4.56	1.44	1.33
14	H	826	CLA	C3B-C2B	4.56	1.46	1.40
14	a	812	CLA	CHD-C1D	4.56	1.47	1.38
14	a	810	CLA	C3C-C2C	4.56	1.46	1.36
14	G	828	CLA	C3D-C4D	-4.56	1.33	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	807	CLA	C3C-C2C	4.56	1.46	1.36
14	a	832	CLA	C3C-C2C	4.56	1.46	1.36
14	a	836	CLA	C3C-C2C	4.56	1.46	1.36
14	A	833	CLA	CHD-C1D	4.56	1.47	1.38
17	A	849	BCR	C10-C9	-4.56	1.25	1.35
14	K	101	CLA	C3B-C2B	4.56	1.46	1.40
14	b	805	CLA	C3C-C2C	4.56	1.46	1.36
14	H	818	CLA	CHD-C1D	4.55	1.47	1.38
14	J	101	CLA	C3B-C2B	4.55	1.46	1.40
14	b	835	CLA	CHD-C1D	4.55	1.47	1.38
14	A	806	CLA	CHD-C1D	4.55	1.47	1.38
14	b	805	CLA	CHD-C1D	4.55	1.47	1.38
14	G	843	CLA	CHD-C1D	4.55	1.47	1.38
17	b	846	BCR	C10-C9	-4.55	1.25	1.35
14	H	810	CLA	C3C-C2C	4.55	1.46	1.36
14	b	817	CLA	C3B-C2B	4.55	1.46	1.40
17	L	207	BCR	C10-C9	-4.55	1.25	1.35
14	G	817	CLA	CHD-C1D	4.55	1.47	1.38
17	G	849	BCR	C10-C9	-4.55	1.25	1.35
14	H	839	CLA	C3D-C4D	-4.55	1.34	1.44
14	b	824	CLA	C3C-C2C	4.54	1.46	1.36
14	J	101	CLA	CHD-C1D	4.54	1.47	1.38
14	F	1301	CLA	C3B-C2B	4.54	1.46	1.40
14	H	813	CLA	C3D-C4D	-4.54	1.34	1.44
14	A	829	CLA	C3B-C2B	4.54	1.46	1.40
14	B	817	CLA	CHD-C1D	4.54	1.47	1.38
14	H	837	CLA	C3C-C2C	4.54	1.46	1.36
14	B	827	CLA	C3D-C4D	-4.54	1.34	1.44
14	G	834	CLA	CHD-C1D	4.54	1.47	1.38
14	G	817	CLA	C3C-C2C	4.54	1.46	1.36
14	G	834	CLA	C3C-C2C	4.54	1.46	1.36
14	H	806	CLA	C3B-C2B	4.54	1.46	1.40
14	A	829	CLA	C3D-C4D	-4.54	1.34	1.44
14	G	822	CLA	C3C-C2C	4.54	1.46	1.36
14	B	833	CLA	CHD-C1D	4.54	1.47	1.38
14	B	835	CLA	C3C-C2C	4.53	1.46	1.36
14	A	827	CLA	C3B-C2B	4.53	1.46	1.40
14	U	201	CLA	C3B-C2B	4.53	1.46	1.40
17	a	851	BCR	C10-C9	-4.53	1.25	1.35
14	H	818	CLA	C3C-C2C	4.53	1.46	1.36
14	H	811	CLA	CHD-C1D	4.53	1.47	1.38
14	a	811	CLA	CHD-C1D	4.53	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	839	CLA	C3D-C4D	-4.53	1.34	1.44
17	B	843	BCR	C10-C9	-4.53	1.25	1.35
14	H	804	CLA	CHD-C1D	4.53	1.47	1.38
14	J	101	CLA	C3C-C2C	4.53	1.46	1.36
14	b	837	CLA	C3C-C2C	4.53	1.46	1.36
14	b	830	CLA	C3C-C2C	4.53	1.46	1.36
14	A	833	CLA	C3C-C2C	4.53	1.46	1.36
14	G	808	CLA	C3B-C2B	4.53	1.46	1.40
14	a	816	CLA	CHD-C1D	4.53	1.47	1.38
14	A	822	CLA	CHD-C1D	4.52	1.47	1.38
14	G	837	CLA	C3B-C2B	4.52	1.46	1.40
14	B	809	CLA	C3D-C4D	-4.52	1.34	1.44
14	H	811	CLA	C3C-C2C	4.52	1.46	1.36
14	b	839	CLA	C3C-C2C	4.52	1.46	1.36
17	H	846	BCR	C10-C9	-4.52	1.25	1.35
14	a	832	CLA	CHD-C1D	4.52	1.47	1.38
14	A	819	CLA	C3C-C2C	4.52	1.46	1.36
14	b	828	CLA	C3B-C2B	4.52	1.46	1.40
14	b	837	CLA	C3B-C2B	4.52	1.46	1.40
14	F	1303	CLA	C3C-C2C	4.52	1.46	1.36
14	A	804	CLA	C3D-C4D	-4.52	1.34	1.44
14	a	828	CLA	O2D-CGD	4.52	1.44	1.33
14	A	820	CLA	CHD-C1D	4.52	1.47	1.38
14	G	804	CLA	C3C-C2C	4.52	1.46	1.36
14	B	818	CLA	C3C-C2C	4.52	1.46	1.36
14	H	818	CLA	O2D-CGD	4.52	1.44	1.33
14	A	834	CLA	CHD-C1D	4.52	1.47	1.38
14	a	816	CLA	C3C-C2C	4.52	1.46	1.36
14	b	810	CLA	C3C-C2C	4.51	1.46	1.36
17	G	852	BCR	C10-C9	-4.51	1.25	1.35
14	B	830	CLA	C3C-C2C	4.51	1.46	1.36
14	U	206	CLA	CHD-C1D	4.51	1.47	1.38
14	B	824	CLA	C3C-C2C	4.51	1.46	1.36
14	V	1601	CLA	C3D-C4D	-4.51	1.34	1.44
14	l	207	CLA	CHD-C1D	4.51	1.47	1.38
14	B	805	CLA	CHD-C1D	4.51	1.47	1.38
14	A	824	CLA	C3C-C2C	4.51	1.46	1.36
14	G	805	CLA	CHD-C1D	4.51	1.47	1.38
14	H	834	CLA	CHD-C1D	4.51	1.47	1.38
14	G	824	CLA	CHD-C1D	4.51	1.47	1.38
14	H	836	CLA	C3C-C2C	4.51	1.46	1.36
14	a	812	CLA	C3C-C2C	4.51	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	808	CLA	C3C-C2C	4.51	1.46	1.36
14	H	804	CLA	C3C-C2C	4.51	1.46	1.36
14	H	803	CLA	C3B-C2B	4.51	1.46	1.40
14	S	102	CLA	CHD-C1D	4.50	1.47	1.38
14	a	808	CLA	C3C-C2C	4.50	1.46	1.36
14	H	830	CLA	CHD-C1D	4.50	1.47	1.38
14	b	832	CLA	C3C-C2C	4.50	1.46	1.36
14	H	808	CLA	C3D-C4D	-4.50	1.34	1.44
14	a	819	CLA	CHD-C1D	4.50	1.47	1.38
14	B	831	CLA	C3C-C2C	4.50	1.46	1.36
14	H	824	CLA	C3C-C2C	4.50	1.46	1.36
14	b	819	CLA	C3C-C2C	4.50	1.46	1.36
14	b	822	CLA	CHD-C1D	4.50	1.47	1.38
14	B	828	CLA	C3C-C2C	4.50	1.46	1.36
17	Q	202	BCR	C10-C9	-4.50	1.25	1.35
14	A	803	CLA	C3D-C4D	-4.50	1.34	1.44
17	G	850	BCR	C10-C9	-4.50	1.25	1.35
14	B	811	CLA	C3C-C2C	4.50	1.46	1.36
14	a	821	CLA	C3C-C2C	4.50	1.46	1.36
14	a	820	CLA	C3B-C2B	4.49	1.46	1.40
14	G	814	CLA	C3C-C2C	4.49	1.46	1.36
14	K	102	CLA	C3C-C2C	4.49	1.46	1.36
14	S	102	CLA	C3C-C2C	4.49	1.46	1.36
14	b	838	CLA	C3D-C4D	-4.49	1.34	1.44
14	B	840	CLA	C3C-C2C	4.49	1.46	1.36
14	a	831	CLA	C3C-C2C	4.49	1.46	1.36
14	b	820	CLA	C3B-C2B	4.49	1.46	1.40
14	x	1701	CLA	C3C-C2C	4.49	1.46	1.36
14	V	1601	CLA	C3C-C2C	4.49	1.46	1.36
14	A	841	CLA	CHD-C1D	4.49	1.47	1.38
14	B	813	CLA	C3C-C2C	4.49	1.46	1.36
14	B	825	CLA	C3D-C4D	-4.49	1.34	1.44
14	G	839	CLA	CHD-C1D	4.49	1.47	1.38
14	A	843	CLA	C3C-C2C	4.49	1.46	1.36
17	b	847	BCR	C10-C9	-4.49	1.25	1.35
14	b	839	CLA	C3D-C4D	-4.48	1.34	1.44
14	G	813	CLA	C3C-C2C	4.48	1.46	1.36
14	B	839	CLA	C3C-C2C	4.48	1.46	1.36
17	B	850	BCR	C10-C9	-4.48	1.25	1.35
14	A	824	CLA	C3B-C2B	4.48	1.46	1.40
14	V	1601	CLA	CHD-C1D	4.48	1.47	1.38
14	b	806	CLA	C3C-C2C	4.48	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	841	CLA	C3C-C2C	4.48	1.46	1.36
14	b	835	CLA	C3C-C2C	4.48	1.46	1.36
14	B	827	CLA	C3C-C2C	4.48	1.46	1.36
14	i	101	CLA	C3D-C4D	-4.48	1.34	1.44
14	B	833	CLA	C3C-C2C	4.48	1.46	1.36
14	G	835	CLA	CHD-C1D	4.48	1.47	1.38
14	A	817	CLA	C3C-C2C	4.48	1.46	1.36
14	B	805	CLA	C3D-C4D	-4.48	1.34	1.44
14	A	820	CLA	C3C-C2C	4.48	1.46	1.36
14	A	824	CLA	C3D-C4D	-4.48	1.34	1.44
14	a	817	CLA	C3C-C2C	4.48	1.46	1.36
14	b	831	CLA	C3C-C2C	4.47	1.46	1.36
14	j	101	CLA	C3C-C2C	4.47	1.46	1.36
14	L	201	CLA	C3B-C2B	4.47	1.46	1.40
14	A	816	CLA	CHD-C1D	4.47	1.47	1.38
14	b	837	CLA	C3D-C4D	-4.47	1.34	1.44
14	G	806	CLA	CHD-C1D	4.47	1.47	1.38
17	A	852	BCR	C10-C9	-4.47	1.25	1.35
14	b	829	CLA	C3D-C4D	-4.47	1.34	1.44
14	b	811	CLA	C3C-C2C	4.47	1.46	1.36
14	K	102	CLA	CHD-C1D	4.47	1.47	1.38
14	H	821	CLA	C3C-C2C	4.47	1.46	1.36
14	H	807	CLA	C3B-C2B	4.47	1.46	1.40
17	H	847	BCR	C10-C9	-4.47	1.25	1.35
14	Q	201	CLA	C3B-C2B	4.47	1.46	1.40
14	V	1601	CLA	C3B-C2B	4.47	1.46	1.40
14	b	821	CLA	CHD-C1D	4.47	1.47	1.38
17	G	848	BCR	C10-C9	-4.47	1.25	1.35
14	f	202	CLA	CHD-C1D	4.47	1.47	1.38
14	G	831	CLA	CHD-C1D	4.47	1.47	1.38
14	a	834	CLA	CHD-C1D	4.47	1.47	1.38
14	G	840	CLA	C3C-C2C	4.47	1.46	1.36
14	A	830	CLA	C3B-C2B	4.47	1.46	1.40
17	j	103	BCR	C10-C9	-4.46	1.25	1.35
14	A	838	CLA	C3C-C2C	4.46	1.46	1.36
14	A	832	CLA	C3D-C4D	-4.46	1.34	1.44
14	b	811	CLA	C3B-C2B	4.46	1.46	1.40
14	H	819	CLA	C3C-C2C	4.46	1.46	1.36
14	f	202	CLA	C3C-C2C	4.46	1.46	1.36
14	S	101	CLA	C3B-C2B	4.46	1.46	1.40
14	G	833	CLA	C3C-C2C	4.46	1.46	1.36
14	G	822	CLA	C3D-C4D	-4.46	1.34	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	836	CLA	C3C-C2C	4.46	1.46	1.36
14	b	830	CLA	CHD-C1D	4.46	1.47	1.38
14	G	808	CLA	C3C-C2C	4.46	1.46	1.36
14	b	822	CLA	C3C-C2C	4.46	1.46	1.36
14	H	829	CLA	C3D-C4D	-4.46	1.34	1.44
14	G	832	CLA	CHD-C1D	4.46	1.47	1.38
14	A	819	CLA	CHD-C1D	4.46	1.47	1.38
14	m	1601	CLA	CHD-C1D	4.46	1.47	1.38
14	G	824	CLA	C3B-C2B	4.46	1.46	1.40
14	G	829	CLA	C3D-C4D	-4.46	1.34	1.44
14	Q	203	CLA	C3B-C2B	4.46	1.46	1.40
14	G	836	CLA	CHD-C1D	4.46	1.47	1.38
14	b	812	CLA	CHD-C1D	4.46	1.47	1.38
14	G	811	CLA	C3C-C2C	4.46	1.46	1.36
14	a	806	CLA	C3B-C2B	4.46	1.46	1.40
14	b	809	CLA	C3D-C4D	-4.46	1.34	1.44
14	b	803	CLA	C3D-C4D	-4.46	1.34	1.44
14	G	820	CLA	C3C-C2C	4.46	1.46	1.36
14	T	1401	CLA	CHD-C1D	4.45	1.47	1.38
14	G	816	CLA	C3C-C2C	4.45	1.46	1.36
14	a	811	CLA	C3C-C2C	4.45	1.46	1.36
14	a	814	CLA	C3C-C2C	4.45	1.46	1.36
14	m	1601	CLA	C3C-C2C	4.45	1.46	1.36
14	A	839	CLA	CHD-C1D	4.45	1.47	1.38
14	b	808	CLA	C3D-C4D	-4.45	1.34	1.44
14	B	821	CLA	C3C-C2C	4.45	1.46	1.36
14	b	828	CLA	C3C-C2C	4.45	1.46	1.36
14	b	817	CLA	CHD-C1D	4.45	1.47	1.38
14	b	824	CLA	CHD-C1D	4.45	1.47	1.38
14	A	804	CLA	C3C-C2C	4.45	1.46	1.36
14	A	834	CLA	C3C-C2C	4.45	1.46	1.36
14	m	1601	CLA	C3B-C2B	4.45	1.46	1.40
14	G	836	CLA	C3C-C2C	4.45	1.46	1.36
14	a	809	CLA	C3D-C4D	-4.45	1.34	1.44
14	j	102	CLA	C3C-C2C	4.45	1.46	1.36
14	G	827	CLA	CHD-C1D	4.44	1.47	1.38
14	G	835	CLA	C3D-C4D	-4.44	1.34	1.44
14	a	837	CLA	C3C-C2C	4.44	1.46	1.36
14	B	818	CLA	CHD-C1D	4.44	1.47	1.38
14	a	814	CLA	CHD-C1D	4.44	1.47	1.38
14	b	813	CLA	CHD-C1D	4.44	1.47	1.38
14	a	829	CLA	CHD-C1D	4.44	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	817	CLA	CHD-C1D	4.44	1.47	1.38
17	B	847	BCR	C10-C9	-4.44	1.25	1.35
14	A	837	CLA	C3C-C2C	4.44	1.46	1.36
14	A	808	CLA	C3B-C2B	4.44	1.46	1.40
14	H	832	CLA	C3B-C2B	4.44	1.46	1.40
14	G	825	CLA	CHD-C1D	4.44	1.47	1.38
14	a	855	CLA	C3C-C2C	4.44	1.46	1.36
17	B	848	BCR	C10-C9	-4.44	1.25	1.35
14	X	1701	CLA	C3C-C2C	4.44	1.46	1.36
14	b	827	CLA	C3C-C2C	4.44	1.46	1.36
14	A	806	CLA	C3D-C4D	-4.44	1.34	1.44
14	a	832	CLA	C3D-C4D	-4.44	1.34	1.44
14	A	835	CLA	C3B-C2B	4.43	1.46	1.40
14	H	839	CLA	C3C-C2C	4.43	1.46	1.36
14	a	825	CLA	C3D-C4D	-4.43	1.34	1.44
14	B	826	CLA	C3D-C4D	-4.43	1.34	1.44
14	H	827	CLA	C3C-C2C	4.43	1.46	1.36
14	H	838	CLA	C3C-C2C	4.43	1.46	1.36
14	A	835	CLA	CHD-C1D	4.43	1.47	1.38
14	B	832	CLA	CHD-C1D	4.43	1.47	1.38
14	a	826	CLA	C3C-C2C	4.43	1.46	1.36
14	H	810	CLA	CHD-C1D	4.43	1.47	1.38
17	I	101	BCR	C10-C9	-4.43	1.25	1.35
14	b	826	CLA	C3B-C2B	4.43	1.46	1.40
14	A	832	CLA	CHD-C1D	4.43	1.47	1.38
14	b	826	CLA	C3C-C2C	4.43	1.46	1.36
14	G	819	CLA	C3B-C2B	4.43	1.46	1.40
14	b	834	CLA	CHD-C4C	4.43	1.49	1.39
14	G	832	CLA	C3D-C4D	-4.43	1.34	1.44
14	a	835	CLA	CHD-C1D	4.42	1.47	1.38
14	G	823	CLA	C3C-C2C	4.42	1.46	1.36
14	a	838	CLA	CHD-C1D	4.42	1.47	1.38
14	H	827	CLA	C3D-C4D	-4.42	1.34	1.44
14	b	826	CLA	C3D-C4D	-4.42	1.34	1.44
14	H	819	CLA	CHD-C1D	4.42	1.47	1.38
14	a	818	CLA	CHD-C1D	4.42	1.47	1.38
14	a	820	CLA	C3C-C2C	4.42	1.46	1.36
17	B	842	BCR	C10-C9	-4.42	1.25	1.35
14	A	807	CLA	C3D-C4D	-4.42	1.34	1.44
14	A	819	CLA	C3B-C2B	4.42	1.46	1.40
13	A	801	CL0	C3B-C2B	4.42	1.46	1.40
14	A	815	CLA	C3C-C2C	4.42	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	811	CLA	C3B-C2B	4.42	1.46	1.40
17	R	101	BCR	C10-C9	-4.42	1.25	1.35
14	G	810	CLA	CHD-C1D	4.42	1.47	1.38
14	l	205	CLA	C3C-C2C	4.42	1.46	1.36
14	H	820	CLA	C3C-C2C	4.42	1.46	1.36
14	a	804	CLA	CHD-C1D	4.42	1.47	1.38
14	B	815	CLA	C3C-C2C	4.42	1.46	1.36
14	G	809	CLA	C3C-C2C	4.42	1.46	1.36
14	a	818	CLA	C3C-C2C	4.42	1.46	1.36
14	H	836	CLA	CHD-C1D	4.42	1.47	1.38
14	B	814	CLA	C3C-C2C	4.42	1.46	1.36
14	G	807	CLA	C3D-C4D	-4.42	1.34	1.44
14	T	1401	CLA	C3C-C2C	4.42	1.46	1.36
14	W	1701	CLA	C3C-C2C	4.42	1.46	1.36
14	A	813	CLA	C3C-C2C	4.41	1.46	1.36
14	G	808	CLA	CHD-C1D	4.41	1.47	1.38
17	F	1302	BCR	C10-C9	-4.41	1.25	1.35
14	H	839	CLA	C3B-C2B	4.41	1.46	1.40
14	a	833	CLA	C3C-C2C	4.41	1.46	1.36
14	A	831	CLA	CHD-C1D	4.41	1.47	1.38
17	G	853	BCR	C10-C9	-4.41	1.25	1.35
14	H	812	CLA	CHD-C1D	4.41	1.47	1.38
14	G	822	CLA	CHD-C1D	4.41	1.47	1.38
14	b	821	CLA	C3C-C2C	4.41	1.46	1.36
14	B	837	CLA	C3D-C4D	-4.41	1.34	1.44
14	m	1601	CLA	C3D-C4D	-4.41	1.34	1.44
14	G	838	CLA	CHD-C1D	4.41	1.47	1.38
14	b	813	CLA	C3C-C2C	4.41	1.46	1.36
14	H	813	CLA	CHD-C1D	4.41	1.47	1.38
14	a	816	CLA	C3B-C2B	4.41	1.46	1.40
14	H	807	CLA	C3D-C4D	-4.41	1.34	1.44
14	a	839	CLA	CHD-C1D	4.41	1.47	1.38
14	G	842	CLA	C3C-C2C	4.40	1.46	1.36
14	A	841	CLA	C3D-C4D	-4.40	1.34	1.44
14	B	839	CLA	CHD-C1D	4.40	1.47	1.38
14	G	805	CLA	C3C-C2C	4.40	1.46	1.36
14	A	831	CLA	C3B-C2B	4.40	1.46	1.40
14	b	839	CLA	CHD-C1D	4.40	1.47	1.38
14	a	803	CLA	C3C-C2C	4.40	1.46	1.36
14	a	804	CLA	C3C-C2C	4.40	1.46	1.36
17	i	102	BCR	C10-C9	-4.40	1.25	1.35
14	a	839	CLA	C3C-C2C	4.40	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	839	CLA	C3D-C4D	-4.40	1.34	1.44
14	A	814	CLA	C3C-C2C	4.40	1.46	1.36
14	B	820	CLA	C3C-C2C	4.40	1.46	1.36
14	G	839	CLA	C3C-C2C	4.40	1.46	1.36
14	H	825	CLA	C3C-C2C	4.40	1.46	1.36
13	A	801	CL0	C3D-C4D	-4.40	1.34	1.44
14	A	840	CLA	C3C-C2C	4.40	1.46	1.36
17	f	203	BCR	C10-C9	-4.40	1.25	1.35
14	a	842	CLA	CHD-C1D	4.40	1.47	1.38
17	H	843	BCR	C10-C9	-4.40	1.25	1.35
14	a	840	CLA	C3C-C2C	4.40	1.46	1.36
17	A	853	BCR	C10-C9	-4.40	1.25	1.35
14	H	836	CLA	C3D-C4D	-4.40	1.34	1.44
14	A	842	CLA	C3B-C2B	4.40	1.46	1.40
14	K	101	CLA	C3C-C2C	4.40	1.46	1.36
17	a	849	BCR	C10-C9	-4.40	1.25	1.35
14	H	809	CLA	C3D-C4D	-4.40	1.34	1.44
14	H	829	CLA	CHD-C1D	4.40	1.47	1.38
14	b	838	CLA	C3C-C2C	4.39	1.46	1.36
14	b	833	CLA	C3C-C2C	4.39	1.46	1.36
14	A	805	CLA	CHD-C1D	4.39	1.47	1.38
14	a	831	CLA	C3D-C4D	-4.39	1.34	1.44
14	A	830	CLA	CHD-C1D	4.39	1.47	1.38
14	b	838	CLA	C3B-C2B	4.39	1.46	1.40
14	H	813	CLA	C3C-C2C	4.39	1.46	1.36
14	H	802	CLA	C3D-C4D	-4.39	1.34	1.44
14	H	833	CLA	C3C-C2C	4.39	1.46	1.36
14	M	1601	CLA	C3C-C2C	4.39	1.46	1.36
14	B	834	CLA	CHD-C1D	4.39	1.47	1.38
14	A	814	CLA	CHD-C1D	4.39	1.47	1.38
14	G	812	CLA	C3D-C4D	-4.39	1.34	1.44
14	B	824	CLA	CHD-C1D	4.39	1.47	1.38
14	b	827	CLA	C3D-C4D	-4.39	1.34	1.44
14	L	201	CLA	C3D-C4D	-4.39	1.34	1.44
14	a	821	CLA	C3D-C4D	-4.39	1.34	1.44
17	H	842	BCR	C10-C9	-4.39	1.25	1.35
14	a	843	CLA	C3C-C2C	4.39	1.46	1.36
14	B	837	CLA	C3C-C2C	4.38	1.46	1.36
14	b	835	CLA	C3B-C2B	4.38	1.46	1.40
14	A	827	CLA	C3C-C2C	4.38	1.46	1.36
14	A	836	CLA	C3C-C2C	4.38	1.46	1.36
14	H	826	CLA	C3D-C4D	-4.38	1.34	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	811	CLA	CHD-C1D	4.38	1.47	1.38
14	A	830	CLA	C3D-C4D	-4.38	1.34	1.44
14	H	801	CLA	C3C-C2C	4.38	1.46	1.36
14	A	809	CLA	C3B-C2B	4.38	1.46	1.40
14	A	809	CLA	C3C-C2C	4.38	1.46	1.36
14	A	826	CLA	C3C-C2C	4.38	1.46	1.36
14	A	837	CLA	C3B-C2B	4.38	1.46	1.40
14	G	818	CLA	C3D-C4D	-4.38	1.34	1.44
14	a	813	CLA	CHD-C1D	4.38	1.47	1.38
14	G	824	CLA	C3C-C2C	4.38	1.46	1.36
14	A	842	CLA	C3C-C2C	4.38	1.46	1.36
14	Q	203	CLA	C3C-C2C	4.38	1.46	1.36
18	A	855	LHG	O8-C23	4.38	1.46	1.33
14	B	814	CLA	C3D-C4D	-4.38	1.34	1.44
14	a	830	CLA	C3B-C2B	4.38	1.46	1.40
14	i	101	CLA	C3B-C2B	4.38	1.46	1.40
14	G	808	CLA	C3D-C4D	-4.37	1.34	1.44
14	a	825	CLA	C3C-C2C	4.37	1.46	1.36
14	k	1401	CLA	CHD-C1D	4.37	1.47	1.38
14	A	821	CLA	C3C-C2C	4.37	1.46	1.36
14	S	101	CLA	C3C-C2C	4.37	1.46	1.36
14	G	838	CLA	C3D-C4D	-4.37	1.34	1.44
14	H	816	CLA	CHD-C1D	4.37	1.47	1.38
14	G	815	CLA	C3C-C2C	4.37	1.46	1.36
14	B	810	CLA	C3D-C4D	-4.37	1.34	1.44
14	a	829	CLA	C3D-C4D	-4.37	1.34	1.44
14	B	838	CLA	C3B-C2B	4.37	1.46	1.40
14	B	813	CLA	C3D-C4D	-4.37	1.34	1.44
14	G	837	CLA	C3C-C2C	4.37	1.46	1.36
14	H	823	CLA	C3D-C4D	-4.37	1.34	1.44
14	A	825	CLA	CHD-C1D	4.37	1.46	1.38
14	b	807	CLA	C3D-C4D	-4.37	1.34	1.44
14	B	832	CLA	C3C-C2C	4.37	1.46	1.36
14	G	814	CLA	CHD-C1D	4.37	1.46	1.38
17	b	843	BCR	C10-C9	-4.37	1.25	1.35
14	B	807	CLA	C3C-C2C	4.37	1.46	1.36
14	H	838	CLA	CHD-C1D	4.37	1.46	1.38
14	Q	203	CLA	CHD-C1D	4.37	1.46	1.38
14	a	805	CLA	CHD-C1D	4.37	1.46	1.38
14	a	806	CLA	C3D-C4D	-4.37	1.34	1.44
14	B	821	CLA	C3B-C2B	4.37	1.46	1.40
14	a	831	CLA	C3B-C2B	4.37	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	803	CLA	CHD-C1D	4.37	1.46	1.38
14	a	808	CLA	C3B-C2B	4.37	1.46	1.40
18	a	854	LHG	O8-C23	4.37	1.46	1.33
14	a	805	CLA	C3D-C4D	-4.36	1.34	1.44
14	b	810	CLA	C3D-C4D	-4.36	1.34	1.44
14	a	841	CLA	CHD-C1D	4.36	1.46	1.38
14	B	806	CLA	C3D-C4D	-4.36	1.34	1.44
14	G	841	CLA	C3D-C4D	-4.36	1.34	1.44
14	a	807	CLA	C3D-C4D	-4.36	1.34	1.44
14	G	821	CLA	C3D-C4D	-4.36	1.34	1.44
14	H	835	CLA	C3B-C2B	4.36	1.46	1.40
14	b	826	CLA	CHD-C1D	4.36	1.46	1.38
14	G	819	CLA	C3C-C2C	4.36	1.46	1.36
14	a	822	CLA	C3C-C2C	4.36	1.46	1.36
14	H	838	CLA	C3D-C4D	-4.36	1.34	1.44
14	H	805	CLA	C3C-C2C	4.36	1.46	1.36
17	A	850	BCR	C10-C9	-4.36	1.25	1.35
14	A	844	CLA	C3D-C4D	-4.36	1.34	1.44
14	x	1701	CLA	CHD-C1D	4.36	1.46	1.38
14	A	840	CLA	C3D-C4D	-4.36	1.34	1.44
14	b	818	CLA	C3D-C4D	-4.36	1.34	1.44
14	A	840	CLA	CHD-C1D	4.36	1.46	1.38
14	b	833	CLA	CHD-C1D	4.36	1.46	1.38
14	l	207	CLA	C3C-C2C	4.36	1.46	1.36
14	A	821	CLA	CHD-C1D	4.36	1.46	1.38
14	G	806	CLA	C3D-C4D	-4.36	1.34	1.44
14	A	820	CLA	C3D-C4D	-4.36	1.34	1.44
14	B	829	CLA	C3D-C4D	-4.36	1.34	1.44
14	A	819	CLA	C3D-C4D	-4.35	1.34	1.44
14	a	820	CLA	CHD-C1D	4.35	1.46	1.38
14	B	817	CLA	C3D-C4D	-4.35	1.34	1.44
14	A	843	CLA	C3D-C4D	-4.35	1.34	1.44
14	G	810	CLA	C3D-C4D	-4.35	1.34	1.44
14	a	817	CLA	C3D-C4D	-4.35	1.34	1.44
13	G	801	CL0	C3D-C4D	-4.35	1.34	1.44
14	M	1601	CLA	C3D-C4D	-4.35	1.34	1.44
14	G	841	CLA	CHD-C1D	4.35	1.46	1.38
14	A	835	CLA	C3D-C4D	-4.35	1.34	1.44
14	b	835	CLA	C3D-C4D	-4.35	1.34	1.44
14	U	205	CLA	C3D-C4D	-4.35	1.34	1.44
14	H	840	CLA	C3C-C2C	4.35	1.46	1.36
17	H	849	BCR	C10-C9	-4.35	1.25	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Q	201	CLA	C3D-C4D	-4.35	1.34	1.44
14	G	824	CLA	C3D-C4D	-4.35	1.34	1.44
14	B	838	CLA	C3C-C2C	4.35	1.46	1.36
14	l	205	CLA	CHD-C1D	4.35	1.46	1.38
14	L	204	CLA	C3C-C2C	4.35	1.46	1.36
14	B	812	CLA	C3D-C4D	-4.35	1.34	1.44
14	a	823	CLA	CHD-C1D	4.35	1.46	1.38
14	H	833	CLA	C3D-C4D	-4.35	1.34	1.44
14	B	807	CLA	C3D-C4D	-4.35	1.34	1.44
14	a	802	CLA	CHD-C1D	4.35	1.46	1.38
14	B	838	CLA	C3D-C4D	-4.35	1.34	1.44
14	K	102	CLA	C3D-C4D	-4.35	1.34	1.44
13	a	801	CL0	C3D-C4D	-4.35	1.34	1.44
14	U	201	CLA	C3D-C4D	-4.35	1.34	1.44
14	H	810	CLA	C3D-C4D	-4.35	1.34	1.44
14	B	819	CLA	C3C-C2C	4.34	1.46	1.36
14	G	820	CLA	C3D-C4D	-4.34	1.34	1.44
14	A	803	CLA	CHD-C1D	4.34	1.46	1.38
14	G	834	CLA	C3D-C4D	-4.34	1.34	1.44
14	B	836	CLA	CHD-C1D	4.34	1.46	1.38
14	M	1601	CLA	CHD-C1D	4.34	1.46	1.38
14	A	812	CLA	C3C-C2C	4.34	1.46	1.36
14	G	841	CLA	C3C-C2C	4.34	1.46	1.36
14	B	815	CLA	CHD-C1D	4.34	1.46	1.38
14	A	827	CLA	C3D-C4D	-4.34	1.34	1.44
14	H	824	CLA	C3D-C4D	-4.34	1.34	1.44
14	a	837	CLA	C3D-C4D	-4.34	1.34	1.44
14	A	813	CLA	CHD-C1D	4.34	1.46	1.38
14	G	807	CLA	C3C-C2C	4.34	1.46	1.36
14	a	819	CLA	C3C-C2C	4.34	1.46	1.36
14	A	823	CLA	C3C-C2C	4.34	1.46	1.36
14	a	837	CLA	CHD-C1D	4.34	1.46	1.38
14	H	831	CLA	C3D-C4D	-4.34	1.34	1.44
14	A	844	CLA	CHD-C1D	4.34	1.46	1.38
14	L	206	CLA	CHD-C1D	4.34	1.46	1.38
14	G	823	CLA	C3D-C4D	-4.34	1.34	1.44
14	A	832	CLA	C3C-C2C	4.34	1.46	1.36
14	B	814	CLA	CHD-C1D	4.34	1.46	1.38
14	A	826	CLA	CHD-C1D	4.34	1.46	1.38
14	A	826	CLA	C3D-C4D	-4.34	1.34	1.44
14	H	825	CLA	C3D-C4D	-4.34	1.34	1.44
14	H	839	CLA	CHD-C1D	4.34	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	836	CLA	C3B-C2B	4.34	1.46	1.40
14	L	206	CLA	C3C-C2C	4.33	1.46	1.36
14	A	834	CLA	C3D-C4D	-4.33	1.34	1.44
14	B	804	CLA	C3C-C2C	4.33	1.46	1.36
14	b	814	CLA	C3C-C2C	4.33	1.46	1.36
14	G	838	CLA	C3C-C2C	4.33	1.46	1.36
14	b	815	CLA	C3C-C2C	4.33	1.46	1.36
14	l	207	CLA	C3D-C4D	-4.33	1.34	1.44
14	G	831	CLA	C3D-C4D	-4.33	1.34	1.44
14	G	827	CLA	C3D-C4D	-4.33	1.34	1.44
14	G	833	CLA	C3D-C4D	-4.33	1.34	1.44
14	H	826	CLA	C3C-C2C	4.33	1.46	1.36
14	H	835	CLA	C3C-C2C	4.33	1.46	1.36
14	b	813	CLA	C3D-C4D	-4.33	1.34	1.44
14	a	823	CLA	C3B-C2B	4.33	1.46	1.40
14	b	832	CLA	CHD-C1D	4.33	1.46	1.38
14	A	839	CLA	C3C-C2C	4.33	1.46	1.36
14	A	816	CLA	C3C-C2C	4.33	1.46	1.36
14	G	818	CLA	CHD-C1D	4.33	1.46	1.38
14	A	835	CLA	C3C-C2C	4.33	1.46	1.36
14	G	821	CLA	C3C-C2C	4.33	1.46	1.36
17	b	849	BCR	C10-C9	-4.33	1.25	1.35
14	B	827	CLA	CHD-C1D	4.33	1.46	1.38
14	a	840	CLA	C3D-C4D	-4.33	1.34	1.44
14	A	811	CLA	CHD-C1D	4.32	1.46	1.38
17	B	844	BCR	C10-C9	-4.32	1.25	1.35
14	b	809	CLA	C3C-C2C	4.32	1.46	1.36
14	a	824	CLA	CHD-C1D	4.32	1.46	1.38
14	B	804	CLA	CHD-C1D	4.32	1.46	1.38
14	b	831	CLA	CHD-C1D	4.32	1.46	1.38
17	m	1602	BCR	C10-C9	-4.32	1.25	1.35
14	a	842	CLA	C3B-C2B	4.32	1.46	1.40
14	H	806	CLA	C3C-C2C	4.32	1.46	1.36
14	G	830	CLA	C3D-C4D	-4.32	1.34	1.44
14	a	811	CLA	C3D-C4D	-4.32	1.34	1.44
14	l	202	CLA	C3D-C4D	-4.32	1.34	1.44
18	G	855	LHG	O8-C23	4.32	1.45	1.33
14	b	816	CLA	CHD-C1D	4.32	1.46	1.38
14	a	818	CLA	C3D-C4D	-4.32	1.34	1.44
14	G	832	CLA	C3C-C2C	4.32	1.46	1.36
14	B	839	CLA	C3B-C2B	4.32	1.46	1.40
14	b	805	CLA	C3D-C4D	-4.32	1.34	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	834	CLA	C3C-C2C	4.32	1.46	1.36
14	G	823	CLA	CHD-C1D	4.32	1.46	1.38
14	l	206	CLA	C3C-C2C	4.32	1.46	1.36
14	Q	201	CLA	C3C-C2C	4.32	1.46	1.36
14	G	839	CLA	C3B-C2B	4.31	1.46	1.40
14	a	822	CLA	C3D-C4D	-4.31	1.34	1.44
17	a	847	BCR	C10-C9	-4.31	1.25	1.35
14	a	835	CLA	C3C-C2C	4.31	1.46	1.36
14	l	206	CLA	C3D-C4D	-4.31	1.34	1.44
14	a	834	CLA	C3C-C2C	4.31	1.46	1.36
14	B	819	CLA	CHD-C1D	4.31	1.46	1.38
14	b	840	CLA	C3D-C4D	-4.31	1.34	1.44
14	b	807	CLA	C3C-C2C	4.31	1.46	1.36
14	G	812	CLA	C3C-C2C	4.31	1.46	1.36
17	l	208	BCR	C10-C9	-4.31	1.25	1.35
14	W	1701	CLA	CHD-C1D	4.31	1.46	1.38
14	H	816	CLA	C3C-C2C	4.31	1.46	1.36
14	H	806	CLA	C3D-C4D	-4.31	1.34	1.44
14	b	819	CLA	C3D-C4D	-4.31	1.34	1.44
14	B	821	CLA	CHD-C1D	4.31	1.46	1.38
14	B	818	CLA	C3D-C4D	-4.31	1.34	1.44
14	G	826	CLA	C3D-C4D	-4.31	1.34	1.44
14	A	817	CLA	C3B-C2B	4.31	1.46	1.40
14	a	819	CLA	C3D-C4D	-4.31	1.34	1.44
14	B	831	CLA	CHD-C1D	4.31	1.46	1.38
14	a	842	CLA	C3D-C4D	-4.31	1.34	1.44
14	G	839	CLA	C3D-C4D	-4.31	1.34	1.44
14	B	829	CLA	CHD-C1D	4.31	1.46	1.38
14	G	842	CLA	C3D-C4D	-4.31	1.34	1.44
14	b	833	CLA	C3D-C4D	-4.30	1.34	1.44
14	B	801	CLA	C3C-C2C	4.30	1.46	1.36
14	b	839	CLA	C3B-C2B	4.30	1.46	1.40
14	B	806	CLA	C3C-C2C	4.30	1.46	1.36
14	a	802	CLA	C3C-C2C	4.30	1.46	1.36
14	b	820	CLA	C3C-C2C	4.30	1.46	1.36
14	B	824	CLA	C3D-C4D	-4.30	1.34	1.44
14	b	825	CLA	C3D-C4D	-4.30	1.34	1.44
14	b	814	CLA	C3D-C4D	-4.30	1.34	1.44
14	a	834	CLA	C3D-C4D	-4.30	1.34	1.44
17	H	844	BCR	C10-C9	-4.30	1.25	1.35
14	a	841	CLA	C3D-C4D	-4.30	1.34	1.44
14	a	843	CLA	C3D-C4D	-4.30	1.34	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	204	CLA	C3D-C4D	-4.30	1.34	1.44
14	H	817	CLA	C3C-C2C	4.30	1.46	1.36
14	b	829	CLA	CHD-C1D	4.30	1.46	1.38
14	T	1401	CLA	C3D-C4D	-4.30	1.34	1.44
14	A	836	CLA	C3B-C2B	4.30	1.46	1.40
14	G	842	CLA	CHD-C1D	4.30	1.46	1.38
14	U	201	CLA	C3C-C2C	4.30	1.46	1.36
14	a	828	CLA	C3D-C4D	-4.30	1.34	1.44
17	b	842	BCR	C10-C9	-4.30	1.25	1.35
14	A	809	CLA	C3D-C4D	-4.30	1.34	1.44
14	l	205	CLA	C3D-C4D	-4.30	1.34	1.44
14	G	804	CLA	C3D-C4D	-4.30	1.34	1.44
14	U	206	CLA	C3C-C2C	4.30	1.46	1.36
14	B	829	CLA	C3C-C2C	4.30	1.46	1.36
14	A	842	CLA	CHD-C1D	4.29	1.46	1.38
14	G	833	CLA	CHD-C1D	4.29	1.46	1.38
14	a	803	CLA	C3D-C4D	-4.29	1.34	1.44
14	a	810	CLA	C3D-C4D	-4.29	1.34	1.44
14	H	815	CLA	C3C-C2C	4.29	1.46	1.36
14	B	832	CLA	C3D-C4D	-4.29	1.34	1.44
14	H	815	CLA	C3D-C4D	-4.29	1.34	1.44
14	b	840	CLA	CHD-C1D	4.29	1.46	1.38
17	a	852	BCR	C10-C9	-4.29	1.25	1.35
14	A	805	CLA	C3C-C2C	4.29	1.46	1.36
14	B	838	CLA	CHD-C1D	4.29	1.46	1.38
19	H	848	LMG	O8-C28	4.29	1.45	1.33
14	G	844	CLA	C3C-C2C	4.29	1.46	1.36
14	G	843	CLA	C3D-C4D	-4.29	1.34	1.44
14	A	807	CLA	CHD-C1D	4.29	1.46	1.38
14	H	809	CLA	CHD-C1D	4.29	1.46	1.38
14	H	821	CLA	CHD-C1D	4.29	1.46	1.38
14	H	818	CLA	C3D-C4D	-4.29	1.34	1.44
14	b	806	CLA	CHD-C1D	4.29	1.46	1.38
18	A	854	LHG	O7-C7	4.29	1.46	1.34
14	U	204	CLA	CHD-C1D	4.29	1.46	1.38
14	G	835	CLA	C3C-C2C	4.28	1.46	1.36
14	H	815	CLA	CHD-C1D	4.28	1.46	1.38
14	G	844	CLA	C3D-C4D	-4.28	1.34	1.44
14	a	806	CLA	CHD-C1D	4.28	1.46	1.38
14	A	818	CLA	C3D-C4D	-4.28	1.34	1.44
14	B	833	CLA	C3D-C4D	-4.28	1.34	1.44
14	G	816	CLA	C3D-C4D	-4.28	1.34	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	836	CLA	C3D-C4D	-4.28	1.34	1.44
14	X	1701	CLA	C3D-C4D	-4.28	1.34	1.44
14	H	803	CLA	C1D-ND	-4.28	1.32	1.37
14	a	823	CLA	C3D-C4D	-4.28	1.34	1.44
14	b	837	CLA	CHD-C1D	4.28	1.46	1.38
14	b	817	CLA	C3D-C4D	-4.28	1.34	1.44
14	H	820	CLA	CHD-C1D	4.28	1.46	1.38
14	B	802	CLA	C3D-C4D	-4.28	1.34	1.44
14	L	201	CLA	CHD-C1D	4.28	1.46	1.38
14	b	807	CLA	CHD-C1D	4.28	1.46	1.38
14	A	833	CLA	C3D-C4D	-4.28	1.34	1.44
14	A	812	CLA	C3D-C4D	-4.28	1.34	1.44
14	B	831	CLA	C3D-C4D	-4.27	1.34	1.44
14	G	814	CLA	C3D-C4D	-4.27	1.34	1.44
14	B	815	CLA	C3D-C4D	-4.27	1.34	1.44
14	H	804	CLA	C3D-C4D	-4.27	1.34	1.44
14	a	841	CLA	C3C-C2C	4.27	1.46	1.36
14	b	824	CLA	C3D-C4D	-4.27	1.34	1.44
14	a	809	CLA	CHD-C1D	4.27	1.46	1.38
14	b	802	CLA	C3D-C4D	-4.27	1.34	1.44
14	A	811	CLA	C3D-C4D	-4.27	1.34	1.44
14	B	840	CLA	C3D-C4D	-4.27	1.34	1.44
14	B	830	CLA	C3D-C4D	-4.27	1.34	1.44
14	H	806	CLA	CHD-C1D	4.27	1.46	1.38
14	G	825	CLA	C3C-C2C	4.27	1.46	1.36
14	a	833	CLA	C3D-C4D	-4.27	1.34	1.44
14	b	820	CLA	C3D-C4D	-4.27	1.34	1.44
14	A	807	CLA	C3C-C2C	4.26	1.46	1.36
14	G	819	CLA	C3D-C4D	-4.26	1.34	1.44
14	b	812	CLA	C3D-C4D	-4.26	1.34	1.44
14	a	844	CLA	CHD-C1D	4.26	1.46	1.38
14	A	831	CLA	C3D-C4D	-4.26	1.34	1.44
14	B	835	CLA	C3D-C4D	-4.26	1.34	1.44
14	x	1701	CLA	C3D-C4D	-4.26	1.34	1.44
14	B	809	CLA	C3C-C2C	4.26	1.46	1.36
14	G	840	CLA	C3D-C4D	-4.26	1.34	1.44
14	k	1401	CLA	C3D-C4D	-4.26	1.34	1.44
14	a	806	CLA	C3C-C2C	4.26	1.46	1.36
14	G	813	CLA	C3D-C4D	-4.26	1.34	1.44
14	G	837	CLA	C3D-C4D	-4.26	1.34	1.44
14	b	827	CLA	CHD-C1D	4.26	1.46	1.38
14	b	816	CLA	C3D-C4D	-4.26	1.34	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	816	CLA	C3D-C4D	-4.26	1.34	1.44
14	L	205	CLA	C3D-C4D	-4.26	1.34	1.44
14	G	811	CLA	C3D-C4D	-4.26	1.34	1.44
14	H	840	CLA	C3D-C4D	-4.26	1.34	1.44
14	b	831	CLA	C3D-C4D	-4.26	1.34	1.44
14	A	838	CLA	C3D-C4D	-4.26	1.34	1.44
14	H	816	CLA	C3D-C4D	-4.26	1.34	1.44
14	H	834	CLA	C3D-C4D	-4.26	1.34	1.44
13	a	801	CL0	C3C-C2C	4.26	1.46	1.36
14	a	829	CLA	C3C-C2C	4.26	1.45	1.36
14	B	808	CLA	C1D-ND	-4.25	1.32	1.37
14	a	835	CLA	C3D-C4D	-4.25	1.34	1.44
14	H	822	CLA	C3C-C2C	4.25	1.45	1.36
14	G	809	CLA	C3D-C4D	-4.25	1.34	1.44
14	j	101	CLA	C3D-C4D	-4.25	1.34	1.44
14	b	802	CLA	CHD-C1D	4.25	1.46	1.38
14	i	101	CLA	CHD-C1D	4.25	1.46	1.38
14	A	839	CLA	C3D-C4D	-4.25	1.34	1.44
14	a	838	CLA	C3C-C2C	4.25	1.45	1.36
14	a	826	CLA	C3D-C4D	-4.25	1.34	1.44
14	B	840	CLA	CHD-C1D	4.25	1.46	1.38
14	H	835	CLA	C3D-C4D	-4.25	1.34	1.44
14	G	819	CLA	CHD-C1D	4.25	1.46	1.38
14	A	830	CLA	C3C-C2C	4.25	1.45	1.36
14	A	808	CLA	C3D-C4D	-4.25	1.34	1.44
14	a	855	CLA	C3B-C2B	4.25	1.46	1.40
14	U	201	CLA	CHD-C1D	4.25	1.46	1.38
14	G	817	CLA	C3B-C2B	4.25	1.46	1.40
14	A	837	CLA	C3D-C4D	-4.25	1.34	1.44
14	a	818	CLA	C3B-C2B	4.25	1.46	1.40
14	H	829	CLA	C3C-C2C	4.25	1.45	1.36
14	A	822	CLA	C3D-C4D	-4.25	1.34	1.44
14	B	823	CLA	C3D-C4D	-4.25	1.34	1.44
14	H	832	CLA	C3D-C4D	-4.25	1.34	1.44
14	a	817	CLA	C3B-C2B	4.24	1.46	1.40
14	A	804	CLA	CHD-C1D	4.24	1.46	1.38
14	G	826	CLA	CHD-C1D	4.24	1.46	1.38
14	H	807	CLA	CHD-C1D	4.24	1.46	1.38
14	L	206	CLA	C3D-C4D	-4.24	1.34	1.44
14	G	815	CLA	C3D-C4D	-4.24	1.34	1.44
14	a	838	CLA	C3D-C4D	-4.24	1.34	1.44
14	b	836	CLA	C3D-C4D	-4.24	1.34	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	808	CLA	C3C-C2C	4.24	1.45	1.36
14	a	836	CLA	C3D-C4D	-4.24	1.34	1.44
14	a	811	CLA	C3B-C2B	4.24	1.46	1.40
14	G	809	CLA	C3B-C2B	4.24	1.46	1.40
14	a	830	CLA	CHD-C1D	4.24	1.46	1.38
14	A	845	CLA	C3D-C4D	-4.24	1.34	1.44
14	H	814	CLA	C3C-C2C	4.24	1.45	1.36
14	A	802	CLA	C3C-C2C	4.24	1.45	1.36
14	B	803	CLA	C3B-C2B	4.24	1.46	1.40
14	G	807	CLA	CHD-C1D	4.23	1.46	1.38
14	a	808	CLA	C3D-C4D	-4.23	1.34	1.44
14	G	840	CLA	CHD-C1D	4.23	1.46	1.38
17	R	103	BCR	C10-C9	-4.23	1.26	1.35
14	A	818	CLA	CHD-C1D	4.23	1.46	1.38
14	A	821	CLA	C3D-C4D	-4.23	1.34	1.44
14	H	812	CLA	C3D-C4D	-4.23	1.34	1.44
14	F	1303	CLA	C3D-C4D	-4.23	1.34	1.44
14	a	815	CLA	C3D-C4D	-4.23	1.34	1.44
14	H	820	CLA	C3D-C4D	-4.23	1.34	1.44
14	A	818	CLA	C3C-C2C	4.23	1.45	1.36
14	G	809	CLA	CHD-C1D	4.23	1.46	1.38
14	H	818	CLA	C3B-C2B	4.23	1.46	1.40
14	H	827	CLA	CHD-C1D	4.23	1.46	1.38
14	A	842	CLA	C3D-C4D	-4.23	1.34	1.44
14	A	805	CLA	C3D-C4D	-4.23	1.34	1.44
17	V	1602	BCR	C10-C9	-4.23	1.26	1.35
14	G	830	CLA	CHD-C1D	4.23	1.46	1.38
14	A	813	CLA	C3D-C4D	-4.22	1.34	1.44
14	H	832	CLA	C3C-C2C	4.22	1.45	1.36
14	H	811	CLA	C3D-C4D	-4.22	1.34	1.44
14	A	838	CLA	CHD-C1D	4.22	1.46	1.38
14	B	836	CLA	C3D-C4D	-4.22	1.34	1.44
14	H	826	CLA	CHD-C1D	4.22	1.46	1.38
14	A	814	CLA	C3D-C4D	-4.22	1.34	1.44
14	A	803	CLA	C3C-C2C	4.22	1.45	1.36
14	S	102	CLA	C3D-C4D	-4.22	1.34	1.44
14	B	837	CLA	CHD-C1D	4.22	1.46	1.38
14	H	840	CLA	CHD-C1D	4.22	1.46	1.38
14	L	201	CLA	C3C-C2C	4.22	1.45	1.36
14	B	834	CLA	C3B-C2B	4.22	1.46	1.40
14	A	817	CLA	C3D-C4D	-4.22	1.34	1.44
14	A	845	CLA	CHD-C1D	4.22	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	l	202	CLA	CHD-C1D	4.22	1.46	1.38
14	f	202	CLA	C3D-C4D	-4.22	1.34	1.44
17	A	848	BCR	C10-C9	-4.22	1.26	1.35
14	U	206	CLA	C3D-C4D	-4.22	1.34	1.44
14	H	807	CLA	C3C-C2C	4.22	1.45	1.36
17	I	102	BCR	C10-C9	-4.21	1.26	1.35
14	B	807	CLA	C3B-C2B	4.21	1.46	1.40
14	a	855	CLA	C3D-C4D	-4.21	1.34	1.44
14	j	102	CLA	C3D-C4D	-4.21	1.34	1.44
14	l	202	CLA	C3C-C2C	4.21	1.45	1.36
14	a	813	CLA	C3C-C2C	4.21	1.45	1.36
14	G	817	CLA	C3D-C4D	-4.21	1.34	1.44
14	U	204	CLA	C3D-C4D	-4.21	1.34	1.44
14	A	810	CLA	CHD-C1D	4.21	1.46	1.38
14	b	820	CLA	CHD-C1D	4.21	1.46	1.38
14	b	830	CLA	C3D-C4D	-4.21	1.34	1.44
14	b	811	CLA	C3D-C4D	-4.21	1.34	1.44
14	b	814	CLA	CHD-C1D	4.21	1.46	1.38
14	H	817	CLA	C3D-C4D	-4.21	1.34	1.44
14	F	1301	CLA	CHD-C1D	4.21	1.46	1.38
14	b	832	CLA	C3D-C4D	-4.21	1.34	1.44
14	A	809	CLA	CHD-C1D	4.21	1.46	1.38
14	a	814	CLA	C3D-C4D	-4.21	1.34	1.44
14	b	822	CLA	C3D-C4D	-4.21	1.34	1.44
14	A	806	CLA	C3C-C2C	4.20	1.45	1.36
14	B	816	CLA	C3C-C2C	4.20	1.45	1.36
14	M	1601	CLA	C3B-C2B	4.20	1.46	1.40
14	H	822	CLA	C3D-C4D	-4.20	1.34	1.44
14	Q	203	CLA	C3D-C4D	-4.20	1.34	1.44
14	i	101	CLA	C3C-C2C	4.20	1.45	1.36
14	A	810	CLA	C3D-C4D	-4.20	1.34	1.44
14	B	819	CLA	C3D-C4D	-4.20	1.34	1.44
14	b	836	CLA	C3C-C2C	4.20	1.45	1.36
14	b	829	CLA	C3C-C2C	4.20	1.45	1.36
14	B	808	CLA	CHD-C1D	4.20	1.46	1.38
13	A	801	CL0	C3C-C2C	4.20	1.45	1.36
17	J	103	BCR	C10-C9	-4.20	1.26	1.35
14	X	1701	CLA	CHD-C1D	4.20	1.46	1.38
14	A	827	CLA	CHD-C1D	4.19	1.46	1.38
14	H	823	CLA	CHD-C1D	4.19	1.46	1.38
14	b	815	CLA	C3D-C4D	-4.19	1.34	1.44
14	B	826	CLA	C3C-C2C	4.19	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	806	CLA	C3C-C2C	4.19	1.45	1.36
14	H	808	CLA	C3C-C2C	4.19	1.45	1.36
14	B	816	CLA	C3D-C4D	-4.19	1.34	1.44
14	B	822	CLA	C3C-C2C	4.19	1.45	1.36
14	A	840	CLA	C3B-C2B	4.19	1.46	1.40
14	G	805	CLA	C3D-C4D	-4.19	1.34	1.44
14	F	1301	CLA	C3D-C4D	-4.19	1.34	1.44
14	A	843	CLA	CHD-C1D	4.19	1.46	1.38
14	H	830	CLA	C3D-C4D	-4.19	1.34	1.44
14	b	808	CLA	CHD-C1D	4.18	1.46	1.38
14	B	821	CLA	C3D-C4D	-4.18	1.34	1.44
14	b	832	CLA	C3B-C2B	4.18	1.46	1.40
17	M	1602	BCR	C10-C9	-4.18	1.26	1.35
14	B	808	CLA	C3C-C2C	4.18	1.45	1.36
14	a	803	CLA	CHD-C1D	4.18	1.46	1.38
14	G	812	CLA	C3B-C2B	4.18	1.46	1.40
14	B	804	CLA	C3D-C4D	-4.18	1.34	1.44
14	H	821	CLA	C3D-C4D	-4.18	1.34	1.44
14	A	839	CLA	C3B-C2B	4.17	1.46	1.40
13	G	801	CL0	C3C-C2C	4.17	1.45	1.36
14	B	828	CLA	C3B-C2B	4.17	1.46	1.40
14	a	820	CLA	C3D-C4D	-4.17	1.34	1.44
14	G	825	CLA	C3D-C4D	-4.17	1.34	1.44
14	G	803	CLA	C3C-C2C	4.17	1.45	1.36
14	B	809	CLA	CHD-C1D	4.17	1.46	1.38
14	B	820	CLA	C3D-C4D	-4.17	1.34	1.44
14	a	830	CLA	C3D-C4D	-4.17	1.34	1.44
14	H	838	CLA	C3B-C2B	4.17	1.46	1.40
14	B	812	CLA	CHD-C1D	4.17	1.46	1.38
14	K	101	CLA	C3D-C4D	-4.17	1.34	1.44
14	Q	201	CLA	CHD-C1D	4.17	1.46	1.38
14	a	831	CLA	CHD-C1D	4.17	1.46	1.38
14	b	803	CLA	C3C-C2C	4.17	1.45	1.36
14	A	836	CLA	CHD-C1D	4.17	1.46	1.38
14	H	819	CLA	C3D-C4D	-4.16	1.34	1.44
17	b	844	BCR	C10-C9	-4.16	1.26	1.35
14	H	823	CLA	C3C-C2C	4.16	1.45	1.36
14	b	838	CLA	CHD-C1D	4.16	1.46	1.38
14	A	802	CLA	C3D-C4D	-4.16	1.34	1.44
14	B	811	CLA	C3D-C4D	-4.16	1.34	1.44
14	B	826	CLA	CHD-C1D	4.16	1.46	1.38
14	J	101	CLA	C3D-C4D	-4.16	1.34	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	854	LHG	O8-C23	4.16	1.45	1.33
14	b	816	CLA	C3C-C2C	4.16	1.45	1.36
14	b	819	CLA	CHD-C1D	4.16	1.46	1.38
14	G	804	CLA	CHD-C1D	4.16	1.46	1.38
14	H	812	CLA	C3C-C2C	4.15	1.45	1.36
14	A	825	CLA	C3D-C4D	-4.15	1.34	1.44
14	H	809	CLA	C3C-C2C	4.15	1.45	1.36
14	B	823	CLA	C3C-C2C	4.15	1.45	1.36
14	B	822	CLA	CHD-C1D	4.15	1.46	1.38
14	G	832	CLA	C3B-C2B	4.15	1.46	1.40
14	G	845	CLA	C3D-C4D	-4.15	1.34	1.44
14	G	829	CLA	CHD-C1D	4.15	1.46	1.38
14	H	831	CLA	CHD-C1D	4.15	1.46	1.38
14	a	808	CLA	CHD-C1D	4.14	1.46	1.38
14	a	844	CLA	C3D-C4D	-4.14	1.34	1.44
14	a	825	CLA	C1D-ND	-4.14	1.32	1.37
14	B	810	CLA	CHD-C4C	4.14	1.48	1.39
14	H	814	CLA	C3D-C4D	-4.14	1.34	1.44
14	A	815	CLA	C3D-C4D	-4.14	1.34	1.44
14	A	823	CLA	C3D-C4D	-4.14	1.34	1.44
14	b	821	CLA	C3D-C4D	-4.14	1.34	1.44
19	b	848	LMG	O8-C28	4.14	1.45	1.33
14	H	835	CLA	CHD-C1D	4.14	1.46	1.38
14	a	821	CLA	CHD-C4C	4.14	1.48	1.39
14	a	810	CLA	CHD-C4C	4.14	1.48	1.39
14	B	835	CLA	C3B-C2B	4.14	1.46	1.40
14	a	816	CLA	C3D-C4D	-4.13	1.34	1.44
14	H	808	CLA	CHD-C1D	4.13	1.46	1.38
14	a	812	CLA	C3D-C4D	-4.13	1.34	1.44
14	b	815	CLA	CHD-C1D	4.13	1.46	1.38
14	b	818	CLA	CHD-C4C	4.13	1.48	1.39
13	A	801	CL0	C1D-ND	-4.13	1.32	1.37
14	G	843	CLA	C3C-C2C	4.13	1.45	1.36
14	K	101	CLA	CHD-C4C	4.13	1.48	1.39
14	H	801	CLA	C3D-C4D	-4.13	1.34	1.44
14	B	817	CLA	C3C-C2C	4.13	1.45	1.36
14	A	825	CLA	C3C-C2C	4.13	1.45	1.36
14	L	204	CLA	CHD-C1D	4.13	1.46	1.38
14	B	822	CLA	C3D-C4D	-4.13	1.34	1.44
14	B	834	CLA	C3D-C4D	-4.13	1.34	1.44
14	a	843	CLA	CHD-C4C	4.13	1.48	1.39
14	G	802	CLA	C3C-C2C	4.13	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	802	CLA	C3D-C4D	-4.12	1.34	1.44
14	W	1701	CLA	C3D-C4D	-4.12	1.34	1.44
14	G	836	CLA	C3B-C2B	4.12	1.46	1.40
17	Q	204	BCR	C10-C9	-4.12	1.26	1.35
14	S	101	CLA	C3D-C4D	-4.12	1.34	1.44
14	b	823	CLA	C3D-C4D	-4.12	1.34	1.44
14	a	804	CLA	C3D-C4D	-4.12	1.34	1.44
14	A	832	CLA	C3B-C2B	4.12	1.45	1.40
14	G	840	CLA	C3B-C2B	4.12	1.45	1.40
14	a	813	CLA	C3D-C4D	-4.12	1.34	1.44
14	B	806	CLA	CHD-C1D	4.11	1.46	1.38
14	A	818	CLA	C3B-C2B	4.11	1.45	1.40
14	B	813	CLA	CHD-C1D	4.11	1.46	1.38
14	A	802	CLA	C1D-ND	-4.11	1.32	1.37
14	H	837	CLA	CHD-C4C	4.11	1.48	1.39
14	b	834	CLA	C3D-C4D	-4.11	1.34	1.44
14	H	805	CLA	CHD-C1D	4.11	1.46	1.38
14	G	829	CLA	C3C-C2C	4.11	1.45	1.36
14	A	824	CLA	CHD-C4C	4.11	1.48	1.39
14	b	812	CLA	C3C-C2C	4.10	1.45	1.36
14	A	829	CLA	C3C-C2C	4.10	1.45	1.36
14	a	828	CLA	C3C-C2C	4.10	1.45	1.36
14	a	822	CLA	CHD-C1D	4.10	1.46	1.38
14	G	810	CLA	C3C-C2C	4.10	1.45	1.36
14	a	824	CLA	C3D-C4D	-4.10	1.35	1.44
14	A	817	CLA	CHD-C4C	4.10	1.48	1.39
14	b	817	CLA	C3C-C2C	4.10	1.45	1.36
14	b	831	CLA	CHD-C4C	4.09	1.48	1.39
14	G	845	CLA	CHD-C1D	4.09	1.46	1.38
14	H	814	CLA	CHD-C1D	4.09	1.46	1.38
19	B	849	LMG	O8-C28	4.09	1.45	1.33
14	a	824	CLA	C3C-C2C	4.09	1.45	1.36
18	a	853	LHG	O8-C23	4.09	1.45	1.33
14	b	809	CLA	C1D-ND	-4.09	1.32	1.37
14	B	805	CLA	CHD-C4C	4.08	1.48	1.39
14	G	818	CLA	C3C-C2C	4.08	1.45	1.36
14	A	837	CLA	CHD-C4C	4.08	1.48	1.39
14	a	825	CLA	CHD-C1D	4.08	1.46	1.38
14	A	836	CLA	C3D-C4D	-4.08	1.35	1.44
14	A	844	CLA	C3C-C2C	4.07	1.45	1.36
14	G	844	CLA	CHD-C4C	4.07	1.48	1.39
13	A	801	CL0	CHD-C1D	4.07	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	831	CLA	CHD-C4C	4.07	1.48	1.39
18	A	854	LHG	O8-C23	4.07	1.45	1.33
14	a	839	CLA	C3B-C2B	4.07	1.45	1.40
14	A	834	CLA	CHD-C4C	4.07	1.48	1.39
14	i	101	CLA	CHD-C4C	4.07	1.48	1.39
14	b	801	CLA	C1D-ND	-4.07	1.32	1.37
14	H	822	CLA	CHD-C1D	4.07	1.46	1.38
14	A	829	CLA	CHD-C1D	4.07	1.46	1.38
14	a	840	CLA	CHD-C4C	4.06	1.48	1.39
14	b	810	CLA	CHD-C4C	4.06	1.48	1.39
14	b	801	CLA	C3C-C2C	4.06	1.45	1.36
14	b	823	CLA	C3C-C2C	4.06	1.45	1.36
14	B	820	CLA	CHD-C1D	4.06	1.46	1.38
14	F	1303	CLA	CHD-C4C	4.06	1.48	1.39
14	G	821	CLA	CHD-C1D	4.06	1.46	1.38
14	A	811	CLA	C3C-C2C	4.06	1.45	1.36
14	H	802	CLA	CHD-C1D	4.06	1.46	1.38
14	L	205	CLA	C1D-ND	-4.06	1.32	1.37
14	A	822	CLA	CHD-C4C	4.05	1.48	1.39
14	a	807	CLA	CHD-C4C	4.05	1.48	1.39
14	A	833	CLA	CHD-C4C	4.05	1.48	1.39
14	B	803	CLA	C3D-C4D	-4.05	1.35	1.44
14	B	816	CLA	CHD-C1D	4.05	1.46	1.38
14	a	812	CLA	CHD-C4C	4.05	1.48	1.39
14	A	810	CLA	C3C-C2C	4.05	1.45	1.36
14	A	814	CLA	O2D-CGD	4.04	1.43	1.33
14	G	826	CLA	C3C-C2C	4.04	1.45	1.36
14	B	817	CLA	CHD-C4C	4.04	1.48	1.39
14	a	826	CLA	CHD-C1D	4.04	1.46	1.38
14	l	207	CLA	CHD-C4C	4.04	1.48	1.39
14	B	801	CLA	C3D-C4D	-4.04	1.35	1.44
14	A	814	CLA	OBD-CAD	4.04	1.29	1.22
14	G	820	CLA	CHD-C4C	4.04	1.48	1.39
18	a	854	LHG	O7-C7	4.04	1.45	1.34
14	G	806	CLA	CHD-C4C	4.03	1.48	1.39
14	H	811	CLA	CHD-C4C	4.03	1.48	1.39
13	a	801	CL0	C1D-ND	-4.03	1.32	1.37
14	b	804	CLA	C3D-C4D	-4.03	1.35	1.44
14	H	803	CLA	C3D-C4D	-4.03	1.35	1.44
14	B	802	CLA	C3C-C2C	4.03	1.45	1.36
14	b	825	CLA	CHD-C1D	4.03	1.46	1.38
14	B	812	CLA	C3C-C2C	4.03	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	833	CLA	CHD-C4C	4.03	1.48	1.39
14	A	806	CLA	CHD-C4C	4.03	1.48	1.39
14	B	807	CLA	CHD-C1D	4.03	1.46	1.38
14	b	802	CLA	C3C-C2C	4.03	1.45	1.36
14	a	836	CLA	CHD-C4C	4.03	1.48	1.39
14	A	812	CLA	CHD-C4C	4.02	1.48	1.39
14	a	805	CLA	C3C-C2C	4.02	1.45	1.36
14	a	832	CLA	CHD-C4C	4.02	1.48	1.39
14	a	816	CLA	CHD-C4C	4.02	1.48	1.39
14	G	811	CLA	CHD-C1D	4.02	1.46	1.38
14	B	831	CLA	CHD-C4C	4.02	1.48	1.39
14	G	815	CLA	CHD-C4C	4.02	1.48	1.39
18	G	855	LHG	O7-C7	4.01	1.45	1.34
14	B	833	CLA	CHD-C4C	4.01	1.48	1.39
13	G	801	CL0	CHD-C1D	4.01	1.46	1.38
14	b	837	CLA	CHD-C4C	4.01	1.48	1.39
14	H	830	CLA	CHD-C4C	4.01	1.48	1.39
14	b	835	CLA	CHD-C4C	4.01	1.48	1.39
14	A	815	CLA	CHD-C4C	4.01	1.48	1.39
18	a	853	LHG	O7-C7	4.01	1.45	1.34
14	G	812	CLA	CHD-C4C	4.01	1.48	1.39
14	G	817	CLA	CHD-C4C	4.00	1.48	1.39
14	j	102	CLA	CHD-C4C	4.00	1.48	1.39
14	b	811	CLA	CHD-C4C	4.00	1.48	1.39
14	a	835	CLA	C3B-C2B	4.00	1.45	1.40
13	G	801	CL0	C1D-ND	-4.00	1.32	1.37
14	B	803	CLA	C1D-ND	-4.00	1.32	1.37
14	b	803	CLA	CHD-C1D	3.99	1.46	1.38
14	a	819	CLA	CHD-C4C	3.99	1.48	1.39
14	A	808	CLA	CHD-C4C	3.99	1.48	1.39
14	H	833	CLA	CHD-C4C	3.99	1.48	1.39
14	a	817	CLA	CHD-C4C	3.99	1.48	1.39
14	B	835	CLA	CHD-C4C	3.99	1.48	1.39
14	G	835	CLA	CHD-C4C	3.98	1.48	1.39
14	G	837	CLA	CHD-C4C	3.98	1.48	1.39
14	H	828	CLA	CHD-C4C	3.98	1.48	1.39
14	b	804	CLA	C1D-ND	-3.98	1.32	1.37
14	H	818	CLA	CHD-C4C	3.97	1.48	1.39
14	b	836	CLA	CHD-C1D	3.97	1.46	1.38
14	a	828	CLA	CHD-C1D	3.97	1.46	1.38
14	G	822	CLA	CHD-C4C	3.97	1.48	1.39
14	b	827	CLA	C3B-C2B	3.96	1.45	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	815	CLA	CHD-C4C	3.96	1.48	1.39
14	b	806	CLA	CHD-C4C	3.96	1.48	1.39
14	H	802	CLA	C1D-ND	-3.96	1.32	1.37
14	G	802	CLA	C1D-ND	-3.96	1.32	1.37
14	b	804	CLA	C3C-C2C	3.96	1.45	1.36
14	H	801	CLA	C1D-ND	-3.96	1.32	1.37
14	A	820	CLA	CHD-C4C	3.96	1.48	1.39
14	a	809	CLA	C3C-C2C	3.96	1.45	1.36
14	a	811	CLA	CHD-C4C	3.95	1.48	1.39
14	B	832	CLA	C3B-C2B	3.95	1.45	1.40
14	U	206	CLA	CHD-C4C	3.95	1.48	1.39
18	A	855	LHG	O7-C7	3.95	1.45	1.34
14	A	841	CLA	CHD-C4C	3.95	1.48	1.39
14	S	102	CLA	CHD-C4C	3.95	1.48	1.39
13	a	801	CL0	CHD-C1D	3.95	1.46	1.38
14	G	805	CLA	CHD-C4C	3.94	1.48	1.39
14	B	818	CLA	CHD-C4C	3.94	1.48	1.39
14	G	836	CLA	CHD-C4C	3.94	1.48	1.39
14	H	809	CLA	C3B-C2B	3.94	1.45	1.40
14	H	824	CLA	CHD-C4C	3.94	1.48	1.39
14	G	834	CLA	CHD-C4C	3.94	1.48	1.39
17	j	104	BCR	C10-C9	-3.94	1.26	1.35
14	B	824	CLA	CHD-C4C	3.94	1.48	1.39
14	j	101	CLA	CHD-C4C	3.94	1.48	1.39
14	a	855	CLA	CHD-C1D	3.93	1.46	1.38
14	B	825	CLA	CHD-C1D	3.93	1.46	1.38
14	H	807	CLA	CHD-C4C	3.93	1.48	1.39
14	U	205	CLA	C1D-ND	-3.93	1.32	1.37
14	a	818	CLA	CHD-C4C	3.93	1.48	1.39
14	b	828	CLA	CHD-C4C	3.92	1.48	1.39
14	b	817	CLA	CHD-C4C	3.92	1.48	1.39
14	H	810	CLA	CHD-C4C	3.92	1.48	1.39
14	K	102	CLA	CHD-C4C	3.92	1.48	1.39
14	B	830	CLA	CHD-C4C	3.92	1.48	1.39
14	A	813	CLA	CHD-C4C	3.92	1.48	1.39
14	b	833	CLA	CHD-C4C	3.92	1.48	1.39
14	G	824	CLA	CHD-C4C	3.92	1.48	1.39
14	B	809	CLA	C1D-ND	-3.92	1.32	1.37
14	H	804	CLA	CHD-C4C	3.92	1.48	1.39
14	G	813	CLA	CHD-C4C	3.92	1.48	1.39
14	B	828	CLA	CHD-C4C	3.92	1.48	1.39
14	Q	203	CLA	CHD-C4C	3.92	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	U	205	CLA	CHD-C4C	3.92	1.48	1.39
18	G	854	LHG	O7-C7	3.91	1.45	1.34
14	H	802	CLA	C3C-C2C	3.91	1.45	1.36
14	b	830	CLA	CHD-C4C	3.91	1.48	1.39
14	J	101	CLA	CHD-C4C	3.91	1.48	1.39
14	b	820	CLA	CHD-C4C	3.91	1.48	1.39
14	b	821	CLA	CHD-C4C	3.91	1.48	1.39
14	b	809	CLA	CHD-C1D	3.91	1.46	1.38
14	G	827	CLA	CHD-C4C	3.91	1.48	1.39
14	H	834	CLA	CHD-C4C	3.91	1.48	1.39
14	H	835	CLA	C1D-ND	-3.91	1.32	1.37
14	a	820	CLA	CHD-C4C	3.90	1.48	1.39
14	G	839	CLA	CHD-C4C	3.90	1.48	1.39
14	A	819	CLA	CHD-C4C	3.90	1.48	1.39
14	a	805	CLA	CHD-C4C	3.90	1.48	1.39
14	b	805	CLA	CHD-C4C	3.90	1.48	1.39
14	b	824	CLA	CHD-C4C	3.90	1.48	1.39
14	H	817	CLA	CHD-C4C	3.90	1.48	1.39
14	a	814	CLA	CHD-C4C	3.90	1.48	1.39
14	k	1401	CLA	CHD-C4C	3.89	1.48	1.39
14	H	819	CLA	CHD-C4C	3.89	1.48	1.39
14	B	815	CLA	CHD-C4C	3.89	1.48	1.39
14	G	840	CLA	CHD-C4C	3.89	1.48	1.39
14	B	807	CLA	CHD-C4C	3.89	1.48	1.39
14	A	835	CLA	CHD-C4C	3.89	1.48	1.39
14	G	831	CLA	CHD-C4C	3.88	1.48	1.39
14	a	804	CLA	CHD-C4C	3.88	1.48	1.39
14	b	801	CLA	C3D-C4D	-3.88	1.35	1.44
14	U	204	CLA	CHD-C4C	3.88	1.48	1.39
14	b	815	CLA	CHD-C4C	3.88	1.48	1.39
14	B	811	CLA	CHD-C4C	3.88	1.48	1.39
14	G	843	CLA	CHD-C4C	3.88	1.48	1.39
14	H	838	CLA	CHD-C4C	3.88	1.48	1.39
14	A	840	CLA	CHD-C4C	3.88	1.48	1.39
14	S	101	CLA	CHD-C4C	3.87	1.48	1.39
14	B	801	CLA	C1D-ND	-3.87	1.32	1.37
14	a	834	CLA	CHD-C4C	3.87	1.48	1.39
14	G	816	CLA	CHD-C4C	3.87	1.48	1.39
17	a	850	BCR	C11-C12	-3.87	1.24	1.34
14	H	803	CLA	C3C-C2C	3.87	1.45	1.36
14	l	206	CLA	C1D-ND	-3.87	1.32	1.37
14	B	802	CLA	C1D-ND	-3.87	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	832	CLA	CHD-C4C	3.87	1.48	1.39
14	T	1401	CLA	CHD-C4C	3.87	1.48	1.39
14	a	839	CLA	CHD-C4C	3.86	1.48	1.39
14	A	839	CLA	CHD-C4C	3.86	1.48	1.39
14	G	830	CLA	C3C-C2C	3.86	1.45	1.36
14	H	806	CLA	CHD-C4C	3.86	1.48	1.39
14	H	840	CLA	C3B-C2B	3.86	1.45	1.40
14	a	842	CLA	CHD-C4C	3.86	1.48	1.39
14	b	829	CLA	CHD-C4C	3.85	1.48	1.39
14	b	832	CLA	CHD-C4C	3.85	1.48	1.39
14	f	202	CLA	CHD-C4C	3.85	1.48	1.39
14	B	840	CLA	C3B-C2B	3.85	1.45	1.40
14	A	816	CLA	CHD-C4C	3.85	1.48	1.39
14	H	820	CLA	CHD-C4C	3.85	1.48	1.39
14	B	838	CLA	CHD-C4C	3.85	1.48	1.39
14	G	808	CLA	CHD-C4C	3.85	1.48	1.39
14	b	834	CLA	C3B-C2B	3.84	1.45	1.40
14	B	827	CLA	C3B-C2B	3.84	1.45	1.40
14	G	803	CLA	CHD-C4C	3.84	1.47	1.39
14	B	823	CLA	CHD-C1D	3.84	1.45	1.38
14	G	819	CLA	CHD-C4C	3.84	1.47	1.39
14	A	830	CLA	C1D-ND	-3.84	1.32	1.37
14	b	834	CLA	C1D-ND	-3.84	1.32	1.37
14	L	205	CLA	CHD-C4C	3.84	1.47	1.39
14	a	808	CLA	CHD-C4C	3.84	1.47	1.39
14	G	809	CLA	CHD-C4C	3.84	1.47	1.39
14	G	838	CLA	CHD-C4C	3.84	1.47	1.39
14	G	823	CLA	CHD-C4C	3.84	1.47	1.39
14	b	823	CLA	CHD-C1D	3.84	1.45	1.38
19	b	848	LMG	O7-C10	3.84	1.45	1.34
14	G	841	CLA	CHD-C4C	3.83	1.47	1.39
14	G	825	CLA	CHD-C4C	3.83	1.47	1.39
14	B	827	CLA	CHD-C4C	3.83	1.47	1.39
14	B	832	CLA	CHD-C4C	3.83	1.47	1.39
14	A	825	CLA	CHD-C4C	3.83	1.47	1.39
14	H	816	CLA	CHD-C4C	3.83	1.47	1.39
14	A	805	CLA	CHD-C4C	3.83	1.47	1.39
14	A	823	CLA	C1D-ND	-3.83	1.32	1.37
14	a	817	CLA	OBD-CAD	3.83	1.29	1.22
14	b	823	CLA	C1D-ND	-3.82	1.32	1.37
14	G	815	CLA	OBD-CAD	3.82	1.29	1.22
14	a	816	CLA	OBD-CAD	3.82	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	l	205	CLA	CHD-C4C	3.82	1.47	1.39
14	b	822	CLA	CHD-C4C	3.82	1.47	1.39
14	H	805	CLA	CHD-C4C	3.82	1.47	1.39
14	a	838	CLA	CHD-C4C	3.82	1.47	1.39
14	A	838	CLA	CHD-C4C	3.82	1.47	1.39
14	L	204	CLA	CHD-C4C	3.81	1.47	1.39
14	L	206	CLA	CHD-C4C	3.81	1.47	1.39
14	x	1701	CLA	CHD-C4C	3.81	1.47	1.39
14	H	827	CLA	C3B-C2B	3.81	1.45	1.40
14	H	815	CLA	CHD-C4C	3.81	1.47	1.39
14	a	855	CLA	C1D-ND	-3.81	1.32	1.37
14	B	839	CLA	CHD-C4C	3.81	1.47	1.39
14	G	828	CLA	C3C-C2C	3.81	1.45	1.36
14	m	1601	CLA	CHD-C4C	3.81	1.47	1.39
14	V	1601	CLA	CHD-C4C	3.81	1.47	1.39
14	H	825	CLA	CHD-C1D	3.81	1.45	1.38
14	a	840	CLA	OBD-CAD	3.80	1.29	1.22
14	B	819	CLA	OBD-CAD	3.80	1.29	1.22
14	A	803	CLA	CHD-C4C	3.80	1.47	1.39
14	B	808	CLA	MG-ND	-3.80	1.98	2.05
14	a	802	CLA	CHD-C4C	3.80	1.47	1.39
14	b	839	CLA	CHD-C4C	3.80	1.47	1.39
14	b	807	CLA	CHD-C4C	3.80	1.47	1.39
14	H	834	CLA	C3B-C2B	3.80	1.45	1.40
14	l	206	CLA	CHD-C4C	3.80	1.47	1.39
14	H	808	CLA	C3B-C2B	3.80	1.45	1.40
14	H	829	CLA	CHD-C4C	3.80	1.47	1.39
14	G	807	CLA	CHD-C4C	3.79	1.47	1.39
14	J	101	CLA	OBD-CAD	3.79	1.29	1.22
14	B	829	CLA	CHD-C4C	3.79	1.47	1.39
14	A	826	CLA	CHD-C4C	3.79	1.47	1.39
19	B	849	LMG	O7-C10	3.79	1.45	1.34
14	b	826	CLA	CHD-C4C	3.79	1.47	1.39
14	B	837	CLA	CHD-C4C	3.79	1.47	1.39
14	H	820	CLA	OBD-CAD	3.79	1.29	1.22
14	b	818	CLA	OBD-CAD	3.79	1.29	1.22
14	B	831	CLA	OBD-CAD	3.79	1.29	1.22
14	G	804	CLA	CHD-C4C	3.79	1.47	1.39
17	f	201	BCR	C11-C12	-3.79	1.24	1.34
14	b	813	CLA	CHD-C4C	3.78	1.47	1.39
14	b	816	CLA	CHD-C4C	3.78	1.47	1.39
14	G	837	CLA	OBD-CAD	3.78	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	824	CLA	CHD-C4C	3.78	1.47	1.39
14	a	827	CLA	C3C-C2C	3.78	1.44	1.36
14	b	838	CLA	CHD-C4C	3.78	1.47	1.39
14	b	803	CLA	C1D-ND	-3.78	1.32	1.37
14	a	837	CLA	CHD-C4C	3.78	1.47	1.39
14	H	836	CLA	CHD-C4C	3.78	1.47	1.39
14	a	835	CLA	CHD-C4C	3.78	1.47	1.39
14	W	1701	CLA	CHD-C4C	3.78	1.47	1.39
14	b	827	CLA	CHD-C4C	3.77	1.47	1.39
14	B	821	CLA	CHD-C4C	3.77	1.47	1.39
14	G	810	CLA	CHD-C4C	3.77	1.47	1.39
19	H	848	LMG	O7-C10	3.77	1.44	1.34
19	b	848	LMG	C40-C39	-3.77	1.33	1.51
14	a	806	CLA	CHD-C4C	3.76	1.47	1.39
14	a	812	CLA	OBD-CAD	3.76	1.29	1.22
14	B	809	CLA	C3B-C2B	3.76	1.45	1.40
14	a	830	CLA	C1D-ND	-3.76	1.32	1.37
14	G	818	CLA	CHD-C4C	3.76	1.47	1.39
14	a	827	CLA	CHD-C1D	3.76	1.45	1.38
14	A	821	CLA	CHD-C4C	3.76	1.47	1.39
14	A	809	CLA	CHD-C4C	3.75	1.47	1.39
14	H	809	CLA	C1D-ND	-3.75	1.32	1.37
14	B	801	CLA	OBD-CAD	3.75	1.28	1.22
14	H	839	CLA	CHD-C4C	3.75	1.47	1.39
14	A	827	CLA	CHD-C4C	3.75	1.47	1.39
14	H	813	CLA	CHD-C4C	3.75	1.47	1.39
14	B	814	CLA	CHD-C4C	3.75	1.47	1.39
14	B	803	CLA	C3C-C2C	3.75	1.44	1.36
14	G	832	CLA	CHD-C4C	3.75	1.47	1.39
14	B	804	CLA	CHD-C4C	3.75	1.47	1.39
14	k	1401	CLA	OBD-CAD	3.75	1.28	1.22
14	B	813	CLA	OBD-CAD	3.75	1.28	1.22
14	a	807	CLA	OBD-CAD	3.75	1.28	1.22
14	H	833	CLA	OBD-CAD	3.75	1.28	1.22
17	J	102	BCR	C11-C12	-3.74	1.24	1.34
14	G	845	CLA	OBD-CAD	3.74	1.28	1.22
14	B	801	CLA	CHD-C1D	3.74	1.45	1.38
14	B	820	CLA	CHD-C4C	3.74	1.47	1.39
14	B	802	CLA	CHD-C1D	3.74	1.45	1.38
14	G	826	CLA	OBD-CAD	3.74	1.28	1.22
14	b	817	CLA	OBD-CAD	3.74	1.28	1.22
14	B	834	CLA	CHD-C4C	3.74	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	823	CLA	C1D-ND	-3.74	1.32	1.37
14	a	822	CLA	CHD-C4C	3.74	1.47	1.39
14	A	808	CLA	OBD-CAD	3.74	1.28	1.22
14	A	807	CLA	CHD-C4C	3.74	1.47	1.39
14	B	819	CLA	CHD-C4C	3.74	1.47	1.39
14	G	817	CLA	OBD-CAD	3.74	1.28	1.22
14	G	829	CLA	OBD-CAD	3.74	1.28	1.22
14	b	834	CLA	OBD-CAD	3.74	1.28	1.22
14	B	815	CLA	OBD-CAD	3.74	1.28	1.22
19	H	848	LMG	C40-C39	-3.74	1.33	1.51
14	A	826	CLA	OBD-CAD	3.73	1.28	1.22
14	H	834	CLA	OBD-CAD	3.73	1.28	1.22
14	K	102	CLA	OBD-CAD	3.73	1.28	1.22
14	B	824	CLA	OBD-CAD	3.73	1.28	1.22
14	G	820	CLA	OBD-CAD	3.73	1.28	1.22
14	G	808	CLA	OBD-CAD	3.73	1.28	1.22
14	B	806	CLA	CHD-C4C	3.73	1.47	1.39
14	a	823	CLA	CHD-C4C	3.73	1.47	1.39
14	a	809	CLA	OBD-CAD	3.73	1.28	1.22
17	A	851	BCR	C11-C12	-3.73	1.24	1.34
14	a	819	CLA	OBD-CAD	3.73	1.28	1.22
14	a	824	CLA	OBD-CAD	3.73	1.28	1.22
17	S	103	BCR	C11-C12	-3.73	1.24	1.34
14	H	832	CLA	OBD-CAD	3.73	1.28	1.22
14	a	810	CLA	OBD-CAD	3.73	1.28	1.22
19	H	848	LMG	C19-C18	-3.73	1.33	1.51
14	T	1401	CLA	OBD-CAD	3.72	1.28	1.22
14	G	833	CLA	CHD-C4C	3.72	1.47	1.39
14	G	842	CLA	CHD-C4C	3.72	1.47	1.39
14	G	803	CLA	OBD-CAD	3.72	1.28	1.22
14	H	812	CLA	OBD-CAD	3.72	1.28	1.22
14	H	826	CLA	CHD-C4C	3.72	1.47	1.39
14	B	835	CLA	OBD-CAD	3.72	1.28	1.22
14	B	820	CLA	OBD-CAD	3.72	1.28	1.22
14	A	845	CLA	OBD-CAD	3.71	1.28	1.22
17	G	851	BCR	C11-C12	-3.71	1.25	1.34
14	H	801	CLA	CHD-C1D	3.71	1.45	1.38
14	a	803	CLA	CHD-C4C	3.71	1.47	1.39
17	l	203	BCR	C11-C12	-3.71	1.25	1.34
14	H	809	CLA	CHD-C4C	3.71	1.47	1.39
14	a	822	CLA	OBD-CAD	3.71	1.28	1.22
14	G	823	CLA	OBD-CAD	3.71	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	829	CLA	CHD-C4C	3.71	1.47	1.39
14	b	832	CLA	OBD-CAD	3.71	1.28	1.22
14	A	817	CLA	OBD-CAD	3.71	1.28	1.22
14	A	820	CLA	OBD-CAD	3.71	1.28	1.22
14	a	813	CLA	OBD-CAD	3.71	1.28	1.22
14	B	811	CLA	OBD-CAD	3.71	1.28	1.22
14	H	801	CLA	OBD-CAD	3.71	1.28	1.22
14	b	809	CLA	C3B-C2B	3.71	1.45	1.40
14	A	841	CLA	OBD-CAD	3.71	1.28	1.22
14	B	836	CLA	CHD-C4C	3.71	1.47	1.39
14	M	1601	CLA	CHD-C4C	3.71	1.47	1.39
14	G	811	CLA	OBD-CAD	3.70	1.28	1.22
14	a	804	CLA	OBD-CAD	3.70	1.28	1.22
14	S	101	CLA	OBD-CAD	3.70	1.28	1.22
14	a	825	CLA	OBD-CAD	3.70	1.28	1.22
14	b	840	CLA	CHD-C4C	3.70	1.47	1.39
14	A	837	CLA	OBD-CAD	3.70	1.28	1.22
14	A	812	CLA	C3B-C2B	3.70	1.45	1.40
14	G	830	CLA	C1D-ND	-3.70	1.33	1.37
14	b	828	CLA	OBD-CAD	3.70	1.28	1.22
19	B	849	LMG	C40-C39	-3.70	1.33	1.51
14	H	804	CLA	OBD-CAD	3.70	1.28	1.22
14	A	818	CLA	CHD-C4C	3.70	1.47	1.39
14	H	814	CLA	OBD-CAD	3.70	1.28	1.22
14	B	832	CLA	OBD-CAD	3.70	1.28	1.22
14	H	821	CLA	CHD-C4C	3.70	1.47	1.39
14	b	815	CLA	OBD-CAD	3.69	1.28	1.22
14	a	813	CLA	CHD-C4C	3.69	1.47	1.39
14	G	818	CLA	OBD-CAD	3.69	1.28	1.22
17	R	102	BCR	C11-C12	-3.69	1.25	1.34
14	a	809	CLA	CHD-C4C	3.69	1.47	1.39
14	X	1701	CLA	CHD-C4C	3.69	1.47	1.39
14	H	823	CLA	C1D-ND	-3.69	1.33	1.37
14	b	802	CLA	C1D-ND	-3.69	1.33	1.37
14	b	814	CLA	CHD-C4C	3.69	1.47	1.39
14	A	815	CLA	OBD-CAD	3.69	1.28	1.22
14	G	826	CLA	CHD-C4C	3.69	1.47	1.39
14	A	811	CLA	CHD-C4C	3.69	1.47	1.39
14	A	816	CLA	OBD-CAD	3.69	1.28	1.22
14	a	831	CLA	CHD-C4C	3.69	1.47	1.39
14	A	821	CLA	OBD-CAD	3.69	1.28	1.22
14	b	814	CLA	OBD-CAD	3.69	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	849	LMG	C19-C18	-3.69	1.33	1.51
14	A	845	CLA	CHD-C4C	3.69	1.47	1.39
14	b	801	CLA	OBD-CAD	3.69	1.28	1.22
14	H	840	CLA	CHD-C4C	3.69	1.47	1.39
14	V	1601	CLA	OBD-CAD	3.68	1.28	1.22
14	B	833	CLA	OBD-CAD	3.68	1.28	1.22
14	G	810	CLA	OBD-CAD	3.68	1.28	1.22
14	b	830	CLA	OBD-CAD	3.68	1.28	1.22
19	b	848	LMG	C19-C18	-3.68	1.33	1.51
14	a	808	CLA	OBD-CAD	3.68	1.28	1.22
14	H	801	CLA	C3B-C2B	3.68	1.45	1.40
14	G	829	CLA	CHD-C4C	3.68	1.47	1.39
14	G	802	CLA	CHD-C1D	3.68	1.45	1.38
14	a	829	CLA	CHD-C4C	3.68	1.47	1.39
14	A	810	CLA	CHD-C4C	3.68	1.47	1.39
14	b	808	CLA	CHD-C4C	3.68	1.47	1.39
14	G	809	CLA	OBD-CAD	3.68	1.28	1.22
14	A	802	CLA	CHD-C1D	3.68	1.45	1.38
14	A	831	CLA	CHD-C4C	3.68	1.47	1.39
14	A	836	CLA	CHD-C4C	3.68	1.47	1.39
14	a	826	CLA	OBD-CAD	3.67	1.28	1.22
14	G	821	CLA	CHD-C4C	3.67	1.47	1.39
14	H	815	CLA	OBD-CAD	3.67	1.28	1.22
14	H	835	CLA	OBD-CAD	3.67	1.28	1.22
14	A	804	CLA	CHD-C4C	3.67	1.47	1.39
14	A	814	CLA	CHD-C4C	3.67	1.47	1.39
14	a	844	CLA	CHD-C4C	3.67	1.47	1.39
14	a	855	CLA	OBD-CAD	3.67	1.28	1.22
14	H	831	CLA	OBD-CAD	3.67	1.28	1.22
14	G	814	CLA	CHD-C4C	3.67	1.47	1.39
14	A	811	CLA	OBD-CAD	3.67	1.28	1.22
14	B	817	CLA	OBD-CAD	3.67	1.28	1.22
14	b	831	CLA	OBD-CAD	3.67	1.28	1.22
14	H	811	CLA	OBD-CAD	3.67	1.28	1.22
14	b	835	CLA	OBD-CAD	3.67	1.28	1.22
14	A	832	CLA	CHD-C4C	3.67	1.47	1.39
14	Q	201	CLA	CHD-C4C	3.67	1.47	1.39
14	a	836	CLA	OBD-CAD	3.67	1.28	1.22
14	b	802	CLA	CHD-C4C	3.67	1.47	1.39
14	a	844	CLA	OBD-CAD	3.67	1.28	1.22
14	A	843	CLA	CHD-C4C	3.67	1.47	1.39
14	H	814	CLA	CHD-C4C	3.67	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	826	CLA	CHD-C4C	3.67	1.47	1.39
14	A	813	CLA	OBD-CAD	3.67	1.28	1.22
14	B	816	CLA	CHD-C4C	3.67	1.47	1.39
14	A	802	CLA	CHD-C4C	3.66	1.47	1.39
14	l	206	CLA	CHD-C1D	3.66	1.45	1.38
14	a	820	CLA	OBD-CAD	3.66	1.28	1.22
14	U	201	CLA	CHD-C4C	3.66	1.47	1.39
14	G	827	CLA	OBD-CAD	3.66	1.28	1.22
14	j	101	CLA	OBD-CAD	3.66	1.28	1.22
14	H	813	CLA	OBD-CAD	3.66	1.28	1.22
13	G	801	CL0	OBD-CAD	3.66	1.28	1.22
19	b	848	LMG	C37-C36	-3.66	1.33	1.51
14	B	827	CLA	OBD-CAD	3.66	1.28	1.22
14	a	835	CLA	OBD-CAD	3.66	1.28	1.22
14	b	824	CLA	OBD-CAD	3.66	1.28	1.22
14	b	833	CLA	OBD-CAD	3.66	1.28	1.22
14	A	830	CLA	MG-ND	-3.66	1.98	2.05
14	A	844	CLA	CHD-C4C	3.66	1.47	1.39
14	b	812	CLA	OBD-CAD	3.65	1.28	1.22
14	l	206	CLA	OBD-CAD	3.65	1.28	1.22
14	F	1301	CLA	CHD-C4C	3.65	1.47	1.39
17	S	104	BCR	C11-C12	-3.65	1.25	1.34
19	b	848	LMG	C43-C42	-3.65	1.33	1.51
14	A	830	CLA	CHD-C4C	3.65	1.47	1.39
17	L	207	BCR	C11-C12	-3.65	1.25	1.34
14	b	840	CLA	C3B-C2B	3.65	1.45	1.40
14	B	830	CLA	OBD-CAD	3.65	1.28	1.22
19	H	848	LMG	C43-C42	-3.65	1.33	1.51
14	A	844	CLA	C1D-ND	-3.65	1.33	1.37
14	H	827	CLA	C1D-ND	-3.65	1.33	1.37
14	a	825	CLA	CHD-C4C	3.65	1.47	1.39
14	B	813	CLA	CHD-C4C	3.65	1.47	1.39
14	B	808	CLA	OBD-CAD	3.65	1.28	1.22
14	G	830	CLA	OBD-CAD	3.64	1.28	1.22
13	a	801	CL0	OBD-CAD	3.64	1.28	1.22
14	G	812	CLA	OBD-CAD	3.64	1.28	1.22
14	B	840	CLA	CHD-C4C	3.64	1.47	1.39
14	A	842	CLA	CHD-C4C	3.64	1.47	1.39
14	b	840	CLA	OBD-CAD	3.64	1.28	1.22
14	a	841	CLA	CHD-C4C	3.64	1.47	1.39
14	A	818	CLA	OBD-CAD	3.64	1.28	1.22
17	G	850	BCR	C11-C12	-3.64	1.25	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	814	CLA	OBD-CAD	3.64	1.28	1.22
14	l	207	CLA	OBD-CAD	3.64	1.28	1.22
14	B	810	CLA	OBD-CAD	3.64	1.28	1.22
14	H	824	CLA	OBD-CAD	3.64	1.28	1.22
14	A	829	CLA	OBD-CAD	3.64	1.28	1.22
14	A	803	CLA	OBD-CAD	3.63	1.28	1.22
14	L	206	CLA	OBD-CAD	3.63	1.28	1.22
14	a	842	CLA	OBD-CAD	3.63	1.28	1.22
14	U	206	CLA	OBD-CAD	3.63	1.28	1.22
14	H	827	CLA	OBD-CAD	3.63	1.28	1.22
14	A	828	CLA	CHD-C1D	3.63	1.45	1.38
19	B	849	LMG	C37-C36	-3.63	1.33	1.51
14	H	840	CLA	OBD-CAD	3.63	1.28	1.22
19	B	849	LMG	C43-C42	-3.63	1.33	1.51
14	A	840	CLA	OBD-CAD	3.63	1.28	1.22
14	H	829	CLA	OBD-CAD	3.63	1.28	1.22
14	L	205	CLA	OBD-CAD	3.63	1.28	1.22
14	b	836	CLA	C1D-ND	-3.63	1.33	1.37
14	B	827	CLA	C1D-ND	-3.63	1.33	1.37
14	G	842	CLA	OBD-CAD	3.62	1.28	1.22
14	b	803	CLA	OBD-CAD	3.62	1.28	1.22
13	A	801	CL0	OBD-CAD	3.62	1.28	1.22
14	A	825	CLA	OBD-CAD	3.62	1.28	1.22
14	a	834	CLA	OBD-CAD	3.62	1.28	1.22
14	H	805	CLA	C1D-ND	-3.62	1.33	1.37
14	U	205	CLA	CHD-C1D	3.62	1.45	1.38
14	G	819	CLA	OBD-CAD	3.62	1.28	1.22
14	H	810	CLA	OBD-CAD	3.62	1.28	1.22
14	H	830	CLA	OBD-CAD	3.62	1.28	1.22
14	a	831	CLA	OBD-CAD	3.62	1.28	1.22
14	B	826	CLA	CHD-C4C	3.62	1.47	1.39
14	f	202	CLA	OBD-CAD	3.62	1.28	1.22
14	Q	201	CLA	OBD-CAD	3.62	1.28	1.22
17	B	846	BCR	C11-C12	-3.62	1.25	1.34
14	G	834	CLA	OBD-CAD	3.62	1.28	1.22
17	U	202	BCR	C11-C12	-3.61	1.25	1.34
14	b	805	CLA	OBD-CAD	3.61	1.28	1.22
14	b	813	CLA	OBD-CAD	3.61	1.28	1.22
14	G	814	CLA	OBD-CAD	3.61	1.28	1.22
14	b	811	CLA	OBD-CAD	3.61	1.28	1.22
14	a	829	CLA	OBD-CAD	3.61	1.28	1.22
19	H	848	LMG	C37-C36	-3.61	1.33	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Q	203	CLA	OBD-CAD	3.61	1.28	1.22
14	A	823	CLA	OBD-CAD	3.61	1.28	1.22
14	B	816	CLA	OBD-CAD	3.61	1.28	1.22
14	H	817	CLA	OBD-CAD	3.61	1.28	1.22
14	B	828	CLA	OBD-CAD	3.61	1.28	1.22
14	H	808	CLA	OBD-CAD	3.61	1.28	1.22
14	B	808	CLA	CHD-C4C	3.61	1.47	1.39
14	B	834	CLA	OBD-CAD	3.61	1.28	1.22
14	H	819	CLA	OBD-CAD	3.61	1.28	1.22
14	a	830	CLA	CHD-C4C	3.60	1.47	1.39
14	G	825	CLA	OBD-CAD	3.60	1.28	1.22
14	b	819	CLA	OBD-CAD	3.60	1.28	1.22
14	b	827	CLA	OBD-CAD	3.60	1.28	1.22
14	G	802	CLA	OBD-CAD	3.60	1.28	1.22
14	W	1701	CLA	OBD-CAD	3.60	1.28	1.22
14	A	839	CLA	OBD-CAD	3.60	1.28	1.22
14	a	833	CLA	OBD-CAD	3.60	1.28	1.22
14	B	807	CLA	C1D-ND	-3.60	1.33	1.37
14	A	819	CLA	OBD-CAD	3.60	1.28	1.22
14	A	829	CLA	C1D-ND	-3.60	1.33	1.37
14	L	201	CLA	CHD-C4C	3.60	1.47	1.39
14	b	810	CLA	OBD-CAD	3.60	1.28	1.22
17	G	852	BCR	C11-C12	-3.60	1.25	1.34
14	G	833	CLA	OBD-CAD	3.60	1.28	1.22
14	b	826	CLA	OBD-CAD	3.60	1.28	1.22
14	A	836	CLA	OBD-CAD	3.59	1.28	1.22
14	G	836	CLA	OBD-CAD	3.59	1.28	1.22
14	b	819	CLA	CHD-C4C	3.59	1.47	1.39
14	b	816	CLA	OBD-CAD	3.59	1.28	1.22
14	G	835	CLA	OBD-CAD	3.59	1.28	1.22
14	A	831	CLA	C1D-ND	-3.59	1.33	1.37
17	H	846	BCR	C11-C12	-3.59	1.25	1.34
14	B	803	CLA	CHD-C4C	3.59	1.47	1.39
14	B	826	CLA	OBD-CAD	3.59	1.28	1.22
14	a	803	CLA	OBD-CAD	3.58	1.28	1.22
14	a	839	CLA	OBD-CAD	3.58	1.28	1.22
14	B	829	CLA	OBD-CAD	3.58	1.28	1.22
14	a	829	CLA	C1D-ND	-3.58	1.33	1.37
14	G	830	CLA	CHD-C4C	3.58	1.47	1.39
14	B	804	CLA	OBD-CAD	3.58	1.28	1.22
17	a	848	BCR	C11-C12	-3.58	1.25	1.34
14	H	827	CLA	CHD-C4C	3.58	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	202	BCR	C11-C12	-3.58	1.25	1.34
14	B	807	CLA	OBD-CAD	3.58	1.28	1.22
14	G	845	CLA	CHD-C4C	3.58	1.47	1.39
14	G	802	CLA	CHD-C4C	3.58	1.47	1.39
14	A	827	CLA	OBD-CAD	3.58	1.28	1.22
14	b	829	CLA	OBD-CAD	3.58	1.28	1.22
14	B	840	CLA	OBD-CAD	3.58	1.28	1.22
14	H	816	CLA	OBD-CAD	3.58	1.28	1.22
14	b	829	CLA	C1D-ND	-3.58	1.33	1.37
17	l	201	BCR	C11-C12	-3.58	1.25	1.34
14	G	843	CLA	C1D-ND	-3.58	1.33	1.37
14	H	802	CLA	OBD-CAD	3.57	1.28	1.22
14	b	808	CLA	C3B-C2B	3.57	1.45	1.40
14	a	837	CLA	OBD-CAD	3.57	1.28	1.22
14	A	802	CLA	OBD-CAD	3.57	1.28	1.22
14	H	826	CLA	OBD-CAD	3.57	1.28	1.22
14	b	808	CLA	OBD-CAD	3.57	1.28	1.22
14	B	802	CLA	OBD-CAD	3.57	1.28	1.22
14	M	1601	CLA	OBD-CAD	3.57	1.28	1.22
14	a	811	CLA	OBD-CAD	3.57	1.28	1.22
14	B	822	CLA	CHD-C4C	3.57	1.47	1.39
14	a	802	CLA	OBD-CAD	3.57	1.28	1.22
14	b	827	CLA	C1D-ND	-3.57	1.33	1.37
14	A	832	CLA	OBD-CAD	3.57	1.28	1.22
14	H	836	CLA	OBD-CAD	3.57	1.28	1.22
14	A	835	CLA	OBD-CAD	3.57	1.28	1.22
14	G	840	CLA	OBD-CAD	3.56	1.28	1.22
14	a	831	CLA	C1D-ND	-3.56	1.33	1.37
17	G	849	BCR	C11-C12	-3.56	1.25	1.34
14	U	205	CLA	OBD-CAD	3.56	1.28	1.22
17	L	202	BCR	C11-C12	-3.56	1.25	1.34
14	b	825	CLA	CHD-C4C	3.56	1.47	1.39
14	A	830	CLA	OBD-CAD	3.56	1.28	1.22
14	H	828	CLA	OBD-CAD	3.56	1.28	1.22
17	b	846	BCR	C11-C12	-3.56	1.25	1.34
14	b	822	CLA	OBD-CAD	3.56	1.28	1.22
14	A	809	CLA	OBD-CAD	3.55	1.28	1.22
14	b	802	CLA	OBD-CAD	3.55	1.28	1.22
14	x	1701	CLA	OBD-CAD	3.55	1.28	1.22
14	A	838	CLA	OBD-CAD	3.55	1.28	1.22
14	b	812	CLA	CHD-C4C	3.55	1.47	1.39
14	B	825	CLA	CHD-C4C	3.54	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	833	CLA	OBD-CAD	3.54	1.28	1.22
14	H	802	CLA	CHD-C4C	3.54	1.47	1.39
14	A	843	CLA	OBD-CAD	3.54	1.28	1.22
14	a	828	CLA	OBD-CAD	3.54	1.28	1.22
14	H	808	CLA	CHD-C4C	3.54	1.47	1.39
14	B	808	CLA	C3B-C2B	3.54	1.45	1.40
14	G	805	CLA	OBD-CAD	3.54	1.28	1.22
14	H	803	CLA	OBD-CAD	3.54	1.28	1.22
14	G	811	CLA	CHD-C4C	3.54	1.47	1.39
14	H	826	CLA	C1D-ND	-3.54	1.33	1.37
14	l	202	CLA	CHD-C4C	3.54	1.47	1.39
13	G	801	CL0	CHD-C4C	3.54	1.47	1.39
17	a	851	BCR	C11-C12	-3.54	1.25	1.34
14	b	828	CLA	C1D-ND	-3.53	1.33	1.37
14	H	822	CLA	CHD-C4C	3.53	1.47	1.39
14	A	824	CLA	OBD-CAD	3.53	1.28	1.22
14	H	828	CLA	MG-ND	-3.53	1.98	2.05
17	B	847	BCR	C11-C12	-3.53	1.25	1.34
17	B	843	BCR	C11-C12	-3.53	1.25	1.34
14	m	1601	CLA	OBD-CAD	3.53	1.28	1.22
14	b	809	CLA	MG-ND	-3.53	1.98	2.05
14	H	812	CLA	CHD-C4C	3.53	1.47	1.39
14	H	818	CLA	OBD-CAD	3.52	1.28	1.22
14	G	826	CLA	C1D-ND	-3.52	1.33	1.37
14	b	801	CLA	CHD-C1D	3.52	1.45	1.38
17	A	849	BCR	C11-C12	-3.52	1.25	1.34
14	G	832	CLA	OBD-CAD	3.52	1.28	1.22
14	B	836	CLA	OBD-CAD	3.52	1.28	1.22
13	A	801	CL0	MG-ND	-3.51	1.98	2.05
14	b	839	CLA	OBD-CAD	3.51	1.28	1.22
17	b	847	BCR	C11-C12	-3.51	1.25	1.34
14	A	823	CLA	CHD-C1D	3.51	1.45	1.38
17	i	102	BCR	C11-C12	-3.51	1.25	1.34
14	a	828	CLA	CHD-C4C	3.51	1.47	1.39
14	a	823	CLA	OBD-CAD	3.51	1.28	1.22
14	B	803	CLA	CHD-C1D	3.51	1.45	1.38
17	G	848	BCR	C11-C12	-3.51	1.25	1.34
14	B	809	CLA	MG-ND	-3.51	1.98	2.05
14	A	834	CLA	OBD-CAD	3.51	1.28	1.22
14	B	803	CLA	OBD-CAD	3.50	1.28	1.22
17	I	101	BCR	C11-C12	-3.50	1.25	1.34
14	G	816	CLA	OBD-CAD	3.50	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	804	CLA	CHD-C4C	3.50	1.47	1.39
17	B	848	BCR	C11-C12	-3.50	1.25	1.34
14	G	807	CLA	OBD-CAD	3.50	1.28	1.22
14	A	805	CLA	OBD-CAD	3.50	1.28	1.22
14	a	838	CLA	OBD-CAD	3.50	1.28	1.22
14	H	839	CLA	OBD-CAD	3.50	1.28	1.22
14	H	838	CLA	OBD-CAD	3.50	1.28	1.22
14	G	841	CLA	OBD-CAD	3.49	1.28	1.22
14	B	814	CLA	OBD-CAD	3.49	1.28	1.22
14	L	204	CLA	OBD-CAD	3.49	1.28	1.22
14	A	813	CLA	C1D-ND	-3.49	1.33	1.37
14	G	828	CLA	CHD-C1D	3.49	1.45	1.38
14	G	824	CLA	OBD-CAD	3.49	1.28	1.22
14	G	832	CLA	C1D-ND	-3.48	1.33	1.37
14	B	818	CLA	OBD-CAD	3.48	1.28	1.22
14	a	855	CLA	CHD-C4C	3.48	1.47	1.39
13	a	801	CL0	CHD-C4C	3.48	1.47	1.39
14	H	823	CLA	CHD-C4C	3.48	1.47	1.39
17	A	852	BCR	C11-C12	-3.48	1.25	1.34
14	A	832	CLA	C1D-ND	-3.48	1.33	1.37
14	G	829	CLA	C1D-ND	-3.48	1.33	1.37
14	l	205	CLA	OBD-CAD	3.48	1.28	1.22
17	R	101	BCR	C11-C12	-3.48	1.25	1.34
14	L	205	CLA	CHD-C1D	3.48	1.45	1.38
17	H	842	BCR	C11-C12	-3.48	1.25	1.34
14	b	820	CLA	OBD-CAD	3.47	1.28	1.22
14	a	855	CLA	C3D-C2D	3.47	1.48	1.39
17	A	850	BCR	C11-C12	-3.47	1.25	1.34
14	G	803	CLA	MG-ND	-3.47	1.98	2.05
14	i	101	CLA	OBD-CAD	3.47	1.28	1.22
14	b	802	CLA	C3B-C2B	3.47	1.45	1.40
14	G	843	CLA	OBD-CAD	3.47	1.28	1.22
17	a	847	BCR	C11-C12	-3.47	1.25	1.34
14	H	829	CLA	C1D-ND	-3.47	1.33	1.37
14	a	828	CLA	C1D-ND	-3.47	1.33	1.37
17	j	103	BCR	C11-C12	-3.47	1.25	1.34
14	B	822	CLA	OBD-CAD	3.46	1.28	1.22
14	H	803	CLA	CHD-C4C	3.46	1.47	1.39
14	H	822	CLA	OBD-CAD	3.46	1.28	1.22
17	H	843	BCR	C11-C12	-3.46	1.25	1.34
14	A	844	CLA	C3B-C2B	3.46	1.45	1.40
14	a	818	CLA	OBD-CAD	3.46	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	801	CLA	CHD-C4C	3.46	1.47	1.39
14	B	821	CLA	OBD-CAD	3.46	1.28	1.22
14	b	836	CLA	CHD-C4C	3.45	1.47	1.39
14	b	804	CLA	CHD-C1D	3.45	1.45	1.38
14	H	801	CLA	CHD-C4C	3.45	1.47	1.39
17	H	847	BCR	C11-C12	-3.45	1.25	1.34
14	a	806	CLA	OBD-CAD	3.45	1.28	1.22
14	G	831	CLA	C1D-ND	-3.45	1.33	1.37
14	G	821	CLA	OBD-CAD	3.45	1.28	1.22
14	b	804	CLA	OBD-CAD	3.45	1.28	1.22
17	B	842	BCR	C11-C12	-3.45	1.25	1.34
14	B	812	CLA	OBD-CAD	3.44	1.28	1.22
14	B	801	CLA	C3B-C2B	3.44	1.45	1.40
14	B	828	CLA	MG-ND	-3.44	1.99	2.05
14	A	829	CLA	MG-ND	-3.44	1.99	2.05
13	A	801	CL0	CHD-C4C	3.44	1.47	1.39
17	a	849	BCR	C11-C12	-3.44	1.25	1.34
14	b	824	CLA	C3D-C2D	3.43	1.48	1.39
14	G	839	CLA	OBD-CAD	3.43	1.28	1.22
14	a	832	CLA	OBD-CAD	3.43	1.28	1.22
14	a	802	CLA	C1D-ND	-3.43	1.33	1.37
17	b	843	BCR	C11-C12	-3.43	1.25	1.34
14	H	807	CLA	OBD-CAD	3.43	1.28	1.22
14	b	828	CLA	MG-ND	-3.43	1.99	2.05
14	G	803	CLA	C3B-C2B	3.43	1.45	1.40
14	a	830	CLA	OBD-CAD	3.43	1.28	1.22
14	G	843	CLA	C3D-C2D	3.43	1.48	1.39
14	B	802	CLA	CHD-C4C	3.43	1.47	1.39
14	H	828	CLA	C1D-ND	-3.42	1.33	1.37
14	b	826	CLA	C1D-ND	-3.42	1.33	1.37
14	G	843	CLA	C3B-C2B	3.42	1.45	1.40
14	H	808	CLA	C1D-ND	-3.42	1.33	1.37
14	b	829	CLA	C3B-C2B	3.42	1.45	1.40
14	A	823	CLA	CHD-C4C	3.42	1.47	1.39
14	b	807	CLA	OBD-CAD	3.42	1.28	1.22
14	F	1301	CLA	OBD-CAD	3.42	1.28	1.22
14	G	804	CLA	OBD-CAD	3.42	1.28	1.22
14	b	826	CLA	MG-ND	-3.42	1.99	2.05
14	a	829	CLA	MG-ND	-3.41	1.99	2.05
14	G	838	CLA	OBD-CAD	3.41	1.28	1.22
14	B	828	CLA	C1D-ND	-3.41	1.33	1.37
14	b	803	CLA	CHD-C4C	3.41	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	829	CLA	MG-ND	-3.41	1.99	2.05
14	B	801	CLA	CHD-C4C	3.41	1.47	1.39
14	H	809	CLA	MG-ND	-3.40	1.99	2.05
14	A	806	CLA	OBD-CAD	3.40	1.28	1.22
17	G	853	BCR	C11-C12	-3.40	1.25	1.34
14	B	801	CLA	C3D-C2D	3.40	1.48	1.39
14	H	835	CLA	CHD-C4C	3.40	1.46	1.39
14	G	813	CLA	OBD-CAD	3.40	1.28	1.22
14	B	809	CLA	CHD-C4C	3.39	1.46	1.39
14	B	839	CLA	C1D-ND	-3.39	1.33	1.37
14	a	815	CLA	OBD-CAD	3.39	1.28	1.22
14	H	839	CLA	C1D-ND	-3.39	1.33	1.37
17	b	842	BCR	C11-C12	-3.39	1.25	1.34
14	B	829	CLA	C1D-ND	-3.39	1.33	1.37
14	G	803	CLA	C1D-ND	-3.39	1.33	1.37
14	A	810	CLA	OBD-CAD	3.38	1.28	1.22
14	b	808	CLA	C1D-ND	-3.38	1.33	1.37
14	F	1301	CLA	C3D-C2D	3.38	1.48	1.39
14	A	803	CLA	C1D-ND	-3.38	1.33	1.37
14	b	806	CLA	C1D-ND	-3.38	1.33	1.37
14	H	801	CLA	C3D-C2D	3.37	1.48	1.39
14	U	204	CLA	OBD-CAD	3.37	1.28	1.22
14	B	839	CLA	OBD-CAD	3.37	1.28	1.22
14	b	817	CLA	C1D-ND	-3.37	1.33	1.37
14	A	844	CLA	OBD-CAD	3.37	1.28	1.22
14	b	836	CLA	OBD-CAD	3.37	1.28	1.22
14	B	827	CLA	MG-ND	-3.37	1.99	2.05
17	B	844	BCR	C11-C12	-3.37	1.25	1.34
17	l	208	BCR	C11-C12	-3.37	1.25	1.34
14	B	838	CLA	OBD-CAD	3.37	1.28	1.22
14	b	809	CLA	OBD-CAD	3.36	1.28	1.22
14	G	830	CLA	MG-ND	-3.36	1.99	2.05
17	H	844	BCR	C11-C12	-3.36	1.25	1.34
14	B	826	CLA	MG-ND	-3.36	1.99	2.05
14	H	826	CLA	MG-ND	-3.36	1.99	2.05
14	a	827	CLA	CHD-C4C	3.36	1.46	1.39
14	H	823	CLA	MG-ND	-3.35	1.99	2.05
14	B	819	CLA	C1D-ND	-3.35	1.33	1.37
14	A	803	CLA	C3B-C2B	3.35	1.44	1.40
14	b	823	CLA	MG-ND	-3.35	1.99	2.05
14	b	836	CLA	MG-ND	-3.35	1.99	2.05
14	a	841	CLA	OBD-CAD	3.35	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	823	CLA	CHD-C4C	3.35	1.46	1.39
14	a	802	CLA	C3B-C2B	3.35	1.44	1.40
14	B	826	CLA	C1D-ND	-3.35	1.33	1.37
14	a	802	CLA	MG-ND	-3.35	1.99	2.05
17	A	853	BCR	C11-C12	-3.35	1.25	1.34
14	A	807	CLA	OBD-CAD	3.35	1.28	1.22
14	A	831	CLA	OBD-CAD	3.34	1.28	1.22
14	B	812	CLA	CHD-C4C	3.34	1.46	1.39
14	A	822	CLA	OBD-CAD	3.34	1.28	1.22
14	H	803	CLA	MG-ND	-3.34	1.99	2.05
14	H	803	CLA	C1C-NC	-3.34	1.32	1.37
14	H	824	CLA	C3D-C2D	3.34	1.48	1.39
17	b	849	BCR	C11-C12	-3.34	1.26	1.34
14	U	201	CLA	OBD-CAD	3.34	1.28	1.22
14	A	831	CLA	C3D-C2D	3.34	1.48	1.39
14	b	837	CLA	OBD-CAD	3.34	1.28	1.22
14	Q	203	CLA	C3D-C2D	3.34	1.48	1.39
14	G	829	CLA	MG-ND	-3.33	1.99	2.05
14	b	803	CLA	MG-ND	-3.33	1.99	2.05
14	X	1701	CLA	OBD-CAD	3.33	1.28	1.22
17	H	849	BCR	C11-C12	-3.33	1.26	1.34
14	F	1301	CLA	C1D-ND	-3.33	1.33	1.37
17	a	852	BCR	C11-C12	-3.33	1.26	1.34
14	i	101	CLA	C1D-ND	-3.32	1.33	1.37
14	H	825	CLA	CHD-C4C	3.32	1.46	1.39
14	B	806	CLA	OBD-CAD	3.32	1.28	1.22
13	G	801	CL0	MG-ND	-3.32	1.99	2.05
14	B	823	CLA	OBD-CAD	3.32	1.28	1.22
17	b	844	BCR	C11-C12	-3.32	1.26	1.34
14	H	803	CLA	CHD-C1D	3.31	1.44	1.38
14	A	804	CLA	OBD-CAD	3.31	1.28	1.22
14	a	830	CLA	C3D-C2D	3.31	1.48	1.39
14	A	842	CLA	OBD-CAD	3.31	1.28	1.22
14	H	809	CLA	C3D-C2D	3.31	1.48	1.39
14	a	825	CLA	MG-ND	-3.31	1.99	2.05
14	H	835	CLA	C1C-NC	-3.31	1.32	1.37
14	l	202	CLA	C1C-NC	-3.31	1.32	1.37
14	b	823	CLA	C3D-C2D	3.30	1.48	1.39
14	a	821	CLA	OBD-CAD	3.30	1.28	1.22
14	b	839	CLA	C1D-ND	-3.30	1.33	1.37
14	H	802	CLA	MG-ND	-3.30	1.99	2.05
14	a	855	CLA	MG-ND	-3.30	1.99	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	m	1602	BCR	C11-C12	-3.30	1.26	1.34
14	b	836	CLA	MG-NC	3.30	2.14	2.06
14	G	831	CLA	OBD-CAD	3.29	1.28	1.22
17	A	848	BCR	C11-C12	-3.29	1.26	1.34
14	H	811	CLA	C1D-ND	-3.29	1.33	1.37
14	H	831	CLA	C1D-ND	-3.29	1.33	1.37
14	b	825	CLA	OBD-CAD	3.29	1.28	1.22
14	B	805	CLA	C1D-ND	-3.28	1.33	1.37
14	A	828	CLA	C3C-C2C	3.28	1.43	1.36
14	b	829	CLA	MG-ND	-3.28	1.99	2.05
14	H	823	CLA	OBD-CAD	3.28	1.28	1.22
17	J	103	BCR	C11-C12	-3.28	1.26	1.34
14	b	821	CLA	OBD-CAD	3.28	1.28	1.22
14	A	818	CLA	C1D-ND	-3.28	1.33	1.37
14	B	824	CLA	C3D-C2D	3.28	1.47	1.39
14	l	202	CLA	OBD-CAD	3.28	1.28	1.22
14	B	836	CLA	C1D-ND	-3.28	1.33	1.37
14	b	819	CLA	C1D-ND	-3.27	1.33	1.37
17	I	102	BCR	C11-C12	-3.27	1.26	1.34
14	H	801	CLA	MG-ND	-3.27	1.99	2.05
14	a	805	CLA	OBD-CAD	3.26	1.28	1.22
14	A	844	CLA	C3D-C2D	3.26	1.47	1.39
17	B	850	BCR	C11-C12	-3.26	1.26	1.34
14	B	821	CLA	C1D-ND	-3.26	1.33	1.37
14	B	823	CLA	MG-ND	-3.26	1.99	2.05
14	G	826	CLA	MG-ND	-3.26	1.99	2.05
14	A	843	CLA	C1D-ND	-3.26	1.33	1.37
14	a	825	CLA	MG-NC	3.25	2.14	2.06
14	a	834	CLA	C3D-C2D	3.25	1.47	1.39
14	A	835	CLA	C3D-C2D	3.25	1.47	1.39
14	A	838	CLA	C1D-ND	-3.25	1.33	1.37
14	a	822	CLA	C1D-ND	-3.25	1.33	1.37
14	B	825	CLA	MG-ND	-3.25	1.99	2.05
14	H	821	CLA	C1D-ND	-3.25	1.33	1.37
14	G	806	CLA	OBD-CAD	3.25	1.28	1.22
14	H	837	CLA	OBD-CAD	3.25	1.28	1.22
14	G	828	CLA	C1D-ND	-3.25	1.33	1.37
14	B	801	CLA	MG-ND	-3.25	1.99	2.05
14	f	202	CLA	MG-NC	3.24	2.14	2.06
14	b	831	CLA	C1D-ND	-3.24	1.33	1.37
14	B	812	CLA	C1D-ND	-3.24	1.33	1.37
14	H	806	CLA	OBD-CAD	3.24	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	834	CLA	C1D-ND	-3.24	1.33	1.37
14	H	809	CLA	OBD-CAD	3.24	1.28	1.22
14	A	831	CLA	MG-ND	-3.24	1.99	2.05
14	b	840	CLA	C1C-NC	-3.24	1.32	1.37
14	b	817	CLA	C3D-C2D	3.24	1.47	1.39
14	B	837	CLA	OBD-CAD	3.24	1.28	1.22
14	a	835	CLA	C1D-ND	-3.24	1.33	1.37
14	B	803	CLA	MG-ND	-3.24	1.99	2.05
14	a	819	CLA	C1D-ND	-3.23	1.33	1.37
14	b	801	CLA	C3D-C2D	3.23	1.47	1.39
14	G	822	CLA	OBD-CAD	3.23	1.28	1.22
14	B	829	CLA	MG-ND	-3.23	1.99	2.05
14	a	830	CLA	MG-ND	-3.23	1.99	2.05
13	a	801	CL0	MG-ND	-3.23	1.99	2.05
17	M	1602	BCR	C11-C12	-3.23	1.26	1.34
14	G	832	CLA	MG-ND	-3.23	1.99	2.05
14	B	817	CLA	C1D-ND	-3.23	1.33	1.37
14	b	812	CLA	C1D-ND	-3.23	1.33	1.37
17	f	203	BCR	C11-C12	-3.23	1.26	1.34
14	A	803	CLA	MG-ND	-3.23	1.99	2.05
14	H	819	CLA	MG-NC	3.23	2.13	2.06
14	H	822	CLA	C1D-ND	-3.22	1.33	1.37
14	b	804	CLA	C1C-NC	-3.22	1.32	1.37
14	B	829	CLA	C3B-C2B	3.22	1.44	1.40
14	G	821	CLA	C1D-ND	-3.22	1.33	1.37
14	L	201	CLA	OBD-CAD	3.22	1.28	1.22
14	G	834	CLA	C1D-ND	-3.22	1.33	1.37
14	H	827	CLA	MG-ND	-3.22	1.99	2.05
14	A	820	CLA	C1D-ND	-3.21	1.33	1.37
14	H	808	CLA	MG-ND	-3.21	1.99	2.05
17	j	104	BCR	C11-C12	-3.21	1.26	1.34
14	a	828	CLA	MG-ND	-3.21	1.99	2.05
14	b	823	CLA	CHD-C4C	3.21	1.46	1.39
14	B	840	CLA	C1C-NC	-3.21	1.32	1.37
14	A	812	CLA	OBD-CAD	3.21	1.28	1.22
17	Q	204	BCR	C11-C12	-3.21	1.26	1.34
14	j	102	CLA	MG-NC	3.21	2.13	2.06
14	b	808	CLA	MG-ND	-3.21	1.99	2.05
14	B	803	CLA	C1C-NC	-3.21	1.32	1.37
14	b	825	CLA	C1D-ND	-3.21	1.33	1.37
14	G	845	CLA	C1D-ND	-3.21	1.33	1.37
14	H	812	CLA	C1D-ND	-3.21	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	823	CLA	OBD-CAD	3.20	1.28	1.22
14	A	826	CLA	MG-NC	3.20	2.13	2.06
14	G	802	CLA	MG-ND	-3.20	1.99	2.05
17	R	103	BCR	C11-C12	-3.20	1.26	1.34
14	W	1701	CLA	MG-NC	3.20	2.13	2.06
14	Q	201	CLA	C1D-ND	-3.20	1.33	1.37
14	A	820	CLA	MG-ND	-3.20	1.99	2.05
14	G	819	CLA	C1D-ND	-3.19	1.33	1.37
14	G	826	CLA	MG-NC	3.19	2.13	2.06
14	L	204	CLA	C1D-ND	-3.19	1.33	1.37
14	H	821	CLA	OBD-CAD	3.19	1.28	1.22
14	A	842	CLA	C1D-ND	-3.18	1.33	1.37
14	K	101	CLA	C3D-C2D	3.18	1.47	1.39
14	B	802	CLA	MG-ND	-3.18	1.99	2.05
14	H	822	CLA	C3D-C2D	3.18	1.47	1.39
14	B	822	CLA	C1D-ND	-3.18	1.33	1.37
14	A	841	CLA	C1D-ND	-3.18	1.33	1.37
14	A	827	CLA	C1D-ND	-3.18	1.33	1.37
14	G	806	CLA	C1D-ND	-3.17	1.33	1.37
14	A	836	CLA	C1D-ND	-3.17	1.33	1.37
14	b	809	CLA	CHD-C4C	3.17	1.46	1.39
14	a	830	CLA	C1C-NC	-3.17	1.32	1.37
14	S	101	CLA	MG-NC	3.16	2.13	2.06
14	L	201	CLA	C1C-NC	-3.16	1.32	1.37
14	A	828	CLA	C1C-NC	-3.16	1.32	1.37
14	b	804	CLA	MG-ND	-3.16	1.99	2.05
14	b	820	CLA	C1D-ND	-3.16	1.33	1.37
14	A	826	CLA	C1D-ND	-3.16	1.33	1.37
14	b	825	CLA	MG-ND	-3.16	1.99	2.05
14	A	835	CLA	C1D-ND	-3.16	1.33	1.37
14	G	804	CLA	C1D-ND	-3.16	1.33	1.37
14	b	802	CLA	C3D-C2D	3.16	1.47	1.39
14	B	824	CLA	C1D-ND	-3.15	1.33	1.37
14	H	813	CLA	C1D-ND	-3.15	1.33	1.37
14	H	837	CLA	C1D-ND	-3.15	1.33	1.37
14	G	835	CLA	C3D-C2D	3.15	1.47	1.39
14	a	841	CLA	C1D-ND	-3.15	1.33	1.37
14	G	828	CLA	CHD-C4C	3.15	1.46	1.39
14	H	820	CLA	C1D-ND	-3.15	1.33	1.37
14	B	822	CLA	C3D-C2D	3.15	1.47	1.39
14	A	845	CLA	C1C-NC	-3.15	1.32	1.37
14	k	1401	CLA	C1D-ND	-3.15	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	803	CLA	C3D-C2D	3.15	1.47	1.39
14	B	831	CLA	C1D-ND	-3.15	1.33	1.37
14	b	817	CLA	MG-ND	-3.15	1.99	2.05
14	A	823	CLA	C3D-C2D	3.14	1.47	1.39
14	H	805	CLA	MG-ND	-3.14	1.99	2.05
14	L	206	CLA	C1D-ND	-3.14	1.33	1.37
14	H	840	CLA	C1D-ND	-3.14	1.33	1.37
14	H	811	CLA	C3D-C2D	3.14	1.47	1.39
14	S	102	CLA	MG-NC	3.14	2.13	2.06
14	a	829	CLA	MG-NC	3.14	2.13	2.06
14	b	821	CLA	MG-NC	3.14	2.13	2.06
14	B	819	CLA	MG-ND	-3.14	1.99	2.05
14	G	802	CLA	C3D-C2D	3.14	1.47	1.39
14	A	822	CLA	C3D-C2D	3.13	1.47	1.39
14	B	827	CLA	MG-NC	3.13	2.13	2.06
14	H	807	CLA	C1D-ND	-3.13	1.33	1.37
14	l	202	CLA	C3D-C2D	3.13	1.47	1.39
14	G	829	CLA	MG-NC	3.13	2.13	2.06
14	j	101	CLA	MG-NC	3.13	2.13	2.06
17	V	1602	BCR	C11-C12	-3.13	1.26	1.34
14	H	834	CLA	C1D-ND	-3.13	1.33	1.37
14	A	844	CLA	MG-ND	-3.13	1.99	2.05
14	a	819	CLA	C3D-C2D	3.13	1.47	1.39
14	V	1601	CLA	MG-NC	3.13	2.13	2.06
14	T	1401	CLA	MG-NC	3.13	2.13	2.06
14	b	837	CLA	C1D-ND	-3.13	1.33	1.37
14	A	810	CLA	C1D-ND	-3.13	1.33	1.37
14	G	828	CLA	MG-ND	-3.13	1.99	2.05
14	H	821	CLA	C3D-C2D	3.13	1.47	1.39
14	a	802	CLA	C3D-C2D	3.13	1.47	1.39
14	a	835	CLA	C3D-C2D	3.13	1.47	1.39
14	G	843	CLA	MG-ND	-3.13	1.99	2.05
14	H	820	CLA	C3D-C2D	3.13	1.47	1.39
14	a	838	CLA	MG-NC	3.12	2.13	2.06
14	b	802	CLA	MG-ND	-3.12	1.99	2.05
14	U	201	CLA	C1C-NC	-3.12	1.33	1.37
14	G	810	CLA	C1D-ND	-3.12	1.33	1.37
14	b	815	CLA	C1D-ND	-3.12	1.33	1.37
14	b	835	CLA	MG-NC	3.12	2.13	2.06
14	a	803	CLA	C1D-ND	-3.12	1.33	1.37
14	m	1601	CLA	MG-NC	3.12	2.13	2.06
14	l	207	CLA	C1D-ND	-3.12	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	201	CLA	C3D-C2D	3.12	1.47	1.39
14	A	823	CLA	MG-ND	-3.12	1.99	2.05
14	G	828	CLA	MG-NC	3.12	2.13	2.06
14	H	830	CLA	C3D-C2D	3.12	1.47	1.39
14	B	840	CLA	C1D-ND	-3.12	1.33	1.37
14	M	1601	CLA	MG-NC	3.12	2.13	2.06
14	A	837	CLA	C3D-C2D	3.12	1.47	1.39
14	A	840	CLA	C1D-ND	-3.12	1.33	1.37
14	A	802	CLA	C3D-C2D	3.12	1.47	1.39
14	a	823	CLA	C1D-ND	-3.11	1.33	1.37
14	a	833	CLA	C1D-ND	-3.11	1.33	1.37
14	b	822	CLA	C3D-C2D	3.11	1.47	1.39
14	f	202	CLA	C3D-C2D	3.11	1.47	1.39
14	U	201	CLA	C3D-C2D	3.11	1.47	1.39
14	B	825	CLA	C1D-ND	-3.11	1.33	1.37
14	A	833	CLA	MG-NC	3.11	2.13	2.06
14	x	1701	CLA	MG-NC	3.11	2.13	2.06
14	A	814	CLA	C3D-C2D	3.11	1.47	1.39
14	b	819	CLA	MG-NC	3.11	2.13	2.06
14	b	807	CLA	C1D-ND	-3.11	1.33	1.37
14	G	836	CLA	C1D-ND	-3.11	1.33	1.37
14	A	802	CLA	MG-ND	-3.11	1.99	2.05
14	A	832	CLA	MG-ND	-3.11	1.99	2.05
14	b	827	CLA	MG-ND	-3.11	1.99	2.05
14	B	836	CLA	C3D-C2D	3.11	1.47	1.39
14	B	815	CLA	C1D-ND	-3.11	1.33	1.37
14	B	814	CLA	MG-ND	-3.10	1.99	2.05
14	G	831	CLA	MG-ND	-3.10	1.99	2.05
14	B	804	CLA	C1D-ND	-3.10	1.33	1.37
14	B	813	CLA	C1D-ND	-3.10	1.33	1.37
14	b	813	CLA	C1D-ND	-3.10	1.33	1.37
14	B	821	CLA	C3D-C2D	3.10	1.47	1.39
14	b	821	CLA	C3D-C2D	3.10	1.47	1.39
14	G	839	CLA	C1D-ND	-3.10	1.33	1.37
14	G	831	CLA	C3D-C2D	3.10	1.47	1.39
14	H	819	CLA	C3D-C2D	3.10	1.47	1.39
14	U	206	CLA	C3D-C2D	3.10	1.47	1.39
14	G	820	CLA	MG-ND	-3.10	1.99	2.05
14	B	803	CLA	C3D-C2D	3.10	1.47	1.39
14	A	820	CLA	C3D-C2D	3.10	1.47	1.39
14	K	102	CLA	MG-NC	3.09	2.13	2.06
14	b	825	CLA	MG-NC	3.09	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	835	CLA	C1D-ND	-3.09	1.33	1.37
14	G	837	CLA	C3D-C2D	3.09	1.47	1.39
14	b	809	CLA	C1C-NC	-3.09	1.33	1.37
14	a	843	CLA	C3D-C2D	3.09	1.47	1.39
14	a	826	CLA	C1D-ND	-3.09	1.33	1.37
14	H	821	CLA	MG-NC	3.09	2.13	2.06
14	B	808	CLA	MG-NC	3.09	2.13	2.06
14	X	1701	CLA	MG-NC	3.09	2.13	2.06
14	H	817	CLA	C3D-C2D	3.09	1.47	1.39
14	G	839	CLA	MG-NC	3.09	2.13	2.06
14	B	801	CLA	MG-NC	3.09	2.13	2.06
14	k	1401	CLA	C3D-C2D	3.08	1.47	1.39
14	B	837	CLA	C1D-ND	-3.08	1.33	1.37
14	b	840	CLA	C1D-ND	-3.08	1.33	1.37
14	S	101	CLA	C4D-CHA	3.08	1.49	1.38
14	G	844	CLA	MG-NC	3.08	2.13	2.06
14	b	818	CLA	C3D-C2D	3.08	1.47	1.39
14	B	809	CLA	OBD-CAD	3.08	1.27	1.22
14	A	828	CLA	MG-ND	-3.08	1.99	2.05
14	A	804	CLA	C1D-ND	-3.08	1.33	1.37
14	H	819	CLA	C1D-ND	-3.08	1.33	1.37
14	a	831	CLA	MG-ND	-3.08	1.99	2.05
14	G	842	CLA	C1D-ND	-3.08	1.33	1.37
14	j	102	CLA	C3D-C2D	3.08	1.47	1.39
14	H	810	CLA	MG-NC	3.08	2.13	2.06
17	F	1302	BCR	C11-C12	-3.08	1.26	1.34
14	A	839	CLA	C1D-ND	-3.08	1.33	1.37
14	a	828	CLA	MG-NC	3.08	2.13	2.06
14	a	844	CLA	C1D-ND	-3.08	1.33	1.37
14	B	836	CLA	MG-NC	3.08	2.13	2.06
14	H	838	CLA	C1D-ND	-3.08	1.33	1.37
14	a	843	CLA	MG-NC	3.07	2.13	2.06
14	k	1401	CLA	MG-NC	3.07	2.13	2.06
14	K	102	CLA	C3D-C2D	3.07	1.47	1.39
14	U	204	CLA	C1D-ND	-3.07	1.33	1.37
14	B	812	CLA	MG-ND	-3.07	1.99	2.05
14	G	823	CLA	C1D-ND	-3.07	1.33	1.37
14	H	804	CLA	C1D-ND	-3.07	1.33	1.37
14	G	816	CLA	MG-NC	3.07	2.13	2.06
14	W	1701	CLA	C3D-C2D	3.07	1.47	1.39
14	a	814	CLA	MG-NC	3.07	2.13	2.06
14	B	835	CLA	MG-NC	3.07	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	827	CLA	MG-NC	3.07	2.13	2.06
14	H	834	CLA	MG-NC	3.07	2.13	2.06
14	a	812	CLA	C3D-C2D	3.07	1.47	1.39
14	B	817	CLA	C3D-C2D	3.07	1.47	1.39
14	B	821	CLA	MG-NC	3.07	2.13	2.06
14	a	810	CLA	C3D-C2D	3.07	1.47	1.39
14	H	825	CLA	OBD-CAD	3.07	1.27	1.22
14	H	840	CLA	C1C-NC	-3.07	1.33	1.37
14	G	839	CLA	C3D-C2D	3.06	1.47	1.39
14	A	829	CLA	MG-NC	3.06	2.13	2.06
14	J	101	CLA	MG-NC	3.06	2.13	2.06
14	H	801	CLA	MG-NC	3.06	2.13	2.06
14	b	840	CLA	C3D-C2D	3.06	1.47	1.39
14	S	101	CLA	C3D-C2D	3.06	1.47	1.39
14	G	836	CLA	C3D-C2D	3.06	1.47	1.39
14	H	817	CLA	C1D-ND	-3.06	1.33	1.37
14	B	823	CLA	C3D-C2D	3.06	1.47	1.39
14	G	820	CLA	C1D-ND	-3.06	1.33	1.37
14	b	836	CLA	C3D-C2D	3.06	1.47	1.39
14	H	811	CLA	MG-NC	3.06	2.13	2.06
14	A	833	CLA	C3D-C2D	3.06	1.47	1.39
14	L	206	CLA	C3D-C2D	3.06	1.47	1.39
14	a	832	CLA	C3D-C2D	3.06	1.47	1.39
14	a	812	CLA	MG-NC	3.06	2.13	2.06
14	B	820	CLA	C1D-ND	-3.06	1.33	1.37
14	H	824	CLA	C1D-ND	-3.06	1.33	1.37
14	G	844	CLA	C3D-C2D	3.06	1.47	1.39
14	a	805	CLA	C1D-ND	-3.06	1.33	1.37
14	G	816	CLA	C4D-CHA	3.05	1.48	1.38
14	a	827	CLA	MG-NC	3.05	2.13	2.06
14	H	816	CLA	C3D-C2D	3.05	1.47	1.39
14	A	810	CLA	C3D-C2D	3.05	1.47	1.39
14	H	825	CLA	MG-ND	-3.05	1.99	2.05
14	b	831	CLA	MG-NC	3.05	2.13	2.06
14	H	804	CLA	C3D-C2D	3.05	1.47	1.39
14	a	837	CLA	C1D-ND	-3.05	1.33	1.37
14	G	820	CLA	C3D-C2D	3.05	1.47	1.39
14	b	824	CLA	C1D-ND	-3.05	1.33	1.37
14	G	840	CLA	C3D-C2D	3.05	1.47	1.39
14	F	1301	CLA	MG-ND	-3.05	1.99	2.05
14	b	834	CLA	MG-ND	-3.05	1.99	2.05
14	T	1401	CLA	C3D-C2D	3.05	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	812	CLA	C3D-C2D	3.05	1.47	1.39
14	H	840	CLA	C3D-C2D	3.05	1.47	1.39
14	H	814	CLA	C1D-ND	-3.04	1.33	1.37
14	A	824	CLA	MG-NC	3.04	2.13	2.06
14	b	806	CLA	MG-ND	-3.04	1.99	2.05
14	a	837	CLA	MG-NC	3.04	2.13	2.06
14	a	834	CLA	C1D-ND	-3.04	1.33	1.37
14	H	836	CLA	C1D-ND	-3.04	1.33	1.37
14	A	805	CLA	C3D-C2D	3.04	1.47	1.39
14	b	814	CLA	MG-NC	3.04	2.13	2.06
14	B	825	CLA	C4D-CHA	3.04	1.48	1.38
14	B	830	CLA	C3D-C2D	3.04	1.47	1.39
14	S	102	CLA	C3D-C2D	3.04	1.47	1.39
14	B	836	CLA	MG-ND	-3.04	1.99	2.05
14	H	803	CLA	C3D-C2D	3.04	1.47	1.39
14	a	815	CLA	C3D-C2D	3.04	1.47	1.39
14	A	821	CLA	C1D-ND	-3.04	1.33	1.37
14	G	827	CLA	C1D-ND	-3.04	1.33	1.37
14	l	205	CLA	C3D-C2D	3.04	1.47	1.39
14	l	205	CLA	C1D-ND	-3.04	1.33	1.37
14	B	810	CLA	C3D-C2D	3.04	1.47	1.39
14	a	804	CLA	C3D-C2D	3.04	1.47	1.39
14	T	1401	CLA	C1D-ND	-3.04	1.33	1.37
14	A	806	CLA	C1D-ND	-3.04	1.33	1.37
14	H	836	CLA	MG-ND	-3.04	1.99	2.05
14	m	1601	CLA	C4D-CHA	3.03	1.48	1.38
14	a	815	CLA	MG-NC	3.03	2.13	2.06
14	G	827	CLA	C3D-C2D	3.03	1.47	1.39
14	G	837	CLA	MG-NC	3.03	2.13	2.06
14	H	834	CLA	MG-ND	-3.03	1.99	2.05
14	G	833	CLA	MG-NC	3.03	2.13	2.06
14	l	207	CLA	C3D-C2D	3.03	1.47	1.39
14	H	823	CLA	C3D-C2D	3.03	1.47	1.39
14	F	1303	CLA	C3D-C2D	3.03	1.47	1.39
14	b	834	CLA	MG-NC	3.03	2.13	2.06
14	B	838	CLA	C1D-ND	-3.03	1.33	1.37
14	H	833	CLA	C1D-ND	-3.03	1.33	1.37
14	G	833	CLA	C3D-C2D	3.03	1.47	1.39
14	A	833	CLA	C1D-ND	-3.03	1.33	1.37
13	a	801	CL0	C3D-C2D	3.03	1.47	1.39
14	B	810	CLA	MG-NC	3.03	2.13	2.06
14	H	832	CLA	MG-NC	3.03	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	805	CLA	C1D-ND	-3.03	1.33	1.37
14	A	816	CLA	MG-NC	3.03	2.13	2.06
14	B	814	CLA	C1D-ND	-3.03	1.33	1.37
14	G	822	CLA	C1D-ND	-3.03	1.33	1.37
14	G	828	CLA	OBD-CAD	3.02	1.27	1.22
14	H	818	CLA	MG-NC	3.02	2.13	2.06
14	B	812	CLA	C3D-C2D	3.02	1.47	1.39
14	a	815	CLA	C4D-CHA	3.02	1.48	1.38
14	A	819	CLA	MG-NC	3.02	2.13	2.06
14	A	813	CLA	C3D-C2D	3.02	1.47	1.39
14	G	806	CLA	C3D-C2D	3.02	1.47	1.39
14	G	814	CLA	C3D-C2D	3.02	1.47	1.39
14	G	829	CLA	C3D-C2D	3.02	1.47	1.39
14	a	836	CLA	C3D-C2D	3.02	1.47	1.39
14	B	819	CLA	MG-NC	3.02	2.13	2.06
14	b	834	CLA	C4D-CHA	3.02	1.48	1.38
14	A	840	CLA	C3D-C2D	3.02	1.47	1.39
14	A	815	CLA	C3D-C2D	3.02	1.47	1.39
14	b	821	CLA	C4D-CHA	3.02	1.48	1.38
14	A	831	CLA	C1C-NC	-3.02	1.33	1.37
14	B	812	CLA	C1C-NC	-3.02	1.33	1.37
14	Q	203	CLA	C4D-CHA	3.02	1.48	1.38
14	a	840	CLA	C1D-ND	-3.02	1.33	1.37
14	j	101	CLA	C4D-CHA	3.02	1.48	1.38
14	a	855	CLA	MG-NC	3.02	2.13	2.06
14	B	819	CLA	C3D-C2D	3.02	1.47	1.39
14	b	820	CLA	C3D-C2D	3.02	1.47	1.39
14	B	807	CLA	MG-ND	-3.02	1.99	2.05
13	G	801	CL0	C3D-C2D	3.02	1.47	1.39
14	B	837	CLA	C3D-C2D	3.02	1.47	1.39
14	H	821	CLA	MG-ND	-3.02	1.99	2.05
14	U	205	CLA	C3D-C2D	3.01	1.47	1.39
14	A	842	CLA	C3D-C2D	3.01	1.47	1.39
14	A	837	CLA	C4D-CHA	3.01	1.48	1.38
14	G	809	CLA	C1D-ND	-3.01	1.33	1.37
14	H	814	CLA	C4D-CHA	3.01	1.48	1.38
14	A	837	CLA	MG-NC	3.01	2.13	2.06
14	H	829	CLA	MG-NC	3.01	2.13	2.06
13	A	801	CL0	C3D-C2D	3.01	1.47	1.39
14	U	201	CLA	MG-ND	-3.01	1.99	2.05
14	B	834	CLA	MG-NC	3.01	2.13	2.06
14	a	803	CLA	MG-NC	3.01	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	833	CLA	C1D-ND	-3.01	1.33	1.37
14	G	841	CLA	C1D-ND	-3.01	1.33	1.37
14	G	825	CLA	C1D-ND	-3.01	1.33	1.37
14	B	835	CLA	C3D-C2D	3.01	1.47	1.39
14	A	804	CLA	MG-ND	-3.01	1.99	2.05
14	a	837	CLA	MG-ND	-3.01	1.99	2.05
14	G	814	CLA	MG-NC	3.01	2.13	2.06
14	A	836	CLA	C3D-C2D	3.01	1.47	1.39
14	H	804	CLA	MG-NC	3.01	2.13	2.06
14	A	830	CLA	C3D-C2D	3.01	1.47	1.39
14	H	816	CLA	C1D-ND	-3.01	1.33	1.37
14	A	817	CLA	MG-NC	3.01	2.13	2.06
14	a	816	CLA	C4D-CHA	3.01	1.48	1.38
14	H	838	CLA	C1C-NC	-3.01	1.33	1.37
14	A	843	CLA	MG-ND	-3.00	1.99	2.05
14	B	807	CLA	C3D-C2D	3.00	1.47	1.39
14	a	804	CLA	MG-NC	3.00	2.13	2.06
14	b	826	CLA	C3D-C2D	3.00	1.47	1.39
14	b	838	CLA	OBD-CAD	3.00	1.27	1.22
14	G	815	CLA	MG-NC	3.00	2.13	2.06
14	B	830	CLA	MG-NC	3.00	2.13	2.06
14	F	1301	CLA	C4D-CHA	3.00	1.48	1.38
14	A	834	CLA	C3D-C2D	3.00	1.47	1.39
14	A	815	CLA	MG-NC	3.00	2.13	2.06
14	B	820	CLA	C3D-C2D	3.00	1.47	1.39
14	K	101	CLA	MG-NC	3.00	2.13	2.06
14	Q	203	CLA	MG-NC	3.00	2.13	2.06
14	G	813	CLA	C3D-C2D	3.00	1.47	1.39
14	H	815	CLA	C1D-ND	-3.00	1.33	1.37
14	L	206	CLA	MG-NC	3.00	2.13	2.06
14	G	821	CLA	MG-ND	-3.00	1.99	2.05
14	a	809	CLA	C1D-ND	-3.00	1.33	1.37
14	a	839	CLA	C1D-ND	-3.00	1.33	1.37
14	B	817	CLA	MG-ND	-3.00	1.99	2.05
14	b	819	CLA	MG-ND	-3.00	1.99	2.05
14	G	834	CLA	MG-NC	3.00	2.13	2.06
14	A	828	CLA	CHD-C4C	3.00	1.46	1.39
14	a	812	CLA	C1D-ND	-3.00	1.33	1.37
14	B	824	CLA	C4D-CHA	3.00	1.48	1.38
14	B	840	CLA	C3D-C2D	3.00	1.47	1.39
14	b	816	CLA	C3D-C2D	3.00	1.47	1.39
14	G	840	CLA	C1D-ND	-3.00	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	810	CLA	C3D-C2D	3.00	1.47	1.39
14	b	812	CLA	C3D-C2D	3.00	1.47	1.39
14	G	803	CLA	C3D-C2D	3.00	1.47	1.39
14	H	826	CLA	C3D-C2D	3.00	1.47	1.39
14	L	204	CLA	C3D-C2D	2.99	1.47	1.39
14	b	811	CLA	C3D-C2D	2.99	1.47	1.39
14	U	204	CLA	C3D-C2D	2.99	1.47	1.39
14	H	821	CLA	C4D-CHA	2.99	1.48	1.38
14	A	826	CLA	MG-ND	-2.99	1.99	2.05
14	F	1301	CLA	MG-NC	2.99	2.13	2.06
14	a	833	CLA	MG-NC	2.99	2.13	2.06
14	b	805	CLA	C3D-C2D	2.99	1.47	1.39
14	H	825	CLA	C1C-NC	-2.99	1.33	1.37
14	b	806	CLA	OBD-CAD	2.99	1.27	1.22
14	b	826	CLA	MG-NC	2.99	2.13	2.06
14	b	830	CLA	C3D-C2D	2.99	1.47	1.39
14	a	827	CLA	MG-ND	-2.99	1.99	2.05
14	b	838	CLA	C1D-ND	-2.99	1.33	1.37
14	B	829	CLA	MG-NC	2.99	2.13	2.06
14	G	805	CLA	C4D-CHA	2.99	1.48	1.38
14	H	825	CLA	C1D-ND	-2.99	1.33	1.37
14	H	830	CLA	MG-NC	2.99	2.13	2.06
14	G	817	CLA	C3D-C2D	2.99	1.47	1.39
14	G	816	CLA	MG-ND	-2.99	1.99	2.05
14	G	821	CLA	MG-NC	2.99	2.13	2.06
14	a	813	CLA	C3D-C2D	2.99	1.47	1.39
14	a	844	CLA	C3D-C2D	2.99	1.47	1.39
14	G	830	CLA	C3D-C2D	2.99	1.47	1.39
14	W	1701	CLA	C4D-CHA	2.99	1.48	1.38
14	G	804	CLA	MG-NC	2.99	2.13	2.06
14	a	820	CLA	MG-NC	2.99	2.13	2.06
14	H	838	CLA	C3D-C2D	2.99	1.47	1.39
14	A	815	CLA	C4D-CHA	2.99	1.48	1.38
14	l	202	CLA	MG-ND	-2.98	1.99	2.05
14	G	826	CLA	C3D-C2D	2.98	1.47	1.39
14	G	825	CLA	C3D-C2D	2.98	1.47	1.39
14	b	811	CLA	MG-NC	2.98	2.13	2.06
14	a	838	CLA	C3D-C2D	2.98	1.47	1.39
14	G	842	CLA	MG-NC	2.98	2.13	2.06
14	M	1601	CLA	C4D-CHA	2.98	1.48	1.38
14	b	838	CLA	MG-NC	2.98	2.13	2.06
14	a	816	CLA	C3D-C2D	2.98	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	831	CLA	MG-NC	2.98	2.13	2.06
14	B	829	CLA	C3D-C2D	2.98	1.47	1.39
14	G	816	CLA	C3D-C2D	2.98	1.47	1.39
14	X	1701	CLA	C3D-C2D	2.98	1.47	1.39
14	b	814	CLA	C4D-CHA	2.98	1.48	1.38
14	G	824	CLA	MG-NC	2.98	2.13	2.06
14	a	821	CLA	C3D-C2D	2.98	1.47	1.39
14	a	829	CLA	C4D-CHA	2.98	1.48	1.38
14	A	805	CLA	MG-NC	2.98	2.13	2.06
14	A	841	CLA	MG-ND	-2.98	1.99	2.05
14	a	819	CLA	MG-ND	-2.98	1.99	2.05
14	A	807	CLA	C1D-ND	-2.98	1.34	1.37
14	A	829	CLA	C3D-C2D	2.98	1.47	1.39
14	A	821	CLA	MG-NC	2.97	2.13	2.06
14	G	811	CLA	MG-NC	2.97	2.13	2.06
14	B	833	CLA	C1D-ND	-2.97	1.34	1.37
14	b	804	CLA	C3D-C2D	2.97	1.47	1.39
14	B	834	CLA	C4D-CHA	2.97	1.48	1.38
14	B	814	CLA	C4D-CHA	2.97	1.48	1.38
14	H	834	CLA	C4D-CHA	2.97	1.48	1.38
14	A	814	CLA	MG-NC	2.97	2.13	2.06
14	H	829	CLA	C3B-C2B	2.97	1.44	1.40
14	G	825	CLA	MG-NC	2.97	2.13	2.06
14	X	1701	CLA	C4D-CHA	2.97	1.48	1.38
14	B	811	CLA	C1D-ND	-2.97	1.34	1.37
14	a	817	CLA	C1D-ND	-2.97	1.34	1.37
14	B	814	CLA	MG-NC	2.97	2.13	2.06
14	H	824	CLA	C4D-CHA	2.97	1.48	1.38
14	b	823	CLA	C1C-NC	-2.97	1.33	1.37
14	a	838	CLA	C1D-ND	-2.97	1.34	1.37
14	H	836	CLA	MG-NC	2.97	2.13	2.06
14	a	823	CLA	MG-NC	2.97	2.13	2.06
14	b	831	CLA	C3D-C2D	2.97	1.47	1.39
14	A	828	CLA	C1D-ND	-2.97	1.34	1.37
14	H	817	CLA	MG-ND	-2.97	1.99	2.05
14	F	1303	CLA	MG-NC	2.97	2.13	2.06
14	A	837	CLA	C1D-ND	-2.97	1.34	1.37
14	G	820	CLA	C4D-CHA	2.97	1.48	1.38
14	A	830	CLA	MG-NC	2.97	2.13	2.06
14	a	828	CLA	C3D-C2D	2.97	1.47	1.39
14	a	804	CLA	C1D-ND	-2.97	1.34	1.37
14	a	821	CLA	C1D-ND	-2.97	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	825	CLA	OBD-CAD	2.97	1.27	1.22
14	G	808	CLA	MG-NC	2.97	2.13	2.06
14	B	811	CLA	C3D-C2D	2.97	1.47	1.39
14	G	836	CLA	MG-ND	-2.97	1.99	2.05
14	b	814	CLA	MG-ND	-2.97	1.99	2.05
14	a	807	CLA	C3D-C2D	2.97	1.47	1.39
14	b	835	CLA	C3D-C2D	2.97	1.47	1.39
14	a	827	CLA	C4D-CHA	2.97	1.48	1.38
14	Q	203	CLA	C1D-ND	-2.96	1.34	1.37
14	B	820	CLA	C4D-CHA	2.96	1.48	1.38
14	H	814	CLA	C3D-C2D	2.96	1.47	1.39
14	a	803	CLA	C3D-C2D	2.96	1.47	1.39
14	A	811	CLA	C1D-ND	-2.96	1.34	1.37
14	H	830	CLA	C1D-ND	-2.96	1.34	1.37
14	K	102	CLA	C1D-ND	-2.96	1.34	1.37
14	a	842	CLA	C1D-ND	-2.96	1.34	1.37
14	H	824	CLA	MG-NC	2.96	2.13	2.06
14	b	828	CLA	C1C-NC	-2.96	1.33	1.37
14	a	804	CLA	C4D-CHA	2.96	1.48	1.38
14	b	816	CLA	C1D-ND	-2.96	1.34	1.37
14	a	833	CLA	C3D-C2D	2.96	1.47	1.39
14	A	838	CLA	MG-NC	2.96	2.13	2.06
14	G	822	CLA	C3D-C2D	2.96	1.47	1.39
14	b	829	CLA	MG-NC	2.96	2.13	2.06
14	A	841	CLA	C3D-C2D	2.96	1.47	1.39
14	a	812	CLA	C4D-CHA	2.96	1.48	1.38
14	a	855	CLA	C4D-CHA	2.96	1.48	1.38
14	H	817	CLA	C4D-CHA	2.96	1.48	1.38
14	j	101	CLA	C3D-C2D	2.96	1.47	1.39
14	A	843	CLA	MG-NC	2.96	2.13	2.06
14	G	823	CLA	C3D-C2D	2.96	1.47	1.39
14	H	832	CLA	C4D-CHA	2.96	1.48	1.38
14	a	821	CLA	MG-NC	2.96	2.13	2.06
14	A	836	CLA	C4D-CHA	2.96	1.48	1.38
14	B	809	CLA	C1C-NC	-2.96	1.33	1.37
14	b	814	CLA	C1D-ND	-2.96	1.34	1.37
14	G	837	CLA	C4D-CHA	2.96	1.48	1.38
14	b	834	CLA	C4C-C3C	2.96	1.50	1.45
14	B	815	CLA	MG-NC	2.96	2.13	2.06
14	A	811	CLA	C3D-C2D	2.96	1.47	1.39
14	G	805	CLA	C3D-C2D	2.96	1.47	1.39
14	a	842	CLA	MG-NC	2.95	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	822	CLA	C1D-ND	-2.95	1.34	1.37
14	H	825	CLA	C4D-CHA	2.95	1.48	1.38
14	A	844	CLA	C1C-NC	-2.95	1.33	1.37
14	B	811	CLA	MG-NC	2.95	2.13	2.06
14	V	1601	CLA	C1D-ND	-2.95	1.34	1.37
14	B	805	CLA	C3D-C2D	2.95	1.47	1.39
14	b	824	CLA	C4D-CHA	2.95	1.48	1.38
14	A	808	CLA	C3D-C2D	2.95	1.47	1.39
14	H	807	CLA	C3D-C2D	2.95	1.47	1.39
14	b	824	CLA	MG-NC	2.95	2.13	2.06
14	H	834	CLA	C3D-C2D	2.95	1.47	1.39
14	G	818	CLA	C1D-ND	-2.95	1.34	1.37
14	a	806	CLA	C1D-ND	-2.95	1.34	1.37
14	A	804	CLA	MG-NC	2.95	2.13	2.06
14	b	840	CLA	C4D-CHA	2.95	1.48	1.38
14	A	817	CLA	C3D-C2D	2.95	1.47	1.39
14	A	821	CLA	C4D-CHA	2.95	1.48	1.38
14	A	832	CLA	C3D-C2D	2.95	1.47	1.39
14	B	825	CLA	MG-NC	2.95	2.13	2.06
14	A	805	CLA	C1D-ND	-2.95	1.34	1.37
14	a	824	CLA	C3D-C2D	2.95	1.47	1.39
14	B	840	CLA	C4D-CHA	2.95	1.48	1.38
14	b	825	CLA	C4D-CHA	2.95	1.48	1.38
14	G	834	CLA	C3D-C2D	2.95	1.47	1.39
14	x	1701	CLA	C3D-C2D	2.95	1.47	1.39
14	B	826	CLA	MG-NC	2.95	2.13	2.06
14	H	815	CLA	C3D-C2D	2.95	1.47	1.39
14	G	804	CLA	C3D-C2D	2.95	1.47	1.39
14	J	101	CLA	C4D-CHA	2.95	1.48	1.38
14	a	825	CLA	C3D-C2D	2.95	1.47	1.39
14	a	839	CLA	MG-NC	2.95	2.13	2.06
14	b	801	CLA	MG-ND	-2.94	1.99	2.05
14	G	819	CLA	MG-NC	2.94	2.13	2.06
14	B	809	CLA	C3D-C2D	2.94	1.47	1.39
14	L	201	CLA	MG-ND	-2.94	2.00	2.05
14	G	838	CLA	MG-NC	2.94	2.13	2.06
14	a	832	CLA	MG-NC	2.94	2.13	2.06
14	G	807	CLA	C1D-ND	-2.94	1.34	1.37
14	S	102	CLA	C1D-ND	-2.94	1.34	1.37
14	a	816	CLA	MG-NC	2.94	2.13	2.06
14	H	813	CLA	MG-ND	-2.94	2.00	2.05
14	G	818	CLA	MG-NC	2.94	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	832	CLA	C1D-ND	-2.94	1.34	1.37
14	U	201	CLA	C4D-CHA	2.94	1.48	1.38
14	a	813	CLA	C4D-CHA	2.94	1.48	1.38
13	G	801	CL0	MG-NC	2.94	2.13	2.06
14	B	804	CLA	MG-NC	2.94	2.13	2.06
14	G	805	CLA	C1D-ND	-2.94	1.34	1.37
14	a	810	CLA	MG-NC	2.94	2.13	2.06
14	b	834	CLA	CHD-C1D	2.94	1.44	1.38
14	G	836	CLA	C4D-CHA	2.94	1.48	1.38
14	B	832	CLA	MG-NC	2.94	2.13	2.06
14	A	826	CLA	C4D-CHA	2.94	1.48	1.38
14	m	1601	CLA	MG-ND	-2.94	2.00	2.05
14	G	808	CLA	C1D-ND	-2.94	1.34	1.37
14	G	811	CLA	C1D-ND	-2.94	1.34	1.37
14	b	833	CLA	C1D-ND	-2.94	1.34	1.37
14	l	202	CLA	C1D-ND	-2.94	1.34	1.37
14	G	813	CLA	C4D-CHA	2.94	1.48	1.38
14	A	839	CLA	MG-NC	2.94	2.13	2.06
14	b	820	CLA	C4D-CHA	2.94	1.48	1.38
14	A	805	CLA	C4D-CHA	2.94	1.48	1.38
14	b	827	CLA	MG-NC	2.94	2.13	2.06
14	B	804	CLA	C4D-CHA	2.94	1.48	1.38
14	a	814	CLA	C4D-CHA	2.94	1.48	1.38
14	A	813	CLA	MG-ND	-2.94	2.00	2.05
14	H	812	CLA	C1C-NC	-2.94	1.33	1.37
14	H	833	CLA	C3D-C2D	2.93	1.47	1.39
14	G	838	CLA	C1D-ND	-2.93	1.34	1.37
14	a	836	CLA	C1D-ND	-2.93	1.34	1.37
14	b	811	CLA	C1D-ND	-2.93	1.34	1.37
14	B	816	CLA	C3D-C2D	2.93	1.47	1.39
14	B	830	CLA	MG-ND	-2.93	2.00	2.05
14	l	206	CLA	C3D-C2D	2.93	1.47	1.39
14	A	834	CLA	MG-NC	2.93	2.13	2.06
14	B	804	CLA	C3D-C2D	2.93	1.47	1.39
14	b	816	CLA	MG-NC	2.93	2.13	2.06
14	A	840	CLA	MG-NC	2.93	2.13	2.06
14	A	817	CLA	C4D-CHA	2.93	1.48	1.38
14	a	818	CLA	MG-NC	2.93	2.13	2.06
14	a	844	CLA	C4D-CHA	2.93	1.48	1.38
14	a	821	CLA	MG-ND	-2.93	2.00	2.05
14	b	821	CLA	C1D-ND	-2.93	1.34	1.37
14	G	805	CLA	MG-NC	2.93	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	826	CLA	C4D-CHA	2.93	1.48	1.38
14	H	812	CLA	C4D-CHA	2.93	1.48	1.38
14	A	823	CLA	MG-NC	2.93	2.13	2.06
14	A	816	CLA	MG-ND	-2.93	2.00	2.05
14	A	828	CLA	C4D-CHA	2.93	1.48	1.38
14	a	805	CLA	C3D-C2D	2.93	1.47	1.39
14	a	830	CLA	C4D-CHA	2.93	1.48	1.38
14	b	805	CLA	MG-NC	2.93	2.13	2.06
14	B	831	CLA	C3D-C2D	2.93	1.47	1.39
14	a	826	CLA	C3D-C2D	2.93	1.47	1.39
14	b	812	CLA	MG-NC	2.93	2.13	2.06
14	L	205	CLA	MG-ND	-2.93	2.00	2.05
14	H	804	CLA	C4D-CHA	2.92	1.48	1.38
14	B	815	CLA	C3D-C2D	2.92	1.47	1.39
14	a	817	CLA	C3D-C2D	2.92	1.47	1.39
14	H	820	CLA	C4D-CHA	2.92	1.48	1.38
14	b	840	CLA	MG-ND	-2.92	2.00	2.05
14	G	808	CLA	C3D-C2D	2.92	1.47	1.39
14	A	835	CLA	C4D-CHA	2.92	1.48	1.38
14	G	830	CLA	C4D-CHA	2.92	1.48	1.38
14	j	102	CLA	OBD-CAD	2.92	1.29	1.23
14	l	205	CLA	MG-ND	-2.92	2.00	2.05
14	b	810	CLA	C1D-ND	-2.92	1.34	1.37
14	H	823	CLA	MG-NC	2.92	2.13	2.06
14	B	819	CLA	C4D-CHA	2.92	1.48	1.38
14	A	803	CLA	MG-NC	2.92	2.13	2.06
14	a	813	CLA	MG-NC	2.92	2.13	2.06
14	a	837	CLA	C4D-CHA	2.92	1.48	1.38
14	H	831	CLA	C3D-C2D	2.92	1.47	1.39
14	G	831	CLA	C1C-NC	-2.92	1.33	1.37
14	b	830	CLA	MG-NC	2.92	2.13	2.06
14	A	816	CLA	C3D-C2D	2.92	1.47	1.39
14	a	806	CLA	C3D-C2D	2.92	1.47	1.39
14	H	806	CLA	C4D-CHA	2.92	1.48	1.38
14	H	832	CLA	C3D-C2D	2.92	1.47	1.39
14	a	819	CLA	C4D-CHA	2.92	1.48	1.38
14	G	817	CLA	C4D-CHA	2.92	1.48	1.38
14	H	810	CLA	C3D-C2D	2.92	1.46	1.39
14	A	841	CLA	C4D-CHA	2.92	1.48	1.38
14	b	812	CLA	C4D-CHA	2.92	1.48	1.38
14	A	816	CLA	C4D-CHA	2.92	1.48	1.38
14	A	827	CLA	C3D-C2D	2.92	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	832	CLA	MG-NC	2.92	2.13	2.06
14	B	831	CLA	MG-NC	2.92	2.13	2.06
14	L	205	CLA	C3D-C2D	2.92	1.46	1.39
14	b	817	CLA	C4D-CHA	2.92	1.48	1.38
14	A	809	CLA	C1D-ND	-2.92	1.34	1.37
14	A	814	CLA	C1D-ND	-2.92	1.34	1.37
14	M	1601	CLA	MG-ND	-2.92	2.00	2.05
14	G	839	CLA	C4D-CHA	2.92	1.48	1.38
14	H	818	CLA	C3D-C2D	2.91	1.46	1.39
14	i	101	CLA	MG-NC	2.91	2.13	2.06
14	b	839	CLA	MG-ND	-2.91	2.00	2.05
14	a	829	CLA	C3D-C2D	2.91	1.46	1.39
14	G	835	CLA	C4D-CHA	2.91	1.48	1.38
14	L	206	CLA	C4D-CHA	2.91	1.48	1.38
14	G	830	CLA	MG-NC	2.91	2.13	2.06
14	B	834	CLA	C3D-C2D	2.91	1.46	1.39
14	B	801	CLA	C4D-CHA	2.91	1.48	1.38
14	G	815	CLA	C4D-CHA	2.91	1.48	1.38
14	B	838	CLA	C3D-C2D	2.91	1.46	1.39
14	a	840	CLA	C4D-CHA	2.91	1.48	1.38
14	G	842	CLA	C3D-C2D	2.91	1.46	1.39
14	A	814	CLA	C4D-CHA	2.91	1.48	1.38
14	B	823	CLA	MG-NC	2.91	2.13	2.06
14	A	830	CLA	C4D-CHA	2.91	1.48	1.38
14	A	810	CLA	MG-ND	-2.91	2.00	2.05
14	Q	201	CLA	MG-NC	2.91	2.13	2.06
14	A	838	CLA	MG-ND	-2.91	2.00	2.05
14	G	823	CLA	C4D-CHA	2.91	1.48	1.38
14	G	825	CLA	MG-ND	-2.91	2.00	2.05
14	b	838	CLA	MG-ND	-2.91	2.00	2.05
14	H	835	CLA	MG-ND	-2.91	2.00	2.05
14	V	1601	CLA	MG-ND	-2.91	2.00	2.05
14	A	838	CLA	C3D-C2D	2.91	1.46	1.39
14	b	819	CLA	C4D-CHA	2.91	1.48	1.38
14	H	812	CLA	MG-ND	-2.91	2.00	2.05
14	G	840	CLA	MG-NC	2.91	2.13	2.06
14	B	832	CLA	C3D-C2D	2.91	1.46	1.39
14	a	832	CLA	C1D-ND	-2.91	1.34	1.37
14	a	836	CLA	C4D-CHA	2.91	1.48	1.38
14	a	820	CLA	C4D-CHA	2.91	1.48	1.38
14	A	834	CLA	MG-ND	-2.91	2.00	2.05
14	B	839	CLA	MG-ND	-2.91	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	826	CLA	MG-NC	2.91	2.13	2.06
14	a	834	CLA	C4D-CHA	2.91	1.48	1.38
14	G	813	CLA	MG-NC	2.91	2.13	2.06
14	G	815	CLA	C3D-C2D	2.91	1.46	1.39
14	J	101	CLA	C3D-C2D	2.90	1.46	1.39
14	L	201	CLA	C4D-CHA	2.90	1.48	1.38
14	G	814	CLA	MG-ND	-2.90	2.00	2.05
14	Q	201	CLA	MG-ND	-2.90	2.00	2.05
14	B	821	CLA	C4D-CHA	2.90	1.48	1.38
14	b	822	CLA	MG-NC	2.90	2.13	2.06
14	G	825	CLA	C4D-CHA	2.90	1.48	1.38
14	a	824	CLA	MG-NC	2.90	2.13	2.06
14	F	1301	CLA	C1C-NC	-2.90	1.33	1.37
14	G	838	CLA	C3D-C2D	2.90	1.46	1.39
14	H	811	CLA	MG-ND	-2.90	2.00	2.05
14	M	1601	CLA	C1D-ND	-2.90	1.34	1.37
14	l	202	CLA	C4D-CHA	2.90	1.48	1.38
14	a	823	CLA	C3D-C2D	2.90	1.46	1.39
14	b	822	CLA	C4D-CHA	2.90	1.48	1.38
14	A	812	CLA	C4D-CHA	2.90	1.48	1.38
14	B	821	CLA	MG-ND	-2.90	2.00	2.05
14	G	819	CLA	C3D-C2D	2.90	1.46	1.39
14	a	814	CLA	C3D-C2D	2.90	1.46	1.39
14	G	845	CLA	C1C-NC	-2.90	1.33	1.37
14	b	815	CLA	C3D-C2D	2.90	1.46	1.39
14	A	845	CLA	C3D-C2D	2.90	1.46	1.39
14	G	821	CLA	C4D-CHA	2.90	1.48	1.38
14	G	809	CLA	C3D-C2D	2.90	1.46	1.39
14	a	837	CLA	C3D-C2D	2.90	1.46	1.39
14	G	814	CLA	C1D-ND	-2.90	1.34	1.37
14	H	819	CLA	C4D-CHA	2.90	1.48	1.38
14	a	835	CLA	MG-ND	-2.89	2.00	2.05
14	b	818	CLA	MG-NC	2.89	2.13	2.06
14	B	814	CLA	C3D-C2D	2.89	1.46	1.39
14	A	808	CLA	MG-NC	2.89	2.13	2.06
14	b	810	CLA	MG-NC	2.89	2.13	2.06
14	B	827	CLA	C3D-C2D	2.89	1.46	1.39
14	B	839	CLA	MG-NC	2.89	2.13	2.06
14	A	833	CLA	C4D-CHA	2.89	1.48	1.38
14	B	812	CLA	C4D-CHA	2.89	1.48	1.38
14	b	836	CLA	C4D-CHA	2.89	1.48	1.38
14	x	1701	CLA	C4D-CHA	2.89	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	814	CLA	C1C-NC	-2.89	1.33	1.37
14	G	841	CLA	C4D-CHA	2.89	1.48	1.38
14	H	830	CLA	MG-ND	-2.89	2.00	2.05
14	B	807	CLA	MG-NC	2.89	2.13	2.06
14	G	812	CLA	C4D-CHA	2.89	1.48	1.38
14	H	824	CLA	MG-ND	-2.89	2.00	2.05
14	a	803	CLA	C4D-CHA	2.89	1.48	1.38
14	H	822	CLA	MG-NC	2.89	2.13	2.06
14	A	807	CLA	C3D-C2D	2.89	1.46	1.39
14	A	816	CLA	C1D-ND	-2.89	1.34	1.37
14	Q	201	CLA	C4D-CHA	2.89	1.48	1.38
14	l	205	CLA	MG-NC	2.89	2.13	2.06
14	A	810	CLA	C4D-CHA	2.89	1.48	1.38
14	B	818	CLA	C3D-C2D	2.89	1.46	1.39
14	G	834	CLA	C4D-CHA	2.89	1.48	1.38
14	B	816	CLA	C1D-ND	-2.89	1.34	1.37
14	G	838	CLA	C4D-CHA	2.89	1.48	1.38
14	a	842	CLA	C4D-CHA	2.89	1.48	1.38
14	a	839	CLA	C3D-C2D	2.89	1.46	1.39
14	a	832	CLA	C4D-CHA	2.89	1.48	1.38
14	A	825	CLA	C1D-ND	-2.89	1.34	1.37
14	B	805	CLA	C4D-CHA	2.89	1.48	1.38
14	b	805	CLA	C4D-CHA	2.89	1.48	1.38
14	a	840	CLA	MG-ND	-2.88	2.00	2.05
14	B	820	CLA	MG-NC	2.88	2.13	2.06
14	l	205	CLA	C4D-CHA	2.88	1.48	1.38
14	B	830	CLA	C1D-ND	-2.88	1.34	1.37
14	a	810	CLA	C4D-CHA	2.88	1.48	1.38
14	a	809	CLA	MG-ND	-2.88	2.00	2.05
14	b	819	CLA	C3D-C2D	2.88	1.46	1.39
14	A	811	CLA	C4D-CHA	2.88	1.48	1.38
14	G	841	CLA	MG-NC	2.88	2.13	2.06
14	B	830	CLA	C4D-CHA	2.88	1.48	1.38
14	A	809	CLA	C3D-C2D	2.88	1.46	1.39
14	U	205	CLA	MG-NC	2.88	2.13	2.06
14	b	830	CLA	C4D-CHA	2.88	1.48	1.38
14	H	808	CLA	C1C-NC	-2.88	1.33	1.37
14	U	205	CLA	MG-ND	-2.88	2.00	2.05
14	B	818	CLA	C1D-ND	-2.88	1.34	1.37
14	b	834	CLA	C3D-C2D	2.88	1.46	1.39
14	B	838	CLA	MG-NC	2.88	2.13	2.06
14	H	840	CLA	MG-ND	-2.88	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	833	CLA	MG-ND	-2.88	2.00	2.05
14	U	204	CLA	MG-NC	2.88	2.13	2.06
14	j	101	CLA	MG-ND	-2.88	2.00	2.05
14	U	201	CLA	MG-NC	2.88	2.13	2.06
14	A	827	CLA	MG-ND	-2.88	2.00	2.05
14	a	835	CLA	MG-NC	2.88	2.13	2.06
14	G	832	CLA	C3D-C2D	2.88	1.46	1.39
14	G	813	CLA	C1D-ND	-2.88	1.34	1.37
14	A	811	CLA	MG-NC	2.88	2.13	2.06
14	B	818	CLA	MG-NC	2.88	2.13	2.06
14	a	818	CLA	C3D-C2D	2.88	1.46	1.39
14	G	843	CLA	C4D-CHA	2.88	1.48	1.38
14	A	831	CLA	C4D-CHA	2.88	1.48	1.38
14	V	1601	CLA	C4D-CHA	2.88	1.48	1.38
14	A	825	CLA	C3D-C2D	2.88	1.46	1.39
14	G	841	CLA	C3D-C2D	2.88	1.46	1.39
14	B	824	CLA	MG-ND	-2.88	2.00	2.05
14	A	813	CLA	MG-NC	2.88	2.13	2.06
14	b	832	CLA	C4D-CHA	2.88	1.48	1.38
14	A	806	CLA	C3D-C2D	2.88	1.46	1.39
14	H	814	CLA	MG-ND	-2.88	2.00	2.05
14	A	814	CLA	C1C-NC	-2.88	1.33	1.37
14	A	813	CLA	C4D-CHA	2.88	1.48	1.38
14	G	814	CLA	C4D-CHA	2.88	1.48	1.38
14	A	839	CLA	C3D-C2D	2.88	1.46	1.39
14	B	805	CLA	MG-NC	2.88	2.13	2.06
14	J	101	CLA	C1D-ND	-2.88	1.34	1.37
14	b	808	CLA	C1C-NC	-2.88	1.33	1.37
14	S	102	CLA	OBD-CAD	2.87	1.28	1.23
14	a	834	CLA	MG-ND	-2.87	2.00	2.05
13	A	801	CL0	MG-NC	2.87	2.13	2.06
14	m	1601	CLA	C3D-C2D	2.87	1.46	1.39
14	G	833	CLA	C4D-CHA	2.87	1.48	1.38
14	a	841	CLA	MG-NC	2.87	2.13	2.06
14	b	816	CLA	C4D-CHA	2.87	1.48	1.38
14	G	810	CLA	C3D-C2D	2.87	1.46	1.39
14	A	825	CLA	C4D-CHA	2.87	1.48	1.38
14	U	204	CLA	C4D-CHA	2.87	1.48	1.38
14	A	843	CLA	C3D-C2D	2.87	1.46	1.39
14	B	826	CLA	C3D-C2D	2.87	1.46	1.39
14	G	843	CLA	MG-NC	2.87	2.13	2.06
14	a	809	CLA	MG-NC	2.87	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	809	CLA	C1C-NC	-2.87	1.33	1.37
14	G	807	CLA	C3D-C2D	2.87	1.46	1.39
14	A	802	CLA	C4D-CHA	2.87	1.48	1.38
14	A	810	CLA	MG-NC	2.87	2.13	2.06
14	b	814	CLA	C3D-C2D	2.87	1.46	1.39
14	b	812	CLA	MG-ND	-2.87	2.00	2.05
14	B	836	CLA	C4D-CHA	2.87	1.48	1.38
14	X	1701	CLA	C1D-ND	-2.87	1.34	1.37
14	a	808	CLA	C1D-ND	-2.87	1.34	1.37
14	A	828	CLA	OBD-CAD	2.87	1.27	1.22
14	L	204	CLA	C4D-CHA	2.87	1.48	1.38
14	a	825	CLA	C4D-CHA	2.87	1.48	1.38
14	A	841	CLA	MG-NC	2.87	2.13	2.06
14	H	835	CLA	MG-NC	2.87	2.13	2.06
14	G	828	CLA	C4B-CHC	2.87	1.49	1.41
14	b	822	CLA	C1D-ND	-2.87	1.34	1.37
14	B	832	CLA	C4D-CHA	2.87	1.48	1.38
14	a	809	CLA	C4D-CHA	2.87	1.48	1.38
14	A	834	CLA	C4D-CHA	2.87	1.48	1.38
14	b	823	CLA	C4D-CHA	2.87	1.48	1.38
14	B	806	CLA	C1D-ND	-2.87	1.34	1.37
14	f	202	CLA	C4D-CHA	2.87	1.48	1.38
14	H	830	CLA	C4D-CHA	2.87	1.48	1.38
14	H	836	CLA	C4D-CHA	2.87	1.48	1.38
14	A	839	CLA	C4D-CHA	2.87	1.48	1.38
14	H	835	CLA	C3D-C2D	2.87	1.46	1.39
14	a	840	CLA	C3D-C2D	2.87	1.46	1.39
14	b	826	CLA	C4D-CHA	2.87	1.48	1.38
14	U	206	CLA	C1D-ND	-2.87	1.34	1.37
14	G	832	CLA	MG-NC	2.87	2.13	2.06
14	G	833	CLA	MG-ND	-2.87	2.00	2.05
14	A	845	CLA	C4D-CHA	2.87	1.48	1.38
14	B	833	CLA	C3D-C2D	2.87	1.46	1.39
14	B	808	CLA	C1C-NC	-2.87	1.33	1.37
14	m	1601	CLA	C1D-ND	-2.87	1.34	1.37
14	B	835	CLA	C4D-CHA	2.87	1.48	1.38
14	B	805	CLA	MG-ND	-2.86	2.00	2.05
14	a	822	CLA	MG-NC	2.86	2.13	2.06
14	G	813	CLA	MG-ND	-2.86	2.00	2.05
14	a	838	CLA	C4D-CHA	2.86	1.48	1.38
14	H	801	CLA	C4D-CHA	2.86	1.48	1.38
14	G	839	CLA	MG-ND	-2.86	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	809	CLA	C4D-CHA	2.86	1.48	1.38
14	a	839	CLA	C4D-CHA	2.86	1.48	1.38
14	B	813	CLA	MG-ND	-2.86	2.00	2.05
14	a	842	CLA	C3D-C2D	2.86	1.46	1.39
14	L	204	CLA	MG-NC	2.86	2.13	2.06
14	b	809	CLA	C3D-C2D	2.86	1.46	1.39
14	H	810	CLA	C1D-ND	-2.86	1.34	1.37
14	a	833	CLA	C4D-CHA	2.86	1.48	1.38
14	H	838	CLA	MG-ND	-2.86	2.00	2.05
14	H	817	CLA	MG-NC	2.86	2.13	2.06
14	b	832	CLA	C3D-C2D	2.86	1.46	1.39
14	a	818	CLA	C4D-CHA	2.86	1.48	1.38
14	B	840	CLA	MG-ND	-2.86	2.00	2.05
14	B	826	CLA	C4D-CHA	2.86	1.48	1.38
14	H	840	CLA	C4D-CHA	2.86	1.48	1.38
14	H	816	CLA	C4D-CHA	2.86	1.48	1.38
14	G	809	CLA	C4D-CHA	2.86	1.48	1.38
14	T	1401	CLA	MG-ND	-2.86	2.00	2.05
14	a	811	CLA	C1D-ND	-2.85	1.34	1.37
14	H	833	CLA	C4D-CHA	2.85	1.48	1.38
14	H	818	CLA	C4D-CHA	2.85	1.48	1.38
14	l	206	CLA	MG-ND	-2.85	2.00	2.05
14	b	825	CLA	C3D-C2D	2.85	1.46	1.39
14	a	806	CLA	C4D-CHA	2.85	1.48	1.38
14	a	820	CLA	C1D-ND	-2.85	1.34	1.37
14	B	824	CLA	MG-NC	2.85	2.13	2.06
14	B	822	CLA	C4D-CHA	2.85	1.48	1.38
14	a	824	CLA	C4D-CHA	2.85	1.48	1.38
14	L	206	CLA	MG-ND	-2.85	2.00	2.05
14	B	810	CLA	C4D-CHA	2.85	1.48	1.38
14	b	813	CLA	MG-ND	-2.85	2.00	2.05
14	x	1701	CLA	C1D-ND	-2.85	1.34	1.37
14	G	806	CLA	MG-ND	-2.85	2.00	2.05
14	H	839	CLA	MG-ND	-2.85	2.00	2.05
14	A	820	CLA	C4D-CHA	2.85	1.48	1.38
14	G	806	CLA	C4D-CHA	2.85	1.48	1.38
14	b	835	CLA	C4D-CHA	2.85	1.48	1.38
14	H	802	CLA	C3D-C2D	2.85	1.46	1.39
14	B	817	CLA	C4D-CHA	2.85	1.48	1.38
14	F	1303	CLA	OBD-CAD	2.85	1.28	1.23
14	i	101	CLA	C3D-C2D	2.85	1.46	1.39
14	H	838	CLA	MG-NC	2.85	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	840	CLA	MG-NC	2.85	2.13	2.06
14	b	803	CLA	C1C-NC	-2.85	1.33	1.37
14	G	823	CLA	MG-ND	-2.85	2.00	2.05
14	G	820	CLA	MG-NC	2.85	2.13	2.06
14	B	827	CLA	C4D-CHA	2.85	1.48	1.38
14	G	810	CLA	MG-ND	-2.85	2.00	2.05
14	f	202	CLA	C1D-ND	-2.84	1.34	1.37
14	a	802	CLA	MG-NC	2.84	2.13	2.06
14	a	839	CLA	MG-ND	-2.84	2.00	2.05
14	H	828	CLA	C1C-NC	-2.84	1.33	1.37
14	B	823	CLA	C4D-CHA	2.84	1.48	1.38
14	a	808	CLA	C3D-C2D	2.84	1.46	1.39
14	a	822	CLA	MG-ND	-2.84	2.00	2.05
14	a	827	CLA	C1D-ND	-2.84	1.34	1.37
14	A	809	CLA	C1C-NC	-2.84	1.33	1.37
14	Q	203	CLA	MG-ND	-2.84	2.00	2.05
14	G	842	CLA	C4D-CHA	2.84	1.48	1.38
14	a	841	CLA	C4D-CHA	2.84	1.48	1.38
14	B	822	CLA	MG-ND	-2.84	2.00	2.05
14	B	829	CLA	C4D-CHA	2.84	1.48	1.38
14	A	812	CLA	C3D-C2D	2.84	1.46	1.39
14	a	820	CLA	C3D-C2D	2.84	1.46	1.39
14	B	816	CLA	MG-NC	2.84	2.13	2.06
14	G	828	CLA	C4D-CHA	2.84	1.48	1.38
14	b	812	CLA	C1C-NC	-2.84	1.33	1.37
14	L	201	CLA	C1D-ND	-2.84	1.34	1.37
14	a	824	CLA	C1D-ND	-2.84	1.34	1.37
14	B	812	CLA	MG-NC	2.84	2.13	2.06
14	b	813	CLA	C3D-C2D	2.84	1.46	1.39
14	a	822	CLA	C3D-C2D	2.84	1.46	1.39
14	B	828	CLA	C1C-NC	-2.84	1.33	1.37
14	b	802	CLA	MG-NC	2.84	2.13	2.06
14	A	840	CLA	MG-ND	-2.83	2.00	2.05
14	a	826	CLA	MG-ND	-2.83	2.00	2.05
14	G	803	CLA	MG-NC	2.83	2.13	2.06
14	b	837	CLA	MG-NC	2.83	2.13	2.06
14	G	834	CLA	MG-ND	-2.83	2.00	2.05
14	G	802	CLA	C4D-CHA	2.83	1.48	1.38
14	H	822	CLA	C1C-NC	-2.83	1.33	1.37
14	b	838	CLA	C3D-C2D	2.83	1.46	1.39
14	A	836	CLA	MG-NC	2.83	2.13	2.06
14	H	811	CLA	C4D-CHA	2.83	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	837	CLA	MG-NC	2.83	2.13	2.06
14	a	841	CLA	C3D-C2D	2.83	1.46	1.39
14	A	819	CLA	C1D-ND	-2.83	1.34	1.37
14	G	831	CLA	C4D-CHA	2.83	1.48	1.38
14	H	813	CLA	MG-NC	2.83	2.13	2.06
14	b	815	CLA	MG-NC	2.83	2.13	2.06
14	G	819	CLA	MG-ND	-2.83	2.00	2.05
14	a	832	CLA	MG-ND	-2.83	2.00	2.05
14	a	844	CLA	MG-ND	-2.83	2.00	2.05
14	b	818	CLA	C1D-ND	-2.83	1.34	1.37
14	G	824	CLA	C4D-CHA	2.83	1.48	1.38
14	B	802	CLA	C3D-C2D	2.83	1.46	1.39
14	a	836	CLA	MG-NC	2.83	2.13	2.06
14	G	811	CLA	C3D-C2D	2.83	1.46	1.39
14	G	827	CLA	C4D-CHA	2.83	1.48	1.38
14	W	1701	CLA	C1D-ND	-2.83	1.34	1.37
14	G	845	CLA	C4D-CHA	2.83	1.48	1.38
14	G	822	CLA	MG-NC	2.83	2.13	2.06
14	a	833	CLA	MG-ND	-2.83	2.00	2.05
14	G	810	CLA	C4D-CHA	2.83	1.48	1.38
14	H	823	CLA	C4D-CHA	2.83	1.48	1.38
14	A	829	CLA	C4D-CHA	2.82	1.48	1.38
14	A	838	CLA	C4D-CHA	2.82	1.48	1.38
14	H	825	CLA	MG-NC	2.82	2.13	2.06
14	G	835	CLA	MG-ND	-2.82	2.00	2.05
14	H	820	CLA	MG-NC	2.82	2.13	2.06
14	A	824	CLA	C1D-ND	-2.82	1.34	1.37
14	H	810	CLA	C4D-CHA	2.82	1.48	1.38
14	H	837	CLA	MG-ND	-2.82	2.00	2.05
14	X	1701	CLA	MG-ND	-2.82	2.00	2.05
14	a	824	CLA	MG-ND	-2.82	2.00	2.05
14	a	810	CLA	MG-ND	-2.82	2.00	2.05
14	L	205	CLA	MG-NC	2.82	2.13	2.06
14	G	829	CLA	C4D-CHA	2.82	1.48	1.38
14	G	807	CLA	C4D-CHA	2.82	1.48	1.38
14	H	836	CLA	C3D-C2D	2.82	1.46	1.39
14	a	823	CLA	C4D-CHA	2.82	1.48	1.38
14	B	825	CLA	C1C-NC	-2.82	1.33	1.37
14	b	802	CLA	C4D-CHA	2.82	1.48	1.38
14	a	807	CLA	C1D-ND	-2.82	1.34	1.37
14	b	806	CLA	C4D-CHA	2.82	1.48	1.38
13	A	801	CL0	C4D-CHA	2.82	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	814	CLA	C1D-ND	-2.82	1.34	1.37
14	A	836	CLA	MG-ND	-2.82	2.00	2.05
14	a	835	CLA	C4D-CHA	2.82	1.48	1.38
14	A	804	CLA	C4D-CHA	2.82	1.48	1.38
14	b	807	CLA	C3D-C2D	2.82	1.46	1.39
14	A	807	CLA	MG-ND	-2.82	2.00	2.05
14	b	839	CLA	MG-NC	2.82	2.13	2.06
14	B	822	CLA	C1C-NC	-2.82	1.33	1.37
14	A	808	CLA	C1D-ND	-2.82	1.34	1.37
14	B	835	CLA	C1D-ND	-2.82	1.34	1.37
14	A	811	CLA	MG-ND	-2.82	2.00	2.05
14	A	821	CLA	C3D-C2D	2.82	1.46	1.39
14	A	807	CLA	C4D-CHA	2.82	1.48	1.38
14	G	812	CLA	C1D-ND	-2.82	1.34	1.37
14	A	832	CLA	C4D-CHA	2.81	1.48	1.38
14	A	818	CLA	C3D-C2D	2.81	1.46	1.39
14	H	818	CLA	C1D-ND	-2.81	1.34	1.37
14	a	844	CLA	MG-NC	2.81	2.13	2.06
14	A	823	CLA	C4D-CHA	2.81	1.48	1.38
14	b	810	CLA	C4D-CHA	2.81	1.48	1.38
14	H	822	CLA	C4D-CHA	2.81	1.48	1.38
14	K	101	CLA	OBD-CAD	2.81	1.28	1.23
14	B	805	CLA	OBD-CAD	2.81	1.27	1.22
14	U	206	CLA	C4D-CHA	2.81	1.48	1.38
14	G	845	CLA	C3D-C2D	2.81	1.46	1.39
14	B	811	CLA	C4D-CHA	2.81	1.48	1.38
14	b	833	CLA	C3D-C2D	2.81	1.46	1.39
14	G	840	CLA	C4D-CHA	2.81	1.48	1.38
14	b	824	CLA	MG-ND	-2.81	2.00	2.05
14	H	839	CLA	MG-NC	2.81	2.12	2.06
14	B	828	CLA	C4D-CHA	2.81	1.48	1.38
14	a	828	CLA	C4D-CHA	2.81	1.48	1.38
14	A	822	CLA	MG-NC	2.81	2.12	2.06
14	b	806	CLA	MG-NC	2.81	2.12	2.06
14	G	818	CLA	C4D-CHA	2.81	1.48	1.38
14	G	808	CLA	C4D-CHA	2.81	1.48	1.38
14	b	829	CLA	C1C-NC	-2.81	1.33	1.37
14	G	832	CLA	C4D-CHA	2.81	1.48	1.38
14	H	802	CLA	C4D-CHA	2.81	1.48	1.38
14	A	842	CLA	MG-ND	-2.81	2.00	2.05
14	a	805	CLA	MG-ND	-2.81	2.00	2.05
14	M	1601	CLA	C3D-C2D	2.81	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	845	CLA	C1D-ND	-2.81	1.34	1.37
14	A	804	CLA	C3D-C2D	2.81	1.46	1.39
14	A	820	CLA	MG-NC	2.81	2.12	2.06
14	G	827	CLA	MG-NC	2.81	2.12	2.06
14	H	809	CLA	MG-NC	2.81	2.12	2.06
14	G	824	CLA	C3D-C2D	2.81	1.46	1.39
14	b	813	CLA	C4D-CHA	2.81	1.48	1.38
14	A	825	CLA	MG-ND	-2.81	2.00	2.05
14	G	812	CLA	MG-ND	-2.81	2.00	2.05
14	A	835	CLA	MG-ND	-2.80	2.00	2.05
14	H	829	CLA	C4D-CHA	2.80	1.48	1.38
14	B	803	CLA	C4D-CHA	2.80	1.48	1.38
14	G	823	CLA	MG-NC	2.80	2.12	2.06
14	b	838	CLA	C1C-NC	-2.80	1.33	1.37
14	B	815	CLA	C4D-CHA	2.80	1.48	1.38
14	G	817	CLA	C1D-ND	-2.80	1.34	1.37
14	A	844	CLA	MG-NC	2.80	2.12	2.06
14	a	815	CLA	MG-ND	-2.80	2.00	2.05
14	B	818	CLA	C4D-CHA	2.80	1.48	1.38
14	l	207	CLA	MG-ND	-2.80	2.00	2.05
14	G	804	CLA	C4D-CHA	2.80	1.48	1.38
14	b	807	CLA	MG-NC	2.80	2.12	2.06
14	H	827	CLA	C4D-CHA	2.80	1.48	1.38
14	b	829	CLA	C4D-CHA	2.80	1.48	1.38
14	a	811	CLA	C4D-CHA	2.80	1.48	1.38
14	A	827	CLA	C4D-CHA	2.80	1.48	1.38
14	a	831	CLA	MG-NC	2.80	2.12	2.06
14	B	813	CLA	C1C-NC	-2.80	1.33	1.37
14	A	806	CLA	MG-ND	-2.80	2.00	2.05
14	T	1401	CLA	C4D-CHA	2.80	1.48	1.38
14	a	822	CLA	C4D-CHA	2.80	1.48	1.38
14	H	816	CLA	MG-NC	2.80	2.12	2.06
14	a	841	CLA	MG-ND	-2.80	2.00	2.05
14	H	822	CLA	MG-ND	-2.80	2.00	2.05
14	b	823	CLA	MG-NC	2.80	2.12	2.06
14	G	809	CLA	MG-NC	2.80	2.12	2.06
13	G	801	CL0	C4D-CHA	2.80	1.48	1.38
14	H	819	CLA	MG-ND	-2.80	2.00	2.05
14	b	828	CLA	C4D-CHA	2.79	1.48	1.38
14	b	818	CLA	C4D-CHA	2.79	1.48	1.38
14	f	202	CLA	MG-ND	-2.79	2.00	2.05
14	H	806	CLA	C1D-ND	-2.79	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	805	CLA	MG-ND	-2.79	2.00	2.05
14	a	844	CLA	C1C-NC	-2.79	1.33	1.37
14	B	832	CLA	MG-ND	-2.79	2.00	2.05
14	B	834	CLA	C1D-ND	-2.79	1.34	1.37
14	G	837	CLA	C1D-ND	-2.79	1.34	1.37
14	G	841	CLA	MG-ND	-2.79	2.00	2.05
14	S	101	CLA	MG-ND	-2.79	2.00	2.05
14	G	824	CLA	C1D-ND	-2.79	1.34	1.37
14	A	842	CLA	C4D-CHA	2.79	1.48	1.38
14	a	824	CLA	C1C-NC	-2.79	1.33	1.37
14	H	806	CLA	C3D-C2D	2.79	1.46	1.39
14	A	824	CLA	C4D-CHA	2.79	1.48	1.38
14	B	816	CLA	C4D-CHA	2.79	1.48	1.38
14	A	825	CLA	MG-NC	2.79	2.12	2.06
14	A	839	CLA	MG-ND	-2.79	2.00	2.05
14	L	204	CLA	MG-ND	-2.79	2.00	2.05
14	b	808	CLA	C4D-CHA	2.79	1.48	1.38
14	B	834	CLA	MG-ND	-2.79	2.00	2.05
14	a	803	CLA	MG-ND	-2.79	2.00	2.05
14	b	811	CLA	C4D-CHA	2.79	1.47	1.38
14	A	808	CLA	C4D-CHA	2.79	1.47	1.38
14	G	845	CLA	MG-ND	-2.79	2.00	2.05
14	A	842	CLA	MG-NC	2.79	2.12	2.06
14	G	817	CLA	MG-NC	2.79	2.12	2.06
14	B	815	CLA	MG-ND	-2.79	2.00	2.05
14	A	843	CLA	C4D-CHA	2.79	1.47	1.38
14	H	826	CLA	C4D-CHA	2.79	1.47	1.38
14	A	842	CLA	C4B-CHC	2.79	1.48	1.41
14	b	803	CLA	C3D-C2D	2.79	1.46	1.39
14	A	812	CLA	MG-NC	2.79	2.12	2.06
14	H	812	CLA	MG-NC	2.79	2.12	2.06
14	H	815	CLA	C4D-CHA	2.78	1.47	1.38
14	b	809	CLA	MG-NC	2.78	2.12	2.06
14	a	842	CLA	MG-ND	-2.78	2.00	2.05
14	b	829	CLA	C3D-C2D	2.78	1.46	1.39
14	G	844	CLA	C1D-ND	-2.78	1.34	1.37
14	j	102	CLA	C1D-ND	-2.78	1.34	1.37
14	A	835	CLA	C1C-NC	-2.78	1.33	1.37
14	H	814	CLA	MG-NC	2.78	2.12	2.06
14	b	835	CLA	C1D-ND	-2.78	1.34	1.37
14	G	842	CLA	MG-ND	-2.78	2.00	2.05
14	H	801	CLA	C4B-CHC	2.78	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	811	CLA	C1B-CHB	2.78	1.48	1.41
14	a	815	CLA	C1D-ND	-2.78	1.34	1.37
14	B	806	CLA	C4D-CHA	2.78	1.47	1.38
14	a	805	CLA	C4D-CHA	2.78	1.47	1.38
14	G	836	CLA	MG-NC	2.78	2.12	2.06
14	H	808	CLA	MG-NC	2.78	2.12	2.06
14	H	804	CLA	MG-ND	-2.78	2.00	2.05
14	a	821	CLA	C4D-CHA	2.78	1.47	1.38
14	b	815	CLA	C4D-CHA	2.78	1.47	1.38
14	b	833	CLA	MG-NC	2.78	2.12	2.06
14	a	806	CLA	MG-ND	-2.78	2.00	2.05
14	A	815	CLA	MG-ND	-2.78	2.00	2.05
14	B	809	CLA	C4D-CHA	2.78	1.47	1.38
14	a	808	CLA	C4D-CHA	2.78	1.47	1.38
14	a	831	CLA	C3D-C2D	2.78	1.46	1.39
14	H	833	CLA	MG-NC	2.78	2.12	2.06
14	A	832	CLA	MG-NC	2.78	2.12	2.06
14	b	813	CLA	C1C-NC	-2.78	1.33	1.37
14	a	816	CLA	C1D-ND	-2.77	1.34	1.37
14	A	830	CLA	C1C-NC	-2.77	1.33	1.37
14	B	825	CLA	C3D-C2D	2.77	1.46	1.39
14	b	839	CLA	C4D-CHA	2.77	1.47	1.38
13	a	801	CL0	C4D-CHA	2.77	1.47	1.38
14	l	207	CLA	C4D-CHA	2.77	1.47	1.38
14	H	836	CLA	C1C-NC	-2.77	1.33	1.37
14	A	844	CLA	C4D-CHA	2.77	1.47	1.38
14	A	831	CLA	MG-NC	2.77	2.12	2.06
14	H	829	CLA	C3D-C2D	2.77	1.46	1.39
14	a	817	CLA	C4D-CHA	2.77	1.47	1.38
14	B	822	CLA	MG-NC	2.77	2.12	2.06
14	G	822	CLA	MG-ND	-2.77	2.00	2.05
14	b	801	CLA	C4D-CHA	2.77	1.47	1.38
14	A	819	CLA	C3D-C2D	2.77	1.46	1.39
14	b	821	CLA	MG-ND	-2.77	2.00	2.05
14	G	827	CLA	MG-ND	-2.77	2.00	2.05
14	G	838	CLA	MG-ND	-2.77	2.00	2.05
14	b	830	CLA	MG-ND	-2.77	2.00	2.05
14	a	807	CLA	MG-NC	2.77	2.12	2.06
14	G	819	CLA	C4B-CHC	2.77	1.48	1.41
14	a	809	CLA	C3D-C2D	2.77	1.46	1.39
14	a	843	CLA	OBD-CAD	2.77	1.28	1.23
14	A	822	CLA	MG-ND	-2.77	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	820	CLA	MG-ND	-2.77	2.00	2.05
14	H	828	CLA	C4D-CHA	2.77	1.47	1.38
14	H	825	CLA	C3D-C2D	2.77	1.46	1.39
14	A	840	CLA	C4D-CHA	2.77	1.47	1.38
14	B	833	CLA	C4D-CHA	2.77	1.47	1.38
14	b	832	CLA	C1C-NC	-2.77	1.33	1.37
14	A	806	CLA	C4D-CHA	2.76	1.47	1.38
14	a	838	CLA	MG-ND	-2.76	2.00	2.05
14	U	206	CLA	MG-NC	2.76	2.12	2.06
14	H	806	CLA	MG-NC	2.76	2.12	2.06
14	b	802	CLA	C1C-NC	-2.76	1.33	1.37
14	j	101	CLA	C1D-ND	-2.76	1.34	1.37
14	b	806	CLA	C3D-C2D	2.76	1.46	1.39
14	G	808	CLA	MG-ND	-2.76	2.00	2.05
14	H	832	CLA	MG-ND	-2.76	2.00	2.05
14	B	831	CLA	MG-ND	-2.76	2.00	2.05
14	b	807	CLA	C4D-CHA	2.76	1.47	1.38
14	A	819	CLA	C4D-CHA	2.76	1.47	1.38
14	a	811	CLA	MG-ND	-2.76	2.00	2.05
14	b	822	CLA	C1C-NC	-2.76	1.33	1.37
14	a	811	CLA	MG-NC	2.76	2.12	2.06
14	B	839	CLA	C4D-CHA	2.76	1.47	1.38
14	U	201	CLA	C1D-ND	-2.76	1.34	1.37
14	b	805	CLA	MG-ND	-2.76	2.00	2.05
14	A	817	CLA	C1D-ND	-2.76	1.34	1.37
14	H	805	CLA	C4D-CHA	2.76	1.47	1.38
14	b	838	CLA	C4D-CHA	2.76	1.47	1.38
14	J	101	CLA	MG-ND	-2.76	2.00	2.05
14	H	826	CLA	C1C-NC	-2.76	1.33	1.37
14	x	1701	CLA	MG-ND	-2.76	2.00	2.05
14	H	827	CLA	C3D-C2D	2.76	1.46	1.39
14	i	101	CLA	MG-ND	-2.76	2.00	2.05
14	A	812	CLA	MG-ND	-2.75	2.00	2.05
14	G	818	CLA	C3D-C2D	2.75	1.46	1.39
14	b	808	CLA	MG-NC	2.75	2.12	2.06
14	G	837	CLA	MG-ND	-2.75	2.00	2.05
14	A	803	CLA	C4D-CHA	2.75	1.47	1.38
14	H	813	CLA	C1C-NC	-2.75	1.33	1.37
14	B	809	CLA	MG-NC	2.75	2.12	2.06
14	A	818	CLA	MG-ND	-2.75	2.00	2.05
14	A	837	CLA	MG-ND	-2.75	2.00	2.05
14	G	811	CLA	MG-ND	-2.75	2.00	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	S	101	CLA	C1D-ND	-2.75	1.34	1.37
14	a	807	CLA	C4D-CHA	2.75	1.47	1.38
14	b	831	CLA	C4D-CHA	2.75	1.47	1.38
14	b	808	CLA	C3D-C2D	2.75	1.46	1.39
14	G	816	CLA	C1D-ND	-2.75	1.34	1.37
14	a	834	CLA	MG-NC	2.75	2.12	2.06
14	a	818	CLA	C1D-ND	-2.75	1.34	1.37
14	B	838	CLA	C4D-CHA	2.75	1.47	1.38
14	K	102	CLA	MG-ND	-2.75	2.00	2.05
14	A	822	CLA	C4D-CHA	2.75	1.47	1.38
14	G	818	CLA	MG-ND	-2.75	2.00	2.05
13	a	801	CL0	MG-NC	2.75	2.12	2.06
14	b	837	CLA	MG-ND	-2.75	2.00	2.05
14	a	802	CLA	C4D-CHA	2.75	1.47	1.38
14	a	817	CLA	MG-ND	-2.75	2.00	2.05
14	H	828	CLA	MG-NC	2.75	2.12	2.06
14	G	821	CLA	C3D-C2D	2.75	1.46	1.39
14	b	827	CLA	C4D-CHA	2.75	1.47	1.38
14	a	820	CLA	MG-ND	-2.74	2.00	2.05
14	H	813	CLA	C4D-CHA	2.74	1.47	1.38
14	G	822	CLA	C4D-CHA	2.74	1.47	1.38
14	k	1401	CLA	MG-ND	-2.74	2.00	2.05
14	k	1401	CLA	C4D-CHA	2.74	1.47	1.38
14	H	805	CLA	C3D-C2D	2.74	1.46	1.39
14	A	818	CLA	C4D-CHA	2.74	1.47	1.38
14	B	831	CLA	C4D-CHA	2.74	1.47	1.38
14	b	831	CLA	MG-ND	-2.74	2.00	2.05
14	A	818	CLA	MG-NC	2.74	2.12	2.06
14	F	1303	CLA	C1D-ND	-2.74	1.34	1.37
14	H	815	CLA	MG-NC	2.74	2.12	2.06
14	l	206	CLA	MG-NC	2.74	2.12	2.06
14	B	838	CLA	MG-ND	-2.74	2.00	2.05
14	B	802	CLA	C4D-CHA	2.74	1.47	1.38
14	K	102	CLA	C4D-CHA	2.74	1.47	1.38
14	b	803	CLA	MG-NC	2.73	2.12	2.06
14	a	814	CLA	MG-ND	-2.73	2.00	2.05
14	A	814	CLA	MG-ND	-2.73	2.00	2.05
14	G	807	CLA	MG-ND	-2.73	2.00	2.05
14	B	833	CLA	MG-NC	2.73	2.12	2.06
14	b	827	CLA	C1C-NC	-2.73	1.33	1.37
14	G	811	CLA	CHB-C4A	2.73	1.35	1.33
14	B	813	CLA	C4D-CHA	2.73	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	W	1701	CLA	MG-ND	-2.73	2.00	2.05
14	a	811	CLA	C1C-NC	-2.73	1.33	1.37
14	b	830	CLA	C1D-ND	-2.73	1.34	1.37
14	L	201	CLA	MG-NC	2.73	2.12	2.06
14	b	803	CLA	C4D-CHA	2.73	1.47	1.38
14	Q	201	CLA	C3D-C2D	2.73	1.46	1.39
14	a	823	CLA	MG-ND	-2.73	2.00	2.05
14	H	808	CLA	C4D-CHA	2.73	1.47	1.38
14	G	840	CLA	C1C-NC	-2.73	1.33	1.37
14	a	831	CLA	C4D-CHA	2.73	1.47	1.38
14	A	812	CLA	C1C-NC	-2.73	1.33	1.37
14	a	826	CLA	C4D-CHA	2.73	1.47	1.38
14	A	845	CLA	MG-ND	-2.72	2.00	2.05
14	G	819	CLA	C4D-CHA	2.72	1.47	1.38
14	A	821	CLA	MG-ND	-2.72	2.00	2.05
14	U	206	CLA	MG-ND	-2.72	2.00	2.05
14	a	827	CLA	C3D-C2D	2.72	1.46	1.39
14	A	809	CLA	C4D-CHA	2.72	1.47	1.38
14	b	816	CLA	MG-ND	-2.72	2.00	2.05
14	H	807	CLA	C1C-NC	-2.72	1.33	1.37
14	H	807	CLA	MG-ND	-2.72	2.00	2.05
14	a	830	CLA	MG-NC	2.72	2.12	2.06
14	l	207	CLA	MG-NC	2.72	2.12	2.06
14	b	826	CLA	C1C-NC	-2.72	1.33	1.37
14	B	813	CLA	MG-NC	2.72	2.12	2.06
14	a	810	CLA	C1D-ND	-2.72	1.34	1.37
14	b	815	CLA	MG-ND	-2.72	2.00	2.05
14	b	827	CLA	C3D-C2D	2.72	1.46	1.39
14	B	802	CLA	MG-NC	2.72	2.12	2.06
14	b	839	CLA	C3D-C2D	2.71	1.46	1.39
14	b	820	CLA	MG-NC	2.71	2.12	2.06
14	G	840	CLA	MG-ND	-2.71	2.00	2.05
14	A	827	CLA	MG-NC	2.71	2.12	2.06
14	B	814	CLA	C1C-NC	-2.71	1.33	1.37
14	H	831	CLA	C4B-CHC	2.71	1.48	1.41
14	G	812	CLA	C1C-NC	-2.71	1.33	1.37
14	G	810	CLA	MG-NC	2.71	2.12	2.06
14	B	816	CLA	C4B-CHC	2.71	1.48	1.41
14	A	815	CLA	C1C-NC	-2.71	1.33	1.37
14	b	833	CLA	C4D-CHA	2.71	1.47	1.38
14	A	842	CLA	C1C-NC	-2.71	1.33	1.37
14	H	829	CLA	C1C-NC	-2.71	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	835	CLA	MG-NC	2.71	2.12	2.06
14	b	837	CLA	C3D-C2D	2.71	1.46	1.39
14	A	826	CLA	C3D-C2D	2.71	1.46	1.39
14	B	818	CLA	MG-ND	-2.71	2.00	2.05
14	G	803	CLA	C4D-CHA	2.71	1.47	1.38
14	H	837	CLA	C3D-C2D	2.71	1.46	1.39
14	A	819	CLA	C4B-CHC	2.71	1.48	1.41
14	H	803	CLA	C4D-CHA	2.70	1.47	1.38
14	H	807	CLA	MG-NC	2.70	2.12	2.06
14	B	838	CLA	C1C-NC	-2.70	1.33	1.37
14	a	843	CLA	MG-ND	-2.70	2.00	2.05
14	H	818	CLA	MG-ND	-2.70	2.00	2.05
14	B	837	CLA	C4D-CHA	2.70	1.47	1.38
14	G	841	CLA	C1C-NC	-2.70	1.33	1.37
14	H	823	CLA	C1C-NC	-2.70	1.33	1.37
14	B	839	CLA	C3D-C2D	2.70	1.46	1.39
14	B	837	CLA	MG-ND	-2.70	2.00	2.05
14	B	826	CLA	C1C-NC	-2.70	1.33	1.37
14	B	813	CLA	C3D-C2D	2.70	1.46	1.39
14	G	844	CLA	MG-ND	-2.70	2.00	2.05
14	G	804	CLA	MG-ND	-2.70	2.00	2.05
14	H	832	CLA	C1D-ND	-2.70	1.34	1.37
14	b	837	CLA	C4D-CHA	2.70	1.47	1.38
14	a	843	CLA	C1D-ND	-2.70	1.34	1.37
14	A	815	CLA	C1D-ND	-2.70	1.34	1.37
14	B	804	CLA	MG-ND	-2.70	2.00	2.05
14	B	833	CLA	MG-ND	-2.70	2.00	2.05
14	a	813	CLA	C1C-NC	-2.70	1.33	1.37
14	H	831	CLA	C4D-CHA	2.69	1.47	1.38
14	B	808	CLA	C4D-CHA	2.69	1.47	1.38
14	b	804	CLA	C4D-CHA	2.69	1.47	1.38
14	A	806	CLA	MG-NC	2.69	2.12	2.06
14	a	807	CLA	C1D-C2D	2.69	1.50	1.45
14	G	805	CLA	MG-ND	-2.69	2.00	2.05
14	B	817	CLA	C1C-NC	-2.69	1.33	1.37
14	A	827	CLA	C1C-NC	-2.69	1.33	1.37
14	H	817	CLA	C1C-NC	-2.69	1.33	1.37
14	B	806	CLA	MG-NC	2.69	2.12	2.06
14	G	811	CLA	C4D-CHA	2.69	1.47	1.38
14	A	816	CLA	C1C-NC	-2.69	1.33	1.37
14	B	802	CLA	C1C-NC	-2.69	1.33	1.37
14	a	834	CLA	C1C-NC	-2.69	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	839	CLA	C3D-C2D	2.69	1.46	1.39
14	H	837	CLA	C4D-CHA	2.69	1.47	1.38
14	G	804	CLA	C4B-CHC	2.69	1.48	1.41
14	a	804	CLA	MG-ND	-2.69	2.00	2.05
14	b	813	CLA	MG-NC	2.68	2.12	2.06
14	G	812	CLA	MG-NC	2.68	2.12	2.06
14	G	807	CLA	MG-NC	2.68	2.12	2.06
14	H	802	CLA	MG-NC	2.68	2.12	2.06
14	H	827	CLA	C1C-NC	-2.68	1.33	1.37
14	a	808	CLA	C1C-NC	-2.68	1.33	1.37
14	a	813	CLA	MG-ND	-2.68	2.00	2.05
14	A	824	CLA	C3D-C2D	2.68	1.46	1.39
14	H	808	CLA	C3D-C2D	2.68	1.46	1.39
14	G	844	CLA	OBD-CAD	2.68	1.28	1.23
14	a	817	CLA	MG-NC	2.68	2.12	2.06
14	K	101	CLA	C1D-ND	-2.68	1.34	1.37
14	b	832	CLA	C1D-ND	-2.68	1.34	1.37
14	b	835	CLA	MG-ND	-2.68	2.00	2.05
14	A	828	CLA	C4B-CHC	2.68	1.48	1.41
14	B	806	CLA	MG-ND	-2.68	2.00	2.05
14	H	815	CLA	MG-ND	-2.68	2.00	2.05
14	B	801	CLA	C4B-CHC	2.68	1.48	1.41
14	A	824	CLA	MG-ND	-2.68	2.00	2.05
14	a	841	CLA	C1C-NC	-2.67	1.33	1.37
14	H	838	CLA	C4D-CHA	2.67	1.47	1.38
14	G	824	CLA	MG-ND	-2.67	2.00	2.05
14	a	818	CLA	C4B-CHC	2.67	1.48	1.41
14	B	810	CLA	C1D-ND	-2.67	1.34	1.37
14	B	807	CLA	C4D-CHA	2.67	1.47	1.38
14	a	819	CLA	MG-NC	2.67	2.12	2.06
14	B	827	CLA	C1C-NC	-2.67	1.33	1.37
14	l	202	CLA	MG-NC	2.67	2.12	2.06
14	b	809	CLA	C4D-CHA	2.67	1.47	1.38
14	a	826	CLA	C1C-NC	-2.67	1.33	1.37
14	H	839	CLA	C4D-CHA	2.67	1.47	1.38
14	A	818	CLA	C4B-CHC	2.67	1.48	1.41
14	a	809	CLA	C1C-NC	-2.67	1.33	1.37
14	H	805	CLA	OBD-CAD	2.66	1.27	1.22
14	A	819	CLA	MG-ND	-2.66	2.00	2.05
14	b	822	CLA	MG-ND	-2.66	2.00	2.05
14	b	816	CLA	C4B-CHC	2.66	1.48	1.41
14	H	805	CLA	MG-NC	2.66	2.12	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	812	CLA	C3D-C2D	2.66	1.46	1.39
14	A	828	CLA	MG-NC	2.66	2.12	2.06
14	b	817	CLA	MG-NC	2.66	2.12	2.06
14	A	812	CLA	C1D-ND	-2.66	1.34	1.37
14	x	1701	CLA	C4B-CHC	2.66	1.48	1.41
14	a	818	CLA	MG-ND	-2.66	2.00	2.05
14	B	811	CLA	MG-ND	-2.66	2.00	2.05
14	B	828	CLA	MG-NC	2.66	2.12	2.06
14	H	807	CLA	C4D-CHA	2.66	1.47	1.38
14	a	806	CLA	MG-NC	2.66	2.12	2.06
14	A	843	CLA	C4B-CHC	2.66	1.48	1.41
14	A	840	CLA	C4B-CHC	2.66	1.48	1.41
14	B	829	CLA	C1C-NC	-2.65	1.33	1.37
14	H	833	CLA	MG-ND	-2.65	2.00	2.05
14	j	102	CLA	MG-ND	-2.65	2.00	2.05
14	H	832	CLA	C1C-NC	-2.65	1.33	1.37
14	a	827	CLA	OBD-CAD	2.65	1.27	1.22
14	H	816	CLA	MG-ND	-2.65	2.00	2.05
14	A	835	CLA	MG-NC	2.65	2.12	2.06
14	B	806	CLA	C3D-C2D	2.65	1.46	1.39
14	U	206	CLA	C1C-NC	-2.65	1.33	1.37
14	H	831	CLA	MG-ND	-2.65	2.00	2.05
14	G	835	CLA	C1C-NC	-2.65	1.33	1.37
14	G	843	CLA	C1C-NC	-2.65	1.33	1.37
14	b	834	CLA	C1C-NC	-2.65	1.33	1.37
14	a	813	CLA	C1D-ND	-2.65	1.34	1.37
14	B	835	CLA	MG-ND	-2.65	2.00	2.05
14	b	828	CLA	MG-NC	2.64	2.12	2.06
14	H	835	CLA	C1D-C2D	2.64	1.50	1.45
14	H	839	CLA	C1C-NC	-2.64	1.33	1.37
14	a	826	CLA	MG-NC	2.64	2.12	2.06
14	a	808	CLA	C4B-CHC	2.64	1.48	1.41
14	A	811	CLA	C1C-NC	-2.64	1.33	1.37
14	a	810	CLA	C1C-NC	-2.64	1.33	1.37
14	K	101	CLA	MG-ND	-2.64	2.00	2.05
14	a	836	CLA	C4B-CHC	2.64	1.48	1.41
14	Q	201	CLA	C4B-CHC	2.64	1.48	1.41
14	b	811	CLA	C4B-CHC	2.64	1.48	1.41
14	G	809	CLA	MG-ND	-2.64	2.00	2.05
14	a	816	CLA	MG-ND	-2.64	2.00	2.05
14	V	1601	CLA	C3D-C2D	2.63	1.46	1.39
14	H	835	CLA	C4D-CHA	2.63	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	832	CLA	C1C-NC	-2.63	1.33	1.37
14	H	820	CLA	MG-ND	-2.63	2.00	2.05
14	S	102	CLA	MG-ND	-2.63	2.00	2.05
14	B	834	CLA	C1C-NC	-2.63	1.33	1.37
14	H	802	CLA	C1C-NC	-2.63	1.33	1.37
14	b	806	CLA	C1C-NC	-2.63	1.33	1.37
14	H	816	CLA	C4B-CHC	2.63	1.48	1.41
14	A	832	CLA	C1C-NC	-2.63	1.33	1.37
14	G	815	CLA	C1D-ND	-2.63	1.34	1.37
14	b	810	CLA	MG-ND	-2.63	2.00	2.05
14	a	855	CLA	C4B-CHC	2.63	1.48	1.41
14	a	802	CLA	C1C-NC	-2.63	1.33	1.37
14	a	807	CLA	C1C-NC	-2.63	1.33	1.37
14	F	1303	CLA	MG-ND	-2.63	2.00	2.05
14	b	833	CLA	MG-ND	-2.63	2.00	2.05
14	a	831	CLA	C1C-NC	-2.63	1.33	1.37
14	b	818	CLA	C1D-C2D	2.62	1.50	1.45
14	a	828	CLA	C4B-CHC	2.62	1.48	1.41
14	b	807	CLA	MG-ND	-2.62	2.00	2.05
14	A	807	CLA	C1C-NC	-2.62	1.33	1.37
14	G	810	CLA	C1C-NC	-2.62	1.33	1.37
14	A	839	CLA	C1C-NC	-2.62	1.33	1.37
14	B	823	CLA	C1C-NC	-2.62	1.33	1.37
14	A	802	CLA	MG-NC	2.62	2.12	2.06
14	a	841	CLA	C4B-CHC	2.62	1.48	1.41
14	b	825	CLA	C4B-CHC	2.62	1.48	1.41
14	b	820	CLA	MG-ND	-2.62	2.00	2.05
14	b	824	CLA	C4B-CHC	2.62	1.48	1.41
14	b	809	CLA	C1B-CHB	2.62	1.48	1.41
14	B	810	CLA	MG-ND	-2.62	2.00	2.05
14	A	828	CLA	C3D-C2D	2.62	1.46	1.39
14	A	820	CLA	C1C-NC	-2.62	1.33	1.37
14	B	816	CLA	MG-ND	-2.62	2.00	2.05
14	b	811	CLA	MG-ND	-2.62	2.00	2.05
14	G	840	CLA	C4B-CHC	2.62	1.48	1.41
14	H	811	CLA	C4B-CHC	2.62	1.48	1.41
14	b	831	CLA	C4B-CHC	2.62	1.48	1.41
14	b	817	CLA	C1C-NC	-2.62	1.33	1.37
14	H	810	CLA	C1B-CHB	2.62	1.48	1.41
14	B	811	CLA	C4B-CHC	2.61	1.48	1.41
14	a	805	CLA	MG-NC	2.61	2.12	2.06
14	G	827	CLA	C1C-NC	-2.61	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	840	CLA	MG-NC	2.61	2.12	2.06
14	A	836	CLA	C1C-NC	-2.61	1.33	1.37
14	a	808	CLA	MG-NC	2.61	2.12	2.06
14	b	839	CLA	C1C-NC	-2.61	1.33	1.37
14	W	1701	CLA	C4B-CHC	2.61	1.48	1.41
14	H	810	CLA	MG-ND	-2.61	2.00	2.05
14	H	835	CLA	C4C-C3C	2.61	1.49	1.45
14	A	824	CLA	C1D-C2D	2.61	1.50	1.45
14	a	814	CLA	C1C-NC	-2.61	1.33	1.37
14	B	817	CLA	MG-NC	2.61	2.12	2.06
14	A	822	CLA	C1C-NC	-2.60	1.33	1.37
14	S	102	CLA	C4B-CHC	2.60	1.48	1.41
14	b	804	CLA	MG-NC	2.60	2.12	2.06
14	G	820	CLA	C1C-NC	-2.60	1.33	1.37
14	b	835	CLA	C4B-CHC	2.60	1.48	1.41
14	H	813	CLA	C3D-C2D	2.60	1.46	1.39
14	A	807	CLA	MG-NC	2.60	2.12	2.06
14	G	813	CLA	C1C-NC	-2.60	1.33	1.37
14	G	825	CLA	C1C-NC	-2.60	1.33	1.37
14	l	206	CLA	C4D-CHA	2.60	1.47	1.38
14	B	840	CLA	MG-NC	2.60	2.12	2.06
14	G	831	CLA	MG-NC	2.60	2.12	2.06
14	b	818	CLA	MG-ND	-2.60	2.00	2.05
14	G	816	CLA	C1C-NC	-2.60	1.33	1.37
14	i	101	CLA	C4D-CHA	2.59	1.47	1.38
14	a	823	CLA	C1C-NC	-2.59	1.33	1.37
14	a	835	CLA	C1C-NC	-2.59	1.33	1.37
14	G	815	CLA	C1D-C2D	2.59	1.50	1.45
14	B	824	CLA	C4B-CHC	2.59	1.48	1.41
14	A	825	CLA	C1C-NC	-2.59	1.33	1.37
14	B	803	CLA	MG-NC	2.59	2.12	2.06
14	b	832	CLA	MG-ND	-2.59	2.00	2.05
14	H	814	CLA	C1C-NC	-2.59	1.33	1.37
14	a	839	CLA	C4B-CHC	2.59	1.48	1.41
14	G	808	CLA	C1C-NC	-2.59	1.33	1.37
14	H	833	CLA	C1C-NC	-2.59	1.33	1.37
14	a	815	CLA	C1C-NC	-2.59	1.33	1.37
14	B	839	CLA	C4B-CHC	2.59	1.48	1.41
14	B	807	CLA	C1C-NC	-2.59	1.33	1.37
14	B	810	CLA	C1D-C2D	2.59	1.50	1.45
14	A	808	CLA	MG-ND	-2.59	2.00	2.05
13	G	801	CL0	C1B-CHB	2.58	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	817	CLA	MG-ND	-2.58	2.00	2.05
14	B	836	CLA	C1C-NC	-2.58	1.33	1.37
14	a	839	CLA	C1C-NC	-2.58	1.33	1.37
14	H	839	CLA	C4B-CHC	2.58	1.48	1.41
14	a	807	CLA	MG-ND	-2.58	2.00	2.05
14	B	838	CLA	C4B-CHC	2.58	1.48	1.41
14	A	837	CLA	C1C-NC	-2.58	1.33	1.37
14	B	809	CLA	C1B-CHB	2.58	1.48	1.41
14	G	822	CLA	C1C-NC	-2.58	1.33	1.37
14	b	825	CLA	C1C-NC	-2.57	1.33	1.37
14	b	836	CLA	C1C-NC	-2.57	1.33	1.37
14	G	815	CLA	MG-ND	-2.57	2.00	2.05
14	A	823	CLA	C1B-CHB	2.57	1.48	1.41
14	A	841	CLA	C1C-NC	-2.57	1.33	1.37
14	A	804	CLA	C4B-CHC	2.57	1.48	1.41
14	a	803	CLA	C4B-CHC	2.57	1.48	1.41
14	b	833	CLA	C4B-CHC	2.57	1.48	1.41
14	G	809	CLA	C4B-CHC	2.57	1.48	1.41
14	A	843	CLA	C1C-NC	-2.57	1.33	1.37
14	A	821	CLA	C4B-CHC	2.57	1.48	1.41
14	a	819	CLA	C1C-NC	-2.57	1.33	1.37
14	H	810	CLA	C4B-CHC	2.57	1.48	1.41
14	G	805	CLA	C4B-CHC	2.57	1.48	1.41
14	H	819	CLA	C4B-CHC	2.56	1.48	1.41
14	a	817	CLA	C1C-NC	-2.56	1.33	1.37
14	A	845	CLA	MG-NC	2.56	2.12	2.06
14	T	1401	CLA	C4B-CHC	2.56	1.48	1.41
14	G	809	CLA	C1C-NC	-2.56	1.33	1.37
14	a	812	CLA	MG-ND	-2.56	2.00	2.05
14	a	811	CLA	C3D-C2D	2.56	1.46	1.39
14	a	836	CLA	MG-ND	-2.56	2.00	2.05
14	a	843	CLA	C4C-C3C	2.56	1.49	1.45
14	a	827	CLA	C1C-NC	-2.56	1.33	1.37
14	H	832	CLA	C1B-CHB	2.56	1.48	1.41
14	L	205	CLA	C1C-NC	-2.56	1.33	1.37
14	U	204	CLA	MG-ND	-2.56	2.00	2.05
14	A	803	CLA	C4B-CHC	2.56	1.48	1.41
14	A	840	CLA	C1C-NC	-2.56	1.33	1.37
14	G	802	CLA	C1C-NC	-2.56	1.33	1.37
14	A	817	CLA	MG-ND	-2.56	2.00	2.05
14	A	810	CLA	C1B-CHB	2.56	1.48	1.41
14	a	804	CLA	C4B-CHC	2.56	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	806	CLA	C1C-NC	-2.56	1.33	1.37
14	U	205	CLA	C1C-NC	-2.55	1.33	1.37
14	b	838	CLA	C4B-CHC	2.55	1.48	1.41
14	b	801	CLA	MG-NC	2.55	2.12	2.06
14	B	811	CLA	C1C-NC	-2.55	1.33	1.37
14	U	205	CLA	C4D-CHA	2.55	1.47	1.38
14	a	843	CLA	C1D-C2D	2.55	1.50	1.45
14	b	836	CLA	C4B-CHC	2.55	1.48	1.41
14	G	824	CLA	C1C-NC	-2.55	1.33	1.37
14	H	815	CLA	C4B-CHC	2.55	1.48	1.41
14	H	803	CLA	MG-NC	2.55	2.12	2.06
14	a	838	CLA	C1C-NC	-2.55	1.33	1.37
14	a	805	CLA	C1C-NC	-2.55	1.33	1.37
14	l	206	CLA	C1C-NC	-2.55	1.33	1.37
14	Q	203	CLA	C4B-CHC	2.55	1.48	1.41
14	G	807	CLA	C1C-NC	-2.55	1.33	1.37
14	G	811	CLA	C1C-NC	-2.55	1.33	1.37
14	a	842	CLA	C1C-NC	-2.55	1.33	1.37
14	a	817	CLA	C4B-CHC	2.54	1.48	1.41
14	b	804	CLA	C4B-CHC	2.54	1.48	1.41
14	B	815	CLA	C4B-CHC	2.54	1.48	1.41
14	B	831	CLA	C4B-CHC	2.54	1.48	1.41
14	G	828	CLA	C3D-C2D	2.54	1.45	1.39
14	A	803	CLA	C1C-NC	-2.54	1.33	1.37
14	B	839	CLA	C1C-NC	-2.54	1.33	1.37
14	F	1303	CLA	C1D-C2D	2.54	1.50	1.45
14	H	805	CLA	C4B-CHC	2.54	1.48	1.41
14	f	202	CLA	C4B-CHC	2.54	1.48	1.41
14	A	810	CLA	C1C-NC	-2.54	1.33	1.37
14	L	205	CLA	C4D-CHA	2.54	1.47	1.38
14	A	841	CLA	C4B-CHC	2.54	1.48	1.41
14	L	205	CLA	C4B-CHC	2.54	1.48	1.41
14	a	840	CLA	C4B-CHC	2.54	1.48	1.41
14	a	840	CLA	C1C-NC	-2.54	1.33	1.37
14	H	814	CLA	C1B-CHB	2.54	1.48	1.41
14	X	1701	CLA	C4B-CHC	2.54	1.48	1.41
14	A	806	CLA	C4B-CHC	2.54	1.48	1.41
14	b	839	CLA	C4B-CHC	2.54	1.48	1.41
14	B	804	CLA	C4B-CHC	2.54	1.48	1.41
14	J	101	CLA	C4B-CHC	2.54	1.48	1.41
14	H	806	CLA	MG-ND	-2.53	2.00	2.05
14	A	837	CLA	C4B-CHC	2.53	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	826	CLA	C1C-NC	-2.53	1.33	1.37
14	H	837	CLA	C1D-C2D	2.53	1.50	1.45
14	A	836	CLA	C4B-CHC	2.53	1.48	1.41
14	G	845	CLA	MG-NC	2.53	2.12	2.06
14	G	833	CLA	C4B-CHC	2.53	1.48	1.41
14	k	1401	CLA	C4B-CHC	2.53	1.48	1.41
14	G	836	CLA	C1C-NC	-2.53	1.33	1.37
14	l	205	CLA	C1C-NC	-2.53	1.33	1.37
14	b	801	CLA	C1C-NC	-2.53	1.33	1.37
14	B	806	CLA	C1B-CHB	2.53	1.48	1.41
14	a	855	CLA	C1C-NC	-2.53	1.33	1.37
14	G	827	CLA	C4B-CHC	2.53	1.48	1.41
14	H	806	CLA	C1C-NC	-2.53	1.33	1.37
14	H	834	CLA	C1C-NC	-2.52	1.33	1.37
14	a	829	CLA	C1C-NC	-2.52	1.33	1.37
14	G	803	CLA	C1C-NC	-2.52	1.33	1.37
14	G	806	CLA	MG-NC	2.52	2.12	2.06
14	S	101	CLA	C4B-CHC	2.52	1.48	1.41
14	G	839	CLA	C1C-NC	-2.52	1.33	1.37
14	A	824	CLA	C4C-C3C	2.52	1.49	1.45
14	A	823	CLA	C1C-NC	-2.52	1.33	1.37
14	b	805	CLA	C1C-NC	-2.52	1.33	1.37
14	a	810	CLA	C4C-C3C	2.52	1.49	1.45
14	A	833	CLA	C4B-CHC	2.52	1.48	1.41
14	i	101	CLA	C1B-CHB	2.52	1.48	1.41
14	a	812	CLA	C4B-CHC	2.51	1.48	1.41
14	a	828	CLA	C1C-NC	-2.51	1.33	1.37
14	G	824	CLA	C1D-C2D	2.51	1.50	1.45
14	b	801	CLA	C4B-CHC	2.51	1.48	1.41
14	G	802	CLA	MG-NC	2.51	2.12	2.06
14	b	807	CLA	C1B-CHB	2.51	1.48	1.41
14	A	806	CLA	C1C-NC	-2.51	1.33	1.37
14	G	822	CLA	C4B-CHC	2.51	1.48	1.41
14	L	206	CLA	C1C-NC	-2.51	1.33	1.37
14	G	842	CLA	C4B-CHC	2.51	1.48	1.41
14	H	809	CLA	C1B-CHB	2.51	1.48	1.41
14	H	822	CLA	C1B-CHB	2.51	1.48	1.41
14	G	815	CLA	C1C-NC	-2.51	1.33	1.37
14	a	832	CLA	C1C-NC	-2.51	1.33	1.37
14	V	1601	CLA	C1C-NC	-2.51	1.33	1.37
14	a	821	CLA	C4C-C3C	2.51	1.49	1.45
14	G	844	CLA	C1D-C2D	2.51	1.50	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	j	102	CLA	C1B-CHB	2.51	1.48	1.41
14	G	832	CLA	C1C-NC	-2.51	1.33	1.37
14	a	810	CLA	C1D-C2D	2.51	1.50	1.45
14	K	101	CLA	C4C-C3C	2.51	1.49	1.45
14	H	804	CLA	C4B-CHC	2.51	1.48	1.41
14	H	805	CLA	C1C-NC	-2.51	1.34	1.37
14	B	821	CLA	C4B-CHC	2.51	1.48	1.41
14	G	828	CLA	C1B-CHB	2.50	1.48	1.41
14	A	811	CLA	C1B-CHB	2.50	1.48	1.41
14	H	837	CLA	C4B-CHC	2.50	1.48	1.41
14	b	840	CLA	C1B-CHB	2.50	1.47	1.41
14	H	821	CLA	C4B-CHC	2.50	1.47	1.41
14	H	822	CLA	C4B-CHC	2.50	1.47	1.41
14	a	806	CLA	C1C-NC	-2.50	1.34	1.37
14	X	1701	CLA	C1C-NC	-2.50	1.34	1.37
14	B	829	CLA	C1B-CHB	2.50	1.47	1.41
14	K	101	CLA	C1D-C2D	2.50	1.50	1.45
14	G	818	CLA	C1C-NC	-2.50	1.34	1.37
14	G	821	CLA	C1B-CHB	2.50	1.47	1.41
14	a	823	CLA	C4B-CHC	2.50	1.47	1.41
14	A	809	CLA	MG-ND	-2.50	2.00	2.05
14	A	805	CLA	C4B-CHC	2.50	1.47	1.41
14	B	837	CLA	MG-NC	2.50	2.12	2.06
14	a	832	CLA	C1D-C2D	2.50	1.50	1.45
14	H	815	CLA	C1C-NC	-2.49	1.34	1.37
14	A	812	CLA	C1D-C2D	2.49	1.50	1.45
14	B	835	CLA	C1D-C2D	2.49	1.50	1.45
14	G	829	CLA	C4B-CHC	2.49	1.47	1.41
13	A	801	CL0	C1C-NC	-2.49	1.34	1.37
14	G	842	CLA	C1B-CHB	2.49	1.47	1.41
14	m	1601	CLA	C1C-NC	-2.49	1.34	1.37
14	G	842	CLA	C1C-NC	-2.49	1.34	1.37
14	x	1701	CLA	C1C-NC	-2.49	1.34	1.37
14	b	818	CLA	C4B-CHC	2.49	1.47	1.41
14	l	207	CLA	C1C-NC	-2.49	1.34	1.37
14	G	814	CLA	C4B-CHC	2.49	1.47	1.41
14	b	819	CLA	C4B-CHC	2.49	1.47	1.41
14	b	836	CLA	C1B-CHB	2.49	1.47	1.41
14	U	204	CLA	C4B-CHC	2.49	1.47	1.41
13	a	801	CL0	C1C-NC	-2.49	1.34	1.37
14	A	808	CLA	C1C-NC	-2.49	1.34	1.37
14	b	814	CLA	C1C-NC	-2.49	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	833	CLA	C4B-CHC	2.49	1.47	1.41
14	A	829	CLA	C4B-CHC	2.49	1.47	1.41
14	L	204	CLA	C1C-NC	-2.49	1.34	1.37
14	b	830	CLA	C1C-NC	-2.49	1.34	1.37
14	K	102	CLA	C4B-CHC	2.49	1.47	1.41
14	A	802	CLA	C4B-CHC	2.48	1.47	1.41
14	a	835	CLA	C4B-CHC	2.48	1.47	1.41
14	i	101	CLA	C1C-NC	-2.48	1.34	1.37
14	a	811	CLA	C1D-C2D	2.48	1.50	1.45
14	G	824	CLA	C4B-CHC	2.48	1.47	1.41
14	B	818	CLA	C4B-CHC	2.48	1.47	1.41
14	B	833	CLA	C1D-C2D	2.48	1.50	1.45
14	k	1401	CLA	C1B-CHB	2.48	1.47	1.41
14	B	806	CLA	C1C-NC	-2.48	1.34	1.37
14	B	805	CLA	C4C-C3C	2.48	1.49	1.45
14	H	827	CLA	C4B-CHC	2.48	1.47	1.41
14	B	803	CLA	C4B-CHC	2.48	1.47	1.41
14	H	825	CLA	C4B-CHC	2.48	1.47	1.41
14	B	836	CLA	C1B-CHB	2.48	1.47	1.41
14	a	844	CLA	C4B-CHC	2.48	1.47	1.41
14	H	840	CLA	MG-NC	2.48	2.12	2.06
14	A	819	CLA	C1B-CHB	2.47	1.47	1.41
14	G	833	CLA	C1C-NC	-2.47	1.34	1.37
14	H	824	CLA	C1C-NC	-2.47	1.34	1.37
14	B	813	CLA	C4B-CHC	2.47	1.47	1.41
14	f	202	CLA	C1C-NC	-2.47	1.34	1.37
14	H	807	CLA	C1B-CHB	2.47	1.47	1.41
14	U	205	CLA	C4B-CHC	2.47	1.47	1.41
13	G	801	CL0	C1C-NC	-2.47	1.34	1.37
14	G	837	CLA	C4B-CHC	2.47	1.47	1.41
14	a	838	CLA	C4B-CHC	2.47	1.47	1.41
14	a	831	CLA	C4B-CHC	2.47	1.47	1.41
14	B	810	CLA	C4B-CHC	2.47	1.47	1.41
14	a	838	CLA	C1B-CHB	2.47	1.47	1.41
14	B	827	CLA	C4B-CHC	2.47	1.47	1.41
14	G	821	CLA	C4B-CHC	2.47	1.47	1.41
14	b	815	CLA	C4B-CHC	2.47	1.47	1.41
14	B	814	CLA	C1B-CHB	2.47	1.47	1.41
14	a	827	CLA	C4B-CHC	2.47	1.47	1.41
14	G	844	CLA	C1B-CHB	2.47	1.47	1.41
14	B	819	CLA	C4B-CHC	2.47	1.47	1.41
14	j	101	CLA	C1C-NC	-2.47	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	817	CLA	C1D-C2D	2.47	1.50	1.45
14	a	821	CLA	C4B-CHC	2.47	1.47	1.41
14	a	822	CLA	C4B-CHC	2.47	1.47	1.41
14	B	831	CLA	C1C-NC	-2.47	1.34	1.37
14	G	841	CLA	C4B-CHC	2.46	1.47	1.41
14	b	810	CLA	C4B-CHC	2.46	1.47	1.41
14	A	826	CLA	C1C-NC	-2.46	1.34	1.37
14	G	829	CLA	C1C-NC	-2.46	1.34	1.37
14	b	815	CLA	C1C-NC	-2.46	1.34	1.37
14	A	823	CLA	C4B-CHC	2.46	1.47	1.41
14	G	835	CLA	C1D-C2D	2.46	1.50	1.45
14	a	821	CLA	C1D-C2D	2.46	1.50	1.45
14	G	813	CLA	C4B-CHC	2.46	1.47	1.41
14	H	833	CLA	C4B-CHC	2.46	1.47	1.41
14	A	808	CLA	C4B-CHC	2.46	1.47	1.41
14	B	834	CLA	C4B-CHC	2.46	1.47	1.41
14	G	823	CLA	C4B-CHC	2.46	1.47	1.41
14	b	824	CLA	C1C-NC	-2.46	1.34	1.37
14	b	810	CLA	C1B-CHB	2.46	1.47	1.41
14	G	808	CLA	C4B-CHC	2.46	1.47	1.41
14	B	804	CLA	C1C-NC	-2.46	1.34	1.37
14	K	102	CLA	C1B-CHB	2.46	1.47	1.41
14	B	828	CLA	C3D-C2D	2.46	1.45	1.39
14	A	824	CLA	C4B-CHC	2.46	1.47	1.41
14	B	802	CLA	C1B-CHB	2.46	1.47	1.41
14	A	813	CLA	C1C-NC	-2.45	1.34	1.37
14	b	835	CLA	C1D-C2D	2.45	1.50	1.45
14	a	836	CLA	C1C-NC	-2.45	1.34	1.37
14	b	810	CLA	C1D-C2D	2.45	1.50	1.45
14	L	206	CLA	C4B-CHC	2.45	1.47	1.41
14	X	1701	CLA	C1B-CHB	2.45	1.47	1.41
14	a	818	CLA	C1D-C2D	2.45	1.50	1.45
14	a	825	CLA	C4B-CHC	2.45	1.47	1.41
14	b	804	CLA	C4C-C3C	2.45	1.49	1.45
14	a	826	CLA	C4B-CHC	2.45	1.47	1.41
14	G	804	CLA	C1C-NC	-2.45	1.34	1.37
14	V	1601	CLA	C4B-CHC	2.45	1.47	1.41
14	A	819	CLA	C1D-C2D	2.45	1.50	1.45
14	A	837	CLA	C4C-C3C	2.45	1.49	1.45
13	A	801	CL0	C1B-CHB	2.45	1.47	1.41
14	a	820	CLA	C4B-CHC	2.45	1.47	1.41
14	a	842	CLA	C4B-CHC	2.45	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	816	CLA	C4C-C3C	2.45	1.49	1.45
14	A	814	CLA	C1D-C2D	2.45	1.50	1.45
14	B	805	CLA	C1C-NC	-2.45	1.34	1.37
14	A	822	CLA	C4B-CHC	2.45	1.47	1.41
14	H	819	CLA	C1B-CHB	2.45	1.47	1.41
14	a	825	CLA	C1C-NC	-2.45	1.34	1.37
14	A	837	CLA	C1D-C2D	2.45	1.50	1.45
14	B	801	CLA	C1C-NC	-2.44	1.34	1.37
14	G	818	CLA	C1B-CHB	2.44	1.47	1.41
14	A	833	CLA	C4C-C3C	2.44	1.49	1.45
14	H	815	CLA	C1B-CHB	2.44	1.47	1.41
14	H	818	CLA	C4B-CHC	2.44	1.47	1.41
14	M	1601	CLA	C4B-CHC	2.44	1.47	1.41
14	b	828	CLA	C3D-C2D	2.44	1.45	1.39
14	B	808	CLA	C3D-C2D	2.44	1.45	1.39
14	H	803	CLA	C4C-C3C	2.44	1.49	1.45
14	a	822	CLA	C1B-CHB	2.44	1.47	1.41
14	B	818	CLA	C1D-C2D	2.44	1.50	1.45
14	G	837	CLA	C1C-NC	-2.44	1.34	1.37
14	H	804	CLA	C1C-NC	-2.44	1.34	1.37
14	b	833	CLA	C1C-NC	-2.44	1.34	1.37
14	b	821	CLA	C1B-CHB	2.44	1.47	1.41
14	B	833	CLA	C1C-NC	-2.44	1.34	1.37
14	a	837	CLA	C4B-CHC	2.44	1.47	1.41
14	b	803	CLA	C1B-CHB	2.44	1.47	1.41
14	B	820	CLA	C1B-CHB	2.44	1.47	1.41
14	J	101	CLA	C1C-NC	-2.44	1.34	1.37
14	B	825	CLA	C4B-CHC	2.44	1.47	1.41
14	B	840	CLA	C1B-CHB	2.44	1.47	1.41
14	b	802	CLA	C1B-CHB	2.44	1.47	1.41
14	a	803	CLA	C1C-NC	-2.44	1.34	1.37
14	b	807	CLA	C4B-CHC	2.44	1.47	1.41
14	H	832	CLA	C1D-C2D	2.44	1.50	1.45
14	J	101	CLA	C1D-C2D	2.44	1.50	1.45
14	B	820	CLA	C4B-CHC	2.44	1.47	1.41
14	B	818	CLA	C1C-NC	-2.44	1.34	1.37
14	G	811	CLA	C4B-CHC	2.44	1.47	1.41
14	b	814	CLA	C1B-CHB	2.44	1.47	1.41
14	a	833	CLA	C1D-C2D	2.44	1.50	1.45
14	H	828	CLA	C3D-C2D	2.44	1.45	1.39
14	H	831	CLA	C1D-C2D	2.44	1.50	1.45
14	A	804	CLA	C1C-NC	-2.43	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	830	CLA	C1C-NC	-2.43	1.34	1.37
14	a	816	CLA	C1C-NC	-2.43	1.34	1.37
14	l	206	CLA	C4B-CHC	2.43	1.47	1.41
14	B	835	CLA	C4C-C3C	2.43	1.49	1.45
14	F	1303	CLA	C4B-CHC	2.43	1.47	1.41
14	B	832	CLA	C1B-CHB	2.43	1.47	1.41
14	b	831	CLA	C1D-C2D	2.43	1.50	1.45
14	A	829	CLA	C1C-NC	-2.43	1.34	1.37
14	F	1303	CLA	C1C-NC	-2.43	1.34	1.37
14	A	838	CLA	C1C-NC	-2.43	1.34	1.37
14	H	820	CLA	C1C-NC	-2.43	1.34	1.37
14	G	803	CLA	C4B-CHC	2.43	1.47	1.41
14	H	813	CLA	C1B-CHB	2.43	1.47	1.41
17	H	846	BCR	C30-C25	-2.43	1.50	1.53
14	b	820	CLA	C1C-NC	-2.43	1.34	1.37
14	G	839	CLA	C4C-C3C	2.43	1.49	1.45
14	B	810	CLA	C1C-NC	-2.43	1.34	1.37
14	B	808	CLA	C1B-CHB	2.43	1.47	1.41
14	H	815	CLA	C1D-C2D	2.42	1.50	1.45
14	B	807	CLA	C1B-CHB	2.42	1.47	1.41
14	H	838	CLA	C4B-CHC	2.42	1.47	1.41
14	B	820	CLA	C1C-NC	-2.42	1.34	1.37
14	A	822	CLA	C1D-C2D	2.42	1.50	1.45
14	a	821	CLA	C1C-NC	-2.42	1.34	1.37
14	a	836	CLA	C1D-C2D	2.42	1.50	1.45
14	K	101	CLA	C4B-CHC	2.42	1.47	1.41
14	b	822	CLA	C4B-CHC	2.42	1.47	1.41
14	H	808	CLA	C1B-CHB	2.42	1.47	1.41
14	a	808	CLA	MG-ND	-2.42	2.01	2.05
14	j	101	CLA	C1D-C2D	2.42	1.50	1.45
14	a	802	CLA	C4B-CHC	2.42	1.47	1.41
14	a	807	CLA	C4B-CHC	2.42	1.47	1.41
14	B	833	CLA	C4B-CHC	2.42	1.47	1.41
14	G	825	CLA	C4B-CHC	2.42	1.47	1.41
14	H	832	CLA	C4C-C3C	2.42	1.49	1.45
14	H	833	CLA	C1D-C2D	2.42	1.50	1.45
14	B	835	CLA	C1B-CHB	2.42	1.47	1.41
14	H	808	CLA	C4B-CHC	2.42	1.47	1.41
14	b	819	CLA	C1B-CHB	2.42	1.47	1.41
14	H	818	CLA	C1D-C2D	2.42	1.50	1.45
14	H	830	CLA	C1D-C2D	2.42	1.50	1.45
14	G	834	CLA	C4B-CHC	2.42	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	805	CLA	C4B-CHC	2.42	1.47	1.41
14	a	813	CLA	C4B-CHC	2.42	1.47	1.41
14	j	102	CLA	C1D-C2D	2.42	1.50	1.45
14	b	834	CLA	C1B-CHB	2.42	1.47	1.41
14	f	202	CLA	C1B-CHB	2.42	1.47	1.41
14	H	810	CLA	C1C-NC	-2.42	1.34	1.37
14	H	824	CLA	C4B-CHC	2.42	1.47	1.41
14	a	815	CLA	C4C-C3C	2.42	1.49	1.45
14	Q	201	CLA	C1C-NC	-2.42	1.34	1.37
14	G	834	CLA	C1C-NC	-2.42	1.34	1.37
14	W	1701	CLA	C1C-NC	-2.42	1.34	1.37
14	G	838	CLA	C4B-CHC	2.42	1.47	1.41
14	A	809	CLA	C4B-CHC	2.42	1.47	1.41
14	H	802	CLA	C1B-CHB	2.42	1.47	1.41
14	H	820	CLA	C1B-CHB	2.42	1.47	1.41
14	G	833	CLA	C1B-CHB	2.42	1.47	1.41
14	a	809	CLA	C4B-CHC	2.42	1.47	1.41
14	G	837	CLA	C4C-C3C	2.41	1.49	1.45
14	G	836	CLA	C4B-CHC	2.41	1.47	1.41
14	H	820	CLA	C4B-CHC	2.41	1.47	1.41
14	A	809	CLA	MG-NC	2.41	2.12	2.06
14	a	842	CLA	C1B-CHB	2.41	1.47	1.41
14	b	829	CLA	C1B-CHB	2.41	1.47	1.41
14	G	821	CLA	C1C-NC	-2.41	1.34	1.37
14	G	844	CLA	C4B-CHC	2.41	1.47	1.41
14	A	834	CLA	C4B-CHC	2.41	1.47	1.41
14	F	1301	CLA	C1B-CHB	2.41	1.47	1.41
14	T	1401	CLA	C1B-CHB	2.41	1.47	1.41
14	j	102	CLA	C4C-C3C	2.41	1.49	1.45
14	B	822	CLA	C4B-CHC	2.41	1.47	1.41
14	H	840	CLA	C1B-CHB	2.41	1.47	1.41
14	l	207	CLA	C1D-C2D	2.41	1.50	1.45
14	B	813	CLA	C1B-CHB	2.41	1.47	1.41
14	H	813	CLA	C4B-CHC	2.41	1.47	1.41
14	A	839	CLA	C1B-CHB	2.41	1.47	1.41
14	S	102	CLA	C1B-CHB	2.41	1.47	1.41
14	B	810	CLA	C4C-C3C	2.40	1.49	1.45
14	b	827	CLA	C4B-CHC	2.40	1.47	1.41
14	B	821	CLA	C1C-NC	-2.40	1.34	1.37
14	B	823	CLA	C1B-CHB	2.40	1.47	1.41
14	B	810	CLA	C1B-CHB	2.40	1.47	1.41
14	a	823	CLA	C1B-CHB	2.40	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	828	CLA	C1C-NC	-2.40	1.34	1.37
14	J	101	CLA	C4C-C3C	2.40	1.49	1.45
14	a	814	CLA	C1D-C2D	2.40	1.50	1.45
14	b	837	CLA	C4B-CHC	2.40	1.47	1.41
14	M	1601	CLA	C1B-CHB	2.40	1.47	1.41
14	l	205	CLA	C4B-CHC	2.40	1.47	1.41
14	V	1601	CLA	C1B-CHB	2.40	1.47	1.41
14	b	805	CLA	C4B-CHC	2.40	1.47	1.41
14	G	805	CLA	C1D-C2D	2.40	1.50	1.45
14	A	808	CLA	C1D-C2D	2.40	1.50	1.45
14	A	821	CLA	C1C-NC	-2.40	1.34	1.37
14	A	828	CLA	C1C-C2C	2.40	1.49	1.44
14	G	817	CLA	C1C-NC	-2.40	1.34	1.37
14	H	803	CLA	C4B-CHC	2.39	1.47	1.41
13	a	801	CL0	C1B-CHB	2.39	1.47	1.41
14	H	835	CLA	C1B-CHB	2.39	1.47	1.41
14	b	811	CLA	C1D-C2D	2.39	1.50	1.45
14	j	101	CLA	C4B-CHC	2.39	1.47	1.41
14	B	816	CLA	C1C-NC	-2.39	1.34	1.37
14	A	838	CLA	C4B-CHC	2.39	1.47	1.41
14	L	204	CLA	C4B-CHC	2.39	1.47	1.41
14	A	832	CLA	C4B-CHC	2.39	1.47	1.41
14	H	825	CLA	C1B-CHB	2.39	1.47	1.41
14	B	824	CLA	C1C-NC	-2.39	1.34	1.37
14	Q	203	CLA	C1C-NC	-2.39	1.34	1.37
14	b	810	CLA	C1C-NC	-2.39	1.34	1.37
14	B	835	CLA	C4B-CHC	2.39	1.47	1.41
14	j	102	CLA	C4B-CHC	2.39	1.47	1.41
14	G	812	CLA	C1D-C2D	2.39	1.50	1.45
14	H	810	CLA	C1D-C2D	2.39	1.50	1.45
14	a	814	CLA	C4B-CHC	2.39	1.47	1.41
14	a	833	CLA	C1C-NC	-2.39	1.34	1.37
14	A	844	CLA	C1B-CHB	2.39	1.47	1.41
14	G	807	CLA	C1B-CHB	2.39	1.47	1.41
14	H	806	CLA	C1B-CHB	2.39	1.47	1.41
14	i	101	CLA	C4C-C3C	2.39	1.49	1.45
14	B	837	CLA	C4B-CHC	2.39	1.47	1.41
14	A	813	CLA	C4B-CHC	2.39	1.47	1.41
14	A	817	CLA	C4B-CHC	2.39	1.47	1.41
14	a	803	CLA	C1B-CHB	2.39	1.47	1.41
14	U	205	CLA	C4C-C3C	2.39	1.49	1.45
14	A	802	CLA	C1C-NC	-2.39	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	816	CLA	C1B-CHB	2.39	1.47	1.41
14	j	101	CLA	C4C-C3C	2.39	1.49	1.45
14	a	809	CLA	C1B-CHB	2.39	1.47	1.41
14	a	816	CLA	C4B-CHC	2.39	1.47	1.41
14	B	822	CLA	C1B-CHB	2.39	1.47	1.41
14	G	810	CLA	C1B-CHB	2.39	1.47	1.41
14	b	812	CLA	C4C-C3C	2.38	1.49	1.45
14	G	819	CLA	C1C-NC	-2.38	1.34	1.37
14	G	817	CLA	C4B-CHC	2.38	1.47	1.41
14	b	815	CLA	C1B-CHB	2.38	1.47	1.41
14	H	818	CLA	C1C-NC	-2.38	1.34	1.37
14	b	832	CLA	C1B-CHB	2.38	1.47	1.41
14	x	1701	CLA	C1B-CHB	2.38	1.47	1.41
14	B	837	CLA	C1D-C2D	2.38	1.50	1.45
14	G	818	CLA	C4B-CHC	2.38	1.47	1.41
14	G	839	CLA	C1B-CHB	2.38	1.47	1.41
14	A	824	CLA	C1B-CHB	2.38	1.47	1.41
14	H	811	CLA	C1C-NC	-2.38	1.34	1.37
14	H	806	CLA	C4B-CHC	2.38	1.47	1.41
14	k	1401	CLA	C1C-NC	-2.38	1.34	1.37
14	H	801	CLA	C1C-NC	-2.38	1.34	1.37
14	A	827	CLA	C4B-CHC	2.38	1.47	1.41
14	A	817	CLA	C1D-C2D	2.38	1.50	1.45
14	B	831	CLA	C1D-C2D	2.38	1.50	1.45
14	A	817	CLA	C1C-NC	-2.38	1.34	1.37
14	G	830	CLA	C1C-NC	-2.38	1.34	1.37
14	H	835	CLA	C4B-CHC	2.38	1.47	1.41
14	a	823	CLA	C1D-C2D	2.38	1.50	1.45
14	a	816	CLA	C4C-C3C	2.38	1.49	1.45
14	a	843	CLA	C1C-NC	-2.37	1.34	1.37
14	G	823	CLA	C1B-CHB	2.37	1.47	1.41
14	Q	201	CLA	C1B-CHB	2.37	1.47	1.41
14	G	815	CLA	C1B-CHB	2.37	1.47	1.41
14	G	808	CLA	C1B-CHB	2.37	1.47	1.41
14	H	821	CLA	C1C-NC	-2.37	1.34	1.37
14	a	832	CLA	C4B-CHC	2.37	1.47	1.41
14	A	839	CLA	C4B-CHC	2.37	1.47	1.41
14	B	834	CLA	C1B-CHB	2.37	1.47	1.41
14	A	822	CLA	C4C-C3C	2.37	1.49	1.45
14	B	807	CLA	C4C-C3C	2.37	1.49	1.45
14	a	843	CLA	C4B-CHC	2.37	1.47	1.41
14	m	1601	CLA	C4B-CHC	2.37	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	835	CLA	C1C-NC	-2.37	1.34	1.37
14	U	206	CLA	C1B-CHB	2.37	1.47	1.41
14	K	102	CLA	C1D-C2D	2.37	1.50	1.45
14	a	816	CLA	C1D-C2D	2.37	1.50	1.45
14	M	1601	CLA	C1C-NC	-2.37	1.34	1.37
14	A	816	CLA	C1B-CHB	2.37	1.47	1.41
14	B	816	CLA	C1B-CHB	2.37	1.47	1.41
14	B	837	CLA	C1B-CHB	2.37	1.47	1.41
14	b	807	CLA	C1C-NC	-2.37	1.34	1.37
14	A	807	CLA	C4B-CHC	2.37	1.47	1.41
14	H	830	CLA	C4B-CHC	2.37	1.47	1.41
14	A	808	CLA	C4C-C3C	2.36	1.49	1.45
14	a	838	CLA	C4C-C3C	2.36	1.49	1.45
14	A	814	CLA	C4B-CHC	2.36	1.47	1.41
14	B	823	CLA	C4B-CHC	2.36	1.47	1.41
14	G	839	CLA	C4B-CHC	2.36	1.47	1.41
14	b	830	CLA	C4B-CHC	2.36	1.47	1.41
14	a	820	CLA	C1C-NC	-2.36	1.34	1.37
14	a	824	CLA	C1B-CHB	2.36	1.47	1.41
14	b	808	CLA	C1B-CHB	2.36	1.47	1.41
14	A	812	CLA	C4C-C3C	2.36	1.49	1.45
14	G	845	CLA	C4B-CHC	2.36	1.47	1.41
14	a	806	CLA	C4B-CHC	2.36	1.47	1.41
14	b	837	CLA	C1B-CHB	2.36	1.47	1.41
14	U	206	CLA	C1D-C2D	2.36	1.50	1.45
14	A	819	CLA	C1C-NC	-2.36	1.34	1.37
14	U	206	CLA	C4B-CHC	2.36	1.47	1.41
14	A	821	CLA	C1B-CHB	2.36	1.47	1.41
14	i	101	CLA	C4B-CHC	2.36	1.47	1.41
14	H	834	CLA	C1B-CHB	2.36	1.47	1.41
14	b	838	CLA	C1B-CHB	2.36	1.47	1.41
14	a	830	CLA	C1B-CHB	2.36	1.47	1.41
14	b	821	CLA	C1C-NC	-2.36	1.34	1.37
14	A	815	CLA	C4C-C3C	2.36	1.49	1.45
14	b	833	CLA	C1D-C2D	2.36	1.50	1.45
14	b	818	CLA	C4C-C3C	2.36	1.49	1.45
14	H	836	CLA	C4B-CHC	2.36	1.47	1.41
14	b	814	CLA	C4B-CHC	2.36	1.47	1.41
14	A	817	CLA	C4C-C3C	2.36	1.49	1.45
14	G	806	CLA	C1D-C2D	2.36	1.50	1.45
14	a	811	CLA	C1B-CHB	2.36	1.47	1.41
14	A	833	CLA	C1C-NC	-2.36	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	818	CLA	C1C-NC	-2.36	1.34	1.37
14	W	1701	CLA	C1B-CHB	2.36	1.47	1.41
14	G	815	CLA	C4C-C3C	2.35	1.49	1.45
14	B	815	CLA	C1C-NC	-2.35	1.34	1.37
14	G	844	CLA	C1C-NC	-2.35	1.34	1.37
14	G	837	CLA	C1D-C2D	2.35	1.50	1.45
14	G	819	CLA	C1B-CHB	2.35	1.47	1.41
14	B	830	CLA	C1D-C2D	2.35	1.50	1.45
14	b	811	CLA	C1B-CHB	2.35	1.47	1.41
14	K	102	CLA	C1C-NC	-2.35	1.34	1.37
14	G	844	CLA	C4C-C3C	2.35	1.49	1.45
14	a	813	CLA	C1D-C2D	2.35	1.50	1.45
14	G	827	CLA	C1D-C2D	2.35	1.50	1.45
14	H	827	CLA	C1B-CHB	2.35	1.47	1.41
14	a	825	CLA	C1B-CHB	2.35	1.47	1.41
14	S	101	CLA	C1C-NC	-2.35	1.34	1.37
14	a	834	CLA	C4B-CHC	2.35	1.47	1.41
14	A	817	CLA	C1B-CHB	2.35	1.47	1.41
14	G	806	CLA	C4B-CHC	2.35	1.47	1.41
14	B	811	CLA	C1B-CHB	2.35	1.47	1.41
14	B	838	CLA	C1D-C2D	2.35	1.50	1.45
14	A	806	CLA	C1D-C2D	2.35	1.50	1.45
14	G	838	CLA	C1C-NC	-2.35	1.34	1.37
14	L	204	CLA	C1B-CHB	2.34	1.47	1.41
14	b	822	CLA	C1B-CHB	2.34	1.47	1.41
14	l	207	CLA	C4B-CHC	2.34	1.47	1.41
14	A	811	CLA	C4B-CHC	2.34	1.47	1.41
14	U	205	CLA	C1B-CHB	2.34	1.47	1.41
14	a	807	CLA	C4C-C3C	2.34	1.49	1.45
14	a	817	CLA	C1D-C2D	2.34	1.50	1.45
14	H	821	CLA	C1B-CHB	2.34	1.47	1.41
14	G	822	CLA	C4C-C3C	2.34	1.49	1.45
14	b	817	CLA	C1B-CHB	2.34	1.47	1.41
14	A	833	CLA	C1D-C2D	2.34	1.50	1.45
14	b	832	CLA	C4C-C3C	2.34	1.49	1.45
14	a	815	CLA	C1B-CHB	2.34	1.47	1.41
14	A	818	CLA	C1C-NC	-2.34	1.34	1.37
14	a	806	CLA	C1B-CHB	2.34	1.47	1.41
14	a	843	CLA	C1B-CHB	2.34	1.47	1.41
14	H	831	CLA	C1C-NC	-2.34	1.34	1.37
14	A	814	CLA	C4C-C3C	2.34	1.49	1.45
14	H	811	CLA	C4C-C3C	2.34	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	831	CLA	C4C-C3C	2.34	1.49	1.45
14	b	830	CLA	C1D-C2D	2.34	1.50	1.45
14	b	821	CLA	C4C-C3C	2.34	1.49	1.45
14	G	810	CLA	C4B-CHC	2.34	1.47	1.41
14	B	830	CLA	C4B-CHC	2.34	1.47	1.41
14	G	814	CLA	C1B-CHB	2.34	1.47	1.41
14	F	1301	CLA	C4B-CHC	2.33	1.47	1.41
14	H	830	CLA	C1C-NC	-2.33	1.34	1.37
14	m	1601	CLA	C4C-C3C	2.33	1.49	1.45
14	H	818	CLA	C1B-CHB	2.33	1.47	1.41
14	G	834	CLA	C1D-C2D	2.33	1.50	1.45
14	A	807	CLA	C1B-CHB	2.33	1.47	1.41
14	B	826	CLA	C4B-CHC	2.33	1.47	1.41
14	b	832	CLA	C4B-CHC	2.33	1.47	1.41
14	b	813	CLA	C4B-CHC	2.33	1.47	1.41
14	b	821	CLA	C4B-CHC	2.33	1.47	1.41
14	b	805	CLA	C1D-C2D	2.33	1.49	1.45
14	a	837	CLA	C1C-NC	-2.33	1.34	1.37
14	G	828	CLA	C1C-C2C	2.33	1.49	1.44
14	G	835	CLA	C4B-CHC	2.33	1.47	1.41
14	H	816	CLA	C1C-NC	-2.33	1.34	1.37
14	B	815	CLA	C1B-CHB	2.33	1.47	1.41
14	b	812	CLA	C1B-CHB	2.33	1.47	1.41
14	B	815	CLA	C1D-C2D	2.33	1.49	1.45
14	b	811	CLA	C1C-NC	-2.33	1.34	1.37
14	a	841	CLA	C1B-CHB	2.33	1.47	1.41
14	T	1401	CLA	C1C-NC	-2.33	1.34	1.37
14	a	810	CLA	C4B-CHC	2.33	1.47	1.41
14	b	826	CLA	C4B-CHC	2.33	1.47	1.41
14	B	811	CLA	C4C-C3C	2.33	1.49	1.45
14	G	831	CLA	C4C-C3C	2.33	1.49	1.45
14	a	840	CLA	C4C-C3C	2.33	1.49	1.45
14	G	826	CLA	C4C-C3C	2.32	1.49	1.45
14	a	815	CLA	C1D-C2D	2.32	1.49	1.45
14	b	837	CLA	C1D-C2D	2.32	1.49	1.45
14	A	845	CLA	C1B-CHB	2.32	1.47	1.41
14	a	819	CLA	C4B-CHC	2.32	1.47	1.41
14	H	829	CLA	C1B-CHB	2.32	1.47	1.41
14	A	826	CLA	C1B-CHB	2.32	1.47	1.41
14	H	836	CLA	C1B-CHB	2.32	1.47	1.41
14	k	1401	CLA	C1D-C2D	2.32	1.49	1.45
14	j	102	CLA	C1C-NC	-2.32	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	843	BCR	C30-C25	-2.32	1.50	1.53
14	b	823	CLA	C1B-CHB	2.32	1.47	1.41
14	G	840	CLA	C1B-CHB	2.32	1.47	1.41
14	A	811	CLA	C1D-C2D	2.32	1.49	1.45
14	b	820	CLA	C1B-CHB	2.32	1.47	1.41
14	A	815	CLA	C1D-C2D	2.32	1.49	1.45
14	A	820	CLA	C1D-C2D	2.32	1.49	1.45
14	G	819	CLA	C1D-C2D	2.32	1.49	1.45
14	a	842	CLA	C1D-C2D	2.32	1.49	1.45
14	b	818	CLA	C1C-NC	-2.31	1.34	1.37
14	b	837	CLA	C1C-NC	-2.31	1.34	1.37
14	b	828	CLA	C4C-C3C	2.31	1.49	1.45
14	H	817	CLA	C1B-CHB	2.31	1.47	1.41
14	B	819	CLA	C1B-CHB	2.31	1.47	1.41
14	a	822	CLA	C1C-NC	-2.31	1.34	1.37
14	A	845	CLA	C4B-CHC	2.31	1.47	1.41
14	a	815	CLA	C4B-CHC	2.31	1.47	1.41
14	K	101	CLA	C1C-NC	-2.31	1.34	1.37
14	G	822	CLA	C1D-C2D	2.31	1.49	1.45
14	A	825	CLA	C1B-CHB	2.31	1.47	1.41
14	b	827	CLA	C1B-CHB	2.31	1.47	1.41
14	B	805	CLA	C4B-CHC	2.31	1.47	1.41
14	H	823	CLA	C4B-CHC	2.31	1.47	1.41
14	A	804	CLA	C1B-CHB	2.31	1.47	1.41
14	A	833	CLA	C1B-CHB	2.31	1.47	1.41
14	S	101	CLA	C1D-C2D	2.31	1.49	1.45
14	G	832	CLA	C4B-CHC	2.31	1.47	1.41
14	a	812	CLA	C1C-NC	-2.31	1.34	1.37
14	B	806	CLA	C4B-CHC	2.31	1.47	1.41
14	L	205	CLA	C4C-C3C	2.31	1.49	1.45
14	l	206	CLA	C1B-CHB	2.31	1.47	1.41
14	L	206	CLA	C1B-CHB	2.31	1.47	1.41
14	Q	203	CLA	C1B-CHB	2.31	1.47	1.41
14	G	804	CLA	C1B-CHB	2.31	1.47	1.41
14	H	819	CLA	C1C-NC	-2.30	1.34	1.37
14	A	810	CLA	C4B-CHC	2.30	1.47	1.41
14	B	816	CLA	C1C-C2C	2.30	1.49	1.44
14	B	832	CLA	C4B-CHC	2.30	1.47	1.41
14	G	807	CLA	C4B-CHC	2.30	1.47	1.41
14	a	820	CLA	C1B-CHB	2.30	1.47	1.41
14	a	829	CLA	C1B-CHB	2.30	1.47	1.41
14	A	813	CLA	C1B-CHB	2.30	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	843	CLA	C1B-CHB	2.30	1.47	1.41
14	S	102	CLA	C1D-C2D	2.30	1.49	1.45
14	b	831	CLA	C1C-NC	-2.30	1.34	1.37
14	G	816	CLA	C4B-CHC	2.30	1.47	1.41
17	B	843	BCR	C30-C25	-2.30	1.50	1.53
14	A	838	CLA	C1B-CHB	2.30	1.47	1.41
14	G	808	CLA	C1D-C2D	2.30	1.49	1.45
14	A	825	CLA	C1D-C2D	2.30	1.49	1.45
14	G	826	CLA	C1B-CHB	2.30	1.47	1.41
14	G	804	CLA	C4C-C3C	2.30	1.48	1.45
14	B	837	CLA	C1C-NC	-2.30	1.34	1.37
14	S	102	CLA	C1C-NC	-2.30	1.34	1.37
14	a	844	CLA	C1B-CHB	2.30	1.47	1.41
14	U	204	CLA	C1C-NC	-2.30	1.34	1.37
14	B	836	CLA	C4B-CHC	2.30	1.47	1.41
14	A	816	CLA	C4C-C3C	2.30	1.48	1.45
14	H	838	CLA	C1B-CHB	2.30	1.47	1.41
14	K	101	CLA	C1B-CHB	2.29	1.47	1.41
14	A	830	CLA	C1B-CHB	2.29	1.47	1.41
14	A	840	CLA	C1D-C2D	2.29	1.49	1.45
14	G	824	CLA	C1B-CHB	2.29	1.47	1.41
14	G	814	CLA	C4C-C3C	2.29	1.48	1.45
14	F	1303	CLA	C4C-C3C	2.29	1.48	1.45
14	A	820	CLA	C4B-CHC	2.29	1.47	1.41
14	F	1303	CLA	C1B-CHB	2.29	1.47	1.41
14	G	812	CLA	C1B-CHB	2.29	1.47	1.41
14	b	825	CLA	C1B-CHB	2.29	1.47	1.41
14	G	825	CLA	C1B-CHB	2.29	1.47	1.41
14	B	803	CLA	C4C-C3C	2.29	1.48	1.45
14	B	802	CLA	C4B-CHC	2.29	1.47	1.41
14	m	1601	CLA	C1B-CHB	2.29	1.47	1.41
14	a	812	CLA	C1D-C2D	2.29	1.49	1.45
14	G	820	CLA	C1D-C2D	2.29	1.49	1.45
14	G	813	CLA	C4C-C3C	2.29	1.48	1.45
14	H	805	CLA	C1B-CHB	2.29	1.47	1.41
14	H	804	CLA	C1D-C2D	2.29	1.49	1.45
14	B	812	CLA	C1B-CHB	2.28	1.47	1.41
14	B	825	CLA	C1B-CHB	2.28	1.47	1.41
14	A	826	CLA	C4B-CHC	2.28	1.47	1.41
14	A	812	CLA	C1B-CHB	2.28	1.47	1.41
14	A	835	CLA	C4B-CHC	2.28	1.47	1.41
14	G	834	CLA	C1B-CHB	2.28	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	818	CLA	C1B-CHB	2.28	1.47	1.41
14	a	807	CLA	C1B-CHB	2.28	1.47	1.41
14	H	807	CLA	C4B-CHC	2.28	1.47	1.41
14	H	838	CLA	C1D-C2D	2.28	1.49	1.45
14	H	833	CLA	C4C-C3C	2.28	1.48	1.45
14	f	202	CLA	C4C-C3C	2.28	1.48	1.45
14	H	806	CLA	C1D-C2D	2.28	1.49	1.45
14	b	806	CLA	C4C-C3C	2.28	1.48	1.45
14	H	828	CLA	C4C-C3C	2.28	1.48	1.45
14	l	207	CLA	C1B-CHB	2.28	1.47	1.41
14	F	1301	CLA	C4C-C3C	2.28	1.48	1.45
14	b	832	CLA	C1D-C2D	2.28	1.49	1.45
14	a	836	CLA	C4C-C3C	2.28	1.48	1.45
14	A	814	CLA	C1B-CHB	2.28	1.47	1.41
14	B	804	CLA	C1B-CHB	2.27	1.47	1.41
14	S	101	CLA	C4C-C3C	2.27	1.48	1.45
14	A	834	CLA	C1D-C2D	2.27	1.49	1.45
14	B	812	CLA	C4B-CHC	2.27	1.47	1.41
14	a	804	CLA	C1D-C2D	2.27	1.49	1.45
14	H	811	CLA	C1B-CHB	2.27	1.47	1.41
14	H	824	CLA	C4C-C3C	2.27	1.48	1.45
14	a	814	CLA	C4C-C3C	2.27	1.48	1.45
14	a	804	CLA	C1C-NC	-2.27	1.34	1.37
14	A	834	CLA	C1C-NC	-2.27	1.34	1.37
14	b	807	CLA	C1D-C2D	2.27	1.49	1.45
14	G	820	CLA	C1B-CHB	2.27	1.47	1.41
14	S	102	CLA	C4C-C3C	2.27	1.48	1.45
14	G	807	CLA	C1D-C2D	2.27	1.49	1.45
14	V	1601	CLA	C4C-C3C	2.27	1.48	1.45
14	a	819	CLA	C1D-C2D	2.27	1.49	1.45
14	B	821	CLA	C1B-CHB	2.27	1.47	1.41
14	G	831	CLA	C4B-CHC	2.27	1.47	1.41
14	b	830	CLA	C1B-CHB	2.27	1.47	1.41
14	G	820	CLA	C4C-C3C	2.27	1.48	1.45
14	A	816	CLA	C4B-CHC	2.27	1.47	1.41
14	G	815	CLA	C4B-CHC	2.27	1.47	1.41
14	H	814	CLA	C4B-CHC	2.27	1.47	1.41
14	j	101	CLA	C1B-CHB	2.26	1.47	1.41
14	A	805	CLA	C1D-C2D	2.26	1.49	1.45
14	B	807	CLA	C4B-CHC	2.26	1.47	1.41
14	A	831	CLA	C1B-CHB	2.26	1.47	1.41
14	B	819	CLA	C1C-NC	-2.26	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	806	CLA	C4B-CHC	2.26	1.47	1.41
14	A	824	CLA	C1C-NC	-2.26	1.34	1.37
14	B	830	CLA	C4C-C3C	2.26	1.48	1.45
14	B	830	CLA	C1B-CHB	2.26	1.47	1.41
14	A	809	CLA	C1D-C2D	2.26	1.49	1.45
14	a	835	CLA	C4C-C3C	2.26	1.48	1.45
13	G	801	CL0	CHB-C4A	2.26	1.35	1.33
14	b	835	CLA	C1C-NC	-2.26	1.34	1.37
14	a	824	CLA	C4B-CHC	2.26	1.47	1.41
14	G	840	CLA	C1D-C2D	2.26	1.49	1.45
14	L	206	CLA	C1D-C2D	2.26	1.49	1.45
14	H	831	CLA	C1B-CHB	2.26	1.47	1.41
14	a	833	CLA	C1B-CHB	2.26	1.47	1.41
14	G	843	CLA	C4C-C3C	2.26	1.48	1.45
14	G	805	CLA	C1C-NC	-2.26	1.34	1.37
14	a	840	CLA	C1D-C2D	2.26	1.49	1.45
14	H	812	CLA	C1D-C2D	2.26	1.49	1.45
14	a	810	CLA	C1B-CHB	2.26	1.47	1.41
14	B	827	CLA	C1B-CHB	2.26	1.47	1.41
14	A	808	CLA	C1B-CHB	2.26	1.47	1.41
14	a	835	CLA	C1B-CHB	2.26	1.47	1.41
14	b	816	CLA	C1C-NC	-2.25	1.34	1.37
14	a	839	CLA	C1B-CHB	2.25	1.47	1.41
14	G	822	CLA	C1B-CHB	2.25	1.47	1.41
14	L	205	CLA	C1B-CHB	2.25	1.47	1.41
14	x	1701	CLA	C4C-C3C	2.25	1.48	1.45
14	A	836	CLA	C1B-CHB	2.25	1.47	1.41
14	B	805	CLA	C1D-C2D	2.25	1.49	1.45
14	b	822	CLA	C4C-C3C	2.25	1.48	1.45
14	G	841	CLA	C1B-CHB	2.25	1.47	1.41
14	A	825	CLA	C4B-CHC	2.25	1.47	1.41
14	i	101	CLA	C1D-C2D	2.25	1.49	1.45
14	H	809	CLA	C4C-C3C	2.25	1.48	1.45
14	B	818	CLA	C1B-CHB	2.25	1.47	1.41
14	G	809	CLA	C1D-C2D	2.24	1.49	1.45
14	a	814	CLA	C1B-CHB	2.24	1.47	1.41
14	A	805	CLA	C1C-NC	-2.24	1.34	1.37
14	b	833	CLA	C1B-CHB	2.24	1.47	1.41
14	b	835	CLA	C1B-CHB	2.24	1.47	1.41
14	G	833	CLA	C1D-C2D	2.24	1.49	1.45
14	b	815	CLA	C1D-C2D	2.24	1.49	1.45
14	G	845	CLA	C1B-CHB	2.24	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	838	CLA	C1B-CHB	2.24	1.47	1.41
14	a	813	CLA	C1B-CHB	2.24	1.47	1.41
14	G	823	CLA	C1C-NC	-2.24	1.34	1.37
14	a	805	CLA	C1D-C2D	2.24	1.49	1.45
14	b	816	CLA	C1D-C2D	2.24	1.49	1.45
14	H	836	CLA	C4C-C3C	2.24	1.48	1.45
14	b	835	CLA	C4C-C3C	2.24	1.48	1.45
14	J	101	CLA	C1B-CHB	2.24	1.47	1.41
14	H	837	CLA	C1C-NC	-2.24	1.34	1.37
13	a	801	CL0	C4B-CHC	2.24	1.47	1.41
14	b	806	CLA	C1B-CHB	2.24	1.47	1.41
14	G	843	CLA	C1B-CHB	2.24	1.47	1.41
14	b	813	CLA	C1B-CHB	2.24	1.47	1.41
14	b	823	CLA	C4B-CHC	2.24	1.47	1.41
14	G	813	CLA	C1D-C2D	2.23	1.49	1.45
14	H	807	CLA	C1D-C2D	2.23	1.49	1.45
14	A	834	CLA	C1B-CHB	2.23	1.47	1.41
14	M	1601	CLA	C1A-CHA	2.23	1.52	1.43
14	A	820	CLA	C4C-C3C	2.23	1.48	1.45
14	b	803	CLA	C4B-CHC	2.23	1.47	1.41
14	B	827	CLA	C4C-C3C	2.23	1.48	1.45
14	H	816	CLA	C1D-C2D	2.23	1.49	1.45
14	H	814	CLA	C1A-CHA	2.23	1.52	1.43
14	G	818	CLA	C1D-C2D	2.23	1.49	1.45
14	B	838	CLA	C1B-CHB	2.23	1.47	1.41
14	H	807	CLA	C4C-C3C	2.23	1.48	1.45
14	B	839	CLA	C1D-C2D	2.23	1.49	1.45
14	W	1701	CLA	C4C-C3C	2.23	1.48	1.45
14	H	837	CLA	C1B-CHB	2.23	1.47	1.41
14	U	204	CLA	C1B-CHB	2.23	1.47	1.41
14	b	819	CLA	C1C-NC	-2.23	1.34	1.37
14	b	820	CLA	C4B-CHC	2.23	1.47	1.41
14	S	101	CLA	C1B-CHB	2.22	1.47	1.41
14	a	829	CLA	C4B-CHC	2.22	1.47	1.41
14	G	836	CLA	C4C-C3C	2.22	1.48	1.45
14	b	808	CLA	C4B-CHC	2.22	1.47	1.41
14	U	204	CLA	C1D-C2D	2.22	1.49	1.45
14	B	833	CLA	C4C-C3C	2.22	1.48	1.45
14	A	818	CLA	C1B-CHB	2.22	1.47	1.41
13	G	801	CL0	C4B-CHC	2.22	1.47	1.41
14	a	832	CLA	C1B-CHB	2.22	1.47	1.41
14	B	805	CLA	C1B-CHB	2.22	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	808	CLA	C4C-C3C	2.22	1.48	1.45
14	B	817	CLA	C1D-C2D	2.22	1.49	1.45
14	H	801	CLA	C1C-C2C	2.22	1.49	1.44
14	H	825	CLA	C1A-CHA	2.22	1.52	1.43
14	m	1601	CLA	C1A-CHA	2.22	1.52	1.43
14	a	833	CLA	C4C-C3C	2.22	1.48	1.45
14	l	205	CLA	C1B-CHB	2.22	1.47	1.41
14	G	838	CLA	C1D-C2D	2.22	1.49	1.45
14	H	823	CLA	C1B-CHB	2.22	1.47	1.41
14	B	828	CLA	C4C-C3C	2.21	1.48	1.45
14	G	824	CLA	C4C-C3C	2.21	1.48	1.45
14	H	812	CLA	C4C-C3C	2.21	1.48	1.45
14	A	815	CLA	C1B-CHB	2.21	1.47	1.41
14	B	808	CLA	C4B-CHC	2.21	1.47	1.41
14	G	816	CLA	C1B-CHB	2.21	1.47	1.41
14	a	839	CLA	C1D-C2D	2.21	1.49	1.45
14	A	845	CLA	C1A-CHA	2.21	1.52	1.43
14	G	812	CLA	C4C-C3C	2.21	1.48	1.45
14	G	831	CLA	C1B-CHB	2.21	1.47	1.41
14	b	834	CLA	C1A-CHA	2.21	1.52	1.43
14	A	826	CLA	C4C-C3C	2.21	1.48	1.45
14	B	801	CLA	C1C-C2C	2.21	1.49	1.44
14	b	822	CLA	C1D-C2D	2.21	1.49	1.45
14	B	828	CLA	C1B-CHB	2.21	1.47	1.41
14	b	806	CLA	C1D-C2D	2.21	1.49	1.45
14	A	805	CLA	C1B-CHB	2.21	1.47	1.41
14	x	1701	CLA	C1D-C2D	2.21	1.49	1.45
14	b	811	CLA	C4C-C3C	2.21	1.48	1.45
14	G	830	CLA	C4B-CHC	2.21	1.47	1.41
14	A	816	CLA	C1D-C2D	2.21	1.49	1.45
14	a	834	CLA	C1D-C2D	2.21	1.49	1.45
14	G	813	CLA	C1B-CHB	2.21	1.47	1.41
14	B	821	CLA	C4C-C3C	2.21	1.48	1.45
14	a	812	CLA	C1B-CHB	2.20	1.47	1.41
14	T	1401	CLA	C1D-C2D	2.20	1.49	1.45
14	H	820	CLA	C1D-C2D	2.20	1.49	1.45
14	H	810	CLA	CHB-C4A	2.20	1.35	1.33
14	H	830	CLA	C4C-C3C	2.20	1.48	1.45
14	B	804	CLA	C1D-C2D	2.20	1.49	1.45
14	A	838	CLA	C4C-C3C	2.20	1.48	1.45
14	B	834	CLA	C1D-C2D	2.20	1.49	1.45
14	a	827	CLA	C1B-CHB	2.20	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	839	CLA	C4C-C3C	2.20	1.48	1.45
14	b	821	CLA	C1D-C2D	2.20	1.49	1.45
14	B	833	CLA	C1B-CHB	2.20	1.47	1.41
14	a	816	CLA	C1B-CHB	2.20	1.47	1.41
14	a	808	CLA	C1D-C2D	2.20	1.49	1.45
14	A	825	CLA	C1A-CHA	2.20	1.52	1.43
14	b	824	CLA	C1D-C2D	2.20	1.49	1.45
14	a	828	CLA	C1B-CHB	2.20	1.47	1.41
14	H	832	CLA	C4B-CHC	2.20	1.47	1.41
14	b	838	CLA	C1D-C2D	2.20	1.49	1.45
14	G	820	CLA	C1A-CHA	2.19	1.52	1.43
14	H	834	CLA	C4B-CHC	2.19	1.47	1.41
14	G	829	CLA	C1B-CHB	2.19	1.47	1.41
14	A	813	CLA	C4C-C3C	2.19	1.48	1.45
14	b	812	CLA	C4B-CHC	2.19	1.47	1.41
14	b	828	CLA	C1B-CHB	2.19	1.47	1.41
14	b	805	CLA	C4C-C3C	2.19	1.48	1.45
14	G	809	CLA	C1B-CHB	2.19	1.47	1.41
14	B	826	CLA	C1B-CHB	2.19	1.47	1.41
14	B	831	CLA	C1B-CHB	2.19	1.47	1.41
14	H	829	CLA	C4C-C3C	2.19	1.48	1.45
14	B	811	CLA	C1D-C2D	2.19	1.49	1.45
14	B	825	CLA	C1A-CHA	2.19	1.52	1.43
14	A	840	CLA	C1B-CHB	2.19	1.47	1.41
14	H	826	CLA	C4B-CHC	2.19	1.47	1.41
14	B	806	CLA	C1D-C2D	2.18	1.49	1.45
14	H	819	CLA	C4C-C3C	2.18	1.48	1.45
14	G	820	CLA	C4B-CHC	2.18	1.47	1.41
14	G	839	CLA	C1D-C2D	2.18	1.49	1.45
14	a	830	CLA	C4B-CHC	2.18	1.47	1.41
14	A	845	CLA	C1D-C2D	2.18	1.49	1.45
14	G	804	CLA	C1D-C2D	2.18	1.49	1.45
14	H	828	CLA	C4B-CHC	2.18	1.47	1.41
14	a	830	CLA	C4C-C3C	2.18	1.48	1.45
14	b	834	CLA	C4B-CHC	2.18	1.47	1.41
14	H	834	CLA	C1D-C2D	2.18	1.49	1.45
14	A	815	CLA	C4B-CHC	2.18	1.47	1.41
14	H	818	CLA	C4C-C3C	2.18	1.48	1.45
14	a	824	CLA	C1A-CHA	2.18	1.52	1.43
14	H	810	CLA	C4C-C3C	2.18	1.48	1.45
14	G	837	CLA	C1B-CHB	2.18	1.47	1.41
14	A	835	CLA	C1D-C2D	2.18	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	814	CLA	C1D-C2D	2.18	1.49	1.45
14	H	824	CLA	C1D-C2D	2.18	1.49	1.45
14	B	834	CLA	C1A-CHA	2.18	1.52	1.43
14	b	812	CLA	C1D-C2D	2.18	1.49	1.45
14	a	844	CLA	C1A-CHA	2.17	1.52	1.43
14	G	802	CLA	C1A-CHA	2.17	1.52	1.43
14	L	201	CLA	C4B-CHC	2.17	1.47	1.41
14	a	832	CLA	C4C-C3C	2.17	1.48	1.45
14	A	839	CLA	C1D-C2D	2.17	1.49	1.45
14	l	202	CLA	C1B-CHB	2.17	1.47	1.41
14	B	824	CLA	C1D-C2D	2.17	1.49	1.45
14	b	805	CLA	C1B-CHB	2.17	1.47	1.41
14	S	102	CLA	C3A-C2A	-2.17	1.52	1.54
14	A	820	CLA	C1B-CHB	2.17	1.47	1.41
14	B	817	CLA	C1B-CHB	2.17	1.47	1.41
14	T	1401	CLA	C4C-C3C	2.17	1.48	1.45
14	A	807	CLA	C1D-C2D	2.17	1.49	1.45
14	G	817	CLA	C4C-C3C	2.17	1.48	1.45
14	b	820	CLA	C1D-C2D	2.16	1.49	1.45
13	A	801	CL0	C4B-CHC	2.16	1.47	1.41
14	G	826	CLA	C4B-CHC	2.16	1.47	1.41
14	a	811	CLA	C4B-CHC	2.16	1.47	1.41
14	G	830	CLA	C1B-CHB	2.16	1.47	1.41
14	H	817	CLA	C1D-C2D	2.16	1.49	1.45
14	G	826	CLA	C1A-CHA	2.16	1.52	1.43
14	a	805	CLA	C1B-CHB	2.16	1.47	1.41
14	a	840	CLA	C1A-CHA	2.16	1.52	1.43
14	a	838	CLA	C1D-C2D	2.16	1.49	1.45
14	A	841	CLA	C1D-C2D	2.16	1.49	1.45
14	G	802	CLA	C4B-CHC	2.16	1.47	1.41
14	H	812	CLA	C1B-CHB	2.16	1.47	1.41
14	a	804	CLA	C1A-CHA	2.16	1.52	1.43
14	B	832	CLA	C4C-C3C	2.16	1.48	1.45
14	A	830	CLA	C4C-C3C	2.16	1.48	1.45
14	A	809	CLA	C1B-CHB	2.16	1.47	1.41
14	H	803	CLA	C1A-CHA	2.16	1.52	1.43
14	G	841	CLA	C1D-C2D	2.16	1.49	1.45
14	H	802	CLA	C4B-CHC	2.16	1.47	1.41
14	a	823	CLA	C4C-C3C	2.16	1.48	1.45
14	H	833	CLA	C1B-CHB	2.16	1.47	1.41
14	G	816	CLA	C1D-C2D	2.16	1.49	1.45
14	b	839	CLA	C1D-C2D	2.15	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	816	CLA	C1A-CHA	2.15	1.52	1.43
14	G	832	CLA	C1B-CHB	2.15	1.47	1.41
14	U	201	CLA	C1B-CHB	2.15	1.47	1.41
14	b	821	CLA	C1A-CHA	2.15	1.52	1.43
14	B	840	CLA	C1A-CHA	2.15	1.52	1.43
14	A	831	CLA	C4B-CHC	2.15	1.47	1.41
14	H	826	CLA	C4C-C3C	2.15	1.48	1.45
14	B	812	CLA	C4C-C3C	2.15	1.48	1.45
14	b	827	CLA	C4C-C3C	2.15	1.48	1.45
14	a	814	CLA	C1A-CHA	2.15	1.51	1.43
14	k	1401	CLA	C4C-C3C	2.15	1.48	1.45
14	H	839	CLA	C1B-CHB	2.15	1.47	1.41
14	G	830	CLA	C1A-CHA	2.15	1.51	1.43
14	G	817	CLA	C1B-CHB	2.15	1.47	1.41
14	a	816	CLA	C1A-CHA	2.15	1.51	1.43
14	b	825	CLA	C1A-CHA	2.15	1.51	1.43
14	b	801	CLA	C1A-CHA	2.14	1.51	1.43
14	A	842	CLA	C1B-CHB	2.14	1.47	1.41
14	a	825	CLA	C4C-C3C	2.14	1.48	1.45
14	H	824	CLA	C1B-CHB	2.14	1.46	1.41
14	H	804	CLA	C4C-C3C	2.14	1.48	1.45
14	H	804	CLA	C1B-CHB	2.14	1.46	1.41
14	a	837	CLA	C1B-CHB	2.14	1.46	1.41
14	Q	203	CLA	C4C-C3C	2.14	1.48	1.45
14	H	811	CLA	C1D-C2D	2.14	1.49	1.45
14	A	815	CLA	C1A-CHA	2.14	1.51	1.43
14	G	845	CLA	C1A-CHA	2.14	1.51	1.43
14	A	828	CLA	C1B-CHB	2.14	1.46	1.41
14	B	807	CLA	C1D-C2D	2.14	1.49	1.45
14	W	1701	CLA	C1A-CHA	2.14	1.51	1.43
14	H	828	CLA	C1B-CHB	2.14	1.46	1.41
14	a	828	CLA	C1C-C2C	2.14	1.48	1.44
14	H	838	CLA	C4C-C3C	2.14	1.48	1.45
14	B	838	CLA	C4C-C3C	2.14	1.48	1.45
14	A	826	CLA	C1A-CHA	2.14	1.51	1.43
14	H	826	CLA	C1B-CHB	2.13	1.46	1.41
14	b	824	CLA	C1B-CHB	2.13	1.46	1.41
14	K	102	CLA	C4C-C3C	2.13	1.48	1.45
14	H	830	CLA	C1B-CHB	2.13	1.46	1.41
14	H	834	CLA	C1A-CHA	2.13	1.51	1.43
14	G	825	CLA	C1A-CHA	2.13	1.51	1.43
14	G	812	CLA	C1A-CHA	2.13	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	823	CLA	C1A-CHA	2.13	1.51	1.43
14	B	832	CLA	C1D-C2D	2.13	1.49	1.45
14	H	814	CLA	CHB-C4A	2.13	1.35	1.33
14	b	831	CLA	C1B-CHB	2.13	1.46	1.41
14	H	816	CLA	C1B-CHB	2.13	1.46	1.41
14	B	814	CLA	C4B-CHC	2.13	1.46	1.41
14	B	828	CLA	C4B-CHC	2.13	1.46	1.41
14	b	829	CLA	C4B-CHC	2.13	1.46	1.41
14	l	202	CLA	C4B-CHC	2.13	1.46	1.41
14	a	804	CLA	C1B-CHB	2.13	1.46	1.41
14	a	821	CLA	C1B-CHB	2.13	1.46	1.41
14	H	837	CLA	C4C-C3C	2.13	1.48	1.45
14	H	819	CLA	C1D-C2D	2.12	1.49	1.45
14	G	840	CLA	C4C-C3C	2.12	1.48	1.45
14	b	814	CLA	C1A-CHA	2.12	1.51	1.43
14	a	820	CLA	C1A-CHA	2.12	1.51	1.43
14	B	821	CLA	C1A-CHA	2.12	1.51	1.43
14	G	821	CLA	C1A-CHA	2.12	1.51	1.43
14	a	820	CLA	C1D-C2D	2.12	1.49	1.45
14	A	832	CLA	C1B-CHB	2.12	1.46	1.41
14	b	819	CLA	C1A-CHA	2.12	1.51	1.43
14	B	820	CLA	C1D-C2D	2.12	1.49	1.45
14	A	844	CLA	C4C-C3C	2.12	1.48	1.45
14	m	1601	CLA	C1D-C2D	2.12	1.49	1.45
14	b	820	CLA	C1A-CHA	2.12	1.51	1.43
14	b	840	CLA	C1D-C2D	2.12	1.49	1.45
14	G	825	CLA	C1D-C2D	2.12	1.49	1.45
14	H	840	CLA	C1D-C2D	2.12	1.49	1.45
14	H	817	CLA	C4B-CHC	2.12	1.46	1.41
14	a	829	CLA	C4C-C3C	2.12	1.48	1.45
14	a	818	CLA	C4C-C3C	2.12	1.48	1.45
14	H	803	CLA	C1B-CHB	2.12	1.46	1.41
14	G	842	CLA	C1D-C2D	2.11	1.49	1.45
14	a	824	CLA	C1D-C2D	2.11	1.49	1.45
14	G	834	CLA	C4C-C3C	2.11	1.48	1.45
14	A	802	CLA	C1A-CHA	2.11	1.51	1.43
14	a	808	CLA	C1B-CHB	2.11	1.46	1.41
14	H	832	CLA	CHB-C4A	2.11	1.35	1.33
14	U	201	CLA	C4B-CHC	2.11	1.46	1.41
14	f	202	CLA	C1D-C2D	2.11	1.49	1.45
14	J	101	CLA	C1A-CHA	2.11	1.51	1.43
14	b	818	CLA	C1B-CHB	2.11	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	816	CLA	C1D-C2D	2.11	1.49	1.45
14	a	844	CLA	C1D-C2D	2.11	1.49	1.45
14	G	805	CLA	C1A-CHA	2.11	1.51	1.43
14	a	825	CLA	C1A-CHA	2.11	1.51	1.43
14	A	812	CLA	C1A-CHA	2.11	1.51	1.43
14	a	831	CLA	C1B-CHB	2.11	1.46	1.41
14	a	827	CLA	C1C-C2C	2.11	1.48	1.44
14	H	821	CLA	C1A-CHA	2.11	1.51	1.43
14	b	816	CLA	C1C-C2C	2.11	1.48	1.44
14	b	817	CLA	C1D-C2D	2.11	1.49	1.45
14	b	830	CLA	C4C-C3C	2.11	1.48	1.45
14	a	812	CLA	C4C-C3C	2.11	1.48	1.45
14	A	844	CLA	C4B-CHC	2.10	1.46	1.41
14	a	806	CLA	C1D-C2D	2.10	1.49	1.45
14	a	826	CLA	C1D-C2D	2.10	1.49	1.45
14	S	101	CLA	C1A-CHA	2.10	1.51	1.43
14	A	816	CLA	C1A-CHA	2.10	1.51	1.43
14	b	824	CLA	C4C-C3C	2.10	1.48	1.45
14	H	817	CLA	C1A-CHA	2.10	1.51	1.43
14	G	811	CLA	C1C-C2C	2.10	1.48	1.44
14	B	818	CLA	C4C-C3C	2.10	1.48	1.45
14	A	806	CLA	C1B-CHB	2.10	1.46	1.41
14	G	828	CLA	C1A-CHA	2.10	1.51	1.43
14	a	831	CLA	C4C-C3C	2.10	1.48	1.45
14	A	830	CLA	C1A-CHA	2.10	1.51	1.43
14	L	201	CLA	C1B-CHB	2.10	1.46	1.41
14	B	839	CLA	C1B-CHB	2.10	1.46	1.41
14	A	836	CLA	C1A-CHA	2.10	1.51	1.43
14	A	831	CLA	C4C-C3C	2.10	1.48	1.45
14	G	805	CLA	C1B-CHB	2.09	1.46	1.41
14	G	837	CLA	C1A-CHA	2.09	1.51	1.43
14	H	827	CLA	C4C-C3C	2.09	1.48	1.45
14	b	836	CLA	C4C-C3C	2.09	1.48	1.45
14	G	845	CLA	C1D-C2D	2.09	1.49	1.45
14	G	836	CLA	C1D-C2D	2.09	1.49	1.45
14	H	831	CLA	C4C-C3C	2.09	1.48	1.45
14	B	839	CLA	C4C-C3C	2.09	1.48	1.45
14	b	809	CLA	CHB-C4A	2.09	1.35	1.33
14	a	837	CLA	C1A-CHA	2.09	1.51	1.43
14	f	202	CLA	C1A-CHA	2.09	1.51	1.43
14	F	1303	CLA	C3A-C2A	-2.09	1.52	1.54
14	a	815	CLA	C1A-CHA	2.09	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	814	CLA	C1A-CHA	2.09	1.51	1.43
14	b	804	CLA	C1B-CHB	2.08	1.46	1.41
14	A	805	CLA	C1A-CHA	2.08	1.51	1.43
14	l	205	CLA	C4C-C3C	2.08	1.48	1.45
14	B	804	CLA	C1A-CHA	2.08	1.51	1.43
14	B	801	CLA	C1A-CHA	2.08	1.51	1.43
14	b	838	CLA	C4C-C3C	2.08	1.48	1.45
14	G	823	CLA	C1D-C2D	2.08	1.49	1.45
14	b	840	CLA	C1A-CHA	2.08	1.51	1.43
14	b	839	CLA	C4C-C3C	2.08	1.48	1.45
14	a	813	CLA	C1A-CHA	2.08	1.51	1.43
17	j	104	BCR	C1-C6	-2.08	1.51	1.53
14	A	818	CLA	C1D-C2D	2.08	1.49	1.45
14	V	1601	CLA	C1A-CHA	2.08	1.51	1.43
14	B	831	CLA	C4C-C3C	2.08	1.48	1.45
14	B	819	CLA	C1A-CHA	2.08	1.51	1.43
14	H	813	CLA	C4C-C3C	2.08	1.48	1.45
14	A	819	CLA	C1C-C2C	2.08	1.48	1.44
14	b	802	CLA	C4B-CHC	2.08	1.46	1.41
14	H	836	CLA	C1D-C2D	2.07	1.49	1.45
14	l	205	CLA	C1D-C2D	2.07	1.49	1.45
14	H	831	CLA	C1C-C2C	2.07	1.48	1.44
14	b	810	CLA	C4C-C3C	2.07	1.48	1.45
14	A	821	CLA	C1A-CHA	2.07	1.51	1.43
14	G	825	CLA	C4C-C3C	2.07	1.48	1.45
14	M	1601	CLA	C4C-C3C	2.07	1.48	1.45
14	b	828	CLA	C4B-CHC	2.07	1.46	1.41
14	A	823	CLA	C1C-C2C	2.07	1.48	1.44
14	A	822	CLA	C1B-CHB	2.07	1.46	1.41
14	b	814	CLA	C1D-C2D	2.07	1.49	1.45
14	B	803	CLA	C1B-CHB	2.07	1.46	1.41
14	l	202	CLA	C4C-C3C	2.07	1.48	1.45
14	a	811	CLA	C1A-CHA	2.07	1.51	1.43
14	a	829	CLA	C1A-CHA	2.07	1.51	1.43
14	B	804	CLA	C1C-C2C	2.06	1.48	1.44
14	B	817	CLA	C4B-CHC	2.06	1.46	1.41
14	H	819	CLA	C1A-CHA	2.06	1.51	1.43
14	H	840	CLA	C1A-CHA	2.06	1.51	1.43
14	a	836	CLA	C1B-CHB	2.06	1.46	1.41
14	G	841	CLA	C4C-C3C	2.06	1.48	1.45
14	G	829	CLA	C1C-C2C	2.06	1.48	1.44
14	S	102	CLA	C1C-C2C	2.06	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	805	CLA	C1C-C2C	2.06	1.48	1.44
14	H	818	CLA	C1A-CHA	2.06	1.51	1.43
14	X	1701	CLA	C1A-CHA	2.06	1.51	1.43
14	G	843	CLA	C4B-CHC	2.06	1.46	1.41
14	L	204	CLA	C1D-C2D	2.06	1.49	1.45
14	B	840	CLA	C4B-CHC	2.06	1.46	1.41
14	B	820	CLA	C1A-CHA	2.06	1.51	1.43
14	H	821	CLA	C4C-C3C	2.06	1.48	1.45
14	A	829	CLA	C1B-CHB	2.06	1.46	1.41
14	A	804	CLA	C1D-C2D	2.06	1.49	1.45
14	B	819	CLA	C1C-C2C	2.06	1.48	1.44
14	a	812	CLA	C1A-CHA	2.06	1.51	1.43
14	B	803	CLA	C1A-CHA	2.06	1.51	1.43
14	G	832	CLA	C1D-C2D	2.06	1.49	1.45
14	a	819	CLA	C1A-CHA	2.06	1.51	1.43
14	b	830	CLA	C1A-CHA	2.06	1.51	1.43
14	A	841	CLA	C4C-C3C	2.06	1.48	1.45
14	b	822	CLA	C1A-CHA	2.06	1.51	1.43
14	B	801	CLA	C1B-CHB	2.06	1.46	1.41
14	b	836	CLA	C1A-CHA	2.05	1.51	1.43
14	B	809	CLA	CMB-C2B	-2.05	1.47	1.51
17	I	101	BCR	C30-C25	-2.05	1.51	1.53
14	L	206	CLA	C4C-C3C	2.05	1.48	1.45
14	H	840	CLA	C4B-CHC	2.05	1.46	1.41
14	b	835	CLA	C1C-C2C	2.05	1.48	1.44
14	B	836	CLA	C1A-CHA	2.05	1.51	1.43
14	A	841	CLA	C1A-CHA	2.05	1.51	1.43
14	U	206	CLA	C4C-C3C	2.05	1.48	1.45
14	a	811	CLA	C4C-C3C	2.05	1.48	1.45
14	a	855	CLA	C1C-C2C	2.05	1.48	1.44
14	G	809	CLA	C1A-CHA	2.05	1.51	1.43
14	G	810	CLA	C1D-C2D	2.05	1.49	1.45
14	b	839	CLA	C1B-CHB	2.05	1.46	1.41
14	b	832	CLA	C1A-CHA	2.05	1.51	1.43
14	U	201	CLA	C1D-C2D	2.05	1.49	1.45
14	A	834	CLA	C4C-C3C	2.05	1.48	1.45
14	B	824	CLA	C4C-C3C	2.05	1.48	1.45
14	G	819	CLA	C1C-C2C	2.04	1.48	1.44
14	B	829	CLA	C4C-C3C	2.04	1.48	1.45
14	H	829	CLA	C4B-CHC	2.04	1.46	1.41
14	a	826	CLA	C1B-CHB	2.04	1.46	1.41
14	A	839	CLA	C1A-CHA	2.04	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	809	CLA	C1A-CHA	2.04	1.51	1.43
14	H	809	CLA	CMB-C2B	-2.04	1.47	1.51
14	A	827	CLA	C1D-C2D	2.04	1.49	1.45
14	b	833	CLA	C4C-C3C	2.04	1.48	1.45
14	G	841	CLA	C1A-CHA	2.04	1.51	1.43
14	a	817	CLA	C4C-C3C	2.04	1.48	1.45
14	G	833	CLA	C1A-CHA	2.04	1.51	1.43
14	l	207	CLA	C4C-C3C	2.04	1.48	1.45
14	G	806	CLA	C1B-CHB	2.04	1.46	1.41
14	U	201	CLA	C4C-C3C	2.04	1.48	1.45
14	j	102	CLA	C1A-CHA	2.04	1.51	1.43
14	b	817	CLA	C1A-CHA	2.04	1.51	1.43
14	b	826	CLA	C1B-CHB	2.04	1.46	1.41
14	b	817	CLA	C4B-CHC	2.04	1.46	1.41
14	j	101	CLA	C1A-CHA	2.04	1.51	1.43
14	H	817	CLA	C4C-C3C	2.03	1.48	1.45
14	G	827	CLA	C1C-C2C	2.03	1.48	1.44
14	G	811	CLA	C1D-C2D	2.03	1.49	1.45
14	G	814	CLA	C1A-CHA	2.03	1.51	1.43
14	G	838	CLA	C1A-CHA	2.03	1.51	1.43
14	a	808	CLA	C1A-CHA	2.03	1.51	1.43
14	H	820	CLA	C1A-CHA	2.03	1.51	1.43
14	H	832	CLA	C1A-CHA	2.03	1.51	1.43
14	H	812	CLA	C4B-CHC	2.03	1.46	1.41
14	A	817	CLA	C1A-CHA	2.03	1.51	1.43
14	U	201	CLA	C1A-CHA	2.03	1.51	1.43
14	X	1701	CLA	C4C-C3C	2.03	1.48	1.45
14	G	817	CLA	C1A-CHA	2.03	1.51	1.43
14	B	829	CLA	C1A-CHA	2.03	1.51	1.43
14	a	842	CLA	C1A-CHA	2.03	1.51	1.43
14	a	819	CLA	C1B-CHB	2.03	1.46	1.41
14	A	838	CLA	C1D-C2D	2.03	1.49	1.45
14	A	842	CLA	C1D-C2D	2.03	1.49	1.45
14	H	828	CLA	C1D-C2D	2.03	1.49	1.45
14	W	1701	CLA	C1D-C2D	2.03	1.49	1.45
14	B	809	CLA	C4C-C3C	2.03	1.48	1.45
14	a	834	CLA	C1B-CHB	2.03	1.46	1.41
14	X	1701	CLA	C1D-C2D	2.02	1.49	1.45
14	b	831	CLA	C1C-C2C	2.02	1.48	1.44
14	a	855	CLA	C1B-CHB	2.02	1.46	1.41
14	H	839	CLA	C1D-C2D	2.02	1.49	1.45
14	H	801	CLA	C1B-CHB	2.02	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	204	CLA	C1A-CHA	2.02	1.51	1.43
14	G	836	CLA	C1A-CHA	2.02	1.51	1.43
14	H	819	CLA	C1C-C2C	2.02	1.48	1.44
14	b	819	CLA	C1C-C2C	2.02	1.48	1.44
14	T	1401	CLA	C1C-C2C	2.02	1.48	1.44
14	a	822	CLA	C1A-CHA	2.02	1.51	1.43
14	A	821	CLA	C1D-C2D	2.02	1.49	1.45
14	b	815	CLA	C1A-CHA	2.02	1.51	1.43
14	B	821	CLA	C1D-C2D	2.02	1.49	1.45
14	B	817	CLA	C1A-CHA	2.02	1.51	1.43
14	b	826	CLA	C4C-C3C	2.02	1.48	1.45
14	U	204	CLA	C1A-CHA	2.02	1.51	1.43
14	b	812	CLA	C1A-CHA	2.02	1.51	1.43
14	B	821	CLA	C1C-C2C	2.02	1.48	1.44
14	b	804	CLA	C1A-CHA	2.02	1.51	1.43
14	A	828	CLA	C1A-CHA	2.02	1.51	1.43
14	A	819	CLA	C4C-C3C	2.02	1.48	1.45
14	A	838	CLA	C1A-CHA	2.02	1.51	1.43
13	A	801	CL0	CHB-C4A	2.02	1.34	1.33
14	G	819	CLA	C4C-C3C	2.01	1.48	1.45
14	b	825	CLA	C1C-C2C	2.01	1.48	1.44
14	G	842	CLA	C1A-CHA	2.01	1.51	1.43
14	b	811	CLA	C1C-C2C	2.01	1.48	1.44
14	b	802	CLA	C4C-C3C	2.01	1.48	1.45
14	b	805	CLA	C1A-CHA	2.01	1.51	1.43
14	G	827	CLA	C1B-CHB	2.01	1.46	1.41
14	B	832	CLA	C1A-CHA	2.01	1.51	1.43
14	A	840	CLA	C4C-C3C	2.01	1.48	1.45
14	a	839	CLA	C4C-C3C	2.01	1.48	1.45
14	H	804	CLA	C1C-C2C	2.01	1.48	1.44
14	A	812	CLA	C4B-CHC	2.01	1.46	1.41
14	b	829	CLA	C4C-C3C	2.01	1.48	1.45
14	A	820	CLA	C1A-CHA	2.01	1.51	1.43
14	H	830	CLA	C1A-CHA	2.01	1.51	1.43
14	L	201	CLA	C1D-C2D	2.01	1.49	1.45
14	A	837	CLA	C1B-CHB	2.01	1.46	1.41
14	A	804	CLA	C1C-C2C	2.01	1.48	1.44
14	b	826	CLA	C1A-CHA	2.01	1.51	1.43
14	B	813	CLA	C1A-CHA	2.00	1.51	1.43
14	b	840	CLA	CHB-C4A	2.00	1.34	1.33
14	G	835	CLA	C1B-CHB	2.00	1.46	1.41
14	B	808	CLA	C1A-CHA	2.00	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	818	CLA	C1A-CHA	2.00	1.51	1.43
14	A	810	CLA	CHB-C4A	2.00	1.34	1.33
14	b	813	CLA	C1A-CHA	2.00	1.51	1.43
14	a	802	CLA	C1B-CHB	2.00	1.46	1.41

All (8181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	849	BCR	C20-C21-C22	25.63	163.23	127.28
17	J	103	BCR	C16-C17-C18	25.34	162.82	127.28
17	A	849	BCR	C20-C21-C22	25.16	162.56	127.28
17	A	853	BCR	C20-C21-C22	24.52	161.67	127.28
17	H	847	BCR	C20-C21-C22	24.46	161.58	127.28
17	a	848	BCR	C20-C21-C22	24.02	160.96	127.28
17	b	847	BCR	C20-C21-C22	24.02	160.96	127.28
17	a	850	BCR	C20-C21-C22	23.67	160.47	127.28
17	S	104	BCR	C16-C17-C18	23.35	160.03	127.28
17	B	848	BCR	C20-C21-C22	23.23	159.85	127.28
17	G	851	BCR	C20-C21-C22	23.01	159.55	127.28
17	G	853	BCR	C20-C21-C22	23.00	159.54	127.28
17	S	104	BCR	C20-C21-C22	22.93	159.44	127.28
17	G	852	BCR	C20-C21-C22	22.88	159.37	127.28
17	J	103	BCR	C20-C21-C22	22.80	159.26	127.28
17	I	101	BCR	C20-C21-C22	22.72	159.15	127.28
17	b	845	BCR	C20-C21-C22	22.57	158.93	127.28
17	B	845	BCR	C20-C21-C22	22.46	158.78	127.28
17	B	842	BCR	C20-C21-C22	22.41	158.70	127.28
17	b	843	BCR	C20-C21-C22	22.37	158.65	127.28
17	R	101	BCR	C20-C21-C22	22.37	158.64	127.28
17	Q	202	BCR	C15-C16-C17	22.28	169.12	123.52
17	H	843	BCR	C20-C21-C22	22.21	158.42	127.28
17	f	201	BCR	C15-C16-C17	22.16	168.86	123.52
17	j	104	BCR	C16-C17-C18	22.14	158.32	127.28
17	M	1602	BCR	C20-C21-C22	22.06	158.21	127.28
17	A	852	BCR	C20-C21-C22	22.03	158.17	127.28
17	b	849	BCR	C20-C21-C22	21.94	158.05	127.28
17	A	853	BCR	C16-C17-C18	21.90	157.99	127.28
17	B	847	BCR	C15-C16-C17	21.86	168.25	123.52
17	a	852	BCR	C20-C21-C22	21.86	157.93	127.28
17	j	104	BCR	C20-C21-C22	21.82	157.88	127.28
17	H	845	BCR	C20-C21-C22	21.81	157.86	127.28
17	b	842	BCR	C20-C21-C22	21.78	157.82	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	852	BCR	C15-C16-C17	21.77	168.07	123.52
17	j	103	BCR	C20-C21-C22	21.76	157.80	127.28
17	G	849	BCR	C15-C16-C17	21.64	167.79	123.52
17	A	851	BCR	C20-C21-C22	21.60	157.58	127.28
17	B	850	BCR	C20-C21-C22	21.56	157.51	127.28
17	a	848	BCR	C15-C16-C17	21.55	167.62	123.52
17	H	847	BCR	C15-C16-C17	21.43	167.37	123.52
17	H	849	BCR	C20-C21-C22	21.42	157.32	127.28
17	G	851	BCR	C15-C16-C17	21.38	167.26	123.52
17	R	103	BCR	C20-C21-C22	21.37	157.25	127.28
17	f	203	BCR	C20-C21-C22	21.36	157.24	127.28
17	i	102	BCR	C20-C21-C22	21.36	157.23	127.28
17	V	1602	BCR	C16-C17-C18	21.33	157.19	127.28
17	m	1602	BCR	C16-C17-C18	21.31	157.16	127.28
17	V	1602	BCR	C20-C21-C22	21.30	157.15	127.28
17	b	846	BCR	C20-C21-C22	21.27	157.11	127.28
17	M	1602	BCR	C16-C17-C18	21.24	157.06	127.28
17	m	1602	BCR	C20-C21-C22	21.22	157.04	127.28
17	G	852	BCR	C15-C16-C17	21.20	166.90	123.52
17	B	846	BCR	C20-C21-C22	21.18	156.98	127.28
17	f	201	BCR	C20-C21-C22	21.14	156.93	127.28
17	a	851	BCR	C20-C21-C22	21.11	156.88	127.28
17	m	1602	BCR	C15-C16-C17	21.07	166.62	123.52
17	A	851	BCR	C16-C17-C18	21.06	156.81	127.28
17	Q	202	BCR	C20-C21-C22	21.04	156.79	127.28
17	H	843	BCR	C15-C16-C17	21.03	166.54	123.52
17	S	103	BCR	C20-C21-C22	21.01	156.74	127.28
17	j	103	BCR	C15-C16-C17	21.01	166.50	123.52
17	B	843	BCR	C16-C17-C18	20.97	156.69	127.28
17	a	850	BCR	C16-C17-C18	20.97	156.69	127.28
17	A	848	BCR	C16-C17-C18	20.95	156.66	127.28
17	b	842	BCR	C15-C16-C17	20.94	166.37	123.52
17	B	843	BCR	C20-C21-C22	20.90	156.59	127.28
17	B	850	BCR	C16-C17-C18	20.90	156.59	127.28
17	b	843	BCR	C15-C16-C17	20.87	166.22	123.52
17	F	1302	BCR	C20-C21-C22	20.87	156.55	127.28
17	l	201	BCR	C15-C16-C17	20.87	166.22	123.52
17	Q	204	BCR	C16-C17-C18	20.86	156.53	127.28
17	G	850	BCR	C20-C21-C22	20.84	156.51	127.28
17	B	842	BCR	C15-C16-C17	20.83	166.15	123.52
17	R	101	BCR	C16-C17-C18	20.81	156.47	127.28
17	J	102	BCR	C15-C16-C17	20.81	166.10	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	853	BCR	C16-C17-C18	20.81	156.46	127.28
17	H	846	BCR	C20-C21-C22	20.79	156.44	127.28
17	b	849	BCR	C16-C17-C18	20.76	156.40	127.28
17	H	845	BCR	C16-C17-C18	20.76	156.40	127.28
17	I	102	BCR	C20-C21-C22	20.76	156.39	127.28
17	U	202	BCR	C16-C17-C18	20.75	156.38	127.28
17	f	203	BCR	C15-C16-C17	20.74	165.96	123.52
17	a	850	BCR	C15-C16-C17	20.74	165.95	123.52
17	a	852	BCR	C15-C16-C17	20.71	165.90	123.52
17	H	842	BCR	C20-C21-C22	20.71	156.32	127.28
17	R	103	BCR	C15-C16-C17	20.70	165.88	123.52
17	b	844	BCR	C16-C17-C18	20.70	156.31	127.28
17	J	102	BCR	C20-C21-C22	20.69	156.30	127.28
17	l	208	BCR	C20-C21-C22	20.66	156.25	127.28
17	G	848	BCR	C16-C17-C18	20.65	156.24	127.28
17	i	102	BCR	C16-C17-C18	20.65	156.23	127.28
17	b	847	BCR	C15-C16-C17	20.64	165.76	123.52
17	a	851	BCR	C15-C16-C17	20.59	165.65	123.52
17	a	847	BCR	C16-C17-C18	20.59	156.15	127.28
17	G	852	BCR	C16-C17-C18	20.56	156.12	127.28
17	B	847	BCR	C20-C21-C22	20.55	156.09	127.28
17	M	1602	BCR	C15-C16-C17	20.53	165.52	123.52
17	R	102	BCR	C15-C16-C17	20.52	165.51	123.52
17	A	848	BCR	C20-C21-C22	20.52	156.06	127.28
17	L	207	BCR	C15-C16-C17	20.48	165.43	123.52
17	V	1602	BCR	C15-C16-C17	20.47	165.40	123.52
17	H	844	BCR	C16-C17-C18	20.44	155.95	127.28
17	I	102	BCR	C16-C17-C18	20.40	155.89	127.28
17	a	849	BCR	C20-C21-C22	20.40	155.89	127.28
17	L	202	BCR	C15-C16-C17	20.39	165.25	123.52
17	I	101	BCR	C16-C17-C18	20.37	155.84	127.28
17	A	851	BCR	C15-C16-C17	20.32	165.10	123.52
17	S	103	BCR	C15-C16-C17	20.32	165.09	123.52
17	G	853	BCR	C15-C16-C17	20.31	165.08	123.52
17	a	847	BCR	C20-C21-C22	20.31	155.76	127.28
17	Q	204	BCR	C15-C16-C17	20.30	165.06	123.52
17	H	842	BCR	C15-C16-C17	20.28	165.02	123.52
17	G	850	BCR	C16-C17-C18	20.28	155.72	127.28
17	b	845	BCR	C16-C17-C18	20.28	155.72	127.28
17	L	202	BCR	C16-C17-C18	20.28	155.71	127.28
17	F	1302	BCR	C15-C16-C17	20.25	164.96	123.52
17	l	203	BCR	C16-C17-C18	20.25	155.68	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	844	BCR	C20-C21-C22	20.22	155.64	127.28
17	a	849	BCR	C16-C17-C18	20.22	155.64	127.28
17	B	845	BCR	C16-C17-C18	20.22	155.63	127.28
17	l	203	BCR	C15-C16-C17	20.19	164.84	123.52
17	F	1302	BCR	C16-C17-C18	20.16	155.55	127.28
17	A	850	BCR	C20-C21-C22	20.14	155.52	127.28
17	B	845	BCR	C15-C16-C17	20.13	164.71	123.52
17	i	102	BCR	C15-C16-C17	20.13	164.70	123.52
17	A	849	BCR	C15-C16-C17	20.11	164.66	123.52
17	l	208	BCR	C15-C16-C17	20.11	164.66	123.52
17	B	843	BCR	C15-C16-C17	20.09	164.62	123.52
17	b	846	BCR	C16-C17-C18	20.09	155.45	127.28
17	U	202	BCR	C15-C16-C17	20.08	164.60	123.52
17	A	850	BCR	C15-C16-C17	20.05	164.54	123.52
17	R	102	BCR	C16-C17-C18	20.02	155.36	127.28
17	a	849	BCR	C15-C16-C17	20.00	164.45	123.52
17	I	101	BCR	C15-C16-C17	20.00	164.44	123.52
17	Q	204	BCR	C20-C21-C22	19.99	155.32	127.28
17	A	849	BCR	C16-C17-C18	19.96	155.27	127.28
17	H	846	BCR	C16-C17-C18	19.95	155.26	127.28
17	B	848	BCR	C16-C17-C18	19.95	155.26	127.28
17	B	848	BCR	C15-C16-C17	19.92	164.28	123.52
17	H	844	BCR	C15-C16-C17	19.91	164.26	123.52
17	B	844	BCR	C15-C16-C17	19.91	164.26	123.52
17	A	852	BCR	C16-C17-C18	19.88	155.16	127.28
17	B	844	BCR	C16-C17-C18	19.87	155.14	127.28
17	G	851	BCR	C16-C17-C18	19.86	155.13	127.28
17	Q	202	BCR	C16-C17-C18	19.83	155.09	127.28
17	b	844	BCR	C15-C16-C17	19.82	164.08	123.52
17	a	851	BCR	C16-C17-C18	19.80	155.04	127.28
17	B	846	BCR	C15-C16-C17	19.78	164.00	123.52
17	b	843	BCR	C16-C17-C18	19.78	155.02	127.28
17	a	852	BCR	C16-C17-C18	19.78	155.02	127.28
17	l	208	BCR	C16-C17-C18	19.76	154.99	127.28
17	b	844	BCR	C20-C21-C22	19.71	154.93	127.28
17	G	848	BCR	C20-C21-C22	19.71	154.92	127.28
17	I	102	BCR	C15-C16-C17	19.69	163.82	123.52
17	R	101	BCR	C15-C16-C17	19.66	163.75	123.52
17	B	846	BCR	C16-C17-C18	19.65	154.84	127.28
17	b	846	BCR	C15-C16-C17	19.55	163.51	123.52
17	H	846	BCR	C15-C16-C17	19.54	163.50	123.52
17	b	845	BCR	C15-C16-C17	19.53	163.49	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	850	BCR	C15-C16-C17	19.42	163.25	123.52
17	A	850	BCR	C16-C17-C18	19.39	154.47	127.28
17	S	104	BCR	C15-C16-C17	19.31	163.03	123.52
17	G	848	BCR	C15-C16-C17	19.31	163.02	123.52
17	f	203	BCR	C16-C17-C18	19.29	154.33	127.28
17	R	101	BCR	C10-C11-C12	19.20	178.82	123.20
17	j	103	BCR	C16-C17-C18	19.18	154.18	127.28
17	a	847	BCR	C10-C11-C12	19.17	178.75	123.20
17	b	847	BCR	C16-C17-C18	19.10	154.06	127.28
17	H	843	BCR	C16-C17-C18	19.05	153.99	127.28
17	R	103	BCR	C16-C17-C18	19.05	153.99	127.28
17	H	844	BCR	C20-C21-C22	19.03	153.96	127.28
17	J	102	BCR	C10-C11-C12	19.02	178.31	123.20
17	H	849	BCR	C16-C17-C18	19.01	153.93	127.28
17	j	104	BCR	C10-C11-C12	19.00	178.24	123.20
17	b	849	BCR	C15-C16-C17	18.99	162.38	123.52
17	R	102	BCR	C20-C21-C22	18.99	153.91	127.28
17	A	853	BCR	C15-C16-C17	18.98	162.35	123.52
17	a	847	BCR	C15-C16-C17	18.97	162.33	123.52
17	H	846	BCR	C10-C11-C12	18.97	178.15	123.20
17	L	207	BCR	C10-C11-C12	18.97	178.15	123.20
17	S	103	BCR	C10-C11-C12	18.96	178.13	123.20
17	B	847	BCR	C16-C17-C18	18.95	153.86	127.28
17	H	845	BCR	C15-C16-C17	18.95	162.28	123.52
17	Q	204	BCR	C10-C11-C12	18.94	178.08	123.20
17	G	848	BCR	C10-C11-C12	18.90	177.96	123.20
17	A	848	BCR	C15-C16-C17	18.88	162.16	123.52
17	l	201	BCR	C10-C11-C12	18.88	177.90	123.20
17	B	842	BCR	C10-C11-C12	18.87	177.89	123.20
17	J	102	BCR	C16-C17-C18	18.87	153.75	127.28
17	G	850	BCR	C10-C11-C12	18.84	177.79	123.20
17	L	202	BCR	C20-C21-C22	18.83	153.68	127.28
17	H	847	BCR	C10-C11-C12	18.82	177.74	123.20
17	b	846	BCR	C10-C11-C12	18.76	177.56	123.20
17	H	849	BCR	C10-C11-C12	18.76	177.55	123.20
17	H	844	BCR	C10-C11-C12	18.74	177.50	123.20
17	a	849	BCR	C10-C11-C12	18.72	177.44	123.20
17	A	851	BCR	C10-C11-C12	18.72	177.44	123.20
17	A	848	BCR	C10-C11-C12	18.72	177.43	123.20
17	I	102	BCR	C10-C11-C12	18.71	177.43	123.20
17	b	847	BCR	C10-C11-C12	18.71	177.43	123.20
17	H	849	BCR	C15-C16-C17	18.71	161.81	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	850	BCR	C15-C16-C17	18.70	161.78	123.52
17	A	850	BCR	C10-C11-C12	18.69	177.36	123.20
17	H	847	BCR	C16-C17-C18	18.66	153.45	127.28
17	b	849	BCR	C10-C11-C12	18.66	177.27	123.20
17	B	844	BCR	C10-C11-C12	18.61	177.11	123.20
17	m	1602	BCR	C10-C11-C12	18.59	177.07	123.20
17	S	104	BCR	C10-C11-C12	18.56	176.97	123.20
17	i	102	BCR	C10-C11-C12	18.52	176.86	123.20
17	f	201	BCR	C16-C17-C18	18.48	153.19	127.28
17	M	1602	BCR	C10-C11-C12	18.47	176.73	123.20
17	J	103	BCR	C10-C11-C12	18.47	176.71	123.20
17	b	842	BCR	C10-C11-C12	18.46	176.68	123.20
17	S	103	BCR	C16-C17-C18	18.46	153.16	127.28
17	R	103	BCR	C10-C11-C12	18.42	176.56	123.20
17	B	850	BCR	C10-C11-C12	18.39	176.50	123.20
17	H	842	BCR	C16-C17-C18	18.39	153.07	127.28
17	H	842	BCR	C10-C11-C12	18.38	176.46	123.20
17	B	847	BCR	C10-C11-C12	18.38	176.45	123.20
17	V	1602	BCR	C10-C11-C12	18.36	176.39	123.20
17	G	851	BCR	C10-C11-C12	18.35	176.38	123.20
17	a	848	BCR	C10-C11-C12	18.33	176.32	123.20
17	L	207	BCR	C16-C17-C18	18.32	152.97	127.28
17	B	848	BCR	C10-C11-C12	18.31	176.25	123.20
17	B	846	BCR	C10-C11-C12	18.30	176.22	123.20
17	A	852	BCR	C10-C11-C12	18.22	176.00	123.20
17	a	851	BCR	C10-C11-C12	18.19	175.91	123.20
17	J	103	BCR	C15-C16-C17	18.19	160.74	123.52
17	H	843	BCR	C10-C11-C12	18.16	175.83	123.20
17	B	843	BCR	C10-C11-C12	18.16	175.81	123.20
17	l	203	BCR	C10-C11-C12	18.15	175.79	123.20
17	a	850	BCR	C10-C11-C12	18.14	175.77	123.20
17	L	202	BCR	C10-C11-C12	18.13	175.73	123.20
17	I	101	BCR	C10-C11-C12	18.11	175.66	123.20
17	b	843	BCR	C10-C11-C12	18.09	175.62	123.20
17	G	849	BCR	C10-C11-C12	18.09	175.61	123.20
17	b	842	BCR	C16-C17-C18	18.09	152.64	127.28
17	a	852	BCR	C10-C11-C12	18.08	175.59	123.20
17	j	103	BCR	C10-C11-C12	18.07	175.56	123.20
17	l	201	BCR	C16-C17-C18	18.06	152.61	127.28
17	b	844	BCR	C10-C11-C12	18.06	175.53	123.20
17	G	852	BCR	C10-C11-C12	18.01	175.38	123.20
17	l	208	BCR	C10-C11-C12	17.96	175.24	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	853	BCR	C10-C11-C12	17.91	175.09	123.20
17	U	202	BCR	C10-C11-C12	17.90	175.08	123.20
17	f	201	BCR	C10-C11-C12	17.90	175.05	123.20
17	B	842	BCR	C16-C17-C18	17.86	152.32	127.28
17	A	849	BCR	C10-C11-C12	17.85	174.92	123.20
17	l	203	BCR	C20-C21-C22	17.84	152.30	127.28
17	R	102	BCR	C10-C11-C12	17.77	174.70	123.20
17	Q	202	BCR	C10-C11-C12	17.75	174.65	123.20
17	L	207	BCR	C20-C21-C22	17.74	152.16	127.28
17	a	848	BCR	C16-C17-C18	17.41	151.69	127.28
17	A	853	BCR	C10-C11-C12	17.40	173.62	123.20
17	U	202	BCR	C20-C21-C22	17.17	151.35	127.28
17	l	201	BCR	C20-C21-C22	16.92	151.01	127.28
17	f	203	BCR	C10-C11-C12	16.76	171.77	123.20
17	j	104	BCR	C15-C16-C17	16.54	157.36	123.52
17	G	849	BCR	C16-C17-C18	16.51	150.44	127.28
17	B	848	BCR	C21-C20-C19	16.44	170.83	123.20
17	R	101	BCR	C21-C20-C19	16.22	170.19	123.20
17	H	847	BCR	C21-C20-C19	16.12	169.90	123.20
17	i	102	BCR	C21-C20-C19	15.65	168.56	123.20
17	U	202	BCR	C21-C20-C19	15.36	167.71	123.20
17	I	101	BCR	C21-C20-C19	15.21	167.28	123.20
17	b	847	BCR	C21-C20-C19	15.16	167.12	123.20
17	b	844	BCR	C11-C10-C9	15.07	148.41	127.28
17	L	207	BCR	C21-C20-C19	15.05	166.79	123.20
17	H	842	BCR	C21-C20-C19	15.00	166.67	123.20
17	B	847	BCR	C21-C20-C19	14.88	166.32	123.20
17	G	848	BCR	C21-C20-C19	14.87	166.30	123.20
17	A	848	BCR	C21-C20-C19	14.87	166.28	123.20
17	a	847	BCR	C21-C20-C19	14.83	166.18	123.20
17	J	103	BCR	C16-C15-C14	14.82	153.84	123.52
17	J	103	BCR	C11-C10-C9	14.67	147.84	127.28
17	f	201	BCR	C21-C20-C19	14.66	165.69	123.20
17	b	844	BCR	C21-C20-C19	14.65	165.65	123.20
17	Q	202	BCR	C21-C20-C19	14.56	165.38	123.20
17	G	850	BCR	C21-C20-C19	14.55	165.35	123.20
17	a	849	BCR	C21-C20-C19	14.47	165.13	123.20
17	L	202	BCR	C21-C20-C19	14.46	165.08	123.20
17	A	853	BCR	C11-C10-C9	14.44	147.53	127.28
17	l	203	BCR	C21-C20-C19	14.43	165.00	123.20
17	A	850	BCR	C21-C20-C19	14.41	164.96	123.20
17	B	844	BCR	C21-C20-C19	14.41	164.96	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	844	BCR	C21-C20-C19	14.40	164.93	123.20
17	A	848	BCR	C16-C15-C14	14.38	152.94	123.52
17	j	104	BCR	C11-C10-C9	14.37	147.44	127.28
17	R	102	BCR	C21-C20-C19	14.35	164.78	123.20
17	l	201	BCR	C21-C20-C19	14.34	164.75	123.20
17	G	853	BCR	C11-C10-C9	14.32	147.36	127.28
17	j	104	BCR	C21-C20-C19	14.28	164.57	123.20
17	l	208	BCR	C21-C20-C19	14.28	164.56	123.20
17	B	850	BCR	C21-C20-C19	14.26	164.51	123.20
17	B	848	BCR	C11-C10-C9	14.24	147.24	127.28
17	Q	204	BCR	C21-C20-C19	14.22	164.41	123.20
17	I	102	BCR	C21-C20-C19	14.21	164.37	123.20
17	a	847	BCR	C16-C15-C14	14.20	152.57	123.52
17	A	849	BCR	C11-C10-C9	14.20	147.19	127.28
17	b	842	BCR	C21-C20-C19	14.18	164.29	123.20
17	A	848	BCR	C11-C10-C9	14.15	147.12	127.28
17	B	842	BCR	C21-C20-C19	14.05	163.90	123.20
17	i	102	BCR	C11-C10-C9	14.02	146.94	127.28
17	H	845	BCR	C16-C15-C14	14.00	152.16	123.52
17	S	104	BCR	C11-C10-C9	13.98	146.89	127.28
17	F	1302	BCR	C21-C20-C19	13.98	163.70	123.20
17	f	203	BCR	C21-C20-C19	13.97	163.69	123.20
17	A	849	BCR	C21-C20-C19	13.96	163.65	123.20
17	l	208	BCR	C11-C10-C9	13.94	146.83	127.28
17	R	103	BCR	C21-C20-C19	13.92	163.54	123.20
17	G	852	BCR	C11-C10-C9	13.91	146.78	127.28
17	b	849	BCR	C21-C20-C19	13.91	163.50	123.20
17	b	846	BCR	C21-C20-C19	13.90	163.49	123.20
17	H	846	BCR	C21-C20-C19	13.88	163.42	123.20
17	a	852	BCR	C11-C10-C9	13.84	146.68	127.28
17	Q	202	BCR	C11-C10-C9	13.81	146.65	127.28
17	m	1602	BCR	C21-C20-C19	13.80	163.19	123.20
17	a	851	BCR	C21-C20-C19	13.79	163.14	123.20
17	G	848	BCR	C16-C15-C14	13.78	151.72	123.52
17	B	850	BCR	C16-C15-C14	13.78	151.71	123.52
17	B	845	BCR	C21-C20-C19	13.77	163.11	123.20
17	b	849	BCR	C16-C15-C14	13.76	151.68	123.52
17	H	849	BCR	C21-C20-C19	13.76	163.06	123.20
17	m	1602	BCR	C11-C10-C9	13.74	146.55	127.28
17	V	1602	BCR	C11-C10-C9	13.70	146.50	127.28
17	a	848	BCR	C11-C10-C9	13.70	146.49	127.28
17	S	103	BCR	C21-C20-C19	13.69	162.88	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	j	104	BCR	C16-C15-C14	13.68	151.51	123.52
17	G	849	BCR	C11-C10-C9	13.68	146.46	127.28
17	j	103	BCR	C11-C10-C9	13.68	146.46	127.28
17	H	842	BCR	C11-C10-C9	13.65	146.42	127.28
17	I	102	BCR	C11-C10-C9	13.64	146.40	127.28
17	J	102	BCR	C21-C20-C19	13.64	162.71	123.20
17	H	849	BCR	C16-C15-C14	13.63	151.41	123.52
17	U	202	BCR	C11-C10-C9	13.62	146.38	127.28
17	R	103	BCR	C11-C10-C9	13.62	146.38	127.28
17	b	843	BCR	C11-C10-C9	13.62	146.37	127.28
17	b	842	BCR	C11-C10-C9	13.59	146.34	127.28
17	G	852	BCR	C21-C20-C19	13.53	162.42	123.20
17	S	104	BCR	C16-C15-C14	13.52	151.19	123.52
17	I	101	BCR	C11-C10-C9	13.52	146.24	127.28
17	b	845	BCR	C16-C15-C14	13.50	151.14	123.52
17	H	843	BCR	C21-C20-C19	13.47	162.24	123.20
17	a	850	BCR	C11-C10-C9	13.47	146.16	127.28
17	a	848	BCR	C21-C20-C19	13.46	162.20	123.20
17	B	843	BCR	C21-C20-C19	13.45	162.18	123.20
17	f	201	BCR	C11-C10-C9	13.42	146.10	127.28
17	B	847	BCR	C11-C10-C9	13.41	146.08	127.28
17	l	203	BCR	C11-C10-C9	13.40	146.07	127.28
17	G	851	BCR	C11-C10-C9	13.38	146.04	127.28
17	R	102	BCR	C11-C10-C9	13.35	146.01	127.28
17	F	1302	BCR	C10-C11-C12	13.35	161.88	123.20
17	a	851	BCR	C11-C10-C9	13.34	145.99	127.28
17	H	843	BCR	C11-C10-C9	13.34	145.99	127.28
17	a	852	BCR	C21-C20-C19	13.34	161.84	123.20
17	V	1602	BCR	C21-C20-C19	13.34	161.84	123.20
17	H	847	BCR	C11-C10-C9	13.32	145.96	127.28
17	M	1602	BCR	C21-C20-C19	13.29	161.72	123.20
17	H	842	BCR	C16-C15-C14	13.27	150.67	123.52
17	G	853	BCR	C21-C20-C19	13.27	161.64	123.20
17	I	102	BCR	C16-C15-C14	13.26	150.65	123.52
17	b	845	BCR	C21-C20-C19	13.22	161.52	123.20
17	B	843	BCR	C11-C10-C9	13.22	145.82	127.28
17	B	846	BCR	C21-C20-C19	13.22	161.50	123.20
17	a	847	BCR	C11-C10-C9	13.22	145.81	127.28
17	H	846	BCR	C16-C15-C14	13.16	150.46	123.52
17	A	851	BCR	C21-C20-C19	13.15	161.29	123.20
17	j	103	BCR	C21-C20-C19	13.14	161.27	123.20
17	A	852	BCR	C21-C20-C19	13.14	161.26	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	851	BCR	C21-C20-C19	13.13	161.25	123.20
17	L	202	BCR	C11-C10-C9	13.11	145.66	127.28
17	b	846	BCR	C16-C15-C14	13.10	150.33	123.52
17	B	845	BCR	C16-C15-C14	13.09	150.30	123.52
17	b	847	BCR	C11-C10-C9	13.08	145.62	127.28
17	H	845	BCR	C21-C20-C19	13.06	161.05	123.20
17	b	843	BCR	C21-C20-C19	13.03	160.97	123.20
17	A	852	BCR	C11-C10-C9	13.03	145.56	127.28
17	A	853	BCR	C16-C15-C14	13.00	150.12	123.52
17	S	104	BCR	C21-C20-C19	12.90	160.59	123.20
17	G	850	BCR	C11-C10-C9	12.87	145.32	127.28
17	A	850	BCR	C16-C15-C14	12.84	149.79	123.52
17	M	1602	BCR	C11-C10-C9	12.82	145.26	127.28
17	G	848	BCR	C11-C10-C9	12.81	145.25	127.28
17	l	208	BCR	C16-C15-C14	12.80	149.71	123.52
17	B	844	BCR	C16-C15-C14	12.77	149.65	123.52
17	B	846	BCR	C11-C10-C9	12.76	145.17	127.28
17	B	842	BCR	C11-C10-C9	12.73	145.13	127.28
17	Q	204	BCR	C11-C10-C9	12.69	145.08	127.28
17	b	844	BCR	C16-C15-C14	12.65	149.41	123.52
17	B	848	BCR	C16-C15-C14	12.65	149.40	123.52
17	J	103	BCR	C21-C20-C19	12.65	159.85	123.20
17	B	846	BCR	C16-C15-C14	12.63	149.35	123.52
17	V	1602	BCR	C16-C15-C14	12.62	149.35	123.52
17	B	844	BCR	C11-C10-C9	12.62	144.98	127.28
17	F	1302	BCR	C16-C15-C14	12.61	149.31	123.52
17	a	849	BCR	C11-C10-C9	12.60	144.95	127.28
17	H	844	BCR	C11-C10-C9	12.59	144.93	127.28
17	b	847	BCR	C16-C15-C14	12.54	149.17	123.52
17	S	103	BCR	C11-C10-C9	12.54	144.86	127.28
17	G	850	BCR	C16-C15-C14	12.53	149.16	123.52
17	G	849	BCR	C21-C20-C19	12.52	159.48	123.20
17	H	844	BCR	C16-C15-C14	12.48	149.05	123.52
17	A	853	BCR	C21-C20-C19	12.46	159.30	123.20
17	b	842	BCR	C16-C15-C14	12.41	148.91	123.52
17	L	207	BCR	C16-C15-C14	12.39	148.87	123.52
17	R	101	BCR	C16-C15-C14	12.36	148.82	123.52
17	a	850	BCR	C21-C20-C19	12.33	158.94	123.20
17	a	851	BCR	C16-C15-C14	12.31	148.71	123.52
17	U	202	BCR	C11-C12-C13	12.28	160.04	126.36
17	A	851	BCR	C11-C10-C9	12.27	144.49	127.28
17	S	103	BCR	C16-C15-C14	12.26	148.60	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	m	1602	BCR	C16-C15-C14	12.25	148.58	123.52
17	A	851	BCR	C16-C15-C14	12.24	148.56	123.52
17	B	842	BCR	C16-C15-C14	12.22	148.52	123.52
17	Q	204	BCR	C16-C15-C14	12.20	148.48	123.52
17	M	1602	BCR	C16-C15-C14	12.17	148.43	123.52
17	R	102	BCR	C11-C12-C13	12.16	159.72	126.36
17	i	102	BCR	C16-C15-C14	12.09	148.27	123.52
17	U	202	BCR	C16-C15-C14	12.09	148.26	123.52
17	A	853	BCR	C11-C12-C13	12.06	159.43	126.36
17	b	846	BCR	C11-C10-C9	12.02	144.14	127.28
17	I	101	BCR	C11-C12-C13	11.99	159.23	126.36
17	R	103	BCR	C16-C15-C14	11.98	148.04	123.52
17	a	852	BCR	C16-C15-C14	11.97	148.00	123.52
17	L	202	BCR	C11-C12-C13	11.95	159.13	126.36
17	R	102	BCR	C16-C15-C14	11.93	147.93	123.52
17	a	849	BCR	C16-C15-C14	11.93	147.93	123.52
17	l	203	BCR	C16-C15-C14	11.93	147.93	123.52
17	j	103	BCR	C11-C12-C13	11.91	159.02	126.36
17	G	853	BCR	C16-C15-C14	11.91	147.88	123.52
17	L	207	BCR	C11-C10-C9	11.90	143.97	127.28
17	I	101	BCR	C16-C15-C14	11.88	147.82	123.52
17	l	201	BCR	C11-C10-C9	11.86	143.91	127.28
17	R	101	BCR	C11-C10-C9	11.86	143.91	127.28
17	A	849	BCR	C16-C15-C14	11.85	147.76	123.52
17	a	852	BCR	C11-C12-C13	11.84	158.83	126.36
17	f	203	BCR	C16-C15-C14	11.82	147.69	123.52
17	G	853	BCR	C11-C12-C13	11.79	158.69	126.36
17	H	847	BCR	C16-C15-C14	11.77	147.61	123.52
17	B	843	BCR	C11-C12-C13	11.77	158.64	126.36
17	l	201	BCR	C16-C15-C14	11.77	147.60	123.52
17	B	850	BCR	C11-C12-C13	11.76	158.62	126.36
17	b	849	BCR	C11-C10-C9	11.75	143.75	127.28
17	M	1602	BCR	C11-C12-C13	11.74	158.57	126.36
17	l	208	BCR	C11-C12-C13	11.73	158.53	126.36
17	A	852	BCR	C11-C12-C13	11.72	158.51	126.36
17	G	849	BCR	C11-C12-C13	11.71	158.47	126.36
17	B	847	BCR	C11-C12-C13	11.70	158.45	126.36
17	b	843	BCR	C11-C12-C13	11.70	158.43	126.36
17	B	843	BCR	C16-C15-C14	11.69	147.44	123.52
17	a	851	BCR	C11-C12-C13	11.68	158.40	126.36
17	L	202	BCR	C16-C15-C14	11.67	147.39	123.52
17	H	843	BCR	C11-C12-C13	11.66	158.33	126.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	843	BCR	C16-C15-C14	11.65	147.36	123.52
17	H	846	BCR	C11-C10-C9	11.63	143.59	127.28
17	a	850	BCR	C16-C15-C14	11.58	147.21	123.52
17	H	843	BCR	C16-C15-C14	11.54	147.13	123.52
17	A	849	BCR	C11-C12-C13	11.54	158.00	126.36
17	j	103	BCR	C16-C15-C14	11.48	147.00	123.52
17	G	852	BCR	C11-C12-C13	11.45	157.75	126.36
17	G	852	BCR	C16-C15-C14	11.44	146.93	123.52
17	B	844	BCR	C11-C12-C13	11.44	157.72	126.36
17	b	844	BCR	C11-C12-C13	11.40	157.62	126.36
17	J	102	BCR	C16-C15-C14	11.40	146.84	123.52
17	A	850	BCR	C11-C10-C9	11.39	143.25	127.28
17	b	849	BCR	C11-C12-C13	11.38	157.58	126.36
17	f	201	BCR	C11-C12-C13	11.36	157.51	126.36
17	i	102	BCR	C11-C12-C13	11.34	157.45	126.36
17	R	103	BCR	C11-C12-C13	11.33	157.43	126.36
17	l	203	BCR	C11-C12-C13	11.32	157.40	126.36
17	B	842	BCR	C11-C12-C13	11.25	157.21	126.36
17	b	846	BCR	C11-C12-C13	11.22	157.13	126.36
17	G	851	BCR	C16-C15-C14	11.21	146.45	123.52
17	A	852	BCR	C16-C15-C14	11.18	146.40	123.52
17	Q	202	BCR	C11-C12-C13	11.16	156.96	126.36
17	G	851	BCR	C11-C12-C13	11.16	156.96	126.36
17	a	848	BCR	C16-C15-C14	11.14	146.32	123.52
17	G	849	BCR	C16-C15-C14	11.13	146.30	123.52
17	J	102	BCR	C11-C10-C9	11.09	142.82	127.28
17	a	848	BCR	C11-C12-C13	11.06	156.68	126.36
17	H	844	BCR	C11-C12-C13	11.05	156.65	126.36
17	l	201	BCR	C11-C12-C13	11.04	156.65	126.36
17	V	1602	BCR	C11-C12-C13	11.03	156.60	126.36
17	a	850	BCR	C11-C12-C13	11.02	156.57	126.36
17	B	850	BCR	C11-C10-C9	10.95	142.64	127.28
17	R	101	BCR	C11-C12-C13	10.93	156.33	126.36
17	B	848	BCR	C11-C12-C13	10.87	156.18	126.36
17	H	846	BCR	C11-C12-C13	10.86	156.14	126.36
17	J	102	BCR	C11-C12-C13	10.81	156.01	126.36
17	H	849	BCR	C11-C12-C13	10.81	155.99	126.36
17	B	846	BCR	C11-C12-C13	10.72	155.77	126.36
17	b	842	BCR	C11-C12-C13	10.68	155.65	126.36
17	B	847	BCR	C16-C15-C14	10.65	145.31	123.52
17	H	849	BCR	C11-C10-C9	10.60	142.14	127.28
17	a	849	BCR	C11-C12-C13	10.58	155.38	126.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	848	BCR	C11-C12-C13	10.58	155.38	126.36
17	A	851	BCR	C11-C12-C13	10.57	155.35	126.36
17	L	207	BCR	C11-C12-C13	10.57	155.34	126.36
17	H	847	BCR	C11-C12-C13	10.49	155.12	126.36
17	m	1602	BCR	C11-C12-C13	10.48	155.10	126.36
17	G	848	BCR	C11-C12-C13	10.42	154.93	126.36
17	b	847	BCR	C11-C12-C13	10.40	154.88	126.36
17	S	103	BCR	C11-C12-C13	10.40	154.87	126.36
17	a	847	BCR	C11-C12-C13	10.40	154.87	126.36
17	I	102	BCR	C11-C12-C13	10.39	154.84	126.36
17	Q	202	BCR	C16-C15-C14	10.36	144.73	123.52
17	f	201	BCR	C16-C15-C14	10.32	144.64	123.52
17	G	850	BCR	C11-C12-C13	10.10	154.05	126.36
17	H	842	BCR	C11-C12-C13	9.99	153.76	126.36
17	j	104	BCR	C11-C12-C13	9.83	153.31	126.36
17	Q	204	BCR	C11-C12-C13	9.67	152.88	126.36
14	a	811	CLA	CMD-C2D-C1D	9.48	141.43	124.73
17	J	103	BCR	C11-C12-C13	9.34	151.98	126.36
14	G	812	CLA	CMD-C2D-C1D	9.22	140.96	124.73
14	A	824	CLA	CMD-C2D-C1D	9.19	140.91	124.73
14	H	837	CLA	CMD-C2D-C1D	9.10	140.76	124.73
14	H	828	CLA	CMD-C2D-C1D	9.06	140.69	124.73
14	A	819	CLA	CMD-C2D-C1D	8.94	140.47	124.73
17	A	850	BCR	C11-C12-C13	8.88	150.71	126.36
14	A	812	CLA	CMD-C2D-C1D	8.87	140.35	124.73
17	G	849	BCR	C20-C19-C18	8.85	150.63	126.36
14	H	835	CLA	CMD-C2D-C1D	8.84	140.29	124.73
14	b	837	CLA	CMD-C2D-C1D	8.83	140.27	124.73
14	B	828	CLA	CMD-C2D-C1D	8.82	140.25	124.73
14	a	818	CLA	CMD-C2D-C1D	8.81	140.25	124.73
14	G	824	CLA	CMD-C2D-C1D	8.78	140.19	124.73
14	b	828	CLA	CMD-C2D-C1D	8.74	140.12	124.73
14	H	806	CLA	CMD-C2D-C1D	8.71	140.06	124.73
14	B	806	CLA	CMD-C2D-C1D	8.66	139.98	124.73
14	G	815	CLA	CMD-C2D-C1D	8.64	139.95	124.73
17	a	850	BCR	C20-C19-C18	8.63	150.04	126.36
17	S	104	BCR	C11-C12-C13	8.62	150.01	126.36
17	J	103	BCR	C20-C19-C18	8.60	149.94	126.36
14	a	807	CLA	CMD-C2D-C1D	8.59	139.86	124.73
14	B	839	CLA	CMD-C2D-C1D	8.58	139.83	124.73
14	J	101	CLA	CMD-C2D-C1D	8.54	139.76	124.73
14	G	818	CLA	CMD-C2D-C1D	8.44	139.60	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	831	CLA	CMD-C2D-C1D	8.44	139.59	124.73
14	a	814	CLA	CMD-C2D-C1D	8.42	139.56	124.73
14	b	838	CLA	CMD-C2D-C1D	8.42	139.55	124.73
14	j	101	CLA	CMD-C2D-C1D	8.41	139.54	124.73
14	a	823	CLA	CMD-C2D-C1D	8.40	139.52	124.73
14	B	833	CLA	CMD-C2D-C1D	8.40	139.51	124.73
14	B	818	CLA	CMD-C2D-C1D	8.39	139.51	124.73
14	A	806	CLA	CMD-C2D-C1D	8.39	139.51	124.73
14	a	813	CLA	CMD-C2D-C1D	8.39	139.50	124.73
14	b	839	CLA	CMD-C2D-C1D	8.39	139.50	124.73
14	b	806	CLA	CMD-C2D-C1D	8.38	139.49	124.73
14	a	817	CLA	CMD-C2D-C1D	8.37	139.47	124.73
17	S	104	BCR	C20-C19-C18	8.36	149.29	126.36
14	V	1601	CLA	CMD-C2D-C1D	8.36	139.45	124.73
14	H	818	CLA	CMD-C2D-C1D	8.31	139.37	124.73
14	b	832	CLA	CMD-C2D-C1D	8.30	139.35	124.73
14	B	810	CLA	CMD-C2D-C1D	8.29	139.33	124.73
14	b	835	CLA	CMD-C2D-C1D	8.29	139.33	124.73
14	B	831	CLA	CMD-C2D-C1D	8.29	139.33	124.73
14	b	834	CLA	CMD-C2D-C1D	8.28	139.31	124.73
14	b	833	CLA	CMD-C2D-C1D	8.28	139.31	124.73
14	G	807	CLA	CMD-C2D-C1D	8.28	139.31	124.73
14	G	819	CLA	CMD-C2D-C1D	8.28	139.31	124.73
14	H	813	CLA	CMD-C2D-C1D	8.28	139.30	124.73
14	G	844	CLA	CMD-C2D-C1D	8.28	139.30	124.73
14	a	816	CLA	CMD-C2D-C1D	8.28	139.30	124.73
14	a	842	CLA	CMD-C2D-C1D	8.27	139.29	124.73
14	G	834	CLA	CMD-C2D-C1D	8.27	139.29	124.73
14	G	805	CLA	CMD-C2D-C1D	8.27	139.28	124.73
14	H	810	CLA	CMD-C2D-C1D	8.25	139.25	124.73
14	b	818	CLA	CMD-C2D-C1D	8.25	139.25	124.73
14	B	815	CLA	CMD-C2D-C1D	8.24	139.24	124.73
14	H	832	CLA	CMD-C2D-C1D	8.24	139.24	124.73
14	b	807	CLA	CMD-C2D-C1D	8.24	139.24	124.73
14	A	825	CLA	CMD-C2D-C1D	8.24	139.24	124.73
14	B	838	CLA	CMD-C2D-C1D	8.24	139.24	124.73
14	a	840	CLA	CMD-C2D-C1D	8.23	139.23	124.73
14	b	830	CLA	CMD-C2D-C1D	8.22	139.21	124.73
14	H	815	CLA	CMD-C2D-C1D	8.22	139.20	124.73
14	a	839	CLA	CMD-C2D-C1D	8.21	139.19	124.73
14	G	809	CLA	CMD-C2D-C1D	8.21	139.18	124.73
14	a	810	CLA	CMD-C2D-C1D	8.21	139.18	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	845	CLA	CMD-C2D-C1D	8.20	139.17	124.73
14	A	817	CLA	CMD-C2D-C1D	8.18	139.14	124.73
14	a	808	CLA	CMD-C2D-C1D	8.18	139.13	124.73
14	A	808	CLA	CMD-C2D-C1D	8.17	139.12	124.73
14	G	808	CLA	CMD-C2D-C1D	8.16	139.11	124.73
14	F	1303	CLA	CMD-C2D-C1D	8.16	139.10	124.73
14	H	833	CLA	CMD-C2D-C1D	8.16	139.10	124.73
17	f	203	BCR	C11-C10-C9	8.16	138.72	127.28
14	A	814	CLA	CMD-C2D-C1D	8.15	139.09	124.73
14	a	827	CLA	CMD-C2D-C1D	8.15	139.09	124.73
14	B	835	CLA	CMD-C2D-C1D	8.15	139.08	124.73
14	a	832	CLA	CMD-C2D-C1D	8.15	139.08	124.73
14	b	805	CLA	CMD-C2D-C1D	8.14	139.07	124.73
14	G	817	CLA	CMD-C2D-C1D	8.14	139.06	124.73
14	b	810	CLA	CMD-C2D-C1D	8.14	139.06	124.73
14	G	837	CLA	CMD-C2D-C1D	8.14	139.06	124.73
14	A	811	CLA	CMD-C2D-C1D	8.14	139.06	124.73
17	l	208	BCR	C24-C23-C22	-8.14	114.20	126.23
14	B	813	CLA	CMD-C2D-C1D	8.14	139.05	124.73
14	Q	201	CLA	CMD-C2D-C1D	8.12	139.02	124.73
14	A	807	CLA	CMD-C2D-C1D	8.11	139.02	124.73
14	G	822	CLA	CMD-C2D-C1D	8.11	139.01	124.73
14	H	839	CLA	CMD-C2D-C1D	8.11	139.01	124.73
14	a	843	CLA	CMD-C2D-C1D	8.11	139.01	124.73
14	b	831	CLA	CMD-C2D-C1D	8.11	139.00	124.73
17	F	1302	BCR	C11-C10-C9	8.11	138.65	127.28
14	G	838	CLA	CMD-C2D-C1D	8.10	139.00	124.73
17	V	1602	BCR	C20-C19-C18	8.10	148.59	126.36
14	G	835	CLA	CMD-C2D-C1D	8.10	139.00	124.73
14	a	805	CLA	CMD-C2D-C1D	8.10	139.00	124.73
14	m	1601	CLA	CMD-C2D-C1D	8.10	138.99	124.73
14	a	820	CLA	CMD-C2D-C1D	8.10	138.99	124.73
14	G	827	CLA	CMD-C2D-C1D	8.10	138.99	124.73
14	A	834	CLA	CMD-C2D-C1D	8.09	138.98	124.73
17	B	843	BCR	C20-C19-C18	8.09	148.56	126.36
14	M	1601	CLA	CMD-C2D-C1D	8.09	138.97	124.73
14	b	814	CLA	CMD-C2D-C1D	8.09	138.97	124.73
14	H	830	CLA	CMD-C2D-C1D	8.09	138.97	124.73
14	A	804	CLA	CMD-C2D-C1D	8.08	138.96	124.73
14	G	845	CLA	CMD-C2D-C1D	8.08	138.96	124.73
14	A	805	CLA	CMD-C2D-C1D	8.08	138.95	124.73
14	a	821	CLA	CMD-C2D-C1D	8.07	138.94	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	828	CLA	CMD-C2D-C1D	8.06	138.93	124.73
14	B	830	CLA	CMD-C2D-C1D	8.06	138.92	124.73
14	G	810	CLA	CMD-C2D-C1D	8.06	138.91	124.73
14	G	811	CLA	CMD-C2D-C1D	8.06	138.91	124.73
14	b	815	CLA	CMD-C2D-C1D	8.05	138.90	124.73
14	a	833	CLA	CMD-C2D-C1D	8.05	138.90	124.73
14	a	836	CLA	CMD-C2D-C1D	8.05	138.90	124.73
14	G	816	CLA	CMD-C2D-C1D	8.05	138.90	124.73
14	B	837	CLA	CMD-C2D-C1D	8.04	138.89	124.73
14	G	820	CLA	CMD-C2D-C1D	8.03	138.87	124.73
14	G	841	CLA	CMD-C2D-C1D	8.02	138.85	124.73
14	i	101	CLA	CMD-C2D-C1D	8.02	138.85	124.73
17	b	843	BCR	C20-C19-C18	8.01	148.33	126.36
17	f	203	BCR	C11-C12-C13	8.01	148.32	126.36
14	H	807	CLA	CMD-C2D-C1D	8.01	138.83	124.73
14	A	816	CLA	CMD-C2D-C1D	8.01	138.83	124.73
14	B	834	CLA	CMD-C2D-C1D	8.00	138.82	124.73
17	j	103	BCR	C20-C19-C18	7.99	148.28	126.36
14	B	832	CLA	CMD-C2D-C1D	7.99	138.81	124.73
14	b	816	CLA	CMD-C2D-C1D	7.99	138.80	124.73
14	a	844	CLA	CMD-C2D-C1D	7.99	138.79	124.73
14	A	809	CLA	CMD-C2D-C1D	7.99	138.79	124.73
14	U	204	CLA	CMD-C2D-C1D	7.98	138.78	124.73
14	H	836	CLA	CMD-C2D-C1D	7.98	138.78	124.73
14	a	806	CLA	CMD-C2D-C1D	7.97	138.77	124.73
14	A	841	CLA	CMD-C2D-C1D	7.97	138.77	124.73
14	H	816	CLA	CMD-C2D-C1D	7.97	138.76	124.73
14	l	207	CLA	CMD-C2D-C1D	7.97	138.76	124.73
14	G	842	CLA	CMD-C2D-C1D	7.96	138.75	124.73
17	F	1302	BCR	C11-C12-C13	7.96	148.18	126.36
14	A	826	CLA	CMD-C2D-C1D	7.95	138.73	124.73
14	a	837	CLA	CMD-C2D-C1D	7.93	138.70	124.73
17	A	851	BCR	C20-C19-C18	7.93	148.12	126.36
14	x	1701	CLA	CMD-C2D-C1D	7.93	138.69	124.73
14	j	102	CLA	CMD-C2D-C1D	7.92	138.68	124.73
14	A	821	CLA	CMD-C2D-C1D	7.92	138.68	124.73
14	a	815	CLA	CMD-C2D-C1D	7.92	138.68	124.73
14	b	820	CLA	CMD-C2D-C1D	7.92	138.67	124.73
14	A	815	CLA	CMD-C2D-C1D	7.92	138.67	124.73
14	G	814	CLA	CMD-C2D-C1D	7.91	138.66	124.73
14	H	805	CLA	CMD-C2D-C1D	7.91	138.65	124.73
14	a	804	CLA	CMD-C2D-C1D	7.91	138.65	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	804	CLA	CMD-C2D-C1D	7.91	138.65	124.73
17	G	851	BCR	C20-C19-C18	7.90	148.03	126.36
14	B	805	CLA	CMD-C2D-C1D	7.90	138.63	124.73
17	M	1602	BCR	C20-C19-C18	7.90	148.01	126.36
14	H	838	CLA	CMD-C2D-C1D	7.89	138.63	124.73
14	a	809	CLA	CMD-C2D-C1D	7.89	138.63	124.73
14	G	833	CLA	CMD-C2D-C1D	7.89	138.62	124.73
14	a	824	CLA	CMD-C2D-C1D	7.88	138.61	124.73
14	S	101	CLA	CMD-C2D-C1D	7.87	138.59	124.73
14	H	812	CLA	CMD-C2D-C1D	7.87	138.59	124.73
14	A	840	CLA	CMD-C2D-C1D	7.87	138.59	124.73
14	A	839	CLA	CMD-C2D-C1D	7.87	138.59	124.73
14	S	102	CLA	CMD-C2D-C1D	7.87	138.59	124.73
14	A	837	CLA	CMD-C2D-C1D	7.87	138.58	124.73
14	H	834	CLA	CMD-C2D-C1D	7.87	138.58	124.73
14	L	206	CLA	CMD-C2D-C1D	7.86	138.58	124.73
14	a	826	CLA	CMD-C2D-C1D	7.86	138.56	124.73
14	b	840	CLA	CMD-C2D-C1D	7.85	138.56	124.73
14	B	804	CLA	CMD-C2D-C1D	7.85	138.55	124.73
14	U	206	CLA	CMD-C2D-C1D	7.84	138.53	124.73
14	G	813	CLA	CMD-C2D-C1D	7.83	138.52	124.73
14	G	806	CLA	CMD-C2D-C1D	7.82	138.51	124.73
14	A	833	CLA	CMD-C2D-C1D	7.82	138.50	124.73
14	G	823	CLA	CMD-C2D-C1D	7.82	138.49	124.73
14	G	828	CLA	CMD-C2D-C1D	7.81	138.49	124.73
14	G	821	CLA	CMD-C2D-C1D	7.81	138.49	124.73
14	L	204	CLA	CMD-C2D-C1D	7.81	138.48	124.73
14	B	816	CLA	CMD-C2D-C1D	7.81	138.48	124.73
14	K	101	CLA	CMD-C2D-C1D	7.81	138.48	124.73
14	a	822	CLA	CMD-C2D-C1D	7.81	138.47	124.73
14	a	838	CLA	CMD-C2D-C1D	7.78	138.43	124.73
14	b	812	CLA	CMD-C2D-C1D	7.78	138.42	124.73
14	B	814	CLA	CMD-C2D-C1D	7.77	138.42	124.73
14	b	829	CLA	CMD-C2D-C1D	7.76	138.40	124.73
14	X	1701	CLA	CMD-C2D-C1D	7.75	138.38	124.73
14	a	819	CLA	CMD-C2D-C1D	7.75	138.37	124.73
17	S	103	BCR	C20-C19-C18	7.74	147.58	126.36
14	H	804	CLA	CMD-C2D-C1D	7.73	138.34	124.73
17	J	102	BCR	C20-C19-C18	7.72	147.53	126.36
14	B	817	CLA	CMD-C2D-C1D	7.72	138.32	124.73
14	U	201	CLA	CMD-C2D-C1D	7.71	138.31	124.73
14	A	822	CLA	CMD-C2D-C1D	7.71	138.31	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	840	CLA	CMD-C2D-C1D	7.71	138.31	124.73
14	a	812	CLA	CMD-C2D-C1D	7.71	138.30	124.73
14	A	838	CLA	CMD-C2D-C1D	7.70	138.28	124.73
17	a	848	BCR	C20-C19-C18	7.70	147.46	126.36
14	a	841	CLA	CMD-C2D-C1D	7.69	138.28	124.73
14	B	829	CLA	CMD-C2D-C1D	7.69	138.26	124.73
14	A	818	CLA	CMD-C2D-C1D	7.69	138.26	124.73
14	B	840	CLA	CMD-C2D-C1D	7.68	138.26	124.73
14	K	102	CLA	CMD-C2D-C1D	7.68	138.26	124.73
14	l	205	CLA	CMD-C2D-C1D	7.68	138.25	124.73
14	H	817	CLA	CMD-C2D-C1D	7.67	138.24	124.73
14	A	827	CLA	CMD-C2D-C1D	7.67	138.23	124.73
14	G	825	CLA	CMD-C2D-C1D	7.66	138.22	124.73
14	b	811	CLA	CMD-C2D-C1D	7.65	138.20	124.73
14	H	808	CLA	CMD-C2D-C1D	7.65	138.20	124.73
14	H	820	CLA	CMD-C2D-C1D	7.65	138.19	124.73
14	H	814	CLA	CMD-C2D-C1D	7.64	138.19	124.73
14	B	825	CLA	CMD-C2D-C1D	7.64	138.19	124.73
14	B	811	CLA	CMD-C2D-C1D	7.64	138.19	124.73
14	G	832	CLA	CMD-C2D-C1D	7.64	138.18	124.73
14	B	826	CLA	CMD-C2D-C1D	7.64	138.18	124.73
14	A	820	CLA	CMD-C2D-C1D	7.63	138.17	124.73
14	G	839	CLA	CMD-C2D-C1D	7.61	138.13	124.73
14	a	834	CLA	CMD-C2D-C1D	7.61	138.13	124.73
14	G	840	CLA	CMD-C2D-C1D	7.60	138.11	124.73
14	b	821	CLA	CMD-C2D-C1D	7.60	138.11	124.73
14	B	820	CLA	CMD-C2D-C1D	7.59	138.10	124.73
14	b	808	CLA	CMD-C2D-C1D	7.58	138.08	124.73
14	B	807	CLA	CMD-C2D-C1D	7.58	138.08	124.73
14	H	803	CLA	C4A-NA-C1A	7.57	110.13	106.68
14	G	836	CLA	CMD-C2D-C1D	7.56	138.05	124.73
17	B	846	BCR	C20-C19-C18	7.56	147.10	126.36
14	b	819	CLA	CMD-C2D-C1D	7.56	138.04	124.73
17	A	853	BCR	C20-C19-C18	7.55	147.06	126.36
14	b	813	CLA	CMD-C2D-C1D	7.54	138.00	124.73
14	H	819	CLA	CMD-C2D-C1D	7.53	137.98	124.73
17	A	852	BCR	C20-C19-C18	7.52	146.98	126.36
14	L	201	CLA	CMD-C2D-C1D	7.50	137.93	124.73
14	A	835	CLA	CMD-C2D-C1D	7.49	137.92	124.73
17	H	843	BCR	C20-C19-C18	7.49	146.90	126.36
14	H	829	CLA	CMD-C2D-C1D	7.47	137.89	124.73
14	T	1401	CLA	CMD-C2D-C1D	7.47	137.88	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	W	1701	CLA	CMD-C2D-C1D	7.45	137.85	124.73
14	B	809	CLA	CMD-C2D-C1D	7.45	137.85	124.73
14	b	822	CLA	CMD-C2D-C1D	7.44	137.83	124.73
14	b	834	CLA	C2C-C1C-NC	7.44	117.79	109.98
14	a	831	CLA	CMD-C2D-C1D	7.43	137.81	124.73
14	a	803	CLA	CMD-C2D-C1D	7.42	137.80	124.73
14	A	832	CLA	CMD-C2D-C1D	7.41	137.78	124.73
17	F	1302	BCR	C20-C19-C18	7.39	146.64	126.36
14	f	202	CLA	CMD-C2D-C1D	7.38	137.72	124.73
14	A	843	CLA	CMD-C2D-C1D	7.36	137.69	124.73
14	k	1401	CLA	CMD-C2D-C1D	7.34	137.65	124.73
14	b	829	CLA	C2C-C1C-NC	7.33	117.68	109.98
14	H	825	CLA	CMD-C2D-C1D	7.33	137.63	124.73
14	G	803	CLA	CMD-C2D-C1D	7.31	137.61	124.73
14	A	842	CLA	CMD-C2D-C1D	7.31	137.61	124.73
14	b	827	CLA	CMD-C2D-C1D	7.31	137.60	124.73
14	b	826	CLA	CMD-C2D-C1D	7.31	137.59	124.73
17	b	845	BCR	C20-C19-C18	7.30	146.39	126.36
14	B	812	CLA	CMD-C2D-C1D	7.28	137.55	124.73
14	B	840	CLA	C4A-NA-C1A	7.27	110.00	106.68
14	l	202	CLA	CMD-C2D-C1D	7.26	137.51	124.73
14	l	206	CLA	CMD-C2D-C1D	7.25	137.49	124.73
14	b	825	CLA	CMD-C2D-C1D	7.25	137.49	124.73
14	H	840	CLA	C4A-NA-C1A	7.23	109.98	106.68
14	H	821	CLA	CMD-C2D-C1D	7.21	137.43	124.73
14	L	205	CLA	CMD-C2D-C1D	7.21	137.42	124.73
14	b	817	CLA	CMD-C2D-C1D	7.18	137.37	124.73
14	H	809	CLA	C2C-C1C-NC	7.17	117.52	109.98
17	G	852	BCR	C20-C19-C18	7.17	146.04	126.36
14	a	828	CLA	CMD-C2D-C1D	7.17	137.35	124.73
17	j	104	BCR	C20-C19-C18	7.17	146.02	126.36
14	A	803	CLA	CMD-C2D-C1D	7.15	137.33	124.73
17	H	849	BCR	C20-C19-C18	7.14	145.94	126.36
14	b	809	CLA	CMD-C2D-C1D	7.13	137.29	124.73
14	H	826	CLA	CMD-C2D-C1D	7.13	137.28	124.73
17	m	1602	BCR	C20-C19-C18	7.12	145.89	126.36
14	B	821	CLA	CMD-C2D-C1D	7.12	137.27	124.73
14	B	809	CLA	C2C-C1C-NC	7.12	117.46	109.98
14	A	829	CLA	CMD-C2D-C1D	7.09	137.21	124.73
17	H	845	BCR	C20-C19-C18	7.08	145.76	126.36
14	B	824	CLA	CMD-C2D-C1D	7.07	137.19	124.73
14	A	813	CLA	CMD-C2D-C1D	7.07	137.18	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	840	CLA	C2C-C1C-NC	7.07	117.40	109.98
17	Q	204	BCR	C20-C19-C18	7.06	145.73	126.36
14	G	831	CLA	CMD-C2D-C1D	7.06	137.15	124.73
17	b	846	BCR	C20-C19-C18	7.05	145.68	126.36
14	U	205	CLA	CMD-C2D-C1D	7.04	137.12	124.73
14	B	829	CLA	C2C-C1C-NC	7.04	117.37	109.98
14	H	824	CLA	CMD-C2D-C1D	7.03	137.11	124.73
14	G	829	CLA	CMD-C2D-C1D	7.03	137.11	124.73
14	H	829	CLA	C2C-C1C-NC	7.01	117.35	109.98
14	H	814	CLA	C4A-NA-C1A	7.00	109.87	106.68
14	G	845	CLA	O2D-CGD-CBD	6.99	123.44	111.23
14	A	836	CLA	CMD-C2D-C1D	6.98	137.02	124.73
17	b	843	BCR	C24-C23-C22	-6.97	115.92	126.23
17	a	851	BCR	C20-C19-C18	6.94	145.40	126.36
14	B	819	CLA	CMD-C2D-C1D	6.94	136.96	124.73
14	l	202	CLA	C2C-C1C-NC	6.94	117.27	109.98
17	H	844	BCR	C20-C19-C18	6.93	145.38	126.36
14	A	810	CLA	CMD-C2D-C1D	6.93	136.93	124.73
14	B	822	CLA	CMD-C2D-C1D	6.93	136.93	124.73
17	B	845	BCR	C20-C19-C18	6.92	145.34	126.36
14	B	827	CLA	CMD-C2D-C1D	6.92	136.91	124.73
14	B	802	CLA	C4A-NA-C1A	6.89	109.82	106.68
17	U	202	BCR	C7-C8-C9	-6.89	116.04	126.23
14	b	809	CLA	C2C-C1C-NC	6.88	117.21	109.98
14	a	844	CLA	O2D-CGD-CBD	6.87	123.24	111.23
14	a	802	CLA	CMD-C2D-C1D	6.86	136.82	124.73
14	H	811	CLA	CMD-C2D-C1D	6.84	136.78	124.73
17	R	102	BCR	C20-C19-C18	6.84	145.13	126.36
14	B	840	CLA	C2C-C1C-NC	6.84	117.16	109.98
17	A	849	BCR	C20-C19-C18	6.84	145.11	126.36
14	a	829	CLA	CMD-C2D-C1D	6.83	136.75	124.73
14	b	811	CLA	O2D-CGD-CBD	6.82	123.16	111.23
14	b	840	CLA	C4A-NA-C1A	6.82	109.79	106.68
17	l	201	BCR	C20-C19-C18	6.82	145.07	126.36
14	b	804	CLA	CAC-C3C-C4C	6.82	133.67	124.79
14	A	844	CLA	C2C-C1C-NC	6.82	117.14	109.98
14	H	827	CLA	CMD-C2D-C1D	6.81	136.73	124.73
17	b	849	BCR	C20-C19-C18	6.79	144.99	126.36
14	B	836	CLA	CMD-C2D-C1D	6.79	136.69	124.73
14	H	803	CLA	CAC-C3C-C4C	6.79	133.63	124.79
17	H	846	BCR	C20-C19-C18	6.79	144.98	126.36
17	B	843	BCR	C24-C23-C22	-6.79	116.19	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	802	CLA	C4A-NA-C1A	6.79	109.78	106.68
17	I	102	BCR	C24-C23-C22	-6.76	116.23	126.23
14	H	835	CLA	C2C-C1C-NC	6.76	117.08	109.98
17	f	203	BCR	C20-C19-C18	6.75	144.88	126.36
14	G	845	CLA	C4A-NA-C1A	6.74	109.75	106.68
14	H	811	CLA	O2D-CGD-CBD	6.74	123.01	111.23
17	I	102	BCR	C20-C19-C18	6.74	144.84	126.36
14	B	837	CLA	C1C-C2C-C3C	-6.74	99.90	106.98
17	B	844	BCR	C20-C19-C18	6.73	144.81	126.36
14	b	801	CLA	C2D-C1D-ND	6.72	116.78	110.13
14	A	830	CLA	O2D-CGD-CBD	6.72	122.98	111.23
14	H	840	CLA	C2C-C1C-NC	6.72	117.03	109.98
14	H	838	CLA	C2C-C1C-NC	6.69	117.00	109.98
17	l	203	BCR	C20-C19-C18	6.68	144.67	126.36
14	b	824	CLA	CMD-C2D-C1D	6.68	136.48	124.73
17	A	853	BCR	C24-C23-C22	-6.67	116.36	126.23
14	a	835	CLA	CMD-C2D-C1D	6.67	136.47	124.73
14	H	803	CLA	C2D-C1D-ND	6.67	116.72	110.13
14	U	201	CLA	C2C-C1C-NC	6.67	116.98	109.98
14	A	830	CLA	C2C-C1C-NC	6.66	116.98	109.98
17	l	201	BCR	C7-C8-C9	-6.65	116.40	126.23
14	L	205	CLA	C2D-C1D-ND	6.65	116.71	110.13
14	B	814	CLA	O2D-CGD-CBD	6.65	122.85	111.23
14	a	827	CLA	O2D-CGD-CBD	6.64	122.84	111.23
14	b	808	CLA	C4A-NA-C1A	6.64	109.71	106.68
14	L	201	CLA	C2C-C1C-NC	6.63	116.95	109.98
14	A	845	CLA	C4A-NA-C1A	6.63	109.70	106.68
14	V	1601	CLA	C2C-C1C-NC	6.63	116.95	109.98
17	a	852	BCR	C20-C19-C18	6.63	144.54	126.36
14	G	843	CLA	C2C-C1C-NC	6.62	116.94	109.98
17	b	842	BCR	C20-C19-C18	6.62	144.51	126.36
14	A	844	CLA	CMD-C2D-C1D	6.62	136.38	124.73
14	b	829	CLA	C1C-C2C-C3C	-6.61	100.03	106.98
14	H	814	CLA	O2D-CGD-CBD	6.61	122.78	111.23
14	m	1601	CLA	C2C-C1C-NC	6.60	116.91	109.98
14	b	805	CLA	O2D-CGD-CBD	6.59	122.74	111.23
14	a	855	CLA	O2D-CGD-CBD	6.58	122.74	111.23
14	a	830	CLA	O2D-CGD-CBD	6.56	122.70	111.23
14	H	822	CLA	CMD-C2D-C1D	6.56	136.28	124.73
14	b	824	CLA	O2D-CGD-CBD	6.55	122.69	111.23
14	A	815	CLA	C2C-C1C-NC	6.54	116.86	109.98
17	A	850	BCR	C15-C14-C13	-6.54	118.10	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	j	101	CLA	O2D-CGD-CBD	6.53	122.65	111.23
17	G	853	BCR	C20-C19-C18	6.53	144.27	126.36
14	b	802	CLA	CMD-C2D-C1D	6.52	136.21	124.73
14	H	801	CLA	O2D-CGD-CBD	6.52	122.63	111.23
17	A	848	BCR	C20-C19-C18	6.52	144.24	126.36
14	H	822	CLA	O2D-CGD-CBD	6.52	122.62	111.23
17	i	102	BCR	C20-C19-C18	6.51	144.22	126.36
14	A	831	CLA	C2C-C1C-NC	6.51	116.82	109.98
14	G	820	CLA	O2D-CGD-CBD	6.51	122.61	111.23
14	G	802	CLA	C4A-NA-C1A	6.51	109.65	106.68
14	A	809	CLA	C4A-NA-C1A	6.50	109.65	106.68
14	B	836	CLA	C2C-C1C-NC	6.49	116.80	109.98
17	B	842	BCR	C7-C8-C9	-6.48	116.64	126.23
17	L	202	BCR	C20-C19-C18	6.48	144.13	126.36
17	R	103	BCR	C20-C19-C18	6.48	144.13	126.36
14	G	812	CLA	C4A-NA-C1A	6.47	109.63	106.68
14	B	802	CLA	CMD-C2D-C1D	6.47	136.12	124.73
17	a	847	BCR	C20-C19-C18	6.47	144.09	126.36
14	b	814	CLA	O2D-CGD-CBD	6.47	122.53	111.23
17	H	846	BCR	C24-C23-C22	-6.46	116.68	126.23
14	b	804	CLA	CMD-C2D-C1D	6.46	136.10	124.73
14	A	823	CLA	C2D-C1D-ND	6.45	116.51	110.13
14	H	801	CLA	C2D-C1D-ND	6.45	116.51	110.13
14	H	817	CLA	C2C-C1C-NC	6.45	116.75	109.98
14	b	828	CLA	C2C-C1C-NC	6.45	116.75	109.98
14	B	803	CLA	CAC-C3C-C4C	6.44	133.17	124.79
14	G	829	CLA	O2D-CGD-CBD	6.42	122.46	111.23
17	A	850	BCR	C20-C19-C18	6.42	143.96	126.36
14	b	804	CLA	C2D-C1D-ND	6.42	116.48	110.13
14	G	826	CLA	C2C-C1C-NC	6.42	116.72	109.98
14	A	809	CLA	O2D-CGD-CBD	6.42	122.45	111.23
17	Q	202	BCR	C20-C19-C18	6.42	143.95	126.36
14	A	811	CLA	O2D-CGD-CBD	6.41	122.44	111.23
14	b	803	CLA	C4A-NA-C1A	6.41	109.60	106.68
14	b	803	CLA	CMD-C2D-C1D	6.41	136.01	124.73
14	H	825	CLA	C4A-NA-C1A	6.40	109.60	106.68
17	I	101	BCR	C20-C19-C18	6.40	143.91	126.36
14	a	830	CLA	C2C-C1C-NC	6.40	116.70	109.98
14	a	834	CLA	O2D-CGD-CBD	6.39	122.41	111.23
14	b	832	CLA	O2D-CGD-CBD	6.39	122.41	111.23
14	G	812	CLA	C2C-C1C-NC	6.39	116.70	109.98
14	b	817	CLA	C2C-C1C-NC	6.39	116.70	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	805	CLA	O2D-CGD-CBD	6.39	122.40	111.23
14	b	827	CLA	C2C-C1C-NC	6.38	116.69	109.98
14	H	804	CLA	O2D-CGD-CBD	6.38	122.38	111.23
14	b	834	CLA	C2D-C1D-ND	6.38	116.44	110.13
14	B	817	CLA	C2C-C1C-NC	6.36	116.67	109.98
14	H	832	CLA	C2C-C1C-NC	6.36	116.66	109.98
17	H	847	BCR	C20-C19-C18	6.36	143.79	126.36
17	a	849	BCR	C20-C19-C18	6.36	143.79	126.36
14	b	838	CLA	C2C-C1C-NC	6.35	116.66	109.98
14	A	839	CLA	C2C-C1C-NC	6.35	116.65	109.98
14	A	828	CLA	O2D-CGD-CBD	6.35	122.33	111.23
17	R	101	BCR	C20-C19-C18	6.35	143.77	126.36
14	b	821	CLA	C2C-C1C-NC	6.34	116.64	109.98
14	B	803	CLA	CMD-C2D-C1D	6.34	135.90	124.73
14	A	837	CLA	C2C-C1C-NC	6.33	116.64	109.98
17	b	844	BCR	C20-C19-C18	6.33	143.73	126.36
14	L	201	CLA	O2A-CGA-O1A	-6.33	107.78	123.63
13	a	801	CL0	C4A-NA-C1A	6.33	109.57	106.68
14	G	835	CLA	O2D-CGD-CBD	6.33	122.30	111.23
14	b	834	CLA	C1C-C2C-C3C	-6.33	100.33	106.98
17	B	850	BCR	C20-C19-C18	6.33	143.71	126.36
14	B	814	CLA	C2C-C1C-NC	6.32	116.62	109.98
14	H	809	CLA	CMD-C2D-C1D	6.32	135.86	124.73
14	H	802	CLA	CMD-C2D-C1D	6.31	135.85	124.73
14	B	807	CLA	C2C-C1C-NC	6.31	116.61	109.98
14	l	206	CLA	C4A-NA-C1A	6.31	109.56	106.68
14	B	804	CLA	O2D-CGD-CBD	6.31	122.26	111.23
14	A	821	CLA	O2D-CGD-CBD	6.30	122.25	111.23
17	J	102	BCR	C24-C23-C22	-6.30	116.91	126.23
17	B	848	BCR	C20-C19-C18	6.30	143.65	126.36
14	b	825	CLA	O2D-CGD-CBD	6.30	122.25	111.23
14	H	834	CLA	C2C-C1C-NC	6.30	116.60	109.98
17	G	848	BCR	C7-C8-C9	-6.30	116.92	126.23
14	B	813	CLA	C4A-NA-C1A	6.30	109.55	106.68
14	A	831	CLA	O2D-CGD-CBD	6.30	122.24	111.23
14	A	805	CLA	O2D-CGD-CBD	6.30	122.23	111.23
14	G	843	CLA	CMD-C2D-C1D	6.29	135.81	124.73
14	B	829	CLA	C4A-NA-C1A	6.29	109.55	106.68
14	H	826	CLA	C2C-C1C-NC	6.29	116.59	109.98
14	B	829	CLA	C1C-C2C-C3C	-6.29	100.37	106.98
14	B	808	CLA	CMD-C2D-C1D	6.29	135.80	124.73
17	U	202	BCR	C20-C19-C18	6.29	143.60	126.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	812	CLA	C2C-C1C-NC	6.28	116.58	109.98
14	a	843	CLA	C2C-C1C-NC	6.28	116.58	109.98
14	a	810	CLA	C2C-C1C-NC	6.28	116.58	109.98
14	H	824	CLA	O2D-CGD-CBD	6.27	122.20	111.23
14	H	807	CLA	C2C-C1C-NC	6.27	116.57	109.98
14	G	820	CLA	C2C-C1C-NC	6.27	116.57	109.98
14	a	827	CLA	C3D-C2D-C1D	-6.27	97.28	105.83
14	G	837	CLA	C2C-C1C-NC	6.27	116.57	109.98
14	G	830	CLA	CMD-C2D-C1D	6.27	135.76	124.73
14	a	803	CLA	O2D-CGD-CBD	6.27	122.18	111.23
14	b	801	CLA	C4A-NA-C1A	6.26	109.54	106.68
14	H	808	CLA	O2D-CGD-CBD	6.26	122.17	111.23
17	A	850	BCR	C24-C23-C22	-6.26	116.97	126.23
14	l	202	CLA	C4A-NA-C1A	6.26	109.53	106.68
14	j	101	CLA	C2C-C1C-NC	6.26	116.56	109.98
14	G	815	CLA	C2C-C1C-NC	6.25	116.54	109.98
14	A	832	CLA	O2D-CGD-CBD	6.25	122.15	111.23
14	G	816	CLA	C2C-C1C-NC	6.24	116.54	109.98
13	G	801	CL0	C2C-C1C-NC	6.24	116.53	109.98
14	B	828	CLA	C2C-C1C-NC	6.23	116.53	109.98
14	a	838	CLA	O2D-CGD-CBD	6.23	122.12	111.23
14	H	835	CLA	C2D-C1D-ND	6.23	116.29	110.13
14	a	804	CLA	O2D-CGD-CBD	6.23	122.12	111.23
17	G	848	BCR	C20-C19-C18	6.23	143.44	126.36
14	b	802	CLA	C2C-C1C-NC	6.23	116.52	109.98
14	a	841	CLA	C2C-C1C-NC	6.22	116.52	109.98
14	a	838	CLA	C2C-C1C-NC	6.22	116.52	109.98
14	B	838	CLA	C2C-C1C-NC	6.22	116.51	109.98
17	l	208	BCR	C20-C19-C18	6.21	143.40	126.36
14	G	830	CLA	C2C-C1C-NC	6.21	116.51	109.98
14	H	823	CLA	CMD-C2D-C1D	6.21	135.67	124.73
14	U	205	CLA	O2D-CGD-CBD	6.21	122.09	111.23
14	a	811	CLA	C4A-NA-C1A	6.21	109.51	106.68
17	B	842	BCR	C20-C19-C18	6.21	143.38	126.36
14	H	828	CLA	C2C-C1C-NC	6.20	116.50	109.98
14	j	102	CLA	C2C-C1C-NC	6.20	116.49	109.98
14	U	205	CLA	C2D-C1D-ND	6.20	116.26	110.13
13	A	801	CL0	C2C-C1C-NC	6.20	116.49	109.98
14	b	820	CLA	C2C-C1C-NC	6.20	116.49	109.98
14	G	838	CLA	C2C-C1C-NC	6.20	116.49	109.98
14	a	820	CLA	O2D-CGD-CBD	6.19	122.06	111.23
14	H	827	CLA	C2C-C1C-NC	6.19	116.48	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	830	CLA	C2C-C1C-NC	6.18	116.47	109.98
14	K	101	CLA	C2C-C1C-NC	6.18	116.47	109.98
14	B	817	CLA	C1C-C2C-C3C	-6.18	100.48	106.98
14	A	835	CLA	O2D-CGD-CBD	6.17	122.02	111.23
14	M	1601	CLA	C2C-C1C-NC	6.17	116.46	109.98
14	b	836	CLA	CMD-C2D-C1D	6.16	135.58	124.73
14	b	812	CLA	C2C-C1C-NC	6.16	116.45	109.98
14	B	835	CLA	C2C-C1C-NC	6.16	116.45	109.98
14	H	812	CLA	C2C-C1C-NC	6.15	116.45	109.98
13	A	801	CL0	C4A-NA-C1A	6.15	109.49	106.68
14	G	828	CLA	C2D-C1D-ND	6.15	116.22	110.13
14	B	812	CLA	O2D-CGD-CBD	6.15	121.98	111.23
14	G	839	CLA	O2D-CGD-CBD	6.15	121.98	111.23
14	b	820	CLA	C1C-C2C-C3C	-6.15	100.51	106.98
14	H	836	CLA	C2C-C1C-NC	6.15	116.44	109.98
14	B	808	CLA	C2C-C1C-NC	6.15	116.44	109.98
14	H	835	CLA	C3D-C2D-C1D	-6.15	97.44	105.83
14	G	831	CLA	C2C-C1C-NC	6.14	116.44	109.98
14	i	101	CLA	C2C-C1C-NC	6.14	116.44	109.98
14	L	205	CLA	C1D-ND-C4D	-6.14	102.00	106.31
14	B	803	CLA	C2D-C1D-ND	6.14	116.20	110.13
17	a	849	BCR	C24-C23-C22	-6.14	117.16	126.23
14	a	815	CLA	C2C-C1C-NC	6.13	116.42	109.98
14	b	817	CLA	C1C-C2C-C3C	-6.13	100.53	106.98
14	B	801	CLA	C2D-C1D-ND	6.13	116.19	110.13
14	G	826	CLA	CMD-C2D-C1D	6.13	135.52	124.73
14	A	828	CLA	CMC-C2C-C1C	6.13	134.61	125.03
14	b	809	CLA	C4A-NA-C1A	6.13	109.47	106.68
14	B	805	CLA	C2C-C1C-NC	6.12	116.41	109.98
14	A	830	CLA	CMD-C2D-C1D	6.12	135.50	124.73
14	G	839	CLA	C2C-C1C-NC	6.11	116.40	109.98
14	G	821	CLA	C2C-C1C-NC	6.11	116.40	109.98
14	a	833	CLA	C2C-C1C-NC	6.11	116.40	109.98
14	a	808	CLA	O2D-CGD-CBD	6.10	121.90	111.23
14	X	1701	CLA	C2C-C1C-NC	6.10	116.39	109.98
14	A	817	CLA	C2C-C1C-NC	6.10	116.39	109.98
14	a	820	CLA	C2C-C1C-NC	6.10	116.39	109.98
14	B	827	CLA	C2C-C1C-NC	6.10	116.38	109.98
14	G	844	CLA	C2C-C1C-NC	6.09	116.38	109.98
14	H	819	CLA	C2C-C1C-NC	6.09	116.38	109.98
14	l	202	CLA	O2A-CGA-O1A	-6.09	108.39	123.63
14	H	805	CLA	O2D-CGD-CBD	6.08	121.86	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	829	CLA	C1C-C2C-C3C	-6.08	100.59	106.98
14	A	816	CLA	C2C-C1C-NC	6.08	116.37	109.98
14	S	101	CLA	C2C-C1C-NC	6.08	116.37	109.98
14	B	803	CLA	C4A-NA-C1A	6.08	109.45	106.68
14	a	811	CLA	C2C-C1C-NC	6.07	116.36	109.98
14	a	814	CLA	C2C-C1C-NC	6.07	116.36	109.98
14	B	808	CLA	O2D-CGD-CBD	6.06	121.83	111.23
17	a	847	BCR	C7-C8-C9	-6.06	117.27	126.23
14	a	842	CLA	C2C-C1C-NC	6.06	116.34	109.98
14	B	820	CLA	C4A-NA-C1A	6.05	109.44	106.68
14	a	814	CLA	O2D-CGD-CBD	6.05	121.81	111.23
14	G	802	CLA	C2D-C1D-ND	6.05	116.11	110.13
14	A	838	CLA	C2C-C1C-NC	6.05	116.33	109.98
14	A	825	CLA	C4A-NA-C1A	6.05	109.44	106.68
14	G	840	CLA	C2C-C1C-NC	6.04	116.33	109.98
14	A	812	CLA	C4A-NA-C1A	6.04	109.43	106.68
14	G	821	CLA	C4A-NA-C1A	6.04	109.43	106.68
14	B	806	CLA	C2C-C1C-NC	6.04	116.32	109.98
14	a	829	CLA	C2C-C1C-NC	6.03	116.32	109.98
17	G	850	BCR	C15-C14-C13	-6.03	118.82	127.28
14	A	815	CLA	O2D-CGD-CBD	6.03	121.77	111.23
14	B	834	CLA	C2C-C1C-NC	6.03	116.31	109.98
14	a	837	CLA	O2D-CGD-CBD	6.02	121.75	111.23
14	l	206	CLA	C2D-C1D-ND	6.01	116.08	110.13
17	f	201	BCR	C20-C19-C18	6.01	142.85	126.36
14	b	806	CLA	C2C-C1C-NC	6.01	116.30	109.98
17	G	853	BCR	C7-C8-C9	-6.01	117.35	126.23
14	B	808	CLA	C4A-NA-C1A	6.01	109.42	106.68
14	a	825	CLA	C2C-C1C-NC	6.00	116.29	109.98
14	A	831	CLA	CMD-C2D-C1D	6.00	135.30	124.73
14	A	820	CLA	C2C-C1C-NC	6.00	116.29	109.98
14	B	832	CLA	C2C-C1C-NC	6.00	116.28	109.98
14	A	802	CLA	CMD-C2D-C1D	6.00	135.29	124.73
14	f	202	CLA	C2C-C1C-NC	6.00	116.28	109.98
14	b	814	CLA	C2C-C1C-NC	6.00	116.28	109.98
17	R	103	BCR	C24-C23-C22	-5.99	117.37	126.23
13	G	801	CL0	C4A-NA-C1A	5.99	109.41	106.68
14	U	201	CLA	O2A-CGA-O1A	-5.99	108.65	123.63
14	a	823	CLA	C2C-C1C-NC	5.99	116.27	109.98
14	Q	203	CLA	CMD-C2D-C1D	5.98	135.27	124.73
13	G	801	CL0	C1C-C2C-C3C	-5.98	100.69	106.98
14	B	837	CLA	C2C-C1C-NC	5.98	116.26	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	826	CLA	C2C-C1C-NC	5.98	116.26	109.98
14	a	816	CLA	C2C-C1C-NC	5.98	116.26	109.98
14	J	101	CLA	C2C-C1C-NC	5.98	116.26	109.98
14	B	801	CLA	O2D-CGD-CBD	5.98	121.68	111.23
14	b	808	CLA	C2C-C1C-NC	5.98	116.26	109.98
14	W	1701	CLA	C2C-C1C-NC	5.98	116.26	109.98
14	A	826	CLA	C2C-C1C-NC	5.97	116.26	109.98
14	G	813	CLA	C2C-C1C-NC	5.97	116.26	109.98
14	B	819	CLA	C2C-C1C-NC	5.97	116.25	109.98
14	B	811	CLA	C2C-C1C-NC	5.97	116.25	109.98
14	A	821	CLA	C2C-C1C-NC	5.97	116.25	109.98
14	a	837	CLA	C2C-C1C-NC	5.97	116.25	109.98
14	b	819	CLA	C2C-C1C-NC	5.97	116.25	109.98
14	l	202	CLA	C1C-C2C-C3C	-5.97	100.70	106.98
14	B	823	CLA	C4A-NA-C1A	5.97	109.40	106.68
14	G	811	CLA	C2C-C1C-NC	5.96	116.25	109.98
14	B	817	CLA	C4A-NA-C1A	5.96	109.40	106.68
14	G	828	CLA	C3D-C2D-C1D	-5.96	97.70	105.83
14	G	811	CLA	C4A-NA-C1A	5.96	109.40	106.68
14	b	823	CLA	C4A-NA-C1A	5.96	109.40	106.68
17	B	847	BCR	C20-C19-C18	5.96	142.70	126.36
14	H	820	CLA	C2C-C1C-NC	5.96	116.24	109.98
14	a	829	CLA	O2D-CGD-CBD	5.96	121.64	111.23
14	b	806	CLA	O2D-CGD-CBD	5.96	121.64	111.23
14	b	808	CLA	O2D-CGD-CBD	5.95	121.64	111.23
14	l	206	CLA	O2D-CGD-CBD	5.95	121.64	111.23
14	A	802	CLA	C2D-C1D-ND	5.95	116.02	110.13
17	Q	204	BCR	C24-C23-C22	-5.95	117.43	126.23
17	A	853	BCR	C7-C8-C9	-5.95	117.43	126.23
14	A	810	CLA	C2C-C1C-NC	5.95	116.23	109.98
14	a	832	CLA	C2C-C1C-NC	5.95	116.23	109.98
14	B	811	CLA	O2D-CGD-CBD	5.95	121.63	111.23
14	A	844	CLA	C1C-C2C-C3C	-5.95	100.72	106.98
14	A	845	CLA	C2C-C1C-NC	5.95	116.23	109.98
14	G	831	CLA	O2D-CGD-CBD	5.94	121.62	111.23
14	S	101	CLA	O2D-CGD-CBD	5.94	121.62	111.23
14	B	821	CLA	C2C-C1C-NC	5.94	116.22	109.98
14	G	824	CLA	C2C-C1C-NC	5.94	116.22	109.98
14	H	818	CLA	C2C-C1C-NC	5.94	116.22	109.98
14	A	824	CLA	C2C-C1C-NC	5.94	116.22	109.98
14	H	821	CLA	C2C-C1C-NC	5.94	116.22	109.98
14	G	834	CLA	C2C-C1C-NC	5.94	116.22	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1601	CLA	C4A-NA-C1A	5.93	109.39	106.68
14	b	832	CLA	C2C-C1C-NC	5.93	116.21	109.98
14	b	830	CLA	C2C-C1C-NC	5.93	116.21	109.98
14	b	834	CLA	C3D-C2D-C1D	-5.93	97.74	105.83
14	a	841	CLA	C1C-C2C-C3C	-5.93	100.75	106.98
14	b	814	CLA	C4A-NA-C1A	5.93	109.38	106.68
14	H	814	CLA	C2C-C1C-NC	5.93	116.21	109.98
14	H	838	CLA	O2D-CGD-CBD	5.92	121.58	111.23
17	H	842	BCR	C7-C8-C9	-5.92	117.48	126.23
14	H	838	CLA	C1C-C2C-C3C	-5.92	100.76	106.98
17	G	850	BCR	C20-C19-C18	5.92	142.59	126.36
14	a	839	CLA	C2C-C1C-NC	5.92	116.20	109.98
14	H	840	CLA	C1C-C2C-C3C	-5.91	100.76	106.98
14	A	836	CLA	C2C-C1C-NC	5.91	116.19	109.98
14	x	1701	CLA	C2C-C1C-NC	5.91	116.19	109.98
14	a	844	CLA	C4A-NA-C1A	5.91	109.38	106.68
14	K	102	CLA	C2C-C1C-NC	5.91	116.19	109.98
14	A	828	CLA	C3D-C2D-C1D	-5.91	97.77	105.83
14	B	825	CLA	O2D-CGD-CBD	5.91	121.56	111.23
14	U	201	CLA	C1C-C2C-C3C	-5.91	100.77	106.98
14	A	823	CLA	C4A-NA-C1A	5.91	109.37	106.68
14	F	1303	CLA	C2C-C1C-NC	5.90	116.18	109.98
14	B	806	CLA	C1C-C2C-C3C	-5.90	100.77	106.98
14	F	1301	CLA	CMD-C2D-C1D	5.90	135.12	124.73
14	b	819	CLA	O2D-CGD-CBD	5.90	121.55	111.23
14	U	204	CLA	O2D-CGD-CBD	5.90	121.54	111.23
14	B	825	CLA	C2C-C1C-NC	5.90	116.17	109.98
14	k	1401	CLA	C2C-C1C-NC	5.90	116.17	109.98
14	a	820	CLA	C4A-NA-C1A	5.89	109.37	106.68
14	H	836	CLA	O2D-CGD-CBD	5.89	121.52	111.23
14	H	820	CLA	C1C-C2C-C3C	-5.89	100.79	106.98
14	B	820	CLA	C2C-C1C-NC	5.89	116.16	109.98
14	L	201	CLA	C1C-C2C-C3C	-5.89	100.79	106.98
14	A	837	CLA	O2D-CGD-CBD	5.88	121.51	111.23
14	a	835	CLA	C2C-C1C-NC	5.88	116.16	109.98
14	G	821	CLA	O2D-CGD-CBD	5.88	121.50	111.23
14	B	804	CLA	C4A-NA-C1A	5.88	109.36	106.68
14	U	206	CLA	C2C-C1C-NC	5.88	116.15	109.98
14	G	830	CLA	C1C-C2C-C3C	-5.88	100.80	106.98
14	b	819	CLA	C4A-NA-C1A	5.87	109.36	106.68
14	G	802	CLA	CMD-C2D-C1D	5.87	135.07	124.73
14	G	838	CLA	C1C-C2C-C3C	-5.87	100.81	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	801	CL0	CMD-C2D-C1D	5.87	135.06	124.73
14	b	840	CLA	C1C-C2C-C3C	-5.87	100.81	106.98
14	b	825	CLA	C2C-C1C-NC	5.86	116.14	109.98
14	B	819	CLA	O2D-CGD-CBD	5.86	121.48	111.23
14	H	810	CLA	C2C-C1C-NC	5.86	116.13	109.98
14	b	804	CLA	C4A-NA-C1A	5.86	109.35	106.68
14	b	836	CLA	C2C-C1C-NC	5.86	116.13	109.98
14	A	833	CLA	C2C-C1C-NC	5.85	116.13	109.98
14	H	803	CLA	CMD-C2D-C1D	5.85	135.03	124.73
14	B	810	CLA	C2C-C1C-NC	5.84	116.12	109.98
14	H	802	CLA	C2C-C1C-NC	5.84	116.12	109.98
14	L	204	CLA	C2C-C1C-NC	5.84	116.12	109.98
14	b	805	CLA	C2C-C1C-NC	5.84	116.12	109.98
14	b	839	CLA	C2C-C1C-NC	5.84	116.12	109.98
14	b	820	CLA	O2D-CGD-CBD	5.84	121.44	111.23
14	G	841	CLA	C2C-C1C-NC	5.84	116.11	109.98
14	b	808	CLA	O2A-CGA-O1A	-5.84	109.03	123.63
14	a	836	CLA	C2C-C1C-NC	5.83	116.11	109.98
14	A	822	CLA	C2C-C1C-NC	5.83	116.11	109.98
14	a	803	CLA	C2C-C1C-NC	5.83	116.11	109.98
14	H	817	CLA	C4A-NA-C1A	5.83	109.34	106.68
14	A	814	CLA	C2C-C1C-NC	5.83	116.10	109.98
14	G	808	CLA	C2C-C1C-NC	5.82	116.10	109.98
14	b	820	CLA	C4A-NA-C1A	5.82	109.33	106.68
14	A	804	CLA	O2D-CGD-CBD	5.82	121.41	111.23
14	b	813	CLA	O2D-CGD-CBD	5.82	121.40	111.23
14	B	836	CLA	C1C-C2C-C3C	-5.82	100.86	106.98
13	A	801	CL0	C1C-C2C-C3C	-5.82	100.86	106.98
13	a	801	CL0	C2C-C1C-NC	5.82	116.09	109.98
14	A	825	CLA	C2C-C1C-NC	5.81	116.09	109.98
14	A	813	CLA	C2C-C1C-NC	5.81	116.09	109.98
14	G	841	CLA	C4A-NA-C1A	5.81	109.33	106.68
14	B	825	CLA	C3D-C2D-C1D	-5.81	97.90	105.83
14	b	819	CLA	C1C-C2C-C3C	-5.81	100.87	106.98
14	b	821	CLA	C4A-NA-C1A	5.81	109.33	106.68
14	b	838	CLA	O2D-CGD-CBD	5.81	121.38	111.23
14	m	1601	CLA	C4A-NA-C1A	5.81	109.33	106.68
14	H	830	CLA	C2C-C1C-NC	5.81	116.08	109.98
14	G	817	CLA	C2C-C1C-NC	5.80	116.08	109.98
14	A	839	CLA	O2D-CGD-CBD	5.80	121.38	111.23
14	a	827	CLA	C2D-C1D-ND	5.80	115.87	110.13
14	G	816	CLA	O2D-CGD-CBD	5.80	121.37	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	823	CLA	C2C-C1C-NC	5.80	116.07	109.98
14	I	205	CLA	O2D-CGD-CBD	5.80	121.37	111.23
14	A	829	CLA	C2C-C1C-NC	5.80	116.07	109.98
14	H	814	CLA	C1C-C2C-C3C	-5.80	100.88	106.98
14	H	817	CLA	C1C-C2C-C3C	-5.80	100.88	106.98
14	G	835	CLA	C2C-C1C-NC	5.80	116.07	109.98
14	G	812	CLA	C1C-C2C-C3C	-5.80	100.88	106.98
14	b	801	CLA	O2A-CGA-CBA	5.80	129.51	111.83
14	I	205	CLA	C2C-C1C-NC	5.79	116.06	109.98
14	A	841	CLA	C2C-C1C-NC	5.79	116.06	109.98
14	B	812	CLA	C2C-C1C-NC	5.79	116.06	109.98
14	a	806	CLA	C2C-C1C-NC	5.78	116.05	109.98
14	b	818	CLA	C2C-C1C-NC	5.78	116.05	109.98
14	G	823	CLA	C1C-C2C-C3C	-5.77	100.91	106.98
14	H	832	CLA	O2D-CGD-CBD	5.77	121.32	111.23
14	G	833	CLA	C2C-C1C-NC	5.77	116.05	109.98
14	G	836	CLA	C2C-C1C-NC	5.77	116.05	109.98
14	G	842	CLA	C2C-C1C-NC	5.77	116.05	109.98
14	G	802	CLA	C2C-C1C-NC	5.77	116.04	109.98
14	B	820	CLA	C1C-C2C-C3C	-5.76	100.92	106.98
14	B	837	CLA	C4A-NA-C1A	5.76	109.31	106.68
17	H	843	BCR	C24-C23-C22	-5.76	117.71	126.23
14	A	827	CLA	C1C-C2C-C3C	-5.76	100.92	106.98
14	B	809	CLA	C1C-C2C-C3C	-5.76	100.92	106.98
14	A	834	CLA	C2C-C1C-NC	5.76	116.03	109.98
14	a	844	CLA	C2C-C1C-NC	5.76	116.03	109.98
13	a	801	CL0	CMD-C2D-C1D	5.76	134.87	124.73
14	A	832	CLA	C2C-C1C-NC	5.76	116.03	109.98
14	B	818	CLA	C2C-C1C-NC	5.76	116.03	109.98
17	L	207	BCR	C20-C19-C18	5.75	142.14	126.36
14	H	825	CLA	C3D-C2D-C1D	-5.75	97.98	105.83
14	B	814	CLA	C4A-NA-C1A	5.75	109.30	106.68
14	H	823	CLA	C2C-C1C-NC	5.75	116.03	109.98
14	U	205	CLA	C2C-C1C-NC	5.75	116.02	109.98
14	G	843	CLA	C1C-C2C-C3C	-5.75	100.93	106.98
14	b	827	CLA	C1C-C2C-C3C	-5.75	100.93	106.98
14	L	201	CLA	O2A-CGA-CBA	5.75	129.36	111.83
14	G	829	CLA	C2C-C1C-NC	5.75	116.02	109.98
14	A	841	CLA	O2D-CGD-CBD	5.75	121.28	111.23
14	G	818	CLA	C2C-C1C-NC	5.75	116.02	109.98
17	B	846	BCR	C24-C23-C22	-5.75	117.73	126.23
14	B	825	CLA	C4A-NA-C1A	5.74	109.30	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	855	CLA	C2D-C1D-ND	5.74	115.81	110.13
14	A	823	CLA	C2C-C1C-NC	5.74	116.01	109.98
14	B	819	CLA	C1C-C2C-C3C	-5.74	100.94	106.98
14	a	824	CLA	C4A-NA-C1A	5.74	109.30	106.68
14	b	812	CLA	C4A-NA-C1A	5.74	109.30	106.68
14	a	821	CLA	C2C-C1C-NC	5.74	116.01	109.98
14	T	1401	CLA	C2C-C1C-NC	5.74	116.01	109.98
14	a	808	CLA	C4A-NA-C1A	5.73	109.29	106.68
14	a	833	CLA	C1C-C2C-C3C	-5.73	100.95	106.98
14	G	832	CLA	C2C-C1C-NC	5.73	116.00	109.98
14	G	821	CLA	C1C-C2C-C3C	-5.73	100.95	106.98
14	A	828	CLA	C2D-C1D-ND	5.73	115.80	110.13
14	L	205	CLA	O2D-CGD-CBD	5.73	121.24	111.23
14	b	803	CLA	C2C-C1C-NC	5.73	116.00	109.98
14	H	837	CLA	C2C-C1C-NC	5.72	116.00	109.98
14	H	808	CLA	C4A-NA-C1A	5.72	109.29	106.68
14	A	806	CLA	O2D-CGD-CBD	5.72	121.23	111.23
14	l	206	CLA	C1C-C2C-C3C	-5.72	100.96	106.98
14	B	823	CLA	C2D-C1D-ND	5.72	115.79	110.13
14	G	822	CLA	C2C-C1C-NC	5.72	115.99	109.98
14	A	802	CLA	C4A-NA-C1A	5.72	109.29	106.68
14	a	813	CLA	C3D-C2D-C1D	-5.72	98.03	105.83
14	A	835	CLA	C2C-C1C-NC	5.72	115.99	109.98
14	Q	201	CLA	C2C-C1C-NC	5.72	115.98	109.98
14	A	814	CLA	C3D-C2D-C1D	-5.71	98.03	105.83
14	J	101	CLA	O2D-CGD-CBD	5.71	121.22	111.23
14	G	811	CLA	C1C-C2C-C3C	-5.71	100.97	106.98
14	H	834	CLA	C1C-C2C-C3C	-5.71	100.97	106.98
14	H	819	CLA	O2D-CGD-CBD	5.71	121.21	111.23
14	a	812	CLA	C2C-C1C-NC	5.71	115.98	109.98
14	B	826	CLA	C2C-C1C-NC	5.71	115.97	109.98
14	b	837	CLA	C2C-C1C-NC	5.71	115.97	109.98
14	H	824	CLA	C2C-C1C-NC	5.70	115.97	109.98
14	a	806	CLA	C1C-C2C-C3C	-5.70	100.98	106.98
14	G	804	CLA	O2D-CGD-CBD	5.70	121.19	111.23
14	b	810	CLA	C2C-C1C-NC	5.70	115.97	109.98
14	a	808	CLA	C1D-ND-C4D	-5.70	102.31	106.31
14	H	825	CLA	O2D-CGD-CBD	5.70	121.19	111.23
14	V	1601	CLA	C1C-C2C-C3C	-5.70	100.99	106.98
14	b	806	CLA	C4A-NA-C1A	5.69	109.28	106.68
14	S	102	CLA	C2C-C1C-NC	5.69	115.96	109.98
14	a	822	CLA	C2C-C1C-NC	5.69	115.96	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	829	CLA	O2D-CGD-CBD	5.69	121.18	111.23
14	A	829	CLA	O2D-CGD-CBD	5.69	121.17	111.23
14	G	806	CLA	C2C-C1C-NC	5.69	115.95	109.98
14	H	839	CLA	O2D-CGD-CBD	5.68	121.17	111.23
14	a	806	CLA	O2A-CGA-O1A	-5.68	109.41	123.63
17	S	103	BCR	C24-C23-C22	-5.68	117.83	126.23
14	a	820	CLA	C1C-C2C-C3C	-5.68	101.01	106.98
14	a	824	CLA	C2C-C1C-NC	5.68	115.94	109.98
14	b	823	CLA	C2D-C1D-ND	5.68	115.74	110.13
14	H	803	CLA	C3D-C2D-C1D	-5.67	98.09	105.83
14	a	808	CLA	C2D-C1D-ND	5.67	115.74	110.13
14	a	802	CLA	C2C-C1C-NC	5.67	115.94	109.98
14	A	823	CLA	CMD-C2D-C1D	5.67	134.71	124.73
14	U	201	CLA	C3D-C2D-C1D	-5.67	98.09	105.83
14	H	812	CLA	O2A-CGA-O1A	-5.67	109.45	123.63
14	A	809	CLA	C2C-C1C-NC	5.66	115.93	109.98
14	b	813	CLA	C4A-NA-C1A	5.66	109.26	106.68
14	G	806	CLA	C1C-C2C-C3C	-5.66	101.02	106.98
14	b	802	CLA	C4A-NA-C1A	5.66	109.26	106.68
17	j	104	BCR	C24-C23-C22	-5.66	117.86	126.23
14	H	802	CLA	C1C-C2C-C3C	-5.66	101.03	106.98
14	L	205	CLA	C3D-C2D-C1D	-5.66	98.11	105.83
14	V	1601	CLA	O2D-CGD-CBD	5.65	121.11	111.23
14	B	823	CLA	C2C-C1C-NC	5.65	115.92	109.98
17	b	847	BCR	C20-C19-C18	5.65	141.86	126.36
14	U	204	CLA	C2C-C1C-NC	5.65	115.92	109.98
14	b	811	CLA	C2C-C1C-NC	5.65	115.92	109.98
14	a	840	CLA	C2C-C1C-NC	5.65	115.91	109.98
14	A	826	CLA	C4A-NA-C1A	5.65	109.25	106.68
14	a	819	CLA	O2D-CGD-CBD	5.65	121.10	111.23
14	l	207	CLA	C2C-C1C-NC	5.64	115.91	109.98
13	a	801	CL0	C1C-C2C-C3C	-5.64	101.04	106.98
14	B	840	CLA	C1C-C2C-C3C	-5.64	101.04	106.98
14	U	204	CLA	C4A-NA-C1A	5.64	109.25	106.68
14	U	205	CLA	C1D-ND-C4D	-5.64	102.35	106.31
14	H	825	CLA	C2D-C1D-ND	5.64	115.71	110.13
14	L	201	CLA	C3D-C2D-C1D	-5.64	98.13	105.83
14	G	806	CLA	O2D-CGD-CBD	5.64	121.09	111.23
14	A	805	CLA	C2C-C1C-NC	5.64	115.91	109.98
14	H	804	CLA	C2C-C1C-NC	5.64	115.91	109.98
14	H	809	CLA	C1C-C2C-C3C	-5.64	101.05	106.98
14	F	1301	CLA	C2C-C1C-NC	5.64	115.91	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	845	CLA	C2C-C1C-NC	5.64	115.90	109.98
14	G	815	CLA	C4A-NA-C1A	5.64	109.25	106.68
14	A	807	CLA	C2C-C1C-NC	5.64	115.90	109.98
14	H	812	CLA	O2D-CGD-CBD	5.64	121.08	111.23
13	A	801	CL0	O2D-CGD-CBD	5.64	121.08	111.23
14	G	826	CLA	C4A-NA-C1A	5.64	109.25	106.68
14	A	843	CLA	C2C-C1C-NC	5.63	115.90	109.98
14	a	831	CLA	O2D-CGD-CBD	5.63	121.08	111.23
17	G	852	BCR	C24-C23-C22	-5.63	117.90	126.23
14	A	808	CLA	C2C-C1C-NC	5.63	115.90	109.98
14	G	811	CLA	C2D-C1D-ND	5.63	115.70	110.13
14	a	826	CLA	C2D-C1D-ND	5.63	115.70	110.13
14	A	827	CLA	C2C-C1C-NC	5.63	115.90	109.98
14	L	206	CLA	C2C-C1C-NC	5.63	115.89	109.98
14	b	838	CLA	C1C-C2C-C3C	-5.63	101.06	106.98
14	G	809	CLA	O2D-CGD-CBD	5.63	121.06	111.23
14	a	842	CLA	C4A-NA-C1A	5.62	109.25	106.68
14	l	202	CLA	C3D-C2D-C1D	-5.62	98.16	105.83
14	b	803	CLA	O2D-CGD-CBD	5.62	121.06	111.23
14	A	811	CLA	O1D-CGD-CBD	-5.62	113.44	124.52
14	A	816	CLA	C4A-NA-C1A	5.62	109.24	106.68
14	b	826	CLA	O2D-CGD-CBD	5.62	121.05	111.23
14	G	807	CLA	O2A-CGA-O1A	-5.62	109.58	123.63
14	A	840	CLA	C2C-C1C-NC	5.62	115.88	109.98
14	b	804	CLA	C3D-C2D-C1D	-5.62	98.17	105.83
14	G	835	CLA	C1C-C2C-C3C	-5.61	101.08	106.98
14	a	834	CLA	C2C-C1C-NC	5.61	115.88	109.98
14	m	1601	CLA	C1C-C2C-C3C	-5.61	101.08	106.98
14	B	816	CLA	C2D-C1D-ND	5.61	115.68	110.13
17	S	104	BCR	C24-C23-C22	-5.61	117.93	126.23
14	A	836	CLA	C1C-C2C-C3C	-5.61	101.08	106.98
14	H	837	CLA	C1C-C2C-C3C	-5.61	101.08	106.98
14	H	825	CLA	C2C-C1C-NC	5.61	115.87	109.98
14	b	828	CLA	C1C-C2C-C3C	-5.61	101.08	106.98
14	a	842	CLA	O2D-CGD-CBD	5.61	121.04	111.23
14	Q	203	CLA	C2C-C1C-NC	5.61	115.87	109.98
14	L	204	CLA	C4A-NA-C1A	5.61	109.24	106.68
17	A	851	BCR	C24-C23-C22	-5.61	117.94	126.23
14	G	825	CLA	C2C-C1C-NC	5.61	115.87	109.98
14	a	830	CLA	C4A-NA-C1A	5.60	109.24	106.68
14	B	803	CLA	C3D-C2D-C1D	-5.60	98.18	105.83
14	A	842	CLA	C2C-C1C-NC	5.60	115.87	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	204	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
14	a	830	CLA	CMD-C2D-C1D	5.60	134.59	124.73
14	G	804	CLA	C2C-C1C-NC	5.60	115.87	109.98
14	Q	201	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
14	H	818	CLA	O2D-CGD-CBD	5.60	121.02	111.23
14	H	807	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
14	H	829	CLA	O2D-CGD-CBD	5.59	121.01	111.23
14	A	836	CLA	C4A-NA-C1A	5.59	109.23	106.68
14	H	819	CLA	C1C-C2C-C3C	-5.59	101.10	106.98
14	G	830	CLA	O2D-CGD-CBD	5.59	121.00	111.23
14	B	820	CLA	O2D-CGD-CBD	5.59	121.00	111.23
17	L	207	BCR	C7-C8-C9	-5.59	117.97	126.23
14	a	826	CLA	C3D-C2D-C1D	-5.59	98.21	105.83
14	B	806	CLA	C3D-C2D-C1D	-5.58	98.21	105.83
14	A	831	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
14	a	842	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
14	F	1301	CLA	C2D-C1D-ND	5.58	115.65	110.13
14	G	837	CLA	O2D-CGD-CBD	5.58	120.99	111.23
17	V	1602	BCR	C24-C23-C22	-5.58	117.98	126.23
14	b	823	CLA	C2C-C1C-NC	5.58	115.84	109.98
14	b	807	CLA	C2C-C1C-NC	5.57	115.84	109.98
14	U	204	CLA	C1C-C2C-C3C	-5.57	101.12	106.98
14	B	832	CLA	O2D-CGD-CBD	5.57	120.97	111.23
14	B	831	CLA	C2C-C1C-NC	5.57	115.83	109.98
14	a	812	CLA	O2D-CGD-CBD	5.57	120.97	111.23
14	B	829	CLA	O2D-CGD-CBD	5.57	120.97	111.23
14	A	807	CLA	O2A-CGA-O1A	-5.57	109.70	123.63
14	H	811	CLA	C2C-C1C-NC	5.57	115.83	109.98
14	H	826	CLA	O2D-CGD-CBD	5.57	120.96	111.23
14	a	824	CLA	O2A-CGA-O1A	-5.57	109.70	123.63
14	l	206	CLA	C2C-C1C-NC	5.57	115.83	109.98
14	B	805	CLA	O2A-CGA-O1A	-5.57	109.71	123.63
14	A	823	CLA	O2D-CGD-CBD	5.56	120.96	111.23
14	G	832	CLA	O2D-CGD-CBD	5.56	120.96	111.23
14	B	805	CLA	C1C-C2C-C3C	-5.56	101.13	106.98
14	K	101	CLA	C1C-C2C-C3C	-5.56	101.13	106.98
14	B	807	CLA	C1C-C2C-C3C	-5.56	101.13	106.98
14	a	807	CLA	C2C-C1C-NC	5.56	115.82	109.98
14	G	837	CLA	C1C-C2C-C3C	-5.56	101.14	106.98
17	A	848	BCR	C7-C8-C9	-5.56	118.01	126.23
14	b	806	CLA	O2A-CGA-O1A	-5.56	109.73	123.63
14	A	815	CLA	C1C-C2C-C3C	-5.56	101.14	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	U	201	CLA	C4A-NA-C1A	5.55	109.21	106.68
14	B	804	CLA	C2C-C1C-NC	5.55	115.81	109.98
14	G	845	CLA	C2D-C1D-ND	5.55	115.62	110.13
14	A	810	CLA	C4A-NA-C1A	5.55	109.21	106.68
14	H	834	CLA	C4A-NA-C1A	5.55	109.21	106.68
14	L	201	CLA	C4A-NA-C1A	5.55	109.21	106.68
14	H	814	CLA	C3D-C2D-C1D	-5.55	98.26	105.83
14	A	815	CLA	C4A-NA-C1A	5.55	109.21	106.68
14	A	845	CLA	C3D-C2D-C1D	-5.55	98.26	105.83
14	G	807	CLA	C2C-C1C-NC	5.55	115.81	109.98
14	A	823	CLA	C3D-C2D-C1D	-5.55	98.26	105.83
14	b	815	CLA	C2D-C1D-ND	5.55	115.61	110.13
14	B	839	CLA	C2C-C1C-NC	5.55	115.81	109.98
14	A	804	CLA	O2A-CGA-O1A	-5.54	109.76	123.63
14	a	822	CLA	C1C-C2C-C3C	-5.54	101.15	106.98
14	b	817	CLA	O2D-CGD-CBD	5.54	120.92	111.23
14	B	801	CLA	C4A-NA-C1A	5.54	109.21	106.68
14	B	826	CLA	O2D-CGD-CBD	5.54	120.92	111.23
14	A	821	CLA	C1C-C2C-C3C	-5.54	101.15	106.98
14	B	823	CLA	CMD-C2D-C1D	5.54	134.48	124.73
14	a	819	CLA	C2C-C1C-NC	5.54	115.80	109.98
14	a	815	CLA	O2D-CGD-CBD	5.54	120.91	111.23
14	A	839	CLA	C1C-C2C-C3C	-5.54	101.16	106.98
14	a	837	CLA	C1C-C2C-C3C	-5.54	101.16	106.98
14	b	807	CLA	C1C-C2C-C3C	-5.54	101.16	106.98
14	G	817	CLA	C4A-NA-C1A	5.53	109.20	106.68
14	G	809	CLA	C2C-C1C-NC	5.53	115.80	109.98
14	H	808	CLA	O2A-CGA-O1A	-5.53	109.78	123.63
14	B	828	CLA	C1C-C2C-C3C	-5.53	101.16	106.98
14	A	809	CLA	C1D-ND-C4D	-5.53	102.43	106.31
14	B	812	CLA	C4A-NA-C1A	5.53	109.20	106.68
14	A	845	CLA	O2D-CGD-CBD	5.53	120.90	111.23
14	i	101	CLA	O2D-CGD-CBD	5.53	120.90	111.23
14	b	821	CLA	C1C-C2C-C3C	-5.53	101.17	106.98
14	G	811	CLA	C3D-C2D-C1D	-5.53	98.29	105.83
14	B	807	CLA	C2D-C1D-ND	5.52	115.59	110.13
14	A	804	CLA	C2C-C1C-NC	5.52	115.78	109.98
14	a	826	CLA	C2C-C1C-NC	5.52	115.78	109.98
14	a	831	CLA	C2C-C1C-NC	5.52	115.78	109.98
14	H	828	CLA	O2D-CGD-CBD	5.52	120.88	111.23
14	B	823	CLA	O2A-CGA-O1A	-5.52	109.82	123.63
14	A	838	CLA	C1C-C2C-C3C	-5.52	101.17	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	838	CLA	O2D-CGD-CBD	5.52	120.88	111.23
14	i	101	CLA	C1C-C2C-C3C	-5.52	101.18	106.98
14	H	831	CLA	C3D-C2D-C1D	-5.52	98.30	105.83
14	L	206	CLA	O2D-CGD-CBD	5.52	120.87	111.23
14	A	837	CLA	C1C-C2C-C3C	-5.51	101.18	106.98
14	b	814	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
14	B	836	CLA	C4A-NA-C1A	5.51	109.19	106.68
14	G	810	CLA	C2C-C1C-NC	5.51	115.77	109.98
14	H	806	CLA	C2C-C1C-NC	5.51	115.77	109.98
14	b	831	CLA	C2C-C1C-NC	5.51	115.77	109.98
14	a	826	CLA	C1C-C2C-C3C	-5.51	101.18	106.98
14	H	814	CLA	C2D-C1D-ND	5.51	115.58	110.13
14	A	834	CLA	C1C-C2C-C3C	-5.51	101.19	106.98
14	U	205	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
14	A	825	CLA	O2A-CGA-O1A	-5.51	109.85	123.63
14	A	841	CLA	C1C-C2C-C3C	-5.51	101.19	106.98
14	G	820	CLA	C1C-C2C-C3C	-5.51	101.19	106.98
14	H	832	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	a	810	CLA	C1C-C2C-C3C	-5.50	101.19	106.98
14	B	825	CLA	C2D-C1D-ND	5.50	115.57	110.13
14	H	812	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	a	816	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	A	839	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	B	834	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	G	818	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	G	842	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	b	822	CLA	C2C-C1C-NC	5.50	115.76	109.98
14	l	206	CLA	C3D-C2D-C1D	-5.50	98.33	105.83
14	b	829	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	H	806	CLA	C3D-C2D-C1D	-5.50	98.33	105.83
14	B	838	CLA	C1C-C2C-C3C	-5.50	101.20	106.98
17	l	203	BCR	C7-C8-C9	-5.49	118.11	126.23
14	G	802	CLA	C1C-C2C-C3C	-5.49	101.20	106.98
14	A	809	CLA	C2D-C1D-ND	5.49	115.56	110.13
14	B	840	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
14	B	805	CLA	O2D-CGD-CBD	5.49	120.83	111.23
14	H	835	CLA	C1D-ND-C4D	-5.49	102.46	106.31
14	b	839	CLA	O2D-CGD-CBD	5.49	120.83	111.23
14	a	843	CLA	C1C-C2C-C3C	-5.49	101.20	106.98
14	B	806	CLA	C4A-NA-C1A	5.49	109.18	106.68
14	H	833	CLA	C2C-C1C-NC	5.48	115.74	109.98
14	B	830	CLA	C1C-C2C-C3C	-5.48	101.21	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	820	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
14	B	802	CLA	C2D-C1D-ND	5.48	115.55	110.13
14	b	817	CLA	C4A-NA-C1A	5.48	109.18	106.68
14	A	830	CLA	C1C-C2C-C3C	-5.48	101.22	106.98
17	B	847	BCR	C24-C23-C22	-5.48	118.13	126.23
14	b	835	CLA	C2C-C1C-NC	5.48	115.73	109.98
13	A	801	CL0	CMD-C2D-C1D	5.48	134.37	124.73
14	H	801	CLA	C3D-C2D-C1D	-5.48	98.36	105.83
14	H	823	CLA	O2D-CGD-CBD	5.47	120.80	111.23
14	B	815	CLA	C2C-C1C-NC	5.47	115.73	109.98
14	A	843	CLA	O2D-CGD-CBD	5.47	120.80	111.23
14	G	810	CLA	C4A-NA-C1A	5.47	109.18	106.68
17	H	842	BCR	C24-C23-C22	-5.47	118.14	126.23
14	H	806	CLA	C4A-NA-C1A	5.47	109.17	106.68
14	B	820	CLA	C2D-C1D-ND	5.47	115.54	110.13
14	H	808	CLA	C2C-C1C-NC	5.47	115.72	109.98
14	X	1701	CLA	C3D-C2D-C1D	-5.47	98.37	105.83
14	b	813	CLA	C2C-C1C-NC	5.47	115.72	109.98
14	A	805	CLA	C1C-C2C-C3C	-5.47	101.23	106.98
14	a	832	CLA	C1C-C2C-C3C	-5.47	101.23	106.98
14	a	804	CLA	C2C-C1C-NC	5.47	115.72	109.98
14	G	838	CLA	O2D-CGD-CBD	5.46	120.78	111.23
17	b	842	BCR	C7-C8-C9	-5.46	118.15	126.23
14	B	815	CLA	C4A-NA-C1A	5.46	109.17	106.68
14	b	839	CLA	C4A-NA-C1A	5.46	109.17	106.68
14	H	822	CLA	C2D-C1D-ND	5.46	115.53	110.13
14	B	822	CLA	C4A-NA-C1A	5.46	109.17	106.68
14	a	811	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
14	B	813	CLA	C2C-C1C-NC	5.46	115.72	109.98
14	b	802	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
14	A	805	CLA	C4A-NA-C1A	5.46	109.17	106.68
14	G	803	CLA	C2C-C1C-NC	5.46	115.71	109.98
14	b	810	CLA	C1C-C2C-C3C	-5.45	101.24	106.98
14	l	206	CLA	C1D-ND-C4D	-5.45	102.48	106.31
14	b	818	CLA	O2D-CGD-CBD	5.45	120.77	111.23
14	G	840	CLA	O2D-CGD-CBD	5.45	120.76	111.23
14	b	801	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
14	b	801	CLA	C1D-ND-C4D	-5.45	102.49	106.31
14	B	807	CLA	O2D-CGD-CBD	5.45	120.76	111.23
14	b	815	CLA	C4A-NA-C1A	5.45	109.17	106.68
14	G	845	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
17	j	103	BCR	C24-C23-C22	-5.45	118.17	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	844	CLA	C1C-C2C-C3C	-5.45	101.25	106.98
14	b	815	CLA	C2C-C1C-NC	5.45	115.71	109.98
14	b	805	CLA	C1C-C2C-C3C	-5.45	101.25	106.98
14	B	802	CLA	C2C-C1C-NC	5.45	115.70	109.98
14	B	802	CLA	O2D-CGD-CBD	5.45	120.75	111.23
14	M	1601	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
14	j	101	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
14	A	807	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
14	H	840	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
14	B	809	CLA	C4A-NA-C1A	5.44	109.16	106.68
14	G	834	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
14	b	836	CLA	C2D-C1D-ND	5.43	115.50	110.13
14	B	835	CLA	O2D-CGD-CBD	5.43	120.73	111.23
14	G	834	CLA	O2A-CGA-O1A	-5.43	110.04	123.63
14	G	807	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
14	V	1601	CLA	C4A-NA-C1A	5.43	109.16	106.68
14	H	828	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
14	H	818	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
14	A	802	CLA	C3D-C2D-C1D	-5.43	98.43	105.83
14	B	806	CLA	C2D-C1D-ND	5.42	115.50	110.13
14	H	839	CLA	C2C-C1C-NC	5.42	115.68	109.98
14	A	835	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
17	I	101	BCR	C24-C23-C22	-5.42	118.22	126.23
14	b	838	CLA	C3D-C2D-C1D	-5.42	98.43	105.83
14	G	842	CLA	O2D-CGD-CBD	5.42	120.70	111.23
14	A	836	CLA	C2D-C1D-ND	5.42	115.49	110.13
14	H	831	CLA	C2D-C1D-ND	5.42	115.49	110.13
14	B	812	CLA	C3D-C2D-C1D	-5.42	98.44	105.83
14	F	1301	CLA	C3D-C2D-C1D	-5.41	98.44	105.83
17	L	202	BCR	C7-C8-C9	-5.41	118.22	126.23
14	A	842	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
14	G	809	CLA	C2D-C1D-ND	5.41	115.48	110.13
14	G	813	CLA	O2D-CGD-CBD	5.41	120.69	111.23
17	B	847	BCR	C3-C4-C5	-5.41	104.40	114.06
14	G	827	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
14	b	839	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
14	A	812	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
14	A	803	CLA	C2C-C1C-NC	5.41	115.67	109.98
14	a	823	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
14	L	204	CLA	C2D-C1D-ND	5.41	115.48	110.13
14	a	828	CLA	C2D-C1D-ND	5.41	115.48	110.13
14	B	833	CLA	C2C-C1C-NC	5.41	115.66	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	205	CLA	C2C-C1C-NC	5.41	115.66	109.98
14	B	839	CLA	O2D-CGD-CBD	5.41	120.68	111.23
14	b	837	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
14	A	833	CLA	O2D-CGD-CBD	5.41	120.68	111.23
14	G	826	CLA	O2D-CGD-CBD	5.41	120.68	111.23
14	B	822	CLA	C2D-C1D-ND	5.40	115.47	110.13
14	G	807	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
14	A	817	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
14	H	835	CLA	O2D-CGD-CBD	5.40	120.67	111.23
14	B	817	CLA	O2D-CGD-CBD	5.40	120.67	111.23
14	a	825	CLA	C4A-NA-C1A	5.40	109.14	106.68
14	G	818	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
14	G	827	CLA	C2C-C1C-NC	5.40	115.65	109.98
14	l	202	CLA	O2A-CGA-CBA	5.40	128.30	111.83
17	F	1302	BCR	C24-C23-C22	-5.40	118.25	126.23
14	G	809	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
14	A	823	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
14	B	816	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
14	K	102	CLA	O2D-CGD-CBD	5.40	120.67	111.23
14	b	840	CLA	O2A-CGA-O1A	-5.40	110.13	123.63
14	a	828	CLA	C2C-C1C-NC	5.40	115.65	109.98
14	a	832	CLA	O2D-CGD-CBD	5.40	120.66	111.23
14	b	828	CLA	O2D-CGD-CBD	5.40	120.66	111.23
14	H	821	CLA	C4A-NA-C1A	5.39	109.14	106.68
14	G	823	CLA	O2D-CGD-CBD	5.39	120.66	111.23
14	G	814	CLA	C2C-C1C-NC	5.39	115.64	109.98
14	G	815	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
14	G	817	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
18	A	854	LHG	O7-C7-C8	5.39	123.14	111.48
14	B	838	CLA	C3D-C2D-C1D	-5.39	98.48	105.83
14	G	806	CLA	C4A-NA-C1A	5.39	109.14	106.68
14	a	804	CLA	C4A-NA-C1A	5.39	109.14	106.68
14	b	820	CLA	C3D-C2D-C1D	-5.39	98.48	105.83
14	H	820	CLA	O2D-CGD-CBD	5.39	120.65	111.23
14	A	810	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
14	B	819	CLA	C4A-NA-C1A	5.39	109.14	106.68
14	H	816	CLA	C3D-C2D-C1D	-5.38	98.48	105.83
14	a	813	CLA	C2D-C1D-ND	5.38	115.45	110.13
14	G	824	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
14	H	806	CLA	C2D-C1D-ND	5.38	115.45	110.13
14	b	827	CLA	O2D-CGD-CBD	5.38	120.64	111.23
14	H	820	CLA	C3D-C2D-C1D	-5.38	98.49	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	U	201	CLA	O2A-CGA-CBA	5.38	128.25	111.83
14	b	832	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
14	b	818	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
14	l	202	CLA	C2D-C1D-ND	5.38	115.45	110.13
14	L	206	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
14	B	831	CLA	C4A-NA-C1A	5.38	109.13	106.68
14	A	835	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
14	A	845	CLA	C2D-C1D-ND	5.38	115.45	110.13
14	k	1401	CLA	O2D-CGD-CBD	5.38	120.63	111.23
14	G	802	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
14	a	834	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
14	H	810	CLA	C4A-NA-C1A	5.37	109.13	106.68
14	l	207	CLA	O2D-CGD-CBD	5.37	120.62	111.23
14	a	808	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
14	U	206	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
14	L	204	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
14	b	811	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
14	G	805	CLA	C4A-NA-C1A	5.37	109.13	106.68
14	a	809	CLA	C4A-NA-C1A	5.37	109.13	106.68
14	b	815	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
14	a	844	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
14	a	806	CLA	C3D-C2D-C1D	-5.37	98.51	105.83
14	H	813	CLA	C2C-C1C-NC	5.37	115.62	109.98
14	H	827	CLA	C1C-C2C-C3C	-5.37	101.34	106.98
14	b	840	CLA	C3D-C2D-C1D	-5.37	98.51	105.83
14	H	826	CLA	O2A-CGA-O1A	-5.36	110.21	123.63
14	a	839	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
14	B	812	CLA	O2A-CGA-O1A	-5.36	110.22	123.63
14	b	831	CLA	C3D-C2D-C1D	-5.36	98.51	105.83
14	K	102	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
14	W	1701	CLA	C2D-C1D-ND	5.36	115.43	110.13
14	A	811	CLA	C4A-NA-C1A	5.36	109.12	106.68
14	H	828	CLA	O2A-CGA-O1A	-5.36	110.23	123.63
14	B	814	CLA	C1C-C2C-C3C	-5.36	101.35	106.98
14	A	805	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
14	H	835	CLA	CHD-C1D-ND	-5.35	117.27	124.80
14	A	809	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
14	G	835	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
14	B	837	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
14	G	840	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
14	b	825	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
14	a	828	CLA	C3D-C2D-C1D	-5.35	98.53	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	819	CLA	C2C-C1C-NC	5.35	115.60	109.98
14	H	805	CLA	C2C-C1C-NC	5.35	115.60	109.98
14	j	102	CLA	C1C-C2C-C3C	-5.35	101.36	106.98
14	b	828	CLA	O2A-CGA-O1A	-5.35	110.25	123.63
14	H	809	CLA	C4A-NA-C1A	5.35	109.12	106.68
14	G	814	CLA	C3D-C2D-C1D	-5.35	98.54	105.83
14	a	816	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
14	B	838	CLA	O2D-CGD-CBD	5.34	120.57	111.23
14	B	821	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
14	W	1701	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
14	b	836	CLA	O2A-CGA-O1A	-5.34	110.26	123.63
14	B	831	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
14	X	1701	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
14	G	821	CLA	C2D-C1D-ND	5.34	115.41	110.13
14	b	834	CLA	C4A-NA-C1A	5.34	109.12	106.68
14	B	837	CLA	O2A-CGA-O1A	-5.34	110.27	123.63
14	B	808	CLA	O2A-CGA-O1A	-5.34	110.27	123.63
14	b	812	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
14	b	801	CLA	CMD-C2D-C1D	5.34	134.13	124.73
14	B	810	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
14	H	807	CLA	C3D-C2D-C1D	-5.34	98.55	105.83
14	H	807	CLA	C2D-C1D-ND	5.34	115.41	110.13
14	G	840	CLA	C3D-C2D-C1D	-5.34	98.55	105.83
14	H	806	CLA	C1C-C2C-C3C	-5.34	101.37	106.98
14	a	805	CLA	C2C-C1C-NC	5.34	115.59	109.98
14	b	808	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
14	b	826	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
14	X	1701	CLA	C2D-C1D-ND	5.33	115.40	110.13
14	a	817	CLA	O2D-CGD-CBD	5.33	120.54	111.23
14	A	807	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
14	a	803	CLA	C1C-C2C-C3C	-5.33	101.38	106.98
14	B	807	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
14	A	834	CLA	O2A-CGA-O1A	-5.33	110.31	123.63
14	H	832	CLA	O2A-CGA-O1A	-5.32	110.31	123.63
14	G	821	CLA	C3D-C2D-C1D	-5.32	98.56	105.83
14	H	805	CLA	C4A-NA-C1A	5.32	109.11	106.68
14	A	820	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
14	b	814	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
14	m	1601	CLA	O2D-CGD-CBD	5.32	120.53	111.23
14	A	817	CLA	C4A-NA-C1A	5.32	109.11	106.68
14	a	813	CLA	C4A-NA-C1A	5.32	109.11	106.68
14	B	812	CLA	C2D-C1D-ND	5.32	115.39	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	U	204	CLA	C2D-C1D-ND	5.32	115.39	110.13
14	A	811	CLA	C2C-C1C-NC	5.32	115.57	109.98
14	a	836	CLA	C1C-C2C-C3C	-5.32	101.39	106.98
14	a	855	CLA	C2C-C1C-NC	5.32	115.57	109.98
14	G	804	CLA	O2A-CGA-O1A	-5.32	110.32	123.63
14	a	824	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
14	H	837	CLA	O2D-CGD-CBD	5.32	120.53	111.23
14	b	807	CLA	C2D-C1D-ND	5.32	115.39	110.13
14	H	807	CLA	C4A-NA-C1A	5.32	109.11	106.68
14	b	805	CLA	C4A-NA-C1A	5.32	109.11	106.68
14	B	816	CLA	C1D-ND-C4D	-5.32	102.58	106.31
14	A	806	CLA	C2C-C1C-NC	5.32	115.57	109.98
14	x	1701	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
14	b	812	CLA	O2A-CGA-O1A	-5.32	110.33	123.63
14	L	205	CLA	C4A-NA-C1A	5.32	109.10	106.68
14	a	823	CLA	C4A-NA-C1A	5.31	109.10	106.68
17	G	850	BCR	C24-C23-C22	-5.31	118.38	126.23
14	A	825	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
14	A	819	CLA	O2D-CGD-CBD	5.31	120.52	111.23
14	A	809	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
14	a	822	CLA	C2D-C1D-ND	5.31	115.38	110.13
14	A	840	CLA	C1C-C2C-C3C	-5.31	101.40	106.98
14	B	815	CLA	C1C-C2C-C3C	-5.31	101.40	106.98
14	A	814	CLA	C2D-C1D-ND	5.31	115.38	110.13
14	G	833	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
14	b	824	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
14	B	831	CLA	C1C-C2C-C3C	-5.31	101.40	106.98
14	B	834	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
14	H	826	CLA	C1C-C2C-C3C	-5.31	101.40	106.98
14	b	807	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
14	G	810	CLA	O2D-CGD-CBD	5.30	120.50	111.23
14	B	827	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
14	T	1401	CLA	O2D-CGD-CBD	5.30	120.50	111.23
14	H	821	CLA	C2D-C1D-ND	5.30	115.38	110.13
14	U	205	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
14	a	817	CLA	C2C-C1C-NC	5.30	115.55	109.98
14	B	835	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
14	H	840	CLA	O2A-CGA-O1A	-5.30	110.37	123.63
14	A	832	CLA	O2A-CGA-O1A	-5.30	110.38	123.63
14	S	101	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
14	H	816	CLA	O2D-CGD-CBD	5.29	120.49	111.23
14	H	817	CLA	O2D-CGD-CBD	5.29	120.49	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	X	1701	CLA	C4A-NA-C1A	5.29	109.09	106.68
14	a	855	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
14	B	831	CLA	O2D-CGD-CBD	5.29	120.48	111.23
14	B	818	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
14	G	840	CLA	C2D-C1D-ND	5.29	115.36	110.13
14	H	821	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
14	H	821	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
14	b	813	CLA	O2A-CGA-O1A	-5.29	110.40	123.63
14	a	813	CLA	C2C-C1C-NC	5.29	115.54	109.98
14	L	204	CLA	O2D-CGD-CBD	5.29	120.47	111.23
14	G	805	CLA	C2C-C1C-NC	5.29	115.53	109.98
14	W	1701	CLA	C4A-NA-C1A	5.29	109.09	106.68
14	G	804	CLA	C2D-C1D-ND	5.29	115.36	110.13
14	B	801	CLA	C3D-C2D-C1D	-5.29	98.62	105.83
14	A	810	CLA	O2D-CGD-CBD	5.29	120.47	111.23
14	b	812	CLA	O2D-CGD-CBD	5.28	120.47	111.23
14	H	804	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
14	G	836	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
14	G	842	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
14	b	817	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
14	a	805	CLA	O2D-CGD-CBD	5.28	120.46	111.23
14	a	823	CLA	C2D-C1D-ND	5.28	115.35	110.13
14	U	205	CLA	C4A-NA-C1A	5.28	109.09	106.68
14	A	810	CLA	C2D-C1D-ND	5.28	115.35	110.13
14	m	1601	CLA	C3D-C2D-C1D	-5.27	98.63	105.83
14	B	821	CLA	O2D-CGD-CBD	5.27	120.45	111.23
14	a	819	CLA	C1C-C2C-C3C	-5.27	101.43	106.98
14	b	816	CLA	C3D-C2D-C1D	-5.27	98.63	105.83
14	a	816	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
14	H	810	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
14	H	804	CLA	O2A-CGA-O1A	-5.27	110.44	123.63
14	F	1303	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
14	a	806	CLA	C2D-C1D-ND	5.27	115.34	110.13
14	l	205	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
14	H	812	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
14	a	804	CLA	O2A-CGA-O1A	-5.27	110.45	123.63
14	G	833	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
14	H	836	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
14	G	819	CLA	O2D-CGD-CBD	5.27	120.44	111.23
14	U	206	CLA	O2D-CGD-CBD	5.27	120.44	111.23
14	a	825	CLA	O2D-CGD-CBD	5.27	120.44	111.23
14	B	826	CLA	O2A-CGA-O1A	-5.27	110.45	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	813	CLA	O2A-CGA-O1A	-5.27	110.46	123.63
14	B	815	CLA	C3D-C2D-C1D	-5.27	98.65	105.83
14	b	805	CLA	O2A-CGA-O1A	-5.26	110.46	123.63
14	a	822	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
14	A	804	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
14	a	839	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
14	B	840	CLA	C2D-C1D-ND	5.26	115.33	110.13
14	A	824	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
14	b	809	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
14	L	201	CLA	C2D-C1D-ND	5.26	115.33	110.13
14	B	828	CLA	O2A-CGA-O1A	-5.26	110.48	123.63
14	H	822	CLA	C2C-C1C-NC	5.26	115.50	109.98
14	G	841	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
14	a	842	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
14	G	819	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
14	A	825	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
17	G	849	BCR	C3-C4-C5	-5.25	104.69	114.06
14	H	831	CLA	C2C-C1C-NC	5.25	115.50	109.98
14	a	804	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
14	G	804	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
14	b	830	CLA	C4A-NA-C1A	5.25	109.07	106.68
14	G	825	CLA	O2A-CGA-O1A	-5.25	110.51	123.63
14	a	830	CLA	C1C-C2C-C3C	-5.24	101.46	106.98
14	A	819	CLA	C3D-C2D-C1D	-5.24	98.67	105.83
14	A	830	CLA	O2A-CGA-O1A	-5.24	110.51	123.63
14	H	815	CLA	C2C-C1C-NC	5.24	115.49	109.98
14	a	844	CLA	C2D-C1D-ND	5.24	115.31	110.13
14	b	825	CLA	C2D-C1D-ND	5.24	115.31	110.13
14	a	814	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
14	G	805	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
17	i	102	BCR	C24-C23-C22	-5.24	118.48	126.23
14	A	838	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
14	H	820	CLA	C4A-NA-C1A	5.24	109.07	106.68
14	A	806	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
14	J	101	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
14	B	822	CLA	O2D-CGD-CBD	5.24	120.39	111.23
14	H	820	CLA	C2D-C1D-ND	5.24	115.31	110.13
14	A	829	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
14	B	837	CLA	C2D-C1D-ND	5.24	115.31	110.13
14	a	803	CLA	O2A-CGA-O1A	-5.24	110.53	123.63
14	U	204	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
14	G	809	CLA	C1C-C2C-C3C	-5.24	101.47	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	816	CLA	O2D-CGD-CBD	5.24	120.39	111.23
14	H	815	CLA	C3D-C2D-C1D	-5.24	98.69	105.83
14	k	1401	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
14	G	831	CLA	C1C-C2C-C3C	-5.23	101.47	106.98
14	J	101	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
14	a	807	CLA	O2D-CGD-CBD	5.23	120.38	111.23
14	G	816	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
14	i	101	CLA	C1D-ND-C4D	-5.23	102.64	106.31
14	A	811	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
14	B	824	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
14	H	836	CLA	O2A-CGA-O1A	-5.23	110.54	123.63
14	a	835	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
14	a	814	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
14	b	815	CLA	C1D-ND-C4D	-5.23	102.64	106.31
17	m	1602	BCR	C24-C23-C22	-5.23	118.50	126.23
14	a	823	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
14	b	820	CLA	C2D-C1D-ND	5.23	115.30	110.13
14	a	803	CLA	C2D-C1D-ND	5.22	115.30	110.13
14	a	805	CLA	C4A-NA-C1A	5.22	109.06	106.68
14	A	810	CLA	C3D-C2D-C1D	-5.22	98.70	105.83
14	H	835	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
14	b	815	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
14	B	814	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
14	b	819	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
14	A	831	CLA	C4A-NA-C1A	5.22	109.06	106.68
14	H	817	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
14	a	838	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
14	B	816	CLA	C4A-NA-C1A	5.22	109.06	106.68
14	a	835	CLA	O2D-CGD-CBD	5.22	120.35	111.23
14	H	822	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
14	H	809	CLA	O2D-CGD-CBD	5.21	120.35	111.23
14	b	806	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
14	A	812	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
14	b	831	CLA	O2D-CGD-CBD	5.21	120.34	111.23
14	a	808	CLA	C2C-C1C-NC	5.21	115.46	109.98
14	H	819	CLA	C4A-NA-C1A	5.21	109.06	106.68
14	G	828	CLA	O2D-CGD-CBD	5.21	120.34	111.23
14	B	804	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
14	H	810	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
14	G	807	CLA	C2D-C1D-ND	5.21	115.28	110.13
14	a	836	CLA	O2D-CGD-CBD	5.21	120.34	111.23
14	a	812	CLA	C1C-C2C-C3C	-5.21	101.50	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	804	CLA	C1D-ND-C4D	-5.21	102.66	106.31
14	a	824	CLA	C2D-C1D-ND	5.21	115.28	110.13
14	b	821	CLA	O2D-CGD-CBD	5.21	120.33	111.23
14	F	1303	CLA	C3D-C2D-C1D	-5.21	98.73	105.83
14	A	838	CLA	C2D-C1D-ND	5.21	115.28	110.13
14	U	206	CLA	C3D-C2D-C1D	-5.21	98.73	105.83
14	G	839	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
14	b	814	CLA	C2D-C1D-ND	5.20	115.28	110.13
14	i	101	CLA	C2D-C1D-ND	5.20	115.28	110.13
14	A	827	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	A	840	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	B	801	CLA	CMD-C2D-C1D	5.20	133.89	124.73
14	G	827	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
14	a	815	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
14	a	814	CLA	C4A-NA-C1A	5.20	109.05	106.68
14	U	201	CLA	C2D-C1D-ND	5.20	115.27	110.13
14	b	806	CLA	C1C-C2C-C3C	-5.20	101.52	106.98
14	A	821	CLA	C4A-NA-C1A	5.19	109.05	106.68
14	a	815	CLA	C4A-NA-C1A	5.19	109.05	106.68
14	G	819	CLA	C2D-C1D-ND	5.19	115.27	110.13
14	A	836	CLA	C3D-C2D-C1D	-5.19	98.74	105.83
14	G	822	CLA	C3D-C2D-C1D	-5.19	98.74	105.83
14	l	207	CLA	C3D-C2D-C1D	-5.19	98.74	105.83
14	B	815	CLA	C2D-C1D-ND	5.19	115.27	110.13
14	G	841	CLA	O2D-CGD-CBD	5.19	120.31	111.23
14	H	807	CLA	O2D-CGD-CBD	5.19	120.31	111.23
14	a	812	CLA	C4A-NA-C1A	5.19	109.05	106.68
14	a	805	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
14	H	840	CLA	C2D-C1D-ND	5.19	115.26	110.13
14	G	832	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
14	l	205	CLA	C4A-NA-C1A	5.19	109.05	106.68
14	H	821	CLA	O2A-CGA-O1A	-5.19	110.65	123.63
14	B	822	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
14	H	816	CLA	C2D-C1D-ND	5.19	115.26	110.13
14	a	819	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
14	A	808	CLA	O2D-CGD-CBD	5.19	120.30	111.23
14	B	804	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
14	a	832	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
14	B	802	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
14	S	101	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	B	832	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	l	207	CLA	C1C-C2C-C3C	-5.18	101.53	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	807	CLA	C1D-ND-C4D	-5.18	102.67	106.31
14	G	813	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
14	x	1701	CLA	C2D-C1D-ND	5.18	115.25	110.13
14	G	842	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
13	G	801	CL0	O2A-CGA-O1A	-5.18	110.67	123.63
17	b	847	BCR	C24-C23-C22	-5.18	118.57	126.23
14	b	822	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	A	813	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
14	G	811	CLA	C1D-ND-C4D	-5.18	102.68	106.31
14	H	819	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
14	B	811	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
14	W	1701	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
14	S	102	CLA	C1C-C2C-C3C	-5.18	101.54	106.98
14	a	840	CLA	C1C-C2C-C3C	-5.18	101.54	106.98
14	a	821	CLA	C1C-C2C-C3C	-5.18	101.54	106.98
14	a	818	CLA	C2C-C1C-NC	5.17	115.42	109.98
14	A	843	CLA	C1C-C2C-C3C	-5.17	101.54	106.98
14	A	805	CLA	O2A-CGA-O1A	-5.17	110.69	123.63
14	b	823	CLA	O2A-CGA-O1A	-5.17	110.69	123.63
14	a	803	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
14	G	836	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
14	A	818	CLA	O2D-CGD-CBD	5.17	120.27	111.23
14	b	832	CLA	C2D-C1D-ND	5.17	115.24	110.13
17	Q	202	BCR	C24-C23-C22	-5.17	118.59	126.23
14	b	830	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
14	a	826	CLA	C4A-NA-C1A	5.17	109.04	106.68
14	G	842	CLA	C2D-C1D-ND	5.17	115.24	110.13
14	G	830	CLA	C4A-NA-C1A	5.17	109.04	106.68
14	a	818	CLA	C3D-C2D-C1D	-5.16	98.78	105.83
14	B	801	CLA	C2C-C1C-NC	5.16	115.41	109.98
14	A	818	CLA	C4A-NA-C1A	5.16	109.03	106.68
14	H	831	CLA	O2D-CGD-CBD	5.16	120.26	111.23
14	b	830	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
14	S	102	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	A	822	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
14	x	1701	CLA	C1C-C2C-C3C	-5.16	101.55	106.98
14	G	821	CLA	O2A-CGA-O1A	-5.16	110.72	123.63
14	G	811	CLA	O2D-CGD-CBD	5.16	120.25	111.23
14	G	808	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	A	802	CLA	CMB-C2B-C3B	5.16	134.99	124.68
14	G	824	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	G	845	CLA	C1C-C2C-C3C	-5.16	101.56	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	824	CLA	C2C-C1C-NC	5.16	115.40	109.98
14	H	807	CLA	C1D-ND-C4D	-5.16	102.69	106.31
14	b	833	CLA	C1D-ND-C4D	-5.16	102.69	106.31
14	G	810	CLA	O2A-CGA-O1A	-5.15	110.73	123.63
14	H	811	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
14	H	813	CLA	O2A-CGA-O1A	-5.15	110.74	123.63
14	b	837	CLA	O2A-CGA-O1A	-5.15	110.74	123.63
14	H	815	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
14	G	841	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
14	A	818	CLA	C2D-C1D-ND	5.15	115.22	110.13
14	G	823	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
14	b	826	CLA	O2A-CGA-O1A	-5.15	110.75	123.63
14	a	820	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
14	B	804	CLA	C2D-C1D-ND	5.15	115.22	110.13
14	G	816	CLA	C4A-NA-C1A	5.15	109.03	106.68
14	H	813	CLA	O2D-CGD-CBD	5.15	120.23	111.23
14	B	818	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
14	T	1401	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
14	B	828	CLA	C4A-NA-C1A	5.14	109.03	106.68
14	A	819	CLA	O2A-CGA-O1A	-5.14	110.76	123.63
14	A	823	CLA	C1D-ND-C4D	-5.14	102.70	106.31
14	H	803	CLA	C1D-ND-C4D	-5.14	102.70	106.31
14	b	822	CLA	C4A-NA-C1A	5.14	109.03	106.68
14	G	832	CLA	O2A-CGA-O1A	-5.14	110.77	123.63
14	A	842	CLA	C2D-C1D-ND	5.14	115.22	110.13
14	H	830	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
14	b	821	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
14	B	813	CLA	O2D-CGD-CBD	5.14	120.22	111.23
14	i	101	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
14	H	823	CLA	C4A-NA-C1A	5.14	109.02	106.68
14	a	804	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
14	A	832	CLA	C1C-C2C-C3C	-5.14	101.58	106.98
14	A	834	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
14	G	807	CLA	O2A-CGA-CBA	5.14	127.50	111.83
14	B	815	CLA	O2D-CGD-CBD	5.14	120.21	111.23
14	A	833	CLA	C1C-C2C-C3C	-5.14	101.58	106.98
14	b	831	CLA	C1C-C2C-C3C	-5.14	101.58	106.98
14	a	837	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
17	H	842	BCR	C20-C19-C18	5.14	140.44	126.36
14	a	831	CLA	O2A-CGA-O1A	-5.14	110.78	123.63
14	b	824	CLA	C2C-C1C-NC	5.13	115.38	109.98
14	H	824	CLA	C3D-C2D-C1D	-5.13	98.82	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	828	CLA	O2D-CGD-CBD	5.13	120.20	111.23
14	G	822	CLA	C1C-C2C-C3C	-5.13	101.58	106.98
14	b	803	CLA	C1C-C2C-C3C	-5.13	101.58	106.98
14	B	838	CLA	C2D-C1D-ND	5.13	115.20	110.13
14	G	823	CLA	C2D-C1D-ND	5.13	115.20	110.13
14	a	804	CLA	C2D-C1D-ND	5.13	115.20	110.13
14	b	831	CLA	C2D-C1D-ND	5.13	115.20	110.13
14	B	824	CLA	O2D-CGD-CBD	5.13	120.20	111.23
14	H	818	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
14	j	102	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
14	H	815	CLA	C2D-C1D-ND	5.13	115.20	110.13
14	H	831	CLA	C1C-C2C-C3C	-5.13	101.59	106.98
14	H	838	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
14	A	803	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
14	b	812	CLA	C2D-C1D-ND	5.13	115.20	110.13
14	b	816	CLA	C2D-C1D-ND	5.12	115.20	110.13
14	B	836	CLA	O2A-CGA-O1A	-5.12	110.81	123.63
14	G	815	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	A	822	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	B	835	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	A	817	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	G	837	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	M	1601	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
14	b	836	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
14	H	812	CLA	C2D-C1D-ND	5.12	115.19	110.13
14	A	833	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
14	M	1601	CLA	O2D-CGD-CBD	5.12	120.17	111.23
14	A	807	CLA	C2D-C1D-ND	5.12	115.19	110.13
14	B	817	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
14	H	839	CLA	C1C-C2C-C3C	-5.12	101.60	106.98
14	a	809	CLA	O2D-CGD-CBD	5.12	120.17	111.23
14	a	838	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
14	A	805	CLA	C2D-C1D-ND	5.11	115.19	110.13
14	b	825	CLA	C1C-C2C-C3C	-5.11	101.60	106.98
14	G	807	CLA	C4A-NA-C1A	5.11	109.01	106.68
14	G	814	CLA	O2D-CGD-CBD	5.11	120.17	111.23
14	B	804	CLA	O2A-CGA-O1A	-5.11	110.84	123.63
14	G	808	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
14	A	835	CLA	C4A-NA-C1A	5.11	109.01	106.68
14	b	810	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
14	B	832	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
14	H	805	CLA	C1C-C2C-C3C	-5.11	101.61	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	832	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
14	G	815	CLA	O2D-CGD-CBD	5.11	120.16	111.23
14	G	819	CLA	O2A-CGA-O1A	-5.11	110.85	123.63
14	G	826	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
14	G	828	CLA	C1D-ND-C4D	-5.11	102.73	106.31
14	H	830	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
14	G	805	CLA	O2A-CGA-O1A	-5.11	110.86	123.63
14	A	821	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
14	H	832	CLA	C3D-C2D-C1D	-5.10	98.86	105.83
14	B	831	CLA	C2D-C1D-ND	5.10	115.18	110.13
14	A	820	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	H	833	CLA	C4A-NA-C1A	5.10	109.01	106.68
14	a	827	CLA	C4A-NA-C1A	5.10	109.01	106.68
14	l	205	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	b	810	CLA	O2D-CGD-CBD	5.10	120.15	111.23
14	G	838	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	b	805	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	G	824	CLA	C4A-NA-C1A	5.10	109.01	106.68
14	b	807	CLA	C4A-NA-C1A	5.10	109.01	106.68
14	b	823	CLA	O2D-CGD-CBD	5.10	120.15	111.23
14	B	839	CLA	C1C-C2C-C3C	-5.10	101.62	106.98
14	b	833	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	B	822	CLA	C2C-C1C-NC	5.10	115.34	109.98
14	A	820	CLA	O2D-CGD-CBD	5.10	120.14	111.23
14	B	834	CLA	C1C-C2C-C3C	-5.10	101.62	106.98
14	b	802	CLA	O2A-CGA-O1A	-5.10	110.88	123.63
14	b	824	CLA	C2D-C1D-ND	5.10	115.17	110.13
14	A	808	CLA	C1C-C2C-C3C	-5.10	101.62	106.98
14	H	826	CLA	C4A-NA-C1A	5.10	109.00	106.68
14	A	807	CLA	O2A-CGA-CBA	5.10	127.37	111.83
14	a	840	CLA	O2A-CGA-O1A	-5.10	110.88	123.63
14	H	819	CLA	C2D-C1D-ND	5.09	115.17	110.13
14	b	833	CLA	C4A-NA-C1A	5.09	109.00	106.68
14	a	826	CLA	C1D-ND-C4D	-5.09	102.74	106.31
14	j	101	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
14	B	826	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
14	G	825	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
14	B	806	CLA	C1D-ND-C4D	-5.09	102.74	106.31
14	a	855	CLA	CMD-C2D-C1D	5.09	133.69	124.73
14	B	816	CLA	O2D-CGD-CBD	5.09	120.13	111.23
14	A	827	CLA	C2D-C1D-ND	5.09	115.16	110.13
14	A	816	CLA	C3D-C2D-C1D	-5.09	98.89	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	836	CLA	O2D-CGD-CBD	5.09	120.12	111.23
14	K	102	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
14	B	807	CLA	C4A-NA-C1A	5.09	109.00	106.68
14	B	832	CLA	C4A-NA-C1A	5.09	109.00	106.68
14	H	822	CLA	C4A-NA-C1A	5.09	109.00	106.68
14	H	834	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
14	H	804	CLA	C4A-NA-C1A	5.09	109.00	106.68
14	b	832	CLA	C4A-NA-C1A	5.09	109.00	106.68
14	H	829	CLA	C4A-NA-C1A	5.08	109.00	106.68
14	G	828	CLA	O2A-CGA-O1A	-5.08	110.92	123.63
14	B	807	CLA	C1D-ND-C4D	-5.08	102.75	106.31
14	H	835	CLA	C4A-NA-C1A	5.08	109.00	106.68
14	A	828	CLA	O2A-CGA-O1A	-5.08	110.92	123.63
14	B	837	CLA	C1D-ND-C4D	-5.08	102.75	106.31
14	H	826	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
14	B	823	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
14	G	808	CLA	O2D-CGD-CBD	5.08	120.11	111.23
14	B	823	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
14	a	815	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
17	b	847	BCR	C7-C8-C9	-5.08	118.73	126.23
14	B	821	CLA	C2D-C1D-ND	5.07	115.15	110.13
14	A	818	CLA	C1D-ND-C4D	-5.07	102.75	106.31
14	b	835	CLA	C1C-C2C-C3C	-5.07	101.64	106.98
14	b	832	CLA	O2A-CGA-O1A	-5.07	110.94	123.63
14	H	816	CLA	CMB-C2B-C3B	5.07	134.82	124.68
13	a	801	CL0	C2D-C1D-ND	5.07	115.14	110.13
14	L	206	CLA	C2D-C1D-ND	5.07	115.14	110.13
14	b	819	CLA	C2D-C1D-ND	5.07	115.14	110.13
14	b	833	CLA	C2D-C1D-ND	5.07	115.14	110.13
14	H	824	CLA	C1C-C2C-C3C	-5.07	101.65	106.98
14	b	837	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	f	202	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	Q	201	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	a	834	CLA	C1C-C2C-C3C	-5.07	101.65	106.98
14	a	806	CLA	O2A-CGA-CBA	5.07	127.28	111.83
14	B	810	CLA	C3D-C2D-C1D	-5.07	98.92	105.83
14	a	822	CLA	O2D-CGD-CBD	5.07	120.09	111.23
14	G	825	CLA	C4A-NA-C1A	5.07	108.99	106.68
14	G	829	CLA	C4A-NA-C1A	5.07	108.99	106.68
14	b	825	CLA	C4A-NA-C1A	5.07	108.99	106.68
14	H	836	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
14	Q	203	CLA	C2D-C1D-ND	5.06	115.14	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	S	102	CLA	C2D-C1D-ND	5.06	115.14	110.13
14	H	831	CLA	C1D-ND-C4D	-5.06	102.76	106.31
14	b	809	CLA	C2D-C1D-ND	5.06	115.14	110.13
14	A	842	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
14	b	838	CLA	C2D-C1D-ND	5.06	115.14	110.13
14	b	828	CLA	C4A-NA-C1A	5.06	108.99	106.68
14	B	834	CLA	C2D-C1D-ND	5.06	115.13	110.13
14	a	816	CLA	O2A-CGA-O1A	-5.06	110.32	123.33
14	a	841	CLA	C4A-NA-C1A	5.06	108.99	106.68
14	H	806	CLA	C1D-ND-C4D	-5.06	102.76	106.31
14	G	817	CLA	C3D-C2D-C1D	-5.05	98.93	105.83
14	a	838	CLA	C4A-NA-C1A	5.05	108.98	106.68
14	B	809	CLA	O2A-CGA-O1A	-5.05	110.98	123.63
14	G	813	CLA	C3D-C2D-C1D	-5.05	98.93	105.83
14	a	830	CLA	C2D-C1D-ND	5.05	115.13	110.13
14	k	1401	CLA	C3D-C2D-C1D	-5.05	98.93	105.83
14	B	808	CLA	C1C-C2C-C3C	-5.05	101.67	106.98
13	a	801	CL0	O2A-CGA-O1A	-5.05	110.99	123.63
14	b	835	CLA	O2D-CGD-CBD	5.05	120.06	111.23
14	b	835	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
14	a	805	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
13	a	801	CL0	O2D-CGD-CBD	5.05	120.06	111.23
14	a	822	CLA	C4A-NA-C1A	5.05	108.98	106.68
14	b	833	CLA	C2C-C1C-NC	5.05	115.29	109.98
14	G	812	CLA	O2A-CGA-O1A	-5.05	111.00	123.63
14	U	206	CLA	O2A-CGA-O1A	-5.05	111.00	123.63
14	H	801	CLA	CMD-C2D-C1D	5.05	133.62	124.73
14	b	802	CLA	C2D-C1D-ND	5.05	115.12	110.13
14	A	802	CLA	C1C-C2C-C3C	-5.05	101.67	106.98
14	G	829	CLA	C1C-C2C-C3C	-5.05	101.67	106.98
14	a	818	CLA	O2A-CGA-O1A	-5.05	111.00	123.63
14	G	810	CLA	C1C-C2C-C3C	-5.05	101.67	106.98
14	B	840	CLA	O2A-CGA-O1A	-5.05	111.01	123.63
14	B	830	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
14	a	817	CLA	C1C-C2C-C3C	-5.04	101.68	106.98
14	A	808	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
14	G	820	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
14	H	823	CLA	C1C-C2C-C3C	-5.04	101.68	106.98
14	a	827	CLA	C1-C2-C3	-5.04	117.94	126.20
14	G	806	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
14	k	1401	CLA	C2D-C1D-ND	5.04	115.11	110.13
14	b	823	CLA	C3D-C2D-C1D	-5.04	98.95	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	844	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
14	b	822	CLA	O2D-CGD-CBD	5.04	120.04	111.23
14	G	827	CLA	O2A-CGA-O1A	-5.04	111.03	123.63
14	a	816	CLA	C2D-C1D-ND	5.03	115.11	110.13
14	G	814	CLA	C2D-C1D-ND	5.03	115.11	110.13
14	L	206	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
14	A	815	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
14	f	202	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
14	a	811	CLA	O2A-CGA-O1A	-5.03	111.04	123.63
14	G	833	CLA	C2D-C1D-ND	5.03	115.11	110.13
14	H	810	CLA	C2D-C1D-ND	5.03	115.11	110.13
14	F	1301	CLA	O2D-CGD-CBD	5.03	120.02	111.23
14	H	815	CLA	O2D-CGD-CBD	5.03	120.02	111.23
14	G	805	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
14	b	840	CLA	O2D-CGD-CBD	5.03	120.02	111.23
17	a	852	BCR	C7-C8-C9	-5.03	118.80	126.23
14	G	802	CLA	O2D-CGD-CBD	5.03	120.02	111.23
14	B	821	CLA	C4A-NA-C1A	5.03	108.97	106.68
14	B	811	CLA	C2D-C1D-ND	5.03	115.10	110.13
13	G	801	CL0	O2D-CGD-CBD	5.03	120.02	111.23
17	H	846	BCR	C38-C26-C25	-5.02	119.00	124.48
14	B	826	CLA	C1C-C2C-C3C	-5.02	101.69	106.98
14	A	841	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
14	A	827	CLA	C4A-NA-C1A	5.02	108.97	106.68
14	H	815	CLA	C4A-NA-C1A	5.02	108.97	106.68
14	a	802	CLA	O2D-CGD-CBD	5.02	120.01	111.23
14	a	825	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
14	b	818	CLA	O2A-CGA-O1A	-5.02	111.06	123.63
14	B	823	CLA	O2D-CGD-CBD	5.02	120.01	111.23
14	G	839	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
14	a	812	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
14	a	813	CLA	O2A-CGA-O1A	-5.02	111.07	123.63
14	A	804	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
14	l	202	CLA	O2D-CGD-CBD	5.02	120.00	111.23
14	G	809	CLA	C1D-ND-C4D	-5.02	102.79	106.31
14	H	805	CLA	O2A-CGA-O1A	-5.02	111.08	123.63
14	a	844	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
14	A	808	CLA	C4A-NA-C1A	5.02	108.97	106.68
14	B	818	CLA	O2A-CGA-O1A	-5.01	111.08	123.63
14	A	829	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	a	809	CLA	C2C-C1C-NC	5.01	115.25	109.98
14	A	825	CLA	C2D-C1D-ND	5.01	115.09	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	833	CLA	O2D-CGD-CBD	5.01	119.99	111.23
14	A	810	CLA	O2A-CGA-O1A	-5.01	111.10	123.63
14	b	802	CLA	O2D-CGD-CBD	5.01	119.99	111.23
14	H	838	CLA	C4A-NA-C1A	5.01	108.96	106.68
14	B	821	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
14	A	839	CLA	O2A-CGA-O1A	-5.01	111.10	123.63
14	B	829	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
14	G	834	CLA	O2D-CGD-CBD	5.01	119.98	111.23
14	A	802	CLA	C2C-C1C-NC	5.01	115.24	109.98
14	H	823	CLA	O2A-CGA-O1A	-5.01	111.11	123.63
14	A	834	CLA	O2D-CGD-CBD	5.01	119.98	111.23
14	a	807	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
14	b	809	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
14	A	843	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
14	a	836	CLA	O2A-CGA-O1A	-5.00	110.47	123.33
14	A	841	CLA	O2A-CGA-O1A	-5.00	111.12	123.63
14	a	802	CLA	C1C-C2C-C3C	-5.00	101.72	106.98
14	B	819	CLA	C2D-C1D-ND	5.00	115.07	110.13
14	a	834	CLA	C2D-C1D-ND	5.00	115.07	110.13
14	W	1701	CLA	O2D-CGD-CBD	5.00	119.97	111.23
14	B	805	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
14	b	802	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
14	a	810	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
14	A	812	CLA	O2A-CGA-O1A	-5.00	111.13	123.63
14	B	832	CLA	C2D-C1D-ND	5.00	115.07	110.13
14	G	820	CLA	C4A-NA-C1A	5.00	108.96	106.68
14	H	833	CLA	O2D-CGD-CBD	4.99	119.96	111.23
14	H	840	CLA	O2D-CGD-CBD	4.99	119.95	111.23
14	A	839	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
14	Q	203	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
14	A	841	CLA	C4A-NA-C1A	4.99	108.95	106.68
14	A	824	CLA	O2D-CGD-CBD	4.99	119.95	111.23
14	T	1401	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
14	A	840	CLA	O2D-CGD-CBD	4.99	119.95	111.23
14	b	840	CLA	C2D-C1D-ND	4.99	115.06	110.13
14	G	803	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
14	G	834	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
14	H	826	CLA	C2D-C1D-ND	4.98	115.06	110.13
14	G	804	CLA	C1C-C2C-C3C	-4.98	101.74	106.98
14	F	1301	CLA	C4A-NA-C1A	4.98	108.95	106.68
14	A	811	CLA	C2D-C1D-ND	4.98	115.05	110.13
14	b	818	CLA	C3D-C2D-C1D	-4.98	99.04	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	813	CLA	C1D-ND-C4D	-4.98	102.82	106.31
14	G	816	CLA	C1C-C2C-C3C	-4.98	101.75	106.98
14	a	820	CLA	C2D-C1D-ND	4.97	115.05	110.13
14	B	813	CLA	C2D-C1D-ND	4.97	115.05	110.13
14	H	808	CLA	C1C-C2C-C3C	-4.97	101.75	106.98
14	A	806	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
14	H	804	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
14	H	813	CLA	C4A-NA-C1A	4.97	108.95	106.68
14	H	839	CLA	C4A-NA-C1A	4.97	108.95	106.68
14	A	843	CLA	C2D-C1D-ND	4.97	115.04	110.13
14	Q	201	CLA	C2D-C1D-ND	4.96	115.04	110.13
14	a	808	CLA	C1C-C2C-C3C	-4.96	101.76	106.98
14	G	813	CLA	O2A-CGA-O1A	-4.96	111.21	123.63
14	a	836	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
14	G	831	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
14	B	811	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
14	b	801	CLA	C1C-C2C-C3C	-4.96	101.76	106.98
14	H	818	CLA	O2A-CGA-O1A	-4.96	111.22	123.63
14	A	821	CLA	C2D-C1D-ND	4.96	115.03	110.13
14	H	816	CLA	O2A-CGA-O1A	-4.96	111.23	123.63
14	G	841	CLA	O2A-CGA-O1A	-4.96	111.23	123.63
14	U	206	CLA	C2D-C1D-ND	4.96	115.03	110.13
14	A	813	CLA	C2D-C1D-ND	4.96	115.03	110.13
14	b	822	CLA	C2D-C1D-ND	4.95	115.03	110.13
14	a	802	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
14	H	838	CLA	C2D-C1D-ND	4.95	115.03	110.13
14	a	829	CLA	C1C-C2C-C3C	-4.95	101.77	106.98
14	G	805	CLA	C2D-C1D-ND	4.95	115.03	110.13
14	A	802	CLA	O2D-CGD-CBD	4.95	119.89	111.23
14	B	824	CLA	C2D-C1D-ND	4.95	115.03	110.13
14	A	838	CLA	C4A-NA-C1A	4.95	108.94	106.68
14	G	829	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
14	A	804	CLA	C2D-C1D-ND	4.95	115.02	110.13
14	b	833	CLA	O2A-CGA-O1A	-4.95	110.61	123.33
14	A	814	CLA	O2A-CGA-O1A	-4.95	111.25	123.63
14	b	837	CLA	C4A-NA-C1A	4.95	108.94	106.68
14	H	815	CLA	C1D-ND-C4D	-4.95	102.84	106.31
14	B	833	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
14	A	819	CLA	C1C-C2C-C3C	-4.94	101.78	106.98
14	G	841	CLA	C2D-C1D-ND	4.94	115.02	110.13
14	G	843	CLA	O2A-CGA-O1A	-4.94	111.26	123.63
14	a	806	CLA	O2D-CGD-CBD	4.94	119.87	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	816	CLA	C2C-C1C-NC	4.94	115.17	109.98
14	b	813	CLA	C1C-C2C-C3C	-4.94	101.78	106.98
14	A	845	CLA	O2A-CGA-O1A	-4.94	110.62	123.33
14	Q	203	CLA	C1C-C2C-C3C	-4.94	101.78	106.98
14	A	816	CLA	O2D-CGD-CBD	4.94	119.87	111.23
14	j	102	CLA	C4A-NA-C1A	4.94	108.93	106.68
14	L	205	CLA	C1C-C2C-C3C	-4.94	101.78	106.98
14	A	826	CLA	C1C-C2C-C3C	-4.94	101.78	106.98
14	H	817	CLA	C2D-C1D-ND	4.94	115.02	110.13
14	a	829	CLA	O2A-CGA-O1A	-4.94	111.27	123.63
14	A	840	CLA	C2D-C1D-ND	4.94	115.01	110.13
14	b	817	CLA	C2D-C1D-ND	4.94	115.01	110.13
14	G	837	CLA	C4A-NA-C1A	4.94	108.93	106.68
14	A	835	CLA	C2D-C1D-ND	4.94	115.01	110.13
14	a	843	CLA	C3D-C2D-C1D	-4.94	99.10	105.83
14	b	807	CLA	O2A-CGA-O1A	-4.93	111.28	123.63
14	a	841	CLA	C2D-C1D-ND	4.93	115.01	110.13
14	H	805	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
14	H	812	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
14	H	835	CLA	O2A-CGA-O1A	-4.93	110.64	123.33
14	B	813	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
14	A	818	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
14	B	824	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
14	a	825	CLA	CMD-C2D-C1D	4.93	133.41	124.73
14	b	826	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
14	f	202	CLA	C2D-C1D-ND	4.93	115.00	110.13
14	b	811	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
14	A	808	CLA	C2D-C1D-ND	4.93	115.00	110.13
14	H	810	CLA	O2D-CGD-CBD	4.93	119.84	111.23
14	b	834	CLA	C1D-ND-C4D	-4.93	102.86	106.31
14	B	810	CLA	O2D-CGD-CBD	4.92	119.84	111.23
14	a	841	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
14	a	833	CLA	O2A-CGA-O1A	-4.92	111.31	123.63
14	A	808	CLA	C1D-ND-C4D	-4.92	102.86	106.31
14	b	811	CLA	C1D-ND-C4D	-4.92	102.86	106.31
14	b	801	CLA	CMB-C2B-C3B	4.92	134.52	124.68
14	a	833	CLA	O2D-CGD-CBD	4.92	119.83	111.23
14	H	811	CLA	O2A-CGA-O1A	-4.92	110.68	123.33
14	G	814	CLA	O2A-CGA-O1A	-4.92	111.33	123.63
14	a	809	CLA	O2A-CGA-O1A	-4.92	111.33	123.63
14	G	808	CLA	C2D-C1D-ND	4.91	114.99	110.13
14	a	810	CLA	O2D-CGD-CBD	4.91	119.82	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	840	CLA	C1D-ND-C4D	-4.91	102.86	106.31
14	A	822	CLA	C2D-C1D-ND	4.91	114.99	110.13
14	G	819	CLA	C2C-C1C-NC	4.91	115.14	109.98
14	a	809	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
14	b	811	CLA	C2D-C1D-ND	4.91	114.99	110.13
14	a	828	CLA	C1C-C2C-C3C	-4.91	101.81	106.98
14	G	822	CLA	C2D-C1D-ND	4.91	114.99	110.13
14	G	837	CLA	O2A-CGA-O1A	-4.91	110.70	123.33
14	A	807	CLA	C4A-NA-C1A	4.91	108.92	106.68
14	a	838	CLA	C2D-C1D-ND	4.91	114.98	110.13
14	a	839	CLA	C2D-C1D-ND	4.91	114.98	110.13
14	A	813	CLA	O2A-CGA-O1A	-4.91	111.35	123.63
14	G	845	CLA	O2A-CGA-O1A	-4.91	110.72	123.33
14	H	810	CLA	C1D-ND-C4D	-4.91	102.87	106.31
14	A	830	CLA	C4A-NA-C1A	4.91	108.92	106.68
14	A	837	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
14	H	827	CLA	O2A-CGA-O1A	-4.90	111.36	123.63
13	G	801	CL0	C2D-C1D-ND	4.90	114.98	110.13
14	a	835	CLA	C2D-C1D-ND	4.90	114.98	110.13
14	G	802	CLA	O2A-CGA-CBA	4.90	126.78	111.83
14	f	202	CLA	O2A-CGA-O1A	-4.90	110.72	123.33
14	l	207	CLA	C2D-C1D-ND	4.90	114.98	110.13
14	U	204	CLA	C1D-ND-C4D	-4.90	102.87	106.31
14	G	830	CLA	O2A-CGA-O1A	-4.90	111.37	123.63
14	l	205	CLA	C2D-C1D-ND	4.90	114.98	110.13
14	A	829	CLA	C4A-NA-C1A	4.90	108.91	106.68
14	H	801	CLA	C1D-ND-C4D	-4.90	102.88	106.31
14	B	825	CLA	C1C-C2C-C3C	-4.90	101.83	106.98
14	G	818	CLA	O2D-CGD-CBD	4.90	119.79	111.23
14	l	205	CLA	O2A-CGA-O1A	-4.90	111.38	123.63
14	G	836	CLA	C2D-C1D-ND	4.90	114.97	110.13
14	B	818	CLA	O2D-CGD-CBD	4.89	119.78	111.23
14	G	810	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
14	B	833	CLA	C1C-C2C-C3C	-4.89	101.83	106.98
14	a	805	CLA	C2D-C1D-ND	4.89	114.97	110.13
14	b	838	CLA	C4A-NA-C1A	4.89	108.91	106.68
14	G	825	CLA	C2D-C1D-ND	4.89	114.97	110.13
14	B	803	CLA	O2A-CGA-O1A	-4.89	111.39	123.63
14	a	828	CLA	C4A-NA-C1A	4.89	108.91	106.68
14	a	823	CLA	O2D-CGD-CBD	4.89	119.78	111.23
14	a	833	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
14	A	819	CLA	C2D-C1D-ND	4.89	114.96	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	806	CLA	C4A-NA-C1A	4.89	108.91	106.68
14	G	818	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
14	G	833	CLA	O2D-CGD-CBD	4.89	119.77	111.23
14	B	813	CLA	C3D-C2D-C1D	-4.88	99.16	105.83
14	A	811	CLA	O2A-CGA-O1A	-4.88	110.77	123.33
14	K	101	CLA	O2A-CGA-O1A	-4.88	110.77	123.33
14	b	830	CLA	O2A-CGA-O1A	-4.88	110.77	123.33
14	a	817	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
14	H	801	CLA	C2C-C1C-NC	4.88	115.11	109.98
14	H	833	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
14	a	844	CLA	O2A-CGA-O1A	-4.88	110.78	123.33
14	K	101	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
14	G	804	CLA	C1D-ND-C4D	-4.88	102.89	106.31
14	b	821	CLA	C2D-C1D-ND	4.88	114.96	110.13
14	B	802	CLA	C1D-ND-C4D	-4.88	102.89	106.31
14	B	805	CLA	O2A-CGA-CBA	4.88	126.71	111.83
14	G	803	CLA	C1C-C2C-C3C	-4.88	101.85	106.98
14	J	101	CLA	C2D-C1D-ND	4.88	114.95	110.13
14	A	845	CLA	C1C-C2C-C3C	-4.88	101.85	106.98
14	b	832	CLA	C1C-C2C-C3C	-4.88	101.85	106.98
14	K	102	CLA	O2A-CGA-O1A	-4.88	110.79	123.33
14	A	813	CLA	O2D-CGD-CBD	4.87	119.75	111.23
14	a	818	CLA	O2D-CGD-CBD	4.87	119.75	111.23
14	G	817	CLA	C2D-C1D-ND	4.87	114.95	110.13
14	B	836	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
14	A	813	CLA	C4A-NA-C1A	4.87	108.90	106.68
14	k	1401	CLA	C1D-ND-C4D	-4.87	102.89	106.31
14	H	816	CLA	C2C-C1C-NC	4.87	115.10	109.98
14	G	819	CLA	C1D-ND-C4D	-4.87	102.89	106.31
14	a	812	CLA	O2A-CGA-O1A	-4.87	111.45	123.63
14	B	819	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
14	G	845	CLA	C1D-ND-C4D	-4.87	102.90	106.31
14	a	811	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
14	B	815	CLA	C1D-ND-C4D	-4.87	102.90	106.31
14	A	816	CLA	C1C-C2C-C3C	-4.87	101.86	106.98
14	B	820	CLA	O2A-CGA-O1A	-4.87	110.82	123.33
17	A	852	BCR	C24-C23-C22	-4.87	119.04	126.23
14	B	830	CLA	O2D-CGD-CBD	4.87	119.73	111.23
14	G	807	CLA	C1D-ND-C4D	-4.86	102.90	106.31
14	A	803	CLA	C1C-C2C-C3C	-4.86	101.86	106.98
14	H	837	CLA	O2A-CGA-O1A	-4.86	111.47	123.63
14	G	843	CLA	O2D-CGD-CBD	4.86	119.73	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	809	CLA	O2A-CGA-O1A	-4.86	111.47	123.63
14	b	806	CLA	O2A-CGA-CBA	4.86	126.65	111.83
14	a	820	CLA	O2A-CGA-O1A	-4.86	111.47	123.63
14	M	1601	CLA	C2D-C1D-ND	4.86	114.94	110.13
14	b	816	CLA	O2A-CGA-O1A	-4.86	111.47	123.63
14	b	836	CLA	O2D-CGD-CBD	4.86	119.72	111.23
13	A	801	CL0	O2A-CGA-O1A	-4.86	111.48	123.63
14	H	822	CLA	O2A-CGA-O1A	-4.86	110.84	123.33
14	b	810	CLA	O2A-CGA-O1A	-4.86	110.84	123.33
14	B	802	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
14	H	820	CLA	O2A-CGA-O1A	-4.85	110.85	123.33
14	a	824	CLA	C1C-C2C-C3C	-4.85	101.88	106.98
14	G	840	CLA	O2A-CGA-O1A	-4.85	110.85	123.33
14	a	842	CLA	C2D-C1D-ND	4.85	114.93	110.13
14	b	811	CLA	C4A-NA-C1A	4.85	108.89	106.68
14	a	814	CLA	C2D-C1D-ND	4.85	114.93	110.13
14	a	803	CLA	C4A-NA-C1A	4.85	108.89	106.68
14	G	835	CLA	O2A-CGA-O1A	-4.85	111.50	123.63
14	a	830	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
14	a	812	CLA	C2D-C1D-ND	4.85	114.92	110.13
14	H	809	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
14	S	101	CLA	C2D-C1D-ND	4.84	114.92	110.13
14	L	204	CLA	O2A-CGA-O1A	-4.84	111.51	123.63
14	a	827	CLA	C2C-C1C-NC	4.84	115.07	109.98
14	H	833	CLA	C1C-C2C-C3C	-4.84	101.89	106.98
14	a	837	CLA	C2D-C1D-ND	4.84	114.92	110.13
14	b	837	CLA	C1D-ND-C4D	-4.84	102.92	106.31
14	G	836	CLA	O2D-CGD-CBD	4.84	119.69	111.23
14	H	802	CLA	O2D-CGD-CBD	4.84	119.69	111.23
14	B	836	CLA	C2D-C1D-ND	4.84	114.91	110.13
14	A	803	CLA	C2D-C1D-ND	4.84	114.91	110.13
14	b	812	CLA	C1C-C2C-C3C	-4.83	101.89	106.98
14	b	833	CLA	C1C-C2C-C3C	-4.83	101.89	106.98
14	G	828	CLA	CMC-C2C-C1C	4.83	132.59	125.03
14	b	837	CLA	C2D-C1D-ND	4.83	114.91	110.13
14	a	823	CLA	C1D-ND-C4D	-4.83	102.92	106.31
14	a	835	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
14	G	808	CLA	C4A-NA-C1A	4.83	108.88	106.68
14	H	803	CLA	O2A-CGA-O1A	-4.83	111.54	123.63
14	b	807	CLA	O2D-CGD-CBD	4.83	119.67	111.23
14	A	806	CLA	O2A-CGA-O1A	-4.83	110.91	123.33
14	b	827	CLA	O2A-CGA-O1A	-4.83	111.55	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	844	CLA	O2D-CGD-CBD	4.83	119.67	111.23
14	a	835	CLA	O2A-CGA-O1A	-4.83	110.91	123.33
14	G	825	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
14	G	823	CLA	O2A-CGA-O1A	-4.83	110.91	123.33
14	W	1701	CLA	O2A-CGA-O1A	-4.83	110.91	123.33
14	X	1701	CLA	O2A-CGA-O1A	-4.83	110.91	123.33
14	A	802	CLA	O2A-CGA-CBA	4.83	126.56	111.83
14	A	813	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
14	G	823	CLA	C4A-NA-C1A	4.82	108.88	106.68
14	H	833	CLA	O2A-CGA-O1A	-4.82	110.92	123.33
14	G	831	CLA	C2D-C1D-ND	4.82	114.90	110.13
14	Q	201	CLA	O2A-CGA-O1A	-4.82	110.93	123.33
14	b	834	CLA	O2A-CGA-O1A	-4.82	110.93	123.33
14	B	835	CLA	C4A-NA-C1A	4.82	108.88	106.68
14	G	831	CLA	O2A-CGA-O1A	-4.82	111.57	123.63
14	G	827	CLA	C2D-C1D-ND	4.82	114.90	110.13
14	A	844	CLA	O2A-CGA-O1A	-4.82	111.57	123.63
14	B	818	CLA	C2D-C1D-ND	4.82	114.90	110.13
14	B	811	CLA	C1D-ND-C4D	-4.82	102.93	106.31
14	l	207	CLA	C4A-NA-C1A	4.82	108.88	106.68
14	a	815	CLA	O2A-CGA-O1A	-4.82	110.94	123.33
14	A	826	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
14	H	822	CLA	O2D-CGD-O1D	-4.81	114.48	123.85
14	A	831	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
14	a	806	CLA	C1D-ND-C4D	-4.81	102.94	106.31
14	b	821	CLA	O2A-CGA-O1A	-4.81	111.59	123.63
14	b	805	CLA	C2D-C1D-ND	4.81	114.89	110.13
14	G	806	CLA	O2A-CGA-O1A	-4.81	110.95	123.33
14	b	816	CLA	C1C-C2C-C3C	-4.81	101.92	106.98
14	K	102	CLA	C2D-C1D-ND	4.81	114.89	110.13
14	b	801	CLA	C2C-C1C-NC	4.81	115.03	109.98
14	a	855	CLA	O2A-CGA-O1A	-4.81	111.60	123.63
14	A	836	CLA	O2A-CGA-O1A	-4.81	110.96	123.33
14	V	1601	CLA	O2A-CGA-O1A	-4.81	110.97	123.33
14	A	829	CLA	C2D-C1D-ND	4.81	114.89	110.13
14	a	807	CLA	C1C-C2C-C3C	-4.81	101.92	106.98
14	a	822	CLA	C1D-ND-C4D	-4.81	102.94	106.31
14	G	816	CLA	O2A-CGA-O1A	-4.81	110.97	123.33
14	a	840	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
14	G	836	CLA	O2A-CGA-O1A	-4.80	110.97	123.33
14	x	1701	CLA	O2A-CGA-O1A	-4.80	110.99	123.33
14	B	818	CLA	C4A-NA-C1A	4.80	108.87	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	802	CLA	O2A-CGA-O1A	-4.79	111.63	123.63
14	a	818	CLA	C1-C2-C3	-4.79	119.00	126.76
17	J	102	BCR	C4-C5-C6	-4.79	116.23	122.70
14	G	813	CLA	C4A-NA-C1A	4.79	108.87	106.68
14	F	1303	CLA	C2D-C1D-ND	4.79	114.87	110.13
14	b	810	CLA	C2D-C1D-ND	4.79	114.87	110.13
14	B	809	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
14	A	832	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
17	G	849	BCR	C36-C18-C17	-4.79	115.05	122.82
14	a	817	CLA	O2A-CGA-O1A	-4.79	111.01	123.33
14	b	839	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
14	a	838	CLA	O2A-CGA-O1A	-4.79	111.65	123.63
14	A	845	CLA	C1D-ND-C4D	-4.79	102.95	106.31
14	H	837	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
14	a	842	CLA	O2A-CGA-O1A	-4.79	111.65	123.63
14	a	819	CLA	C2D-C1D-ND	4.79	114.86	110.13
14	H	822	CLA	C1D-ND-C4D	-4.79	102.95	106.31
14	L	204	CLA	C1D-ND-C4D	-4.79	102.95	106.31
14	a	807	CLA	O2A-CGA-O1A	-4.79	111.02	123.33
17	H	845	BCR	C24-C23-C22	-4.79	119.15	126.23
14	H	839	CLA	O2A-CGA-O1A	-4.79	111.66	123.63
14	A	816	CLA	O2A-CGA-O1A	-4.79	111.02	123.33
14	H	818	CLA	C2D-C1D-ND	4.79	114.86	110.13
14	G	802	CLA	C1D-ND-C4D	-4.79	102.95	106.31
14	A	827	CLA	O2A-CGA-O1A	-4.79	111.66	123.63
14	A	843	CLA	C4A-NA-C1A	4.78	108.86	106.68
14	H	830	CLA	O2A-CGA-O1A	-4.78	111.03	123.33
14	a	831	CLA	C1C-C2C-C3C	-4.78	101.95	106.98
14	B	822	CLA	O2A-CGA-O1A	-4.78	111.03	123.33
14	B	801	CLA	O2A-CGA-O1A	-4.78	111.67	123.63
14	B	840	CLA	O2D-CGD-CBD	4.78	119.59	111.23
14	a	837	CLA	O2A-CGA-O1A	-4.78	111.67	123.63
14	H	830	CLA	C4A-NA-C1A	4.78	108.86	106.68
14	Q	203	CLA	O2A-CGA-O1A	-4.78	111.05	123.33
14	a	810	CLA	O2A-CGA-O1A	-4.78	111.05	123.33
14	B	829	CLA	O2A-CGA-O1A	-4.78	111.05	123.33
17	S	104	BCR	C31-C1-C6	4.78	117.73	110.24
14	i	101	CLA	C4A-NA-C1A	4.78	108.86	106.68
14	H	834	CLA	O2D-CGD-CBD	4.77	119.58	111.23
14	G	809	CLA	C4A-NA-C1A	4.77	108.86	106.68
14	L	201	CLA	O2D-CGD-CBD	4.77	119.58	111.23
14	B	814	CLA	C2D-C1D-ND	4.77	114.85	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	818	CLA	C2D-C1D-ND	4.77	114.85	110.13
14	A	819	CLA	C1D-ND-C4D	-4.77	102.96	106.31
14	b	832	CLA	C1D-ND-C4D	-4.77	102.96	106.31
14	B	834	CLA	O2A-CGA-O1A	-4.77	111.06	123.33
14	G	838	CLA	C4A-NA-C1A	4.77	108.86	106.68
14	H	815	CLA	O2A-CGA-O1A	-4.77	111.06	123.33
14	A	818	CLA	C2C-C1C-NC	4.77	114.99	109.98
14	m	1601	CLA	C2D-C1D-ND	4.77	114.85	110.13
14	S	101	CLA	O2A-CGA-O1A	-4.77	111.06	123.33
14	G	812	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
14	H	838	CLA	C1D-ND-C4D	-4.77	102.97	106.31
17	f	203	BCR	C24-C23-C22	-4.77	119.19	126.23
14	b	808	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
14	f	202	CLA	O2D-CGD-CBD	4.76	119.56	111.23
14	l	206	CLA	O2A-CGA-O1A	-4.76	111.71	123.63
14	a	821	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
14	A	802	CLA	O2A-CGA-O1A	-4.76	111.72	123.63
14	U	204	CLA	O2A-CGA-O1A	-4.76	111.72	123.63
14	A	833	CLA	O2A-CGA-O1A	-4.76	111.72	123.63
14	G	823	CLA	C1D-ND-C4D	-4.76	102.97	106.31
14	A	817	CLA	C2D-C1D-ND	4.76	114.84	110.13
14	b	830	CLA	C2D-C1D-ND	4.76	114.84	110.13
14	A	818	CLA	C1C-C2C-C3C	-4.76	101.97	106.98
14	G	806	CLA	C2D-C1D-ND	4.76	114.84	110.13
14	T	1401	CLA	C2D-C1D-ND	4.76	114.84	110.13
14	A	838	CLA	O2A-CGA-O1A	-4.76	111.73	123.63
14	B	838	CLA	C1D-ND-C4D	-4.76	102.97	106.31
14	a	839	CLA	O2D-CGD-CBD	4.76	119.55	111.23
14	X	1701	CLA	O2D-CGD-CBD	4.76	119.55	111.23
14	M	1601	CLA	O2A-CGA-O1A	-4.76	111.10	123.33
14	j	102	CLA	C2D-C1D-ND	4.76	114.83	110.13
14	A	823	CLA	O2A-CGA-O1A	-4.76	111.10	123.33
14	b	837	CLA	O2D-CGD-CBD	4.75	119.54	111.23
14	a	827	CLA	CMC-C2C-C1C	4.75	132.46	125.03
14	A	826	CLA	O2D-CGD-CBD	4.75	119.54	111.23
14	G	827	CLA	O2D-CGD-CBD	4.75	119.54	111.23
14	H	802	CLA	C2D-C1D-ND	4.75	114.83	110.13
14	a	802	CLA	C2D-C1D-ND	4.75	114.83	110.13
14	A	828	CLA	C1D-ND-C4D	-4.75	102.98	106.31
14	B	810	CLA	O2A-CGA-O1A	-4.75	111.11	123.33
14	b	833	CLA	O2D-CGD-CBD	4.75	119.53	111.23
14	a	818	CLA	C4A-NA-C1A	4.75	108.85	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	838	CLA	C2D-C1D-ND	4.75	114.83	110.13
14	G	812	CLA	O2D-CGD-CBD	4.75	119.53	111.23
13	A	801	CL0	C2D-C1D-ND	4.75	114.82	110.13
17	G	853	BCR	C38-C26-C25	-4.75	119.31	124.48
14	G	829	CLA	C2D-C1D-ND	4.74	114.82	110.13
14	a	843	CLA	O2A-CGA-O1A	-4.74	111.13	123.33
14	G	832	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
14	G	844	CLA	O2A-CGA-O1A	-4.74	111.13	123.33
14	A	821	CLA	O2A-CGA-O1A	-4.74	111.77	123.63
14	G	814	CLA	C4A-NA-C1A	4.74	108.84	106.68
14	b	836	CLA	C4A-NA-C1A	4.74	108.84	106.68
14	a	814	CLA	O2A-CGA-O1A	-4.74	111.14	123.33
14	a	822	CLA	O2A-CGA-O1A	-4.74	111.14	123.33
14	H	811	CLA	C2D-C1D-ND	4.74	114.82	110.13
14	A	839	CLA	C2D-C1D-ND	4.74	114.82	110.13
14	H	834	CLA	O2A-CGA-O1A	-4.74	111.15	123.33
14	a	829	CLA	C4A-NA-C1A	4.74	108.84	106.68
14	b	820	CLA	O2A-CGA-O1A	-4.74	111.15	123.33
14	G	809	CLA	O2A-CGA-O1A	-4.74	111.78	123.63
14	G	810	CLA	C2D-C1D-ND	4.74	114.81	110.13
14	G	818	CLA	O2A-CGA-O1A	-4.73	111.16	123.33
14	A	833	CLA	C2D-C1D-ND	4.73	114.81	110.13
14	m	1601	CLA	O2A-CGA-O1A	-4.73	111.16	123.33
14	a	809	CLA	C2D-C1D-ND	4.73	114.81	110.13
14	b	803	CLA	C2D-C1D-ND	4.73	114.81	110.13
14	G	828	CLA	C4A-NA-C1A	4.73	108.84	106.68
14	a	855	CLA	C1C-C2C-C3C	-4.73	102.00	106.98
14	b	824	CLA	C1C-C2C-C3C	-4.73	102.00	106.98
14	B	821	CLA	O2A-CGA-O1A	-4.73	111.80	123.63
14	A	814	CLA	C4A-NA-C1A	4.73	108.84	106.68
14	A	834	CLA	C2D-C1D-ND	4.73	114.81	110.13
14	B	826	CLA	C2D-C1D-ND	4.73	114.81	110.13
14	G	802	CLA	O2A-CGA-O1A	-4.73	111.80	123.63
14	B	809	CLA	O2D-CGD-CBD	4.73	119.49	111.23
17	U	202	BCR	C24-C23-C22	-4.73	119.24	126.23
14	A	831	CLA	C2D-C1D-ND	4.73	114.80	110.13
14	B	833	CLA	O2A-CGA-O1A	-4.73	111.18	123.33
14	H	829	CLA	O2A-CGA-O1A	-4.73	111.18	123.33
14	B	837	CLA	O2D-CGD-CBD	4.72	119.49	111.23
14	A	824	CLA	O2A-CGA-O1A	-4.72	111.18	123.33
14	G	839	CLA	C2D-C1D-ND	4.72	114.80	110.13
14	H	808	CLA	C2D-C1D-ND	4.72	114.80	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	816	CLA	O2A-CGA-O1A	-4.72	111.82	123.63
14	A	837	CLA	O2A-CGA-O1A	-4.72	111.19	123.33
14	b	824	CLA	O2A-CGA-O1A	-4.72	111.19	123.33
14	H	805	CLA	C2D-C1D-ND	4.72	114.80	110.13
14	j	101	CLA	O2A-CGA-O1A	-4.72	111.19	123.33
14	G	813	CLA	C2D-C1D-ND	4.72	114.80	110.13
14	A	806	CLA	C1D-ND-C4D	-4.72	103.00	106.31
14	U	206	CLA	C4A-NA-C1A	4.72	108.83	106.68
14	A	806	CLA	C2D-C1D-ND	4.72	114.80	110.13
14	B	829	CLA	C2D-C1D-ND	4.72	114.80	110.13
14	G	817	CLA	O2A-CGA-O1A	-4.72	111.20	123.33
14	B	819	CLA	O2A-CGA-O1A	-4.72	111.20	123.33
14	Q	203	CLA	O2D-CGD-CBD	4.72	119.47	111.23
14	L	205	CLA	O2A-CGA-O1A	-4.71	111.83	123.63
14	b	830	CLA	O2D-CGD-CBD	4.71	119.47	111.23
14	F	1301	CLA	O2A-CGA-O1A	-4.71	111.21	123.33
14	b	815	CLA	O2D-CGD-CBD	4.71	119.47	111.23
14	b	823	CLA	CMD-C2D-C1D	4.71	133.02	124.73
14	a	840	CLA	C4A-NA-C1A	4.71	108.83	106.68
14	B	827	CLA	O2A-CGA-O1A	-4.71	111.85	123.63
14	A	807	CLA	C1D-ND-C4D	-4.71	103.01	106.31
14	G	811	CLA	O2A-CGA-O1A	-4.71	111.22	123.33
14	A	824	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
14	a	815	CLA	C2D-C1D-ND	4.71	114.78	110.13
14	A	842	CLA	C1D-ND-C4D	-4.71	103.01	106.31
14	x	1701	CLA	C1D-ND-C4D	-4.71	103.01	106.31
14	G	824	CLA	C2D-C1D-ND	4.70	114.78	110.13
14	a	832	CLA	O2A-CGA-O1A	-4.70	111.86	123.63
14	H	824	CLA	C2D-C1D-ND	4.70	114.78	110.13
14	b	829	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
14	A	844	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
14	b	839	CLA	O2A-CGA-O1A	-4.70	111.88	123.63
14	B	838	CLA	O2A-CGA-O1A	-4.70	111.25	123.33
14	a	841	CLA	O2A-CGA-O1A	-4.70	111.25	123.33
14	B	814	CLA	O2A-CGA-O1A	-4.70	111.25	123.33
14	G	843	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
14	a	836	CLA	C2D-C1D-ND	4.70	114.77	110.13
14	A	842	CLA	O2A-CGA-O1A	-4.69	111.26	123.33
14	T	1401	CLA	O2A-CGA-O1A	-4.69	111.27	123.33
14	G	808	CLA	C1D-ND-C4D	-4.69	103.02	106.31
14	G	824	CLA	O2A-CGA-O1A	-4.69	111.27	123.33
14	b	814	CLA	O2A-CGA-O1A	-4.69	111.27	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	839	CLA	O2A-CGA-O1A	-4.69	111.90	123.63
14	b	838	CLA	O2A-CGA-O1A	-4.69	111.28	123.33
14	H	808	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
14	H	823	CLA	C2D-C1D-ND	4.69	114.77	110.13
14	G	808	CLA	O2A-CGA-O1A	-4.69	111.28	123.33
17	R	101	BCR	C7-C8-C9	-4.69	119.30	126.23
14	A	819	CLA	C1-C2-C3	-4.69	119.18	126.76
14	b	806	CLA	C2D-C1D-ND	4.69	114.76	110.13
14	a	831	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
14	B	823	CLA	C1D-ND-C4D	-4.68	103.03	106.31
14	b	835	CLA	O2A-CGA-O1A	-4.68	111.29	123.33
14	F	1303	CLA	CAA-C2A-C3A	-4.68	105.50	116.23
14	G	804	CLA	C4A-NA-C1A	4.68	108.81	106.68
14	Q	201	CLA	C4A-NA-C1A	4.68	108.81	106.68
14	a	840	CLA	O2D-CGD-CBD	4.68	119.41	111.23
14	B	830	CLA	O2A-CGA-O1A	-4.68	111.30	123.33
14	G	837	CLA	C2D-C1D-ND	4.68	114.76	110.13
14	H	809	CLA	O2A-CGA-O1A	-4.68	111.93	123.63
14	S	102	CLA	CAA-C2A-C3A	-4.68	105.50	116.23
14	G	822	CLA	C1D-ND-C4D	-4.68	103.03	106.31
14	B	806	CLA	O2A-CGA-O1A	-4.68	111.93	123.63
14	H	804	CLA	C2D-C1D-ND	4.68	114.75	110.13
17	B	850	BCR	C7-C8-C9	-4.67	119.32	126.23
14	B	835	CLA	O2A-CGA-O1A	-4.67	111.31	123.33
14	G	817	CLA	C1D-ND-C4D	-4.67	103.03	106.31
14	G	815	CLA	O2A-CGA-O1A	-4.67	111.31	123.33
14	a	831	CLA	C2D-C1D-ND	4.67	114.75	110.13
14	A	816	CLA	C2D-C1D-ND	4.67	114.75	110.13
14	A	840	CLA	O2A-CGA-O1A	-4.67	111.32	123.33
14	a	803	CLA	C1D-ND-C4D	-4.67	103.03	106.31
14	b	838	CLA	C1D-ND-C4D	-4.67	103.03	106.31
14	a	826	CLA	O2A-CGA-O1A	-4.67	111.95	123.63
14	a	830	CLA	O2A-CGA-O1A	-4.67	111.95	123.63
14	a	837	CLA	CMB-C2B-C3B	4.67	134.01	124.68
14	H	816	CLA	C1C-C2C-C3C	-4.66	102.07	106.98
14	b	829	CLA	O2A-CGA-O1A	-4.66	111.34	123.33
14	A	812	CLA	C2D-C1D-ND	4.66	114.74	110.13
14	A	841	CLA	C2D-C1D-ND	4.66	114.74	110.13
14	B	817	CLA	C2D-C1D-ND	4.66	114.74	110.13
14	k	1401	CLA	O2A-CGA-O1A	-4.66	111.34	123.33
14	H	801	CLA	O2A-CGA-O1A	-4.66	111.96	123.63
14	B	835	CLA	C2D-C1D-ND	4.66	114.74	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	805	CLA	O2A-CGA-O1A	-4.66	111.34	123.33
14	G	833	CLA	C4A-NA-C1A	4.66	108.81	106.68
14	B	839	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
14	S	102	CLA	C1D-ND-C4D	-4.66	103.04	106.31
14	B	822	CLA	C1D-ND-C4D	-4.66	103.05	106.31
14	H	836	CLA	C2D-C1D-ND	4.66	114.73	110.13
14	b	804	CLA	O2A-CGA-O1A	-4.66	111.98	123.63
14	H	834	CLA	C2D-C1D-ND	4.65	114.73	110.13
14	a	805	CLA	C1D-ND-C4D	-4.65	103.05	106.31
14	a	807	CLA	C1D-ND-C4D	-4.65	103.05	106.31
14	B	811	CLA	O2A-CGA-O1A	-4.65	111.36	123.33
14	H	809	CLA	C2D-C1D-ND	4.65	114.73	110.13
14	b	808	CLA	C2D-C1D-ND	4.65	114.73	110.13
14	G	834	CLA	C2D-C1D-ND	4.65	114.73	110.13
14	a	802	CLA	O2A-CGA-O1A	-4.65	112.00	123.63
14	B	833	CLA	C2D-C1D-ND	4.65	114.73	110.13
14	B	820	CLA	C1D-ND-C4D	-4.65	103.05	106.31
14	G	833	CLA	O2A-CGA-O1A	-4.65	112.00	123.63
14	H	831	CLA	CMB-C2B-C3B	4.64	133.97	124.68
14	A	822	CLA	C1D-ND-C4D	-4.64	103.05	106.31
14	B	811	CLA	C4A-NA-C1A	4.64	108.80	106.68
14	A	817	CLA	O2A-CGA-O1A	-4.64	111.39	123.33
14	H	810	CLA	O2A-CGA-O1A	-4.64	111.39	123.33
14	b	836	CLA	C1C-C2C-C3C	-4.64	102.10	106.98
14	b	816	CLA	C1D-ND-C4D	-4.64	103.06	106.31
14	H	803	CLA	C2C-C1C-NC	4.64	114.85	109.98
14	A	817	CLA	O2D-CGD-CBD	4.64	119.34	111.23
14	a	826	CLA	CAA-C2A-C3A	-4.64	100.47	113.00
14	B	803	CLA	CAA-C2A-C3A	-4.64	100.47	113.00
17	H	845	BCR	C23-C22-C21	4.63	126.30	119.01
14	H	824	CLA	O2A-CGA-O1A	-4.63	111.41	123.33
14	B	815	CLA	O2A-CGA-O1A	-4.63	111.42	123.33
14	B	824	CLA	O2A-CGA-O1A	-4.63	111.42	123.33
14	B	803	CLA	C1D-ND-C4D	-4.63	103.06	106.31
14	B	805	CLA	C4A-NA-C1A	4.63	108.79	106.68
14	F	1303	CLA	C4A-NA-C1A	4.63	108.79	106.68
17	M	1602	BCR	C7-C8-C9	-4.63	119.39	126.23
14	G	818	CLA	C2D-C1D-ND	4.63	114.71	110.13
14	H	801	CLA	C4A-NA-C1A	4.63	108.79	106.68
14	b	803	CLA	O2A-CGA-O1A	-4.63	112.05	123.63
14	G	807	CLA	CAA-C2A-C3A	-4.63	100.49	113.00
14	a	819	CLA	C4A-NA-C1A	4.63	108.79	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Q	203	CLA	C4A-NA-C1A	4.62	108.79	106.68
14	H	823	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
14	b	809	CLA	O2D-CGD-CBD	4.62	119.31	111.23
14	A	814	CLA	CED-O2D-CGD	-4.62	105.43	115.92
17	M	1602	BCR	C24-C23-C22	-4.62	119.40	126.23
14	b	813	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
14	G	816	CLA	C2D-C1D-ND	4.62	114.70	110.13
14	A	831	CLA	O2A-CGA-O1A	-4.62	112.07	123.63
14	b	835	CLA	C2D-C1D-ND	4.62	114.70	110.13
14	A	807	CLA	CAA-C2A-C3A	-4.62	100.52	113.00
14	a	823	CLA	O2A-CGA-O1A	-4.62	111.45	123.33
14	b	813	CLA	C2D-C1D-ND	4.62	114.70	110.13
14	G	830	CLA	C2D-C1D-ND	4.62	114.69	110.13
14	a	839	CLA	O2A-CGA-O1A	-4.62	111.46	123.33
14	H	811	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
14	B	825	CLA	O2A-CGA-O1A	-4.61	112.09	123.63
14	G	838	CLA	O2A-CGA-O1A	-4.61	112.09	123.63
14	H	832	CLA	C2D-C1D-ND	4.61	114.69	110.13
14	G	807	CLA	O2D-CGD-CBD	4.61	119.29	111.23
14	B	833	CLA	C1D-ND-C4D	-4.61	103.08	106.31
14	A	826	CLA	C2D-C1D-ND	4.61	114.69	110.13
14	b	811	CLA	O2A-CGA-O1A	-4.61	111.47	123.33
14	b	819	CLA	O2A-CGA-O1A	-4.61	111.48	123.33
14	G	803	CLA	O2A-CGA-O1A	-4.61	112.10	123.63
14	L	206	CLA	O2A-C1-C2	4.61	125.84	108.11
14	A	818	CLA	O2A-CGA-O1A	-4.61	111.48	123.33
14	H	814	CLA	O2A-CGA-O1A	-4.61	111.48	123.33
14	B	832	CLA	O2A-CGA-O1A	-4.61	112.11	123.63
14	B	818	CLA	C1D-ND-C4D	-4.61	103.08	106.31
14	K	102	CLA	C1D-ND-C4D	-4.61	103.08	106.31
14	A	815	CLA	O2A-CGA-O1A	-4.61	111.49	123.33
14	b	831	CLA	C4A-NA-C1A	4.61	108.78	106.68
14	G	827	CLA	CAA-C2A-C3A	-4.60	100.56	113.00
14	B	812	CLA	C1C-C2C-C3C	-4.60	102.14	106.98
14	a	835	CLA	C4A-NA-C1A	4.60	108.78	106.68
14	A	808	CLA	O2A-CGA-O1A	-4.60	111.50	123.33
14	G	844	CLA	C2D-C1D-ND	4.60	114.68	110.13
14	B	826	CLA	C4A-NA-C1A	4.60	108.78	106.68
14	G	835	CLA	C2D-C1D-ND	4.60	114.68	110.13
14	K	101	CLA	C2D-C1D-ND	4.60	114.68	110.13
14	H	819	CLA	O2A-CGA-O1A	-4.60	111.51	123.33
17	b	844	BCR	C7-C8-C9	-4.60	119.44	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	831	CLA	C1D-ND-C4D	-4.60	103.09	106.31
14	G	815	CLA	C2D-C1D-ND	4.60	114.67	110.13
14	H	825	CLA	O2A-CGA-O1A	-4.60	112.13	123.63
14	V	1601	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
14	G	821	CLA	C1D-ND-C4D	-4.59	103.09	106.31
14	G	842	CLA	C1D-ND-C4D	-4.59	103.09	106.31
14	A	827	CLA	C1D-ND-C4D	-4.59	103.09	106.31
14	H	818	CLA	O2D-CGD-O1D	-4.59	114.91	123.85
14	b	818	CLA	C2D-C1D-ND	4.59	114.67	110.13
17	J	103	BCR	C24-C23-C22	-4.59	119.44	126.23
14	H	830	CLA	C2D-C1D-ND	4.59	114.67	110.13
14	a	834	CLA	O2A-CGA-O1A	-4.59	112.15	123.63
14	G	822	CLA	O2D-CGD-CBD	4.59	119.25	111.23
14	A	815	CLA	C2D-C1D-ND	4.59	114.67	110.13
14	B	810	CLA	C2D-C1D-ND	4.59	114.67	110.13
14	G	842	CLA	O2A-CGA-O1A	-4.59	112.16	123.63
14	a	841	CLA	C1D-ND-C4D	-4.58	103.09	106.31
14	B	805	CLA	C2D-C1D-ND	4.58	114.66	110.13
14	a	839	CLA	C4A-NA-C1A	4.58	108.77	106.68
14	b	822	CLA	C1C-C2C-C3C	-4.58	102.16	106.98
14	b	822	CLA	O2A-CGA-O1A	-4.58	111.56	123.33
14	A	820	CLA	C2D-C1D-ND	4.58	114.66	110.13
14	B	804	CLA	C1D-ND-C4D	-4.57	103.10	106.31
14	b	818	CLA	C1D-ND-C4D	-4.57	103.10	106.31
14	H	825	CLA	C1C-C2C-C3C	-4.57	102.17	106.98
14	H	839	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
14	G	836	CLA	C4A-NA-C1A	4.57	108.77	106.68
14	B	839	CLA	O2A-CGA-O1A	-4.57	112.19	123.63
14	U	205	CLA	O2A-CGA-O1A	-4.57	112.19	123.63
14	J	101	CLA	C4A-NA-C1A	4.57	108.76	106.68
14	B	833	CLA	C4A-NA-C1A	4.57	108.76	106.68
14	b	810	CLA	C1D-ND-C4D	-4.57	103.11	106.31
14	A	835	CLA	O2A-CGA-O1A	-4.57	112.20	123.63
14	A	844	CLA	C2D-C1D-ND	4.57	114.65	110.13
14	b	827	CLA	C4A-NA-C1A	4.57	108.76	106.68
14	A	836	CLA	C1D-ND-C4D	-4.57	103.11	106.31
14	a	818	CLA	C1D-ND-C4D	-4.56	103.11	106.31
14	a	818	CLA	C1C-C2C-C3C	-4.56	102.18	106.98
14	a	824	CLA	C1D-ND-C4D	-4.56	103.11	106.31
14	G	830	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
14	b	826	CLA	C2D-C1D-ND	4.56	114.64	110.13
14	H	833	CLA	C2D-C1D-ND	4.56	114.64	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	807	CLA	C2D-C1D-ND	4.56	114.64	110.13
14	A	814	CLA	C1C-C2C-C3C	-4.56	102.19	106.98
14	W	1701	CLA	C1D-ND-C4D	-4.56	103.12	106.31
14	J	101	CLA	O2A-CGA-O1A	-4.55	111.63	123.33
14	A	819	CLA	C4A-NA-C1A	4.55	108.75	106.68
14	A	811	CLA	C1C-C2C-C3C	-4.55	102.20	106.98
14	H	806	CLA	O2A-CGA-O1A	-4.55	112.25	123.63
14	B	801	CLA	C1D-ND-C4D	-4.55	103.12	106.31
14	A	838	CLA	C1D-ND-C4D	-4.55	103.12	106.31
14	G	824	CLA	C1D-ND-C4D	-4.55	103.12	106.31
14	H	811	CLA	C1D-ND-C4D	-4.54	103.12	106.31
14	f	202	CLA	C4A-NA-C1A	4.54	108.75	106.68
14	b	815	CLA	O2A-CGA-O1A	-4.54	111.65	123.33
14	G	834	CLA	C4A-NA-C1A	4.54	108.75	106.68
14	b	831	CLA	C1D-ND-C4D	-4.54	103.13	106.31
14	a	833	CLA	C2D-C1D-ND	4.54	114.62	110.13
14	a	827	CLA	C1D-ND-C4D	-4.54	103.13	106.31
14	G	818	CLA	C1D-ND-C4D	-4.54	103.13	106.31
14	U	206	CLA	C1D-ND-C4D	-4.54	103.13	106.31
14	j	101	CLA	C2D-C1D-ND	4.54	114.61	110.13
14	j	101	CLA	C4A-NA-C1A	4.54	108.75	106.68
14	a	842	CLA	O2A-CGA-CBA	4.53	125.66	111.83
14	a	827	CLA	O2A-CGA-O1A	-4.53	112.29	123.63
14	Q	201	CLA	C1D-ND-C4D	-4.53	103.13	106.31
14	a	834	CLA	C4A-NA-C1A	4.53	108.75	106.68
14	A	832	CLA	O2A-CGA-CBA	4.53	125.64	111.83
14	A	807	CLA	O2D-CGD-CBD	4.53	119.15	111.23
14	a	808	CLA	O2A-CGA-O1A	-4.53	112.30	123.63
17	B	844	BCR	C7-C8-C9	-4.52	119.54	126.23
14	X	1701	CLA	C1D-ND-C4D	-4.52	103.14	106.31
14	H	816	CLA	C1D-ND-C4D	-4.52	103.14	106.31
14	B	810	CLA	C1D-ND-C4D	-4.52	103.14	106.31
14	B	832	CLA	C1D-ND-C4D	-4.52	103.14	106.31
17	A	851	BCR	C7-C8-C9	-4.52	119.55	126.23
17	a	850	BCR	C3-C4-C5	-4.52	106.00	114.06
14	b	813	CLA	C1D-ND-C4D	-4.52	103.14	106.31
14	H	837	CLA	C4A-NA-C1A	4.52	108.74	106.68
14	B	809	CLA	C2D-C1D-ND	4.52	114.60	110.13
14	G	803	CLA	C2D-C1D-ND	4.52	114.59	110.13
14	H	837	CLA	C1D-ND-C4D	-4.52	103.14	106.31
14	a	827	CLA	C1C-C2C-C3C	-4.51	102.23	106.98
14	G	831	CLA	C4A-NA-C1A	4.51	108.74	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	841	CLA	C1D-ND-C4D	-4.51	103.15	106.31
14	A	832	CLA	C2D-C1D-ND	4.51	114.59	110.13
14	b	840	CLA	O2A-C1-C2	4.51	125.46	108.11
14	G	819	CLA	C4A-NA-C1A	4.51	108.74	106.68
14	x	1701	CLA	C4A-NA-C1A	4.51	108.74	106.68
14	G	803	CLA	O2D-CGD-CBD	4.51	119.11	111.23
14	H	821	CLA	O2D-CGD-CBD	4.51	119.11	111.23
14	H	818	CLA	C1D-ND-C4D	-4.51	103.15	106.31
14	H	808	CLA	C1D-ND-C4D	-4.50	103.15	106.31
14	G	820	CLA	C2D-C1D-ND	4.50	114.58	110.13
14	S	102	CLA	C4A-NA-C1A	4.50	108.73	106.68
14	a	832	CLA	C2D-C1D-ND	4.50	114.58	110.13
14	l	207	CLA	C1D-ND-C4D	-4.50	103.16	106.31
14	a	811	CLA	C1D-ND-C4D	-4.49	103.16	106.31
14	A	826	CLA	O2A-CGA-O1A	-4.49	112.39	123.63
14	G	826	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
14	G	826	CLA	C2D-C1D-ND	4.49	114.57	110.13
17	A	851	BCR	C15-C14-C13	-4.49	120.98	127.28
14	H	832	CLA	O2A-C1-C2	4.49	125.39	108.11
14	B	801	CLA	C1C-C2C-C3C	-4.49	102.26	106.98
14	A	844	CLA	C4A-NA-C1A	4.49	108.73	106.68
14	H	832	CLA	O2A-CGA-CBA	4.49	125.52	111.83
14	B	830	CLA	C2D-C1D-ND	4.49	114.57	110.13
14	G	843	CLA	C2D-C1D-ND	4.49	114.57	110.13
14	i	101	CLA	O2A-CGA-O1A	-4.49	112.41	123.63
14	G	835	CLA	C4A-NA-C1A	4.48	108.72	106.68
14	b	823	CLA	C1C-C2C-C3C	-4.48	102.26	106.98
14	H	836	CLA	C4A-NA-C1A	4.48	108.72	106.68
14	A	803	CLA	O2A-CGA-O1A	-4.48	112.42	123.63
17	a	847	BCR	C15-C14-C13	-4.48	120.99	127.28
14	H	813	CLA	C1C-C2C-C3C	-4.48	102.27	106.98
14	a	810	CLA	C4A-NA-C1A	4.48	108.72	106.68
14	G	829	CLA	O2A-C1-C2	4.48	125.35	108.11
14	a	824	CLA	O2A-CGA-CBA	4.48	125.49	111.83
14	b	808	CLA	O2A-CGA-CBA	4.48	125.49	111.83
14	B	803	CLA	C2C-C1C-NC	4.48	114.68	109.98
14	a	828	CLA	O2A-C1-C2	4.47	125.32	108.11
17	A	849	BCR	C3-C4-C5	-4.47	106.08	114.06
14	b	801	CLA	O2A-CGA-O1A	-4.47	112.44	123.63
14	a	804	CLA	O2A-CGA-CBA	4.47	125.47	111.83
14	a	837	CLA	C4A-NA-C1A	4.47	108.72	106.68
14	b	840	CLA	O2A-CGA-CBA	4.47	125.46	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	840	CLA	C1D-ND-C4D	-4.47	103.18	106.31
14	A	811	CLA	C1D-ND-C4D	-4.47	103.18	106.31
13	a	801	CL0	C3D-C2D-C1D	-4.47	99.74	105.83
14	A	825	CLA	C1D-ND-C4D	-4.47	103.18	106.31
14	G	819	CLA	C1-C2-C3	-4.46	119.55	126.76
14	B	830	CLA	C4A-NA-C1A	4.46	108.71	106.68
14	a	817	CLA	C2D-C1D-ND	4.46	114.54	110.13
14	a	810	CLA	C2D-C1D-ND	4.46	114.54	110.13
17	H	842	BCR	C19-C18-C17	4.46	126.02	119.01
14	H	830	CLA	O2D-CGD-CBD	4.45	119.02	111.23
14	A	812	CLA	O2D-CGD-CBD	4.45	119.02	111.23
14	H	802	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
14	H	801	CLA	O2A-C1-C2	4.45	125.24	108.11
14	Q	201	CLA	O2D-CGD-CBD	4.45	119.01	111.23
14	k	1401	CLA	C4A-NA-C1A	4.45	108.71	106.68
14	A	810	CLA	C1D-ND-C4D	-4.45	103.19	106.31
14	H	838	CLA	O2A-CGA-O1A	-4.45	111.89	123.33
14	a	813	CLA	O2D-CGD-CBD	4.45	119.01	111.23
17	B	846	BCR	C38-C26-C25	-4.45	119.63	124.48
14	a	826	CLA	O2D-CGD-CBD	4.45	119.00	111.23
14	A	810	CLA	O2A-CGA-CBA	4.44	125.38	111.83
14	b	826	CLA	O2A-CGA-CBA	4.44	125.38	111.83
14	b	836	CLA	O2A-CGA-CBA	4.44	125.38	111.83
14	a	816	CLA	C1D-ND-C4D	-4.44	103.19	106.31
14	L	201	CLA	O2A-C1-C2	4.44	125.20	108.11
17	H	847	BCR	C7-C8-C9	-4.44	119.67	126.23
14	a	813	CLA	C1D-ND-C4D	-4.44	103.20	106.31
14	B	839	CLA	C4A-NA-C1A	4.44	108.70	106.68
14	H	806	CLA	O2D-CGD-CBD	4.44	118.99	111.23
14	a	843	CLA	OBD-CAD-C3D	-4.43	121.39	128.60
14	H	801	CLA	C1C-C2C-C3C	-4.43	102.32	106.98
13	G	801	CL0	C3D-C2D-C1D	-4.43	99.79	105.83
14	H	818	CLA	C4A-NA-C1A	4.43	108.70	106.68
14	A	804	CLA	C1D-ND-C4D	-4.43	103.20	106.31
17	B	848	BCR	C7-C8-C9	-4.43	119.68	126.23
14	A	837	CLA	C2D-C1D-ND	4.43	114.51	110.13
14	A	824	CLA	C1D-ND-C4D	-4.43	103.21	106.31
14	a	821	CLA	O2A-CGA-O1A	-4.43	112.56	123.63
14	a	811	CLA	C2D-C1D-ND	4.43	114.51	110.13
14	A	806	CLA	C4A-NA-C1A	4.42	108.70	106.68
17	R	101	BCR	C24-C23-C22	-4.42	119.69	126.23
14	A	827	CLA	O2A-C1-C2	4.42	125.12	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	843	CLA	C1D-ND-C4D	-4.42	103.21	106.31
14	A	824	CLA	C4A-NA-C1A	4.42	108.69	106.68
14	a	819	CLA	O2A-CGA-CBA	4.42	125.31	111.83
14	b	802	CLA	O2A-CGA-CBA	4.42	125.31	111.83
14	A	805	CLA	O2A-CGA-CBA	4.42	125.30	111.83
14	B	826	CLA	O2A-CGA-CBA	4.42	125.30	111.83
14	A	827	CLA	O2D-CGD-CBD	4.42	118.95	111.23
14	a	804	CLA	C1D-ND-C4D	-4.41	103.22	106.31
14	A	820	CLA	C4A-NA-C1A	4.41	108.69	106.68
14	H	839	CLA	C1D-ND-C4D	-4.41	103.22	106.31
14	G	833	CLA	C1D-ND-C4D	-4.41	103.22	106.31
17	b	843	BCR	C33-C5-C6	-4.41	119.67	124.48
14	H	828	CLA	CMB-C2B-C3B	4.41	133.49	124.68
14	a	825	CLA	O2A-CGA-O1A	-4.41	112.60	123.63
14	H	812	CLA	C1D-ND-C4D	-4.41	103.22	106.31
17	a	848	BCR	C7-C8-C9	-4.41	119.72	126.23
14	H	812	CLA	O2A-CGA-CBA	4.41	125.27	111.83
14	j	102	CLA	CAA-C2A-C3A	-4.41	106.13	116.23
14	F	1303	CLA	C1D-ND-C4D	-4.41	103.22	106.31
14	H	826	CLA	O2A-CGA-CBA	4.41	125.27	111.83
14	a	806	CLA	CAA-C2A-C3A	-4.41	101.09	113.00
14	G	839	CLA	C4A-NA-C1A	4.40	108.69	106.68
14	a	820	CLA	C1D-ND-C4D	-4.40	103.22	106.31
14	a	813	CLA	C1C-C2C-C3C	-4.40	102.35	106.98
14	H	828	CLA	O2A-CGA-CBA	4.40	125.25	111.83
13	a	801	CL0	C1D-ND-C4D	-4.40	103.22	106.31
14	G	819	CLA	C1C-C2C-C3C	-4.40	102.35	106.98
14	A	838	CLA	CMB-C2B-C3B	4.40	133.47	124.68
14	G	822	CLA	O2A-CGA-O1A	-4.40	112.62	123.63
14	a	839	CLA	C1D-ND-C4D	-4.40	103.23	106.31
14	b	835	CLA	C1D-ND-C4D	-4.40	103.23	106.31
14	A	836	CLA	O2D-CGD-CBD	4.40	118.92	111.23
14	b	829	CLA	C2D-C1D-ND	4.40	114.48	110.13
14	H	814	CLA	C1D-ND-C4D	-4.40	103.23	106.31
14	A	833	CLA	C4A-NA-C1A	4.39	108.68	106.68
14	A	829	CLA	O2A-C1-C2	4.39	125.01	108.11
14	H	833	CLA	C1D-ND-C4D	-4.39	103.23	106.31
17	j	104	BCR	C38-C26-C25	-4.39	119.69	124.48
14	b	803	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
14	a	809	CLA	C1D-ND-C4D	-4.39	103.23	106.31
14	A	802	CLA	C1D-ND-C4D	-4.39	103.23	106.31
14	K	101	CLA	C1D-ND-C4D	-4.38	103.24	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	835	CLA	C1D-ND-C4D	-4.38	103.24	106.31
14	G	832	CLA	C2D-C1D-ND	4.38	114.46	110.13
14	L	206	CLA	C4A-NA-C1A	4.38	108.68	106.68
14	H	836	CLA	O2A-CGA-CBA	4.38	125.19	111.83
14	B	821	CLA	C1D-ND-C4D	-4.38	103.24	106.31
14	H	827	CLA	C2D-C1D-ND	4.38	114.46	110.13
14	G	804	CLA	O2A-C1-C2	4.38	124.97	108.11
14	G	810	CLA	C1D-ND-C4D	-4.38	103.24	106.31
14	H	839	CLA	C2D-C1D-ND	4.38	114.46	110.13
14	H	840	CLA	O2A-C1-C2	4.37	124.94	108.11
14	A	803	CLA	O2D-CGD-CBD	4.37	118.88	111.23
14	B	801	CLA	O2A-CGA-CBA	4.37	125.17	111.83
17	R	102	BCR	C7-C8-C9	-4.37	119.77	126.23
14	A	830	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
14	G	842	CLA	O2A-C1-C2	4.37	124.93	108.11
14	B	827	CLA	O2D-CGD-CBD	4.37	118.87	111.23
14	H	820	CLA	C1D-ND-C4D	-4.36	103.25	106.31
14	B	812	CLA	O2A-CGA-CBA	4.36	125.14	111.83
14	G	806	CLA	C1D-ND-C4D	-4.36	103.25	106.31
14	a	836	CLA	C1D-ND-C4D	-4.36	103.25	106.31
14	b	803	CLA	C1D-ND-C4D	-4.36	103.25	106.31
14	a	840	CLA	C2D-C1D-ND	4.36	114.44	110.13
14	A	825	CLA	O2A-CGA-CBA	4.36	125.12	111.83
14	H	829	CLA	C3D-C2D-C1D	-4.36	99.89	105.83
14	a	843	CLA	C2D-C1D-ND	4.36	114.44	110.13
17	A	850	BCR	C28-C27-C26	-4.36	106.29	114.06
14	b	828	CLA	O2A-CGA-CBA	4.36	125.12	111.83
14	G	810	CLA	O2A-CGA-CBA	4.35	125.11	111.83
14	H	840	CLA	O2A-CGA-CBA	4.35	125.10	111.83
14	A	813	CLA	C1D-ND-C4D	-4.35	103.26	106.31
14	G	832	CLA	O2A-CGA-CBA	4.35	125.10	111.83
14	A	814	CLA	C1D-ND-C4D	-4.35	103.26	106.31
14	A	822	CLA	O2A-CGA-O1A	-4.35	112.75	123.63
14	B	812	CLA	C1D-ND-C4D	-4.35	103.26	106.31
14	B	813	CLA	O2A-CGA-CBA	4.35	125.09	111.83
14	b	805	CLA	C1D-ND-C4D	-4.35	103.26	106.31
14	b	820	CLA	C1D-ND-C4D	-4.34	103.26	106.31
14	f	202	CLA	C1D-ND-C4D	-4.34	103.26	106.31
14	B	807	CLA	O2A-CGA-O1A	-4.34	112.77	123.63
14	H	807	CLA	O2A-CGA-O1A	-4.34	112.77	123.63
14	l	207	CLA	O2A-CGA-O1A	-4.34	112.77	123.63
14	T	1401	CLA	C1D-ND-C4D	-4.34	103.27	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	815	CLA	C1D-ND-C4D	-4.34	103.27	106.31
14	a	828	CLA	C1D-ND-C4D	-4.34	103.27	106.31
17	J	102	BCR	C7-C8-C9	-4.34	119.82	126.23
14	a	841	CLA	O2D-CGD-CBD	4.34	118.81	111.23
14	a	842	CLA	O2A-C1-C2	4.33	124.79	108.11
14	G	844	CLA	C1D-ND-C4D	-4.33	103.27	106.31
14	B	827	CLA	O2A-C1-C2	4.33	124.78	108.11
14	a	803	CLA	O2A-CGA-CBA	4.33	125.05	111.83
17	L	202	BCR	C38-C26-C25	-4.33	119.76	124.48
14	a	838	CLA	C1D-ND-C4D	-4.33	103.27	106.31
14	a	836	CLA	C4A-NA-C1A	4.33	108.66	106.68
14	b	831	CLA	CMB-C2B-C3B	4.33	133.34	124.68
14	B	838	CLA	C4A-NA-C1A	4.33	108.65	106.68
14	G	805	CLA	O2A-CGA-CBA	4.32	125.02	111.83
14	a	814	CLA	C1D-ND-C4D	-4.32	103.28	106.31
14	B	840	CLA	O2A-C1-C2	4.32	124.75	108.11
17	R	101	BCR	C33-C5-C6	-4.32	119.77	124.48
14	G	838	CLA	C1D-ND-C4D	-4.32	103.28	106.31
14	b	822	CLA	C1D-ND-C4D	-4.32	103.28	106.31
17	a	851	BCR	C24-C23-C22	-4.32	119.84	126.23
17	H	842	BCR	C15-C14-C13	-4.32	121.22	127.28
14	B	834	CLA	C1D-ND-C4D	-4.32	103.28	106.31
14	a	832	CLA	CMB-C2B-C3B	4.32	133.31	124.68
14	A	805	CLA	C1D-ND-C4D	-4.32	103.28	106.31
14	a	844	CLA	C1D-ND-C4D	-4.32	103.28	106.31
14	b	839	CLA	C2D-C1D-ND	4.32	114.40	110.13
14	G	842	CLA	O2A-CGA-CBA	4.31	124.99	111.83
14	A	844	CLA	O2A-CGA-CBA	4.31	124.99	111.83
14	H	825	CLA	C1D-ND-C4D	-4.31	103.29	106.31
14	U	201	CLA	O2D-CGD-CBD	4.31	118.77	111.23
14	A	830	CLA	O2A-CGA-CBA	4.31	124.98	111.83
14	B	828	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
14	l	202	CLA	C1D-ND-C4D	-4.31	103.29	106.31
14	A	821	CLA	C1D-ND-C4D	-4.31	103.29	106.31
14	B	816	CLA	C2C-C1C-NC	4.31	114.51	109.98
14	H	813	CLA	C1D-ND-C4D	-4.31	103.29	106.31
14	a	842	CLA	C1D-ND-C4D	-4.31	103.29	106.31
14	A	817	CLA	C1D-ND-C4D	-4.31	103.29	106.31
14	G	843	CLA	C4A-NA-C1A	4.30	108.64	106.68
14	H	801	CLA	O2A-CGA-CBA	4.30	124.96	111.83
14	a	829	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
14	L	206	CLA	O2A-CGA-O1A	-4.30	112.87	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	804	CLA	C4A-NA-C1A	4.30	108.64	106.68
17	a	850	BCR	C24-C23-C22	-4.30	119.88	126.23
14	A	804	CLA	O2A-CGA-CBA	4.30	124.94	111.83
14	G	827	CLA	C1D-ND-C4D	-4.30	103.30	106.31
14	H	805	CLA	C1D-ND-C4D	-4.30	103.30	106.31
13	A	801	CL0	C3D-C2D-C1D	-4.30	99.97	105.83
14	a	821	CLA	C2D-C1D-ND	4.29	114.38	110.13
14	H	806	CLA	O2A-C1-C2	4.29	124.63	108.11
14	G	824	CLA	O2D-CGD-CBD	4.29	118.73	111.23
14	G	805	CLA	C1D-ND-C4D	-4.29	103.30	106.31
14	B	830	CLA	CMB-C2B-C3B	4.29	133.25	124.68
14	a	807	CLA	C4A-NA-C1A	4.29	108.64	106.68
14	a	819	CLA	CMB-C2B-C3B	4.29	133.25	124.68
14	L	206	CLA	C1-C2-C3	-4.29	119.17	126.20
14	H	819	CLA	C1D-ND-C4D	-4.29	103.30	106.31
17	R	102	BCR	C38-C26-C25	-4.29	119.81	124.48
14	A	827	CLA	CAA-C2A-C3A	-4.28	101.42	113.00
14	A	834	CLA	C1-C2-C3	-4.28	119.18	126.20
17	B	846	BCR	C3-C4-C5	-4.28	106.42	114.06
14	B	806	CLA	O2D-CGD-CBD	4.28	118.71	111.23
14	a	827	CLA	O2A-C1-C2	4.28	124.56	108.11
14	B	840	CLA	O2A-CGA-CBA	4.27	124.87	111.83
14	A	812	CLA	C1D-ND-C4D	-4.27	103.31	106.31
14	H	837	CLA	C2D-C1D-ND	4.27	114.35	110.13
14	G	828	CLA	C2C-C1C-NC	4.27	114.47	109.98
14	H	813	CLA	O2A-CGA-CBA	4.27	124.85	111.83
14	H	813	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
14	G	812	CLA	C2D-C1D-ND	4.26	114.35	110.13
14	A	839	CLA	C1D-ND-C4D	-4.26	103.32	106.31
14	B	819	CLA	C1D-ND-C4D	-4.26	103.32	106.31
14	A	809	CLA	CAA-C2A-C1A	-4.26	98.01	111.97
14	G	814	CLA	C1D-ND-C4D	-4.26	103.32	106.31
14	a	817	CLA	C1D-ND-C4D	-4.26	103.32	106.31
14	H	821	CLA	C1D-ND-C4D	-4.26	103.32	106.31
17	L	207	BCR	C37-C22-C21	-4.26	115.92	122.82
14	a	831	CLA	C1D-ND-C4D	-4.26	103.33	106.31
14	B	836	CLA	O2A-CGA-CBA	4.26	124.81	111.83
14	l	205	CLA	C1D-ND-C4D	-4.26	103.33	106.31
17	A	848	BCR	C15-C14-C13	-4.25	121.31	127.28
14	a	832	CLA	C4A-NA-C1A	4.25	108.62	106.68
14	a	809	CLA	O2A-CGA-CBA	4.25	124.81	111.83
14	b	810	CLA	C4A-NA-C1A	4.25	108.62	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	821	CLA	O2A-CGA-CBA	4.25	124.80	111.83
14	b	825	CLA	O2A-CGA-O1A	-4.25	112.99	123.63
14	b	814	CLA	C1D-ND-C4D	-4.25	103.33	106.31
14	H	822	CLA	C1C-C2C-C3C	-4.25	102.51	106.98
14	J	101	CLA	C1D-ND-C4D	-4.25	103.33	106.31
14	B	816	CLA	C1C-C2C-C3C	-4.25	102.51	106.98
14	H	802	CLA	O2A-CGA-O1A	-4.25	113.00	123.63
14	G	844	CLA	C4A-NA-C1A	4.25	108.62	106.68
14	B	827	CLA	C3D-C2D-C1D	-4.25	100.04	105.83
14	S	101	CLA	C4A-NA-C1A	4.24	108.61	106.68
14	b	827	CLA	C2D-C1D-ND	4.24	114.33	110.13
14	a	828	CLA	O2D-CGD-CBD	4.24	118.64	111.23
14	B	802	CLA	C1-C2-C3	-4.24	119.25	126.20
14	G	826	CLA	O2A-CGA-O1A	-4.24	113.02	123.63
14	G	817	CLA	O2D-CGD-CBD	4.24	118.64	111.23
14	b	808	CLA	C1D-ND-C4D	-4.24	103.34	106.31
14	L	201	CLA	C1D-ND-C4D	-4.24	103.34	106.31
14	a	812	CLA	C1D-ND-C4D	-4.24	103.34	106.31
14	H	840	CLA	C1D-ND-C4D	-4.23	103.34	106.31
14	A	806	CLA	CMB-C2B-C3B	4.23	133.14	124.68
14	G	812	CLA	C1D-ND-C4D	-4.23	103.34	106.31
14	b	823	CLA	C1D-ND-C4D	-4.23	103.34	106.31
14	b	836	CLA	C1D-ND-C4D	-4.23	103.34	106.31
14	H	824	CLA	CAA-C2A-C3A	-4.23	101.56	113.00
14	a	820	CLA	O2A-CGA-CBA	4.23	124.74	111.83
14	b	804	CLA	C2C-C1C-NC	4.23	114.42	109.98
14	B	803	CLA	O2A-CGA-CBA	4.23	124.73	111.83
14	b	813	CLA	O2A-CGA-CBA	4.23	124.73	111.83
14	B	823	CLA	O2A-C1-C2	4.23	124.38	108.11
14	a	825	CLA	C2D-C1D-ND	4.23	114.31	110.13
14	B	824	CLA	C4A-NA-C1A	4.23	108.61	106.68
14	H	827	CLA	C4A-NA-C1A	4.23	108.61	106.68
14	G	830	CLA	C1-C2-C3	-4.22	119.28	126.20
14	B	839	CLA	C2D-C1D-ND	4.22	114.31	110.13
14	b	812	CLA	C1D-ND-C4D	-4.22	103.35	106.31
14	a	821	CLA	C1D-ND-C4D	-4.22	103.35	106.31
14	F	1301	CLA	C1D-ND-C4D	-4.22	103.35	106.31
17	b	849	BCR	C38-C26-C25	-4.22	119.88	124.48
14	b	823	CLA	O2A-C1-C2	4.22	124.34	108.11
14	b	826	CLA	C4A-NA-C1A	4.22	108.60	106.68
17	A	853	BCR	C38-C26-C25	-4.21	119.89	124.48
14	B	822	CLA	C1C-C2C-C3C	-4.21	102.55	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	805	CLA	O2A-CGA-CBA	4.21	124.68	111.83
14	G	843	CLA	O2A-CGA-CBA	4.21	124.67	111.83
14	A	841	CLA	CMB-C2B-C3B	4.21	133.10	124.68
14	b	831	CLA	C1-O2A-CGA	4.21	126.84	116.65
14	M	1601	CLA	C1D-ND-C4D	-4.21	103.36	106.31
14	j	102	CLA	C1D-ND-C4D	-4.21	103.36	106.31
14	H	827	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
14	B	835	CLA	C1D-ND-C4D	-4.21	103.36	106.31
14	G	825	CLA	C1D-ND-C4D	-4.21	103.36	106.31
14	H	816	CLA	O2A-CGA-CBA	4.20	124.65	111.83
14	a	855	CLA	O2A-CGA-CBA	4.20	124.65	111.83
14	A	809	CLA	O2A-CGA-O1A	-4.20	113.12	123.63
14	V	1601	CLA	C2D-C1D-ND	4.20	114.28	110.13
14	b	830	CLA	C1D-ND-C4D	-4.20	103.37	106.31
17	f	201	BCR	C24-C23-C22	-4.20	120.03	126.23
14	B	824	CLA	CAA-C2A-C3A	-4.19	101.66	113.00
14	Q	203	CLA	C1D-ND-C4D	-4.19	103.37	106.31
14	a	826	CLA	O2A-C1-C2	4.19	124.24	108.11
14	G	834	CLA	C1D-ND-C4D	-4.19	103.37	106.31
13	G	801	CL0	C1D-ND-C4D	-4.19	103.37	106.31
17	A	851	BCR	C38-C26-C25	-4.19	119.91	124.48
17	U	202	BCR	C37-C22-C21	-4.19	116.03	122.82
14	a	809	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
14	a	831	CLA	C4A-NA-C1A	4.19	108.59	106.68
17	b	846	BCR	C24-C23-C22	-4.19	120.04	126.23
17	B	847	BCR	C7-C8-C9	-4.18	120.04	126.23
14	a	833	CLA	C1D-ND-C4D	-4.18	103.38	106.31
14	G	813	CLA	C1D-ND-C4D	-4.18	103.38	106.31
14	H	832	CLA	C1D-ND-C4D	-4.18	103.38	106.31
14	A	830	CLA	C2D-C1D-ND	4.18	114.26	110.13
14	H	827	CLA	O2A-C1-C2	4.18	124.19	108.11
14	A	842	CLA	O2D-CGD-CBD	4.18	118.53	111.23
14	G	838	CLA	CMB-C2B-C3B	4.18	133.03	124.68
18	a	853	LHG	O7-C7-C8	4.18	120.52	111.48
14	a	855	CLA	O2A-C1-C2	4.17	124.17	108.11
14	A	834	CLA	C4A-NA-C1A	4.17	108.58	106.68
14	L	206	CLA	C1D-ND-C4D	-4.17	103.39	106.31
14	F	1301	CLA	C1C-C2C-C3C	-4.16	102.60	106.98
14	b	827	CLA	C3D-C2D-C1D	-4.16	100.15	105.83
17	S	103	BCR	C7-C8-C9	-4.16	120.08	126.23
14	H	821	CLA	O2A-CGA-CBA	4.16	124.51	111.83
14	B	840	CLA	C1D-ND-C4D	-4.16	103.39	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	831	CLA	CMB-C2B-C3B	4.16	132.99	124.68
14	H	831	CLA	CHD-C1D-ND	-4.15	118.96	124.80
14	b	832	CLA	O2A-CGA-CBA	4.15	124.49	111.83
14	H	831	CLA	C1-O2A-CGA	4.15	126.69	116.65
14	B	808	CLA	O2A-CGA-CBA	4.15	124.48	111.83
14	b	816	CLA	C4A-NA-C1A	4.15	108.57	106.68
14	a	819	CLA	O2A-CGA-O1A	-4.14	113.26	123.63
14	b	824	CLA	C1D-ND-C4D	-4.14	103.41	106.31
14	a	804	CLA	CMB-C2B-C3B	4.14	132.96	124.68
14	B	801	CLA	O2A-C1-C2	4.14	124.05	108.11
14	a	813	CLA	O2A-CGA-CBA	4.14	124.46	111.83
14	b	817	CLA	O2A-CGA-CBA	4.14	124.46	111.83
14	G	830	CLA	O2A-C1-C2	4.14	124.04	108.11
14	G	802	CLA	CMB-C2B-C3B	4.14	132.95	124.68
17	a	848	BCR	C3-C4-C5	-4.14	106.68	114.06
17	G	850	BCR	C28-C27-C26	-4.14	106.68	114.06
17	G	848	BCR	C15-C14-C13	-4.14	121.48	127.28
17	b	844	BCR	C33-C5-C6	-4.14	119.97	124.48
14	A	824	CLA	C2D-C1D-ND	4.13	114.22	110.13
14	b	802	CLA	C1D-ND-C4D	-4.13	103.41	106.31
14	a	833	CLA	C4A-NA-C1A	4.13	108.56	106.68
17	A	851	BCR	C3-C4-C5	-4.13	106.69	114.06
17	B	846	BCR	C15-C14-C13	-4.13	121.49	127.28
14	b	818	CLA	C4A-NA-C1A	4.13	108.56	106.68
14	b	833	CLA	CMB-C2B-C3B	4.12	132.92	124.68
14	A	842	CLA	C4A-NA-C1A	4.12	108.56	106.68
14	G	840	CLA	C4A-NA-C1A	4.12	108.56	106.68
14	a	811	CLA	O2A-CGA-CBA	4.12	124.40	111.83
14	H	836	CLA	C1D-ND-C4D	-4.12	103.42	106.31
14	A	828	CLA	O2A-CGA-CBA	4.12	124.39	111.83
17	B	843	BCR	C33-C5-C6	-4.12	119.99	124.48
14	G	825	CLA	O2A-CGA-CBA	4.12	124.39	111.83
14	H	836	CLA	CMB-C2B-C3B	4.12	132.91	124.68
14	b	827	CLA	C1D-ND-C4D	-4.11	103.42	106.31
14	H	808	CLA	O2A-CGA-CBA	4.11	124.38	111.83
14	H	830	CLA	CMB-C2B-C3B	4.11	132.90	124.68
17	S	104	BCR	C38-C26-C25	-4.11	120.00	124.48
14	a	844	CLA	CMB-C2B-C3B	4.11	132.90	124.68
14	G	802	CLA	O2A-C1-C2	4.11	123.92	108.11
14	A	840	CLA	C4A-NA-C1A	4.11	108.55	106.68
17	G	849	BCR	C19-C18-C17	4.11	125.47	119.01
14	a	831	CLA	O2A-CGA-CBA	4.11	124.36	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	820	CLA	CMB-C2B-C3B	4.11	132.89	124.68
14	b	816	CLA	CMC-C2C-C1C	4.11	131.45	125.03
17	G	850	BCR	C7-C8-C9	-4.11	120.16	126.23
14	H	823	CLA	CMB-C2B-C3B	4.11	132.89	124.68
14	a	829	CLA	C2D-C1D-ND	4.11	114.19	110.13
14	A	826	CLA	C1D-ND-C4D	-4.11	103.43	106.31
13	G	801	CL0	O2A-CGA-CBA	4.10	124.34	111.83
14	G	820	CLA	CBA-CAA-C2A	4.10	126.00	113.79
14	G	813	CLA	O2A-CGA-CBA	4.10	124.34	111.83
14	B	804	CLA	O2A-CGA-CBA	4.10	124.34	111.83
14	H	804	CLA	C1D-ND-C4D	-4.10	103.44	106.31
14	b	806	CLA	C1D-ND-C4D	-4.10	103.44	106.31
14	b	827	CLA	O2A-C1-C2	4.10	123.87	108.11
14	V	1601	CLA	C1D-ND-C4D	-4.10	103.44	106.31
14	A	819	CLA	O2A-CGA-CBA	4.09	124.32	111.83
14	b	812	CLA	O2A-CGA-CBA	4.09	124.32	111.83
14	B	805	CLA	C1D-ND-C4D	-4.09	103.44	106.31
14	B	801	CLA	O2D-CGD-O1D	-4.09	115.88	123.85
14	U	201	CLA	C1D-ND-C4D	-4.09	103.44	106.31
14	H	824	CLA	C4A-NA-C1A	4.09	108.54	106.68
14	B	839	CLA	C1D-ND-C4D	-4.09	103.44	106.31
14	A	828	CLA	C4A-NA-C1A	4.09	108.54	106.68
14	A	833	CLA	C1D-ND-C4D	-4.08	103.45	106.31
14	B	809	CLA	O2A-CGA-CBA	4.08	124.29	111.83
14	H	827	CLA	O2D-CGD-CBD	4.08	118.37	111.23
14	H	804	CLA	O2A-CGA-CBA	4.08	124.28	111.83
14	b	808	CLA	O2A-C1-C2	4.08	123.81	108.11
14	G	839	CLA	C1D-ND-C4D	-4.08	103.45	106.31
14	H	817	CLA	C1D-ND-C4D	-4.08	103.45	106.31
14	b	819	CLA	C1D-ND-C4D	-4.08	103.45	106.31
14	G	828	CLA	O2A-CGA-CBA	4.08	124.27	111.83
14	G	812	CLA	O2A-CGA-CBA	4.08	124.27	111.83
14	A	813	CLA	C1-C2-C3	-4.08	120.16	126.76
14	A	814	CLA	O2A-CGA-CBA	4.08	124.27	111.83
14	S	101	CLA	C1D-ND-C4D	-4.08	103.45	106.31
17	S	103	BCR	C36-C18-C17	-4.08	116.21	122.82
14	B	836	CLA	C1D-ND-C4D	-4.07	103.45	106.31
14	a	840	CLA	CMB-C2B-C3B	4.07	132.82	124.68
17	m	1602	BCR	C7-C8-C9	-4.07	120.21	126.23
14	B	816	CLA	O2A-CGA-CBA	4.07	124.24	111.83
14	H	802	CLA	C1D-ND-C4D	-4.07	103.46	106.31
17	a	852	BCR	C38-C26-C25	-4.07	120.05	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	810	CLA	C1D-ND-C4D	-4.07	103.46	106.31
14	a	843	CLA	C1D-ND-C4D	-4.07	103.46	106.31
14	b	825	CLA	CMB-C2B-C3B	4.06	132.81	124.68
14	G	809	CLA	O2A-CGA-CBA	4.06	124.22	111.83
14	A	803	CLA	C1D-ND-C4D	-4.06	103.46	106.31
17	H	845	BCR	C37-C22-C23	-4.06	111.88	118.09
14	b	817	CLA	O2A-CGA-O1A	-4.06	113.47	123.63
14	A	812	CLA	O2A-CGA-CBA	4.06	124.22	111.83
14	A	833	CLA	CMB-C2B-C3B	4.06	132.79	124.68
14	a	818	CLA	O2A-C1-C2	4.06	123.72	108.11
14	B	828	CLA	O2A-CGA-CBA	4.06	124.21	111.83
17	b	846	BCR	C38-C26-C25	-4.06	120.06	124.48
14	a	814	CLA	CMB-C2B-C3B	4.06	132.79	124.68
14	H	803	CLA	O2A-C1-C2	4.05	123.70	108.11
14	G	836	CLA	C1D-ND-C4D	-4.05	103.47	106.31
14	a	817	CLA	C4A-NA-C1A	4.05	108.53	106.68
17	M	1602	BCR	C33-C5-C6	-4.05	120.06	124.48
14	G	822	CLA	C4A-NA-C1A	4.05	108.53	106.68
14	G	831	CLA	C1D-ND-C4D	-4.05	103.47	106.31
14	b	816	CLA	O2A-CGA-CBA	4.05	124.17	111.83
14	H	828	CLA	C4A-NA-C1A	4.04	108.52	106.68
14	A	828	CLA	CAC-C3C-C4C	4.04	130.05	124.79
14	b	812	CLA	CAC-C3C-C4C	4.04	130.04	124.79
14	a	837	CLA	C1D-ND-C4D	-4.03	103.48	106.31
17	j	104	BCR	C15-C14-C13	-4.03	121.62	127.28
14	b	823	CLA	CMB-C2B-C3B	4.03	132.74	124.68
14	b	809	CLA	C1D-ND-C4D	-4.03	103.48	106.31
14	L	205	CLA	CHD-C1D-ND	-4.03	119.13	124.80
14	b	801	CLA	O2D-CGD-CBD	4.03	118.28	111.23
14	H	811	CLA	O2D-CGD-O1D	-4.03	116.00	123.85
14	A	813	CLA	O2A-CGA-CBA	4.03	124.13	111.83
14	H	827	CLA	C1D-ND-C4D	-4.03	103.48	106.31
14	b	804	CLA	O2A-C1-C2	4.03	123.61	108.11
14	B	810	CLA	C4A-NA-C1A	4.03	108.52	106.68
14	A	827	CLA	C1-C2-C3	-4.03	119.60	126.20
14	a	855	CLA	C4A-NA-C1A	4.03	108.52	106.68
14	b	834	CLA	CHD-C1D-ND	-4.03	119.14	124.80
14	B	817	CLA	O2A-CGA-O1A	-4.03	113.56	123.63
14	a	816	CLA	O2D-CGD-CBD	4.02	118.27	111.23
14	B	825	CLA	C1D-ND-C4D	-4.02	103.49	106.31
14	H	804	CLA	CMB-C2B-C3B	4.02	132.71	124.68
14	H	831	CLA	O2A-C1-C2	4.01	123.56	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	841	CLA	O2A-CGA-CBA	4.01	124.07	111.83
14	H	823	CLA	O2A-C1-C2	4.01	123.55	108.11
14	K	102	CLA	C4A-NA-C1A	4.01	108.51	106.68
14	b	821	CLA	C1D-ND-C4D	-4.01	103.50	106.31
14	a	818	CLA	O2A-CGA-CBA	4.01	124.06	111.83
14	l	206	CLA	CHD-C1D-ND	-4.01	119.16	124.80
14	b	825	CLA	C1D-ND-C4D	-4.01	103.50	106.31
14	B	817	CLA	O2A-CGA-CBA	4.01	124.06	111.83
17	B	844	BCR	C33-C5-C6	-4.01	120.11	124.48
17	b	844	BCR	C38-C26-C25	-4.01	120.11	124.48
14	H	826	CLA	C1D-ND-C4D	-4.01	103.50	106.31
14	G	837	CLA	C1D-ND-C4D	-4.01	103.50	106.31
17	B	842	BCR	C19-C18-C17	4.01	125.31	119.01
14	G	826	CLA	O2A-C1-C2	4.01	123.52	108.11
14	A	832	CLA	C4A-NA-C1A	4.00	108.51	106.68
14	a	812	CLA	O2A-CGA-CBA	4.00	124.05	111.83
14	b	840	CLA	C1D-ND-C4D	-4.00	103.50	106.31
14	b	805	CLA	O2A-CGA-CBA	4.00	124.04	111.83
14	b	839	CLA	C1D-ND-C4D	-4.00	103.50	106.31
14	G	834	CLA	O2A-CGA-CBA	4.00	124.03	111.83
19	b	848	LMG	O7-C10-C11	4.00	120.13	111.48
14	G	841	CLA	O2A-CGA-CBA	4.00	124.02	111.83
14	H	813	CLA	C2D-C1D-ND	4.00	114.08	110.13
14	a	855	CLA	C1D-ND-C4D	-3.99	103.51	106.31
14	H	829	CLA	C2D-C1D-ND	3.99	114.08	110.13
14	b	824	CLA	C4A-NA-C1A	3.99	108.50	106.68
14	a	802	CLA	C1D-ND-C4D	-3.99	103.51	106.31
14	a	830	CLA	O2A-C1-C2	3.99	123.47	108.11
13	a	801	CL0	O2A-CGA-CBA	3.99	124.00	111.83
14	H	805	CLA	CMB-C2B-C3B	3.99	132.66	124.68
14	H	828	CLA	C3D-C2D-C1D	-3.99	100.39	105.83
14	x	1701	CLA	O2D-CGD-CBD	3.99	118.20	111.23
14	G	814	CLA	C1C-C2C-C3C	-3.99	102.79	106.98
14	a	821	CLA	O2D-CGD-CBD	3.99	118.20	111.23
14	a	833	CLA	O2A-CGA-CBA	3.98	123.98	111.83
17	b	849	BCR	C24-C23-C22	-3.98	120.34	126.23
14	A	816	CLA	C1D-ND-C4D	-3.98	103.52	106.31
14	b	829	CLA	CBC-CAC-C3C	-3.98	101.63	112.42
14	U	204	CLA	O2A-C1-C2	3.98	123.42	108.11
14	a	833	CLA	C1-C2-C3	-3.97	119.69	126.20
14	H	827	CLA	O2A-CGA-CBA	3.97	123.95	111.83
17	A	850	BCR	C7-C8-C9	-3.97	120.36	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	841	CLA	C1D-ND-C4D	-3.97	103.53	106.31
14	A	834	CLA	C1D-ND-C4D	-3.97	103.53	106.31
14	U	206	CLA	O2A-CGA-CBA	3.97	123.93	111.83
14	B	824	CLA	C1D-ND-C4D	-3.97	103.53	106.31
14	G	833	CLA	CMB-C2B-C3B	3.97	132.61	124.68
17	H	844	BCR	C33-C5-C6	-3.97	120.16	124.48
14	H	831	CLA	C1-C2-C3	-3.96	119.70	126.20
14	L	206	CLA	CMB-C2B-C3B	3.96	132.60	124.68
14	a	834	CLA	C1D-ND-C4D	-3.96	103.53	106.31
14	G	819	CLA	O2A-CGA-CBA	3.96	123.91	111.83
14	A	823	CLA	OBD-CAD-C3D	-3.96	119.16	128.42
14	a	807	CLA	CHD-C1D-ND	-3.96	119.23	124.80
14	B	837	CLA	CHD-C1D-ND	-3.96	119.23	124.80
17	H	849	BCR	C38-C26-C25	-3.96	120.17	124.48
15	B	841	PQN	C11-C12-C13	-3.95	120.02	126.83
14	G	809	CLA	O2A-C1-C2	3.95	123.31	108.11
17	b	844	BCR	C34-C9-C10	-3.95	116.42	122.82
14	H	803	CLA	O2A-CGA-CBA	3.95	123.87	111.83
14	T	1401	CLA	C4A-NA-C1A	3.95	108.48	106.68
14	b	816	CLA	C1-C2-C3	-3.95	119.73	126.20
14	b	831	CLA	CHD-C1D-ND	-3.95	119.25	124.80
14	B	806	CLA	O2A-C1-C2	3.94	123.28	108.11
14	G	827	CLA	C4A-NA-C1A	3.94	108.48	106.68
14	a	832	CLA	C1D-ND-C4D	-3.94	103.55	106.31
14	H	816	CLA	O2A-C1-C2	3.94	123.27	108.11
17	H	846	BCR	C15-C14-C13	-3.94	121.75	127.28
14	a	803	CLA	O2A-C1-C2	3.94	123.27	108.11
14	B	820	CLA	CMB-C2B-C3B	3.94	132.56	124.68
14	b	813	CLA	CMB-C2B-C3B	3.94	132.55	124.68
14	A	814	CLA	CHD-C1D-ND	-3.94	119.26	124.80
17	B	843	BCR	C7-C8-C9	-3.94	120.41	126.23
14	G	827	CLA	O2A-CGA-CBA	3.94	123.84	111.83
14	B	827	CLA	C2D-C1D-ND	3.94	114.02	110.13
17	l	201	BCR	C24-C23-C22	-3.94	120.41	126.23
14	G	843	CLA	O2A-C1-C2	3.93	123.25	108.11
14	G	820	CLA	O2A-CGA-O1A	-3.93	113.79	123.63
14	a	840	CLA	O2A-CGA-CBA	3.93	123.81	111.83
17	B	848	BCR	C3-C4-C5	-3.93	107.05	114.06
14	m	1601	CLA	C1D-ND-C4D	-3.93	103.56	106.31
14	G	804	CLA	O2A-CGA-CBA	3.93	123.80	111.83
14	A	810	CLA	O2A-C1-C2	3.92	123.21	108.11
14	A	815	CLA	C1D-ND-C4D	-3.92	103.56	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	809	CLA	O2A-C1-C2	3.92	123.20	108.11
14	A	822	CLA	O2D-CGD-CBD	3.92	118.09	111.23
14	a	815	CLA	C1D-ND-C4D	-3.92	103.56	106.31
14	a	819	CLA	C1D-ND-C4D	-3.92	103.56	106.31
17	G	851	BCR	C3-C4-C5	-3.92	107.07	114.06
14	b	807	CLA	C1-C2-C3	-3.92	119.78	126.20
14	A	837	CLA	C4A-NA-C1A	3.92	108.47	106.68
14	K	101	CLA	C4A-NA-C1A	3.92	108.47	106.68
14	B	831	CLA	CHD-C1D-ND	-3.92	119.29	124.80
14	G	831	CLA	O2A-CGA-CBA	3.92	123.78	111.83
14	j	101	CLA	C1D-ND-C4D	-3.92	103.56	106.31
14	G	803	CLA	C1D-ND-C4D	-3.91	103.57	106.31
14	B	827	CLA	O2A-CGA-CBA	3.91	123.77	111.83
14	G	814	CLA	O2A-CGA-CBA	3.91	123.77	111.83
14	B	834	CLA	O2D-CGD-CBD	3.91	118.07	111.23
18	a	854	LHG	O7-C7-C8	3.91	119.94	111.48
14	B	836	CLA	O2A-C1-C2	3.91	123.16	108.11
14	G	835	CLA	CHD-C1D-ND	-3.91	119.30	124.80
17	I	102	BCR	C38-C26-C25	-3.91	120.22	124.48
14	A	816	CLA	CMB-C2B-C3B	3.91	132.49	124.68
17	a	848	BCR	C36-C18-C17	-3.90	116.49	122.82
14	G	832	CLA	C4A-NA-C1A	3.90	108.46	106.68
14	H	816	CLA	C4A-NA-C1A	3.90	108.46	106.68
14	b	834	CLA	CBC-CAC-C3C	-3.90	101.84	112.42
17	J	103	BCR	C38-C26-C25	-3.90	120.23	124.48
14	A	828	CLA	C3C-C4C-NC	3.90	115.42	110.43
14	A	803	CLA	O2A-CGA-CBA	3.89	123.71	111.83
14	A	834	CLA	O2A-CGA-CBA	3.89	123.71	111.83
14	a	843	CLA	C4A-NA-C1A	3.89	108.45	106.68
14	b	828	CLA	C3D-C2D-C1D	-3.89	100.52	105.83
14	a	840	CLA	C1D-ND-C4D	-3.89	103.58	106.31
14	H	803	CLA	CAA-C2A-C3A	-3.89	102.49	113.00
17	S	103	BCR	C3-C4-C5	-3.89	107.12	114.06
14	a	828	CLA	CMC-C2C-C1C	3.89	131.11	125.03
14	a	820	CLA	O2A-C1-C2	3.89	123.07	108.11
14	G	830	CLA	O2A-CGA-CBA	3.89	123.68	111.83
17	F	1302	BCR	C33-C5-C6	-3.89	120.24	124.48
14	a	811	CLA	O2D-CGD-CBD	3.89	118.02	111.23
14	G	813	CLA	O2A-C1-C2	3.88	123.05	108.11
14	a	829	CLA	O2A-CGA-CBA	3.88	123.67	111.83
14	A	821	CLA	O2A-CGA-CBA	3.88	123.67	111.83
17	B	848	BCR	C38-C26-C25	-3.88	120.25	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	853	BCR	C33-C5-C6	-3.88	120.25	124.48
14	B	804	CLA	CMB-C2B-C3B	3.88	132.43	124.68
15	A	846	PQN	C14-C13-C15	3.88	121.96	115.23
14	b	836	CLA	O2A-C1-C2	3.88	123.03	108.11
14	A	824	CLA	CHD-C1D-ND	-3.88	119.35	124.80
14	a	825	CLA	CMB-C2B-C3B	3.88	132.43	124.68
14	G	831	CLA	CMB-C2B-C3B	3.87	132.43	124.68
14	B	824	CLA	CMB-C2B-C3B	3.87	132.42	124.68
14	H	805	CLA	C1-C2-C3	-3.87	119.85	126.20
14	G	825	CLA	O2D-CGD-CBD	3.87	118.00	111.23
14	H	837	CLA	CHD-C1D-ND	-3.87	119.35	124.80
14	b	811	CLA	O2D-CGD-O1D	-3.87	116.31	123.85
14	U	205	CLA	O2A-CGA-CBA	3.87	123.64	111.83
14	A	843	CLA	O2A-CGA-O1A	-3.87	113.95	123.63
14	B	833	CLA	CHD-C1D-ND	-3.86	119.36	124.80
14	b	827	CLA	O2A-CGA-CBA	3.86	123.61	111.83
17	j	104	BCR	C33-C5-C6	-3.86	120.27	124.48
14	b	835	CLA	C4A-NA-C1A	3.86	108.44	106.68
14	l	202	CLA	O2A-C1-C2	3.86	122.97	108.11
13	A	801	CL0	C1D-ND-C4D	-3.86	103.60	106.31
14	A	804	CLA	O2A-C1-C2	3.86	122.96	108.11
14	G	805	CLA	CMB-C2B-C3B	3.86	132.39	124.68
14	H	817	CLA	O2A-CGA-O1A	-3.86	113.98	123.63
17	a	850	BCR	C7-C8-C9	-3.86	120.53	126.23
14	G	844	CLA	OBD-CAD-C3D	-3.85	122.33	128.60
14	A	806	CLA	CHD-C1D-ND	-3.85	119.38	124.80
14	a	811	CLA	CHD-C1D-ND	-3.85	119.38	124.80
14	A	832	CLA	C1D-ND-C4D	-3.85	103.61	106.31
14	a	830	CLA	C1D-ND-C4D	-3.85	103.61	106.31
17	H	842	BCR	C28-C27-C26	-3.85	107.19	114.06
14	A	839	CLA	O2A-CGA-CBA	3.85	123.57	111.83
14	b	837	CLA	O2A-CGA-CBA	3.85	123.57	111.83
14	A	844	CLA	C1D-ND-C4D	-3.85	103.61	106.31
14	A	843	CLA	O2A-C1-C2	3.85	122.92	108.11
14	a	825	CLA	C3D-C2D-C1D	-3.85	100.58	105.83
14	b	807	CLA	O2A-CGA-CBA	3.85	123.56	111.83
14	b	802	CLA	O2A-C1-C2	3.85	122.91	108.11
19	B	849	LMG	O7-C10-C11	3.85	119.80	111.48
14	G	829	CLA	CMC-C2C-C1C	3.85	131.04	125.03
14	A	822	CLA	C1-C2-C3	-3.84	119.90	126.20
14	G	835	CLA	O2A-C1-C2	3.84	122.90	108.11
14	B	829	CLA	C1D-ND-C4D	-3.84	103.61	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	825	CLA	O2A-CGA-CBA	3.84	123.55	111.83
14	B	803	CLA	O2A-C1-C2	3.84	122.89	108.11
14	b	818	CLA	CMB-C2B-C3B	3.84	132.36	124.68
14	H	825	CLA	O2A-C1-C2	3.84	122.88	108.11
17	H	845	BCR	C15-C14-C13	-3.84	121.62	127.48
14	G	834	CLA	C1-C2-C3	-3.84	119.91	126.20
14	B	804	CLA	O2A-C1-C2	3.84	122.87	108.11
14	H	815	CLA	CHD-C1D-ND	-3.84	119.40	124.80
17	b	847	BCR	C38-C26-C25	-3.84	120.30	124.48
14	b	818	CLA	O2A-CGA-CBA	3.83	123.53	111.83
14	H	818	CLA	O2A-CGA-CBA	3.83	123.52	111.83
14	b	826	CLA	O2A-C1-C2	3.83	122.85	108.11
17	B	845	BCR	C38-C26-C25	-3.83	120.31	124.48
14	A	826	CLA	O2A-C1-C2	3.83	122.84	108.11
14	A	819	CLA	CHD-C1D-ND	-3.83	119.42	124.80
14	b	837	CLA	CHD-C1D-ND	-3.83	119.42	124.80
14	B	831	CLA	C1-O2A-CGA	3.83	125.91	116.65
14	G	825	CLA	O2A-C1-C2	3.83	122.83	108.11
14	B	817	CLA	C1D-ND-C4D	-3.83	103.63	106.31
14	B	807	CLA	CHD-C1D-ND	-3.83	119.42	124.80
14	b	804	CLA	CAA-C2A-C3A	-3.82	102.66	113.00
14	a	823	CLA	CHD-C1D-ND	-3.82	119.42	124.80
14	b	817	CLA	C4-C3-C5	3.82	121.87	115.23
14	A	837	CLA	C1D-ND-C4D	-3.82	103.63	106.31
14	H	828	CLA	CMD-C2D-C3D	-3.82	118.92	127.69
14	b	822	CLA	CMB-C2B-C3B	3.82	132.32	124.68
14	A	835	CLA	C1D-ND-C4D	-3.82	103.63	106.31
17	A	852	BCR	C33-C5-C6	-3.82	120.32	124.48
14	A	843	CLA	O2A-CGA-CBA	3.82	123.47	111.83
17	a	848	BCR	C38-C26-C25	-3.81	120.32	124.48
17	a	848	BCR	C24-C23-C22	-3.81	120.60	126.23
15	a	845	PQN	C14-C13-C15	3.81	121.84	115.23
17	f	201	BCR	C12-C13-C14	-3.81	113.02	119.01
14	b	825	CLA	O2A-CGA-CBA	3.81	123.45	111.83
14	a	825	CLA	O2A-C1-C2	3.81	122.76	108.11
14	G	828	CLA	C3C-C4C-NC	3.81	115.31	110.43
17	a	849	BCR	C15-C14-C13	-3.80	121.94	127.28
14	b	816	CLA	CMB-C2B-C3B	3.80	132.29	124.68
17	R	103	BCR	C19-C18-C17	3.80	124.99	119.01
14	B	823	CLA	CMB-C2B-C3B	3.80	132.28	124.68
14	b	809	CLA	O2A-CGA-CBA	3.80	123.43	111.83
14	G	819	CLA	O2A-C1-C2	3.80	122.74	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	823	CLA	C1D-ND-C4D	-3.80	103.64	106.31
14	G	806	CLA	CMB-C2B-C3B	3.80	132.28	124.68
17	I	101	BCR	C33-C5-C6	-3.80	120.34	124.48
14	H	833	CLA	CMB-C2B-C3B	3.80	132.28	124.68
14	A	843	CLA	C4-C3-C5	3.80	121.82	115.23
17	l	201	BCR	C37-C22-C21	-3.80	116.66	122.82
14	B	837	CLA	O2A-CGA-CBA	3.80	123.42	111.83
14	A	812	CLA	CHD-C1D-ND	-3.80	119.46	124.80
14	b	829	CLA	C1D-ND-C4D	-3.80	103.65	106.31
14	b	818	CLA	CHD-C1D-ND	-3.80	119.46	124.80
17	j	103	BCR	C3-C4-C5	-3.80	107.29	114.06
14	B	808	CLA	C4D-C3D-CAD	3.80	112.23	108.11
17	B	850	BCR	C38-C26-C25	-3.80	120.34	124.48
17	l	203	BCR	C38-C26-C25	-3.79	120.34	124.48
14	H	834	CLA	C1D-ND-C4D	-3.79	103.65	106.31
14	a	826	CLA	C1-C2-C3	-3.79	119.98	126.20
14	G	823	CLA	CMB-C2B-C3B	3.79	132.26	124.68
14	b	807	CLA	O2A-C1-C2	3.79	122.69	108.11
14	B	810	CLA	CHD-C1D-ND	-3.79	119.47	124.80
14	b	805	CLA	O2A-C1-C2	3.79	122.68	108.11
14	B	830	CLA	C1D-ND-C4D	-3.78	103.66	106.31
14	U	205	CLA	CHD-C1D-ND	-3.78	119.48	124.80
14	a	827	CLA	O2A-CGA-CBA	3.78	123.37	111.83
17	b	847	BCR	C33-C5-C6	-3.78	120.36	124.48
14	G	806	CLA	CHD-C1D-ND	-3.78	119.48	124.80
14	H	812	CLA	CHD-C1D-ND	-3.78	119.48	124.80
14	H	809	CLA	O2A-CGA-CBA	3.78	123.36	111.83
14	l	207	CLA	CHD-C1D-ND	-3.78	119.48	124.80
14	A	834	CLA	CHD-C1D-ND	-3.78	119.48	124.80
14	G	826	CLA	CAC-C3C-C4C	3.78	129.71	124.79
14	a	831	CLA	C1-C2-C3	-3.78	120.65	126.76
14	b	821	CLA	O2A-CGA-CBA	3.78	123.36	111.83
17	a	849	BCR	C28-C27-C26	-3.78	107.32	114.06
14	A	820	CLA	C1D-ND-C4D	-3.78	103.66	106.31
13	A	801	CL0	O2A-CGA-CBA	3.78	123.35	111.83
14	a	832	CLA	CHD-C1D-ND	-3.78	119.49	124.80
14	G	830	CLA	CMC-C2C-C1C	3.77	130.93	125.03
14	A	825	CLA	CMB-C2B-C3B	3.77	132.22	124.68
17	U	202	BCR	C1-C6-C5	-3.77	117.49	122.64
14	G	829	CLA	C1D-ND-C4D	-3.77	103.67	106.31
17	j	104	BCR	C3-C4-C5	-3.77	107.34	114.06
14	a	819	CLA	CHD-C1D-ND	-3.77	119.50	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	810	CLA	CHD-C1D-ND	-3.77	119.50	124.80
14	a	802	CLA	O2A-CGA-CBA	3.76	123.31	111.83
17	Q	204	BCR	C38-C26-C25	-3.76	120.38	124.48
14	B	815	CLA	CHD-C1D-ND	-3.76	119.51	124.80
14	H	831	CLA	C4A-NA-C1A	3.76	108.39	106.68
17	G	851	BCR	C24-C23-C22	-3.76	120.67	126.23
14	B	812	CLA	CMB-C2B-C3B	3.76	132.19	124.68
14	A	830	CLA	C1-C2-C3	-3.75	120.05	126.20
14	U	204	CLA	CHD-C1D-ND	-3.75	119.52	124.80
14	B	818	CLA	O2A-CGA-CBA	3.75	123.28	111.83
14	G	832	CLA	C1D-ND-C4D	-3.75	103.68	106.31
14	G	830	CLA	CMB-C2B-C3B	3.75	132.18	124.68
14	U	204	CLA	O2A-CGA-CBA	3.75	123.27	111.83
14	G	806	CLA	O2D-CGD-O1D	-3.75	116.55	123.85
17	i	102	BCR	C33-C5-C6	-3.75	120.39	124.48
14	A	819	CLA	O2A-C1-C2	3.75	122.53	108.11
17	R	102	BCR	C3-C4-C5	-3.75	107.38	114.06
14	b	804	CLA	O2A-CGA-CBA	3.75	123.25	111.83
14	G	845	CLA	CAC-C3C-C2C	3.74	134.44	127.56
14	a	815	CLA	CMB-C2B-C3B	3.74	132.17	124.68
14	a	811	CLA	C4D-C3D-CAD	3.74	112.17	108.11
14	B	815	CLA	CMB-C2B-C3B	3.74	132.16	124.68
14	a	834	CLA	CMB-C2B-C3B	3.74	132.16	124.68
14	a	818	CLA	CHD-C1D-ND	-3.74	119.54	124.80
14	a	824	CLA	CMB-C2B-C3B	3.74	132.16	124.68
14	G	824	CLA	CHD-C1D-ND	-3.74	119.54	124.80
14	A	831	CLA	O2A-CGA-CBA	3.74	123.23	111.83
14	G	819	CLA	CHD-C1D-ND	-3.73	119.55	124.80
14	b	823	CLA	O2A-CGA-CBA	3.73	123.22	111.83
14	B	825	CLA	O2A-CGA-CBA	3.73	123.22	111.83
14	H	808	CLA	O2A-C1-C2	3.73	122.47	108.11
14	a	813	CLA	O2A-C1-C2	3.73	122.46	108.11
14	B	817	CLA	CHD-C1D-ND	-3.73	119.56	124.80
14	A	838	CLA	O2A-CGA-CBA	3.73	123.20	111.83
14	H	813	CLA	O2A-C1-C2	3.73	122.45	108.11
14	a	829	CLA	CMB-C2B-C3B	3.73	132.13	124.68
14	B	826	CLA	C1D-ND-C4D	-3.73	103.70	106.31
17	f	201	BCR	C3-C4-C5	-3.72	107.42	114.06
17	f	203	BCR	C33-C5-C6	-3.72	120.42	124.48
14	G	803	CLA	O2A-CGA-CBA	3.72	123.19	111.83
14	B	814	CLA	C1D-ND-C4D	-3.72	103.70	106.31
14	G	807	CLA	O2A-C1-C2	3.72	122.43	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	842	CLA	C4-C3-C5	3.72	121.69	115.23
14	B	817	CLA	C4-C3-C5	3.72	121.69	115.23
14	A	805	CLA	CMB-C2B-C3B	3.72	132.12	124.68
14	A	823	CLA	CMB-C2B-C3B	3.72	132.11	124.68
14	a	826	CLA	CHD-C1D-ND	-3.72	119.57	124.80
14	b	833	CLA	CHD-C1D-ND	-3.72	119.57	124.80
14	U	206	CLA	CMB-C2B-C3B	3.72	132.11	124.68
17	B	848	BCR	C24-C23-C22	-3.71	120.75	126.23
14	a	831	CLA	O2A-C1-C2	3.71	122.39	108.11
14	b	820	CLA	CHD-C1D-ND	-3.71	119.58	124.80
14	B	816	CLA	C1-C2-C3	-3.71	120.12	126.20
14	B	818	CLA	C1-C2-C3	-3.71	120.12	126.20
14	b	828	CLA	CMB-C2B-C3B	3.71	132.09	124.68
14	H	830	CLA	C1D-ND-C4D	-3.71	103.71	106.31
14	A	827	CLA	O2A-CGA-CBA	3.71	123.14	111.83
14	G	827	CLA	CHD-C1D-ND	-3.71	119.59	124.80
14	b	834	CLA	O2D-CGD-CBD	3.70	117.71	111.23
14	H	807	CLA	CHD-C1D-ND	-3.70	119.59	124.80
14	G	835	CLA	C1D-ND-C4D	-3.70	103.71	106.31
14	B	816	CLA	O2A-C1-C2	3.70	122.35	108.11
14	a	805	CLA	CMB-C2B-C3B	3.70	132.08	124.68
14	A	835	CLA	O2A-C1-C2	3.70	122.35	108.11
14	b	817	CLA	C1D-ND-C4D	-3.70	103.72	106.31
14	A	833	CLA	O2A-CGA-CBA	3.70	123.12	111.83
14	a	821	CLA	CMB-C2B-C3B	3.70	132.08	124.68
14	H	811	CLA	C4A-NA-C1A	3.70	108.37	106.68
17	b	849	BCR	C7-C8-C9	-3.70	120.76	126.23
14	H	807	CLA	O2A-CGA-CBA	3.70	123.11	111.83
17	L	207	BCR	C4-C5-C6	-3.70	117.71	122.70
14	G	828	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
14	H	802	CLA	C1-C2-C3	-3.70	120.14	126.20
14	B	808	CLA	O2A-C1-C2	3.70	122.34	108.11
14	G	839	CLA	O2A-CGA-CBA	3.70	123.10	111.83
14	H	804	CLA	O2A-C1-C2	3.70	122.33	108.11
14	G	835	CLA	O2A-CGA-CBA	3.69	123.10	111.83
14	b	815	CLA	CHD-C1D-ND	-3.69	119.60	124.80
17	b	847	BCR	C19-C18-C17	3.69	124.82	119.01
14	B	805	CLA	CHD-C1D-ND	-3.69	119.61	124.80
14	a	813	CLA	CHD-C1D-ND	-3.69	119.61	124.80
14	H	824	CLA	C1D-ND-C4D	-3.69	103.72	106.31
14	F	1303	CLA	CHD-C1D-ND	-3.69	119.61	124.80
14	a	837	CLA	O2A-CGA-CBA	3.69	123.08	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	828	CLA	C4D-C3D-CAD	3.69	112.11	108.11
14	A	820	CLA	O2A-CGA-O1A	-3.69	114.40	123.63
14	H	838	CLA	CHD-C1D-ND	-3.69	119.61	124.80
14	B	838	CLA	CHD-C1D-ND	-3.69	119.61	124.80
14	H	826	CLA	C1-C2-C3	-3.68	120.16	126.20
14	G	820	CLA	CMB-C2B-C3B	3.68	132.05	124.68
14	L	205	CLA	O2A-CGA-CBA	3.68	123.07	111.83
14	A	807	CLA	O2A-C1-C2	3.68	122.28	108.11
14	a	808	CLA	C1-C2-C3	-3.68	120.17	126.20
14	A	822	CLA	CHD-C1D-ND	-3.68	119.62	124.80
14	a	844	CLA	CMA-C3A-C4A	3.68	121.65	111.77
14	a	834	CLA	O2A-C1-C2	3.67	122.24	108.11
14	b	835	CLA	CHD-C1D-ND	-3.67	119.63	124.80
14	B	812	CLA	CAC-C3C-C4C	3.67	129.57	124.79
14	A	808	CLA	CHD-C1D-ND	-3.67	119.64	124.80
13	A	801	CL0	C1-C2-C3	-3.67	120.19	126.20
14	G	805	CLA	O2A-C1-C2	3.67	122.23	108.11
14	A	822	CLA	C4A-NA-C1A	3.67	108.35	106.68
14	A	829	CLA	C1D-ND-C4D	-3.67	103.74	106.31
14	G	815	CLA	CHD-C1D-ND	-3.67	119.64	124.80
14	G	820	CLA	C1D-ND-C4D	-3.66	103.74	106.31
14	G	832	CLA	O2A-C1-C2	3.66	122.21	108.11
14	B	816	CLA	CMB-C2B-C3B	3.66	132.00	124.68
14	B	823	CLA	O2A-CGA-CBA	3.66	123.00	111.83
14	b	810	CLA	CMB-C2B-C3B	3.66	132.00	124.68
14	b	807	CLA	CHD-C1D-ND	-3.66	119.65	124.80
14	l	206	CLA	O2A-CGA-CBA	3.66	122.99	111.83
14	l	207	CLA	CMB-C2B-C3B	3.66	131.99	124.68
17	L	207	BCR	C1-C6-C5	-3.66	117.64	122.64
14	A	831	CLA	O2A-C1-C2	3.66	122.18	108.11
14	a	814	CLA	CHD-C1D-ND	-3.65	119.66	124.80
14	G	825	CLA	CMB-C2B-C3B	3.65	131.99	124.68
14	a	821	CLA	CHD-C1D-ND	-3.65	119.66	124.80
14	i	101	CLA	CHD-C1D-ND	-3.65	119.66	124.80
14	G	805	CLA	C1-C2-C3	-3.65	120.21	126.20
14	H	837	CLA	O2A-CGA-CBA	3.65	122.97	111.83
14	G	810	CLA	O2A-C1-C2	3.65	122.16	108.11
14	l	205	CLA	O2A-CGA-CBA	3.65	122.96	111.83
14	H	828	CLA	C4D-C3D-CAD	3.65	112.07	108.11
14	G	812	CLA	CHD-C1D-ND	-3.65	119.67	124.80
14	G	807	CLA	CHD-C1D-ND	-3.65	119.67	124.80
14	a	805	CLA	CHD-C1D-ND	-3.65	119.67	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	831	CLA	O2A-CGA-CBA	3.65	122.95	111.83
14	b	825	CLA	O2A-C1-C2	3.65	122.14	108.11
14	A	814	CLA	O2A-C1-C2	3.65	122.14	108.11
14	a	812	CLA	C1-C2-C3	-3.65	120.86	126.76
14	H	806	CLA	CHD-C1D-ND	-3.64	119.67	124.80
17	V	1602	BCR	C3-C4-C5	-3.64	107.56	114.06
14	B	802	CLA	O2A-CGA-CBA	3.64	122.94	111.83
14	B	828	CLA	C2D-C1D-ND	3.64	113.73	110.13
14	b	817	CLA	CHD-C1D-ND	-3.64	119.68	124.80
14	A	829	CLA	O2A-CGA-O1A	-3.64	114.52	123.63
14	G	829	CLA	O1D-CGD-CBD	-3.64	117.34	124.52
14	A	825	CLA	O2A-C1-C2	3.64	122.12	108.11
14	A	844	CLA	O2A-C1-C2	3.64	122.12	108.11
14	B	806	CLA	C1-C2-C3	-3.64	120.23	126.20
14	G	843	CLA	C1-C2-C3	-3.64	120.23	126.20
14	a	830	CLA	O2A-CGA-CBA	3.64	122.93	111.83
14	G	810	CLA	CMB-C2B-C3B	3.64	131.95	124.68
17	A	852	BCR	C38-C26-C25	-3.64	120.52	124.48
14	a	829	CLA	O2A-C1-C2	3.64	122.11	108.11
14	U	201	CLA	C1-O2A-CGA	3.64	125.45	116.65
14	H	806	CLA	C1-C2-C3	-3.63	120.24	126.20
14	b	828	CLA	CMD-C2D-C3D	-3.63	119.36	127.69
14	A	820	CLA	CHD-C1D-ND	-3.63	119.69	124.80
14	H	820	CLA	CHD-C1D-ND	-3.63	119.69	124.80
14	b	838	CLA	CHD-C1D-ND	-3.63	119.69	124.80
14	A	845	CLA	CMB-C2B-C3B	3.63	131.94	124.68
17	a	852	BCR	C33-C5-C6	-3.63	120.52	124.48
14	H	813	CLA	CMB-C2B-C3B	3.63	131.94	124.68
13	G	801	CL0	C1-C2-C3	-3.63	120.25	126.20
14	A	813	CLA	O2A-C1-C2	3.63	122.07	108.11
14	G	816	CLA	C1D-ND-C4D	-3.63	103.77	106.31
14	A	835	CLA	CHD-C1D-ND	-3.63	119.70	124.80
14	L	204	CLA	O2A-CGA-CBA	3.63	122.89	111.83
14	B	826	CLA	O1D-CGD-CBD	-3.62	117.37	124.52
17	a	848	BCR	C19-C18-C17	3.62	124.71	119.01
14	L	204	CLA	O2A-C1-C2	3.62	122.04	108.11
17	b	843	BCR	C7-C8-C9	-3.62	120.88	126.23
14	a	811	CLA	CMD-C2D-C3D	-3.62	119.39	127.69
14	G	830	CLA	C1D-ND-C4D	-3.62	103.77	106.31
14	a	840	CLA	O2A-C1-C2	3.62	122.03	108.11
14	a	828	CLA	CMB-C2B-C3B	3.61	131.90	124.68
14	B	831	CLA	O2A-C1-C2	3.61	122.01	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	809	CLA	CHD-C1D-ND	-3.61	119.72	124.80
14	G	805	CLA	CHD-C1D-ND	-3.61	119.72	124.80
14	H	833	CLA	CHD-C1D-ND	-3.61	119.72	124.80
14	U	206	CLA	CHD-C1D-ND	-3.61	119.72	124.80
14	G	837	CLA	CHD-C1D-ND	-3.61	119.72	124.80
14	a	833	CLA	CHD-C1D-ND	-3.61	119.72	124.80
14	a	826	CLA	O2A-CGA-CBA	3.61	122.84	111.83
14	b	805	CLA	CMB-C2B-C3B	3.61	131.90	124.68
14	a	819	CLA	CAA-C2A-C1A	-3.61	100.15	111.97
14	b	813	CLA	C1-C2-C3	-3.61	120.28	126.20
17	a	852	BCR	C30-C25-C24	3.61	125.44	115.65
14	H	835	CLA	C3C-C4C-NC	3.61	115.05	110.43
14	a	812	CLA	CHD-C1D-ND	-3.61	119.73	124.80
14	b	830	CLA	O2A-CGA-CBA	3.61	125.39	114.00
14	A	834	CLA	O2A-C1-C2	3.60	121.98	108.11
14	b	824	CLA	CMB-C2B-C3B	3.60	131.89	124.68
14	G	813	CLA	C1-C2-C3	-3.60	120.93	126.76
14	B	824	CLA	CHD-C1D-ND	-3.60	119.73	124.80
14	a	829	CLA	C1-C2-C3	-3.60	120.29	126.20
14	a	812	CLA	O2A-C1-C2	3.60	121.97	108.11
14	U	204	CLA	C1-C2-C3	-3.60	120.30	126.20
14	G	817	CLA	CHD-C1D-ND	-3.60	119.73	124.80
14	A	826	CLA	O2A-CGA-CBA	3.60	122.82	111.83
14	A	821	CLA	O2A-C1-C2	3.60	121.95	108.11
14	a	830	CLA	CMB-C2B-C3B	3.60	131.87	124.68
14	a	830	CLA	C1-C2-C3	-3.60	120.31	126.20
14	a	832	CLA	O2A-CGA-CBA	3.60	122.80	111.83
17	A	853	BCR	C33-C5-C6	-3.60	120.56	124.48
14	A	841	CLA	O2A-C1-C2	3.59	121.94	108.11
17	m	1602	BCR	C28-C27-C26	-3.59	107.65	114.06
14	A	829	CLA	CMC-C2C-C1C	3.59	130.64	125.03
17	H	849	BCR	C24-C23-C22	-3.59	120.93	126.23
14	G	845	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
14	a	817	CLA	CHD-C1D-ND	-3.59	119.76	124.80
14	a	826	CLA	CMB-C2B-C3B	3.58	131.85	124.68
14	b	805	CLA	CHD-C1D-ND	-3.58	119.76	124.80
14	B	809	CLA	C1D-ND-C4D	-3.58	103.80	106.31
14	H	830	CLA	CHD-C1D-ND	-3.58	119.76	124.80
14	a	808	CLA	CHD-C1D-ND	-3.58	119.76	124.80
14	B	805	CLA	CMB-C2B-C3B	3.58	131.84	124.68
17	I	101	BCR	C7-C8-C9	-3.58	120.94	126.23
14	G	833	CLA	O2A-CGA-CBA	3.58	122.75	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	836	CLA	CHD-C1D-ND	-3.58	119.77	124.80
14	B	810	CLA	CMB-C2B-C3B	3.58	131.84	124.68
14	B	806	CLA	CHD-C1D-ND	-3.58	119.77	124.80
17	H	843	BCR	C7-C8-C9	-3.58	120.94	126.23
17	H	847	BCR	C19-C18-C17	3.58	124.63	119.01
14	A	831	CLA	C1D-ND-C4D	-3.57	103.80	106.31
14	a	828	CLA	O2A-CGA-O1A	-3.57	114.69	123.63
14	b	824	CLA	CHD-C1D-ND	-3.57	119.78	124.80
14	B	816	CLA	CMC-C2C-C1C	3.57	130.61	125.03
17	f	203	BCR	C35-C13-C14	-3.57	117.03	122.82
14	G	844	CLA	CHD-C1D-ND	-3.57	119.78	124.80
17	a	847	BCR	C33-C5-C6	-3.57	120.59	124.48
14	K	101	CLA	CHD-C1D-ND	-3.57	119.78	124.80
14	G	826	CLA	C1D-ND-C4D	-3.57	103.81	106.31
17	i	102	BCR	C7-C8-C9	-3.57	120.96	126.23
17	G	853	BCR	C24-C23-C22	-3.57	120.96	126.23
17	B	850	BCR	C19-C18-C17	3.57	124.62	119.01
14	G	821	CLA	C4D-C3D-CAD	3.57	111.98	108.11
14	b	839	CLA	O2A-CGA-CBA	3.57	122.71	111.83
14	B	803	CLA	CED-O2D-CGD	3.56	124.00	115.92
13	G	801	CL0	CMC-C2C-C1C	3.56	130.60	125.03
14	A	825	CLA	CHD-C1D-ND	-3.56	119.79	124.80
17	a	852	BCR	C24-C23-C22	-3.56	120.97	126.23
14	H	816	CLA	C1-C2-C3	-3.56	120.36	126.20
14	b	831	CLA	O2A-CGA-CBA	3.56	122.69	111.83
14	G	804	CLA	CHD-C1D-ND	-3.56	119.79	124.80
14	A	822	CLA	CMB-C2B-C3B	3.56	131.80	124.68
14	G	821	CLA	O2A-C1-C2	3.56	121.80	108.11
14	G	818	CLA	CMC-C2C-C1C	3.56	130.59	125.03
14	b	826	CLA	C1D-ND-C4D	-3.56	103.82	106.31
14	a	816	CLA	CHD-C1D-ND	-3.56	119.80	124.80
14	A	812	CLA	O2A-C1-C2	3.56	121.79	108.11
17	J	103	BCR	C15-C14-C13	-3.55	122.30	127.28
14	G	842	CLA	C4-C3-C5	3.55	121.39	115.23
14	A	809	CLA	O2A-CGA-CBA	3.55	122.67	111.83
14	A	803	CLA	O2A-C1-C2	3.55	121.78	108.11
17	H	843	BCR	C33-C5-C6	-3.55	120.61	124.48
14	A	845	CLA	CAC-C3C-C2C	3.55	134.08	127.56
14	b	806	CLA	CHD-C1D-ND	-3.55	119.81	124.80
17	H	847	BCR	C33-C5-C6	-3.55	120.61	124.48
14	a	842	CLA	CHD-C1D-ND	-3.55	119.81	124.80
14	G	834	CLA	CHD-C1D-ND	-3.55	119.81	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	809	CLA	C1-C2-C3	-3.55	120.39	126.20
14	G	831	CLA	O2A-C1-C2	3.55	121.75	108.11
14	a	825	CLA	C1D-ND-C4D	-3.54	103.83	106.31
14	b	814	CLA	CMB-C2B-C3B	3.54	131.76	124.68
14	B	825	CLA	CMB-C2B-C3B	3.54	131.76	124.68
14	B	806	CLA	O2A-CGA-CBA	3.54	122.63	111.83
14	H	817	CLA	CHD-C1D-ND	-3.54	119.82	124.80
14	H	816	CLA	CHD-C1D-ND	-3.54	119.82	124.80
14	a	804	CLA	CHD-C1D-ND	-3.54	119.82	124.80
17	l	208	BCR	C38-C26-C25	-3.54	120.62	124.48
14	H	812	CLA	O2A-C1-C2	3.54	121.73	108.11
14	a	855	CLA	O2D-CGD-O1D	-3.54	116.96	123.85
17	Q	202	BCR	C12-C13-C14	-3.54	113.44	119.01
14	H	801	CLA	O2D-CGD-O1D	-3.54	116.96	123.85
14	H	824	CLA	CHD-C1D-ND	-3.54	119.83	124.80
14	a	843	CLA	CHD-C1D-ND	-3.54	119.83	124.80
14	A	833	CLA	CHD-C1D-ND	-3.54	119.83	124.80
14	H	804	CLA	C1-C2-C3	-3.54	120.41	126.20
14	B	821	CLA	O2A-CGA-CBA	3.53	122.61	111.83
14	b	828	CLA	C4D-C3D-CAD	3.53	111.94	108.11
17	B	850	BCR	C24-C23-C22	-3.53	121.01	126.23
19	H	848	LMG	O7-C10-C11	3.53	119.12	111.48
17	J	103	BCR	C33-C5-C6	-3.53	120.63	124.48
14	b	836	CLA	CMB-C2B-C3B	3.53	131.74	124.68
14	A	818	CLA	C4D-C3D-CAD	3.53	111.94	108.11
14	B	826	CLA	CMB-C2B-C3B	3.53	131.74	124.68
14	A	805	CLA	O2A-C1-C2	3.53	121.68	108.11
14	G	826	CLA	CMB-C2B-C3B	3.53	131.73	124.68
14	B	818	CLA	CMB-C2B-C3B	3.53	131.73	124.68
17	V	1602	BCR	C38-C26-C25	-3.53	120.64	124.48
14	b	830	CLA	CMB-C2B-C3B	3.53	131.73	124.68
14	l	205	CLA	CMB-C2B-C3B	3.53	131.73	124.68
14	A	829	CLA	CMB-C2B-C3B	3.52	131.73	124.68
14	J	101	CLA	CHD-C1D-ND	-3.52	119.84	124.80
14	b	816	CLA	O2A-C1-C2	3.52	121.67	108.11
14	G	803	CLA	CAA-C2A-C3A	-3.52	103.48	113.00
14	A	809	CLA	C1-C2-C3	-3.52	120.42	126.20
14	B	818	CLA	CHD-C1D-ND	-3.52	119.84	124.80
14	a	806	CLA	CHD-C1D-ND	-3.52	119.85	124.80
17	U	202	BCR	C4-C5-C6	-3.52	117.94	122.70
14	H	839	CLA	O2A-CGA-CBA	3.52	122.57	111.83
14	i	101	CLA	CAC-C3C-C4C	3.52	129.37	124.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	802	CLA	C1-O2A-CGA	3.52	125.17	116.65
14	G	822	CLA	CHD-C1D-ND	-3.52	119.85	124.80
14	H	810	CLA	CHD-C1D-ND	-3.52	119.85	124.80
14	B	801	CLA	C3C-C4C-NC	3.52	114.94	110.43
14	a	833	CLA	O2A-C1-C2	3.52	121.64	108.11
14	H	835	CLA	CAC-C3C-C4C	3.51	129.36	124.79
14	a	809	CLA	CAC-C3C-C4C	3.51	129.36	124.79
14	a	806	CLA	C4-C3-C5	3.51	121.32	115.23
14	A	803	CLA	CHD-C1D-ND	-3.51	119.86	124.80
18	G	855	LHG	O7-C7-C8	3.51	119.07	111.48
14	M	1601	CLA	CMA-C3A-C4A	3.51	121.20	111.77
14	B	812	CLA	O2A-C1-C2	3.51	121.61	108.11
14	B	805	CLA	O2A-C1-C2	3.51	121.61	108.11
14	G	822	CLA	C1-C2-C3	-3.51	120.45	126.20
14	A	830	CLA	O2A-C1-C2	3.51	121.60	108.11
14	A	805	CLA	CMC-C2C-C1C	3.50	130.51	125.03
14	b	809	CLA	CHD-C1D-ND	-3.50	119.87	124.80
14	A	811	CLA	CHD-C1D-ND	-3.50	119.87	124.80
14	G	809	CLA	CHD-C1D-ND	-3.50	119.87	124.80
14	b	831	CLA	O2A-C1-C2	3.50	121.58	108.11
14	B	836	CLA	CMB-C2B-C3B	3.50	131.68	124.68
14	G	838	CLA	O2A-CGA-CBA	3.50	122.51	111.83
14	H	817	CLA	C1-C2-C3	-3.50	120.46	126.20
14	H	810	CLA	CMB-C2B-C3B	3.50	131.68	124.68
14	A	835	CLA	CAA-C2A-C3A	-3.50	103.54	113.00
17	a	852	BCR	C3-C4-C5	-3.50	107.81	114.06
17	B	842	BCR	C24-C23-C22	-3.50	121.06	126.23
17	H	846	BCR	C7-C8-C9	-3.50	121.06	126.23
14	A	835	CLA	O2A-CGA-CBA	3.50	122.50	111.83
17	j	104	BCR	C8-C7-C6	-3.50	117.65	127.00
17	G	850	BCR	C3-C4-C5	-3.50	107.82	114.06
14	A	840	CLA	CHD-C1D-ND	-3.50	119.88	124.80
14	G	826	CLA	O2A-CGA-CBA	3.50	122.50	111.83
14	H	818	CLA	CHD-C1D-ND	-3.50	119.88	124.80
14	H	826	CLA	O2A-C1-C2	3.50	121.56	108.11
14	a	832	CLA	O2A-C1-C2	3.50	121.56	108.11
14	G	840	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	A	824	CLA	CMD-C2D-C3D	-3.49	119.68	127.69
14	H	825	CLA	CMB-C2B-C3B	3.49	131.66	124.68
14	A	805	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	a	810	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	H	811	CLA	O2A-CGA-CBA	3.49	125.03	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	823	CLA	O2A-CGA-CBA	3.49	125.02	114.00
14	G	803	CLA	CHD-C1D-ND	-3.49	119.90	124.80
14	l	205	CLA	O2A-C1-C2	3.49	121.52	108.11
17	G	848	BCR	C30-C25-C26	-3.49	117.87	122.64
14	A	820	CLA	CMA-C3A-C4A	3.49	121.14	111.77
14	a	834	CLA	CHD-C1D-ND	-3.48	119.90	124.80
14	A	810	CLA	C1-C2-C3	-3.48	120.49	126.20
14	A	837	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
14	B	803	CLA	CMA-C3A-C4A	3.48	121.13	111.77
14	H	812	CLA	CAC-C3C-C4C	3.48	129.32	124.79
14	B	828	CLA	C1D-ND-C4D	-3.48	103.87	106.31
14	H	813	CLA	C4D-C3D-CAD	3.48	111.89	108.11
14	G	834	CLA	O2A-C1-C2	3.48	121.50	108.11
14	G	812	CLA	C4D-C3D-CAD	3.48	111.89	108.11
14	k	1401	CLA	CHD-C1D-ND	-3.48	119.91	124.80
14	H	831	CLA	O2A-CGA-CBA	3.48	122.44	111.83
14	H	840	CLA	CHD-C1D-ND	-3.48	119.91	124.80
14	A	831	CLA	CMB-C2B-C3B	3.48	131.63	124.68
14	G	812	CLA	CMD-C2D-C3D	-3.48	119.72	127.69
14	L	206	CLA	CHD-C1D-ND	-3.48	119.91	124.80
17	R	101	BCR	C38-C26-C25	-3.48	120.69	124.48
14	j	101	CLA	CHD-C1D-ND	-3.47	119.91	124.80
14	b	809	CLA	CAA-C2A-C3A	-3.47	103.61	113.00
14	B	825	CLA	O2A-C1-C2	3.47	121.47	108.11
14	a	828	CLA	O2A-CGA-CBA	3.47	122.42	111.83
17	S	104	BCR	C15-C14-C13	-3.47	122.41	127.28
17	L	207	BCR	C19-C18-C17	3.47	124.47	119.01
14	b	812	CLA	CMB-C2B-C3B	3.47	131.62	124.68
14	H	821	CLA	CMB-C2B-C3B	3.47	131.61	124.68
14	b	839	CLA	CHD-C1D-ND	-3.47	119.92	124.80
14	B	830	CLA	CHD-C1D-ND	-3.47	119.92	124.80
14	B	813	CLA	CMB-C2B-C3B	3.47	131.61	124.68
14	j	101	CLA	CMA-C3A-C4A	3.47	121.09	111.77
14	A	809	CLA	CHD-C1D-ND	-3.46	119.93	124.80
17	H	849	BCR	C19-C18-C17	3.46	124.46	119.01
14	b	824	CLA	CAA-C2A-C3A	-3.46	103.64	113.00
14	b	803	CLA	O2A-CGA-CBA	3.46	122.39	111.83
14	a	802	CLA	C4A-NA-C1A	3.46	108.26	106.68
14	G	820	CLA	O2A-C1-C2	3.46	121.42	108.11
14	K	102	CLA	CHD-C1D-ND	-3.46	119.93	124.80
15	G	846	PQN	C14-C13-C15	3.46	121.23	115.23
14	G	845	CLA	CHD-C1D-ND	-3.46	119.94	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	804	CLA	CMB-C2B-C3B	3.45	131.59	124.68
14	a	834	CLA	CAA-C2A-C3A	-3.45	103.66	113.00
14	a	839	CLA	CHD-C1D-ND	-3.45	119.94	124.80
14	G	820	CLA	CHD-C1D-ND	-3.45	119.94	124.80
14	G	843	CLA	C1D-ND-C4D	-3.45	103.89	106.31
14	G	803	CLA	O2A-C1-C2	3.45	121.39	108.11
14	A	838	CLA	O2A-C1-C2	3.45	121.39	108.11
14	G	816	CLA	CMB-C2B-C3B	3.45	131.58	124.68
14	G	841	CLA	CMB-C2B-C3B	3.45	131.57	124.68
14	S	102	CLA	CHD-C1D-ND	-3.45	119.95	124.80
17	G	852	BCR	C33-C5-C6	-3.45	120.72	124.48
14	A	802	CLA	O2A-C1-C2	3.45	121.38	108.11
14	B	820	CLA	CHD-C1D-ND	-3.45	119.95	124.80
14	B	811	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
14	A	817	CLA	CHD-C1D-ND	-3.45	119.95	124.80
14	a	844	CLA	CHD-C1D-ND	-3.45	119.95	124.80
14	A	832	CLA	O2A-C1-C2	3.44	121.36	108.11
14	U	201	CLA	O2A-C1-C2	3.44	121.36	108.11
14	B	828	CLA	CMD-C2D-C3D	-3.44	119.79	127.69
14	A	824	CLA	C4D-C3D-CAD	3.44	111.84	108.11
14	A	803	CLA	CAA-C2A-C3A	-3.44	103.70	113.00
14	A	825	CLA	O2D-CGD-CBD	3.44	117.25	111.23
17	b	845	BCR	C38-C26-C25	-3.44	120.73	124.48
14	A	829	CLA	O2A-CGA-CBA	3.44	122.32	111.83
14	a	824	CLA	O2A-C1-C2	3.44	121.34	108.11
14	b	813	CLA	O2A-C1-C2	3.44	121.34	108.11
14	H	812	CLA	C1-C2-C3	-3.44	120.57	126.20
14	H	801	CLA	CMC-C2C-C1C	3.44	130.40	125.03
14	H	836	CLA	O2A-C1-C2	3.44	121.33	108.11
14	A	830	CLA	O2D-CGD-O1D	-3.43	117.16	123.85
14	A	827	CLA	CHD-C1D-ND	-3.43	119.97	124.80
14	b	812	CLA	CHD-C1D-ND	-3.43	119.97	124.80
14	G	833	CLA	O2A-C1-C2	3.43	121.32	108.11
17	H	844	BCR	C7-C8-C9	-3.43	121.16	126.23
14	H	805	CLA	CHD-C1D-ND	-3.43	119.97	124.80
14	b	811	CLA	CHD-C1D-ND	-3.43	119.97	124.80
14	H	833	CLA	O2A-CGA-CBA	3.43	124.84	114.00
14	l	202	CLA	C1-C2-C3	-3.43	120.58	126.20
14	G	808	CLA	CHD-C1D-ND	-3.43	119.97	124.80
14	a	844	CLA	CAC-C3C-C2C	3.43	133.86	127.56
14	b	818	CLA	O2A-C1-C2	3.43	121.30	108.11
17	G	848	BCR	C33-C5-C6	-3.43	120.75	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	848	BCR	C24-C23-C22	-3.43	121.17	126.23
17	Q	204	BCR	C35-C13-C14	-3.43	117.27	122.82
14	A	807	CLA	CHD-C1D-ND	-3.42	119.98	124.80
14	b	832	CLA	C4-C3-C5	3.42	121.17	115.23
14	G	843	CLA	CAC-C3C-C4C	3.42	129.24	124.79
14	G	835	CLA	CMB-C2B-C3B	3.42	131.52	124.68
14	B	804	CLA	CMC-C2C-C1C	3.42	130.38	125.03
14	A	811	CLA	O2A-CGA-CBA	3.42	124.81	114.00
14	a	825	CLA	O2A-CGA-CBA	3.42	122.27	111.83
14	G	820	CLA	C1-C2-C3	-3.42	120.59	126.20
14	H	819	CLA	CHD-C1D-ND	-3.42	119.99	124.80
14	U	204	CLA	CMB-C2B-C3B	3.42	131.52	124.68
14	b	816	CLA	CHD-C1D-ND	-3.42	119.99	124.80
14	U	205	CLA	CMB-C2B-C3B	3.42	131.52	124.68
14	a	821	CLA	C1-C2-C3	-3.42	120.59	126.20
14	H	817	CLA	O2A-CGA-CBA	3.42	122.26	111.83
17	H	847	BCR	C38-C26-C25	-3.42	120.76	124.48
17	H	844	BCR	C24-C23-C22	-3.42	121.18	126.23
14	G	827	CLA	CMB-C2B-C3B	3.42	131.51	124.68
14	A	818	CLA	CMC-C2C-C1C	3.42	130.37	125.03
14	H	837	CLA	CMB-C2B-C3B	3.41	131.51	124.68
14	H	801	CLA	C3C-C4C-NC	3.41	114.80	110.43
14	G	845	CLA	CMB-C2B-C3B	3.41	131.50	124.68
17	a	850	BCR	C38-C26-C25	-3.41	120.76	124.48
14	H	809	CLA	C1D-ND-C4D	-3.41	103.92	106.31
14	j	102	CLA	CHD-C1D-ND	-3.41	120.00	124.80
14	B	835	CLA	CHD-C1D-ND	-3.41	120.00	124.80
14	b	837	CLA	C4D-C3D-CAD	3.41	111.81	108.11
14	A	845	CLA	CMA-C3A-C4A	3.41	120.94	111.77
17	B	842	BCR	C36-C18-C17	-3.41	117.30	122.82
14	B	839	CLA	CHD-C1D-ND	-3.41	120.01	124.80
14	b	826	CLA	CMB-C2B-C3B	3.41	131.49	124.68
14	B	809	CLA	O2A-C1-C2	3.41	121.21	108.11
17	A	853	BCR	C3-C4-C5	-3.40	107.98	114.06
14	H	837	CLA	C4D-C3D-CAD	3.40	111.80	108.11
17	H	846	BCR	C3-C4-C5	-3.40	107.98	114.06
17	A	853	BCR	C24-C25-C26	-3.40	113.72	121.56
14	K	101	CLA	OBD-CAD-C3D	-3.40	123.06	128.60
14	B	801	CLA	CMC-C2C-C1C	3.40	130.35	125.03
14	i	101	CLA	O2A-CGA-CBA	3.40	122.20	111.83
15	A	846	PQN	C12-C11-C3	-3.40	103.71	112.08
17	b	842	BCR	C36-C18-C17	-3.40	117.31	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	845	BCR	C15-C14-C13	-3.40	122.29	127.48
14	G	833	CLA	C4-C3-C5	3.40	121.13	115.23
14	A	845	CLA	CHD-C1D-ND	-3.40	120.02	124.80
14	b	830	CLA	CHD-C1D-ND	-3.40	120.02	124.80
14	a	809	CLA	CMB-C2B-C3B	3.40	131.47	124.68
14	H	829	CLA	C1D-ND-C4D	-3.40	103.93	106.31
14	a	806	CLA	O2A-C1-C2	3.40	121.17	108.11
14	A	833	CLA	O2A-C1-C2	3.39	121.17	108.11
14	a	824	CLA	CMA-C3A-C4A	3.39	120.90	111.77
14	U	205	CLA	O2A-C1-C2	3.39	121.17	108.11
14	B	827	CLA	C1D-ND-C4D	-3.39	103.93	106.31
14	a	808	CLA	CAA-C2A-C1A	-3.39	100.86	111.97
14	A	841	CLA	CHD-C1D-ND	-3.39	120.03	124.80
14	L	204	CLA	CHD-C1D-ND	-3.39	120.03	124.80
17	j	104	BCR	C1-C6-C5	-3.39	118.00	122.64
14	B	813	CLA	O2A-C1-C2	3.39	121.15	108.11
14	H	830	CLA	O2A-CGA-CBA	3.39	124.70	114.00
14	H	814	CLA	CHD-C1D-ND	-3.39	120.04	124.80
14	H	802	CLA	CMC-C2C-C1C	3.39	130.32	125.03
14	B	817	CLA	CMB-C2B-C3B	3.38	131.45	124.68
14	a	823	CLA	CMA-C3A-C4A	3.38	120.87	111.77
14	G	808	CLA	O2A-CGA-CBA	3.38	124.69	114.00
14	B	804	CLA	C1-C2-C3	-3.38	120.65	126.20
14	b	826	CLA	C1-C2-C3	-3.38	120.65	126.20
14	a	827	CLA	CHD-C4C-C3C	-3.38	119.84	124.77
14	l	205	CLA	CHD-C1D-ND	-3.38	120.04	124.80
17	a	851	BCR	C33-C5-C6	-3.38	120.79	124.48
17	f	201	BCR	C35-C13-C12	3.38	123.25	118.09
14	A	824	CLA	CMA-C3A-C4A	3.38	120.86	111.77
14	G	819	CLA	CMC-C2C-C1C	3.38	130.32	125.03
14	G	835	CLA	CAA-C2A-C3A	-3.38	103.87	113.00
14	G	831	CLA	CHD-C1D-ND	-3.38	120.05	124.80
14	G	836	CLA	CHD-C1D-ND	-3.38	120.05	124.80
14	b	826	CLA	O1D-CGD-CBD	-3.38	117.85	124.52
14	H	804	CLA	CHD-C1D-ND	-3.38	120.05	124.80
14	a	840	CLA	CHD-C1D-ND	-3.38	120.05	124.80
14	H	837	CLA	CMD-C2D-C3D	-3.38	119.95	127.69
14	A	833	CLA	C1-C2-C3	-3.38	120.67	126.20
14	H	805	CLA	O2A-C1-C2	3.37	121.09	108.11
14	H	831	CLA	CMA-C3A-C4A	3.37	120.84	111.77
14	a	805	CLA	CAA-C2A-C3A	-3.37	103.89	113.00
17	R	103	BCR	C38-C26-C25	-3.37	120.81	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	102	BCR	C38-C26-C25	-3.37	120.81	124.48
14	G	818	CLA	CHD-C1D-ND	-3.37	120.06	124.80
14	B	826	CLA	C1-C2-C3	-3.37	120.68	126.20
14	b	836	CLA	C3C-C4C-NC	3.37	114.75	110.43
17	b	843	BCR	C38-C26-C25	-3.37	120.81	124.48
14	G	825	CLA	CHD-C1D-ND	-3.37	120.06	124.80
14	b	818	CLA	C4-C3-C5	3.37	121.07	115.23
14	b	803	CLA	C1-C2-C3	-3.37	120.68	126.20
18	G	854	LHG	O7-C7-C8	3.37	118.77	111.48
14	x	1701	CLA	CHD-C1D-ND	-3.37	120.06	124.80
14	A	837	CLA	CHD-C1D-ND	-3.37	120.06	124.80
14	b	832	CLA	CHD-C1D-ND	-3.37	120.06	124.80
14	B	832	CLA	O2A-CGA-CBA	3.37	122.10	111.83
14	L	204	CLA	C1-C2-C3	-3.37	120.68	126.20
14	b	801	CLA	CMC-C2C-C1C	3.37	130.29	125.03
14	V	1601	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
14	b	834	CLA	CMA-C3A-C4A	3.36	120.81	111.77
14	a	829	CLA	CMA-C3A-C4A	3.36	120.81	111.77
17	b	842	BCR	C15-C14-C13	-3.36	122.56	127.28
14	b	840	CLA	CHD-C1D-ND	-3.36	120.07	124.80
14	a	844	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
14	a	822	CLA	O2A-CGA-CBA	3.36	124.62	114.00
15	a	845	PQN	C12-C11-C3	-3.36	103.81	112.08
14	a	837	CLA	O2A-C1-C2	3.36	121.04	108.11
14	a	802	CLA	CAA-C2A-C3A	-3.36	103.92	113.00
14	F	1301	CLA	O2A-CGA-CBA	3.36	124.61	114.00
17	J	102	BCR	C36-C18-C17	-3.36	117.38	122.82
14	B	828	CLA	O2A-C1-C2	3.36	121.02	108.11
14	H	806	CLA	O2A-CGA-CBA	3.35	122.06	111.83
14	a	838	CLA	O2A-CGA-CBA	3.35	122.06	111.83
17	l	208	BCR	C15-C14-C13	-3.35	122.57	127.28
14	G	829	CLA	O2A-CGA-O1A	-3.35	115.24	123.63
14	A	818	CLA	CHD-C1D-ND	-3.35	120.08	124.80
17	H	845	BCR	C38-C26-C25	-3.35	120.83	124.48
14	U	206	CLA	O2A-C1-C2	3.35	121.01	108.11
14	G	806	CLA	O2A-CGA-CBA	3.35	124.59	114.00
17	S	104	BCR	C32-C1-C31	-3.35	99.04	108.63
14	A	803	CLA	C1-C2-C3	-3.35	120.71	126.20
14	B	802	CLA	CMC-C2C-C1C	3.35	130.27	125.03
14	a	832	CLA	C4-C3-C5	3.35	121.04	115.23
14	b	806	CLA	OBD-CAD-C3D	-3.35	120.59	128.42
14	a	844	CLA	O2A-CGA-CBA	3.35	124.57	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	841	CLA	CAA-C2A-C3A	-3.34	103.96	113.00
14	a	804	CLA	O2A-C1-C2	3.34	120.97	108.11
14	G	833	CLA	CHD-C1D-ND	-3.34	120.10	124.80
14	B	810	CLA	CAA-C2A-C3A	-3.34	103.97	113.00
14	a	824	CLA	CHD-C1D-ND	-3.34	120.10	124.80
14	B	840	CLA	C1-C2-C3	-3.34	120.72	126.20
14	G	827	CLA	O2A-C1-C2	3.34	120.97	108.11
17	Q	202	BCR	C28-C27-C26	-3.34	108.10	114.06
14	l	206	CLA	O2A-C1-C2	3.34	120.96	108.11
14	B	830	CLA	O2A-CGA-CBA	3.34	124.55	114.00
14	A	842	CLA	CHD-C1D-ND	-3.34	120.10	124.80
14	a	810	CLA	O2A-CGA-CBA	3.34	124.55	114.00
14	B	829	CLA	CHD-C1D-ND	-3.34	120.11	124.80
14	b	823	CLA	C1-C2-C3	-3.34	121.36	126.76
14	H	826	CLA	CMB-C2B-C3B	3.34	131.35	124.68
14	B	804	CLA	CHD-C1D-ND	-3.34	120.11	124.80
14	a	802	CLA	CHD-C1D-ND	-3.33	120.11	124.80
14	G	813	CLA	CHD-C1D-ND	-3.33	120.11	124.80
14	b	804	CLA	CMA-C3A-C4A	3.33	120.73	111.77
14	L	201	CLA	C1-O2A-CGA	3.33	124.71	116.65
14	a	819	CLA	O2A-C1-C2	3.33	120.92	108.11
14	H	825	CLA	C3C-C4C-NC	3.33	114.69	110.43
14	A	842	CLA	O2A-CGA-CBA	3.33	124.51	114.00
14	G	840	CLA	O2A-CGA-CBA	3.33	124.51	114.00
14	H	823	CLA	C1-C2-C3	-3.33	121.38	126.76
17	R	102	BCR	C35-C13-C12	3.32	123.17	118.09
14	G	823	CLA	CHD-C1D-ND	-3.32	120.13	124.80
14	a	834	CLA	O2A-CGA-CBA	3.32	121.96	111.83
14	S	101	CLA	CHD-C1D-ND	-3.32	120.13	124.80
14	V	1601	CLA	C4D-C3D-CAD	3.32	111.71	108.11
14	G	842	CLA	CHD-C1D-ND	-3.32	120.13	124.80
14	b	822	CLA	CHD-C1D-ND	-3.32	120.13	124.80
17	f	203	BCR	C28-C27-C26	-3.31	108.15	114.06
14	H	823	CLA	O2A-CGA-CBA	3.31	121.94	111.83
14	A	806	CLA	CAA-C2A-C3A	-3.31	104.05	113.00
17	b	849	BCR	C19-C18-C17	3.31	124.22	119.01
14	a	807	CLA	O2A-CGA-CBA	3.31	124.47	114.00
13	a	801	CL0	CAA-C2A-C3A	-3.31	104.05	113.00
14	a	827	CLA	OBD-CAD-C3D	-3.31	120.68	128.42
14	H	822	CLA	O2A-CGA-CBA	3.31	124.46	114.00
14	b	825	CLA	C3C-C4C-NC	3.31	114.67	110.43
17	b	842	BCR	C19-C18-C17	3.31	124.22	119.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	827	CLA	C4D-C3D-CAD	3.31	111.70	108.11
14	H	822	CLA	CMA-C3A-C4A	3.31	120.66	111.77
14	Q	201	CLA	CMC-C2C-C1C	3.31	130.20	125.03
14	H	824	CLA	O2A-CGA-CBA	3.31	124.45	114.00
14	a	814	CLA	O2A-CGA-CBA	3.31	124.44	114.00
14	A	815	CLA	CMB-C2B-C3B	3.30	131.29	124.68
14	H	832	CLA	CHD-C1D-ND	-3.30	120.15	124.80
14	b	829	CLA	C4D-C3D-CAD	3.30	111.69	108.11
14	T	1401	CLA	CMA-C3A-C4A	3.30	120.65	111.77
14	B	815	CLA	CMC-C2C-C1C	3.30	130.20	125.03
14	A	804	CLA	C4-C3-C5	3.30	120.96	115.23
14	G	820	CLA	O2A-CGA-CBA	3.30	121.90	111.83
14	B	831	CLA	O2A-CGA-O1A	-3.30	115.37	123.63
14	A	844	CLA	C4-C3-C5	3.30	120.96	115.23
14	G	810	CLA	CHD-C1D-ND	-3.30	120.16	124.80
14	b	833	CLA	O2A-CGA-CBA	3.30	124.42	114.00
14	S	101	CLA	O2A-CGA-CBA	3.30	124.42	114.00
14	a	808	CLA	O2A-C1-C2	3.30	120.80	108.11
14	b	822	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
14	K	101	CLA	O2A-CGA-CBA	3.29	124.41	114.00
14	a	836	CLA	O2A-CGA-CBA	3.29	124.41	114.00
14	A	830	CLA	CMB-C2B-C3B	3.29	131.26	124.68
17	A	853	BCR	C30-C25-C24	3.29	124.58	115.65
14	G	818	CLA	C4D-C3D-CAD	3.29	111.68	108.11
14	b	821	CLA	CHD-C1D-ND	-3.29	120.17	124.80
14	Q	201	CLA	O2A-CGA-CBA	3.29	124.39	114.00
14	A	843	CLA	C1-O2A-CGA	3.29	124.61	116.65
14	b	810	CLA	CAA-C2A-C3A	-3.29	104.11	113.00
14	H	801	CLA	OBD-CAD-C3D	-3.29	120.73	128.42
14	a	841	CLA	O2A-CGA-CBA	3.29	124.38	114.00
14	B	820	CLA	O2A-CGA-CBA	3.28	124.38	114.00
14	B	828	CLA	C1-C2-C3	-3.28	120.82	126.20
14	H	803	CLA	C4C-C3C-C2C	-3.28	102.11	106.89
14	H	829	CLA	C4D-C3D-CAD	3.28	111.67	108.11
17	l	201	BCR	C1-C6-C5	-3.28	118.15	122.64
17	G	853	BCR	C40-C30-C25	3.28	115.39	110.24
14	A	815	CLA	CHD-C1D-ND	-3.28	120.19	124.80
14	b	801	CLA	O2A-C1-C2	3.28	120.73	108.11
14	a	809	CLA	C1-C2-C3	-3.28	120.82	126.20
14	B	822	CLA	CMB-C2B-C3B	3.28	131.24	124.68
14	M	1601	CLA	O2A-CGA-CBA	3.28	124.36	114.00
14	B	835	CLA	O2A-CGA-CBA	3.28	124.36	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	845	CLA	O2A-CGA-CBA	3.28	124.36	114.00
13	A	801	CL0	O2A-C1-C2	3.28	120.72	108.11
14	K	102	CLA	CMA-C3A-C4A	3.27	120.58	111.77
14	T	1401	CLA	O2A-CGA-CBA	3.27	124.35	114.00
14	b	805	CLA	C1-C2-C3	-3.27	120.83	126.20
14	l	206	CLA	CBC-CAC-C3C	-3.27	103.55	112.42
14	H	838	CLA	O2A-CGA-CBA	3.27	124.34	114.00
14	a	820	CLA	C4D-C3D-CAD	3.27	111.66	108.11
14	G	821	CLA	OBD-CAD-C3D	-3.27	120.77	128.42
14	H	826	CLA	O1D-CGD-CBD	-3.27	118.06	124.52
14	b	809	CLA	C3C-C4C-NC	3.27	114.62	110.43
14	G	803	CLA	C1-C2-C3	-3.27	120.84	126.20
17	a	847	BCR	C37-C22-C21	-3.27	117.52	122.82
14	b	804	CLA	C4C-C3C-C2C	-3.27	102.13	106.89
14	S	102	CLA	CMB-C2B-C3B	3.27	131.22	124.68
14	G	825	CLA	C1-C2-C3	-3.27	120.84	126.20
17	H	849	BCR	C7-C8-C9	-3.27	121.40	126.23
14	A	828	CLA	CMB-C2B-C3B	3.27	131.22	124.68
14	b	817	CLA	CMB-C2B-C3B	3.27	131.22	124.68
14	H	817	CLA	C4-C3-C5	3.27	120.90	115.23
14	G	829	CLA	CMB-C2B-C3B	3.27	131.21	124.68
14	A	826	CLA	C1-C2-C3	-3.27	120.85	126.20
14	b	806	CLA	CMB-C2B-C3B	3.27	131.21	124.68
14	b	834	CLA	O2A-CGA-CBA	3.26	124.31	114.00
17	G	849	BCR	C24-C23-C22	-3.26	121.41	126.23
14	b	810	CLA	O2A-CGA-CBA	3.26	124.31	114.00
17	A	849	BCR	C24-C23-C22	-3.26	121.41	126.23
14	X	1701	CLA	O2A-CGA-CBA	3.26	124.31	114.00
14	a	817	CLA	C4D-C3D-CAD	3.26	111.65	108.11
14	a	827	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
14	b	832	CLA	O2A-C1-C2	3.26	120.66	108.11
14	H	809	CLA	O2A-C1-C2	3.26	120.66	108.11
14	A	823	CLA	O2A-CGA-CBA	3.26	124.30	114.00
14	B	840	CLA	C6-C5-C3	-3.26	105.53	113.47
14	H	809	CLA	CAA-C2A-C3A	-3.26	104.19	113.00
14	B	816	CLA	CHD-C1D-ND	-3.26	120.22	124.80
14	G	845	CLA	CMA-C3A-C4A	3.26	120.53	111.77
14	H	817	CLA	O2A-C1-C2	3.26	120.65	108.11
14	A	838	CLA	CHD-C1D-ND	-3.26	120.22	124.80
14	a	830	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
14	G	841	CLA	CHD-C1D-ND	-3.26	120.22	124.80
14	G	832	CLA	C1-C2-C3	-3.26	121.49	126.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	834	CLA	CMA-C3A-C4A	3.26	120.53	111.77
17	B	848	BCR	C19-C18-C17	3.26	124.13	119.01
14	G	811	CLA	O2A-CGA-CBA	3.26	124.29	114.00
14	H	815	CLA	O2A-CGA-CBA	3.26	124.29	114.00
14	A	804	CLA	CHD-C1D-ND	-3.26	120.22	124.80
14	B	813	CLA	CHD-C1D-ND	-3.26	120.22	124.80
14	B	827	CLA	C4A-NA-C1A	3.25	108.16	106.68
14	l	207	CLA	C1-C2-C3	-3.25	120.86	126.20
14	B	825	CLA	C3C-C4C-NC	3.25	114.60	110.43
14	a	835	CLA	O2A-CGA-CBA	3.25	124.28	114.00
14	A	840	CLA	CMC-C2C-C1C	3.25	130.12	125.03
14	L	206	CLA	O2A-CGA-CBA	3.25	121.75	111.83
17	a	847	BCR	C30-C25-C26	-3.25	118.19	122.64
14	A	802	CLA	CHD-C1D-ND	-3.25	120.22	124.80
14	V	1601	CLA	O2A-CGA-CBA	3.25	124.28	114.00
14	A	826	CLA	CMB-C2B-C3B	3.25	131.18	124.68
14	A	816	CLA	O2A-CGA-CBA	3.25	124.28	114.00
17	b	846	BCR	C3-C4-C5	-3.25	108.26	114.06
14	G	838	CLA	CHD-C1D-ND	-3.25	120.23	124.80
14	a	822	CLA	CMB-C2B-C3B	3.25	131.18	124.68
17	G	848	BCR	C37-C22-C21	-3.25	117.55	122.82
14	a	855	CLA	OBD-CAD-C3D	-3.25	120.82	128.42
17	I	102	BCR	C19-C18-C17	3.25	124.12	119.01
17	m	1602	BCR	C33-C5-C6	-3.25	120.94	124.48
14	B	815	CLA	O2A-CGA-CBA	3.25	124.26	114.00
14	G	829	CLA	C1-O2A-CGA	3.25	124.51	116.65
17	V	1602	BCR	C7-C8-C9	-3.25	121.43	126.23
14	H	814	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
14	B	802	CLA	O2A-C1-C2	3.24	120.59	108.11
14	A	808	CLA	O2A-CGA-CBA	3.24	124.24	114.00
14	A	836	CLA	O2A-CGA-CBA	3.24	124.24	114.00
14	x	1701	CLA	O2A-CGA-CBA	3.24	124.24	114.00
14	H	808	CLA	C4D-C3D-CAD	3.24	111.63	108.11
14	j	101	CLA	CAA-C2A-C3A	-3.24	104.24	113.00
14	a	822	CLA	CHD-C1D-ND	-3.24	120.24	124.80
14	H	834	CLA	CHD-C1D-ND	-3.24	120.24	124.80
14	A	828	CLA	CHD-C4C-C3C	-3.24	120.05	124.77
14	B	828	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
14	a	843	CLA	O2A-CGA-CBA	3.24	124.23	114.00
14	B	837	CLA	CMB-C2B-C3B	3.24	131.15	124.68
14	G	815	CLA	O2A-CGA-CBA	3.24	124.22	114.00
14	m	1601	CLA	CMA-C3A-C4A	3.23	120.47	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	846	BCR	C33-C5-C6	-3.23	120.95	124.48
14	A	844	CLA	CHD-C1D-ND	-3.23	120.25	124.80
14	B	811	CLA	O2A-CGA-CBA	3.23	124.22	114.00
14	a	819	CLA	CBA-CAA-C2A	3.23	123.41	113.79
14	H	820	CLA	CMA-C3A-C4A	3.23	120.46	111.77
14	G	805	CLA	C4D-C3D-CAD	3.23	111.61	108.11
14	A	839	CLA	C4D-C3D-CAD	3.23	111.61	108.11
14	b	835	CLA	O2A-CGA-CBA	3.23	124.20	114.00
14	G	811	CLA	CHD-C1D-ND	-3.23	120.26	124.80
14	a	815	CLA	CHD-C1D-ND	-3.23	120.26	124.80
14	V	1601	CLA	CMA-C3A-C4A	3.23	120.45	111.77
14	B	819	CLA	CMC-C2C-C1C	3.23	130.08	125.03
14	j	101	CLA	O2A-CGA-CBA	3.23	124.19	114.00
14	A	809	CLA	O2A-C1-C2	3.23	120.52	108.11
14	B	822	CLA	O2A-CGA-CBA	3.22	124.18	114.00
14	A	844	CLA	CMA-C3A-C4A	3.22	120.43	111.77
14	B	834	CLA	CHD-C1D-ND	-3.22	120.27	124.80
17	a	852	BCR	C24-C25-C26	-3.22	114.13	121.56
14	S	102	CLA	CMA-C3A-C4A	3.22	120.43	111.77
14	b	824	CLA	O2A-CGA-CBA	3.22	124.18	114.00
14	G	839	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
14	A	845	CLA	O2A-CGA-CBA	3.22	124.18	114.00
14	b	814	CLA	O2A-CGA-CBA	3.22	124.17	114.00
14	B	839	CLA	O2A-CGA-CBA	3.22	121.65	111.83
14	G	835	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
14	B	805	CLA	C1-C2-C3	-3.22	120.92	126.20
14	b	831	CLA	O2A-CGA-O1A	-3.22	115.58	123.63
14	T	1401	CLA	CHD-C1D-ND	-3.22	120.27	124.80
14	b	839	CLA	CMB-C2B-C3B	3.22	131.11	124.68
17	A	849	BCR	C7-C8-C9	-3.22	121.48	126.23
14	H	812	CLA	CMB-C2B-C3B	3.22	131.11	124.68
14	K	102	CLA	O2A-CGA-CBA	3.22	124.16	114.00
17	G	853	BCR	C3-C4-C5	-3.22	108.32	114.06
14	G	816	CLA	O2A-CGA-CBA	3.22	124.16	114.00
14	A	819	CLA	C4D-C3D-CAD	3.22	111.60	108.11
14	H	839	CLA	C4D-C3D-CAD	3.22	111.60	108.11
14	a	811	CLA	O2A-C1-C2	3.21	120.48	108.11
14	B	832	CLA	CHD-C1D-ND	-3.21	120.28	124.80
17	G	849	BCR	C38-C26-C25	-3.21	120.98	124.48
14	a	802	CLA	O2A-C1-C2	3.21	120.47	108.11
14	H	824	CLA	CMB-C2B-C3B	3.21	131.10	124.68
18	A	855	LHG	O7-C7-C8	3.21	118.43	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	838	CLA	O2A-CGA-CBA	3.21	124.15	114.00
14	m	1601	CLA	O2A-CGA-CBA	3.21	124.15	114.00
14	B	811	CLA	CHD-C1D-ND	-3.21	120.28	124.80
17	J	103	BCR	C3-C4-C5	-3.21	108.33	114.06
14	A	835	CLA	C1-C2-C3	-3.21	120.94	126.20
14	H	827	CLA	C4D-C3D-CAD	3.21	111.59	108.11
14	A	826	CLA	C4D-C3D-CAD	3.21	111.59	108.11
14	A	811	CLA	CED-O2D-CGD	3.21	123.19	115.92
14	H	816	CLA	CMC-C2C-C1C	3.21	130.05	125.03
14	B	829	CLA	O2A-CGA-CBA	3.21	124.14	114.00
14	H	829	CLA	O2A-CGA-CBA	3.21	124.13	114.00
14	a	821	CLA	C4A-NA-C1A	3.21	108.14	106.68
17	A	850	BCR	C38-C26-C25	-3.21	120.98	124.48
14	G	828	CLA	CHD-C4C-C3C	-3.21	120.10	124.77
17	R	103	BCR	C33-C5-C6	-3.21	120.99	124.48
14	b	828	CLA	C1-C2-C3	-3.21	120.94	126.20
14	A	828	CLA	O2A-C1-C2	3.21	120.44	108.11
14	a	827	CLA	C4-C3-C5	3.20	120.79	115.23
14	i	101	CLA	CMC-C2C-C1C	3.20	130.04	125.03
14	H	820	CLA	O2A-CGA-CBA	3.20	124.12	114.00
14	G	831	CLA	CAA-C2A-C3A	-3.20	104.34	113.00
14	a	815	CLA	O2A-CGA-CBA	3.20	124.12	114.00
14	A	813	CLA	CHD-C1D-ND	-3.20	120.30	124.80
17	Q	204	BCR	C33-C5-C6	-3.20	120.99	124.48
14	B	833	CLA	CMB-C2B-C3B	3.20	131.08	124.68
14	H	818	CLA	O2A-C1-C2	3.20	120.42	108.11
14	B	829	CLA	CMB-C2B-C1B	3.20	133.14	128.46
14	a	814	CLA	CMA-C3A-C4A	3.20	120.37	111.77
14	a	844	CLA	C3C-C4C-NC	3.20	114.53	110.43
14	A	839	CLA	CHD-C1D-ND	-3.20	120.30	124.80
14	H	826	CLA	CHD-C1D-ND	-3.20	120.30	124.80
14	a	841	CLA	CHD-C1D-ND	-3.20	120.30	124.80
14	b	839	CLA	C1-C2-C3	-3.20	120.96	126.20
17	B	844	BCR	C38-C26-C25	-3.20	121.00	124.48
14	B	826	CLA	O2A-C1-C2	3.20	120.41	108.11
14	a	827	CLA	CMB-C2B-C3B	3.20	131.07	124.68
14	A	815	CLA	O2A-CGA-CBA	3.20	124.10	114.00
14	G	837	CLA	O2A-CGA-CBA	3.20	124.09	114.00
14	A	806	CLA	CMC-C2C-C1C	3.19	130.03	125.03
14	G	832	CLA	CHD-C1D-ND	-3.19	120.31	124.80
14	B	808	CLA	CAA-C2A-C3A	-3.19	104.37	113.00
17	H	843	BCR	C38-C26-C25	-3.19	121.00	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	W	1701	CLA	O2A-CGA-CBA	3.19	124.09	114.00
14	A	832	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
14	B	837	CLA	CMC-C2C-C1C	3.19	130.02	125.03
14	G	805	CLA	CMC-C2C-C1C	3.19	130.02	125.03
14	M	1601	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
14	l	206	CLA	CAA-C2A-C3A	-3.19	104.38	113.00
14	G	844	CLA	O2A-CGA-CBA	3.19	124.08	114.00
14	A	822	CLA	CAA-C2A-C3A	-3.19	104.38	113.00
14	A	831	CLA	CAA-C2A-C3A	-3.19	104.38	113.00
14	a	821	CLA	O2A-CGA-CBA	3.19	121.56	111.83
14	B	822	CLA	CHD-C1D-ND	-3.19	120.32	124.80
14	Q	201	CLA	CHD-C1D-ND	-3.19	120.32	124.80
14	G	829	CLA	O2A-CGA-CBA	3.19	121.55	111.83
14	H	835	CLA	O2A-CGA-CBA	3.19	124.07	114.00
14	B	807	CLA	O2A-CGA-CBA	3.19	121.55	111.83
14	G	824	CLA	O2A-CGA-CBA	3.19	124.07	114.00
14	G	820	CLA	CAA-C2A-C1A	-3.19	101.53	111.97
14	B	812	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
17	F	1302	BCR	C38-C26-C25	-3.18	121.01	124.48
14	J	101	CLA	O2A-CGA-CBA	3.18	124.06	114.00
14	b	836	CLA	C1-C2-C3	-3.18	120.98	126.20
14	B	818	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
14	B	838	CLA	O2A-CGA-CBA	3.18	124.06	114.00
14	G	822	CLA	CMB-C2B-C3B	3.18	131.04	124.68
14	H	828	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
14	B	809	CLA	CAA-C2A-C3A	-3.18	104.40	113.00
14	b	819	CLA	O2A-CGA-CBA	3.18	124.05	114.00
14	l	202	CLA	C1-O2A-CGA	3.18	124.35	116.65
17	Q	202	BCR	C35-C13-C12	3.18	122.94	118.09
14	H	828	CLA	C1-C2-C3	-3.18	120.99	126.20
14	B	834	CLA	O2A-CGA-CBA	3.18	124.04	114.00
14	b	828	CLA	C2D-C1D-ND	3.18	113.27	110.13
17	B	847	BCR	C28-C27-C26	-3.18	108.39	114.06
14	b	827	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
14	H	834	CLA	O2A-CGA-CBA	3.18	124.03	114.00
14	A	821	CLA	C1-C2-C3	-3.17	121.62	126.76
14	a	839	CLA	O2A-CGA-CBA	3.17	124.03	114.00
14	a	828	CLA	CHD-C1D-ND	-3.17	120.33	124.80
14	H	815	CLA	CMC-C2C-C1C	3.17	129.99	125.03
14	H	802	CLA	O2A-C1-C2	3.17	120.32	108.11
17	G	852	BCR	C38-C26-C25	-3.17	121.02	124.48
14	a	805	CLA	O2A-CGA-CBA	3.17	124.03	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	832	CLA	CAC-C3C-C4C	3.17	128.92	124.79
14	A	840	CLA	O2A-CGA-CBA	3.17	124.03	114.00
14	b	827	CLA	C1-C2-C3	-3.17	121.00	126.20
14	b	839	CLA	O2A-C1-C2	3.17	120.32	108.11
14	L	205	CLA	CMB-C2B-C3B	3.17	131.02	124.68
14	G	811	CLA	C4D-C3D-CAD	3.17	111.55	108.11
17	L	207	BCR	C15-C14-C13	-3.17	122.83	127.28
14	B	828	CLA	CHD-C1D-ND	-3.17	120.34	124.80
14	H	839	CLA	CHD-C1D-ND	-3.17	120.34	124.80
14	b	804	CLA	CHD-C1D-ND	-3.17	120.34	124.80
17	H	842	BCR	C36-C18-C17	-3.17	117.68	122.82
14	A	805	CLA	C1-C2-C3	-3.17	121.00	126.20
14	A	820	CLA	C1-C2-C3	-3.17	121.00	126.20
14	A	841	CLA	C1-C2-C3	-3.17	121.00	126.20
14	l	206	CLA	CMB-C2B-C3B	3.17	131.02	124.68
14	Q	203	CLA	CHD-C1D-ND	-3.17	120.34	124.80
14	B	821	CLA	CHD-C1D-ND	-3.17	120.34	124.80
17	F	1302	BCR	C28-C27-C26	-3.17	108.40	114.06
14	G	803	CLA	CMC-C2C-C1C	3.17	129.99	125.03
14	a	820	CLA	CHD-C1D-ND	-3.17	120.34	124.80
14	G	841	CLA	O2A-C1-C2	3.17	120.30	108.11
14	G	839	CLA	CHD-C1D-ND	-3.17	120.35	124.80
14	B	824	CLA	O2A-CGA-CBA	3.17	124.00	114.00
17	m	1602	BCR	C38-C26-C25	-3.17	121.03	124.48
14	a	843	CLA	OBD-CAD-CBD	-3.17	119.59	125.94
17	L	202	BCR	C3-C4-C5	-3.16	108.41	114.06
14	b	811	CLA	O2A-CGA-CBA	3.16	124.00	114.00
14	B	819	CLA	O2A-CGA-CBA	3.16	124.00	114.00
17	I	102	BCR	C33-C5-C6	-3.16	121.03	124.48
14	H	835	CLA	CMA-C3A-C4A	3.16	120.28	111.77
14	a	826	CLA	CAA-C2A-C1A	-3.16	101.61	111.97
14	a	841	CLA	CMC-C2C-C1C	3.16	129.98	125.03
14	A	815	CLA	CMA-C3A-C4A	3.16	120.27	111.77
14	A	831	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
14	B	808	CLA	C1D-ND-C4D	-3.16	104.09	106.31
14	H	819	CLA	CMA-C3A-C4A	3.16	120.27	111.77
14	a	829	CLA	C1D-ND-C4D	-3.16	104.09	106.31
14	a	803	CLA	CHD-C1D-ND	-3.16	120.35	124.80
14	b	839	CLA	C4D-C3D-CAD	3.16	111.54	108.11
14	a	808	CLA	O2A-CGA-CBA	3.16	121.47	111.83
14	G	836	CLA	O2A-CGA-CBA	3.16	123.98	114.00
14	a	820	CLA	O2D-CGD-O1D	-3.16	117.70	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	841	PQN	C11-C12-C13	-3.16	121.39	126.83
17	a	849	BCR	C3-C4-C5	-3.16	108.42	114.06
17	a	851	BCR	C38-C26-C25	-3.16	121.04	124.48
15	H	841	PQN	C11-C12-C13	-3.16	121.39	126.83
17	J	102	BCR	C38-C26-C25	-3.16	121.04	124.48
14	a	813	CLA	C1-C2-C3	-3.16	121.03	126.20
14	G	839	CLA	CMA-C3A-C4A	3.16	120.25	111.77
14	H	808	CLA	CAA-C2A-C3A	-3.16	104.47	113.00
14	b	803	CLA	O2A-C1-C2	3.16	120.25	108.11
14	H	827	CLA	CMA-C3A-C4A	3.15	120.25	111.77
14	A	806	CLA	O2A-CGA-CBA	3.15	123.96	114.00
14	B	810	CLA	O2A-CGA-CBA	3.15	123.96	114.00
14	b	828	CLA	C1D-ND-C4D	-3.15	104.10	106.31
14	A	842	CLA	CAA-C2A-C3A	-3.15	104.48	113.00
14	H	821	CLA	CHD-C1D-ND	-3.15	120.37	124.80
14	B	833	CLA	O2A-CGA-CBA	3.15	123.96	114.00
17	A	851	BCR	C38-C26-C27	3.15	120.31	113.60
14	A	830	CLA	CMA-C3A-C4A	3.15	120.24	111.77
14	B	813	CLA	C4D-C3D-CAD	3.15	111.53	108.11
14	B	839	CLA	C1-C2-C3	-3.15	121.04	126.20
15	G	846	PQN	C12-C11-C3	-3.15	104.33	112.08
14	b	829	CLA	O2A-CGA-CBA	3.15	123.95	114.00
14	A	828	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
14	A	810	CLA	CMA-C3A-C4A	3.15	120.23	111.77
14	H	819	CLA	O2A-CGA-CBA	3.15	123.94	114.00
14	G	817	CLA	O2A-CGA-CBA	3.15	123.94	114.00
14	b	826	CLA	CHD-C1D-ND	-3.15	120.38	124.80
14	G	820	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
14	A	803	CLA	CMC-C2C-C1C	3.15	129.95	125.03
17	F	1302	BCR	C34-C9-C10	-3.14	117.72	122.82
14	G	838	CLA	O2A-C1-C2	3.14	120.20	108.11
14	H	827	CLA	C1-C2-C3	-3.14	121.05	126.20
17	I	101	BCR	C38-C26-C25	-3.14	121.06	124.48
14	a	855	CLA	CMB-C2B-C3B	3.14	130.96	124.68
14	b	817	CLA	O2A-C1-C2	3.14	120.20	108.11
14	G	814	CLA	CHD-C1D-ND	-3.14	120.38	124.80
14	A	828	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
14	B	840	CLA	CHD-C1D-ND	-3.14	120.39	124.80
14	a	827	CLA	C3C-C4C-NC	3.14	114.45	110.43
14	H	814	CLA	O2A-CGA-CBA	3.14	123.92	114.00
14	a	816	CLA	O2A-CGA-CBA	3.14	123.92	114.00
14	b	830	CLA	C4D-C3D-CAD	3.14	111.51	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	838	CLA	CMA-C3A-C4A	3.14	120.21	111.77
14	X	1701	CLA	CHD-C1D-ND	-3.14	120.39	124.80
14	G	837	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
17	A	849	BCR	C38-C26-C27	3.14	120.28	113.60
14	G	820	CLA	CMA-C3A-C4A	3.14	120.20	111.77
14	G	828	CLA	OBD-CAD-C3D	-3.14	121.09	128.42
17	j	104	BCR	C33-C5-C4	3.13	120.28	113.60
14	a	825	CLA	C4D-C3D-CAD	3.13	111.51	108.11
14	a	838	CLA	CHD-C1D-ND	-3.13	120.39	124.80
17	B	850	BCR	C34-C9-C10	-3.13	117.74	122.82
14	b	820	CLA	O2A-CGA-CBA	3.13	123.89	114.00
14	G	804	CLA	C1-C2-C3	-3.13	121.07	126.20
14	H	811	CLA	CHD-C1D-ND	-3.13	120.40	124.80
14	b	815	CLA	O2A-CGA-CBA	3.13	123.89	114.00
17	f	201	BCR	C34-C9-C8	3.13	122.87	118.09
14	B	832	CLA	C4-C3-C5	3.13	120.66	115.23
14	H	803	CLA	CMB-C2B-C3B	3.13	130.94	124.68
14	B	839	CLA	CMB-C2B-C3B	3.13	130.93	124.68
14	H	802	CLA	CBC-CAC-C3C	-3.13	103.94	112.42
14	b	833	CLA	CMC-C2C-C1C	3.13	129.92	125.03
14	G	802	CLA	CHD-C1D-ND	-3.13	120.40	124.80
14	W	1701	CLA	CHD-C1D-ND	-3.13	120.40	124.80
14	a	809	CLA	C4D-C3D-CAD	3.13	111.50	108.11
17	b	843	BCR	C34-C9-C10	-3.13	117.75	122.82
14	b	806	CLA	O2A-C1-C2	3.13	120.14	108.11
14	B	817	CLA	O2A-C1-C2	3.12	120.13	108.11
14	G	814	CLA	CMB-C2B-C3B	3.12	130.93	124.68
17	G	852	BCR	C34-C9-C8	3.12	122.86	118.09
14	A	827	CLA	CMC-C2C-C1C	3.12	129.91	125.03
14	a	855	CLA	C3C-C4C-NC	3.12	114.42	110.43
14	H	818	CLA	C4D-C3D-CAD	3.12	111.49	108.11
17	J	103	BCR	C1-C6-C5	-3.12	118.38	122.64
14	B	803	CLA	CHD-C1D-ND	-3.12	120.42	124.80
14	A	817	CLA	O2A-CGA-CBA	3.12	123.84	114.00
14	b	831	CLA	CMA-C3A-C4A	3.12	120.15	111.77
14	b	805	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
14	B	819	CLA	CHD-C1D-ND	-3.11	120.42	124.80
17	A	849	BCR	C38-C26-C25	-3.11	121.09	124.48
14	H	802	CLA	O2A-CGA-CBA	3.11	121.33	111.83
14	b	815	CLA	CMC-C2C-C1C	3.11	129.90	125.03
14	A	837	CLA	O2A-CGA-CBA	3.11	123.83	114.00
14	a	807	CLA	CAA-C2A-C3A	-3.11	104.59	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	801	CL0	C1-C2-C3	-3.11	121.10	126.20
14	B	808	CLA	C2D-C1D-ND	3.11	113.20	110.13
14	H	805	CLA	CMC-C2C-C1C	3.11	129.89	125.03
14	a	834	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
14	B	801	CLA	OBD-CAD-C3D	-3.11	121.16	128.42
14	U	205	CLA	CMA-C3A-C4A	3.11	120.12	111.77
14	H	840	CLA	C1-O2A-CGA	3.11	124.17	116.65
14	b	808	CLA	CAA-C2A-C3A	-3.10	104.61	113.00
14	a	820	CLA	C1-C2-C3	-3.10	121.74	126.76
14	B	828	CLA	CMB-C2B-C3B	3.10	130.88	124.68
14	H	836	CLA	CHD-C1D-ND	-3.10	120.44	124.80
14	b	814	CLA	CHD-C1D-ND	-3.10	120.44	124.80
14	H	813	CLA	C1-C2-C3	-3.10	121.12	126.20
14	A	827	CLA	CMB-C2B-C3B	3.10	130.88	124.68
14	a	812	CLA	CMB-C2B-C3B	3.10	130.88	124.68
14	H	804	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
14	b	813	CLA	C4D-C3D-CAD	3.10	111.47	108.11
14	a	811	CLA	CMA-C3A-C4A	3.10	120.10	111.77
14	A	816	CLA	CHD-C1D-ND	-3.10	120.44	124.80
14	A	832	CLA	CHD-C1D-ND	-3.10	120.44	124.80
17	A	849	BCR	C12-C13-C14	-3.10	114.14	119.01
14	a	814	CLA	C4D-C3D-CAD	3.10	111.47	108.11
18	a	853	LHG	C5-O7-C7	-3.10	110.39	117.80
14	G	826	CLA	C1-O2A-CGA	3.10	124.14	116.65
17	A	850	BCR	C19-C18-C17	3.09	123.88	119.01
14	H	828	CLA	C1D-ND-C4D	-3.09	104.14	106.31
14	b	822	CLA	O2A-CGA-CBA	3.09	123.78	114.00
14	b	823	CLA	C3C-C4C-NC	3.09	114.39	110.43
14	b	819	CLA	CHD-C1D-ND	-3.09	120.45	124.80
14	A	805	CLA	C4D-C3D-CAD	3.09	111.46	108.11
14	a	804	CLA	C4D-C3D-CAD	3.09	111.46	108.11
17	H	849	BCR	C33-C5-C6	-3.09	121.11	124.48
14	a	812	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
14	G	821	CLA	CHD-C1D-ND	-3.09	120.45	124.80
14	U	201	CLA	CHD-C1D-ND	-3.09	120.45	124.80
14	a	824	CLA	O2D-CGD-CBD	3.09	116.63	111.23
14	B	814	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
14	H	828	CLA	C2D-C1D-ND	3.09	113.18	110.13
14	G	811	CLA	CMC-C2C-C1C	3.09	129.86	125.03
14	b	813	CLA	CHD-C1D-ND	-3.08	120.46	124.80
14	B	823	CLA	CMC-C2C-C1C	3.08	129.85	125.03
14	b	812	CLA	C1-C2-C3	-3.08	121.15	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	812	CLA	CMA-C3A-C4A	3.08	120.06	111.77
14	b	801	CLA	C1-O2A-CGA	3.08	124.11	116.65
14	a	838	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
14	B	814	CLA	O2A-CGA-CBA	3.08	123.73	114.00
14	A	843	CLA	CMA-C3A-C4A	3.08	120.05	111.77
14	b	829	CLA	CHD-C1D-ND	-3.08	120.47	124.80
14	A	824	CLA	O2A-CGA-CBA	3.08	123.73	114.00
14	G	815	CLA	CMB-C2B-C3B	3.08	130.84	124.68
17	J	102	BCR	C1-C6-C5	-3.08	118.43	122.64
14	J	101	CLA	C4D-C3D-CAD	3.08	111.45	108.11
14	a	838	CLA	C4D-C3D-CAD	3.08	111.45	108.11
14	a	843	CLA	CAC-C3C-C4C	3.08	128.79	124.79
17	a	848	BCR	C38-C26-C27	3.08	120.16	113.60
14	b	809	CLA	C4D-C3D-CAD	3.08	111.45	108.11
14	A	841	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
14	B	832	CLA	C1-O2A-CGA	3.08	124.09	116.65
14	B	839	CLA	C4D-C3D-CAD	3.08	111.45	108.11
14	B	826	CLA	CHD-C1D-ND	-3.07	120.48	124.80
14	a	831	CLA	CMB-C2B-C3B	3.07	130.82	124.68
14	a	832	CLA	C1-C2-C3	-3.07	121.17	126.20
17	b	842	BCR	C24-C23-C22	-3.07	121.69	126.23
14	b	802	CLA	CHD-C1D-ND	-3.07	120.48	124.80
17	H	846	BCR	C36-C18-C17	-3.07	117.84	122.82
14	H	817	CLA	CMB-C2B-C3B	3.07	130.81	124.68
14	A	810	CLA	CHD-C1D-ND	-3.07	120.48	124.80
14	A	837	CLA	CMB-C2B-C3B	3.07	130.81	124.68
14	H	813	CLA	CAA-C2A-C3A	-3.07	104.71	113.00
14	A	823	CLA	C3C-C4C-NC	3.07	114.36	110.43
14	b	831	CLA	CMC-C2C-C1C	3.07	129.83	125.03
14	b	806	CLA	C4D-C3D-CAD	3.07	111.44	108.11
14	k	1401	CLA	O2A-CGA-CBA	3.06	123.68	114.00
14	G	812	CLA	CMA-C3A-C4A	3.06	120.01	111.77
17	B	845	BCR	C24-C23-C22	-3.06	121.70	126.23
17	U	202	BCR	C33-C5-C4	3.06	120.13	113.60
14	G	807	CLA	CMB-C2B-C3B	3.06	130.81	124.68
14	B	802	CLA	CAA-C2A-C3A	-3.06	104.72	113.00
14	H	806	CLA	C4-C3-C5	3.06	120.54	115.23
14	a	834	CLA	C1-C2-C3	-3.06	121.18	126.20
14	b	825	CLA	OBD-CAD-C3D	-3.06	121.26	128.42
14	H	813	CLA	CMD-C2D-C3D	-3.06	120.67	127.69
14	b	805	CLA	C4D-C3D-CAD	3.06	111.43	108.11
14	A	821	CLA	CHD-C1D-ND	-3.06	120.50	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	803	CLA	CAA-C2A-C3A	-3.06	104.73	113.00
14	a	830	CLA	CAA-C2A-C3A	-3.06	104.73	113.00
14	a	822	CLA	C4D-C3D-CAD	3.06	111.43	108.11
14	B	808	CLA	C3D-C2D-C1D	-3.06	101.66	105.83
17	b	846	BCR	C8-C7-C6	-3.06	118.83	127.00
14	H	815	CLA	CMB-C2B-C3B	3.06	130.79	124.68
14	A	825	CLA	CMA-C3A-C4A	3.06	119.99	111.77
14	B	803	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
17	A	849	BCR	C35-C13-C12	3.06	122.76	118.09
14	b	825	CLA	C4D-C3D-CAD	3.06	111.42	108.11
14	G	814	CLA	O2A-C1-C2	3.06	119.86	108.11
14	a	826	CLA	CMC-C2C-C1C	3.06	129.81	125.03
17	H	844	BCR	C38-C26-C25	-3.05	121.15	124.48
14	G	843	CLA	CHD-C1D-ND	-3.05	120.51	124.80
14	k	1401	CLA	C3D-C4D-ND	3.05	114.95	109.99
14	A	839	CLA	CMA-C3A-C4A	3.05	119.97	111.77
14	a	819	CLA	CMA-C3A-C4A	3.05	119.97	111.77
17	A	848	BCR	C33-C5-C6	-3.05	121.16	124.48
14	b	821	CLA	CMA-C3A-C4A	3.05	119.97	111.77
14	B	839	CLA	CMD-C2D-C3D	-3.05	120.70	127.69
17	l	208	BCR	C19-C18-C17	3.05	123.80	119.01
14	a	805	CLA	CMC-C2C-C1C	3.05	129.80	125.03
14	A	818	CLA	O2A-CGA-CBA	3.05	123.63	114.00
14	A	821	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
14	f	202	CLA	O2A-CGA-CBA	3.05	123.63	114.00
17	G	848	BCR	C19-C18-C17	3.04	123.80	119.01
14	b	814	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
17	B	850	BCR	C33-C5-C6	-3.04	121.16	124.48
14	a	817	CLA	O2A-CGA-CBA	3.04	123.61	114.00
14	B	829	CLA	C4D-C3D-CAD	3.04	111.41	108.11
14	H	814	CLA	CMA-C3A-C4A	3.04	119.95	111.77
14	Q	201	CLA	CAA-C2A-C3A	-3.04	104.78	113.00
14	l	207	CLA	O2A-CGA-CBA	3.04	121.10	111.83
14	B	837	CLA	O2A-C1-C2	3.04	119.80	108.11
14	B	825	CLA	C1-C2-C3	-3.04	121.22	126.20
14	H	809	CLA	CHD-C1D-ND	-3.04	120.53	124.80
14	b	828	CLA	O2A-C1-C2	3.04	119.80	108.11
14	a	802	CLA	C6-C5-C3	-3.04	106.07	113.47
14	a	804	CLA	CMC-C2C-C1C	3.04	129.78	125.03
14	l	202	CLA	C6-C5-C3	-3.04	106.07	113.47
14	H	836	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
17	b	844	BCR	C15-C14-C13	-3.03	123.02	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	845	CLA	C3C-C4C-NC	3.03	114.32	110.43
14	H	837	CLA	O2A-C1-C2	3.03	119.78	108.11
17	H	849	BCR	C36-C18-C17	-3.03	117.90	122.82
14	H	822	CLA	CHD-C1D-ND	-3.03	120.54	124.80
14	b	801	CLA	CHD-C1D-ND	-3.03	120.54	124.80
14	H	805	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
17	a	848	BCR	C30-C25-C26	-3.03	118.50	122.64
14	a	837	CLA	CHD-C1D-ND	-3.03	120.54	124.80
17	B	845	BCR	C36-C18-C17	-3.03	117.91	122.82
14	G	828	CLA	O2A-C1-C2	3.03	119.77	108.11
14	a	810	CLA	CMB-C2B-C3B	3.03	130.74	124.68
14	G	806	CLA	CMC-C2C-C1C	3.03	129.76	125.03
17	l	201	BCR	C4-C5-C6	-3.03	118.61	122.70
14	H	825	CLA	OBD-CAD-C3D	-3.03	121.34	128.42
17	L	202	BCR	C37-C22-C23	3.03	122.71	118.09
14	b	809	CLA	O2A-C1-C2	3.03	119.76	108.11
14	b	803	CLA	C4D-C3D-CAD	3.03	111.39	108.11
14	a	840	CLA	C4D-C3D-CAD	3.02	111.39	108.11
13	G	801	CL0	O2A-C1-C2	3.02	119.75	108.11
14	H	828	CLA	CMB-C2B-C1B	-3.02	124.03	128.46
14	H	828	CLA	CHD-C1D-ND	-3.02	120.55	124.80
14	G	842	CLA	CMC-C2C-C1C	3.02	129.76	125.03
14	L	205	CLA	C3D-C4D-ND	3.02	114.90	109.99
14	l	206	CLA	CMC-C2C-C1C	3.02	129.75	125.03
14	A	843	CLA	CHD-C1D-ND	-3.02	120.55	124.80
14	B	821	CLA	CMC-C2C-C1C	3.02	129.75	125.03
14	B	818	CLA	O2A-C1-C2	3.02	119.72	108.11
17	B	845	BCR	C19-C18-C17	3.02	123.75	119.01
17	A	849	BCR	C27-C26-C25	-3.02	118.63	122.70
14	H	810	CLA	O2A-CGA-CBA	3.02	123.53	114.00
14	a	831	CLA	CHD-C1D-ND	-3.02	120.56	124.80
14	H	831	CLA	O2A-CGA-O1A	-3.01	116.09	123.63
17	f	201	BCR	C2-C1-C6	3.01	114.82	110.44
14	a	803	CLA	C1-C2-C3	-3.01	121.26	126.20
14	b	818	CLA	C1-C2-C3	-3.01	121.26	126.20
14	A	821	CLA	C4D-C3D-CAD	3.01	111.38	108.11
14	G	812	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
14	H	803	CLA	CHD-C1D-ND	-3.01	120.56	124.80
14	B	812	CLA	CHD-C1D-ND	-3.01	120.56	124.80
14	a	807	CLA	C3D-C4D-ND	3.01	114.88	109.99
14	a	822	CLA	CMC-C2C-C1C	3.01	129.74	125.03
14	b	835	CLA	CMC-C2C-C1C	3.01	129.74	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	1301	CLA	C3C-C4C-NC	3.01	114.29	110.43
14	B	820	CLA	CMC-C2C-C1C	3.01	129.74	125.03
14	A	833	CLA	CMA-C3A-C4A	3.01	119.86	111.77
14	G	814	CLA	C3C-C4C-NC	3.01	114.28	110.43
14	a	831	CLA	C4D-C3D-CAD	3.01	111.37	108.11
14	G	822	CLA	O2A-CGA-CBA	3.01	121.00	111.83
17	I	102	BCR	C15-C14-C13	-3.01	123.06	127.28
14	a	802	CLA	CMC-C2C-C1C	3.01	129.73	125.03
14	G	838	CLA	C4D-C3D-CAD	3.00	111.37	108.11
14	G	802	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	A	805	CLA	OBD-CAD-C3D	-3.00	121.40	128.42
14	A	823	CLA	CMC-C2C-C1C	3.00	129.73	125.03
14	a	844	CLA	CAA-C2A-C3A	-3.00	104.89	113.00
14	A	831	CLA	C1-C2-C3	-3.00	121.28	126.20
14	b	828	CLA	CHD-C1D-ND	-3.00	120.58	124.80
14	G	818	CLA	O2A-CGA-CBA	3.00	123.48	114.00
14	G	821	CLA	CMC-C2C-C1C	3.00	129.72	125.03
14	b	832	CLA	O1D-CGD-CBD	-3.00	118.60	124.52
17	L	207	BCR	C24-C23-C22	-3.00	121.80	126.23
17	j	103	BCR	C7-C8-C9	-3.00	121.80	126.23
14	H	825	CLA	C1-C2-C3	-3.00	121.28	126.20
14	B	827	CLA	C1-C2-C3	-3.00	121.28	126.20
14	b	837	CLA	CMD-C2D-C3D	-3.00	120.81	127.69
14	A	805	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
14	b	808	CLA	CHD-C1D-ND	-3.00	120.58	124.80
17	B	844	BCR	C15-C14-C13	-3.00	123.08	127.28
14	A	845	CLA	C3C-C4C-NC	3.00	114.27	110.43
14	b	802	CLA	C4-C3-C5	3.00	120.43	115.23
14	b	828	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
14	A	811	CLA	CMB-C2B-C3B	3.00	130.67	124.68
14	a	836	CLA	CMB-C2B-C3B	3.00	130.67	124.68
14	a	808	CLA	C4D-C3D-CAD	3.00	111.36	108.11
14	j	102	CLA	CMA-C3A-C4A	2.99	119.82	111.77
14	G	811	CLA	CMA-C3A-C2A	-2.99	102.41	113.98
14	Q	203	CLA	O2A-CGA-CBA	2.99	123.46	114.00
14	H	804	CLA	CMC-C2C-C1C	2.99	129.71	125.03
14	G	816	CLA	CHD-C1D-ND	-2.99	120.59	124.80
14	H	832	CLA	C1-C2-C3	-2.99	121.29	126.20
13	a	801	CL0	CMC-C2C-C1C	2.99	129.71	125.03
14	L	201	CLA	CHD-C1D-ND	-2.99	120.59	124.80
14	G	837	CLA	CMB-C2B-C3B	2.99	130.66	124.68
14	F	1301	CLA	CHD-C1D-ND	-2.99	120.59	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	831	CLA	CHD-C1D-ND	-2.99	120.59	124.80
14	b	808	CLA	C4D-C3D-CAD	2.99	111.35	108.11
14	M	1601	CLA	C4D-C3D-CAD	2.99	111.35	108.11
14	A	820	CLA	CBA-CAA-C2A	2.99	122.69	113.79
14	B	812	CLA	OBD-CAD-C3D	-2.99	121.43	128.42
14	a	823	CLA	C4D-C3D-CAD	2.99	111.35	108.11
14	b	840	CLA	C1-C2-C3	-2.99	121.30	126.20
14	G	805	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
17	j	103	BCR	C35-C13-C12	2.99	122.65	118.09
14	G	829	CLA	CHD-C1D-ND	-2.99	120.60	124.80
14	G	808	CLA	C4D-C3D-CAD	2.98	111.35	108.11
14	G	819	CLA	C4D-C3D-CAD	2.98	111.35	108.11
14	U	205	CLA	C3D-C4D-ND	2.98	114.84	109.99
14	A	819	CLA	CMD-C2D-C3D	-2.98	120.85	127.69
14	B	837	CLA	C3D-C4D-ND	2.98	114.84	109.99
13	A	801	CL0	CMC-C2C-C1C	2.98	129.69	125.03
14	M	1601	CLA	CHD-C1D-ND	-2.98	120.61	124.80
14	a	814	CLA	O1D-CGD-CBD	-2.98	118.64	124.52
17	a	848	BCR	C30-C25-C24	2.98	123.73	115.65
14	U	205	CLA	CAA-C2A-C3A	-2.98	104.95	113.00
14	H	808	CLA	CHD-C1D-ND	-2.98	120.61	124.80
14	B	832	CLA	C4D-C3D-CAD	2.98	111.34	108.11
14	G	810	CLA	C1-C2-C3	-2.98	121.32	126.20
14	A	836	CLA	CHD-C1D-ND	-2.98	120.61	124.80
17	B	846	BCR	C36-C18-C17	-2.98	117.99	122.82
14	A	807	CLA	C4-C3-C5	2.98	120.39	115.23
14	U	205	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
14	H	823	CLA	C1-O2A-CGA	2.98	123.85	116.65
14	i	101	CLA	C3D-C4D-ND	2.98	114.82	109.99
14	G	838	CLA	CMC-C2C-C1C	2.98	129.68	125.03
17	J	102	BCR	C33-C5-C4	2.97	119.94	113.60
14	B	812	CLA	CMC-C2C-C1C	2.97	129.68	125.03
14	a	817	CLA	CMB-C2B-C3B	2.97	130.62	124.68
14	a	840	CLA	CED-O2D-CGD	2.97	122.66	115.92
17	G	850	BCR	C38-C26-C25	-2.97	121.24	124.48
17	F	1302	BCR	C12-C13-C14	2.97	123.68	119.01
14	A	822	CLA	C3D-C4D-ND	2.97	114.81	109.99
14	a	828	CLA	C3C-C4C-NC	2.97	114.23	110.43
14	a	855	CLA	CMC-C2C-C1C	2.97	129.67	125.03
14	b	811	CLA	C3D-C4D-ND	2.97	114.81	109.99
14	A	845	CLA	CMC-C2C-C3C	2.97	134.18	126.15
14	G	813	CLA	CMB-C2B-C3B	2.97	130.61	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	818	CLA	C3D-C4D-ND	2.97	114.81	109.99
14	a	833	CLA	CMB-C2B-C3B	2.97	130.61	124.68
14	L	204	CLA	C4D-C3D-CAD	2.97	111.33	108.11
14	G	822	CLA	CAA-C2A-C3A	-2.97	104.99	113.00
14	a	827	CLA	CHD-C1D-ND	-2.96	120.63	124.80
14	A	841	CLA	CMC-C2C-C1C	2.96	129.66	125.03
17	B	846	BCR	C7-C8-C9	-2.96	121.85	126.23
14	b	821	CLA	C1-O2A-CGA	2.96	123.82	116.65
14	G	813	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
14	G	811	CLA	C3C-C4C-NC	2.96	114.22	110.43
14	l	205	CLA	C1-C2-C3	-2.96	121.35	126.20
14	G	828	CLA	C4D-C3D-CAD	2.96	111.32	108.11
14	G	803	CLA	C4A-NA-C1A	2.96	108.03	106.68
17	H	846	BCR	C19-C18-C17	2.96	123.66	119.01
14	l	202	CLA	CHD-C1D-ND	-2.96	120.64	124.80
14	m	1601	CLA	CHD-C1D-ND	-2.96	120.64	124.80
14	A	804	CLA	C4D-C3D-CAD	2.96	111.32	108.11
17	I	101	BCR	C35-C13-C12	2.96	122.61	118.09
17	L	207	BCR	C23-C22-C21	2.96	123.66	119.01
14	B	823	CLA	C3C-C4C-NC	2.96	114.22	110.43
14	G	833	CLA	CMA-C3A-C4A	2.96	119.72	111.77
14	K	102	CLA	C3D-C4D-ND	2.96	114.79	109.99
14	A	822	CLA	C6-C5-C3	-2.96	106.27	113.47
17	a	849	BCR	C38-C26-C25	-2.96	121.26	124.48
14	B	836	CLA	CHD-C1D-ND	-2.96	120.64	124.80
14	B	812	CLA	C3C-C4C-NC	2.96	114.22	110.43
14	G	802	CLA	CAA-CBA-CGA	-2.96	104.81	113.21
14	a	805	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
14	H	818	CLA	C1-C2-C3	-2.95	121.36	126.20
14	b	803	CLA	C4-C3-C5	2.95	120.36	115.23
14	B	834	CLA	C4D-C3D-CAD	2.95	111.31	108.11
14	A	839	CLA	O2A-C1-C2	2.95	119.47	108.11
14	H	834	CLA	CMA-C3A-C4A	2.95	119.71	111.77
14	H	819	CLA	CMC-C2C-C1C	2.95	129.65	125.03
14	a	825	CLA	CMA-C3A-C4A	2.95	119.71	111.77
14	b	811	CLA	C4D-C3D-CAD	2.95	111.31	108.11
14	a	815	CLA	CMA-C3A-C4A	2.95	119.71	111.77
17	b	846	BCR	C33-C5-C6	-2.95	121.26	124.48
14	b	814	CLA	CMA-C3A-C4A	2.95	119.71	111.77
14	H	839	CLA	O2A-C1-C2	2.95	119.47	108.11
14	B	826	CLA	CMC-C2C-C1C	2.95	129.65	125.03
14	b	807	CLA	CMC-C2C-C1C	2.95	129.65	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	851	BCR	C23-C24-C25	-2.95	119.12	127.00
17	J	103	BCR	C8-C7-C6	-2.95	119.12	127.00
14	b	824	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
14	H	838	CLA	C3D-C4D-ND	2.95	114.78	109.99
14	B	812	CLA	C1-C2-C3	-2.95	121.37	126.20
14	B	814	CLA	CHD-C1D-ND	-2.95	120.65	124.80
14	A	820	CLA	O2A-C1-C2	2.95	119.45	108.11
17	H	843	BCR	C34-C9-C10	-2.95	118.04	122.82
14	A	844	CLA	CAC-C3C-C4C	2.95	128.62	124.79
14	B	827	CLA	CMA-C3A-C4A	2.95	119.69	111.77
18	G	855	LHG	O8-C23-C24	2.95	120.09	111.15
14	A	812	CLA	CMD-C2D-C3D	-2.95	120.93	127.69
14	H	835	CLA	C3D-C4D-ND	2.95	114.78	109.99
14	f	202	CLA	CHD-C1D-ND	-2.95	120.66	124.80
14	G	834	CLA	CMB-C2B-C3B	2.94	130.57	124.68
14	H	817	CLA	CMA-C3A-C4A	2.94	119.69	111.77
14	G	803	CLA	C6-C5-C3	-2.94	106.30	113.47
14	a	828	CLA	C1-O2A-CGA	2.94	123.78	116.65
14	H	830	CLA	CMA-C3A-C4A	2.94	119.68	111.77
14	A	836	CLA	CMC-C2C-C1C	2.94	129.63	125.03
14	l	206	CLA	C3D-C4D-ND	2.94	114.77	109.99
14	A	814	CLA	CAA-C2A-C3A	-2.94	105.05	113.00
14	a	819	CLA	CAA-C2A-C3A	-2.94	105.05	113.00
14	W	1701	CLA	CMC-C2C-C1C	2.94	129.63	125.03
14	b	815	CLA	CMA-C3A-C4A	2.94	119.68	111.77
14	G	844	CLA	C4D-C3D-CAD	2.94	111.37	107.69
14	a	829	CLA	C3C-C4C-NC	2.94	114.20	110.43
14	H	811	CLA	C3D-C4D-ND	2.94	114.77	109.99
14	H	820	CLA	CMB-C2B-C3B	2.94	130.56	124.68
14	a	835	CLA	CHD-C1D-ND	-2.94	120.67	124.80
14	B	832	CLA	CMA-C3A-C4A	2.94	119.67	111.77
14	G	810	CLA	C4D-C3D-CAD	2.94	111.30	108.11
14	f	202	CLA	CMA-C3A-C4A	2.94	119.67	111.77
14	A	803	CLA	C4A-NA-C1A	2.93	108.02	106.68
14	l	207	CLA	O2A-C1-C2	2.93	119.40	108.11
14	A	814	CLA	C1-C2-C3	-2.93	121.39	126.20
17	B	843	BCR	C34-C9-C10	-2.93	118.06	122.82
17	B	845	BCR	C28-C27-C26	-2.93	108.83	114.06
14	a	818	CLA	CMD-C2D-C3D	-2.93	120.97	127.69
14	B	839	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
14	A	827	CLA	CBC-CAC-C3C	-2.93	104.47	112.42
14	A	802	CLA	CMB-C2B-C1B	-2.93	124.16	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	809	CLA	C4D-C3D-CAD	2.93	111.29	108.11
14	H	813	CLA	CHD-C1D-ND	-2.93	120.68	124.80
14	B	820	CLA	CMA-C3A-C4A	2.93	119.65	111.77
14	A	809	CLA	C3D-C4D-ND	2.93	114.75	109.99
14	A	809	CLA	C4D-C3D-CAD	2.93	111.29	108.11
17	A	850	BCR	C3-C4-C5	-2.93	108.83	114.06
14	a	803	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
14	b	806	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
14	B	821	CLA	O2A-C1-C2	2.93	119.37	108.11
14	G	825	CLA	CMA-C3A-C4A	2.93	119.64	111.77
14	A	829	CLA	CHD-C1D-ND	-2.93	120.68	124.80
18	A	855	LHG	O8-C23-C24	2.93	120.03	111.15
14	b	819	CLA	C4D-C3D-CAD	2.93	111.28	108.11
14	a	813	CLA	CAC-C3C-C4C	2.93	128.60	124.79
14	A	839	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
14	a	837	CLA	C4D-C3D-CAD	2.92	111.28	108.11
14	H	807	CLA	C3D-C4D-ND	2.92	114.74	109.99
14	a	803	CLA	CMA-C3A-C4A	2.92	119.63	111.77
14	b	817	CLA	CMA-C3A-C4A	2.92	119.63	111.77
14	j	101	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
14	a	803	CLA	CMC-C2C-C1C	2.92	129.60	125.03
14	V	1601	CLA	CMD-C2D-C3D	-2.92	120.99	127.69
14	B	815	CLA	C4D-C3D-CAD	2.92	111.28	108.11
14	A	808	CLA	C3D-C4D-ND	2.92	114.73	109.99
14	l	206	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
14	B	806	CLA	C4-C3-C5	2.92	120.29	115.23
14	G	824	CLA	CMA-C3A-C4A	2.92	119.61	111.77
17	M	1602	BCR	C38-C26-C25	-2.92	121.30	124.48
17	J	102	BCR	C35-C13-C12	2.92	122.54	118.09
14	B	830	CLA	C4D-C3D-CAD	2.92	111.27	108.11
14	H	832	CLA	C4-C3-C5	2.92	120.29	115.23
14	B	835	CLA	CMA-C3A-C4A	2.92	119.61	111.77
18	a	854	LHG	O8-C23-C24	2.92	120.00	111.15
17	b	847	BCR	C15-C14-C13	-2.92	123.19	127.28
14	a	839	CLA	CMC-C2C-C1C	2.91	129.59	125.03
14	G	843	CLA	C4-C3-C5	2.91	120.29	115.23
14	H	836	CLA	C1-C2-C3	-2.91	121.42	126.20
17	A	849	BCR	C19-C18-C17	2.91	123.59	119.01
17	B	847	BCR	C12-C13-C14	-2.91	114.43	119.01
17	H	847	BCR	C36-C18-C17	-2.91	118.10	122.82
14	b	816	CLA	C4D-C3D-CAD	2.91	111.27	108.11
14	G	827	CLA	CMC-C2C-C1C	2.91	129.59	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	812	CLA	O2A-C1-C2	2.91	119.32	108.11
14	B	807	CLA	C3D-C4D-ND	2.91	114.72	109.99
14	G	814	CLA	CMA-C3A-C4A	2.91	119.60	111.77
14	b	802	CLA	CMC-C2C-C1C	2.91	129.58	125.03
17	H	845	BCR	C36-C18-C17	-2.91	118.10	122.82
14	G	824	CLA	CMD-C2D-C3D	-2.91	121.01	127.69
14	G	829	CLA	C3C-C4C-NC	2.91	114.16	110.43
14	b	812	CLA	C4-C3-C5	2.91	120.28	115.23
14	A	810	CLA	CMC-C2C-C1C	2.91	129.58	125.03
14	L	205	CLA	O2A-C1-C2	2.91	119.31	108.11
14	A	835	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
14	A	802	CLA	C1-O2A-CGA	2.91	123.69	116.65
17	l	203	BCR	C3-C4-C5	-2.91	108.87	114.06
14	G	845	CLA	C4D-C3D-CAD	2.91	111.27	108.11
14	A	816	CLA	CMA-C3A-C4A	2.91	119.59	111.77
14	G	832	CLA	CMC-C2C-C1C	2.91	129.58	125.03
14	H	839	CLA	C1-C2-C3	-2.91	121.43	126.20
14	A	826	CLA	CHD-C1D-ND	-2.91	120.71	124.80
14	H	820	CLA	CMC-C2C-C1C	2.91	129.58	125.03
14	a	823	CLA	C3C-C4C-NC	2.91	114.15	110.43
14	A	834	CLA	CMB-C2B-C3B	2.91	130.49	124.68
17	a	850	BCR	C38-C26-C27	2.91	119.79	113.60
14	A	810	CLA	CMB-C2B-C3B	2.91	130.49	124.68
14	H	832	CLA	C1-O2A-CGA	2.91	123.69	116.65
14	A	806	CLA	C3D-C4D-ND	2.91	114.71	109.99
17	l	201	BCR	C15-C14-C13	-2.90	123.20	127.28
14	a	824	CLA	C4D-C3D-CAD	2.90	111.26	108.11
14	b	809	CLA	OBD-CAD-C3D	-2.90	121.63	128.42
14	a	835	CLA	CAA-C2A-C3A	-2.90	105.16	113.00
14	L	201	CLA	C1-C2-C3	-2.90	121.44	126.20
14	G	817	CLA	C4D-C3D-CAD	2.90	111.26	108.11
14	G	842	CLA	C1-O2A-CGA	2.90	123.67	116.65
14	G	830	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
14	a	804	CLA	C1-C2-C3	-2.90	121.44	126.20
14	b	825	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
14	B	817	CLA	CMA-C3A-C4A	2.90	119.57	111.77
14	A	835	CLA	CMB-C2B-C3B	2.90	130.48	124.68
14	b	833	CLA	C3D-C4D-ND	2.90	114.70	109.99
14	B	805	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
14	B	803	CLA	CMB-C2B-C3B	2.90	130.47	124.68
14	H	828	CLA	O2A-C1-C2	2.90	119.26	108.11
14	A	825	CLA	C1-C2-C3	-2.90	121.45	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	821	CLA	C3D-C4D-ND	2.90	114.70	109.99
14	H	832	CLA	CMA-C3A-C4A	2.90	119.56	111.77
14	G	815	CLA	CMA-C3A-C4A	2.90	119.56	111.77
14	B	832	CLA	O2A-C1-C2	2.90	119.25	108.11
14	A	804	CLA	C3C-C4C-NC	2.89	114.14	110.43
14	A	832	CLA	C1-C2-C3	-2.89	122.08	126.76
14	B	834	CLA	C3C-C4C-NC	2.89	114.14	110.43
14	b	820	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
14	H	831	CLA	C3D-C4D-ND	2.89	114.69	109.99
14	H	837	CLA	C3D-C4D-ND	2.89	114.69	109.99
14	L	205	CLA	CAA-C2A-C3A	-2.89	105.18	113.00
14	B	808	CLA	CAC-C3C-C4C	2.89	128.55	124.79
14	k	1401	CLA	CMA-C3A-C4A	2.89	119.55	111.77
14	B	836	CLA	CMA-C3A-C4A	2.89	119.54	111.77
14	B	833	CLA	C3D-C4D-ND	2.89	114.69	109.99
14	a	827	CLA	CMA-C3A-C4A	2.89	119.54	111.77
14	A	807	CLA	CMB-C2B-C3B	2.89	130.46	124.68
14	B	818	CLA	CAA-C2A-C3A	-2.89	105.19	113.00
17	a	851	BCR	C38-C26-C27	2.89	119.76	113.60
14	A	809	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
14	B	816	CLA	C3C-C4C-NC	2.89	114.13	110.43
17	L	202	BCR	C35-C13-C12	2.89	122.50	118.09
17	b	845	BCR	C28-C27-C26	-2.89	108.91	114.06
14	b	818	CLA	CAA-C2A-C3A	-2.89	105.19	113.00
17	a	851	BCR	C34-C9-C8	2.89	122.50	118.09
14	H	803	CLA	CMA-C3A-C4A	2.89	119.53	111.77
14	a	833	CLA	C4D-C3D-CAD	2.89	111.24	108.11
14	a	802	CLA	OBD-CAD-C3D	-2.89	121.67	128.42
14	b	833	CLA	C4D-C3D-CAD	2.89	111.24	108.11
14	T	1401	CLA	CMB-C2B-C3B	2.89	130.45	124.68
17	b	849	BCR	C33-C5-C6	-2.89	121.34	124.48
14	A	808	CLA	CMC-C2C-C1C	2.88	129.54	125.03
14	A	803	CLA	C6-C5-C3	-2.88	106.44	113.47
14	G	822	CLA	C6-C5-C3	-2.88	106.44	113.47
14	U	204	CLA	C4D-C3D-CAD	2.88	111.24	108.11
14	a	818	CLA	C4D-C3D-CAD	2.88	111.24	108.11
14	a	840	CLA	C1-C2-C3	-2.88	121.47	126.20
17	a	847	BCR	C27-C26-C25	-2.88	118.81	122.70
14	a	808	CLA	C3D-C4D-ND	2.88	114.67	109.99
14	A	821	CLA	CMC-C2C-C1C	2.88	129.54	125.03
14	B	807	CLA	C1-O2A-CGA	2.88	123.62	116.65
17	U	202	BCR	C23-C22-C21	2.88	123.54	119.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	207	BCR	C36-C18-C17	-2.88	118.15	122.82
14	a	809	CLA	CMA-C3A-C4A	2.88	119.51	111.77
14	a	838	CLA	C6-C5-C3	-2.88	106.46	113.47
14	a	809	CLA	CHD-C1D-ND	-2.88	120.75	124.80
14	S	101	CLA	CMC-C2C-C1C	2.88	129.53	125.03
14	A	822	CLA	O2A-CGA-CBA	2.88	120.61	111.83
14	B	808	CLA	C3C-C4C-NC	2.88	114.12	110.43
14	a	825	CLA	C1-C2-C3	-2.88	121.48	126.20
14	G	823	CLA	CMC-C2C-C1C	2.88	129.53	125.03
14	L	205	CLA	C4-C3-C5	2.88	120.22	115.23
14	a	802	CLA	C4-C3-C5	2.88	120.22	115.23
14	U	205	CLA	C1-C2-C3	-2.88	121.48	126.20
14	S	101	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
14	B	831	CLA	C4D-C3D-CAD	2.88	111.23	108.11
14	B	816	CLA	C4D-C3D-CAD	2.87	111.23	108.11
14	b	819	CLA	CMA-C3A-C4A	2.87	119.49	111.77
17	G	850	BCR	C38-C26-C27	2.87	119.72	113.60
17	R	102	BCR	C33-C5-C6	-2.87	121.35	124.48
14	H	839	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
14	G	835	CLA	C1-C2-C3	-2.87	121.49	126.20
14	A	802	CLA	CMC-C2C-C1C	2.87	129.52	125.03
14	A	839	CLA	C1-C2-C3	-2.87	121.49	126.20
14	H	808	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
14	A	842	CLA	CMC-C2C-C1C	2.87	129.52	125.03
14	L	204	CLA	CED-O2D-CGD	2.87	122.42	115.92
17	U	202	BCR	C35-C13-C12	2.87	122.47	118.09
14	a	823	CLA	O2A-CGA-CBA	2.87	123.06	114.00
14	a	815	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
14	B	810	CLA	C3D-C4D-ND	2.87	114.65	109.99
14	T	1401	CLA	CMC-C2C-C1C	2.87	129.51	125.03
14	G	826	CLA	C4D-C3D-CAD	2.87	111.22	108.11
14	a	832	CLA	CAA-C2A-C3A	-2.87	105.25	113.00
14	H	807	CLA	O2A-C1-C2	2.87	119.14	108.11
14	H	835	CLA	CHD-C4C-NC	-2.87	119.79	124.23
14	b	811	CLA	CMC-C2C-C1C	2.87	129.51	125.03
17	Q	202	BCR	C3-C4-C5	-2.86	108.95	114.06
14	G	844	CLA	CAC-C3C-C4C	2.86	128.52	124.79
17	b	846	BCR	C33-C5-C4	2.86	119.70	113.60
14	b	802	CLA	C1-C2-C3	-2.86	121.50	126.20
14	H	808	CLA	CMC-C2C-C1C	2.86	129.51	125.03
14	b	825	CLA	C4-C3-C5	2.86	120.20	115.23
14	b	827	CLA	CMA-C3A-C4A	2.86	119.47	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	803	CLA	C4-C3-C5	2.86	120.20	115.23
14	B	825	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
14	H	802	CLA	CAA-CBA-CGA	-2.86	105.08	113.21
17	G	851	BCR	C38-C26-C25	-2.86	121.36	124.48
14	W	1701	CLA	C4D-C3D-CAD	2.86	111.21	108.11
17	a	847	BCR	C36-C18-C17	-2.86	118.18	122.82
14	A	828	CLA	C2C-C1C-NC	2.86	112.98	109.98
14	A	830	CLA	C1D-ND-C4D	-2.86	104.31	106.31
14	G	812	CLA	O2A-C1-C2	2.86	119.10	108.11
17	S	104	BCR	C34-C9-C8	2.86	122.45	118.09
14	G	837	CLA	CMA-C3A-C4A	2.86	119.45	111.77
13	G	801	CL0	CAA-C2A-C3A	-2.86	105.28	113.00
14	a	807	CLA	CMD-C2D-C3D	-2.86	121.14	127.69
14	b	830	CLA	CMA-C3A-C4A	2.85	119.45	111.77
14	A	820	CLA	O2A-CGA-CBA	2.85	120.54	111.83
14	b	803	CLA	CMC-C2C-C1C	2.85	129.49	125.03
14	a	824	CLA	CAC-C3C-C4C	2.85	128.50	124.79
19	H	848	LMG	O8-C28-C29	2.85	120.53	111.83
14	W	1701	CLA	CMA-C3A-C4A	2.85	119.44	111.77
15	b	841	PQN	C14-C13-C15	2.85	120.18	115.23
17	B	846	BCR	C4-C5-C6	-2.85	118.85	122.70
17	a	847	BCR	C19-C18-C17	2.85	123.49	119.01
14	B	814	CLA	C4D-C3D-CAD	2.85	111.20	108.11
14	A	814	CLA	CAC-C3C-C4C	2.85	128.50	124.79
14	B	806	CLA	C4D-C3D-CAD	2.85	111.20	108.11
14	H	839	CLA	CMB-C2B-C3B	2.85	130.38	124.68
14	a	826	CLA	CMA-C3A-C4A	2.85	119.43	111.77
14	K	101	CLA	C3D-C4D-ND	2.85	114.62	109.99
14	G	816	CLA	CAC-C3C-C4C	2.85	128.50	124.79
14	A	841	CLA	C4D-C3D-CAD	2.85	111.20	108.11
14	b	832	CLA	CMA-C3A-C4A	2.85	119.43	111.77
14	G	804	CLA	CAA-C2A-C3A	-2.85	105.30	113.00
17	j	103	BCR	C36-C18-C17	-2.85	118.20	122.82
17	G	851	BCR	C34-C9-C8	2.85	122.44	118.09
14	B	807	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
17	G	848	BCR	C24-C23-C22	-2.85	122.03	126.23
14	a	838	CLA	CAC-C3C-C4C	2.84	128.49	124.79
17	B	844	BCR	C34-C9-C10	-2.84	118.21	122.82
14	B	808	CLA	CMC-C2C-C1C	2.84	129.48	125.03
14	b	808	CLA	C1-C2-C3	-2.84	121.54	126.20
14	a	804	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
14	H	802	CLA	CAA-C2A-C3A	-2.84	105.31	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	815	CLA	C3D-C4D-ND	2.84	114.61	109.99
17	I	203	BCR	C23-C24-C25	-2.84	119.40	127.00
14	A	838	CLA	C4D-C3D-CAD	2.84	111.19	108.11
14	I	205	CLA	C4D-C3D-CAD	2.84	111.19	108.11
14	A	802	CLA	C1-C2-C3	-2.84	121.54	126.20
14	A	844	CLA	C3D-C4D-ND	2.84	114.61	109.99
14	b	836	CLA	CMC-C2C-C1C	2.84	129.47	125.03
14	B	813	CLA	C1-C2-C3	-2.84	121.54	126.20
14	L	205	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
14	H	822	CLA	CMB-C2B-C3B	2.84	130.36	124.68
14	B	817	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	L	207	BCR	C33-C5-C4	2.84	119.65	113.60
14	A	844	CLA	C1-C2-C3	-2.84	121.55	126.20
14	A	818	CLA	C3D-C4D-ND	2.84	114.60	109.99
14	b	815	CLA	C4D-C3D-CAD	2.84	111.19	108.11
14	U	204	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	I	203	BCR	C35-C13-C12	2.84	122.42	118.09
14	H	821	CLA	C3C-C4C-NC	2.84	114.06	110.43
14	G	840	CLA	C3D-C4D-ND	2.84	114.60	109.99
14	a	818	CLA	CMC-C2C-C1C	2.84	129.47	125.03
17	F	1302	BCR	C36-C18-C17	-2.84	118.22	122.82
14	a	841	CLA	CMA-C3A-C4A	2.84	119.39	111.77
14	b	836	CLA	CMA-C3A-C4A	2.84	119.39	111.77
14	H	822	CLA	C3C-C4C-NC	2.83	114.06	110.43
17	b	849	BCR	C34-C9-C10	-2.83	118.22	122.82
14	G	844	CLA	CMC-C2C-C1C	2.83	129.46	125.03
14	A	814	CLA	CMB-C2B-C3B	2.83	130.35	124.68
14	G	821	CLA	C1-C2-C3	-2.83	122.18	126.76
14	b	802	CLA	CAC-C3C-C4C	2.83	128.48	124.79
14	H	825	CLA	C4D-C3D-CAD	2.83	111.18	108.11
14	L	204	CLA	CMB-C2B-C3B	2.83	130.34	124.68
17	B	847	BCR	C35-C13-C12	2.83	122.41	118.09
14	V	1601	CLA	CHD-C1D-ND	-2.83	120.82	124.80
14	L	206	CLA	C4-C3-C5	2.83	120.14	115.23
17	V	1602	BCR	C28-C27-C26	-2.83	109.01	114.06
14	A	829	CLA	C4-C3-C5	2.83	120.14	115.23
14	A	834	CLA	CMC-C2C-C1C	2.83	129.45	125.03
14	B	807	CLA	C1-C2-C3	-2.83	121.56	126.20
14	b	837	CLA	C4-C3-C5	2.83	120.14	115.23
14	A	808	CLA	CMA-C3A-C4A	2.83	119.37	111.77
14	a	817	CLA	C3D-C4D-ND	2.83	114.58	109.99
17	G	849	BCR	C35-C13-C12	2.83	122.40	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	839	CLA	CMD-C2D-C3D	-2.83	121.21	127.69
14	a	825	CLA	C3C-C4C-NC	2.83	114.05	110.43
14	G	815	CLA	CMD-C2D-C3D	-2.82	121.21	127.69
14	B	802	CLA	C3C-C4C-NC	2.82	114.05	110.43
14	G	830	CLA	CAC-C3C-C4C	2.82	128.46	124.79
14	a	829	CLA	C4D-C3D-CAD	2.82	111.17	108.11
14	a	838	CLA	CMC-C2C-C1C	2.82	129.44	125.03
14	A	804	CLA	CMC-C2C-C1C	2.82	129.44	125.03
17	B	843	BCR	C27-C26-C25	-2.82	118.89	122.70
14	G	804	CLA	C4D-C3D-CAD	2.82	111.17	108.11
14	A	824	CLA	C3D-C4D-ND	2.82	114.57	109.99
14	B	819	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
14	A	821	CLA	CMA-C3A-C4A	2.82	119.34	111.77
14	G	819	CLA	C3D-C4D-ND	2.82	114.56	109.99
14	A	829	CLA	O1D-CGD-CBD	-2.82	118.96	124.52
14	H	821	CLA	CMC-C2C-C1C	2.82	129.43	125.03
14	B	829	CLA	CBC-CAC-C3C	-2.82	104.79	112.42
17	S	104	BCR	C3-C4-C5	-2.82	109.03	114.06
17	H	849	BCR	C34-C9-C10	-2.82	118.25	122.82
17	b	846	BCR	C15-C14-C13	-2.82	123.33	127.28
14	a	837	CLA	CMC-C2C-C1C	2.82	129.43	125.03
13	A	801	CL0	C3C-C4C-NC	2.81	114.04	110.43
14	H	805	CLA	C4D-C3D-CAD	2.81	111.16	108.11
14	G	808	CLA	CAC-C3C-C4C	2.81	128.45	124.79
14	G	825	CLA	CMC-C2C-C1C	2.81	129.43	125.03
14	b	819	CLA	CMC-C2C-C1C	2.81	129.43	125.03
14	A	815	CLA	C4D-C3D-CAD	2.81	111.16	108.11
17	M	1602	BCR	C34-C9-C10	-2.81	118.26	122.82
14	b	819	CLA	C3C-C4C-NC	2.81	114.03	110.43
14	G	829	CLA	CAC-C3C-C4C	2.81	128.45	124.79
14	H	829	CLA	CBC-CAC-C3C	-2.81	104.80	112.42
14	G	803	CLA	CAC-C3C-C4C	2.81	128.45	124.79
14	G	818	CLA	CMD-C2D-C3D	-2.81	121.24	127.69
14	G	808	CLA	CMC-C2C-C1C	2.81	129.43	125.03
14	b	817	CLA	CMC-C2C-C1C	2.81	129.43	125.03
14	G	839	CLA	C6-C5-C3	-2.81	106.62	113.47
14	B	802	CLA	CHD-C1D-ND	-2.81	120.85	124.80
14	H	817	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
14	B	811	CLA	C3D-C4D-ND	2.81	114.55	109.99
14	G	841	CLA	CED-O2D-CGD	2.81	122.29	115.92
14	b	835	CLA	CMA-C3A-C4A	2.81	119.32	111.77
17	U	202	BCR	C3-C4-C5	-2.81	109.05	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	837	CLA	C3D-C4D-ND	2.81	114.55	109.99
14	A	802	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
14	G	843	CLA	CMA-C3A-C4A	2.81	119.32	111.77
14	H	804	CLA	C4D-C3D-CAD	2.81	111.15	108.11
14	M	1601	CLA	C3C-C4C-NC	2.81	114.03	110.43
14	b	803	CLA	C3C-C4C-NC	2.81	114.03	110.43
14	a	807	CLA	CMA-C3A-C4A	2.81	119.31	111.77
14	G	822	CLA	C3D-C4D-ND	2.80	114.55	109.99
14	H	813	CLA	C3D-C4D-ND	2.80	114.55	109.99
14	L	201	CLA	CMC-C2C-C1C	2.80	129.42	125.03
17	b	846	BCR	C34-C9-C8	2.80	122.37	118.09
14	b	807	CLA	C4D-C3D-CAD	2.80	111.15	108.11
14	H	839	CLA	C3D-C4D-ND	2.80	114.54	109.99
14	m	1601	CLA	CED-O2D-CGD	2.80	122.27	115.92
14	U	206	CLA	C3D-C4D-ND	2.80	114.54	109.99
14	B	822	CLA	C3C-C4C-NC	2.80	114.02	110.43
17	a	849	BCR	C38-C26-C27	2.80	119.57	113.60
14	F	1301	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
14	l	207	CLA	C3D-C4D-ND	2.80	114.54	109.99
14	b	817	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
14	A	825	CLA	C4D-C3D-CAD	2.80	111.15	108.11
14	H	821	CLA	O2A-C1-C2	2.80	118.88	108.11
14	a	842	CLA	CMA-C3A-C4A	2.80	119.30	111.77
14	B	804	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
14	b	807	CLA	C3D-C4D-ND	2.80	114.54	109.99
17	f	203	BCR	C19-C18-C17	2.80	123.41	119.01
14	H	825	CLA	CMA-C3A-C4A	2.80	119.30	111.77
14	a	825	CLA	CAC-C3C-C4C	2.80	128.43	124.79
14	W	1701	CLA	C3C-C4C-NC	2.80	114.01	110.43
14	A	804	CLA	CMB-C2B-C3B	2.80	130.27	124.68
14	H	837	CLA	CMC-C2C-C1C	2.80	129.40	125.03
14	G	844	CLA	C3D-C4D-ND	2.80	114.53	109.99
14	G	803	CLA	OBD-CAD-C3D	-2.80	121.88	128.42
14	H	827	CLA	C3C-C4C-NC	2.80	114.01	110.43
14	f	202	CLA	C3C-C4C-NC	2.80	114.01	110.43
14	a	808	CLA	C4-C3-C5	2.80	120.08	115.23
14	A	843	CLA	C4D-C3D-CAD	2.79	111.14	108.11
17	Q	204	BCR	C38-C26-C27	2.79	119.55	113.60
14	B	803	CLA	C1C-C2C-C3C	-2.79	104.04	106.98
14	a	819	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
14	j	101	CLA	C4D-C3D-CAD	2.79	111.14	108.11
17	a	850	BCR	C34-C9-C8	2.79	122.36	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	828	CLA	C4-C3-C5	2.79	120.08	115.23
14	H	836	CLA	CMA-C3A-C4A	2.79	119.28	111.77
14	H	822	CLA	C3D-C4D-ND	2.79	114.53	109.99
17	F	1302	BCR	C35-C13-C14	-2.79	118.29	122.82
14	H	810	CLA	C3D-C4D-ND	2.79	114.52	109.99
14	H	809	CLA	C1-C2-C3	-2.79	121.62	126.20
14	G	826	CLA	C4-C3-C5	2.79	120.07	115.23
14	H	830	CLA	C4D-C3D-CAD	2.79	111.14	108.11
14	A	820	CLA	CAA-C2A-C1A	-2.79	102.84	111.97
14	G	827	CLA	CAA-C2A-C1A	-2.79	102.84	111.97
14	a	833	CLA	CMC-C2C-C1C	2.79	129.39	125.03
14	G	834	CLA	C4D-C3D-CAD	2.79	111.13	108.11
14	l	205	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
14	B	823	CLA	C1-C2-C3	-2.79	122.25	126.76
17	H	849	BCR	C32-C1-C6	-2.79	105.87	110.24
14	A	841	CLA	CED-O2D-CGD	2.79	122.24	115.92
15	H	841	PQN	C16-C15-C13	-2.79	106.68	113.47
14	A	832	CLA	CMB-C2B-C3B	2.79	130.25	124.68
14	G	831	CLA	C4-C3-C5	2.79	120.06	115.23
14	G	833	CLA	CAA-C2A-C3A	-2.79	105.47	113.00
17	B	844	BCR	C35-C13-C12	2.79	122.34	118.09
14	U	206	CLA	C1-C2-C3	-2.79	121.63	126.20
17	l	208	BCR	C7-C8-C9	-2.78	122.11	126.23
17	A	849	BCR	C30-C25-C26	-2.78	118.83	122.64
14	A	842	CLA	C3D-C4D-ND	2.78	114.51	109.99
14	X	1701	CLA	C3C-C4C-NC	2.78	114.00	110.43
13	a	801	CL0	O2A-C1-C2	2.78	118.82	108.11
17	B	846	BCR	C34-C9-C8	2.78	122.34	118.09
14	L	206	CLA	CMC-C2C-C1C	2.78	129.38	125.03
14	a	831	CLA	C3C-C4C-NC	2.78	114.00	110.43
17	l	203	BCR	C33-C5-C6	-2.78	121.45	124.48
14	G	809	CLA	CMA-C3A-C4A	2.78	119.25	111.77
14	A	843	CLA	CMC-C2C-C1C	2.78	129.38	125.03
14	b	840	CLA	C1-O2A-CGA	2.78	123.38	116.65
17	J	102	BCR	C12-C13-C14	-2.78	114.63	119.01
14	A	812	CLA	CAC-C3C-C4C	2.78	128.41	124.79
14	A	811	CLA	C4D-C3D-CAD	2.78	111.13	108.11
14	G	832	CLA	C4D-C3D-CAD	2.78	111.13	108.11
14	A	814	CLA	C3C-C4C-NC	2.78	113.99	110.43
17	a	850	BCR	C15-C14-C13	-2.78	123.38	127.28
17	R	102	BCR	C37-C22-C23	2.78	122.33	118.09
14	a	840	CLA	CMC-C2C-C1C	2.78	129.38	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	833	CLA	C3D-C4D-ND	2.78	114.50	109.99
14	B	826	CLA	C3C-C4C-NC	2.78	113.99	110.43
14	H	801	CLA	CHD-C1D-ND	-2.78	120.89	124.80
14	A	812	CLA	C4D-C3D-CAD	2.78	111.12	108.11
14	H	834	CLA	CMC-C2C-C1C	2.78	129.37	125.03
14	M	1601	CLA	CMC-C2C-C1C	2.78	129.37	125.03
14	b	840	CLA	CMC-C2C-C3C	2.78	133.66	126.15
14	a	803	CLA	C3C-C4C-NC	2.78	113.98	110.43
14	H	806	CLA	C4D-C3D-CAD	2.78	111.12	108.11
14	a	829	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
14	A	844	CLA	CMC-C2C-C1C	2.77	129.37	125.03
14	U	201	CLA	CMC-C2C-C1C	2.77	129.37	125.03
14	a	820	CLA	CMA-C3A-C4A	2.77	119.23	111.77
14	b	827	CLA	CHD-C1D-ND	-2.77	120.90	124.80
13	a	801	CL0	C3C-C4C-NC	2.77	113.98	110.43
14	b	837	CLA	CMA-C3A-C4A	2.77	119.23	111.77
14	G	814	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
14	a	843	CLA	C4D-C3D-CAD	2.77	111.16	107.69
14	H	811	CLA	CMC-C2C-C1C	2.77	129.37	125.03
17	R	103	BCR	C28-C27-C26	-2.77	109.11	114.06
17	l	203	BCR	C24-C23-C22	-2.77	122.14	126.23
14	b	836	CLA	CAC-C3C-C4C	2.77	128.39	124.79
14	H	809	CLA	CHC-C1C-C2C	-2.77	119.10	126.94
14	G	841	CLA	CMC-C2C-C1C	2.77	129.36	125.03
17	f	203	BCR	C38-C26-C25	-2.77	121.46	124.48
14	G	809	CLA	CMC-C2C-C1C	2.77	129.36	125.03
14	H	815	CLA	C4D-C3D-CAD	2.77	111.11	108.11
14	H	823	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
14	b	834	CLA	CMC-C2C-C3C	2.77	133.64	126.15
14	a	821	CLA	CAC-C3C-C4C	2.77	128.39	124.79
14	G	845	CLA	CAA-C2A-C3A	-2.77	105.52	113.00
14	b	815	CLA	C3D-C4D-ND	2.77	114.49	109.99
14	A	808	CLA	C4D-C3D-CAD	2.77	111.11	108.11
14	A	811	CLA	CMC-C2C-C1C	2.77	129.36	125.03
14	B	801	CLA	C4-C3-C5	2.77	120.03	115.23
14	G	808	CLA	C3D-C4D-ND	2.77	114.48	109.99
14	b	810	CLA	C3D-C4D-ND	2.77	114.48	109.99
17	b	847	BCR	C34-C9-C10	-2.77	118.33	122.82
14	B	811	CLA	C4D-C3D-CAD	2.77	111.11	108.11
14	b	813	CLA	CAA-C2A-C3A	-2.77	105.53	113.00
14	H	803	CLA	C3C-C4C-NC	2.76	113.97	110.43
14	a	813	CLA	CMB-C2B-C3B	2.76	130.21	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	838	CLA	C3D-C4D-ND	2.76	114.48	109.99
14	A	833	CLA	CAA-C2A-C3A	-2.76	105.53	113.00
14	A	844	CLA	CAA-C2A-C3A	-2.76	105.53	113.00
14	Q	201	CLA	C4D-C3D-CAD	2.76	111.11	108.11
14	b	814	CLA	C4D-C3D-CAD	2.76	111.11	108.11
14	B	815	CLA	C3D-C4D-ND	2.76	114.48	109.99
14	H	810	CLA	C4D-C3D-CAD	2.76	111.11	108.11
14	a	842	CLA	C1-O2A-CGA	2.76	123.34	116.65
14	B	818	CLA	CMA-C3A-C4A	2.76	119.19	111.77
14	H	834	CLA	C4D-C3D-CAD	2.76	111.11	108.11
14	G	833	CLA	C1-C2-C3	-2.76	121.67	126.20
17	f	201	BCR	C36-C18-C17	-2.76	118.34	122.82
14	H	821	CLA	C1-O2A-CGA	2.76	123.33	116.65
17	a	851	BCR	C19-C18-C17	2.76	123.35	119.01
14	G	814	CLA	C4D-C3D-CAD	2.76	111.10	108.11
14	a	817	CLA	CMD-C2D-C3D	-2.76	121.36	127.69
14	H	809	CLA	OBD-CAD-C3D	-2.76	121.97	128.42
14	G	842	CLA	C4D-C3D-CAD	2.76	111.10	108.11
14	A	822	CLA	O2A-C1-C2	2.76	118.72	108.11
14	a	825	CLA	C1-O2A-CGA	2.76	123.33	116.65
14	A	816	CLA	CAC-C3C-C4C	2.76	128.38	124.79
14	G	814	CLA	CAA-C2A-C3A	-2.76	105.55	113.00
17	B	846	BCR	C33-C5-C4	2.76	119.47	113.60
14	m	1601	CLA	C4D-C3D-CAD	2.76	111.10	108.11
17	A	848	BCR	C19-C18-C17	2.76	123.34	119.01
14	b	830	CLA	OBD-CAD-C3D	-2.76	121.97	128.42
14	X	1701	CLA	CMC-C2C-C1C	2.76	129.34	125.03
14	G	839	CLA	CAC-C3C-C4C	2.76	128.38	124.79
17	l	201	BCR	C19-C18-C17	2.76	123.34	119.01
14	b	821	CLA	O2A-C1-C2	2.75	118.71	108.11
14	a	835	CLA	CAC-C3C-C4C	2.75	128.37	124.79
14	B	828	CLA	C4-C3-C5	2.75	120.01	115.23
14	G	822	CLA	C4-C3-C5	2.75	120.01	115.23
14	a	805	CLA	C3D-C4D-ND	2.75	114.46	109.99
17	A	848	BCR	C36-C18-C17	-2.75	118.36	122.82
14	B	813	CLA	C3D-C4D-ND	2.75	114.46	109.99
14	G	832	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
17	A	852	BCR	C35-C13-C12	2.75	122.29	118.09
14	A	838	CLA	CMC-C2C-C1C	2.75	129.33	125.03
14	B	827	CLA	CHD-C1D-ND	-2.75	120.93	124.80
14	G	806	CLA	C3D-C4D-ND	2.75	114.46	109.99
17	G	852	BCR	C8-C7-C6	-2.75	119.65	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	820	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
14	H	824	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
14	a	807	CLA	CMB-C2B-C3B	2.75	130.17	124.68
14	a	844	CLA	C4D-C3D-CAD	2.75	111.09	108.11
17	B	843	BCR	C38-C26-C27	2.75	119.45	113.60
14	b	814	CLA	C3C-C4C-NC	2.75	113.95	110.43
14	a	855	CLA	CAA-C2A-C3A	-2.75	105.58	113.00
14	l	207	CLA	C6-C5-C3	-2.74	106.78	113.47
14	a	813	CLA	C3C-C4C-NC	2.74	113.95	110.43
14	a	808	CLA	CMA-C3A-C4A	2.74	119.15	111.77
14	a	826	CLA	C3D-C4D-ND	2.74	114.45	109.99
14	G	824	CLA	C4D-C3D-CAD	2.74	111.09	108.11
17	V	1602	BCR	C33-C5-C6	-2.74	121.49	124.48
14	G	811	CLA	CMA-C3A-C4A	2.74	119.14	111.77
17	G	852	BCR	C35-C13-C12	2.74	122.28	118.09
14	B	816	CLA	C3D-C4D-ND	2.74	114.44	109.99
14	H	839	CLA	CMD-C2D-C3D	-2.74	121.40	127.69
14	B	818	CLA	C3D-C4D-ND	2.74	114.44	109.99
14	G	830	CLA	CMA-C3A-C4A	2.74	119.14	111.77
17	R	102	BCR	C23-C24-C25	-2.74	119.67	127.00
14	G	839	CLA	O2A-C1-C2	2.74	118.66	108.11
14	B	809	CLA	C3C-C4C-NC	2.74	113.94	110.43
14	B	833	CLA	CMD-C2D-C3D	-2.74	121.41	127.69
14	b	804	CLA	C3C-C4C-NC	2.74	113.94	110.43
14	B	835	CLA	C4D-C3D-CAD	2.74	111.08	108.11
14	G	802	CLA	CMC-C2C-C1C	2.74	129.31	125.03
14	b	821	CLA	CMC-C2C-C1C	2.74	129.31	125.03
14	A	845	CLA	C4D-C3D-CAD	2.74	111.08	108.11
14	A	819	CLA	CMC-C2C-C1C	2.74	129.31	125.03
14	G	810	CLA	CMC-C2C-C1C	2.74	129.31	125.03
14	B	832	CLA	C1-C2-C3	-2.74	121.71	126.20
14	T	1401	CLA	C3D-C4D-ND	2.74	114.43	109.99
14	A	842	CLA	CMB-C2B-C3B	2.74	130.15	124.68
14	H	811	CLA	CMB-C2B-C3B	2.74	130.15	124.68
14	G	827	CLA	C6-C5-C3	-2.74	106.81	113.47
14	B	831	CLA	C4-C3-C5	2.73	119.97	115.23
14	A	819	CLA	C3D-C4D-ND	2.73	114.43	109.99
14	G	828	CLA	CAC-C3C-C4C	2.73	128.35	124.79
14	b	819	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
14	B	808	CLA	C1-C2-C3	-2.73	121.72	126.20
14	B	836	CLA	C1-C2-C3	-2.73	121.72	126.20
14	G	843	CLA	CMC-C2C-C1C	2.73	129.30	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	843	CLA	C3D-C4D-ND	2.73	114.43	109.99
14	a	806	CLA	CMC-C2C-C1C	2.73	129.30	125.03
14	b	813	CLA	C3D-C4D-ND	2.73	114.43	109.99
14	B	835	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
14	b	838	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
17	B	844	BCR	C36-C18-C17	-2.73	118.39	122.82
14	G	820	CLA	C4D-C3D-CAD	2.73	111.07	108.11
14	a	829	CLA	CAC-C3C-C4C	2.73	128.34	124.79
14	B	831	CLA	CMA-C3A-C4A	2.73	119.11	111.77
17	A	850	BCR	C38-C26-C27	2.73	119.42	113.60
14	A	808	CLA	CAC-C3C-C4C	2.73	128.34	124.79
14	G	821	CLA	CMA-C3A-C4A	2.73	119.11	111.77
14	G	833	CLA	C3C-C4C-NC	2.73	113.93	110.43
14	G	822	CLA	O2A-C1-C2	2.73	118.61	108.11
14	A	812	CLA	C1-C2-C3	-2.73	121.73	126.20
14	A	840	CLA	C3D-C4D-ND	2.73	114.42	109.99
14	a	837	CLA	O1D-CGD-CBD	-2.73	119.14	124.52
14	f	202	CLA	C4D-C3D-CAD	2.73	111.07	108.11
14	a	835	CLA	CMC-C2C-C1C	2.73	129.29	125.03
14	A	827	CLA	CAA-C2A-C1A	-2.73	103.04	111.97
14	G	842	CLA	C3C-C4C-NC	2.73	113.92	110.43
14	H	835	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
14	G	824	CLA	CMC-C2C-C1C	2.73	129.29	125.03
14	A	804	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
14	A	829	CLA	C1-O2A-CGA	2.72	123.25	116.65
14	b	834	CLA	CHC-C1C-C2C	-2.72	119.23	126.94
14	A	806	CLA	CMD-C2D-C3D	-2.72	121.44	127.69
14	G	828	CLA	C4-C3-C5	2.72	119.95	115.23
14	H	831	CLA	CAA-C2A-C3A	-2.72	105.64	113.00
13	G	801	CL0	C6-C5-C3	-2.72	106.84	113.47
14	a	808	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
14	B	808	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
14	H	818	CLA	C1-O2A-CGA	2.72	123.24	116.65
14	G	817	CLA	C3D-C4D-ND	2.72	114.41	109.99
14	G	822	CLA	C4D-C3D-CAD	2.72	111.06	108.11
14	H	831	CLA	C4D-C3D-CAD	2.72	111.06	108.11
14	B	829	CLA	OBD-CAD-C3D	-2.72	122.06	128.42
14	B	806	CLA	CMC-C2C-C1C	2.72	129.28	125.03
14	j	102	CLA	CMC-C2C-C1C	2.72	129.28	125.03
14	b	832	CLA	C4D-C3D-CAD	2.72	111.06	108.11
14	a	835	CLA	C3D-C4D-ND	2.72	114.41	109.99
14	S	102	CLA	CMC-C2C-C1C	2.72	129.28	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	810	CLA	CMC-C2C-C1C	2.72	129.28	125.03
14	G	844	CLA	CAA-C2A-C3A	-2.72	105.65	113.00
14	G	831	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
14	F	1303	CLA	CMA-C3A-C4A	2.72	119.07	111.77
14	a	833	CLA	C3D-C4D-ND	2.72	114.40	109.99
17	b	846	BCR	C4-C5-C6	-2.72	119.03	122.70
17	Q	202	BCR	C34-C9-C8	2.72	122.24	118.09
14	b	820	CLA	CMC-C2C-C1C	2.72	129.28	125.03
17	A	848	BCR	C30-C25-C26	-2.71	118.93	122.64
14	G	816	CLA	CMA-C3A-C4A	2.71	119.07	111.77
14	A	815	CLA	CAC-C3C-C4C	2.71	128.32	124.79
17	G	850	BCR	C27-C26-C25	-2.71	119.04	122.70
17	Q	204	BCR	C37-C22-C21	-2.71	118.42	122.82
14	H	819	CLA	C4D-C3D-CAD	2.71	111.05	108.11
14	H	829	CLA	CHD-C1D-ND	-2.71	120.98	124.80
14	B	833	CLA	C4D-C3D-CAD	2.71	111.05	108.11
14	G	823	CLA	C4D-C3D-CAD	2.71	111.05	108.11
14	B	814	CLA	CMA-C3A-C4A	2.71	119.06	111.77
14	B	807	CLA	O2A-C1-C2	2.71	118.55	108.11
14	G	836	CLA	CMB-C2B-C3B	2.71	130.10	124.68
14	G	803	CLA	CMB-C2B-C3B	2.71	130.10	124.68
14	B	828	CLA	CAC-C3C-C4C	2.71	128.32	124.79
14	a	821	CLA	CAA-C2A-C3A	-2.71	105.68	113.00
14	A	817	CLA	C4D-C3D-CAD	2.71	111.05	108.11
17	F	1302	BCR	C19-C18-C17	2.71	123.27	119.01
14	a	812	CLA	CMC-C2C-C1C	2.71	129.27	125.03
14	B	813	CLA	C3C-C4C-NC	2.71	113.90	110.43
17	B	845	BCR	C15-C14-C13	-2.71	123.34	127.48
14	x	1701	CLA	CMA-C3A-C4A	2.71	119.05	111.77
14	A	824	CLA	CAC-C3C-C4C	2.71	128.31	124.79
14	b	835	CLA	C3D-C4D-ND	2.71	114.39	109.99
14	G	818	CLA	CMB-C2B-C3B	2.71	130.09	124.68
14	G	807	CLA	C4-C3-C5	2.71	119.93	115.23
14	G	840	CLA	CMC-C2C-C1C	2.71	129.26	125.03
14	A	829	CLA	C3C-C4C-NC	2.71	113.90	110.43
14	K	101	CLA	CAC-C3C-C4C	2.71	128.31	124.79
14	A	843	CLA	C3C-C4C-NC	2.71	113.90	110.43
14	B	819	CLA	C4D-C3D-CAD	2.71	111.04	108.11
14	G	841	CLA	C4D-C3D-CAD	2.70	111.04	108.11
14	H	833	CLA	CAC-C3C-C4C	2.70	128.31	124.79
14	j	101	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
14	B	809	CLA	C4-C3-C5	2.70	119.92	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	830	CLA	CHD-C1D-ND	-2.70	121.00	124.80
14	B	836	CLA	C3C-C4C-NC	2.70	113.89	110.43
14	V	1601	CLA	C3C-C4C-NC	2.70	113.89	110.43
14	A	809	CLA	CAA-C2A-C3A	-2.70	105.70	113.00
13	G	801	CL0	C3C-C4C-NC	2.70	113.89	110.43
14	H	821	CLA	CMA-C3A-C4A	2.70	119.03	111.77
14	a	809	CLA	CMC-C2C-C1C	2.70	129.25	125.03
14	H	831	CLA	CMC-C2C-C1C	2.70	129.25	125.03
14	H	803	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
17	L	202	BCR	C33-C5-C6	-2.70	121.54	124.48
14	H	814	CLA	CMC-C2C-C1C	2.70	129.25	125.03
14	a	836	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
14	b	801	CLA	C3D-C4D-ND	2.70	114.38	109.99
14	H	823	CLA	C3C-C4C-NC	2.70	113.89	110.43
14	A	813	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
14	G	833	CLA	C4D-C3D-CAD	2.70	111.04	108.11
14	b	804	CLA	C4-C3-C5	2.70	119.91	115.23
14	a	840	CLA	CMD-C2D-C3D	-2.70	121.50	127.69
14	A	807	CLA	CMC-C2C-C1C	2.70	129.25	125.03
14	A	803	CLA	C3D-C4D-ND	2.70	114.37	109.99
14	A	820	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
17	S	103	BCR	C15-C14-C13	-2.70	123.50	127.28
14	B	831	CLA	C3D-C4D-ND	2.70	114.37	109.99
14	x	1701	CLA	C4D-C3D-CAD	2.70	111.03	108.11
14	A	813	CLA	CMB-C2B-C3B	2.70	130.07	124.68
14	A	815	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
14	B	839	CLA	C3D-C4D-ND	2.70	114.37	109.99
14	S	102	CLA	C3D-C4D-ND	2.70	114.37	109.99
14	H	803	CLA	C1-O2A-CGA	2.70	123.17	116.65
14	B	818	CLA	C4-C3-C5	2.70	119.91	115.23
17	J	102	BCR	C37-C22-C21	-2.69	118.45	122.82
14	A	810	CLA	O1D-CGD-CBD	-2.69	119.20	124.52
14	B	821	CLA	C3C-C4C-NC	2.69	113.88	110.43
14	b	824	CLA	O1D-CGD-CBD	-2.69	119.20	124.52
14	G	827	CLA	C3D-C4D-ND	2.69	114.36	109.99
14	b	812	CLA	C3C-C4C-NC	2.69	113.88	110.43
14	B	802	CLA	C6-C5-C3	-2.69	106.91	113.47
18	a	853	LHG	O8-C23-C24	2.69	120.05	111.83
17	b	845	BCR	C36-C18-C17	-2.69	118.45	122.82
14	B	812	CLA	CAA-C2A-C3A	-2.69	105.72	113.00
14	a	843	CLA	CAA-C2A-C3A	-2.69	105.73	113.00
14	Q	203	CLA	O2D-CGD-O1D	-2.69	118.61	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	827	CLA	C3D-C4D-ND	2.69	114.36	109.99
17	R	101	BCR	C38-C26-C27	2.69	119.33	113.60
14	G	804	CLA	C3D-C4D-ND	2.69	114.36	109.99
14	X	1701	CLA	CMA-C3A-C4A	2.69	119.00	111.77
14	B	818	CLA	C4D-C3D-CAD	2.69	111.03	108.11
17	A	848	BCR	C37-C22-C21	-2.69	118.46	122.82
14	Q	201	CLA	C3C-C4C-NC	2.69	113.87	110.43
14	G	836	CLA	CMC-C2C-C1C	2.69	129.24	125.03
14	B	819	CLA	C3C-C4C-NC	2.69	113.87	110.43
17	a	848	BCR	C33-C5-C6	-2.69	121.55	124.48
14	G	823	CLA	C3D-C4D-ND	2.69	114.35	109.99
14	a	855	CLA	CHD-C1D-ND	-2.69	121.02	124.80
14	J	101	CLA	CMA-C3A-C2A	2.69	124.36	113.98
17	B	848	BCR	C36-C18-C17	-2.68	118.47	122.82
17	A	849	BCR	C33-C5-C6	-2.68	121.56	124.48
14	F	1303	CLA	CMB-C2B-C3B	2.68	130.05	124.68
14	G	804	CLA	C4-C3-C5	2.68	119.89	115.23
14	H	809	CLA	CAC-C3C-C4C	2.68	128.28	124.79
14	B	821	CLA	C1-C2-C3	-2.68	121.80	126.20
14	G	804	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
14	x	1701	CLA	CMC-C2C-C1C	2.68	129.22	125.03
17	G	849	BCR	C38-C26-C27	2.68	119.31	113.60
14	a	836	CLA	C3D-C4D-ND	2.68	114.35	109.99
14	b	827	CLA	C3D-C4D-ND	2.68	114.35	109.99
14	H	802	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
14	a	818	CLA	C3D-C4D-ND	2.68	114.34	109.99
14	a	816	CLA	C4D-C3D-CAD	2.68	111.02	108.11
14	a	828	CLA	C4-C3-C5	2.68	119.88	115.23
14	G	812	CLA	CMB-C2B-C3B	2.68	130.04	124.68
14	G	832	CLA	CMB-C2B-C3B	2.68	130.04	124.68
17	A	853	BCR	C35-C13-C12	2.68	122.18	118.09
14	B	822	CLA	C3D-C4D-ND	2.68	114.34	109.99
14	b	808	CLA	CMB-C2B-C1B	2.68	132.38	128.46
14	G	816	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
14	H	819	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
14	H	808	CLA	C3C-C4C-NC	2.68	113.86	110.43
14	F	1303	CLA	C3D-C4D-ND	2.68	114.34	109.99
14	b	831	CLA	C3D-C4D-ND	2.68	114.34	109.99
14	G	839	CLA	C4D-C3D-CAD	2.68	111.01	108.11
14	J	101	CLA	CMD-C2D-C3D	-2.68	121.55	127.69
14	H	808	CLA	C3D-C4D-ND	2.68	114.34	109.99
14	j	101	CLA	CMB-C2B-C3B	2.68	130.03	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	840	CLA	CHC-C1C-C2C	-2.68	119.36	126.94
13	A	801	CL0	O2D-CGD-O1D	-2.68	118.64	123.85
17	H	845	BCR	C19-C18-C17	2.68	123.22	119.01
14	L	204	CLA	CMC-C2C-C1C	2.68	129.22	125.03
14	l	206	CLA	C1-C2-C3	-2.68	121.81	126.20
14	U	204	CLA	C3D-C4D-ND	2.68	114.34	109.99
13	a	801	CL0	O2D-CGD-O1D	-2.68	118.64	123.85
14	l	207	CLA	CAA-C2A-C3A	-2.68	105.77	113.00
14	G	815	CLA	C4D-C3D-CAD	2.67	111.01	108.11
14	B	809	CLA	CHC-C1C-C2C	-2.67	119.37	126.94
14	b	807	CLA	CAA-C2A-C3A	-2.67	105.77	113.00
14	a	815	CLA	CAC-C3C-C4C	2.67	128.27	124.79
14	A	829	CLA	C4D-C3D-CAD	2.67	111.01	108.11
14	G	803	CLA	C3D-C4D-ND	2.67	114.33	109.99
14	B	835	CLA	CAC-C3C-C4C	2.67	128.27	124.79
14	b	821	CLA	CMB-C2B-C3B	2.67	130.02	124.68
17	F	1302	BCR	C37-C22-C21	-2.67	118.49	122.82
14	b	821	CLA	C4-C3-C5	2.67	119.86	115.23
14	G	824	CLA	C3D-C4D-ND	2.67	114.33	109.99
14	B	815	CLA	CMA-C3A-C4A	2.67	118.95	111.77
14	j	102	CLA	CAC-C3C-C4C	2.67	128.26	124.79
14	H	802	CLA	CHD-C1D-ND	-2.67	121.04	124.80
14	G	815	CLA	CAC-C3C-C4C	2.67	128.26	124.79
14	i	101	CLA	C4D-C3D-CAD	2.67	111.01	108.11
14	a	823	CLA	C3D-C4D-ND	2.67	114.33	109.99
14	H	839	CLA	CMC-C2C-C1C	2.67	129.21	125.03
14	H	818	CLA	C3D-C4D-ND	2.67	114.33	109.99
14	H	810	CLA	CAA-C2A-C3A	-2.67	105.79	113.00
13	a	801	CL0	C3D-C4D-ND	2.67	114.33	109.99
14	b	837	CLA	O2A-C1-C2	2.67	118.38	108.11
14	b	825	CLA	CHD-C1D-ND	-2.67	121.05	124.80
14	A	804	CLA	OBD-CAD-C3D	-2.67	122.18	128.42
14	U	201	CLA	OBD-CAD-C3D	-2.67	122.18	128.42
14	B	803	CLA	C3C-C4C-NC	2.67	113.85	110.43
14	B	826	CLA	C4D-C3D-CAD	2.67	111.00	108.11
14	b	803	CLA	C3D-C4D-ND	2.67	114.32	109.99
14	G	823	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
14	G	826	CLA	CMC-C2C-C1C	2.67	129.20	125.03
14	j	101	CLA	CMD-C2D-C3D	-2.67	121.58	127.69
14	b	818	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
14	A	837	CLA	CAC-C3C-C4C	2.67	128.26	124.79
14	A	816	CLA	C4D-C3D-CAD	2.67	111.00	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	845	BCR	C38-C26-C27	2.67	119.28	113.60
14	G	826	CLA	C1-C2-C3	-2.66	121.83	126.20
14	L	205	CLA	C6-C5-C3	-2.66	106.98	113.47
14	b	802	CLA	C3D-C4D-ND	2.66	114.32	109.99
14	G	844	CLA	CMA-C3A-C4A	2.66	118.93	111.77
14	H	813	CLA	C3C-C4C-NC	2.66	113.84	110.43
14	B	802	CLA	C3D-C4D-ND	2.66	114.32	109.99
14	B	821	CLA	C4D-C3D-CAD	2.66	111.00	108.11
17	A	850	BCR	C37-C22-C21	-2.66	118.50	122.82
14	b	837	CLA	CMC-C2C-C1C	2.66	129.19	125.03
14	H	839	CLA	CMA-C3A-C4A	2.66	118.93	111.77
14	A	833	CLA	C4-C3-C5	2.66	119.85	115.23
14	a	842	CLA	C4D-C3D-CAD	2.66	111.00	108.11
14	G	837	CLA	CMC-C2C-C1C	2.66	129.19	125.03
14	K	102	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
14	A	809	CLA	C4-C3-C5	2.66	119.84	115.23
14	b	835	CLA	CMB-C2B-C3B	2.66	130.00	124.68
14	b	828	CLA	CAC-C3C-C4C	2.66	128.25	124.79
14	G	843	CLA	C3D-C4D-ND	2.66	114.31	109.99
17	G	852	BCR	C23-C24-C25	-2.66	119.90	127.00
17	a	851	BCR	C36-C18-C17	-2.66	118.51	122.82
14	S	101	CLA	CAC-C3C-C4C	2.66	128.25	124.79
17	R	102	BCR	C15-C14-C13	-2.66	123.55	127.28
17	G	848	BCR	C27-C26-C25	-2.66	119.11	122.70
14	b	801	CLA	C3C-C4C-NC	2.66	113.83	110.43
14	H	807	CLA	C4D-C3D-CAD	2.66	110.99	108.11
14	b	803	CLA	O1D-CGD-CBD	-2.66	119.28	124.52
14	A	828	CLA	CHD-C1D-ND	-2.66	121.07	124.80
14	A	823	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
14	G	818	CLA	C3D-C4D-ND	2.65	114.30	109.99
14	b	838	CLA	C3D-C4D-ND	2.65	114.30	109.99
14	k	1401	CLA	C3C-C4C-NC	2.65	113.83	110.43
14	L	205	CLA	CAC-C3C-C4C	2.65	128.24	124.79
17	U	202	BCR	C28-C27-C26	-2.65	109.32	114.06
14	A	826	CLA	C3C-C4C-NC	2.65	113.83	110.43
14	H	806	CLA	CMD-C2D-C3D	-2.65	121.61	127.69
13	a	801	CL0	C4D-C3D-CAD	2.65	110.99	108.11
14	a	824	CLA	CMC-C2C-C1C	2.65	129.18	125.03
17	Q	204	BCR	C28-C27-C26	-2.65	109.33	114.06
14	G	809	CLA	C3D-C4D-ND	2.65	114.30	109.99
14	a	838	CLA	C1-O2A-CGA	2.65	123.07	116.65
14	b	839	CLA	O2D-CGD-O1D	-2.65	118.69	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	849	BCR	C34-C9-C8	2.65	122.14	118.09
14	J	101	CLA	CAC-C3C-C4C	2.65	128.24	124.79
13	A	801	CL0	C4D-C3D-CAD	2.65	110.98	108.11
14	B	807	CLA	C4D-C3D-CAD	2.65	110.98	108.11
14	B	809	CLA	C4D-C3D-CAD	2.65	110.98	108.11
14	b	816	CLA	C3D-C4D-ND	2.65	114.29	109.99
17	l	201	BCR	C3-C4-C5	-2.65	109.33	114.06
14	B	822	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
14	G	834	CLA	C3D-C4D-ND	2.65	114.29	109.99
14	G	840	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
14	b	808	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
14	j	102	CLA	CMB-C2B-C3B	2.65	129.97	124.68
14	a	810	CLA	C4D-C3D-CAD	2.65	110.98	108.11
14	a	831	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
14	G	828	CLA	CMB-C2B-C3B	2.65	129.97	124.68
14	b	837	CLA	CMB-C2B-C3B	2.65	129.97	124.68
14	b	831	CLA	CAC-C3C-C4C	2.65	128.23	124.79
14	H	812	CLA	C3C-C4C-NC	2.65	113.82	110.43
14	G	825	CLA	CAC-C3C-C4C	2.64	128.23	124.79
14	H	824	CLA	O1D-CGD-CBD	-2.64	119.30	124.52
14	b	812	CLA	CAA-C2A-C3A	-2.64	105.85	113.00
17	A	852	BCR	C34-C9-C8	2.64	122.13	118.09
14	G	842	CLA	CMA-C3A-C4A	2.64	118.88	111.77
14	H	826	CLA	CAC-C3C-C4C	2.64	128.23	124.79
14	G	819	CLA	C3C-C4C-NC	2.64	113.82	110.43
14	a	831	CLA	C3D-C4D-ND	2.64	114.28	109.99
14	B	812	CLA	C4D-C3D-CAD	2.64	110.98	108.11
17	Q	204	BCR	C12-C13-C14	2.64	123.16	119.01
14	b	822	CLA	CMA-C3A-C4A	2.64	118.87	111.77
14	G	821	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
14	A	839	CLA	CMC-C2C-C1C	2.64	129.16	125.03
14	A	826	CLA	CAC-C3C-C4C	2.64	128.23	124.79
14	H	816	CLA	C4D-C3D-CAD	2.64	110.97	108.11
14	B	814	CLA	O1D-CGD-CBD	-2.64	119.31	124.52
14	B	819	CLA	CMA-C3A-C4A	2.64	118.87	111.77
14	B	814	CLA	C3C-C4C-NC	2.64	113.81	110.43
17	b	845	BCR	C24-C23-C22	-2.64	122.33	126.23
14	a	811	CLA	C3D-C4D-ND	2.64	114.27	109.99
17	A	851	BCR	C30-C25-C24	2.64	122.80	115.65
14	T	1401	CLA	C3C-C4C-NC	2.64	113.81	110.43
17	j	103	BCR	C39-C30-C25	-2.64	106.11	110.24
17	R	102	BCR	C12-C13-C14	-2.64	114.86	119.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	829	CLA	CMA-C3A-C4A	2.64	118.86	111.77
17	H	842	BCR	C3-C4-C5	-2.64	109.36	114.06
14	i	101	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
14	B	805	CLA	C3D-C4D-ND	2.64	114.27	109.99
14	G	815	CLA	C3D-C4D-ND	2.64	114.27	109.99
14	b	824	CLA	C3D-C4D-ND	2.64	114.27	109.99
14	A	845	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
14	B	837	CLA	CAA-C2A-C3A	-2.64	105.88	113.00
14	G	810	CLA	CMA-C3A-C4A	2.63	118.86	111.77
14	S	101	CLA	CMA-C3A-C4A	2.63	118.85	111.77
14	S	101	CLA	C3C-C4C-NC	2.63	113.80	110.43
14	H	829	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
14	G	829	CLA	C4-C3-C5	2.63	119.80	115.23
14	W	1701	CLA	CAC-C3C-C4C	2.63	128.22	124.79
14	a	812	CLA	C4D-C3D-CAD	2.63	110.97	108.11
14	b	838	CLA	CMC-C2C-C1C	2.63	129.15	125.03
14	B	838	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
14	b	812	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
14	a	802	CLA	C3D-C4D-ND	2.63	114.26	109.99
14	b	834	CLA	CED-O2D-CGD	2.63	121.88	115.92
14	a	855	CLA	C4-C3-C5	2.63	119.80	115.23
14	G	832	CLA	C3C-C4C-NC	2.63	113.80	110.43
14	G	809	CLA	CAA-C2A-C3A	-2.63	105.89	113.00
14	A	809	CLA	O1D-CGD-CBD	-2.63	119.33	124.52
14	Q	203	CLA	CMA-C3A-C4A	2.63	118.84	111.77
14	B	822	CLA	CMA-C3A-C4A	2.63	118.84	111.77
14	G	819	CLA	CMB-C2B-C3B	2.63	129.94	124.68
14	H	815	CLA	CMA-C3A-C4A	2.63	118.84	111.77
14	a	855	CLA	C1-C2-C3	-2.63	121.89	126.20
17	M	1602	BCR	C28-C27-C26	-2.63	109.37	114.06
14	H	833	CLA	C4D-C3D-CAD	2.63	110.96	108.11
14	A	813	CLA	C3D-C4D-ND	2.63	114.26	109.99
14	B	808	CLA	C3D-C4D-ND	2.63	114.26	109.99
17	A	852	BCR	C7-C8-C9	-2.63	122.35	126.23
17	b	843	BCR	C33-C5-C4	2.63	119.20	113.60
14	A	842	CLA	C4D-C3D-CAD	2.63	110.96	108.11
14	a	836	CLA	C4D-C3D-CAD	2.63	110.96	108.11
14	A	823	CLA	CMA-C3A-C4A	2.63	118.83	111.77
14	G	806	CLA	CHB-C4A-NA	2.63	128.19	124.40
14	A	828	CLA	C4D-C3D-CAD	2.63	110.96	108.11
14	x	1701	CLA	C3C-C4C-NC	2.63	113.80	110.43
14	b	809	CLA	C4-C3-C5	2.63	119.79	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	818	CLA	C4-C3-C5	2.63	119.79	115.23
14	Q	201	CLA	CMA-C3A-C4A	2.63	118.83	111.77
14	a	841	CLA	C3D-C4D-ND	2.63	114.25	109.99
14	K	101	CLA	C4D-C3D-CAD	2.63	110.97	107.69
14	B	804	CLA	O1D-CGD-CBD	-2.62	119.34	124.52
14	G	842	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
14	B	801	CLA	C1-C2-C3	-2.62	121.90	126.20
17	a	850	BCR	C35-C13-C12	2.62	122.10	118.09
14	G	829	CLA	C4D-C3D-CAD	2.62	110.96	108.11
14	G	828	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
14	G	812	CLA	C4-C3-C5	2.62	119.78	115.23
14	G	834	CLA	CMD-C2D-C3D	-2.62	121.67	127.69
14	a	810	CLA	C3D-C4D-ND	2.62	114.25	109.99
14	A	843	CLA	CMB-C2B-C3B	2.62	129.92	124.68
17	R	101	BCR	C23-C24-C25	-2.62	120.00	127.00
13	G	801	CL0	C3D-C4D-ND	2.62	114.25	109.99
14	G	814	CLA	C1-C2-C3	-2.62	121.90	126.20
14	G	842	CLA	C1-C2-C3	-2.62	121.90	126.20
14	H	826	CLA	C4D-C3D-CAD	2.62	110.95	108.11
14	B	838	CLA	CMC-C2C-C1C	2.62	129.13	125.03
17	S	103	BCR	C19-C18-C17	2.62	123.13	119.01
14	B	818	CLA	CMD-C2D-C3D	-2.62	121.68	127.69
14	H	832	CLA	C4D-C3D-CAD	2.62	110.95	108.11
18	A	854	LHG	O8-C23-C24	2.62	119.82	111.83
14	H	829	CLA	CMB-C2B-C1B	2.62	132.29	128.46
17	b	843	BCR	C38-C26-C27	2.62	119.18	113.60
14	a	840	CLA	CAC-C3C-C4C	2.62	128.20	124.79
13	G	801	CL0	C4D-C3D-CAD	2.62	110.95	108.11
14	b	801	CLA	C1-C2-C3	-2.62	121.91	126.20
14	a	838	CLA	C4-C3-C5	2.62	119.77	115.23
14	G	831	CLA	C3D-C4D-ND	2.62	114.24	109.99
14	H	805	CLA	C3D-C4D-ND	2.62	114.24	109.99
14	a	822	CLA	C3D-C4D-ND	2.62	114.24	109.99
17	H	846	BCR	C34-C9-C8	2.62	122.09	118.09
14	G	836	CLA	CAC-C3C-C4C	2.62	128.19	124.79
14	A	827	CLA	C4D-C3D-CAD	2.62	110.95	108.11
14	G	819	CLA	CAC-C3C-C4C	2.62	128.19	124.79
14	b	832	CLA	CAC-C3C-C4C	2.62	128.19	124.79
14	a	828	CLA	CHD-C4C-C3C	-2.62	120.96	124.77
14	B	826	CLA	CAA-C2A-C3A	-2.62	105.93	113.00
14	G	838	CLA	C1-C2-C3	-2.62	122.53	126.76
14	b	831	CLA	C4-C3-C5	2.62	119.77	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	f	203	BCR	C36-C18-C17	-2.61	118.58	122.82
17	G	851	BCR	C7-C8-C9	-2.61	122.37	126.23
14	b	814	CLA	CMC-C2C-C1C	2.61	129.12	125.03
14	b	829	CLA	CMC-C2C-C1C	2.61	129.12	125.03
14	G	810	CLA	C3D-C4D-ND	2.61	114.23	109.99
14	L	204	CLA	C3D-C4D-ND	2.61	114.23	109.99
14	A	811	CLA	C3C-C4C-NC	2.61	113.78	110.43
14	B	801	CLA	CHD-C1D-ND	-2.61	121.12	124.80
17	a	849	BCR	C27-C26-C25	-2.61	119.17	122.70
14	b	815	CLA	CMB-C2B-C3B	2.61	129.90	124.68
14	b	839	CLA	C3D-C4D-ND	2.61	114.23	109.99
14	A	804	CLA	CAA-C2A-C3A	-2.61	105.94	113.00
14	J	101	CLA	CMC-C2C-C1C	2.61	129.12	125.03
14	j	101	CLA	CMC-C2C-C1C	2.61	129.12	125.03
14	m	1601	CLA	C3C-C4C-NC	2.61	113.78	110.43
14	G	807	CLA	C3D-C4D-ND	2.61	114.23	109.99
14	G	806	CLA	CAA-C2A-C3A	-2.61	105.94	113.00
14	G	834	CLA	CMC-C2C-C1C	2.61	129.11	125.03
14	S	101	CLA	C4D-C3D-CAD	2.61	110.94	108.11
17	b	846	BCR	C36-C18-C17	-2.61	118.59	122.82
17	G	852	BCR	C38-C26-C27	2.61	119.16	113.60
17	Q	204	BCR	C7-C8-C9	-2.61	122.38	126.23
14	W	1701	CLA	OBD-CAD-C3D	-2.61	122.32	128.42
14	b	819	CLA	CMB-C2B-C3B	2.61	129.90	124.68
14	b	804	CLA	C3D-C4D-ND	2.61	114.23	109.99
14	G	808	CLA	CMA-C3A-C4A	2.61	118.78	111.77
17	b	842	BCR	C33-C5-C6	-2.61	121.64	124.48
14	B	839	CLA	C1-O2A-CGA	2.61	122.96	116.65
17	b	843	BCR	C35-C13-C12	2.61	122.07	118.09
14	A	807	CLA	C4D-C3D-CAD	2.61	110.94	108.11
14	b	834	CLA	C4D-C3D-CAD	2.61	110.94	108.11
14	b	805	CLA	C3D-C4D-ND	2.61	114.22	109.99
14	b	818	CLA	CMD-C2D-C3D	-2.61	121.71	127.69
14	b	820	CLA	CMA-C3A-C4A	2.61	118.78	111.77
14	G	828	CLA	C4C-C3C-C2C	-2.61	103.10	106.89
14	a	835	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
15	A	846	PQN	C11-C12-C13	-2.61	122.34	126.83
14	U	201	CLA	CMB-C2B-C3B	2.61	129.89	124.68
14	B	839	CLA	CMC-C2C-C1C	2.61	129.11	125.03
14	A	830	CLA	C3C-C4C-NC	2.61	113.77	110.43
14	b	839	CLA	CMA-C3A-C2A	2.61	124.06	113.98
14	H	807	CLA	O2D-CGD-O1D	-2.61	118.78	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	l	203	BCR	C37-C22-C23	2.60	122.07	118.09
13	a	801	CL0	CMB-C2B-C3B	2.60	129.89	124.68
14	a	824	CLA	C1-C2-C3	-2.60	121.93	126.20
14	a	832	CLA	C3D-C4D-ND	2.60	114.22	109.99
14	A	819	CLA	C3C-C4C-NC	2.60	113.77	110.43
14	H	825	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
14	V	1601	CLA	CMC-C2C-C1C	2.60	129.10	125.03
14	G	810	CLA	CAC-C3C-C4C	2.60	128.18	124.79
14	G	837	CLA	C4D-C3D-CAD	2.60	110.93	108.11
14	a	821	CLA	C4D-C3D-CAD	2.60	110.93	108.11
14	b	807	CLA	C4-C3-C5	2.60	119.74	115.23
14	A	821	CLA	C3C-C4C-NC	2.60	113.76	110.43
14	A	803	CLA	C3C-C4C-NC	2.60	113.76	110.43
14	H	816	CLA	CMB-C2B-C1B	-2.60	124.65	128.46
14	a	821	CLA	CMD-C2D-C3D	-2.60	121.73	127.69
14	H	803	CLA	C1-C2-C3	-2.60	121.94	126.20
14	A	807	CLA	C3D-C4D-ND	2.60	114.21	109.99
14	H	812	CLA	C3D-C4D-ND	2.60	114.21	109.99
14	b	826	CLA	C3C-C4C-NC	2.60	113.76	110.43
14	b	818	CLA	C1-O2A-CGA	2.60	122.94	116.65
14	S	101	CLA	CMB-C2B-C3B	2.60	129.88	124.68
14	B	836	CLA	C3D-C4D-ND	2.60	114.21	109.99
14	b	804	CLA	C1-C2-C3	-2.60	121.94	126.20
14	b	835	CLA	CMD-C2D-C3D	-2.60	121.73	127.69
14	k	1401	CLA	CMC-C2C-C1C	2.60	129.09	125.03
14	H	833	CLA	CMD-C2D-C3D	-2.60	121.73	127.69
14	b	822	CLA	C3D-C4D-ND	2.60	114.21	109.99
17	B	843	BCR	C38-C26-C25	-2.60	121.65	124.48
14	B	807	CLA	CAC-C3C-C4C	2.60	128.17	124.79
14	a	807	CLA	CAC-C3C-C4C	2.60	128.17	124.79
17	H	843	BCR	C36-C18-C17	-2.60	118.61	122.82
14	A	839	CLA	C3D-C4D-ND	2.60	114.20	109.99
14	B	827	CLA	C4D-C3D-CAD	2.59	110.92	108.11
14	B	821	CLA	C3D-C4D-ND	2.59	114.20	109.99
14	H	816	CLA	C3D-C4D-ND	2.59	114.20	109.99
17	b	849	BCR	C32-C1-C6	-2.59	106.18	110.24
14	H	801	CLA	C1-C2-C3	-2.59	121.95	126.20
14	G	844	CLA	CMD-C2D-C3D	-2.59	121.74	127.69
14	a	814	CLA	CMD-C2D-C3D	-2.59	121.74	127.69
14	A	819	CLA	CMA-C3A-C4A	2.59	118.74	111.77
14	a	807	CLA	C4D-C3D-CAD	2.59	110.92	108.11
17	a	851	BCR	C27-C26-C25	-2.59	119.20	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	804	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
14	A	833	CLA	CAC-C3C-C4C	2.59	128.16	124.79
14	G	826	CLA	CMA-C3A-C2A	2.59	124.00	113.98
14	B	810	CLA	CMD-C2D-C3D	-2.59	121.75	127.69
14	G	825	CLA	C3C-C4C-NC	2.59	113.75	110.43
14	a	822	CLA	CMA-C3A-C4A	2.59	118.73	111.77
18	G	854	LHG	O8-C23-C24	2.59	119.73	111.83
14	B	835	CLA	C3D-C4D-ND	2.59	114.19	109.99
14	A	845	CLA	C4C-C3C-C2C	-2.59	103.12	106.89
14	a	839	CLA	C4D-C3D-CAD	2.59	110.92	108.11
14	Q	203	CLA	CMC-C2C-C1C	2.59	129.08	125.03
14	A	832	CLA	C3C-C4C-NC	2.59	113.74	110.43
14	G	804	CLA	C3C-C4C-NC	2.59	113.74	110.43
14	H	805	CLA	C3C-C4C-NC	2.59	113.74	110.43
17	H	844	BCR	C34-C9-C10	-2.59	118.63	122.82
14	Q	203	CLA	CMB-C2B-C3B	2.59	129.85	124.68
14	H	801	CLA	C4-C3-C5	2.59	119.72	115.23
14	B	825	CLA	CHD-C1D-ND	-2.59	121.16	124.80
14	a	811	CLA	C1-C2-C3	-2.59	121.96	126.20
14	a	816	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
14	a	824	CLA	C4-C3-C5	2.59	119.72	115.23
14	b	826	CLA	C4D-C3D-CAD	2.59	110.91	108.11
17	B	846	BCR	C33-C5-C6	-2.59	121.66	124.48
14	J	101	CLA	CMB-C2B-C3B	2.59	129.85	124.68
17	H	847	BCR	C34-C9-C10	-2.59	118.63	122.82
14	A	843	CLA	C3D-C4D-ND	2.58	114.19	109.99
14	J	101	CLA	C3C-C4C-NC	2.58	113.74	110.43
17	j	103	BCR	C37-C22-C21	-2.58	118.63	122.82
14	a	828	CLA	CAA-CBA-CGA	-2.58	105.87	113.21
14	A	834	CLA	C4D-C3D-CAD	2.58	110.91	108.11
14	H	802	CLA	C4D-C3D-CAD	2.58	110.91	108.11
14	b	829	CLA	CMA-C3A-C4A	2.58	118.72	111.77
14	G	827	CLA	CMA-C3A-C4A	2.58	118.72	111.77
14	B	804	CLA	C4D-C3D-CAD	2.58	110.91	108.11
14	b	802	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
14	k	1401	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
14	B	813	CLA	CMD-C2D-C3D	-2.58	121.77	127.69
14	A	832	CLA	CMC-C2C-C1C	2.58	129.07	125.03
14	G	811	CLA	C3D-C4D-ND	2.58	114.18	109.99
14	a	843	CLA	CMB-C2B-C3B	2.58	129.84	124.68
19	b	848	LMG	O7-C10-O9	-2.58	117.67	123.70
14	H	838	CLA	O2D-CGD-O1D	-2.58	118.83	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	W	1701	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
14	a	806	CLA	C3D-C4D-ND	2.58	114.18	109.99
14	K	102	CLA	CMC-C2C-C1C	2.58	129.06	125.03
14	b	825	CLA	CMA-C3A-C4A	2.58	118.71	111.77
17	B	843	BCR	C23-C22-C21	2.58	123.07	119.01
17	A	851	BCR	C28-C27-C26	-2.58	109.46	114.06
14	a	837	CLA	C3C-C4C-NC	2.58	113.73	110.43
14	H	822	CLA	CAA-C2A-C3A	-2.58	106.03	113.00
14	a	820	CLA	CBC-CAC-C3C	-2.58	105.43	112.42
14	A	811	CLA	C3D-C4D-ND	2.58	114.17	109.99
14	b	832	CLA	C3D-C4D-ND	2.58	114.17	109.99
14	B	837	CLA	C4D-C3D-CAD	2.58	110.90	108.11
14	b	803	CLA	CMB-C2B-C3B	2.58	129.83	124.68
14	B	840	CLA	CMC-C2C-C3C	2.58	133.12	126.15
14	B	837	CLA	CMA-C3A-C4A	2.58	118.69	111.77
14	B	839	CLA	C4-C3-C5	2.57	119.70	115.23
14	A	820	CLA	C3D-C4D-ND	2.57	114.17	109.99
14	B	829	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
14	B	839	CLA	CMA-C3A-C4A	2.57	118.69	111.77
14	j	101	CLA	CMA-C3A-C2A	2.57	123.93	113.98
14	G	833	CLA	C3D-C4D-ND	2.57	114.17	109.99
15	a	845	PQN	C11-C12-C13	-2.57	122.40	126.83
14	a	841	CLA	C4D-C3D-CAD	2.57	110.90	108.11
14	G	808	CLA	CAA-C2A-C3A	-2.57	106.05	113.00
17	H	846	BCR	C33-C5-C4	2.57	119.08	113.60
14	A	814	CLA	OBD-CAD-C3D	-2.57	122.41	128.42
14	l	207	CLA	CAA-CBA-CGA	-2.57	105.91	113.21
14	b	838	CLA	C3C-C4C-NC	2.57	113.72	110.43
14	m	1601	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
14	H	820	CLA	C4D-C3D-CAD	2.57	110.90	108.11
17	R	103	BCR	C36-C18-C17	-2.57	118.65	122.82
14	A	838	CLA	C1-C2-C3	-2.57	122.61	126.76
14	b	806	CLA	CMD-C2D-C3D	-2.57	121.80	127.69
14	G	839	CLA	C3D-C4D-ND	2.57	114.16	109.99
14	A	836	CLA	C3C-C4C-NC	2.57	113.72	110.43
14	a	844	CLA	O1D-CGD-CBD	-2.57	119.45	124.52
17	j	103	BCR	C28-C27-C26	-2.57	109.48	114.06
14	B	832	CLA	C3D-C4D-ND	2.57	114.16	109.99
14	H	830	CLA	OBD-CAD-C3D	-2.57	122.42	128.42
14	H	818	CLA	CMD-C2D-C3D	-2.57	121.80	127.69
14	a	810	CLA	CMD-C2D-C3D	-2.57	121.80	127.69
14	B	840	CLA	CHC-C1C-C2C	-2.57	119.67	126.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	827	CLA	C3D-C4D-ND	2.57	114.16	109.99
14	x	1701	CLA	C3D-C4D-ND	2.57	114.16	109.99
14	B	817	CLA	CMC-C2C-C1C	2.57	129.04	125.03
14	K	101	CLA	CMB-C2B-C3B	2.57	129.81	124.68
14	b	808	CLA	C3D-C4D-ND	2.57	114.16	109.99
14	G	804	CLA	CMB-C2B-C3B	2.57	129.81	124.68
14	a	832	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
14	H	811	CLA	CAC-C3C-C4C	2.56	128.13	124.79
14	B	806	CLA	CMD-C2D-C3D	-2.56	121.81	127.69
14	a	827	CLA	CAA-C2A-C3A	-2.56	106.07	113.00
14	a	804	CLA	C3C-C4C-NC	2.56	113.72	110.43
14	H	837	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
14	a	819	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	G	816	CLA	C3C-C4C-NC	2.56	113.71	110.43
14	b	802	CLA	CMA-C3A-C4A	2.56	118.66	111.77
14	H	807	CLA	CAC-C3C-C4C	2.56	128.12	124.79
14	H	836	CLA	C4D-C3D-CAD	2.56	110.89	108.11
14	a	812	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	a	824	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	H	837	CLA	C1-O2A-CGA	2.56	122.86	116.65
17	B	842	BCR	C35-C13-C12	2.56	122.00	118.09
14	b	805	CLA	O1D-CGD-CBD	-2.56	119.46	124.52
14	B	824	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
14	f	202	CLA	C3D-C4D-ND	2.56	114.15	109.99
17	l	208	BCR	C28-C27-C26	-2.56	109.49	114.06
14	A	838	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	G	838	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	a	825	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	b	833	CLA	CMD-C2D-C3D	-2.56	121.82	127.69
14	a	830	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	H	809	CLA	C4-C3-C5	2.56	119.67	115.23
14	a	808	CLA	CAA-C2A-C3A	-2.56	106.08	113.00
14	B	840	CLA	C3C-C4C-NC	2.56	113.71	110.43
14	j	102	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	b	811	CLA	CMB-C2B-C3B	2.56	129.79	124.68
14	A	828	CLA	OBD-CAD-C3D	-2.56	122.44	128.42
14	G	833	CLA	CMC-C2C-C1C	2.56	129.03	125.03
14	H	804	CLA	C3D-C4D-ND	2.56	114.14	109.99
17	B	844	BCR	C24-C23-C22	-2.56	122.45	126.23
14	A	833	CLA	C3D-C4D-ND	2.56	114.14	109.99
14	l	202	CLA	CMB-C2B-C3B	2.56	129.79	124.68
14	b	831	CLA	C4D-C3D-CAD	2.56	110.88	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	207	BCR	C3-C4-C5	-2.56	109.50	114.06
14	B	804	CLA	C3C-C4C-NC	2.56	113.70	110.43
14	a	803	CLA	C3D-C4D-ND	2.56	114.14	109.99
14	A	811	CLA	CMA-C3A-C4A	2.55	118.64	111.77
14	l	207	CLA	C4D-C3D-CAD	2.55	110.88	108.11
14	H	802	CLA	CMA-C3A-C2A	-2.55	104.11	113.98
14	b	801	CLA	CMB-C2B-C1B	-2.55	124.72	128.46
17	S	103	BCR	C37-C22-C21	-2.55	118.68	122.82
14	G	802	CLA	CBC-CAC-C3C	-2.55	105.50	112.42
14	G	835	CLA	C3D-C4D-ND	2.55	114.13	109.99
14	l	205	CLA	C3D-C4D-ND	2.55	114.13	109.99
14	B	821	CLA	CMA-C3A-C4A	2.55	118.62	111.77
14	B	813	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
14	a	838	CLA	C3D-C4D-ND	2.55	114.13	109.99
14	a	833	CLA	C4-C3-C5	2.55	119.65	115.23
14	A	833	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
14	B	810	CLA	CMC-C2C-C1C	2.55	129.02	125.03
17	R	103	BCR	C7-C8-C9	-2.55	122.47	126.23
14	A	837	CLA	C3D-C4D-ND	2.55	114.13	109.99
14	b	825	CLA	C1-C2-C3	-2.55	122.02	126.20
14	G	812	CLA	C3D-C4D-ND	2.55	114.12	109.99
17	a	852	BCR	C37-C22-C23	2.55	121.98	118.09
14	b	839	CLA	CMC-C2C-C1C	2.55	129.01	125.03
14	A	806	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
14	G	826	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
14	A	825	CLA	CMC-C2C-C1C	2.54	129.01	125.03
14	a	810	CLA	CMA-C3A-C4A	2.54	118.61	111.77
14	H	802	CLA	C3D-C4D-ND	2.54	114.12	109.99
14	H	840	CLA	C1-C2-C3	-2.54	122.03	126.20
14	b	802	CLA	CAA-C2A-C3A	-2.54	106.12	113.00
14	H	838	CLA	CAA-C2A-C3A	-2.54	106.12	113.00
14	H	823	CLA	CMC-C2C-C1C	2.54	129.01	125.03
14	A	802	CLA	C3C-C4C-NC	2.54	113.69	110.43
14	a	839	CLA	C3D-C4D-ND	2.54	114.12	109.99
14	H	819	CLA	C3C-C4C-NC	2.54	113.69	110.43
14	H	806	CLA	CAA-C2A-C3A	-2.54	106.13	113.00
14	a	832	CLA	CMC-C2C-C1C	2.54	129.00	125.03
14	H	827	CLA	C3D-C4D-ND	2.54	114.12	109.99
14	a	838	CLA	C3C-C4C-NC	2.54	113.69	110.43
14	B	829	CLA	CMA-C3A-C4A	2.54	118.60	111.77
14	B	809	CLA	C1-C2-C3	-2.54	122.03	126.20
14	A	826	CLA	CMA-C3A-C4A	2.54	118.60	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	803	CLA	CAA-C2A-C3A	-2.54	106.14	113.00
14	B	839	CLA	C3C-C4C-NC	2.54	113.68	110.43
14	B	804	CLA	C3D-C4D-ND	2.54	114.11	109.99
14	G	813	CLA	C3D-C4D-ND	2.54	114.11	109.99
14	G	804	CLA	CMC-C2C-C1C	2.54	129.00	125.03
14	Q	201	CLA	C3D-C4D-ND	2.54	114.11	109.99
14	A	806	CLA	C4D-C3D-CAD	2.54	110.86	108.11
14	A	807	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
14	H	816	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
14	a	802	CLA	C1-C2-C3	-2.54	122.04	126.20
14	b	829	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
14	A	825	CLA	C4-C3-C5	2.54	119.63	115.23
14	H	839	CLA	C4-C3-C5	2.54	119.63	115.23
14	J	101	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
14	A	829	CLA	CAA-CBA-CGA	-2.54	106.00	113.21
14	A	832	CLA	C3D-C4D-ND	2.54	114.11	109.99
14	G	841	CLA	C3D-C4D-ND	2.54	114.11	109.99
14	H	839	CLA	CAA-C2A-C3A	-2.54	106.15	113.00
14	G	807	CLA	C1-C2-C3	-2.54	122.04	126.20
14	b	809	CLA	C1-C2-C3	-2.54	122.04	126.20
14	H	806	CLA	C3D-C4D-ND	2.53	114.11	109.99
14	B	801	CLA	C4D-C3D-CAD	2.53	110.86	108.11
19	b	848	LMG	O8-C28-C29	2.53	119.56	111.83
14	B	821	CLA	C4-C3-C5	2.53	119.63	115.23
14	G	812	CLA	CAC-C3C-C4C	2.53	128.09	124.79
14	x	1701	CLA	CAA-C2A-C3A	-2.53	106.15	113.00
14	G	808	CLA	C3C-C4C-NC	2.53	113.68	110.43
14	A	825	CLA	C3D-C4D-ND	2.53	114.11	109.99
14	A	816	CLA	C3C-C4C-NC	2.53	113.67	110.43
14	G	842	CLA	C3D-C4D-ND	2.53	114.10	109.99
14	H	830	CLA	C3C-C4C-NC	2.53	113.67	110.43
14	H	806	CLA	C1-O2A-CGA	2.53	122.78	116.65
17	j	104	BCR	C36-C18-C17	-2.53	118.71	122.82
14	A	845	CLA	C3D-C4D-ND	2.53	114.10	109.99
14	G	802	CLA	C3D-C4D-ND	2.53	114.10	109.99
14	H	803	CLA	C3D-C4D-ND	2.53	114.10	109.99
14	L	205	CLA	C3C-C4C-NC	2.53	113.67	110.43
14	G	830	CLA	C4D-C3D-CAD	2.53	110.86	108.11
14	a	842	CLA	C3C-C4C-NC	2.53	113.67	110.43
17	G	850	BCR	C4-C5-C6	-2.53	119.28	122.70
14	B	810	CLA	CMA-C3A-C4A	2.53	118.57	111.77
14	H	809	CLA	C3B-C4B-NB	2.53	112.48	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	f	202	CLA	CMC-C2C-C1C	2.53	128.99	125.03
14	A	803	CLA	CAC-C3C-C4C	2.53	128.08	124.79
14	A	829	CLA	CAC-C3C-C4C	2.53	128.08	124.79
14	j	101	CLA	CAC-C3C-C4C	2.53	128.08	124.79
14	l	202	CLA	CMA-C3A-C4A	2.53	118.57	111.77
17	B	845	BCR	C38-C26-C27	2.53	118.98	113.60
17	H	843	BCR	C19-C18-C17	2.53	122.98	119.01
14	H	832	CLA	CMD-C2D-C3D	-2.53	121.89	127.69
14	H	826	CLA	C3C-C4C-NC	2.53	113.67	110.43
14	A	822	CLA	CAC-C3C-C4C	2.53	128.08	124.79
14	H	828	CLA	CAC-C3C-C4C	2.53	128.08	124.79
14	A	814	CLA	C4D-C3D-CAD	2.53	110.85	108.11
14	b	835	CLA	C4D-C3D-CAD	2.53	110.85	108.11
14	G	845	CLA	CMC-C2C-C3C	2.53	132.98	126.15
14	A	817	CLA	C3D-C4D-ND	2.53	114.09	109.99
14	H	813	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
14	a	843	CLA	CMD-C2D-C3D	-2.53	121.90	127.69
14	a	819	CLA	CMC-C2C-C1C	2.53	128.98	125.03
14	b	823	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
13	A	801	CL0	CAA-C2A-C3A	-2.53	106.17	113.00
14	G	835	CLA	CMC-C2C-C1C	2.53	128.98	125.03
14	l	205	CLA	CMC-C2C-C1C	2.53	128.98	125.03
14	H	812	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
14	a	842	CLA	C3D-C4D-ND	2.52	114.09	109.99
14	A	831	CLA	C3D-C4D-ND	2.52	114.09	109.99
14	b	835	CLA	CAA-C2A-C3A	-2.52	106.18	113.00
14	b	826	CLA	CMC-C2C-C1C	2.52	128.98	125.03
14	G	817	CLA	CMB-C2B-C3B	2.52	129.72	124.68
14	G	825	CLA	C3D-C4D-ND	2.52	114.09	109.99
14	B	811	CLA	CMA-C3A-C4A	2.52	118.55	111.77
14	H	808	CLA	O1D-CGD-CBD	-2.52	119.54	124.52
14	H	804	CLA	C3C-C4C-NC	2.52	113.66	110.43
14	S	101	CLA	CAA-C2A-C3A	-2.52	106.18	113.00
14	G	822	CLA	CAC-C3C-C4C	2.52	128.07	124.79
14	b	814	CLA	O1D-CGD-CBD	-2.52	119.54	124.52
14	a	819	CLA	C4-C3-C5	2.52	119.61	115.23
14	B	811	CLA	CMC-C2C-C1C	2.52	128.97	125.03
14	b	824	CLA	CMC-C2C-C1C	2.52	128.97	125.03
17	m	1602	BCR	C3-C4-C5	-2.52	109.56	114.06
14	G	803	CLA	C4-C3-C5	2.52	119.60	115.23
17	H	845	BCR	C30-C25-C26	-2.52	119.19	122.64
14	a	816	CLA	CMC-C2C-C1C	2.52	128.97	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	819	CLA	C3D-C4D-ND	2.52	114.08	109.99
14	b	816	CLA	C3C-C4C-NC	2.52	113.66	110.43
14	b	832	CLA	C3C-C4C-NC	2.52	113.66	110.43
14	K	101	CLA	OBD-CAD-CBD	-2.52	120.88	125.94
17	B	848	BCR	C2-C1-C6	2.52	114.10	110.44
14	b	825	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
17	B	847	BCR	C33-C5-C6	-2.52	121.73	124.48
14	G	807	CLA	C4D-C3D-CAD	2.52	110.84	108.11
14	a	808	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
14	G	821	CLA	C3C-C4C-NC	2.52	113.66	110.43
14	J	101	CLA	CAA-C2A-C3A	-2.52	106.19	113.00
14	B	836	CLA	CAA-C2A-C3A	-2.52	106.19	113.00
17	B	846	BCR	C8-C7-C6	-2.52	120.27	127.00
14	B	806	CLA	C3D-C4D-ND	2.52	114.08	109.99
14	G	830	CLA	CHD-C1D-ND	-2.52	121.26	124.80
14	S	102	CLA	C3C-C4C-NC	2.52	113.66	110.43
14	H	810	CLA	C3C-C4C-NC	2.52	113.65	110.43
14	a	805	CLA	C4D-C3D-CAD	2.52	110.84	108.11
14	H	832	CLA	C3D-C4D-ND	2.52	114.08	109.99
14	H	828	CLA	CAA-C2A-C3A	-2.52	106.20	113.00
14	U	206	CLA	C4-C3-C5	2.52	119.59	115.23
14	L	201	CLA	CMA-C3A-C4A	2.52	118.53	111.77
14	G	840	CLA	C3C-C4C-NC	2.52	113.65	110.43
14	a	830	CLA	C3C-C4C-NC	2.52	113.65	110.43
14	l	207	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
14	A	820	CLA	C4-C3-C5	2.51	119.59	115.23
14	G	815	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
14	A	826	CLA	C1-O2A-CGA	2.51	122.73	116.65
13	a	801	CL0	CHD-C1D-ND	-2.51	121.27	124.80
14	G	833	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
14	a	815	CLA	C4D-C3D-CAD	2.51	110.83	108.11
14	G	810	CLA	CMD-C2D-C3D	-2.51	121.93	127.69
14	A	837	CLA	CMC-C2C-C1C	2.51	128.96	125.03
14	G	809	CLA	CAA-C2A-C1A	-2.51	103.74	111.97
14	A	804	CLA	CMA-C3A-C4A	2.51	118.52	111.77
14	b	810	CLA	C4D-C3D-CAD	2.51	110.83	108.11
14	a	804	CLA	O1D-CGD-CBD	-2.51	119.56	124.52
14	A	808	CLA	CMD-C2D-C3D	-2.51	121.93	127.69
14	i	101	CLA	O2A-C1-C2	2.51	117.77	108.11
14	G	804	CLA	CMA-C3A-C4A	2.51	118.52	111.77
14	b	831	CLA	C1-C2-C3	-2.51	122.08	126.20
14	a	803	CLA	C4D-C3D-CAD	2.51	110.83	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	821	CLA	O2A-C1-C2	2.51	117.77	108.11
14	H	825	CLA	C4C-C3C-C2C	-2.51	103.24	106.89
14	H	820	CLA	C3D-C4D-ND	2.51	114.07	109.99
14	b	829	CLA	C3D-C4D-ND	2.51	114.07	109.99
17	f	201	BCR	C8-C7-C6	-2.51	120.29	127.00
14	l	207	CLA	CMC-C2C-C1C	2.51	128.96	125.03
14	G	805	CLA	O1D-CGD-CBD	-2.51	119.57	124.52
14	A	824	CLA	CMC-C2C-C1C	2.51	128.96	125.03
14	B	831	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
14	F	1301	CLA	CMB-C2B-C3B	2.51	129.70	124.68
14	A	834	CLA	C3D-C4D-ND	2.51	114.06	109.99
14	B	820	CLA	C3C-C4C-NC	2.51	113.64	110.43
14	a	802	CLA	C3C-C4C-NC	2.51	113.64	110.43
14	K	102	CLA	C3C-C4C-NC	2.51	113.64	110.43
14	H	806	CLA	CMC-C2C-C1C	2.51	128.95	125.03
14	a	818	CLA	CMB-C2B-C3B	2.51	129.69	124.68
17	l	201	BCR	C33-C5-C4	2.51	118.94	113.60
14	G	826	CLA	CMA-C3A-C4A	2.51	118.51	111.77
14	b	821	CLA	C3C-C4C-NC	2.51	113.64	110.43
14	a	833	CLA	CMD-C2D-C3D	-2.51	121.94	127.69
14	A	836	CLA	C4D-C3D-CAD	2.51	110.83	108.11
14	a	818	CLA	C3C-C4C-NC	2.51	113.64	110.43
14	H	823	CLA	C3D-C4D-ND	2.51	114.06	109.99
14	A	837	CLA	C4D-C3D-CAD	2.51	110.83	108.11
14	A	830	CLA	CHC-C1C-C2C	-2.50	119.85	126.94
14	B	809	CLA	C3D-C4D-ND	2.50	114.06	109.99
17	l	208	BCR	C35-C13-C12	2.50	121.91	118.09
14	b	830	CLA	C3D-C4D-ND	2.50	114.06	109.99
14	a	825	CLA	CMC-C2C-C1C	2.50	128.95	125.03
14	a	831	CLA	CAC-C3C-C4C	2.50	128.05	124.79
17	i	102	BCR	C33-C5-C4	2.50	118.93	113.60
17	J	103	BCR	C34-C9-C8	2.50	121.91	118.09
14	H	810	CLA	CMA-C3A-C4A	2.50	118.50	111.77
17	G	853	BCR	C35-C13-C12	2.50	121.91	118.09
17	a	848	BCR	C35-C13-C12	2.50	121.91	118.09
14	L	201	CLA	CMB-C2B-C3B	2.50	129.68	124.68
14	H	809	CLA	C3D-C4D-ND	2.50	114.05	109.99
14	a	814	CLA	C3D-C4D-ND	2.50	114.05	109.99
14	b	832	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
17	H	844	BCR	C36-C18-C17	-2.50	118.77	122.82
14	b	813	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
14	H	825	CLA	CHD-C4C-C3C	-2.50	121.13	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	830	CLA	CAC-C3C-C4C	2.50	128.04	124.79
14	B	807	CLA	CMC-C2C-C1C	2.50	128.94	125.03
14	A	818	CLA	C3C-C4C-NC	2.50	113.63	110.43
14	B	802	CLA	C4-C3-C5	2.50	119.57	115.23
17	U	202	BCR	C12-C13-C14	-2.50	115.08	119.01
13	G	801	CL0	O2D-CGD-O1D	-2.50	118.98	123.85
14	B	811	CLA	CAC-C3C-C4C	2.50	128.04	124.79
14	H	838	CLA	O1D-CGD-CBD	-2.50	119.59	124.52
14	B	817	CLA	C3D-C4D-ND	2.50	114.05	109.99
14	H	802	CLA	CMB-C2B-C3B	2.50	129.68	124.68
14	H	823	CLA	CMA-C3A-C2A	2.50	123.64	113.98
14	a	813	CLA	CMC-C2C-C1C	2.50	128.94	125.03
14	B	808	CLA	O1D-CGD-CBD	-2.50	119.59	124.52
14	H	831	CLA	C4-C3-C5	2.50	119.56	115.23
14	a	821	CLA	C4-C3-C5	2.50	119.56	115.23
14	G	836	CLA	C4D-C3D-CAD	2.50	110.82	108.11
14	B	829	CLA	CMC-C2C-C1C	2.50	128.94	125.03
14	A	842	CLA	CMA-C3A-C4A	2.50	118.48	111.77
14	b	809	CLA	C3D-C4D-ND	2.50	114.04	109.99
14	G	823	CLA	CMA-C3A-C4A	2.50	118.48	111.77
14	H	801	CLA	CAA-C2A-C3A	-2.50	106.25	113.00
17	G	853	BCR	C30-C25-C24	2.50	122.42	115.65
14	A	840	CLA	CMA-C3A-C4A	2.50	118.48	111.77
14	G	832	CLA	C3D-C4D-ND	2.50	114.04	109.99
14	H	832	CLA	O1D-CGD-CBD	-2.49	119.60	124.52
17	B	848	BCR	C15-C14-C13	-2.49	123.78	127.28
14	B	823	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	B	836	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
14	H	810	CLA	CMC-C2C-C1C	2.49	128.93	125.03
14	H	814	CLA	C4D-C3D-CAD	2.49	110.81	108.11
14	F	1301	CLA	CAC-C3C-C4C	2.49	128.03	124.79
14	A	823	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	B	833	CLA	CAC-C3C-C4C	2.49	128.03	124.79
14	A	812	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	H	836	CLA	C3D-C4D-ND	2.49	114.04	109.99
17	H	843	BCR	C33-C5-C4	2.49	118.91	113.60
14	b	819	CLA	CHD-C4C-C3C	-2.49	121.14	124.77
14	b	838	CLA	C4D-C3D-CAD	2.49	110.81	108.11
14	H	817	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	A	834	CLA	CAA-C2A-C3A	-2.49	106.27	113.00
13	G	801	CL0	CMB-C2B-C3B	2.49	129.66	124.68
14	a	804	CLA	C4-C3-C5	2.49	119.55	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	206	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
14	A	823	CLA	CHD-C1D-ND	-2.49	121.30	124.80
14	T	1401	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
14	b	828	CLA	CHC-C1C-C2C	-2.49	119.89	126.94
14	b	828	CLA	CAA-C2A-C3A	-2.49	106.28	113.00
14	G	811	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
14	H	812	CLA	C4D-C3D-CAD	2.49	110.81	108.11
14	a	821	CLA	CMC-C2C-C1C	2.49	128.92	125.03
14	b	805	CLA	CMC-C2C-C1C	2.49	128.92	125.03
14	b	813	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
14	A	812	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
14	H	831	CLA	C6-C5-C3	-2.49	107.41	113.47
14	H	807	CLA	CAA-C2A-C3A	-2.49	106.28	113.00
14	B	824	CLA	C3D-C4D-ND	2.49	114.03	109.99
17	a	847	BCR	C24-C23-C22	-2.49	122.56	126.23
14	a	808	CLA	C6-C5-C3	-2.49	107.41	113.47
14	b	825	CLA	C1-O2A-CGA	2.49	122.67	116.65
14	B	827	CLA	C3C-C4C-NC	2.49	113.61	110.43
14	G	841	CLA	C4-C3-C5	2.49	119.54	115.23
14	Q	203	CLA	C3D-C4D-ND	2.48	114.03	109.99
14	b	815	CLA	CAA-C2A-C3A	-2.48	106.28	113.00
14	a	842	CLA	CMC-C2C-C1C	2.48	128.92	125.03
14	A	815	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
14	a	826	CLA	C4-C3-C5	2.48	119.54	115.23
14	b	809	CLA	CHC-C1C-C2C	-2.48	119.91	126.94
14	A	833	CLA	C4D-C3D-CAD	2.48	110.80	108.11
13	A	801	CL0	C3D-C4D-ND	2.48	114.02	109.99
14	H	824	CLA	CMA-C3A-C4A	2.48	118.45	111.77
14	G	826	CLA	C3C-C4C-NC	2.48	113.61	110.43
14	a	812	CLA	C3C-C4C-NC	2.48	113.61	110.43
14	A	816	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
17	f	203	BCR	C12-C13-C14	2.48	122.91	119.01
14	j	102	CLA	C4D-C3D-CAD	2.48	110.80	107.69
17	f	203	BCR	C38-C26-C27	2.48	118.89	113.60
14	H	835	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
14	L	206	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	a	829	CLA	CMC-C2C-C1C	2.48	128.91	125.03
14	B	811	CLA	C3C-C4C-NC	2.48	113.61	110.43
14	B	840	CLA	C1-O2A-CGA	2.48	122.66	116.65
14	H	818	CLA	CAA-C2A-C3A	-2.48	106.30	113.00
14	L	206	CLA	C3C-C4C-NC	2.48	113.61	110.43
14	A	810	CLA	C3D-C4D-ND	2.48	114.02	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	851	BCR	C35-C13-C12	2.48	121.88	118.09
14	H	819	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	A	818	CLA	OBD-CAD-C3D	-2.48	122.62	128.42
14	B	806	CLA	CMB-C2B-C3B	2.48	129.64	124.68
14	B	818	CLA	CMC-C2C-C1C	2.48	128.91	125.03
17	B	847	BCR	C34-C9-C8	2.48	121.88	118.09
14	G	817	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
14	a	809	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	G	805	CLA	C3C-C4C-NC	2.48	113.61	110.43
17	I	101	BCR	C38-C26-C27	2.48	118.88	113.60
14	b	830	CLA	C3C-C4C-NC	2.48	113.60	110.43
14	A	812	CLA	CHC-C1C-C2C	-2.48	119.92	126.94
14	a	816	CLA	C3D-C4D-ND	2.48	114.01	109.99
17	G	853	BCR	C39-C30-C25	-2.48	106.36	110.24
17	B	842	BCR	C33-C5-C6	-2.48	121.78	124.48
14	G	845	CLA	C3D-C4D-ND	2.48	114.01	109.99
14	H	802	CLA	C1-O2A-CGA	2.48	122.65	116.65
14	A	826	CLA	CMD-C2D-C3D	-2.48	122.01	127.69
14	b	830	CLA	CMD-C2D-C3D	-2.48	122.01	127.69
14	a	843	CLA	CMC-C2C-C1C	2.48	128.90	125.03
14	b	835	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
14	G	820	CLA	O1D-CGD-CBD	-2.48	119.64	124.52
14	A	830	CLA	C4D-C3D-CAD	2.47	110.79	108.11
14	H	803	CLA	CHB-C4A-NA	2.47	127.97	124.40
14	a	814	CLA	C3C-C4C-NC	2.47	113.60	110.43
14	j	101	CLA	C3C-C4C-NC	2.47	113.60	110.43
14	b	838	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
14	A	809	CLA	CMC-C2C-C1C	2.47	128.90	125.03
14	G	819	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
14	G	843	CLA	CHC-C1C-C2C	-2.47	119.94	126.94
14	G	831	CLA	CAC-C3C-C4C	2.47	128.01	124.79
14	a	804	CLA	C3D-C4D-ND	2.47	114.01	109.99
14	H	837	CLA	C4-C3-C5	2.47	119.52	115.23
14	A	817	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
14	a	844	CLA	C4C-C3C-C2C	-2.47	103.29	106.89
14	B	814	CLA	CMB-C2B-C3B	2.47	129.62	124.68
14	B	803	CLA	C3D-C4D-ND	2.47	114.00	109.99
14	H	838	CLA	CMC-C2C-C1C	2.47	128.90	125.03
17	B	843	BCR	C12-C13-C14	-2.47	115.12	119.01
14	a	822	CLA	C3C-C4C-NC	2.47	113.60	110.43
14	A	823	CLA	C4D-C3D-CAD	2.47	110.79	108.11
14	b	822	CLA	CAC-C3C-C4C	2.47	128.00	124.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	832	CLA	C4D-C3D-CAD	2.47	110.79	108.11
14	S	102	CLA	C4D-C3D-CAD	2.47	110.78	107.69
14	b	801	CLA	CBC-CAC-C3C	-2.47	105.73	112.42
14	a	839	CLA	C3C-C4C-NC	2.47	113.59	110.43
14	G	837	CLA	CAC-C3C-C4C	2.47	128.00	124.79
14	B	837	CLA	C1-C2-C3	-2.47	122.15	126.20
14	a	827	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
14	U	205	CLA	CMC-C2C-C1C	2.47	128.89	125.03
14	f	202	CLA	CAC-C3C-C4C	2.47	128.00	124.79
14	G	819	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
14	H	803	CLA	C4-C3-C5	2.47	119.51	115.23
14	H	810	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
14	A	842	CLA	C3C-C4C-NC	2.47	113.59	110.43
14	G	805	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
14	a	823	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
14	b	820	CLA	CMB-C2B-C3B	2.47	129.61	124.68
14	b	808	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
14	b	828	CLA	C3D-C4D-ND	2.47	114.00	109.99
14	i	101	CLA	C1-O2A-CGA	2.47	122.62	116.65
14	B	819	CLA	CMB-C2B-C3B	2.47	129.61	124.68
17	b	843	BCR	C40-C30-C25	-2.46	106.38	110.24
14	B	806	CLA	CAA-C2A-C3A	-2.46	106.34	113.00
14	G	825	CLA	CAA-C2A-C3A	-2.46	106.34	113.00
19	B	849	LMG	O8-C28-C29	2.46	119.35	111.83
14	A	803	CLA	OBD-CAD-C3D	-2.46	122.66	128.42
14	A	840	CLA	CAA-C2A-C3A	-2.46	106.34	113.00
14	K	102	CLA	CMB-C2B-C3B	2.46	129.60	124.68
14	a	836	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
14	H	824	CLA	C3D-C4D-ND	2.46	113.99	109.99
17	A	853	BCR	C34-C9-C10	-2.46	118.83	122.82
17	A	849	BCR	C28-C27-C26	-2.46	109.66	114.06
14	B	825	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
14	A	844	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
17	B	847	BCR	C2-C1-C6	2.46	114.01	110.44
14	b	820	CLA	C4D-C3D-CAD	2.46	110.78	108.11
17	j	103	BCR	C33-C5-C6	-2.46	121.80	124.48
14	a	842	CLA	CMD-C2D-C3D	-2.46	122.05	127.69
14	K	102	CLA	CAA-C2A-C3A	-2.46	106.35	113.00
14	A	805	CLA	C3C-C4C-NC	2.46	113.58	110.43
14	H	809	CLA	C3C-C4C-NC	2.46	113.58	110.43
13	G	801	CL0	CHD-C1D-ND	-2.46	121.34	124.80
14	B	808	CLA	CMA-C3A-C4A	2.46	118.39	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	839	CLA	C4-C3-C5	2.46	119.50	115.23
14	a	830	CLA	C4-C3-C5	2.46	119.50	115.23
14	a	803	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
14	B	832	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
15	a	845	PQN	C11-C3-C2	-2.46	120.67	124.89
14	j	102	CLA	C3C-C4C-NC	2.46	113.58	110.43
14	a	825	CLA	CMA-C3A-C2A	2.46	123.49	113.98
14	H	807	CLA	C1-C2-C3	-2.46	122.17	126.20
14	G	816	CLA	C4D-C3D-CAD	2.46	110.78	108.11
14	a	806	CLA	C4D-C3D-CAD	2.46	110.78	108.11
14	H	840	CLA	CHC-C1C-C2C	-2.46	119.98	126.94
14	H	802	CLA	C3C-C4C-NC	2.46	113.58	110.43
14	B	825	CLA	OBD-CAD-C3D	-2.46	122.67	128.42
14	A	822	CLA	C4D-C3D-CAD	2.46	110.78	108.11
14	H	839	CLA	C3C-C4C-NC	2.46	113.58	110.43
14	b	808	CLA	C3C-C4C-NC	2.46	113.58	110.43
14	a	820	CLA	C1-O2A-CGA	2.46	122.60	116.65
17	J	103	BCR	C1-C6-C7	2.46	122.31	115.65
17	H	843	BCR	C34-C9-C8	2.46	121.84	118.09
14	B	825	CLA	C4-C3-C5	2.46	119.49	115.23
14	L	205	CLA	C4D-C3D-CAD	2.46	110.77	108.11
14	B	820	CLA	C3D-C4D-ND	2.46	113.98	109.99
14	Q	201	CLA	CMD-C2D-C3D	-2.45	122.06	127.69
17	i	102	BCR	C35-C13-C12	2.45	121.84	118.09
14	b	840	CLA	C3C-C4C-NC	2.45	113.57	110.43
14	l	202	CLA	C3C-C4C-NC	2.45	113.57	110.43
14	a	805	CLA	CMD-C2D-C3D	-2.45	122.06	127.69
14	b	805	CLA	CMD-C2D-C3D	-2.45	122.06	127.69
14	G	836	CLA	C3D-C4D-ND	2.45	113.97	109.99
14	H	840	CLA	C3D-C4D-ND	2.45	113.97	109.99
14	Q	203	CLA	C3C-C4C-NC	2.45	113.57	110.43
14	a	816	CLA	CMD-C2D-C3D	-2.45	122.06	127.69
14	B	836	CLA	CMC-C2C-C1C	2.45	128.87	125.03
14	A	814	CLA	C3D-C4D-ND	2.45	113.97	109.99
14	a	840	CLA	C3D-C4D-ND	2.45	113.97	109.99
14	V	1601	CLA	C3D-C4D-ND	2.45	113.97	109.99
14	a	834	CLA	C3D-C4D-ND	2.45	113.97	109.99
14	G	845	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
14	a	843	CLA	CMA-C3A-C4A	2.45	118.36	111.77
14	H	832	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
14	B	810	CLA	C4D-C3D-CAD	2.45	110.77	108.11
14	H	826	CLA	C3D-C4D-ND	2.45	113.97	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	836	CLA	C3C-C4C-NC	2.45	113.57	110.43
14	A	814	CLA	C1-O2A-CGA	2.45	122.58	116.65
13	a	801	CL0	C4-C3-C5	2.45	119.48	115.23
17	Q	202	BCR	C37-C22-C21	-2.45	118.85	122.82
14	B	835	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
14	H	814	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
14	X	1701	CLA	C4D-C3D-CAD	2.45	110.77	108.11
14	A	845	CLA	CAA-C2A-C3A	-2.45	106.38	113.00
14	H	806	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
14	A	811	CLA	CAC-C3C-C4C	2.45	127.97	124.79
14	B	825	CLA	CMA-C3A-C4A	2.45	118.35	111.77
14	G	812	CLA	CHC-C1C-C2C	-2.45	120.01	126.94
14	b	810	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
17	a	849	BCR	C7-C8-C9	-2.45	122.62	126.23
14	b	806	CLA	CAC-C3C-C4C	2.45	127.97	124.79
14	b	839	CLA	CHB-C4A-NA	2.44	127.93	124.40
14	U	201	CLA	C1-C2-C3	-2.44	122.19	126.20
17	B	848	BCR	C34-C9-C10	-2.44	118.86	122.82
14	F	1303	CLA	C4D-C3D-CAD	2.44	110.75	107.69
14	b	828	CLA	C4-C3-C5	2.44	119.47	115.23
14	a	805	CLA	CAC-C3C-C4C	2.44	127.97	124.79
14	X	1701	CLA	CMB-C2B-C3B	2.44	129.56	124.68
14	B	829	CLA	C3D-C4D-ND	2.44	113.96	109.99
14	B	816	CLA	C6-C5-C3	-2.44	107.52	113.47
17	H	843	BCR	C38-C26-C27	2.44	118.80	113.60
14	b	816	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
14	G	809	CLA	O1D-CGD-CBD	-2.44	119.70	124.52
14	A	833	CLA	C3C-C4C-NC	2.44	113.56	110.43
14	a	842	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
14	A	828	CLA	C1-C2-C3	-2.44	122.20	126.20
14	G	828	CLA	CHD-C1D-ND	-2.44	121.37	124.80
14	A	805	CLA	C4-C3-C5	2.44	119.46	115.23
14	a	837	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
14	H	830	CLA	C3D-C4D-ND	2.44	113.95	109.99
14	b	823	CLA	C3D-C4D-ND	2.44	113.95	109.99
17	f	201	BCR	C19-C18-C17	2.44	122.85	119.01
14	G	837	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
14	b	806	CLA	C3D-C4D-ND	2.44	113.95	109.99
14	A	817	CLA	CMC-C2C-C1C	2.44	128.84	125.03
14	a	844	CLA	CMC-C2C-C3C	2.44	132.74	126.15
14	H	826	CLA	C4-C3-C5	2.44	119.46	115.23
14	a	833	CLA	O2D-CGD-O1D	-2.44	119.10	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	837	CLA	C3D-C4D-ND	2.44	113.95	109.99
14	G	839	CLA	CMC-C2C-C1C	2.44	128.84	125.03
14	B	830	CLA	C3D-C4D-ND	2.44	113.95	109.99
14	A	825	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
14	G	827	CLA	C4-C3-C5	2.44	119.46	115.23
14	G	808	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
17	A	852	BCR	C34-C9-C10	-2.44	118.87	122.82
14	A	836	CLA	CMB-C2B-C3B	2.44	129.55	124.68
14	H	814	CLA	CBC-CAC-C3C	-2.44	105.82	112.42
14	H	801	CLA	C3D-C4D-ND	2.44	113.94	109.99
14	H	829	CLA	CMA-C3A-C4A	2.43	118.32	111.77
14	A	802	CLA	C4-C3-C5	2.43	119.45	115.23
14	G	814	CLA	C3D-C4D-ND	2.43	113.94	109.99
14	H	831	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
14	b	830	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
14	A	835	CLA	C3D-C4D-ND	2.43	113.94	109.99
17	R	102	BCR	C33-C5-C4	2.43	118.78	113.60
14	H	809	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
14	G	809	CLA	CAA-CBA-CGA	-2.43	106.30	113.21
17	B	847	BCR	C36-C18-C17	-2.43	118.88	122.82
14	a	817	CLA	CMC-C2C-C1C	2.43	128.84	125.03
14	H	803	CLA	O2D-CGD-CBD	2.43	115.48	111.23
14	B	815	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
14	a	830	CLA	CHC-C1C-C2C	-2.43	120.05	126.94
14	b	809	CLA	C4C-C3C-C2C	-2.43	103.35	106.89
14	A	813	CLA	C4D-C3D-CAD	2.43	110.75	108.11
14	H	815	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
14	a	829	CLA	CHD-C1D-ND	-2.43	121.38	124.80
17	b	844	BCR	C33-C5-C4	2.43	118.78	113.60
14	G	845	CLA	CHD-C4C-C3C	-2.43	121.23	124.77
14	H	819	CLA	CMB-C2B-C3B	2.43	129.54	124.68
14	B	815	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
14	B	835	CLA	CMC-C2C-C1C	2.43	128.83	125.03
14	A	836	CLA	C3D-C4D-ND	2.43	113.94	109.99
17	S	103	BCR	C38-C26-C25	-2.43	121.83	124.48
14	i	101	CLA	C4-C3-C5	2.43	119.44	115.23
14	B	835	CLA	C3C-C4C-NC	2.43	113.54	110.43
14	L	204	CLA	CMA-C3A-C4A	2.43	118.30	111.77
14	f	202	CLA	CMB-C2B-C3B	2.43	129.54	124.68
14	H	828	CLA	C3D-C4D-ND	2.43	113.94	109.99
14	a	838	CLA	O2A-C1-C2	2.43	117.45	108.11
17	G	853	BCR	C34-C9-C10	-2.43	118.88	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	a	851	BCR	C34-C9-C10	-2.43	118.88	122.82
17	B	847	BCR	C19-C18-C17	2.43	122.83	119.01
14	B	840	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
14	G	827	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
15	G	846	PQN	C2M-C2-C3	-2.43	120.46	124.45
14	U	205	CLA	CAC-C3C-C4C	2.43	127.95	124.79
14	a	832	CLA	CMA-C3A-C4A	2.43	118.30	111.77
14	A	832	CLA	C4D-C3D-CAD	2.43	110.74	108.11
14	B	837	CLA	C4-C3-C5	2.43	119.44	115.23
14	B	801	CLA	C4C-C3C-C2C	-2.43	103.36	106.89
14	H	834	CLA	C3C-C4C-NC	2.43	113.54	110.43
14	a	815	CLA	C3C-C4C-NC	2.43	113.54	110.43
14	A	804	CLA	C3D-C4D-ND	2.43	113.93	109.99
14	B	830	CLA	CMA-C3A-C4A	2.43	118.29	111.77
14	U	201	CLA	CMA-C3A-C4A	2.43	118.29	111.77
17	l	203	BCR	C12-C13-C14	-2.43	115.19	119.01
14	L	205	CLA	CMC-C2C-C1C	2.43	128.82	125.03
14	b	809	CLA	CMA-C3A-C4A	2.43	118.29	111.77
14	a	803	CLA	CMB-C2B-C3B	2.43	129.53	124.68
17	j	103	BCR	C34-C9-C8	2.42	121.79	118.09
14	B	830	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
14	a	804	CLA	OBD-CAD-C3D	-2.42	122.75	128.42
14	A	815	CLA	C3D-C4D-ND	2.42	113.93	109.99
14	a	820	CLA	CMC-C2C-C1C	2.42	128.82	125.03
14	B	831	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
14	G	838	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
14	G	835	CLA	CMA-C3A-C4A	2.42	118.29	111.77
14	H	816	CLA	C3C-C4C-NC	2.42	113.53	110.43
14	H	808	CLA	CMA-C3A-C4A	2.42	118.28	111.77
14	b	835	CLA	CAC-C3C-C4C	2.42	127.94	124.79
14	G	844	CLA	OBD-CAD-CBD	-2.42	121.08	125.94
14	A	830	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
14	L	206	CLA	C6-C5-C3	-2.42	107.57	113.47
14	a	842	CLA	C1-C2-C3	-2.42	122.23	126.20
14	A	817	CLA	CAC-C3C-C4C	2.42	127.94	124.79
14	l	206	CLA	C4D-C3D-CAD	2.42	110.73	108.11
14	a	809	CLA	C4-C3-C5	2.42	119.43	115.23
17	l	201	BCR	C35-C13-C12	2.42	121.78	118.09
14	l	205	CLA	C4-C3-C5	2.42	119.43	115.23
14	A	805	CLA	O1D-CGD-CBD	-2.42	119.75	124.52
17	H	844	BCR	C15-C14-C13	-2.42	123.89	127.28
14	A	814	CLA	C4C-C3C-C2C	-2.42	103.37	106.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	b	844	BCR	C24-C23-C22	-2.42	122.66	126.23
17	B	847	BCR	C33-C5-C4	2.42	118.75	113.60
14	b	836	CLA	C4C-C3C-C2C	-2.42	103.38	106.89
14	x	1701	CLA	CAC-C3C-C4C	2.42	127.93	124.79
15	B	841	PQN	C14-C13-C15	2.42	119.42	115.23
15	A	846	PQN	C11-C3-C2	-2.41	120.75	124.89
14	A	833	CLA	CMC-C2C-C1C	2.41	128.81	125.03
14	b	823	CLA	C1-O2A-CGA	2.41	122.50	116.65
14	F	1301	CLA	CMA-C3A-C4A	2.41	118.26	111.77
17	a	848	BCR	C31-C1-C6	-2.41	106.46	110.24
14	B	802	CLA	CMA-C3A-C2A	-2.41	104.65	113.98
14	X	1701	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
14	B	808	CLA	CBA-CAA-C2A	2.41	120.97	113.79
14	G	805	CLA	C3D-C4D-ND	2.41	113.91	109.99
17	Q	204	BCR	C36-C18-C17	-2.41	118.91	122.82
14	H	821	CLA	C4-C3-C5	2.41	119.42	115.23
14	a	839	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
14	a	821	CLA	C1-O2A-CGA	2.41	122.49	116.65
14	b	832	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
14	H	829	CLA	C3D-C4D-ND	2.41	113.91	109.99
17	a	850	BCR	C27-C26-C25	-2.41	119.45	122.70
17	j	104	BCR	C4-C5-C6	-2.41	119.45	122.70
17	a	849	BCR	C35-C13-C12	2.41	121.77	118.09
14	B	818	CLA	C3C-C4C-NC	2.41	113.52	110.43
14	H	840	CLA	C4D-C3D-CAD	2.41	110.72	108.11
14	a	826	CLA	C4D-C3D-CAD	2.41	110.72	108.11
14	l	205	CLA	C3C-C4C-NC	2.41	113.52	110.43
14	G	820	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
17	M	1602	BCR	C35-C13-C12	2.41	121.77	118.09
14	b	804	CLA	CBC-CAC-C3C	2.41	118.95	112.42
14	B	808	CLA	CMB-C2B-C1B	2.41	131.99	128.46
14	B	825	CLA	C4D-C3D-CAD	2.41	110.72	108.11
14	G	809	CLA	C3C-C4C-NC	2.41	113.52	110.43
14	G	834	CLA	C3C-C4C-NC	2.41	113.52	110.43
14	B	820	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
14	A	802	CLA	CHD-C4C-C3C	-2.41	121.26	124.77
14	a	828	CLA	C4D-C3D-CAD	2.41	110.72	108.11
14	b	817	CLA	C3D-C4D-ND	2.41	113.90	109.99
14	F	1303	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
14	b	807	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
14	b	823	CLA	CMA-C3A-C2A	2.41	123.29	113.98
14	B	830	CLA	OBD-CAD-C3D	-2.41	122.79	128.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	808	CLA	CBA-CAA-C2A	2.41	120.96	113.79
14	a	826	CLA	C3C-C4C-NC	2.41	113.51	110.43
14	a	832	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
14	b	816	CLA	C4-C3-C5	2.41	119.41	115.23
14	a	809	CLA	C3C-C4C-NC	2.41	113.51	110.43
14	A	824	CLA	CMB-C2B-C3B	2.41	129.49	124.68
14	A	844	CLA	CHC-C1C-C2C	-2.41	120.13	126.94
14	H	840	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
14	a	824	CLA	C3C-C4C-NC	2.41	113.51	110.43
14	a	813	CLA	CAA-C2A-C3A	-2.40	106.50	113.00
14	a	814	CLA	CMC-C2C-C1C	2.40	128.79	125.03
14	J	101	CLA	C3D-C4D-ND	2.40	113.89	109.99
14	B	831	CLA	CMC-C2C-C1C	2.40	128.79	125.03
14	A	828	CLA	C1C-C2C-C3C	-2.40	104.45	106.98
14	H	822	CLA	CAC-C3C-C4C	2.40	127.92	124.79
14	a	810	CLA	CAC-C3C-C4C	2.40	127.92	124.79
14	A	839	CLA	C6-C5-C3	-2.40	107.61	113.47
17	G	849	BCR	C30-C25-C26	-2.40	119.35	122.64
14	G	838	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
14	M	1601	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
14	H	838	CLA	C4D-C3D-CAD	2.40	110.72	108.11
14	B	821	CLA	CAC-C3C-C4C	2.40	127.92	124.79
14	A	822	CLA	CED-O2D-CGD	2.40	121.36	115.92
14	b	813	CLA	C3C-C4C-NC	2.40	113.51	110.43
14	a	807	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
14	G	815	CLA	CMC-C2C-C1C	2.40	128.79	125.03
14	b	823	CLA	C4C-C3C-C2C	-2.40	103.40	106.89
14	A	840	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
14	l	202	CLA	C3D-C4D-ND	2.40	113.89	109.99
14	H	802	CLA	C4-C3-C5	2.40	119.39	115.23
17	Q	204	BCR	C19-C18-C17	2.40	122.78	119.01
14	a	820	CLA	C3D-C4D-ND	2.40	113.89	109.99
14	b	829	CLA	CMD-C2D-C3D	-2.40	122.19	127.69
17	Q	202	BCR	C2-C1-C6	2.40	113.92	110.44
14	B	833	CLA	CMC-C2C-C1C	2.40	128.78	125.03
14	f	202	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
14	G	813	CLA	CAC-C3C-C4C	2.40	127.91	124.79
17	l	201	BCR	C23-C22-C21	2.40	122.78	119.01
17	A	849	BCR	C23-C24-C25	-2.40	120.59	127.00
14	a	834	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
14	A	805	CLA	C3D-C4D-ND	2.40	113.89	109.99
14	a	806	CLA	O2D-CGD-O1D	-2.40	119.18	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	821	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
14	a	835	CLA	C4D-C3D-CAD	2.40	110.71	108.11
14	B	803	CLA	CMC-C2C-C1C	2.40	128.78	125.03
14	b	812	CLA	CMC-C2C-C1C	2.40	128.78	125.03
14	A	839	CLA	C3C-C4C-NC	2.40	113.50	110.43
17	b	843	BCR	C34-C9-C8	2.40	121.75	118.09
14	a	806	CLA	C1-C2-C3	-2.40	122.27	126.20
14	B	838	CLA	CAA-C2A-C3A	-2.40	106.52	113.00
14	A	824	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
14	A	835	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
14	H	822	CLA	C4C-C3C-C2C	-2.40	103.40	106.89
14	G	843	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
14	b	822	CLA	C3C-C4C-NC	2.40	113.50	110.43
14	B	828	CLA	C3D-C4D-ND	2.40	113.88	109.99
14	b	812	CLA	C3D-C4D-ND	2.40	113.88	109.99
14	a	830	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
14	A	840	CLA	CMB-C2B-C3B	2.40	129.47	124.68
14	B	813	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
14	A	834	CLA	CMD-C2D-C3D	-2.39	122.20	127.69
14	b	840	CLA	C3D-C4D-ND	2.39	113.88	109.99
17	S	103	BCR	C35-C13-C12	2.39	121.74	118.09
14	A	808	CLA	CAA-C2A-C3A	-2.39	106.53	113.00
14	H	821	CLA	C1-C2-C3	-2.39	122.28	126.20
14	U	204	CLA	C3C-C4C-NC	2.39	113.50	110.43
17	j	103	BCR	C12-C13-C14	-2.39	115.25	119.01
14	H	804	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
17	H	847	BCR	C24-C23-C22	-2.39	122.70	126.23
14	H	807	CLA	CMC-C2C-C1C	2.39	128.77	125.03
17	G	851	BCR	C36-C18-C17	-2.39	118.94	122.82
17	i	102	BCR	C37-C22-C21	-2.39	118.94	122.82
14	b	827	CLA	C3C-C4C-NC	2.39	113.49	110.43
14	a	820	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
14	a	828	CLA	C3D-C4D-ND	2.39	113.87	109.99
14	F	1301	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
14	A	810	CLA	CAC-C3C-C4C	2.39	127.90	124.79
14	G	838	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
14	G	807	CLA	CMC-C2C-C1C	2.39	128.77	125.03
14	A	809	CLA	CMA-C3A-C4A	2.39	118.19	111.77
14	G	829	CLA	C3D-C4D-ND	2.39	113.87	109.99
14	G	824	CLA	C3C-C4C-NC	2.39	113.49	110.43
14	G	839	CLA	C3C-C4C-NC	2.39	113.49	110.43
14	A	822	CLA	C4-C3-C5	2.39	119.37	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	807	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
14	W	1701	CLA	C3D-C4D-ND	2.39	113.87	109.99
14	b	820	CLA	C3D-C4D-ND	2.39	113.87	109.99
17	B	843	BCR	C34-C9-C8	2.39	121.73	118.09
14	S	101	CLA	C3D-C4D-ND	2.39	113.87	109.99
14	H	818	CLA	C3C-C4C-NC	2.39	113.49	110.43
17	A	851	BCR	C35-C13-C12	2.39	121.73	118.09
14	G	826	CLA	CHC-C1C-C2C	-2.39	120.18	126.94
14	B	802	CLA	C4D-C3D-CAD	2.39	110.70	108.11
14	H	818	CLA	CMB-C2B-C3B	2.39	129.45	124.68
14	b	838	CLA	CMA-C3A-C4A	2.39	118.19	111.77
14	H	830	CLA	CMD-C2D-C3D	-2.39	122.22	127.69
17	H	844	BCR	C35-C13-C12	2.39	121.73	118.09
14	G	841	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
14	H	816	CLA	C4-C3-C5	2.39	119.37	115.23
14	G	841	CLA	C3C-C4C-NC	2.38	113.48	110.43
14	B	812	CLA	C3D-C4D-ND	2.38	113.86	109.99
14	b	832	CLA	C1-C2-C3	-2.38	122.29	126.20
13	a	801	CL0	C1-O2A-CGA	2.38	122.42	116.65
17	l	203	BCR	C31-C1-C6	-2.38	106.51	110.24
14	G	831	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
14	j	101	CLA	C3D-C4D-ND	2.38	113.86	109.99
17	G	853	BCR	C24-C25-C26	-2.38	116.07	121.56
17	B	847	BCR	C4-C5-C6	-2.38	119.48	122.70
17	b	845	BCR	C19-C18-C17	2.38	122.76	119.01
14	A	810	CLA	C4D-C3D-CAD	2.38	110.69	108.11
14	G	825	CLA	C4D-C3D-CAD	2.38	110.69	108.11
14	a	836	CLA	CMC-C2C-C1C	2.38	128.76	125.03
14	A	808	CLA	CED-O2D-CGD	2.38	121.32	115.92
14	Q	201	CLA	CMB-C2B-C3B	2.38	129.44	124.68
14	b	821	CLA	C3D-C4D-ND	2.38	113.86	109.99
14	H	829	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
14	B	826	CLA	CMA-C3A-C4A	2.38	118.17	111.77
17	Q	204	BCR	C32-C1-C6	-2.38	106.51	110.24
14	b	838	CLA	CAA-C2A-C3A	-2.38	106.57	113.00
17	A	852	BCR	C36-C18-C17	-2.38	118.96	122.82
14	b	837	CLA	OBD-CAD-C3D	-2.38	122.85	128.42
14	A	841	CLA	C3D-C4D-ND	2.38	113.86	109.99
17	G	851	BCR	C38-C26-C27	2.38	118.67	113.60
14	H	801	CLA	C4C-C3C-C2C	-2.38	103.43	106.89
14	B	807	CLA	C4-C3-C5	2.38	119.36	115.23
15	H	841	PQN	C14-C13-C15	2.38	119.36	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	811	CLA	CMB-C2B-C3B	2.38	129.44	124.68
14	A	830	CLA	C4-C3-C5	2.38	119.36	115.23
14	a	809	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
14	b	803	CLA	CMA-C3A-C2A	-2.38	104.79	113.98
14	b	818	CLA	C4D-C3D-CAD	2.38	110.69	108.11
14	G	836	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	B	834	CLA	CED-O2D-CGD	2.38	121.31	115.92
14	a	835	CLA	C3C-C4C-NC	2.38	113.48	110.43
14	A	832	CLA	CAC-C3C-C4C	2.38	127.88	124.79
17	f	203	BCR	C7-C8-C9	-2.38	122.72	126.23
14	A	831	CLA	C3C-C4C-NC	2.38	113.47	110.43
14	A	821	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
14	L	201	CLA	C3D-C4D-ND	2.38	113.85	109.99
14	B	821	CLA	CMB-C2B-C3B	2.38	129.43	124.68
14	G	807	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
14	b	827	CLA	CMD-C2D-C3D	-2.37	122.24	127.69
14	i	101	CLA	CAA-C2A-C3A	-2.37	106.58	113.00
14	G	814	CLA	C4-C3-C5	2.37	119.35	115.23
14	l	206	CLA	C4-C3-C5	2.37	119.35	115.23
14	b	801	CLA	CAA-CBA-CGA	-2.37	106.47	113.21
14	b	818	CLA	CED-O2D-CGD	2.37	121.30	115.92
14	B	820	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
17	B	846	BCR	C19-C18-C17	2.37	122.74	119.01
14	G	813	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
14	b	805	CLA	C1-O2A-CGA	2.37	122.39	116.65
14	a	808	CLA	C3C-C4C-NC	2.37	113.47	110.43
14	a	818	CLA	CMA-C3A-C4A	2.37	118.15	111.77
14	b	826	CLA	C3D-C4D-ND	2.37	113.84	109.99
14	G	822	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
14	U	206	CLA	CMC-C2C-C1C	2.37	128.74	125.03
17	J	102	BCR	C1-C6-C7	2.37	122.09	115.65
14	H	805	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
14	H	834	CLA	C3D-C4D-ND	2.37	113.84	109.99
14	A	837	CLA	CMA-C3A-C4A	2.37	118.15	111.77
14	G	840	CLA	CAC-C3C-C4C	2.37	127.88	124.79
14	A	811	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
14	b	804	CLA	O2D-CGD-CBD	2.37	115.38	111.23
14	B	833	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
14	G	809	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
14	a	844	CLA	C3D-C4D-ND	2.37	113.84	109.99
14	H	818	CLA	CMC-C2C-C1C	2.37	128.74	125.03
14	A	814	CLA	CMA-C3A-C4A	2.37	118.14	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	836	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
14	G	826	CLA	CHD-C1D-ND	-2.37	121.47	124.80
14	A	838	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
14	G	810	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
19	B	849	LMG	C7-O1-C1	-2.37	108.72	113.80
14	B	836	CLA	C4D-C3D-CAD	2.37	110.68	108.11
14	H	817	CLA	C4D-C3D-CAD	2.37	110.68	108.11
14	b	836	CLA	C4D-C3D-CAD	2.37	110.68	108.11
14	b	807	CLA	CMB-C2B-C3B	2.37	129.42	124.68
14	a	818	CLA	CAC-C3C-C4C	2.37	127.87	124.79
14	A	819	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
14	B	832	CLA	C3C-C4C-NC	2.37	113.46	110.43
14	A	841	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
17	A	851	BCR	C33-C5-C6	-2.37	121.90	124.48
14	H	823	CLA	CHD-C1D-ND	-2.37	121.47	124.80
14	a	831	CLA	CMC-C2C-C1C	2.37	128.73	125.03
14	a	820	CLA	C3C-C4C-NC	2.37	113.46	110.43
14	B	801	CLA	C3D-C4D-ND	2.37	113.83	109.99
14	B	840	CLA	CMA-C3A-C4A	2.37	118.14	111.77
14	A	839	CLA	C4-C3-C5	2.37	119.34	115.23
17	B	847	BCR	C37-C22-C21	-2.37	118.98	122.82
14	A	840	CLA	C3C-C4C-NC	2.37	113.46	110.43
14	a	816	CLA	CMB-C2B-C3B	2.37	129.41	124.68
14	b	808	CLA	CBA-CAA-C2A	2.37	120.83	113.79
17	H	846	BCR	C38-C26-C27	2.37	118.64	113.60
14	A	813	CLA	CAA-C2A-C3A	-2.37	106.61	113.00
14	L	201	CLA	CGD-CBD-CAD	-2.37	103.19	110.85
14	H	835	CLA	CMD-C2D-C3D	-2.37	122.27	127.69
14	G	820	CLA	CAC-C3C-C4C	2.37	127.87	124.79
14	U	205	CLA	O1D-CGD-CBD	-2.36	119.85	124.52
14	b	835	CLA	C3C-C4C-NC	2.36	113.46	110.43
14	H	811	CLA	C4D-C3D-CAD	2.36	110.67	108.11
14	F	1301	CLA	C3D-C4D-ND	2.36	113.83	109.99
14	k	1401	CLA	CAA-C2A-C3A	-2.36	106.61	113.00
14	a	802	CLA	CAC-C3C-C4C	2.36	127.86	124.79
14	A	840	CLA	C4D-C3D-CAD	2.36	110.67	108.11
17	H	845	BCR	C28-C27-C26	-2.36	109.84	114.06
14	b	810	CLA	CMA-C3A-C4A	2.36	118.12	111.77
14	B	824	CLA	CMC-C2C-C1C	2.36	128.73	125.03
14	b	840	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
14	G	830	CLA	C3D-C4D-ND	2.36	113.83	109.99
17	a	849	BCR	C37-C22-C21	-2.36	118.99	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	818	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
14	A	838	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
14	H	813	CLA	C4-C3-C5	2.36	119.33	115.23
14	a	837	CLA	C1-C2-C3	-2.36	122.94	126.76
14	b	816	CLA	CAC-C3C-C4C	2.36	127.86	124.79
14	B	838	CLA	CMB-C2B-C3B	2.36	129.40	124.68
17	G	850	BCR	C8-C7-C6	-2.36	120.69	127.00
14	G	827	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
17	B	843	BCR	C35-C13-C12	2.36	121.69	118.09
14	b	824	CLA	C3C-C4C-NC	2.36	113.45	110.43
14	G	808	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
14	B	812	CLA	C4C-C3C-C2C	-2.36	103.46	106.89
14	B	822	CLA	C4C-C3C-C2C	-2.36	103.46	106.89
14	H	828	CLA	CHA-C4D-ND	2.36	137.42	132.55
14	b	829	CLA	CHC-C1C-C2C	-2.36	120.26	126.94
14	A	837	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
14	H	832	CLA	C3C-C4C-NC	2.36	113.45	110.43
14	B	805	CLA	CAC-C3C-C4C	2.36	127.86	124.79
14	k	1401	CLA	CMB-C2B-C3B	2.36	129.40	124.68
14	a	842	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
17	A	849	BCR	C36-C18-C17	-2.36	119.00	122.82
14	B	829	CLA	C3C-C4C-NC	2.36	113.45	110.43
14	H	821	CLA	C3D-C4D-ND	2.36	113.82	109.99
14	A	840	CLA	CAC-C3C-C4C	2.36	127.86	124.79
17	L	202	BCR	C36-C18-C17	-2.36	119.00	122.82
14	x	1701	CLA	CMB-C2B-C3B	2.36	129.39	124.68
14	A	816	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
17	a	848	BCR	C27-C26-C25	-2.36	119.52	122.70
14	J	101	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
14	A	820	CLA	CAC-C3C-C4C	2.36	127.86	124.79
14	B	838	CLA	CMD-C2D-C3D	-2.36	122.29	127.69
14	A	843	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
14	B	810	CLA	CAC-C3C-C4C	2.36	127.85	124.79
14	A	819	CLA	CMB-C2B-C3B	2.35	129.39	124.68
17	b	849	BCR	C36-C18-C17	-2.35	119.00	122.82
14	A	806	CLA	O1D-CGD-CBD	-2.35	119.87	124.52
14	U	206	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
14	G	804	CLA	CAC-C3C-C4C	2.35	127.85	124.79
14	b	837	CLA	C3C-C4C-NC	2.35	113.45	110.43
17	G	848	BCR	C36-C18-C17	-2.35	119.00	122.82
14	B	828	CLA	CHC-C1C-C2C	-2.35	120.27	126.94
17	A	851	BCR	C34-C9-C8	2.35	121.68	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	834	CLA	C3D-C4D-ND	2.35	113.81	109.99
14	a	825	CLA	C14-C13-C15	-2.35	102.88	111.27
14	U	201	CLA	C3C-C4C-NC	2.35	113.44	110.43
14	G	808	CLA	CMB-C2B-C3B	2.35	129.39	124.68
14	a	815	CLA	C3D-C4D-ND	2.35	113.81	109.99
14	b	836	CLA	C3D-C4D-ND	2.35	113.81	109.99
14	H	836	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
14	b	813	CLA	C4-C3-C5	2.35	119.31	115.23
14	A	816	CLA	C3D-C4D-ND	2.35	113.81	109.99
17	G	851	BCR	C35-C13-C12	2.35	121.68	118.09
14	G	839	CLA	CMB-C2B-C3B	2.35	129.38	124.68
14	A	808	CLA	C3C-C4C-NC	2.35	113.44	110.43
17	H	843	BCR	C35-C13-C12	2.35	121.68	118.09
14	A	831	CLA	CHC-C1C-C2C	-2.35	120.28	126.94
14	K	101	CLA	CMC-C2C-C1C	2.35	128.71	125.03
17	I	102	BCR	C34-C9-C8	2.35	121.68	118.09
14	b	811	CLA	CMA-C3A-C4A	2.35	118.09	111.77
14	G	805	CLA	OBD-CAD-C3D	-2.35	122.92	128.42
14	L	201	CLA	C3C-C4C-NC	2.35	113.44	110.43
17	U	202	BCR	C33-C5-C6	-2.35	121.92	124.48
14	a	823	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
14	G	832	CLA	CAA-C2A-C3A	-2.35	106.65	113.00
17	a	852	BCR	C34-C9-C10	-2.35	119.01	122.82
14	b	808	CLA	CMC-C2C-C1C	2.35	128.70	125.03
17	G	853	BCR	C8-C9-C10	2.35	122.70	119.01
14	G	814	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
17	l	203	BCR	C23-C22-C21	-2.35	115.32	119.01
14	A	821	CLA	C3D-C4D-ND	2.35	113.80	109.99
17	j	104	BCR	C1-C6-C7	2.35	122.02	115.65
14	a	828	CLA	CMA-C3A-C4A	2.35	118.08	111.77
14	G	820	CLA	C3D-C4D-ND	2.35	113.80	109.99
14	a	841	CLA	C3C-C4C-NC	2.35	113.44	110.43
17	A	850	BCR	C36-C18-C17	-2.35	119.02	122.82
17	R	103	BCR	C37-C22-C21	-2.35	119.02	122.82
17	f	201	BCR	C37-C22-C21	-2.35	119.02	122.82
14	G	844	CLA	CMB-C2B-C3B	2.35	129.37	124.68
14	a	829	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
14	b	839	CLA	CAA-C2A-C3A	-2.34	106.66	113.00
14	G	834	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
14	b	829	CLA	OBD-CAD-C3D	-2.34	122.94	128.42
14	G	826	CLA	C3D-C4D-ND	2.34	113.80	109.99
14	a	817	CLA	O1D-CGD-CBD	-2.34	119.89	124.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	843	BCR	C37-C22-C21	-2.34	119.02	122.82
17	L	207	BCR	C34-C9-C10	-2.34	119.02	122.82
17	S	104	BCR	C8-C7-C6	-2.34	120.74	127.00
14	H	833	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
15	B	841	PQN	C11-C3-C2	-2.34	120.87	124.89
17	A	849	BCR	C34-C9-C8	2.34	121.67	118.09
14	H	812	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
14	H	832	CLA	CHC-C1C-C2C	-2.34	120.31	126.94
14	U	201	CLA	CAA-C2A-C1A	2.34	119.65	111.97
14	G	805	CLA	C4-C3-C5	2.34	119.29	115.23
14	U	205	CLA	C4-C3-C5	2.34	119.29	115.23
14	G	812	CLA	C3B-C4B-NB	2.34	112.24	109.21
14	a	809	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
14	b	819	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
14	a	816	CLA	CAC-C3C-C4C	2.34	127.83	124.79
14	a	808	CLA	CMC-C2C-C1C	2.34	128.69	125.03
14	B	830	CLA	C3C-C4C-NC	2.34	113.43	110.43
14	B	838	CLA	C3C-C4C-NC	2.34	113.43	110.43
14	H	804	CLA	C6-C5-C3	-2.34	107.77	113.47
17	H	842	BCR	C33-C5-C6	-2.34	121.93	124.48
14	b	829	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
14	b	806	CLA	C3C-C4C-NC	2.34	113.42	110.43
17	j	104	BCR	C37-C22-C21	-2.34	119.03	122.82
14	H	829	CLA	C3C-C4C-NC	2.34	113.42	110.43
14	i	101	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
14	B	813	CLA	C1-O2A-CGA	2.34	122.30	116.65
14	B	807	CLA	CAA-C2A-C3A	-2.34	106.69	113.00
14	H	810	CLA	O2D-CGD-O1D	-2.33	119.30	123.85
14	A	826	CLA	C3D-C4D-ND	2.33	113.78	109.99
14	B	840	CLA	C4D-C3D-CAD	2.33	110.64	108.11
14	B	809	CLA	C3B-C4B-NB	2.33	112.23	109.21
14	H	815	CLA	CAA-C2A-C3A	-2.33	106.69	113.00
14	Q	203	CLA	CAA-C2A-C3A	-2.33	106.69	113.00
14	L	201	CLA	CAC-C3C-C4C	2.33	127.83	124.79
14	l	202	CLA	CAC-C3C-C4C	2.33	127.83	124.79
14	H	815	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
14	H	801	CLA	CHD-C4C-C3C	-2.33	121.37	124.77
14	b	804	CLA	C1-O2A-CGA	2.33	122.30	116.65
14	G	817	CLA	CMC-C2C-C1C	2.33	128.68	125.03
17	b	844	BCR	C37-C22-C23	2.33	121.65	118.09
14	b	803	CLA	CHD-C1D-ND	-2.33	121.52	124.80
14	b	804	CLA	CHB-C4A-NA	2.33	127.76	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	841	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
14	H	821	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
14	B	802	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
17	b	847	BCR	C36-C18-C17	-2.33	119.04	122.82
17	I	102	BCR	C28-C27-C26	-2.33	109.90	114.06
14	J	101	CLA	CMA-C3A-C4A	2.33	118.03	111.77
14	X	1701	CLA	C3D-C4D-ND	2.33	113.77	109.99
14	A	813	CLA	C3C-C4C-NC	2.33	113.41	110.43
14	B	807	CLA	C3C-C4C-NC	2.33	113.41	110.43
14	G	803	CLA	C3C-C4C-NC	2.33	113.41	110.43
14	G	831	CLA	CHC-C1C-C2C	-2.33	120.35	126.94
14	H	840	CLA	C4-C3-C5	2.33	119.27	115.23
14	b	806	CLA	C4-C3-C5	2.33	119.27	115.23
14	H	808	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
14	a	803	CLA	C4-C3-C5	2.33	119.27	115.23
17	B	842	BCR	C15-C14-C13	-2.33	124.01	127.28
14	G	809	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
14	K	101	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
14	B	802	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
14	b	839	CLA	C3C-C4C-NC	2.33	113.41	110.43
14	b	831	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
14	b	809	CLA	CMC-C2C-C3C	2.33	132.44	126.15
14	B	822	CLA	CAC-C3C-C4C	2.33	127.82	124.79
14	l	202	CLA	CMC-C2C-C1C	2.33	128.67	125.03
14	B	805	CLA	CMD-C2D-C3D	-2.33	122.36	127.69
17	H	844	BCR	C34-C9-C8	2.33	121.64	118.09
17	f	203	BCR	C34-C9-C10	-2.33	119.05	122.82
14	A	843	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
17	a	850	BCR	C30-C25-C26	-2.32	119.46	122.64
14	U	204	CLA	CMC-C2C-C1C	2.32	128.66	125.03
18	G	854	LHG	C5-O7-C7	-2.32	112.23	117.80
14	B	802	CLA	CMB-C2B-C3B	2.32	129.33	124.68
14	A	828	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
14	B	826	CLA	C4-C3-C5	2.32	119.26	115.23
14	G	841	CLA	CAC-C3C-C4C	2.32	127.81	124.79
14	a	855	CLA	CHA-C1A-NA	-2.32	121.13	126.39
17	l	208	BCR	C33-C5-C6	-2.32	121.95	124.48
14	B	805	CLA	C4-C3-C5	2.32	119.26	115.23
14	b	836	CLA	CHD-C1D-ND	-2.32	121.54	124.80
14	A	815	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
14	H	828	CLA	CMA-C3A-C4A	2.32	118.01	111.77
14	a	813	CLA	C4D-C3D-CAD	2.32	110.63	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	827	CLA	CMB-C2B-C3B	2.32	129.32	124.68
14	G	811	CLA	CHD-C4C-C3C	-2.32	121.39	124.77
14	B	805	CLA	C6-C5-C3	-2.32	107.82	113.47
14	G	814	CLA	CAC-C3C-C4C	2.32	127.81	124.79
14	T	1401	CLA	C4D-C3D-CAD	2.32	110.62	108.11
14	A	810	CLA	C3C-C4C-NC	2.32	113.40	110.43
14	F	1301	CLA	CAA-C2A-C3A	-2.32	106.73	113.00
14	a	808	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
14	b	836	CLA	OBD-CAD-C3D	-2.32	123.00	128.42
14	B	817	CLA	CHC-C1C-C2C	-2.32	120.38	126.94
14	G	813	CLA	C3C-C4C-NC	2.32	113.40	110.43
14	m	1601	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
14	a	822	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
17	B	844	BCR	C19-C18-C17	2.32	122.65	119.01
14	G	813	CLA	C4D-C3D-CAD	2.32	110.62	108.11
14	H	811	CLA	C3C-C4C-NC	2.32	113.40	110.43
14	a	828	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
14	H	819	CLA	OBD-CAD-C3D	-2.32	123.00	128.42
14	G	830	CLA	C6-C5-C3	-2.32	107.83	113.47
14	a	830	CLA	CMC-C2C-C3C	2.32	132.41	126.15
14	A	802	CLA	C3D-C4D-ND	2.32	113.75	109.99
14	b	815	CLA	O2D-CGD-O1D	-2.31	119.34	123.85
14	A	825	CLA	CAA-C2A-C3A	-2.31	106.75	113.00
14	l	202	CLA	O2D-CGD-O1D	-2.31	119.34	123.85
14	H	823	CLA	C4D-C3D-CAD	2.31	110.62	108.11
14	B	840	CLA	C6-C7-C8	-2.31	108.28	115.97
19	B	849	LMG	O7-C10-O9	-2.31	118.30	123.70
14	b	807	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
14	b	837	CLA	CAA-C2A-C3A	-2.31	106.75	113.00
14	A	804	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
14	G	841	CLA	C1-C2-C3	-2.31	122.41	126.20
17	G	851	BCR	C15-C14-C13	-2.31	124.03	127.28
17	B	845	BCR	C35-C13-C12	2.31	119.91	114.59
14	b	812	CLA	C4D-C3D-CAD	2.31	110.62	108.11
14	B	821	CLA	C1-O2A-CGA	2.31	122.25	116.65
14	A	808	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
14	B	823	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
14	b	821	CLA	CAC-C3C-C4C	2.31	127.80	124.79
14	a	829	CLA	C4-C3-C5	2.31	119.24	115.23
14	A	839	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
17	B	846	BCR	C34-C9-C10	-2.31	119.08	122.82
14	L	204	CLA	C3C-C4C-NC	2.31	113.39	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	832	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
14	H	837	CLA	CMA-C3A-C4A	2.31	117.98	111.77
14	b	802	CLA	C3C-C4C-NC	2.31	113.39	110.43
14	A	844	CLA	CAA-CBA-CGA	-2.31	106.66	113.21
14	G	818	CLA	CED-O2D-CGD	2.31	121.15	115.92
13	A	801	CL0	C4-C3-C5	2.31	119.23	115.23
14	B	803	CLA	C4-C3-C5	2.31	119.23	115.23
14	b	821	CLA	C4D-C3D-CAD	2.31	110.61	108.11
14	a	810	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
14	a	837	CLA	C3D-C4D-ND	2.31	113.73	109.99
17	a	850	BCR	C12-C13-C14	-2.31	115.38	119.01
14	H	816	CLA	CMA-C3A-C4A	2.30	117.97	111.77
14	B	826	CLA	C3D-C4D-ND	2.30	113.73	109.99
14	A	815	CLA	CHC-C1C-C2C	-2.30	120.41	126.94
14	F	1303	CLA	CMC-C2C-C1C	2.30	128.63	125.03
14	A	838	CLA	C3C-C4C-NC	2.30	113.38	110.43
17	A	851	BCR	C30-C25-C26	-2.30	119.49	122.64
17	j	103	BCR	C29-C30-C25	2.30	113.79	110.44
14	U	201	CLA	C3D-C4D-ND	2.30	113.73	109.99
14	H	807	CLA	C1-O2A-CGA	2.30	122.23	116.65
14	b	806	CLA	CHB-C4A-NA	2.30	127.72	124.40
14	b	827	CLA	CMC-C2C-C1C	2.30	128.63	125.03
14	a	841	CLA	CMB-C2B-C3B	2.30	129.28	124.68
14	a	834	CLA	CMC-C2C-C1C	2.30	128.63	125.03
14	a	839	CLA	CMA-C3A-C4A	2.30	117.96	111.77
14	B	815	CLA	C3C-C4C-NC	2.30	113.38	110.43
14	G	842	CLA	C11-C12-C13	-2.30	108.31	115.97
14	H	815	CLA	C3C-C4C-NC	2.30	113.38	110.43
17	G	852	BCR	C28-C27-C26	-2.30	109.95	114.06
14	H	812	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
17	A	850	BCR	C27-C26-C25	-2.30	119.59	122.70
14	G	816	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
14	b	801	CLA	CHD-C4C-C3C	-2.30	121.42	124.77
14	a	802	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
14	b	827	CLA	C1-O2A-CGA	2.30	122.22	116.65
14	G	824	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
17	L	202	BCR	C23-C24-C25	-2.30	120.86	127.00
14	A	808	CLA	CMB-C2B-C3B	2.30	129.28	124.68
14	L	204	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
17	G	849	BCR	C12-C13-C14	-2.30	115.39	119.01
14	A	836	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
14	A	807	CLA	CMD-C2D-C3D	-2.30	122.42	127.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	811	CLA	CMB-C2B-C3B	2.30	129.27	124.68
17	i	102	BCR	C34-C9-C10	-2.30	119.09	122.82
14	H	817	CLA	CMC-C2C-C1C	2.30	128.62	125.03
14	H	814	CLA	CMB-C2B-C3B	2.30	129.27	124.68
14	B	803	CLA	CHB-C4A-NA	2.30	127.71	124.40
17	G	850	BCR	C19-C18-C17	2.29	122.62	119.01
17	R	101	BCR	C34-C9-C10	-2.29	119.10	122.82
14	a	816	CLA	C3C-C4C-NC	2.29	113.37	110.43
17	b	845	BCR	C35-C13-C12	2.29	119.87	114.59
14	G	816	CLA	O1D-CGD-CBD	-2.29	119.99	124.52
14	G	821	CLA	C3D-C4D-ND	2.29	113.72	109.99
14	A	829	CLA	CAA-C2A-C3A	-2.29	106.80	113.00
13	A	801	CL0	CMB-C2B-C3B	2.29	129.27	124.68
14	H	831	CLA	C3C-C4C-NC	2.29	113.37	110.43
14	a	820	CLA	CMB-C2B-C3B	2.29	129.26	124.68
14	A	810	CLA	C4-C3-C5	2.29	119.21	115.23
14	b	840	CLA	C6-C5-C3	-2.29	107.88	113.47
14	Q	203	CLA	CAC-C3C-C4C	2.29	127.77	124.79
14	B	803	CLA	O2D-CGD-CBD	2.29	115.24	111.23
14	B	831	CLA	C6-C7-C8	-2.29	108.35	115.97
14	l	202	CLA	OBD-CAD-C3D	-2.29	123.06	128.42
14	b	825	CLA	C4C-C3C-C2C	-2.29	103.56	106.89
14	U	201	CLA	CGD-CBD-CAD	-2.29	103.43	110.85
14	U	205	CLA	C3C-C4C-NC	2.29	113.36	110.43
14	B	832	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
14	B	829	CLA	CHC-C1C-C2C	-2.29	120.46	126.94
14	H	817	CLA	CHC-C1C-C2C	-2.29	120.46	126.94
14	a	821	CLA	CED-O2D-CGD	2.29	121.10	115.92
14	M	1601	CLA	CED-O2D-CGD	2.29	121.10	115.92
14	G	802	CLA	C3C-C4C-NC	2.29	113.36	110.43
14	a	825	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
17	b	842	BCR	C3-C4-C5	-2.29	109.98	114.06
14	a	825	CLA	C4-C3-C5	2.29	119.19	115.23
14	A	812	CLA	C4-C3-C5	2.28	119.19	115.23
14	B	830	CLA	O2D-CGD-O1D	-2.28	119.40	123.85
14	A	839	CLA	CAC-C3C-C4C	2.28	127.76	124.79
14	G	829	CLA	CAA-C2A-C3A	-2.28	106.83	113.00
14	a	823	CLA	OBD-CAD-C3D	-2.28	123.08	128.42
14	H	827	CLA	CMC-C2C-C1C	2.28	128.60	125.03
17	H	842	BCR	C38-C26-C25	-2.28	121.99	124.48
14	f	202	CLA	OBD-CAD-C3D	-2.28	123.08	128.42
14	B	826	CLA	CAC-C3C-C4C	2.28	127.76	124.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	814	CLA	CAC-C3C-C4C	2.28	127.76	124.79
14	G	821	CLA	C5-C3-C4	2.28	119.84	114.59
14	b	813	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
14	B	809	CLA	CMA-C3A-C4A	2.28	117.91	111.77
17	G	850	BCR	C1-C6-C5	-2.28	119.52	122.64
14	b	833	CLA	CAC-C3C-C4C	2.28	127.76	124.79
14	G	810	CLA	C4-C3-C5	2.28	119.19	115.23
14	b	822	CLA	C4D-C3D-CAD	2.28	110.58	108.11
14	A	821	CLA	CMB-C2B-C3B	2.28	129.24	124.68
14	H	828	CLA	CHC-C1C-C2C	-2.28	120.48	126.94
17	B	844	BCR	C34-C9-C8	2.28	121.57	118.09
14	A	821	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
17	H	845	BCR	C35-C13-C12	2.28	119.84	114.59
14	B	832	CLA	CAC-C3C-C4C	2.28	127.76	124.79
14	H	829	CLA	CHC-C1C-C2C	-2.28	120.48	126.94
14	H	824	CLA	CAA-C2A-C1A	-2.28	104.50	111.97
14	b	815	CLA	C3C-C4C-NC	2.28	113.35	110.43
14	A	827	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
14	B	824	CLA	CMA-C3A-C4A	2.28	117.90	111.77
14	A	817	CLA	C3C-C4C-NC	2.28	113.35	110.43
14	b	811	CLA	C3C-C4C-NC	2.28	113.35	110.43
14	H	838	CLA	CMA-C3A-C4A	2.28	117.90	111.77
14	a	840	CLA	CHB-C4A-NA	2.28	127.69	124.40
17	a	849	BCR	C33-C5-C6	-2.28	122.00	124.48
14	a	834	CLA	CAC-C3C-C4C	2.28	127.75	124.79
14	G	832	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
14	a	816	CLA	CHB-C4A-NA	2.28	127.69	124.40
14	a	855	CLA	C3D-C4D-ND	2.28	113.69	109.99
14	G	835	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
14	H	825	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
14	G	840	CLA	CAA-C2A-C3A	-2.28	106.85	113.00
14	G	822	CLA	CMC-C2C-C1C	2.28	128.59	125.03
14	G	838	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
14	a	838	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
14	B	821	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
14	a	813	CLA	CMD-C2D-C3D	-2.27	122.47	127.69
14	U	205	CLA	C4D-C3D-CAD	2.27	110.58	108.11
17	B	848	BCR	C33-C5-C6	-2.27	122.00	124.48
14	H	820	CLA	OBD-CAD-C3D	-2.27	123.10	128.42
14	b	819	CLA	C3D-C4D-ND	2.27	113.68	109.99
14	b	840	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
14	a	837	CLA	CMD-C2D-C3D	-2.27	122.48	127.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	831	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
14	a	837	CLA	OBD-CAD-C3D	-2.27	123.10	128.42
17	G	850	BCR	C37-C22-C21	-2.27	119.13	122.82
17	L	202	BCR	C31-C1-C6	-2.27	106.68	110.24
14	b	805	CLA	C3C-C4C-NC	2.27	113.34	110.43
14	G	819	CLA	CMA-C3A-C4A	2.27	117.88	111.77
14	G	805	CLA	CHB-C4A-NA	2.27	127.68	124.40
14	b	808	CLA	CMA-C3A-C4A	2.27	117.88	111.77
15	A	846	PQN	C2M-C2-C3	-2.27	120.72	124.45
14	B	808	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
14	j	102	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
14	G	825	CLA	C4-C3-C5	2.27	119.17	115.23
14	a	813	CLA	C3D-C4D-ND	2.27	113.67	109.99
14	G	843	CLA	CAA-C2A-C3A	-2.27	106.87	113.00
17	i	102	BCR	C8-C7-C6	-2.27	120.94	127.00
14	B	824	CLA	C3C-C4C-NC	2.27	113.33	110.43
14	A	804	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
14	l	207	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
14	G	807	CLA	C3C-C4C-NC	2.26	113.33	110.43
14	G	842	CLA	CMB-C2B-C3B	2.26	129.21	124.68
14	G	820	CLA	CHC-C1C-C2C	-2.26	120.53	126.94
14	W	1701	CLA	CMB-C2B-C3B	2.26	129.21	124.68
14	A	841	CLA	C3C-C4C-NC	2.26	113.33	110.43
14	G	811	CLA	OBD-CAD-C3D	-2.26	123.13	128.42
14	K	101	CLA	CAA-C2A-C3A	-2.26	106.88	113.00
14	a	811	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
14	m	1601	CLA	CMB-C2B-C3B	2.26	129.20	124.68
14	H	823	CLA	CHA-C1A-NA	-2.26	121.27	126.39
14	b	810	CLA	C3C-C4C-NC	2.26	113.33	110.43
14	A	827	CLA	C3C-C4C-NC	2.26	113.33	110.43
14	b	833	CLA	C3C-C4C-NC	2.26	113.33	110.43
17	G	850	BCR	C37-C22-C23	2.26	121.54	118.09
17	R	102	BCR	C36-C18-C17	-2.26	119.15	122.82
14	a	843	CLA	CHC-C1C-C2C	-2.26	120.54	126.94
17	f	203	BCR	C27-C26-C25	-2.26	119.65	122.70
14	G	832	CLA	CAC-C3C-C4C	2.26	127.73	124.79
14	a	838	CLA	CMB-C2B-C3B	2.26	129.20	124.68
14	b	831	CLA	C3C-C4C-NC	2.26	113.33	110.43
14	a	805	CLA	CHB-C4A-NA	2.26	127.66	124.40
14	b	839	CLA	C1-O2A-CGA	2.26	122.12	116.65
14	A	844	CLA	C4D-C3D-CAD	2.26	110.56	108.11
17	b	844	BCR	C35-C13-C12	2.26	121.54	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	839	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
17	H	849	BCR	C37-C22-C21	-2.26	119.16	122.82
14	B	830	CLA	CED-O2D-CGD	2.26	121.04	115.92
17	G	850	BCR	C8-C9-C10	-2.26	115.46	119.01
14	G	818	CLA	C3C-C4C-NC	2.26	113.32	110.43
14	b	809	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
14	b	828	CLA	CHA-C4D-ND	2.26	137.21	132.55
14	H	825	CLA	C4-C3-C5	2.26	119.15	115.23
14	B	814	CLA	CHC-C1C-C2C	-2.26	120.55	126.94
14	B	809	CLA	CMC-C2C-C3C	2.26	132.25	126.15
14	G	845	CLA	C4C-C3C-C2C	-2.26	103.61	106.89
14	A	831	CLA	O1D-CGD-CBD	-2.26	120.07	124.52
14	H	823	CLA	CAC-C3C-C4C	2.26	127.72	124.79
14	A	813	CLA	CMC-C2C-C1C	2.26	128.56	125.03
14	B	820	CLA	C4D-C3D-CAD	2.25	110.56	108.11
14	H	838	CLA	C3C-C4C-NC	2.25	113.32	110.43
14	B	823	CLA	CHD-C1D-ND	-2.25	121.63	124.80
14	A	834	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
14	a	806	CLA	CMB-C2B-C3B	2.25	129.19	124.68
14	A	829	CLA	C3D-C4D-ND	2.25	113.65	109.99
14	G	827	CLA	C1-C2-C3	-2.25	122.50	126.20
14	A	805	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
14	B	828	CLA	CHA-C4D-ND	2.25	137.20	132.55
14	G	822	CLA	C3C-C4C-NC	2.25	113.31	110.43
17	B	846	BCR	C37-C22-C21	-2.25	119.17	122.82
14	B	840	CLA	C3D-C4D-ND	2.25	113.64	109.99
14	H	834	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
14	H	803	CLA	C4D-C3D-CAD	2.25	110.55	108.11
14	U	204	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
14	A	822	CLA	C3C-C4C-NC	2.25	113.31	110.43
14	a	810	CLA	CHC-C1C-C2C	-2.25	120.57	126.94
14	G	812	CLA	CBC-CAC-C3C	-2.25	106.32	112.42
14	a	811	CLA	C4-C3-C5	2.25	119.13	115.23
14	H	829	CLA	CMC-C2C-C1C	2.25	128.55	125.03
14	B	837	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
14	H	813	CLA	C4C-C3C-C2C	-2.25	103.62	106.89
14	a	813	CLA	C4C-C3C-C2C	-2.25	103.62	106.89
14	H	816	CLA	CAC-C3C-C4C	2.25	127.71	124.79
14	G	806	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
17	I	203	BCR	C36-C18-C17	-2.25	119.17	122.82
14	B	804	CLA	C4-C3-C5	2.25	119.13	115.23
14	B	805	CLA	CMC-C2C-C1C	2.25	128.54	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	838	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
14	b	838	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
14	a	840	CLA	C4-C3-C5	2.25	119.13	115.23
14	m	1601	CLA	CAC-C3C-C4C	2.25	127.71	124.79
14	G	813	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
14	G	816	CLA	CHC-C1C-C2C	-2.24	120.58	126.94
14	H	826	CLA	CMC-C2C-C1C	2.24	128.54	125.03
14	G	817	CLA	CHB-C4A-NA	2.24	127.64	124.40
14	H	813	CLA	CAC-C3C-C4C	2.24	127.71	124.79
17	I	102	BCR	C36-C18-C17	-2.24	119.18	122.82
14	K	102	CLA	C4D-C3D-CAD	2.24	110.54	108.11
14	B	831	CLA	C1-C2-C3	-2.24	122.52	126.20
14	A	802	CLA	OBD-CAD-C3D	-2.24	123.17	128.42
17	m	1602	BCR	C39-C30-C25	-2.24	106.72	110.24
14	a	811	CLA	CHC-C1C-C2C	-2.24	120.59	126.94
14	B	807	CLA	OBD-CAD-C3D	-2.24	123.17	128.42
17	b	846	BCR	C37-C22-C21	-2.24	119.18	122.82
17	A	853	BCR	C12-C13-C14	-2.24	115.48	119.01
14	B	831	CLA	C3C-C4C-NC	2.24	113.30	110.43
17	L	202	BCR	C12-C13-C14	-2.24	115.48	119.01
14	A	825	CLA	C3C-C4C-NC	2.24	113.30	110.43
18	a	854	LHG	C5-O7-C7	-2.24	112.44	117.80
14	A	844	CLA	C3C-C4C-NC	2.24	113.30	110.43
14	H	814	CLA	C3C-C4C-NC	2.24	113.30	110.43
17	J	103	BCR	C33-C5-C4	2.24	118.37	113.60
17	a	852	BCR	C35-C13-C12	2.24	121.51	118.09
17	A	849	BCR	C37-C22-C23	2.24	121.51	118.09
17	b	846	BCR	C19-C18-C17	2.24	122.53	119.01
14	H	824	CLA	CAC-C3C-C4C	2.24	127.70	124.79
17	B	850	BCR	C37-C22-C21	-2.24	119.19	122.82
14	A	815	CLA	C3C-C4C-NC	2.24	113.30	110.43
14	H	828	CLA	C4-C3-C5	2.24	119.11	115.23
14	a	809	CLA	CAA-C2A-C3A	-2.24	106.95	113.00
17	B	850	BCR	C32-C1-C6	-2.24	106.73	110.24
17	J	102	BCR	C19-C18-C17	2.24	122.53	119.01
14	A	816	CLA	CHC-C1C-C2C	-2.24	120.61	126.94
14	G	823	CLA	C3C-C4C-NC	2.24	113.30	110.43
14	b	817	CLA	CHC-C1C-C2C	-2.24	120.61	126.94
14	L	201	CLA	CMA-C3A-C2A	2.24	122.62	113.98
14	L	201	CLA	OBD-CAD-C3D	-2.24	123.19	128.42
14	G	835	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
14	A	841	CLA	C4-C3-C5	2.24	119.11	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	816	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
17	l	208	BCR	C38-C26-C27	2.23	118.36	113.60
14	G	827	CLA	C4D-C3D-CAD	2.23	110.53	108.11
14	W	1701	CLA	CAA-C2A-C3A	-2.23	106.96	113.00
14	H	824	CLA	CMC-C2C-C1C	2.23	128.53	125.03
14	b	808	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
14	G	812	CLA	C1-O2A-CGA	2.23	122.06	116.65
14	A	845	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
14	B	817	CLA	C4D-C3D-CAD	2.23	110.53	108.11
14	a	814	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
14	A	830	CLA	CHD-C1D-ND	-2.23	121.66	124.80
14	B	816	CLA	CHD-C4C-C3C	-2.23	121.52	124.77
14	a	829	CLA	C3D-C4D-ND	2.23	113.61	109.99
14	H	835	CLA	CMC-C2C-C1C	2.23	128.52	125.03
14	H	808	CLA	C1-C2-C3	-2.23	122.54	126.20
14	U	206	CLA	CAC-C3C-C4C	2.23	127.69	124.79
14	A	812	CLA	CMB-C2B-C3B	2.23	129.14	124.68
14	a	806	CLA	CHB-C4A-NA	2.23	127.62	124.40
14	l	202	CLA	CAA-C2A-C1A	2.23	119.29	111.97
17	F	1302	BCR	C38-C26-C27	2.23	118.35	113.60
14	G	827	CLA	C3C-C4C-NC	2.23	113.29	110.43
14	A	818	CLA	CHB-C4A-NA	2.23	127.62	124.40
14	a	804	CLA	CHB-C4A-NA	2.23	127.62	124.40
14	A	802	CLA	CAA-CBA-CGA	-2.23	106.88	113.21
17	A	852	BCR	C38-C26-C27	2.23	118.35	113.60
14	B	801	CLA	CMA-C3A-C4A	2.23	117.77	111.77
14	a	839	CLA	CAC-C3C-C4C	2.23	127.69	124.79
14	G	809	CLA	C4-C3-C5	2.23	119.10	115.23
14	G	822	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
14	B	821	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
14	L	206	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
14	A	839	CLA	CAA-C2A-C3A	-2.23	106.98	113.00
17	I	102	BCR	C37-C22-C21	-2.23	119.21	122.82
14	m	1601	CLA	CMC-C2C-C1C	2.23	128.51	125.03
14	B	837	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
17	I	101	BCR	C12-C13-C14	-2.23	115.51	119.01
17	A	848	BCR	C34-C9-C10	-2.23	119.21	122.82
17	A	851	BCR	C36-C18-C17	-2.23	119.21	122.82
17	U	202	BCR	C29-C28-C27	-2.23	106.38	111.28
14	S	101	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
14	A	826	CLA	C3B-C4B-NB	2.23	112.09	109.21
14	L	204	CLA	O2D-CGD-O1D	-2.23	119.52	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	815	CLA	CMD-C2D-C3D	-2.23	122.59	127.69
14	a	823	CLA	CMC-C2C-C1C	2.23	128.51	125.03
14	K	101	CLA	CHC-C1C-C2C	-2.22	120.64	126.94
14	H	814	CLA	C3D-C4D-ND	2.22	113.60	109.99
14	B	834	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
17	i	102	BCR	C38-C26-C27	2.22	118.34	113.60
14	H	809	CLA	C4D-C3D-CAD	2.22	110.52	108.11
17	H	846	BCR	C35-C13-C12	2.22	121.49	118.09
14	b	807	CLA	CED-O2D-CGD	2.22	120.96	115.92
14	B	814	CLA	OBD-CAD-C3D	-2.22	123.22	128.42
14	A	810	CLA	CAA-C2A-C3A	-2.22	106.99	113.00
14	H	801	CLA	CMB-C2B-C3B	2.22	129.13	124.68
14	A	835	CLA	CMC-C2C-C1C	2.22	128.51	125.03
14	H	827	CLA	CHD-C1D-ND	-2.22	121.67	124.80
17	a	850	BCR	C30-C25-C24	2.22	121.68	115.65
14	B	801	CLA	CHB-C4A-NA	2.22	127.61	124.40
13	G	801	CL0	CBC-CAC-C3C	-2.22	106.39	112.42
14	G	821	CLA	C1-O2A-CGA	2.22	122.03	116.65
14	G	829	CLA	CAA-CBA-CGA	-2.22	106.90	113.21
14	a	817	CLA	OBD-CAD-C3D	-2.22	123.22	128.42
14	H	809	CLA	C6-C5-C3	-2.22	108.06	113.47
14	b	815	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
14	a	815	CLA	CHC-C1C-C2C	-2.22	120.65	126.94
14	b	821	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
14	A	845	CLA	CHC-C1C-C2C	-2.22	120.65	126.94
14	a	813	CLA	CMA-C3A-C4A	2.22	117.74	111.77
17	j	103	BCR	C2-C1-C6	2.22	113.67	110.44
14	A	842	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
14	U	204	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
14	H	833	CLA	CMC-C2C-C1C	2.22	128.50	125.03
14	A	826	CLA	CMA-C3A-C2A	2.22	122.57	113.98
14	b	809	CLA	C6-C5-C3	-2.22	108.06	113.47
14	H	836	CLA	C4-C3-C5	2.22	119.08	115.23
14	b	821	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
14	a	826	CLA	CBC-CAC-C3C	-2.22	106.40	112.42
14	a	818	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
14	F	1303	CLA	CAC-C3C-C4C	2.22	127.68	124.79
14	a	832	CLA	OBD-CAD-C3D	-2.22	123.23	128.42
14	H	819	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
14	a	817	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
17	Q	202	BCR	C36-C18-C17	-2.22	119.22	122.82
14	A	802	CLA	C4D-C3D-CAD	2.22	110.51	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	844	CLA	CHD-C4C-C3C	-2.22	121.54	124.77
14	a	832	CLA	C3C-C4C-NC	2.22	113.27	110.43
14	G	818	CLA	CAC-C3C-C4C	2.22	127.67	124.79
17	G	849	BCR	C27-C26-C25	-2.22	119.71	122.70
14	G	845	CLA	CAC-C3C-C4C	-2.22	121.91	124.79
14	a	834	CLA	C3C-C4C-NC	2.22	113.27	110.43
17	U	202	BCR	C36-C18-C17	-2.22	119.23	122.82
14	a	825	CLA	O1D-CGD-CBD	-2.22	120.15	124.52
17	b	844	BCR	C19-C18-C17	2.21	122.49	119.01
14	a	830	CLA	CMB-C2B-C1B	-2.21	125.21	128.46
14	H	804	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
14	a	841	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
14	a	855	CLA	C4C-C3C-C2C	-2.21	103.67	106.89
17	V	1602	BCR	C35-C13-C12	2.21	121.47	118.09
14	A	824	CLA	C3C-C4C-NC	2.21	113.27	110.43
17	G	852	BCR	C36-C18-C17	-2.21	119.23	122.82
17	a	847	BCR	C34-C9-C10	-2.21	119.23	122.82
14	i	101	CLA	C1-C2-C3	-2.21	122.57	126.20
14	G	815	CLA	C3C-C4C-NC	2.21	113.26	110.43
14	G	802	CLA	C4-C3-C5	2.21	119.07	115.23
14	H	840	CLA	C6-C5-C3	-2.21	108.08	113.47
14	H	831	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
14	B	810	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
17	b	846	BCR	C35-C13-C12	2.21	121.47	118.09
14	B	819	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
14	A	804	CLA	C1-C2-C3	-2.21	122.58	126.20
14	b	816	CLA	CAA-C2A-C3A	-2.21	107.03	113.00
14	a	824	CLA	CED-O2D-CGD	2.21	120.93	115.92
14	H	805	CLA	C1-O2A-CGA	2.21	122.00	116.65
14	A	809	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
14	H	807	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
14	B	817	CLA	CAA-C2A-C3A	-2.21	107.03	113.00
14	a	807	CLA	C3C-C4C-NC	2.21	113.26	110.43
14	M	1601	CLA	C3D-C4D-ND	2.21	113.58	109.99
14	G	842	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
14	b	840	CLA	C4D-C3D-CAD	2.21	110.50	108.11
14	S	102	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
17	f	203	BCR	C15-C14-C13	-2.21	124.18	127.28
14	S	102	CLA	CAC-C3C-C4C	2.21	127.66	124.79
14	B	837	CLA	CBA-CAA-C2A	2.21	120.36	113.79
14	B	825	CLA	O1D-CGD-CBD	-2.21	120.17	124.52
14	H	825	CLA	CHD-C1D-ND	-2.21	121.70	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	852	BCR	C29-C28-C27	2.21	116.13	111.28
17	H	844	BCR	C39-C30-C25	-2.21	106.78	110.24
14	G	803	CLA	O2D-CGD-O1D	-2.21	119.56	123.85
17	b	844	BCR	C8-C9-C10	2.21	122.48	119.01
14	b	806	CLA	CMC-C2C-C1C	2.21	128.48	125.03
14	b	812	CLA	C11-C10-C8	-2.20	108.64	115.97
14	L	201	CLA	CHA-C1A-NA	-2.20	121.40	126.39
17	S	104	BCR	C35-C13-C12	2.20	121.46	118.09
14	b	807	CLA	C3C-C4C-NC	2.20	113.25	110.43
14	G	813	CLA	C1-O2A-CGA	2.20	121.99	116.65
14	A	818	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
14	H	830	CLA	CMC-C2C-C1C	2.20	128.48	125.03
14	l	207	CLA	C4-C3-C5	2.20	119.05	115.23
17	a	851	BCR	C7-C8-C9	-2.20	122.98	126.23
17	H	846	BCR	C37-C22-C21	-2.20	119.25	122.82
14	G	804	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
14	b	834	CLA	C3D-C4D-ND	2.20	113.57	109.99
14	m	1601	CLA	CHC-C1C-C2C	-2.20	120.70	126.94
14	a	831	CLA	C4C-C3C-C2C	-2.20	103.69	106.89
14	G	824	CLA	CMB-C2B-C3B	2.20	129.08	124.68
14	B	804	CLA	CMA-C3A-C4A	2.20	117.69	111.77
14	H	840	CLA	CMA-C3A-C4A	2.20	117.69	111.77
14	B	816	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
14	H	837	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
17	A	851	BCR	C37-C22-C21	-2.20	119.25	122.82
14	V	1601	CLA	CMB-C2B-C3B	2.20	129.08	124.68
14	A	805	CLA	CMA-C3A-C4A	2.20	117.69	111.77
14	X	1701	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
14	G	813	CLA	CMC-C2C-C1C	2.20	128.47	125.03
14	G	823	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
14	a	830	CLA	C4C-C3C-C2C	-2.20	103.69	106.89
14	b	801	CLA	CHB-C4A-NA	2.20	127.57	124.40
14	b	802	CLA	CHC-C1C-C2C	-2.20	120.71	126.94
17	j	103	BCR	C19-C18-C17	2.20	122.47	119.01
14	G	818	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
14	A	834	CLA	C3C-C4C-NC	2.20	113.25	110.43
14	A	837	CLA	C3C-C4C-NC	2.20	113.25	110.43
15	a	845	PQN	C2M-C2-C3	-2.20	120.84	124.45
14	U	206	CLA	C4D-C3D-CAD	2.20	110.49	108.11
14	A	838	CLA	C5-C3-C4	2.20	119.65	114.59
14	G	838	CLA	C3C-C4C-NC	2.20	113.25	110.43
14	b	810	CLA	O2D-CGD-O1D	-2.20	119.57	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	845	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
14	S	101	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
14	H	805	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
14	A	843	CLA	C16-C15-C13	-2.20	108.67	115.97
14	b	833	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
14	B	804	CLA	CAC-C3C-C4C	2.20	127.65	124.79
14	A	833	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
14	B	835	CLA	CAA-C2A-C3A	-2.20	107.07	113.00
14	G	821	CLA	CBC-CAC-C3C	-2.20	106.47	112.42
14	l	206	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
14	a	810	CLA	CED-O2D-CGD	2.19	120.89	115.92
14	B	829	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
14	G	821	CLA	CMB-C2B-C3B	2.19	129.07	124.68
14	a	826	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
17	I	101	BCR	C34-C9-C8	2.19	121.44	118.09
14	A	826	CLA	CMC-C2C-C1C	2.19	128.46	125.03
17	a	848	BCR	C12-C13-C14	-2.19	115.56	119.01
17	H	846	BCR	C34-C9-C10	-2.19	119.27	122.82
17	J	103	BCR	C34-C9-C10	-2.19	119.27	122.82
14	b	801	CLA	C4D-C3D-CAD	2.19	110.49	108.11
14	H	807	CLA	CHC-C1C-C2C	-2.19	120.74	126.94
14	L	201	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
14	B	834	CLA	C4C-C3C-C2C	-2.19	103.70	106.89
14	B	817	CLA	C3B-C4B-NB	2.19	112.04	109.21
14	B	827	CLA	CMC-C2C-C1C	2.19	128.46	125.03
14	G	807	CLA	CHB-C4A-NA	2.19	127.56	124.40
17	G	849	BCR	C33-C5-C6	-2.19	122.09	124.48
14	H	831	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
14	L	201	CLA	CAA-C2A-C1A	2.19	119.15	111.97
17	a	849	BCR	C23-C24-C25	-2.19	121.15	127.00
14	A	832	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
14	A	837	CLA	CHC-C1C-C2C	-2.19	120.74	126.94
17	G	853	BCR	C31-C1-C6	-2.19	106.81	110.24
17	U	202	BCR	C29-C30-C25	2.19	113.62	110.44
14	H	806	CLA	C3C-C4C-NC	2.19	113.23	110.43
14	b	806	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
14	G	822	CLA	CED-O2D-CGD	2.19	120.88	115.92
14	b	821	CLA	CED-O2D-CGD	2.19	120.88	115.92
14	A	807	CLA	CHB-C4A-NA	2.19	127.56	124.40
14	b	829	CLA	CMB-C2B-C1B	2.19	131.66	128.46
14	B	837	CLA	CHD-C4C-C3C	-2.19	121.59	124.77
14	A	803	CLA	C11-C10-C8	-2.19	108.70	115.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	1301	CLA	CHC-C1C-C2C	-2.19	120.75	126.94
14	A	840	CLA	CMD-C2D-C3D	-2.19	122.68	127.69
14	b	803	CLA	C1-O2A-CGA	2.18	121.94	116.65
14	B	816	CLA	C4-C3-C5	2.18	119.02	115.23
17	A	851	BCR	C34-C9-C10	-2.18	119.28	122.82
14	a	808	CLA	CHB-C4A-NA	2.18	127.55	124.40
17	G	850	BCR	C23-C24-C25	-2.18	121.16	127.00
14	l	205	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
14	G	835	CLA	C1-O2A-CGA	2.18	121.94	116.65
14	H	818	CLA	CMA-C3A-C4A	2.18	117.64	111.77
14	a	855	CLA	CHB-C4A-NA	2.18	127.55	124.40
14	a	804	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
14	B	822	CLA	C4D-C3D-CAD	2.18	110.48	108.11
14	H	816	CLA	OBD-CAD-C3D	-2.18	123.32	128.42
14	G	804	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
14	B	811	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
14	F	1303	CLA	C3C-C4C-NC	2.18	113.22	110.43
14	B	828	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
14	b	801	CLA	C4-C3-C5	2.18	119.01	115.23
14	b	811	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
14	a	820	CLA	OBD-CAD-C3D	-2.18	123.32	128.42
14	B	839	CLA	O2A-C1-C2	2.18	116.50	108.11
14	a	827	CLA	C4D-C3D-CAD	2.18	110.47	108.11
14	A	821	CLA	C5-C3-C4	2.18	119.60	114.59
14	b	814	CLA	C3D-C4D-ND	2.18	113.53	109.99
17	G	853	BCR	C33-C5-C4	2.18	118.24	113.60
14	B	830	CLA	CHC-C1C-C2C	-2.18	120.77	126.94
14	G	802	CLA	CHB-C4A-NA	2.18	127.54	124.40
17	l	208	BCR	C36-C18-C17	-2.18	119.29	122.82
14	a	831	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
14	B	823	CLA	C1-O2A-CGA	2.18	121.92	116.65
14	H	812	CLA	CHC-C1C-C2C	-2.18	120.77	126.94
14	A	819	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
14	b	837	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
14	B	805	CLA	CHB-C4A-NA	2.18	127.54	124.40
14	H	821	CLA	C4D-C3D-CAD	2.18	110.47	108.11
14	b	817	CLA	CBA-CAA-C2A	2.18	120.27	113.79
14	H	812	CLA	CMC-C2C-C1C	2.18	128.44	125.03
14	A	822	CLA	CMC-C2C-C1C	2.18	128.43	125.03
14	B	804	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
14	A	803	CLA	CMB-C2B-C3B	2.18	129.03	124.68
14	B	815	CLA	CAA-C2A-C3A	-2.18	107.12	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	806	CLA	C3C-C4C-NC	2.17	113.22	110.43
14	a	844	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
14	H	808	CLA	CBC-CAC-C3C	-2.17	106.53	112.42
14	G	823	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
14	A	806	CLA	CHB-C4A-NA	2.17	127.54	124.40
14	H	840	CLA	CMC-C2C-C3C	2.17	132.03	126.15
14	a	820	CLA	C5-C3-C4	2.17	119.59	114.59
14	G	810	CLA	C3C-C4C-NC	2.17	113.21	110.43
14	a	820	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
14	b	812	CLA	C4C-C3C-C2C	-2.17	103.73	106.89
14	a	837	CLA	CMA-C3A-C4A	2.17	117.61	111.77
14	a	840	CLA	CMA-C3A-C4A	2.17	117.61	111.77
14	G	817	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
14	a	838	CLA	OBD-CAD-C3D	-2.17	123.34	128.42
15	b	841	PQN	C16-C15-C13	-2.17	108.18	113.47
14	H	833	CLA	CHB-C4A-NA	2.17	127.53	124.40
14	x	1701	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
14	G	833	CLA	OBD-CAD-C3D	-2.17	123.34	128.42
15	B	841	PQN	C2M-C2-C3	-2.17	120.89	124.45
14	H	834	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
14	U	201	CLA	C4D-C3D-CAD	2.17	110.46	108.11
17	A	851	BCR	C27-C26-C25	-2.17	119.77	122.70
17	G	849	BCR	C28-C27-C26	-2.17	110.19	114.06
14	H	809	CLA	C1-O2A-CGA	2.17	121.89	116.65
14	a	812	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
14	a	838	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
14	H	827	CLA	CED-O2D-CGD	2.17	120.83	115.92
14	a	806	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
14	B	809	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
17	V	1602	BCR	C38-C26-C27	2.17	118.21	113.60
14	G	837	CLA	C3C-C4C-NC	2.17	113.20	110.43
17	B	845	BCR	C30-C25-C26	-2.17	119.68	122.64
14	b	814	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
14	H	837	CLA	C1-C2-C3	-2.16	122.65	126.20
17	A	852	BCR	C32-C1-C6	-2.16	106.85	110.24
14	l	207	CLA	C3C-C4C-NC	2.16	113.20	110.43
14	H	805	CLA	OBD-CAD-C3D	-2.16	123.36	128.42
14	B	823	CLA	CMA-C3A-C2A	2.16	122.35	113.98
14	U	201	CLA	CHA-C1A-NA	-2.16	121.49	126.39
14	a	812	CLA	CAC-C3C-C4C	2.16	127.61	124.79
14	a	828	CLA	CAC-C3C-C4C	2.16	127.61	124.79
14	a	819	CLA	CMB-C2B-C1B	-2.16	125.29	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	838	CLA	CMB-C2B-C3B	2.16	129.01	124.68
17	H	846	BCR	C31-C1-C6	-2.16	106.85	110.24
14	b	820	CLA	CHC-C1C-C2C	-2.16	120.82	126.94
17	F	1302	BCR	C7-C8-C9	-2.16	123.04	126.23
14	B	809	CLA	CAC-C3C-C4C	2.16	127.60	124.79
14	A	803	CLA	CAA-CBA-CGA	-2.16	107.07	113.21
17	S	103	BCR	C39-C30-C25	-2.16	106.85	110.24
14	G	820	CLA	CMC-C2C-C1C	2.16	128.41	125.03
17	H	844	BCR	C19-C18-C17	2.16	122.41	119.01
14	x	1701	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
14	b	818	CLA	CAC-C3C-C4C	2.16	127.60	124.79
17	R	102	BCR	C24-C23-C22	-2.16	123.04	126.23
14	A	813	CLA	CAC-C3C-C4C	2.16	127.60	124.79
17	Q	202	BCR	C7-C8-C9	-2.16	123.04	126.23
14	B	810	CLA	C3C-C4C-NC	2.16	113.20	110.43
14	G	843	CLA	C3C-C4C-NC	2.16	113.20	110.43
14	B	829	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
14	G	810	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
17	A	849	BCR	C30-C25-C24	2.16	121.50	115.65
14	A	840	CLA	CAA-CBA-CGA	-2.16	106.73	112.49
17	b	847	BCR	C34-C9-C8	2.16	121.38	118.09
17	A	853	BCR	C33-C5-C4	2.16	118.19	113.60
17	S	103	BCR	C2-C1-C6	2.16	113.57	110.44
14	U	206	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
14	G	838	CLA	C5-C3-C4	2.16	119.55	114.59
13	A	801	CL0	CHB-C4A-NA	2.16	127.51	124.40
14	G	806	CLA	CBC-CAC-C3C	-2.16	106.57	112.42
14	H	829	CLA	O1D-CGD-CBD	-2.16	120.27	124.52
14	H	801	CLA	C4D-C3D-CAD	2.16	110.45	108.11
17	b	843	BCR	C36-C18-C17	-2.16	119.32	122.82
14	b	839	CLA	C4-C3-C5	2.16	118.97	115.23
14	a	828	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
14	A	830	CLA	C3B-C4B-NB	2.15	112.00	109.21
14	H	816	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
14	H	804	CLA	C4-C3-C5	2.15	118.97	115.23
14	L	204	CLA	C4-C3-C5	2.15	118.97	115.23
14	b	803	CLA	CBC-CAC-C3C	-2.15	106.58	112.42
14	A	807	CLA	C3C-C4C-NC	2.15	113.19	110.43
14	B	830	CLA	CMB-C2B-C1B	-2.15	125.30	128.46
14	a	831	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
14	b	816	CLA	C6-C5-C3	-2.15	108.22	113.47
14	l	207	CLA	C11-C10-C8	-2.15	108.81	115.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	851	BCR	C2-C3-C4	-2.15	106.55	111.28
14	A	815	CLA	CMC-C2C-C1C	2.15	128.40	125.03
14	H	813	CLA	CMC-C2C-C1C	2.15	128.40	125.03
14	B	811	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
14	b	818	CLA	CMC-C2C-C1C	2.15	128.40	125.03
14	B	826	CLA	CED-O2D-CGD	2.15	120.79	115.92
14	l	202	CLA	CHC-C1C-C2C	-2.15	120.85	126.94
14	b	829	CLA	C3C-C4C-NC	2.15	113.19	110.43
14	b	803	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
17	A	852	BCR	C23-C24-C25	-2.15	121.25	127.00
13	A	801	CL0	O1D-CGD-CBD	-2.15	120.28	124.52
14	b	822	CLA	C4C-C3C-C2C	-2.15	103.76	106.89
17	G	853	BCR	C1-C6-C7	2.15	121.48	115.65
14	G	805	CLA	CAC-C3C-C4C	2.15	127.59	124.79
14	b	810	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
14	G	816	CLA	C3D-C4D-ND	2.15	113.48	109.99
14	B	805	CLA	C1-O2A-CGA	2.15	121.85	116.65
17	H	849	BCR	C15-C14-C13	-2.15	124.27	127.28
14	A	832	CLA	CAA-C2A-C3A	-2.15	107.19	113.00
17	B	844	BCR	C23-C24-C25	-2.15	121.26	127.00
14	H	822	CLA	CMC-C2C-C1C	2.15	128.39	125.03
17	B	847	BCR	C29-C28-C27	-2.15	106.56	111.28
14	H	825	CLA	C1-O2A-CGA	2.15	121.85	116.65
14	G	820	CLA	C3C-C4C-NC	2.15	113.18	110.43
14	a	855	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
14	A	810	CLA	CAA-CBA-CGA	-2.15	107.11	113.21
13	G	801	CL0	C4-C3-C5	2.15	118.95	115.23
14	H	820	CLA	C3C-C4C-NC	2.15	113.18	110.43
14	H	812	CLA	CMD-C2D-C3D	-2.15	122.77	127.69
17	m	1602	BCR	C36-C18-C17	-2.15	119.34	122.82
14	A	809	CLA	C3C-C4C-NC	2.15	113.18	110.43
14	b	823	CLA	CHA-C1A-NA	-2.14	121.53	126.39
14	B	805	CLA	CHC-C1C-C2C	-2.14	120.87	126.94
14	U	206	CLA	O1D-CGD-CBD	-2.14	120.29	124.52
14	b	806	CLA	CBA-CAA-C2A	2.14	120.17	113.79
14	a	817	CLA	CAA-C2A-C3A	-2.14	107.20	113.00
14	B	838	CLA	C4D-C3D-CAD	2.14	110.44	108.11
14	H	824	CLA	C3C-C4C-NC	2.14	113.18	110.43
14	H	812	CLA	C11-C10-C8	-2.14	108.84	115.97
14	a	837	CLA	CMB-C2B-C1B	-2.14	125.32	128.46
14	H	835	CLA	CHC-C1C-NC	-2.14	121.08	124.31
14	H	806	CLA	CHB-C4A-NA	2.14	127.49	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	820	CLA	C3C-C4C-NC	2.14	113.17	110.43
14	G	836	CLA	C3C-C4C-NC	2.14	113.17	110.43
14	H	812	CLA	C4C-C3C-C2C	-2.14	103.77	106.89
14	l	205	CLA	OBD-CAD-C3D	-2.14	123.41	128.42
14	a	836	CLA	C3C-C4C-NC	2.14	113.17	110.43
14	b	827	CLA	CHC-C1C-C2C	-2.14	120.88	126.94
14	a	840	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
14	i	101	CLA	C3C-C4C-NC	2.14	113.17	110.43
17	H	845	BCR	C23-C24-C25	-2.14	121.28	127.00
14	A	827	CLA	CMA-C3A-C4A	2.14	117.52	111.77
14	A	831	CLA	C4-C3-C5	2.14	118.94	115.23
14	G	820	CLA	C3B-C4B-NB	2.14	111.97	109.21
17	H	847	BCR	C34-C9-C8	2.14	121.36	118.09
14	A	828	CLA	CHA-C4D-ND	2.14	136.96	132.55
17	f	203	BCR	C37-C22-C21	-2.14	119.35	122.82
14	B	816	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
14	b	821	CLA	CHC-C1C-C2C	-2.14	120.89	126.94
17	b	845	BCR	C38-C26-C27	2.14	118.15	113.60
17	I	101	BCR	C36-C18-C17	-2.14	119.36	122.82
17	V	1602	BCR	C37-C22-C21	-2.14	119.36	122.82
14	H	830	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
14	G	837	CLA	CHC-C1C-C2C	-2.14	120.89	126.94
14	a	806	CLA	C3C-C4C-NC	2.14	113.17	110.43
17	i	102	BCR	C34-C9-C8	2.14	121.35	118.09
17	G	852	BCR	C27-C26-C25	-2.13	119.82	122.70
14	H	835	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
14	a	802	CLA	C1-O2A-CGA	2.13	121.82	116.65
14	b	836	CLA	O2D-CGD-O1D	-2.13	119.69	123.85
17	I	101	BCR	C23-C24-C25	-2.13	121.30	127.00
14	G	833	CLA	CMD-C2D-C3D	-2.13	122.79	127.69
14	B	832	CLA	CHC-C1C-C2C	-2.13	120.90	126.94
14	G	827	CLA	CBC-CAC-C3C	-2.13	106.64	112.42
14	b	832	CLA	C4C-C3C-C2C	-2.13	103.79	106.89
17	B	848	BCR	C31-C1-C6	-2.13	106.90	110.24
14	b	813	CLA	CMC-C2C-C1C	2.13	128.37	125.03
14	A	807	CLA	C1-C2-C3	-2.13	122.70	126.20
14	G	811	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
14	U	201	CLA	CAC-C3C-C4C	2.13	127.56	124.79
14	G	831	CLA	C3C-C4C-NC	2.13	113.16	110.43
14	G	814	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
14	b	813	CLA	CHB-C4A-NA	2.13	127.47	124.40
17	G	848	BCR	C34-C9-C10	-2.13	119.36	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	839	CLA	C1-O2A-CGA	2.13	121.81	116.65
14	a	837	CLA	C5-C3-C4	2.13	119.49	114.59
14	b	824	CLA	CAC-C3C-C4C	2.13	127.56	124.79
14	G	826	CLA	C3B-C4B-NB	2.13	111.96	109.21
17	B	843	BCR	C33-C5-C4	2.13	118.14	113.60
14	G	824	CLA	CAC-C3C-C4C	2.13	127.56	124.79
14	G	813	CLA	CHC-C1C-C2C	-2.13	120.91	126.94
14	a	840	CLA	C11-C10-C8	-2.13	108.89	115.97
14	G	809	CLA	C1-O2A-CGA	2.13	121.80	116.65
14	b	806	CLA	CHC-C1C-C2C	-2.13	120.92	126.94
14	a	833	CLA	C3C-C4C-NC	2.13	113.16	110.43
14	G	839	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
17	G	849	BCR	C30-C25-C24	2.13	121.42	115.65
14	B	816	CLA	CED-O2D-CGD	2.13	120.74	115.92
14	G	843	CLA	CED-O2D-CGD	2.13	120.74	115.92
14	m	1601	CLA	C3D-C4D-ND	2.13	113.44	109.99
14	B	816	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
17	B	844	BCR	C33-C5-C4	2.13	118.13	113.60
14	a	824	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
14	B	817	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
14	A	830	CLA	C3D-C4D-ND	2.12	113.44	109.99
14	B	840	CLA	CAA-C2A-C3A	-2.12	107.26	113.00
14	H	803	CLA	CED-O2D-CGD	2.12	120.73	115.92
14	G	817	CLA	C3C-C4C-NC	2.12	113.15	110.43
14	b	812	CLA	C3B-C4B-NB	2.12	111.95	109.21
14	B	801	CLA	CAC-C3C-C4C	2.12	127.55	124.79
14	A	814	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
14	b	837	CLA	C1-O2A-CGA	2.12	121.79	116.65
14	V	1601	CLA	CAC-C3C-C4C	2.12	127.55	124.79
17	A	848	BCR	C23-C22-C21	2.12	122.34	119.01
14	G	838	CLA	OBD-CAD-C3D	-2.12	123.46	128.42
14	A	820	CLA	C4D-C3D-CAD	2.12	110.41	108.11
14	B	802	CLA	CHD-C4C-C3C	-2.12	121.68	124.77
14	a	839	CLA	CAA-CBA-CGA	-2.12	106.84	112.49
14	a	827	CLA	CHA-C4D-ND	2.12	136.92	132.55
17	R	103	BCR	C38-C26-C27	2.12	118.11	113.60
14	l	202	CLA	C4-C3-C5	2.12	118.91	115.23
14	A	841	CLA	CHB-C4A-NA	2.12	127.46	124.40
14	a	804	CLA	CHA-C1A-NA	-2.12	121.59	126.39
14	B	801	CLA	CHD-C4C-C3C	-2.12	121.69	124.77
14	B	806	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
14	b	831	CLA	O2D-CGD-O1D	-2.12	119.73	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	837	CLA	CHA-C1A-NA	-2.12	121.60	126.39
17	B	846	BCR	C38-C26-C27	2.12	118.11	113.60
14	b	840	CLA	C3B-C4B-NB	2.12	111.95	109.21
14	A	820	CLA	CMC-C2C-C1C	2.12	128.34	125.03
17	m	1602	BCR	C19-C18-C17	2.12	122.34	119.01
14	b	833	CLA	CHB-C4A-NA	2.12	127.45	124.40
14	A	806	CLA	CBC-CAC-C3C	-2.12	106.68	112.42
14	H	840	CLA	C3C-C4C-NC	2.12	113.14	110.43
14	G	815	CLA	CHC-C1C-C2C	-2.12	120.95	126.94
14	G	802	CLA	CHC-C1C-C2C	-2.12	120.95	126.94
17	b	842	BCR	C30-C25-C26	-2.12	119.75	122.64
14	G	828	CLA	CHA-C4D-ND	2.11	136.91	132.55
14	b	820	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
14	l	207	CLA	CAC-C3C-C4C	2.11	127.54	124.79
14	A	808	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
14	a	834	CLA	CMA-C3A-C4A	2.11	117.45	111.77
14	G	806	CLA	CAC-C3C-C4C	2.11	127.54	124.79
17	G	849	BCR	C7-C8-C9	-2.11	123.11	126.23
14	A	823	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
17	S	103	BCR	C34-C9-C8	2.11	121.31	118.09
14	a	830	CLA	CAC-C3C-C4C	2.11	127.54	124.79
17	m	1602	BCR	C34-C9-C10	-2.11	119.39	122.82
14	b	830	CLA	CHC-C1C-C2C	-2.11	120.96	126.94
17	B	845	BCR	C23-C24-C25	-2.11	121.36	127.00
14	A	822	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
14	K	102	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
14	b	820	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
14	G	829	CLA	C5-C3-C2	-2.11	116.43	121.17
14	a	829	CLA	C4C-C3C-C2C	-2.11	103.82	106.89
14	G	804	CLA	C1-O2A-CGA	2.11	121.76	116.65
14	A	827	CLA	C4-C3-C5	2.11	118.89	115.23
14	l	205	CLA	CAC-C3C-C4C	2.11	127.53	124.79
14	F	1303	CLA	CHC-C1C-C2C	-2.11	120.97	126.94
17	V	1602	BCR	C34-C9-C10	-2.11	119.40	122.82
14	B	816	CLA	C4C-C3C-C2C	-2.11	103.82	106.89
14	H	807	CLA	C4-C3-C5	2.11	118.89	115.23
17	R	102	BCR	C4-C5-C6	-2.11	119.86	122.70
14	A	820	CLA	CHC-C1C-C2C	-2.11	120.97	126.94
15	b	841	PQN	C2M-C2-C3	-2.11	120.99	124.45
14	B	812	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
14	a	835	CLA	CMB-C2B-C3B	2.11	128.89	124.68
14	G	817	CLA	CHC-C1C-C2C	-2.11	120.98	126.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	838	CLA	CHC-C1C-C2C	-2.11	120.98	126.94
14	B	809	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
14	H	825	CLA	C1D-CHD-C4C	-2.11	121.55	126.02
14	f	202	CLA	CED-O2D-CGD	2.10	120.69	115.92
14	a	825	CLA	CHA-C1A-NA	-2.10	121.62	126.39
15	G	846	PQN	C11-C3-C2	-2.10	121.28	124.89
14	H	807	CLA	OBD-CAD-C3D	-2.10	123.50	128.42
14	H	826	CLA	CHC-C1C-C2C	-2.10	120.98	126.94
14	A	805	CLA	CHA-C1A-NA	-2.10	121.63	126.39
14	G	832	CLA	C5-C3-C4	2.10	119.43	114.59
14	a	819	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
14	A	835	CLA	C1-O2A-CGA	2.10	121.74	116.65
17	b	842	BCR	C37-C22-C21	-2.10	119.41	122.82
14	a	823	CLA	CMB-C2B-C3B	2.10	128.88	124.68
14	A	839	CLA	CHC-C1C-C2C	-2.10	120.99	126.94
14	a	843	CLA	CHA-C1A-NA	-2.10	121.63	126.39
14	A	822	CLA	CAA-CBA-CGA	2.10	119.17	113.21
14	b	823	CLA	CAC-C3C-C4C	2.10	127.52	124.79
14	b	812	CLA	CHB-C4A-NA	2.10	127.43	124.40
14	H	806	CLA	CMB-C2B-C3B	2.10	128.88	124.68
14	B	822	CLA	CMC-C2C-C1C	2.10	128.32	125.03
14	b	834	CLA	CHA-C1A-NA	-2.10	121.64	126.39
17	b	843	BCR	C37-C22-C21	-2.10	119.42	122.82
14	L	206	CLA	C4D-C3D-CAD	2.10	110.39	108.11
14	B	814	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
14	F	1301	CLA	CED-O2D-CGD	2.10	120.67	115.92
14	A	817	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
14	B	835	CLA	CHC-C1C-C2C	-2.10	121.00	126.94
14	i	101	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
14	a	822	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
14	l	205	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
14	B	837	CLA	C1-O2A-CGA	2.10	121.73	116.65
14	A	845	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
17	R	102	BCR	C31-C1-C6	-2.10	106.95	110.24
14	B	805	CLA	CBA-CAA-C2A	2.10	120.03	113.79
14	b	826	CLA	C4-C3-C5	2.10	118.87	115.23
14	H	801	CLA	CHA-C1A-NA	-2.10	121.64	126.39
14	B	817	CLA	CAA-C2A-C1A	-2.10	105.10	111.97
14	l	202	CLA	CED-O2D-CGD	2.10	120.67	115.92
14	L	204	CLA	CBC-CAC-C3C	-2.10	106.74	112.42
14	J	101	CLA	CHB-C4A-NA	2.10	127.42	124.40
14	G	830	CLA	C3C-C4C-NC	2.10	113.11	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	f	201	BCR	C4-C5-C6	-2.10	119.87	122.70
14	l	202	CLA	CMA-C3A-C2A	2.10	122.08	113.98
14	b	817	CLA	C3B-C4B-NB	2.09	111.92	109.21
17	H	845	BCR	C30-C25-C24	2.09	121.33	115.65
14	B	834	CLA	CHC-C1C-C2C	-2.09	121.01	126.94
14	B	830	CLA	CMC-C2C-C1C	2.09	128.31	125.03
14	B	809	CLA	CBC-CAC-C3C	-2.09	106.74	112.42
14	a	809	CLA	C4C-C3C-C2C	-2.09	103.84	106.89
14	a	840	CLA	C11-C12-C13	-2.09	109.01	115.97
14	G	839	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
18	A	854	LHG	O7-C7-O9	-2.09	118.81	123.70
14	A	828	CLA	C6-C5-C3	-2.09	108.37	113.47
17	b	844	BCR	C3-C4-C5	-2.09	110.32	114.06
14	A	817	CLA	CMB-C2B-C3B	2.09	128.87	124.68
14	A	839	CLA	CMB-C2B-C3B	2.09	128.87	124.68
14	G	831	CLA	CMC-C2C-C3C	2.09	131.81	126.15
14	T	1401	CLA	CAA-C2A-C3A	-2.09	107.35	113.00
14	U	206	CLA	CHC-C1C-C2C	-2.09	121.02	126.94
14	B	806	CLA	C1-O2A-CGA	2.09	121.71	116.65
14	G	803	CLA	C1-O2A-CGA	2.09	121.71	116.65
14	b	804	CLA	CMC-C2C-C1C	2.09	128.30	125.03
15	B	841	PQN	C17-C16-C15	-2.09	107.69	113.26
14	H	835	CLA	C4D-C3D-CAD	2.09	110.38	108.11
14	A	809	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
14	b	832	CLA	CHC-C1C-C2C	-2.09	121.02	126.94
14	G	825	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
14	H	801	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
14	j	102	CLA	CHC-C1C-C2C	-2.09	121.03	126.94
14	B	825	CLA	CHA-C1A-NA	-2.09	121.66	126.39
17	A	850	BCR	C1-C6-C5	-2.09	119.78	122.64
17	A	848	BCR	C3-C4-C5	-2.09	110.33	114.06
14	B	833	CLA	C3C-C4C-NC	2.09	113.10	110.43
14	L	205	CLA	CMA-C3A-C4A	2.09	117.38	111.77
14	B	812	CLA	CHB-C4A-NA	2.09	127.41	124.40
14	H	801	CLA	CHB-C4A-NA	2.09	127.41	124.40
17	B	843	BCR	C31-C1-C6	-2.09	106.97	110.24
17	B	842	BCR	C34-C9-C10	-2.09	119.44	122.82
17	H	843	BCR	C37-C22-C21	-2.09	119.44	122.82
14	A	826	CLA	CHC-C1C-C2C	-2.09	121.03	126.94
14	A	821	CLA	C1-O2A-CGA	2.09	121.70	116.65
14	B	814	CLA	C3D-C4D-ND	2.09	113.38	109.99
14	G	819	CLA	C4C-C3C-C2C	-2.09	103.86	106.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	836	CLA	CAC-C3C-C4C	2.09	127.50	124.79
14	G	844	CLA	CHC-C1C-C2C	-2.09	121.03	126.94
14	A	820	CLA	CAA-C2A-C3A	-2.09	107.36	113.00
14	G	816	CLA	C4C-C3C-C2C	-2.08	103.86	106.89
14	T	1401	CLA	CAC-C3C-C4C	2.08	127.50	124.79
14	a	802	CLA	C6-C7-C8	-2.08	109.04	115.97
14	H	816	CLA	CAA-C2A-C3A	-2.08	107.37	113.00
14	A	834	CLA	C4-C3-C5	2.08	118.84	115.23
17	a	848	BCR	C34-C9-C8	2.08	121.27	118.09
14	G	826	CLA	CHA-C1A-NA	-2.08	121.67	126.39
14	a	827	CLA	CHC-C1C-NC	-2.08	121.17	124.31
14	A	816	CLA	C4C-C3C-C2C	-2.08	103.86	106.89
14	H	834	CLA	CHC-C1C-C2C	-2.08	121.04	126.94
14	H	812	CLA	C3B-C4B-NB	2.08	111.90	109.21
17	b	846	BCR	C7-C8-C9	-2.08	123.15	126.23
17	A	850	BCR	C4-C5-C6	-2.08	119.89	122.70
14	H	827	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
14	A	814	CLA	CHA-C1A-NA	-2.08	121.68	126.39
17	J	102	BCR	C39-C30-C25	-2.08	106.98	110.24
17	a	848	BCR	C28-C27-C26	-2.08	110.34	114.06
14	G	842	CLA	C16-C15-C13	-2.08	109.05	115.97
14	l	202	CLA	C11-C10-C8	-2.08	109.05	115.97
14	b	822	CLA	CHC-C1C-C2C	-2.08	121.05	126.94
14	a	823	CLA	C4C-C3C-C2C	-2.08	103.86	106.89
17	l	201	BCR	C34-C9-C10	-2.08	119.44	122.82
14	b	817	CLA	C1-C2-C3	-2.08	122.79	126.20
17	B	844	BCR	C37-C22-C23	2.08	121.27	118.09
14	A	817	CLA	CHC-C1C-C2C	-2.08	121.05	126.94
14	a	840	CLA	C6-C5-C3	-2.08	108.40	113.47
14	G	816	CLA	CHA-C1A-NA	-2.08	121.68	126.39
17	R	101	BCR	C33-C5-C4	2.08	118.03	113.60
14	B	815	CLA	CAC-C3C-C4C	2.08	127.50	124.79
17	R	103	BCR	C35-C13-C12	2.08	121.26	118.09
17	H	845	BCR	C27-C26-C25	-2.08	119.90	122.70
14	b	812	CLA	CHC-C1C-C2C	-2.08	121.06	126.94
14	b	801	CLA	CED-O2D-CGD	2.08	120.63	115.92
14	B	801	CLA	CAA-C2A-C3A	-2.08	107.38	113.00
14	l	207	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
14	H	817	CLA	C3B-C4B-NB	2.08	111.89	109.21
14	G	826	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
14	b	815	CLA	CAC-C3C-C4C	2.08	127.49	124.79
14	G	809	CLA	CBA-CAA-C2A	2.08	119.97	113.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	828	CLA	CHA-C1A-NA	-2.08	121.69	126.39
17	l	203	BCR	C15-C14-C13	-2.08	124.37	127.28
14	A	805	CLA	CHB-C4A-NA	2.08	127.39	124.40
17	a	850	BCR	C28-C27-C26	-2.08	110.36	114.06
14	A	832	CLA	CMD-C2D-C3D	-2.07	122.93	127.69
14	A	812	CLA	C3B-C4B-NB	2.07	111.89	109.21
14	B	808	CLA	C4C-C3C-C2C	-2.07	103.87	106.89
14	a	839	CLA	CAA-C2A-C3A	-2.07	107.39	113.00
14	G	844	CLA	C3C-C4C-NC	2.07	113.09	110.43
14	L	206	CLA	CMD-C2D-C3D	-2.07	122.93	127.69
17	G	848	BCR	C23-C22-C21	2.07	122.27	119.01
14	B	825	CLA	CHA-C4D-ND	2.07	136.83	132.55
14	b	840	CLA	CMD-C2D-C3D	-2.07	122.93	127.69
14	a	810	CLA	C3C-C4C-NC	2.07	113.08	110.43
14	A	802	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
14	G	831	CLA	CMB-C2B-C1B	-2.07	125.42	128.46
14	H	810	CLA	CED-O2D-CGD	2.07	120.62	115.92
14	A	809	CLA	CHB-C4A-NA	2.07	127.39	124.40
14	A	833	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
14	a	819	CLA	C1-C2-C3	-2.07	122.80	126.20
14	G	803	CLA	CMA-C3A-C4A	2.07	117.34	111.77
14	b	836	CLA	CHA-C1A-NA	-2.07	121.70	126.39
14	A	838	CLA	CAC-C3C-C4C	2.07	127.48	124.79
14	b	804	CLA	C4D-C3D-CAD	2.07	110.36	108.11
14	A	826	CLA	C4-C3-C5	2.07	118.82	115.23
17	a	851	BCR	C28-C27-C26	-2.07	110.36	114.06
17	A	849	BCR	C2-C1-C6	2.07	113.45	110.44
14	B	826	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
14	b	834	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
14	L	205	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
14	G	812	CLA	CMC-C2C-C1C	2.07	128.27	125.03
14	a	812	CLA	CAA-C2A-C3A	-2.07	107.41	113.00
14	H	828	CLA	C3C-C4C-NC	2.07	113.08	110.43
14	G	839	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
17	H	844	BCR	C33-C5-C4	2.07	118.00	113.60
14	G	821	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
14	B	828	CLA	C16-C15-C13	-2.07	109.09	115.97
14	b	831	CLA	C6-C7-C8	-2.07	109.10	115.97
14	a	836	CLA	CHC-C1C-C2C	-2.07	121.09	126.94
17	a	852	BCR	C33-C5-C4	2.07	118.00	113.60
14	B	813	CLA	C4C-C3C-C2C	-2.06	103.89	106.89
14	b	840	CLA	CMB-C2B-C1B	2.06	131.48	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	807	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
14	J	101	CLA	CHA-C1A-NA	-2.06	121.72	126.39
17	V	1602	BCR	C30-C25-C24	2.06	121.25	115.65
17	G	851	BCR	C2-C3-C4	-2.06	106.74	111.28
17	Q	204	BCR	C34-C9-C8	2.06	121.24	118.09
17	G	851	BCR	C33-C5-C6	-2.06	122.23	124.48
14	A	820	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
14	A	822	CLA	C1-O2A-CGA	2.06	121.65	116.65
14	j	102	CLA	OBD-CAD-C3D	-2.06	125.24	128.60
14	H	822	CLA	C4D-C3D-CAD	2.06	110.35	108.11
14	m	1601	CLA	CHA-C4D-ND	2.06	136.80	132.55
14	H	801	CLA	CMA-C3A-C4A	2.06	117.32	111.77
17	I	102	BCR	C40-C30-C25	-2.06	107.01	110.24
18	a	854	LHG	O7-C7-O9	-2.06	118.88	123.70
14	B	818	CLA	C1-O2A-CGA	2.06	121.64	116.65
14	a	813	CLA	CHA-C1A-NA	-2.06	121.72	126.39
14	b	805	CLA	CHB-C4A-NA	2.06	127.37	124.40
13	G	801	CL0	C1-O2A-CGA	2.06	121.64	116.65
14	A	826	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
14	H	830	CLA	CHA-C1A-NA	-2.06	121.73	126.39
14	G	810	CLA	CHC-C1C-C2C	-2.06	121.11	126.94
14	b	817	CLA	CAA-C2A-C1A	-2.06	105.23	111.97
14	G	805	CLA	CHA-C1A-NA	-2.06	121.73	126.39
14	B	839	CLA	CAA-C2A-C3A	-2.06	107.44	113.00
17	B	848	BCR	C35-C13-C12	2.06	121.23	118.09
14	H	836	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
14	B	838	CLA	CAC-C3C-C4C	2.06	127.47	124.79
13	A	801	CL0	CHD-C1D-ND	-2.06	121.91	124.80
17	i	102	BCR	C23-C24-C25	-2.06	121.50	127.00
14	b	806	CLA	C6-C5-C3	-2.06	108.46	113.47
14	a	829	CLA	CHC-C1C-C2C	-2.06	121.12	126.94
14	j	101	CLA	CHC-C1C-C2C	-2.06	121.12	126.94
14	T	1401	CLA	CED-O2D-CGD	2.06	120.58	115.92
14	A	829	CLA	O2D-CGD-O1D	-2.06	119.85	123.85
14	a	811	CLA	C3C-C4C-NC	2.06	113.06	110.43
17	B	842	BCR	C32-C1-C6	-2.05	107.02	110.24
14	J	101	CLA	OBD-CAD-C3D	-2.05	123.61	128.42
14	G	839	CLA	CHC-C1C-C2C	-2.05	121.12	126.94
14	A	812	CLA	CED-O2D-CGD	2.05	120.58	115.92
14	A	825	CLA	CHC-C1C-C2C	-2.05	121.12	126.94
13	G	801	CL0	C3B-C4B-NB	2.05	111.86	109.21
14	B	827	CLA	C1-O2A-CGA	2.05	121.62	116.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	V	1601	CLA	CHA-C4D-ND	2.05	136.78	132.55
14	X	1701	CLA	CHA-C1A-NA	-2.05	121.74	126.39
14	b	826	CLA	CHA-C1A-NA	-2.05	121.74	126.39
14	H	833	CLA	C3C-C4C-NC	2.05	113.06	110.43
14	A	839	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
14	B	825	CLA	CHB-C4A-NA	2.05	127.36	124.40
14	G	841	CLA	CMA-C3A-C4A	2.05	117.29	111.77
14	a	819	CLA	C4D-C3D-CAD	2.05	110.33	108.11
14	A	807	CLA	CED-O2D-CGD	2.05	120.57	115.92
14	A	831	CLA	CMC-C2C-C3C	2.05	131.70	126.15
17	R	102	BCR	C23-C22-C21	-2.05	115.78	119.01
14	H	836	CLA	CAC-C3C-C4C	2.05	127.46	124.79
14	A	824	CLA	CHC-C1C-C2C	-2.05	121.13	126.94
14	L	201	CLA	CHC-C1C-C2C	-2.05	121.13	126.94
14	G	811	CLA	CED-O2D-CGD	2.05	120.57	115.92
14	A	818	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
14	b	816	CLA	CMA-C3A-C4A	2.05	117.28	111.77
14	G	840	CLA	C4D-C3D-CAD	2.05	110.33	108.11
14	B	827	CLA	CAC-C3C-C4C	2.05	127.46	124.79
17	a	849	BCR	C19-C18-C17	2.05	122.23	119.01
14	B	806	CLA	CHC-C1C-C2C	-2.05	121.14	126.94
14	b	805	CLA	C4-C3-C5	2.05	118.78	115.23
14	a	827	CLA	CAA-CBA-CGA	-2.05	107.39	113.21
14	B	807	CLA	CHC-C1C-C2C	-2.05	121.14	126.94
17	S	104	BCR	C7-C8-C9	-2.05	123.21	126.23
14	H	809	CLA	CMB-C2B-C3B	2.05	128.77	124.68
14	H	804	CLA	CAA-C2A-C3A	-2.05	107.47	113.00
14	a	822	CLA	OBD-CAD-C3D	-2.05	123.63	128.42
14	L	206	CLA	CAC-C3C-C4C	2.05	127.45	124.79
14	G	830	CLA	CHC-C1C-C2C	-2.05	121.15	126.94
14	G	841	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
14	a	832	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
14	b	839	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
14	A	820	CLA	CMB-C2B-C1B	-2.05	125.46	128.46
14	G	814	CLA	OBD-CAD-C3D	-2.05	123.64	128.42
14	K	101	CLA	CMA-C3A-C4A	2.04	117.27	111.77
14	H	836	CLA	CHC-C1C-C2C	-2.04	121.15	126.94
14	A	844	CLA	CED-O2D-CGD	2.04	120.55	115.92
17	B	848	BCR	C33-C5-C4	2.04	117.95	113.60
17	m	1602	BCR	C37-C22-C21	-2.04	119.51	122.82
14	f	202	CLA	C4C-C3C-C2C	-2.04	103.92	106.89
14	K	101	CLA	CHA-C1A-NA	-2.04	121.77	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	806	CLA	C3B-C4B-NB	2.04	111.85	109.21
14	b	814	CLA	OBD-CAD-C3D	-2.04	123.64	128.42
17	M	1602	BCR	C36-C18-C17	-2.04	119.51	122.82
14	B	830	CLA	CHA-C1A-NA	-2.04	121.77	126.39
19	H	848	LMG	O7-C10-O9	-2.04	118.93	123.70
14	b	811	CLA	CAC-C3C-C4C	2.04	127.45	124.79
14	H	804	CLA	CHB-C4A-NA	2.04	127.35	124.40
14	B	803	CLA	C1-O2A-CGA	2.04	121.59	116.65
14	L	205	CLA	C4C-C3C-C2C	-2.04	103.92	106.89
14	l	206	CLA	C3C-C4C-NC	2.04	113.05	110.43
14	B	828	CLA	C6-C5-C3	-2.04	108.49	113.47
17	S	103	BCR	C4-C5-C6	-2.04	119.94	122.70
14	T	1401	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
14	a	819	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
17	F	1302	BCR	C23-C22-C21	2.04	122.22	119.01
14	H	817	CLA	C3C-C4C-NC	2.04	113.04	110.43
14	M	1601	CLA	CHA-C4D-ND	2.04	136.76	132.55
14	H	805	CLA	CHB-C4A-NA	2.04	127.34	124.40
17	G	849	BCR	C31-C1-C6	-2.04	107.05	110.24
17	I	102	BCR	C23-C22-C21	2.04	122.22	119.01
14	A	814	CLA	CHC-C1C-C2C	-2.04	121.17	126.94
17	M	1602	BCR	C38-C26-C27	2.04	117.94	113.60
19	b	848	LMG	C7-O1-C1	-2.04	109.43	113.80
14	L	204	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
14	H	825	CLA	CHA-C1A-NA	-2.04	121.78	126.39
14	a	840	CLA	CMA-C3A-C2A	2.04	121.86	113.98
14	b	823	CLA	CHD-C1D-ND	-2.04	121.94	124.80
14	G	834	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
14	K	102	CLA	CHA-C1A-NA	-2.04	121.78	126.39
17	a	848	BCR	C2-C1-C6	2.04	113.40	110.44
14	b	812	CLA	CMA-C3A-C4A	2.04	117.25	111.77
14	H	840	CLA	CAA-C2A-C3A	-2.04	107.50	113.00
14	A	810	CLA	CHC-C1C-C2C	-2.04	121.18	126.94
17	b	843	BCR	C23-C22-C21	2.04	122.21	119.01
14	H	806	CLA	CED-O2D-CGD	2.03	120.53	115.92
14	B	823	CLA	CAC-C3C-C4C	2.03	127.44	124.79
18	a	854	LHG	C3-C2-C1	-2.03	104.92	111.77
14	H	840	CLA	C3B-C4B-NB	2.03	111.84	109.21
14	b	809	CLA	C3B-C4B-NB	2.03	111.84	109.21
14	H	835	CLA	CMB-C2B-C3B	2.03	128.75	124.68
14	B	812	CLA	C4-C3-C5	2.03	118.76	115.23
14	A	822	CLA	C16-C15-C13	-2.03	109.21	115.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	U	201	CLA	CHC-C1C-C2C	-2.03	121.19	126.94
14	B	805	CLA	C3C-C4C-NC	2.03	113.03	110.43
14	a	840	CLA	C3C-C4C-NC	2.03	113.03	110.43
14	G	819	CLA	C5-C3-C4	2.03	119.26	114.59
13	a	801	CL0	CBC-CAC-C3C	-2.03	106.92	112.42
14	b	816	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
14	a	814	CLA	CHA-C1A-NA	-2.03	121.79	126.39
14	B	833	CLA	CHB-C4A-NA	2.03	127.33	124.40
14	A	813	CLA	CHC-C1C-C2C	-2.03	121.19	126.94
14	b	811	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
14	B	824	CLA	CAA-C2A-C1A	-2.03	105.33	111.97
14	A	811	CLA	C4C-C3C-C2C	-2.03	103.94	106.89
14	A	827	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
14	b	812	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
14	G	814	CLA	CHA-C1A-NA	-2.03	121.80	126.39
17	G	851	BCR	C27-C26-C25	-2.03	119.96	122.70
14	A	809	CLA	CMB-C2B-C3B	2.03	128.74	124.68
14	b	829	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
14	l	202	CLA	CGD-CBD-CAD	-2.03	104.28	110.85
17	H	846	BCR	C4-C5-C6	-2.03	119.96	122.70
14	A	838	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
14	a	839	CLA	CMB-C2B-C3B	2.03	128.73	124.68
14	G	819	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
14	a	817	CLA	C3C-C4C-NC	2.03	113.03	110.43
17	R	103	BCR	C34-C9-C8	2.03	121.18	118.09
14	H	812	CLA	CHA-C1A-NA	-2.03	121.81	126.39
17	b	844	BCR	C36-C18-C17	-2.03	119.53	122.82
14	A	836	CLA	CED-O2D-CGD	2.03	120.51	115.92
14	k	1401	CLA	O1D-CGD-CBD	-2.02	120.52	124.52
14	A	839	CLA	C6-C7-C8	-2.02	109.23	115.97
14	H	833	CLA	CHC-C1C-C2C	-2.02	121.21	126.94
14	V	1601	CLA	CHC-C1C-C2C	-2.02	121.21	126.94
14	k	1401	CLA	C4D-C3D-CAD	2.02	110.31	108.11
17	l	201	BCR	C39-C30-C25	-2.02	107.07	110.24
17	A	850	BCR	C33-C5-C6	-2.02	122.28	124.48
14	b	825	CLA	C3D-C4D-ND	2.02	113.28	109.99
14	H	817	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
14	H	809	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
14	a	820	CLA	CHC-C1C-C2C	-2.02	121.21	126.94
14	H	831	CLA	C6-C7-C8	-2.02	109.25	115.97
14	B	827	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
14	V	1601	CLA	CED-O2D-CGD	2.02	120.50	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	853	BCR	C12-C13-C14	-2.02	115.83	119.01
14	B	834	CLA	CMB-C2B-C3B	2.02	128.72	124.68
14	B	816	CLA	CMD-C2D-C3D	-2.02	123.06	127.69
14	a	809	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
14	a	816	CLA	CHC-C1C-C2C	-2.02	121.22	126.94
14	b	821	CLA	C1-C2-C3	-2.02	122.89	126.20
14	a	824	CLA	CHC-C1C-C2C	-2.02	121.22	126.94
14	H	813	CLA	C1-O2A-CGA	2.02	121.54	116.65
14	b	825	CLA	CHA-C1A-NA	-2.02	121.82	126.39
14	H	838	CLA	CMB-C2B-C3B	2.02	128.72	124.68
17	R	101	BCR	C27-C26-C25	-2.02	119.98	122.70
17	S	104	BCR	C36-C18-C17	-2.02	119.55	122.82
14	H	809	CLA	CMC-C2C-C3C	2.02	131.61	126.15
14	f	202	CLA	CAA-C2A-C3A	-2.02	107.55	113.00
14	G	843	CLA	C4D-C3D-CAD	2.02	110.30	108.11
14	G	836	CLA	CHA-C1A-NA	-2.02	121.82	126.39
17	a	849	BCR	C8-C7-C6	-2.02	121.61	127.00
14	H	827	CLA	CAC-C3C-C4C	2.02	127.42	124.79
14	H	830	CLA	CHC-C1C-C2C	-2.02	121.23	126.94
14	H	821	CLA	CED-O2D-CGD	2.02	120.49	115.92
14	G	834	CLA	C4-C3-C5	2.02	118.73	115.23
17	R	102	BCR	C34-C9-C8	2.02	121.17	118.09
15	b	841	PQN	C11-C3-C2	-2.02	121.43	124.89
14	G	840	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
14	A	802	CLA	CHB-C4A-NA	2.02	127.31	124.40
14	b	801	CLA	CAA-C2A-C3A	-2.02	107.55	113.00
14	b	823	CLA	CHC-C1C-C2C	-2.02	121.23	126.94
14	A	806	CLA	CAC-C3C-C4C	2.02	127.41	124.79
14	b	814	CLA	CHD-C4C-C3C	-2.02	121.83	124.77
14	B	827	CLA	CHC-C1C-C2C	-2.01	121.24	126.94
14	H	838	CLA	CAC-C3C-C4C	2.01	127.41	124.79
14	a	818	CLA	C4C-C3C-C2C	-2.01	103.96	106.89
14	G	838	CLA	CHC-C1C-C2C	-2.01	121.24	126.94
14	U	201	CLA	C4-C3-C5	2.01	118.72	115.23
14	U	201	CLA	CMA-C3A-C2A	2.01	121.76	113.98
14	a	826	CLA	CAA-CBA-CGA	-2.01	107.49	113.21
14	a	838	CLA	CHC-C1C-C2C	-2.01	121.24	126.94
13	a	801	CL0	CHB-C4A-NA	2.01	127.30	124.40
13	a	801	CL0	C6-C5-C3	-2.01	108.57	113.47
14	G	832	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
14	H	827	CLA	CHC-C1C-C2C	-2.01	121.25	126.94
14	G	822	CLA	C1-O2A-CGA	2.01	121.52	116.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	805	CLA	C4D-C3D-CAD	2.01	110.29	108.11
14	a	825	CLA	C4C-C3C-C2C	-2.01	103.97	106.89
14	B	831	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
14	b	821	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
14	a	829	CLA	CHA-C4D-ND	2.01	136.70	132.55
14	A	835	CLA	C3C-C4C-NC	2.01	113.00	110.43
17	G	850	BCR	C39-C30-C25	-2.01	107.09	110.24
14	H	805	CLA	C6-C5-C3	-2.01	108.57	113.47
14	B	827	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
14	G	842	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
17	b	845	BCR	C39-C30-C25	-2.01	107.09	110.24
14	G	831	CLA	C1-C2-C3	-2.01	122.91	126.20
14	H	817	CLA	CAC-C3C-C4C	2.01	127.40	124.79
14	A	834	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
17	l	208	BCR	C34-C9-C8	2.01	121.16	118.09
14	L	206	CLA	CHA-C1A-NA	-2.01	121.84	126.39
18	A	854	LHG	O8-C23-O10	-2.01	118.61	123.63
14	G	814	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
14	H	814	CLA	CHC-C1C-C2C	-2.01	121.26	126.94
17	F	1302	BCR	C15-C14-C13	-2.01	124.47	127.28
14	a	841	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
14	H	810	CLA	CAC-C3C-C4C	2.01	127.40	124.79
14	B	823	CLA	CHA-C1A-NA	-2.01	121.85	126.39
14	B	836	CLA	CHC-C1C-C2C	-2.01	121.26	126.94
17	a	852	BCR	C1-C6-C7	2.01	121.09	115.65
14	A	826	CLA	C4C-C3C-C2C	-2.01	103.97	106.89
17	L	207	BCR	C28-C27-C26	-2.00	110.48	114.06
14	l	202	CLA	CHA-C1A-NA	-2.00	121.85	126.39
17	S	103	BCR	C33-C5-C6	-2.00	122.30	124.48
14	b	818	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
14	b	830	CLA	CHA-C1A-NA	-2.00	121.85	126.39
14	A	822	CLA	CHC-C1C-C2C	-2.00	121.27	126.94
14	T	1401	CLA	CMD-C2D-C3D	-2.00	123.09	127.69
14	B	819	CLA	CHD-C4C-C3C	-2.00	121.85	124.77
17	b	849	BCR	C37-C22-C21	-2.00	119.57	122.82
17	G	851	BCR	C12-C13-C14	-2.00	115.86	119.01
14	b	840	CLA	C4-C3-C5	2.00	118.70	115.23
14	a	821	CLA	C3C-C4C-NC	2.00	112.99	110.43
14	a	833	CLA	CAA-C2A-C3A	-2.00	107.59	113.00
14	A	825	CLA	C3B-C4B-NB	2.00	111.80	109.21
14	b	828	CLA	CMC-C2C-C3C	2.00	131.56	126.15

All (294) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	NC
13	A	801	CL0	ND
13	A	801	CL0	NA
13	G	801	CL0	NC
13	G	801	CL0	ND
13	G	801	CL0	NA
13	a	801	CL0	NC
13	a	801	CL0	ND
13	a	801	CL0	NA
14	A	802	CLA	ND
14	A	803	CLA	ND
14	A	804	CLA	ND
14	A	805	CLA	ND
14	A	806	CLA	ND
14	A	807	CLA	ND
14	A	808	CLA	ND
14	A	809	CLA	ND
14	A	810	CLA	ND
14	A	811	CLA	ND
14	A	812	CLA	ND
14	A	813	CLA	ND
14	A	814	CLA	ND
14	A	815	CLA	ND
14	A	816	CLA	ND
14	A	817	CLA	ND
14	A	818	CLA	ND
14	A	819	CLA	ND
14	A	820	CLA	ND
14	A	821	CLA	ND
14	A	822	CLA	ND
14	A	823	CLA	ND
14	A	824	CLA	ND
14	A	825	CLA	ND
14	A	826	CLA	ND
14	A	827	CLA	ND
14	A	828	CLA	ND
14	A	829	CLA	ND
14	A	830	CLA	ND
14	A	831	CLA	ND
14	A	832	CLA	ND
14	A	833	CLA	ND
14	A	834	CLA	ND
14	A	835	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
14	A	836	CLA	ND
14	A	837	CLA	ND
14	A	838	CLA	ND
14	A	839	CLA	ND
14	A	840	CLA	ND
14	A	841	CLA	ND
14	A	842	CLA	ND
14	A	843	CLA	ND
14	A	844	CLA	ND
14	A	845	CLA	ND
14	B	801	CLA	ND
14	B	802	CLA	ND
14	B	803	CLA	ND
14	B	804	CLA	ND
14	B	805	CLA	ND
14	B	806	CLA	ND
14	B	807	CLA	ND
14	B	808	CLA	ND
14	B	809	CLA	ND
14	B	810	CLA	ND
14	B	811	CLA	ND
14	B	812	CLA	ND
14	B	813	CLA	ND
14	B	814	CLA	ND
14	B	815	CLA	ND
14	B	816	CLA	ND
14	B	817	CLA	ND
14	B	818	CLA	ND
14	B	819	CLA	ND
14	B	820	CLA	ND
14	B	821	CLA	ND
14	B	822	CLA	ND
14	B	823	CLA	ND
14	B	824	CLA	ND
14	B	825	CLA	ND
14	B	826	CLA	ND
14	B	827	CLA	ND
14	B	828	CLA	ND
14	B	829	CLA	ND
14	B	830	CLA	ND
14	B	831	CLA	ND
14	B	832	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
14	B	833	CLA	ND
14	B	834	CLA	ND
14	B	835	CLA	ND
14	B	836	CLA	ND
14	B	837	CLA	ND
14	B	838	CLA	ND
14	B	839	CLA	ND
14	B	840	CLA	ND
14	F	1301	CLA	ND
14	F	1303	CLA	ND
14	G	802	CLA	ND
14	G	803	CLA	ND
14	G	804	CLA	ND
14	G	805	CLA	ND
14	G	806	CLA	ND
14	G	807	CLA	ND
14	G	808	CLA	ND
14	G	809	CLA	ND
14	G	810	CLA	ND
14	G	811	CLA	ND
14	G	812	CLA	ND
14	G	813	CLA	ND
14	G	814	CLA	ND
14	G	815	CLA	ND
14	G	816	CLA	ND
14	G	817	CLA	ND
14	G	818	CLA	ND
14	G	819	CLA	ND
14	G	820	CLA	ND
14	G	821	CLA	ND
14	G	822	CLA	ND
14	G	823	CLA	ND
14	G	824	CLA	ND
14	G	825	CLA	ND
14	G	826	CLA	ND
14	G	827	CLA	ND
14	G	828	CLA	ND
14	G	829	CLA	ND
14	G	830	CLA	ND
14	G	831	CLA	ND
14	G	832	CLA	ND
14	G	833	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
14	G	834	CLA	ND
14	G	835	CLA	ND
14	G	836	CLA	ND
14	G	837	CLA	ND
14	G	838	CLA	ND
14	G	839	CLA	ND
14	G	840	CLA	ND
14	G	841	CLA	ND
14	G	842	CLA	ND
14	G	843	CLA	ND
14	G	844	CLA	ND
14	G	845	CLA	ND
14	H	801	CLA	ND
14	H	802	CLA	ND
14	H	803	CLA	ND
14	H	804	CLA	ND
14	H	805	CLA	ND
14	H	806	CLA	ND
14	H	807	CLA	ND
14	H	808	CLA	ND
14	H	809	CLA	ND
14	H	810	CLA	ND
14	H	811	CLA	ND
14	H	812	CLA	ND
14	H	813	CLA	ND
14	H	814	CLA	ND
14	H	815	CLA	ND
14	H	816	CLA	ND
14	H	817	CLA	ND
14	H	818	CLA	ND
14	H	819	CLA	ND
14	H	820	CLA	ND
14	H	821	CLA	ND
14	H	822	CLA	ND
14	H	823	CLA	ND
14	H	824	CLA	ND
14	H	825	CLA	ND
14	H	826	CLA	ND
14	H	827	CLA	ND
14	H	828	CLA	ND
14	H	829	CLA	ND
14	H	830	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
14	H	831	CLA	ND
14	H	832	CLA	ND
14	H	833	CLA	ND
14	H	834	CLA	ND
14	H	835	CLA	ND
14	H	836	CLA	ND
14	H	837	CLA	ND
14	H	838	CLA	ND
14	H	839	CLA	ND
14	H	840	CLA	ND
14	J	101	CLA	ND
14	K	101	CLA	ND
14	K	102	CLA	ND
14	L	201	CLA	ND
14	L	204	CLA	ND
14	L	205	CLA	ND
14	L	206	CLA	ND
14	M	1601	CLA	ND
14	Q	201	CLA	ND
14	Q	203	CLA	ND
14	S	101	CLA	ND
14	S	102	CLA	ND
14	T	1401	CLA	ND
14	U	201	CLA	ND
14	U	204	CLA	ND
14	U	205	CLA	ND
14	U	206	CLA	ND
14	V	1601	CLA	ND
14	W	1701	CLA	ND
14	X	1701	CLA	ND
14	a	802	CLA	ND
14	a	803	CLA	ND
14	a	804	CLA	ND
14	a	805	CLA	ND
14	a	806	CLA	ND
14	a	807	CLA	ND
14	a	808	CLA	ND
14	a	809	CLA	ND
14	a	810	CLA	ND
14	a	811	CLA	ND
14	a	812	CLA	ND
14	a	813	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
14	a	814	CLA	ND
14	a	815	CLA	ND
14	a	816	CLA	ND
14	a	817	CLA	ND
14	a	818	CLA	ND
14	a	819	CLA	ND
14	a	820	CLA	ND
14	a	821	CLA	ND
14	a	822	CLA	ND
14	a	823	CLA	ND
14	a	824	CLA	ND
14	a	825	CLA	ND
14	a	826	CLA	ND
14	a	827	CLA	ND
14	a	828	CLA	ND
14	a	829	CLA	ND
14	a	830	CLA	ND
14	a	831	CLA	ND
14	a	832	CLA	ND
14	a	833	CLA	ND
14	a	834	CLA	ND
14	a	835	CLA	ND
14	a	836	CLA	ND
14	a	837	CLA	ND
14	a	838	CLA	ND
14	a	839	CLA	ND
14	a	840	CLA	ND
14	a	841	CLA	ND
14	a	842	CLA	ND
14	a	843	CLA	ND
14	a	844	CLA	ND
14	a	855	CLA	ND
14	b	801	CLA	ND
14	b	802	CLA	ND
14	b	803	CLA	ND
14	b	804	CLA	ND
14	b	805	CLA	ND
14	b	806	CLA	ND
14	b	807	CLA	ND
14	b	808	CLA	ND
14	b	809	CLA	ND
14	b	810	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
14	b	811	CLA	ND
14	b	812	CLA	ND
14	b	813	CLA	ND
14	b	814	CLA	ND
14	b	815	CLA	ND
14	b	816	CLA	ND
14	b	817	CLA	ND
14	b	818	CLA	ND
14	b	819	CLA	ND
14	b	820	CLA	ND
14	b	821	CLA	ND
14	b	822	CLA	ND
14	b	823	CLA	ND
14	b	824	CLA	ND
14	b	825	CLA	ND
14	b	826	CLA	ND
14	b	827	CLA	ND
14	b	828	CLA	ND
14	b	829	CLA	ND
14	b	830	CLA	ND
14	b	831	CLA	ND
14	b	832	CLA	ND
14	b	833	CLA	ND
14	b	834	CLA	ND
14	b	835	CLA	ND
14	b	836	CLA	ND
14	b	837	CLA	ND
14	b	838	CLA	ND
14	b	839	CLA	ND
14	b	840	CLA	ND
14	f	202	CLA	ND
14	i	101	CLA	ND
14	j	101	CLA	ND
14	j	102	CLA	ND
14	k	1401	CLA	ND
14	l	202	CLA	ND
14	l	205	CLA	ND
14	l	206	CLA	ND
14	l	207	CLA	ND
14	m	1601	CLA	ND
14	x	1701	CLA	ND

All (3575) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	802	CLA	CBA-CGA-O2A-C1
14	A	802	CLA	O1A-CGA-O2A-C1
14	A	804	CLA	C2-C1-O2A-CGA
14	A	804	CLA	CHA-CBD-CGD-O1D
14	A	804	CLA	CHA-CBD-CGD-O2D
14	A	805	CLA	C1A-C2A-CAA-CBA
14	A	805	CLA	C3A-C2A-CAA-CBA
14	A	805	CLA	CHA-CBD-CGD-O1D
14	A	805	CLA	CHA-CBD-CGD-O2D
14	A	806	CLA	C1A-C2A-CAA-CBA
14	A	806	CLA	CAD-CBD-CGD-O1D
14	A	806	CLA	CAD-CBD-CGD-O2D
14	A	807	CLA	C1A-C2A-CAA-CBA
14	A	809	CLA	C3A-C2A-CAA-CBA
14	A	809	CLA	CHA-CBD-CGD-O1D
14	A	809	CLA	CHA-CBD-CGD-O2D
14	A	810	CLA	CBD-CGD-O2D-CED
14	A	811	CLA	C1A-C2A-CAA-CBA
14	A	811	CLA	C3A-C2A-CAA-CBA
14	A	811	CLA	CBD-CGD-O2D-CED
14	A	812	CLA	CBD-CGD-O2D-CED
14	A	813	CLA	CBA-CGA-O2A-C1
14	A	813	CLA	O1A-CGA-O2A-C1
14	A	815	CLA	C1A-C2A-CAA-CBA
14	A	815	CLA	C3A-C2A-CAA-CBA
14	A	816	CLA	C3A-C2A-CAA-CBA
14	A	817	CLA	CBD-CGD-O2D-CED
14	A	819	CLA	C3A-C2A-CAA-CBA
14	A	820	CLA	C1A-C2A-CAA-CBA
14	A	820	CLA	C3A-C2A-CAA-CBA
14	A	821	CLA	C1A-C2A-CAA-CBA
14	A	821	CLA	C3A-C2A-CAA-CBA
14	A	823	CLA	CBD-CGD-O2D-CED
14	A	826	CLA	C6-C7-C8-C9
14	A	828	CLA	C6-C7-C8-C9
14	A	831	CLA	CHA-CBD-CGD-O1D
14	A	831	CLA	CHA-CBD-CGD-O2D
14	A	833	CLA	O1A-CGA-O2A-C1
14	A	834	CLA	CBD-CGD-O2D-CED
14	A	835	CLA	CHA-CBD-CGD-O1D
14	A	835	CLA	CHA-CBD-CGD-O2D
14	A	836	CLA	CBD-CGD-O2D-CED
14	A	837	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	837	CLA	C3A-C2A-CAA-CBA
14	A	838	CLA	CBD-CGD-O2D-CED
14	A	841	CLA	CBD-CGD-O2D-CED
14	A	842	CLA	CBD-CGD-O2D-CED
14	A	842	CLA	O1D-CGD-O2D-CED
14	B	801	CLA	CAD-CBD-CGD-O1D
14	B	801	CLA	CAD-CBD-CGD-O2D
14	B	804	CLA	CHA-CBD-CGD-O1D
14	B	804	CLA	CHA-CBD-CGD-O2D
14	B	805	CLA	C1A-C2A-CAA-CBA
14	B	805	CLA	C3A-C2A-CAA-CBA
14	B	808	CLA	CHA-CBD-CGD-O1D
14	B	808	CLA	CHA-CBD-CGD-O2D
14	B	812	CLA	C1A-C2A-CAA-CBA
14	B	812	CLA	C3A-C2A-CAA-CBA
14	B	814	CLA	CHA-CBD-CGD-O1D
14	B	814	CLA	CHA-CBD-CGD-O2D
14	B	816	CLA	C1A-C2A-CAA-CBA
14	B	816	CLA	CBD-CGD-O2D-CED
14	B	817	CLA	C1A-C2A-CAA-CBA
14	B	817	CLA	C3A-C2A-CAA-CBA
14	B	819	CLA	C1A-C2A-CAA-CBA
14	B	819	CLA	C3A-C2A-CAA-CBA
14	B	820	CLA	CHA-CBD-CGD-O1D
14	B	820	CLA	CHA-CBD-CGD-O2D
14	B	821	CLA	CBD-CGD-O2D-CED
14	B	822	CLA	C1A-C2A-CAA-CBA
14	B	822	CLA	C3A-C2A-CAA-CBA
14	B	823	CLA	CHA-CBD-CGD-O1D
14	B	823	CLA	CHA-CBD-CGD-O2D
14	B	824	CLA	CHA-CBD-CGD-O1D
14	B	824	CLA	CHA-CBD-CGD-O2D
14	B	825	CLA	C1A-C2A-CAA-CBA
14	B	825	CLA	C3A-C2A-CAA-CBA
14	B	826	CLA	C1A-C2A-CAA-CBA
14	B	826	CLA	C3A-C2A-CAA-CBA
14	B	827	CLA	C1A-C2A-CAA-CBA
14	B	827	CLA	C3A-C2A-CAA-CBA
14	B	828	CLA	CAD-CBD-CGD-O1D
14	B	828	CLA	CAD-CBD-CGD-O2D
14	B	829	CLA	C3A-C2A-CAA-CBA
14	B	830	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	832	CLA	CHA-CBD-CGD-O1D
14	B	832	CLA	CHA-CBD-CGD-O2D
14	B	834	CLA	C1A-C2A-CAA-CBA
14	B	834	CLA	C3A-C2A-CAA-CBA
14	B	835	CLA	CBD-CGD-O2D-CED
14	B	836	CLA	C1A-C2A-CAA-CBA
14	B	836	CLA	CBD-CGD-O2D-CED
14	B	837	CLA	CBD-CGD-O2D-CED
14	B	840	CLA	C2-C1-O2A-CGA
14	G	802	CLA	CBA-CGA-O2A-C1
14	G	802	CLA	O1A-CGA-O2A-C1
14	G	803	CLA	CBD-CGD-O2D-CED
14	G	804	CLA	CHA-CBD-CGD-O1D
14	G	804	CLA	CHA-CBD-CGD-O2D
14	G	805	CLA	C1A-C2A-CAA-CBA
14	G	806	CLA	C1A-C2A-CAA-CBA
14	G	806	CLA	C3A-C2A-CAA-CBA
14	G	806	CLA	CAD-CBD-CGD-O1D
14	G	806	CLA	CAD-CBD-CGD-O2D
14	G	807	CLA	C1A-C2A-CAA-CBA
14	G	807	CLA	CBD-CGD-O2D-CED
14	G	809	CLA	C3A-C2A-CAA-CBA
14	G	809	CLA	CHA-CBD-CGD-O1D
14	G	809	CLA	CHA-CBD-CGD-O2D
14	G	810	CLA	CBD-CGD-O2D-CED
14	G	811	CLA	C1A-C2A-CAA-CBA
14	G	811	CLA	C3A-C2A-CAA-CBA
14	G	812	CLA	C1A-C2A-CAA-CBA
14	G	812	CLA	C3A-C2A-CAA-CBA
14	G	813	CLA	CBA-CGA-O2A-C1
14	G	813	CLA	O1A-CGA-O2A-C1
14	G	816	CLA	C3A-C2A-CAA-CBA
14	G	819	CLA	C3A-C2A-CAA-CBA
14	G	819	CLA	CBD-CGD-O2D-CED
14	G	820	CLA	C1A-C2A-CAA-CBA
14	G	820	CLA	C3A-C2A-CAA-CBA
14	G	820	CLA	CBD-CGD-O2D-CED
14	G	821	CLA	C1A-C2A-CAA-CBA
14	G	821	CLA	C3A-C2A-CAA-CBA
14	G	830	CLA	C1A-C2A-CAA-CBA
14	G	831	CLA	CHA-CBD-CGD-O1D
14	G	831	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	834	CLA	CBD-CGD-O2D-CED
14	G	835	CLA	CHA-CBD-CGD-O1D
14	G	835	CLA	CHA-CBD-CGD-O2D
14	G	837	CLA	C1A-C2A-CAA-CBA
14	G	837	CLA	C3A-C2A-CAA-CBA
14	G	838	CLA	CBD-CGD-O2D-CED
14	H	801	CLA	CAD-CBD-CGD-O2D
14	H	802	CLA	CBD-CGD-O2D-CED
14	H	804	CLA	CHA-CBD-CGD-O1D
14	H	804	CLA	CHA-CBD-CGD-O2D
14	H	805	CLA	C1A-C2A-CAA-CBA
14	H	805	CLA	C3A-C2A-CAA-CBA
14	H	805	CLA	C6-C7-C8-C9
14	H	808	CLA	CHA-CBD-CGD-O1D
14	H	808	CLA	CHA-CBD-CGD-O2D
14	H	812	CLA	C1A-C2A-CAA-CBA
14	H	812	CLA	C3A-C2A-CAA-CBA
14	H	813	CLA	CBD-CGD-O2D-CED
14	H	814	CLA	CHA-CBD-CGD-O1D
14	H	814	CLA	CHA-CBD-CGD-O2D
14	H	816	CLA	C1A-C2A-CAA-CBA
14	H	816	CLA	C3A-C2A-CAA-CBA
14	H	817	CLA	C1A-C2A-CAA-CBA
14	H	817	CLA	C3A-C2A-CAA-CBA
14	H	819	CLA	C1A-C2A-CAA-CBA
14	H	820	CLA	CHA-CBD-CGD-O1D
14	H	820	CLA	CHA-CBD-CGD-O2D
14	H	823	CLA	CHA-CBD-CGD-O1D
14	H	823	CLA	CHA-CBD-CGD-O2D
14	H	824	CLA	CHA-CBD-CGD-O1D
14	H	824	CLA	CHA-CBD-CGD-O2D
14	H	825	CLA	C3A-C2A-CAA-CBA
14	H	826	CLA	C1A-C2A-CAA-CBA
14	H	826	CLA	C3A-C2A-CAA-CBA
14	H	827	CLA	C1A-C2A-CAA-CBA
14	H	827	CLA	C3A-C2A-CAA-CBA
14	H	828	CLA	CAD-CBD-CGD-O1D
14	H	828	CLA	CAD-CBD-CGD-O2D
14	H	829	CLA	C3A-C2A-CAA-CBA
14	H	830	CLA	C1A-C2A-CAA-CBA
14	H	830	CLA	C3A-C2A-CAA-CBA
14	H	830	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	832	CLA	C2-C1-O2A-CGA
14	H	832	CLA	CHA-CBD-CGD-O1D
14	H	832	CLA	CHA-CBD-CGD-O2D
14	H	834	CLA	C1A-C2A-CAA-CBA
14	H	834	CLA	C3A-C2A-CAA-CBA
14	H	834	CLA	CBD-CGD-O2D-CED
14	H	840	CLA	C2-C1-O2A-CGA
14	H	840	CLA	CBD-CGD-O2D-CED
14	L	204	CLA	C1A-C2A-CAA-CBA
14	L	204	CLA	C3A-C2A-CAA-CBA
14	M	1601	CLA	C1A-C2A-CAA-CBA
14	M	1601	CLA	C3A-C2A-CAA-CBA
14	Q	201	CLA	CBD-CGD-O2D-CED
14	T	1401	CLA	CAD-CBD-CGD-O1D
14	T	1401	CLA	CAD-CBD-CGD-O2D
14	U	204	CLA	C1A-C2A-CAA-CBA
14	U	204	CLA	C3A-C2A-CAA-CBA
14	V	1601	CLA	C1A-C2A-CAA-CBA
14	V	1601	CLA	C3A-C2A-CAA-CBA
14	W	1701	CLA	CBD-CGD-O2D-CED
14	a	803	CLA	CHA-CBD-CGD-O1D
14	a	803	CLA	CHA-CBD-CGD-O2D
14	a	804	CLA	C1A-C2A-CAA-CBA
14	a	804	CLA	C3A-C2A-CAA-CBA
14	a	804	CLA	CHA-CBD-CGD-O1D
14	a	804	CLA	CHA-CBD-CGD-O2D
14	a	805	CLA	C1A-C2A-CAA-CBA
14	a	805	CLA	CAD-CBD-CGD-O1D
14	a	805	CLA	CAD-CBD-CGD-O2D
14	a	806	CLA	C1A-C2A-CAA-CBA
14	a	806	CLA	CBD-CGD-O2D-CED
14	a	808	CLA	C3A-C2A-CAA-CBA
14	a	808	CLA	CHA-CBD-CGD-O1D
14	a	808	CLA	CHA-CBD-CGD-O2D
14	a	809	CLA	CBD-CGD-O2D-CED
14	a	810	CLA	C1A-C2A-CAA-CBA
14	a	810	CLA	C3A-C2A-CAA-CBA
14	a	811	CLA	C1A-C2A-CAA-CBA
14	a	811	CLA	C3A-C2A-CAA-CBA
14	a	811	CLA	CBD-CGD-O2D-CED
14	a	814	CLA	C1A-C2A-CAA-CBA
14	a	814	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	815	CLA	C1A-C2A-CAA-CBA
14	a	815	CLA	C3A-C2A-CAA-CBA
14	a	816	CLA	CBD-CGD-O2D-CED
14	a	818	CLA	C1A-C2A-CAA-CBA
14	a	818	CLA	C3A-C2A-CAA-CBA
14	a	819	CLA	C3A-C2A-CAA-CBA
14	a	820	CLA	C1A-C2A-CAA-CBA
14	a	820	CLA	C3A-C2A-CAA-CBA
14	a	821	CLA	CBD-CGD-O2D-CED
14	a	822	CLA	CBD-CGD-O2D-CED
14	a	827	CLA	C6-C7-C8-C9
14	a	828	CLA	CBD-CGD-O2D-CED
14	a	829	CLA	C1A-C2A-CAA-CBA
14	a	829	CLA	C3A-C2A-CAA-CBA
14	a	830	CLA	CHA-CBD-CGD-O1D
14	a	830	CLA	CHA-CBD-CGD-O2D
14	a	833	CLA	CBD-CGD-O2D-CED
14	a	834	CLA	CHA-CBD-CGD-O1D
14	a	834	CLA	CHA-CBD-CGD-O2D
14	a	835	CLA	CBD-CGD-O2D-CED
14	a	836	CLA	C1A-C2A-CAA-CBA
14	a	836	CLA	C3A-C2A-CAA-CBA
14	a	837	CLA	CBD-CGD-O2D-CED
14	a	841	CLA	CBD-CGD-O2D-CED
14	a	855	CLA	CAD-CBD-CGD-O2D
14	b	801	CLA	CBA-CGA-O2A-C1
14	b	801	CLA	O1A-CGA-O2A-C1
14	b	801	CLA	C14-C13-C15-C16
14	b	803	CLA	CBD-CGD-O2D-CED
14	b	805	CLA	CHA-CBD-CGD-O1D
14	b	805	CLA	CHA-CBD-CGD-O2D
14	b	806	CLA	C1A-C2A-CAA-CBA
14	b	806	CLA	C3A-C2A-CAA-CBA
14	b	807	CLA	CBD-CGD-O2D-CED
14	b	808	CLA	CHA-CBD-CGD-O1D
14	b	808	CLA	CHA-CBD-CGD-O2D
14	b	809	CLA	C1A-C2A-CAA-CBA
14	b	809	CLA	C3A-C2A-CAA-CBA
14	b	812	CLA	C1A-C2A-CAA-CBA
14	b	812	CLA	C3A-C2A-CAA-CBA
14	b	814	CLA	C1A-C2A-CAA-CBA
14	b	814	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	b	814	CLA	CHA-CBD-CGD-O2D
14	b	816	CLA	CBD-CGD-O2D-CED
14	b	817	CLA	C1A-C2A-CAA-CBA
14	b	817	CLA	C3A-C2A-CAA-CBA
14	b	819	CLA	C1A-C2A-CAA-CBA
14	b	819	CLA	C3A-C2A-CAA-CBA
14	b	820	CLA	CHA-CBD-CGD-O1D
14	b	820	CLA	CHA-CBD-CGD-O2D
14	b	821	CLA	CBD-CGD-O2D-CED
14	b	822	CLA	C1A-C2A-CAA-CBA
14	b	823	CLA	CHA-CBD-CGD-O1D
14	b	823	CLA	CHA-CBD-CGD-O2D
14	b	824	CLA	CHA-CBD-CGD-O1D
14	b	824	CLA	CHA-CBD-CGD-O2D
14	b	825	CLA	C3A-C2A-CAA-CBA
14	b	826	CLA	C1A-C2A-CAA-CBA
14	b	826	CLA	C3A-C2A-CAA-CBA
14	b	827	CLA	C1A-C2A-CAA-CBA
14	b	827	CLA	C3A-C2A-CAA-CBA
14	b	828	CLA	CAD-CBD-CGD-O1D
14	b	828	CLA	CAD-CBD-CGD-O2D
14	b	829	CLA	C1A-C2A-CAA-CBA
14	b	829	CLA	CBD-CGD-O2D-CED
14	b	830	CLA	C1A-C2A-CAA-CBA
14	b	830	CLA	C3A-C2A-CAA-CBA
14	b	832	CLA	CHA-CBD-CGD-O1D
14	b	832	CLA	CHA-CBD-CGD-O2D
14	b	833	CLA	C1A-C2A-CAA-CBA
14	b	834	CLA	C1A-C2A-CAA-CBA
14	b	834	CLA	C3A-C2A-CAA-CBA
14	b	836	CLA	CBD-CGD-O2D-CED
14	b	840	CLA	C2-C1-O2A-CGA
14	b	840	CLA	CBD-CGD-O2D-CED
14	f	202	CLA	CBD-CGD-O2D-CED
14	j	101	CLA	CHA-CBD-CGD-O1D
14	j	101	CLA	CHA-CBD-CGD-O2D
14	k	1401	CLA	CBD-CGD-O2D-CED
14	l	205	CLA	C1A-C2A-CAA-CBA
14	l	205	CLA	C3A-C2A-CAA-CBA
14	l	206	CLA	C1A-C2A-CAA-CBA
14	m	1601	CLA	C1A-C2A-CAA-CBA
14	m	1601	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	x	1701	CLA	CHA-CBD-CGD-O1D
14	x	1701	CLA	CHA-CBD-CGD-O2D
15	A	846	PQN	C12-C13-C15-C16
15	A	846	PQN	C14-C13-C15-C16
15	a	845	PQN	C14-C13-C15-C16
17	A	848	BCR	C11-C10-C9-C8
17	A	848	BCR	C11-C10-C9-C34
17	A	848	BCR	C10-C11-C12-C13
17	A	848	BCR	C21-C22-C23-C24
17	A	849	BCR	C7-C8-C9-C10
17	A	849	BCR	C11-C10-C9-C8
17	A	849	BCR	C11-C10-C9-C34
17	A	849	BCR	C10-C11-C12-C13
17	A	849	BCR	C11-C12-C13-C14
17	A	849	BCR	C11-C12-C13-C35
17	A	849	BCR	C17-C18-C19-C20
17	A	849	BCR	C36-C18-C19-C20
17	A	849	BCR	C23-C24-C25-C26
17	A	850	BCR	C7-C8-C9-C10
17	A	850	BCR	C7-C8-C9-C34
17	A	850	BCR	C11-C10-C9-C8
17	A	850	BCR	C11-C10-C9-C34
17	A	850	BCR	C10-C11-C12-C13
17	A	851	BCR	C7-C8-C9-C10
17	A	851	BCR	C7-C8-C9-C34
17	A	851	BCR	C11-C10-C9-C8
17	A	851	BCR	C11-C10-C9-C34
17	A	851	BCR	C10-C11-C12-C13
17	A	851	BCR	C23-C24-C25-C26
17	A	852	BCR	C11-C10-C9-C8
17	A	852	BCR	C11-C10-C9-C34
17	A	852	BCR	C21-C22-C23-C24
17	A	852	BCR	C37-C22-C23-C24
17	A	853	BCR	C11-C10-C9-C8
17	A	853	BCR	C17-C18-C19-C20
17	B	842	BCR	C11-C10-C9-C8
17	B	842	BCR	C11-C10-C9-C34
17	B	842	BCR	C19-C20-C21-C22
17	B	842	BCR	C21-C22-C23-C24
17	B	842	BCR	C37-C22-C23-C24
17	B	843	BCR	C11-C10-C9-C8
17	B	843	BCR	C11-C10-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	844	BCR	C21-C22-C23-C24
17	B	844	BCR	C37-C22-C23-C24
17	B	846	BCR	C11-C10-C9-C8
17	B	846	BCR	C11-C10-C9-C34
17	B	846	BCR	C9-C10-C11-C12
17	B	846	BCR	C17-C18-C19-C20
17	B	847	BCR	C7-C8-C9-C10
17	B	847	BCR	C7-C8-C9-C34
17	B	847	BCR	C11-C10-C9-C8
17	B	847	BCR	C11-C10-C9-C34
17	B	847	BCR	C17-C18-C19-C20
17	B	847	BCR	C36-C18-C19-C20
17	B	848	BCR	C7-C8-C9-C10
17	B	848	BCR	C7-C8-C9-C34
17	B	848	BCR	C11-C10-C9-C8
17	B	848	BCR	C11-C10-C9-C34
17	B	848	BCR	C10-C11-C12-C13
17	B	848	BCR	C18-C19-C20-C21
17	B	850	BCR	C7-C8-C9-C10
17	B	850	BCR	C7-C8-C9-C34
17	F	1302	BCR	C10-C11-C12-C13
17	G	848	BCR	C11-C10-C9-C8
17	G	848	BCR	C11-C10-C9-C34
17	G	849	BCR	C23-C24-C25-C26
17	G	850	BCR	C7-C8-C9-C10
17	G	850	BCR	C7-C8-C9-C34
17	G	850	BCR	C11-C10-C9-C8
17	G	850	BCR	C11-C10-C9-C34
17	G	850	BCR	C10-C11-C12-C13
17	G	850	BCR	C17-C18-C19-C20
17	G	853	BCR	C23-C24-C25-C26
17	G	853	BCR	C23-C24-C25-C30
17	H	842	BCR	C11-C10-C9-C8
17	H	842	BCR	C11-C10-C9-C34
17	H	842	BCR	C21-C22-C23-C24
17	H	842	BCR	C37-C22-C23-C24
17	H	843	BCR	C11-C10-C9-C8
17	H	843	BCR	C11-C10-C9-C34
17	H	843	BCR	C11-C12-C13-C14
17	H	843	BCR	C11-C12-C13-C35
17	H	844	BCR	C21-C22-C23-C24
17	H	846	BCR	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	H	846	BCR	C11-C10-C9-C34
17	H	846	BCR	C17-C18-C19-C20
17	H	847	BCR	C7-C8-C9-C10
17	H	847	BCR	C11-C10-C9-C8
17	H	847	BCR	C11-C10-C9-C34
17	H	847	BCR	C10-C11-C12-C13
17	H	847	BCR	C18-C19-C20-C21
17	H	849	BCR	C7-C8-C9-C10
17	I	101	BCR	C7-C8-C9-C10
17	I	101	BCR	C11-C10-C9-C8
17	I	101	BCR	C11-C10-C9-C34
17	I	102	BCR	C11-C10-C9-C8
17	I	102	BCR	C11-C10-C9-C34
17	I	102	BCR	C10-C11-C12-C13
17	I	102	BCR	C23-C24-C25-C26
17	I	102	BCR	C23-C24-C25-C30
17	J	102	BCR	C7-C8-C9-C10
17	J	102	BCR	C7-C8-C9-C34
17	J	102	BCR	C11-C10-C9-C8
17	J	102	BCR	C11-C10-C9-C34
17	J	102	BCR	C11-C12-C13-C14
17	J	102	BCR	C11-C12-C13-C35
17	J	102	BCR	C21-C22-C23-C24
17	J	103	BCR	C11-C10-C9-C8
17	J	103	BCR	C11-C10-C9-C34
17	J	103	BCR	C10-C11-C12-C13
17	J	103	BCR	C11-C12-C13-C14
17	J	103	BCR	C11-C12-C13-C35
17	J	103	BCR	C15-C16-C17-C18
17	J	103	BCR	C19-C20-C21-C22
17	J	103	BCR	C23-C24-C25-C26
17	L	202	BCR	C7-C8-C9-C10
17	L	202	BCR	C7-C8-C9-C34
17	L	202	BCR	C11-C10-C9-C8
17	L	202	BCR	C11-C10-C9-C34
17	L	207	BCR	C11-C10-C9-C8
17	L	207	BCR	C11-C10-C9-C34
17	M	1602	BCR	C5-C6-C7-C8
17	M	1602	BCR	C7-C8-C9-C10
17	M	1602	BCR	C11-C10-C9-C8
17	M	1602	BCR	C11-C10-C9-C34
17	Q	202	BCR	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	Q	202	BCR	C17-C18-C19-C20
17	R	101	BCR	C7-C8-C9-C10
17	R	101	BCR	C7-C8-C9-C34
17	R	101	BCR	C11-C10-C9-C8
17	R	101	BCR	C11-C10-C9-C34
17	R	101	BCR	C10-C11-C12-C13
17	R	101	BCR	C18-C19-C20-C21
17	R	102	BCR	C7-C8-C9-C10
17	R	102	BCR	C7-C8-C9-C34
17	R	102	BCR	C11-C10-C9-C8
17	R	102	BCR	C11-C10-C9-C34
17	R	103	BCR	C7-C8-C9-C10
17	R	103	BCR	C7-C8-C9-C34
17	R	103	BCR	C23-C24-C25-C26
17	S	103	BCR	C7-C8-C9-C10
17	S	103	BCR	C11-C10-C9-C8
17	S	103	BCR	C11-C10-C9-C34
17	S	103	BCR	C10-C11-C12-C13
17	S	103	BCR	C21-C22-C23-C24
17	S	104	BCR	C11-C10-C9-C8
17	S	104	BCR	C11-C10-C9-C34
17	S	104	BCR	C10-C11-C12-C13
17	S	104	BCR	C19-C20-C21-C22
17	S	104	BCR	C21-C22-C23-C24
17	S	104	BCR	C23-C24-C25-C26
17	U	202	BCR	C11-C10-C9-C8
17	U	202	BCR	C11-C10-C9-C34
17	V	1602	BCR	C5-C6-C7-C8
17	V	1602	BCR	C11-C10-C9-C8
17	V	1602	BCR	C11-C10-C9-C34
17	V	1602	BCR	C10-C11-C12-C13
17	a	847	BCR	C11-C10-C9-C8
17	a	847	BCR	C11-C10-C9-C34
17	a	848	BCR	C7-C8-C9-C10
17	a	848	BCR	C7-C8-C9-C34
17	a	848	BCR	C11-C10-C9-C8
17	a	848	BCR	C11-C10-C9-C34
17	a	848	BCR	C10-C11-C12-C13
17	a	848	BCR	C17-C18-C19-C20
17	a	848	BCR	C36-C18-C19-C20
17	a	848	BCR	C23-C24-C25-C26
17	a	848	BCR	C23-C24-C25-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	a	849	BCR	C7-C8-C9-C10
17	a	849	BCR	C7-C8-C9-C34
17	a	849	BCR	C11-C10-C9-C8
17	a	849	BCR	C11-C10-C9-C34
17	a	849	BCR	C9-C10-C11-C12
17	a	849	BCR	C10-C11-C12-C13
17	a	850	BCR	C7-C8-C9-C10
17	a	850	BCR	C7-C8-C9-C34
17	a	850	BCR	C11-C10-C9-C8
17	a	850	BCR	C11-C10-C9-C34
17	a	850	BCR	C10-C11-C12-C13
17	a	850	BCR	C23-C24-C25-C26
17	a	851	BCR	C11-C10-C9-C8
17	a	851	BCR	C11-C10-C9-C34
17	a	852	BCR	C7-C8-C9-C10
17	a	852	BCR	C7-C8-C9-C34
17	b	842	BCR	C11-C10-C9-C8
17	b	842	BCR	C11-C10-C9-C34
17	b	842	BCR	C21-C22-C23-C24
17	b	843	BCR	C11-C10-C9-C8
17	b	843	BCR	C11-C10-C9-C34
17	b	843	BCR	C11-C12-C13-C14
17	b	843	BCR	C21-C22-C23-C24
17	b	844	BCR	C21-C22-C23-C24
17	b	844	BCR	C37-C22-C23-C24
17	b	846	BCR	C17-C18-C19-C20
17	b	847	BCR	C11-C10-C9-C8
17	b	847	BCR	C11-C10-C9-C34
17	b	847	BCR	C10-C11-C12-C13
17	b	849	BCR	C7-C8-C9-C10
17	b	849	BCR	C11-C10-C9-C8
17	b	849	BCR	C11-C10-C9-C34
17	f	201	BCR	C11-C12-C13-C14
17	f	201	BCR	C11-C12-C13-C35
17	f	201	BCR	C17-C18-C19-C20
17	i	102	BCR	C7-C8-C9-C10
17	i	102	BCR	C11-C10-C9-C8
17	i	102	BCR	C11-C10-C9-C34
17	j	103	BCR	C7-C8-C9-C10
17	j	103	BCR	C11-C10-C9-C8
17	j	103	BCR	C11-C10-C9-C34
17	j	103	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	j	104	BCR	C11-C10-C9-C8
17	j	104	BCR	C11-C10-C9-C34
17	j	104	BCR	C23-C24-C25-C26
17	l	201	BCR	C11-C10-C9-C8
17	l	201	BCR	C11-C10-C9-C34
17	l	203	BCR	C7-C8-C9-C10
17	l	203	BCR	C7-C8-C9-C34
17	l	203	BCR	C11-C10-C9-C8
17	l	203	BCR	C11-C10-C9-C34
17	l	203	BCR	C10-C11-C12-C13
17	l	208	BCR	C7-C8-C9-C10
17	l	208	BCR	C7-C8-C9-C34
17	l	208	BCR	C23-C24-C25-C26
17	m	1602	BCR	C5-C6-C7-C8
17	m	1602	BCR	C7-C8-C9-C10
17	m	1602	BCR	C11-C10-C9-C8
17	m	1602	BCR	C11-C10-C9-C34
17	m	1602	BCR	C10-C11-C12-C13
18	A	854	LHG	O1-C1-C2-O2
18	A	854	LHG	O1-C1-C2-C3
18	A	854	LHG	C3-O3-P-O5
18	A	854	LHG	C3-O3-P-O6
18	A	854	LHG	C4-O6-P-O3
18	A	854	LHG	C4-O6-P-O4
18	A	854	LHG	C4-O6-P-O5
18	A	855	LHG	O2-C2-C3-O3
18	A	855	LHG	O7-C5-C6-O8
18	G	854	LHG	O1-C1-C2-C3
18	G	854	LHG	C3-O3-P-O5
18	G	854	LHG	C4-O6-P-O3
18	G	854	LHG	C4-O6-P-O4
18	G	854	LHG	C4-O6-P-O5
18	G	854	LHG	O7-C5-C6-O8
18	G	855	LHG	O2-C2-C3-O3
18	a	853	LHG	C3-O3-P-O6
18	a	853	LHG	C4-O6-P-O3
18	a	853	LHG	C4-O6-P-O4
18	a	853	LHG	C4-O6-P-O5
18	a	853	LHG	O7-C5-C6-O8
18	a	854	LHG	O1-C1-C2-O2
18	a	854	LHG	O1-C1-C2-C3
18	a	854	LHG	C3-O3-P-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a	854	LHG	C3-O3-P-O5
18	a	854	LHG	C3-O3-P-O6
18	a	854	LHG	C4-O6-P-O3
18	a	854	LHG	C4-O6-P-O4
18	a	854	LHG	O7-C5-C6-O8
14	A	807	CLA	O1D-CGD-O2D-CED
14	A	810	CLA	O1D-CGD-O2D-CED
14	B	802	CLA	O1D-CGD-O2D-CED
14	G	811	CLA	O1D-CGD-O2D-CED
14	G	819	CLA	O1D-CGD-O2D-CED
14	G	841	CLA	O1D-CGD-O2D-CED
14	H	802	CLA	O1D-CGD-O2D-CED
14	H	834	CLA	O1D-CGD-O2D-CED
14	a	809	CLA	O1D-CGD-O2D-CED
14	a	816	CLA	O1D-CGD-O2D-CED
14	a	818	CLA	O1D-CGD-O2D-CED
14	a	821	CLA	O1D-CGD-O2D-CED
14	A	845	CLA	C4C-C3C-CAC-CBC
14	a	844	CLA	C4C-C3C-CAC-CBC
14	A	811	CLA	O1D-CGD-O2D-CED
14	A	817	CLA	O1D-CGD-O2D-CED
14	A	819	CLA	O1D-CGD-O2D-CED
14	A	841	CLA	O1D-CGD-O2D-CED
14	B	810	CLA	O1D-CGD-O2D-CED
14	B	813	CLA	O1D-CGD-O2D-CED
14	B	826	CLA	O1D-CGD-O2D-CED
14	G	807	CLA	O1D-CGD-O2D-CED
14	G	817	CLA	O1D-CGD-O2D-CED
14	H	809	CLA	O1D-CGD-O2D-CED
14	H	830	CLA	O1D-CGD-O2D-CED
14	H	835	CLA	O1D-CGD-O2D-CED
14	Q	201	CLA	O1D-CGD-O2D-CED
14	V	1601	CLA	O1D-CGD-O2D-CED
14	a	806	CLA	O1D-CGD-O2D-CED
14	a	811	CLA	O1D-CGD-O2D-CED
14	a	841	CLA	O1D-CGD-O2D-CED
14	b	803	CLA	O1D-CGD-O2D-CED
14	b	813	CLA	O1D-CGD-O2D-CED
14	b	818	CLA	O1D-CGD-O2D-CED
14	b	830	CLA	O1D-CGD-O2D-CED
14	m	1601	CLA	O1D-CGD-O2D-CED
14	A	806	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	807	CLA	CBD-CGD-O2D-CED
14	A	814	CLA	CBD-CGD-O2D-CED
14	A	815	CLA	CBD-CGD-O2D-CED
14	A	819	CLA	CBD-CGD-O2D-CED
14	A	820	CLA	CBD-CGD-O2D-CED
14	A	824	CLA	CBD-CGD-O2D-CED
14	A	829	CLA	CBD-CGD-O2D-CED
14	A	835	CLA	CBD-CGD-O2D-CED
14	A	844	CLA	CBD-CGD-O2D-CED
14	B	802	CLA	CBD-CGD-O2D-CED
14	B	806	CLA	CBD-CGD-O2D-CED
14	B	810	CLA	CBD-CGD-O2D-CED
14	B	813	CLA	CBD-CGD-O2D-CED
14	B	825	CLA	CBD-CGD-O2D-CED
14	B	826	CLA	CBD-CGD-O2D-CED
14	B	829	CLA	CBD-CGD-O2D-CED
14	B	830	CLA	CBD-CGD-O2D-CED
14	B	831	CLA	CBD-CGD-O2D-CED
14	B	832	CLA	CBD-CGD-O2D-CED
14	B	834	CLA	CBD-CGD-O2D-CED
14	B	840	CLA	CBD-CGD-O2D-CED
14	G	804	CLA	CBD-CGD-O2D-CED
14	G	811	CLA	CBD-CGD-O2D-CED
14	G	812	CLA	CBD-CGD-O2D-CED
14	G	814	CLA	CBD-CGD-O2D-CED
14	G	817	CLA	CBD-CGD-O2D-CED
14	G	822	CLA	CBD-CGD-O2D-CED
14	G	823	CLA	CBD-CGD-O2D-CED
14	G	824	CLA	CBD-CGD-O2D-CED
14	G	829	CLA	CBD-CGD-O2D-CED
14	G	835	CLA	CBD-CGD-O2D-CED
14	G	841	CLA	CBD-CGD-O2D-CED
14	G	843	CLA	CBD-CGD-O2D-CED
14	H	809	CLA	CBD-CGD-O2D-CED
14	H	810	CLA	CBD-CGD-O2D-CED
14	H	814	CLA	CBD-CGD-O2D-CED
14	H	815	CLA	CBD-CGD-O2D-CED
14	H	816	CLA	CBD-CGD-O2D-CED
14	H	823	CLA	CBD-CGD-O2D-CED
14	H	824	CLA	CBD-CGD-O2D-CED
14	H	825	CLA	CBD-CGD-O2D-CED
14	H	826	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	829	CLA	CBD-CGD-O2D-CED
14	H	831	CLA	CBD-CGD-O2D-CED
14	H	835	CLA	CBD-CGD-O2D-CED
14	K	102	CLA	CBD-CGD-O2D-CED
14	M	1601	CLA	CBD-CGD-O2D-CED
14	Q	203	CLA	CBD-CGD-O2D-CED
14	T	1401	CLA	CBD-CGD-O2D-CED
14	V	1601	CLA	CBD-CGD-O2D-CED
14	a	803	CLA	CBD-CGD-O2D-CED
14	a	807	CLA	CBD-CGD-O2D-CED
14	a	810	CLA	CBD-CGD-O2D-CED
14	a	813	CLA	CBD-CGD-O2D-CED
14	a	814	CLA	CBD-CGD-O2D-CED
14	a	815	CLA	CBD-CGD-O2D-CED
14	a	818	CLA	CBD-CGD-O2D-CED
14	a	819	CLA	CBD-CGD-O2D-CED
14	a	823	CLA	CBD-CGD-O2D-CED
14	a	834	CLA	CBD-CGD-O2D-CED
14	b	802	CLA	CBD-CGD-O2D-CED
14	b	805	CLA	CBD-CGD-O2D-CED
14	b	808	CLA	CBD-CGD-O2D-CED
14	b	809	CLA	CBD-CGD-O2D-CED
14	b	810	CLA	CBD-CGD-O2D-CED
14	b	812	CLA	CBD-CGD-O2D-CED
14	b	813	CLA	CBD-CGD-O2D-CED
14	b	818	CLA	CBD-CGD-O2D-CED
14	b	826	CLA	CBD-CGD-O2D-CED
14	b	830	CLA	CBD-CGD-O2D-CED
14	b	831	CLA	CBD-CGD-O2D-CED
14	b	835	CLA	CBD-CGD-O2D-CED
14	l	207	CLA	CBD-CGD-O2D-CED
14	m	1601	CLA	CBD-CGD-O2D-CED
14	A	844	CLA	O1A-CGA-O2A-C1
14	G	845	CLA	C4C-C3C-CAC-CBC
14	b	801	CLA	C8-C10-C11-C12
14	A	845	CLA	C2C-C3C-CAC-CBC
14	A	824	CLA	O1D-CGD-O2D-CED
14	B	806	CLA	O1D-CGD-O2D-CED
14	G	812	CLA	O1D-CGD-O2D-CED
14	G	824	CLA	O1D-CGD-O2D-CED
14	H	810	CLA	O1D-CGD-O2D-CED
14	H	826	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	831	CLA	O1D-CGD-O2D-CED
14	M	1601	CLA	O1D-CGD-O2D-CED
14	a	813	CLA	O1D-CGD-O2D-CED
14	b	810	CLA	O1D-CGD-O2D-CED
14	b	826	CLA	O1D-CGD-O2D-CED
14	b	831	CLA	O1D-CGD-O2D-CED
14	A	844	CLA	CBA-CGA-O2A-C1
14	G	805	CLA	CBA-CGA-O2A-C1
14	G	821	CLA	CBA-CGA-O2A-C1
14	L	204	CLA	CBA-CGA-O2A-C1
14	B	808	CLA	CBD-CGD-O2D-CED
14	H	832	CLA	CBD-CGD-O2D-CED
14	b	832	CLA	CBD-CGD-O2D-CED
14	b	839	CLA	CBD-CGD-O2D-CED
14	A	805	CLA	O1A-CGA-O2A-C1
14	A	821	CLA	O1A-CGA-O2A-C1
14	A	838	CLA	O1A-CGA-O2A-C1
14	G	805	CLA	O1A-CGA-O2A-C1
14	G	821	CLA	O1A-CGA-O2A-C1
14	G	833	CLA	O1A-CGA-O2A-C1
14	G	843	CLA	O1A-CGA-O2A-C1
14	H	828	CLA	O1A-CGA-O2A-C1
14	L	204	CLA	O1A-CGA-O2A-C1
14	L	205	CLA	O1A-CGA-O2A-C1
14	U	204	CLA	O1A-CGA-O2A-C1
14	a	804	CLA	O1A-CGA-O2A-C1
14	a	812	CLA	O1A-CGA-O2A-C1
14	a	820	CLA	O1A-CGA-O2A-C1
14	a	831	CLA	O1A-CGA-O2A-C1
14	a	832	CLA	O1A-CGA-O2A-C1
14	b	802	CLA	O1A-CGA-O2A-C1
14	b	828	CLA	O1A-CGA-O2A-C1
14	a	844	CLA	C2C-C3C-CAC-CBC
14	A	834	CLA	O1D-CGD-O2D-CED
14	B	821	CLA	O1D-CGD-O2D-CED
14	B	831	CLA	O1D-CGD-O2D-CED
14	B	837	CLA	O1D-CGD-O2D-CED
14	B	840	CLA	O1D-CGD-O2D-CED
14	G	810	CLA	O1D-CGD-O2D-CED
14	G	822	CLA	O1D-CGD-O2D-CED
14	G	834	CLA	O1D-CGD-O2D-CED
14	H	813	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	810	CLA	O1D-CGD-O2D-CED
14	a	819	CLA	O1D-CGD-O2D-CED
14	b	807	CLA	O1D-CGD-O2D-CED
14	b	835	CLA	O1D-CGD-O2D-CED
14	b	840	CLA	O1D-CGD-O2D-CED
14	k	1401	CLA	O1D-CGD-O2D-CED
14	A	812	CLA	O1D-CGD-O2D-CED
14	A	823	CLA	O1D-CGD-O2D-CED
14	A	836	CLA	O1D-CGD-O2D-CED
14	A	838	CLA	O1D-CGD-O2D-CED
14	B	816	CLA	O1D-CGD-O2D-CED
14	G	803	CLA	O1D-CGD-O2D-CED
14	G	820	CLA	O1D-CGD-O2D-CED
14	G	838	CLA	O1D-CGD-O2D-CED
14	b	816	CLA	O1D-CGD-O2D-CED
14	b	821	CLA	O1D-CGD-O2D-CED
14	f	202	CLA	O1D-CGD-O2D-CED
14	H	833	CLA	CBD-CGD-O2D-CED
14	G	838	CLA	O1A-CGA-O2A-C1
14	a	837	CLA	O1A-CGA-O2A-C1
14	G	845	CLA	C2C-C3C-CAC-CBC
14	b	829	CLA	O1D-CGD-O2D-CED
14	A	807	CLA	C3-C5-C6-C7
14	A	810	CLA	C3-C5-C6-C7
14	A	814	CLA	C3-C5-C6-C7
14	A	828	CLA	C3-C5-C6-C7
14	A	833	CLA	C3-C5-C6-C7
14	A	844	CLA	C3-C5-C6-C7
14	B	801	CLA	C3-C5-C6-C7
14	B	806	CLA	C3-C5-C6-C7
14	B	821	CLA	C3-C5-C6-C7
14	G	802	CLA	C3-C5-C6-C7
14	G	803	CLA	C3-C5-C6-C7
14	G	814	CLA	C3-C5-C6-C7
14	H	801	CLA	C3-C5-C6-C7
14	H	806	CLA	C3-C5-C6-C7
14	H	809	CLA	C3-C5-C6-C7
14	H	818	CLA	C3-C5-C6-C7
14	H	821	CLA	C3-C5-C6-C7
14	H	839	CLA	C3-C5-C6-C7
14	L	204	CLA	C3-C5-C6-C7
14	L	206	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	U	206	CLA	C3-C5-C6-C7
14	a	808	CLA	C3-C5-C6-C7
14	a	809	CLA	C3-C5-C6-C7
14	a	819	CLA	C3-C5-C6-C7
14	a	825	CLA	C3-C5-C6-C7
14	a	827	CLA	C3-C5-C6-C7
14	a	855	CLA	C3-C5-C6-C7
14	b	807	CLA	C3-C5-C6-C7
14	b	809	CLA	C3-C5-C6-C7
14	l	205	CLA	C3-C5-C6-C7
14	l	207	CLA	C3-C5-C6-C7
14	a	822	CLA	O1D-CGD-O2D-CED
14	A	833	CLA	CBA-CGA-O2A-C1
14	B	828	CLA	CBA-CGA-O2A-C1
14	G	832	CLA	CBA-CGA-O2A-C1
14	G	833	CLA	CBA-CGA-O2A-C1
14	G	843	CLA	CBA-CGA-O2A-C1
14	L	205	CLA	CBA-CGA-O2A-C1
14	U	205	CLA	CBA-CGA-O2A-C1
14	a	820	CLA	CBA-CGA-O2A-C1
14	a	832	CLA	CBA-CGA-O2A-C1
14	b	806	CLA	CBA-CGA-O2A-C1
14	b	813	CLA	CBA-CGA-O2A-C1
14	l	202	CLA	CBA-CGA-O2A-C1
14	A	802	CLA	CBD-CGD-O2D-CED
14	A	803	CLA	CBD-CGD-O2D-CED
14	A	804	CLA	CBD-CGD-O2D-CED
14	A	805	CLA	CBD-CGD-O2D-CED
14	A	809	CLA	CBD-CGD-O2D-CED
14	A	816	CLA	CBD-CGD-O2D-CED
14	A	828	CLA	CBD-CGD-O2D-CED
14	A	843	CLA	CBD-CGD-O2D-CED
14	B	803	CLA	CBD-CGD-O2D-CED
14	B	804	CLA	CBD-CGD-O2D-CED
14	B	812	CLA	CBD-CGD-O2D-CED
14	B	814	CLA	CBD-CGD-O2D-CED
14	B	815	CLA	CBD-CGD-O2D-CED
14	B	817	CLA	CBD-CGD-O2D-CED
14	B	819	CLA	CBD-CGD-O2D-CED
14	B	820	CLA	CBD-CGD-O2D-CED
14	B	822	CLA	CBD-CGD-O2D-CED
14	B	823	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	833	CLA	CBD-CGD-O2D-CED
14	B	839	CLA	CBD-CGD-O2D-CED
14	F	1301	CLA	CBD-CGD-O2D-CED
14	G	809	CLA	CBD-CGD-O2D-CED
14	G	816	CLA	CBD-CGD-O2D-CED
14	G	818	CLA	CBD-CGD-O2D-CED
14	G	832	CLA	CBD-CGD-O2D-CED
14	G	833	CLA	CBD-CGD-O2D-CED
14	G	842	CLA	CBD-CGD-O2D-CED
14	H	804	CLA	CBD-CGD-O2D-CED
14	H	812	CLA	CBD-CGD-O2D-CED
14	H	817	CLA	CBD-CGD-O2D-CED
14	H	819	CLA	CBD-CGD-O2D-CED
14	H	820	CLA	CBD-CGD-O2D-CED
14	H	837	CLA	CBD-CGD-O2D-CED
14	H	838	CLA	CBD-CGD-O2D-CED
14	H	839	CLA	CBD-CGD-O2D-CED
14	J	101	CLA	CBD-CGD-O2D-CED
14	U	201	CLA	CBD-CGD-O2D-CED
14	a	802	CLA	CBD-CGD-O2D-CED
14	a	804	CLA	CBD-CGD-O2D-CED
14	a	805	CLA	CBD-CGD-O2D-CED
14	a	808	CLA	CBD-CGD-O2D-CED
14	a	829	CLA	CBD-CGD-O2D-CED
14	a	830	CLA	CBD-CGD-O2D-CED
14	a	832	CLA	CBD-CGD-O2D-CED
14	a	842	CLA	CBD-CGD-O2D-CED
14	b	814	CLA	CBD-CGD-O2D-CED
14	b	820	CLA	CBD-CGD-O2D-CED
14	b	823	CLA	CBD-CGD-O2D-CED
14	B	834	CLA	O1D-CGD-O2D-CED
14	B	836	CLA	O1D-CGD-O2D-CED
14	H	815	CLA	O1D-CGD-O2D-CED
14	W	1701	CLA	O1D-CGD-O2D-CED
14	a	815	CLA	O1D-CGD-O2D-CED
14	a	828	CLA	O1D-CGD-O2D-CED
14	a	833	CLA	O1D-CGD-O2D-CED
14	a	835	CLA	O1D-CGD-O2D-CED
14	a	837	CLA	O1D-CGD-O2D-CED
14	b	836	CLA	O1D-CGD-O2D-CED
14	b	804	CLA	C2C-C3C-CAC-CBC
14	B	829	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	830	CLA	O1D-CGD-O2D-CED
14	B	835	CLA	O1D-CGD-O2D-CED
14	H	840	CLA	O1D-CGD-O2D-CED
14	A	829	CLA	C4-C3-C5-C6
14	A	843	CLA	C4-C3-C5-C6
14	B	832	CLA	C4-C3-C5-C6
14	G	829	CLA	C4-C3-C5-C6
14	G	833	CLA	C4-C3-C5-C6
14	G	843	CLA	C4-C3-C5-C6
14	H	806	CLA	C4-C3-C5-C6
14	H	817	CLA	C4-C3-C5-C6
14	H	832	CLA	C4-C3-C5-C6
14	a	806	CLA	C4-C3-C5-C6
14	a	828	CLA	C4-C3-C5-C6
14	b	802	CLA	C4-C3-C5-C6
14	b	818	CLA	C4-C3-C5-C6
14	b	832	CLA	C4-C3-C5-C6
14	A	843	CLA	C2-C3-C5-C6
14	B	832	CLA	C2-C3-C5-C6
14	G	843	CLA	C2-C3-C5-C6
14	H	806	CLA	C2-C3-C5-C6
14	H	817	CLA	C2-C3-C5-C6
14	a	806	CLA	C2-C3-C5-C6
14	b	818	CLA	C2-C3-C5-C6
15	a	845	PQN	C12-C13-C15-C16
14	H	807	CLA	CBD-CGD-O2D-CED
14	X	1701	CLA	CBD-CGD-O2D-CED
14	b	817	CLA	CBD-CGD-O2D-CED
14	A	820	CLA	O1D-CGD-O2D-CED
14	A	844	CLA	O1D-CGD-O2D-CED
14	B	825	CLA	O1D-CGD-O2D-CED
14	G	829	CLA	O1D-CGD-O2D-CED
14	A	830	CLA	C2A-CAA-CBA-CGA
14	A	832	CLA	C2A-CAA-CBA-CGA
14	B	816	CLA	C2A-CAA-CBA-CGA
14	b	829	CLA	C2A-CAA-CBA-CGA
14	A	812	CLA	O1A-CGA-O2A-C1
14	B	805	CLA	O1A-CGA-O2A-C1
14	l	205	CLA	O1A-CGA-O2A-C1
14	A	803	CLA	C3-C5-C6-C7
14	B	836	CLA	C3-C5-C6-C7
14	b	801	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	b	806	CLA	C3-C5-C6-C7
14	b	832	CLA	C3-C5-C6-C7
14	b	836	CLA	C3-C5-C6-C7
14	A	805	CLA	CBA-CGA-O2A-C1
14	A	812	CLA	CBA-CGA-O2A-C1
14	A	814	CLA	CBA-CGA-O2A-C1
14	A	821	CLA	CBA-CGA-O2A-C1
14	A	831	CLA	CBA-CGA-O2A-C1
14	A	838	CLA	CBA-CGA-O2A-C1
14	B	805	CLA	CBA-CGA-O2A-C1
14	B	812	CLA	CBA-CGA-O2A-C1
14	G	838	CLA	CBA-CGA-O2A-C1
14	H	805	CLA	CBA-CGA-O2A-C1
14	H	813	CLA	CBA-CGA-O2A-C1
14	H	817	CLA	CBA-CGA-O2A-C1
14	H	828	CLA	CBA-CGA-O2A-C1
14	U	204	CLA	CBA-CGA-O2A-C1
14	a	804	CLA	CBA-CGA-O2A-C1
14	a	812	CLA	CBA-CGA-O2A-C1
14	a	813	CLA	CBA-CGA-O2A-C1
14	a	831	CLA	CBA-CGA-O2A-C1
14	a	837	CLA	CBA-CGA-O2A-C1
14	b	802	CLA	CBA-CGA-O2A-C1
14	b	812	CLA	CBA-CGA-O2A-C1
14	b	828	CLA	CBA-CGA-O2A-C1
14	b	832	CLA	CBA-CGA-O2A-C1
14	b	840	CLA	CBA-CGA-O2A-C1
14	l	206	CLA	CBA-CGA-O2A-C1
19	b	848	LMG	C41-C42-C43-C44
14	H	803	CLA	C2C-C3C-CAC-CBC
17	B	850	BCR	C15-C16-C17-C18
17	F	1302	BCR	C9-C10-C11-C12
17	G	850	BCR	C9-C10-C11-C12
17	G	850	BCR	C13-C14-C15-C16
17	H	842	BCR	C9-C10-C11-C12
17	H	849	BCR	C15-C16-C17-C18
17	b	849	BCR	C15-C16-C17-C18
14	A	809	CLA	O1A-CGA-O2A-C1
14	A	832	CLA	O1A-CGA-O2A-C1
14	a	808	CLA	O1A-CGA-O2A-C1
14	b	832	CLA	O1A-CGA-O2A-C1
14	l	206	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	B	849	LMG	C35-C36-C37-C38
19	B	849	LMG	C41-C42-C43-C44
19	H	848	LMG	C35-C36-C37-C38
19	H	848	LMG	C41-C42-C43-C44
19	b	848	LMG	C35-C36-C37-C38
14	H	825	CLA	O1D-CGD-O2D-CED
14	a	807	CLA	O1D-CGD-O2D-CED
14	A	802	CLA	C3-C5-C6-C7
14	A	826	CLA	C3-C5-C6-C7
14	B	809	CLA	C3-C5-C6-C7
14	B	817	CLA	C3-C5-C6-C7
14	B	818	CLA	C3-C5-C6-C7
14	G	828	CLA	C3-C5-C6-C7
14	a	806	CLA	C3-C5-C6-C7
14	b	817	CLA	C3-C5-C6-C7
14	b	839	CLA	C3-C5-C6-C7
14	G	805	CLA	CBD-CGD-O2D-CED
14	G	821	CLA	CBD-CGD-O2D-CED
14	G	827	CLA	CBD-CGD-O2D-CED
14	H	821	CLA	CBD-CGD-O2D-CED
14	U	206	CLA	CBD-CGD-O2D-CED
14	a	826	CLA	CBD-CGD-O2D-CED
14	b	837	CLA	CBD-CGD-O2D-CED
18	a	854	LHG	O2-C2-C3-O3
14	A	815	CLA	O1D-CGD-O2D-CED
14	A	835	CLA	O1D-CGD-O2D-CED
14	G	804	CLA	O1D-CGD-O2D-CED
14	G	814	CLA	O1D-CGD-O2D-CED
14	H	814	CLA	O1D-CGD-O2D-CED
14	H	824	CLA	O1D-CGD-O2D-CED
14	T	1401	CLA	O1D-CGD-O2D-CED
14	a	803	CLA	O1D-CGD-O2D-CED
14	a	814	CLA	O1D-CGD-O2D-CED
14	b	809	CLA	O1D-CGD-O2D-CED
14	A	809	CLA	CBA-CGA-O2A-C1
14	A	832	CLA	CBA-CGA-O2A-C1
14	B	817	CLA	CBA-CGA-O2A-C1
14	B	818	CLA	CBA-CGA-O2A-C1
14	G	831	CLA	CBA-CGA-O2A-C1
14	H	812	CLA	CBA-CGA-O2A-C1
14	H	832	CLA	CBA-CGA-O2A-C1
14	L	201	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	U	201	CLA	CBA-CGA-O2A-C1
14	b	817	CLA	CBA-CGA-O2A-C1
14	l	205	CLA	CBA-CGA-O2A-C1
14	A	814	CLA	O1A-CGA-O2A-C1
14	B	812	CLA	O1A-CGA-O2A-C1
14	B	828	CLA	O1A-CGA-O2A-C1
14	G	832	CLA	O1A-CGA-O2A-C1
14	U	205	CLA	O1A-CGA-O2A-C1
14	a	811	CLA	O1A-CGA-O2A-C1
14	b	806	CLA	O1A-CGA-O2A-C1
14	b	813	CLA	O1A-CGA-O2A-C1
14	l	202	CLA	O1A-CGA-O2A-C1
14	H	816	CLA	O1D-CGD-O2D-CED
14	b	802	CLA	O1D-CGD-O2D-CED
14	b	824	CLA	CBD-CGD-O2D-CED
14	Q	203	CLA	O1D-CGD-O2D-CED
14	A	806	CLA	O1D-CGD-O2D-CED
14	A	814	CLA	O1D-CGD-O2D-CED
14	A	829	CLA	O1D-CGD-O2D-CED
14	G	843	CLA	O1D-CGD-O2D-CED
14	B	808	CLA	C3-C5-C6-C7
14	G	841	CLA	C3-C5-C6-C7
14	H	805	CLA	C3-C5-C6-C7
14	G	831	CLA	CBD-CGD-O2D-CED
14	b	825	CLA	CBD-CGD-O2D-CED
14	j	101	CLA	CBD-CGD-O2D-CED
14	G	835	CLA	O1D-CGD-O2D-CED
14	H	829	CLA	O1D-CGD-O2D-CED
14	a	834	CLA	O1D-CGD-O2D-CED
14	b	805	CLA	O1D-CGD-O2D-CED
14	b	808	CLA	O1D-CGD-O2D-CED
14	b	812	CLA	O1D-CGD-O2D-CED
14	l	207	CLA	O1D-CGD-O2D-CED
14	B	813	CLA	CBA-CGA-O2A-C1
14	a	808	CLA	CBA-CGA-O2A-C1
14	a	811	CLA	CBA-CGA-O2A-C1
14	A	804	CLA	C4-C3-C5-C6
14	B	801	CLA	C4-C3-C5-C6
14	B	817	CLA	C4-C3-C5-C6
14	a	855	CLA	C4-C3-C5-C6
14	b	803	CLA	C4-C3-C5-C6
14	b	817	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	829	CLA	C2-C3-C5-C6
14	A	844	CLA	C2-C3-C5-C6
14	B	801	CLA	C2-C3-C5-C6
14	B	817	CLA	C2-C3-C5-C6
14	G	829	CLA	C2-C3-C5-C6
14	G	833	CLA	C2-C3-C5-C6
14	G	842	CLA	C2-C3-C5-C6
14	H	832	CLA	C2-C3-C5-C6
14	a	828	CLA	C2-C3-C5-C6
14	a	832	CLA	C2-C3-C5-C6
14	a	855	CLA	C2-C3-C5-C6
14	b	817	CLA	C2-C3-C5-C6
14	G	831	CLA	O1A-CGA-O2A-C1
14	H	812	CLA	O1A-CGA-O2A-C1
14	H	813	CLA	O1A-CGA-O2A-C1
14	H	817	CLA	O1A-CGA-O2A-C1
14	a	813	CLA	O1A-CGA-O2A-C1
14	A	833	CLA	CBD-CGD-O2D-CED
14	b	819	CLA	CBD-CGD-O2D-CED
14	G	823	CLA	O1D-CGD-O2D-CED
14	B	811	CLA	C2A-CAA-CBA-CGA
14	G	810	CLA	C2A-CAA-CBA-CGA
14	a	829	CLA	C2A-CAA-CBA-CGA
14	b	816	CLA	C2A-CAA-CBA-CGA
14	H	833	CLA	O1D-CGD-O2D-CED
14	K	102	CLA	O1D-CGD-O2D-CED
14	A	831	CLA	O1A-CGA-O2A-C1
14	B	813	CLA	O1A-CGA-O2A-C1
14	B	818	CLA	O1A-CGA-O2A-C1
14	H	805	CLA	O1A-CGA-O2A-C1
14	H	832	CLA	O1A-CGA-O2A-C1
14	U	201	CLA	O1A-CGA-O2A-C1
14	b	812	CLA	O1A-CGA-O2A-C1
14	b	840	CLA	O1A-CGA-O2A-C1
14	G	825	CLA	C3-C5-C6-C7
14	a	823	CLA	O1D-CGD-O2D-CED
14	b	839	CLA	O1D-CGD-O2D-CED
14	A	820	CLA	CBA-CGA-O2A-C1
14	A	808	CLA	CBD-CGD-O2D-CED
14	A	831	CLA	CBD-CGD-O2D-CED
14	B	838	CLA	CBD-CGD-O2D-CED
14	G	828	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	806	CLA	CBD-CGD-O2D-CED
14	H	836	CLA	CBD-CGD-O2D-CED
14	S	101	CLA	CBD-CGD-O2D-CED
14	U	204	CLA	CBD-CGD-O2D-CED
14	a	820	CLA	CBD-CGD-O2D-CED
14	a	840	CLA	CBD-CGD-O2D-CED
14	b	815	CLA	CBD-CGD-O2D-CED
14	b	833	CLA	CBD-CGD-O2D-CED
14	b	834	CLA	CBD-CGD-O2D-CED
14	b	838	CLA	CBD-CGD-O2D-CED
19	B	849	LMG	O6-C5-C6-O5
14	L	201	CLA	O1A-CGA-O2A-C1
19	H	848	LMG	O6-C5-C6-O5
14	A	803	CLA	O1D-CGD-O2D-CED
14	B	832	CLA	O1D-CGD-O2D-CED
14	H	823	CLA	O1D-CGD-O2D-CED
14	A	827	CLA	CBD-CGD-O2D-CED
14	G	836	CLA	CBD-CGD-O2D-CED
14	A	843	CLA	O1D-CGD-O2D-CED
17	J	103	BCR	C9-C10-C11-C12
17	j	104	BCR	C15-C16-C17-C18
14	A	827	CLA	O1A-CGA-O2A-C1
14	B	817	CLA	O1A-CGA-O2A-C1
14	B	840	CLA	O1A-CGA-O2A-C1
14	H	840	CLA	O1A-CGA-O2A-C1
14	b	817	CLA	O1A-CGA-O2A-C1
18	A	855	LHG	C1-C2-C3-O3
18	G	855	LHG	C1-C2-C3-O3
14	H	832	CLA	O1D-CGD-O2D-CED
14	A	804	CLA	CBA-CGA-O2A-C1
14	A	827	CLA	CBA-CGA-O2A-C1
14	B	840	CLA	CBA-CGA-O2A-C1
14	G	807	CLA	CBA-CGA-O2A-C1
14	G	809	CLA	CBA-CGA-O2A-C1
14	G	812	CLA	CBA-CGA-O2A-C1
14	G	820	CLA	CBA-CGA-O2A-C1
14	G	827	CLA	CBA-CGA-O2A-C1
14	H	818	CLA	CBA-CGA-O2A-C1
14	H	836	CLA	CBA-CGA-O2A-C1
14	H	840	CLA	CBA-CGA-O2A-C1
14	L	206	CLA	CBA-CGA-O2A-C1
14	a	806	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	819	CLA	CBA-CGA-O2A-C1
14	a	826	CLA	CBA-CGA-O2A-C1
14	a	830	CLA	CBA-CGA-O2A-C1
14	b	818	CLA	CBA-CGA-O2A-C1
19	B	849	LMG	C4-C5-C6-O5
19	H	848	LMG	C4-C5-C6-O5
14	A	816	CLA	O1D-CGD-O2D-CED
14	B	803	CLA	O1D-CGD-O2D-CED
14	B	808	CLA	O1D-CGD-O2D-CED
14	B	820	CLA	O1D-CGD-O2D-CED
14	G	809	CLA	O1D-CGD-O2D-CED
14	G	816	CLA	O1D-CGD-O2D-CED
14	G	833	CLA	O1D-CGD-O2D-CED
14	a	805	CLA	O1D-CGD-O2D-CED
14	a	832	CLA	O1D-CGD-O2D-CED
14	b	832	CLA	O1D-CGD-O2D-CED
14	A	844	CLA	C4-C3-C5-C6
14	B	806	CLA	C4-C3-C5-C6
14	G	842	CLA	C4-C3-C5-C6
14	H	801	CLA	C4-C3-C5-C6
14	a	832	CLA	C4-C3-C5-C6
14	a	842	CLA	C4-C3-C5-C6
14	H	801	CLA	C2-C3-C5-C6
14	a	842	CLA	C2-C3-C5-C6
14	b	802	CLA	C2-C3-C5-C6
14	b	803	CLA	C2-C3-C5-C6
14	b	832	CLA	C2-C3-C5-C6
14	b	804	CLA	CBD-CGD-O2D-CED
14	A	802	CLA	C11-C12-C13-C14
14	A	810	CLA	C11-C10-C8-C9
14	A	814	CLA	C6-C7-C8-C9
14	A	829	CLA	C11-C10-C8-C9
14	A	843	CLA	C11-C10-C8-C9
14	B	805	CLA	C11-C12-C13-C14
14	B	808	CLA	C6-C7-C8-C9
14	B	812	CLA	C14-C13-C15-C16
14	G	807	CLA	C6-C7-C8-C9
14	G	828	CLA	C6-C7-C8-C9
14	G	829	CLA	C11-C10-C8-C9
14	G	842	CLA	C11-C10-C8-C9
14	H	808	CLA	C6-C7-C8-C9
14	H	839	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	825	CLA	C6-C7-C8-C9
14	a	828	CLA	C11-C10-C8-C9
14	b	804	CLA	C6-C7-C8-C9
14	b	808	CLA	C6-C7-C8-C9
14	b	812	CLA	C11-C12-C13-C14
14	b	836	CLA	C11-C10-C8-C9
14	l	207	CLA	C6-C7-C8-C9
14	B	804	CLA	O1D-CGD-O2D-CED
14	B	817	CLA	O1D-CGD-O2D-CED
14	B	839	CLA	O1D-CGD-O2D-CED
14	F	1301	CLA	O1D-CGD-O2D-CED
14	G	832	CLA	O1D-CGD-O2D-CED
14	G	842	CLA	O1D-CGD-O2D-CED
14	H	804	CLA	O1D-CGD-O2D-CED
14	H	817	CLA	O1D-CGD-O2D-CED
14	H	837	CLA	O1D-CGD-O2D-CED
14	b	820	CLA	O1D-CGD-O2D-CED
14	B	819	CLA	O1D-CGD-O2D-CED
14	H	820	CLA	O1D-CGD-O2D-CED
14	a	808	CLA	O1D-CGD-O2D-CED
14	G	812	CLA	O1A-CGA-O2A-C1
14	H	818	CLA	O1A-CGA-O2A-C1
14	L	206	CLA	O1A-CGA-O2A-C1
14	H	808	CLA	CBD-CGD-O2D-CED
14	A	802	CLA	O1D-CGD-O2D-CED
14	B	814	CLA	O1D-CGD-O2D-CED
14	H	812	CLA	O1D-CGD-O2D-CED
14	U	201	CLA	O1D-CGD-O2D-CED
17	A	848	BCR	C7-C8-C9-C34
17	A	848	BCR	C37-C22-C23-C24
17	A	849	BCR	C7-C8-C9-C34
17	A	853	BCR	C7-C8-C9-C34
17	A	853	BCR	C36-C18-C19-C20
17	B	843	BCR	C11-C12-C13-C35
17	B	846	BCR	C36-C18-C19-C20
17	G	848	BCR	C7-C8-C9-C34
17	G	848	BCR	C37-C22-C23-C24
17	G	849	BCR	C36-C18-C19-C20
17	G	850	BCR	C36-C18-C19-C20
17	G	851	BCR	C7-C8-C9-C34
17	G	853	BCR	C7-C8-C9-C34
17	H	844	BCR	C37-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	H	846	BCR	C36-C18-C19-C20
17	H	847	BCR	C7-C8-C9-C34
17	H	849	BCR	C7-C8-C9-C34
17	I	101	BCR	C7-C8-C9-C34
17	I	102	BCR	C37-C22-C23-C24
17	J	102	BCR	C37-C22-C23-C24
17	J	103	BCR	C37-C22-C23-C24
17	L	207	BCR	C7-C8-C9-C34
17	M	1602	BCR	C7-C8-C9-C34
17	Q	202	BCR	C11-C12-C13-C35
17	Q	202	BCR	C36-C18-C19-C20
17	R	103	BCR	C37-C22-C23-C24
17	S	103	BCR	C7-C8-C9-C34
17	S	103	BCR	C37-C22-C23-C24
17	S	104	BCR	C11-C12-C13-C35
17	S	104	BCR	C37-C22-C23-C24
17	V	1602	BCR	C7-C8-C9-C34
17	V	1602	BCR	C37-C22-C23-C24
17	a	847	BCR	C7-C8-C9-C34
17	a	849	BCR	C36-C18-C19-C20
17	b	842	BCR	C7-C8-C9-C34
17	b	842	BCR	C37-C22-C23-C24
17	b	843	BCR	C11-C12-C13-C35
17	b	843	BCR	C37-C22-C23-C24
17	b	846	BCR	C36-C18-C19-C20
17	b	847	BCR	C7-C8-C9-C34
17	b	849	BCR	C7-C8-C9-C34
17	f	201	BCR	C36-C18-C19-C20
17	i	102	BCR	C7-C8-C9-C34
17	j	103	BCR	C7-C8-C9-C34
17	j	103	BCR	C37-C22-C23-C24
17	j	104	BCR	C36-C18-C19-C20
17	l	201	BCR	C7-C8-C9-C34
17	l	208	BCR	C37-C22-C23-C24
17	m	1602	BCR	C7-C8-C9-C34
17	A	853	BCR	C7-C8-C9-C10
17	B	842	BCR	C7-C8-C9-C10
17	G	848	BCR	C7-C8-C9-C10
17	G	849	BCR	C17-C18-C19-C20
17	G	853	BCR	C7-C8-C9-C10
17	H	842	BCR	C7-C8-C9-C10
17	I	102	BCR	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	L	207	BCR	C7-C8-C9-C10
17	Q	202	BCR	C11-C12-C13-C14
17	R	103	BCR	C21-C22-C23-C24
17	b	842	BCR	C7-C8-C9-C10
17	l	201	BCR	C7-C8-C9-C10
17	l	208	BCR	C21-C22-C23-C24
14	A	845	CLA	C2A-CAA-CBA-CGA
14	G	813	CLA	C2A-CAA-CBA-CGA
14	G	844	CLA	C2A-CAA-CBA-CGA
14	H	811	CLA	C2A-CAA-CBA-CGA
14	H	829	CLA	C2A-CAA-CBA-CGA
14	L	206	CLA	C2A-CAA-CBA-CGA
14	b	814	CLA	C2A-CAA-CBA-CGA
19	H	848	LMG	C28-C29-C30-C31
14	A	809	CLA	O1D-CGD-O2D-CED
14	A	804	CLA	O1A-CGA-O2A-C1
14	A	820	CLA	O1A-CGA-O2A-C1
14	G	820	CLA	O1A-CGA-O2A-C1
14	G	827	CLA	O1A-CGA-O2A-C1
14	a	826	CLA	O1A-CGA-O2A-C1
14	G	819	CLA	CBA-CGA-O2A-C1
14	G	828	CLA	CBA-CGA-O2A-C1
14	G	830	CLA	CBA-CGA-O2A-C1
14	B	812	CLA	C5-C6-C7-C8
14	B	817	CLA	C5-C6-C7-C8
14	G	842	CLA	C15-C16-C17-C18
14	H	818	CLA	C5-C6-C7-C8
14	a	825	CLA	C8-C10-C11-C12
14	b	803	CLA	C8-C10-C11-C12
14	A	821	CLA	C2-C1-O2A-CGA
14	A	843	CLA	C2-C1-O2A-CGA
14	B	806	CLA	C2-C1-O2A-CGA
14	B	831	CLA	C2-C1-O2A-CGA
14	G	804	CLA	C2-C1-O2A-CGA
14	G	826	CLA	C2-C1-O2A-CGA
14	H	803	CLA	C2-C1-O2A-CGA
14	H	806	CLA	C2-C1-O2A-CGA
14	H	831	CLA	C2-C1-O2A-CGA
14	a	820	CLA	C2-C1-O2A-CGA
14	a	842	CLA	C2-C1-O2A-CGA
14	b	831	CLA	C2-C1-O2A-CGA
14	b	832	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	818	CLA	O1D-CGD-O2D-CED
14	a	802	CLA	O1D-CGD-O2D-CED
14	a	829	CLA	O1D-CGD-O2D-CED
14	b	823	CLA	O1D-CGD-O2D-CED
14	G	808	CLA	CBD-CGD-O2D-CED
14	B	803	CLA	C2C-C3C-CAC-CBC
14	A	829	CLA	C13-C15-C16-C17
14	B	807	CLA	C13-C15-C16-C17
14	G	803	CLA	C10-C11-C12-C13
14	G	843	CLA	C8-C10-C11-C12
14	H	806	CLA	C13-C15-C16-C17
14	H	836	CLA	C10-C11-C12-C13
14	U	201	CLA	C15-C16-C17-C18
14	a	826	CLA	C5-C6-C7-C8
15	a	845	PQN	C23-C25-C26-C27
14	B	833	CLA	O1D-CGD-O2D-CED
18	A	855	LHG	O1-C1-C2-O2
14	B	812	CLA	O1D-CGD-O2D-CED
14	B	823	CLA	O1D-CGD-O2D-CED
14	H	839	CLA	O1D-CGD-O2D-CED
14	J	101	CLA	O1D-CGD-O2D-CED
14	b	814	CLA	O1D-CGD-O2D-CED
14	B	824	CLA	CBD-CGD-O2D-CED
14	b	827	CLA	CBD-CGD-O2D-CED
14	A	807	CLA	C11-C10-C8-C7
14	B	806	CLA	C11-C10-C8-C7
14	B	831	CLA	C11-C12-C13-C15
14	H	806	CLA	C11-C10-C8-C7
14	H	818	CLA	C6-C7-C8-C10
14	b	807	CLA	C11-C10-C8-C7
14	b	831	CLA	C11-C12-C13-C15
14	G	831	CLA	C4-C3-C5-C6
14	A	826	CLA	C15-C16-C17-C18
14	B	806	CLA	C13-C15-C16-C17
17	A	850	BCR	C9-C10-C11-C12
17	A	850	BCR	C13-C14-C15-C16
17	S	104	BCR	C9-C10-C11-C12
17	S	104	BCR	C15-C16-C17-C18
17	b	842	BCR	C9-C10-C11-C12
17	b	847	BCR	C9-C10-C11-C12
17	j	103	BCR	C19-C20-C21-C22
17	j	104	BCR	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	804	CLA	O1D-CGD-O2D-CED
14	A	805	CLA	O1D-CGD-O2D-CED
14	A	828	CLA	O1D-CGD-O2D-CED
14	H	819	CLA	O1D-CGD-O2D-CED
14	a	830	CLA	O1D-CGD-O2D-CED
19	b	848	LMG	C4-C5-C6-O5
14	B	839	CLA	C3-C5-C6-C7
14	G	810	CLA	C3-C5-C6-C7
14	G	826	CLA	C3-C5-C6-C7
14	b	804	CLA	C3-C5-C6-C7
14	A	839	CLA	C5-C6-C7-C8
14	B	802	CLA	C13-C15-C16-C17
14	B	809	CLA	C10-C11-C12-C13
14	H	807	CLA	O1D-CGD-O2D-CED
14	G	828	CLA	O1A-CGA-O2A-C1
14	H	836	CLA	O1A-CGA-O2A-C1
14	a	806	CLA	O1A-CGA-O2A-C1
14	a	830	CLA	O1A-CGA-O2A-C1
14	a	824	CLA	CBD-CGD-O2D-CED
14	X	1701	CLA	O1D-CGD-O2D-CED
14	a	842	CLA	O1D-CGD-O2D-CED
14	b	817	CLA	O1D-CGD-O2D-CED
14	A	802	CLA	C15-C16-C17-C18
14	A	810	CLA	C13-C15-C16-C17
14	A	820	CLA	C5-C6-C7-C8
14	A	828	CLA	C10-C11-C12-C13
14	A	829	CLA	C8-C10-C11-C12
14	A	830	CLA	C5-C6-C7-C8
14	A	841	CLA	C15-C16-C17-C18
14	B	802	CLA	C8-C10-C11-C12
14	G	826	CLA	C10-C11-C12-C13
14	G	828	CLA	C10-C11-C12-C13
14	G	839	CLA	C15-C16-C17-C18
14	G	842	CLA	C13-C15-C16-C17
14	H	806	CLA	C10-C11-C12-C13
14	H	808	CLA	C8-C10-C11-C12
14	H	817	CLA	C5-C6-C7-C8
14	H	831	CLA	C13-C15-C16-C17
14	a	819	CLA	C13-C15-C16-C17
14	b	801	CLA	C15-C16-C17-C18
14	b	808	CLA	C8-C10-C11-C12
14	i	101	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	802	CLA	C2A-CAA-CBA-CGA
14	A	812	CLA	C2A-CAA-CBA-CGA
14	A	814	CLA	C2A-CAA-CBA-CGA
14	A	816	CLA	C2A-CAA-CBA-CGA
14	A	825	CLA	C2A-CAA-CBA-CGA
14	A	844	CLA	C2A-CAA-CBA-CGA
14	B	804	CLA	C2A-CAA-CBA-CGA
14	B	839	CLA	C2A-CAA-CBA-CGA
14	G	802	CLA	C2A-CAA-CBA-CGA
14	G	809	CLA	C2A-CAA-CBA-CGA
14	G	817	CLA	C2A-CAA-CBA-CGA
14	G	832	CLA	C2A-CAA-CBA-CGA
14	G	843	CLA	C2A-CAA-CBA-CGA
14	H	804	CLA	C2A-CAA-CBA-CGA
14	H	814	CLA	C2A-CAA-CBA-CGA
14	H	839	CLA	C2A-CAA-CBA-CGA
14	K	101	CLA	C2A-CAA-CBA-CGA
14	a	813	CLA	C2A-CAA-CBA-CGA
14	a	824	CLA	C2A-CAA-CBA-CGA
14	a	834	CLA	C2A-CAA-CBA-CGA
14	b	801	CLA	C2A-CAA-CBA-CGA
14	b	805	CLA	C2A-CAA-CBA-CGA
14	b	809	CLA	C2A-CAA-CBA-CGA
14	l	207	CLA	C2A-CAA-CBA-CGA
14	x	1701	CLA	C2A-CAA-CBA-CGA
14	a	804	CLA	O1D-CGD-O2D-CED
17	A	853	BCR	C10-C11-C12-C13
17	f	201	BCR	C10-C11-C12-C13
17	i	102	BCR	C18-C19-C20-C21
14	A	807	CLA	C15-C16-C17-C18
14	A	820	CLA	C13-C15-C16-C17
14	B	837	CLA	C8-C10-C11-C12
14	G	829	CLA	C13-C15-C16-C17
14	H	806	CLA	C5-C6-C7-C8
14	H	831	CLA	C15-C16-C17-C18
14	H	839	CLA	C10-C11-C12-C13
14	a	808	CLA	C5-C6-C7-C8
14	a	811	CLA	C15-C16-C17-C18
14	a	828	CLA	C15-C16-C17-C18
14	a	838	CLA	C8-C10-C11-C12
14	b	817	CLA	C5-C6-C7-C8
14	b	818	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	b	818	CLA	C10-C11-C12-C13
14	b	827	CLA	C15-C16-C17-C18
14	b	828	CLA	C13-C15-C16-C17
14	G	809	CLA	C3-C5-C6-C7
14	b	808	CLA	C3-C5-C6-C7
14	A	826	CLA	CBD-CGD-O2D-CED
14	L	206	CLA	CBD-CGD-O2D-CED
14	B	815	CLA	O1D-CGD-O2D-CED
14	H	838	CLA	O1D-CGD-O2D-CED
14	A	827	CLA	C5-C6-C7-C8
14	A	843	CLA	C5-C6-C7-C8
14	A	844	CLA	C15-C16-C17-C18
14	B	806	CLA	C8-C10-C11-C12
14	B	806	CLA	C10-C11-C12-C13
14	B	808	CLA	C8-C10-C11-C12
14	B	827	CLA	C15-C16-C17-C18
14	B	832	CLA	C5-C6-C7-C8
14	B	836	CLA	C10-C11-C12-C13
14	G	804	CLA	C5-C6-C7-C8
14	G	807	CLA	C10-C11-C12-C13
14	G	807	CLA	C15-C16-C17-C18
14	G	810	CLA	C13-C15-C16-C17
14	G	820	CLA	C13-C15-C16-C17
14	G	826	CLA	C8-C10-C11-C12
14	G	829	CLA	C15-C16-C17-C18
14	G	830	CLA	C8-C10-C11-C12
14	H	808	CLA	C13-C15-C16-C17
14	H	828	CLA	C8-C10-C11-C12
14	L	201	CLA	C10-C11-C12-C13
14	U	205	CLA	C13-C15-C16-C17
14	U	206	CLA	C5-C6-C7-C8
14	a	802	CLA	C10-C11-C12-C13
14	a	828	CLA	C8-C10-C11-C12
14	a	828	CLA	C13-C15-C16-C17
14	a	842	CLA	C15-C16-C17-C18
14	b	804	CLA	C10-C11-C12-C13
14	b	806	CLA	C10-C11-C12-C13
14	b	807	CLA	C10-C11-C12-C13
14	b	807	CLA	C13-C15-C16-C17
14	b	831	CLA	C10-C11-C12-C13
14	b	836	CLA	C10-C11-C12-C13
15	A	846	PQN	C23-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	G	846	PQN	C23-C25-C26-C27
15	H	841	PQN	C23-C25-C26-C27
14	G	814	CLA	CBA-CGA-O2A-C1
14	G	809	CLA	O1A-CGA-O2A-C1
14	b	818	CLA	O1A-CGA-O2A-C1
14	B	818	CLA	C10-C11-C12-C13
14	G	810	CLA	C8-C10-C11-C12
14	G	812	CLA	C15-C16-C17-C18
14	G	839	CLA	C5-C6-C7-C8
14	H	803	CLA	C10-C11-C12-C13
14	H	807	CLA	C13-C15-C16-C17
14	H	826	CLA	C13-C15-C16-C17
14	a	840	CLA	C15-C16-C17-C18
14	b	802	CLA	C15-C16-C17-C18
14	b	808	CLA	C13-C15-C16-C17
14	b	809	CLA	C10-C11-C12-C13
14	b	812	CLA	C15-C16-C17-C18
14	U	206	CLA	O1D-CGD-O2D-CED
14	A	830	CLA	C3-C5-C6-C7
14	B	822	CLA	O1D-CGD-O2D-CED
14	G	805	CLA	O1D-CGD-O2D-CED
14	b	837	CLA	O1D-CGD-O2D-CED
14	B	802	CLA	C15-C16-C17-C18
14	B	812	CLA	C15-C16-C17-C18
14	B	813	CLA	C5-C6-C7-C8
14	B	839	CLA	C10-C11-C12-C13
14	G	828	CLA	C13-C15-C16-C17
14	G	829	CLA	C8-C10-C11-C12
14	H	839	CLA	C13-C15-C16-C17
14	L	206	CLA	C5-C6-C7-C8
14	L	206	CLA	C8-C10-C11-C12
14	b	839	CLA	C13-C15-C16-C17
14	l	207	CLA	C8-C10-C11-C12
14	G	807	CLA	O1A-CGA-O2A-C1
14	G	830	CLA	O1A-CGA-O2A-C1
14	A	804	CLA	C2-C3-C5-C6
14	G	821	CLA	O1D-CGD-O2D-CED
14	G	827	CLA	O1D-CGD-O2D-CED
14	H	821	CLA	O1D-CGD-O2D-CED
14	b	819	CLA	O1D-CGD-O2D-CED
14	A	810	CLA	C8-C10-C11-C12
14	A	829	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	834	CLA	C5-C6-C7-C8
14	B	818	CLA	C5-C6-C7-C8
14	B	839	CLA	C13-C15-C16-C17
14	H	802	CLA	C8-C10-C11-C12
14	H	806	CLA	C8-C10-C11-C12
14	H	809	CLA	C10-C11-C12-C13
14	a	806	CLA	C15-C16-C17-C18
14	A	829	CLA	CBA-CGA-O2A-C1
14	B	836	CLA	CBA-CGA-O2A-C1
14	G	822	CLA	CBA-CGA-O2A-C1
14	H	821	CLA	CBA-CGA-O2A-C1
14	U	206	CLA	CBA-CGA-O2A-C1
14	a	824	CLA	CBA-CGA-O2A-C1
14	L	204	CLA	CBD-CGD-O2D-CED
14	G	814	CLA	O1A-CGA-O2A-C1
14	A	826	CLA	C8-C10-C11-C12
14	A	843	CLA	C15-C16-C17-C18
14	H	827	CLA	C10-C11-C12-C13
14	A	843	CLA	C3-C5-C6-C7
14	G	830	CLA	C3-C5-C6-C7
14	a	813	CLA	C3-C5-C6-C7
17	M	1602	BCR	C19-C20-C21-C22
17	a	849	BCR	C13-C14-C15-C16
14	G	830	CLA	C5-C6-C7-C8
14	a	811	CLA	C10-C11-C12-C13
14	G	819	CLA	O1A-CGA-O2A-C1
14	A	823	CLA	C2A-CAA-CBA-CGA
14	A	835	CLA	C2A-CAA-CBA-CGA
14	G	812	CLA	C2A-CAA-CBA-CGA
14	G	816	CLA	C2A-CAA-CBA-CGA
14	G	823	CLA	C2A-CAA-CBA-CGA
14	G	825	CLA	C2A-CAA-CBA-CGA
14	a	822	CLA	C2A-CAA-CBA-CGA
14	a	831	CLA	C2A-CAA-CBA-CGA
14	b	839	CLA	C2A-CAA-CBA-CGA
14	b	824	CLA	O1D-CGD-O2D-CED
14	B	806	CLA	CBA-CGA-O2A-C1
18	a	853	LHG	C13-C14-C15-C16
14	b	804	CLA	C4C-C3C-CAC-CBC
14	A	826	CLA	C13-C15-C16-C17
14	A	834	CLA	C10-C11-C12-C13
14	B	803	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	806	CLA	C5-C6-C7-C8
14	B	821	CLA	C5-C6-C7-C8
14	B	827	CLA	C13-C15-C16-C17
14	B	831	CLA	C13-C15-C16-C17
14	G	835	CLA	C5-C6-C7-C8
14	H	839	CLA	C8-C10-C11-C12
14	L	201	CLA	C15-C16-C17-C18
14	a	824	CLA	C5-C6-C7-C8
14	a	825	CLA	C13-C15-C16-C17
14	b	802	CLA	C5-C6-C7-C8
14	b	803	CLA	C13-C15-C16-C17
14	b	807	CLA	C5-C6-C7-C8
14	b	807	CLA	C8-C10-C11-C12
14	b	839	CLA	C8-C10-C11-C12
14	A	809	CLA	C5-C6-C7-C8
14	B	831	CLA	C15-C16-C17-C18
14	L	205	CLA	C8-C10-C11-C12
14	U	201	CLA	C10-C11-C12-C13
14	a	838	CLA	C5-C6-C7-C8
14	B	805	CLA	C10-C11-C12-C13
14	B	826	CLA	C13-C15-C16-C17
14	B	839	CLA	C8-C10-C11-C12
14	G	810	CLA	C10-C11-C12-C13
14	H	802	CLA	C13-C15-C16-C17
14	b	827	CLA	C13-C15-C16-C17
14	l	202	CLA	C10-C11-C12-C13
14	A	819	CLA	CBA-CGA-O2A-C1
14	G	804	CLA	CBA-CGA-O2A-C1
14	b	836	CLA	CBA-CGA-O2A-C1
14	G	831	CLA	C2-C3-C5-C6
14	a	826	CLA	O1D-CGD-O2D-CED
14	B	831	CLA	C10-C11-C12-C13
14	a	826	CLA	C8-C10-C11-C12
14	G	843	CLA	C3-C5-C6-C7
14	i	101	CLA	CBD-CGD-O2D-CED
14	B	839	CLA	C14-C13-C15-C16
14	a	802	CLA	C11-C12-C13-C14
14	b	825	CLA	O1D-CGD-O2D-CED
14	B	812	CLA	C13-C15-C16-C17
14	G	827	CLA	C5-C6-C7-C8
14	A	828	CLA	CBA-CGA-O2A-C1
14	G	810	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	802	CLA	C16-C17-C18-C19
14	U	204	CLA	C11-C12-C13-C14
14	U	205	CLA	C16-C17-C18-C20
15	a	845	PQN	C26-C27-C28-C30
14	G	820	CLA	C5-C6-C7-C8
14	G	826	CLA	C5-C6-C7-C8
17	A	853	BCR	C11-C10-C9-C34
17	B	844	BCR	C11-C10-C9-C34
17	B	850	BCR	C11-C10-C9-C34
17	F	1302	BCR	C11-C10-C9-C34
17	G	849	BCR	C11-C10-C9-C34
17	G	851	BCR	C11-C10-C9-C34
17	H	844	BCR	C11-C10-C9-C34
17	H	849	BCR	C11-C10-C9-C34
17	b	846	BCR	C11-C10-C9-C34
14	H	803	CLA	C4C-C3C-CAC-CBC
19	b	848	LMG	O6-C5-C6-O5
14	H	802	CLA	C5-C6-C7-C8
17	A	850	BCR	C36-C18-C19-C20
17	A	853	BCR	C11-C12-C13-C35
17	B	842	BCR	C7-C8-C9-C34
17	G	852	BCR	C11-C12-C13-C35
17	G	852	BCR	C37-C22-C23-C24
17	H	842	BCR	C7-C8-C9-C34
17	H	843	BCR	C37-C22-C23-C24
17	M	1602	BCR	C37-C22-C23-C24
17	U	202	BCR	C7-C8-C9-C34
17	a	847	BCR	C37-C22-C23-C24
17	a	850	BCR	C11-C12-C13-C35
17	a	852	BCR	C36-C18-C19-C20
17	f	203	BCR	C36-C18-C19-C20
17	l	203	BCR	C11-C12-C13-C35
17	A	848	BCR	C7-C8-C9-C10
17	B	843	BCR	C11-C12-C13-C14
17	G	851	BCR	C7-C8-C9-C10
17	S	104	BCR	C11-C12-C13-C14
17	U	202	BCR	C7-C8-C9-C10
17	a	847	BCR	C7-C8-C9-C10
14	A	829	CLA	O1A-CGA-O2A-C1
14	B	806	CLA	O1A-CGA-O2A-C1
14	H	821	CLA	O1A-CGA-O2A-C1
14	a	824	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	829	CLA	C2A-CAA-CBA-CGA
14	G	835	CLA	C2A-CAA-CBA-CGA
14	G	845	CLA	C2A-CAA-CBA-CGA
14	H	826	CLA	C2A-CAA-CBA-CGA
14	M	1601	CLA	C2A-CAA-CBA-CGA
14	a	802	CLA	C2A-CAA-CBA-CGA
14	a	812	CLA	C2A-CAA-CBA-CGA
14	a	815	CLA	C2A-CAA-CBA-CGA
14	G	839	CLA	C8-C10-C11-C12
14	H	825	CLA	C13-C15-C16-C17
14	a	832	CLA	C5-C6-C7-C8
18	A	855	LHG	O1-C1-C2-C3
18	G	855	LHG	O1-C1-C2-C3
18	a	853	LHG	O1-C1-C2-C3
14	G	829	CLA	O2A-C1-C2-C3
14	a	828	CLA	O2A-C1-C2-C3
17	H	846	BCR	C15-C16-C17-C18
14	B	808	CLA	C16-C17-C18-C20
14	B	809	CLA	C16-C17-C18-C19
14	G	835	CLA	C16-C17-C18-C20
14	G	841	CLA	C16-C17-C18-C19
14	H	821	CLA	C6-C7-C8-C9
14	H	821	CLA	C6-C7-C8-C10
14	b	809	CLA	C16-C17-C18-C19
14	b	826	CLA	C16-C17-C18-C19
14	b	831	CLA	C16-C17-C18-C19
14	b	839	CLA	C16-C17-C18-C19
14	G	831	CLA	O1D-CGD-O2D-CED
14	j	101	CLA	O1D-CGD-O2D-CED
14	A	841	CLA	C3-C5-C6-C7
14	G	842	CLA	C3-C5-C6-C7
14	U	204	CLA	C3-C5-C6-C7
14	A	812	CLA	C5-C6-C7-C8
14	B	805	CLA	C15-C16-C17-C18
17	B	844	BCR	C11-C10-C9-C8
17	B	850	BCR	C11-C10-C9-C8
17	F	1302	BCR	C11-C10-C9-C8
17	G	849	BCR	C11-C10-C9-C8
17	G	851	BCR	C11-C10-C9-C8
17	H	844	BCR	C11-C10-C9-C8
17	H	849	BCR	C11-C10-C9-C8
17	b	846	BCR	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	G	854	LHG	C8-C7-O7-C5
14	G	809	CLA	C13-C15-C16-C17
14	a	840	CLA	C8-C10-C11-C12
14	b	834	CLA	O1D-CGD-O2D-CED
18	G	855	LHG	O7-C5-C6-O8
14	A	808	CLA	O1D-CGD-O2D-CED
14	A	833	CLA	O1D-CGD-O2D-CED
14	G	828	CLA	O1D-CGD-O2D-CED
14	H	816	CLA	CBA-CGA-O2A-C1
14	a	828	CLA	CBA-CGA-O2A-C1
14	A	827	CLA	C8-C10-C11-C12
14	H	817	CLA	C8-C10-C11-C12
14	G	806	CLA	CBD-CGD-O2D-CED
18	G	854	LHG	C23-C24-C25-C26
14	A	829	CLA	C2-C1-O2A-CGA
14	B	803	CLA	C2-C1-O2A-CGA
14	B	823	CLA	C2-C1-O2A-CGA
14	G	827	CLA	C2-C1-O2A-CGA
14	G	829	CLA	C2-C1-O2A-CGA
14	G	842	CLA	C2-C1-O2A-CGA
14	a	825	CLA	C2-C1-O2A-CGA
14	a	828	CLA	C2-C1-O2A-CGA
14	b	804	CLA	C2-C1-O2A-CGA
14	B	831	CLA	C16-C17-C18-C20
14	G	843	CLA	C16-C17-C18-C19
14	U	205	CLA	C16-C17-C18-C19
14	a	832	CLA	C6-C7-C8-C10
14	b	807	CLA	C16-C17-C18-C20
15	G	846	PQN	C26-C27-C28-C30
15	a	845	PQN	C26-C27-C28-C29
14	a	819	CLA	O1A-CGA-O2A-C1
14	B	805	CLA	C5-C6-C7-C8
14	B	840	CLA	C13-C15-C16-C17
14	H	825	CLA	C10-C11-C12-C13
14	l	202	CLA	C15-C16-C17-C18
14	b	833	CLA	O1D-CGD-O2D-CED
18	A	854	LHG	C28-C29-C30-C31
18	A	855	LHG	C11-C10-C9-C8
18	G	854	LHG	C11-C10-C9-C8
18	a	854	LHG	C11-C10-C9-C8
14	a	840	CLA	O1D-CGD-O2D-CED
14	b	815	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	829	CLA	C5-C6-C7-C8
14	a	842	CLA	C5-C6-C7-C8
18	a	853	LHG	C11-C12-C13-C14
14	G	804	CLA	O1A-CGA-O2A-C1
14	A	822	CLA	CBA-CGA-O2A-C1
18	a	853	LHG	C28-C29-C30-C31
18	G	854	LHG	O9-C7-O7-C5
18	G	854	LHG	O1-C1-C2-O2
18	G	855	LHG	O1-C1-C2-O2
18	G	854	LHG	C28-C29-C30-C31
14	B	808	CLA	C16-C17-C18-C19
14	B	826	CLA	C16-C17-C18-C19
14	B	831	CLA	C16-C17-C18-C19
14	G	820	CLA	C16-C17-C18-C19
14	G	820	CLA	C16-C17-C18-C20
14	G	833	CLA	C6-C7-C8-C9
14	G	833	CLA	C6-C7-C8-C10
14	G	843	CLA	C16-C17-C18-C20
14	H	806	CLA	C16-C17-C18-C20
14	H	809	CLA	C16-C17-C18-C19
14	H	809	CLA	C16-C17-C18-C20
14	b	826	CLA	C16-C17-C18-C20
14	b	831	CLA	C16-C17-C18-C20
14	b	839	CLA	C16-C17-C18-C20
14	B	836	CLA	O1A-CGA-O2A-C1
14	G	814	CLA	C2A-CAA-CBA-CGA
14	X	1701	CLA	C2A-CAA-CBA-CGA
14	b	802	CLA	C2A-CAA-CBA-CGA
14	A	829	CLA	C10-C11-C12-C13
14	B	828	CLA	C5-C6-C7-C8
14	H	827	CLA	C13-C15-C16-C17
14	a	809	CLA	C8-C10-C11-C12
14	a	826	CLA	C10-C11-C12-C13
14	A	831	CLA	C12-C13-C15-C16
14	G	807	CLA	C11-C10-C8-C7
14	G	834	CLA	C11-C12-C13-C15
14	H	839	CLA	C11-C10-C8-C7
14	H	839	CLA	CBA-CGA-O2A-C1
14	A	820	CLA	C8-C10-C11-C12
14	A	830	CLA	C10-C11-C12-C13
14	a	809	CLA	C10-C11-C12-C13
19	H	848	LMG	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	U	206	CLA	O1A-CGA-O2A-C1
14	G	833	CLA	C3-C5-C6-C7
14	a	832	CLA	C3-C5-C6-C7
14	A	803	CLA	C3A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	806	CLA	C3A-C2A-CAA-CBA
14	A	807	CLA	C3A-C2A-CAA-CBA
14	A	814	CLA	C3A-C2A-CAA-CBA
14	A	833	CLA	C4-C3-C5-C6
14	A	842	CLA	C3A-C2A-CAA-CBA
14	B	835	CLA	C3A-C2A-CAA-CBA
14	B	836	CLA	C3A-C2A-CAA-CBA
14	G	803	CLA	C3A-C2A-CAA-CBA
14	G	804	CLA	C3A-C2A-CAA-CBA
14	G	814	CLA	C3A-C2A-CAA-CBA
14	H	819	CLA	C3A-C2A-CAA-CBA
14	H	835	CLA	C3A-C2A-CAA-CBA
14	H	836	CLA	C3A-C2A-CAA-CBA
14	a	802	CLA	C3A-C2A-CAA-CBA
14	a	803	CLA	C3A-C2A-CAA-CBA
14	a	805	CLA	C3A-C2A-CAA-CBA
14	a	841	CLA	C3A-C2A-CAA-CBA
14	b	822	CLA	C3A-C2A-CAA-CBA
14	b	833	CLA	C3A-C2A-CAA-CBA
14	H	806	CLA	O1D-CGD-O2D-CED
14	A	812	CLA	C15-C16-C17-C18
14	A	831	CLA	C13-C15-C16-C17
14	G	809	CLA	C5-C6-C7-C8
14	a	842	CLA	C8-C10-C11-C12
14	B	824	CLA	O1D-CGD-O2D-CED
14	U	204	CLA	O1D-CGD-O2D-CED
17	b	842	BCR	C19-C20-C21-C22
17	b	844	BCR	C19-C20-C21-C22
13	a	801	CL0	C16-C17-C18-C19
14	b	803	CLA	C16-C17-C18-C20
15	G	846	PQN	C26-C27-C28-C29
14	G	822	CLA	O1A-CGA-O2A-C1
14	G	836	CLA	O1D-CGD-O2D-CED
14	A	832	CLA	CBD-CGD-O2D-CED
14	A	807	CLA	CBA-CGA-O2A-C1
14	a	829	CLA	CBA-CGA-O2A-C1
14	b	826	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	G	854	LHG	C11-C12-C13-C14
18	G	854	LHG	C34-C35-C36-C37
14	H	808	CLA	C3-C5-C6-C7
14	H	817	CLA	C3-C5-C6-C7
14	a	842	CLA	C3-C5-C6-C7
18	a	853	LHG	C23-C24-C25-C26
14	H	806	CLA	C15-C16-C17-C18
14	b	804	CLA	C5-C6-C7-C8
14	b	807	CLA	C15-C16-C17-C18
14	b	817	CLA	C8-C10-C11-C12
18	G	854	LHG	C33-C34-C35-C36
14	A	828	CLA	O1A-CGA-O2A-C1
14	G	810	CLA	O1A-CGA-O2A-C1
14	b	836	CLA	O1A-CGA-O2A-C1
18	G	854	LHG	C10-C11-C12-C13
14	a	820	CLA	O1D-CGD-O2D-CED
18	G	854	LHG	C31-C32-C33-C34
14	B	838	CLA	O1D-CGD-O2D-CED
14	A	833	CLA	C6-C7-C8-C9
14	B	806	CLA	C16-C17-C18-C20
14	B	809	CLA	C16-C17-C18-C20
14	H	806	CLA	C16-C17-C18-C19
14	a	832	CLA	C6-C7-C8-C9
14	b	807	CLA	C16-C17-C18-C19
14	A	819	CLA	O1A-CGA-O2A-C1
17	A	848	BCR	C1-C6-C7-C8
17	A	848	BCR	C5-C6-C7-C8
17	A	849	BCR	C1-C6-C7-C8
17	A	849	BCR	C23-C24-C25-C30
17	A	850	BCR	C1-C6-C7-C8
17	A	850	BCR	C5-C6-C7-C8
17	A	851	BCR	C23-C24-C25-C30
17	A	852	BCR	C1-C6-C7-C8
17	A	853	BCR	C23-C24-C25-C26
17	A	853	BCR	C23-C24-C25-C30
17	B	842	BCR	C1-C6-C7-C8
17	B	848	BCR	C1-C6-C7-C8
17	B	848	BCR	C5-C6-C7-C8
17	B	850	BCR	C23-C24-C25-C26
17	B	850	BCR	C23-C24-C25-C30
17	G	848	BCR	C1-C6-C7-C8
17	G	848	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	G	849	BCR	C23-C24-C25-C30
17	G	850	BCR	C1-C6-C7-C8
17	G	850	BCR	C5-C6-C7-C8
17	G	851	BCR	C23-C24-C25-C26
17	G	851	BCR	C23-C24-C25-C30
17	H	842	BCR	C1-C6-C7-C8
17	H	842	BCR	C5-C6-C7-C8
17	H	842	BCR	C23-C24-C25-C26
17	H	842	BCR	C23-C24-C25-C30
17	H	849	BCR	C23-C24-C25-C26
17	H	849	BCR	C23-C24-C25-C30
17	J	103	BCR	C23-C24-C25-C30
17	L	202	BCR	C23-C24-C25-C30
17	M	1602	BCR	C1-C6-C7-C8
17	R	102	BCR	C23-C24-C25-C26
17	R	102	BCR	C23-C24-C25-C30
17	R	103	BCR	C23-C24-C25-C30
17	S	103	BCR	C1-C6-C7-C8
17	S	103	BCR	C5-C6-C7-C8
17	S	104	BCR	C23-C24-C25-C30
17	V	1602	BCR	C1-C6-C7-C8
17	a	847	BCR	C1-C6-C7-C8
17	a	847	BCR	C5-C6-C7-C8
17	a	848	BCR	C1-C6-C7-C8
17	a	849	BCR	C1-C6-C7-C8
17	a	849	BCR	C5-C6-C7-C8
17	a	850	BCR	C1-C6-C7-C8
17	a	850	BCR	C23-C24-C25-C30
17	a	851	BCR	C1-C6-C7-C8
17	a	851	BCR	C5-C6-C7-C8
17	b	842	BCR	C1-C6-C7-C8
17	b	842	BCR	C5-C6-C7-C8
17	b	844	BCR	C23-C24-C25-C26
17	b	844	BCR	C23-C24-C25-C30
17	b	849	BCR	C23-C24-C25-C26
17	b	849	BCR	C23-C24-C25-C30
17	j	103	BCR	C1-C6-C7-C8
17	j	103	BCR	C5-C6-C7-C8
17	j	104	BCR	C23-C24-C25-C30
17	l	208	BCR	C23-C24-C25-C30
17	m	1602	BCR	C1-C6-C7-C8
14	B	828	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	812	CLA	C15-C16-C17-C18
14	a	827	CLA	C10-C11-C12-C13
14	H	832	CLA	C3-C5-C6-C7
14	S	101	CLA	O1D-CGD-O2D-CED
14	A	813	CLA	C2A-CAA-CBA-CGA
14	B	814	CLA	C2A-CAA-CBA-CGA
14	B	826	CLA	C2A-CAA-CBA-CGA
14	U	206	CLA	C2A-CAA-CBA-CGA
14	W	1701	CLA	C2A-CAA-CBA-CGA
18	a	854	LHG	C7-C8-C9-C10
14	A	841	CLA	C5-C6-C7-C8
18	A	854	LHG	C11-C10-C9-C8
14	H	816	CLA	O1A-CGA-O2A-C1
14	H	839	CLA	O1A-CGA-O2A-C1
14	a	828	CLA	O1A-CGA-O2A-C1
17	B	847	BCR	C10-C11-C12-C13
17	G	851	BCR	C10-C11-C12-C13
17	G	853	BCR	C10-C11-C12-C13
17	H	849	BCR	C10-C11-C12-C13
17	I	101	BCR	C18-C19-C20-C21
17	J	102	BCR	C10-C11-C12-C13
17	L	202	BCR	C10-C11-C12-C13
17	M	1602	BCR	C10-C11-C12-C13
17	R	102	BCR	C10-C11-C12-C13
17	a	847	BCR	C10-C11-C12-C13
17	a	851	BCR	C10-C11-C12-C13
17	b	847	BCR	C18-C19-C20-C21
17	j	104	BCR	C10-C11-C12-C13
14	B	801	CLA	C10-C11-C12-C13
14	A	833	CLA	C2-C3-C5-C6
14	B	806	CLA	C2-C3-C5-C6
14	L	204	CLA	C11-C12-C13-C15
18	A	854	LHG	C31-C32-C33-C34
14	A	830	CLA	CBA-CGA-O2A-C1
14	H	826	CLA	CBA-CGA-O2A-C1
14	a	821	CLA	CBA-CGA-O2A-C1
15	G	846	PQN	C13-C15-C16-C17
14	H	818	CLA	C14-C13-C15-C16
14	U	206	CLA	C6-C7-C8-C9
14	b	812	CLA	C14-C13-C15-C16
14	G	839	CLA	C13-C15-C16-C17
14	L	205	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	822	CLA	C10-C11-C12-C13
14	A	843	CLA	C13-C15-C16-C17
14	H	801	CLA	C10-C11-C12-C13
14	a	828	CLA	C10-C11-C12-C13
14	l	207	CLA	C5-C6-C7-C8
18	A	854	LHG	C11-C12-C13-C14
14	l	206	CLA	C8-C10-C11-C12
14	G	829	CLA	CBA-CGA-O2A-C1
14	l	207	CLA	CBA-CGA-O2A-C1
17	A	848	BCR	C19-C20-C21-C22
17	A	851	BCR	C9-C10-C11-C12
17	B	844	BCR	C19-C20-C21-C22
17	B	850	BCR	C13-C14-C15-C16
17	G	848	BCR	C19-C20-C21-C22
17	H	844	BCR	C19-C20-C21-C22
17	l	203	BCR	C19-C20-C21-C22
14	B	821	CLA	C6-C7-C8-C10
14	G	841	CLA	C16-C17-C18-C20
14	H	802	CLA	C16-C17-C18-C20
14	U	204	CLA	C11-C12-C13-C15
14	b	809	CLA	C16-C17-C18-C20
14	a	855	CLA	C8-C10-C11-C12
14	b	806	CLA	C5-C6-C7-C8
19	b	848	LMG	C31-C32-C33-C34
14	A	843	CLA	C8-C10-C11-C12
17	U	202	BCR	C11-C12-C13-C35
14	H	812	CLA	C3-C5-C6-C7
14	b	818	CLA	C3-C5-C6-C7
14	b	821	CLA	C3-C5-C6-C7
17	a	849	BCR	C17-C18-C19-C20
17	a	852	BCR	C17-C18-C19-C20
17	f	203	BCR	C17-C18-C19-C20
14	A	803	CLA	C2A-CAA-CBA-CGA
13	a	801	CL0	C16-C17-C18-C20
14	A	802	CLA	C16-C17-C18-C20
14	A	833	CLA	C6-C7-C8-C10
14	B	821	CLA	C6-C7-C8-C9
14	B	826	CLA	C16-C17-C18-C20
14	G	835	CLA	C16-C17-C18-C19
14	L	204	CLA	C11-C12-C13-C14
14	b	803	CLA	C16-C17-C18-C19
14	A	807	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	827	CLA	C4-C3-C5-C6
14	a	825	CLA	C4-C3-C5-C6
14	b	831	CLA	C4-C3-C5-C6
14	H	804	CLA	C5-C6-C7-C8
14	U	205	CLA	C8-C10-C11-C12
18	G	855	LHG	C11-C10-C9-C8
14	A	831	CLA	O1D-CGD-O2D-CED
14	A	807	CLA	O1A-CGA-O2A-C1
14	a	829	CLA	O1A-CGA-O2A-C1
19	B	849	LMG	C33-C34-C35-C36
14	b	840	CLA	C2C-C3C-CAC-CBC
14	b	838	CLA	O1D-CGD-O2D-CED
18	a	853	LHG	C29-C30-C31-C32
18	a	853	LHG	C8-C7-O7-C5
14	B	806	CLA	C16-C17-C18-C19
14	G	834	CLA	C16-C17-C18-C20
18	A	854	LHG	C23-C24-C25-C26
19	B	849	LMG	C28-C29-C30-C31
14	B	812	CLA	C8-C10-C11-C12
14	G	841	CLA	C15-C16-C17-C18
14	a	803	CLA	C5-C6-C7-C8
14	a	819	CLA	C5-C6-C7-C8
14	a	819	CLA	C8-C10-C11-C12
14	A	809	CLA	C3-C5-C6-C7
18	A	854	LHG	O7-C5-C6-O8
14	B	826	CLA	CBA-CGA-O2A-C1
14	H	807	CLA	C5-C6-C7-C8
14	H	840	CLA	C13-C15-C16-C17
14	a	833	CLA	C15-C16-C17-C18
14	G	821	CLA	C2-C1-O2A-CGA
14	b	807	CLA	C2-C1-O2A-CGA
14	A	827	CLA	O1D-CGD-O2D-CED
14	A	835	CLA	C16-C17-C18-C20
14	B	839	CLA	C16-C17-C18-C19
14	a	827	CLA	C15-C16-C17-C18
14	a	840	CLA	C5-C6-C7-C8
19	B	849	LMG	C31-C32-C33-C34
15	G	846	PQN	C14-C13-C15-C16
14	b	812	CLA	C3-C5-C6-C7
14	G	834	CLA	C2-C3-C5-C6
14	a	825	CLA	C2-C3-C5-C6
14	b	831	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	a	854	LHG	C1-C2-C3-O3
14	b	809	CLA	C13-C15-C16-C17
14	A	817	CLA	C2A-CAA-CBA-CGA
14	G	803	CLA	C2A-CAA-CBA-CGA
14	a	811	CLA	C2A-CAA-CBA-CGA
14	a	844	CLA	C2A-CAA-CBA-CGA
14	b	826	CLA	C2A-CAA-CBA-CGA
14	b	827	CLA	C2A-CAA-CBA-CGA
13	A	801	CL0	CBD-CGD-O2D-CED
14	H	803	CLA	CBA-CGA-O2A-C1
14	A	826	CLA	O1D-CGD-O2D-CED
14	H	836	CLA	O1D-CGD-O2D-CED
14	A	809	CLA	C15-C16-C17-C18
14	A	833	CLA	C5-C6-C7-C8
14	G	842	CLA	C5-C6-C7-C8
14	L	204	CLA	O1D-CGD-O2D-CED
14	A	822	CLA	O1A-CGA-O2A-C1
14	A	830	CLA	O1A-CGA-O2A-C1
14	b	826	CLA	O1A-CGA-O2A-C1
14	B	812	CLA	C3-C5-C6-C7
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	809	CLA	C1A-C2A-CAA-CBA
14	A	810	CLA	C1A-C2A-CAA-CBA
14	A	812	CLA	C1A-C2A-CAA-CBA
14	A	816	CLA	C1A-C2A-CAA-CBA
14	A	819	CLA	C1A-C2A-CAA-CBA
14	A	822	CLA	C1A-C2A-CAA-CBA
14	A	825	CLA	C1A-C2A-CAA-CBA
14	A	829	CLA	C1A-C2A-CAA-CBA
14	A	830	CLA	C1A-C2A-CAA-CBA
14	A	831	CLA	C1A-C2A-CAA-CBA
14	A	833	CLA	C1A-C2A-CAA-CBA
14	A	835	CLA	C1A-C2A-CAA-CBA
14	A	840	CLA	C1A-C2A-CAA-CBA
14	A	842	CLA	C1A-C2A-CAA-CBA
14	A	843	CLA	C1A-C2A-CAA-CBA
14	B	810	CLA	C1A-C2A-CAA-CBA
14	B	813	CLA	C1A-C2A-CAA-CBA
14	B	818	CLA	C1A-C2A-CAA-CBA
14	B	829	CLA	C1A-C2A-CAA-CBA
14	B	830	CLA	C1A-C2A-CAA-CBA
14	B	838	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	804	CLA	C1A-C2A-CAA-CBA
14	G	809	CLA	C1A-C2A-CAA-CBA
14	G	816	CLA	C1A-C2A-CAA-CBA
14	G	819	CLA	C1A-C2A-CAA-CBA
14	G	822	CLA	C1A-C2A-CAA-CBA
14	G	825	CLA	C1A-C2A-CAA-CBA
14	G	831	CLA	C1A-C2A-CAA-CBA
14	G	833	CLA	C1A-C2A-CAA-CBA
14	G	835	CLA	C1A-C2A-CAA-CBA
14	G	836	CLA	C1A-C2A-CAA-CBA
14	G	840	CLA	C1A-C2A-CAA-CBA
14	G	842	CLA	C1A-C2A-CAA-CBA
14	G	845	CLA	C1A-C2A-CAA-CBA
14	H	810	CLA	C1A-C2A-CAA-CBA
14	H	811	CLA	C1A-C2A-CAA-CBA
14	H	813	CLA	C1A-C2A-CAA-CBA
14	H	814	CLA	C1A-C2A-CAA-CBA
14	H	815	CLA	C1A-C2A-CAA-CBA
14	H	818	CLA	C1A-C2A-CAA-CBA
14	H	825	CLA	C1A-C2A-CAA-CBA
14	H	828	CLA	C1A-C2A-CAA-CBA
14	H	829	CLA	C1A-C2A-CAA-CBA
14	H	838	CLA	C1A-C2A-CAA-CBA
14	K	102	CLA	C1A-C2A-CAA-CBA
14	L	205	CLA	C1A-C2A-CAA-CBA
14	U	205	CLA	C1A-C2A-CAA-CBA
14	U	206	CLA	C1A-C2A-CAA-CBA
14	a	803	CLA	C1A-C2A-CAA-CBA
14	a	807	CLA	C1A-C2A-CAA-CBA
14	a	808	CLA	C1A-C2A-CAA-CBA
14	a	819	CLA	C1A-C2A-CAA-CBA
14	a	821	CLA	C1A-C2A-CAA-CBA
14	a	824	CLA	C1A-C2A-CAA-CBA
14	a	830	CLA	C1A-C2A-CAA-CBA
14	a	832	CLA	C1A-C2A-CAA-CBA
14	a	834	CLA	C1A-C2A-CAA-CBA
14	a	835	CLA	C1A-C2A-CAA-CBA
14	a	839	CLA	C1A-C2A-CAA-CBA
14	a	844	CLA	C1A-C2A-CAA-CBA
14	b	810	CLA	C1A-C2A-CAA-CBA
14	b	815	CLA	C1A-C2A-CAA-CBA
14	b	818	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	b	825	CLA	C1A-C2A-CAA-CBA
14	b	828	CLA	C1A-C2A-CAA-CBA
14	b	838	CLA	C1A-C2A-CAA-CBA
14	k	1401	CLA	C1A-C2A-CAA-CBA
14	G	814	CLA	C5-C6-C7-C8
14	H	836	CLA	C8-C10-C11-C12
18	A	854	LHG	O6-C4-C5-C6
18	G	854	LHG	O6-C4-C5-C6
14	B	831	CLA	C3-C5-C6-C7
14	A	807	CLA	C11-C12-C13-C15
14	A	826	CLA	C6-C7-C8-C10
14	A	828	CLA	C6-C7-C8-C10
14	A	829	CLA	C11-C10-C8-C7
14	A	830	CLA	C12-C13-C15-C16
14	A	844	CLA	C12-C13-C15-C16
14	B	802	CLA	C11-C12-C13-C15
14	B	802	CLA	C12-C13-C15-C16
14	G	809	CLA	C11-C10-C8-C7
14	G	822	CLA	C12-C13-C15-C16
14	G	830	CLA	C12-C13-C15-C16
14	G	831	CLA	C11-C10-C8-C7
14	G	835	CLA	C12-C13-C15-C16
14	G	839	CLA	C12-C13-C15-C16
14	G	842	CLA	C6-C7-C8-C10
14	H	802	CLA	C11-C10-C8-C7
14	H	805	CLA	C6-C7-C8-C10
14	H	817	CLA	C11-C10-C8-C7
14	H	840	CLA	C12-C13-C15-C16
14	L	204	CLA	C6-C7-C8-C10
14	L	205	CLA	C11-C10-C8-C7
14	U	205	CLA	C11-C10-C8-C7
14	a	806	CLA	C11-C10-C8-C7
14	a	806	CLA	C11-C12-C13-C15
14	a	811	CLA	C11-C12-C13-C15
14	a	819	CLA	C11-C12-C13-C15
14	a	825	CLA	C6-C7-C8-C10
14	a	829	CLA	C12-C13-C15-C16
14	a	833	CLA	C12-C13-C15-C16
14	a	842	CLA	C6-C7-C8-C10
14	a	855	CLA	C12-C13-C15-C16
14	b	803	CLA	C11-C10-C8-C7
14	b	806	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	b	807	CLA	C6-C7-C8-C10
14	b	817	CLA	C11-C10-C8-C7
14	b	826	CLA	C11-C12-C13-C15
14	b	840	CLA	C11-C12-C13-C15
14	b	840	CLA	C12-C13-C15-C16
14	l	205	CLA	C6-C7-C8-C10
15	b	841	PQN	C17-C18-C20-C21
14	A	839	CLA	C8-C10-C11-C12
14	A	843	CLA	C10-C11-C12-C13
14	a	829	CLA	C15-C16-C17-C18
14	B	809	CLA	C13-C15-C16-C17
14	B	826	CLA	C5-C6-C7-C8
14	H	813	CLA	C5-C6-C7-C8
14	b	813	CLA	C5-C6-C7-C8
15	G	846	PQN	C25-C26-C27-C28
14	a	833	CLA	C4-C3-C5-C6
14	H	827	CLA	C2-C3-C5-C6
14	U	206	CLA	C2-C3-C5-C6
14	l	207	CLA	O1A-CGA-O2A-C1
14	G	809	CLA	C8-C10-C11-C12
14	a	808	CLA	C8-C10-C11-C12
14	b	803	CLA	C15-C16-C17-C18
14	a	802	CLA	C3-C5-C6-C7
14	A	837	CLA	C2A-CAA-CBA-CGA
14	B	803	CLA	C2A-CAA-CBA-CGA
14	G	819	CLA	C2A-CAA-CBA-CGA
14	H	801	CLA	C2A-CAA-CBA-CGA
14	H	803	CLA	C2A-CAA-CBA-CGA
14	H	830	CLA	C2A-CAA-CBA-CGA
14	a	855	CLA	C2A-CAA-CBA-CGA
14	A	807	CLA	C11-C12-C13-C14
14	A	820	CLA	C11-C12-C13-C14
14	A	830	CLA	C14-C13-C15-C16
14	B	817	CLA	C6-C7-C8-C9
14	B	831	CLA	C11-C12-C13-C14
14	B	837	CLA	C6-C7-C8-C9
14	G	803	CLA	C6-C7-C8-C9
14	G	809	CLA	C11-C10-C8-C9
14	G	820	CLA	C11-C12-C13-C14
14	G	822	CLA	C14-C13-C15-C16
14	G	826	CLA	C11-C12-C13-C14
14	G	826	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	839	CLA	C14-C13-C15-C16
14	H	818	CLA	C6-C7-C8-C9
14	H	837	CLA	C6-C7-C8-C9
14	H	840	CLA	C14-C13-C15-C16
14	L	204	CLA	C6-C7-C8-C9
14	L	205	CLA	C11-C10-C8-C9
14	a	806	CLA	C11-C12-C13-C14
14	a	833	CLA	C14-C13-C15-C16
14	a	842	CLA	C6-C7-C8-C9
14	a	855	CLA	C14-C13-C15-C16
14	b	801	CLA	C11-C10-C8-C9
14	b	803	CLA	C11-C10-C8-C9
14	l	206	CLA	C11-C10-C8-C9
14	G	808	CLA	O1D-CGD-O2D-CED
18	G	854	LHG	C24-C23-O8-C6
18	a	854	LHG	C24-C23-O8-C6
14	B	801	CLA	C5-C6-C7-C8
14	L	205	CLA	C5-C6-C7-C8
14	a	821	CLA	O1A-CGA-O2A-C1
14	G	843	CLA	C5-C6-C7-C8
18	G	855	LHG	C4-C5-C6-O8
18	a	853	LHG	C4-C5-C6-O8
19	b	848	LMG	C18-C19-C20-C21
14	A	839	CLA	CBA-CGA-O2A-C1
14	B	801	CLA	C16-C17-C18-C19
14	A	807	CLA	C10-C11-C12-C13
17	f	203	BCR	C11-C10-C9-C34
14	A	830	CLA	C15-C16-C17-C18
14	H	837	CLA	C3-C5-C6-C7
14	b	840	CLA	C3-C5-C6-C7
14	b	827	CLA	O1D-CGD-O2D-CED
14	G	829	CLA	O1A-CGA-O2A-C1
14	G	834	CLA	C4-C3-C5-C6
14	A	826	CLA	C2-C3-C5-C6
14	H	836	CLA	C2-C3-C5-C6
14	H	827	CLA	C15-C16-C17-C18
14	b	821	CLA	C5-C6-C7-C8
18	a	853	LHG	O9-C7-O7-C5
19	H	848	LMG	C11-C12-C13-C14
17	G	848	BCR	C21-C22-C23-C24
17	V	1602	BCR	C21-C22-C23-C24
17	a	850	BCR	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	j	104	BCR	C17-C18-C19-C20
14	H	826	CLA	O1A-CGA-O2A-C1
14	A	844	CLA	C8-C10-C11-C12
14	B	817	CLA	C8-C10-C11-C12
14	H	837	CLA	C8-C10-C11-C12
14	b	809	CLA	C15-C16-C17-C18
14	B	830	CLA	C2A-CAA-CBA-CGA
14	G	830	CLA	C2A-CAA-CBA-CGA
14	a	809	CLA	C2A-CAA-CBA-CGA
14	A	809	CLA	C8-C10-C11-C12
14	B	806	CLA	C15-C16-C17-C18
14	A	825	CLA	CBA-CGA-O2A-C1
14	a	818	CLA	CBA-CGA-O2A-C1
14	A	829	CLA	O2A-C1-C2-C3
17	R	103	BCR	C10-C11-C12-C13
17	i	102	BCR	C10-C11-C12-C13
14	H	826	CLA	C5-C6-C7-C8
14	L	206	CLA	O1D-CGD-O2D-CED
17	B	848	BCR	C9-C10-C11-C12
17	S	103	BCR	C19-C20-C21-C22
17	a	850	BCR	C9-C10-C11-C12
17	f	203	BCR	C11-C10-C9-C8
18	A	855	LHG	O6-C4-C5-O7
14	G	830	CLA	C10-C11-C12-C13
14	H	804	CLA	CBA-CGA-O2A-C1
14	H	806	CLA	CBA-CGA-O2A-C1
14	a	803	CLA	CBA-CGA-O2A-C1
14	B	826	CLA	O1A-CGA-O2A-C1
14	H	836	CLA	C4-C3-C5-C6
14	U	206	CLA	C4-C3-C5-C6
14	a	830	CLA	C4-C3-C5-C6
14	G	835	CLA	C2-C3-C5-C6
14	H	807	CLA	C2-C3-C5-C6
14	a	833	CLA	C2-C3-C5-C6
18	A	854	LHG	C34-C35-C36-C37
14	G	834	CLA	C16-C17-C18-C19
14	b	807	CLA	CBA-CGA-O2A-C1
18	a	853	LHG	C24-C23-O8-C6
14	G	807	CLA	CAA-CBA-CGA-O2A
14	G	830	CLA	CAA-CBA-CGA-O2A
14	b	805	CLA	C3-C5-C6-C7
14	A	809	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	835	CLA	C16-C17-C18-C19
14	A	844	CLA	C16-C17-C18-C19
14	H	803	CLA	O1A-CGA-O2A-C1
18	G	854	LHG	O10-C23-O8-C6
14	b	804	CLA	O1D-CGD-O2D-CED
14	G	841	CLA	CBA-CGA-O2A-C1
18	a	853	LHG	C35-C36-C37-C38
14	A	826	CLA	C10-C11-C12-C13
14	i	101	CLA	O1D-CGD-O2D-CED
18	A	855	LHG	C7-C8-C9-C10
14	L	201	CLA	C8-C10-C11-C12
14	G	830	CLA	C16-C17-C18-C19
14	H	831	CLA	C16-C17-C18-C19
14	H	839	CLA	C16-C17-C18-C19
19	B	849	LMG	C13-C14-C15-C16
14	A	812	CLA	C4-C3-C5-C6
14	A	826	CLA	C4-C3-C5-C6
14	B	807	CLA	C4-C3-C5-C6
14	H	813	CLA	C4-C3-C5-C6
14	H	831	CLA	C4-C3-C5-C6
14	b	812	CLA	C4-C3-C5-C6
14	b	813	CLA	C4-C3-C5-C6
14	l	205	CLA	C4-C3-C5-C6
14	b	836	CLA	C8-C10-C11-C12
18	a	854	LHG	C9-C10-C11-C12
14	A	803	CLA	C6-C7-C8-C9
14	A	814	CLA	C11-C10-C8-C9
14	A	844	CLA	C14-C13-C15-C16
14	B	802	CLA	C11-C12-C13-C14
14	B	809	CLA	C6-C7-C8-C9
14	B	828	CLA	C6-C7-C8-C9
14	B	840	CLA	C14-C13-C15-C16
14	G	803	CLA	C11-C10-C8-C9
14	G	814	CLA	C6-C7-C8-C9
14	G	828	CLA	C11-C10-C8-C9
14	G	830	CLA	C11-C12-C13-C14
14	G	830	CLA	C14-C13-C15-C16
14	G	831	CLA	C11-C10-C8-C9
14	G	835	CLA	C14-C13-C15-C16
14	G	842	CLA	C6-C7-C8-C9
14	H	802	CLA	C11-C10-C8-C9
14	H	809	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	812	CLA	C11-C12-C13-C14
14	H	817	CLA	C11-C10-C8-C9
14	H	818	CLA	C11-C10-C8-C9
14	U	204	CLA	C6-C7-C8-C9
14	U	205	CLA	C11-C10-C8-C9
14	a	811	CLA	C11-C12-C13-C14
14	a	819	CLA	C11-C12-C13-C14
14	a	829	CLA	C14-C13-C15-C16
14	a	842	CLA	C11-C12-C13-C14
14	b	806	CLA	C11-C10-C8-C9
14	b	807	CLA	C6-C7-C8-C9
14	b	817	CLA	C11-C10-C8-C9
14	b	826	CLA	C11-C12-C13-C14
14	b	828	CLA	C11-C12-C13-C14
14	b	837	CLA	C6-C7-C8-C9
14	b	840	CLA	C11-C10-C8-C9
14	b	840	CLA	C11-C12-C13-C14
14	b	840	CLA	C14-C13-C15-C16
14	l	205	CLA	C6-C7-C8-C9
14	H	808	CLA	O1D-CGD-O2D-CED
14	a	824	CLA	O1D-CGD-O2D-CED
14	U	201	CLA	C8-C10-C11-C12
14	U	204	CLA	C5-C6-C7-C8
14	b	825	CLA	C13-C15-C16-C17
15	B	841	PQN	C23-C25-C26-C27
14	A	812	CLA	C10-C11-C12-C13
14	H	839	CLA	C5-C6-C7-C8
14	A	814	CLA	C11-C12-C13-C15
14	a	825	CLA	C2A-CAA-CBA-CGA
14	A	802	CLA	C11-C12-C13-C15
14	A	803	CLA	C6-C7-C8-C10
14	A	809	CLA	C11-C10-C8-C7
14	A	814	CLA	C11-C10-C8-C7
14	A	820	CLA	C11-C12-C13-C15
14	A	826	CLA	C12-C13-C15-C16
14	A	843	CLA	C6-C7-C8-C10
14	A	844	CLA	C11-C12-C13-C15
14	B	809	CLA	C6-C7-C8-C10
14	B	837	CLA	C6-C7-C8-C10
14	B	840	CLA	C12-C13-C15-C16
14	G	803	CLA	C6-C7-C8-C10
14	G	803	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	807	CLA	C6-C7-C8-C10
14	G	814	CLA	C11-C10-C8-C7
14	G	820	CLA	C11-C12-C13-C15
14	G	822	CLA	C11-C10-C8-C7
14	G	826	CLA	C12-C13-C15-C16
14	G	828	CLA	C11-C10-C8-C7
14	G	830	CLA	C11-C12-C13-C15
14	G	843	CLA	C11-C12-C13-C15
14	H	806	CLA	C6-C7-C8-C10
14	H	809	CLA	C12-C13-C15-C16
14	H	818	CLA	C11-C10-C8-C7
14	H	827	CLA	C11-C10-C8-C7
14	H	836	CLA	C6-C7-C8-C10
14	H	837	CLA	C6-C7-C8-C10
14	U	204	CLA	C6-C7-C8-C10
14	a	808	CLA	C11-C10-C8-C7
14	a	840	CLA	C12-C13-C15-C16
14	b	801	CLA	C11-C10-C8-C7
14	b	804	CLA	C6-C7-C8-C10
14	b	812	CLA	C6-C7-C8-C10
14	b	837	CLA	C6-C7-C8-C10
14	b	839	CLA	C6-C7-C8-C10
14	b	840	CLA	C11-C10-C8-C7
14	l	206	CLA	C11-C10-C8-C7
14	l	207	CLA	C6-C7-C8-C10
15	b	841	PQN	C16-C17-C18-C20
14	A	834	CLA	C8-C10-C11-C12
14	G	841	CLA	C8-C10-C11-C12
14	b	839	CLA	C10-C11-C12-C13
14	G	806	CLA	O1D-CGD-O2D-CED
13	G	801	CL0	C16-C17-C18-C19
14	B	839	CLA	C16-C17-C18-C20
14	A	812	CLA	C3A-C2A-CAA-CBA
14	A	829	CLA	C3A-C2A-CAA-CBA
14	A	830	CLA	C3A-C2A-CAA-CBA
14	A	843	CLA	C3A-C2A-CAA-CBA
14	B	809	CLA	C3A-C2A-CAA-CBA
14	B	816	CLA	C3A-C2A-CAA-CBA
14	G	805	CLA	C3A-C2A-CAA-CBA
14	G	807	CLA	C3A-C2A-CAA-CBA
14	G	815	CLA	C3A-C2A-CAA-CBA
14	G	830	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	835	CLA	C4-C3-C5-C6
14	G	836	CLA	C3A-C2A-CAA-CBA
14	G	842	CLA	C3A-C2A-CAA-CBA
14	H	807	CLA	C4-C3-C5-C6
14	H	814	CLA	C3A-C2A-CAA-CBA
14	L	206	CLA	C3A-C2A-CAA-CBA
14	U	206	CLA	C3A-C2A-CAA-CBA
14	a	827	CLA	C4-C3-C5-C6
14	b	814	CLA	C3A-C2A-CAA-CBA
14	b	829	CLA	C3A-C2A-CAA-CBA
14	a	808	CLA	C13-C15-C16-C17
14	A	835	CLA	C2-C3-C5-C6
14	b	813	CLA	C2-C3-C5-C6
15	G	846	PQN	C12-C13-C15-C16
18	a	854	LHG	O10-C23-O8-C6
17	B	847	BCR	C19-C20-C21-C22
17	H	842	BCR	C19-C20-C21-C22
17	H	849	BCR	C13-C14-C15-C16
17	I	102	BCR	C9-C10-C11-C12
17	Q	202	BCR	C9-C10-C11-C12
17	V	1602	BCR	C9-C10-C11-C12
17	a	847	BCR	C19-C20-C21-C22
17	b	849	BCR	C13-C14-C15-C16
14	B	832	CLA	C3-C5-C6-C7
14	A	814	CLA	C11-C12-C13-C14
14	A	841	CLA	C8-C10-C11-C12
14	b	812	CLA	C13-C15-C16-C17
17	U	202	BCR	C36-C18-C19-C20
18	G	854	LHG	C35-C36-C37-C38
14	A	839	CLA	O1A-CGA-O2A-C1
14	a	803	CLA	O1A-CGA-O2A-C1
14	G	826	CLA	C13-C15-C16-C17
17	A	853	BCR	C11-C12-C13-C14
17	l	203	BCR	C11-C12-C13-C14
18	A	854	LHG	C33-C34-C35-C36
14	B	834	CLA	C2A-CAA-CBA-CGA
14	b	834	CLA	C2A-CAA-CBA-CGA
18	A	854	LHG	C4-C5-C6-O8
18	A	855	LHG	C4-C5-C6-O8
18	a	854	LHG	C4-C5-C6-O8
14	G	830	CLA	C16-C17-C18-C20
14	A	810	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	827	CLA	C10-C11-C12-C13
14	H	805	CLA	C10-C11-C12-C13
14	a	825	CLA	C10-C11-C12-C13
18	A	855	LHG	C9-C10-C11-C12
14	A	835	CLA	C4-C3-C5-C6
14	L	206	CLA	C4-C3-C5-C6
18	a	853	LHG	C34-C35-C36-C37
14	A	812	CLA	C2-C3-C5-C6
14	B	807	CLA	C2-C3-C5-C6
14	H	831	CLA	C2-C3-C5-C6
14	b	812	CLA	C2-C3-C5-C6
14	l	205	CLA	C2-C3-C5-C6
14	H	806	CLA	O1A-CGA-O2A-C1
18	G	854	LHG	O6-C4-C5-O7
18	G	855	LHG	O6-C4-C5-O7
17	A	851	BCR	C1-C6-C7-C8
17	B	842	BCR	C23-C24-C25-C30
17	B	844	BCR	C23-C24-C25-C26
17	B	844	BCR	C23-C24-C25-C30
17	F	1302	BCR	C1-C6-C7-C8
17	G	849	BCR	C1-C6-C7-C8
17	G	851	BCR	C1-C6-C7-C8
17	G	852	BCR	C1-C6-C7-C8
17	H	844	BCR	C23-C24-C25-C30
17	H	847	BCR	C1-C6-C7-C8
17	H	847	BCR	C23-C24-C25-C30
17	H	849	BCR	C1-C6-C7-C8
17	J	102	BCR	C1-C6-C7-C8
17	b	842	BCR	C23-C24-C25-C30
17	b	846	BCR	C23-C24-C25-C30
17	f	203	BCR	C1-C6-C7-C8
17	l	203	BCR	C23-C24-C25-C30
14	l	207	CLA	C13-C15-C16-C17
15	a	845	PQN	C13-C15-C16-C17
14	G	829	CLA	C10-C11-C12-C13
14	b	804	CLA	C8-C10-C11-C12
14	a	827	CLA	CBD-CGD-O2D-CED
14	A	826	CLA	C2A-CAA-CBA-CGA
14	a	829	CLA	C3-C5-C6-C7
14	l	206	CLA	C3-C5-C6-C7
14	b	827	CLA	C5-C6-C7-C8
14	L	206	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	b	848	LMG	C16-C17-C18-C19
14	H	818	CLA	C13-C15-C16-C17
14	A	825	CLA	O1A-CGA-O2A-C1
14	A	809	CLA	C11-C10-C8-C9
14	B	817	CLA	C11-C10-C8-C9
14	G	822	CLA	C11-C10-C8-C9
14	H	801	CLA	C11-C12-C13-C14
14	H	803	CLA	C11-C12-C13-C14
14	H	805	CLA	C11-C12-C13-C14
14	H	827	CLA	C11-C10-C8-C9
14	H	836	CLA	C6-C7-C8-C9
14	b	802	CLA	C6-C7-C8-C9
14	b	806	CLA	C6-C7-C8-C9
14	b	812	CLA	C6-C7-C8-C9
14	b	831	CLA	C11-C12-C13-C14
14	a	818	CLA	O1A-CGA-O2A-C1
14	A	844	CLA	C16-C17-C18-C20
14	H	831	CLA	C16-C17-C18-C20
14	a	838	CLA	C10-C11-C12-C13
14	H	812	CLA	C10-C11-C12-C13
14	b	826	CLA	C5-C6-C7-C8
14	A	834	CLA	CBA-CGA-O2A-C1
14	B	837	CLA	C4-C3-C5-C6
14	L	204	CLA	C4-C3-C5-C6
17	B	850	BCR	C19-C20-C21-C22
17	Q	204	BCR	C9-C10-C11-C12
17	a	852	BCR	C19-C20-C21-C22
14	H	813	CLA	C2-C3-C5-C6
14	a	827	CLA	C2-C3-C5-C6
14	A	802	CLA	C16-C17-C18-C19
14	A	809	CLA	C16-C17-C18-C19
14	B	801	CLA	C16-C17-C18-C20
14	G	803	CLA	C15-C16-C17-C18
17	Q	202	BCR	C11-C10-C9-C34
14	b	807	CLA	O1A-CGA-O2A-C1
14	B	805	CLA	C3-C5-C6-C7
14	B	823	CLA	CBA-CGA-O2A-C1
14	b	804	CLA	CBA-CGA-O2A-C1
14	b	826	CLA	C10-C11-C12-C13
18	G	855	LHG	O6-C4-C5-C6
13	A	801	CL0	O1D-CGD-O2D-CED
14	B	825	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	843	BCR	C37-C22-C23-C24
14	B	801	CLA	C12-C13-C15-C16
14	B	806	CLA	C6-C7-C8-C10
14	G	842	CLA	C11-C10-C8-C7
14	H	801	CLA	C11-C12-C13-C15
14	H	812	CLA	C11-C10-C8-C7
14	H	827	CLA	C12-C13-C15-C16
14	H	831	CLA	C12-C13-C15-C16
14	a	802	CLA	C11-C10-C8-C7
14	a	813	CLA	C11-C10-C8-C7
14	a	825	CLA	C12-C13-C15-C16
14	a	842	CLA	C11-C12-C13-C15
14	b	802	CLA	C6-C7-C8-C10
14	b	809	CLA	C12-C13-C15-C16
14	b	831	CLA	C11-C10-C8-C7
14	B	825	CLA	C10-C11-C12-C13
14	G	835	CLA	C13-C15-C16-C17
14	a	806	CLA	C10-C11-C12-C13
17	A	850	BCR	C17-C18-C19-C20
17	G	852	BCR	C11-C12-C13-C14
17	G	852	BCR	C21-C22-C23-C24
17	H	843	BCR	C21-C22-C23-C24
17	J	103	BCR	C21-C22-C23-C24
17	M	1602	BCR	C21-C22-C23-C24
17	U	202	BCR	C17-C18-C19-C20
17	V	1602	BCR	C7-C8-C9-C10
17	a	847	BCR	C21-C22-C23-C24
17	b	847	BCR	C7-C8-C9-C10
14	b	821	CLA	CBA-CGA-O2A-C1
14	H	804	CLA	O1A-CGA-O2A-C1
18	a	853	LHG	O10-C23-O8-C6
14	b	804	CLA	C13-C15-C16-C17
14	B	827	CLA	C2A-CAA-CBA-CGA
14	G	826	CLA	C2A-CAA-CBA-CGA
14	a	809	CLA	C16-C17-C18-C20
14	a	806	CLA	CAA-CBA-CGA-O2A
14	B	816	CLA	C3-C5-C6-C7
14	a	834	CLA	C3-C5-C6-C7
14	b	840	CLA	C4C-C3C-CAC-CBC
14	G	802	CLA	O2A-C1-C2-C3
14	A	834	CLA	O1A-CGA-O2A-C1
14	B	823	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	841	CLA	O1A-CGA-O2A-C1
14	A	802	CLA	C10-C11-C12-C13
17	H	847	BCR	C9-C10-C11-C12
14	b	801	CLA	C16-C17-C18-C19
14	b	802	CLA	C16-C17-C18-C19
14	b	821	CLA	O1A-CGA-O2A-C1
14	G	822	CLA	C15-C16-C17-C18
14	H	801	CLA	C5-C6-C7-C8
18	A	854	LHG	O6-C4-C5-O7
18	G	854	LHG	C4-C5-C6-O8
14	B	808	CLA	C13-C15-C16-C17
14	G	833	CLA	C5-C6-C7-C8
14	B	837	CLA	C3-C5-C6-C7
19	b	848	LMG	C33-C34-C35-C36
14	G	820	CLA	C4-C3-C5-C6
14	a	816	CLA	C2A-CAA-CBA-CGA
14	b	804	CLA	C2A-CAA-CBA-CGA
14	B	837	CLA	C2-C3-C5-C6
14	L	204	CLA	C2-C3-C5-C6
15	a	845	PQN	C15-C16-C17-C18
14	A	803	CLA	C14-C13-C15-C16
14	B	802	CLA	C14-C13-C15-C16
14	B	806	CLA	C6-C7-C8-C9
14	B	818	CLA	C14-C13-C15-C16
14	B	826	CLA	C14-C13-C15-C16
14	B	828	CLA	C11-C12-C13-C14
14	H	827	CLA	C14-C13-C15-C16
14	H	831	CLA	C14-C13-C15-C16
14	a	825	CLA	C11-C12-C13-C14
14	a	840	CLA	C14-C13-C15-C16
14	b	831	CLA	C11-C10-C8-C9
14	B	840	CLA	C2C-C3C-CAC-CBC
13	a	801	CL0	O1A-CGA-O2A-C1
14	A	844	CLA	C5-C6-C7-C8
15	G	846	PQN	C15-C16-C17-C18
15	b	841	PQN	C23-C25-C26-C27
14	H	802	CLA	C15-C16-C17-C18
14	a	804	CLA	C3-C5-C6-C7
18	G	855	LHG	O8-C23-C24-C25
18	a	854	LHG	O8-C23-C24-C25
14	A	803	CLA	C2-C1-O2A-CGA
14	A	826	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	m	1602	BCR	C9-C10-C11-C12
14	B	825	CLA	C16-C17-C18-C19
14	a	821	CLA	C4-C3-C5-C6
14	H	816	CLA	C3-C5-C6-C7
14	G	820	CLA	C8-C10-C11-C12
14	H	808	CLA	C16-C17-C18-C19
18	A	854	LHG	C35-C36-C37-C38
14	U	201	CLA	C16-C17-C18-C20
14	B	827	CLA	C10-C11-C12-C13
14	A	822	CLA	C3-C5-C6-C7
14	A	813	CLA	C1A-C2A-CAA-CBA
14	B	811	CLA	C1A-C2A-CAA-CBA
14	B	835	CLA	C1A-C2A-CAA-CBA
14	G	814	CLA	C1A-C2A-CAA-CBA
14	H	835	CLA	C1A-C2A-CAA-CBA
14	H	836	CLA	C1A-C2A-CAA-CBA
14	L	206	CLA	C1A-C2A-CAA-CBA
14	a	809	CLA	C1A-C2A-CAA-CBA
14	b	813	CLA	C1A-C2A-CAA-CBA
14	b	816	CLA	C1A-C2A-CAA-CBA
14	A	828	CLA	C4-C3-C5-C6
14	B	831	CLA	C4-C3-C5-C6
14	U	205	CLA	C4-C3-C5-C6
17	G	850	BCR	C11-C12-C13-C14
17	A	848	BCR	C9-C10-C11-C12
14	b	804	CLA	O1A-CGA-O2A-C1
14	b	823	CLA	O1A-CGA-O2A-C1
14	a	843	CLA	C2A-CAA-CBA-CGA
14	b	825	CLA	C10-C11-C12-C13
18	A	855	LHG	O6-C4-C5-C6
18	a	853	LHG	O6-C4-C5-C6
14	A	802	CLA	C11-C10-C8-C7
14	A	822	CLA	C11-C10-C8-C7
14	A	828	CLA	C11-C10-C8-C7
14	A	843	CLA	C11-C10-C8-C7
14	B	808	CLA	C6-C7-C8-C10
14	B	812	CLA	C11-C10-C8-C7
14	B	812	CLA	C12-C13-C15-C16
14	B	826	CLA	C11-C12-C13-C15
14	B	827	CLA	C12-C13-C15-C16
14	G	809	CLA	C12-C13-C15-C16
14	G	842	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	802	CLA	C11-C12-C13-C15
14	H	839	CLA	C6-C7-C8-C10
14	a	827	CLA	C11-C10-C8-C7
14	a	829	CLA	C11-C12-C13-C15
14	b	808	CLA	C6-C7-C8-C10
14	b	827	CLA	C12-C13-C15-C16
14	b	836	CLA	C11-C10-C8-C7
15	b	841	PQN	C22-C23-C25-C26
14	B	803	CLA	C4C-C3C-CAC-CBC
13	G	801	CL0	C16-C17-C18-C20
14	B	816	CLA	C6-C7-C8-C9
14	a	803	CLA	C6-C7-C8-C10
14	G	802	CLA	O1D-CGD-O2D-CED
13	a	801	CL0	CBA-CGA-O2A-C1
14	B	833	CLA	C3A-C2A-CAA-CBA
14	G	802	CLA	C4-C3-C5-C6
14	a	806	CLA	C3A-C2A-CAA-CBA
14	a	803	CLA	C6-C7-C8-C9
18	a	853	LHG	O6-C4-C5-O7
14	B	801	CLA	C14-C13-C15-C16
14	G	843	CLA	C11-C12-C13-C14
14	H	802	CLA	C11-C12-C13-C14
14	H	812	CLA	C11-C10-C8-C9
14	a	802	CLA	C11-C10-C8-C9
14	a	808	CLA	C11-C10-C8-C9
14	a	825	CLA	C14-C13-C15-C16
14	b	809	CLA	C14-C13-C15-C16
14	b	839	CLA	C6-C7-C8-C9
14	l	202	CLA	C6-C7-C8-C9
15	b	841	PQN	C16-C17-C18-C19
14	A	802	CLA	C13-C15-C16-C17
17	A	853	BCR	C19-C20-C21-C22
17	a	848	BCR	C9-C10-C11-C12
17	a	850	BCR	C19-C20-C21-C22
14	a	809	CLA	C16-C17-C18-C19
14	b	831	CLA	C13-C15-C16-C17
14	A	832	CLA	O1D-CGD-O2D-CED
14	H	828	CLA	C3-C5-C6-C7
18	G	855	LHG	O10-C23-C24-C25
14	H	828	CLA	C10-C11-C12-C13
18	a	853	LHG	C15-C16-C17-C18
14	A	807	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	830	CLA	C2-C3-C5-C6
13	G	801	CL0	C3-C5-C6-C7
14	A	814	CLA	CAD-CBD-CGD-O2D
14	A	838	CLA	CAD-CBD-CGD-O2D
14	B	805	CLA	CAD-CBD-CGD-O2D
14	B	812	CLA	CAD-CBD-CGD-O2D
14	B	825	CLA	CAD-CBD-CGD-O2D
14	G	828	CLA	CAD-CBD-CGD-O2D
14	G	839	CLA	CAD-CBD-CGD-O2D
14	G	845	CLA	CAD-CBD-CGD-O2D
14	H	805	CLA	CAD-CBD-CGD-O2D
14	H	825	CLA	CAD-CBD-CGD-O2D
14	H	836	CLA	CAD-CBD-CGD-O2D
14	K	102	CLA	CAD-CBD-CGD-O2D
14	M	1601	CLA	CAD-CBD-CGD-O2D
14	S	101	CLA	CAD-CBD-CGD-O2D
14	V	1601	CLA	CAD-CBD-CGD-O2D
14	a	815	CLA	CAD-CBD-CGD-O2D
14	a	837	CLA	CAD-CBD-CGD-O2D
14	a	838	CLA	CAD-CBD-CGD-O2D
14	a	844	CLA	CAD-CBD-CGD-O2D
14	b	812	CLA	CAD-CBD-CGD-O2D
14	b	825	CLA	CAD-CBD-CGD-O2D
14	k	1401	CLA	CAD-CBD-CGD-O2D
14	B	803	CLA	CBA-CGA-O2A-C1
14	b	823	CLA	CBA-CGA-O2A-C1
14	H	803	CLA	C8-C10-C11-C12
14	A	839	CLA	C16-C17-C18-C19
14	A	839	CLA	C16-C17-C18-C20
14	A	836	CLA	C2A-CAA-CBA-CGA
14	B	801	CLA	C2A-CAA-CBA-CGA
14	b	828	CLA	C10-C11-C12-C13
14	A	814	CLA	CAD-CBD-CGD-O1D
14	A	838	CLA	CAD-CBD-CGD-O1D
14	B	805	CLA	CAD-CBD-CGD-O1D
14	B	812	CLA	CAD-CBD-CGD-O1D
14	B	825	CLA	CAD-CBD-CGD-O1D
14	G	820	CLA	CHA-CBD-CGD-O1D
14	G	820	CLA	CHA-CBD-CGD-O2D
14	G	828	CLA	CAD-CBD-CGD-O1D
14	G	838	CLA	CAD-CBD-CGD-O1D
14	G	839	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	845	CLA	CAD-CBD-CGD-O1D
14	H	801	CLA	CAD-CBD-CGD-O1D
14	H	805	CLA	CAD-CBD-CGD-O1D
14	H	825	CLA	CAD-CBD-CGD-O1D
14	H	836	CLA	CAD-CBD-CGD-O1D
14	K	102	CLA	CAD-CBD-CGD-O1D
14	L	201	CLA	CHA-CBD-CGD-O1D
14	L	201	CLA	CHA-CBD-CGD-O2D
14	M	1601	CLA	CAD-CBD-CGD-O1D
14	S	101	CLA	CAD-CBD-CGD-O1D
14	V	1601	CLA	CAD-CBD-CGD-O1D
14	X	1701	CLA	CHA-CBD-CGD-O1D
14	a	814	CLA	CAD-CBD-CGD-O1D
14	a	815	CLA	CAD-CBD-CGD-O1D
14	a	825	CLA	CHA-CBD-CGD-O1D
14	a	825	CLA	CHA-CBD-CGD-O2D
14	a	827	CLA	CAD-CBD-CGD-O1D
14	a	837	CLA	CAD-CBD-CGD-O1D
14	a	838	CLA	CAD-CBD-CGD-O1D
14	a	844	CLA	CAD-CBD-CGD-O1D
14	a	855	CLA	CAD-CBD-CGD-O1D
14	b	812	CLA	CAD-CBD-CGD-O1D
14	b	825	CLA	CAD-CBD-CGD-O1D
14	b	835	CLA	CHA-CBD-CGD-O1D
14	k	1401	CLA	CAD-CBD-CGD-O1D
14	l	202	CLA	CHA-CBD-CGD-O1D
17	G	848	BCR	C9-C10-C11-C12
17	G	852	BCR	C19-C20-C21-C22
17	R	102	BCR	C19-C20-C21-C22
17	V	1602	BCR	C19-C20-C21-C22
17	b	849	BCR	C19-C20-C21-C22
17	l	203	BCR	C9-C10-C11-C12
18	A	855	LHG	C3-O3-P-O5
18	G	855	LHG	C3-O3-P-O5
18	a	853	LHG	C3-O3-P-O5
18	a	854	LHG	C4-O6-P-O5
14	A	828	CLA	C13-C15-C16-C17
17	B	842	BCR	C23-C24-C25-C26
17	a	848	BCR	C5-C6-C7-C8
17	a	850	BCR	C5-C6-C7-C8
17	b	846	BCR	C23-C24-C25-C26
18	A	855	LHG	O8-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	842	CLA	CAA-CBA-CGA-O2A
14	a	821	CLA	C2-C3-C5-C6
17	F	1302	BCR	C11-C12-C13-C35
17	G	850	BCR	C11-C12-C13-C35
17	S	103	BCR	C11-C12-C13-C35
17	a	848	BCR	C11-C12-C13-C35
14	L	205	CLA	C2C-C3C-CAC-CBC
14	H	840	CLA	C5-C6-C7-C8
15	A	846	PQN	C15-C16-C17-C18
14	H	805	CLA	C16-C17-C18-C19
19	b	848	LMG	C30-C31-C32-C33
14	l	207	CLA	CAA-CBA-CGA-O2A
14	G	826	CLA	O1A-CGA-O2A-C1
18	a	853	LHG	C30-C31-C32-C33
18	A	854	LHG	C30-C31-C32-C33
14	A	830	CLA	C16-C17-C18-C19
14	H	808	CLA	C16-C17-C18-C20
19	b	848	LMG	C28-C29-C30-C31
14	a	855	CLA	C13-C15-C16-C17
14	B	823	CLA	O2A-C1-C2-C3
14	a	834	CLA	C4-C3-C5-C6
14	A	803	CLA	C15-C16-C17-C18
14	a	825	CLA	C5-C6-C7-C8
15	H	841	PQN	C25-C26-C27-C28
14	G	820	CLA	C2-C3-C5-C6
17	J	102	BCR	C19-C20-C21-C22
14	B	816	CLA	C6-C7-C8-C10
14	H	805	CLA	C16-C17-C18-C20
14	H	839	CLA	C16-C17-C18-C20
14	b	802	CLA	C16-C17-C18-C20
15	A	846	PQN	C25-C26-C27-C28
18	a	854	LHG	O10-C23-C24-C25
14	A	826	CLA	C11-C12-C13-C14
14	A	834	CLA	C11-C10-C8-C9
14	A	835	CLA	C14-C13-C15-C16
14	A	843	CLA	C6-C7-C8-C9
14	A	844	CLA	C11-C12-C13-C14
14	G	807	CLA	C11-C10-C8-C9
14	G	834	CLA	C14-C13-C15-C16
14	H	806	CLA	C6-C7-C8-C9
14	a	813	CLA	C11-C10-C8-C9
14	a	821	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	829	CLA	C11-C12-C13-C14
14	a	834	CLA	C14-C13-C15-C16
14	A	814	CLA	C6-C7-C8-C10
14	A	834	CLA	C11-C10-C8-C7
14	A	835	CLA	C12-C13-C15-C16
14	G	802	CLA	C11-C10-C8-C7
14	H	801	CLA	C6-C7-C8-C10
14	a	821	CLA	C11-C10-C8-C7
14	a	834	CLA	C12-C13-C15-C16
15	A	846	PQN	C16-C17-C18-C20
17	Q	202	BCR	C11-C10-C9-C8
17	a	852	BCR	C11-C10-C9-C8
14	A	810	CLA	C2A-CAA-CBA-CGA
14	b	831	CLA	C3-C5-C6-C7
14	b	826	CLA	C4-C3-C5-C6
14	B	803	CLA	O1A-CGA-O2A-C1
14	b	816	CLA	CAA-CBA-CGA-O2A
14	B	831	CLA	C2-C3-C5-C6
14	b	805	CLA	O1A-CGA-O2A-C1
14	H	801	CLA	C15-C16-C17-C18
14	b	805	CLA	CBA-CGA-O2A-C1
17	b	845	BCR	C19-C20-C21-C22
17	l	208	BCR	C13-C14-C15-C16
14	B	840	CLA	C4C-C3C-CAC-CBC
14	G	803	CLA	C2-C1-O2A-CGA
14	b	817	CLA	C2-C1-O2A-CGA
14	A	827	CLA	C4-C3-C5-C6
14	A	819	CLA	CAA-CBA-CGA-O2A
14	G	814	CLA	C4C-C3C-CAC-CBC
15	A	846	PQN	C13-C15-C16-C17
14	G	814	CLA	C2C-C3C-CAC-CBC
14	H	826	CLA	CAA-CBA-CGA-O2A
14	a	818	CLA	CAA-CBA-CGA-O2A
17	G	849	BCR	C11-C12-C13-C35
17	A	848	BCR	C17-C18-C19-C20
17	U	202	BCR	C11-C12-C13-C14
14	G	826	CLA	CBA-CGA-O2A-C1
14	A	807	CLA	CAA-CBA-CGA-O2A
14	B	802	CLA	O1A-CGA-O2A-C1
14	A	819	CLA	C2A-CAA-CBA-CGA
14	H	805	CLA	C2A-CAA-CBA-CGA
14	H	816	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	810	CLA	C2A-CAA-CBA-CGA
14	b	830	CLA	C2A-CAA-CBA-CGA
14	m	1601	CLA	C2A-CAA-CBA-CGA
17	A	852	BCR	C19-C20-C21-C22
17	S	103	BCR	C9-C10-C11-C12
17	m	1602	BCR	C19-C20-C21-C22
14	a	855	CLA	C16-C17-C18-C19
14	b	821	CLA	C6-C7-C8-C10
14	B	826	CLA	C4-C3-C5-C6
14	H	826	CLA	C4-C3-C5-C6
14	b	827	CLA	C10-C11-C12-C13
14	U	205	CLA	C2-C3-C5-C6
14	A	841	CLA	CBA-CGA-O2A-C1
14	A	841	CLA	O1A-CGA-O2A-C1
14	L	201	CLA	C13-C15-C16-C17
14	G	830	CLA	CAA-CBA-CGA-O1A
14	A	820	CLA	C16-C17-C18-C19
14	b	809	CLA	CAA-CBA-CGA-O2A
14	b	826	CLA	CAA-CBA-CGA-O2A
14	A	802	CLA	C11-C10-C8-C9
14	G	814	CLA	C11-C10-C8-C9
14	H	801	CLA	C14-C13-C15-C16
14	b	802	CLA	C14-C13-C15-C16
15	B	841	PQN	C21-C22-C23-C24
14	A	822	CLA	O1D-CGD-O2D-CED
14	G	802	CLA	CBD-CGD-O2D-CED
14	l	206	CLA	C15-C16-C17-C18
14	b	801	CLA	C16-C17-C18-C20
18	A	855	LHG	C24-C23-O8-C6
14	A	804	CLA	C5-C6-C7-C8
18	A	855	LHG	O10-C23-O8-C6
14	A	829	CLA	C2A-CAA-CBA-CGA
14	G	822	CLA	C4-C3-C5-C6
14	G	828	CLA	C4-C3-C5-C6
14	H	837	CLA	C4-C3-C5-C6
14	a	838	CLA	C4-C3-C5-C6
14	b	837	CLA	C4-C3-C5-C6
14	A	828	CLA	C2-C3-C5-C6
14	G	802	CLA	C2-C3-C5-C6
14	b	826	CLA	C2-C3-C5-C6
14	B	830	CLA	CAA-CBA-CGA-O2A
19	b	848	LMG	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	812	CLA	C5-C6-C7-C8
14	B	804	CLA	C6-C7-C8-C9
14	A	830	CLA	CAA-CBA-CGA-O2A
14	A	809	CLA	C6-C7-C8-C10
14	A	831	CLA	C11-C10-C8-C7
14	B	817	CLA	C11-C10-C8-C7
14	B	839	CLA	C11-C10-C8-C7
14	G	834	CLA	C12-C13-C15-C16
14	U	206	CLA	C12-C13-C15-C16
15	B	841	PQN	C21-C22-C23-C25
15	H	841	PQN	C21-C22-C23-C25
15	a	845	PQN	C16-C17-C18-C20
14	H	839	CLA	C15-C16-C17-C18
15	A	846	PQN	C18-C20-C21-C22
13	A	801	CL0	O1A-CGA-O2A-C1
14	A	845	CLA	CAA-CBA-CGA-O2A
18	A	854	LHG	O2-C2-C3-O3
14	H	821	CLA	C5-C6-C7-C8
14	G	841	CLA	C5-C6-C7-C8
14	G	805	CLA	C4-C3-C5-C6
14	G	824	CLA	C3A-C2A-CAA-CBA
14	G	825	CLA	C4-C3-C5-C6
14	Q	201	CLA	C3A-C2A-CAA-CBA
14	a	828	CLA	C3A-C2A-CAA-CBA
14	a	842	CLA	C3A-C2A-CAA-CBA
14	b	807	CLA	C4-C3-C5-C6
14	G	819	CLA	CAA-CBA-CGA-O2A
14	A	827	CLA	C2-C3-C5-C6
14	B	826	CLA	C2-C3-C5-C6
14	G	822	CLA	C2-C3-C5-C6
14	a	834	CLA	C2-C3-C5-C6
18	A	855	LHG	O10-C23-C24-C25
14	H	803	CLA	C16-C17-C18-C19
14	H	836	CLA	C11-C12-C13-C15
17	A	853	BCR	C16-C17-C18-C36
17	B	844	BCR	C20-C21-C22-C37
17	F	1302	BCR	C35-C13-C14-C15
17	G	853	BCR	C11-C10-C9-C34
17	G	853	BCR	C16-C17-C18-C36
17	H	844	BCR	C20-C21-C22-C37
17	L	202	BCR	C20-C21-C22-C37
17	Q	204	BCR	C35-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	R	102	BCR	C20-C21-C22-C37
17	a	852	BCR	C11-C10-C9-C34
17	a	852	BCR	C16-C17-C18-C36
17	b	844	BCR	C20-C21-C22-C37
17	f	203	BCR	C35-C13-C14-C15
17	l	203	BCR	C20-C21-C22-C37
14	G	834	CLA	O1A-CGA-O2A-C1
14	b	840	CLA	C8-C10-C11-C12
14	B	815	CLA	CAA-CBA-CGA-O2A
14	a	836	CLA	CAA-CBA-CGA-O2A
14	L	201	CLA	C2-C1-O2A-CGA
14	U	206	CLA	C2-C1-O2A-CGA
14	a	804	CLA	C2-C1-O2A-CGA
14	a	821	CLA	C2-C1-O2A-CGA
17	A	849	BCR	C9-C10-C11-C12
17	B	846	BCR	C19-C20-C21-C22
17	G	849	BCR	C19-C20-C21-C22
17	Q	202	BCR	C19-C20-C21-C22
17	f	201	BCR	C9-C10-C11-C12
14	A	825	CLA	C3-C5-C6-C7
14	B	836	CLA	C8-C10-C11-C12
14	H	801	CLA	C8-C10-C11-C12
14	B	830	CLA	CAA-CBA-CGA-O1A
14	B	818	CLA	C13-C15-C16-C17
14	A	840	CLA	CAA-CBA-CGA-O1A
14	B	820	CLA	CAA-CBA-CGA-O1A
14	b	833	CLA	CAA-CBA-CGA-O1A
17	S	103	BCR	C11-C12-C13-C14
17	a	848	BCR	C11-C12-C13-C14
14	L	205	CLA	C4-C3-C5-C6
14	b	827	CLA	C4-C3-C5-C6
13	A	801	CL0	C16-C17-C18-C19
14	B	836	CLA	C11-C12-C13-C15
15	b	841	PQN	C25-C26-C27-C28
14	H	838	CLA	CAA-CBA-CGA-O2A
14	H	828	CLA	C13-C15-C16-C17
14	b	812	CLA	C8-C10-C11-C12
14	A	845	CLA	CAA-CBA-CGA-O1A
14	H	815	CLA	CAA-CBA-CGA-O2A
14	A	807	CLA	C11-C10-C8-C9
14	A	822	CLA	C11-C10-C8-C9
14	A	831	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	812	CLA	C11-C10-C8-C9
14	B	825	CLA	C6-C7-C8-C9
14	B	826	CLA	C11-C12-C13-C14
14	H	806	CLA	C11-C10-C8-C9
14	H	808	CLA	C14-C13-C15-C16
14	H	825	CLA	C11-C10-C8-C9
14	L	201	CLA	C11-C10-C8-C9
14	L	206	CLA	C6-C7-C8-C9
14	U	206	CLA	C14-C13-C15-C16
14	a	809	CLA	C11-C12-C13-C14
14	b	801	CLA	C11-C12-C13-C14
14	b	839	CLA	C11-C12-C13-C14
15	H	841	PQN	C21-C22-C23-C24
14	b	806	CLA	C16-C17-C18-C19
14	l	207	CLA	C16-C17-C18-C19
14	B	827	CLA	CBA-CGA-O2A-C1
18	A	854	LHG	C15-C16-C17-C18
14	K	102	CLA	CAA-CBA-CGA-O1A
14	b	819	CLA	CAA-CBA-CGA-O1A
14	a	809	CLA	C5-C6-C7-C8
14	a	809	CLA	C13-C15-C16-C17
14	a	827	CLA	O1D-CGD-O2D-CED
17	a	851	BCR	C19-C20-C21-C22
14	A	840	CLA	CAA-CBA-CGA-O2A
14	G	844	CLA	CAA-CBA-CGA-O2A
14	a	839	CLA	CAA-CBA-CGA-O1A
14	B	809	CLA	C4-C3-C5-C6
14	H	809	CLA	C4-C3-C5-C6
14	a	809	CLA	C4-C3-C5-C6
14	A	830	CLA	C16-C17-C18-C20
14	G	834	CLA	CBA-CGA-O2A-C1
14	H	802	CLA	CAA-CBA-CGA-O2A
14	H	826	CLA	C2-C3-C5-C6
14	H	837	CLA	C2-C3-C5-C6
14	L	205	CLA	C2-C3-C5-C6
14	B	815	CLA	CAA-CBA-CGA-O1A
14	B	820	CLA	CAA-CBA-CGA-O2A
14	H	835	CLA	CAA-CBA-CGA-O2A
14	H	838	CLA	CAA-CBA-CGA-O1A
14	J	101	CLA	CAA-CBA-CGA-O2A
14	V	1601	CLA	CAA-CBA-CGA-O2A
14	a	836	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	844	CLA	CAA-CBA-CGA-O2A
14	G	841	CLA	C2A-CAA-CBA-CGA
14	a	817	CLA	C2A-CAA-CBA-CGA
14	G	807	CLA	CAA-CBA-CGA-O1A
13	G	801	CL0	O1A-CGA-O2A-C1
14	A	803	CLA	C1A-C2A-CAA-CBA
14	A	814	CLA	C1A-C2A-CAA-CBA
14	A	845	CLA	C1A-C2A-CAA-CBA
14	B	801	CLA	C1A-C2A-CAA-CBA
14	B	809	CLA	C1A-C2A-CAA-CBA
14	G	803	CLA	C1A-C2A-CAA-CBA
14	G	813	CLA	C1A-C2A-CAA-CBA
14	H	831	CLA	C1A-C2A-CAA-CBA
14	K	101	CLA	C1A-C2A-CAA-CBA
14	a	802	CLA	C1A-C2A-CAA-CBA
14	b	811	CLA	C1A-C2A-CAA-CBA
14	b	836	CLA	C1A-C2A-CAA-CBA
14	l	207	CLA	C1A-C2A-CAA-CBA
17	A	853	BCR	C16-C17-C18-C19
17	B	844	BCR	C20-C21-C22-C23
17	F	1302	BCR	C12-C13-C14-C15
17	G	853	BCR	C16-C17-C18-C19
17	H	844	BCR	C20-C21-C22-C23
17	L	202	BCR	C20-C21-C22-C23
17	Q	204	BCR	C12-C13-C14-C15
17	R	102	BCR	C20-C21-C22-C23
17	a	852	BCR	C16-C17-C18-C19
17	b	844	BCR	C20-C21-C22-C23
17	f	203	BCR	C12-C13-C14-C15
17	l	203	BCR	C20-C21-C22-C23
14	A	824	CLA	CAA-CBA-CGA-O1A
14	b	838	CLA	CAA-CBA-CGA-O1A
14	a	825	CLA	C15-C16-C17-C18
17	A	849	BCR	C5-C6-C7-C8
17	A	851	BCR	C5-C6-C7-C8
17	A	852	BCR	C5-C6-C7-C8
17	B	842	BCR	C5-C6-C7-C8
17	B	846	BCR	C23-C24-C25-C26
17	B	846	BCR	C23-C24-C25-C30
17	B	850	BCR	C1-C6-C7-C8
17	F	1302	BCR	C5-C6-C7-C8
17	G	849	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	G	851	BCR	C5-C6-C7-C8
17	G	852	BCR	C5-C6-C7-C8
17	G	853	BCR	C1-C6-C7-C8
17	G	853	BCR	C5-C6-C7-C8
17	H	844	BCR	C23-C24-C25-C26
17	H	846	BCR	C23-C24-C25-C30
17	H	847	BCR	C5-C6-C7-C8
17	H	847	BCR	C23-C24-C25-C26
17	H	849	BCR	C5-C6-C7-C8
17	I	101	BCR	C1-C6-C7-C8
17	I	101	BCR	C5-C6-C7-C8
17	J	102	BCR	C5-C6-C7-C8
17	L	202	BCR	C23-C24-C25-C26
17	Q	204	BCR	C1-C6-C7-C8
17	Q	204	BCR	C5-C6-C7-C8
17	a	852	BCR	C1-C6-C7-C8
17	b	842	BCR	C23-C24-C25-C26
17	b	847	BCR	C23-C24-C25-C30
17	f	203	BCR	C5-C6-C7-C8
17	l	203	BCR	C23-C24-C25-C26
17	m	1602	BCR	C23-C24-C25-C26
17	m	1602	BCR	C23-C24-C25-C30
14	A	808	CLA	CAA-CBA-CGA-O2A
14	A	824	CLA	CAA-CBA-CGA-O2A
14	G	844	CLA	CAA-CBA-CGA-O1A
14	H	835	CLA	CAA-CBA-CGA-O1A
14	V	1601	CLA	CAA-CBA-CGA-O1A
14	b	814	CLA	CAA-CBA-CGA-O2A
14	b	833	CLA	CAA-CBA-CGA-O2A
14	a	829	CLA	C8-C10-C11-C12
14	A	803	CLA	C5-C6-C7-C8
14	J	101	CLA	CAA-CBA-CGA-O1A
14	K	101	CLA	CAA-CBA-CGA-O2A
14	a	807	CLA	CAA-CBA-CGA-O1A
14	A	803	CLA	C4-C3-C5-C6
14	B	808	CLA	C4-C3-C5-C6
14	G	826	CLA	C4-C3-C5-C6
14	B	819	CLA	CAA-CBA-CGA-O2A
14	S	101	CLA	CAA-CBA-CGA-O2A
14	b	814	CLA	CAA-CBA-CGA-O1A
14	b	819	CLA	CAA-CBA-CGA-O2A
14	b	822	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	k	1401	CLA	CAA-CBA-CGA-O1A
17	A	853	BCR	C9-C10-C11-C12
14	B	827	CLA	C11-C10-C8-C7
14	B	839	CLA	C6-C7-C8-C10
14	G	810	CLA	C6-C7-C8-C10
14	G	828	CLA	C6-C7-C8-C10
14	G	829	CLA	C11-C12-C13-C15
14	H	801	CLA	C12-C13-C15-C16
14	H	805	CLA	C11-C10-C8-C7
14	H	808	CLA	C6-C7-C8-C10
14	a	809	CLA	C11-C12-C13-C15
14	b	801	CLA	C12-C13-C15-C16
14	b	802	CLA	C11-C12-C13-C15
14	b	802	CLA	C12-C13-C15-C16
14	b	839	CLA	C11-C12-C13-C15
15	G	846	PQN	C16-C17-C18-C20
14	G	811	CLA	C2A-CAA-CBA-CGA
18	A	854	LHG	C19-C20-C21-C22
14	a	844	CLA	CAA-CBA-CGA-O1A
14	b	838	CLA	CAA-CBA-CGA-O2A
14	x	1701	CLA	CAA-CBA-CGA-O1A
14	B	838	CLA	CAA-CBA-CGA-O2A
14	H	815	CLA	CAA-CBA-CGA-O1A
14	W	1701	CLA	CAA-CBA-CGA-O1A
18	A	854	LHG	C26-C27-C28-C29
17	A	848	BCR	C36-C18-C19-C20
17	m	1602	BCR	C37-C22-C23-C24
14	B	819	CLA	CAA-CBA-CGA-O1A
14	G	808	CLA	CAA-CBA-CGA-O1A
14	H	822	CLA	CAA-CBA-CGA-O1A
14	a	843	CLA	CAA-CBA-CGA-O2A
14	A	805	CLA	C4-C3-C5-C6
14	H	808	CLA	C4-C3-C5-C6
14	a	802	CLA	C4-C3-C5-C6
14	a	808	CLA	C4-C3-C5-C6
14	b	808	CLA	C4-C3-C5-C6
14	B	826	CLA	CAA-CBA-CGA-O2A
14	G	805	CLA	C2-C3-C5-C6
14	G	825	CLA	C2-C3-C5-C6
14	G	828	CLA	C2-C3-C5-C6
14	a	838	CLA	C2-C3-C5-C6
14	b	837	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	827	CLA	O1A-CGA-O2A-C1
14	A	805	CLA	C2-C1-O2A-CGA
14	G	802	CLA	C8-C10-C11-C12
14	S	101	CLA	CAA-CBA-CGA-O1A
14	b	834	CLA	CAA-CBA-CGA-O2A
17	F	1302	BCR	C11-C12-C13-C14
14	b	818	CLA	C13-C15-C16-C17
14	B	831	CLA	C2A-CAA-CBA-CGA
14	b	831	CLA	C2A-CAA-CBA-CGA
14	A	808	CLA	CAA-CBA-CGA-O1A
14	B	833	CLA	CAA-CBA-CGA-O2A
14	a	823	CLA	CAA-CBA-CGA-O2A
14	a	839	CLA	CAA-CBA-CGA-O2A
14	B	827	CLA	C11-C10-C8-C9
14	B	831	CLA	C14-C13-C15-C16
14	G	839	CLA	C11-C12-C13-C14
14	H	840	CLA	C11-C12-C13-C14
14	a	821	CLA	C14-C13-C15-C16
14	H	808	CLA	C5-C6-C7-C8
14	U	206	CLA	C10-C11-C12-C13
18	G	855	LHG	C9-C10-C11-C12
14	B	814	CLA	CAA-CBA-CGA-O2A
14	A	802	CLA	C4-C3-C5-C6
14	G	803	CLA	C4-C3-C5-C6
14	G	807	CLA	C4-C3-C5-C6
14	a	819	CLA	C4-C3-C5-C6
14	a	826	CLA	C4-C3-C5-C6
14	b	809	CLA	C4-C3-C5-C6
14	B	838	CLA	CAA-CBA-CGA-O1A
14	H	809	CLA	C2-C3-C5-C6
14	a	802	CLA	C2-C3-C5-C6
14	a	802	CLA	C15-C16-C17-C18
14	a	827	CLA	C13-C15-C16-C17
14	a	819	CLA	C16-C17-C18-C19
14	G	840	CLA	CAA-CBA-CGA-O1A
14	H	822	CLA	CAA-CBA-CGA-O2A
14	X	1701	CLA	CAA-CBA-CGA-O1A
14	x	1701	CLA	CAA-CBA-CGA-O2A
19	B	849	LMG	C10-C11-C12-C13
14	G	818	CLA	CAA-CBA-CGA-O2A
14	K	101	CLA	CAA-CBA-CGA-O1A
14	k	1401	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	H	823	CLA	C2A-CAA-CBA-CGA
14	b	806	CLA	C16-C17-C18-C20
14	G	824	CLA	CAA-CBA-CGA-O2A
14	T	1401	CLA	CAA-CBA-CGA-O2A
14	A	820	CLA	C4-C3-C5-C6
14	b	804	CLA	C4-C3-C5-C6
14	B	834	CLA	CAA-CBA-CGA-O2A
14	B	835	CLA	CAA-CBA-CGA-O2A
14	G	808	CLA	CAA-CBA-CGA-O2A
14	K	102	CLA	CAA-CBA-CGA-O2A
14	b	827	CLA	C2-C3-C5-C6
14	G	831	CLA	C5-C6-C7-C8
14	M	1601	CLA	CAA-CBA-CGA-O2A
14	a	807	CLA	CAA-CBA-CGA-O2A
14	j	101	CLA	CAA-CBA-CGA-O2A
14	G	842	CLA	CAA-CBA-CGA-O2A
14	a	829	CLA	CAA-CBA-CGA-O2A
14	H	831	CLA	O1A-CGA-O2A-C1
14	a	843	CLA	CAA-CBA-CGA-O1A
14	b	835	CLA	CAA-CBA-CGA-O2A
14	m	1601	CLA	CAA-CBA-CGA-O2A
14	H	836	CLA	C11-C12-C13-C14
14	b	821	CLA	C6-C7-C8-C9
14	b	825	CLA	C8-C10-C11-C12
17	R	103	BCR	C11-C10-C9-C34
17	b	844	BCR	C11-C10-C9-C34
13	A	801	CL0	CBA-CGA-O2A-C1
14	G	824	CLA	CAA-CBA-CGA-O1A
14	H	819	CLA	CAA-CBA-CGA-O1A
14	W	1701	CLA	CAA-CBA-CGA-O2A
14	a	804	CLA	C4-C3-C5-C6
14	B	833	CLA	CAA-CBA-CGA-O1A
14	Q	201	CLA	CAA-CBA-CGA-O2A
14	X	1701	CLA	CAA-CBA-CGA-O2A
18	A	854	LHG	C29-C30-C31-C32
14	A	802	CLA	C2-C3-C5-C6
14	b	809	CLA	C2-C3-C5-C6
14	G	829	CLA	C11-C10-C8-C7
14	H	820	CLA	CAA-CBA-CGA-O1A
14	H	834	CLA	CAA-CBA-CGA-O2A
14	b	822	CLA	CAA-CBA-CGA-O2A
18	A	854	LHG	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	b	839	CLA	C5-C6-C7-C8
17	A	851	BCR	C19-C20-C21-C22
17	G	853	BCR	C19-C20-C21-C22
17	H	849	BCR	C19-C20-C21-C22
18	G	854	LHG	C29-C30-C31-C32
14	A	818	CLA	CAA-CBA-CGA-O2A
14	B	829	CLA	CAA-CBA-CGA-O1A
14	M	1601	CLA	CAA-CBA-CGA-O1A
14	b	834	CLA	CAA-CBA-CGA-O1A
14	j	101	CLA	CAA-CBA-CGA-O1A
14	A	826	CLA	C14-C13-C15-C16
14	A	828	CLA	C11-C10-C8-C9
14	A	834	CLA	C14-C13-C15-C16
14	B	806	CLA	C11-C10-C8-C9
14	B	806	CLA	C11-C12-C13-C14
14	G	809	CLA	C14-C13-C15-C16
14	a	830	CLA	C11-C10-C8-C9
14	b	827	CLA	C14-C13-C15-C16
14	b	828	CLA	C6-C7-C8-C9
14	b	831	CLA	C14-C13-C15-C16
14	H	820	CLA	CAA-CBA-CGA-O2A
14	H	827	CLA	C2A-CAA-CBA-CGA
14	a	818	CLA	C2A-CAA-CBA-CGA
14	b	806	CLA	C2A-CAA-CBA-CGA
14	B	817	CLA	C2-C1-O2A-CGA
14	G	807	CLA	C2-C1-O2A-CGA
14	G	814	CLA	C2-C1-O2A-CGA
14	G	831	CLA	C2-C1-O2A-CGA
14	a	806	CLA	C2-C1-O2A-CGA
14	a	818	CLA	C2-C1-O2A-CGA
14	a	830	CLA	C2-C1-O2A-CGA
14	b	839	CLA	C2-C1-O2A-CGA
14	A	830	CLA	C8-C10-C11-C12
14	A	817	CLA	C3A-C2A-CAA-CBA
14	A	818	CLA	C3A-C2A-CAA-CBA
14	B	801	CLA	C3A-C2A-CAA-CBA
14	B	804	CLA	C3A-C2A-CAA-CBA
14	B	821	CLA	C3A-C2A-CAA-CBA
14	G	829	CLA	C3A-C2A-CAA-CBA
14	G	839	CLA	C4-C3-C5-C6
14	H	801	CLA	C3A-C2A-CAA-CBA
14	H	837	CLA	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	a	827	CLA	C3A-C2A-CAA-CBA
14	a	840	CLA	C3A-C2A-CAA-CBA
14	b	816	CLA	C3A-C2A-CAA-CBA
14	b	832	CLA	C3A-C2A-CAA-CBA
14	b	836	CLA	C3A-C2A-CAA-CBA
14	A	823	CLA	CAA-CBA-CGA-O2A
14	B	829	CLA	CAA-CBA-CGA-O2A
14	B	835	CLA	CAA-CBA-CGA-O1A
14	F	1301	CLA	CAA-CBA-CGA-O2A
14	H	814	CLA	CAA-CBA-CGA-O2A
14	H	819	CLA	CAA-CBA-CGA-O2A
14	A	843	CLA	CAA-CBA-CGA-O2A
14	a	808	CLA	C2-C3-C5-C6
14	G	839	CLA	C10-C11-C12-C13
14	b	837	CLA	C3-C5-C6-C7
14	B	814	CLA	CAA-CBA-CGA-O1A
14	G	837	CLA	CAA-CBA-CGA-O2A
14	a	823	CLA	CAA-CBA-CGA-O1A
14	a	835	CLA	CAA-CBA-CGA-O2A
14	b	830	CLA	CAA-CBA-CGA-O2A
14	b	823	CLA	O2A-C1-C2-C3
14	A	837	CLA	CAA-CBA-CGA-O2A
14	H	814	CLA	CAA-CBA-CGA-O1A
14	H	833	CLA	CAA-CBA-CGA-O2A
14	a	855	CLA	C16-C17-C18-C20
14	A	836	CLA	CAA-CBA-CGA-O2A
14	B	834	CLA	CAA-CBA-CGA-O1A
14	T	1401	CLA	CAA-CBA-CGA-O1A
14	b	835	CLA	CAA-CBA-CGA-O1A
14	m	1601	CLA	CAA-CBA-CGA-O1A
14	G	812	CLA	C10-C11-C12-C13
14	A	805	CLA	C3-C5-C6-C7
18	G	854	LHG	C13-C14-C15-C16
14	G	826	CLA	C2-C3-C5-C6
14	a	813	CLA	C5-C6-C7-C8
17	G	853	BCR	C11-C10-C9-C8
17	b	844	BCR	C11-C10-C9-C8
14	a	835	CLA	CAA-CBA-CGA-O1A
14	a	830	CLA	C5-C6-C7-C8
14	a	855	CLA	C10-C11-C12-C13
14	B	802	CLA	CBA-CGA-O2A-C1
14	A	823	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	818	CLA	CAA-CBA-CGA-O1A
14	H	812	CLA	C8-C10-C11-C12
14	G	836	CLA	C2A-CAA-CBA-CGA
14	b	812	CLA	CAA-CBA-CGA-O2A
14	A	836	CLA	CAA-CBA-CGA-O1A
17	H	844	BCR	C13-C14-C15-C16
14	a	842	CLA	C13-C15-C16-C17
14	H	833	CLA	CAA-CBA-CGA-O1A
14	Q	201	CLA	CAA-CBA-CGA-O1A
14	B	826	CLA	C3-C5-C6-C7
14	A	837	CLA	CAA-CBA-CGA-O1A
14	F	1301	CLA	CAA-CBA-CGA-O1A
14	G	845	CLA	CAA-CBA-CGA-O1A
14	H	830	CLA	CAA-CBA-CGA-O1A
14	H	834	CLA	CAA-CBA-CGA-O1A
14	A	834	CLA	C13-C15-C16-C17
14	A	839	CLA	C11-C10-C8-C9
14	B	827	CLA	C14-C13-C15-C16
14	G	834	CLA	C11-C12-C13-C14
14	G	842	CLA	C14-C13-C15-C16
14	H	839	CLA	C6-C7-C8-C9
15	b	841	PQN	C21-C22-C23-C24
15	b	841	PQN	C24-C23-C25-C26
14	B	836	CLA	C11-C12-C13-C14
15	A	846	PQN	C26-C27-C28-C30
14	G	812	CLA	CAA-CBA-CGA-O2A
18	A	854	LHG	O8-C23-C24-C25
15	B	841	PQN	C13-C15-C16-C17
14	U	201	CLA	C13-C15-C16-C17
14	A	834	CLA	C4-C3-C5-C6
14	a	820	CLA	CAA-CBA-CGA-O2A
14	A	803	CLA	C2-C3-C5-C6
14	A	805	CLA	C2-C3-C5-C6
14	A	818	CLA	CAA-CBA-CGA-O1A
14	G	845	CLA	CAA-CBA-CGA-O2A
14	H	830	CLA	CAA-CBA-CGA-O2A
14	G	837	CLA	C2A-CAA-CBA-CGA
14	l	206	CLA	C2A-CAA-CBA-CGA
14	A	810	CLA	C11-C10-C8-C7
14	B	803	CLA	C11-C10-C8-C7
14	B	812	CLA	C6-C7-C8-C10
14	B	825	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	831	CLA	C11-C10-C8-C7
14	B	831	CLA	C12-C13-C15-C16
14	G	839	CLA	C11-C12-C13-C15
14	H	805	CLA	C12-C13-C15-C16
14	H	826	CLA	C11-C12-C13-C15
14	H	840	CLA	C11-C12-C13-C15
14	L	201	CLA	C11-C10-C8-C7
14	a	821	CLA	C12-C13-C15-C16
14	a	827	CLA	C6-C7-C8-C10
14	a	828	CLA	C11-C10-C8-C7
14	b	803	CLA	C11-C12-C13-C15
14	b	831	CLA	C12-C13-C15-C16
15	H	841	PQN	C17-C18-C20-C21
15	b	841	PQN	C21-C22-C23-C25
14	A	818	CLA	O1D-CGD-O2D-CED
17	A	853	BCR	C5-C6-C7-C8
17	B	847	BCR	C1-C6-C7-C8
17	B	848	BCR	C23-C24-C25-C26
17	B	848	BCR	C23-C24-C25-C30
17	B	850	BCR	C5-C6-C7-C8
17	H	846	BCR	C23-C24-C25-C26
17	J	102	BCR	C23-C24-C25-C30
17	S	103	BCR	C23-C24-C25-C26
17	a	852	BCR	C5-C6-C7-C8
17	b	847	BCR	C23-C24-C25-C26
17	l	208	BCR	C5-C6-C7-C8
13	A	801	CL0	CAA-CBA-CGA-O2A
14	b	802	CLA	CAA-CBA-CGA-O2A
14	A	827	CLA	C2-C1-O2A-CGA
14	B	832	CLA	C2-C1-O2A-CGA
14	a	802	CLA	C2-C1-O2A-CGA
14	b	836	CLA	C2-C1-O2A-CGA
14	H	829	CLA	CAA-CBA-CGA-O1A
14	b	818	CLA	CAA-CBA-CGA-O2A
19	b	848	LMG	O7-C10-C11-C12
14	a	817	CLA	CAA-CBA-CGA-O2A
13	G	801	CL0	CBA-CGA-O2A-C1
13	A	801	CL0	C3-C5-C6-C7
14	H	825	CLA	C3-C5-C6-C7
14	B	821	CLA	CAA-CBA-CGA-O2A
14	b	821	CLA	CAA-CBA-CGA-O2A
18	a	853	LHG	O7-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	B	849	LMG	O7-C10-C11-C12
14	A	834	CLA	C2-C3-C5-C6
14	B	813	CLA	C2-C3-C5-C6
14	G	840	CLA	CAA-CBA-CGA-O2A
14	A	841	CLA	C2A-CAA-CBA-CGA
14	U	204	CLA	C2A-CAA-CBA-CGA
14	V	1601	CLA	C2A-CAA-CBA-CGA
14	b	819	CLA	C2A-CAA-CBA-CGA
14	Q	203	CLA	CAA-CBA-CGA-O2A
18	A	854	LHG	C10-C11-C12-C13
14	b	831	CLA	CAA-CBA-CGA-O2A
14	l	207	CLA	C16-C17-C18-C20
14	H	811	CLA	CAA-CBA-CGA-O2A
14	b	830	CLA	CAA-CBA-CGA-O1A
14	B	807	CLA	CAA-CBA-CGA-O2A
14	a	811	CLA	CAA-CBA-CGA-O2A
14	a	827	CLA	CAA-CBA-CGA-O2A
14	B	813	CLA	C4-C3-C5-C6
17	G	848	BCR	C10-C11-C12-C13
14	A	812	CLA	CAA-CBA-CGA-O2A
14	a	838	CLA	CAA-CBA-CGA-O2A
14	G	837	CLA	CAA-CBA-CGA-O1A
14	a	841	CLA	CAA-CBA-CGA-O2A
14	B	811	CLA	CAA-CBA-CGA-O2A
14	H	837	CLA	CAA-CBA-CGA-O2A
19	B	849	LMG	C39-C40-C41-C42
14	a	806	CLA	CAA-CBA-CGA-O1A
14	A	839	CLA	C11-C12-C13-C14
14	B	839	CLA	C6-C7-C8-C9
14	G	802	CLA	C11-C10-C8-C9
14	H	801	CLA	C6-C7-C8-C9
14	H	805	CLA	C14-C13-C15-C16
14	H	812	CLA	C14-C13-C15-C16
14	a	827	CLA	C11-C10-C8-C9
14	b	802	CLA	C11-C12-C13-C14
14	B	831	CLA	CAA-CBA-CGA-O2A
13	A	801	CL0	C1A-C2A-CAA-CBA
14	A	823	CLA	C1A-C2A-CAA-CBA
14	G	815	CLA	C1A-C2A-CAA-CBA
14	G	823	CLA	C1A-C2A-CAA-CBA
14	H	801	CLA	C1A-C2A-CAA-CBA
14	Q	201	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	U	201	CLA	C1A-C2A-CAA-CBA
14	a	822	CLA	C1A-C2A-CAA-CBA
14	a	827	CLA	C1A-C2A-CAA-CBA
14	a	828	CLA	C1A-C2A-CAA-CBA
14	a	841	CLA	C1A-C2A-CAA-CBA
14	b	832	CLA	C1A-C2A-CAA-CBA
14	b	840	CLA	C1A-C2A-CAA-CBA
14	l	202	CLA	C1A-C2A-CAA-CBA
19	B	849	LMG	C16-C17-C18-C19
14	A	809	CLA	C4-C3-C5-C6
14	A	810	CLA	C4-C3-C5-C6
14	B	812	CLA	CAA-CBA-CGA-O2A
19	H	848	LMG	O7-C10-C11-C12
14	B	808	CLA	C2-C3-C5-C6
17	B	843	BCR	C21-C22-C23-C24
17	G	849	BCR	C11-C12-C13-C14
17	m	1602	BCR	C21-C22-C23-C24
17	L	207	BCR	C9-C10-C11-C12
17	b	844	BCR	C13-C14-C15-C16
17	f	201	BCR	C19-C20-C21-C22
14	H	816	CLA	C6-C7-C8-C9
14	A	844	CLA	CAA-CBA-CGA-O2A
14	H	812	CLA	CAA-CBA-CGA-O2A
14	a	828	CLA	C2A-CAA-CBA-CGA
14	A	807	CLA	C16-C17-C18-C19
14	a	804	CLA	C6-C7-C8-C9
14	B	840	CLA	CAA-CBA-CGA-O2A
14	H	821	CLA	CAA-CBA-CGA-O2A
14	b	837	CLA	CAA-CBA-CGA-O2A
18	G	854	LHG	C18-C19-C20-C21
14	Q	203	CLA	CAA-CBA-CGA-O1A
14	A	810	CLA	C5-C6-C7-C8
14	G	814	CLA	C8-C10-C11-C12
14	A	814	CLA	C2-C1-O2A-CGA
14	A	831	CLA	C2-C1-O2A-CGA
14	A	834	CLA	C2-C1-O2A-CGA
14	A	839	CLA	C2-C1-O2A-CGA
14	B	836	CLA	C2-C1-O2A-CGA
14	G	828	CLA	C2-C1-O2A-CGA
14	G	834	CLA	C2-C1-O2A-CGA
14	H	802	CLA	C2-C1-O2A-CGA
14	b	816	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	821	CLA	CAA-CBA-CGA-O2A
14	G	826	CLA	CAA-CBA-CGA-O2A
14	i	101	CLA	CAA-CBA-CGA-O2A
18	G	854	LHG	O7-C7-C8-C9
14	A	834	CLA	C12-C13-C15-C16
14	A	839	CLA	C11-C10-C8-C7
14	A	843	CLA	C11-C12-C13-C15
14	H	802	CLA	C6-C7-C8-C10
14	H	839	CLA	C12-C13-C15-C16
14	a	830	CLA	C11-C10-C8-C7
14	b	809	CLA	C6-C7-C8-C10
14	b	812	CLA	C11-C12-C13-C15
14	b	826	CLA	C6-C7-C8-C10
14	G	807	CLA	C16-C17-C18-C19
14	H	801	CLA	O2A-C1-C2-C3
14	H	823	CLA	O2A-C1-C2-C3
14	A	821	CLA	CAA-CBA-CGA-O2A
14	a	828	CLA	C3-C5-C6-C7
17	L	202	BCR	C19-C20-C21-C22
14	a	819	CLA	C2A-CAA-CBA-CGA
14	a	813	CLA	C8-C10-C11-C12
14	B	805	CLA	C16-C17-C18-C19
14	G	804	CLA	C6-C7-C8-C10
14	G	822	CLA	C16-C17-C18-C20
14	a	808	CLA	C16-C17-C18-C20
14	B	837	CLA	CAA-CBA-CGA-O2A
14	a	811	CLA	CAA-CBA-CGA-O1A
18	A	854	LHG	C13-C14-C15-C16
18	G	855	LHG	O10-C23-O8-C6
14	H	831	CLA	CBA-CGA-O2A-C1
18	a	853	LHG	C26-C27-C28-C29
14	a	855	CLA	C3A-C2A-CAA-CBA
14	b	835	CLA	C3A-C2A-CAA-CBA
14	B	812	CLA	CAA-CBA-CGA-O1A
14	a	820	CLA	CAA-CBA-CGA-O1A
14	A	803	CLA	C10-C11-C12-C13
14	L	201	CLA	C16-C17-C18-C20
14	H	811	CLA	CAA-CBA-CGA-O1A
14	a	817	CLA	CAA-CBA-CGA-O1A
14	b	802	CLA	CAA-CBA-CGA-O1A
18	a	853	LHG	O9-C7-C8-C9
14	b	829	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	821	CLA	CAA-CBA-CGA-O1A
14	a	827	CLA	CAA-CBA-CGA-O1A
14	G	828	CLA	C15-C16-C17-C18
14	B	812	CLA	C16-C17-C18-C19
14	A	811	CLA	C2A-CAA-CBA-CGA
14	B	817	CLA	C2A-CAA-CBA-CGA
14	H	829	CLA	CAA-CBA-CGA-O2A
14	B	803	CLA	C11-C10-C8-C9
14	B	812	CLA	C6-C7-C8-C9
14	G	807	CLA	C11-C12-C13-C14
14	G	810	CLA	C6-C7-C8-C9
14	G	812	CLA	C11-C12-C13-C14
18	A	854	LHG	C24-C25-C26-C27
14	G	812	CLA	CAA-CBA-CGA-O1A
14	b	818	CLA	CAA-CBA-CGA-O1A
14	b	821	CLA	CAA-CBA-CGA-O1A
17	B	846	BCR	C13-C14-C15-C16
14	B	811	CLA	CAA-CBA-CGA-O1A
14	H	803	CLA	C16-C17-C18-C20
14	B	805	CLA	C13-C15-C16-C17
14	B	839	CLA	C5-C6-C7-C8
14	H	837	CLA	C5-C6-C7-C8
19	B	849	LMG	O9-C10-C11-C12
14	b	807	CLA	C2-C3-C5-C6
14	b	812	CLA	CAA-CBA-CGA-O1A
14	i	101	CLA	CAA-CBA-CGA-O1A
19	H	848	LMG	O9-C10-C11-C12
19	b	848	LMG	O9-C10-C11-C12
14	G	823	CLA	CAA-CBA-CGA-O2A
14	a	841	CLA	CAA-CBA-CGA-O1A
14	A	831	CLA	C5-C6-C7-C8
14	H	809	CLA	C15-C16-C17-C18
17	G	853	BCR	C17-C18-C19-C20
14	A	821	CLA	CAA-CBA-CGA-O1A
14	B	807	CLA	CAA-CBA-CGA-O1A
14	G	821	CLA	CAA-CBA-CGA-O1A
14	H	821	CLA	CAA-CBA-CGA-O1A
14	b	831	CLA	CAA-CBA-CGA-O1A
14	G	826	CLA	CAA-CBA-CGA-O1A
14	H	837	CLA	CAA-CBA-CGA-O1A
18	A	854	LHG	O10-C23-C24-C25
14	H	831	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	B	807	CLA	O1D-CGD-O2D-CED
13	A	801	CL0	C16-C17-C18-C20
14	a	824	CLA	C6-C7-C8-C10
18	G	854	LHG	O9-C7-C8-C9
14	A	825	CLA	C4-C3-C5-C6
14	l	205	CLA	C8-C10-C11-C12
14	B	809	CLA	C2-C3-C5-C6
14	a	826	CLA	C2-C3-C5-C6
14	G	829	CLA	C3-C5-C6-C7
14	a	822	CLA	CAA-CBA-CGA-O2A
14	A	812	CLA	CAA-CBA-CGA-O1A
14	a	838	CLA	CAA-CBA-CGA-O1A
14	L	205	CLA	C16-C17-C18-C19
14	a	822	CLA	CAD-CBD-CGD-O2D
14	H	813	CLA	C2C-C3C-CAC-CBC
14	G	827	CLA	C8-C10-C11-C12
14	b	840	CLA	CAA-CBA-CGA-O2A
14	b	831	CLA	C15-C16-C17-C18
14	A	807	CLA	C2-C1-O2A-CGA
14	G	812	CLA	C2-C1-O2A-CGA
14	H	801	CLA	C2-C1-O2A-CGA
14	a	855	CLA	C2-C1-O2A-CGA
14	b	809	CLA	C2-C1-O2A-CGA
14	G	843	CLA	CAA-CBA-CGA-O2A
14	H	816	CLA	CAA-CBA-CGA-O2A
14	A	841	CLA	C16-C17-C18-C19
14	b	812	CLA	C16-C17-C18-C19
14	l	206	CLA	C16-C17-C18-C20
14	B	805	CLA	C2A-CAA-CBA-CGA
14	G	811	CLA	CAA-CBA-CGA-O2A
14	G	830	CLA	CBD-CGD-O2D-CED
14	A	844	CLA	CAA-CBA-CGA-O1A
14	H	812	CLA	CAA-CBA-CGA-O1A
14	b	837	CLA	CAA-CBA-CGA-O1A
14	A	826	CLA	C5-C6-C7-C8
13	G	801	CL0	CAA-CBA-CGA-O2A
14	A	826	CLA	CAA-CBA-CGA-O2A
14	B	825	CLA	CAA-CBA-CGA-O2A
14	H	808	CLA	CAA-CBA-CGA-O2A
14	L	201	CLA	CAA-CBA-CGA-O2A
18	A	854	LHG	O7-C7-C8-C9
14	b	806	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	G	825	CLA	O1A-CGA-O2A-C1
14	H	807	CLA	CAA-CBA-CGA-O2A
14	b	803	CLA	CAA-CBA-CGA-O2A
14	b	808	CLA	C5-C6-C7-C8

There are no ring outliers.

344 monomers are involved in 973 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	S	104	BCR	7	0
14	a	812	CLA	1	0
14	U	204	CLA	3	0
14	B	823	CLA	3	0
14	b	804	CLA	7	0
17	b	847	BCR	9	0
14	j	101	CLA	1	0
14	a	822	CLA	1	0
14	H	817	CLA	5	0
17	B	842	BCR	1	0
14	b	821	CLA	3	0
14	A	820	CLA	10	0
14	A	807	CLA	3	0
17	b	846	BCR	3	0
19	H	848	LMG	2	0
14	X	1701	CLA	1	0
14	G	820	CLA	6	0
14	H	840	CLA	3	0
14	U	201	CLA	6	0
15	B	841	PQN	4	0
14	b	817	CLA	4	0
17	B	846	BCR	2	0
14	H	832	CLA	4	0
14	H	828	CLA	3	0
14	H	830	CLA	2	0
14	Q	203	CLA	3	0
18	A	855	LHG	1	0
14	b	818	CLA	2	0
14	a	825	CLA	5	0
14	m	1601	CLA	3	0
14	b	807	CLA	4	0
14	a	827	CLA	6	0
14	H	808	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	839	CLA	6	0
14	A	837	CLA	2	0
17	R	102	BCR	3	0
14	b	824	CLA	4	0
14	G	810	CLA	2	0
14	a	802	CLA	3	0
14	G	813	CLA	1	0
14	b	806	CLA	8	0
14	j	102	CLA	1	0
14	B	806	CLA	4	0
14	b	836	CLA	3	0
14	A	804	CLA	2	0
14	b	829	CLA	5	0
14	a	833	CLA	7	0
15	A	846	PQN	7	0
14	a	834	CLA	2	0
14	L	205	CLA	6	0
14	H	833	CLA	3	0
14	G	804	CLA	1	0
18	a	853	LHG	1	0
14	G	841	CLA	5	0
14	B	834	CLA	3	0
17	M	1602	BCR	2	0
17	a	849	BCR	3	0
14	G	827	CLA	2	0
17	b	844	BCR	2	0
14	B	815	CLA	4	0
14	G	821	CLA	1	0
14	A	805	CLA	1	0
14	b	815	CLA	2	0
14	a	809	CLA	3	0
14	B	831	CLA	4	0
14	G	809	CLA	4	0
14	G	843	CLA	6	0
14	b	805	CLA	1	0
14	a	855	CLA	7	0
14	a	838	CLA	4	0
14	a	824	CLA	3	0
14	A	839	CLA	2	0
17	B	847	BCR	7	0
17	V	1602	BCR	3	0
14	B	804	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	822	CLA	2	0
19	b	848	LMG	2	0
14	A	810	CLA	7	0
14	G	822	CLA	6	0
14	a	810	CLA	1	0
14	a	826	CLA	4	0
17	G	851	BCR	2	0
14	G	803	CLA	2	0
17	a	851	BCR	4	0
14	a	807	CLA	1	0
14	A	823	CLA	1	0
14	A	825	CLA	6	0
14	A	841	CLA	4	0
14	H	823	CLA	5	0
14	H	825	CLA	3	0
14	b	839	CLA	5	0
14	a	811	CLA	5	0
14	B	818	CLA	2	0
14	B	835	CLA	2	0
14	G	807	CLA	3	0
17	G	853	BCR	4	0
14	A	815	CLA	4	0
14	T	1401	CLA	1	0
14	G	811	CLA	1	0
15	a	845	PQN	4	0
14	A	835	CLA	2	0
14	M	1601	CLA	1	0
14	H	805	CLA	6	0
15	G	846	PQN	6	0
14	H	804	CLA	1	0
14	a	816	CLA	1	0
14	G	802	CLA	6	0
15	H	841	PQN	3	0
14	B	830	CLA	3	0
14	a	832	CLA	2	0
17	R	103	BCR	2	0
14	F	1301	CLA	1	0
14	H	802	CLA	3	0
14	B	816	CLA	3	0
14	b	823	CLA	7	0
14	B	813	CLA	4	0
14	l	202	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	812	CLA	4	0
17	L	207	BCR	5	0
17	B	844	BCR	4	0
14	a	839	CLA	2	0
14	A	829	CLA	10	0
17	G	850	BCR	2	0
14	B	828	CLA	7	0
14	H	835	CLA	2	0
14	U	206	CLA	6	0
14	G	839	CLA	1	0
14	b	838	CLA	5	0
14	G	829	CLA	11	0
14	B	829	CLA	6	0
14	A	834	CLA	2	0
17	A	851	BCR	5	0
17	l	208	BCR	3	0
14	G	838	CLA	4	0
17	b	849	BCR	3	0
14	H	836	CLA	2	0
17	H	842	BCR	3	0
14	G	825	CLA	4	0
14	B	821	CLA	4	0
14	H	806	CLA	5	0
14	l	205	CLA	4	0
14	a	814	CLA	3	0
14	G	836	CLA	4	0
14	A	813	CLA	1	0
14	H	827	CLA	9	0
14	H	813	CLA	1	0
14	b	835	CLA	2	0
14	A	811	CLA	1	0
14	G	826	CLA	4	0
14	H	811	CLA	2	0
17	J	103	BCR	3	0
14	G	828	CLA	5	0
14	A	838	CLA	1	0
14	a	842	CLA	10	0
17	b	843	BCR	2	0
14	b	813	CLA	1	0
14	a	815	CLA	1	0
14	B	802	CLA	5	0
14	a	821	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	829	CLA	10	0
14	W	1701	CLA	1	0
17	G	848	BCR	2	0
14	B	840	CLA	5	0
14	A	803	CLA	4	0
14	B	825	CLA	1	0
14	A	826	CLA	7	0
14	b	831	CLA	11	0
14	G	815	CLA	1	0
17	f	203	BCR	5	0
15	b	841	PQN	4	0
17	A	850	BCR	3	0
17	j	103	BCR	5	0
14	a	844	CLA	3	0
17	H	847	BCR	7	0
14	a	837	CLA	2	0
14	G	833	CLA	1	0
14	a	835	CLA	3	0
17	I	101	BCR	7	0
14	b	834	CLA	5	0
14	B	820	CLA	1	0
14	a	804	CLA	1	0
14	a	806	CLA	2	0
17	F	1302	BCR	3	0
14	H	820	CLA	2	0
14	H	839	CLA	6	0
14	G	814	CLA	4	0
14	A	832	CLA	3	0
14	a	828	CLA	12	0
17	l	203	BCR	2	0
14	b	826	CLA	6	0
14	A	827	CLA	6	0
17	a	850	BCR	6	0
14	V	1601	CLA	1	0
14	G	806	CLA	2	0
14	G	845	CLA	3	0
17	B	850	BCR	4	0
14	G	832	CLA	3	0
14	b	833	CLA	1	0
14	A	809	CLA	4	0
14	a	817	CLA	1	0
14	B	832	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	834	CLA	5	0
14	b	814	CLA	2	0
14	A	843	CLA	10	0
14	A	828	CLA	4	0
14	B	826	CLA	8	0
16	c	102	SF4	1	0
17	S	103	BCR	5	0
17	H	843	BCR	3	0
14	A	817	CLA	1	0
14	f	202	CLA	2	0
18	G	855	LHG	2	0
17	A	848	BCR	2	0
14	A	844	CLA	4	0
14	b	816	CLA	4	0
14	b	809	CLA	7	0
14	B	838	CLA	5	0
14	H	815	CLA	3	0
14	G	819	CLA	5	0
14	L	204	CLA	3	0
14	b	803	CLA	4	0
17	L	202	BCR	1	0
14	i	101	CLA	7	0
17	G	849	BCR	2	0
14	a	836	CLA	2	0
14	b	840	CLA	4	0
14	a	829	CLA	3	0
17	l	201	BCR	1	0
17	A	852	BCR	4	0
14	A	821	CLA	1	0
17	a	852	BCR	6	0
17	B	848	BCR	8	0
14	H	838	CLA	4	0
14	b	825	CLA	3	0
14	B	836	CLA	5	0
14	G	805	CLA	4	0
14	l	206	CLA	7	0
14	H	809	CLA	2	0
14	G	824	CLA	1	0
14	H	824	CLA	2	0
14	b	828	CLA	1	0
14	B	811	CLA	1	0
14	b	830	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	806	CLA	3	0
17	A	853	BCR	4	0
14	A	822	CLA	5	0
14	b	837	CLA	3	0
14	H	826	CLA	6	0
18	G	854	LHG	4	0
14	G	808	CLA	1	0
14	a	803	CLA	2	0
13	A	801	CL0	3	0
14	A	840	CLA	2	0
17	Q	202	BCR	3	0
17	R	101	BCR	5	0
13	a	801	CL0	5	0
14	B	809	CLA	3	0
17	j	104	BCR	6	0
17	J	102	BCR	4	0
14	J	101	CLA	1	0
14	a	819	CLA	4	0
14	A	808	CLA	1	0
14	A	831	CLA	7	0
14	a	831	CLA	2	0
14	G	812	CLA	4	0
14	H	812	CLA	6	0
19	B	849	LMG	3	0
14	G	816	CLA	3	0
14	H	807	CLA	5	0
17	b	842	BCR	2	0
14	B	822	CLA	4	0
17	H	844	BCR	3	0
14	a	820	CLA	2	0
14	U	205	CLA	2	0
14	b	819	CLA	2	0
14	b	832	CLA	5	0
17	m	1602	BCR	4	0
14	H	801	CLA	7	0
14	b	808	CLA	6	0
14	L	206	CLA	6	0
17	a	848	BCR	3	0
14	G	830	CLA	2	0
18	A	854	LHG	5	0
14	b	811	CLA	3	0
17	b	845	BCR	5	0

Continued on next page...

Continued from previous page...

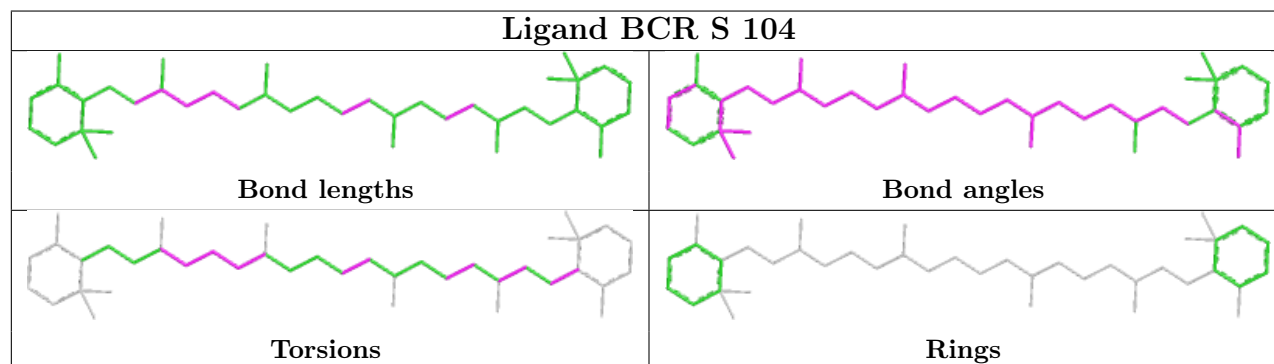
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	G	852	BCR	3	0
17	i	102	BCR	6	0
14	b	801	CLA	6	0
14	B	808	CLA	2	0
14	A	814	CLA	4	0
14	B	837	CLA	3	0
17	B	845	BCR	3	0
14	A	830	CLA	4	0
14	x	1701	CLA	1	0
14	A	819	CLA	3	0
14	a	830	CLA	4	0
14	H	819	CLA	2	0
17	U	202	BCR	3	0
14	B	801	CLA	7	0
17	H	849	BCR	3	0
14	G	831	CLA	7	0
14	A	802	CLA	7	0
14	H	816	CLA	7	0
14	G	817	CLA	1	0
17	I	102	BCR	2	0
14	H	803	CLA	9	0
14	a	818	CLA	2	0
14	A	842	CLA	1	0
14	B	805	CLA	5	0
14	G	842	CLA	9	0
14	b	812	CLA	6	0
14	l	207	CLA	4	0
13	G	801	CL0	6	0
14	a	840	CLA	7	0
17	H	845	BCR	2	0
14	B	803	CLA	7	0
14	G	834	CLA	1	0
16	G	847	SF4	1	0
14	H	814	CLA	1	0
14	A	836	CLA	2	0
14	b	822	CLA	5	0
14	A	833	CLA	1	0
17	A	849	BCR	3	0
14	B	817	CLA	5	0
14	L	201	CLA	4	0
14	B	824	CLA	3	0
14	a	805	CLA	2	0

Continued on next page...

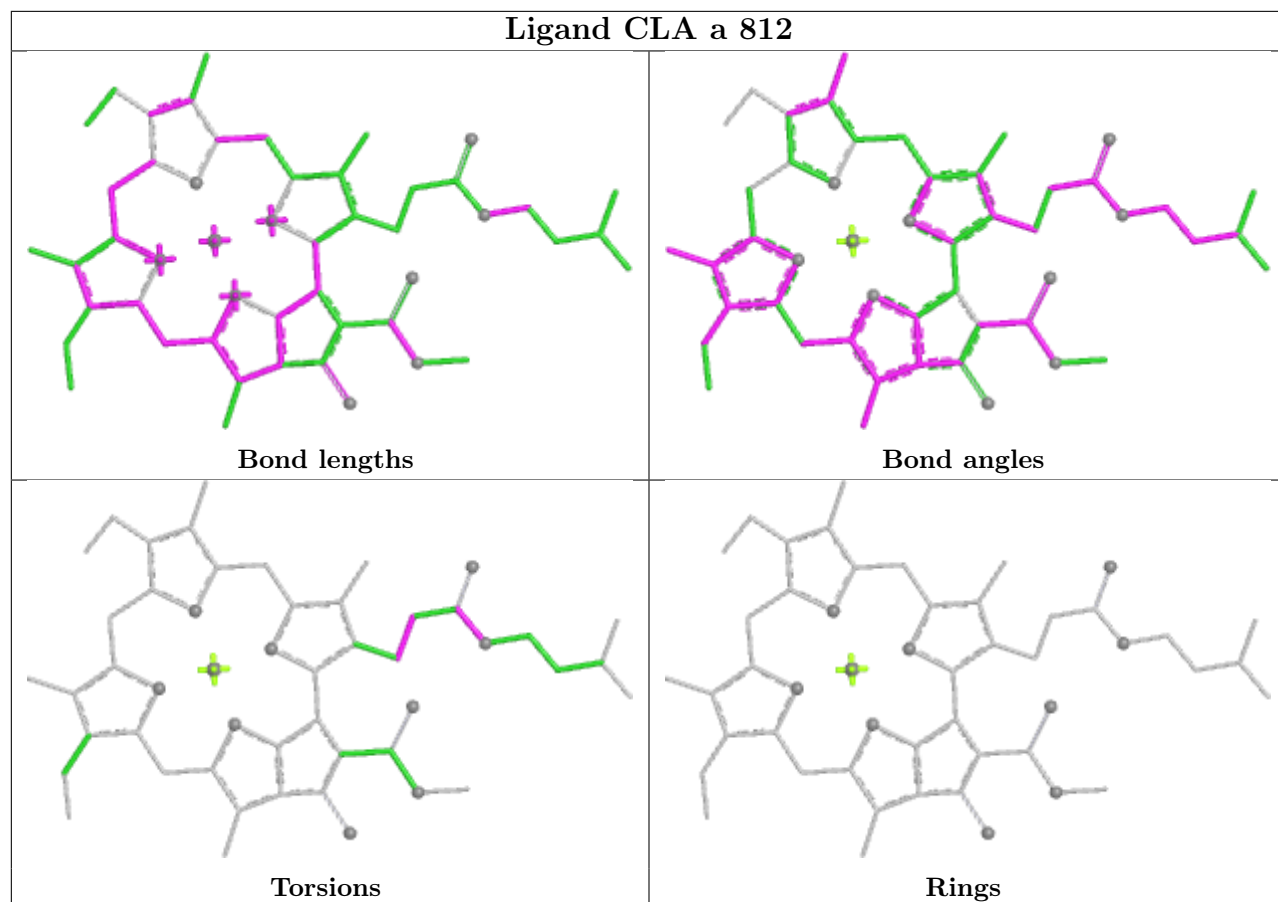
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	802	CLA	5	0
14	H	831	CLA	1	0
17	f	201	BCR	5	0
14	a	808	CLA	5	0
14	H	837	CLA	3	0
14	B	814	CLA	1	0
14	B	819	CLA	2	0
14	A	845	CLA	4	0
14	a	813	CLA	8	0
14	G	835	CLA	1	0
14	b	827	CLA	5	0
14	H	821	CLA	3	0
14	B	812	CLA	5	0
14	B	827	CLA	8	0
17	H	846	BCR	4	0
17	Q	204	BCR	4	0
14	B	807	CLA	2	0

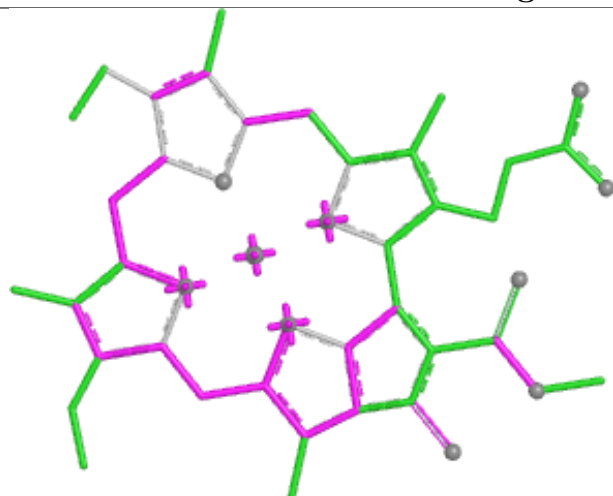
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



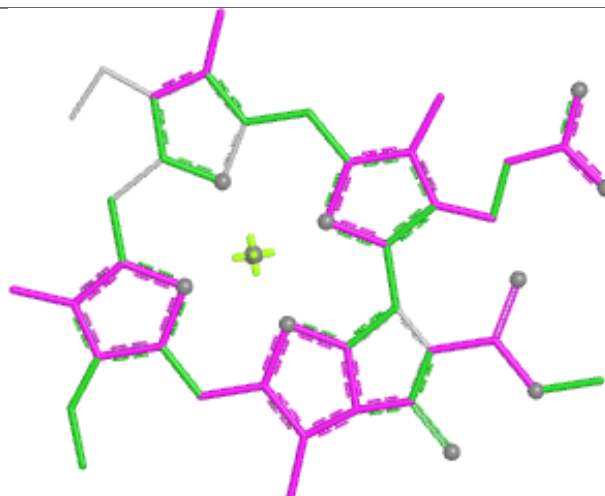
Ligand CLA a 812



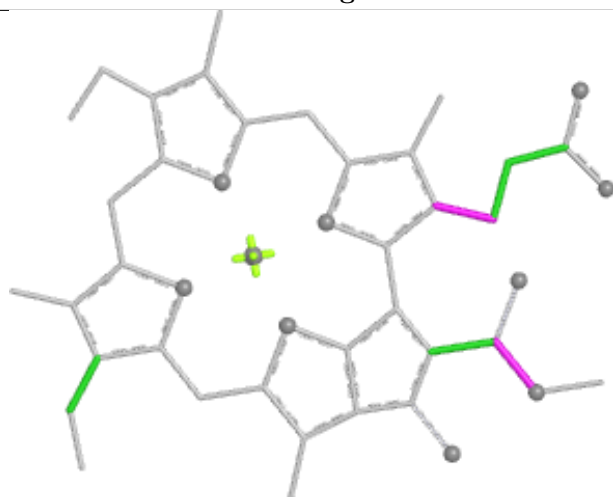
Ligand CLA b 810



Bond lengths



Bond angles

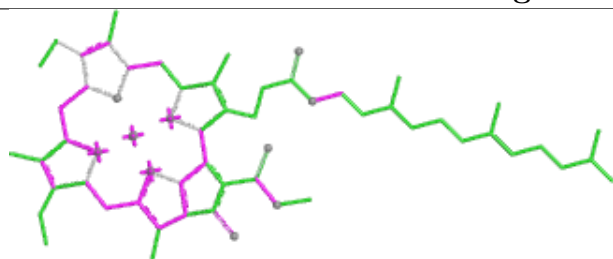


Torsions

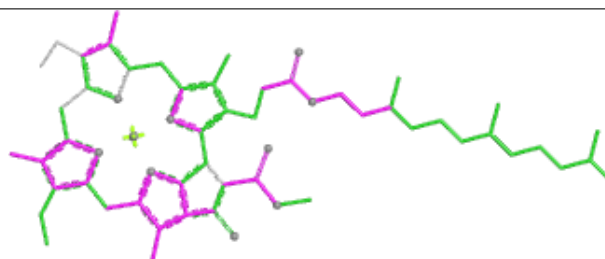


Rings

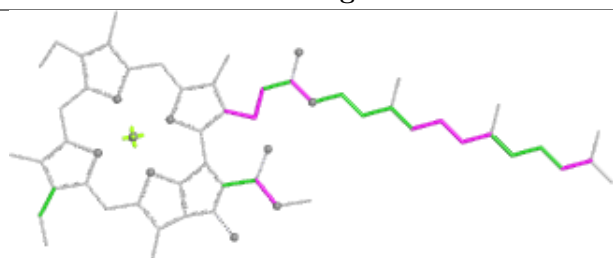
Ligand CLA U 204



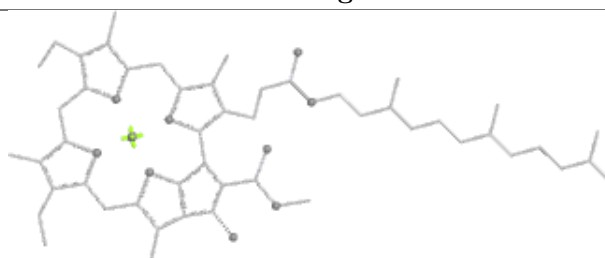
Bond lengths



Bond angles

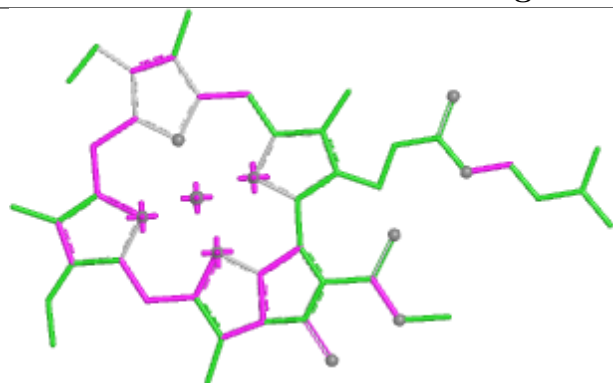


Torsions

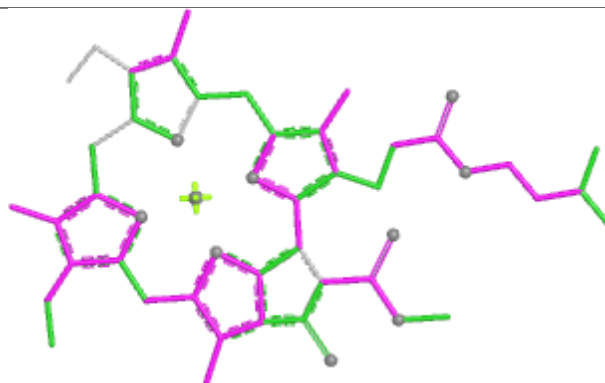


Rings

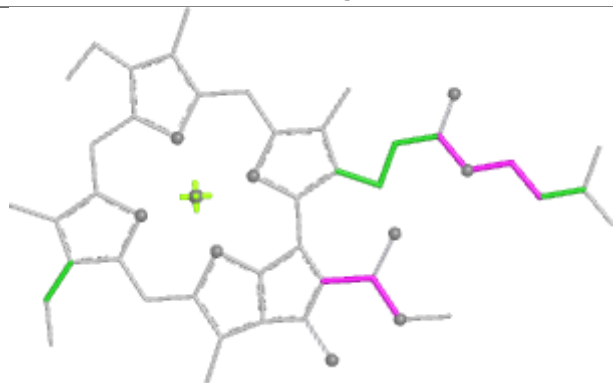
Ligand CLA B 823



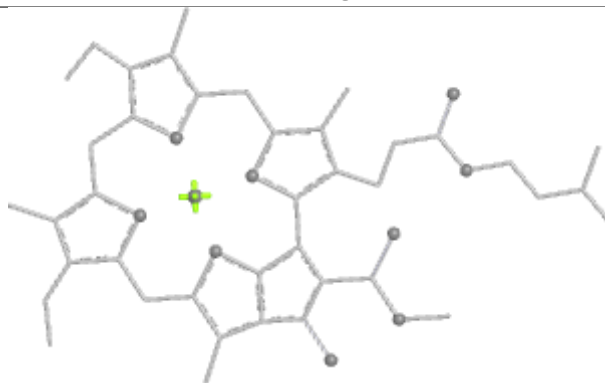
Bond lengths



Bond angles

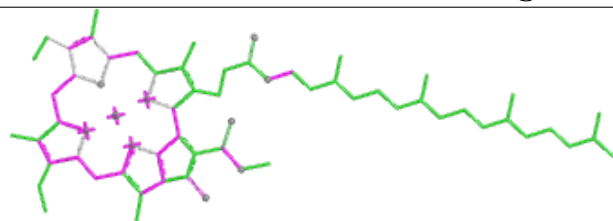


Torsions

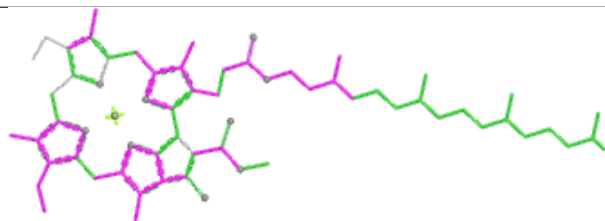


Rings

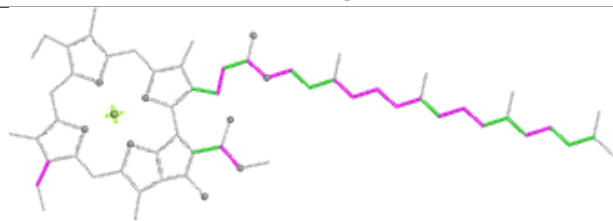
Ligand CLA b 804



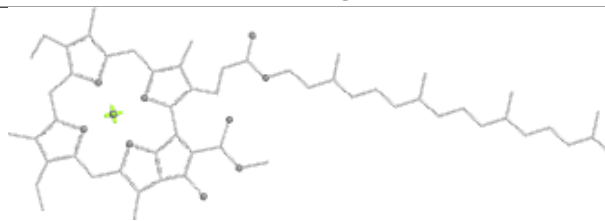
Bond lengths



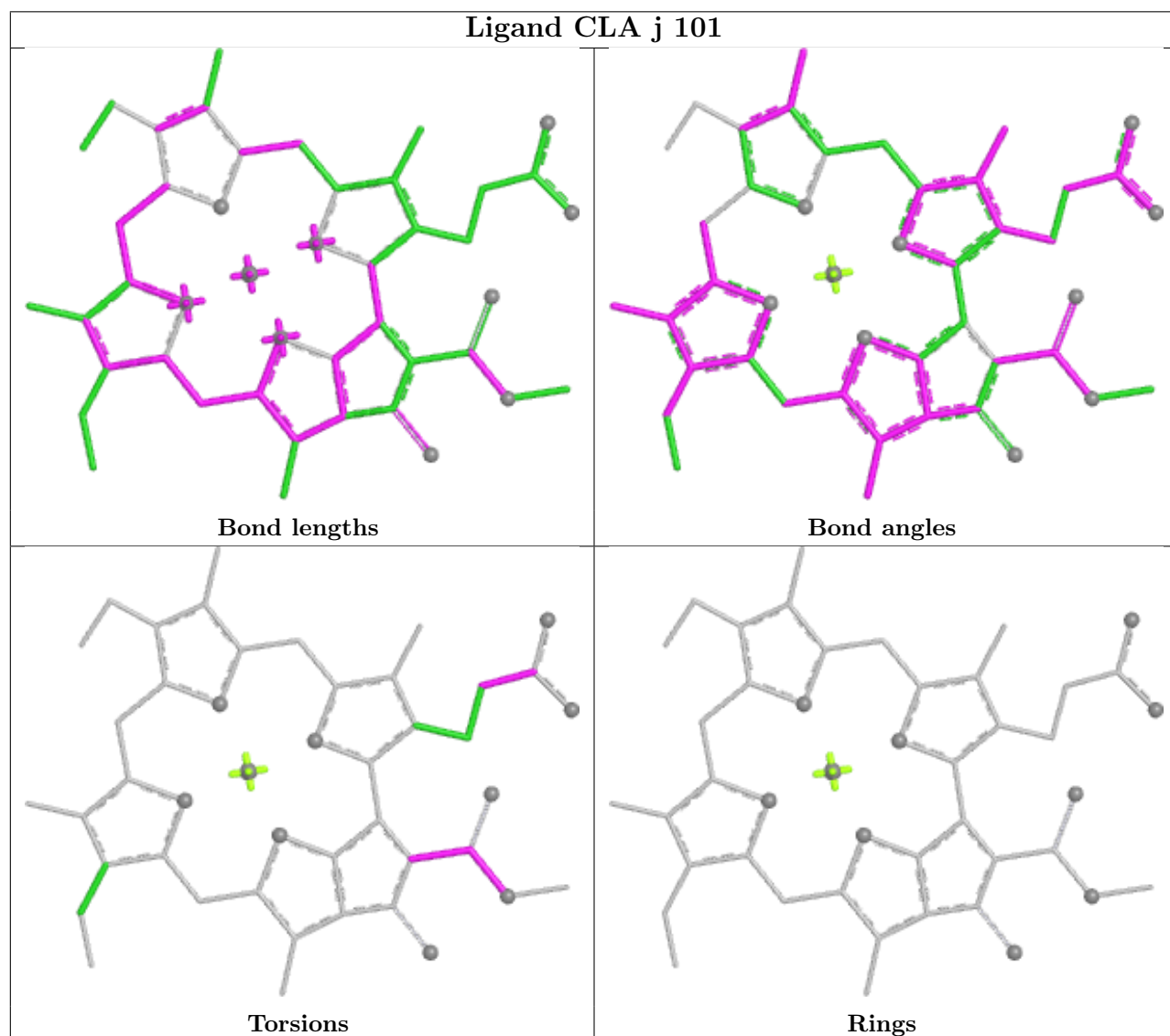
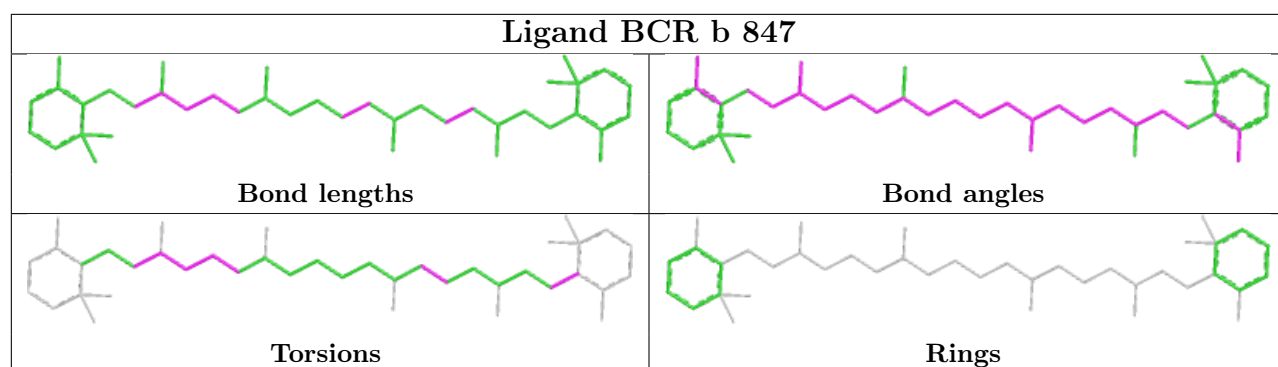
Bond angles



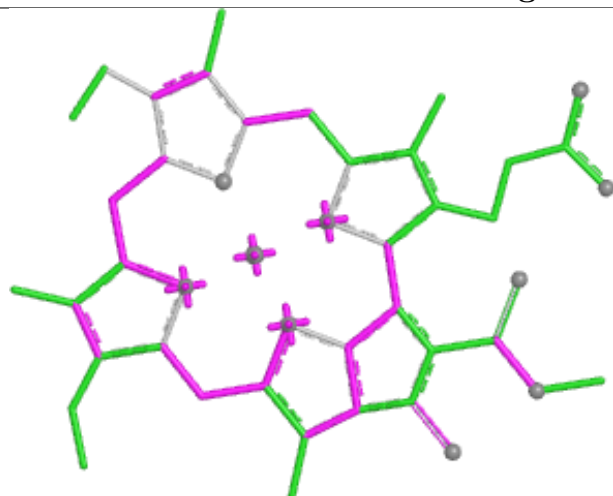
Torsions



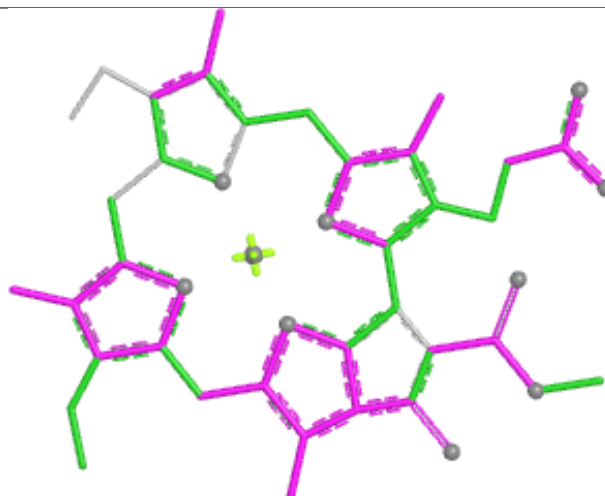
Rings



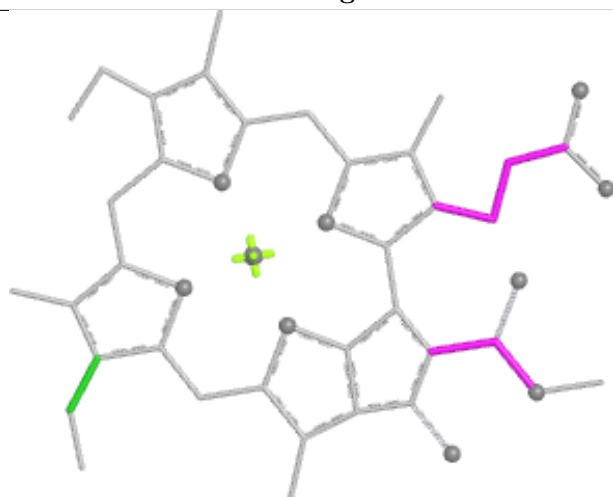
Ligand CLA a 822



Bond lengths



Bond angles

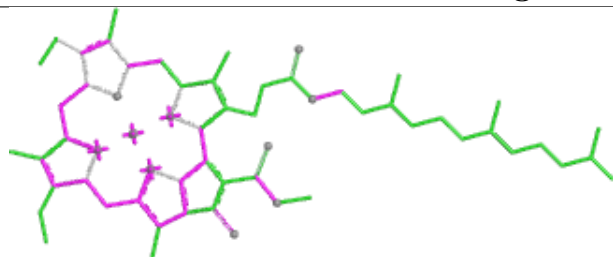


Torsions

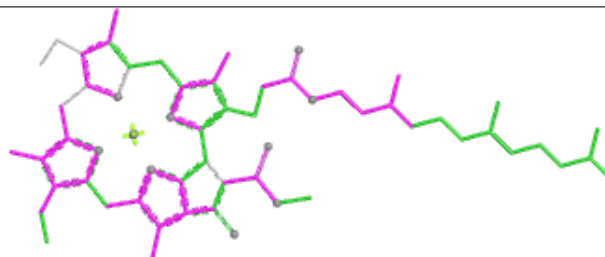


Rings

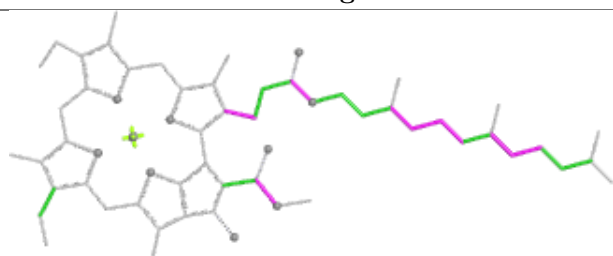
Ligand CLA H 817



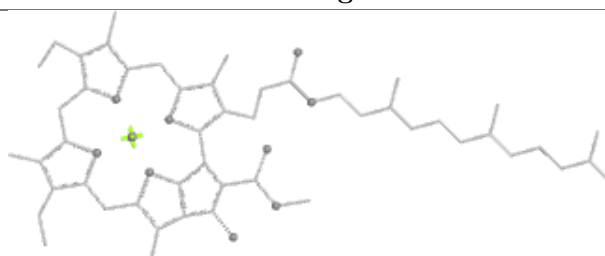
Bond lengths



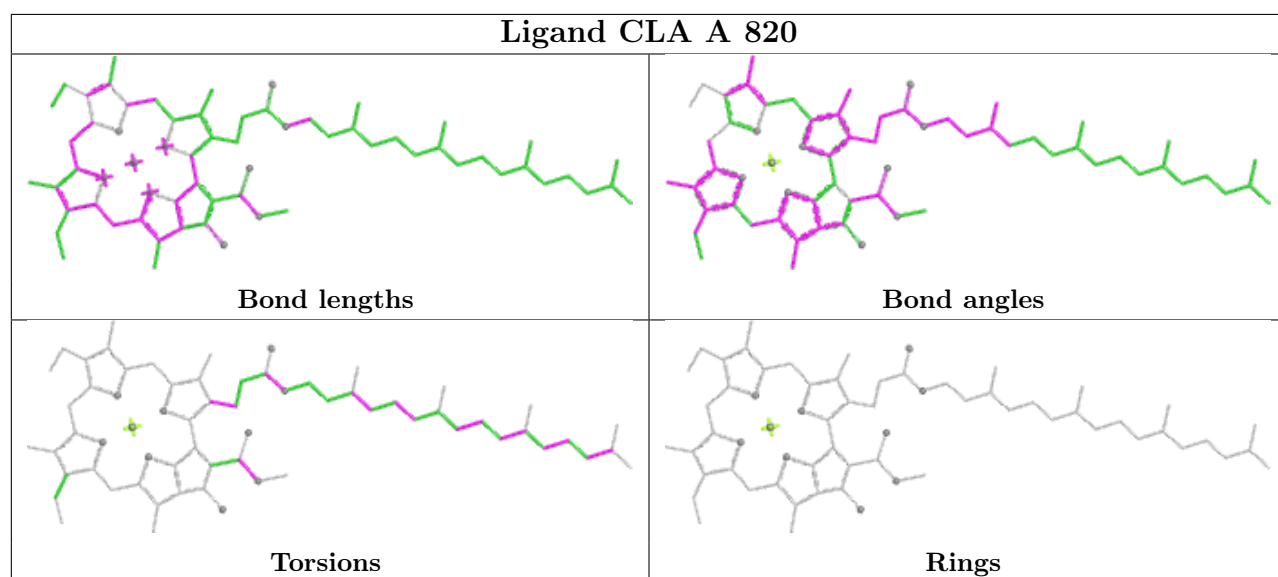
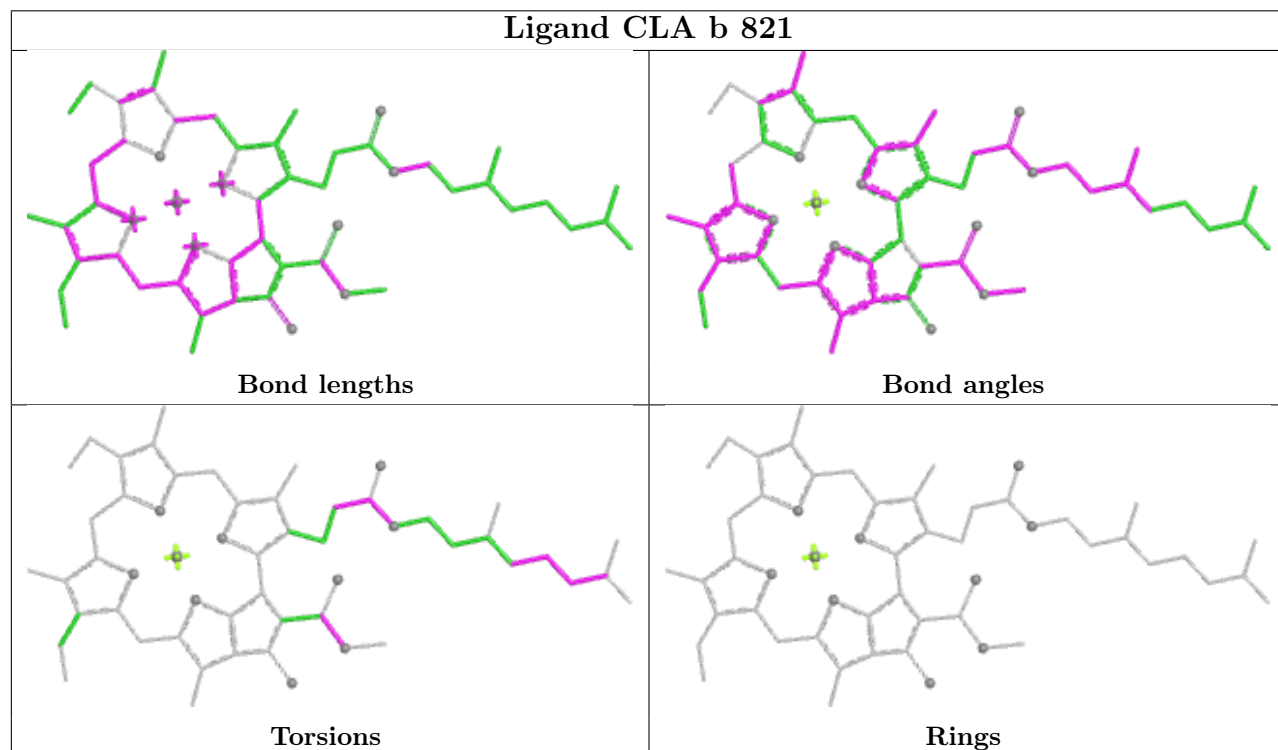
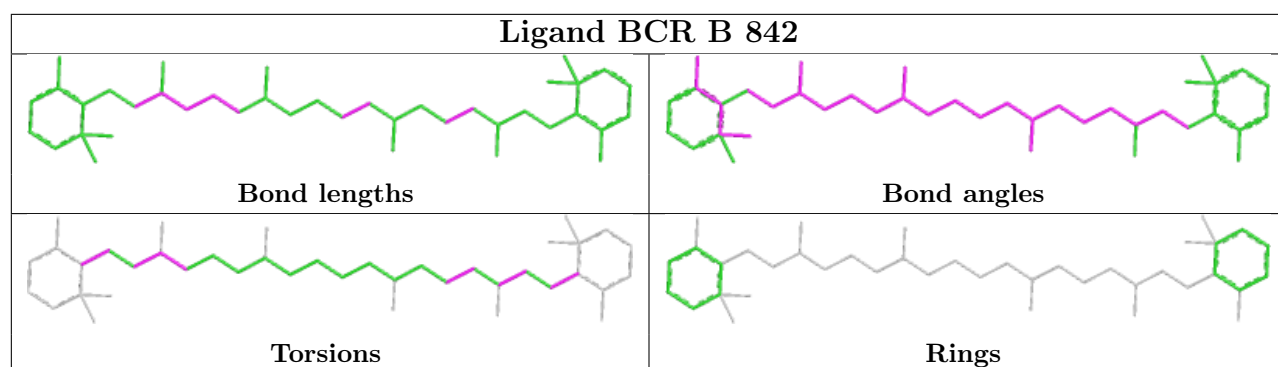
Bond angles

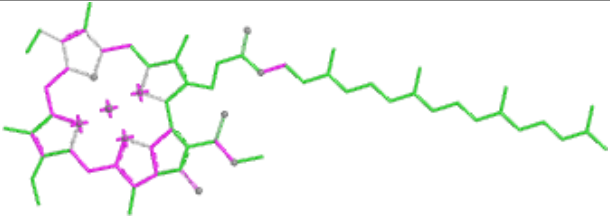
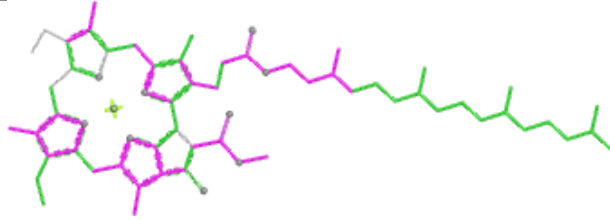
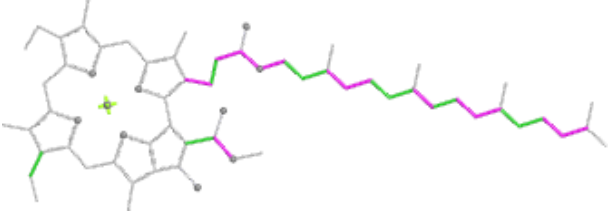
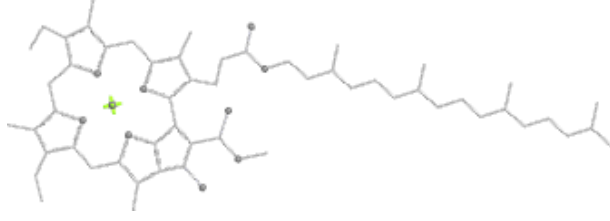
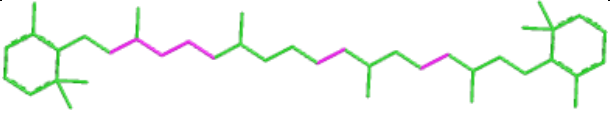
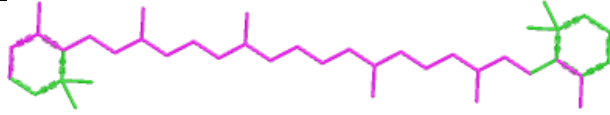
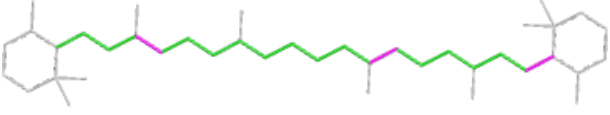
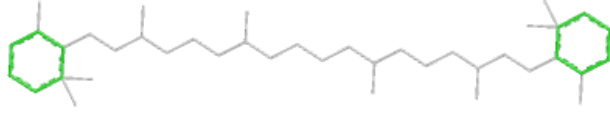
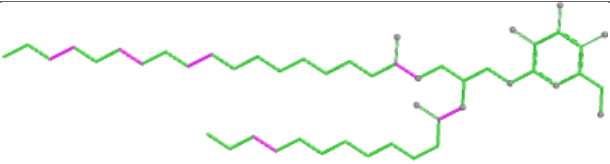
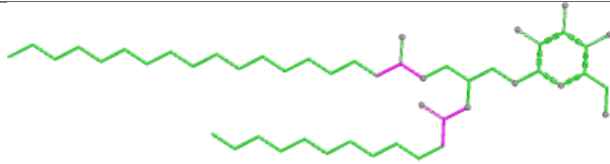
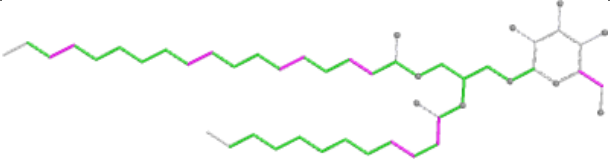



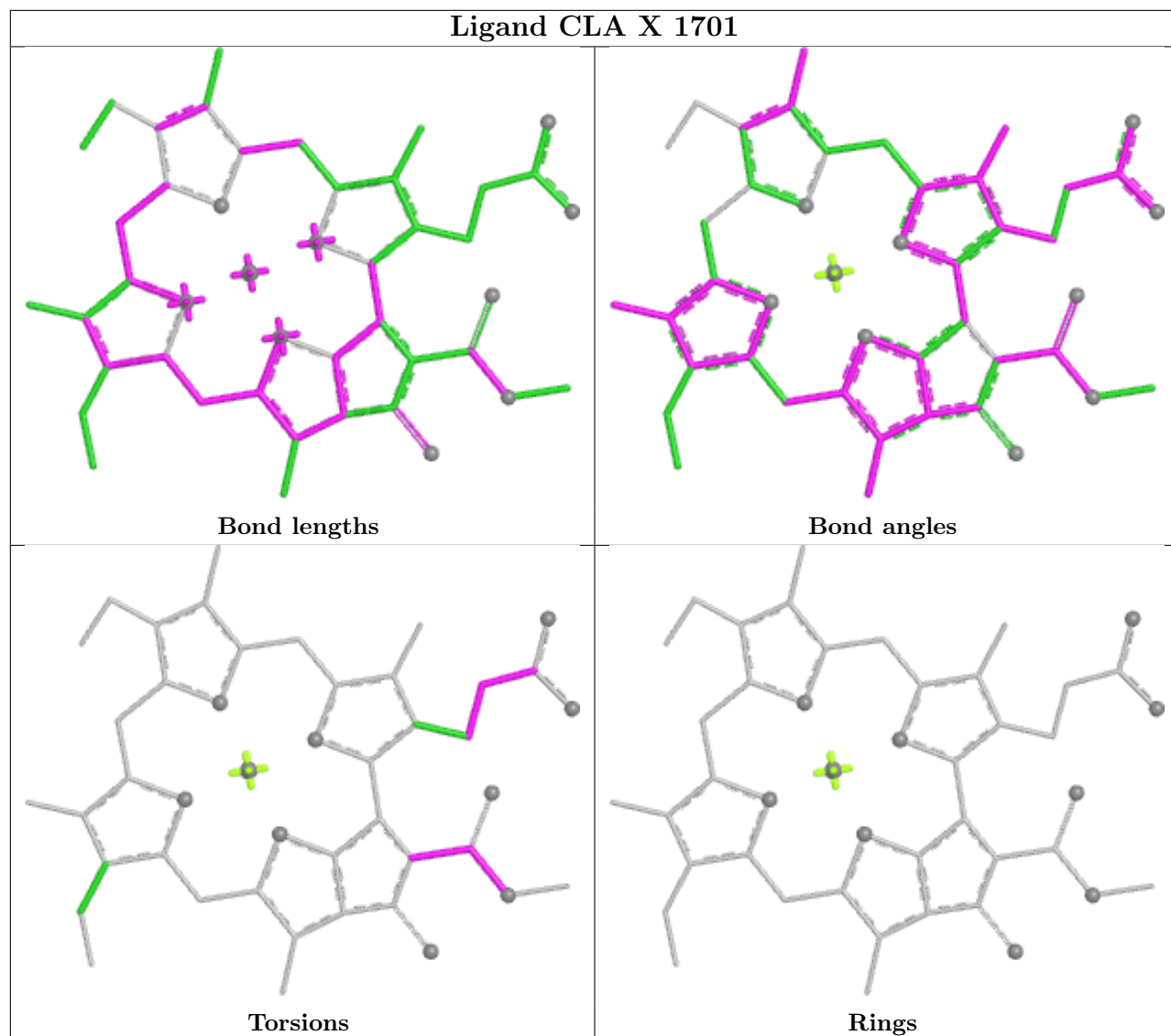
Torsions

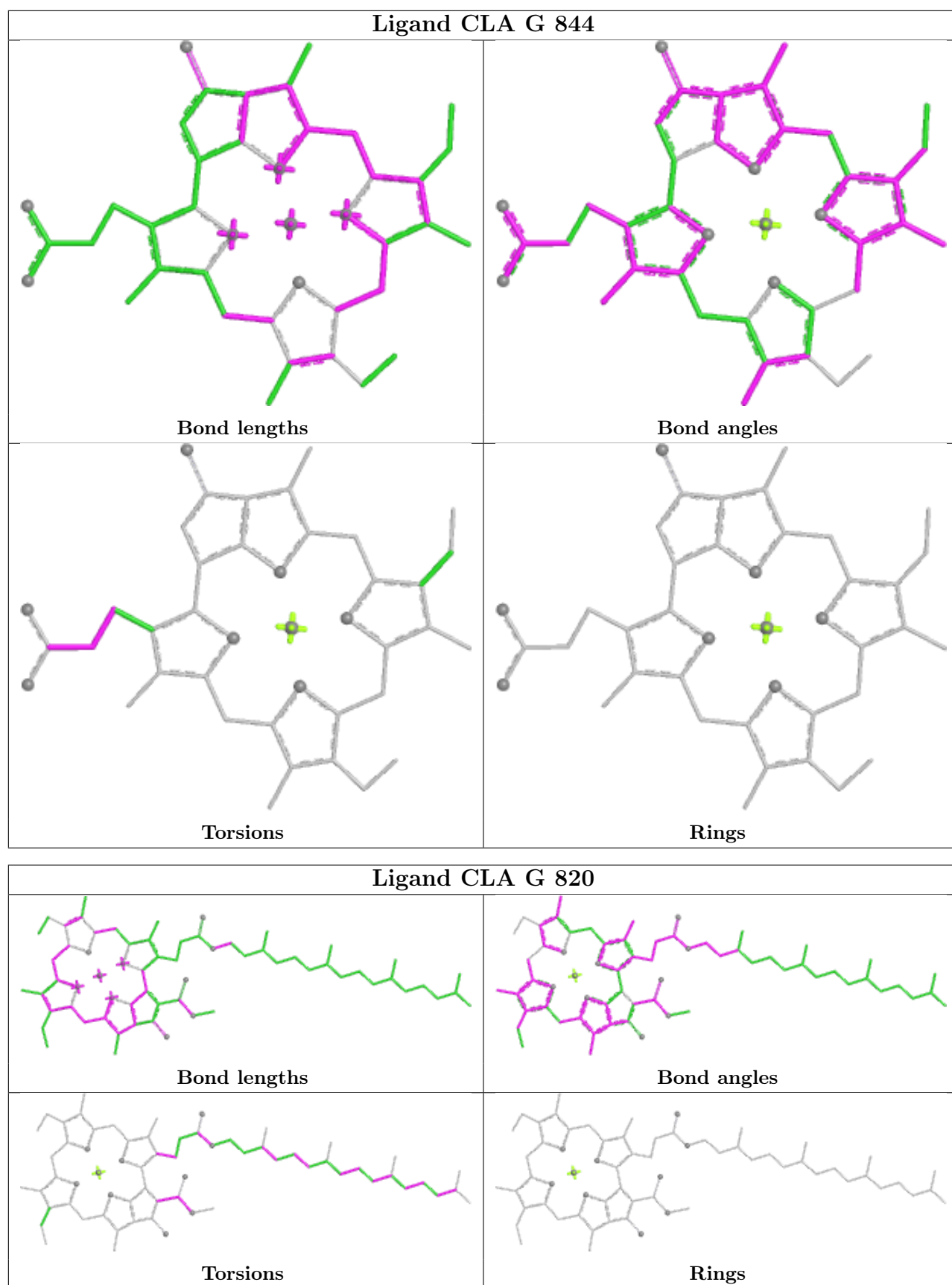


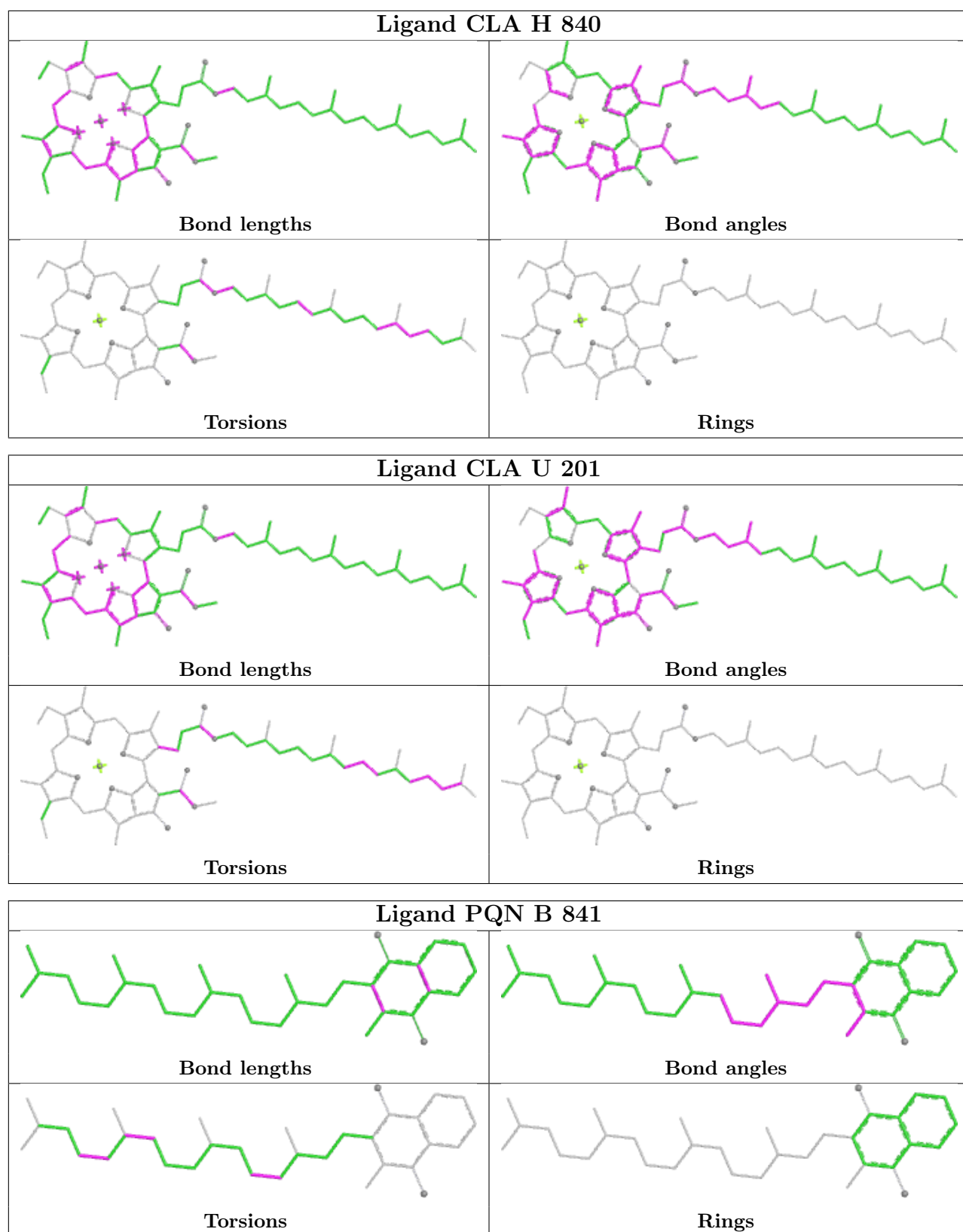
Rings

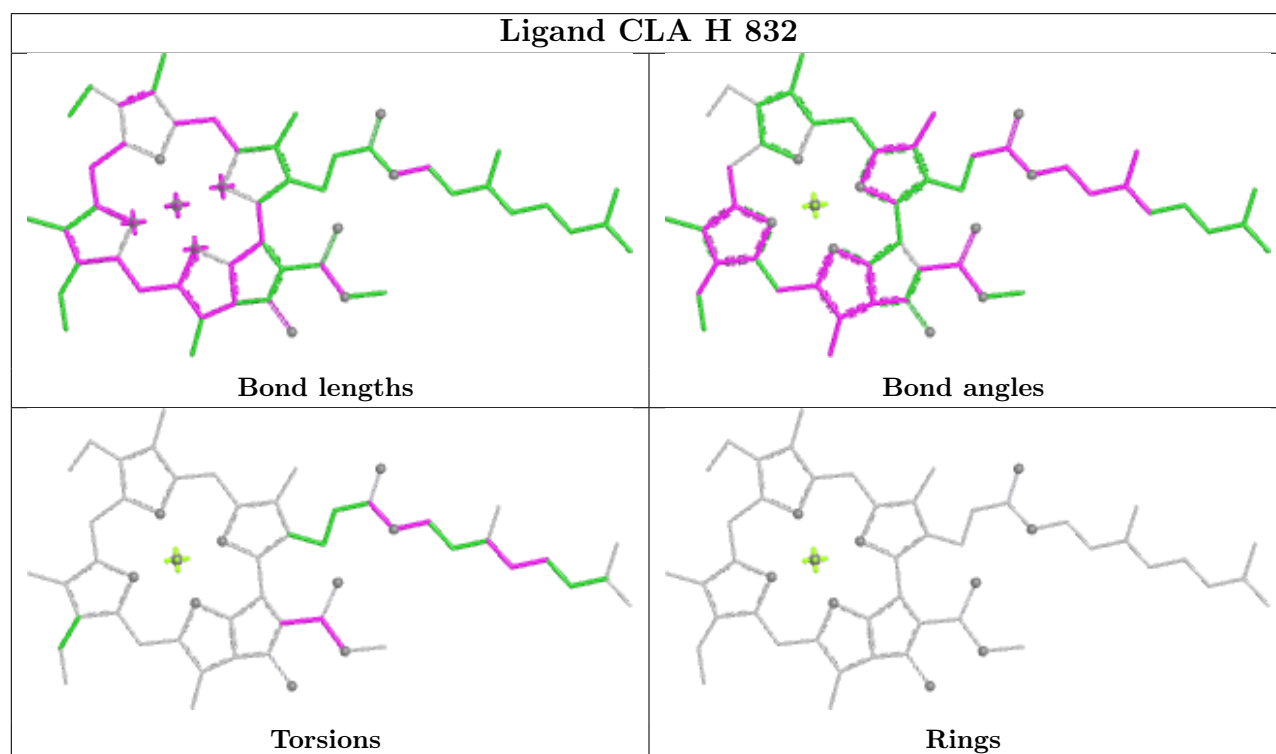
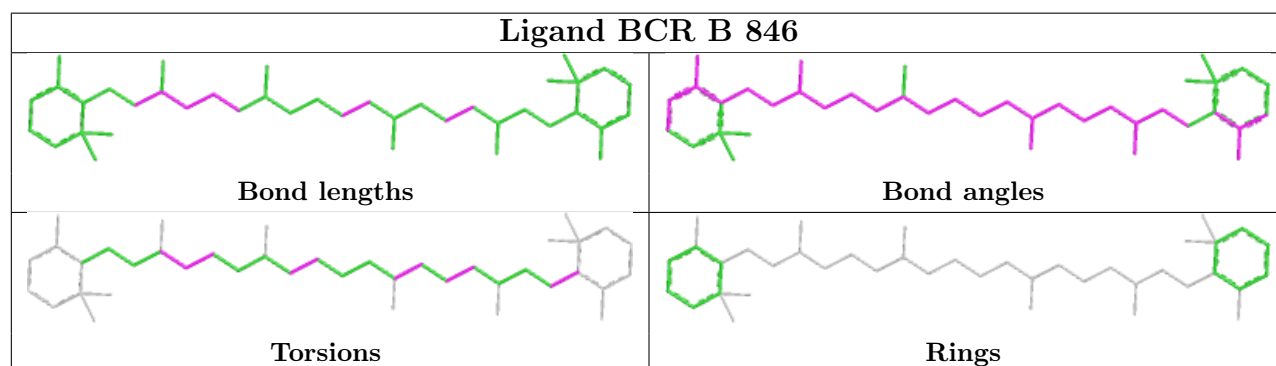
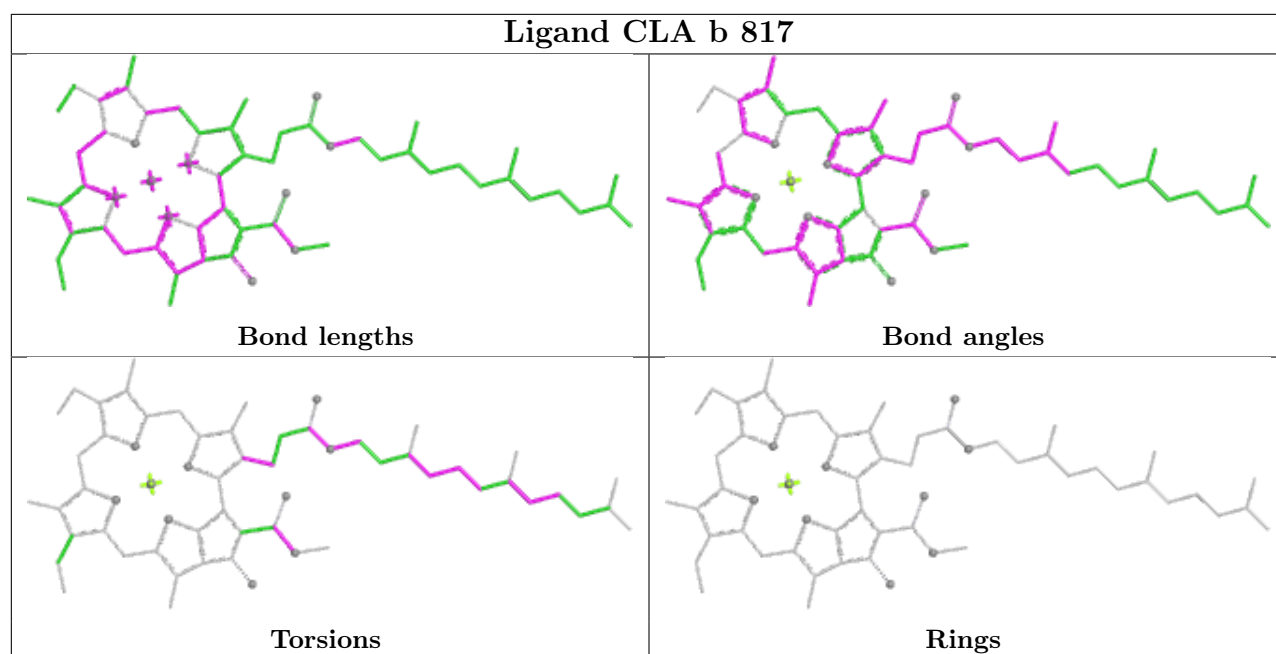


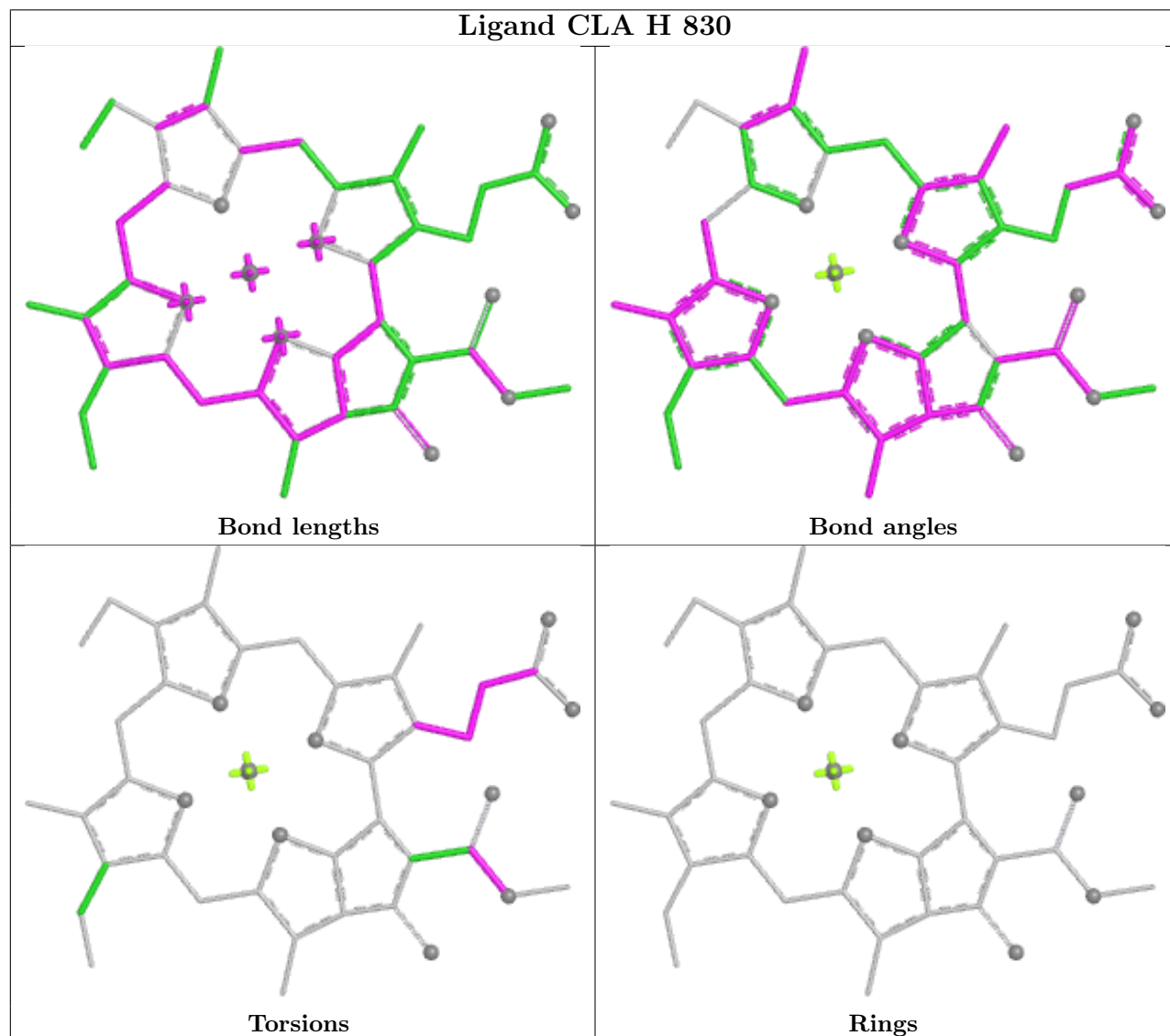
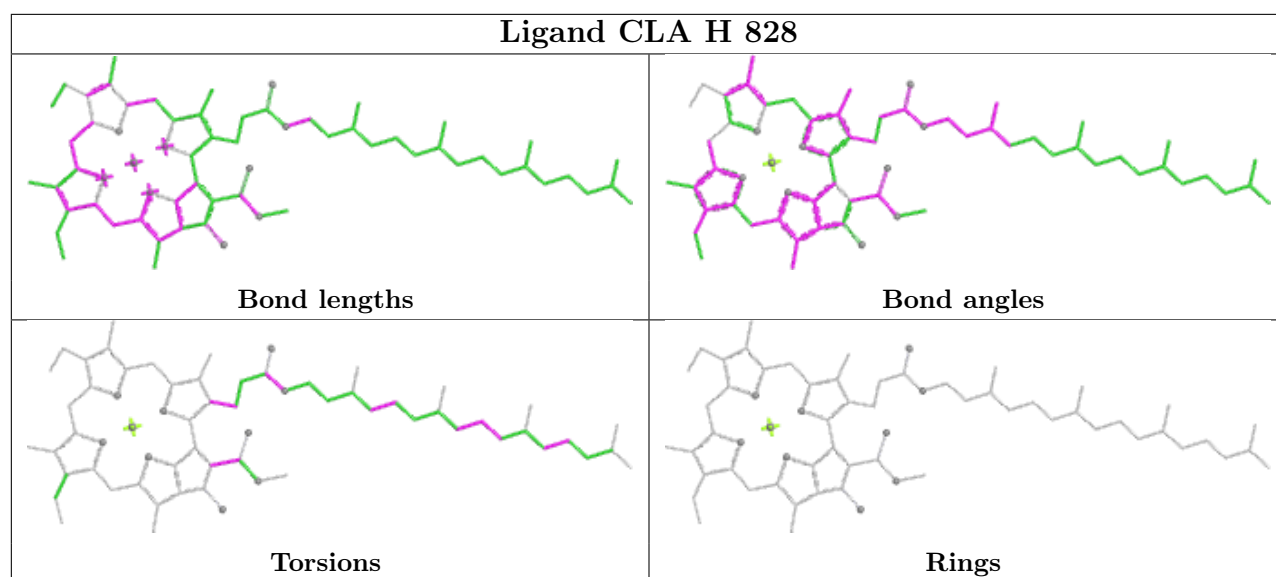
Ligand CLA A 807	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR b 846	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG H 848	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

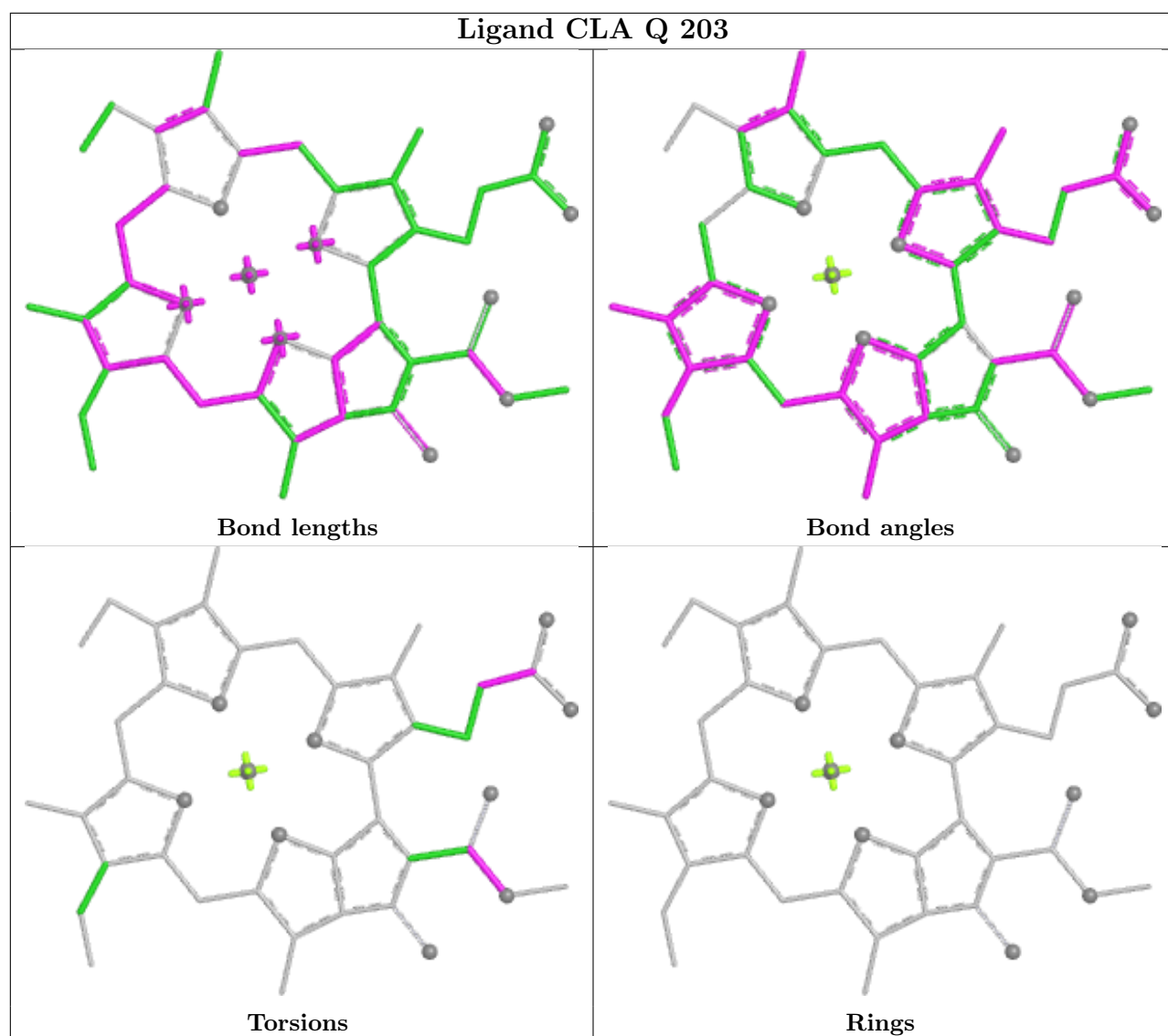


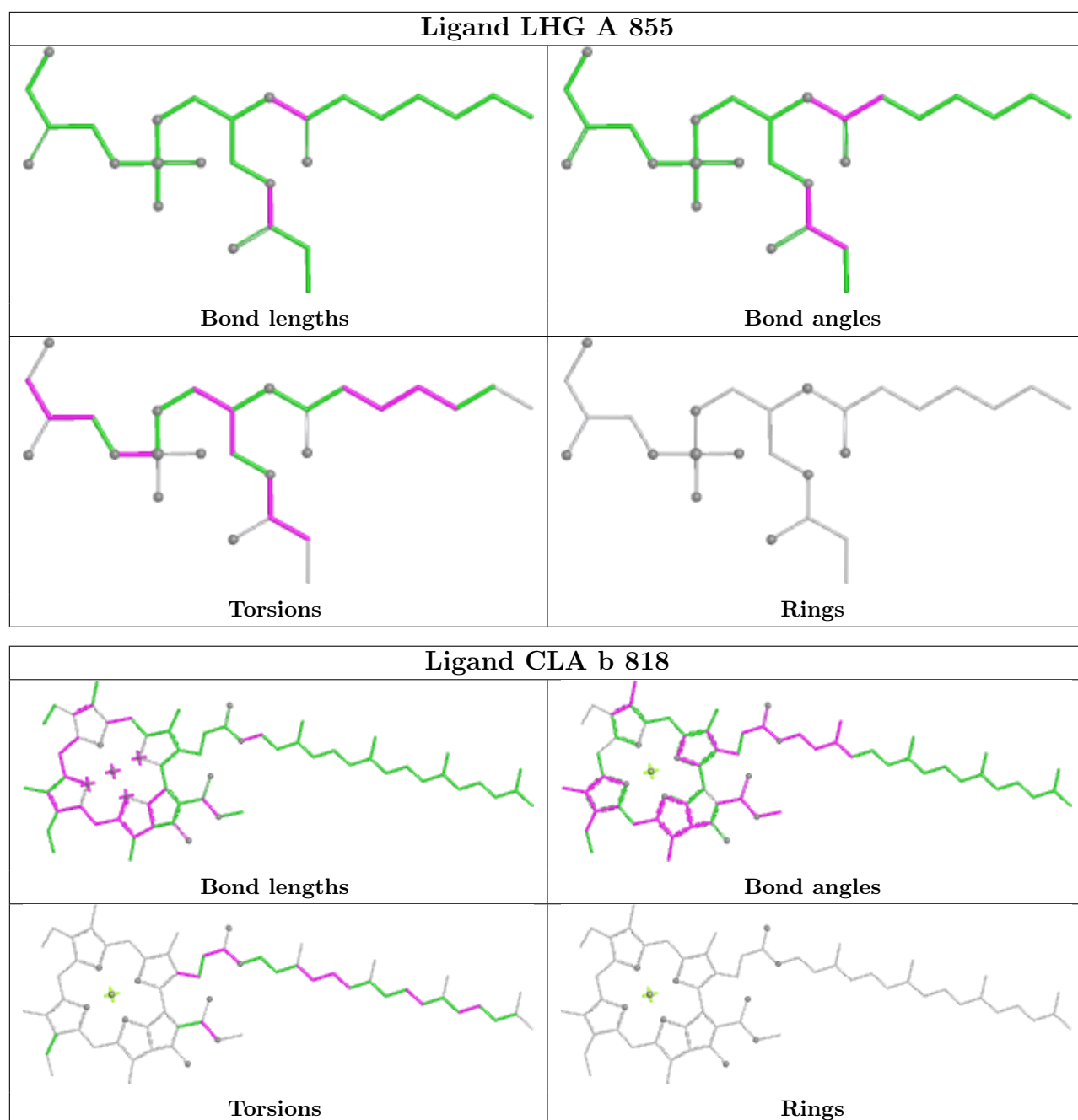


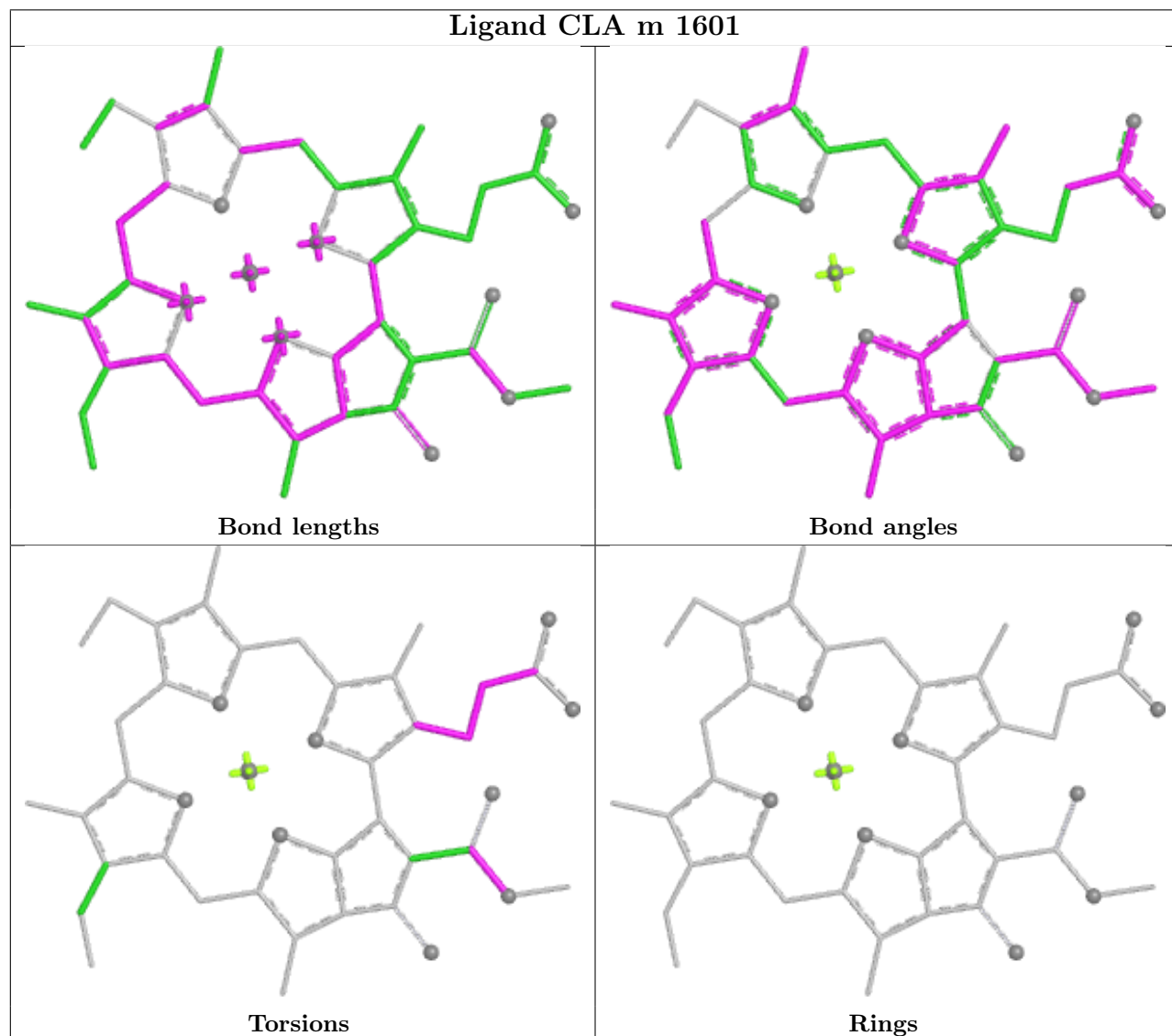
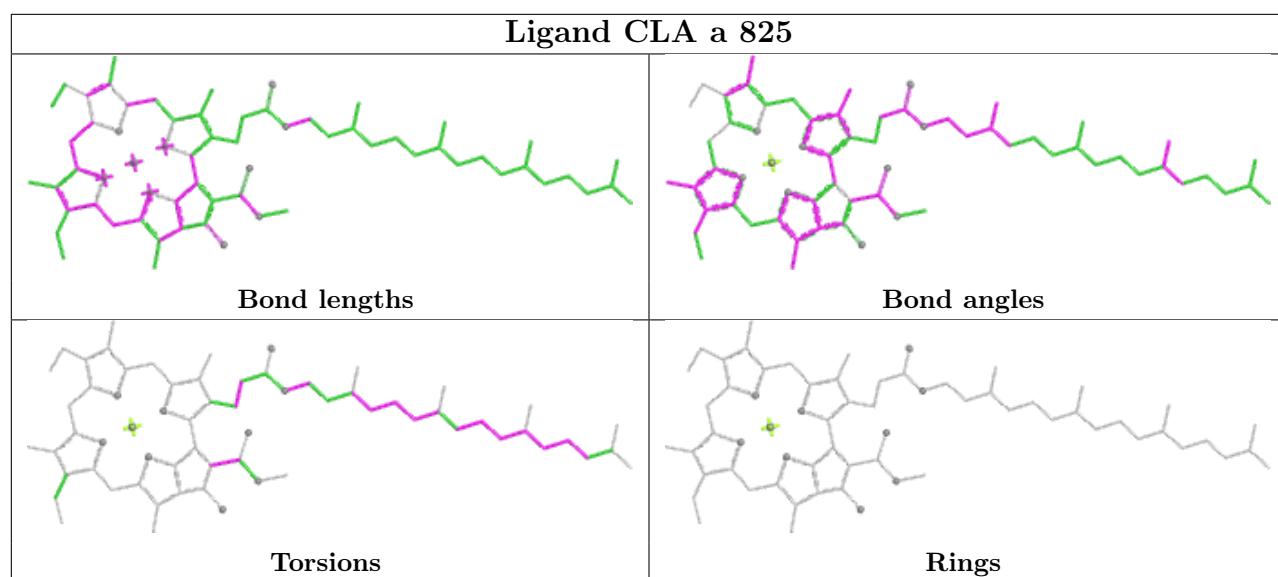




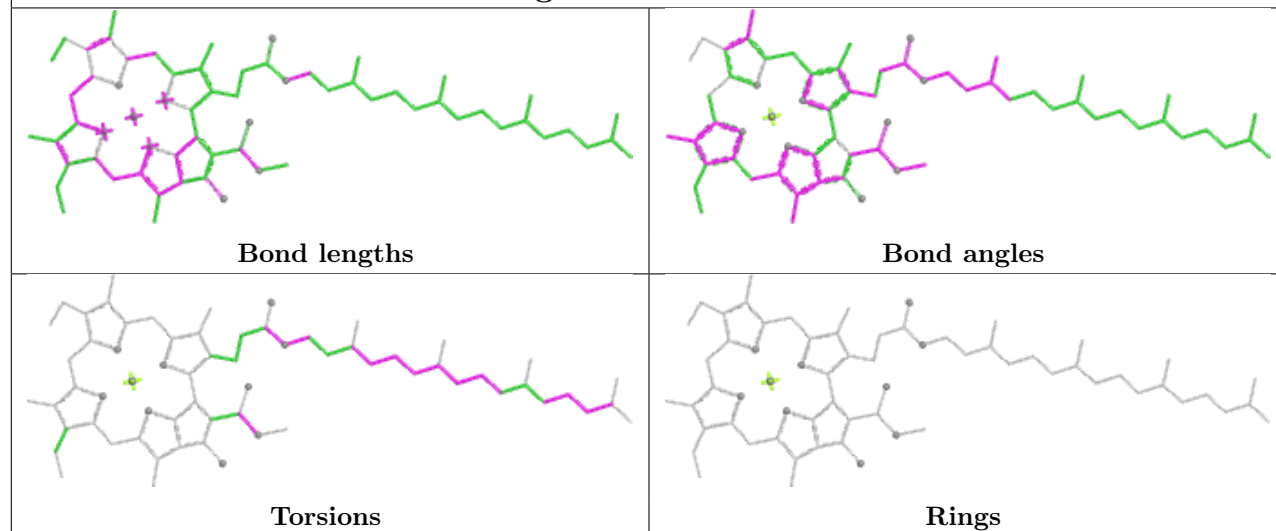




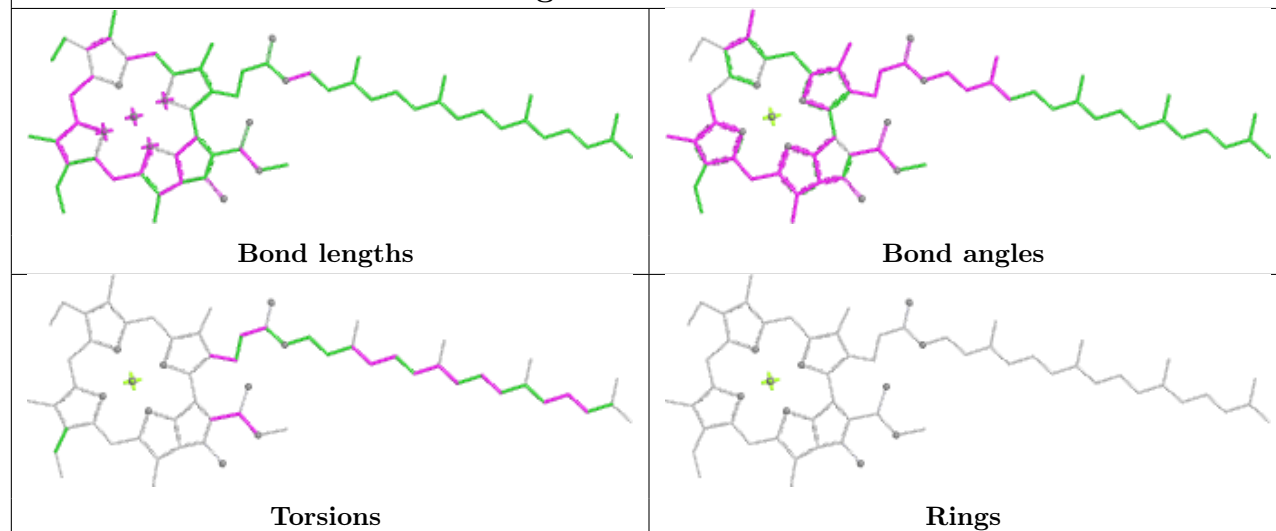




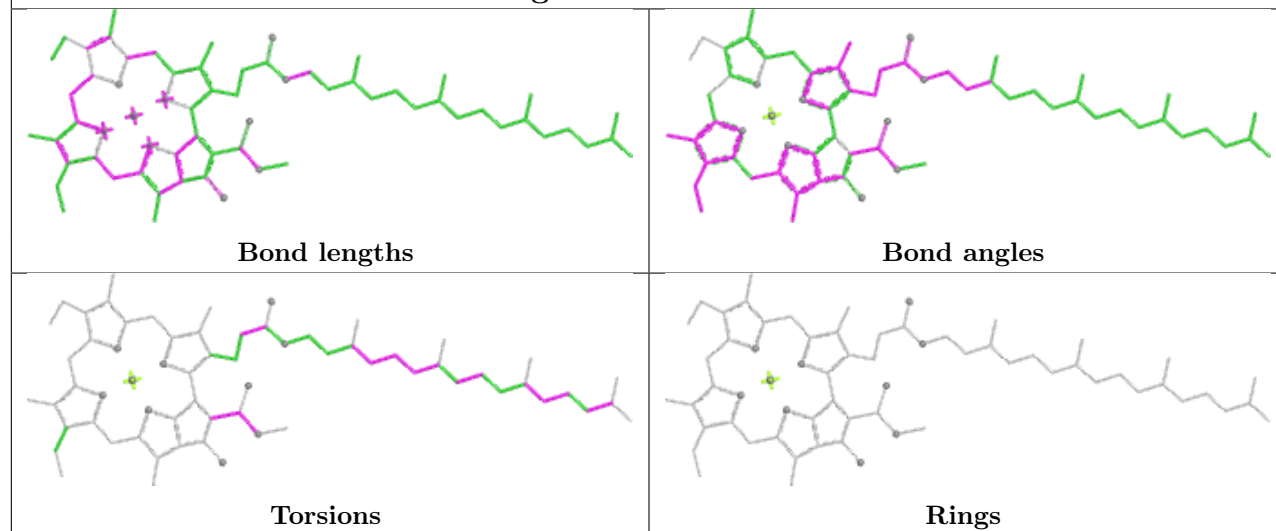
Ligand CLA b 807



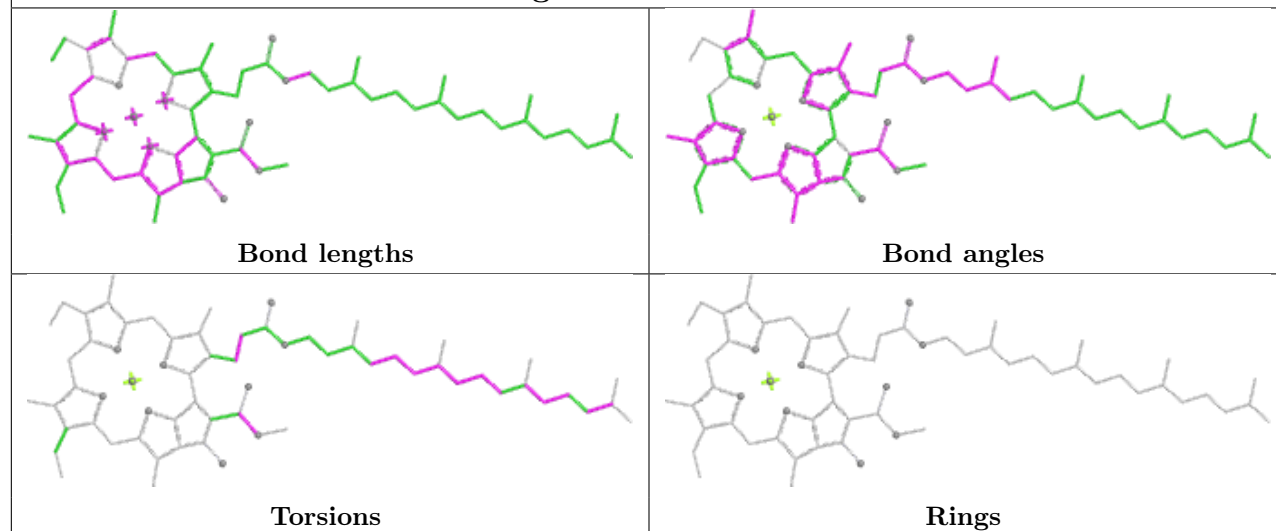
Ligand CLA a 827



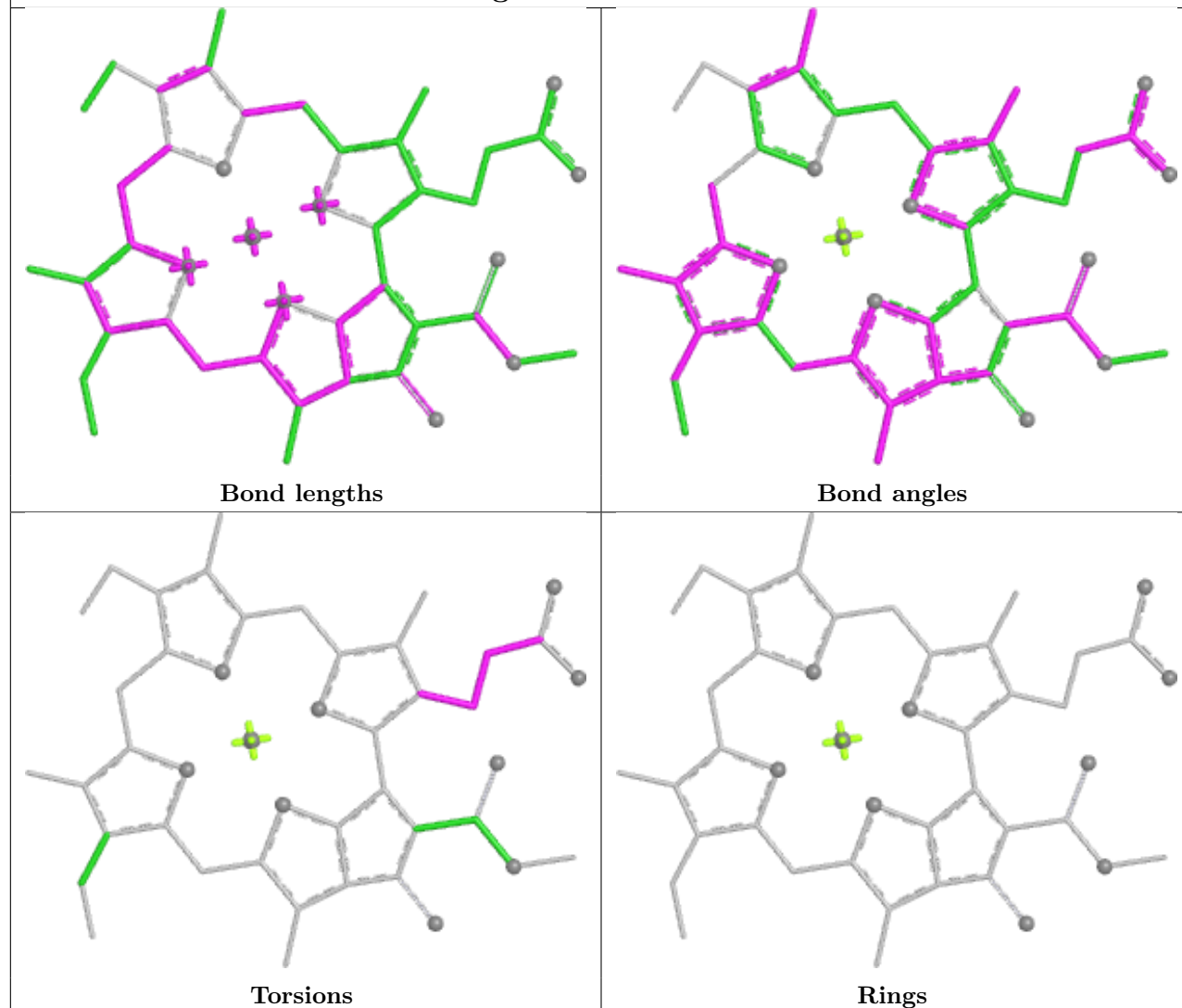
Ligand CLA H 808

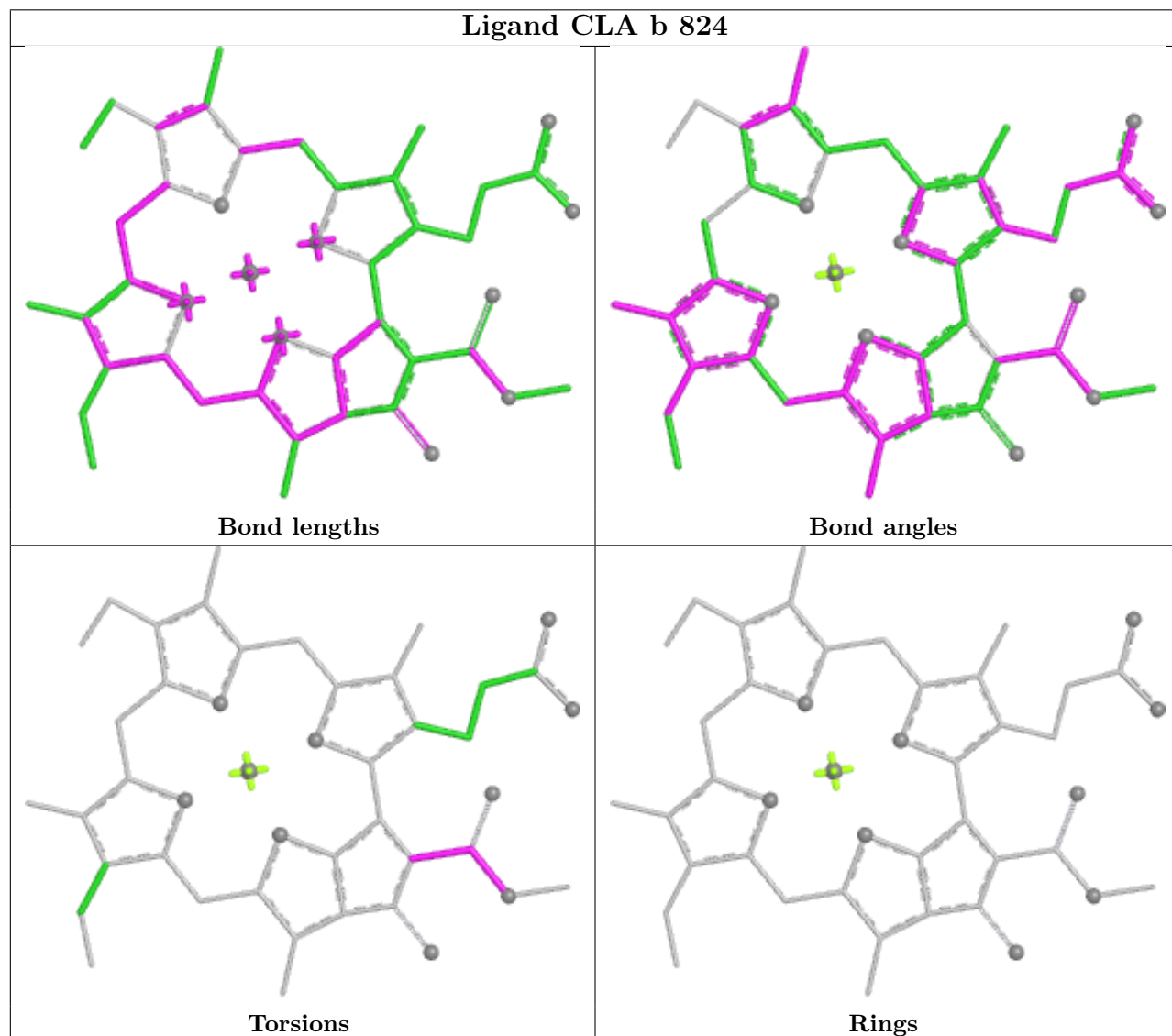
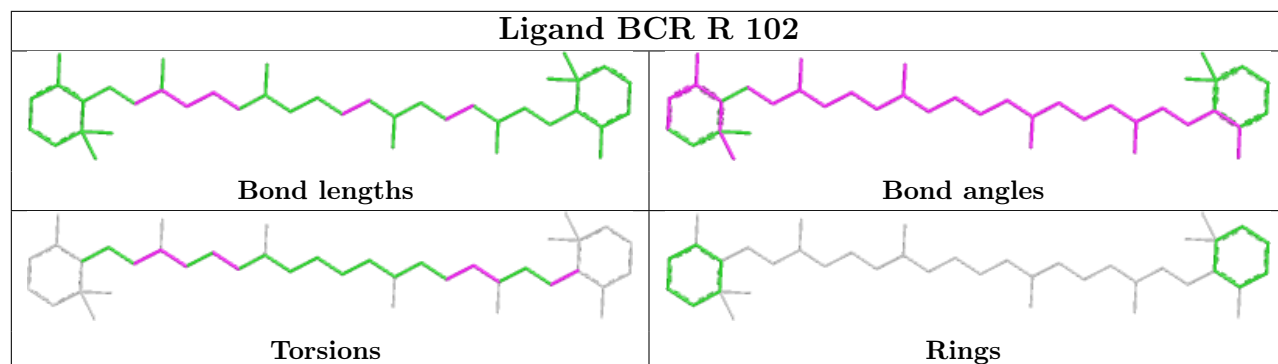


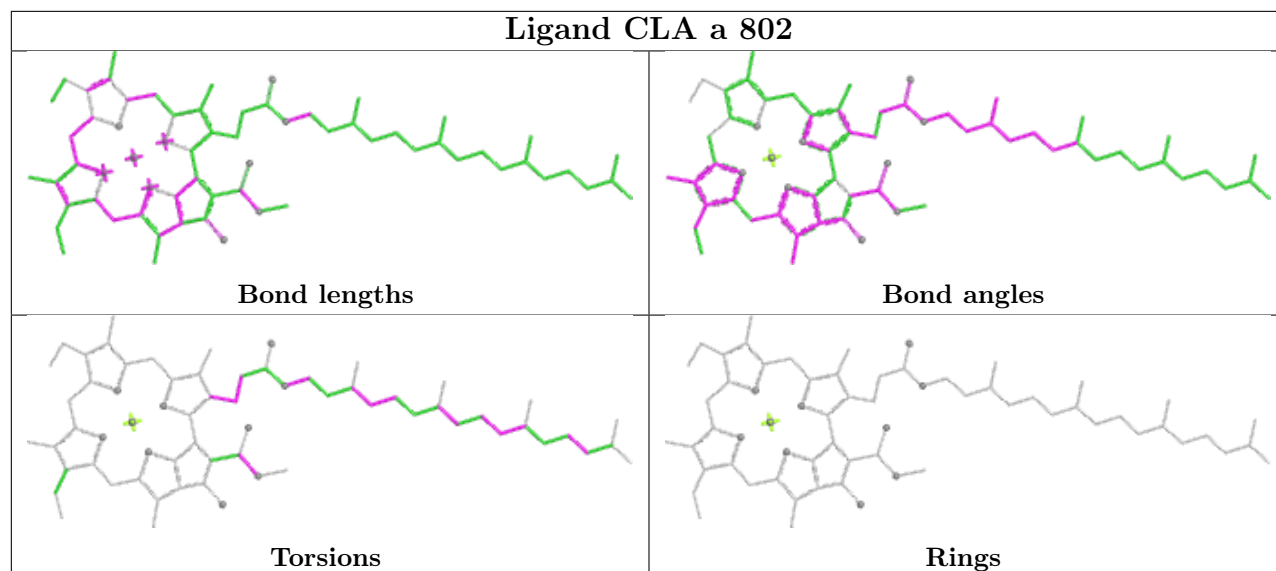
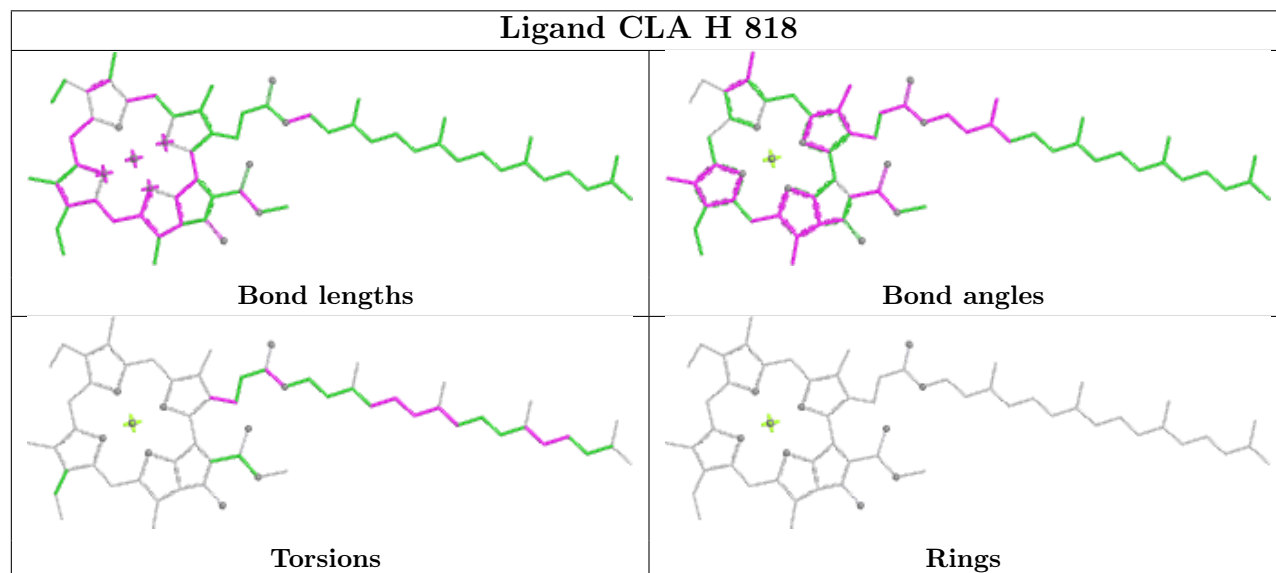
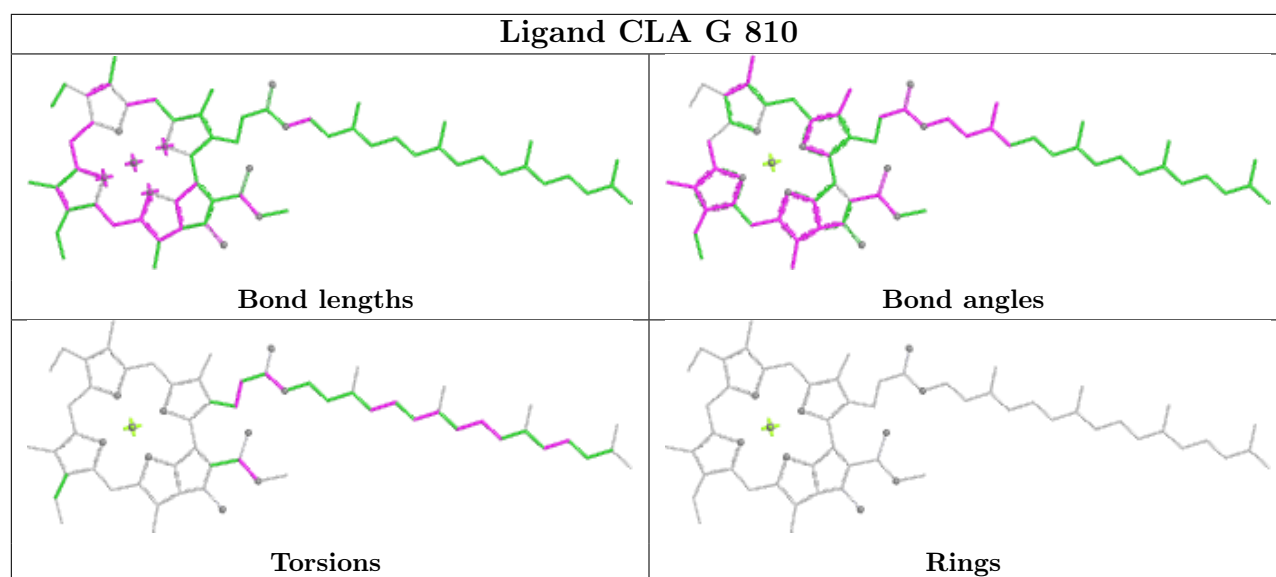
Ligand CLA B 839



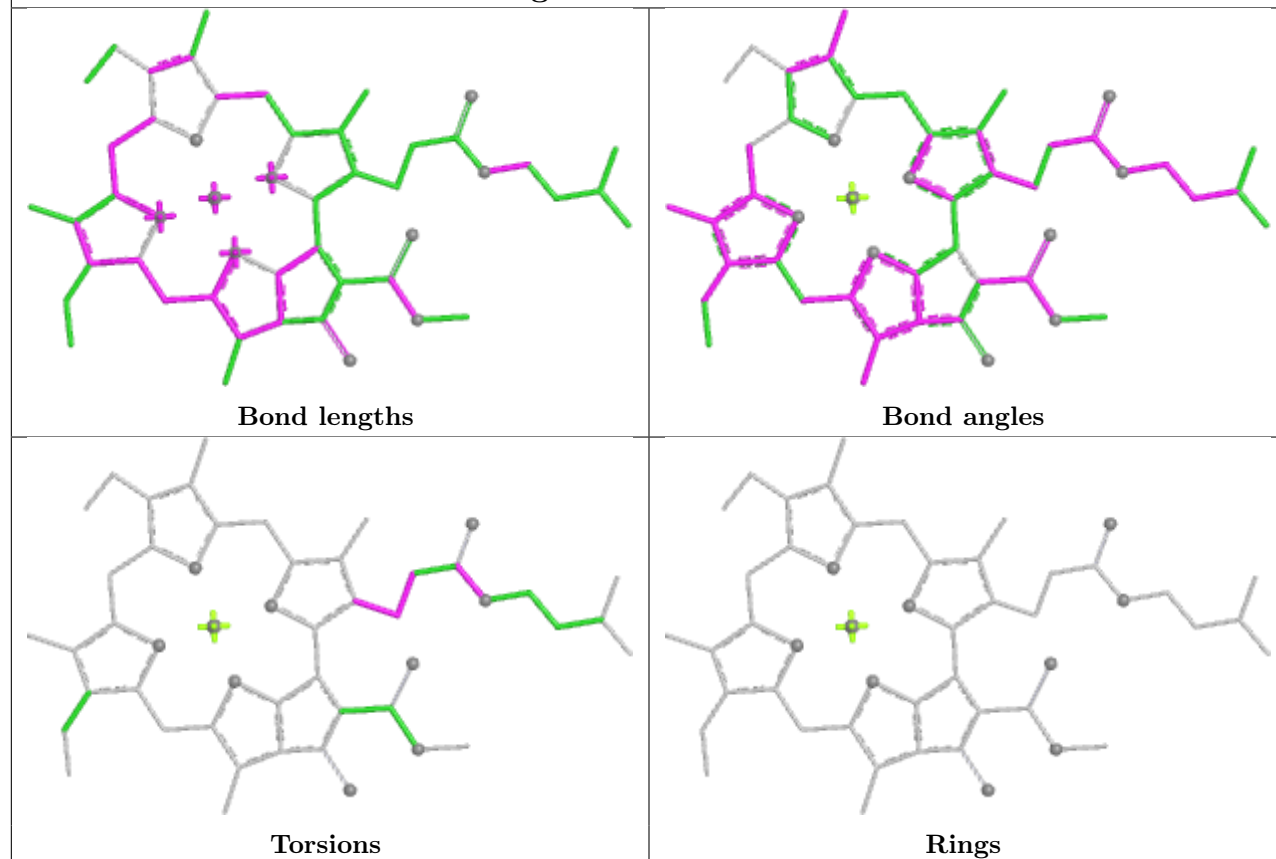
Ligand CLA A 837



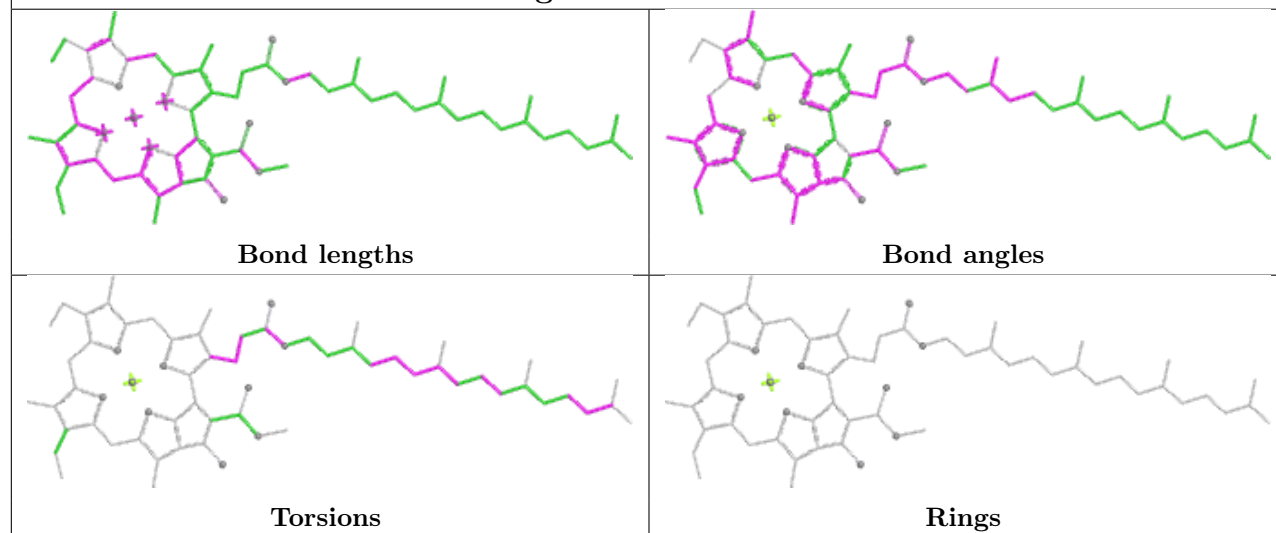




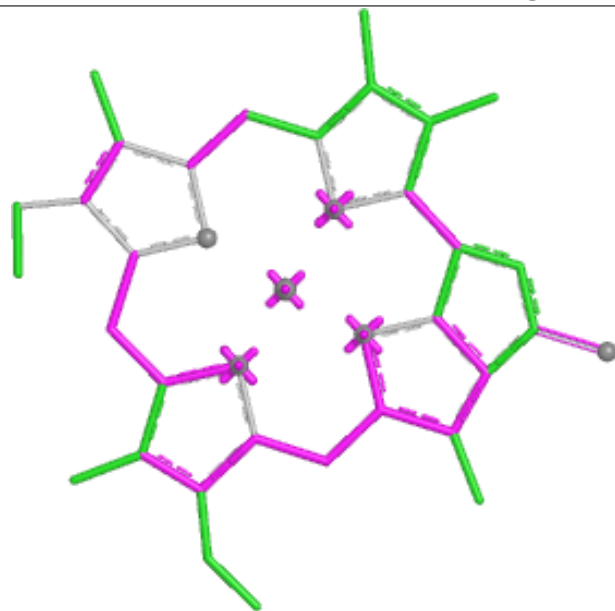
Ligand CLA G 813



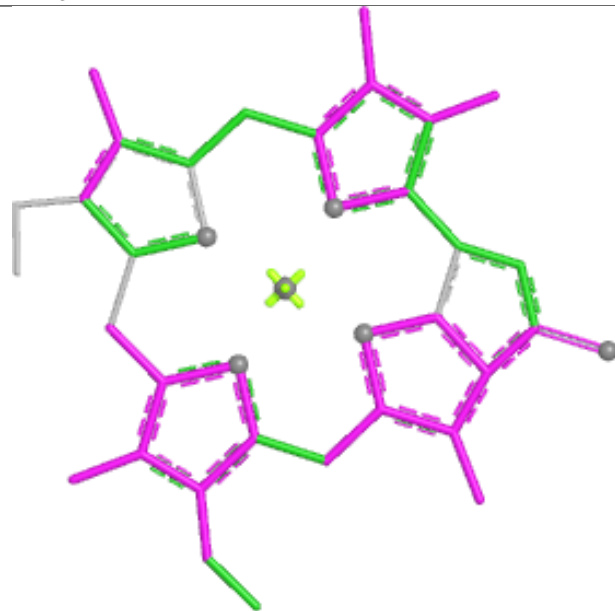
Ligand CLA b 806



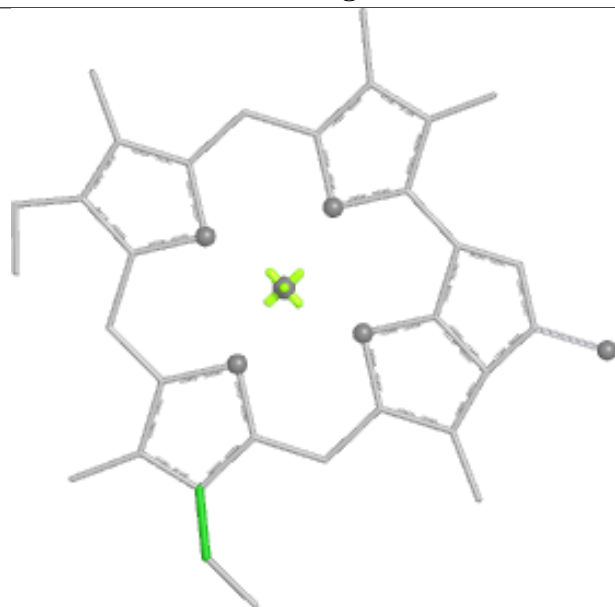
Ligand CLA j 102



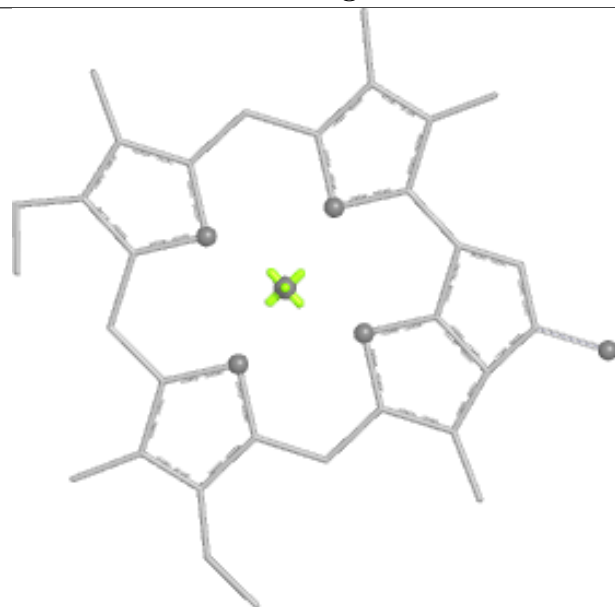
Bond lengths



Bond angles

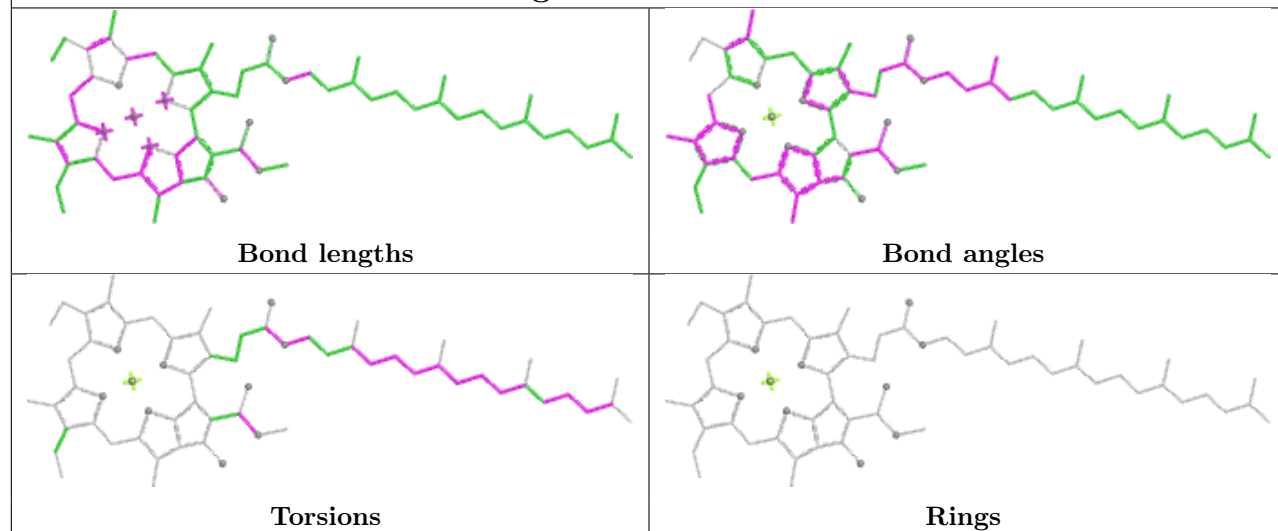


Torsions

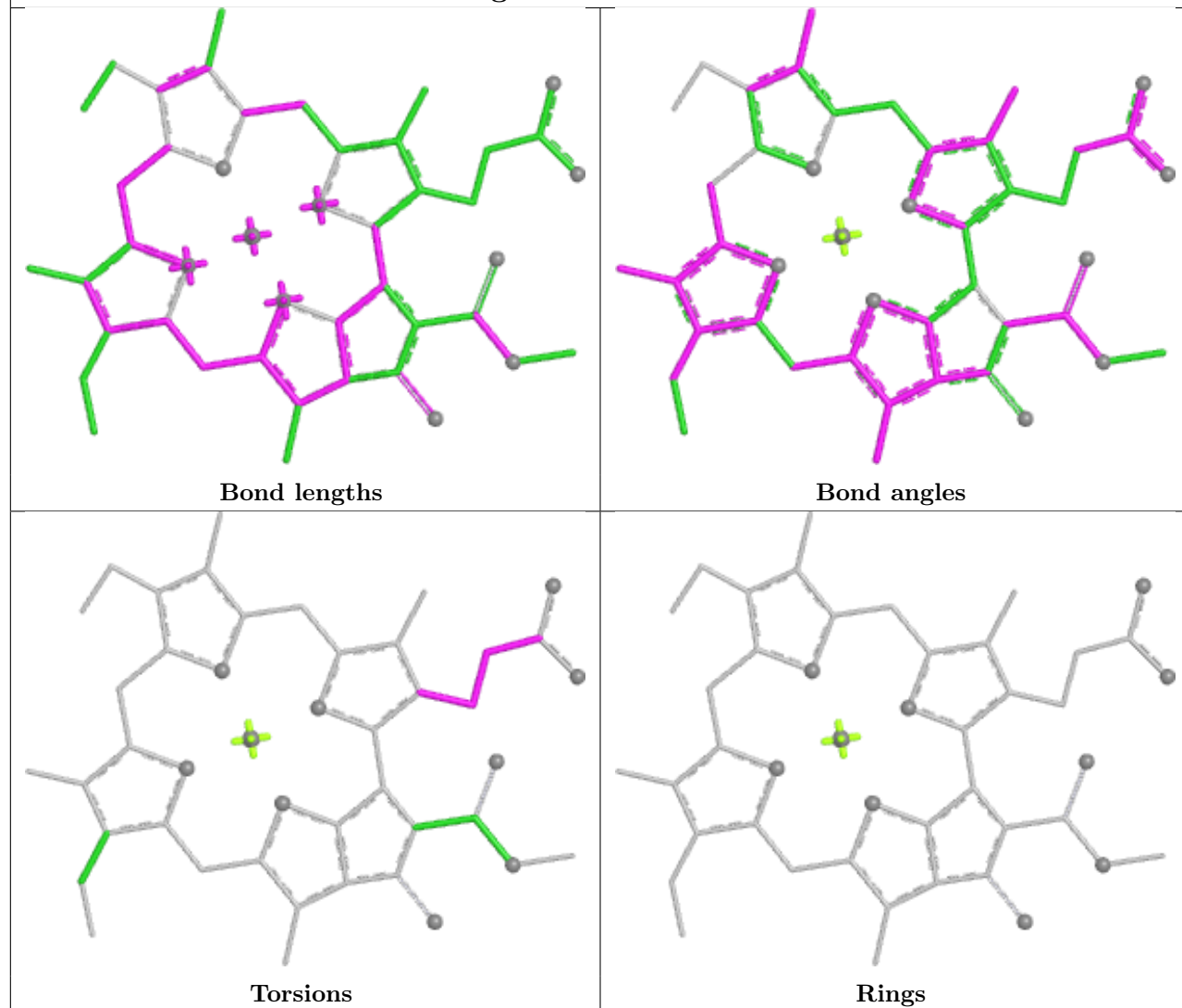


Rings

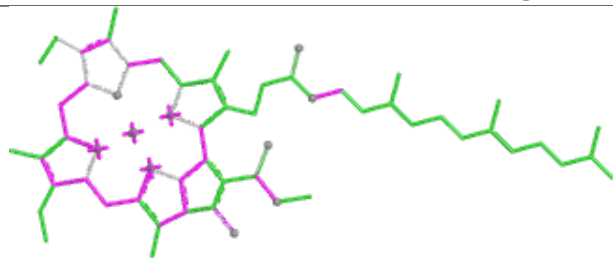
Ligand CLA B 806



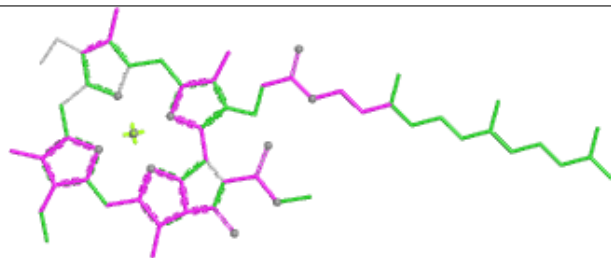
Ligand CLA G 837



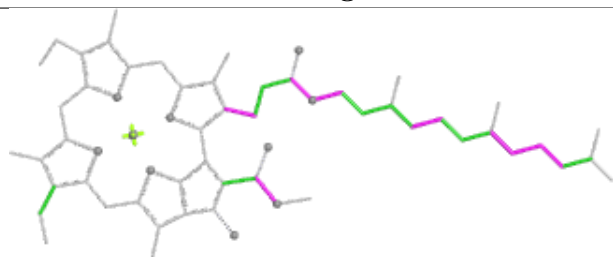
Ligand CLA b 836



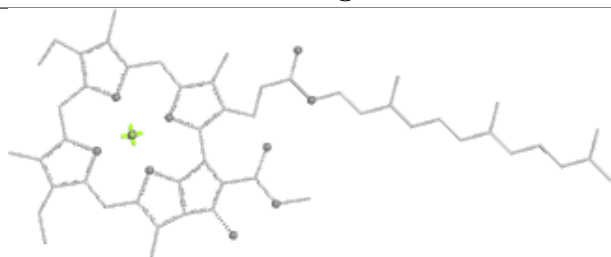
Bond lengths



Bond angles

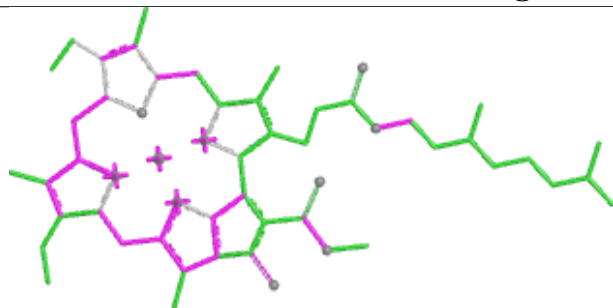


Torsions

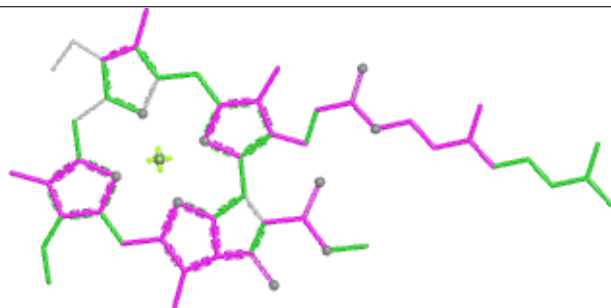


Rings

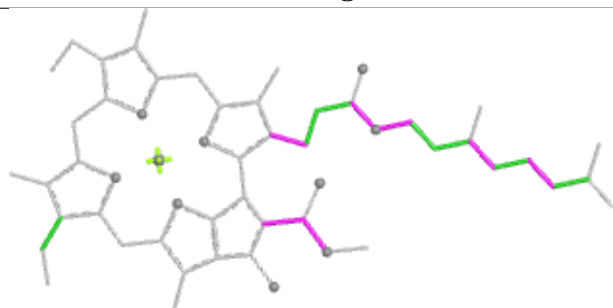
Ligand CLA A 804



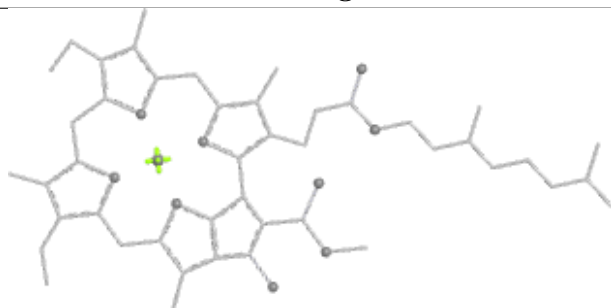
Bond lengths



Bond angles

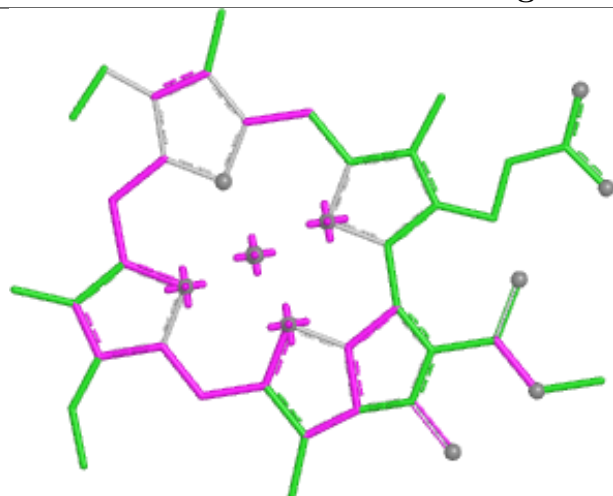


Torsions

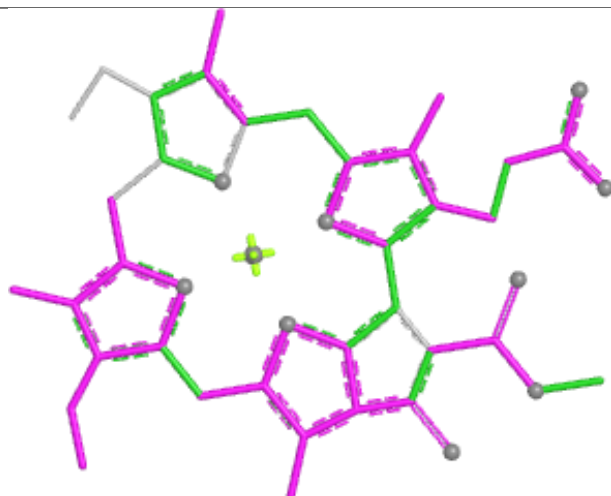


Rings

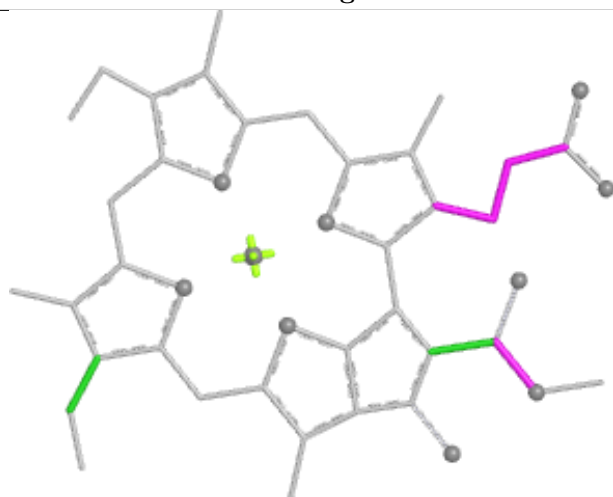
Ligand CLA b 829



Bond lengths



Bond angles

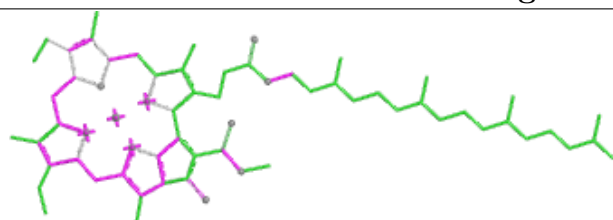


Torsions

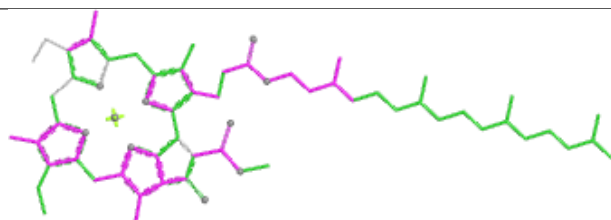


Rings

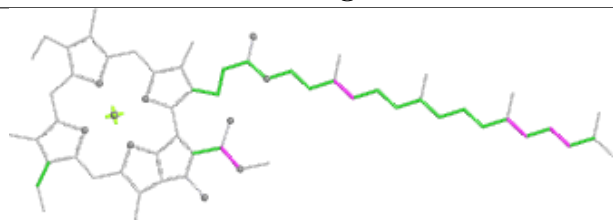
Ligand CLA a 833



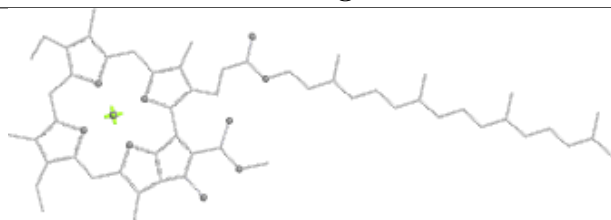
Bond lengths



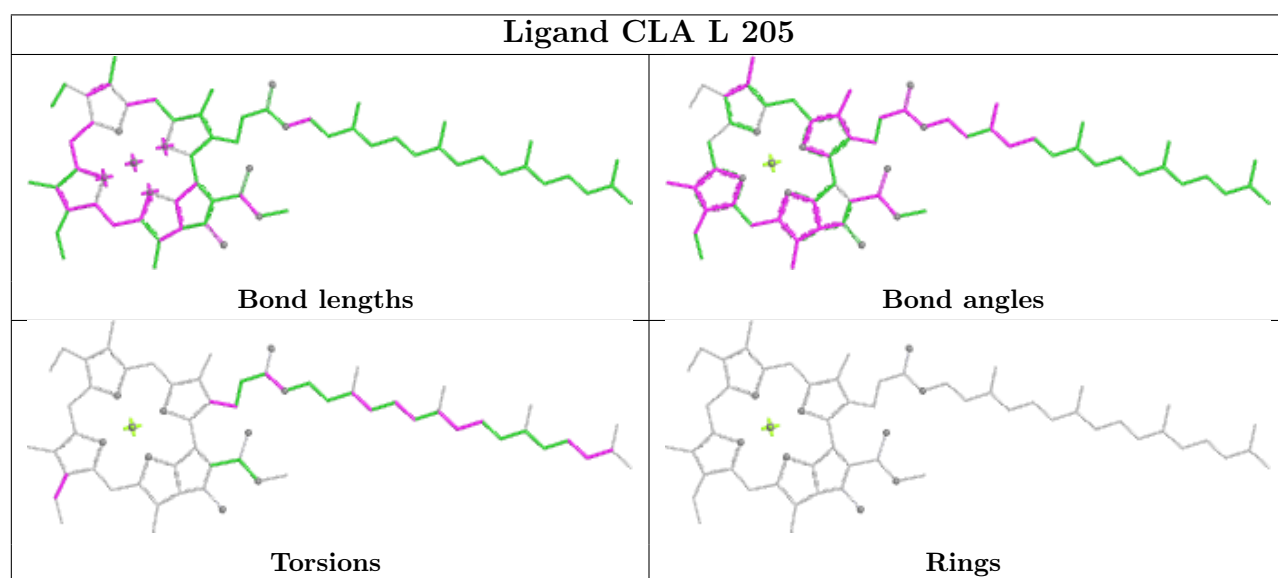
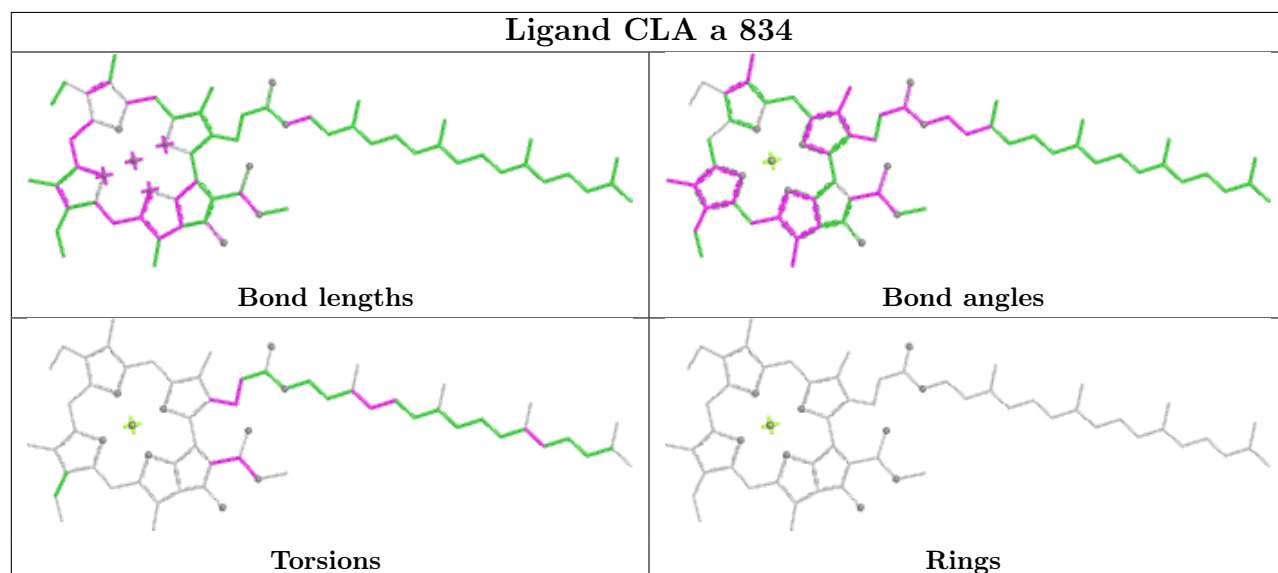
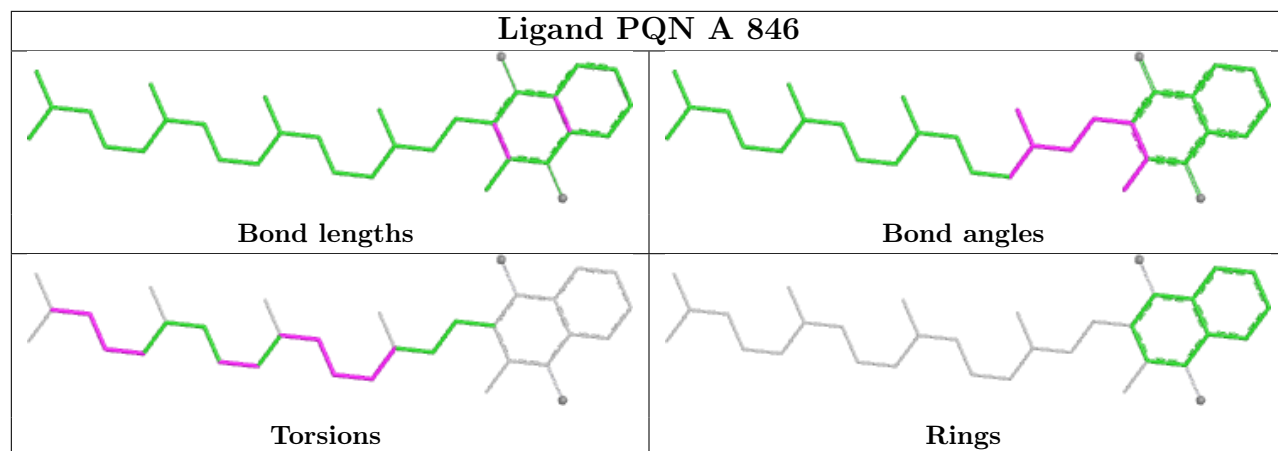
Bond angles

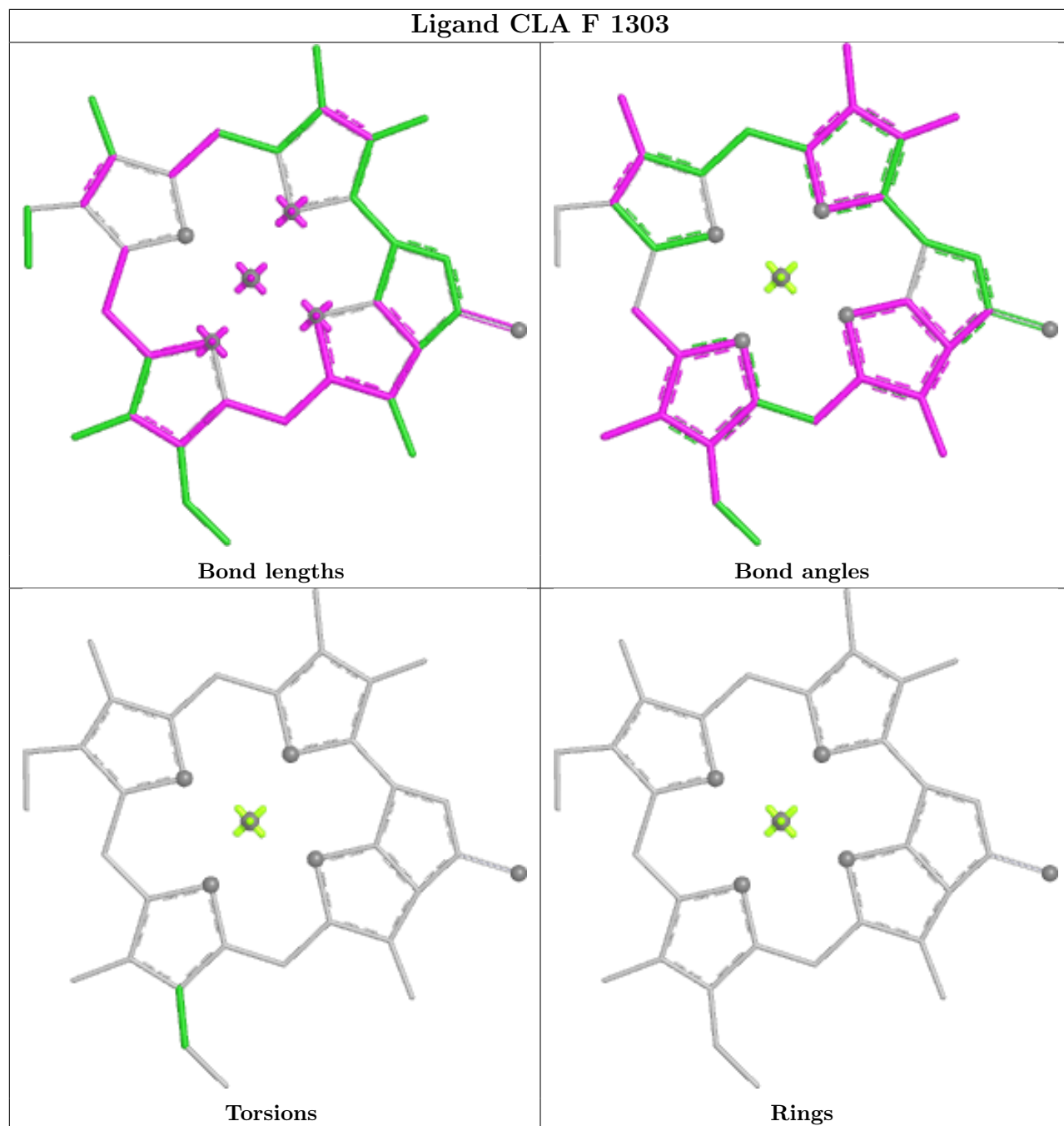


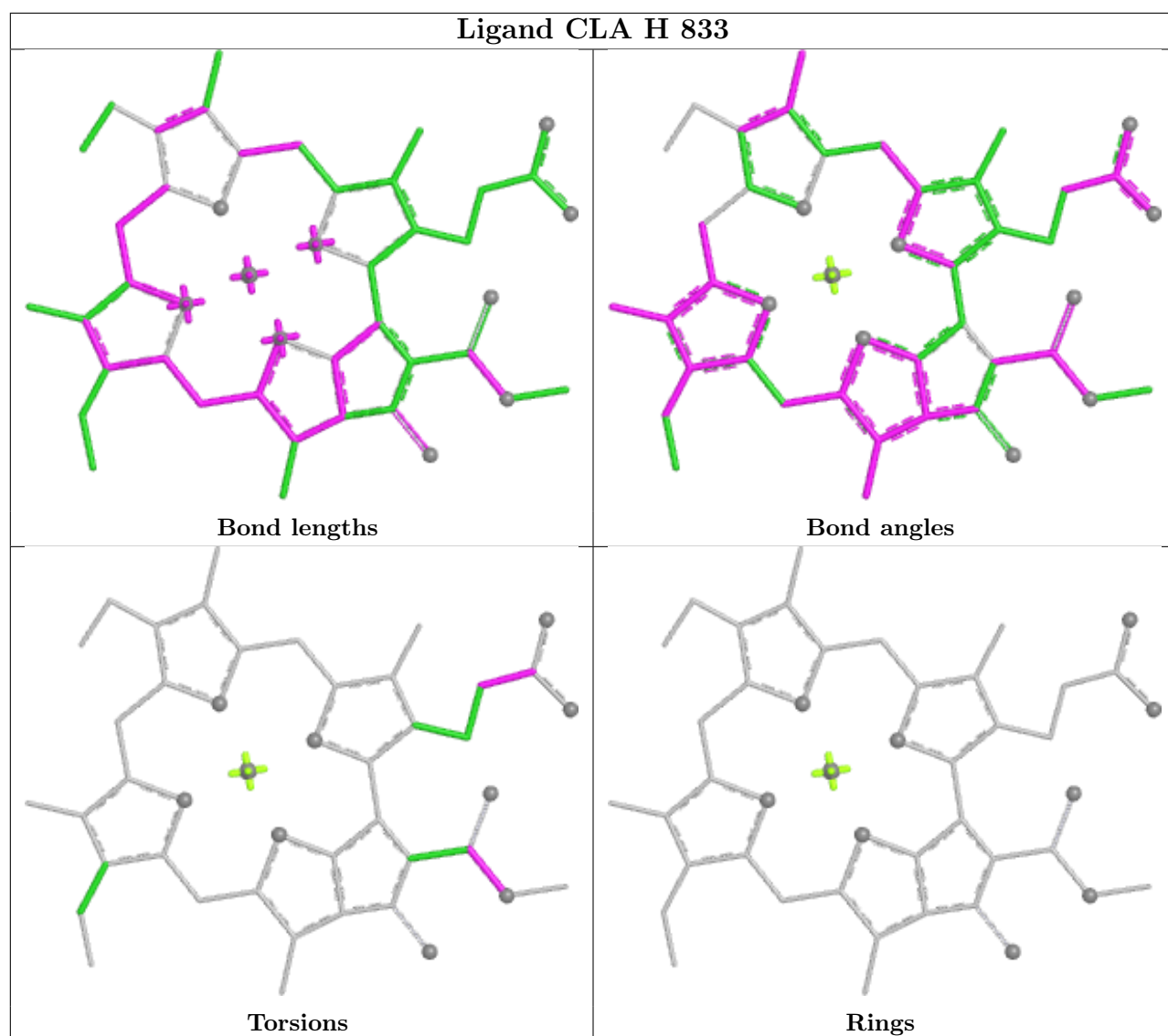
Torsions

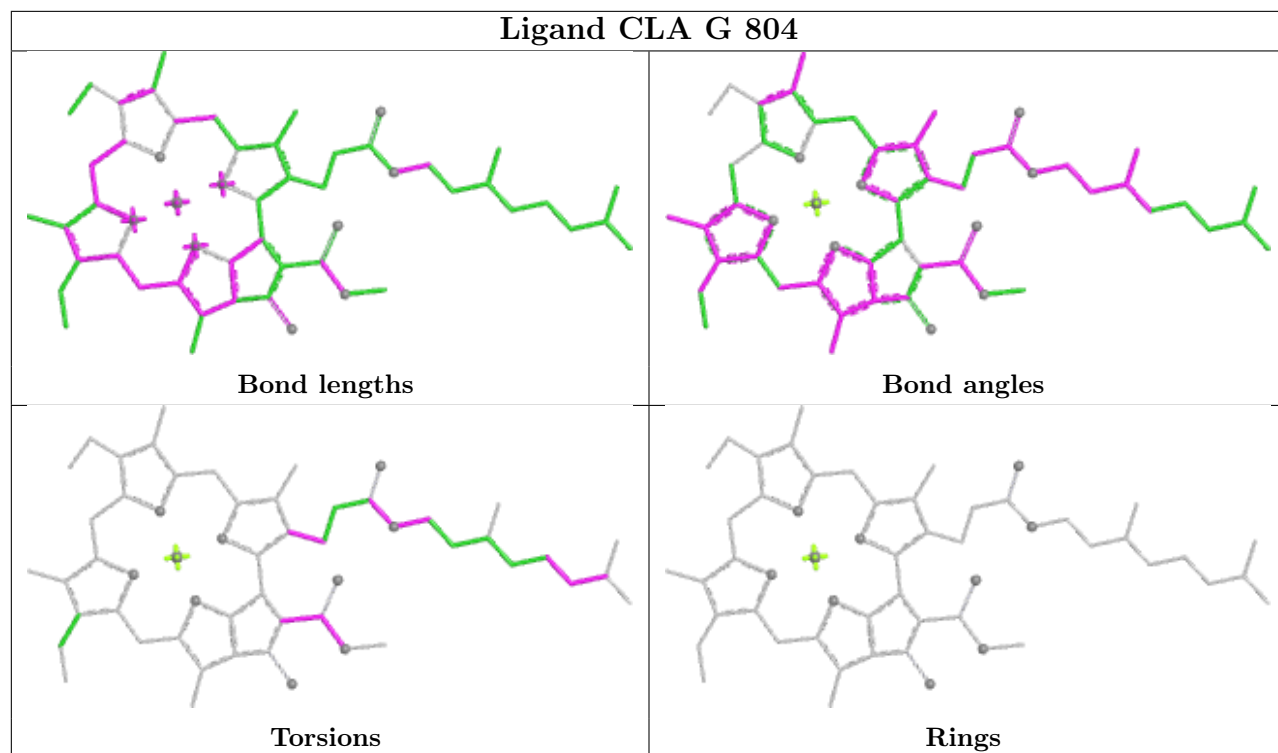


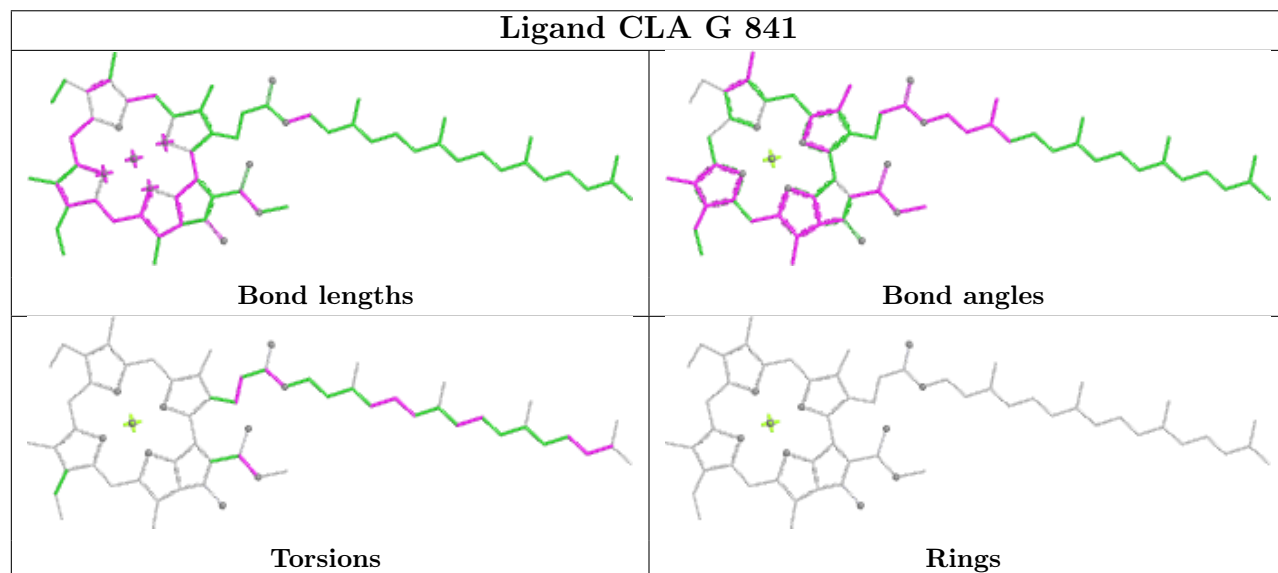
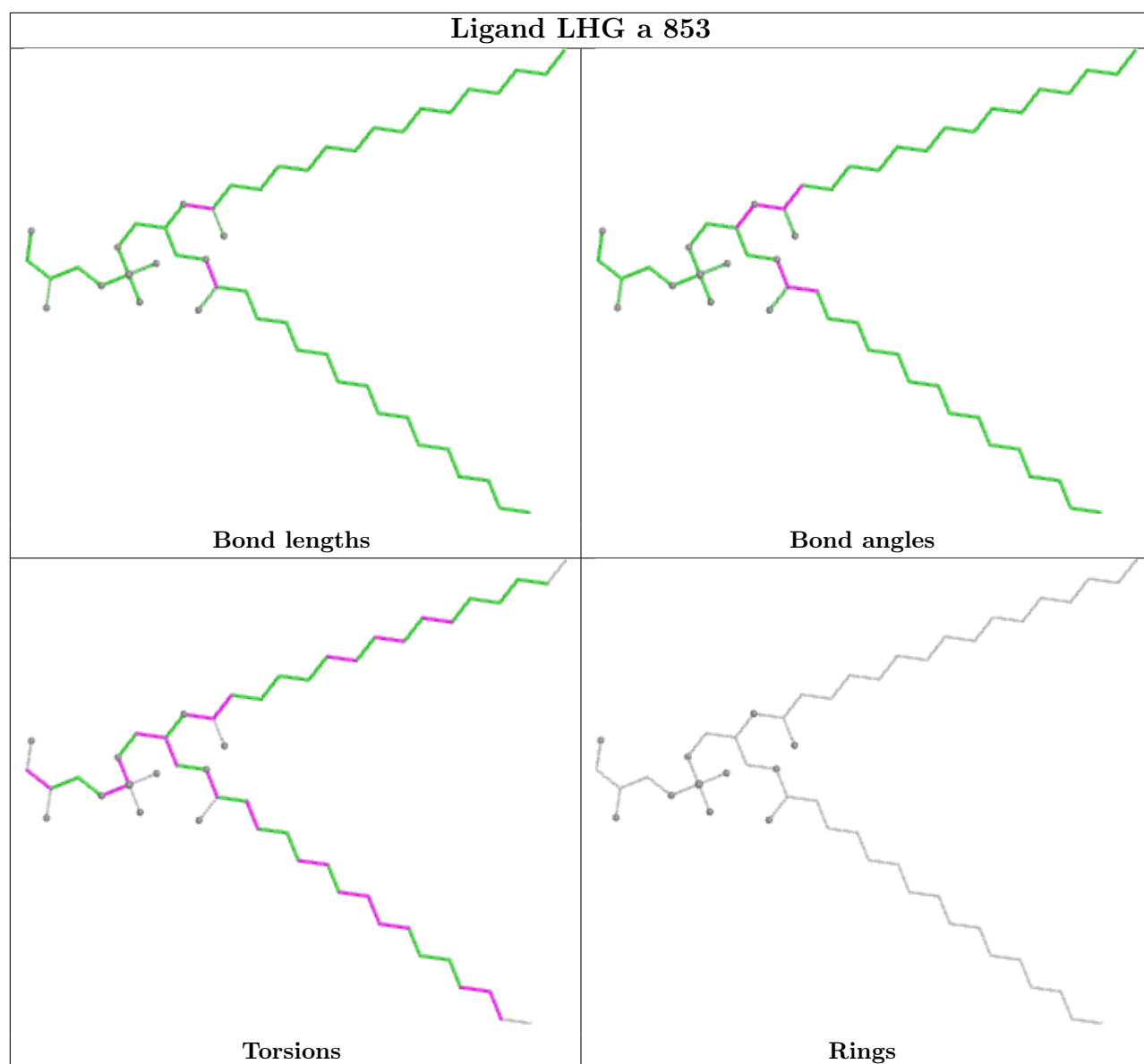
Rings



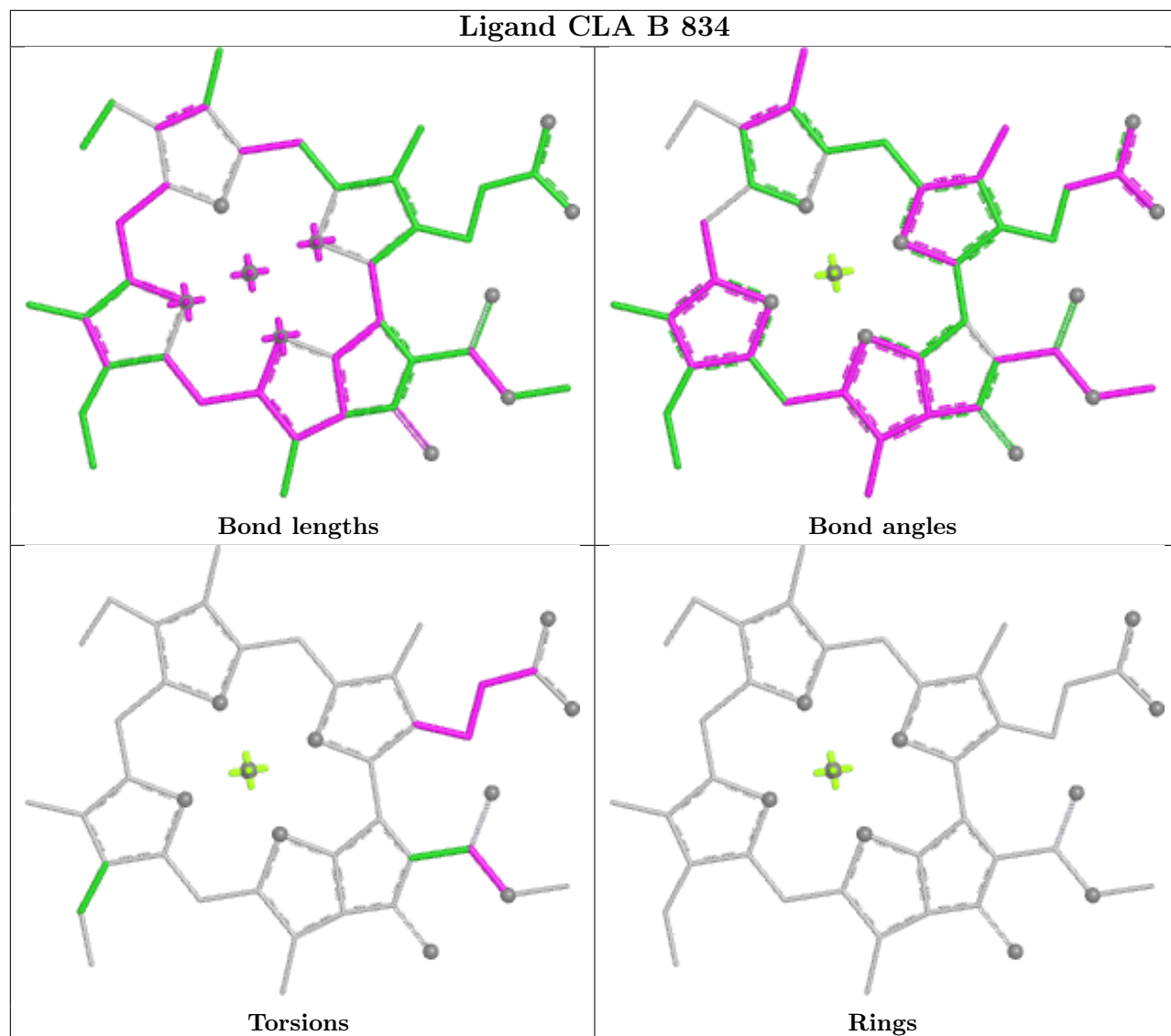




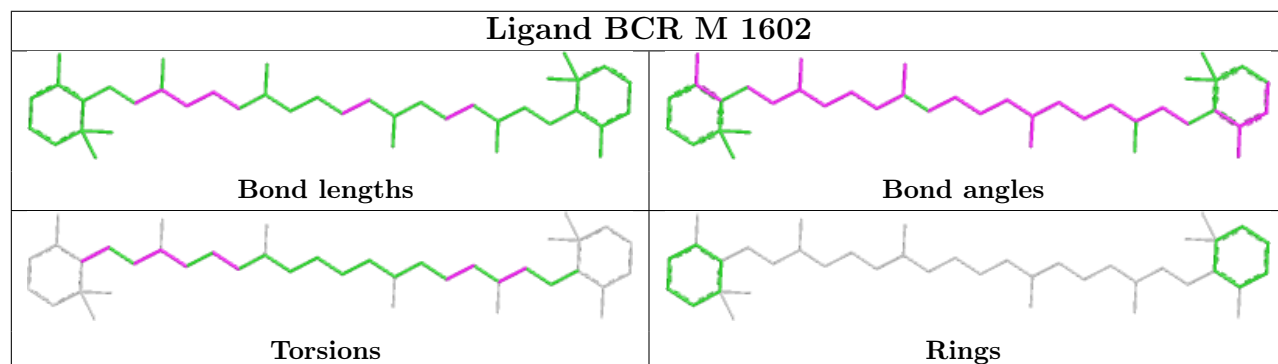


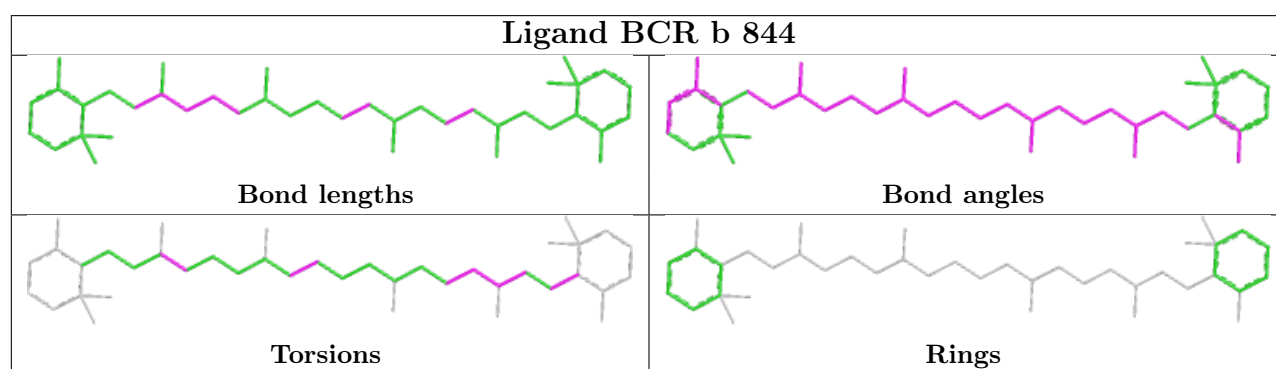
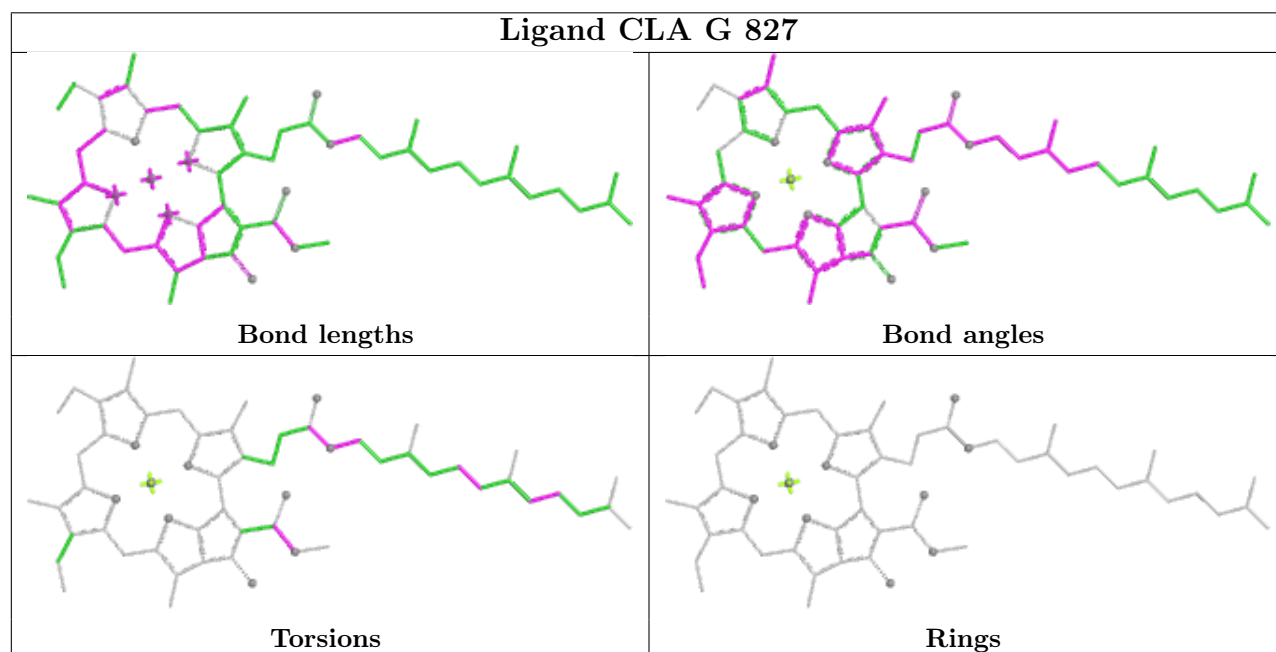
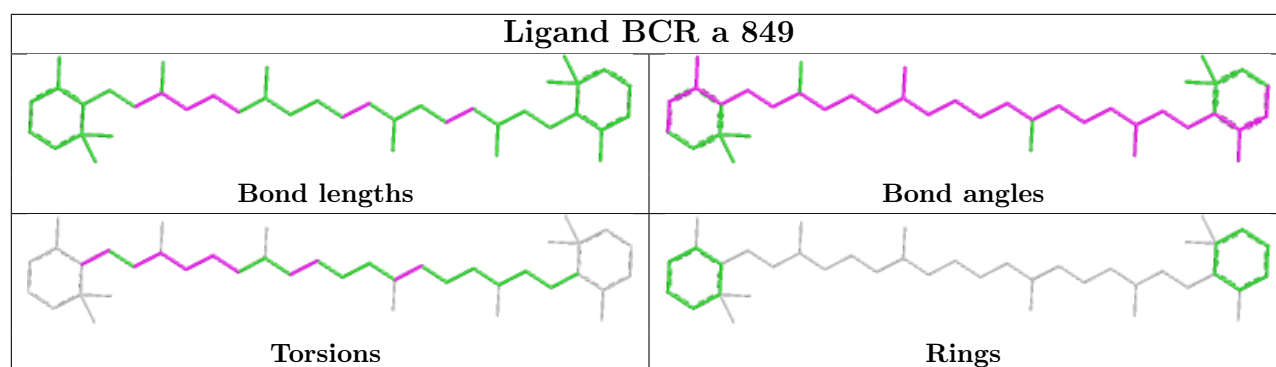


Ligand CLA B 834

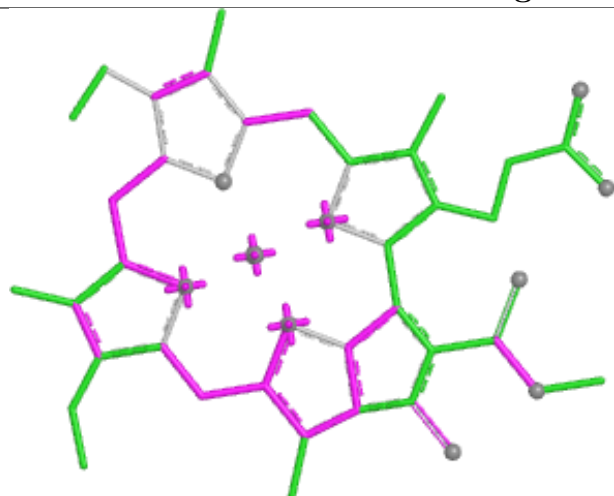


Ligand BCR M 1602

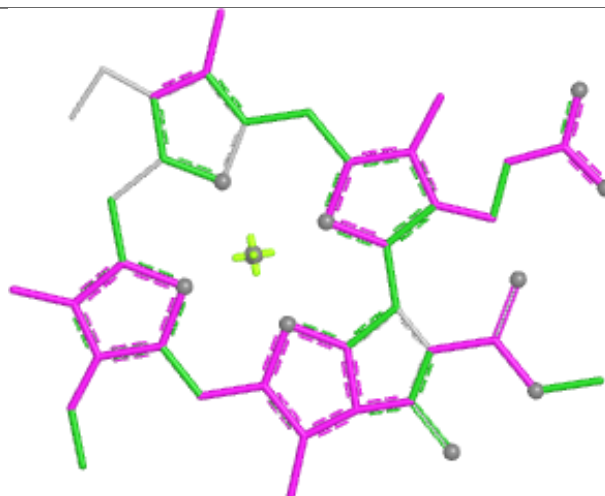




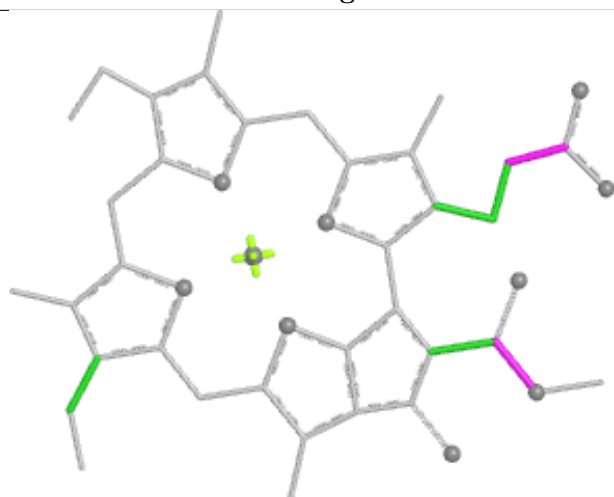
Ligand CLA B 815



Bond lengths



Bond angles

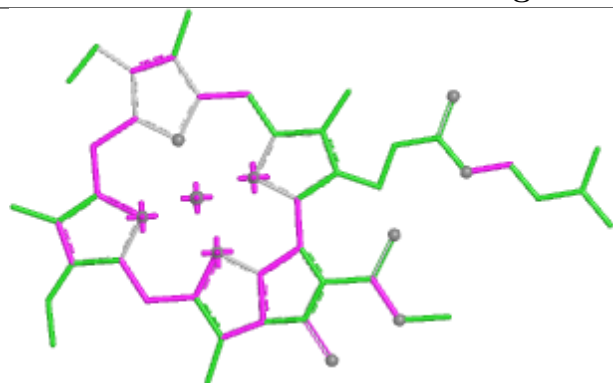


Torsions

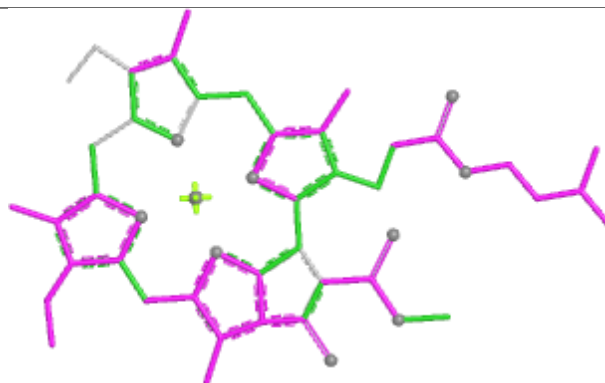


Rings

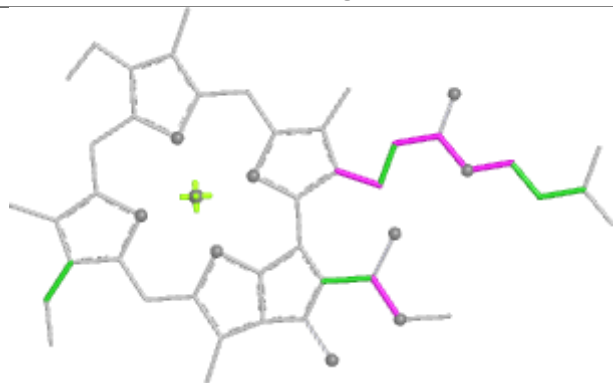
Ligand CLA G 821



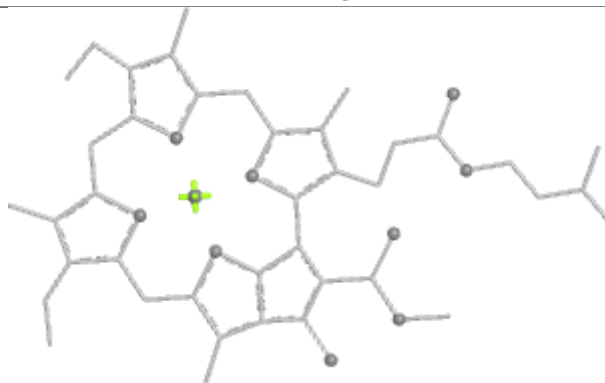
Bond lengths



Bond angles

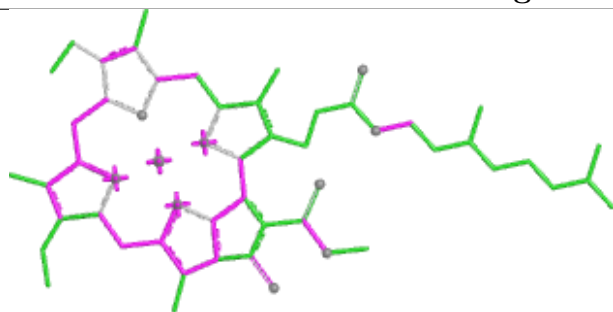


Torsions

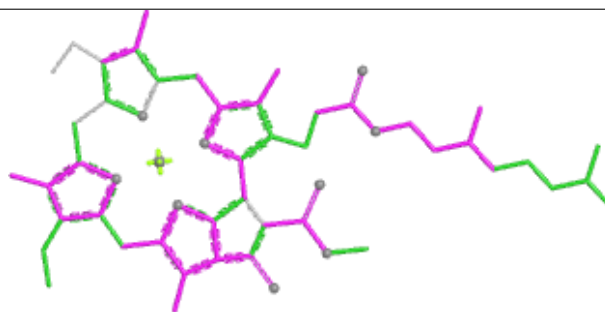


Rings

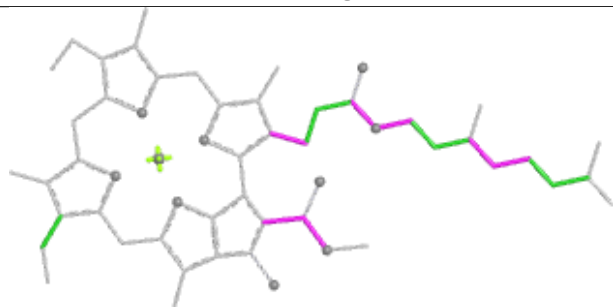
Ligand CLA A 805



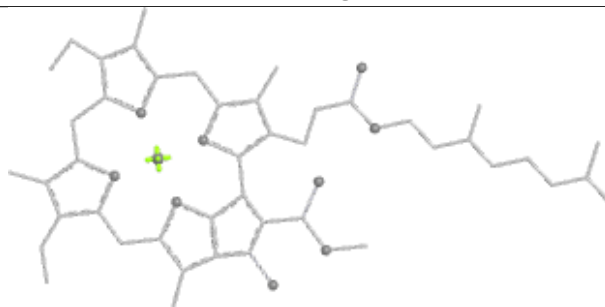
Bond lengths



Bond angles

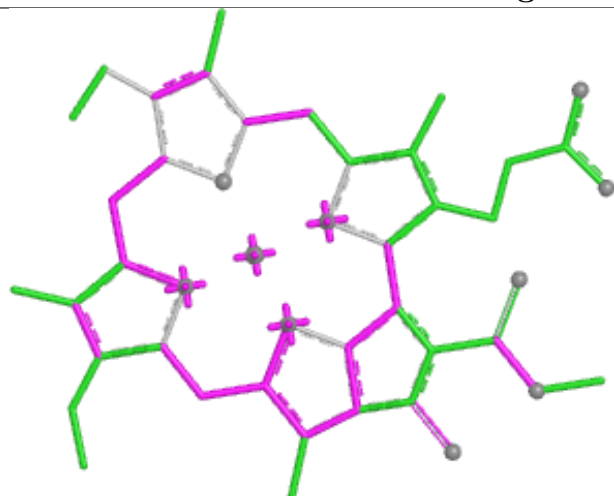


Torsions

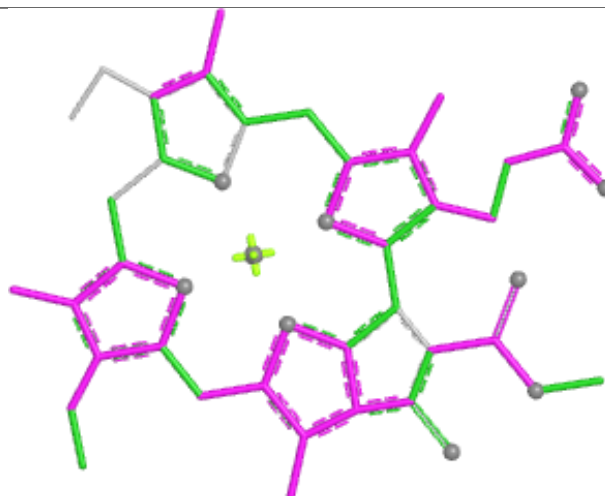


Rings

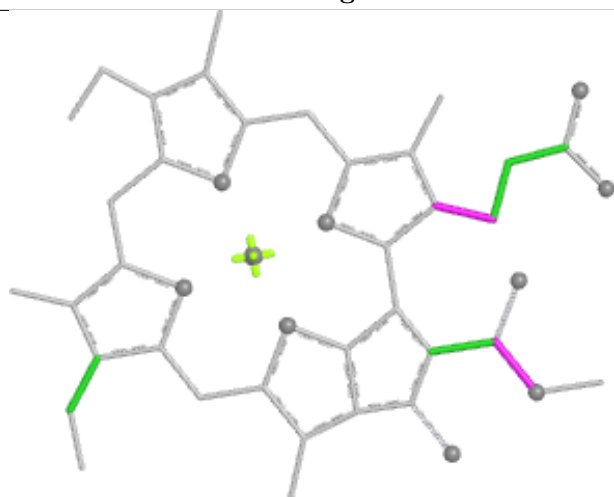
Ligand CLA b 815



Bond lengths



Bond angles

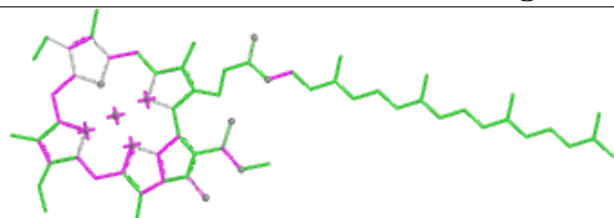


Torsions

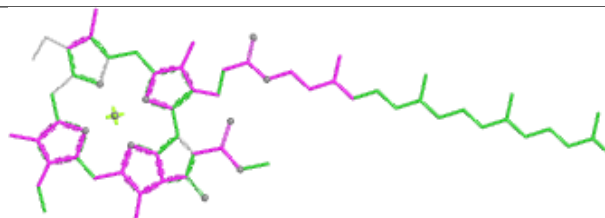


Rings

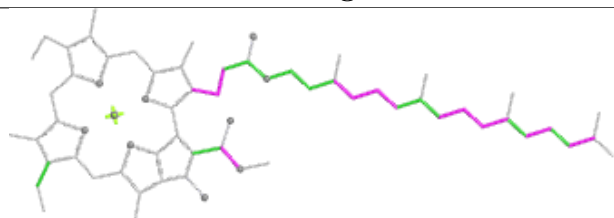
Ligand CLA a 809



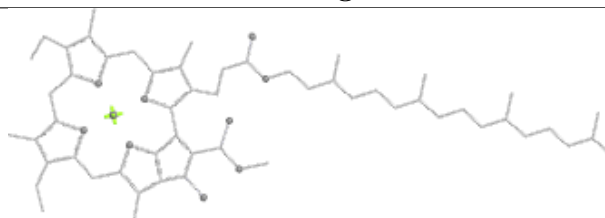
Bond lengths



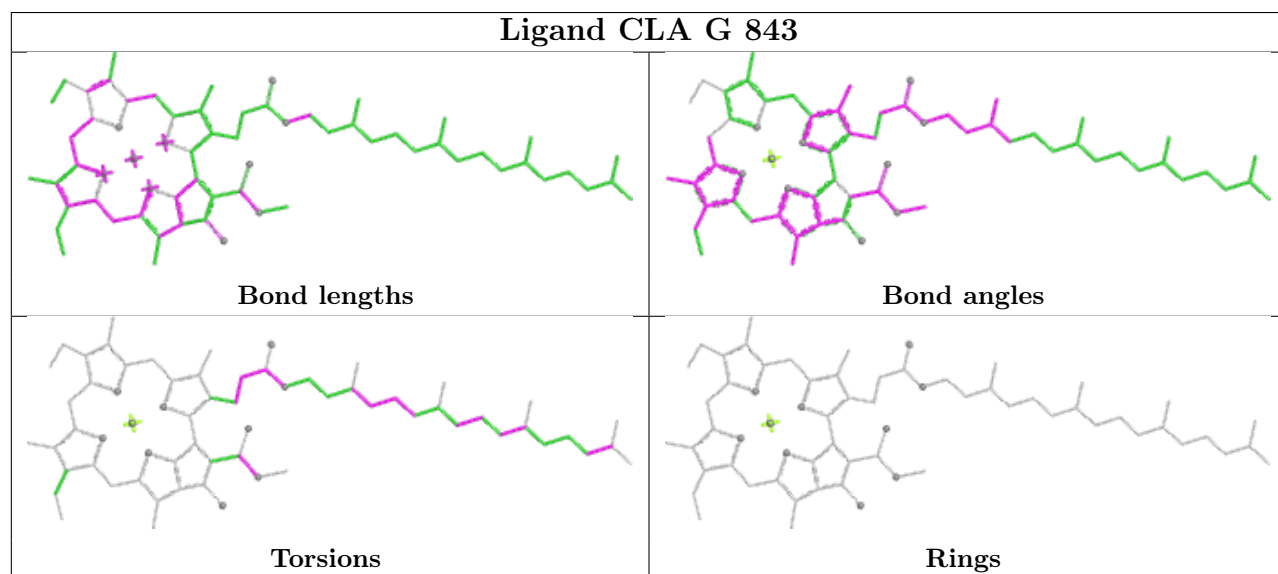
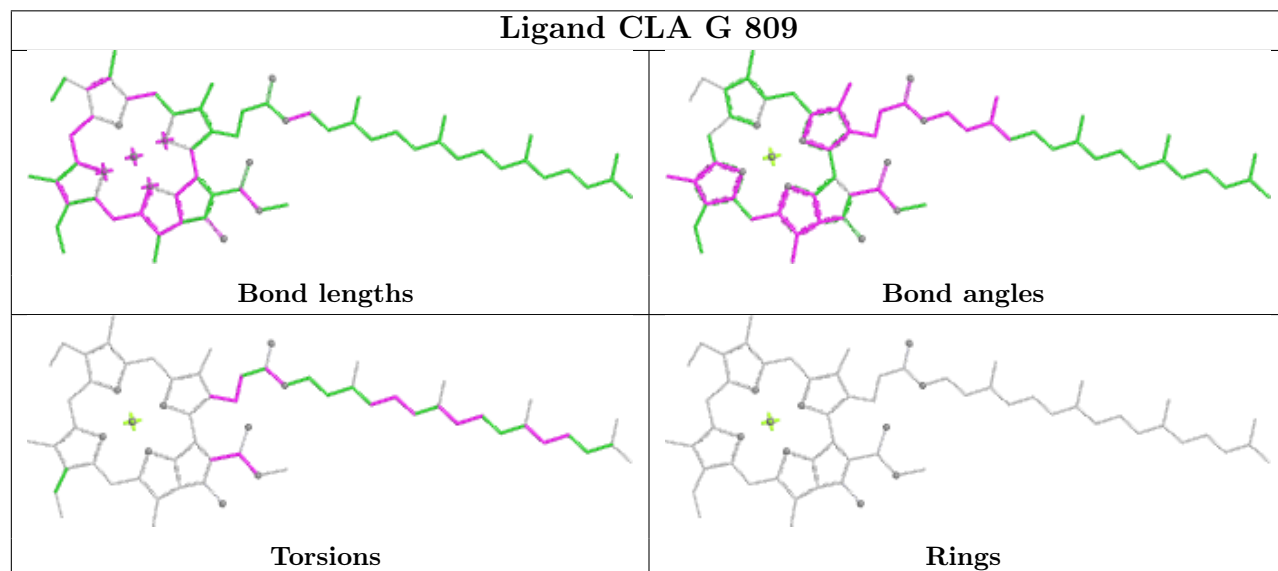
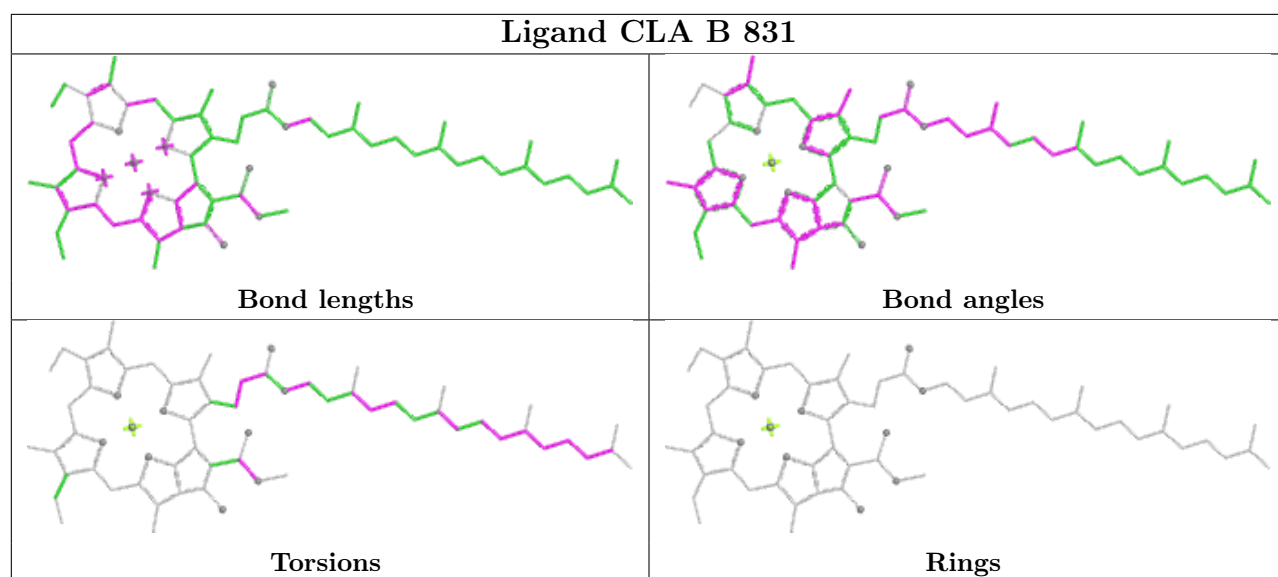
Bond angles

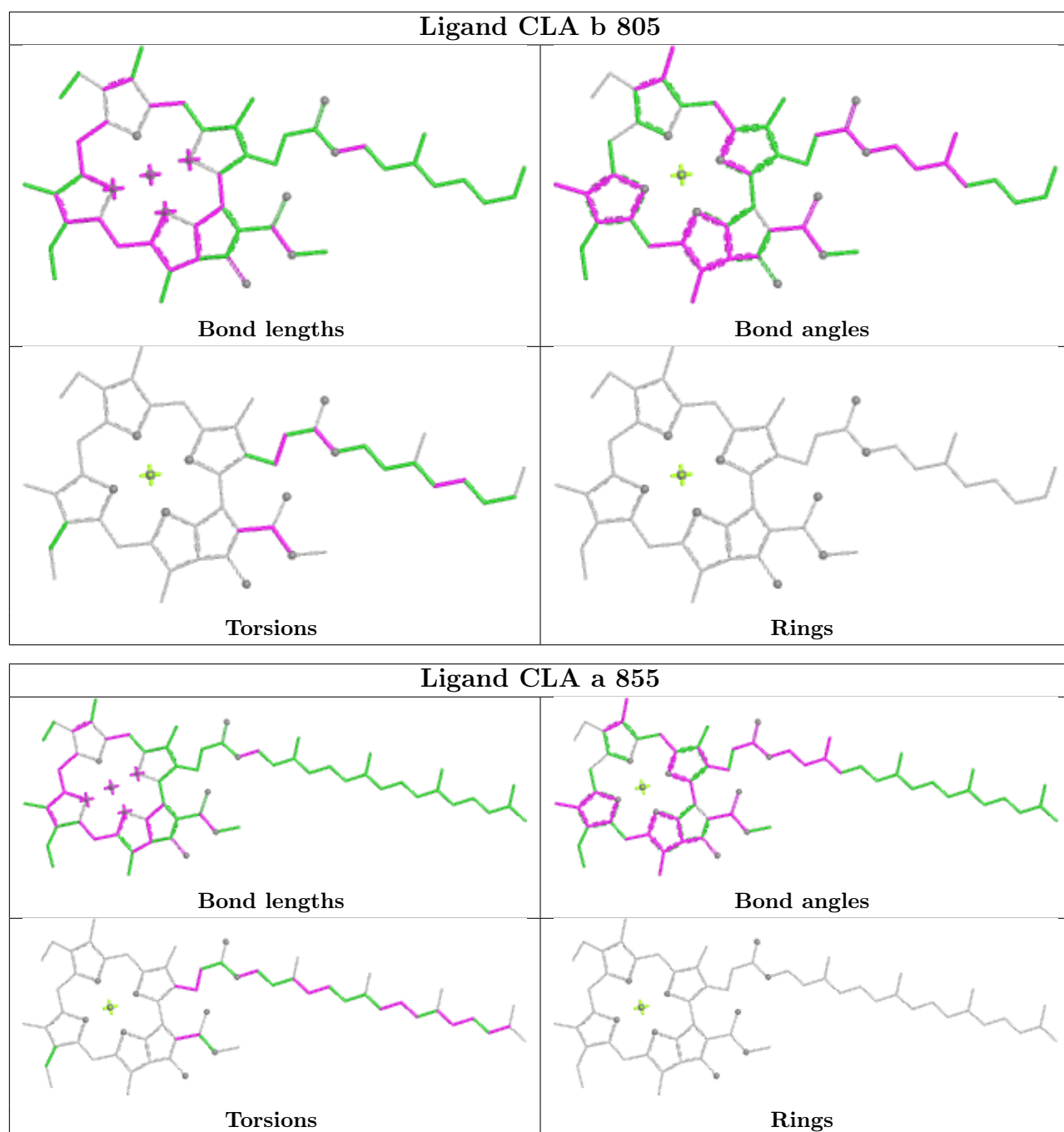


Torsions

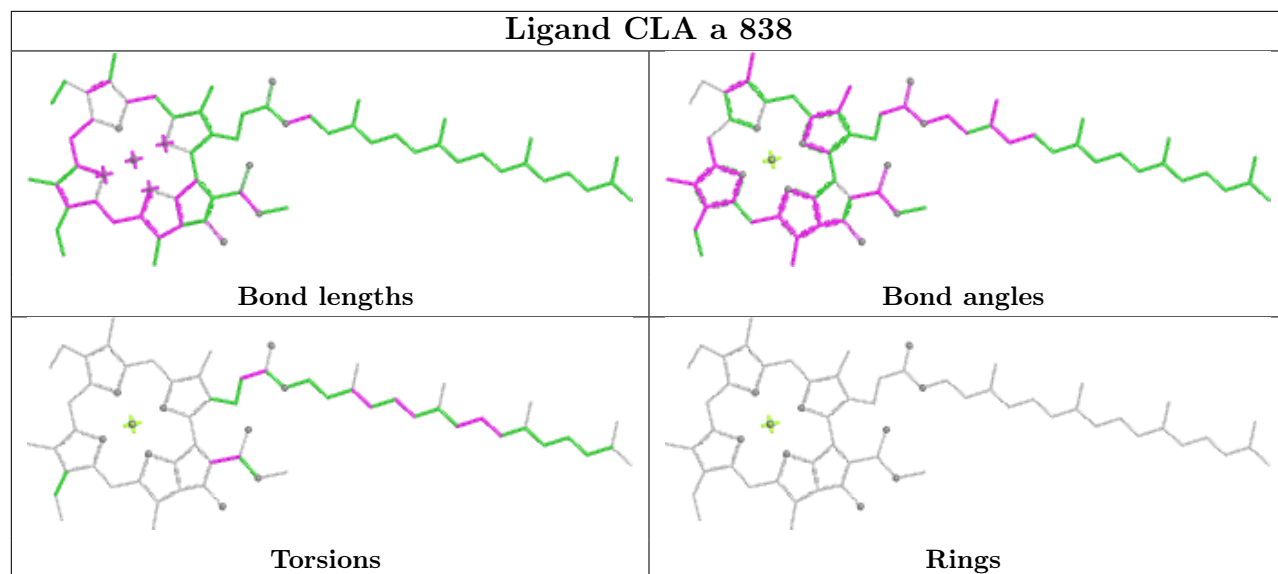


Rings

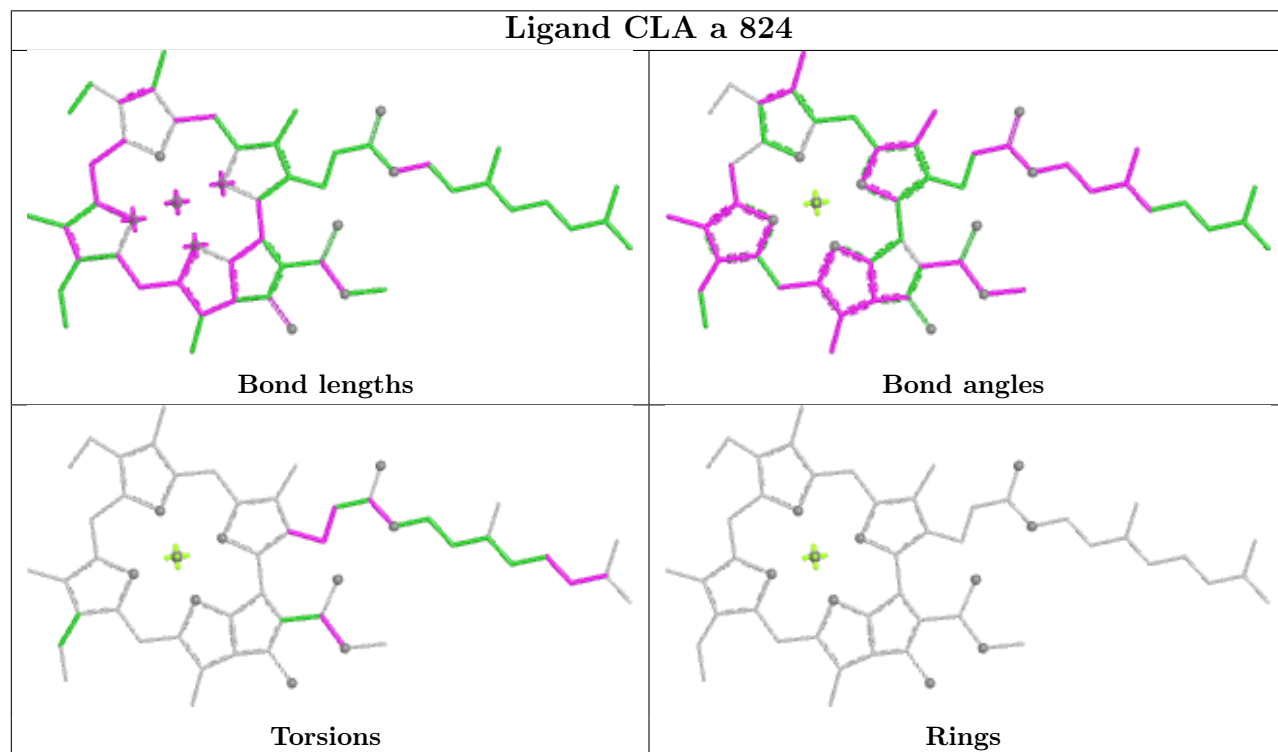


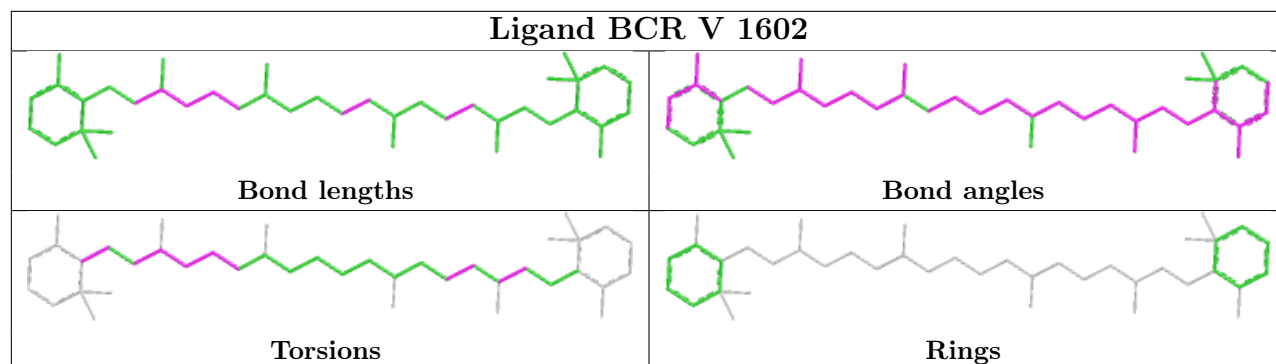
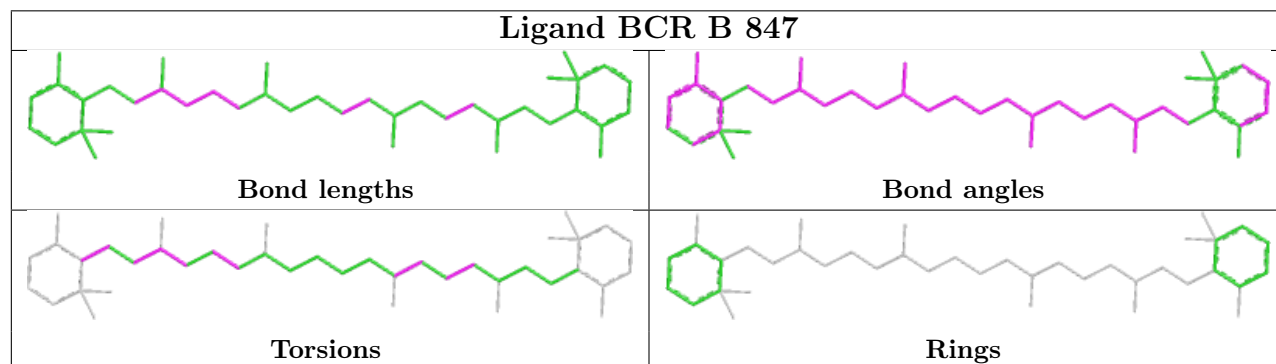
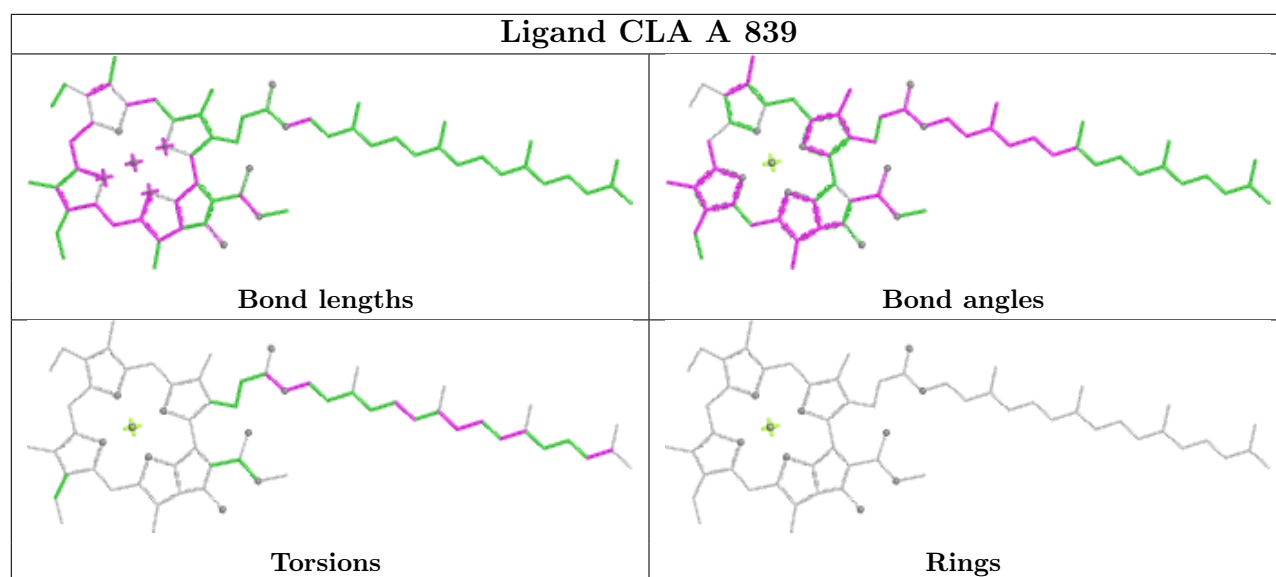


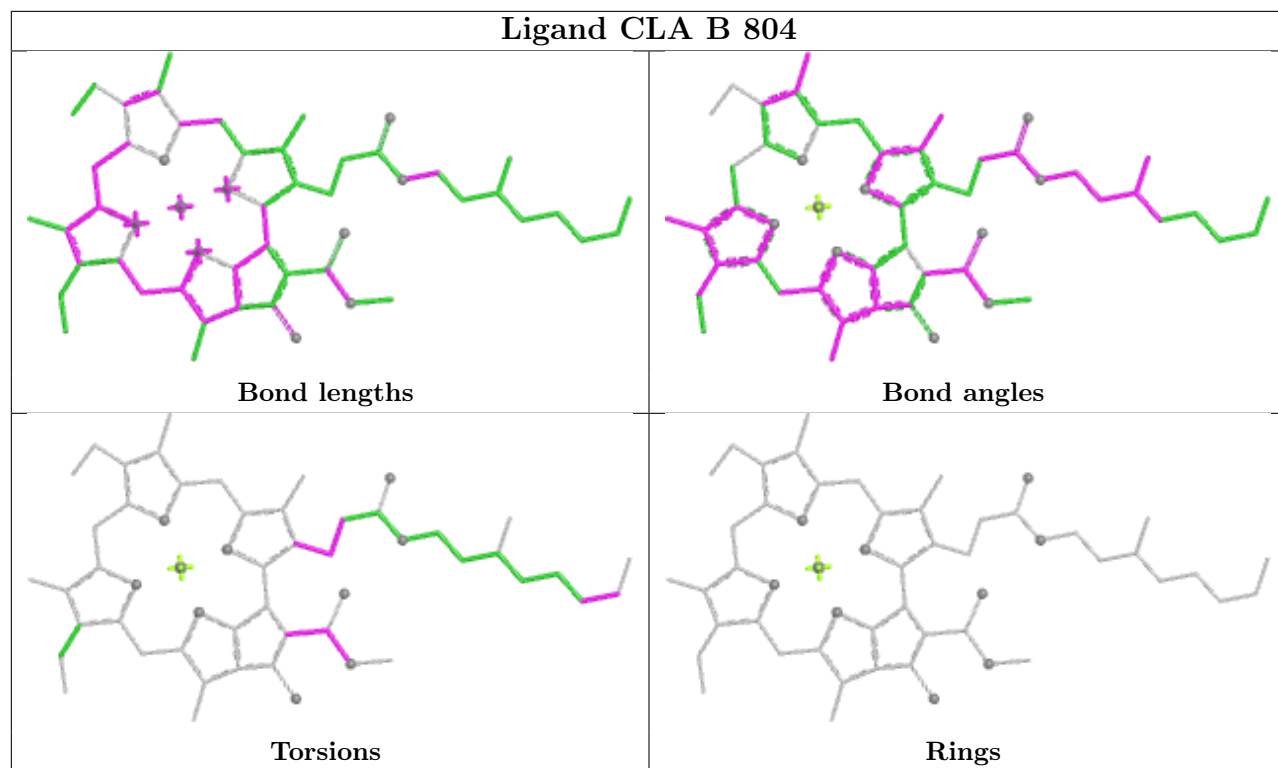
Ligand CLA a 838



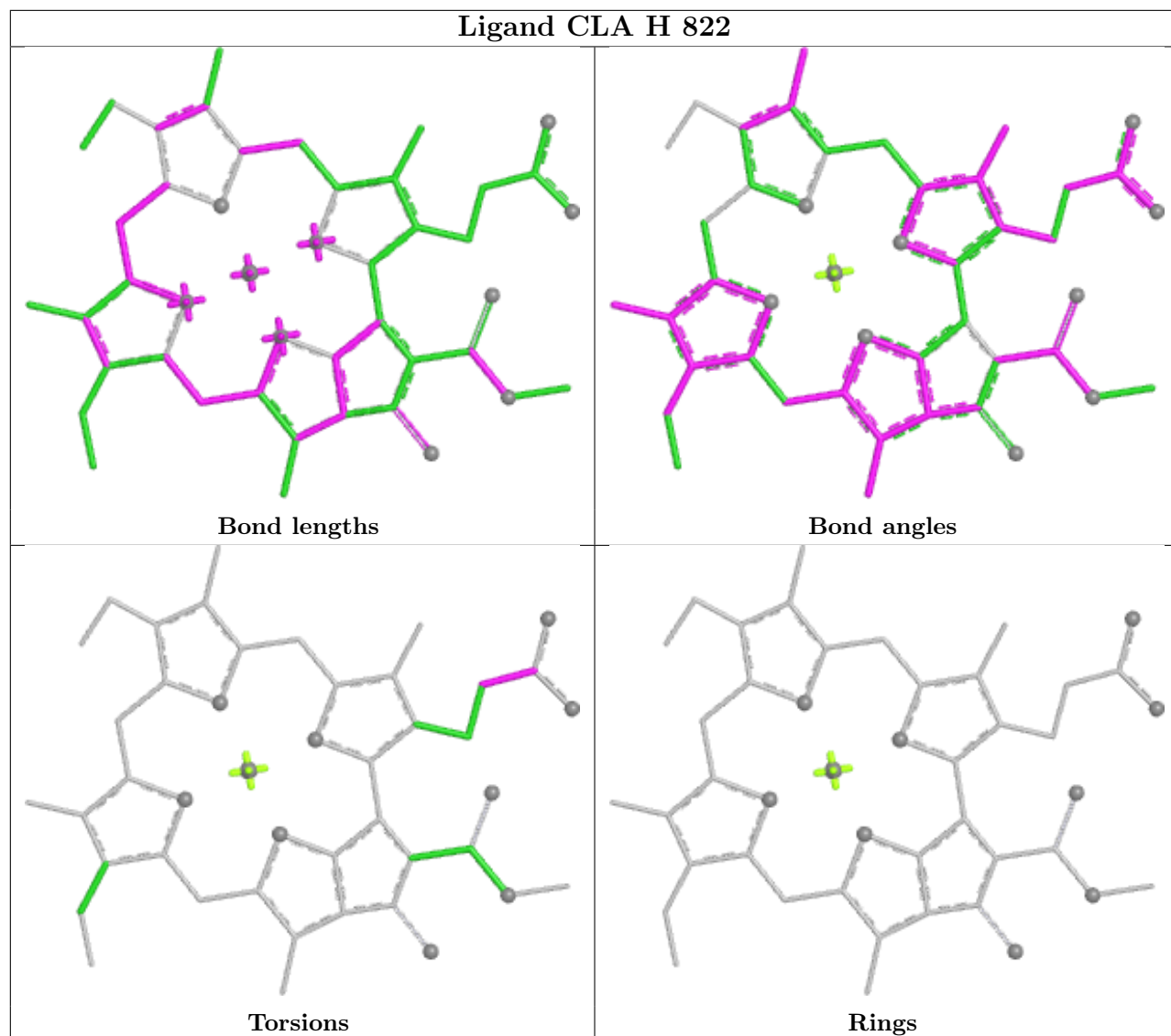
Ligand CLA a 824



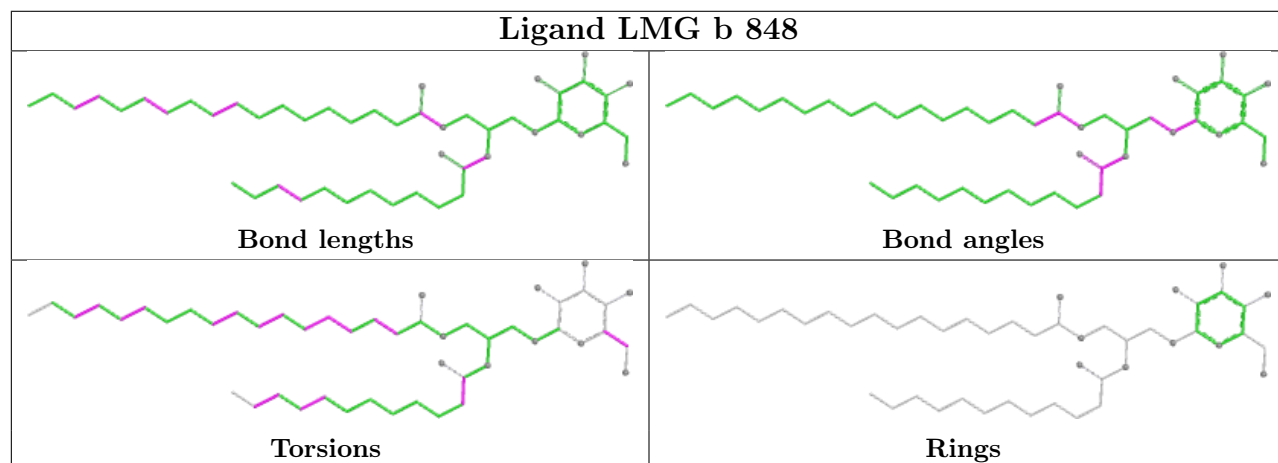


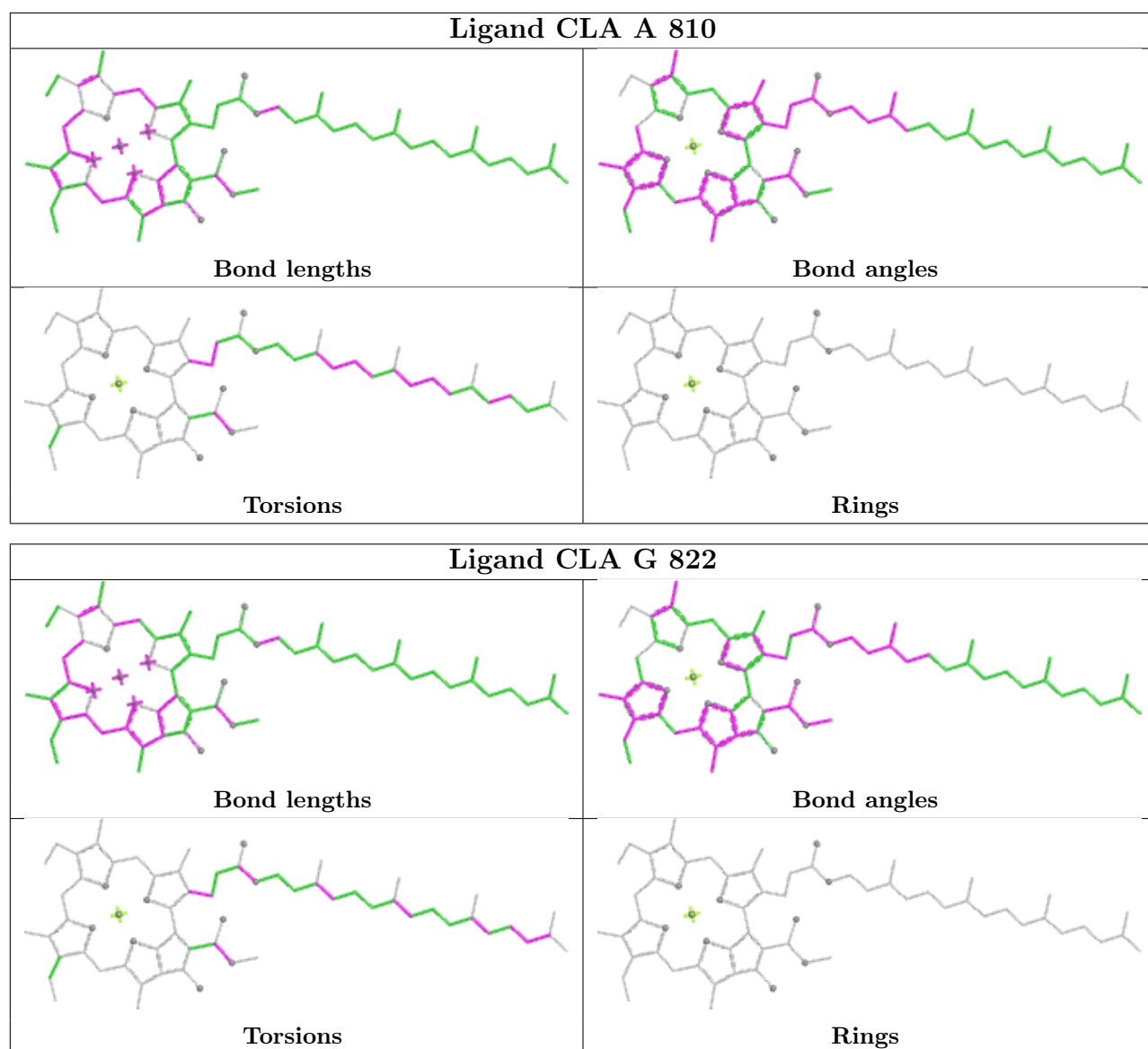


Ligand CLA H 822

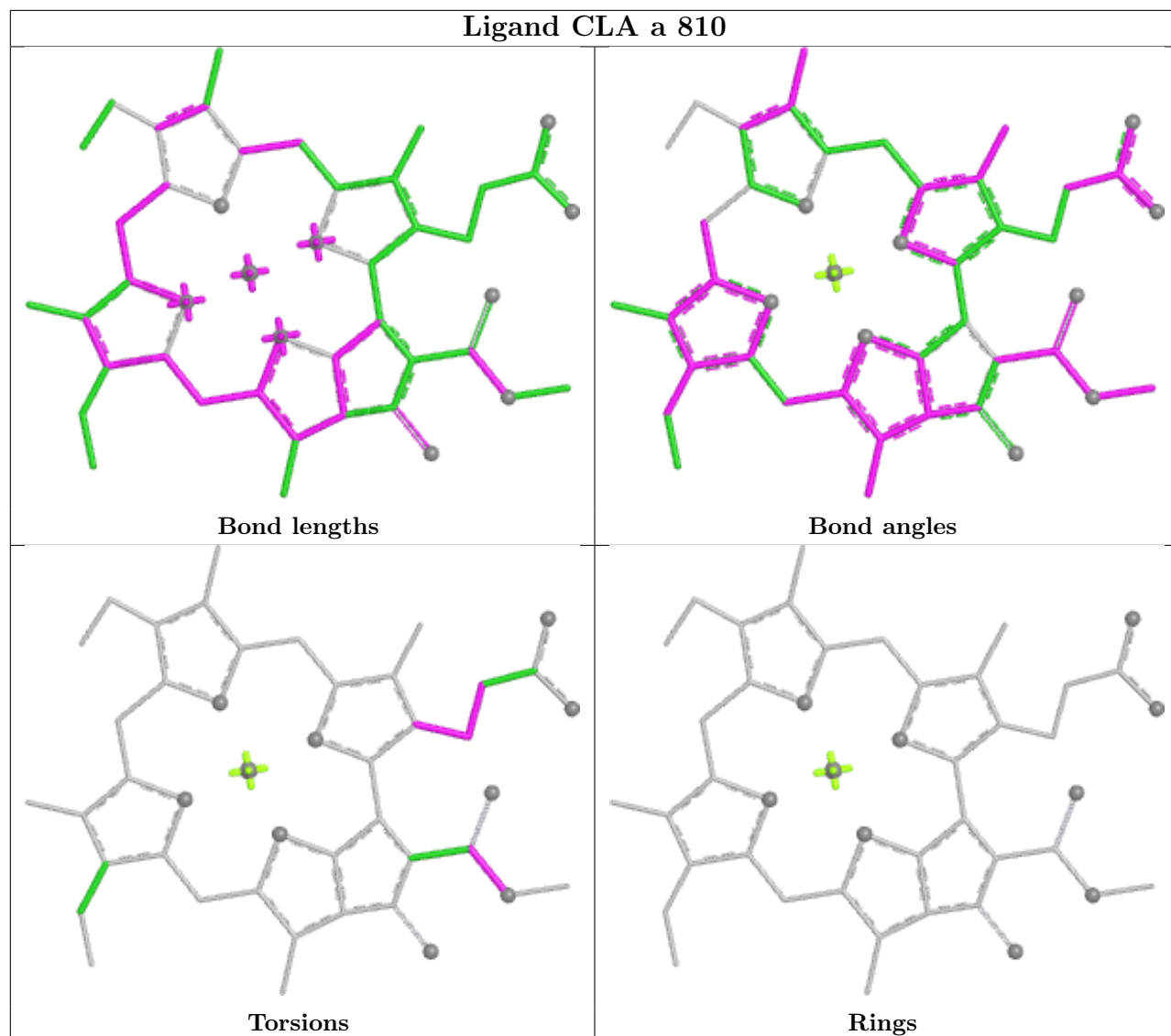


Ligand LMG b 848

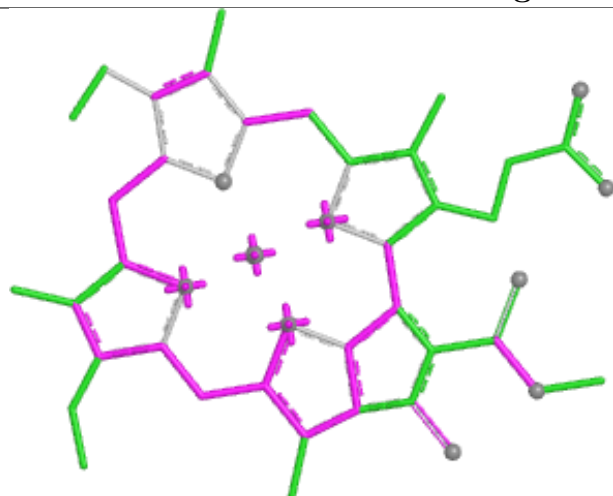




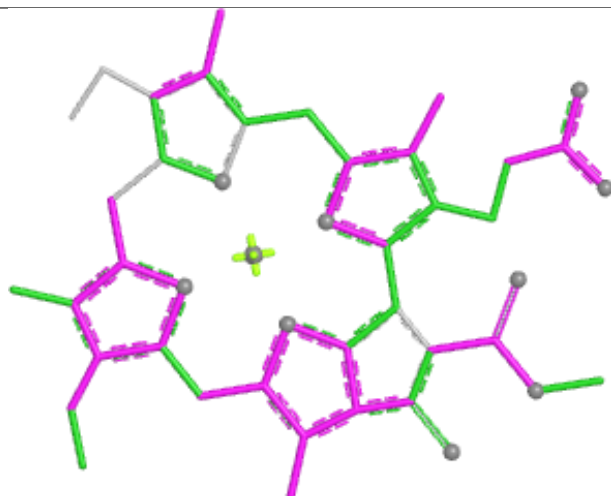
Ligand CLA a 810



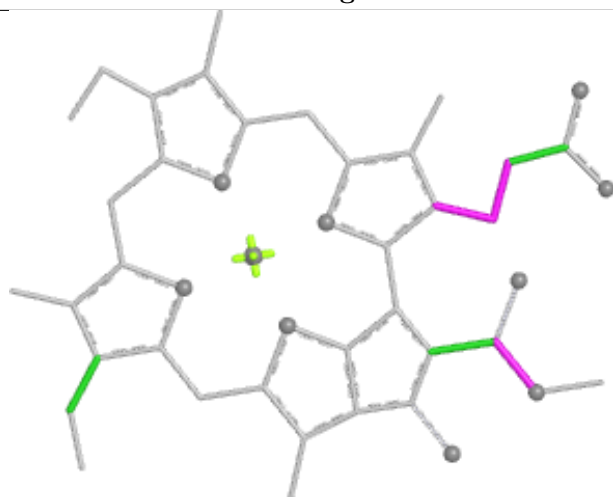
Ligand CLA A 816



Bond lengths



Bond angles

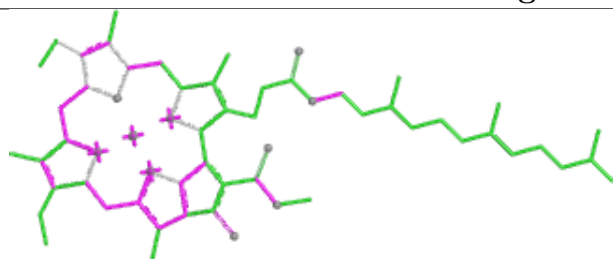


Torsions

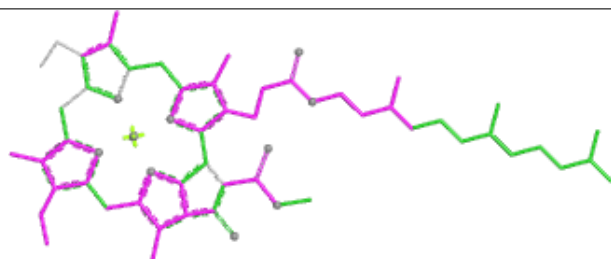


Rings

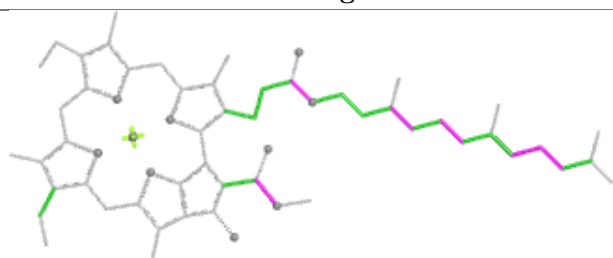
Ligand CLA a 826



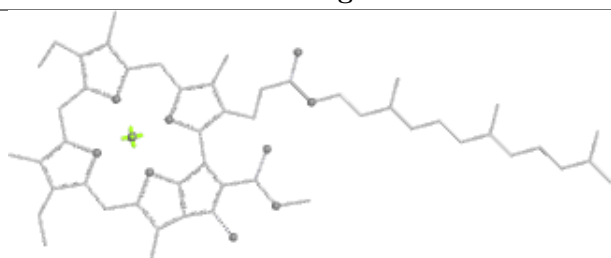
Bond lengths



Bond angles

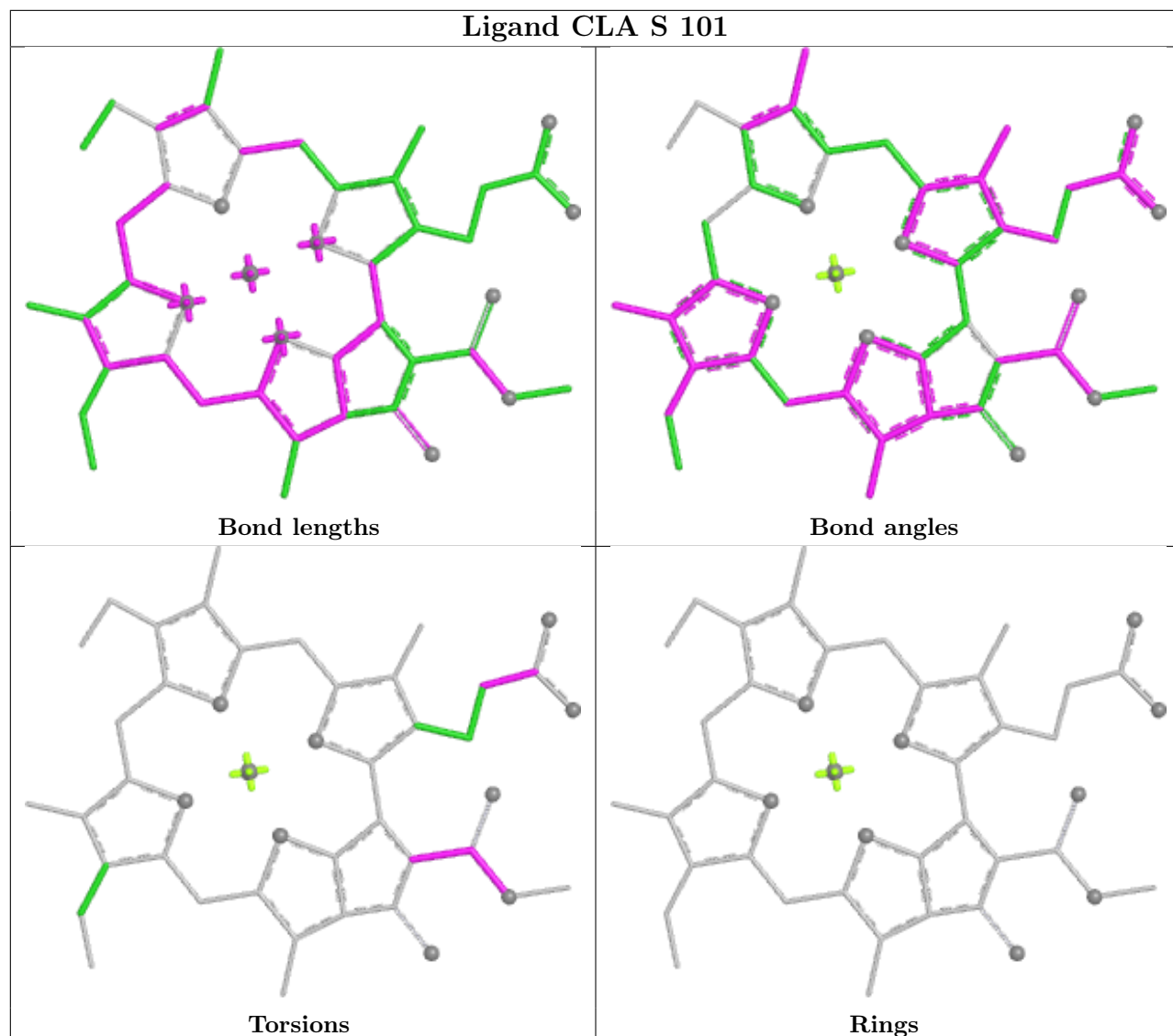


Torsions

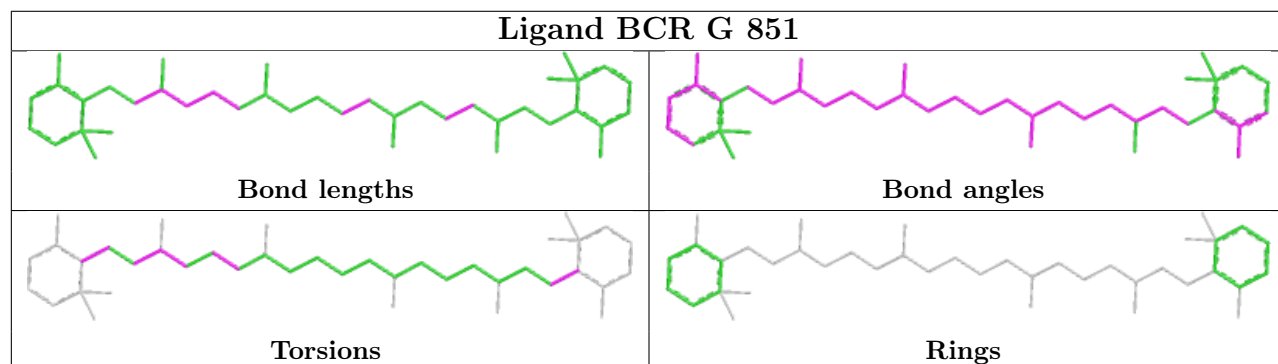


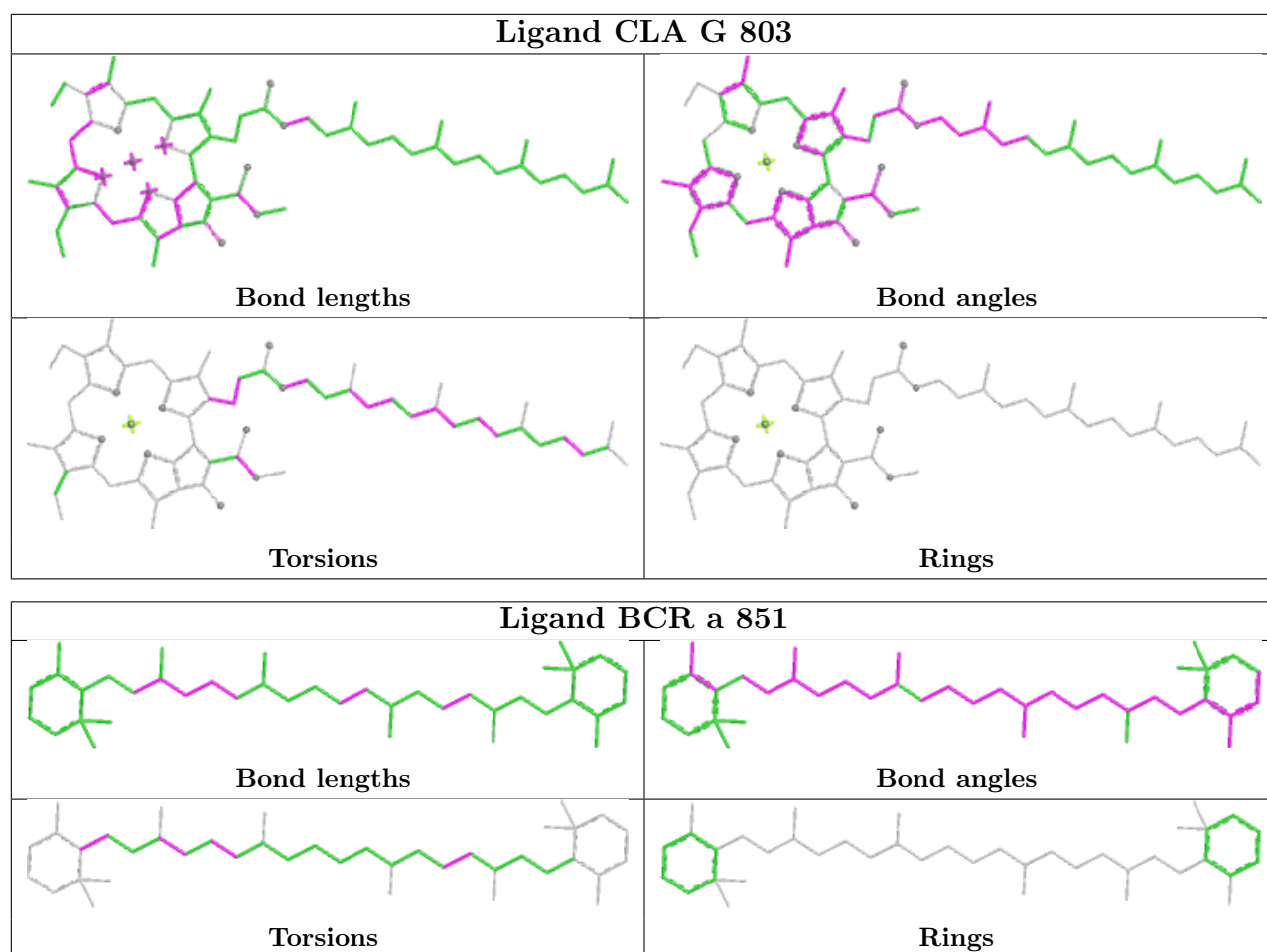
Rings

Ligand CLA S 101

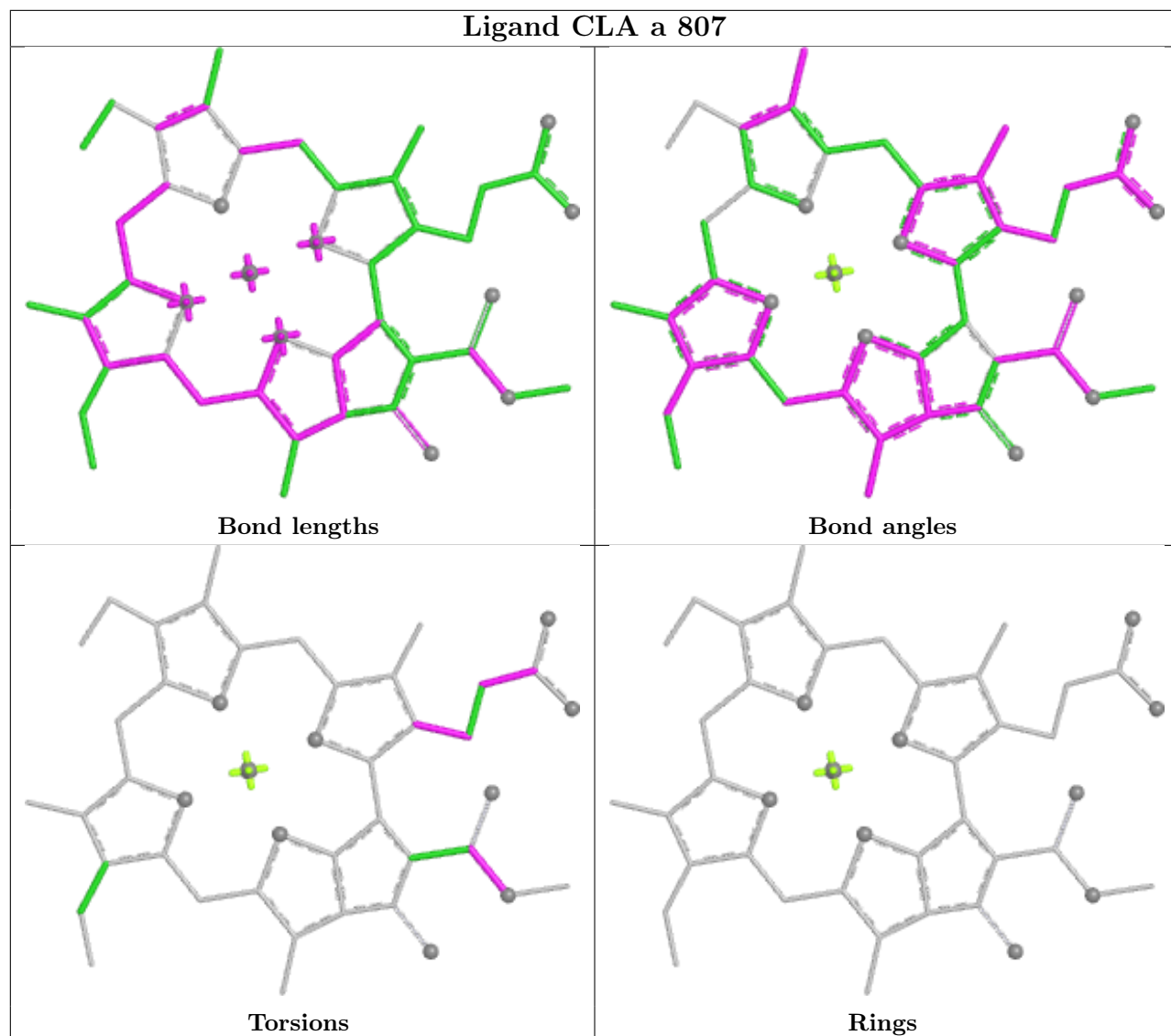


Ligand BCR G 851

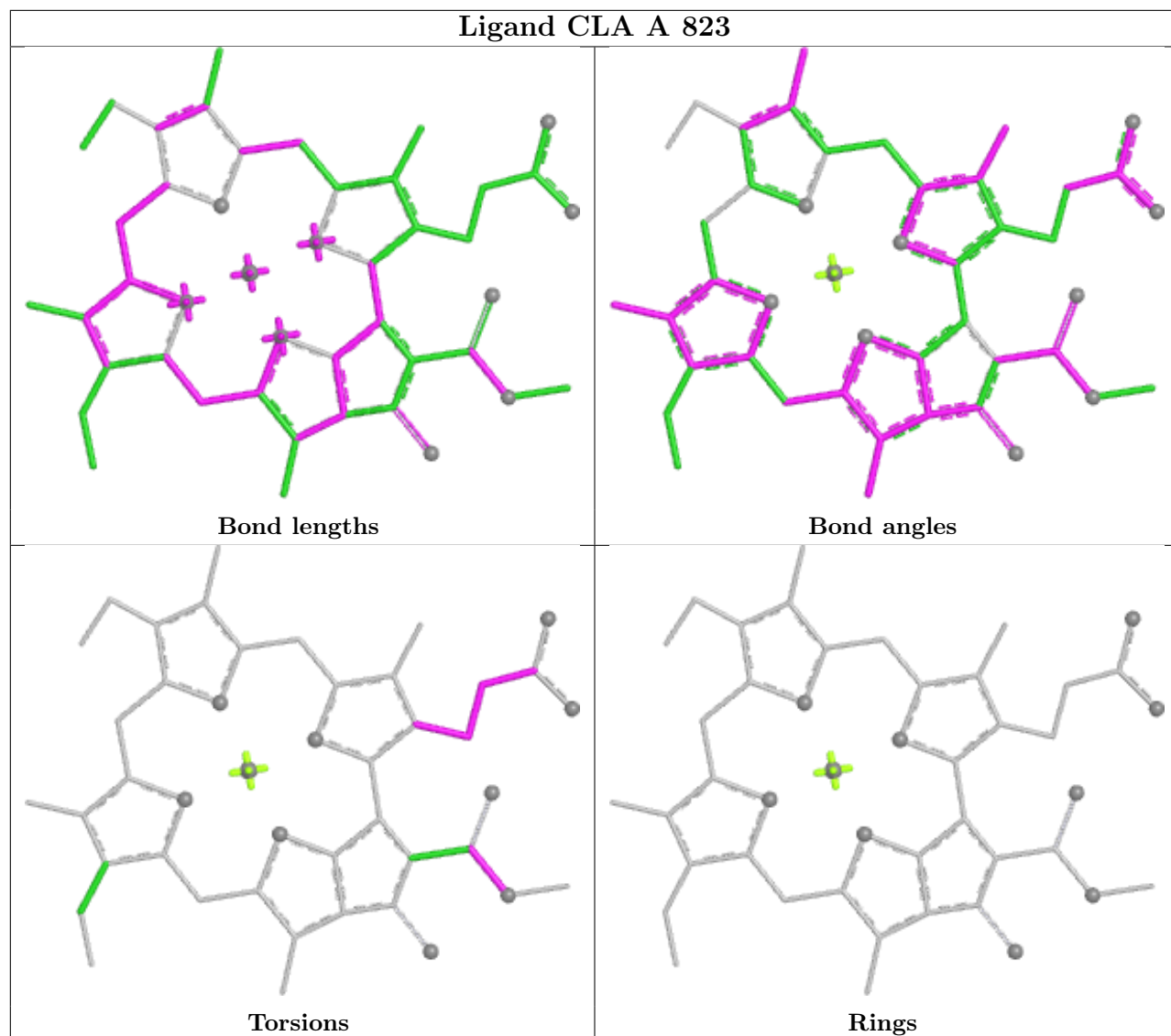




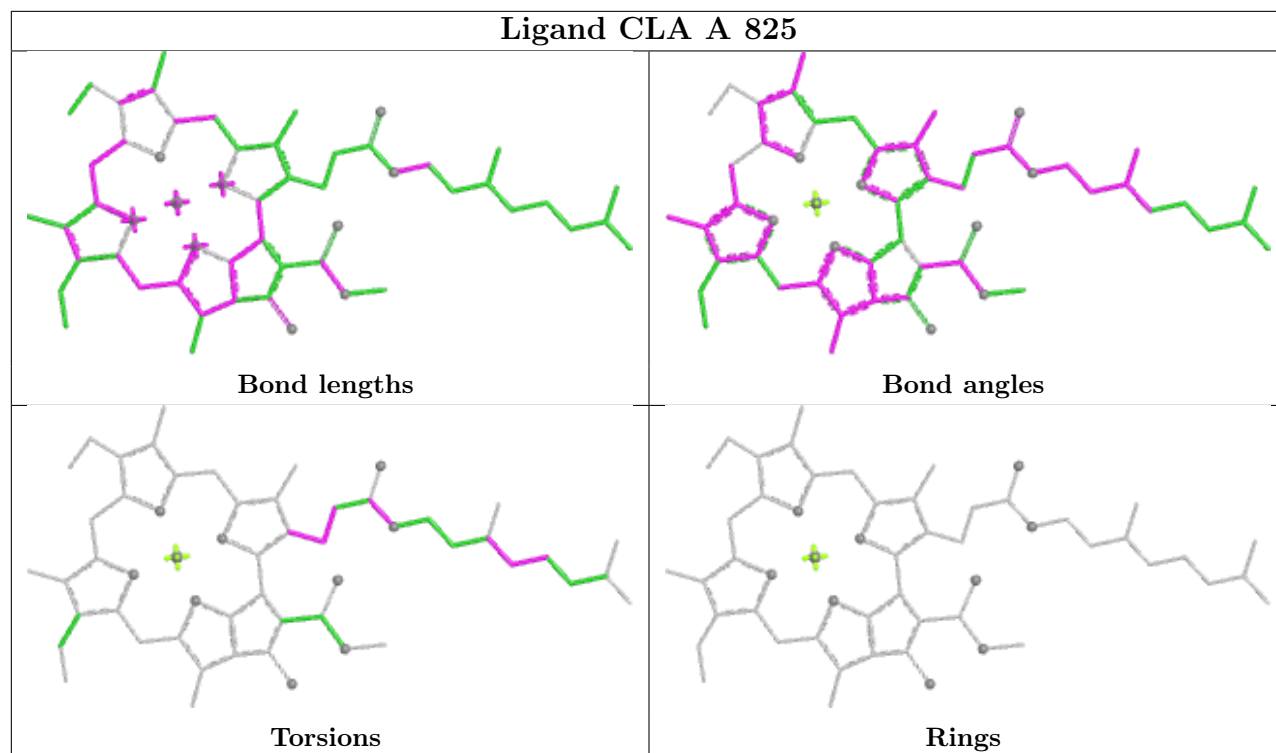
Ligand CLA a 807



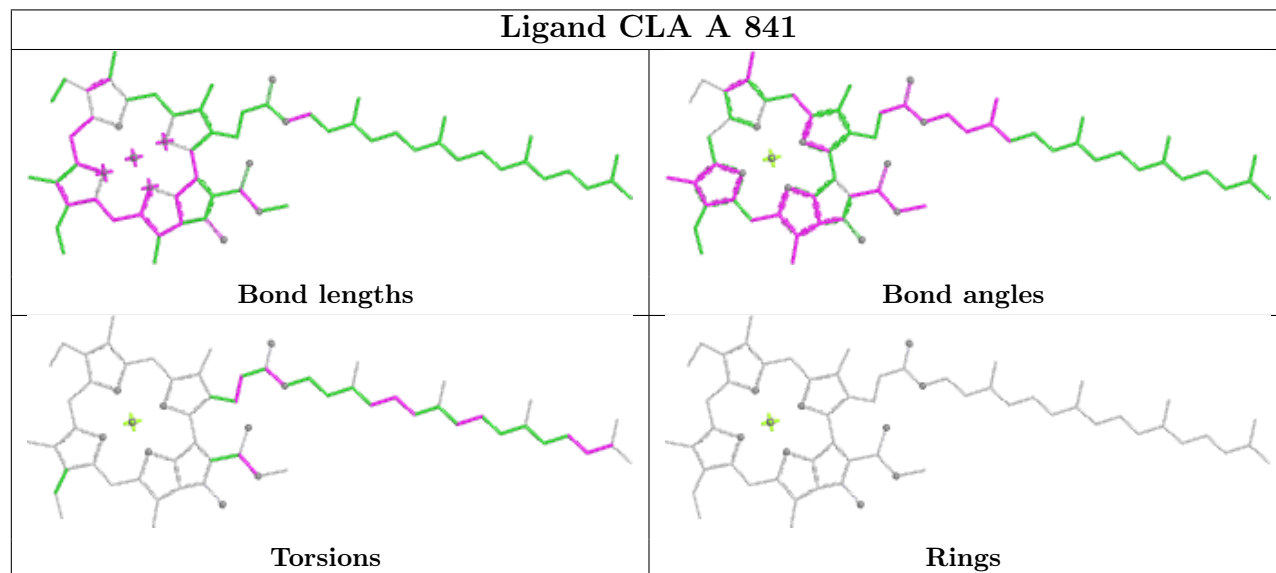
Ligand CLA A 823



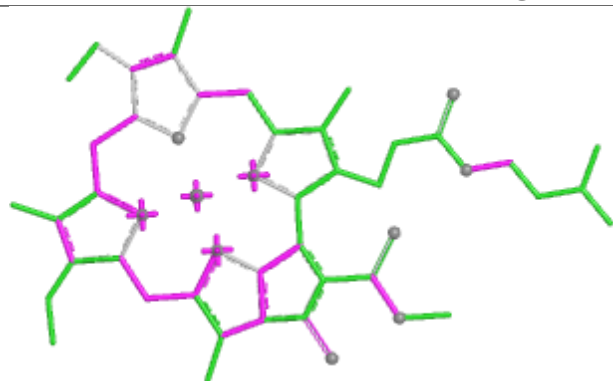
Ligand CLA A 825



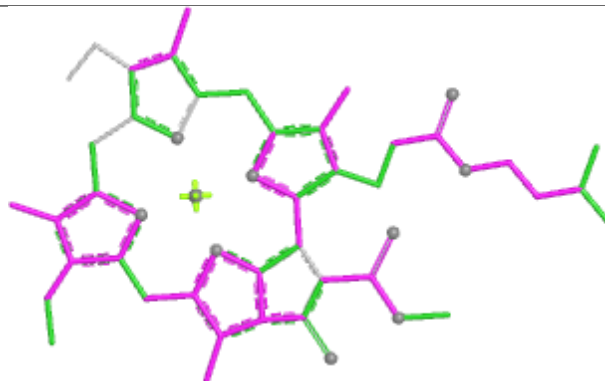
Ligand CLA A 841



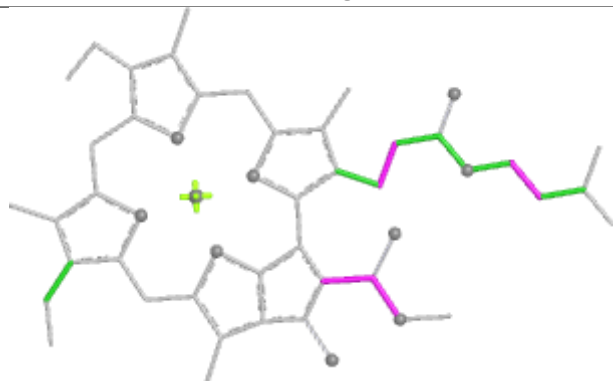
Ligand CLA H 823



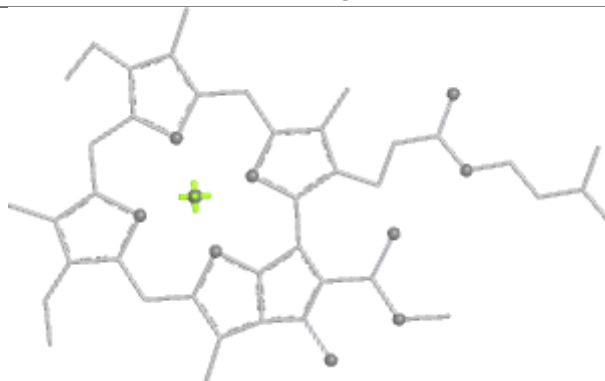
Bond lengths



Bond angles

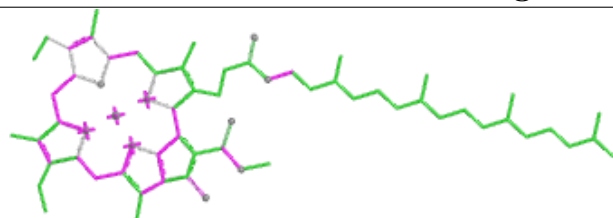


Torsions

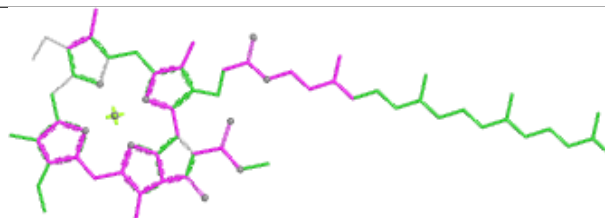


Rings

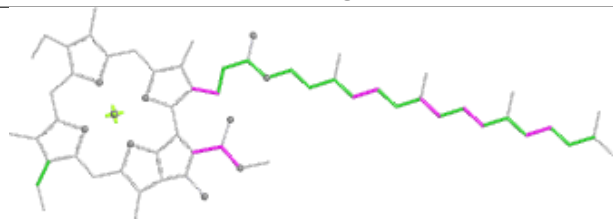
Ligand CLA H 825



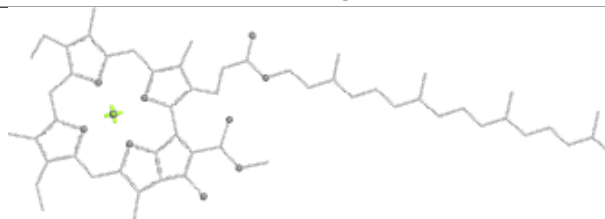
Bond lengths



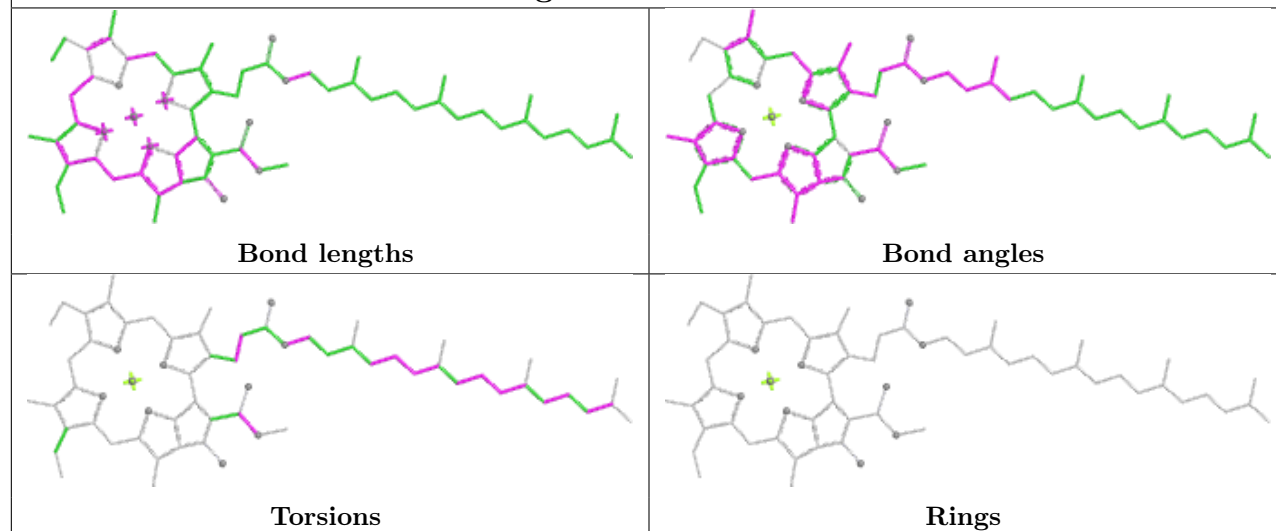
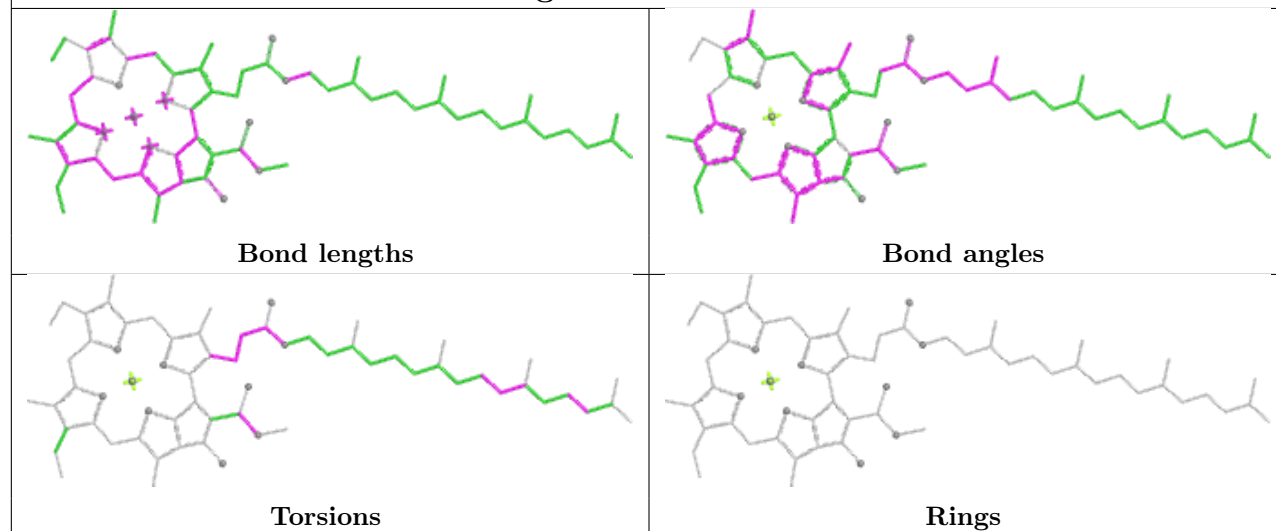
Bond angles



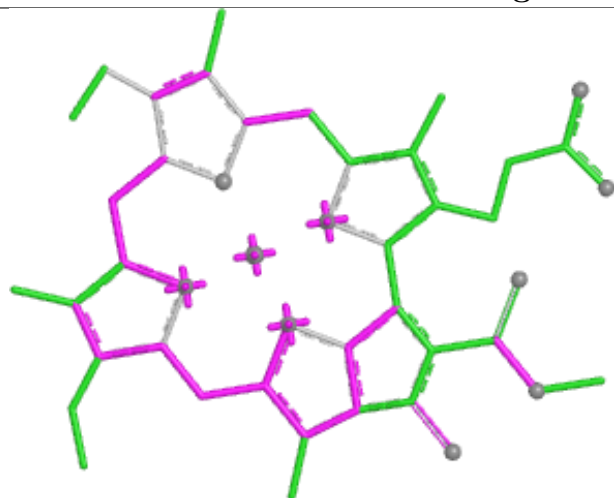
Torsions



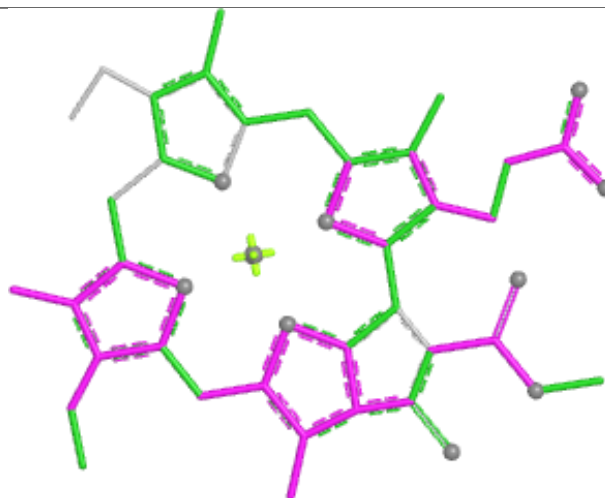
Rings

Ligand CLA b 839**Ligand CLA a 811**

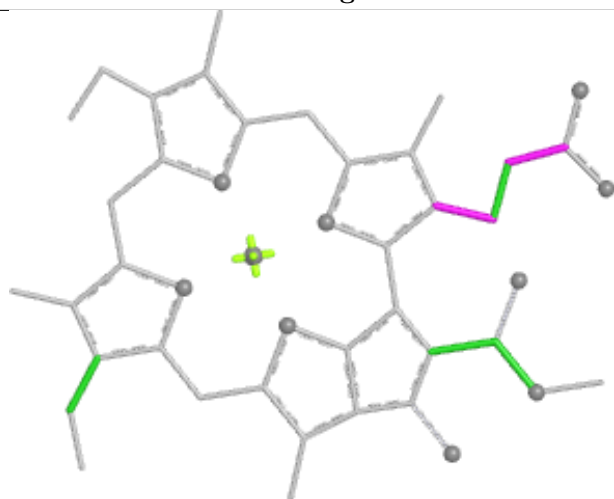
Ligand CLA G 840



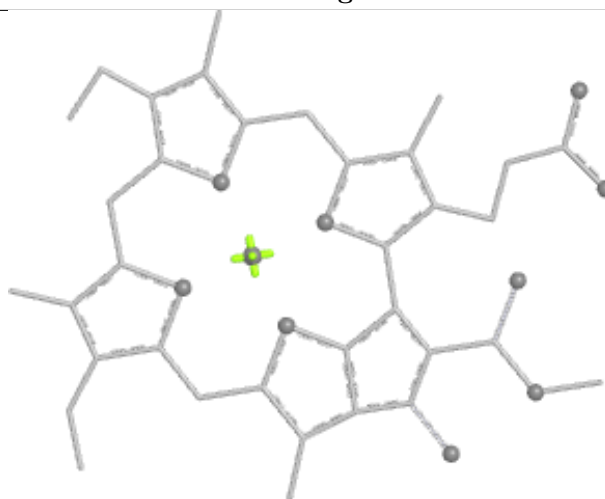
Bond lengths



Bond angles

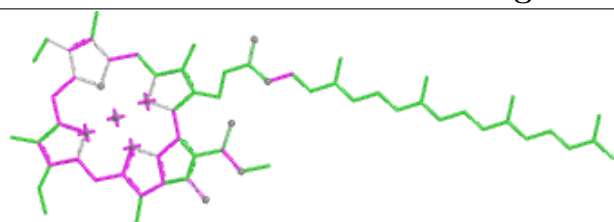


Torsions

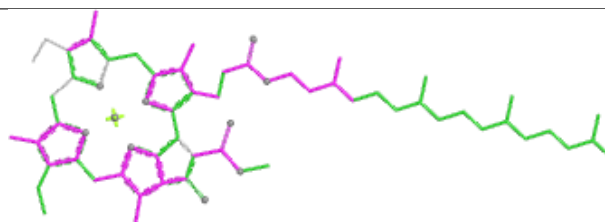


Rings

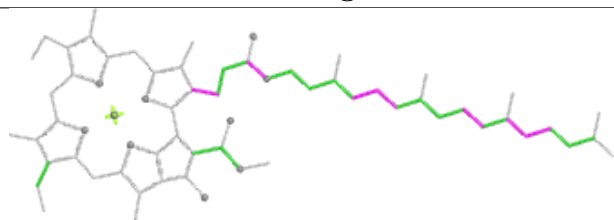
Ligand CLA B 818



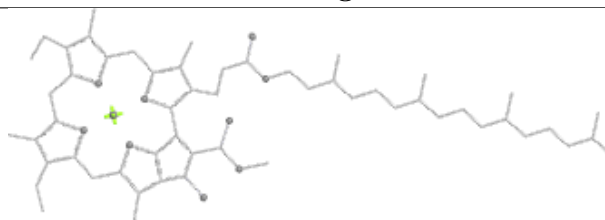
Bond lengths



Bond angles

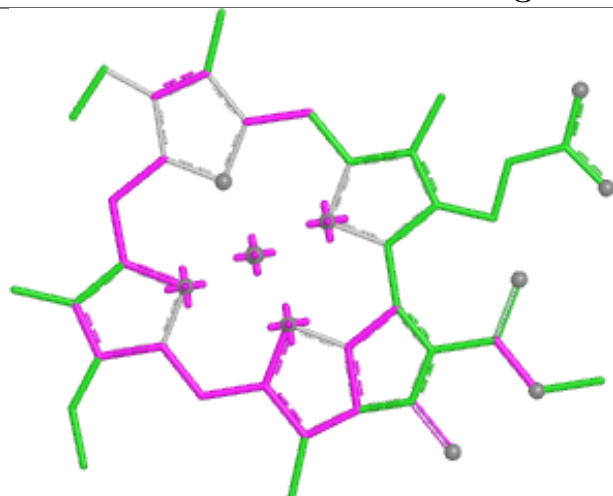


Torsions

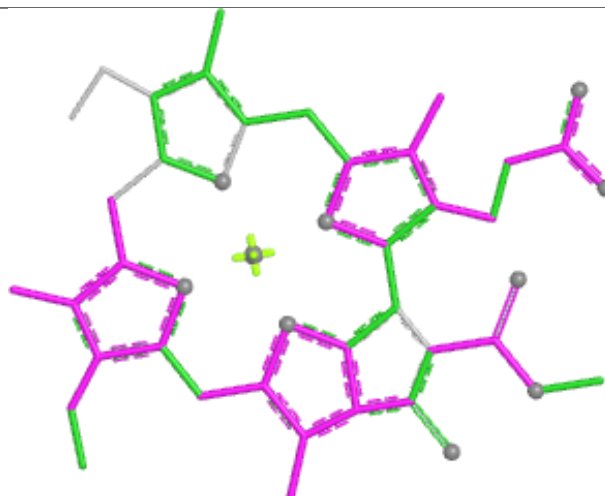


Rings

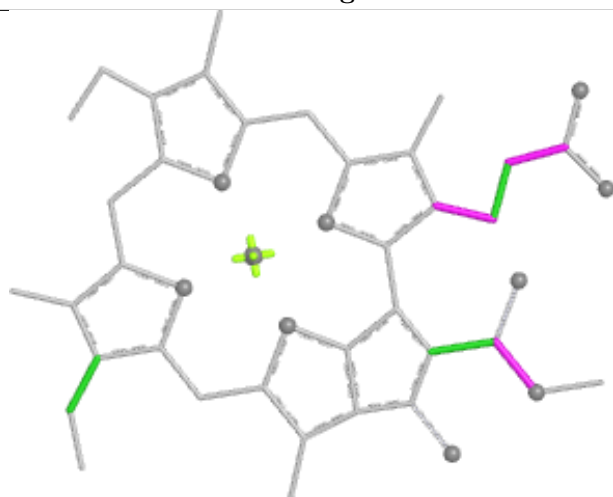
Ligand CLA B 835



Bond lengths



Bond angles

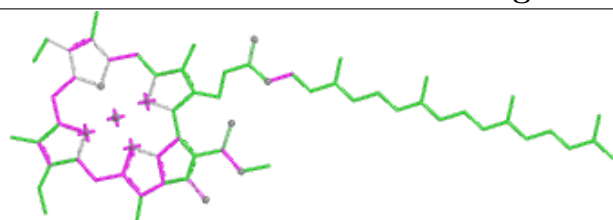


Torsions



Rings

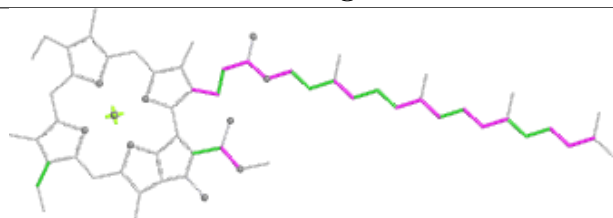
Ligand CLA G 807



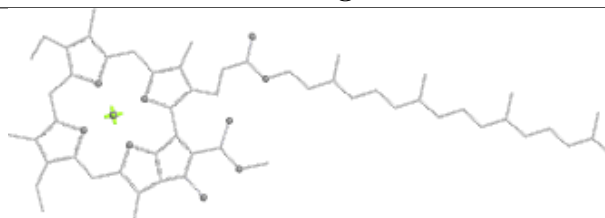
Bond lengths



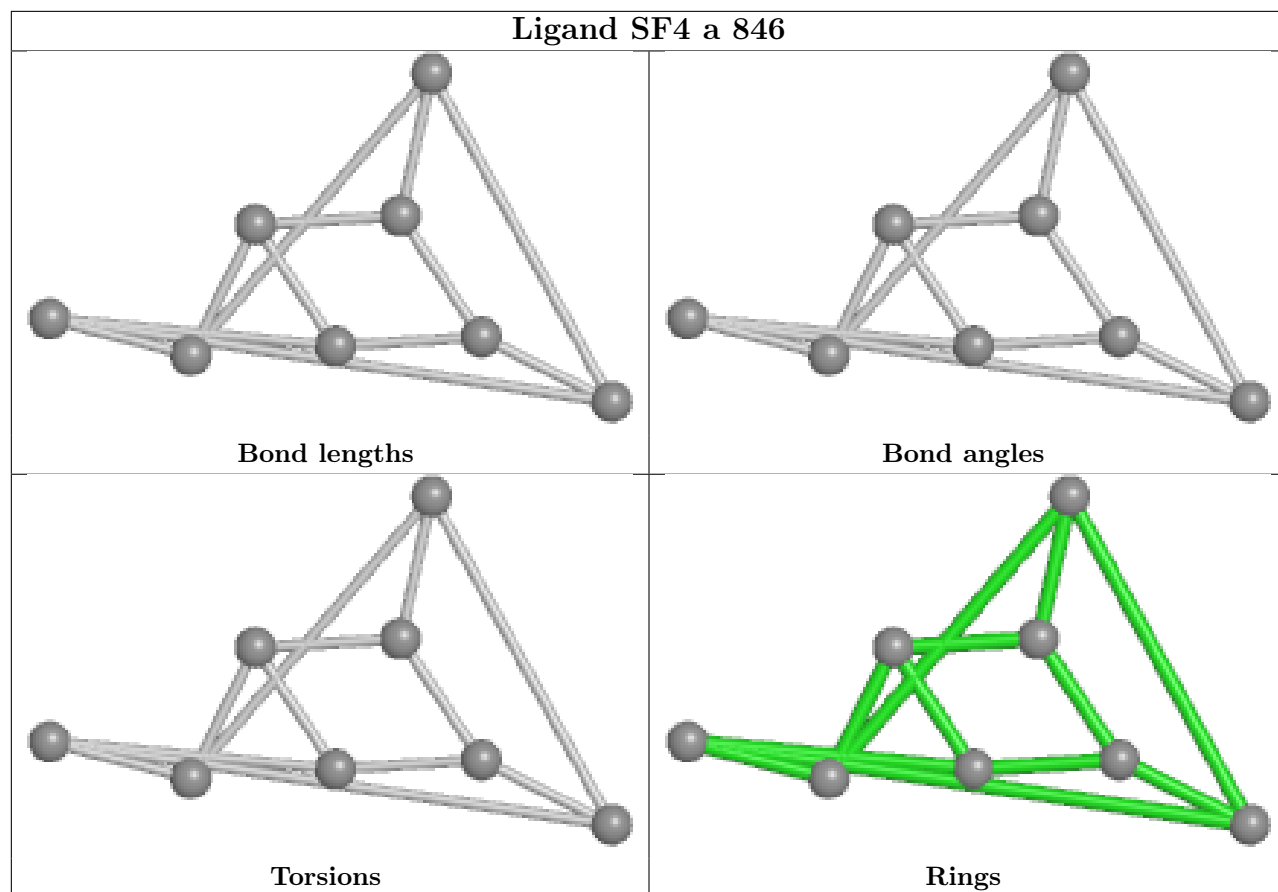
Bond angles



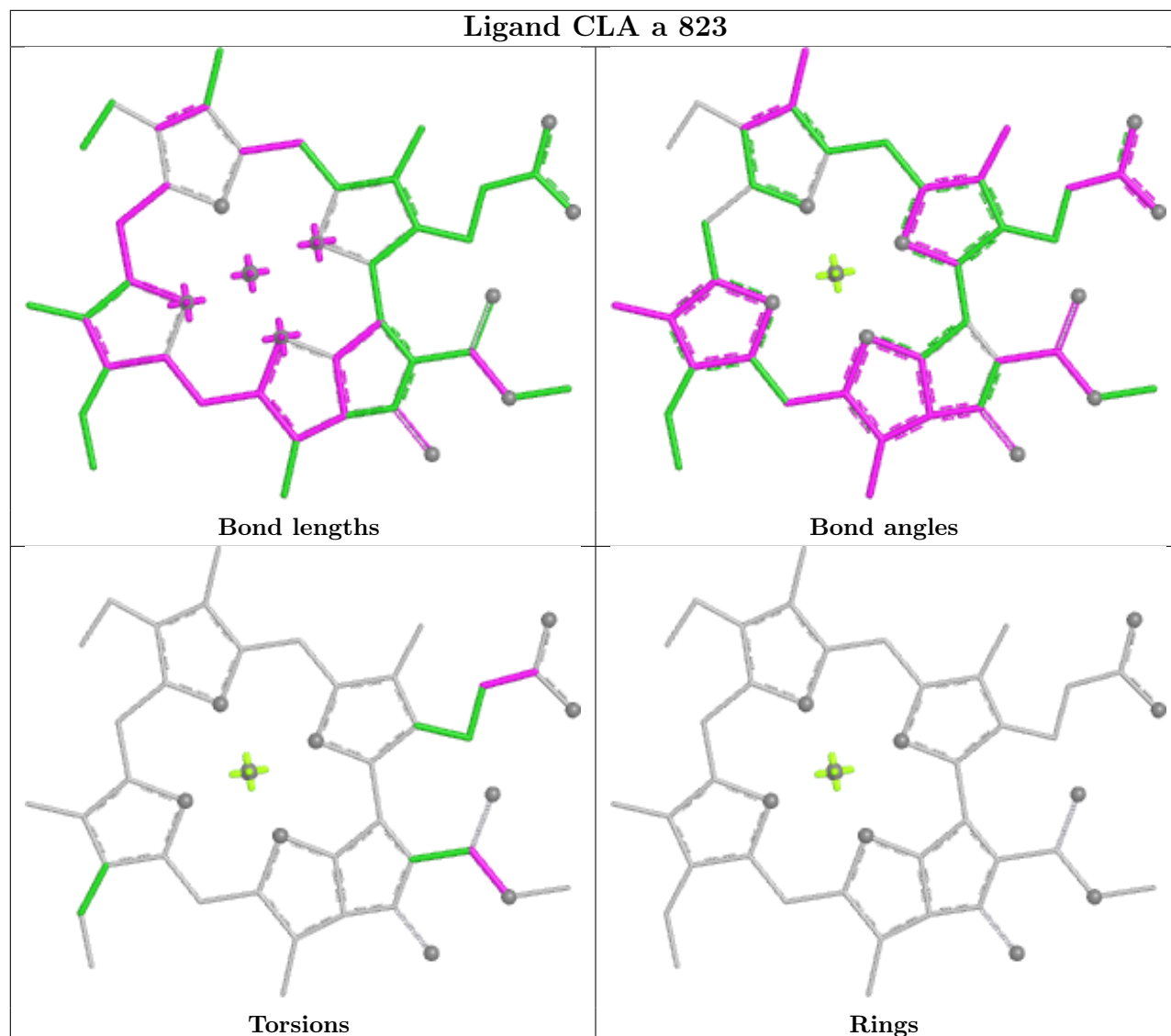
Torsions



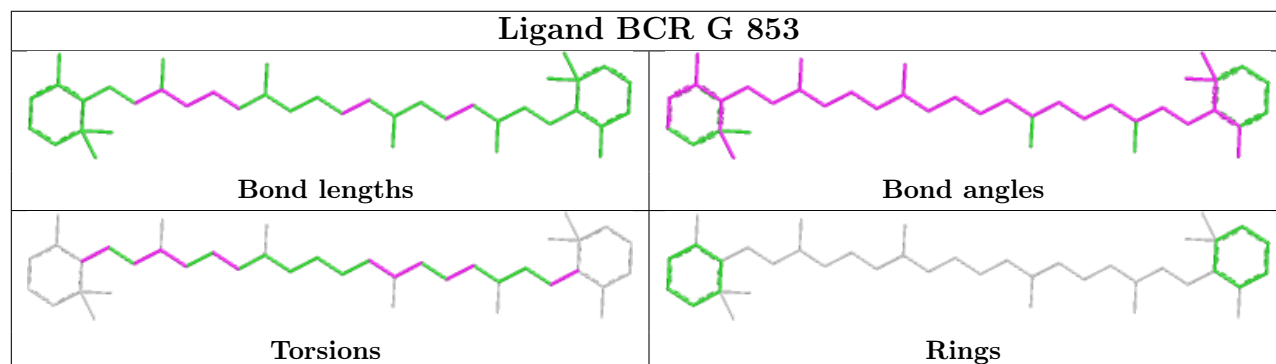
Rings

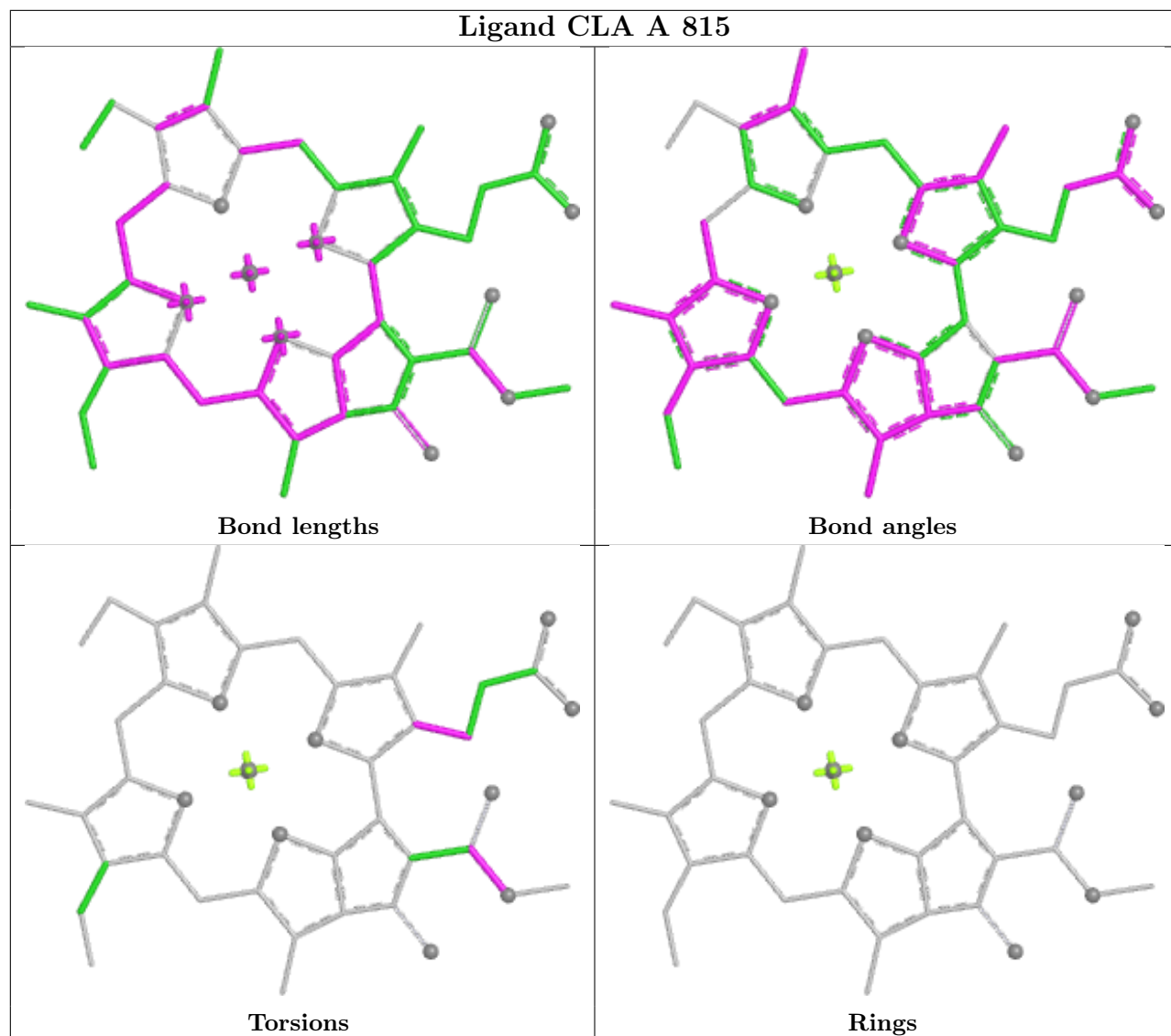


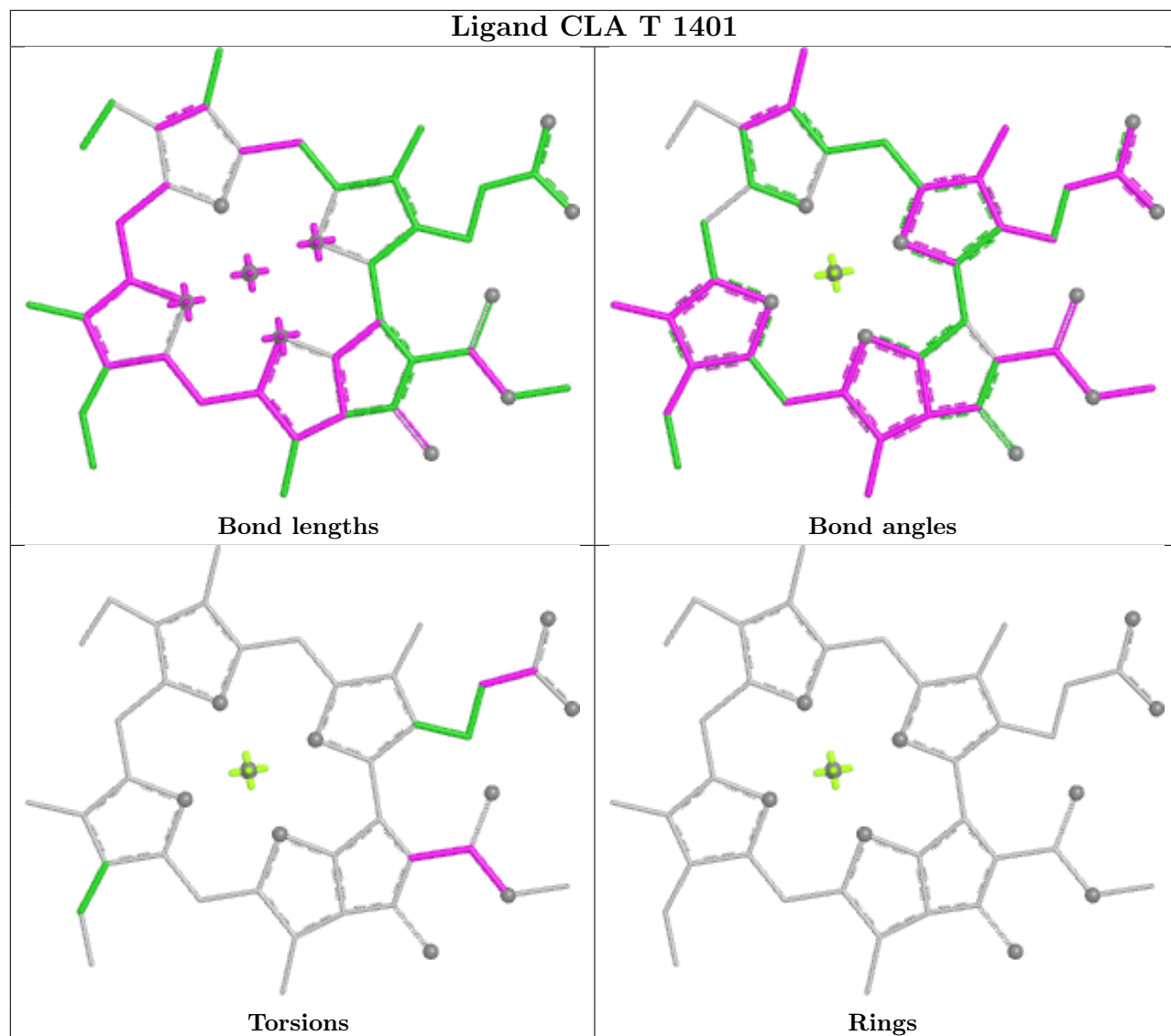
Ligand CLA a 823

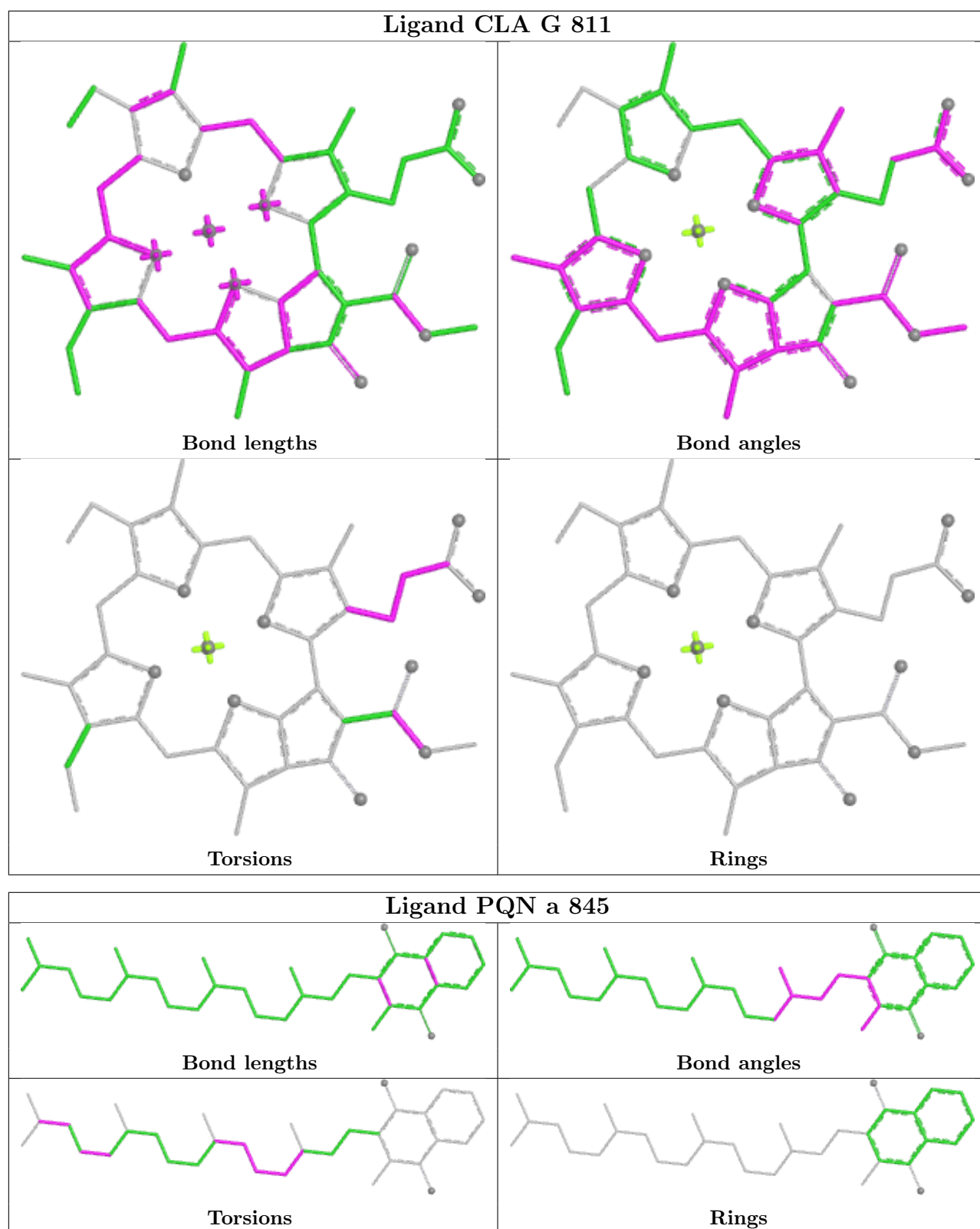


Ligand BCR G 853

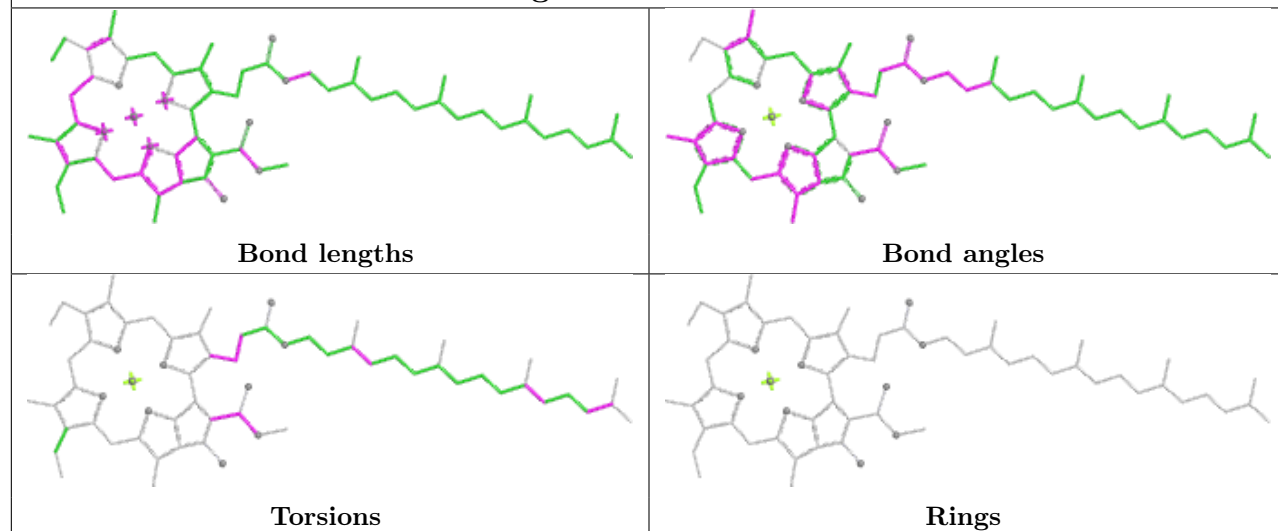




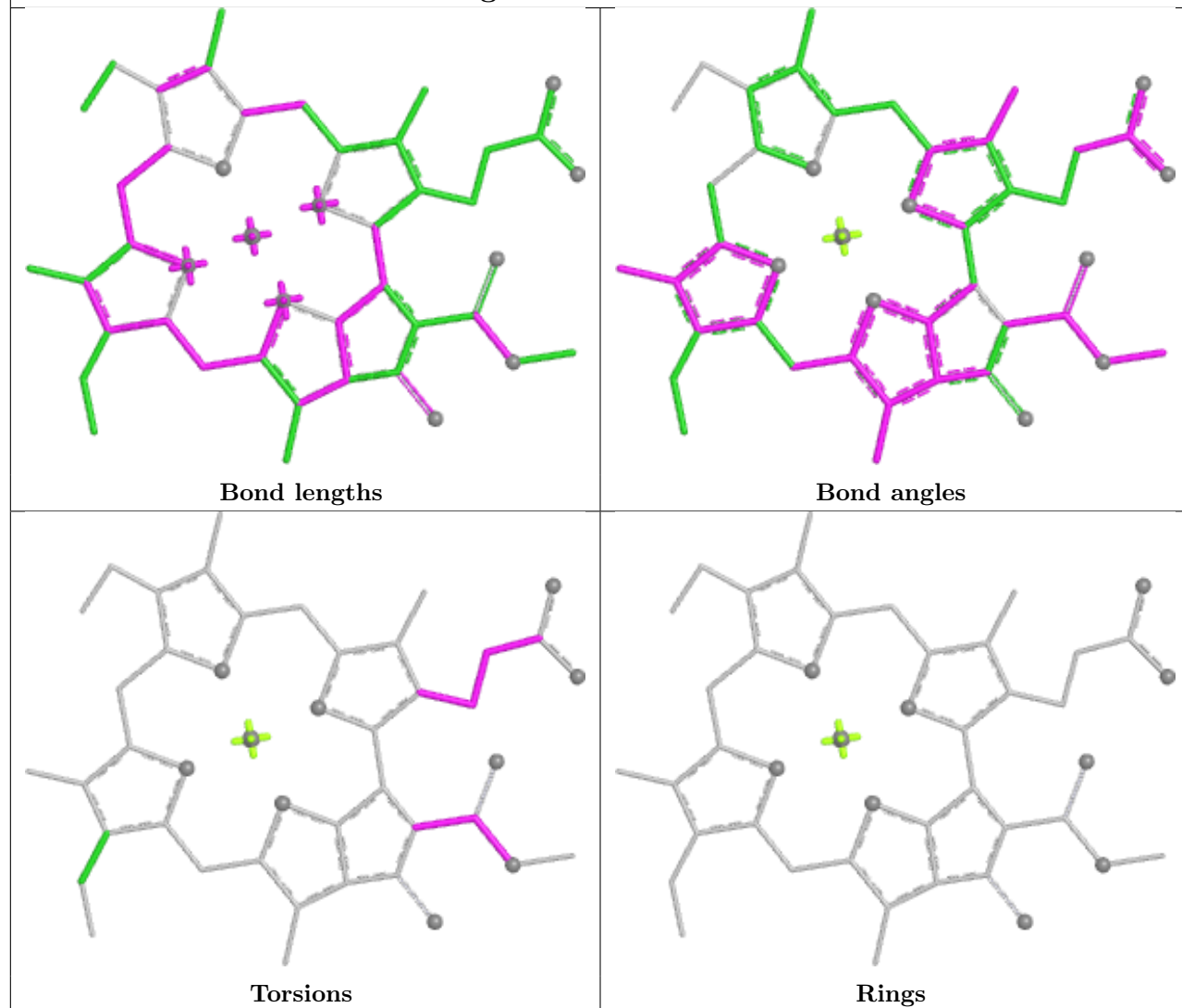


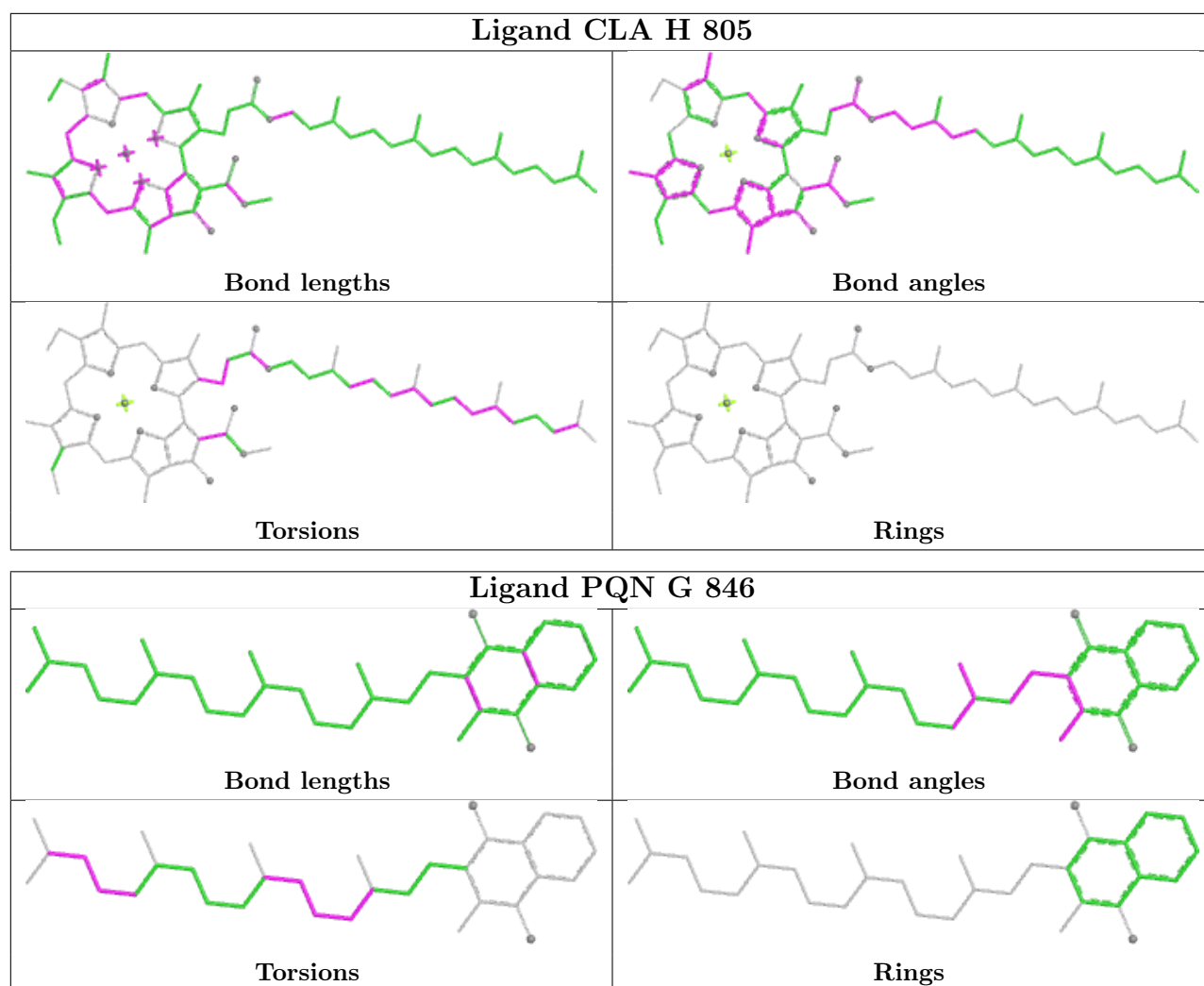


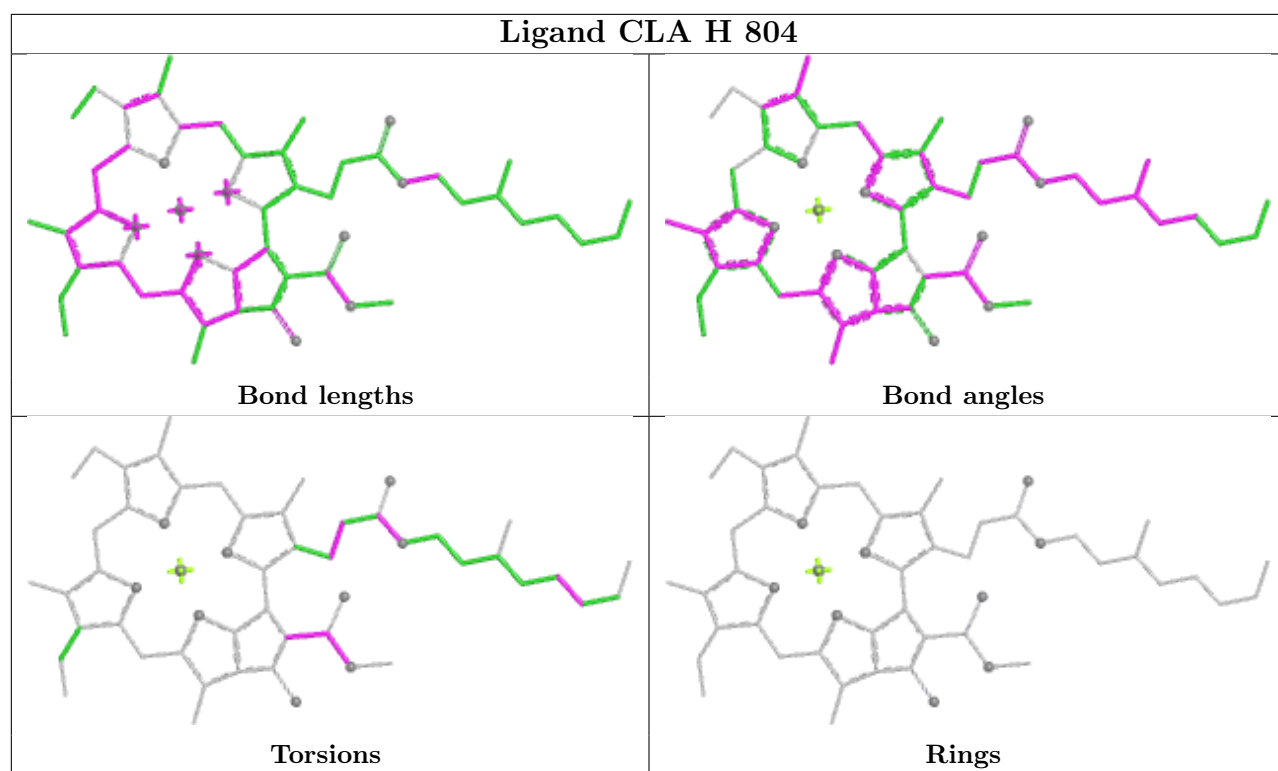
Ligand CLA A 835



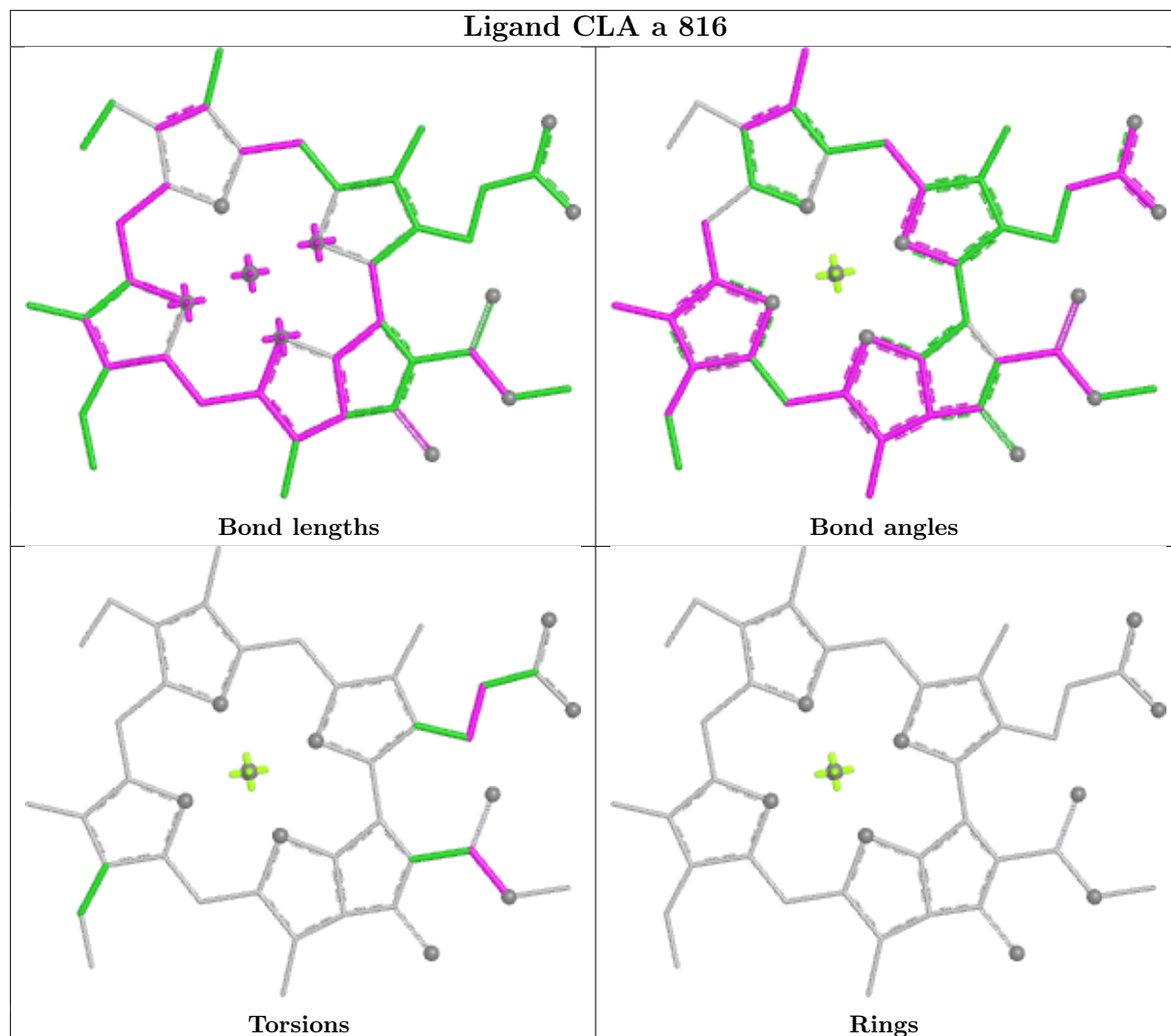
Ligand CLA M 1601



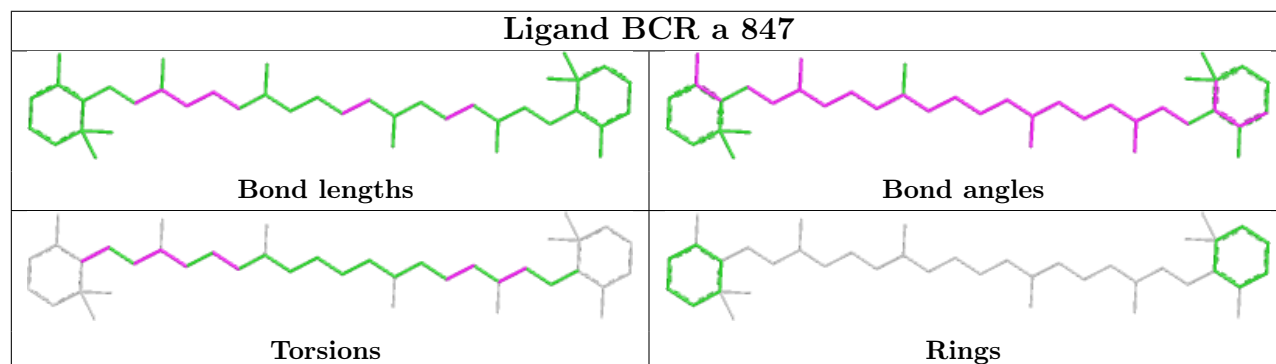


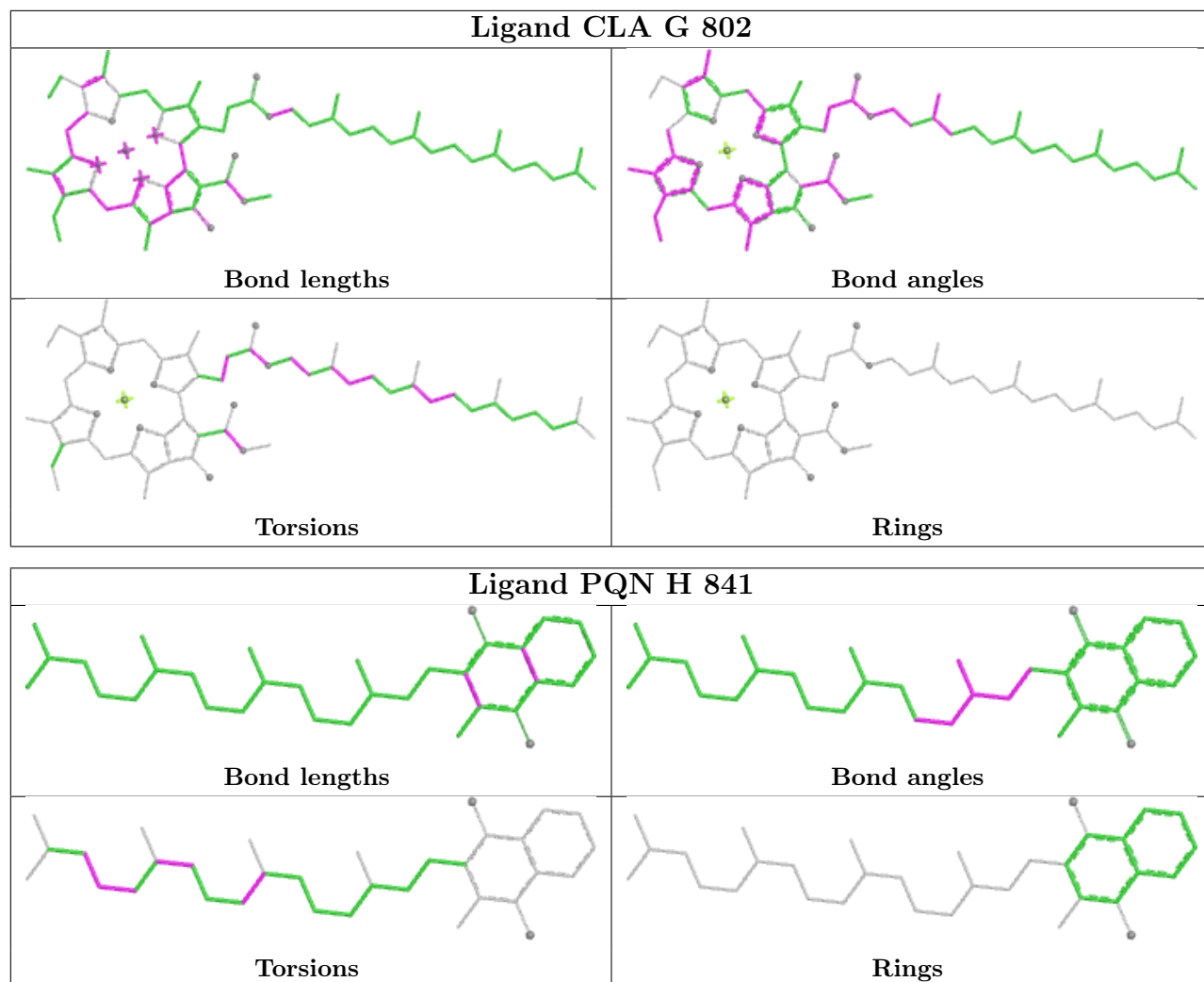


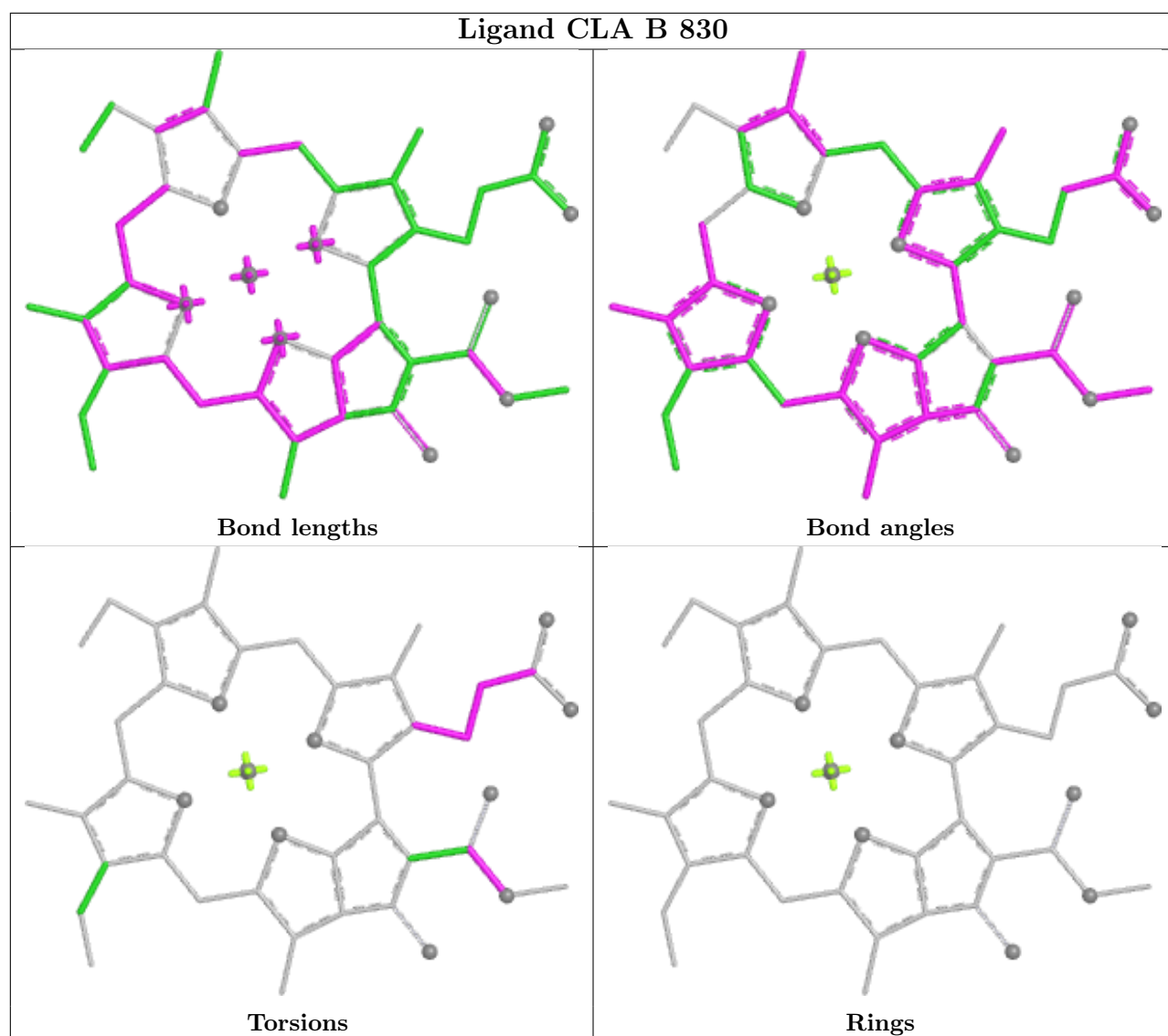
Ligand CLA a 816

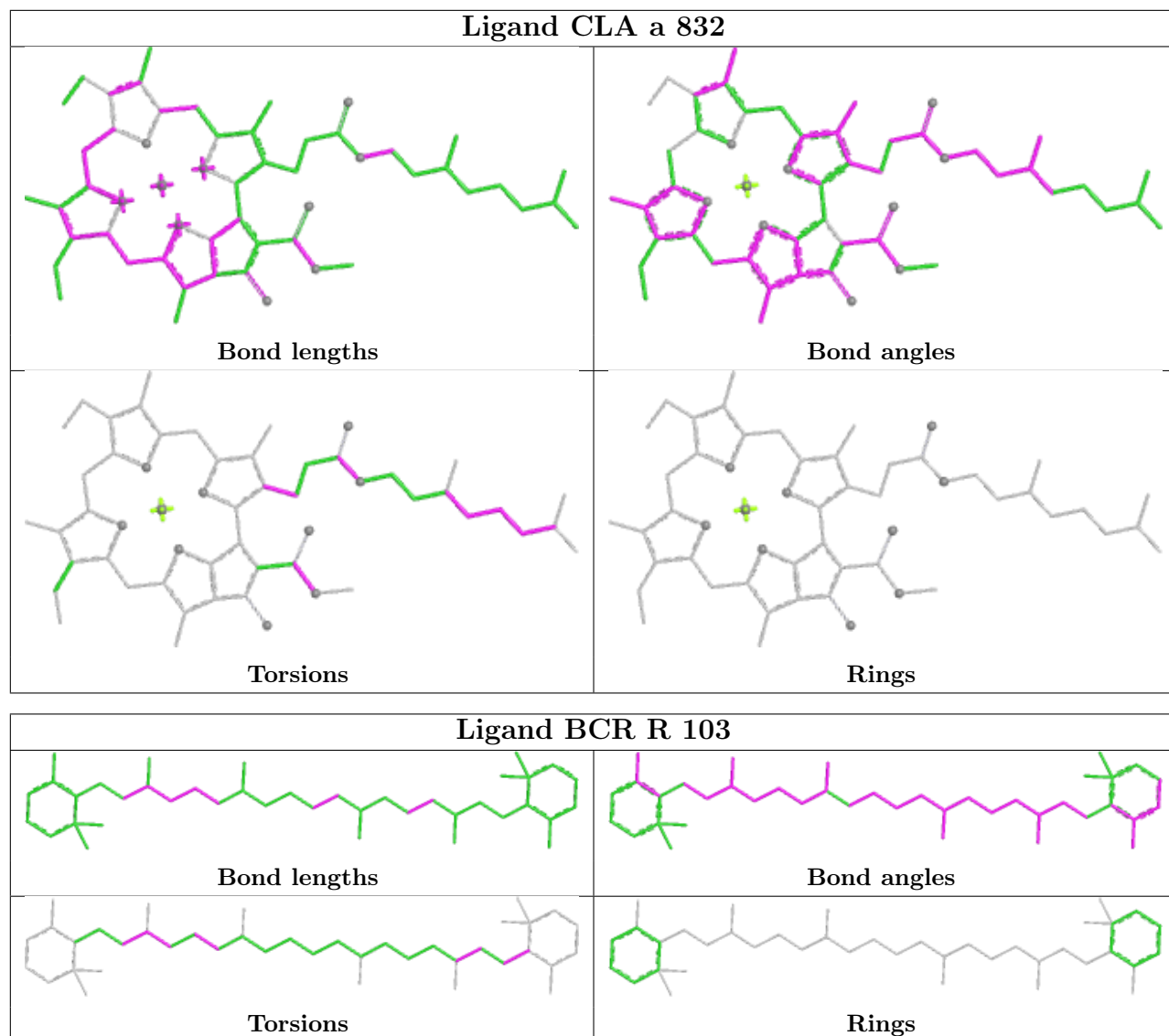


Ligand BCR a 847

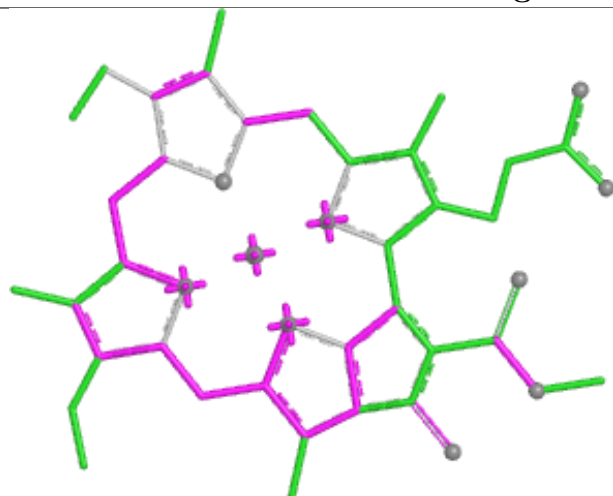




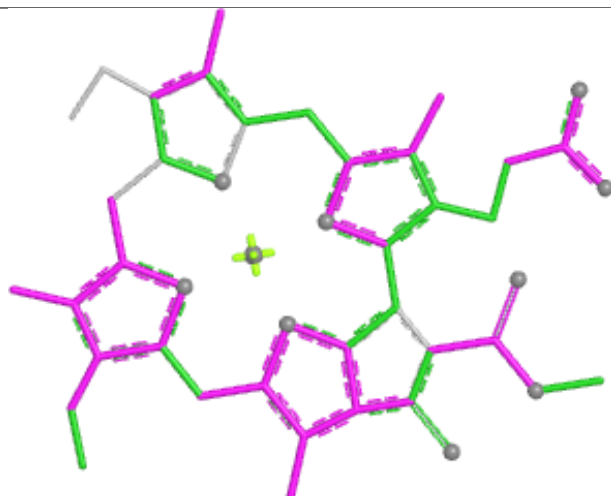




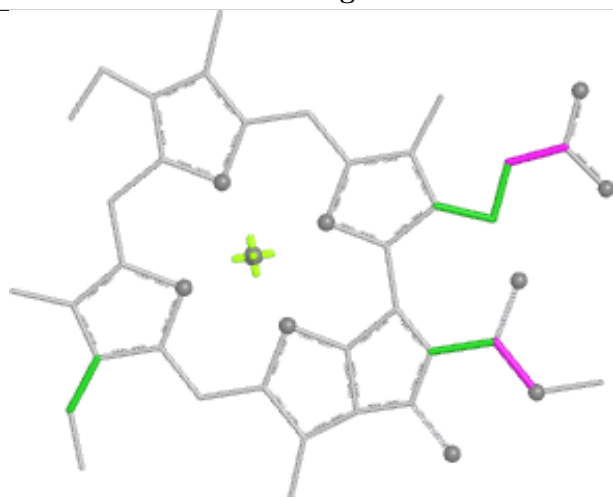
Ligand CLA A 824



Bond lengths



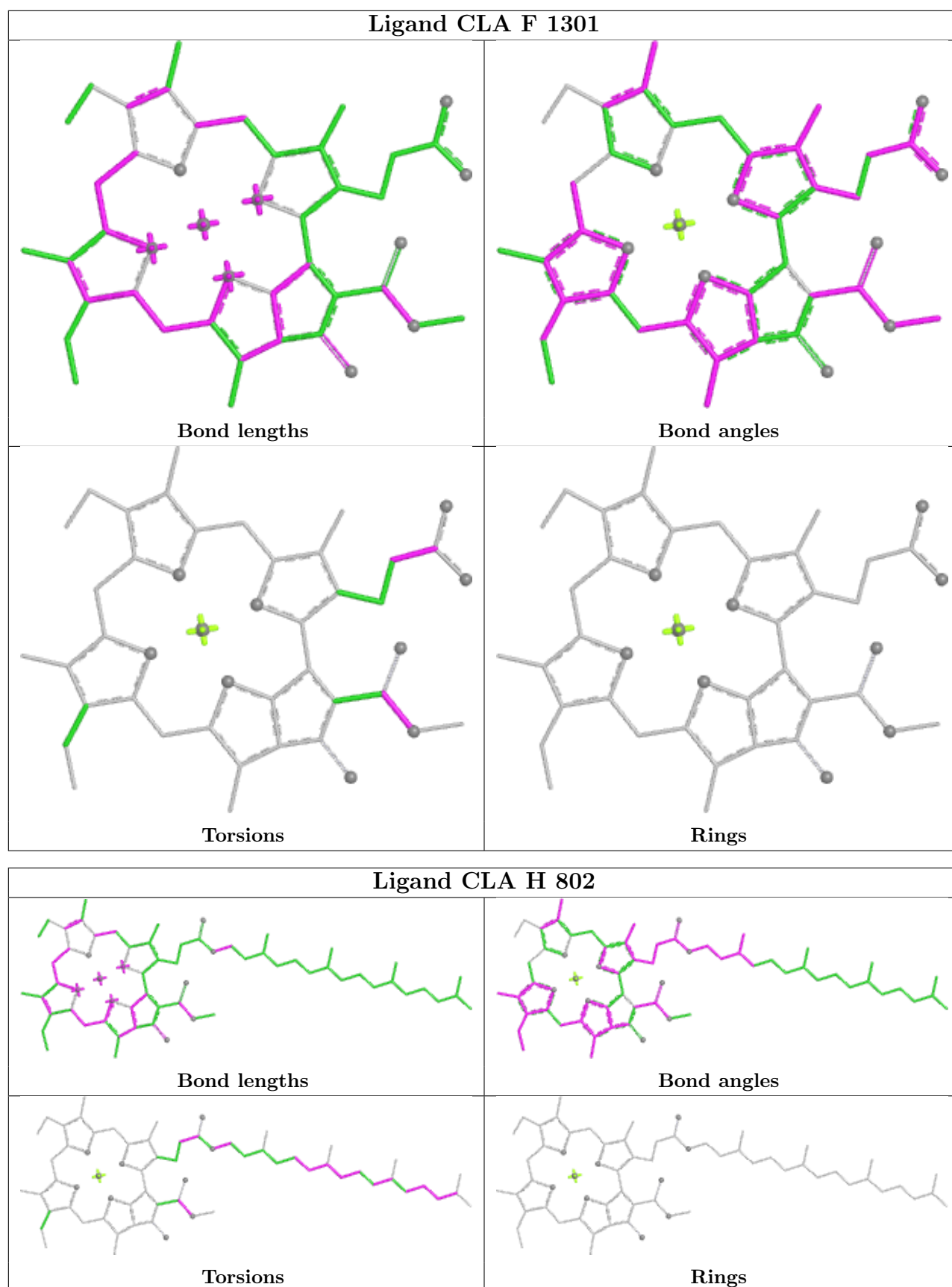
Bond angles



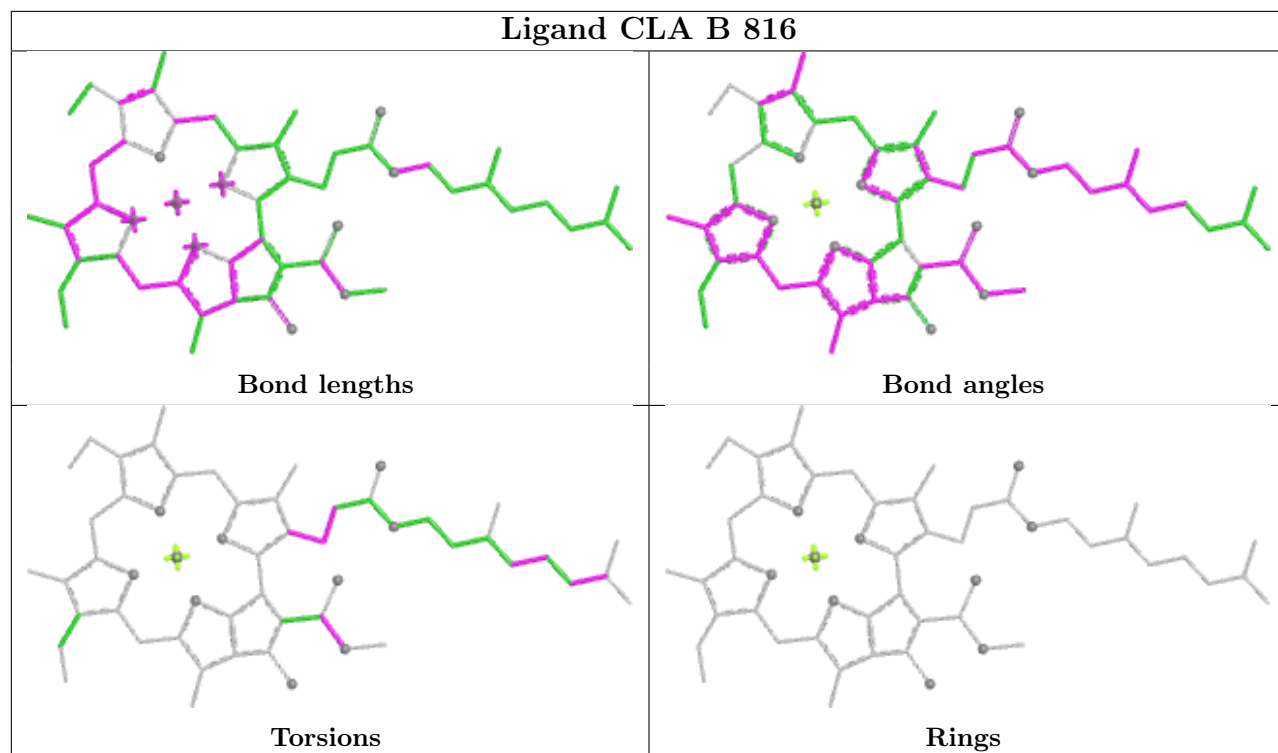
Torsions



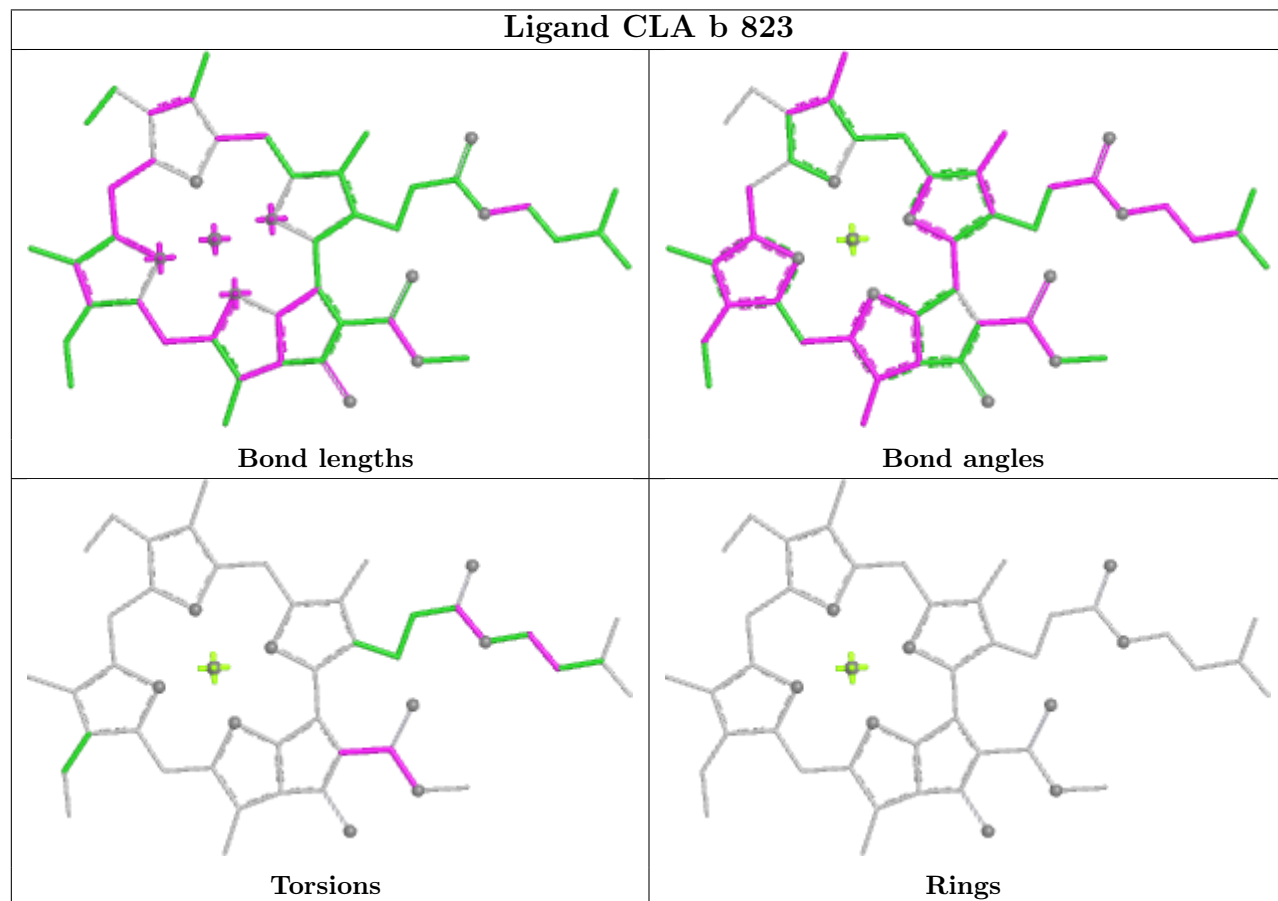
Rings



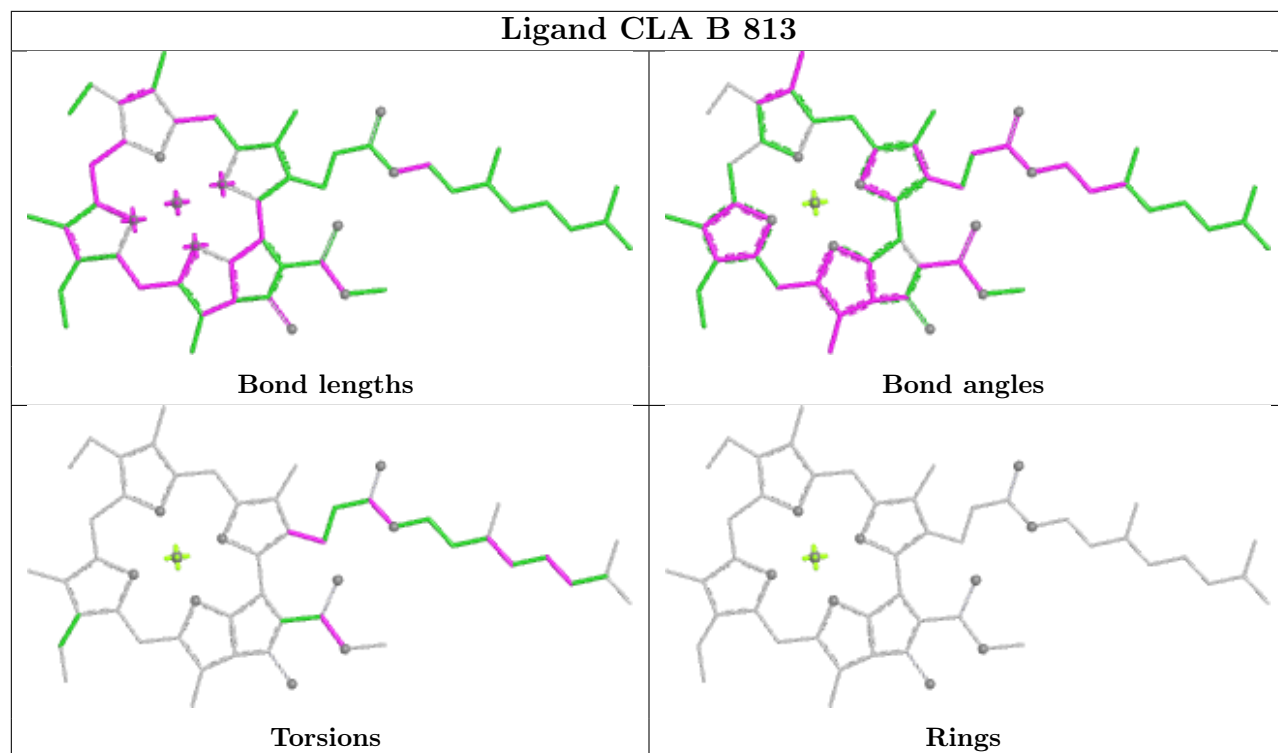
Ligand CLA B 816



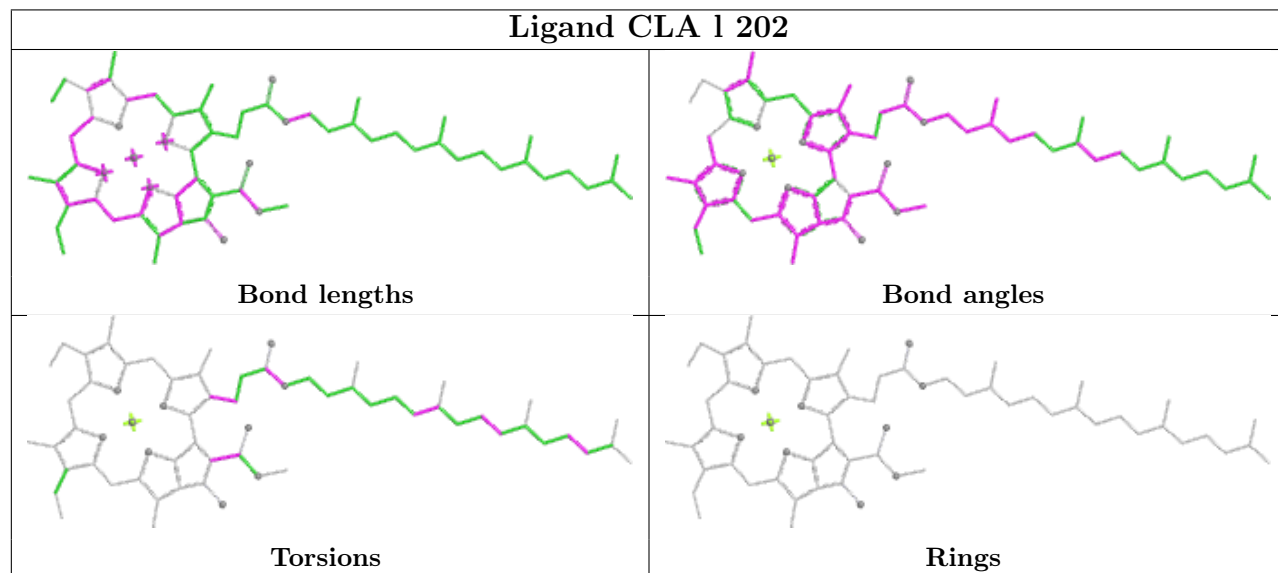
Ligand CLA b 823

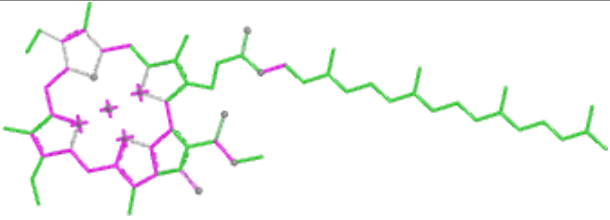
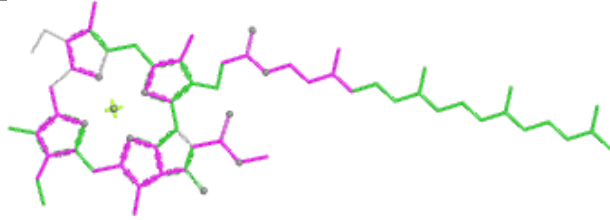
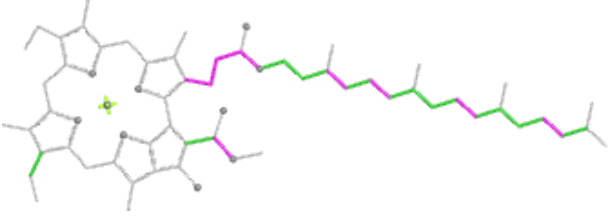
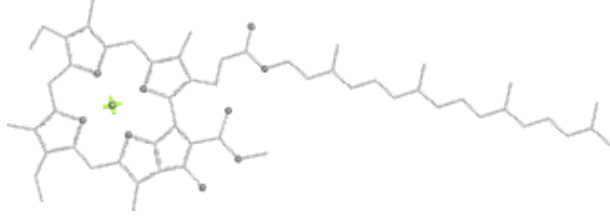
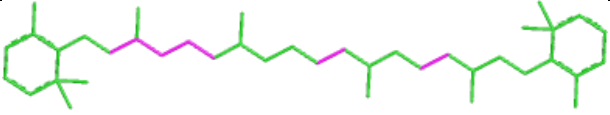
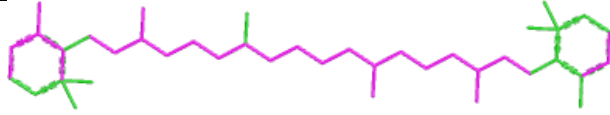
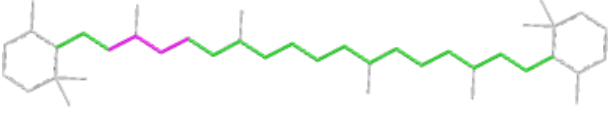
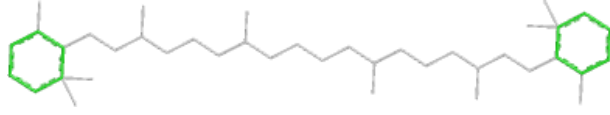
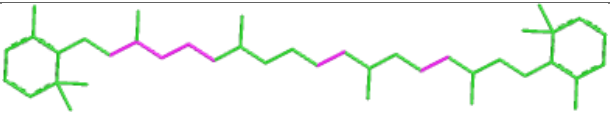
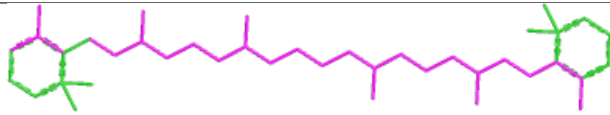
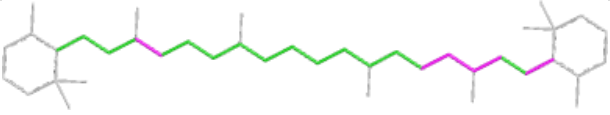
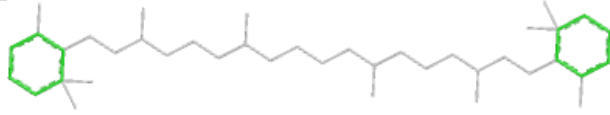


Ligand CLA B 813

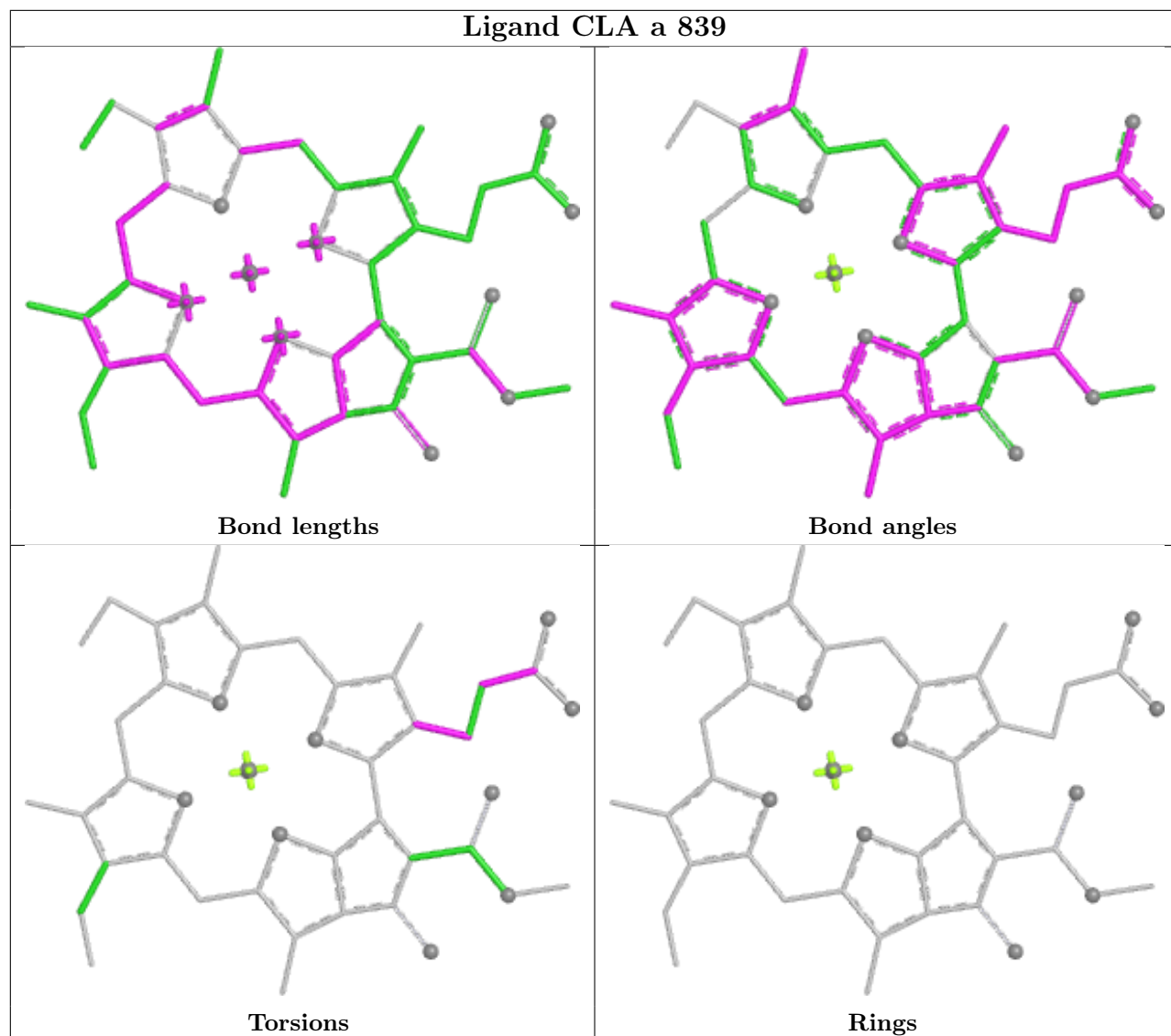


Ligand CLA I 202

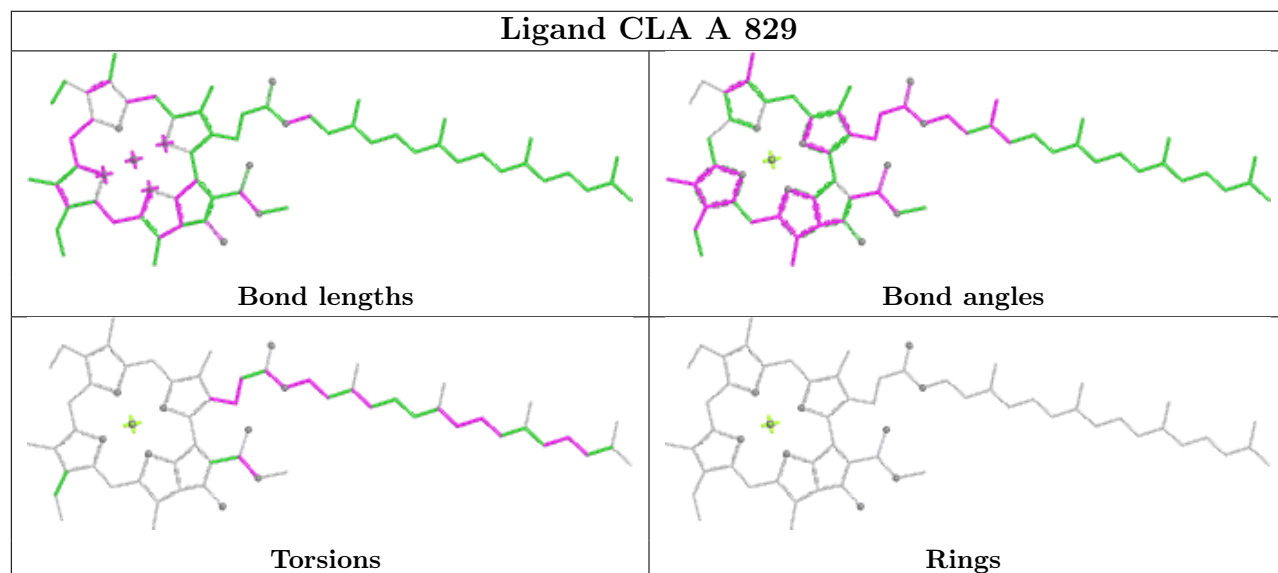


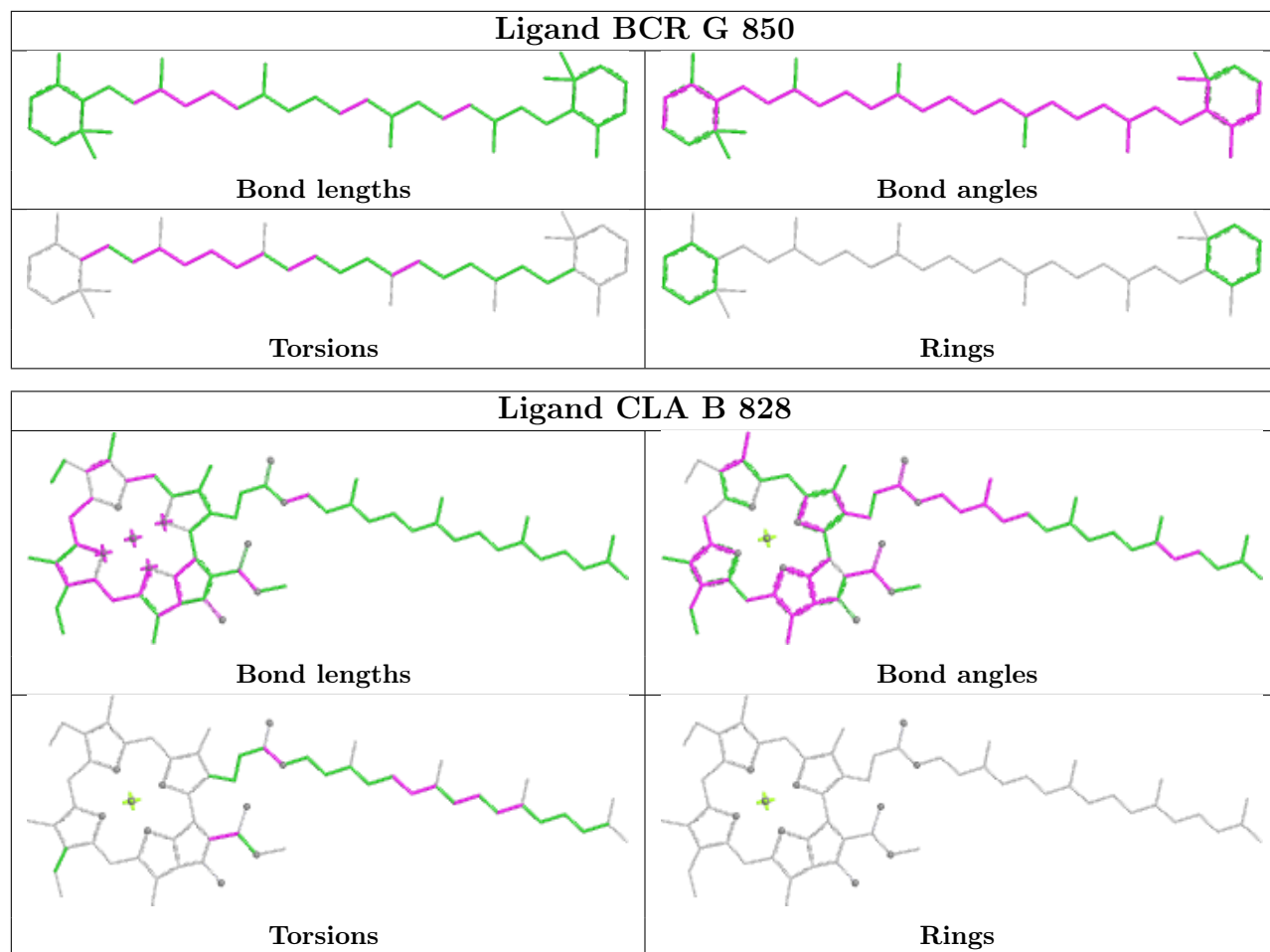
Ligand CLA A 812	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR L 207	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR B 844	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand CLA a 839

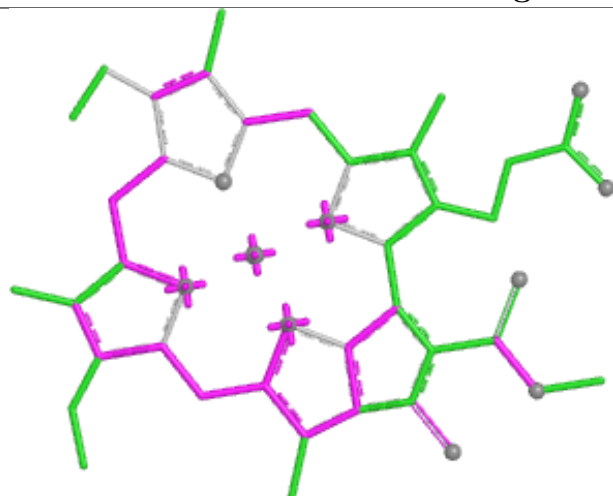


Ligand CLA A 829

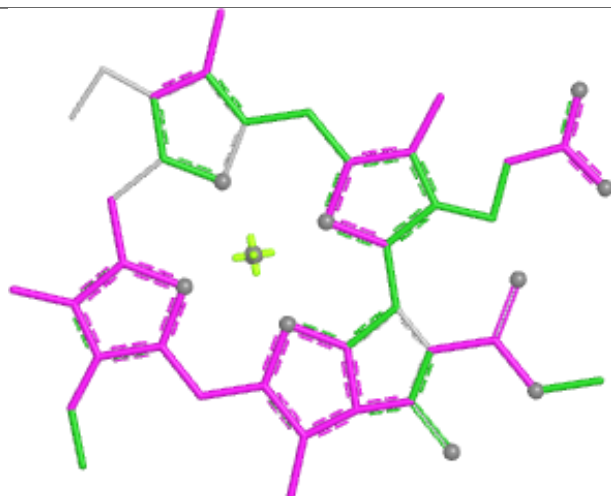




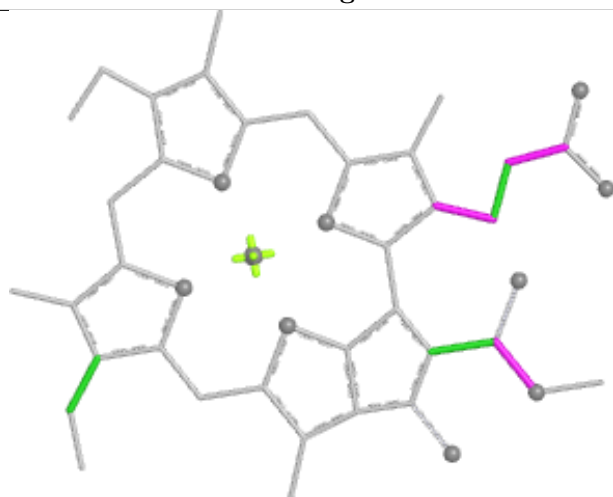
Ligand CLA H 835



Bond lengths



Bond angles

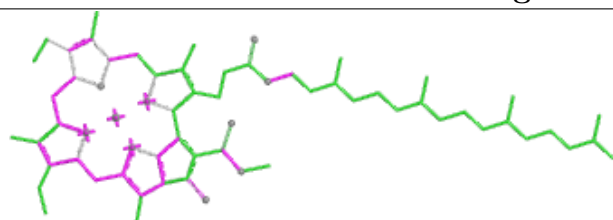


Torsions

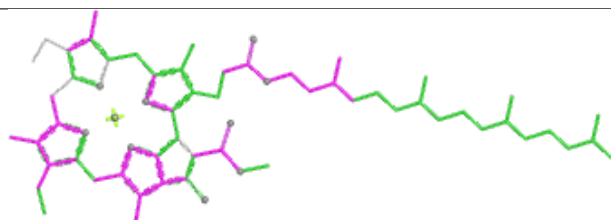


Rings

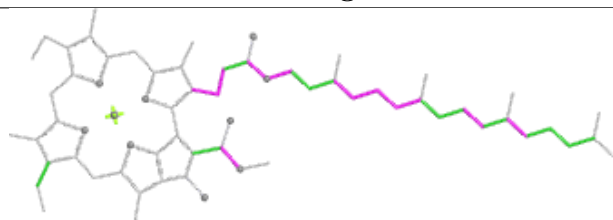
Ligand CLA U 206



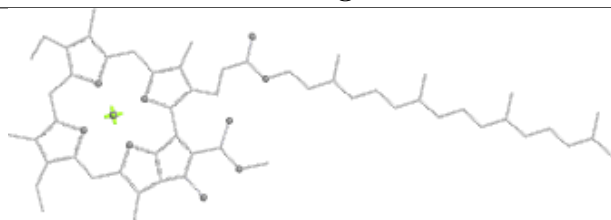
Bond lengths



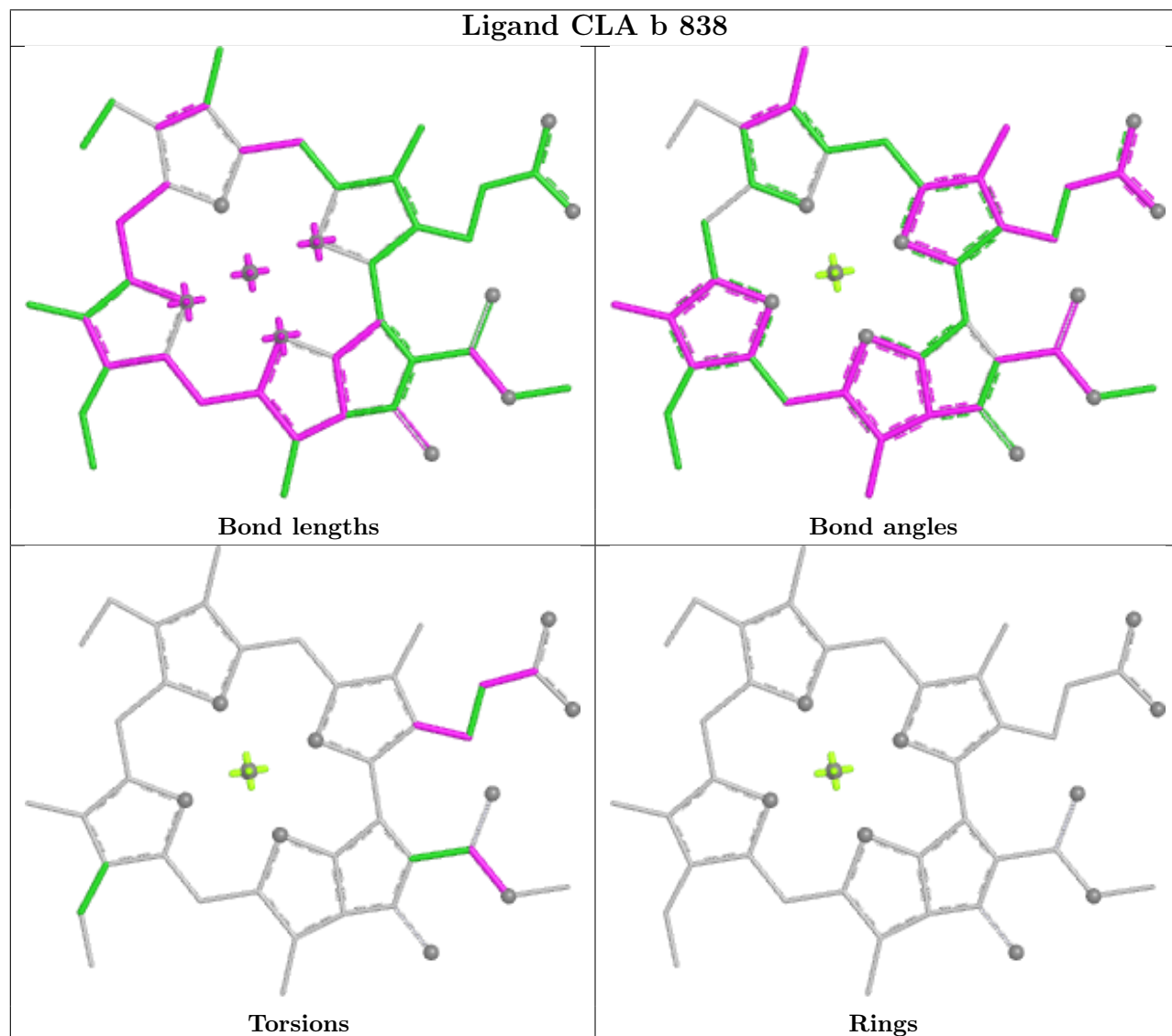
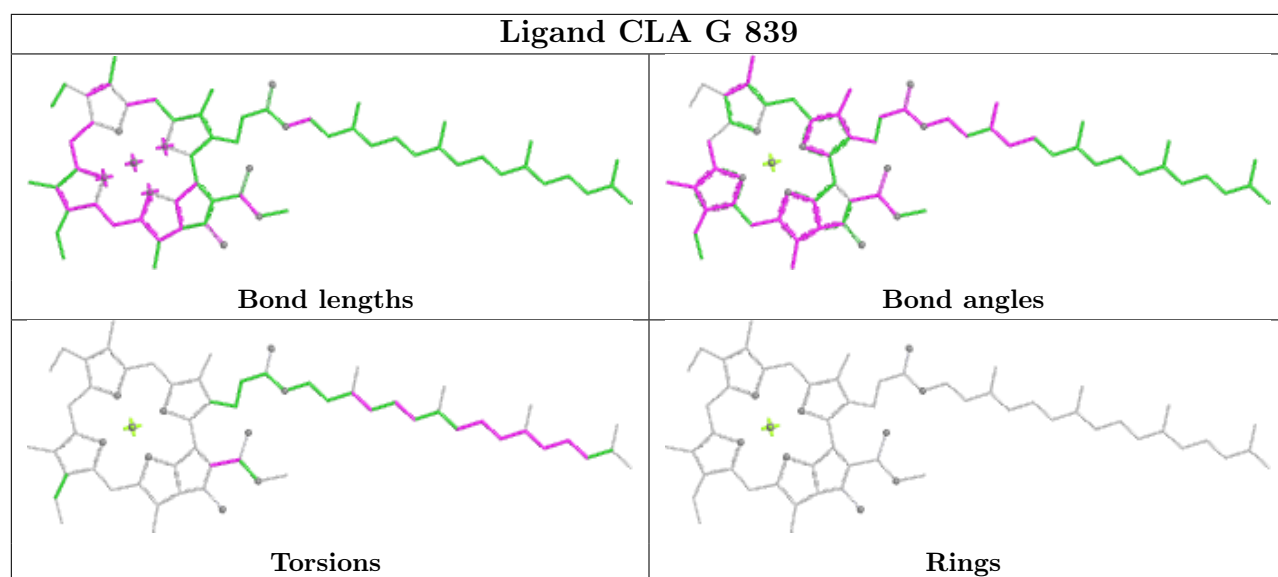
Bond angles

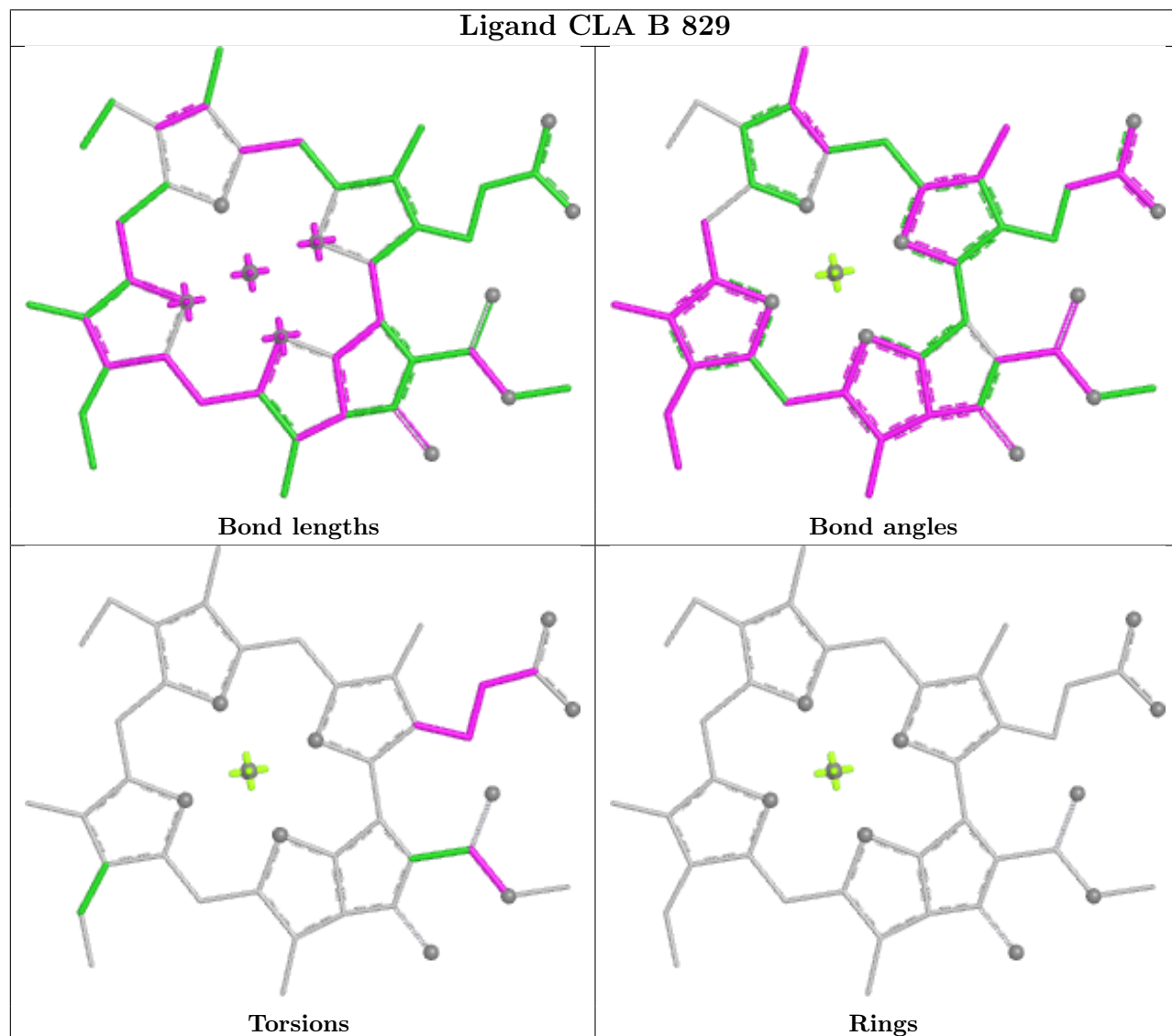
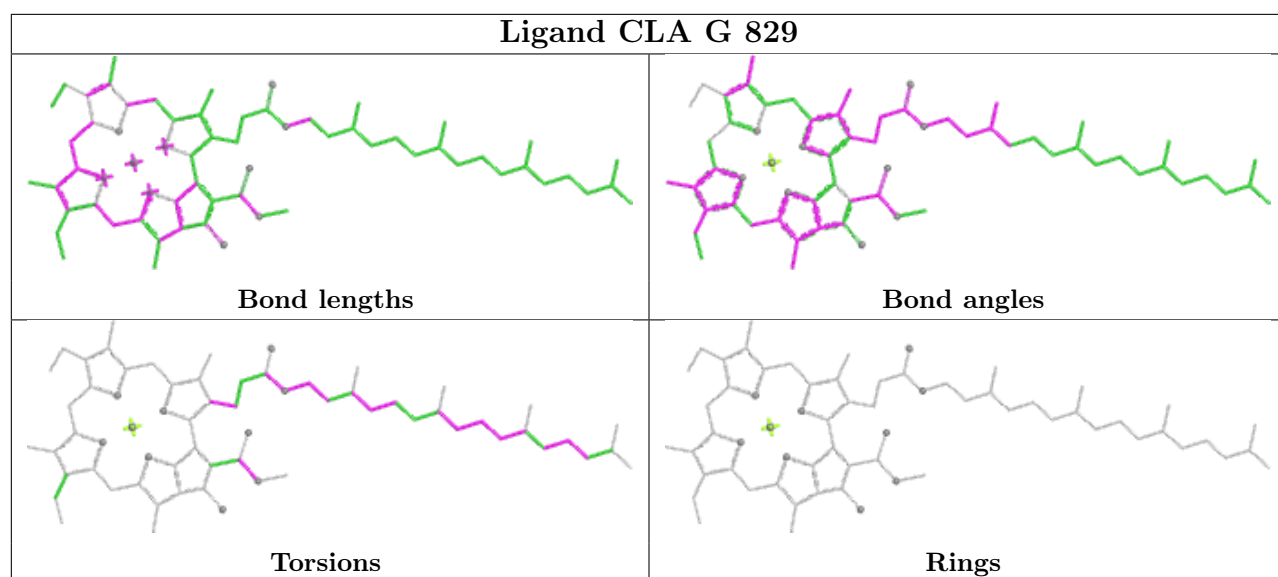


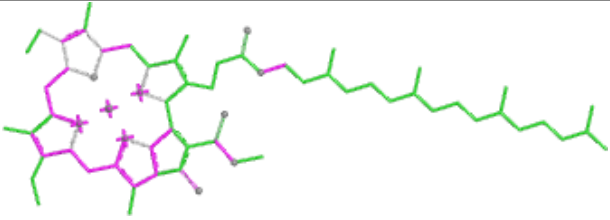
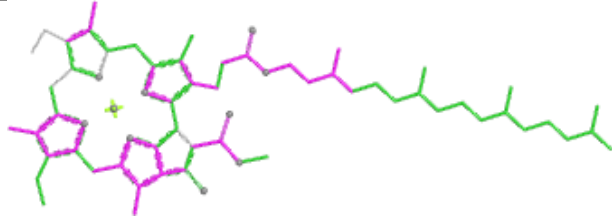
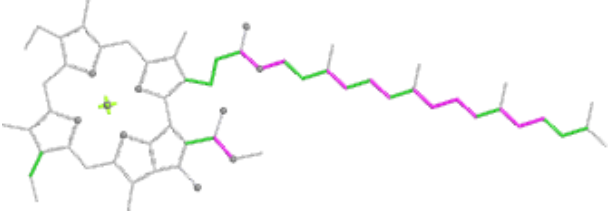
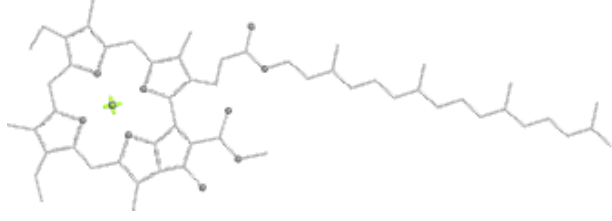
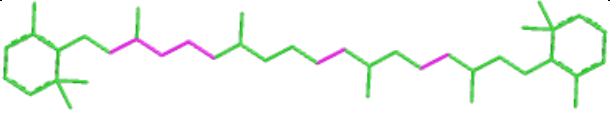
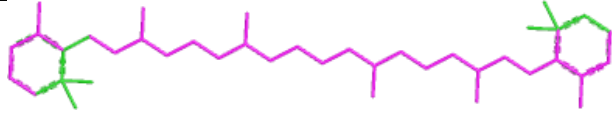
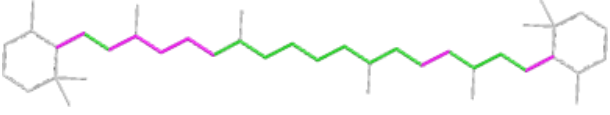
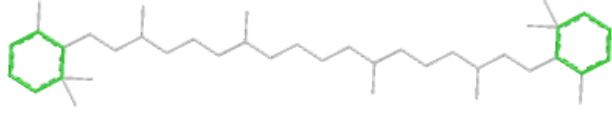
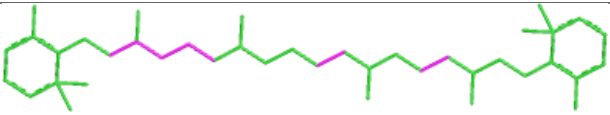
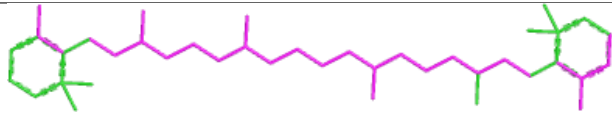
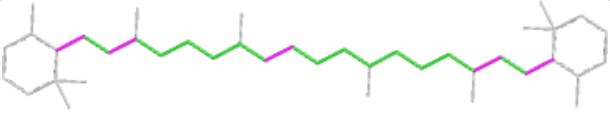
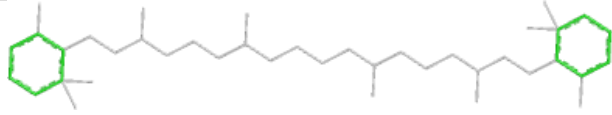
Torsions



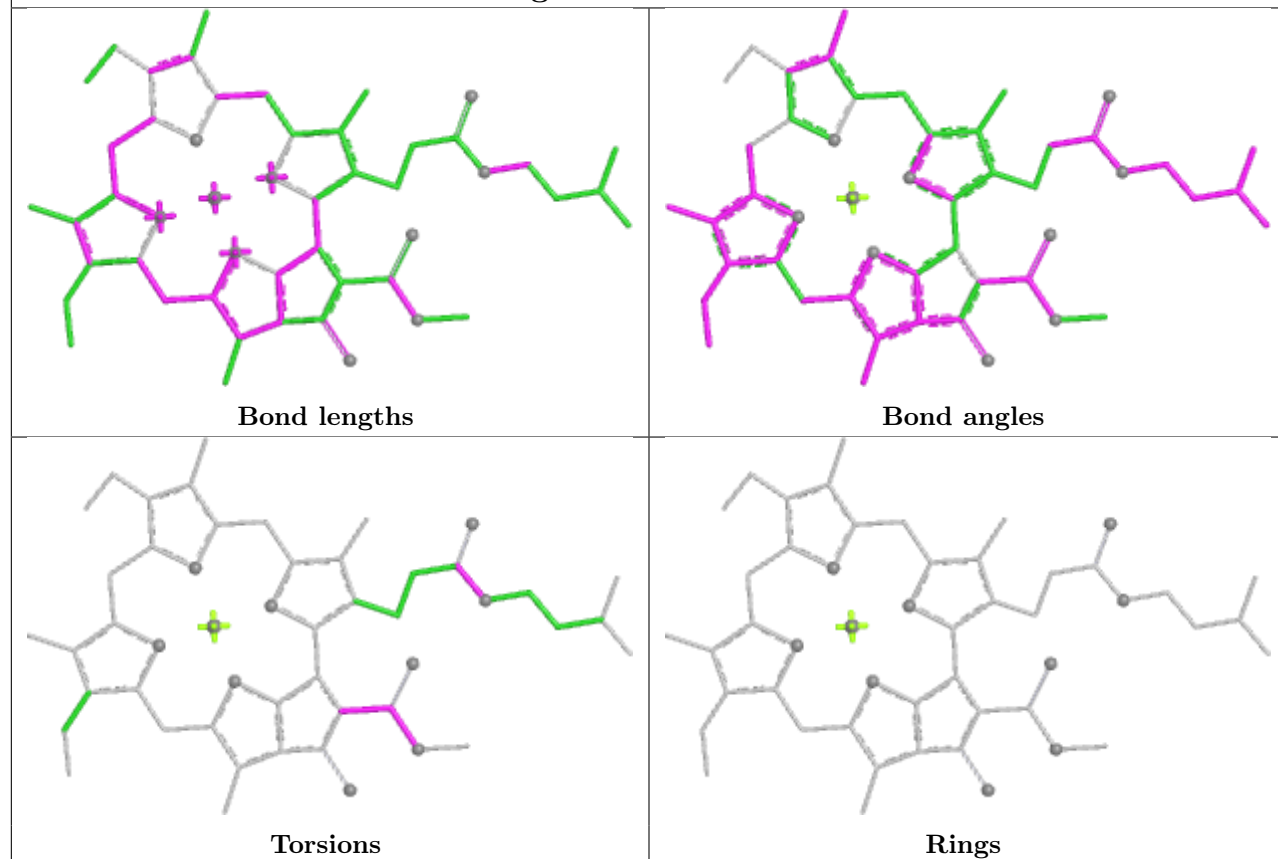
Rings



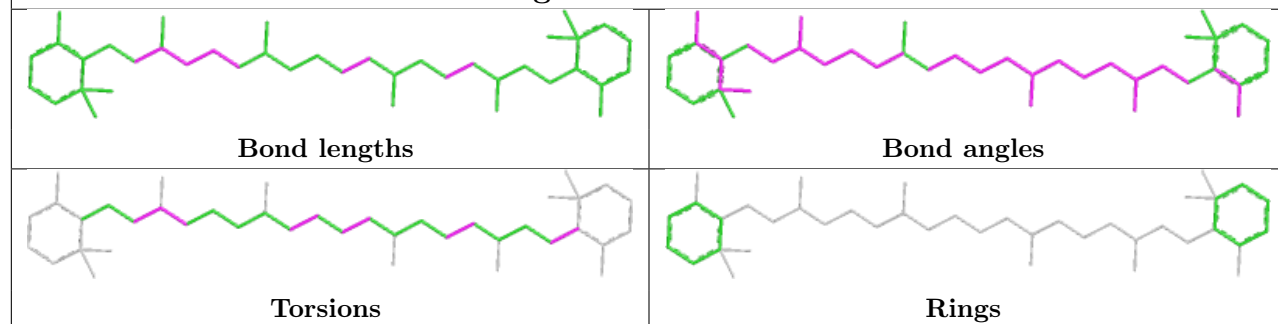


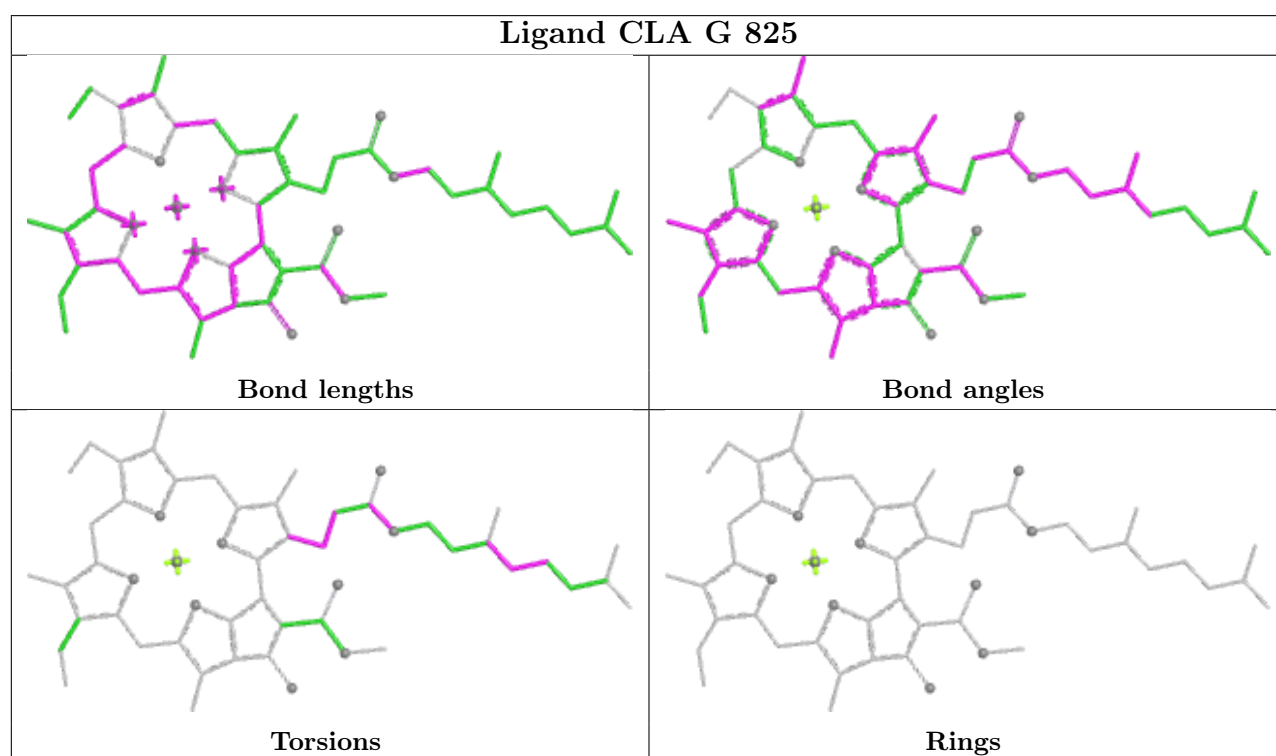
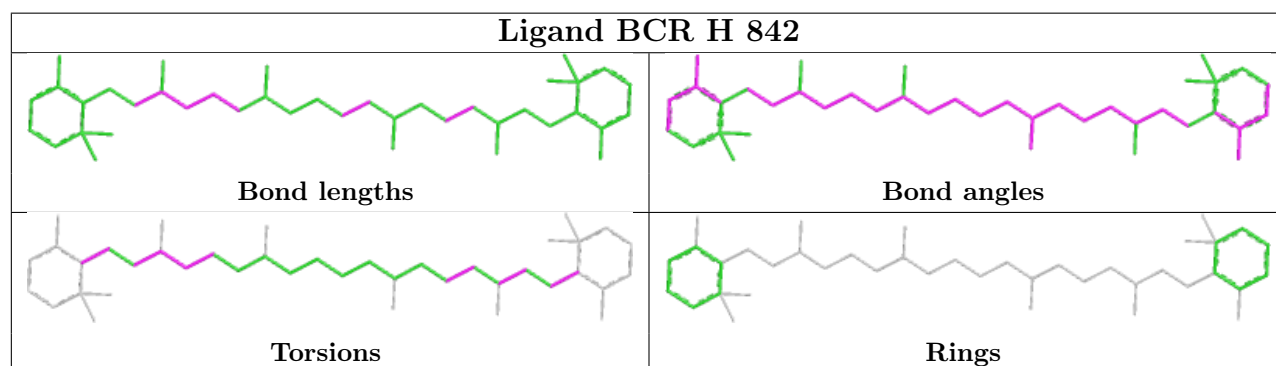
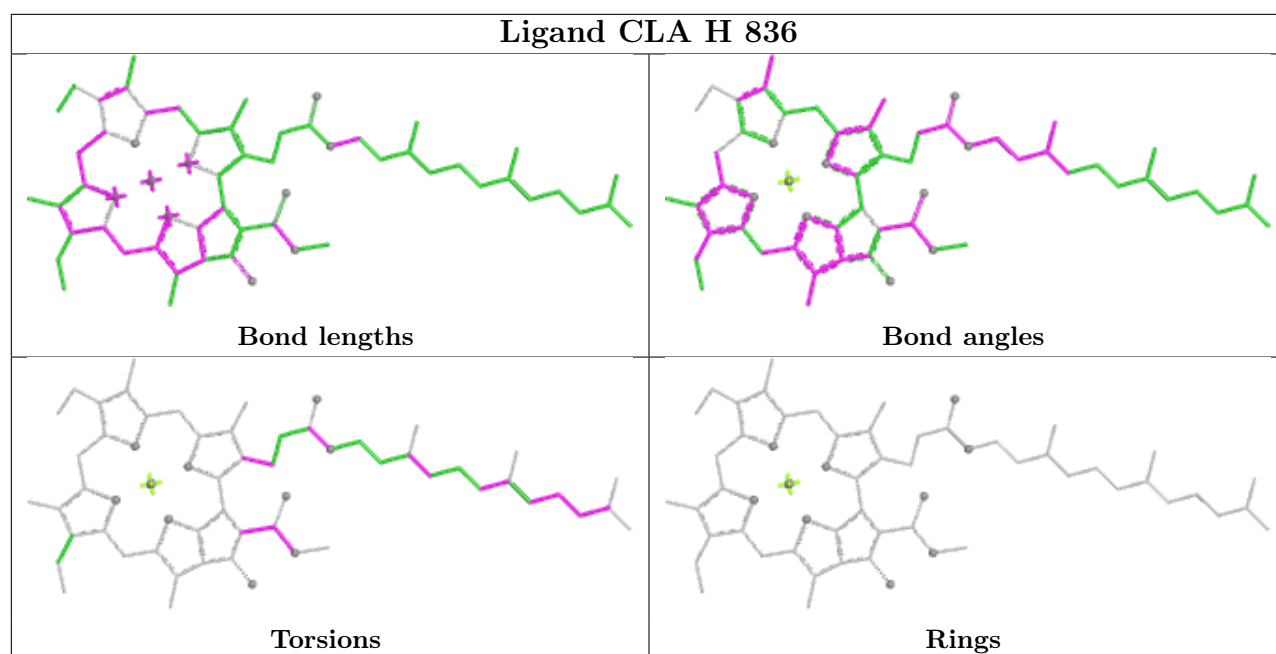
Ligand CLA A 834	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR A 851	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR 1 208	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand CLA G 838

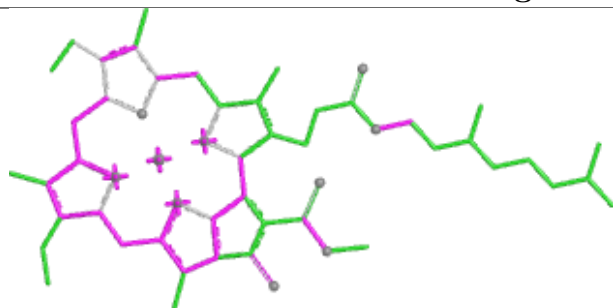


Ligand BCR b 849

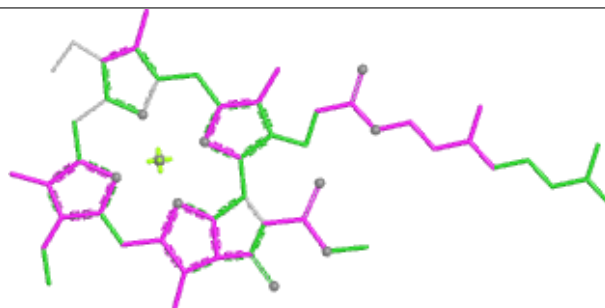




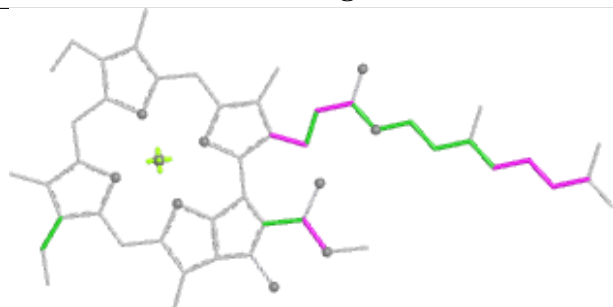
Ligand CLA B 821



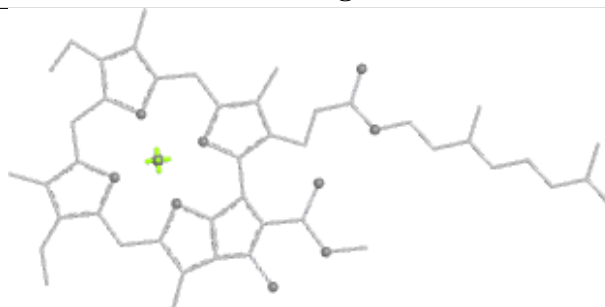
Bond lengths



Bond angles

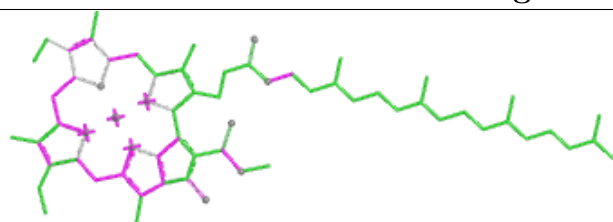


Torsions

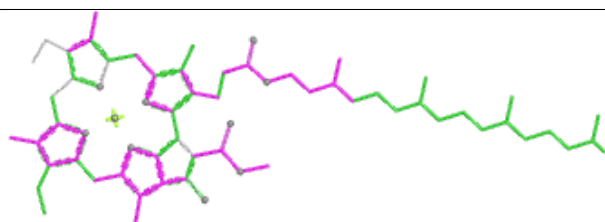


Rings

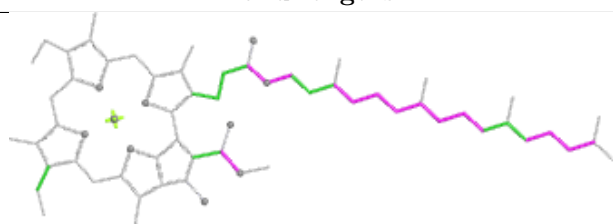
Ligand CLA H 806



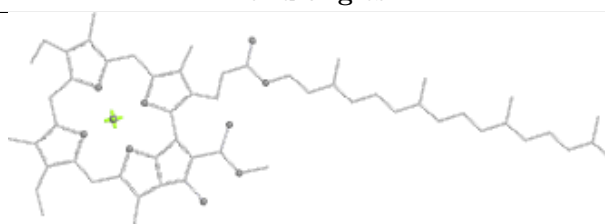
Bond lengths



Bond angles

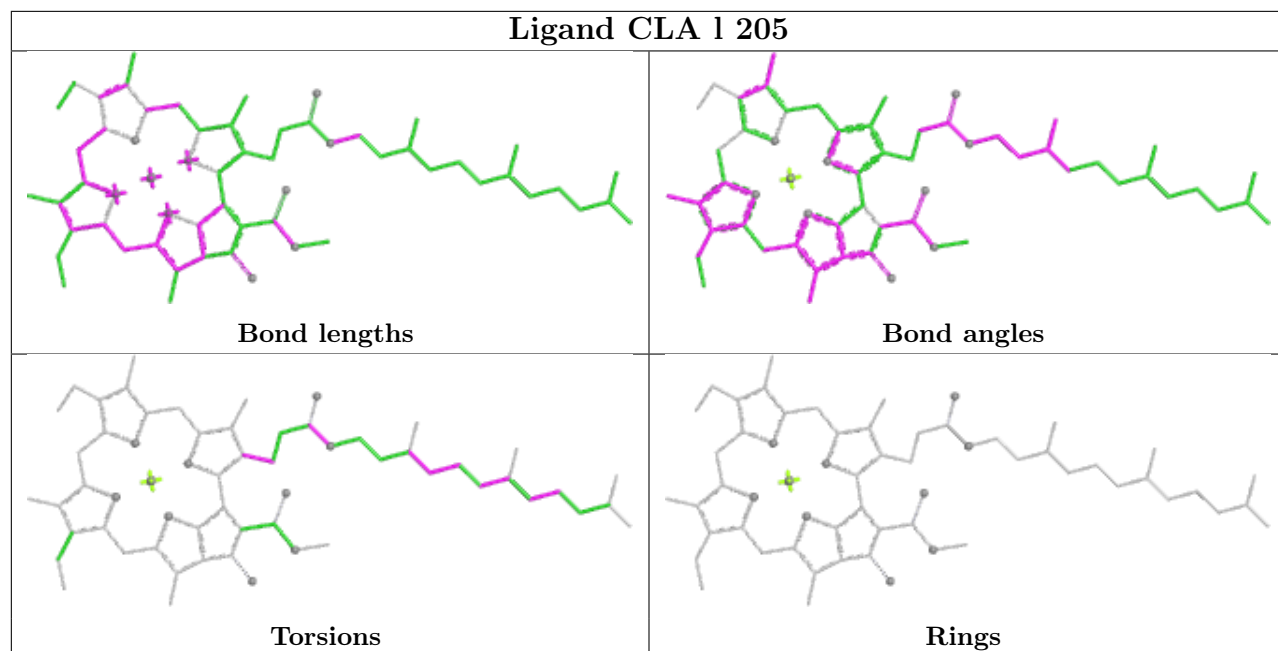


Torsions

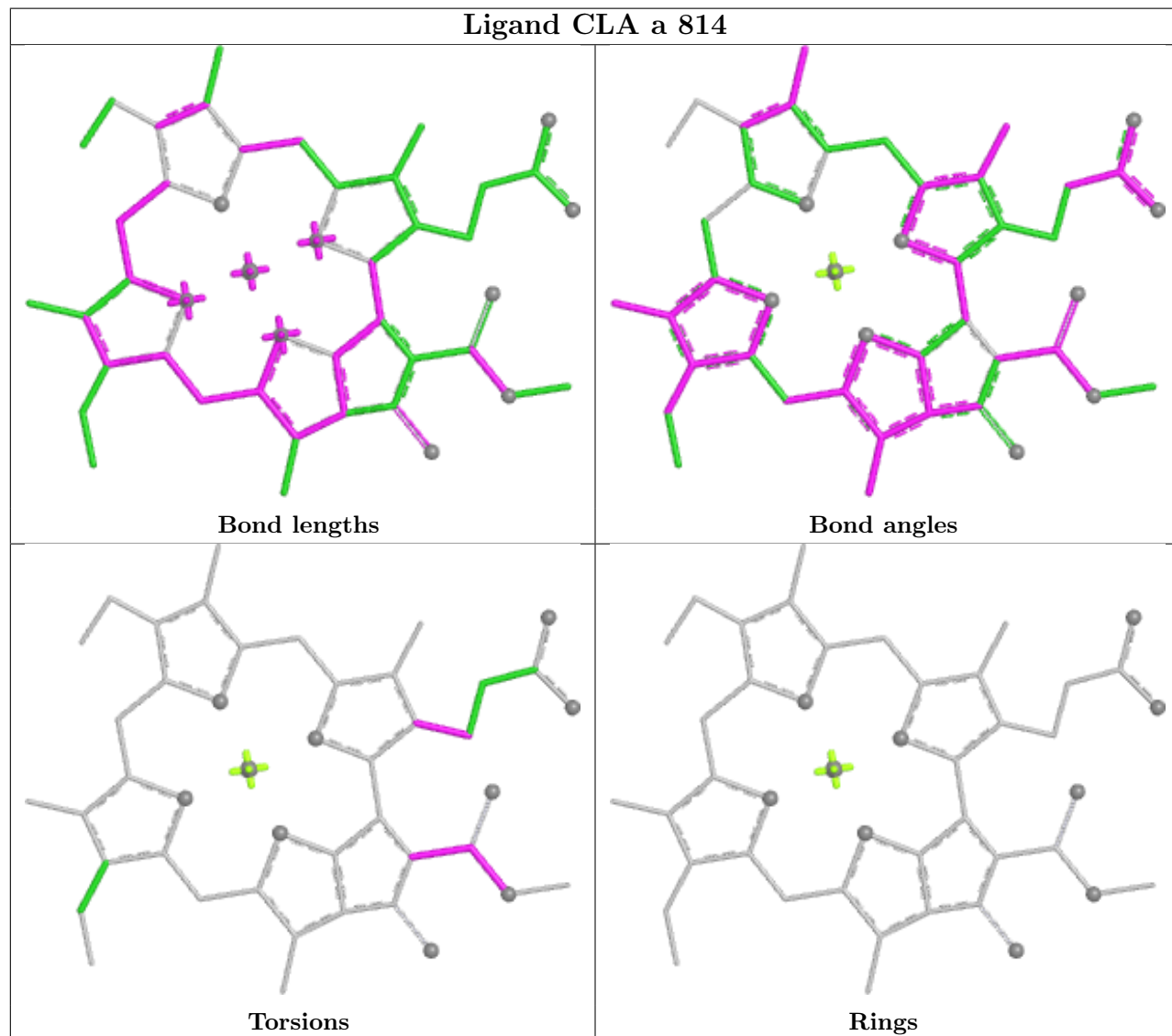


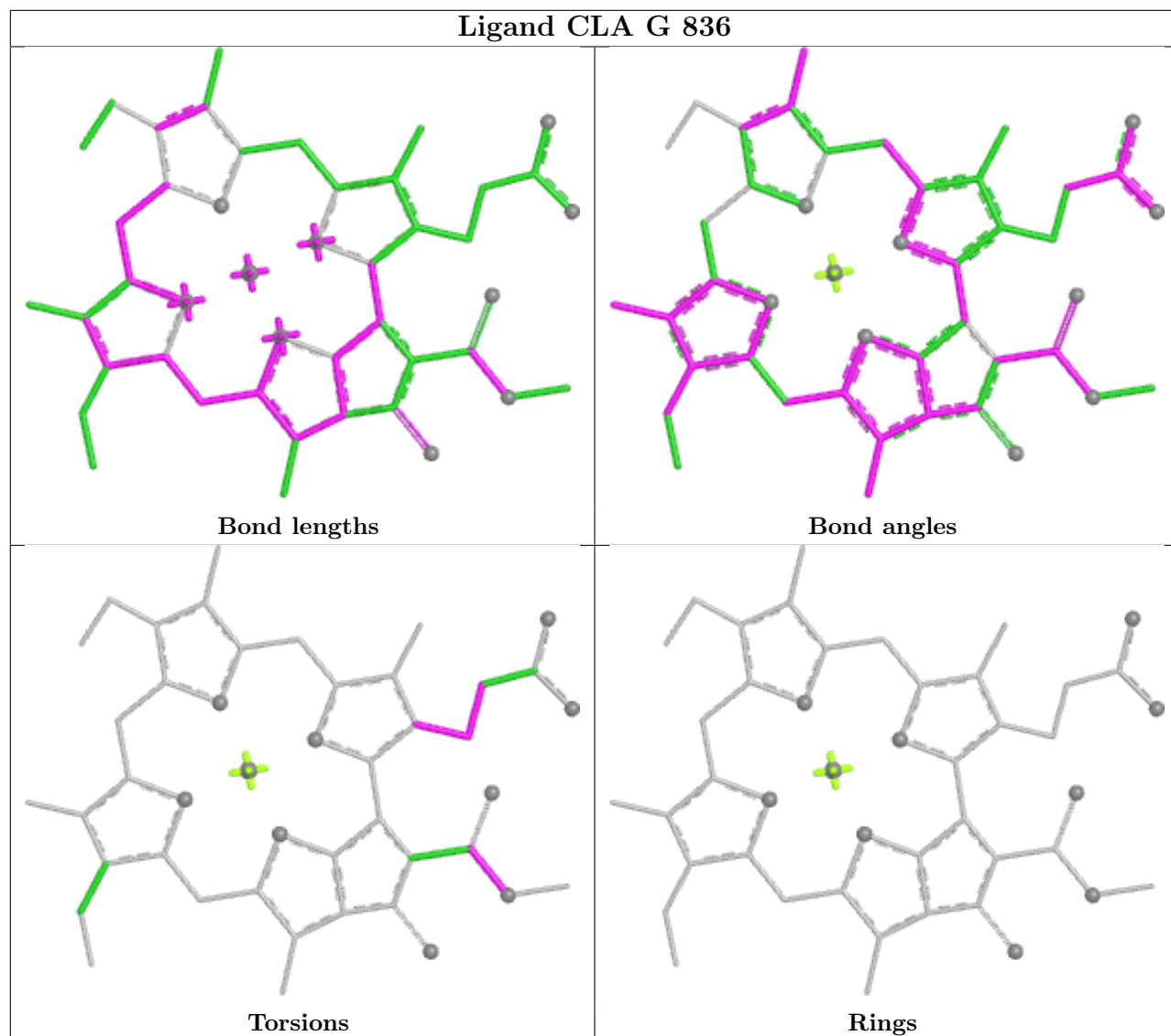
Rings

Ligand CLA 1 205

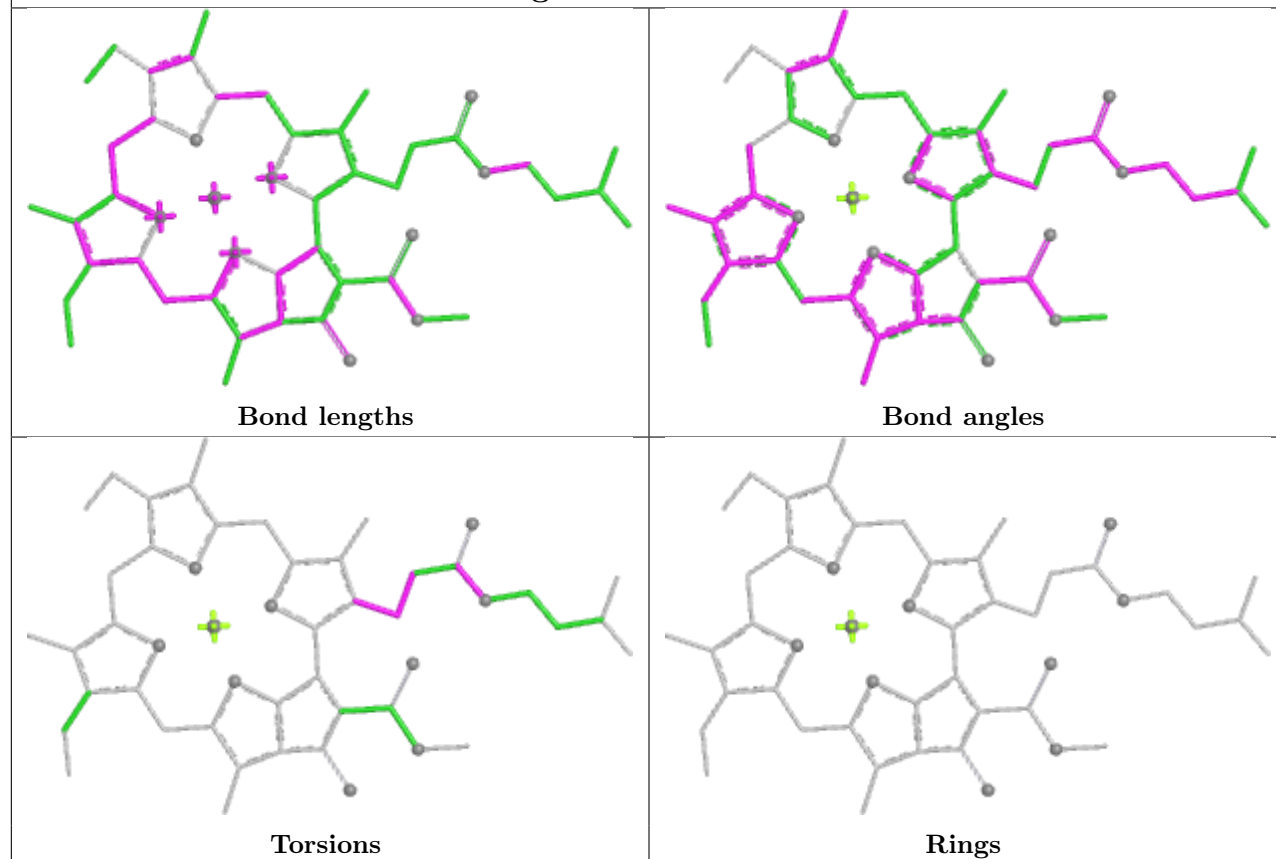


Ligand CLA a 814

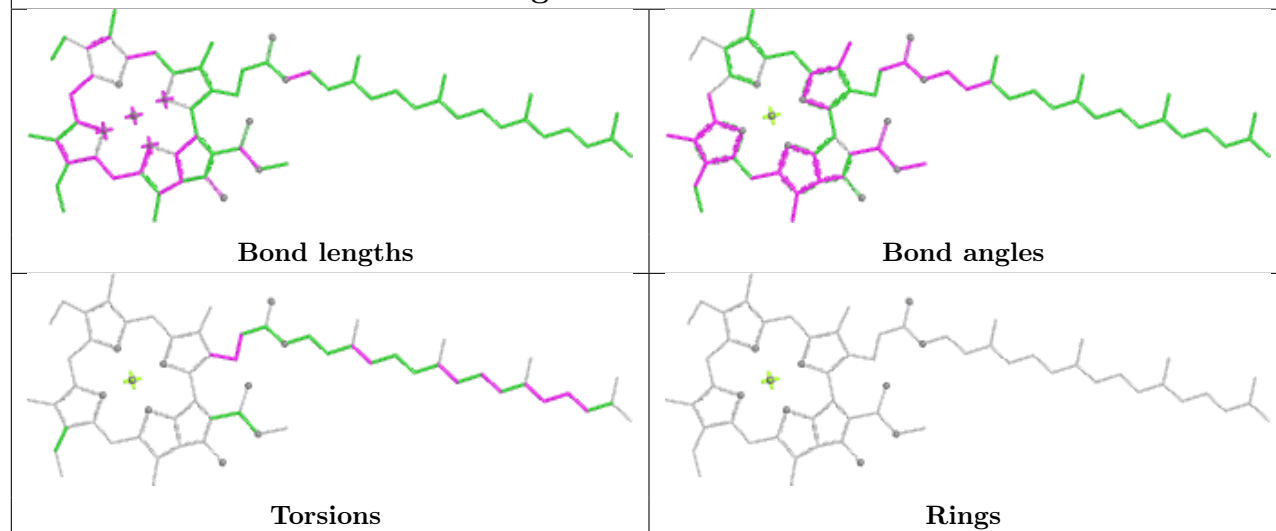


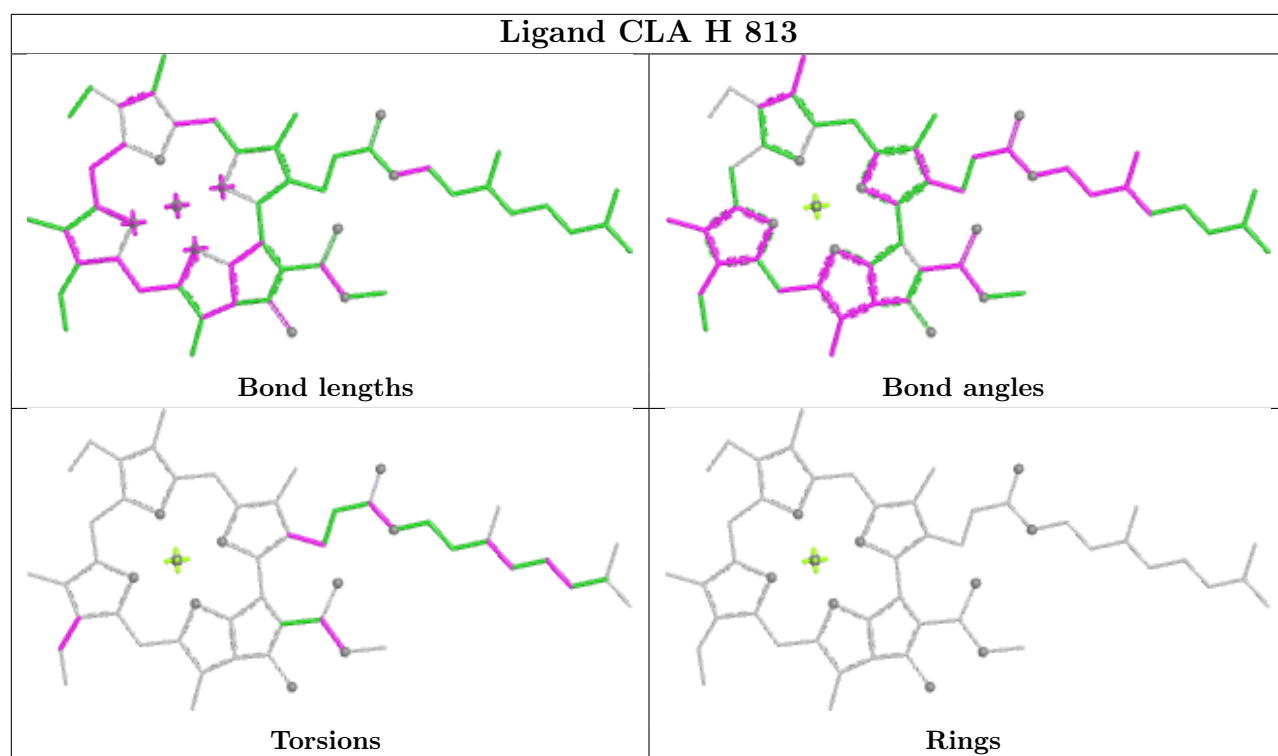


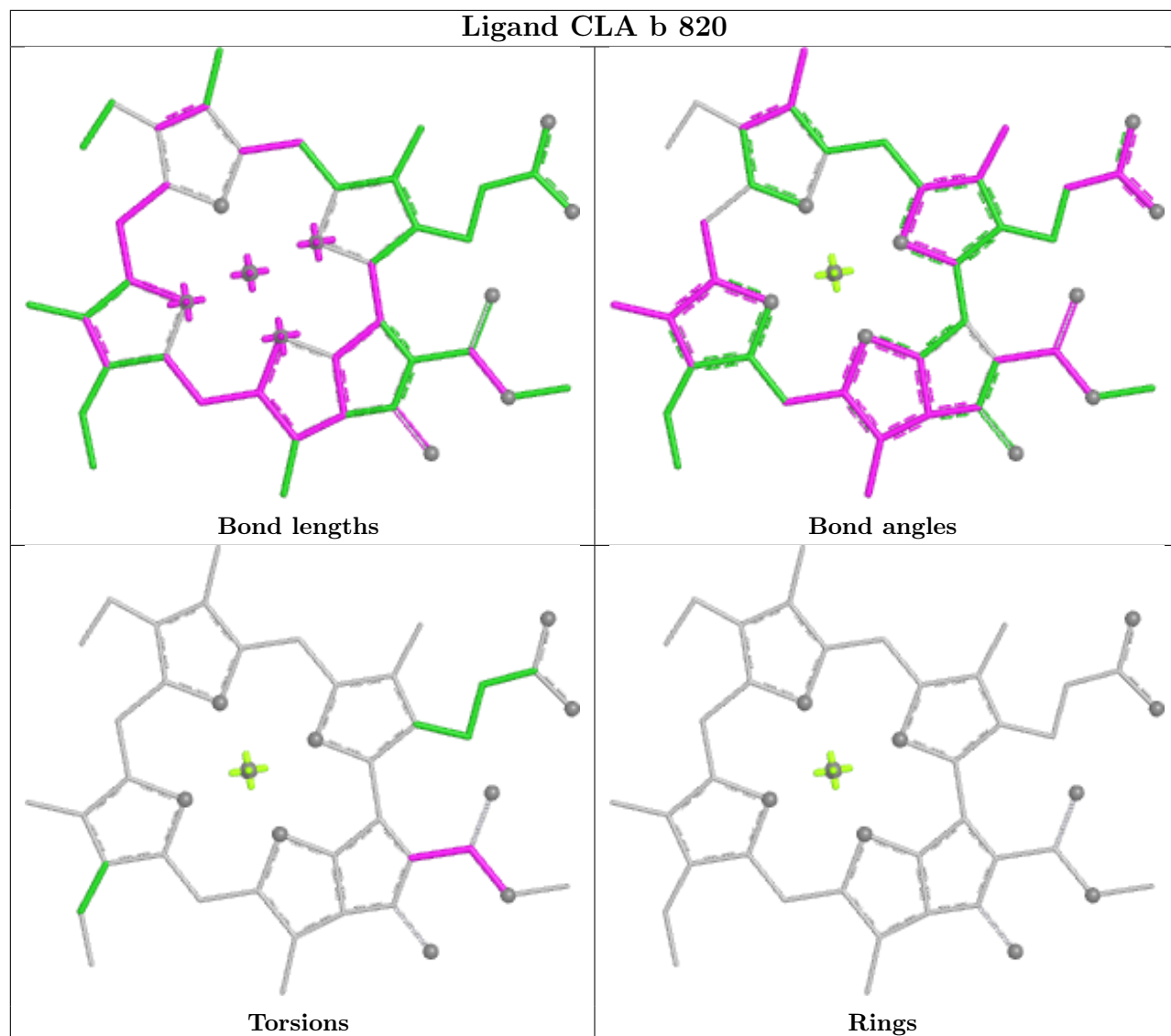
Ligand CLA A 813

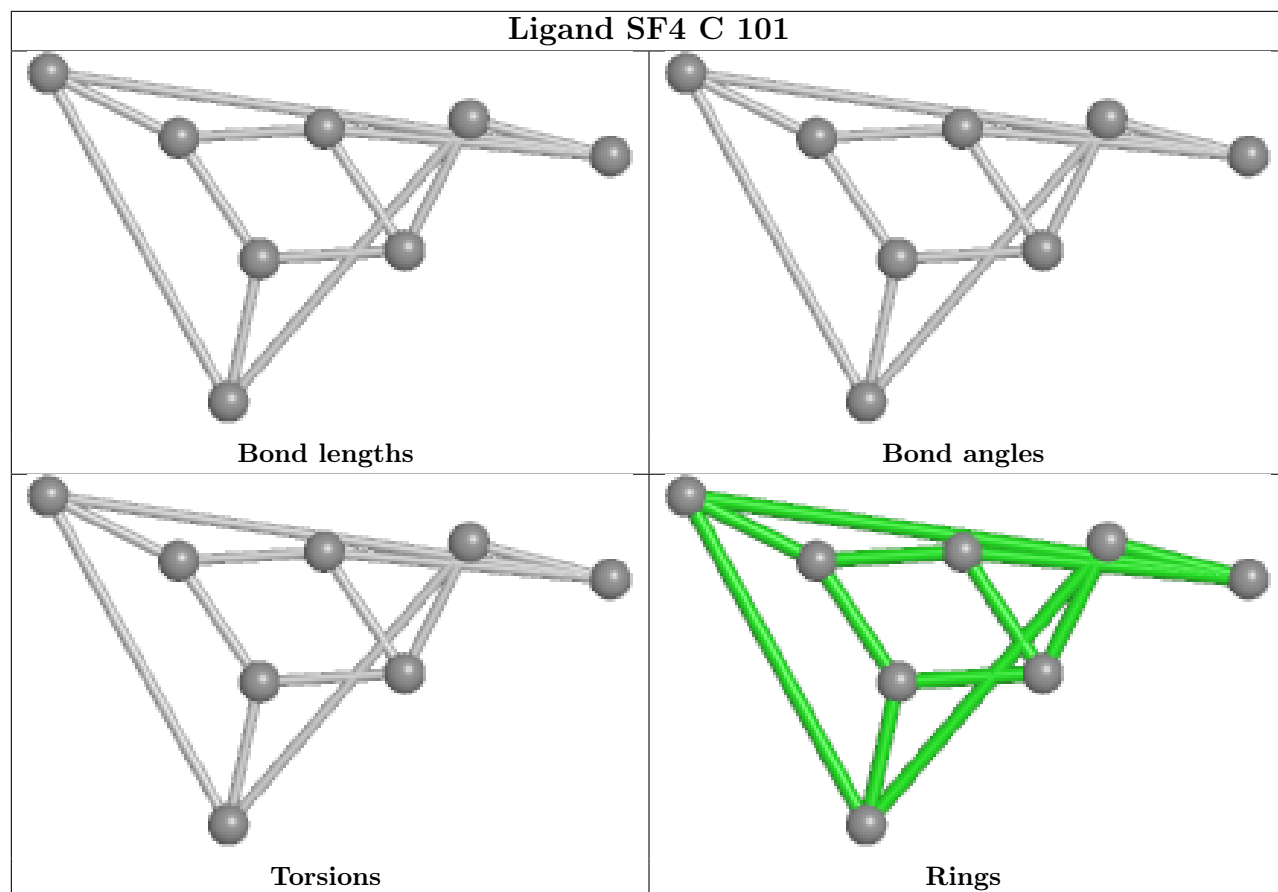


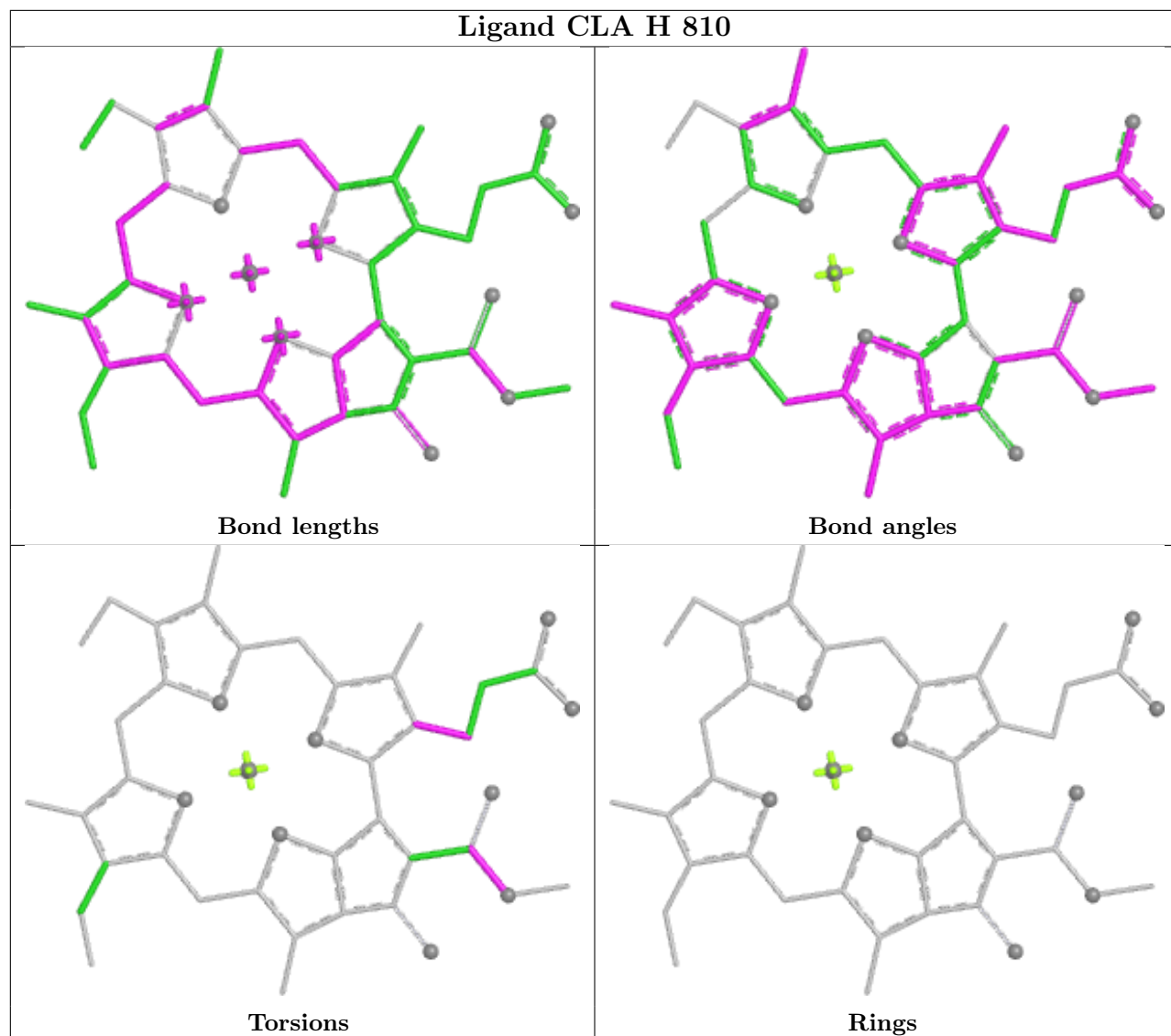
Ligand CLA H 827



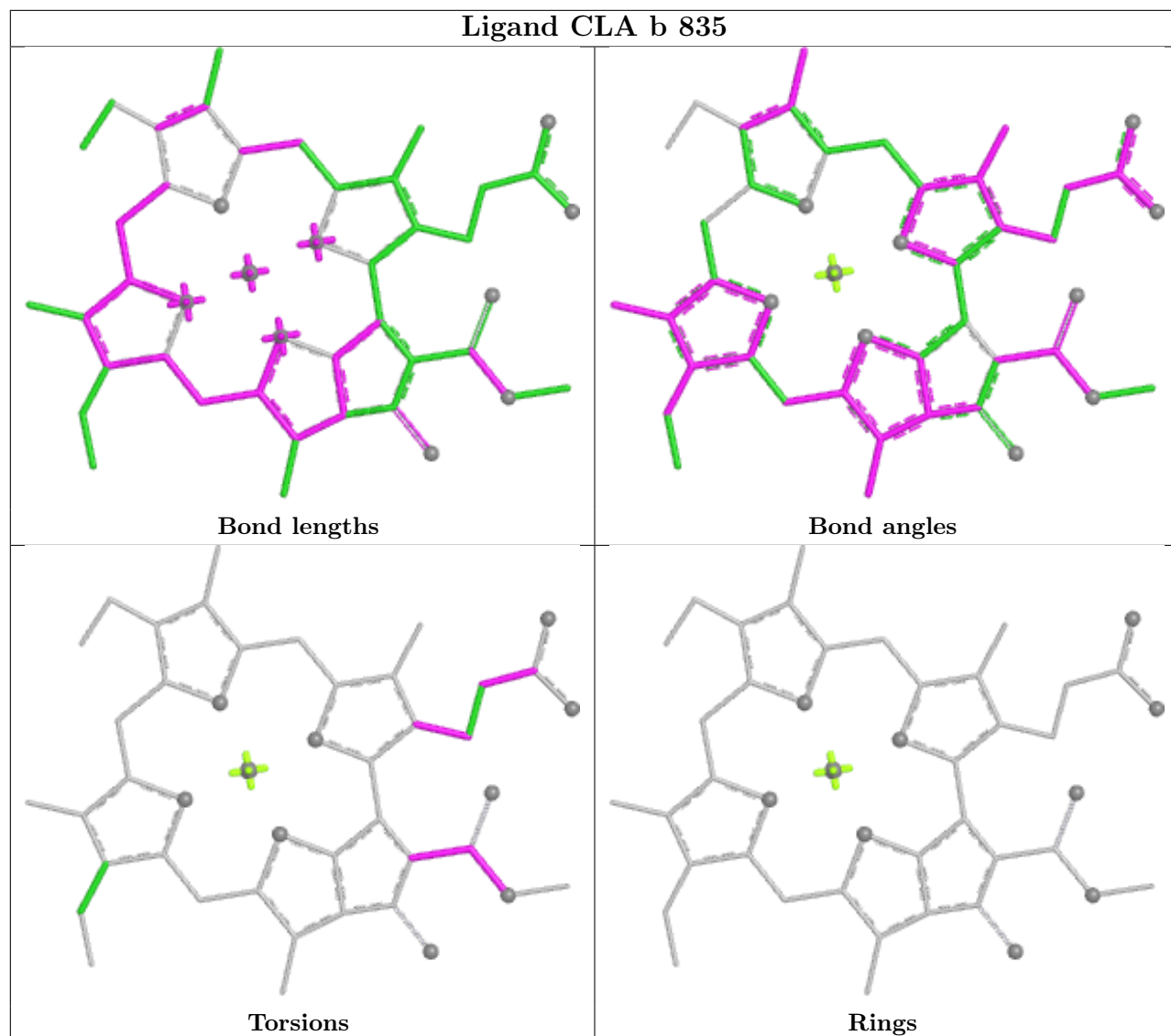




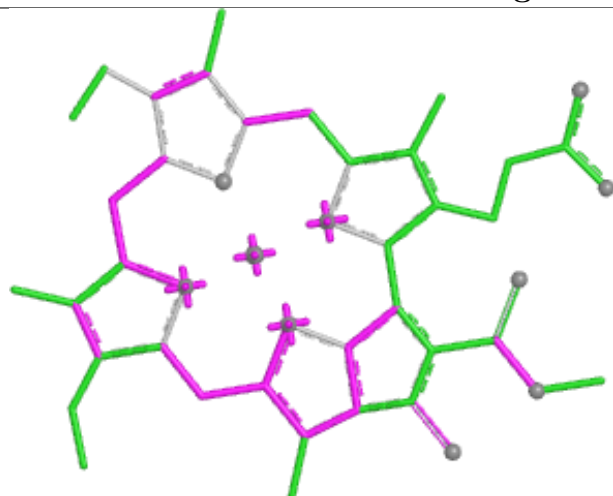




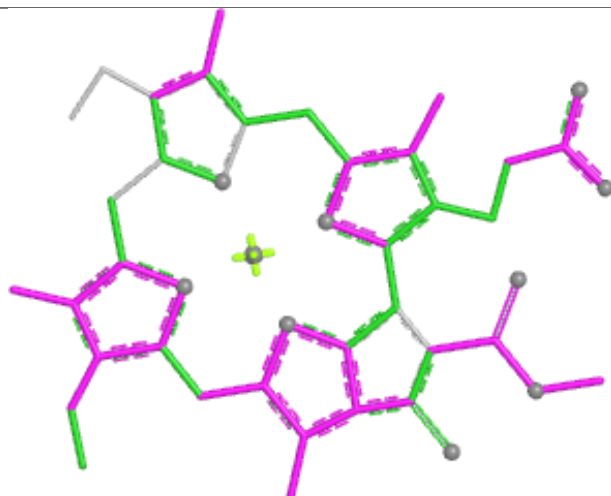
Ligand CLA b 835



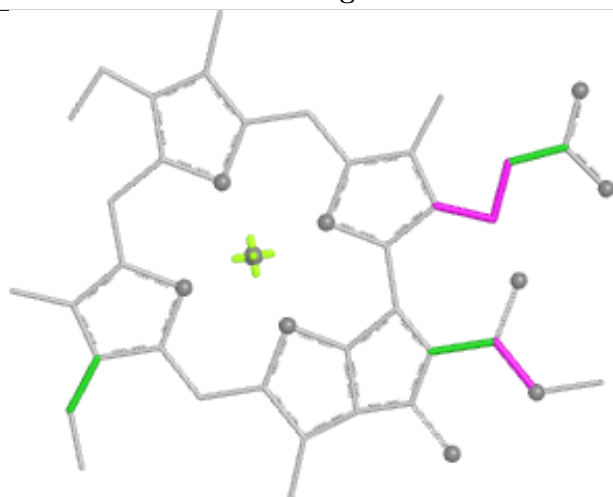
Ligand CLA A 811



Bond lengths



Bond angles

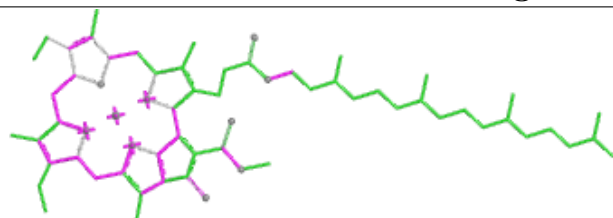


Torsions

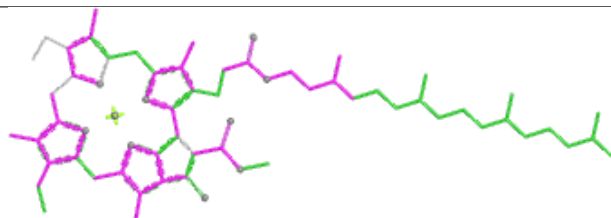


Rings

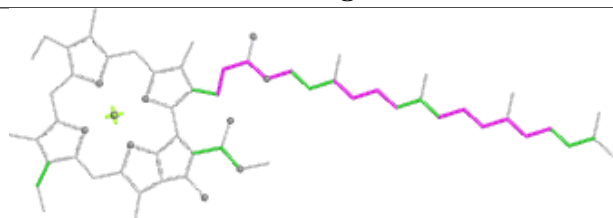
Ligand CLA G 826



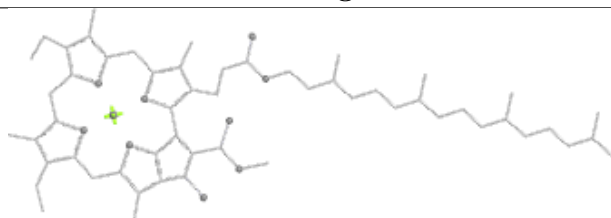
Bond lengths



Bond angles

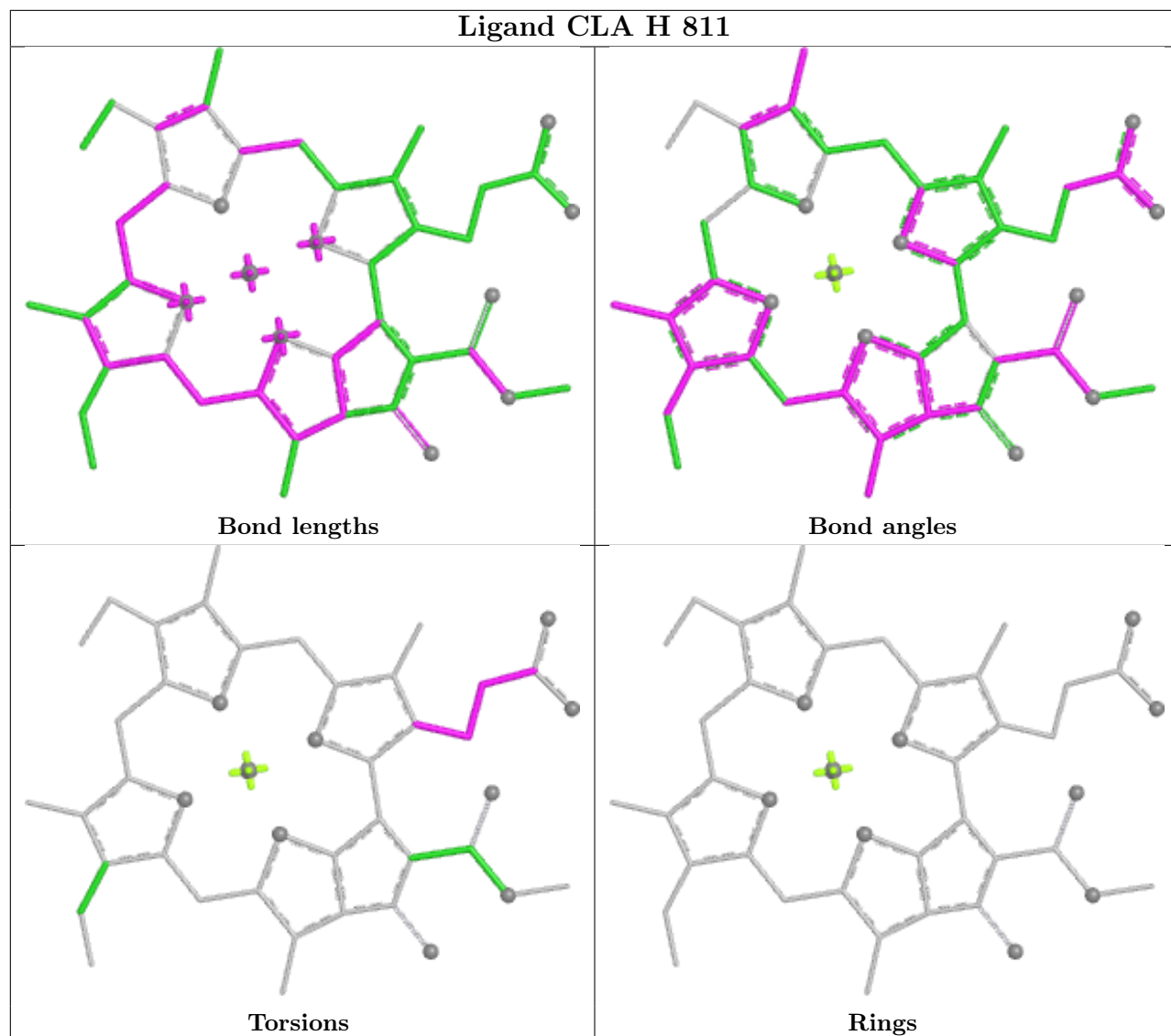


Torsions

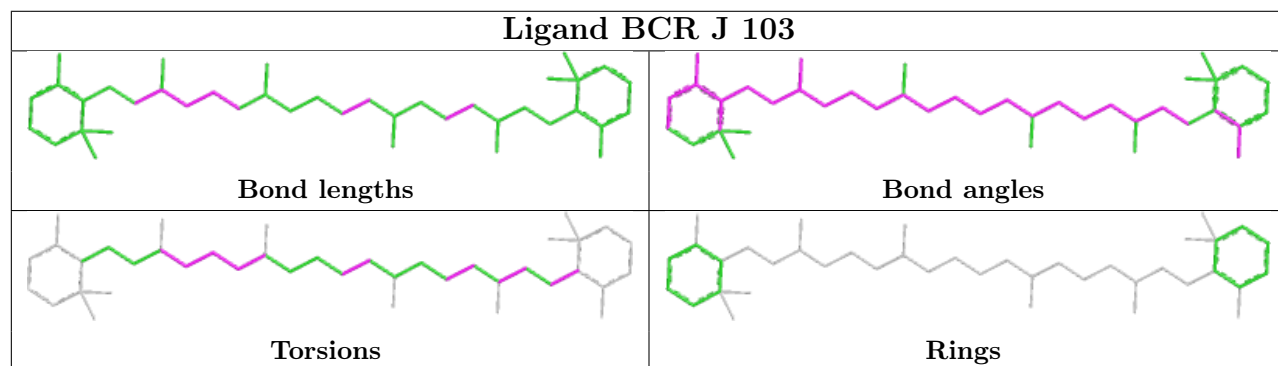


Rings

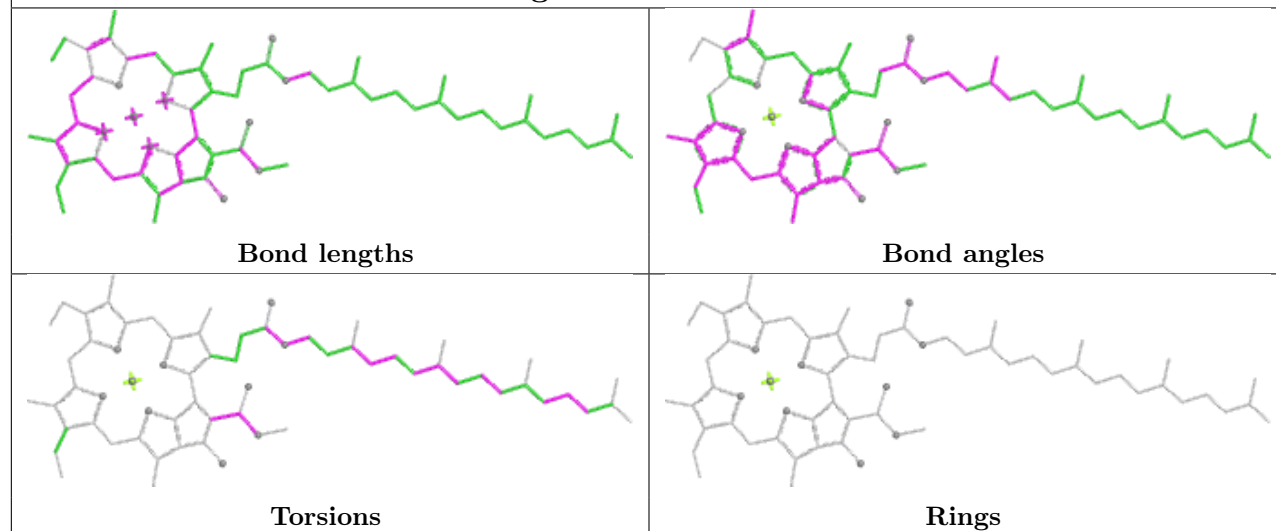
Ligand CLA H 811



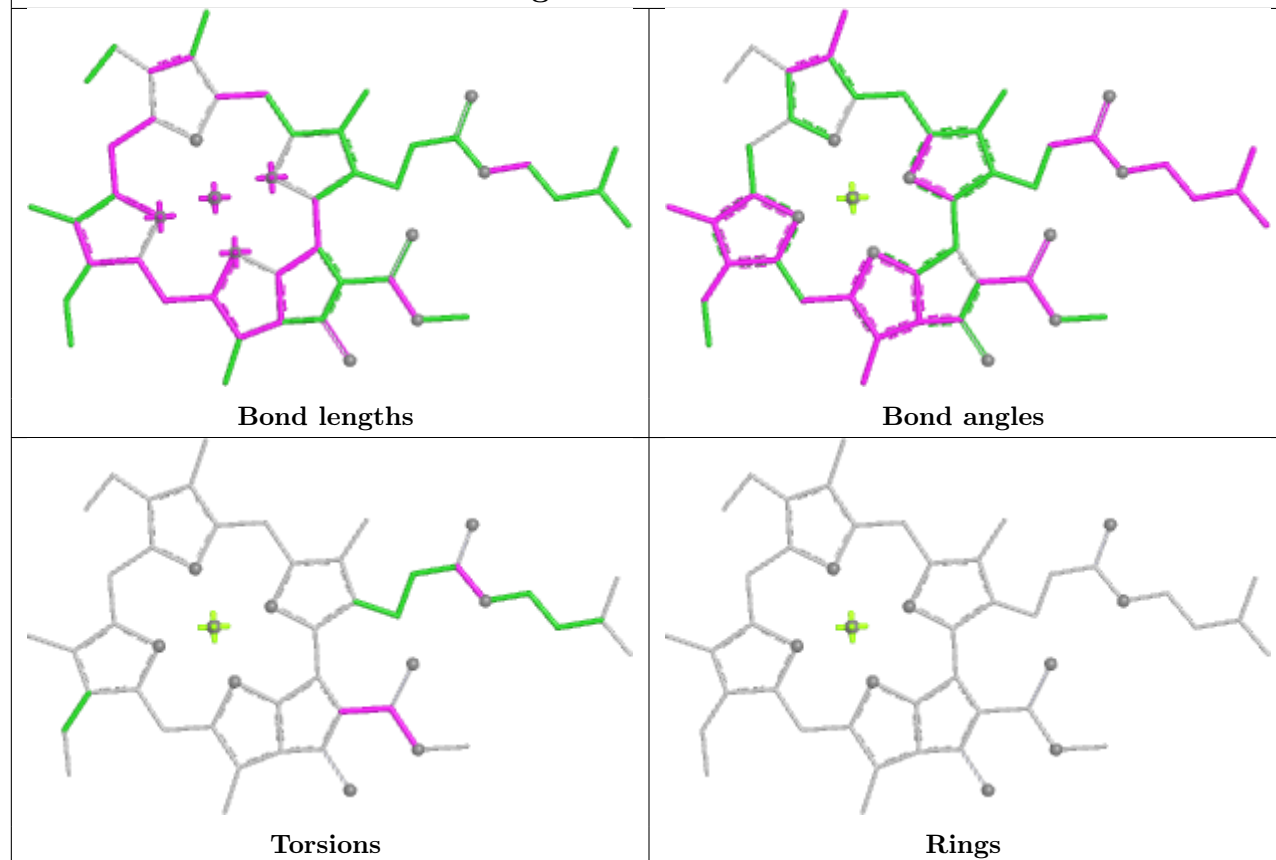
Ligand BCR J 103



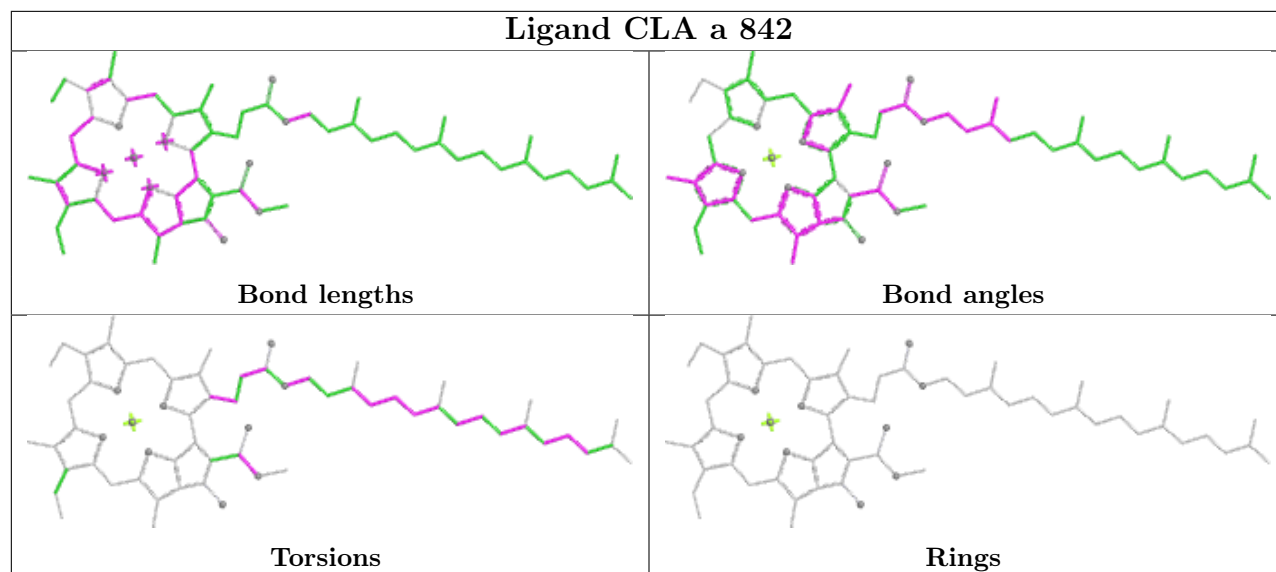
Ligand CLA G 828



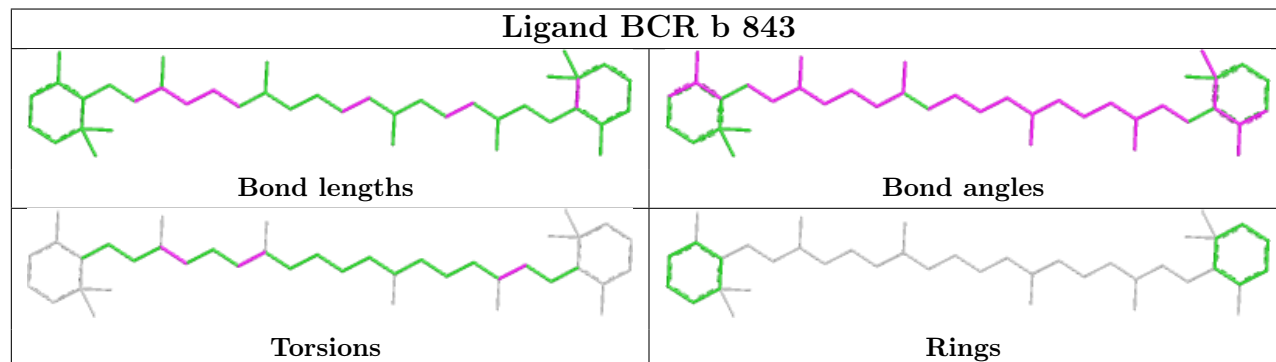
Ligand CLA A 838



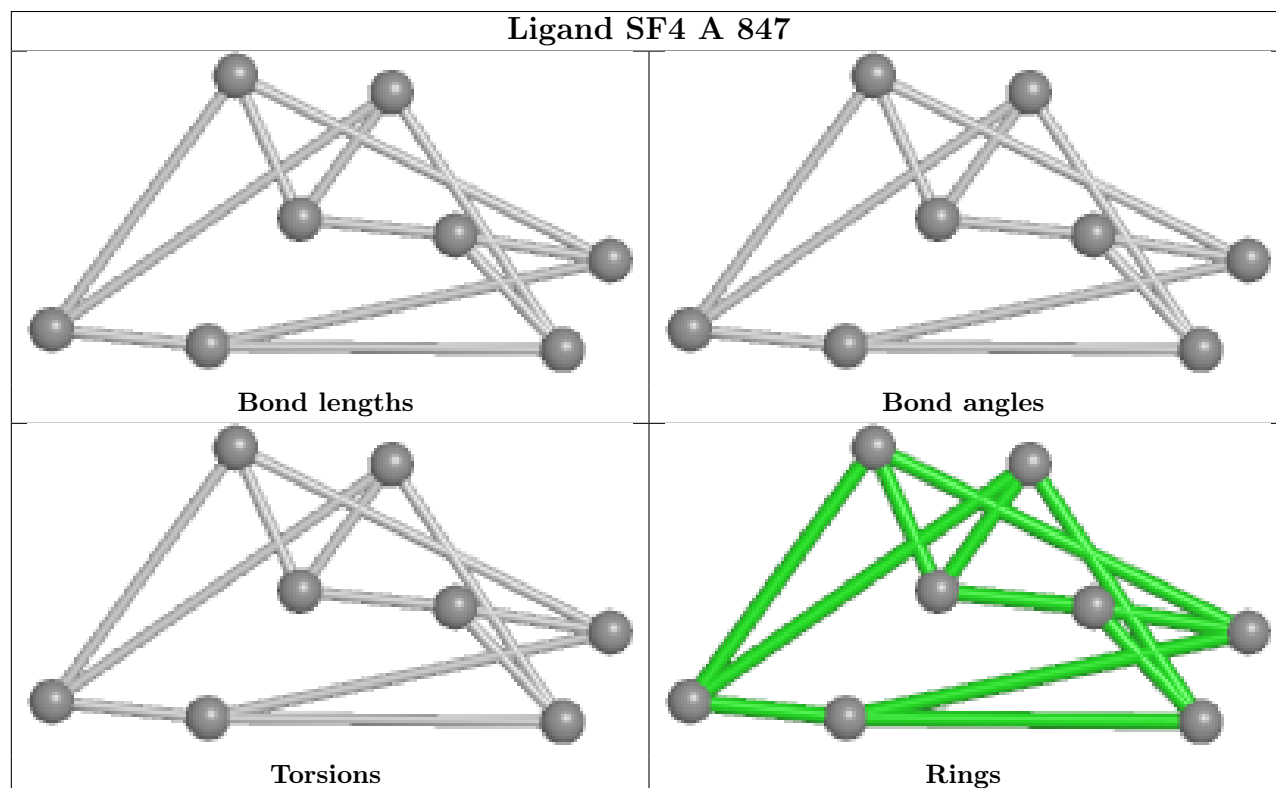
Ligand CLA a 842



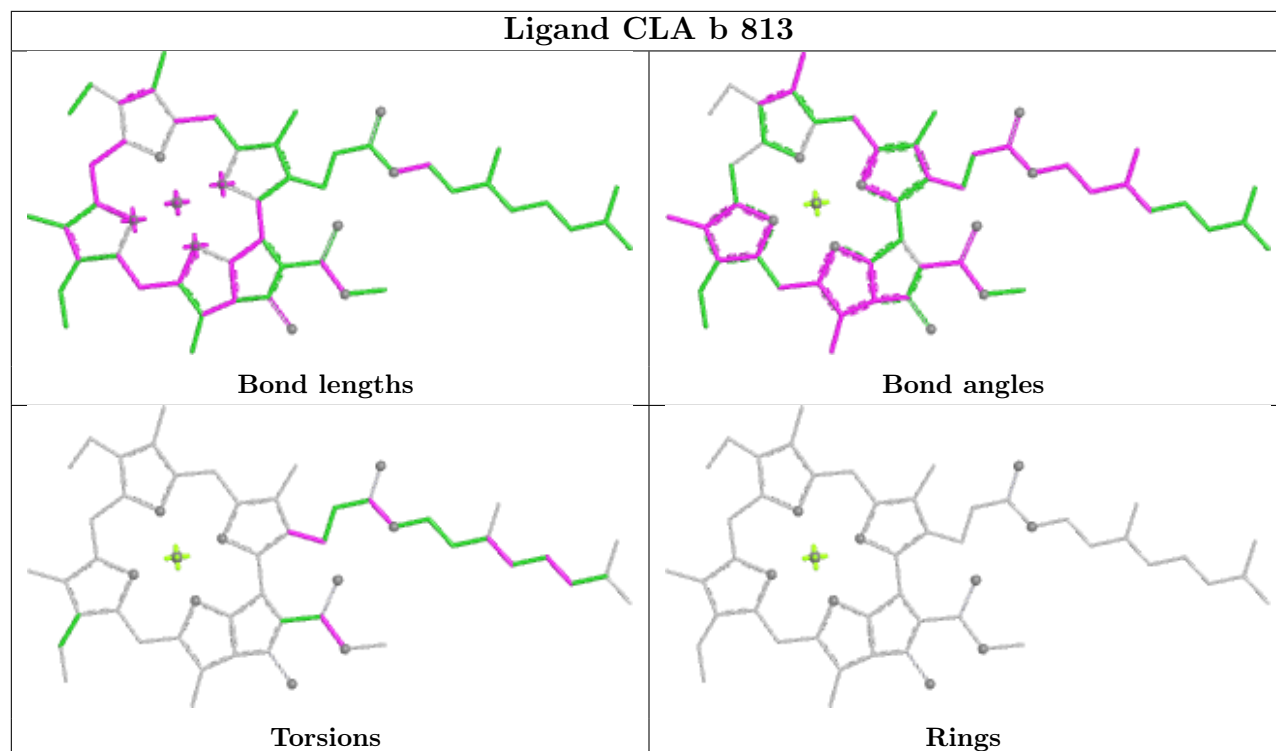
Ligand BCR b 843



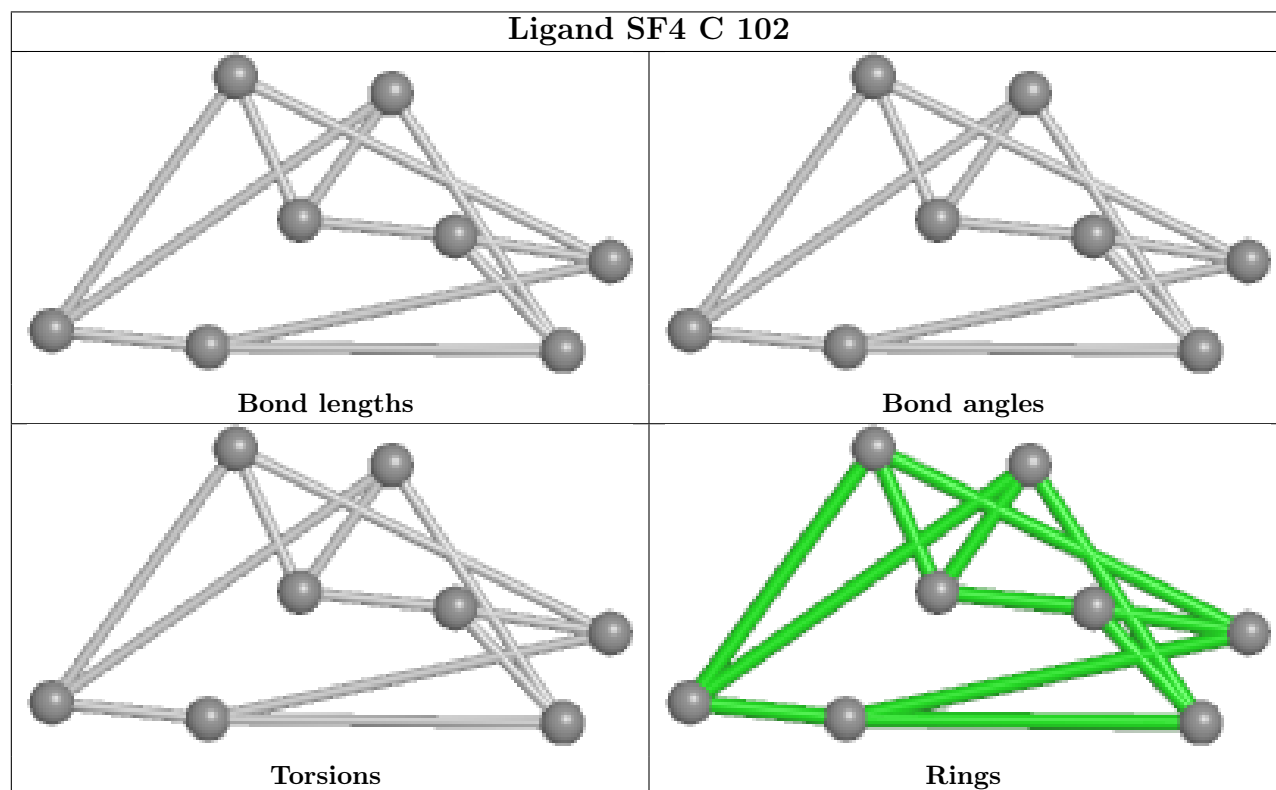
Ligand SF4 A 847



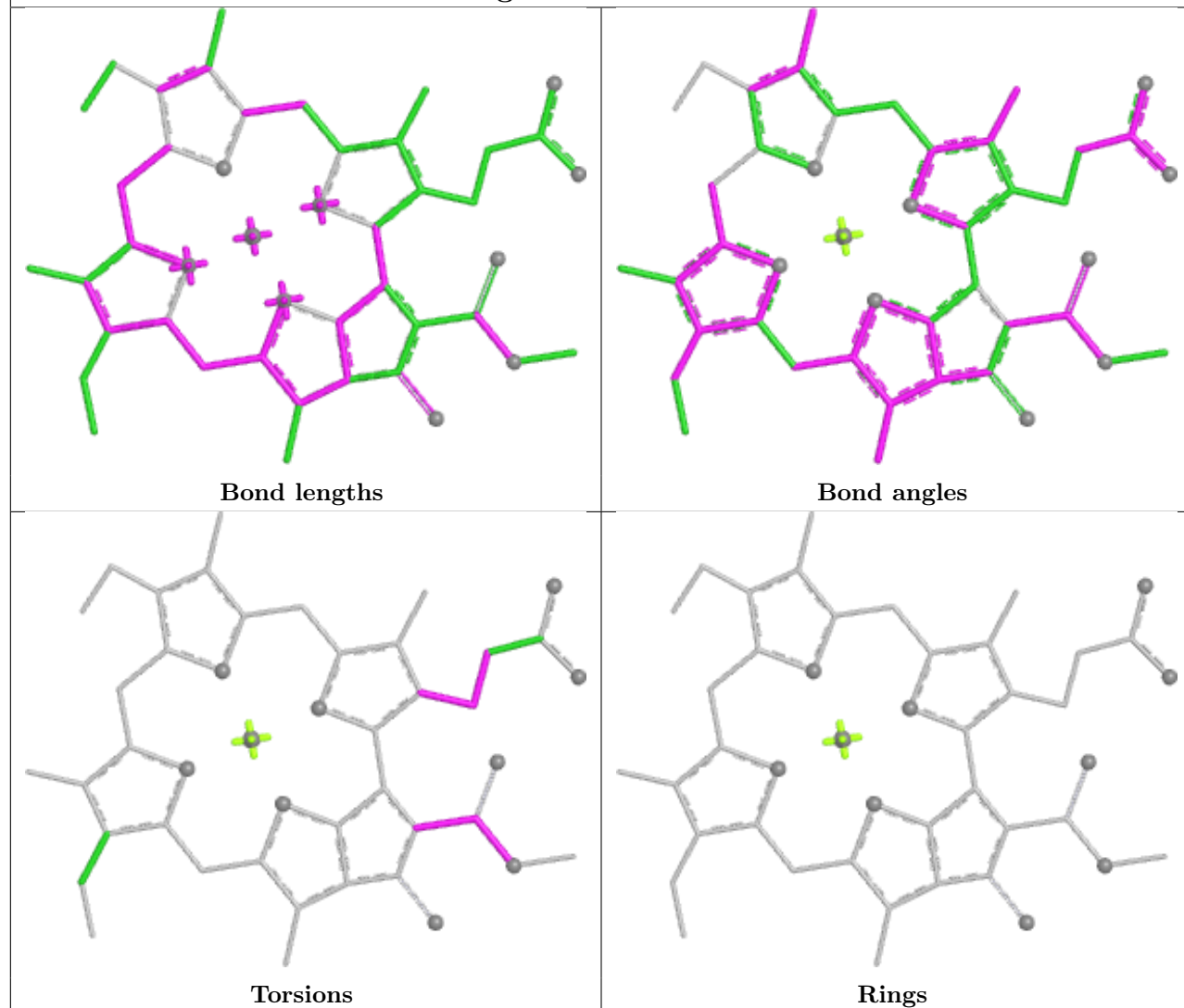
Ligand CLA b 813



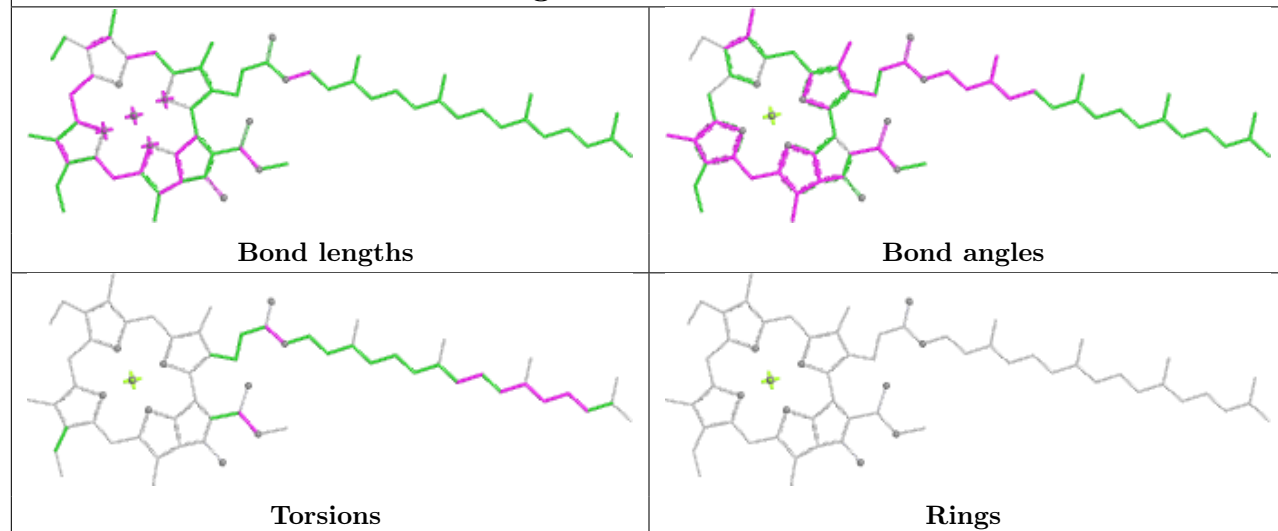
Ligand SF4 C 102



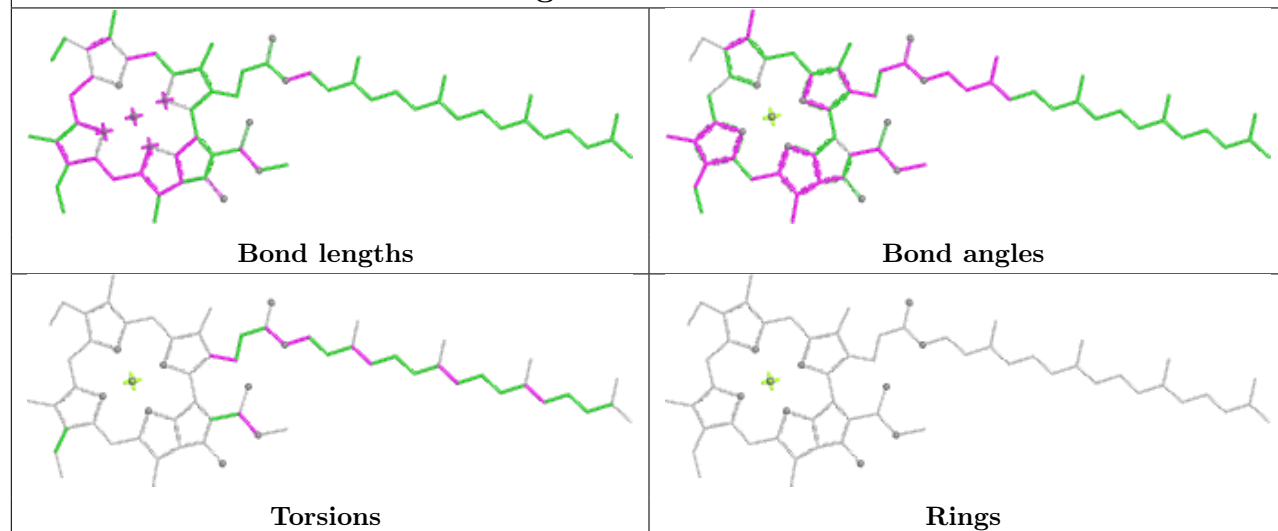
Ligand CLA a 815



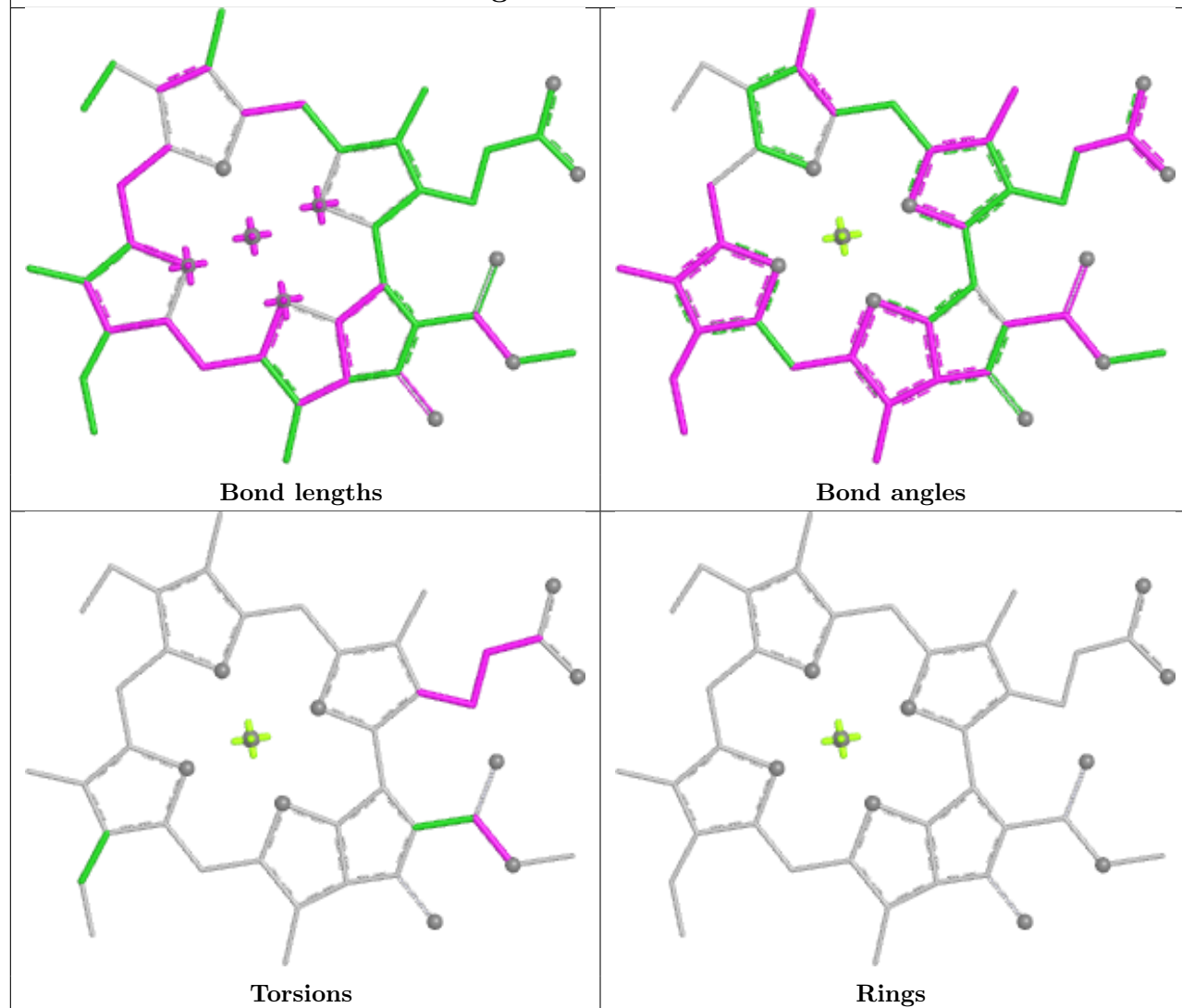
Ligand CLA B 802



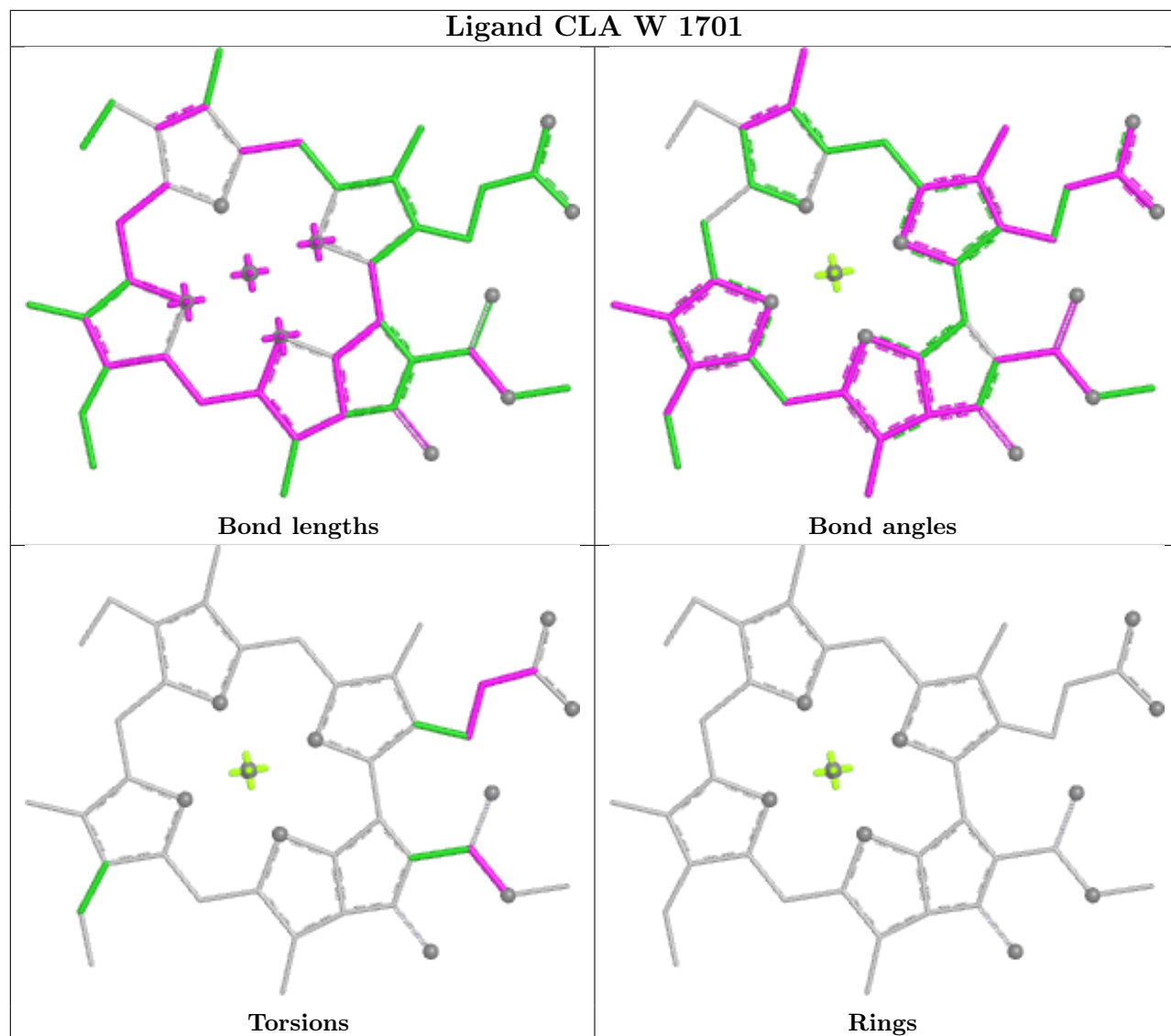
Ligand CLA a 821



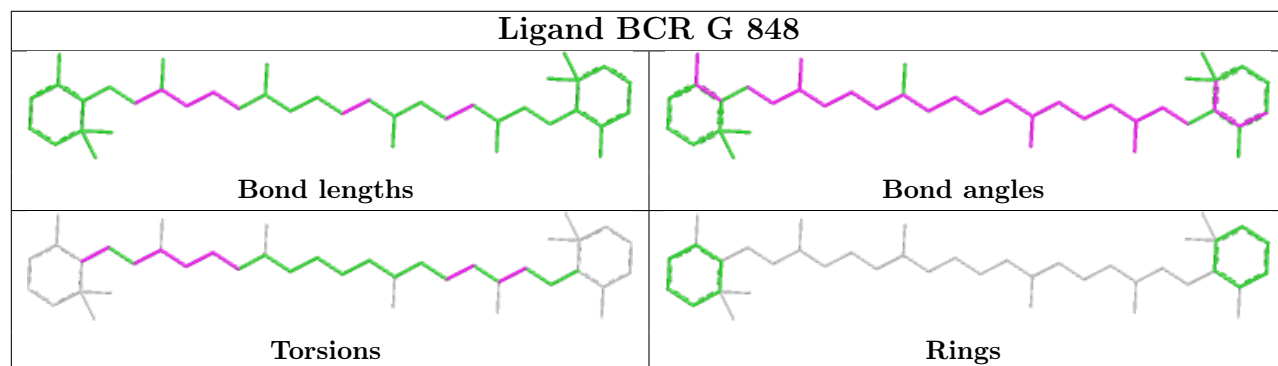
Ligand CLA H 829

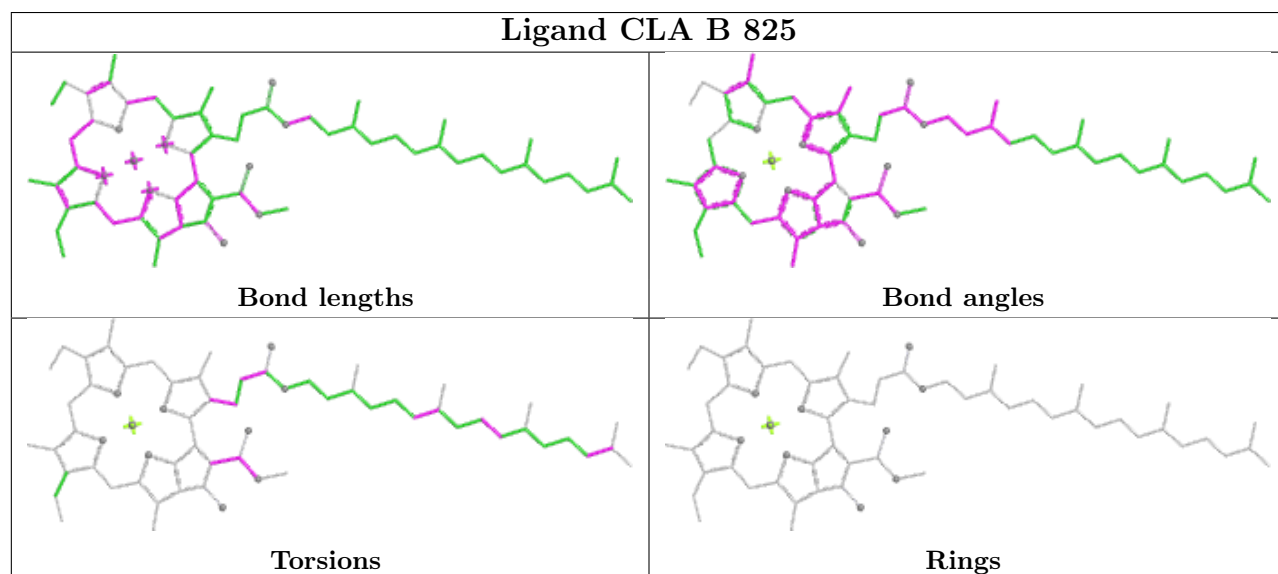
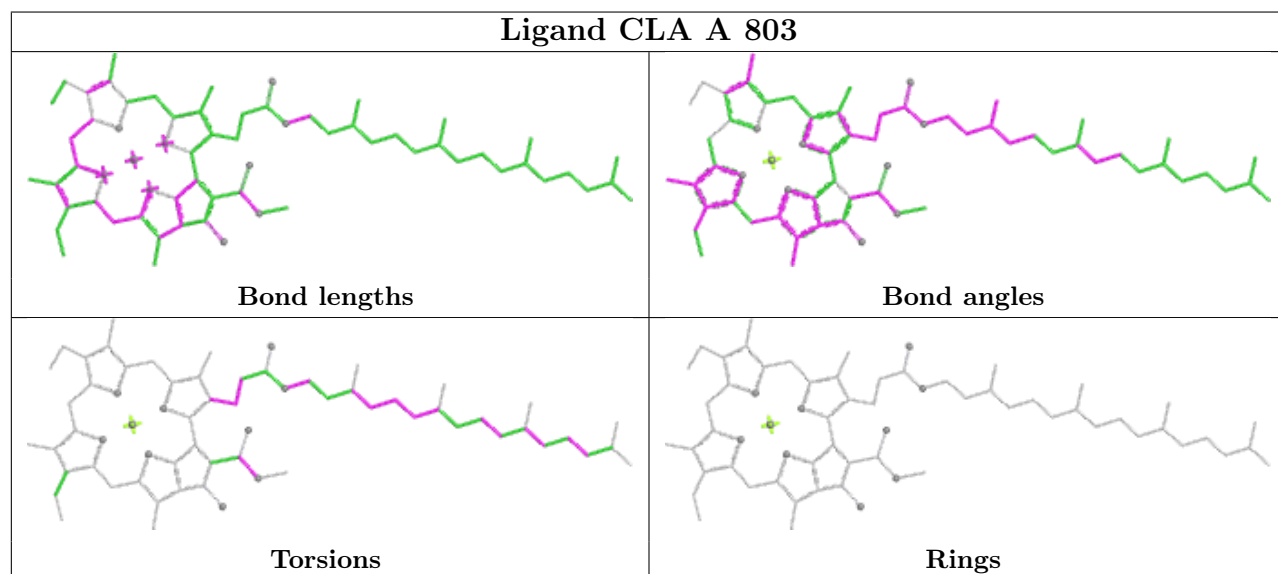
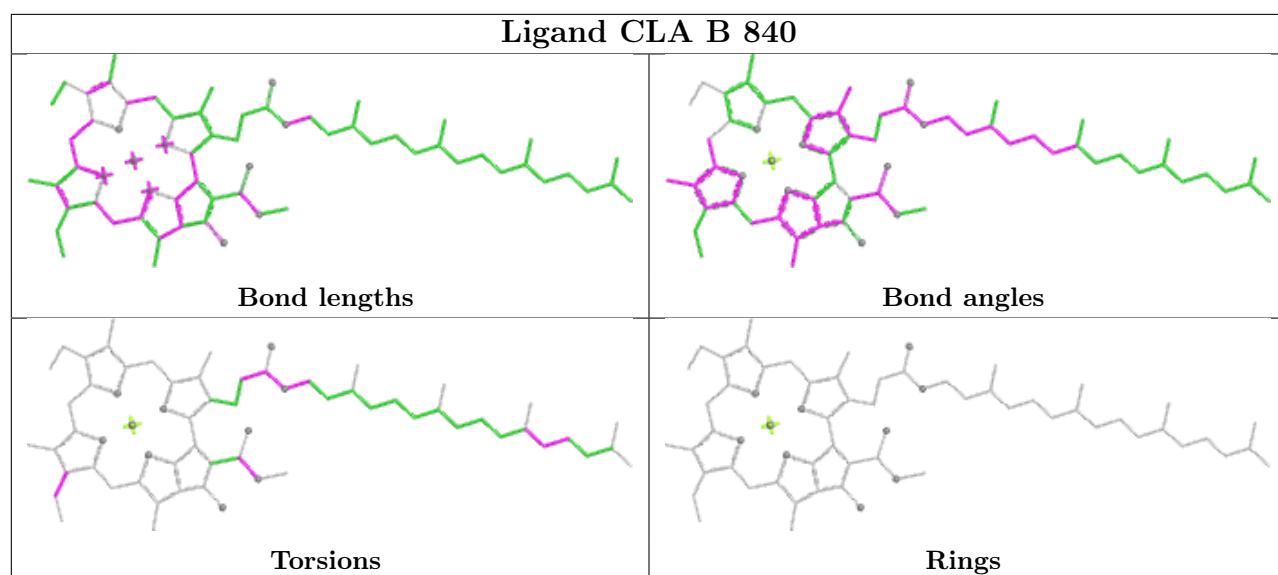


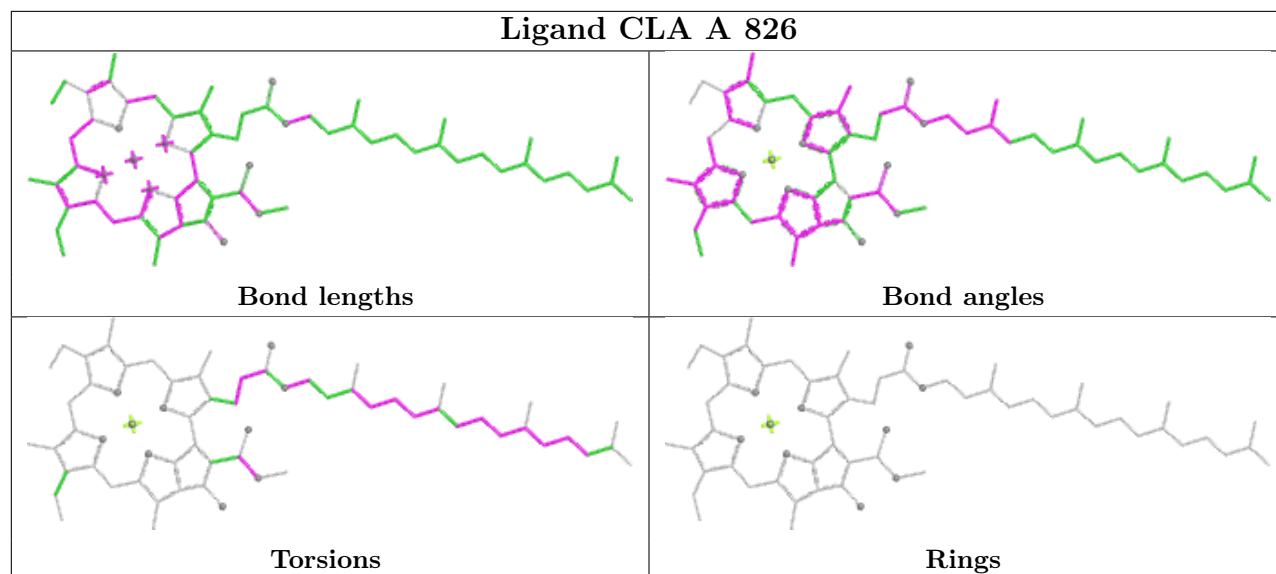
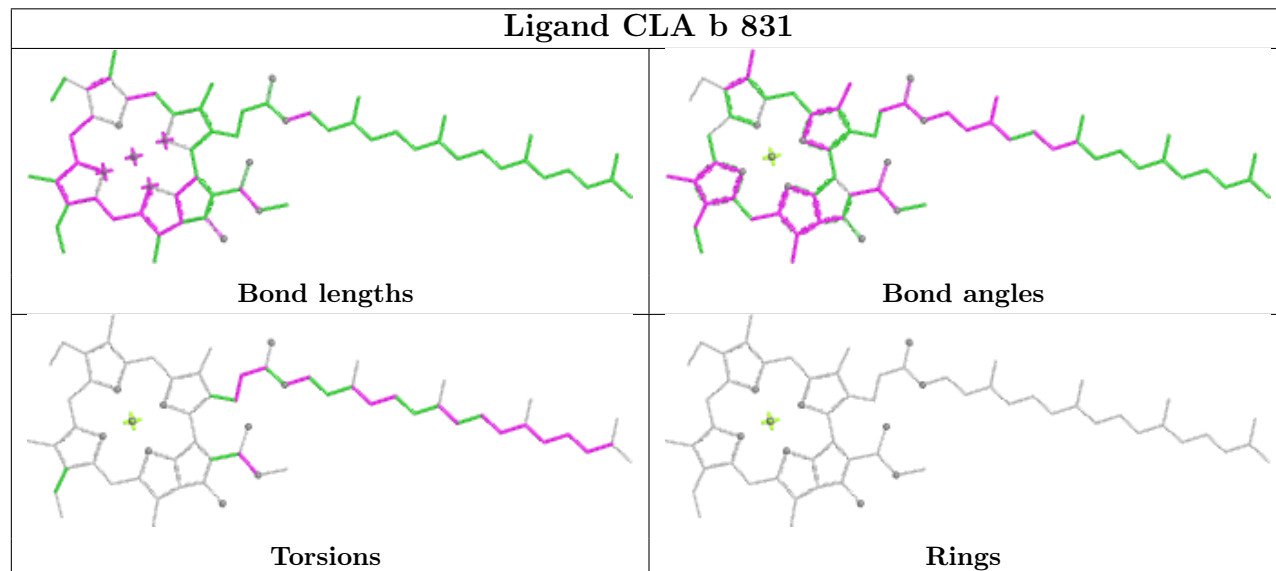
Ligand CLA W 1701



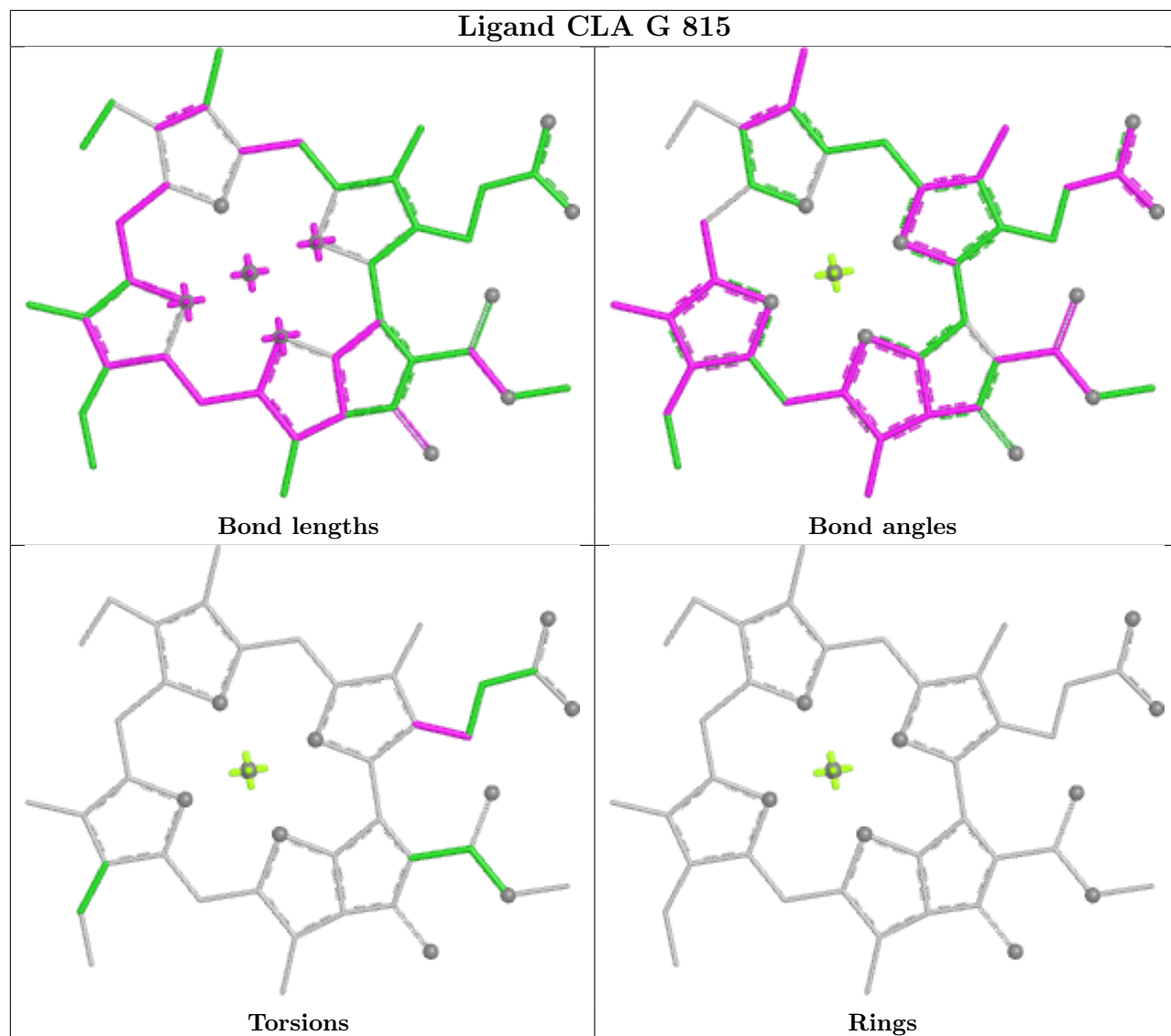
Ligand BCR G 848



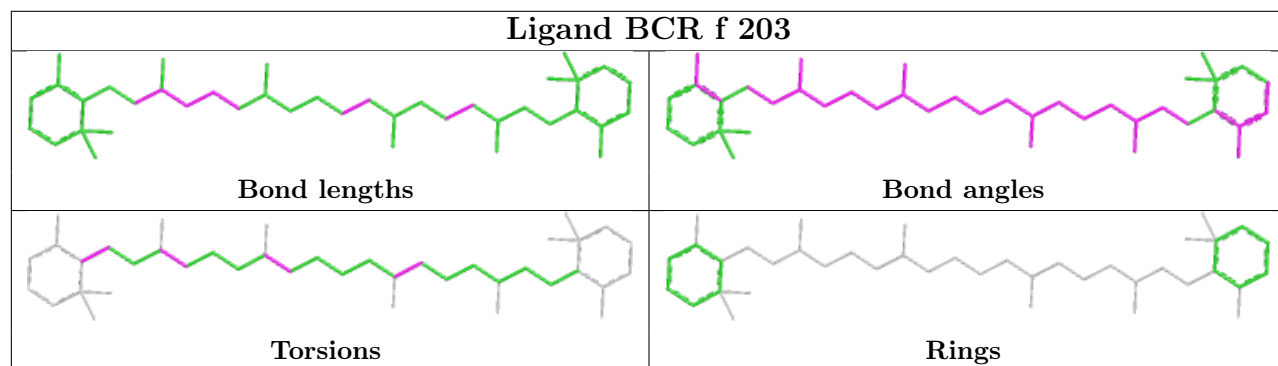


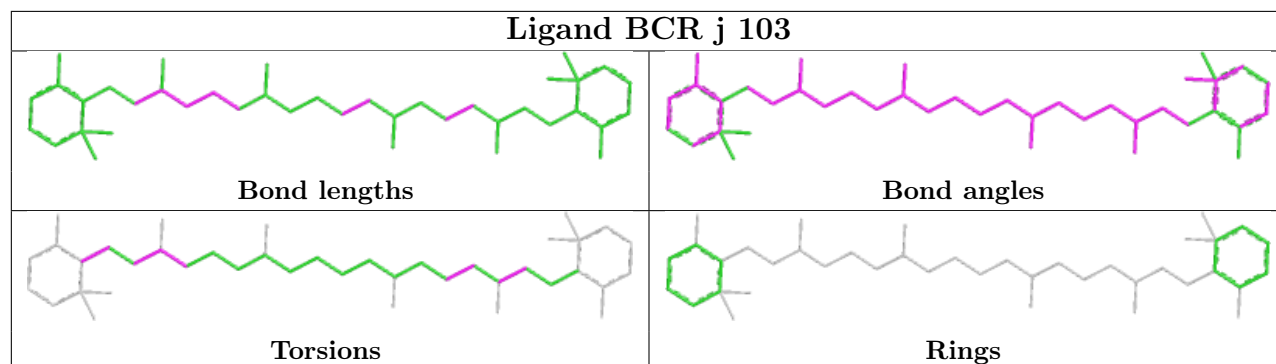
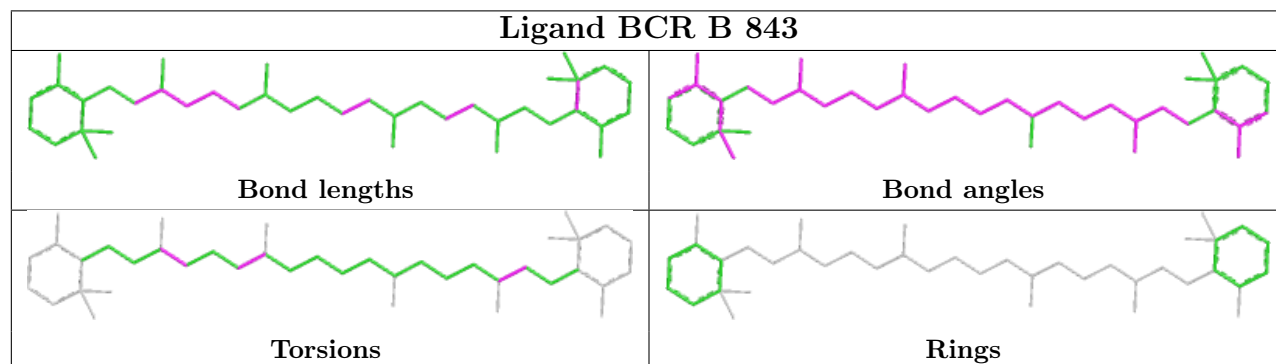
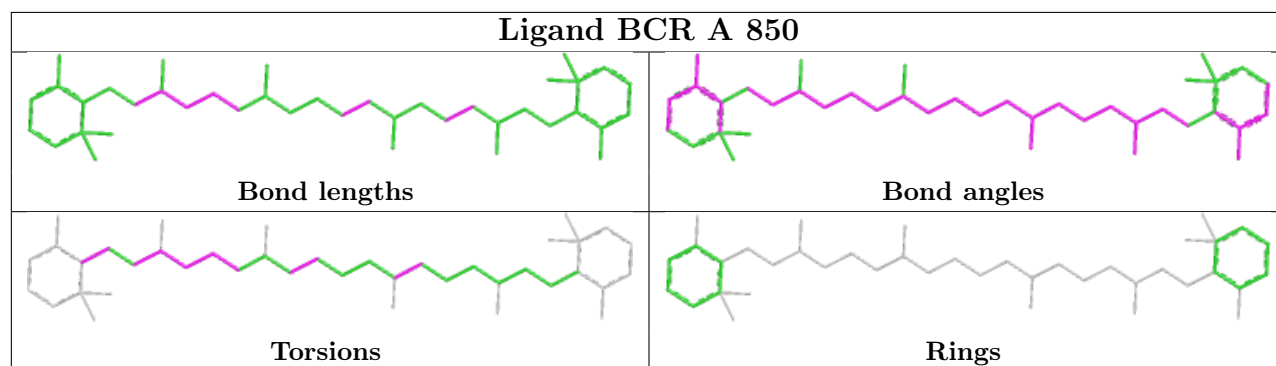
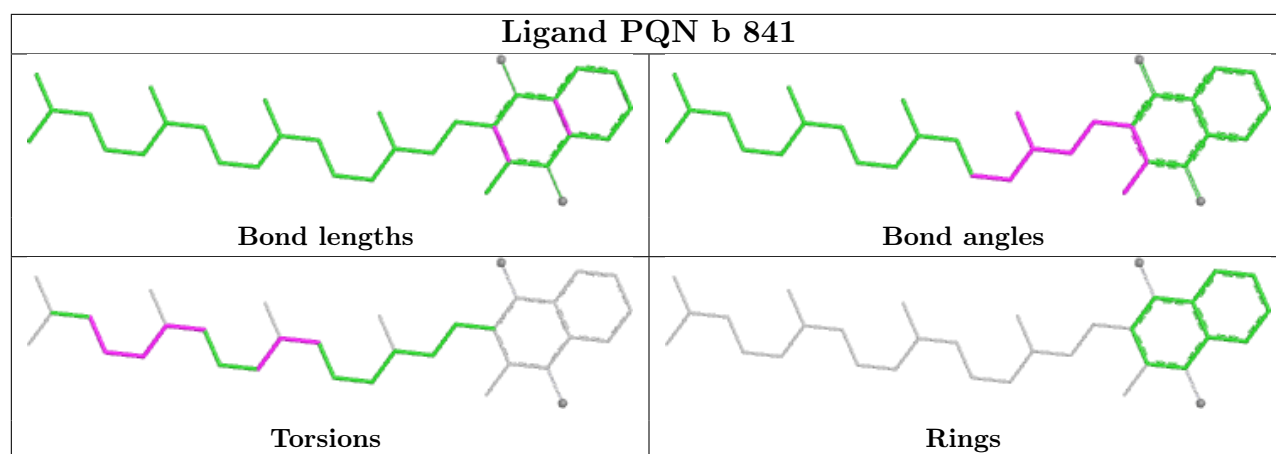
Ligand CLA A 826**Ligand CLA b 831**

Ligand CLA G 815

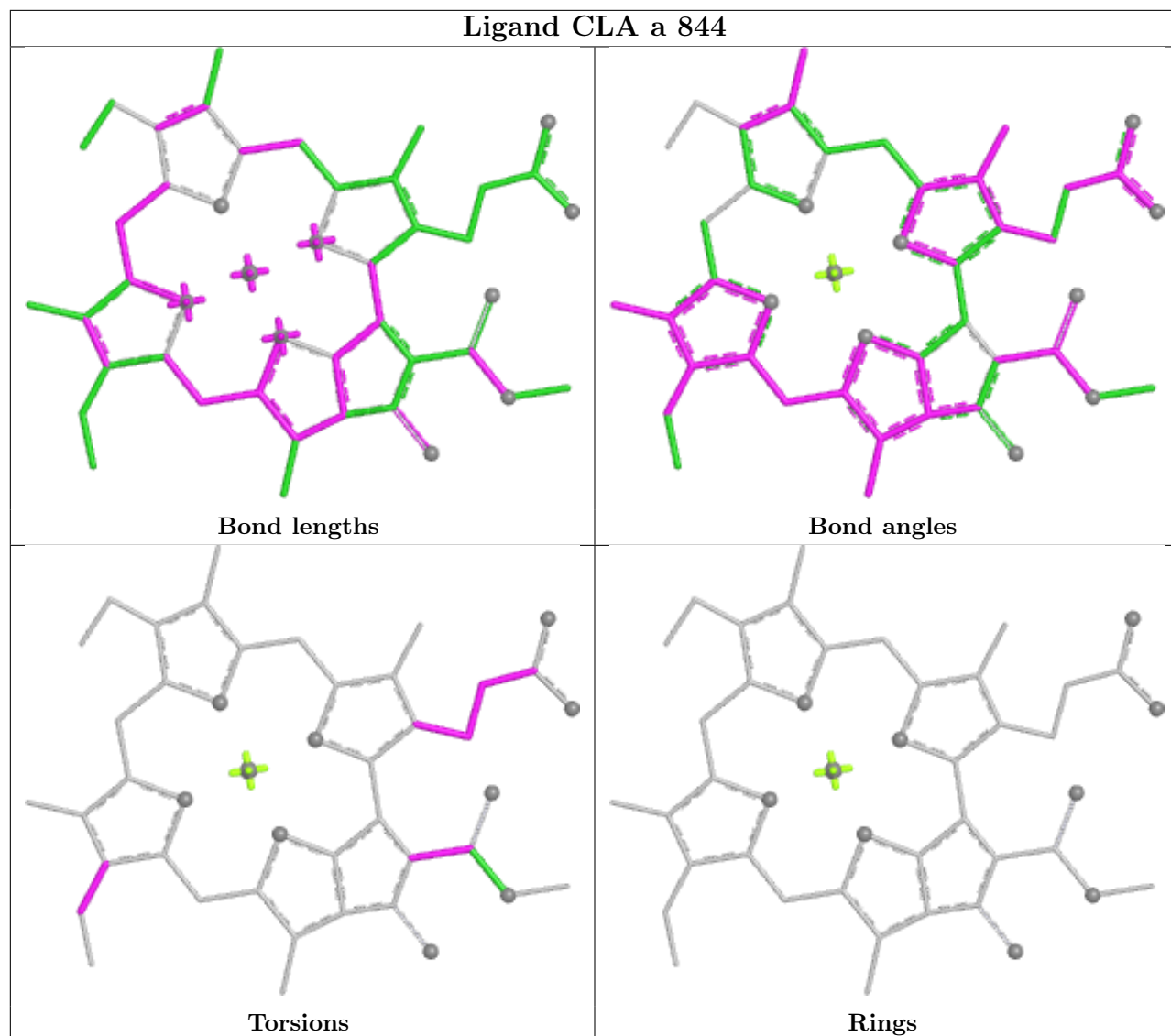


Ligand BCR f 203

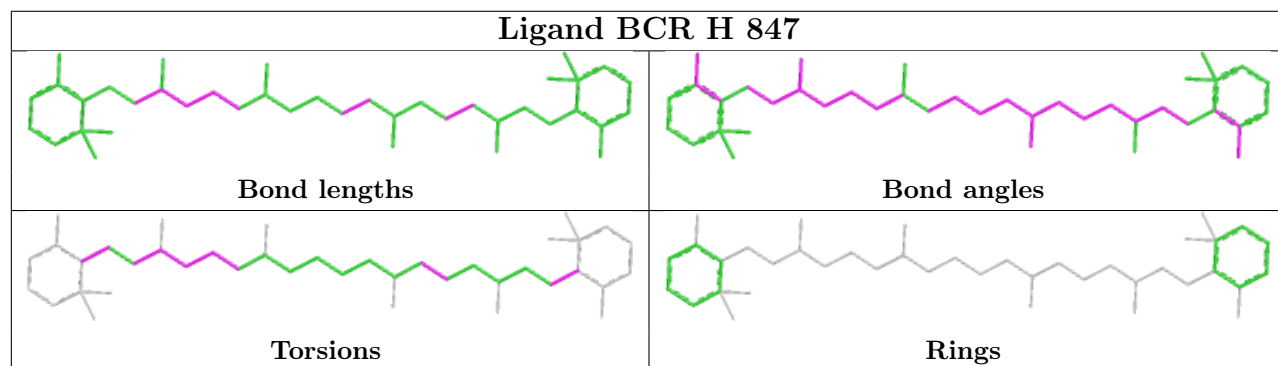




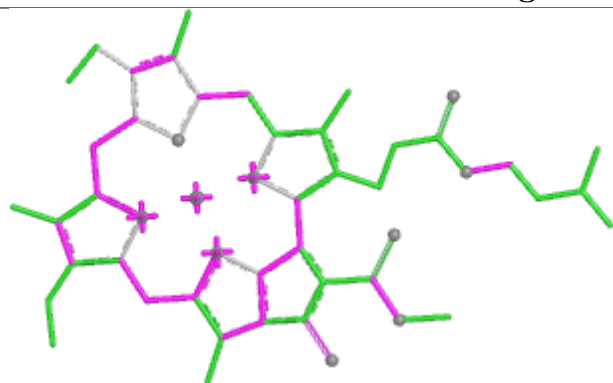
Ligand CLA a 844



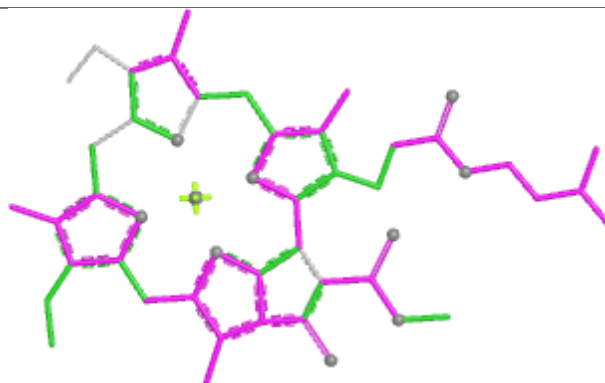
Ligand BCR H 847



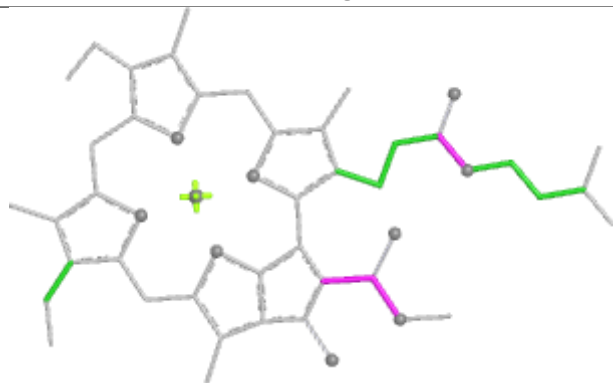
Ligand CLA a 837



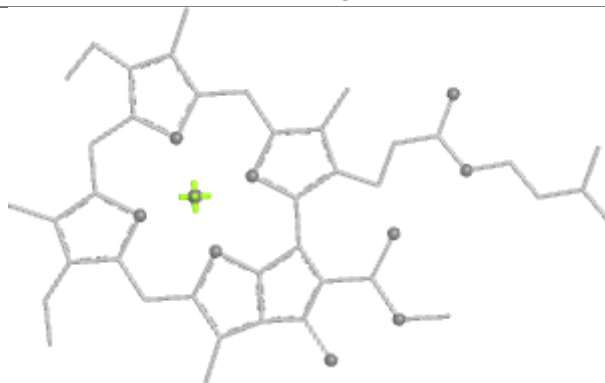
Bond lengths



Bond angles

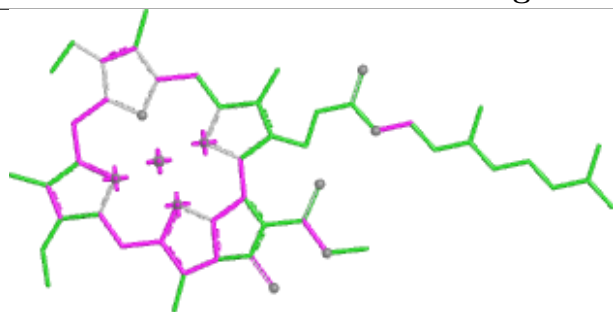


Torsions

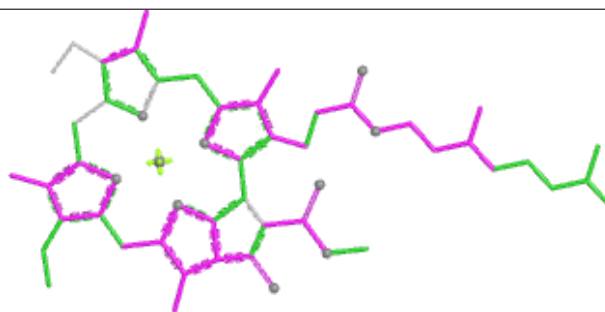


Rings

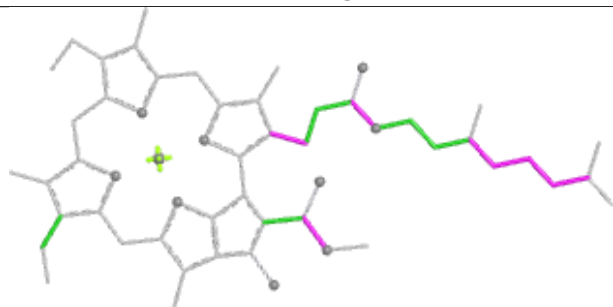
Ligand CLA G 833



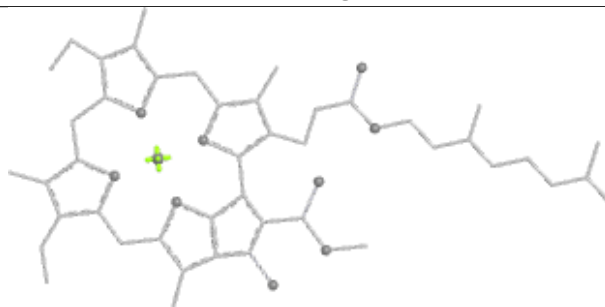
Bond lengths



Bond angles

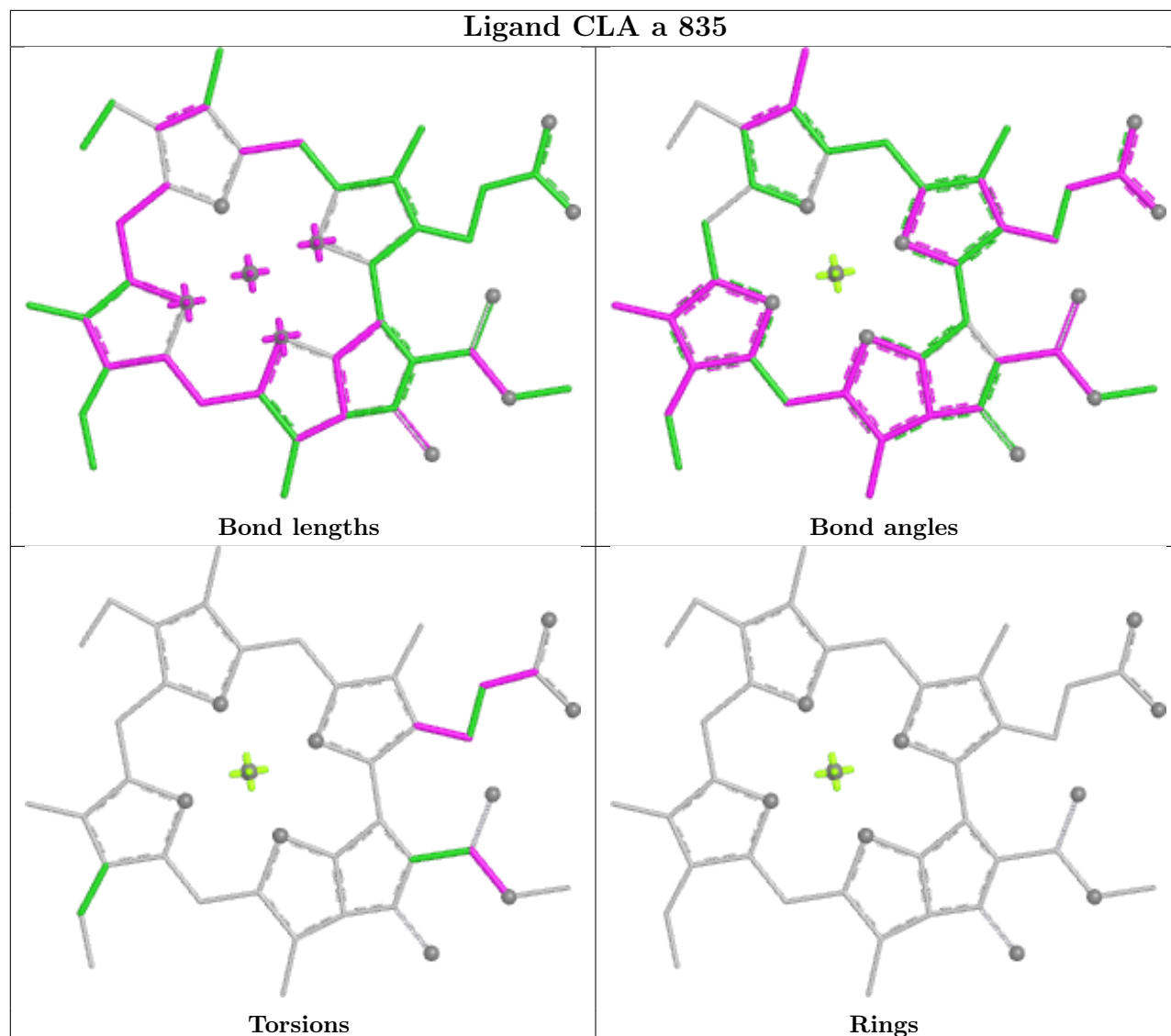


Torsions

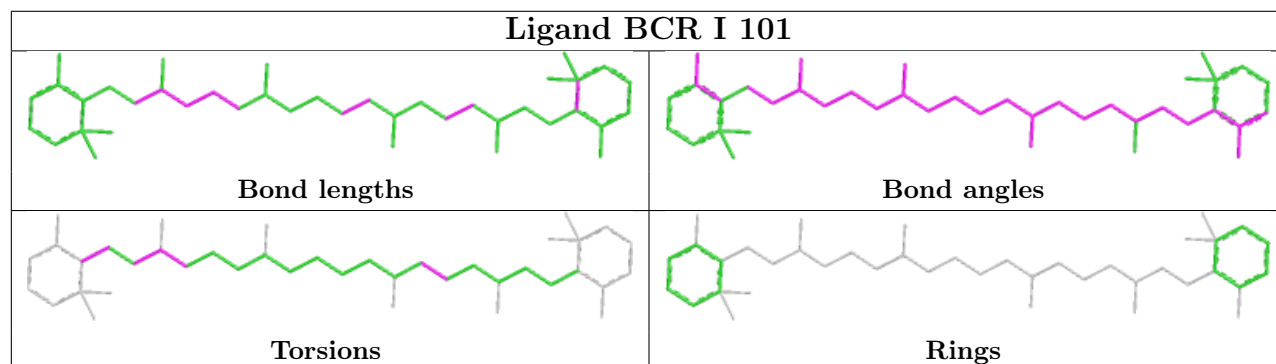


Rings

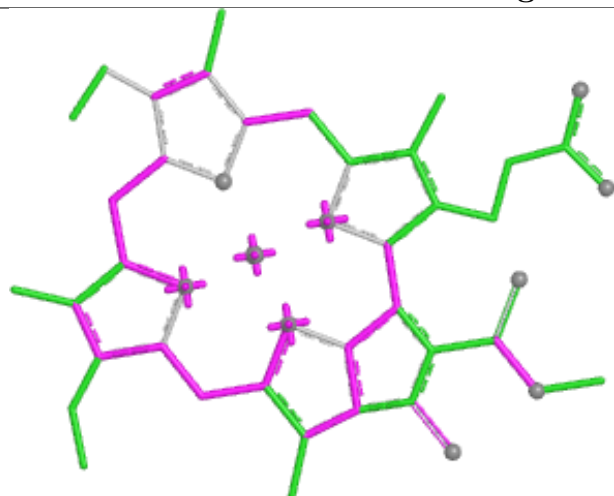
Ligand CLA a 835



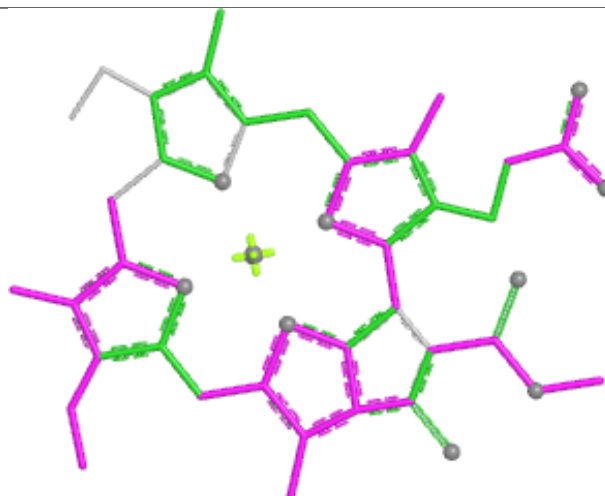
Ligand BCR I 101



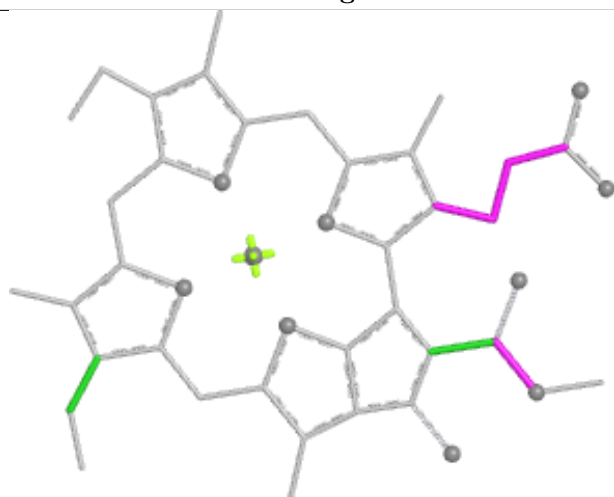
Ligand CLA b 834



Bond lengths



Bond angles

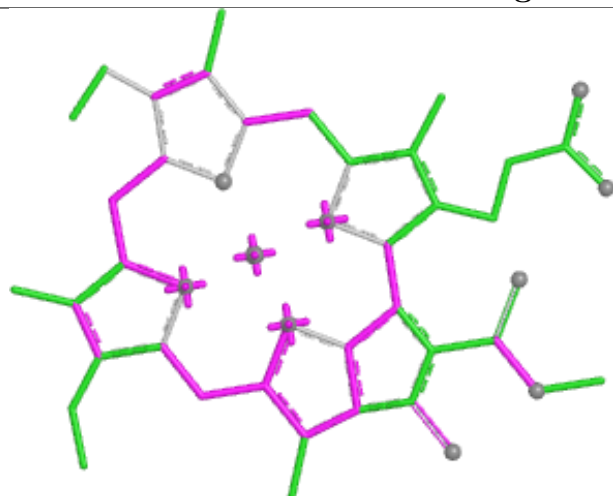


Torsions

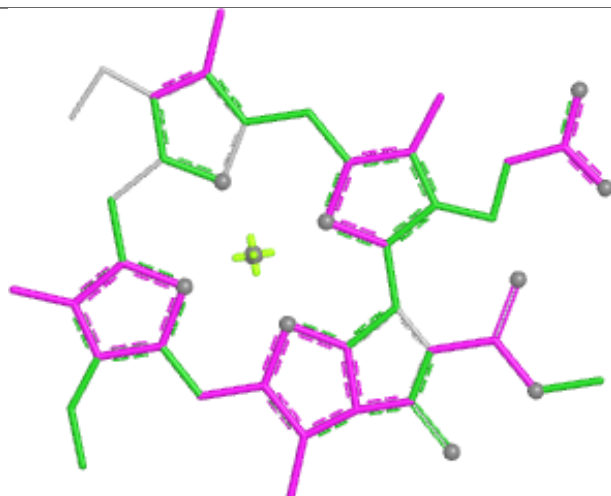


Rings

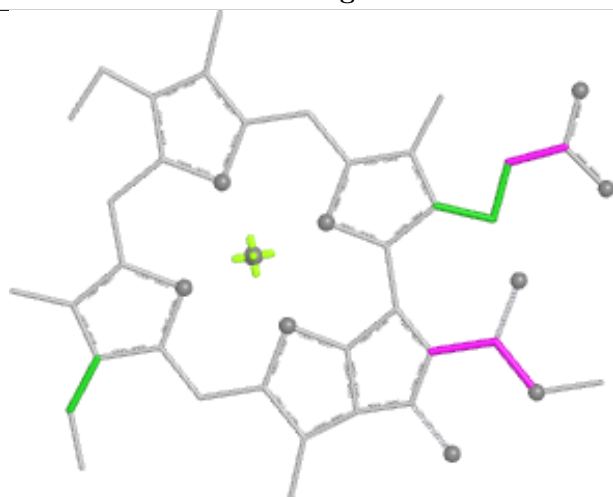
Ligand CLA B 820



Bond lengths



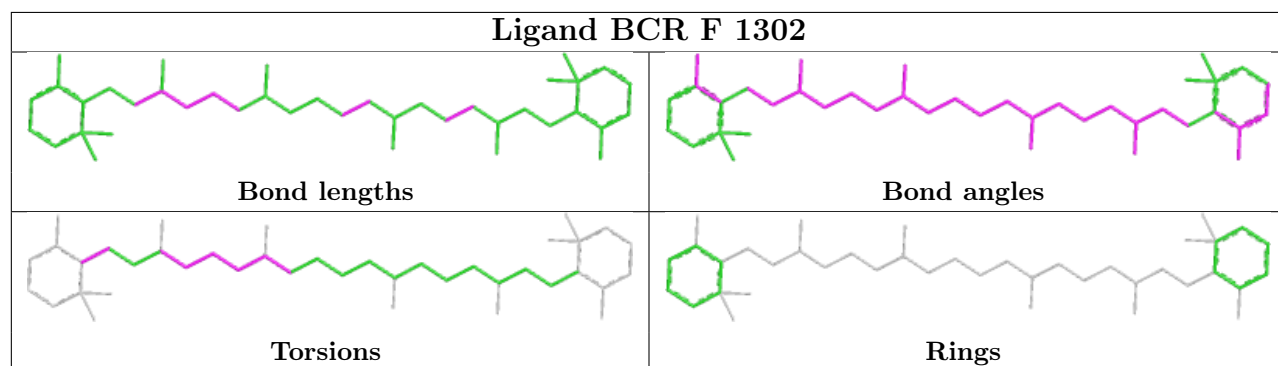
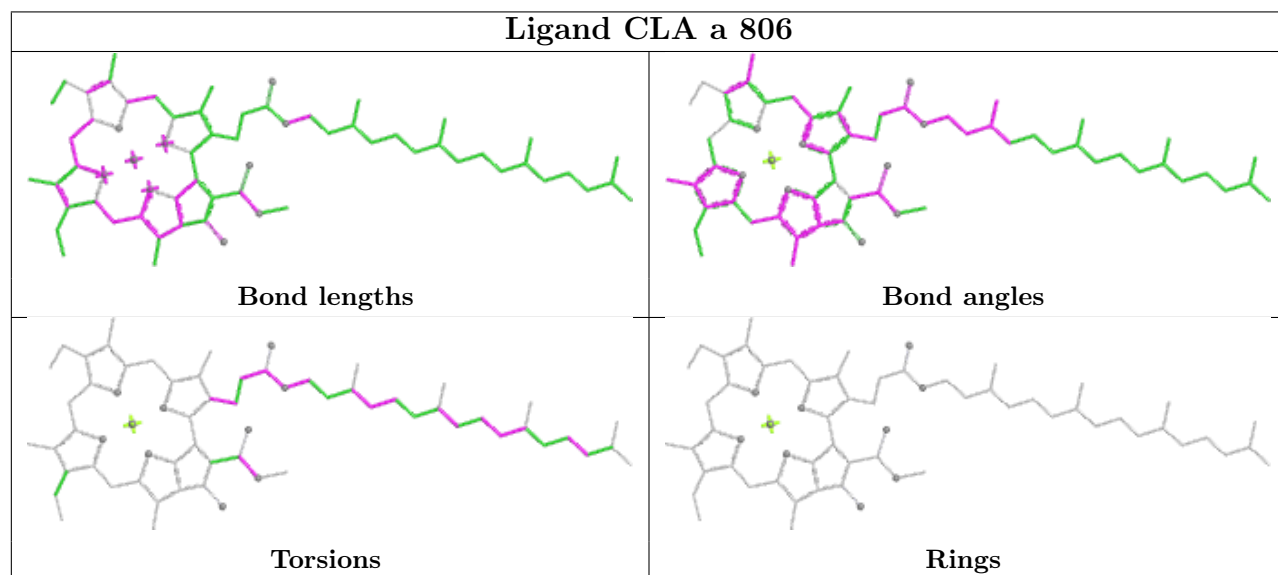
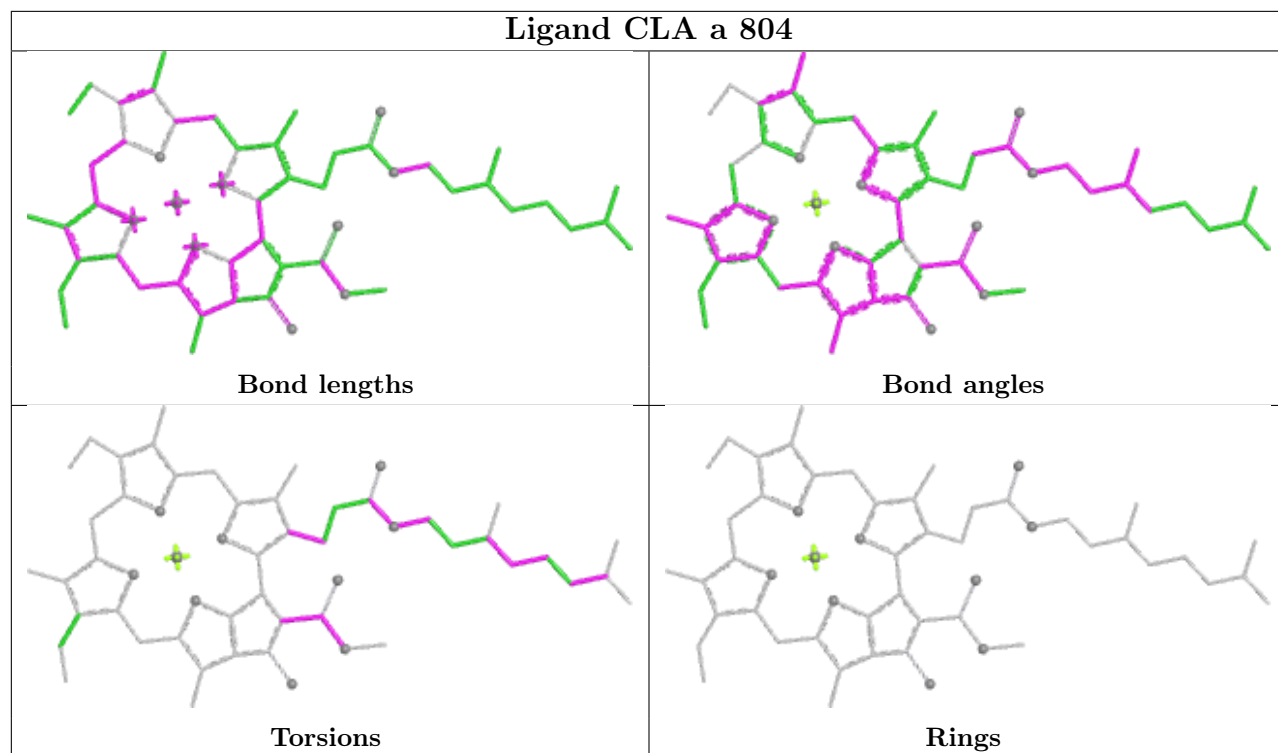
Bond angles



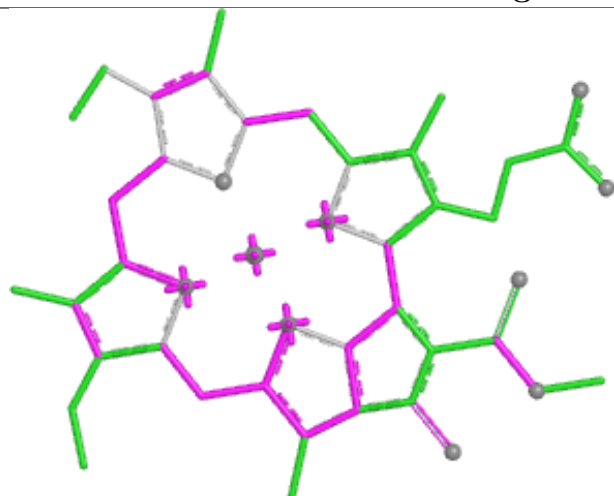
Torsions



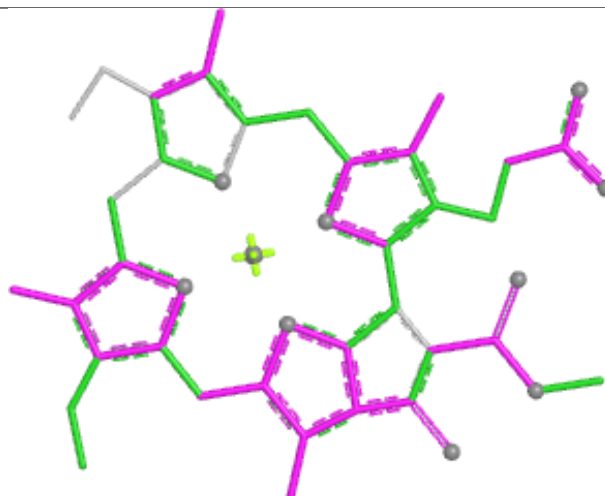
Rings



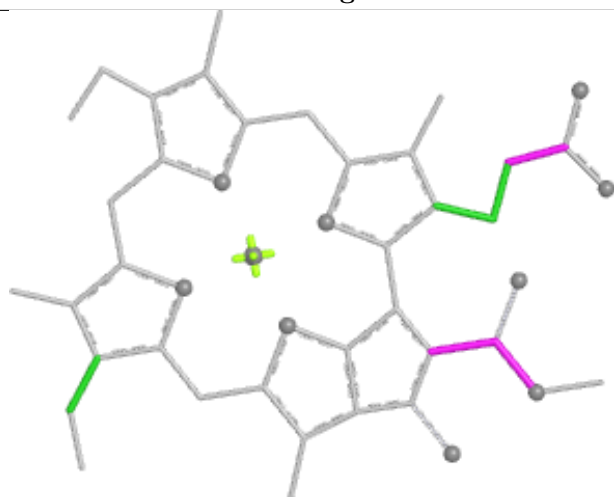
Ligand CLA H 820



Bond lengths



Bond angles

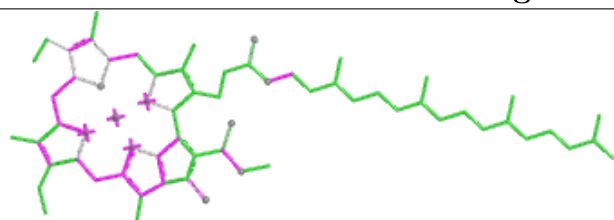


Torsions

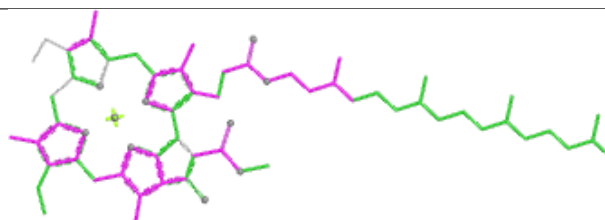


Rings

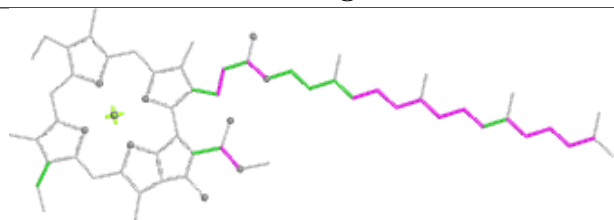
Ligand CLA H 839



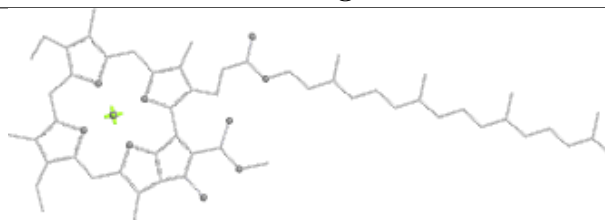
Bond lengths



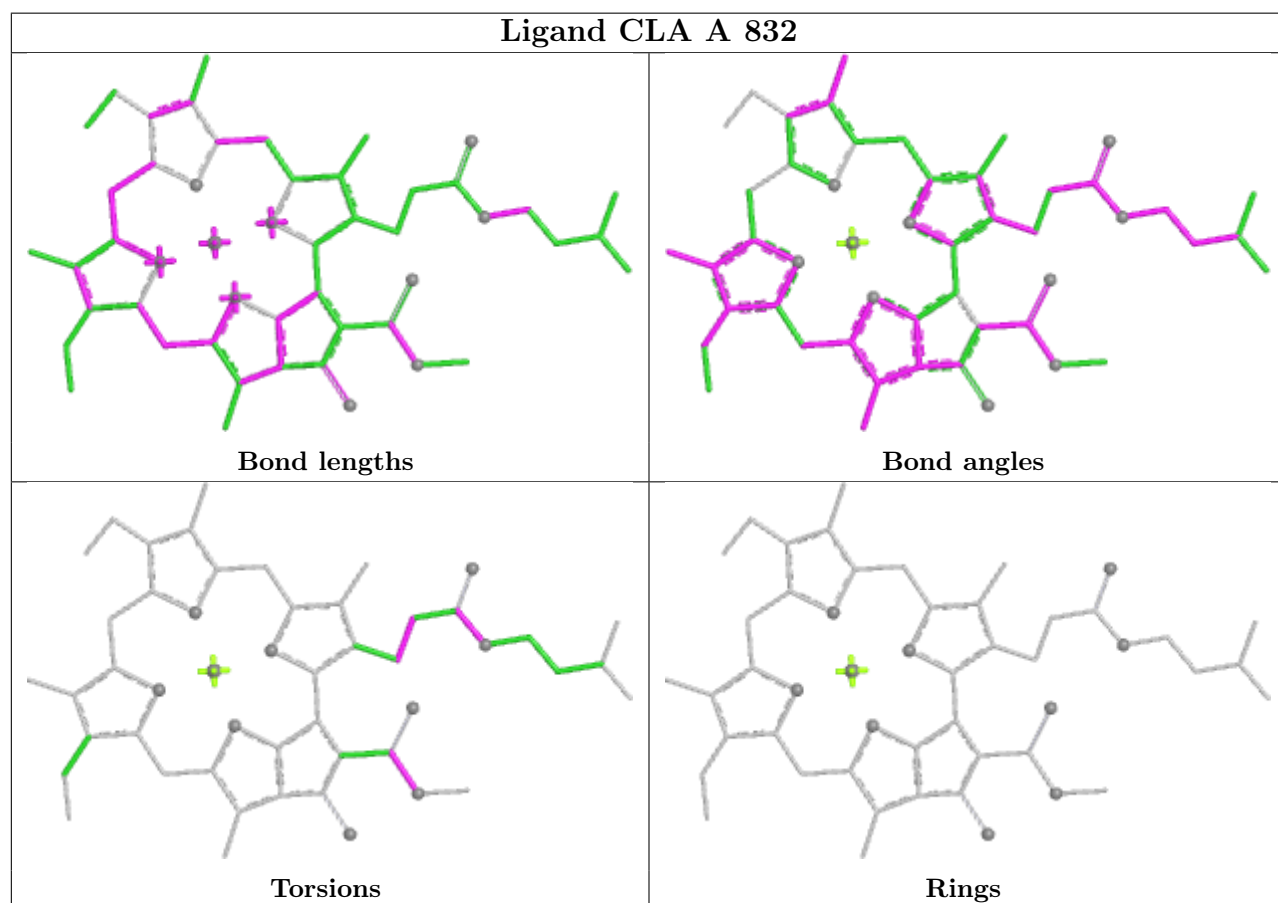
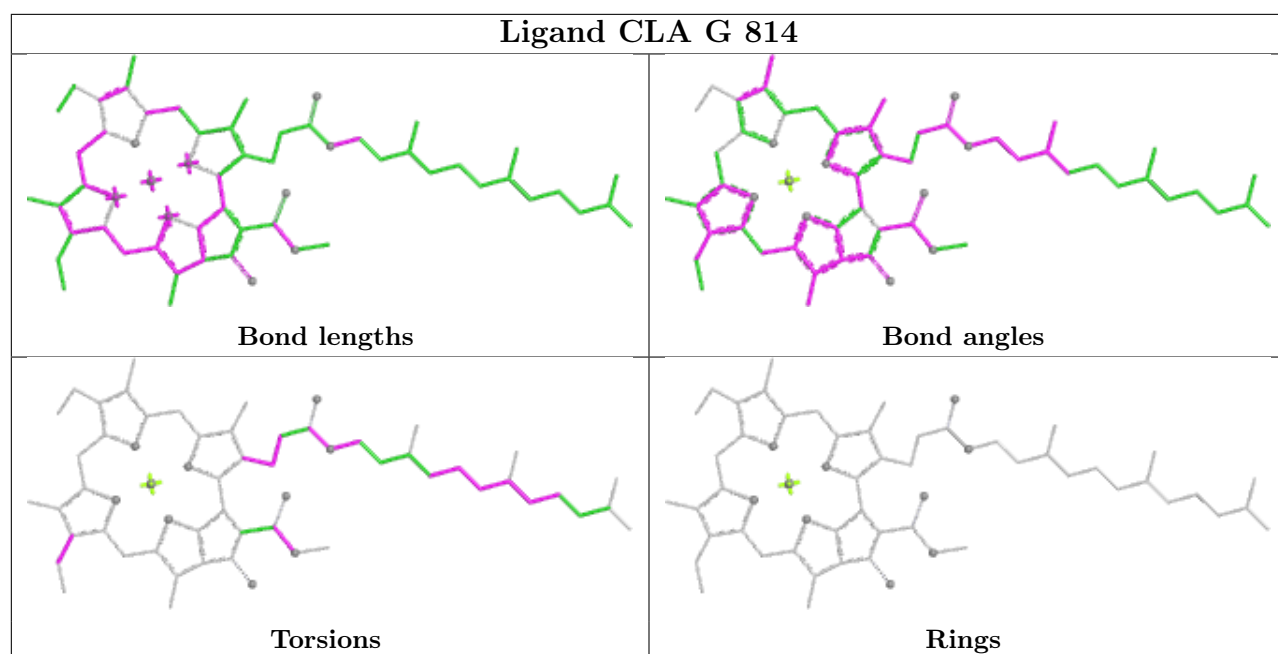
Bond angles

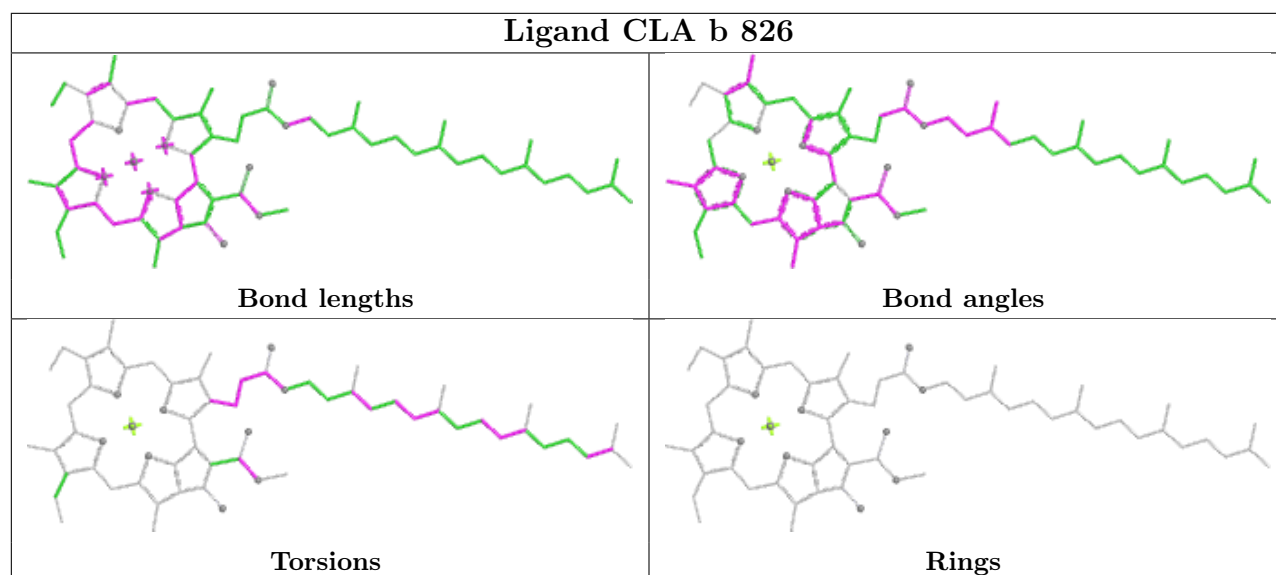
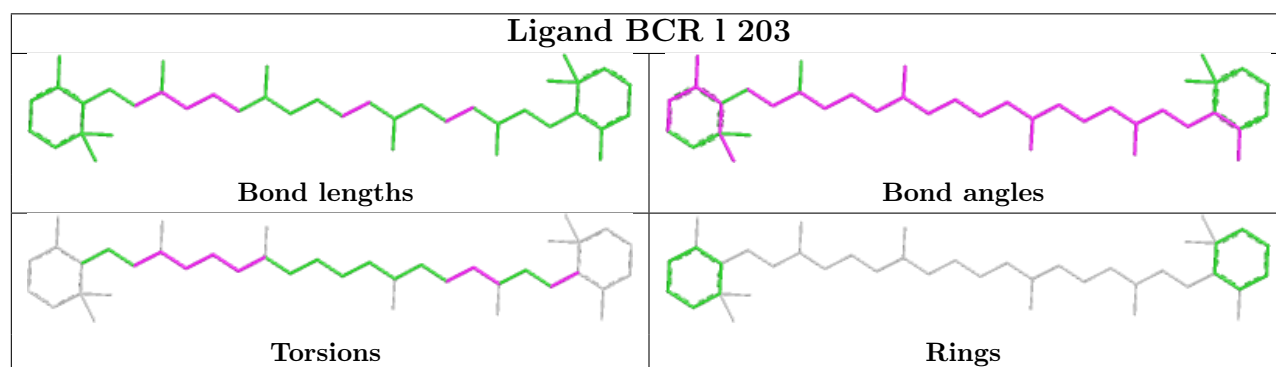
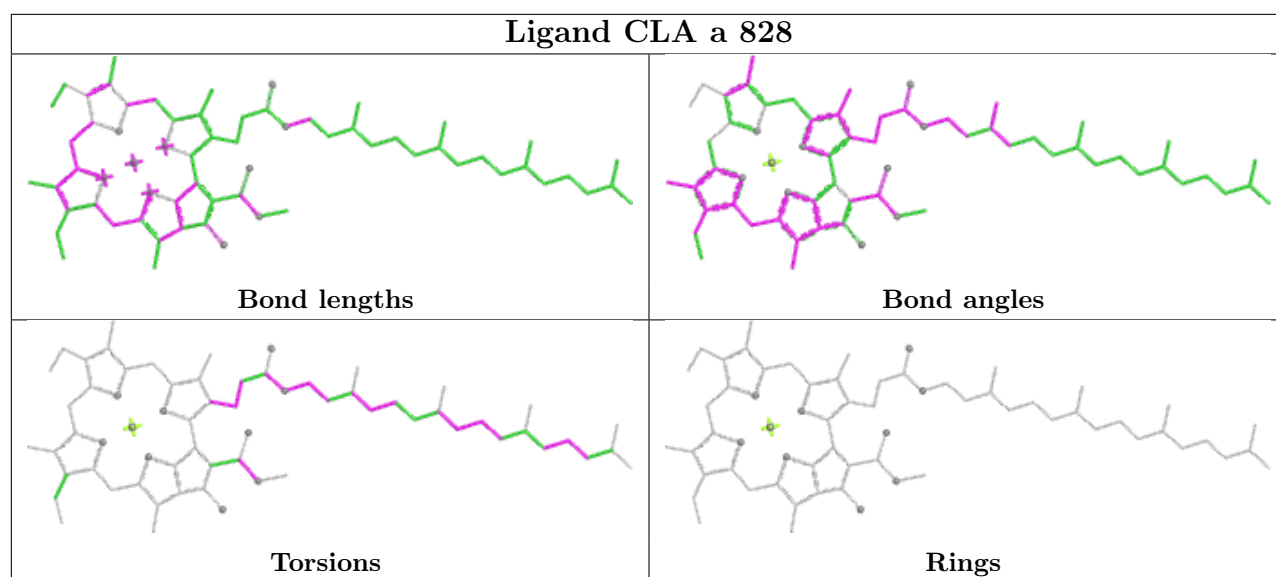


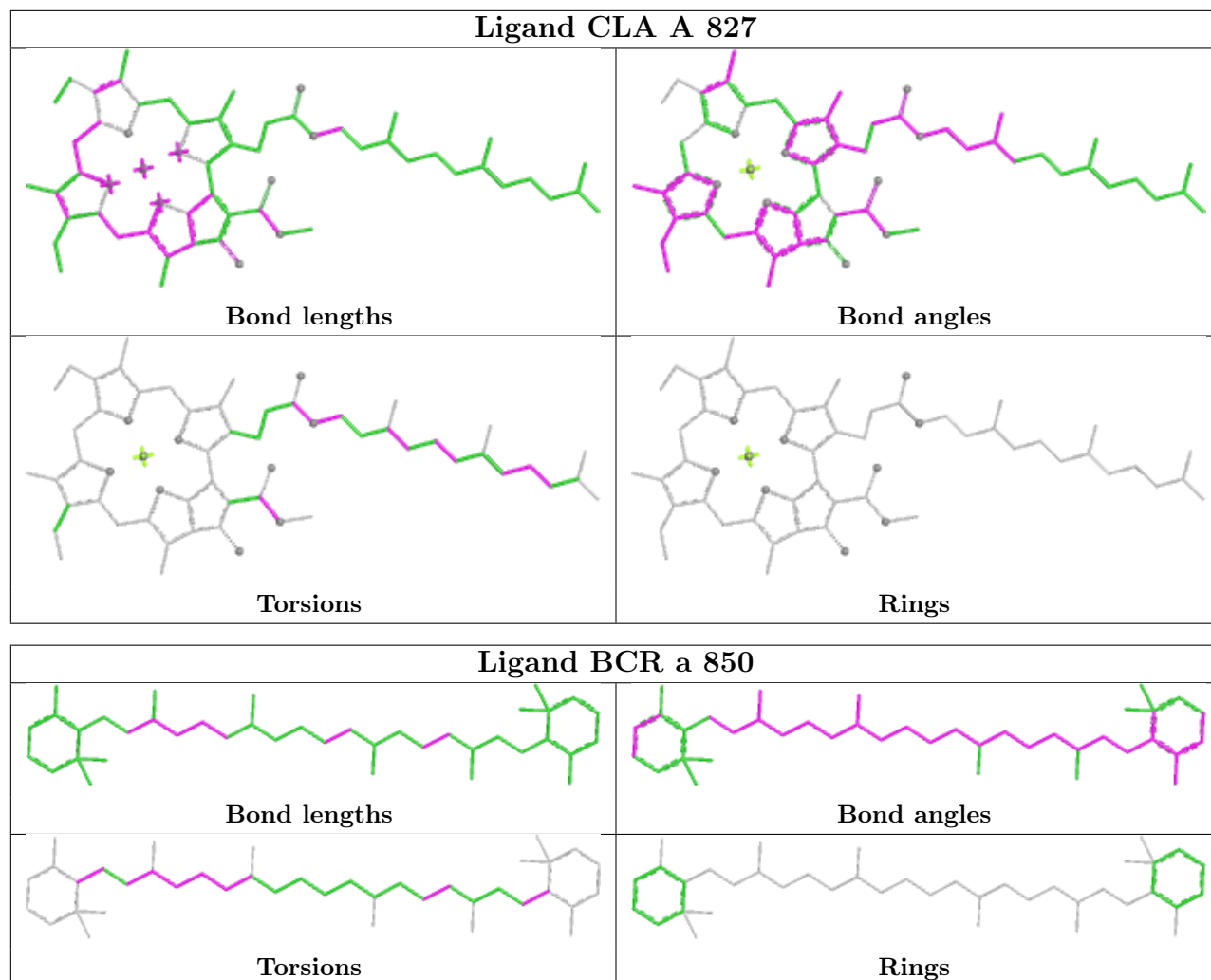
Torsions



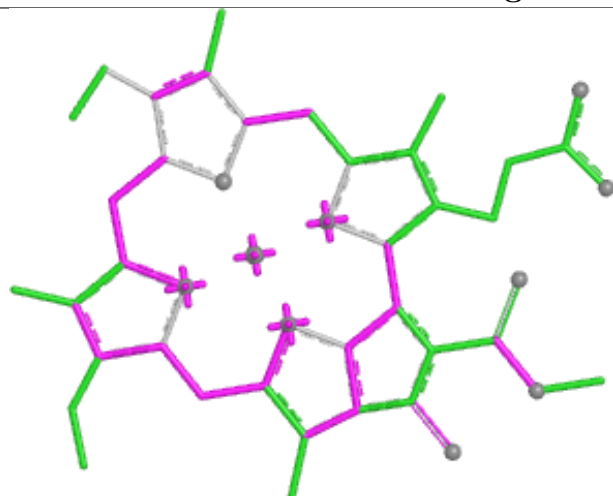
Rings



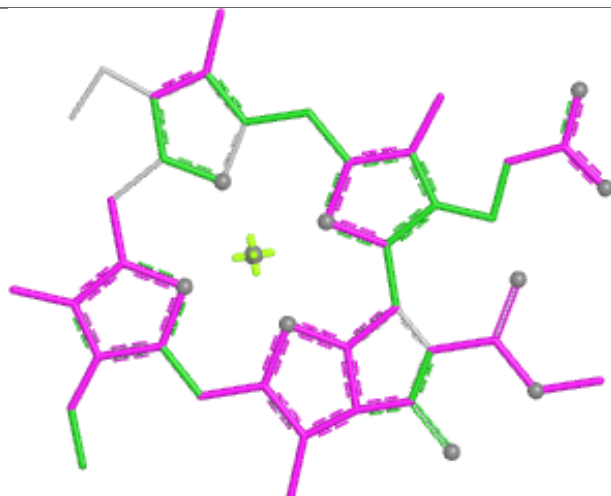




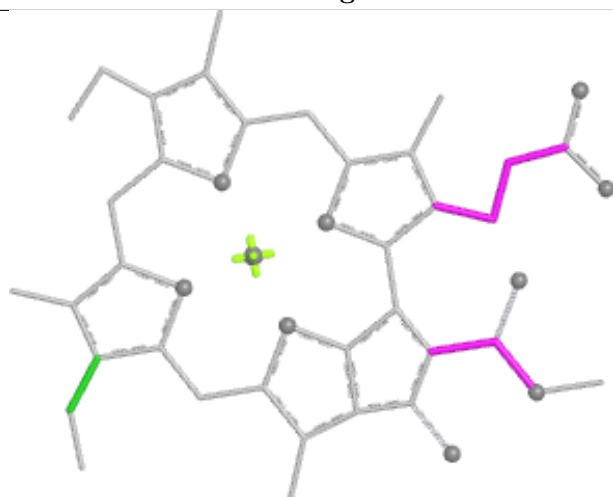
Ligand CLA V 1601



Bond lengths



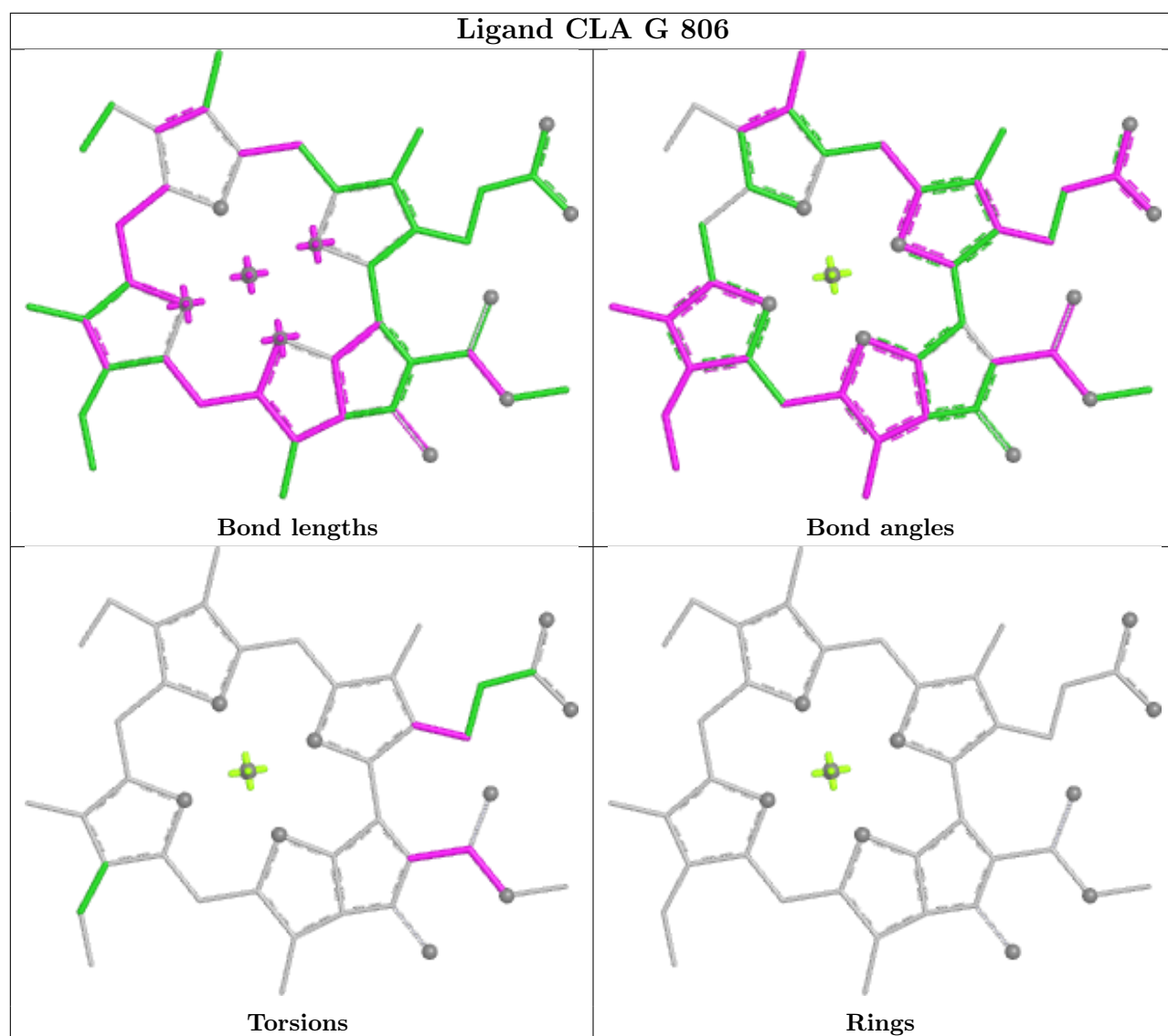
Bond angles

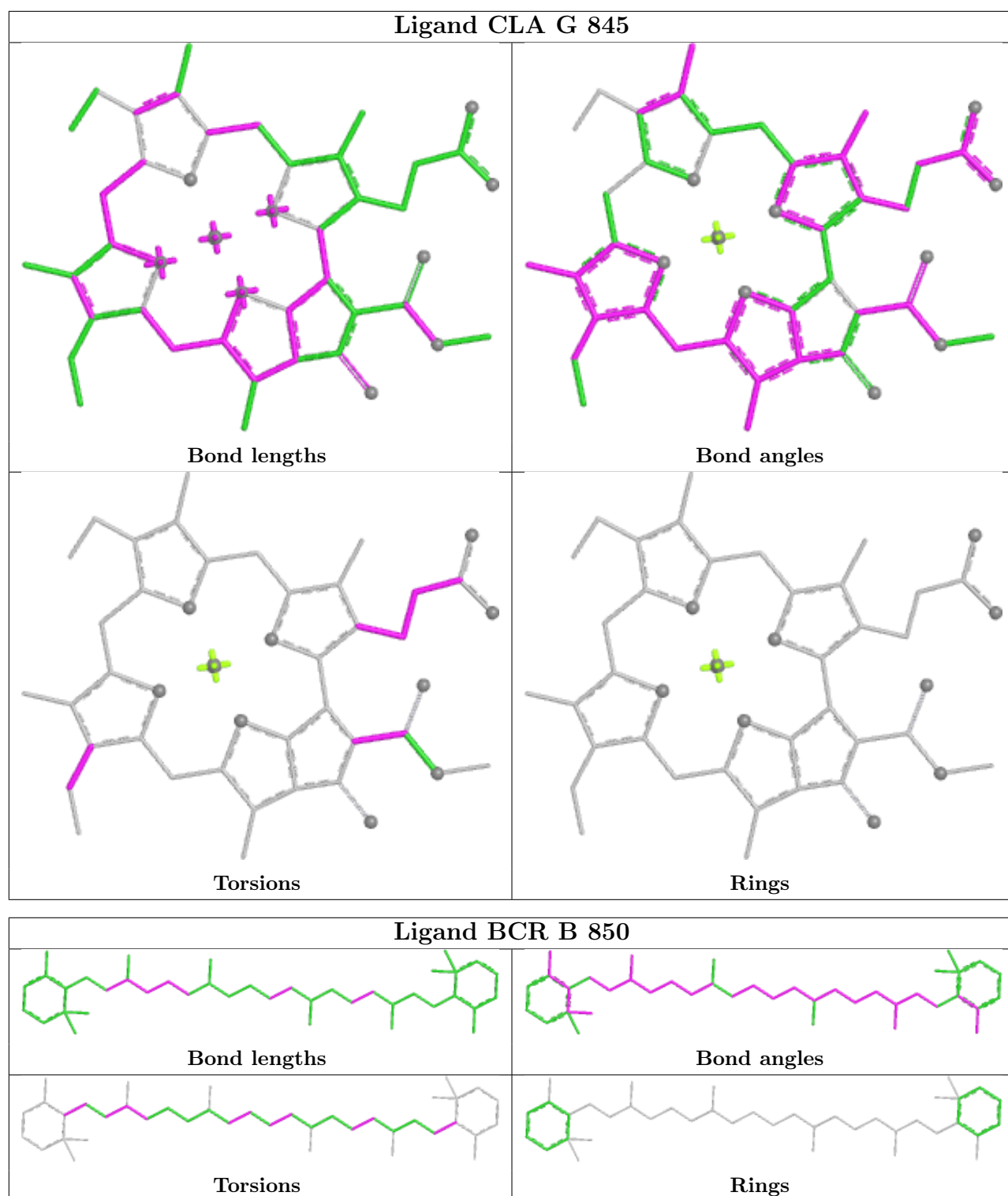


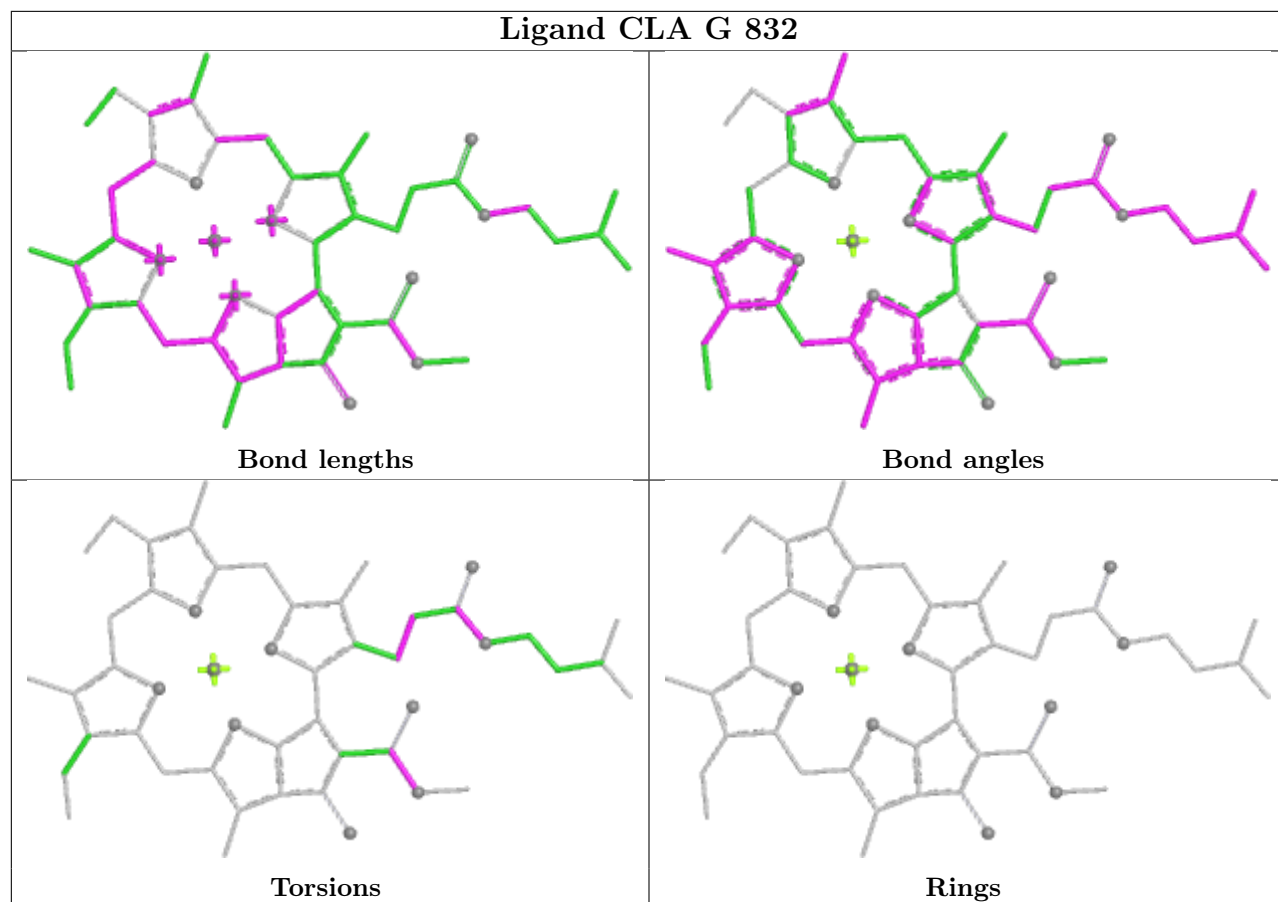
Torsions



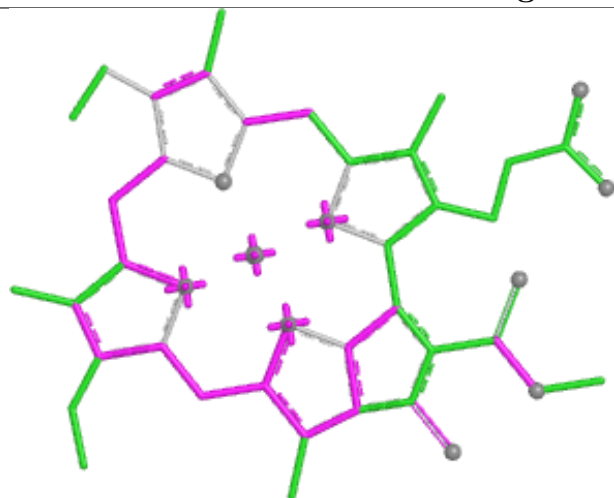
Rings



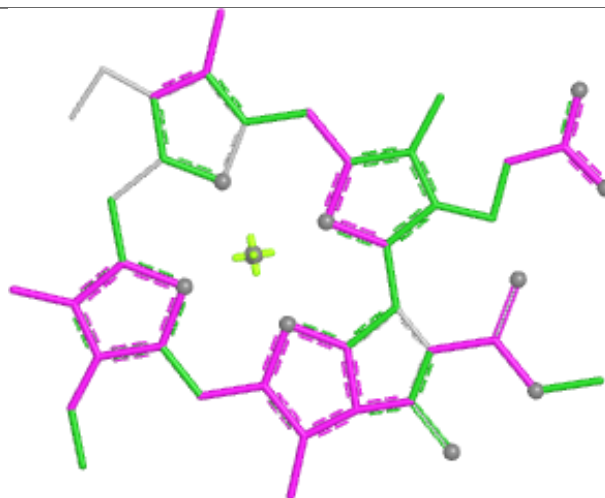




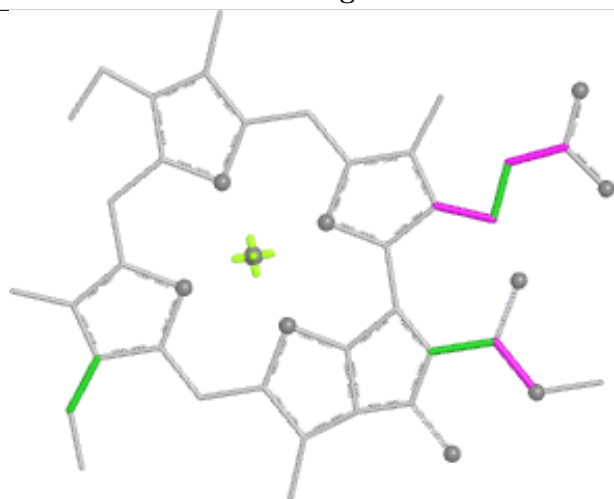
Ligand CLA b 833



Bond lengths



Bond angles

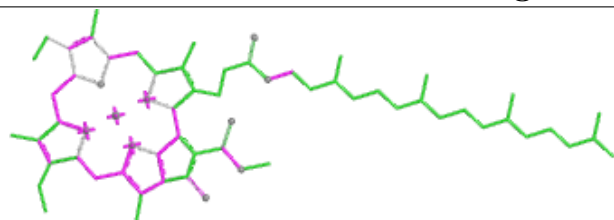


Torsions

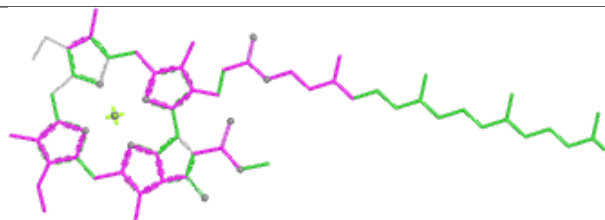


Rings

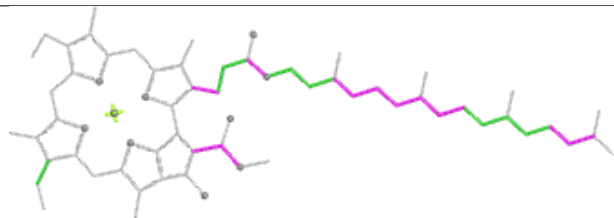
Ligand CLA A 809



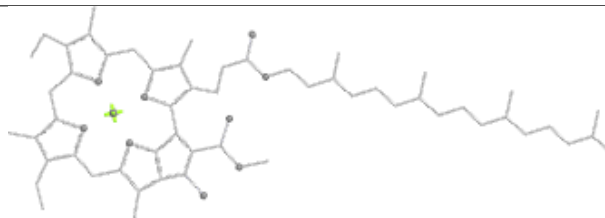
Bond lengths



Bond angles

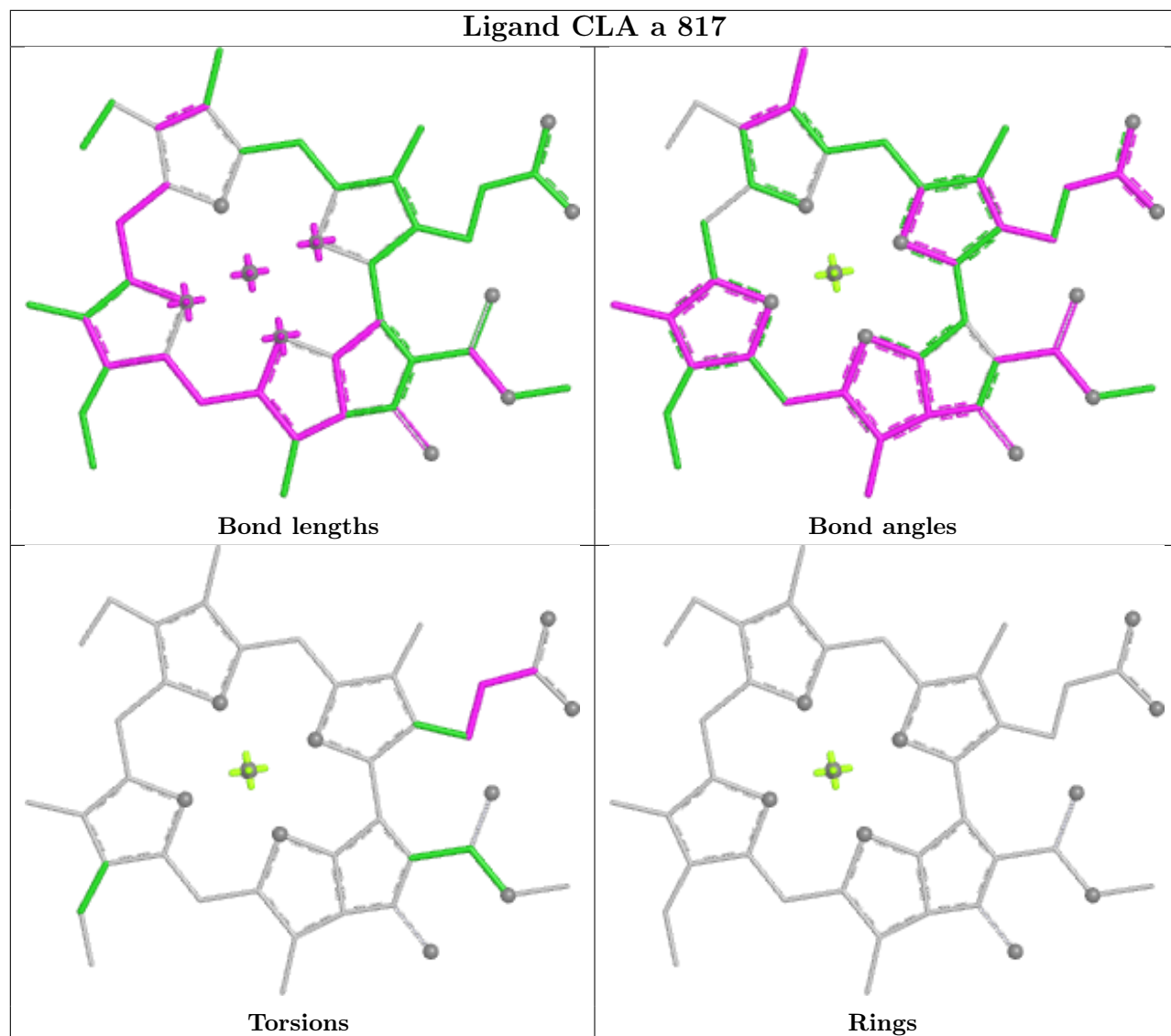


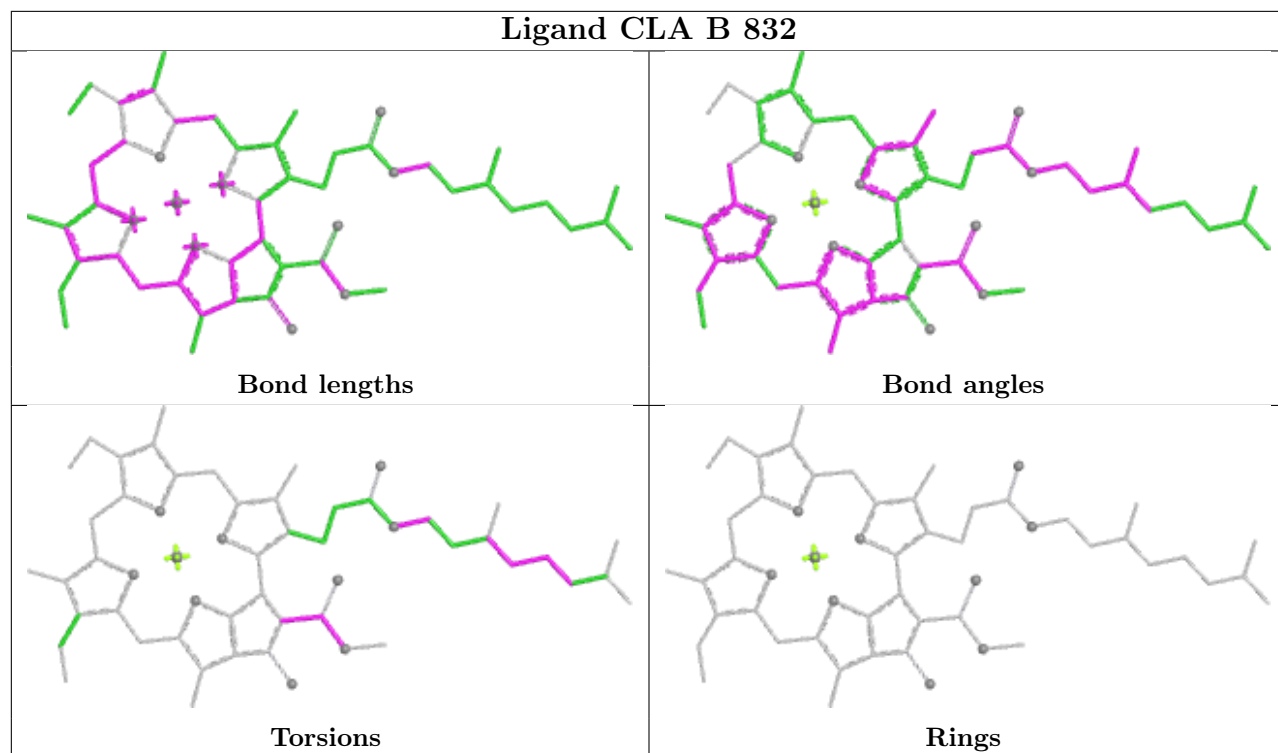
Torsions

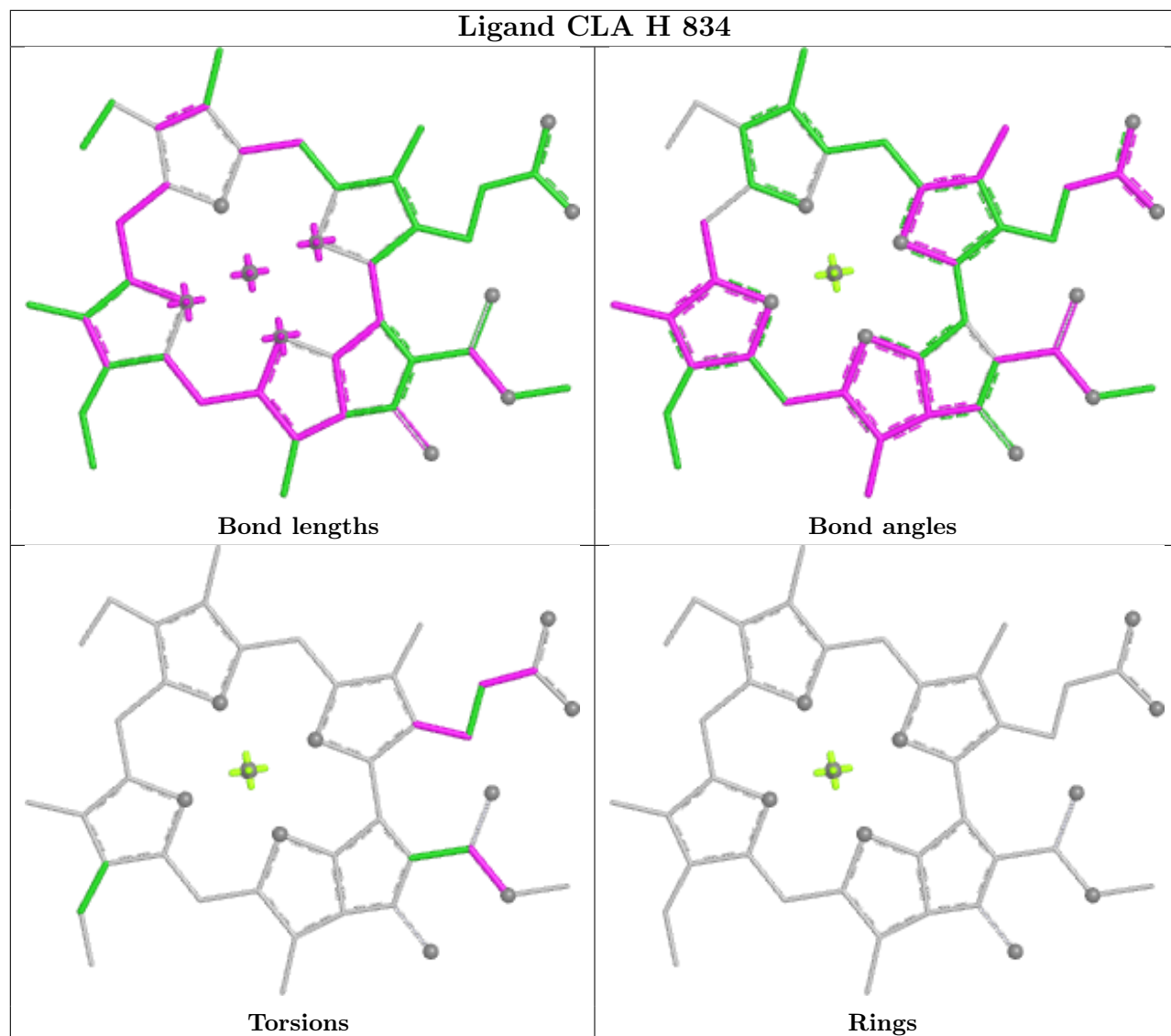


Rings

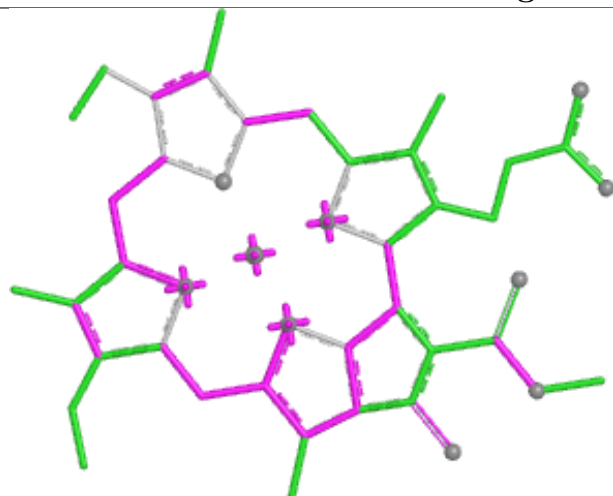
Ligand CLA a 817



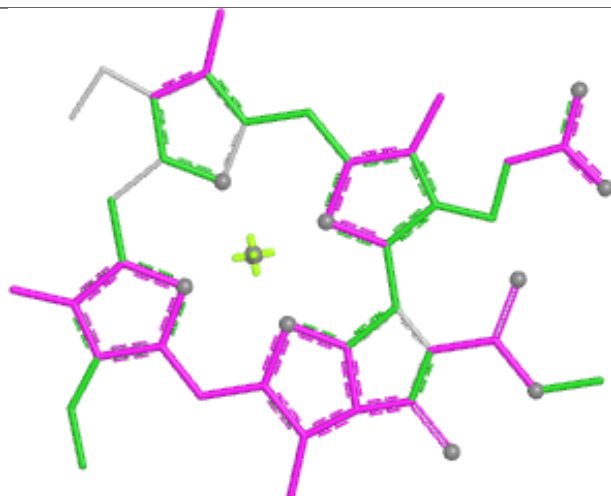




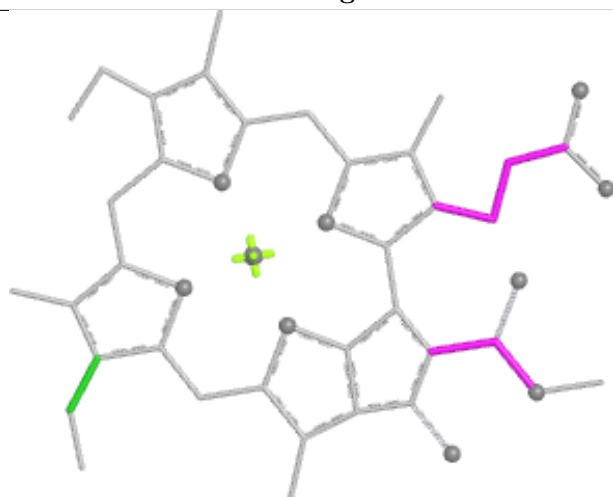
Ligand CLA b 814



Bond lengths



Bond angles

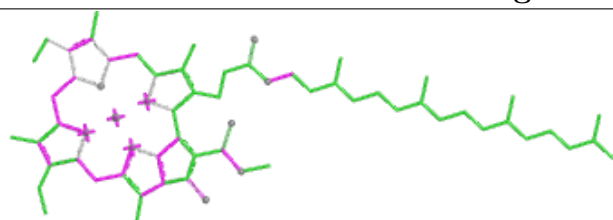


Torsions

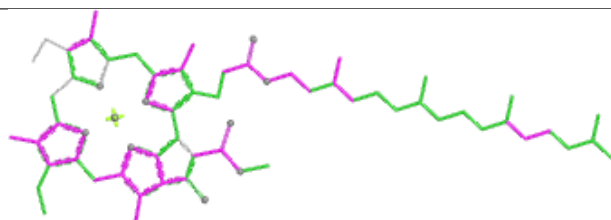


Rings

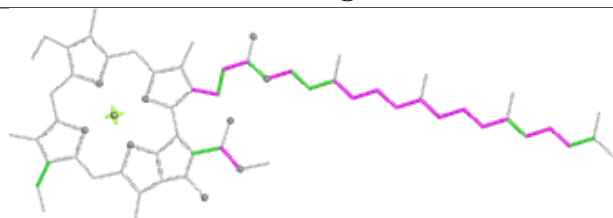
Ligand CLA A 843



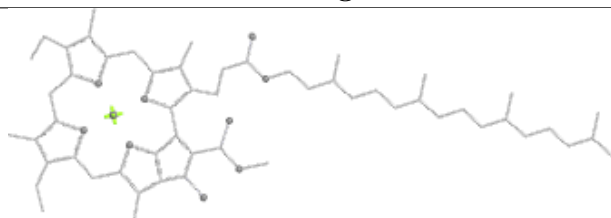
Bond lengths



Bond angles

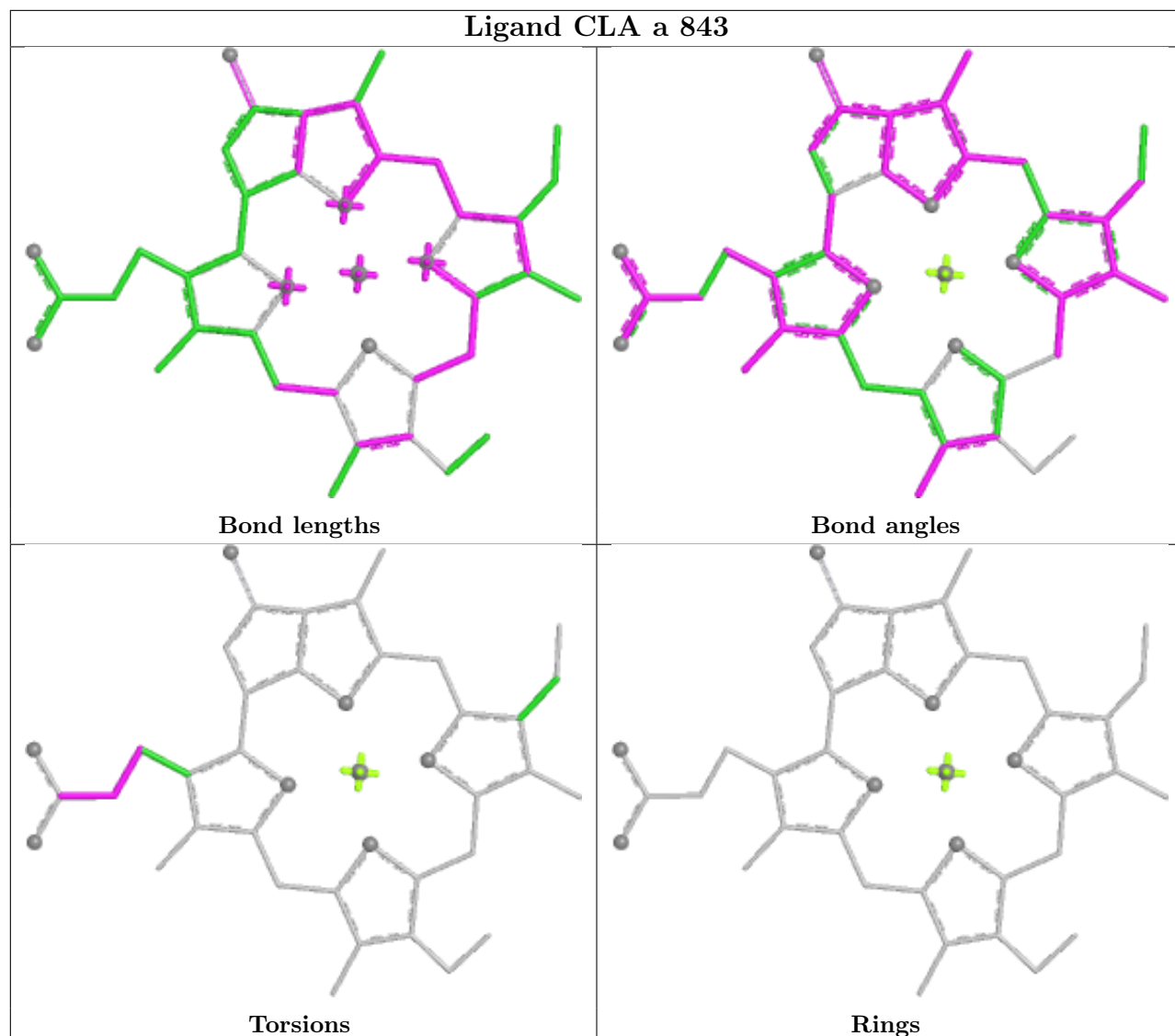


Torsions

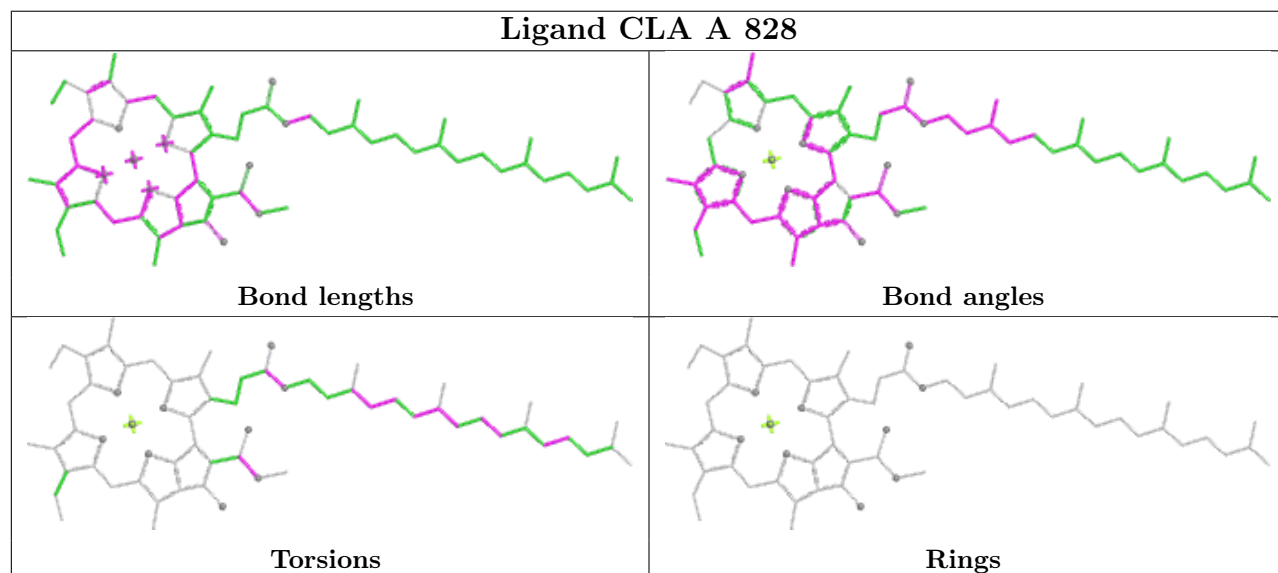


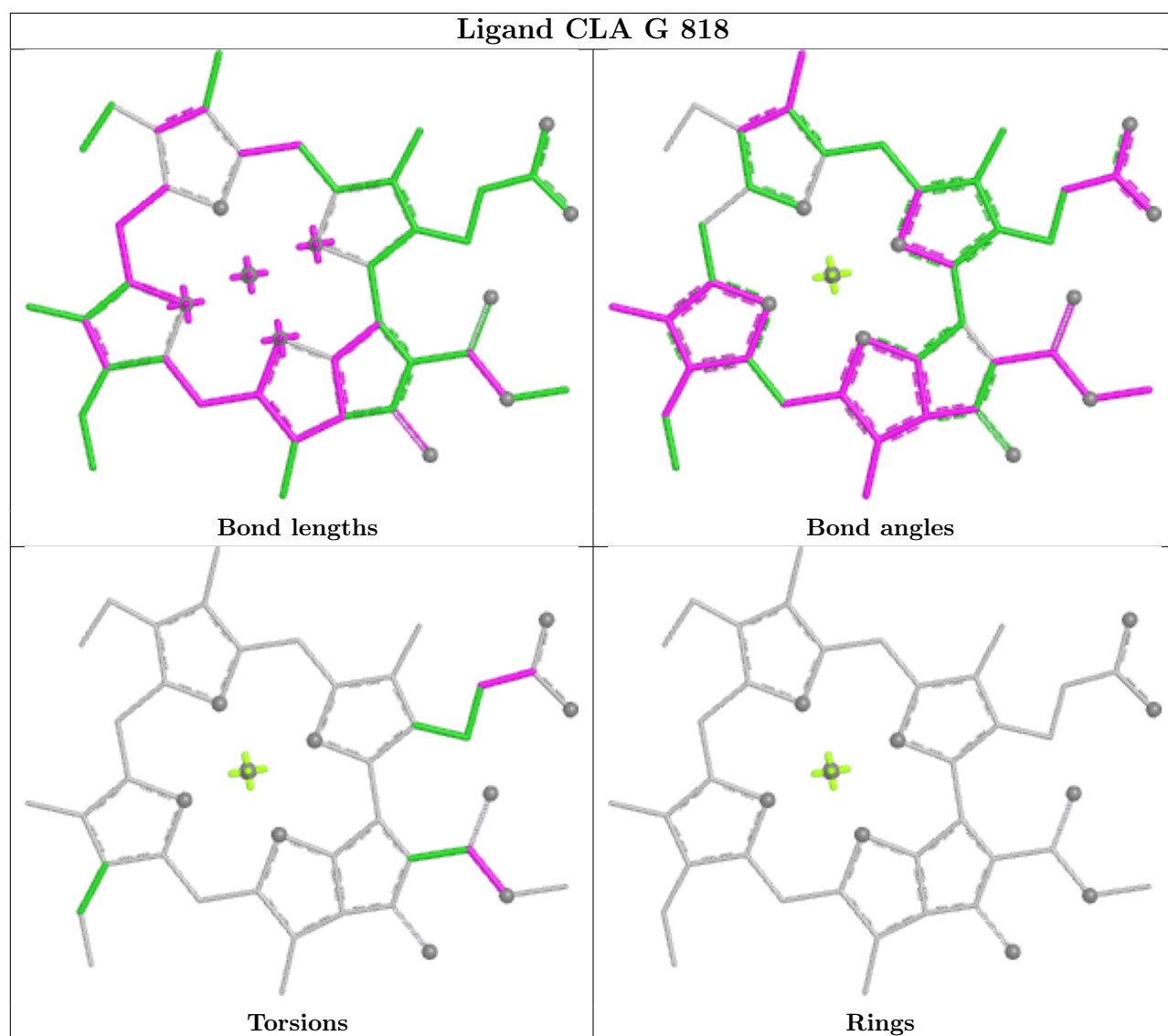
Rings

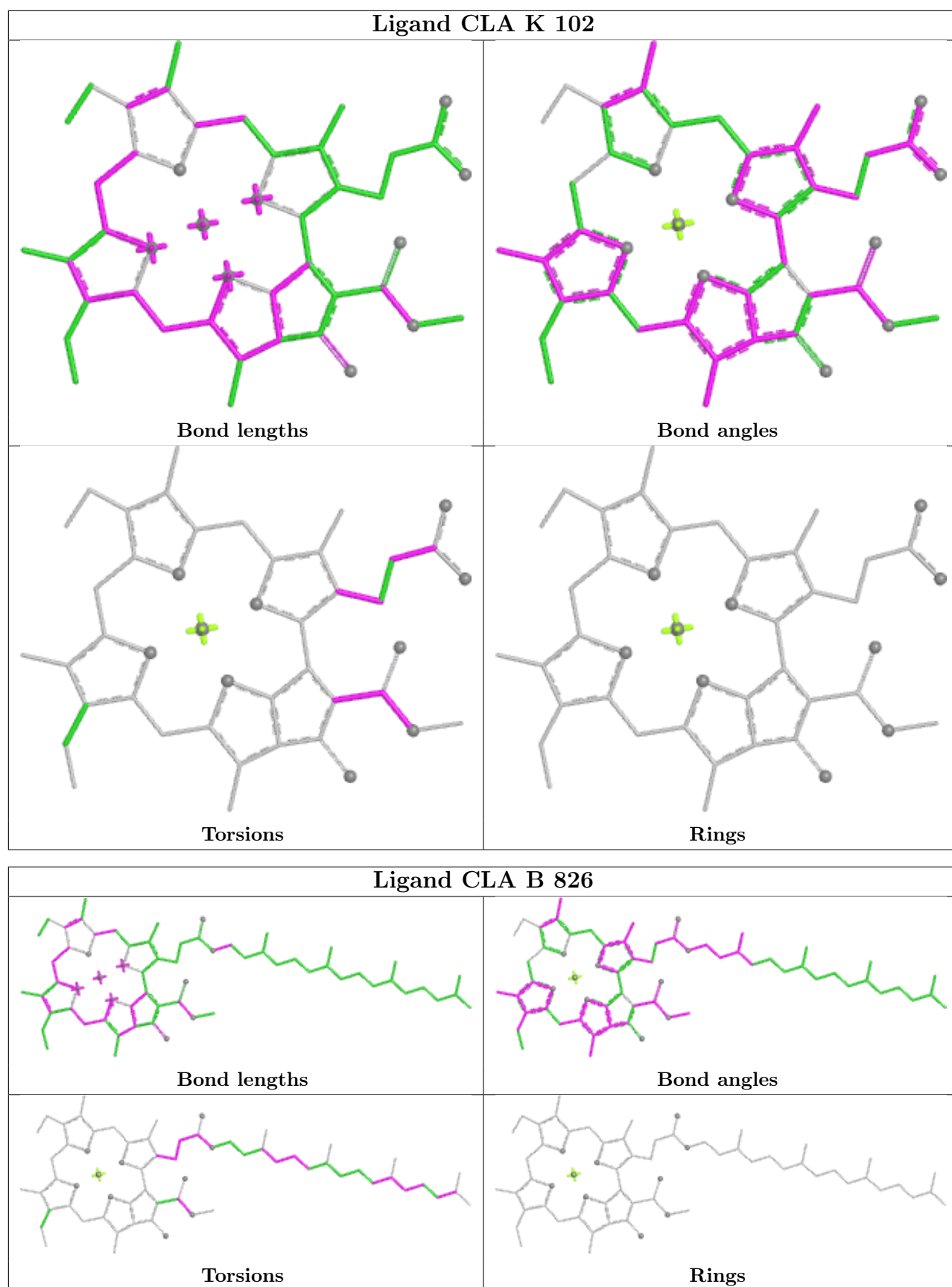
Ligand CLA a 843

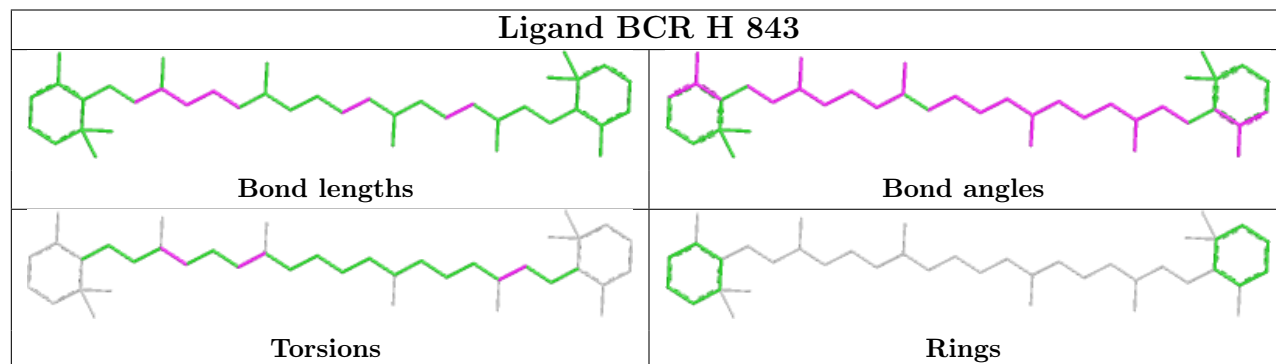
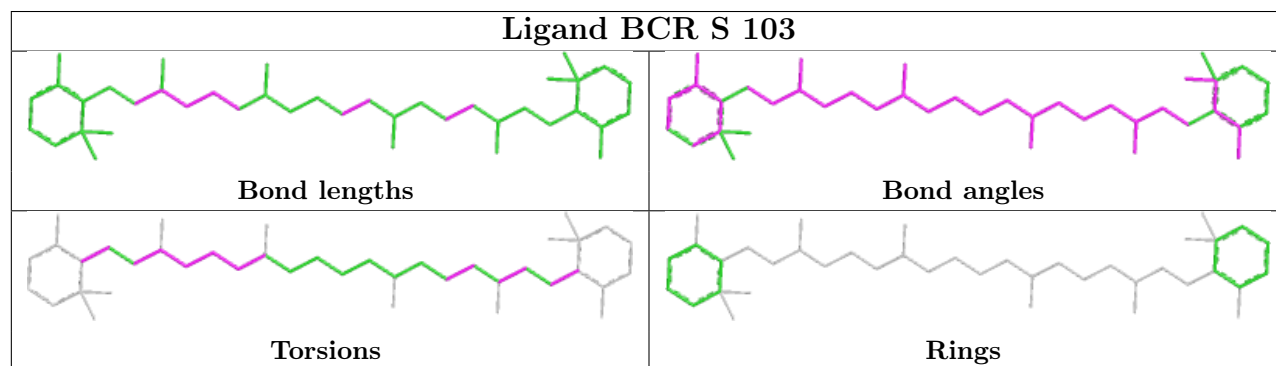
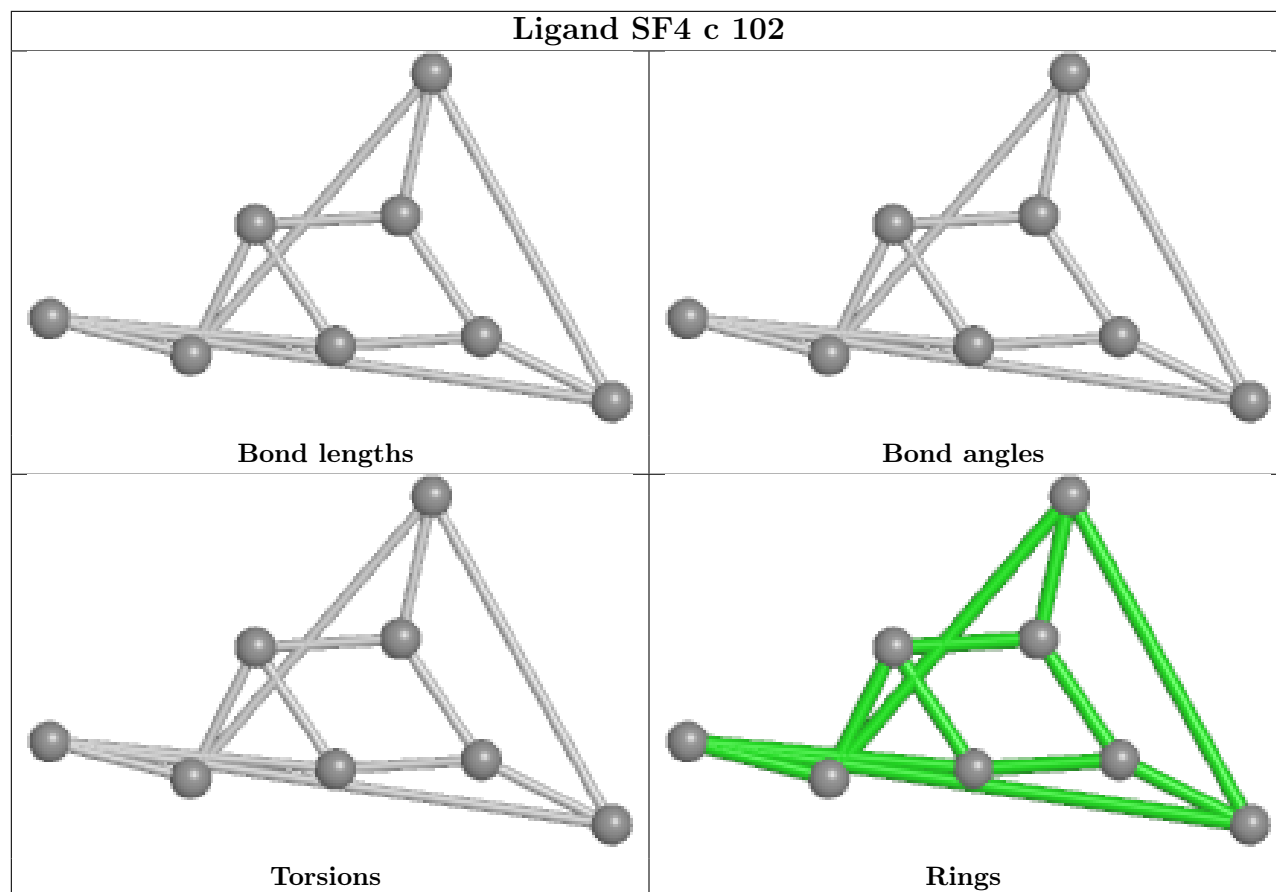


Ligand CLA A 828

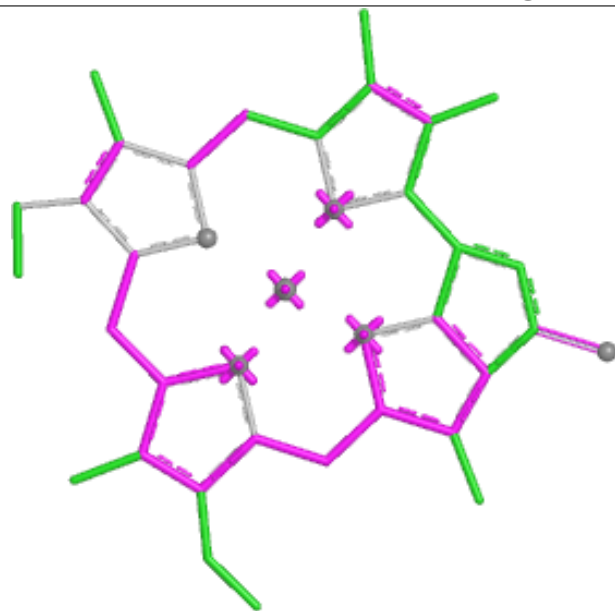




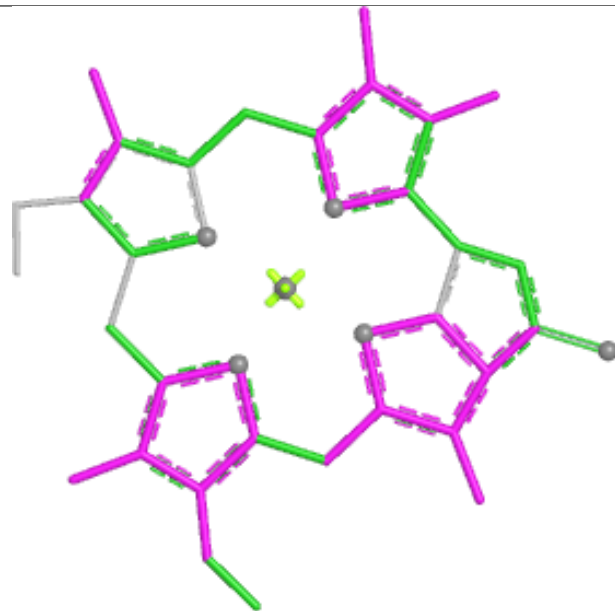




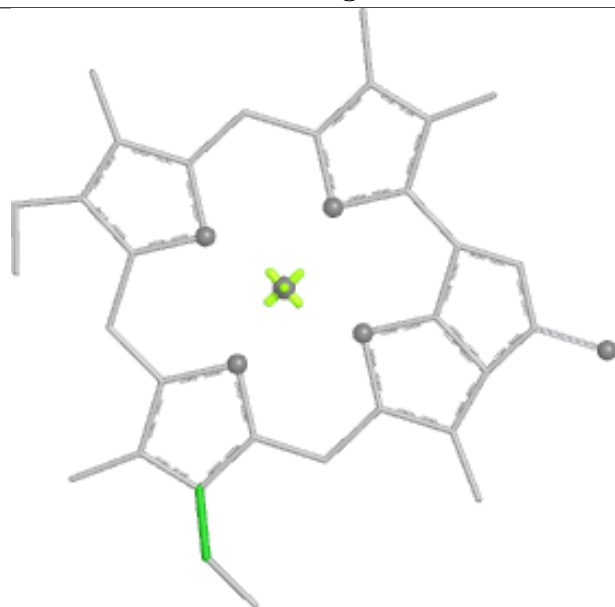
Ligand CLA S 102



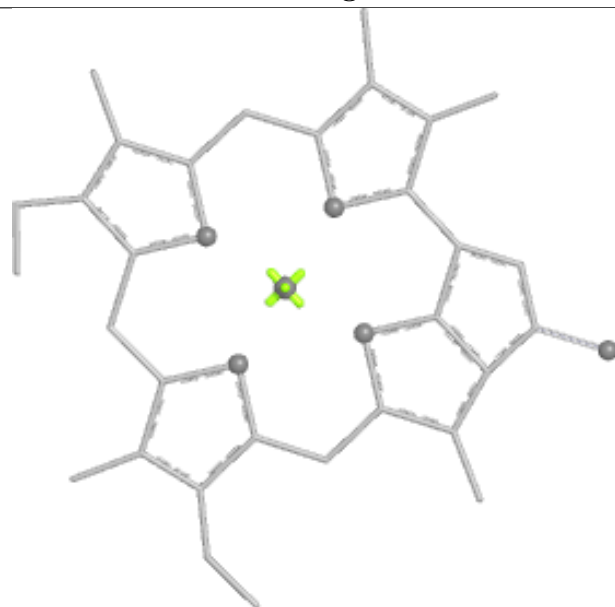
Bond lengths



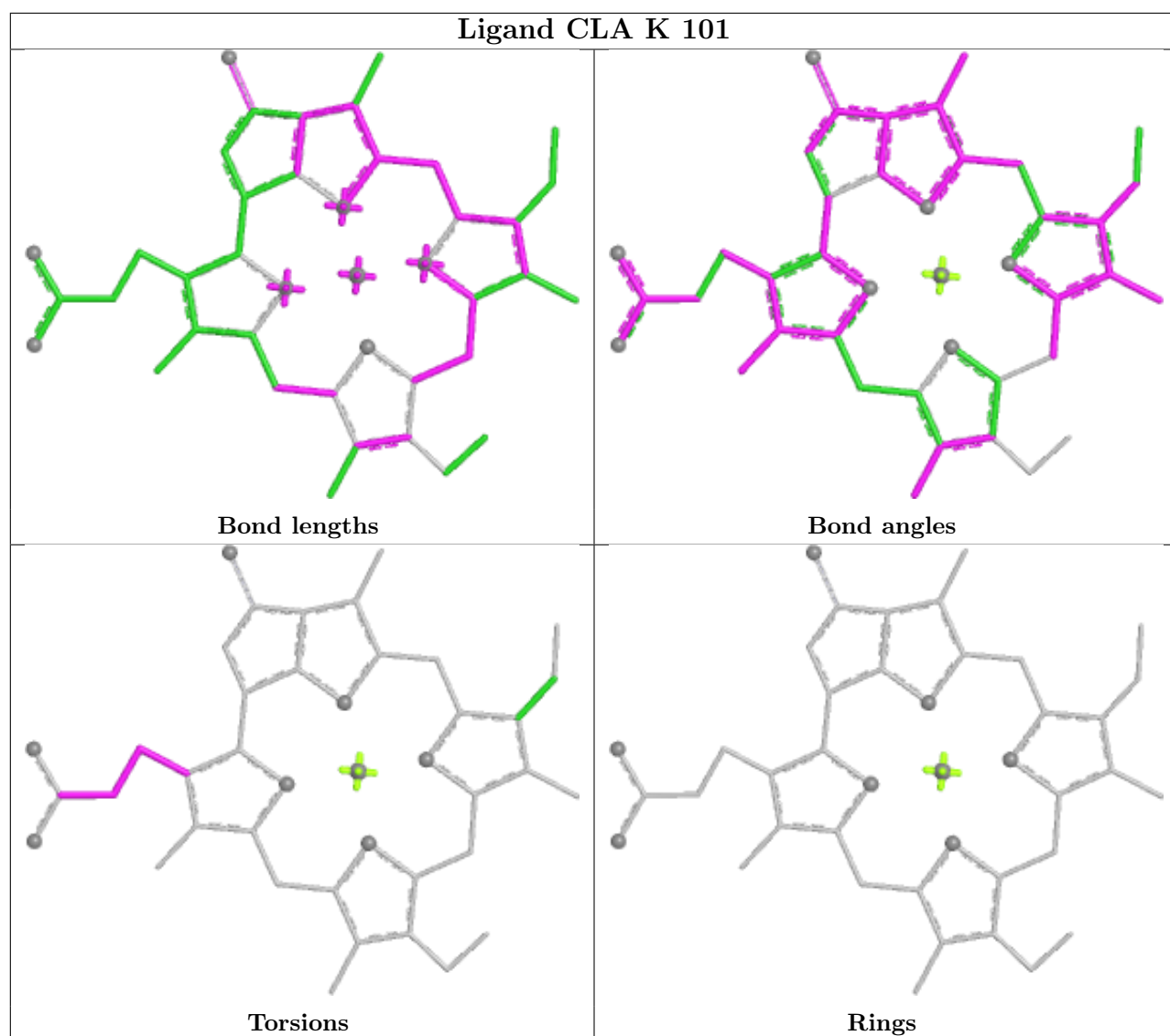
Bond angles

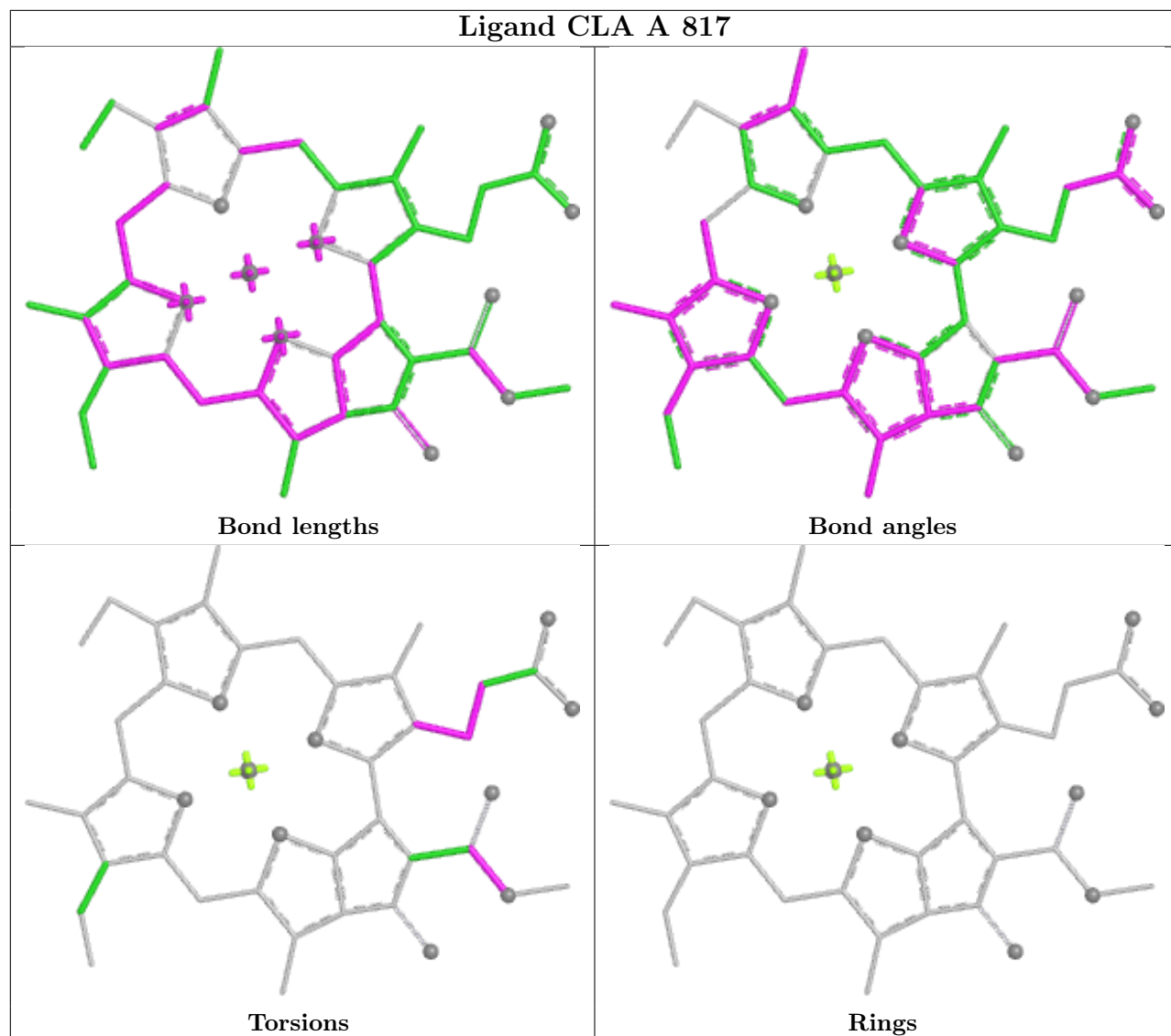


Torsions

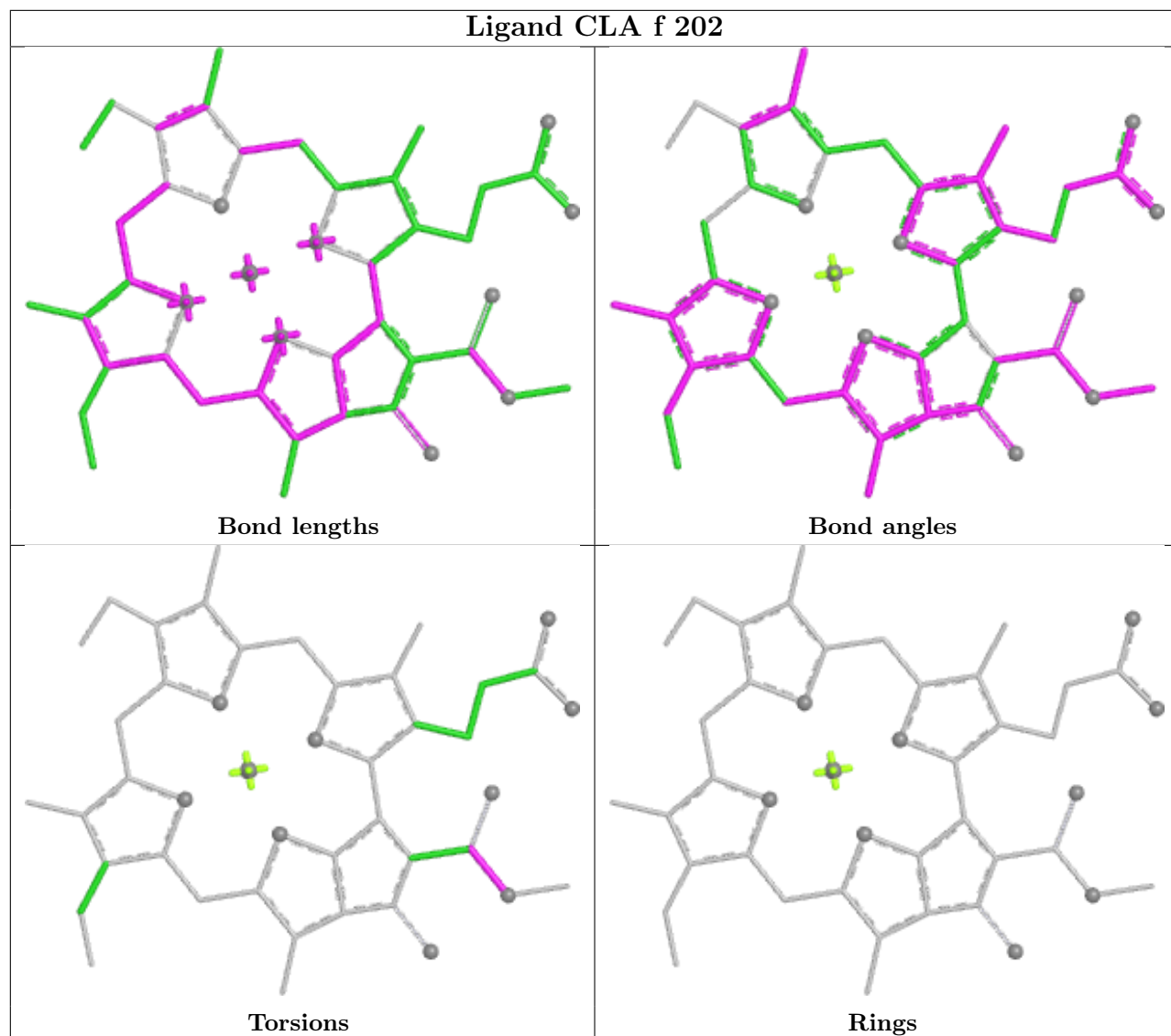


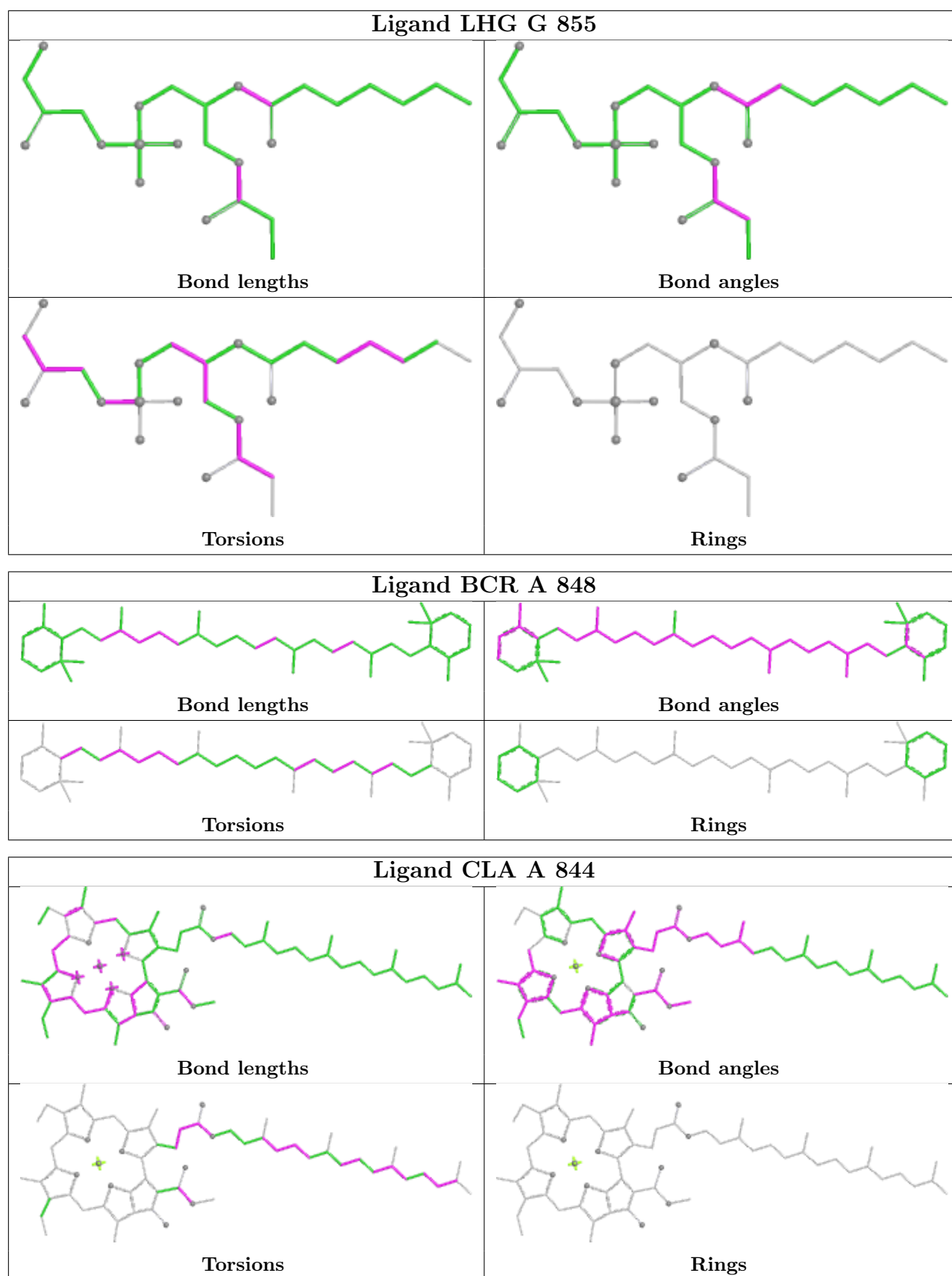
Rings



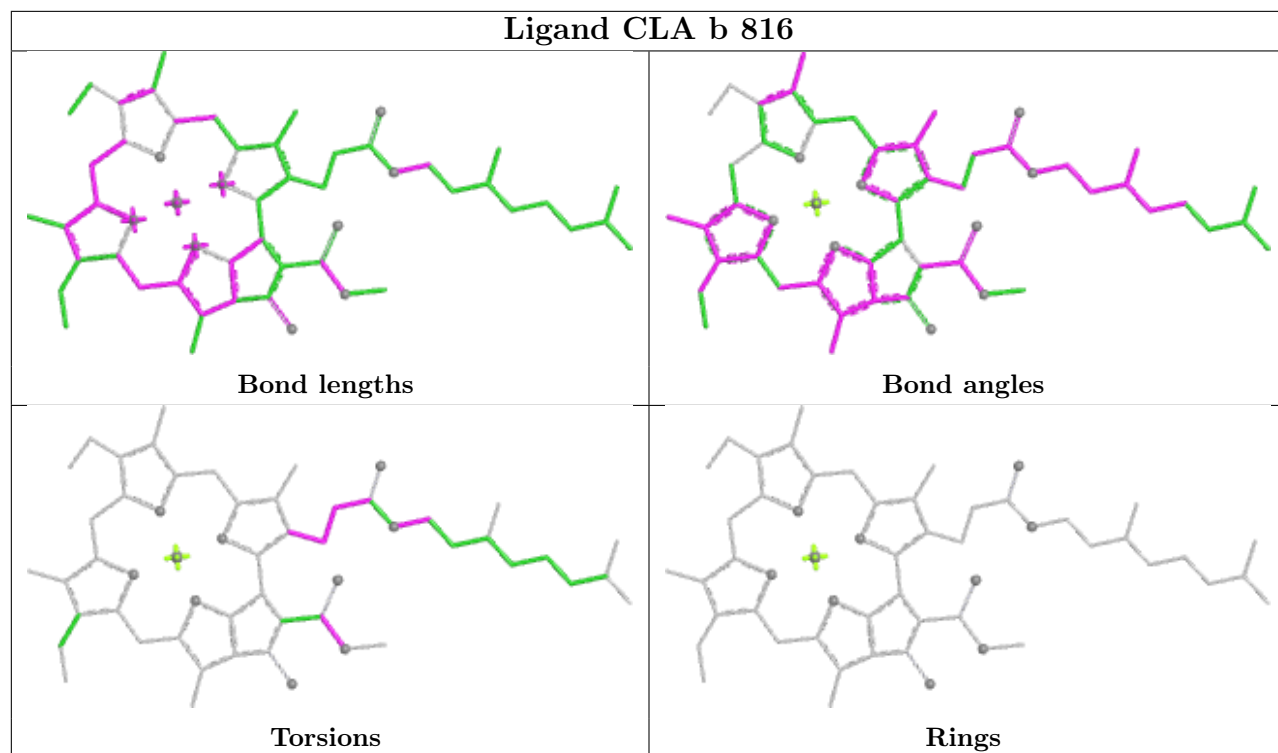


Ligand CLA f 202

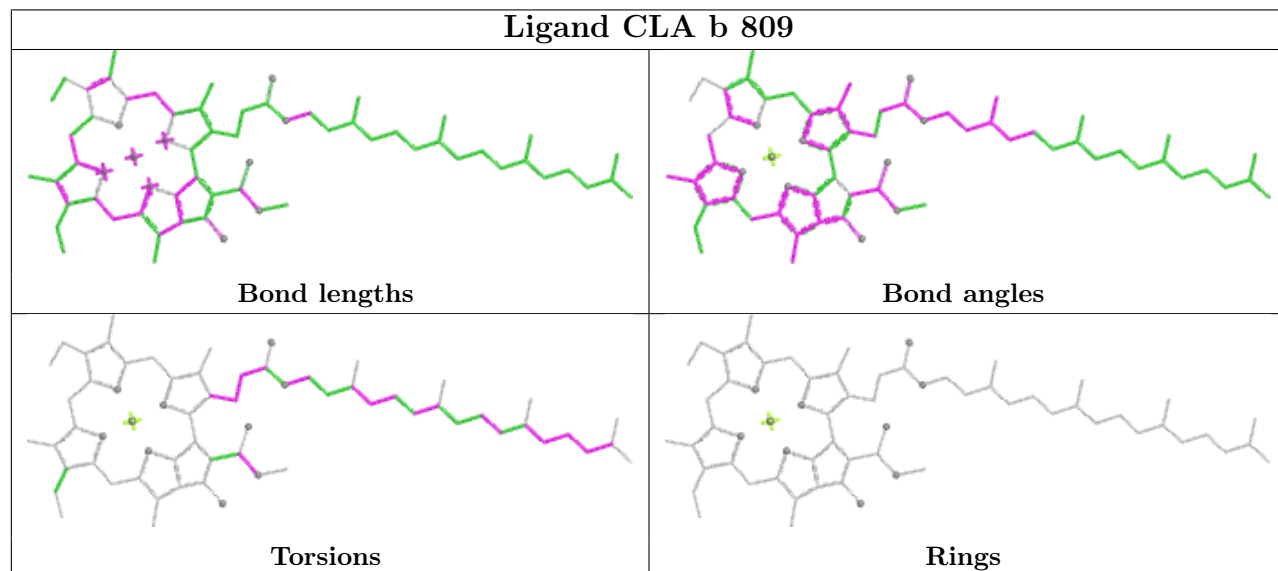




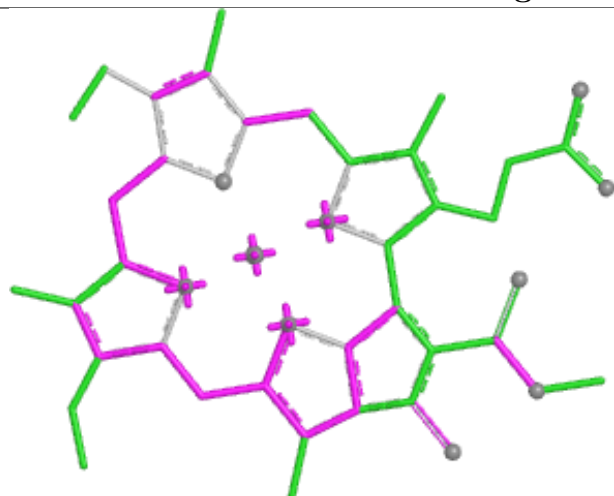
Ligand CLA b 816



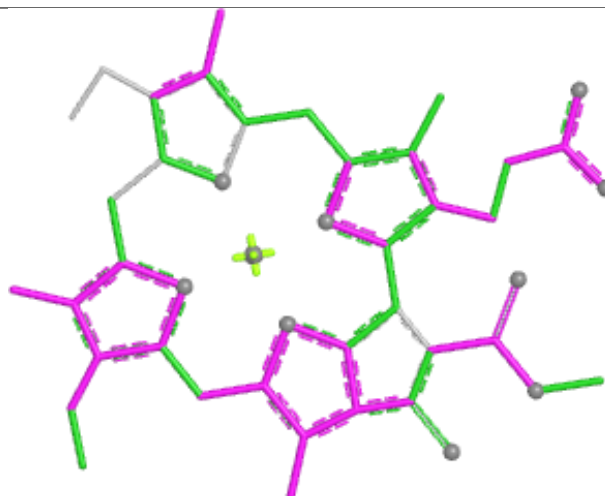
Ligand CLA b 809



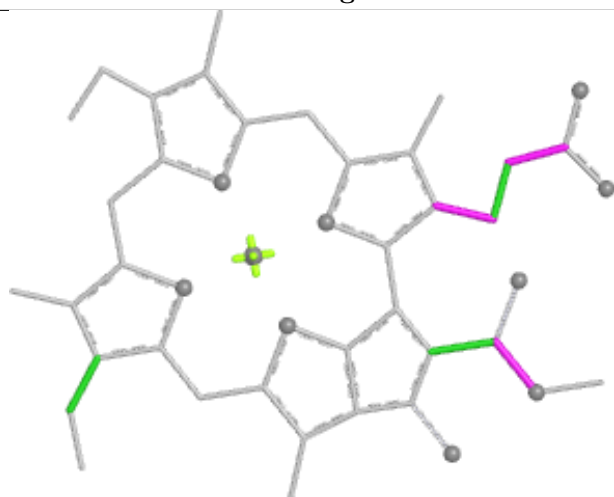
Ligand CLA B 838



Bond lengths



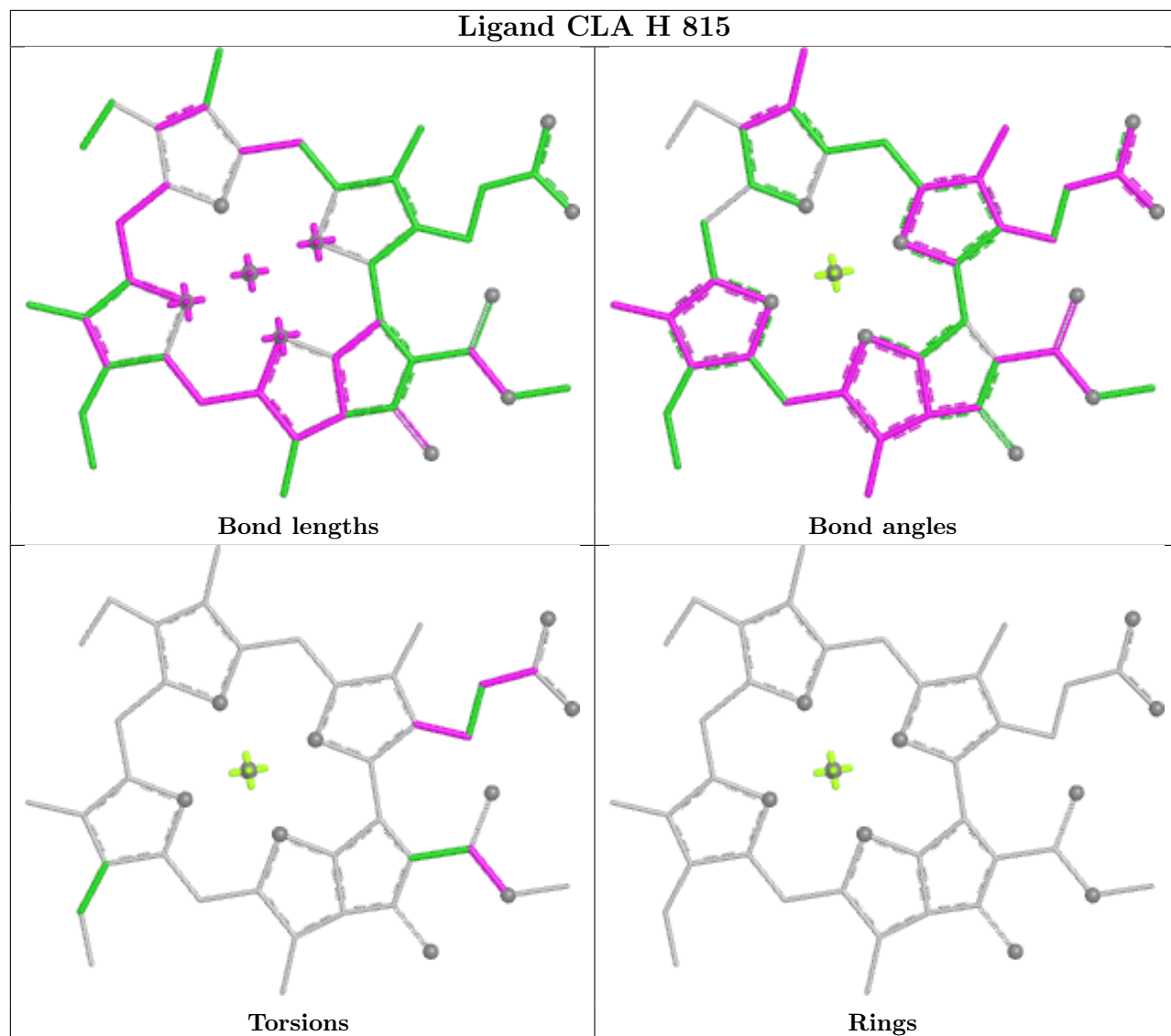
Bond angles



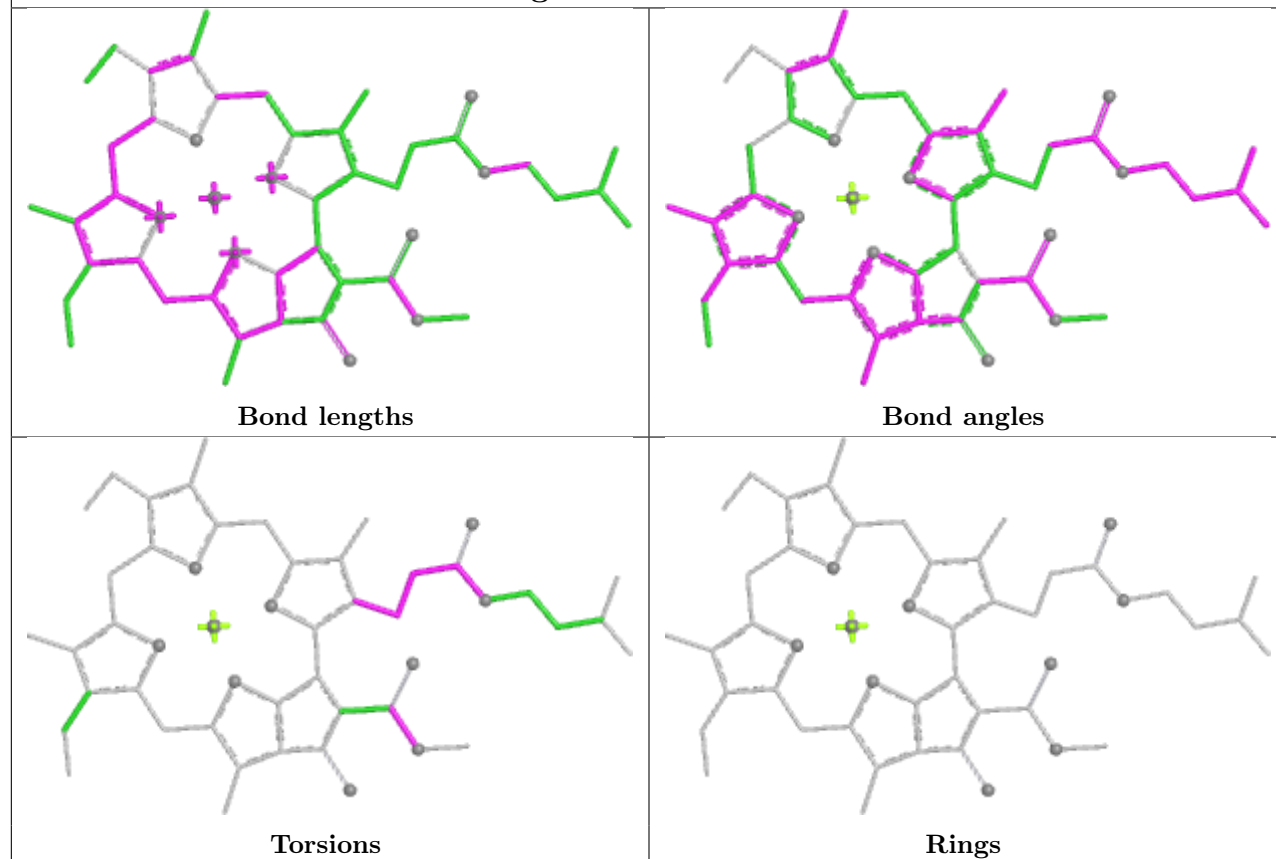
Torsions



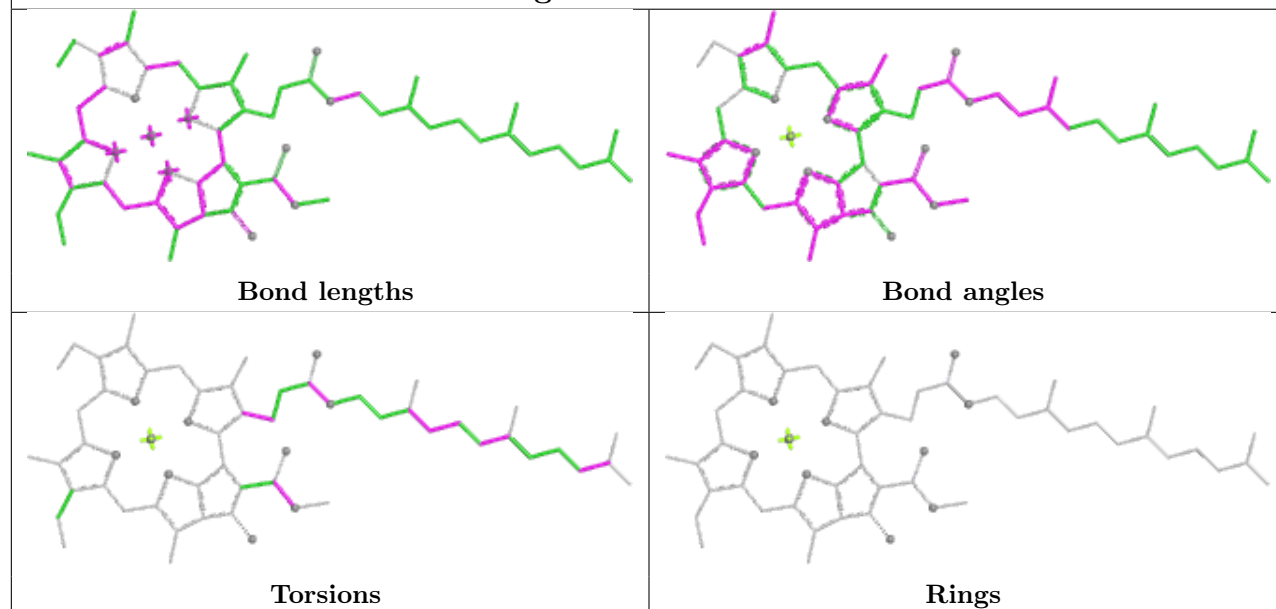
Rings



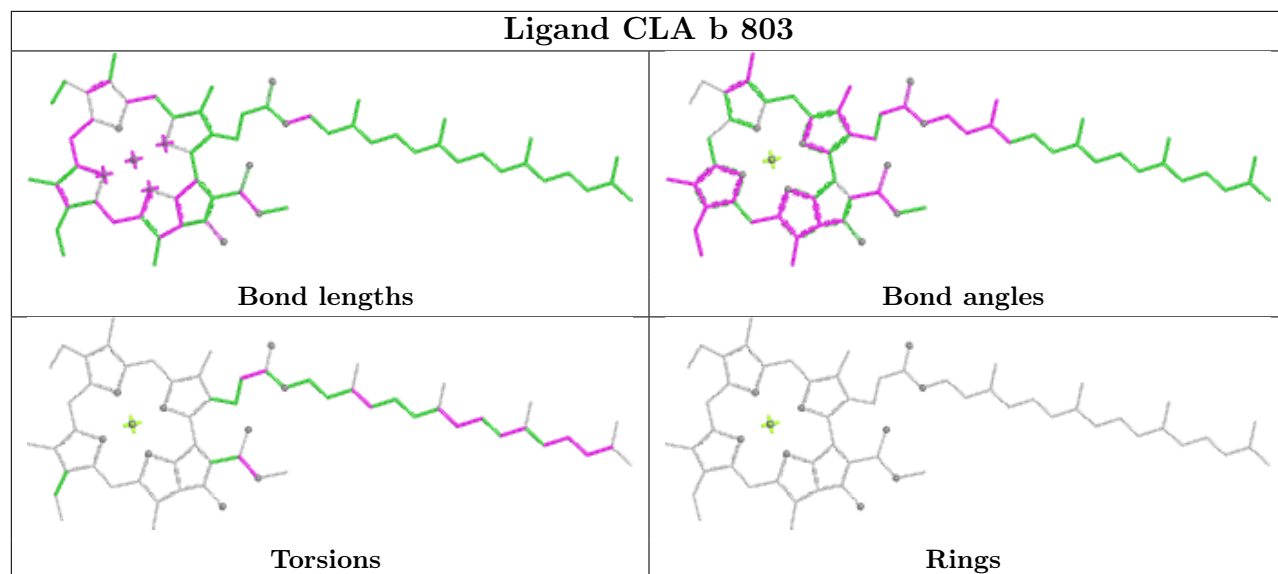
Ligand CLA G 819



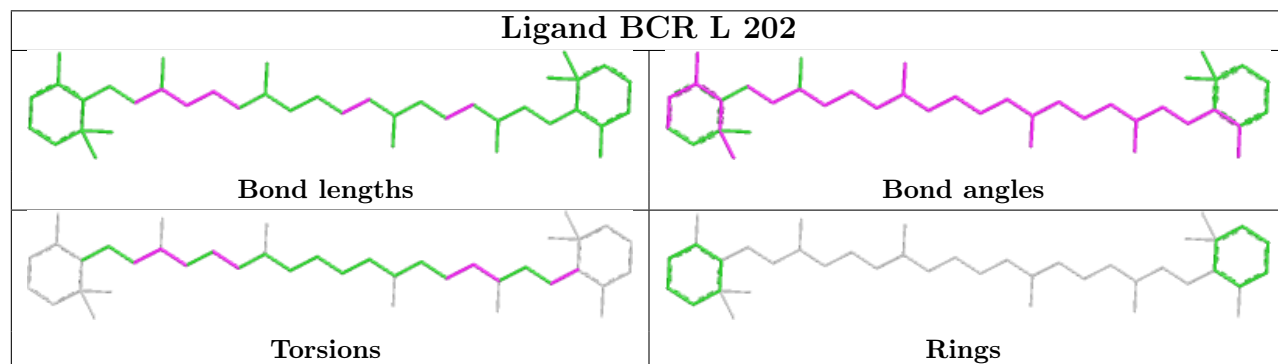
Ligand CLA L 204



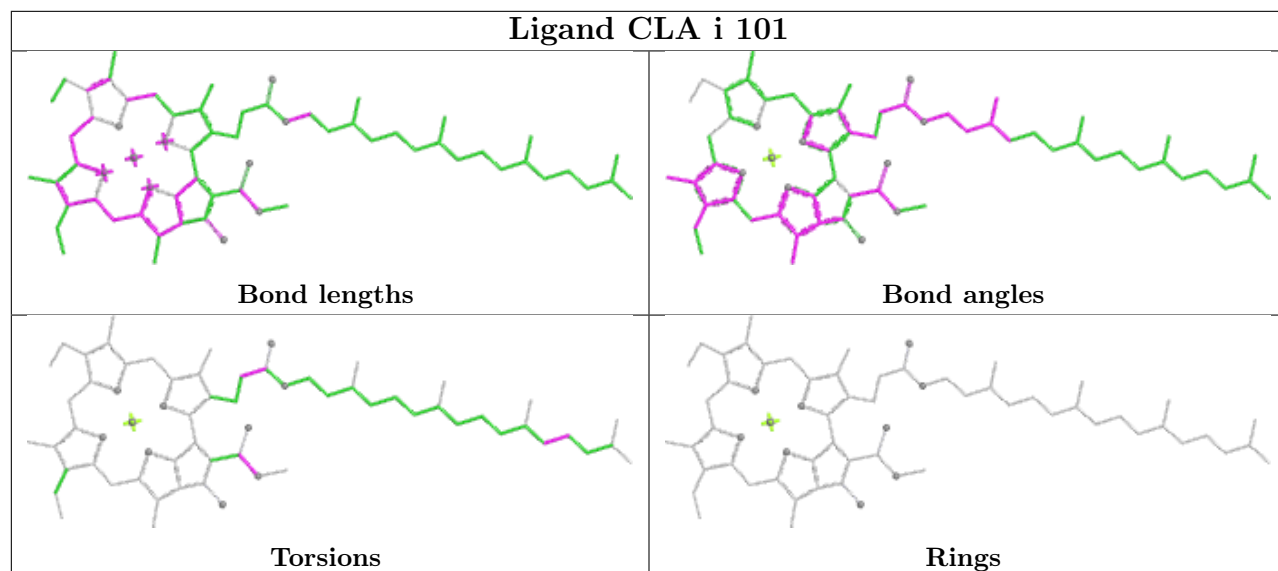
Ligand CLA b 803

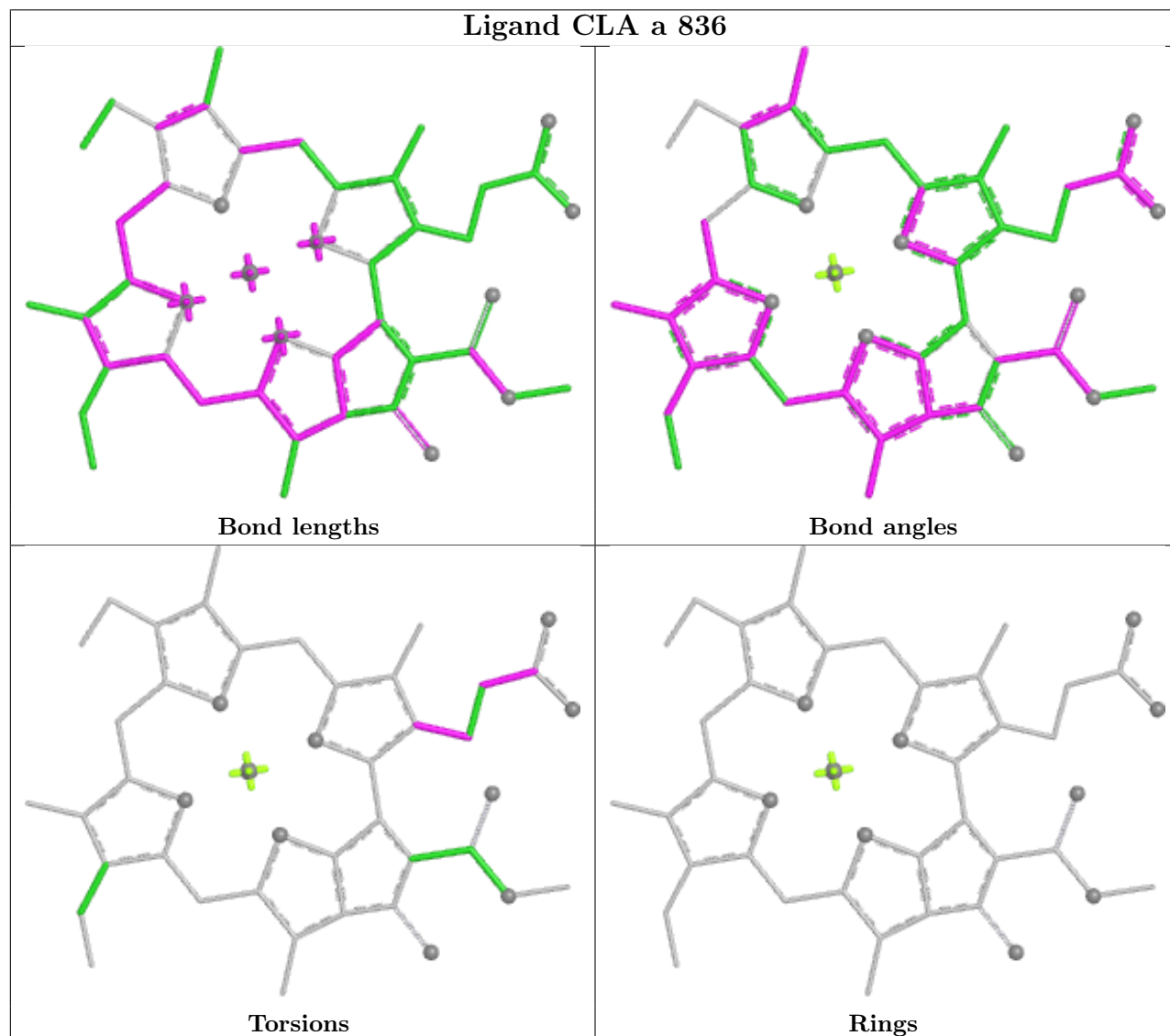
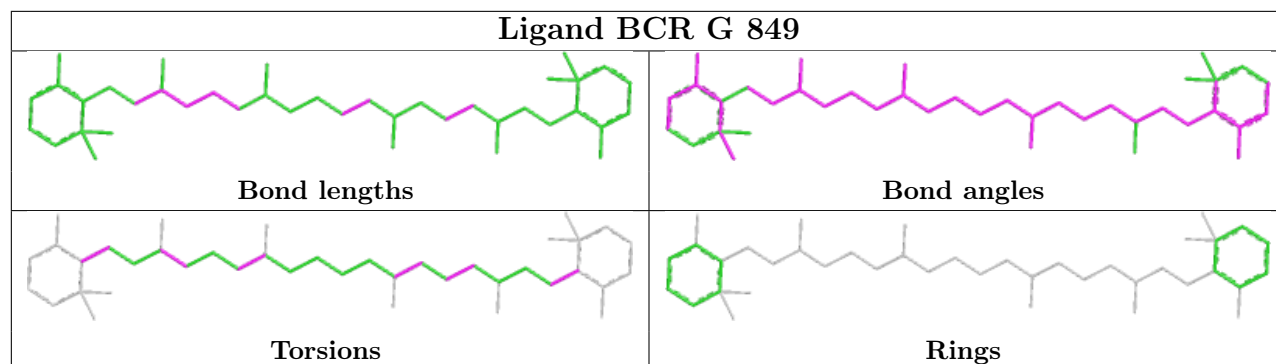


Ligand BCR L 202

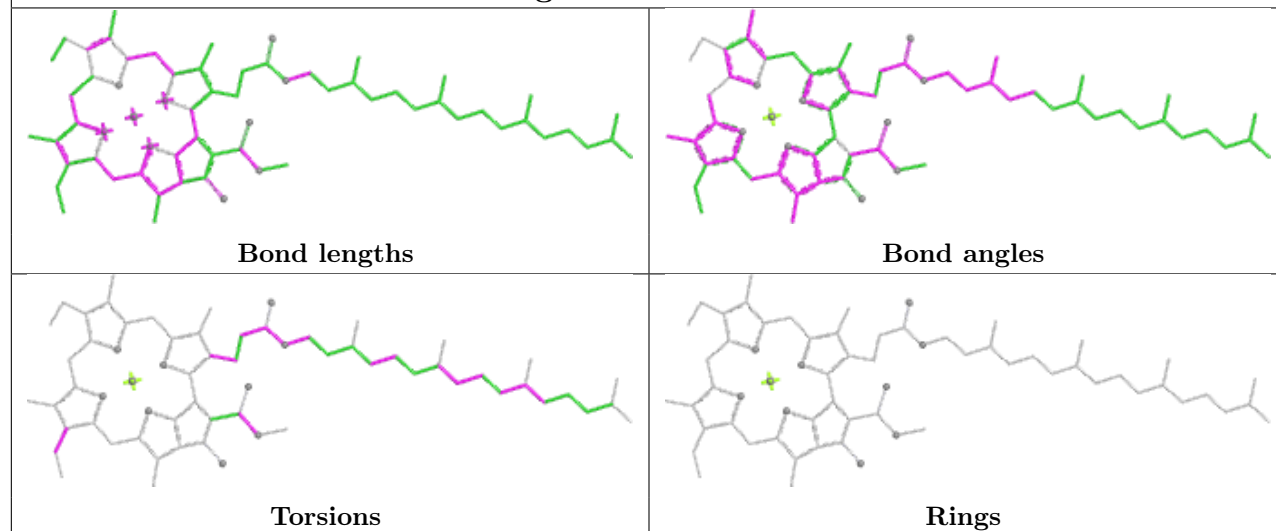


Ligand CLA i 101

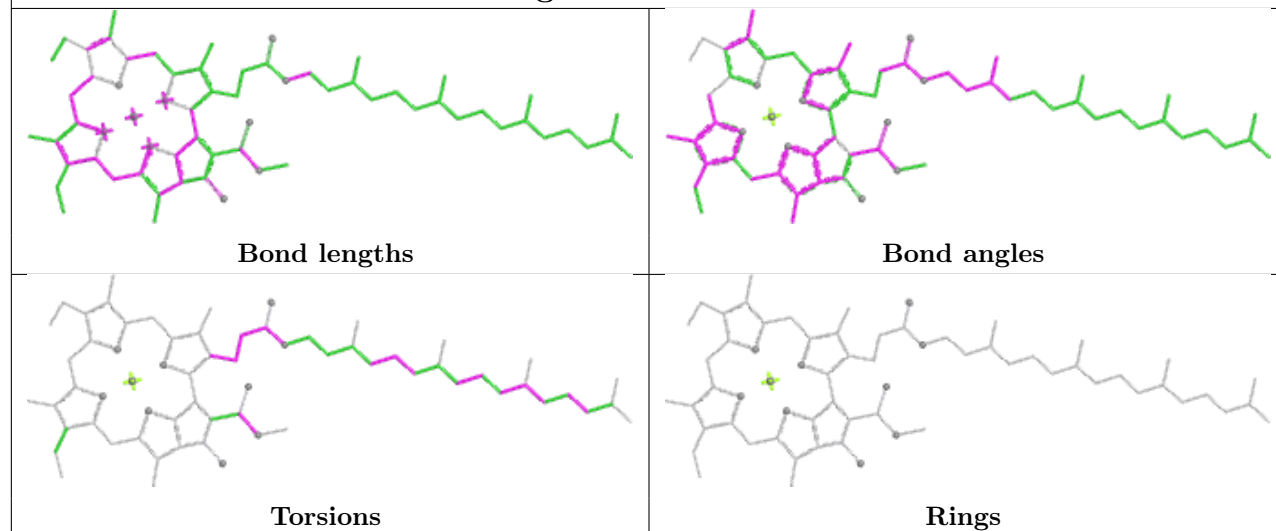




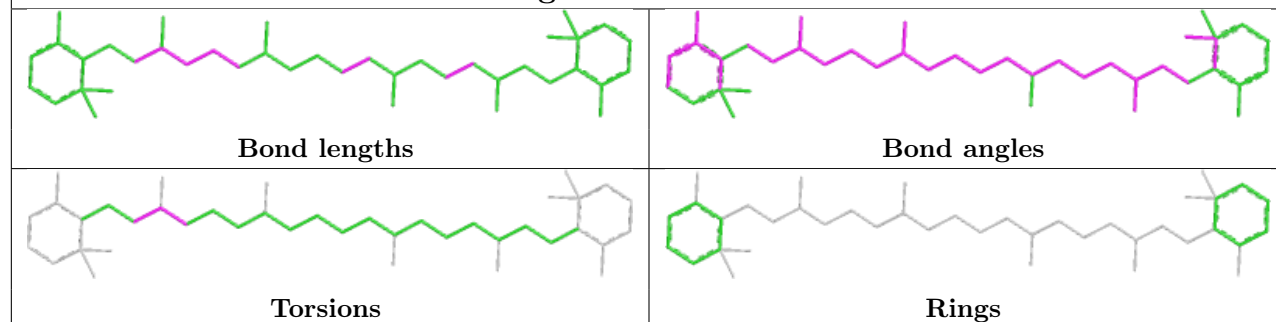
Ligand CLA b 840

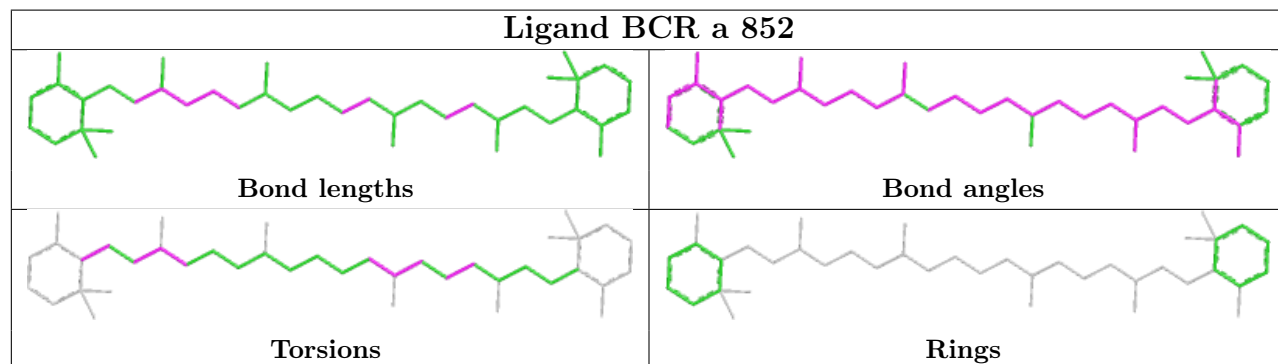
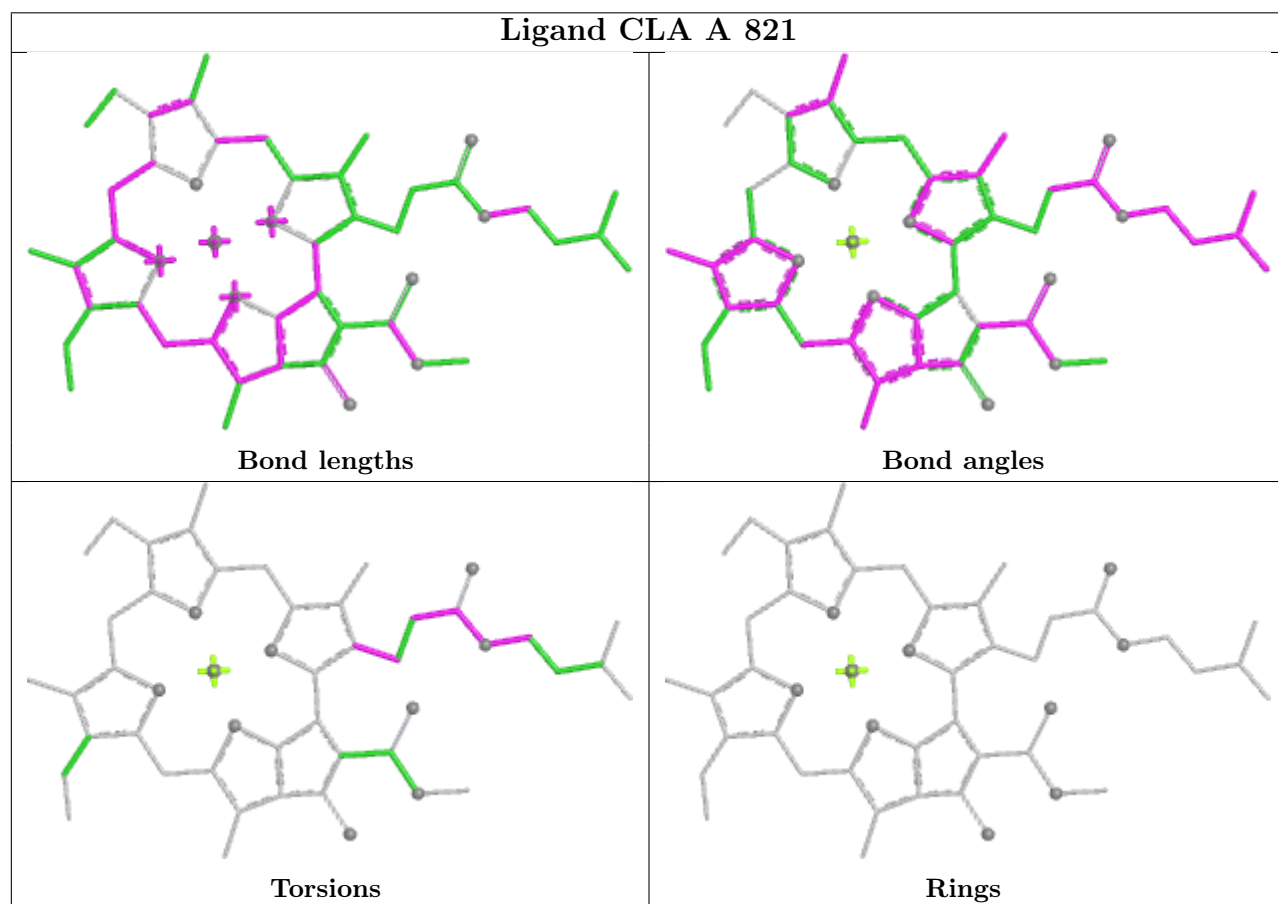
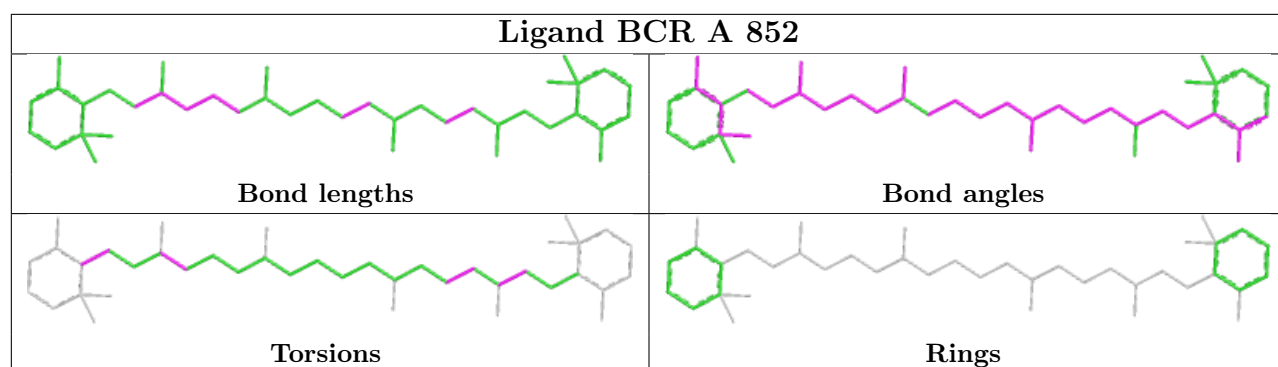


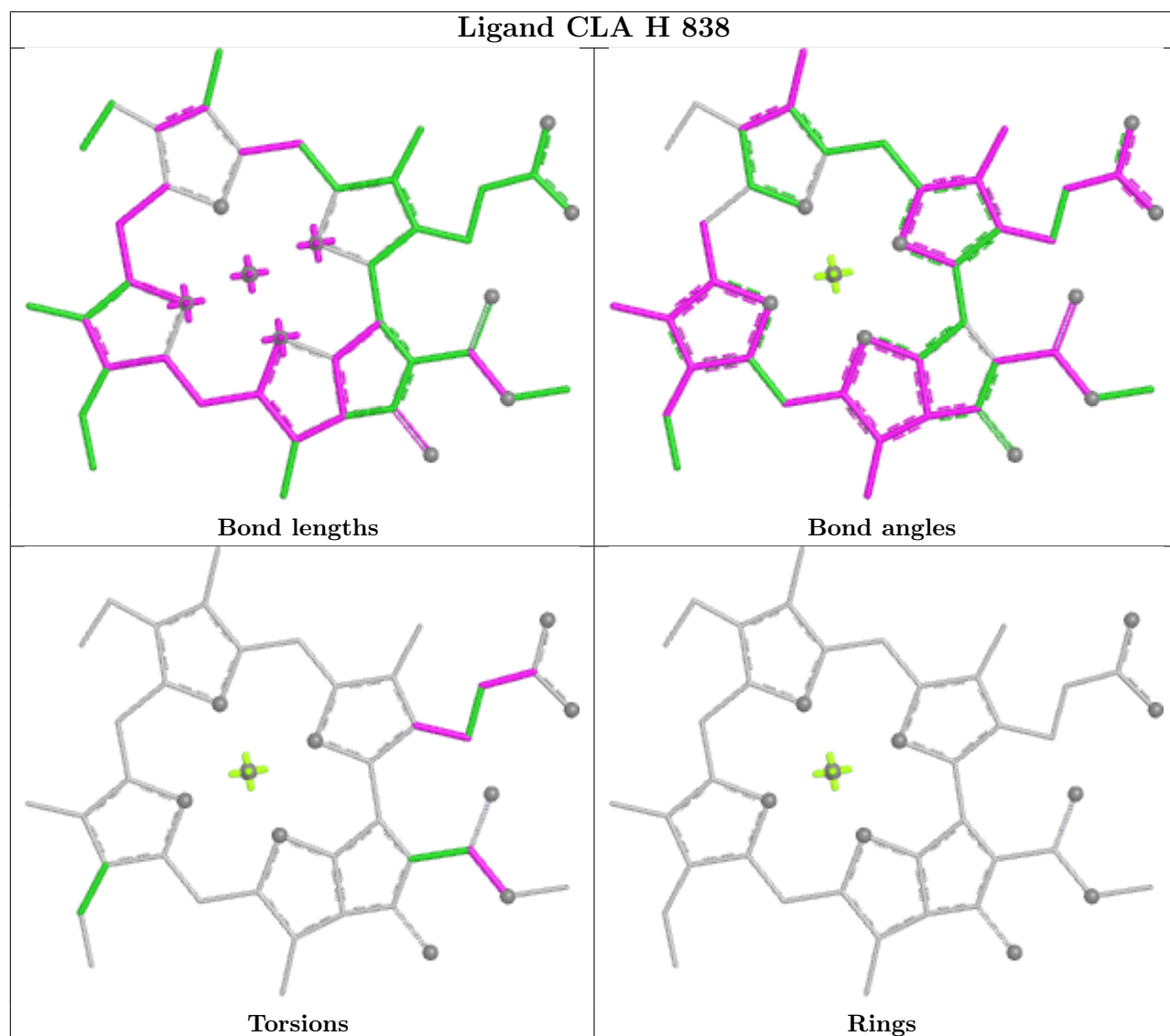
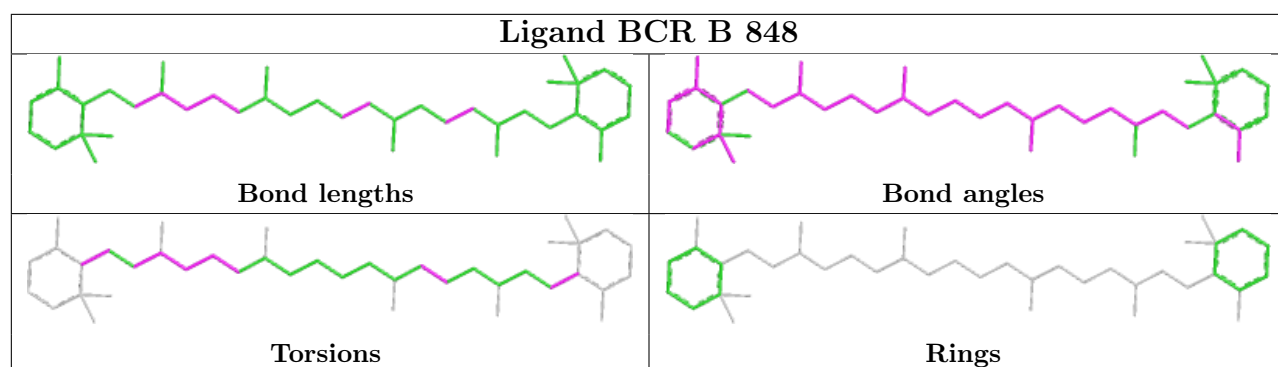
Ligand CLA a 829

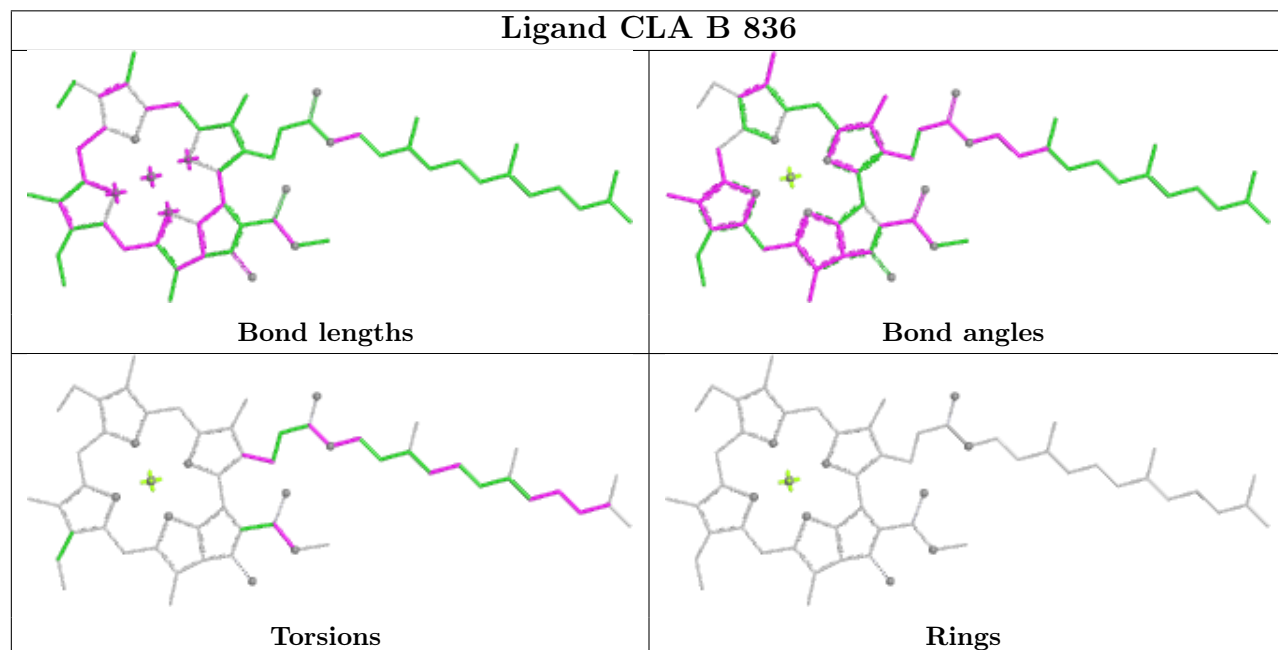
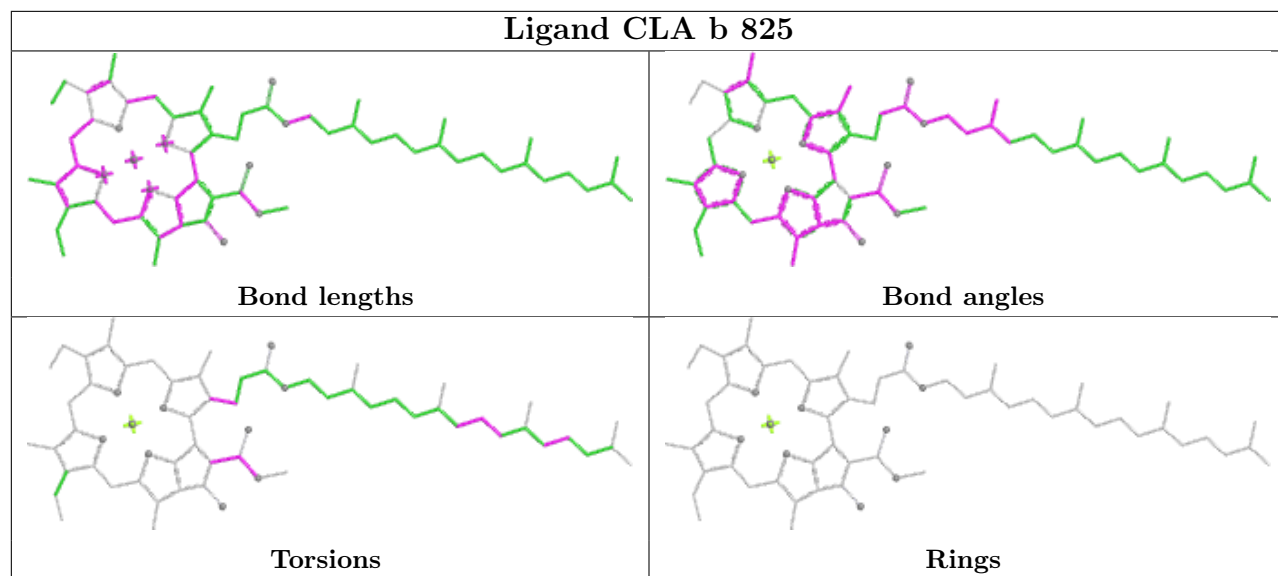


Ligand BCR l 201

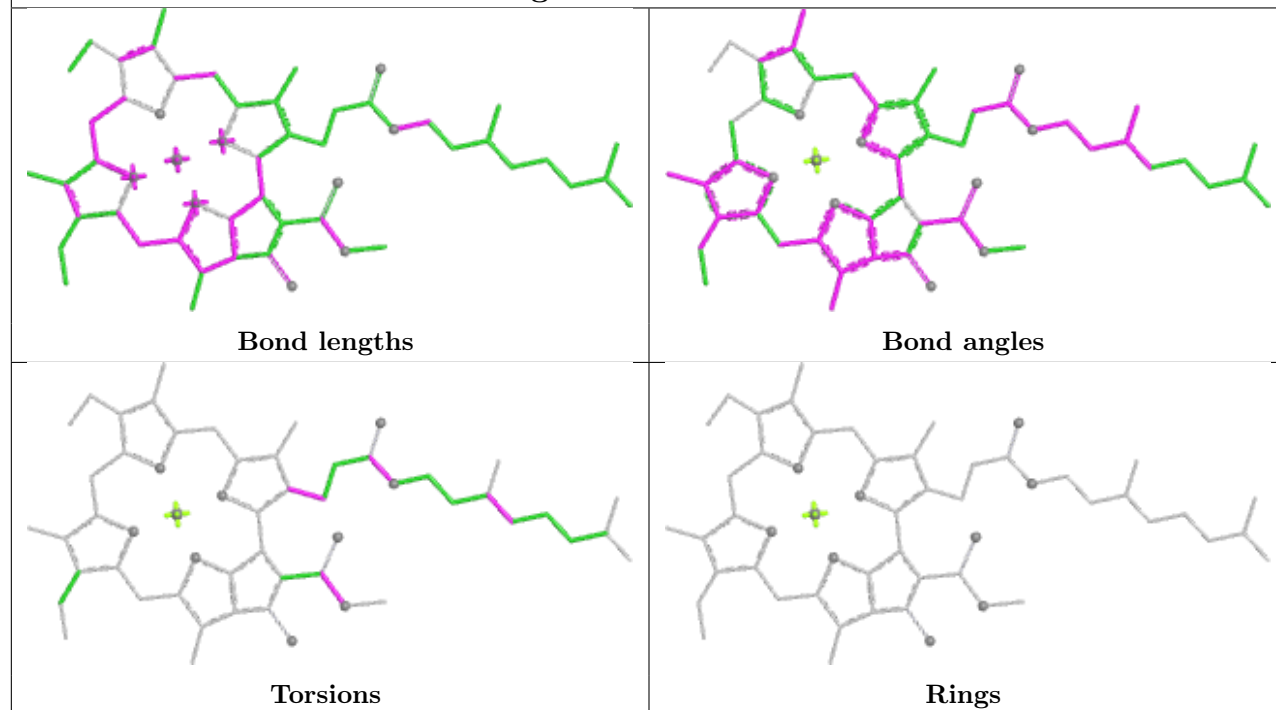




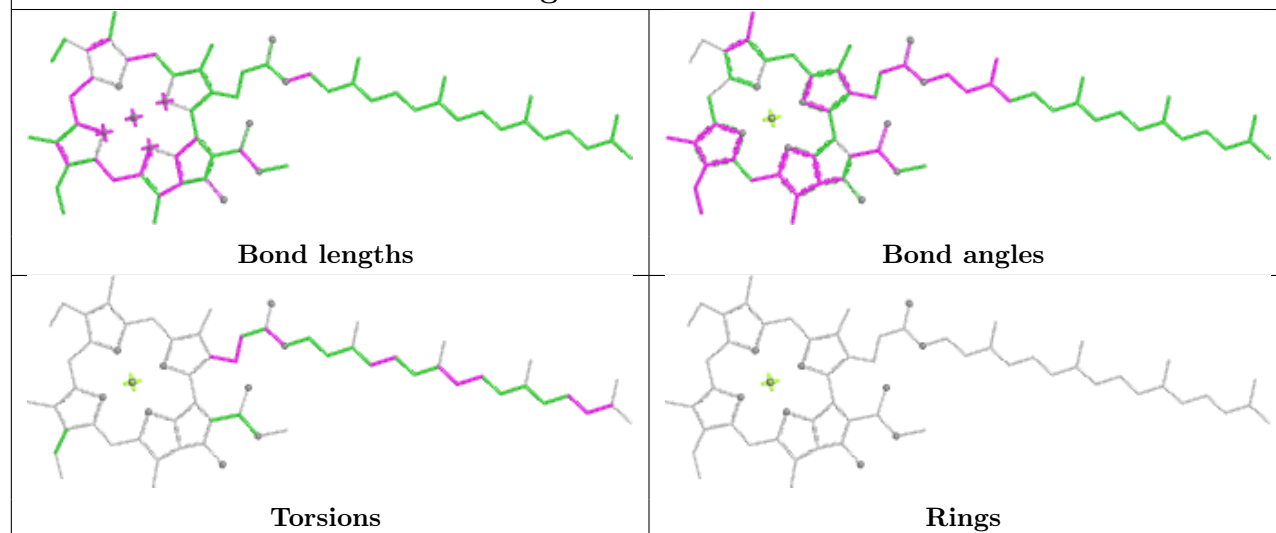


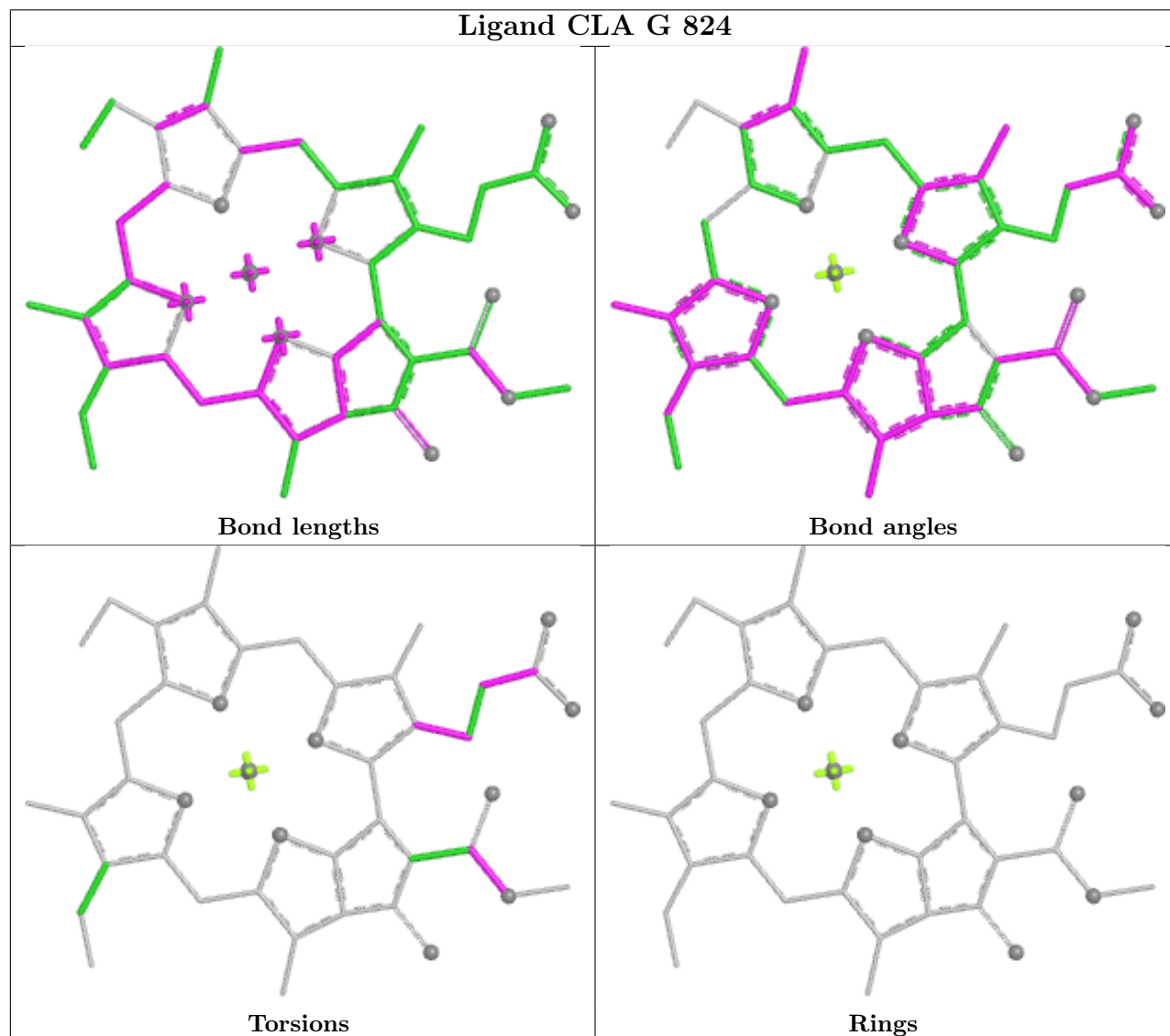
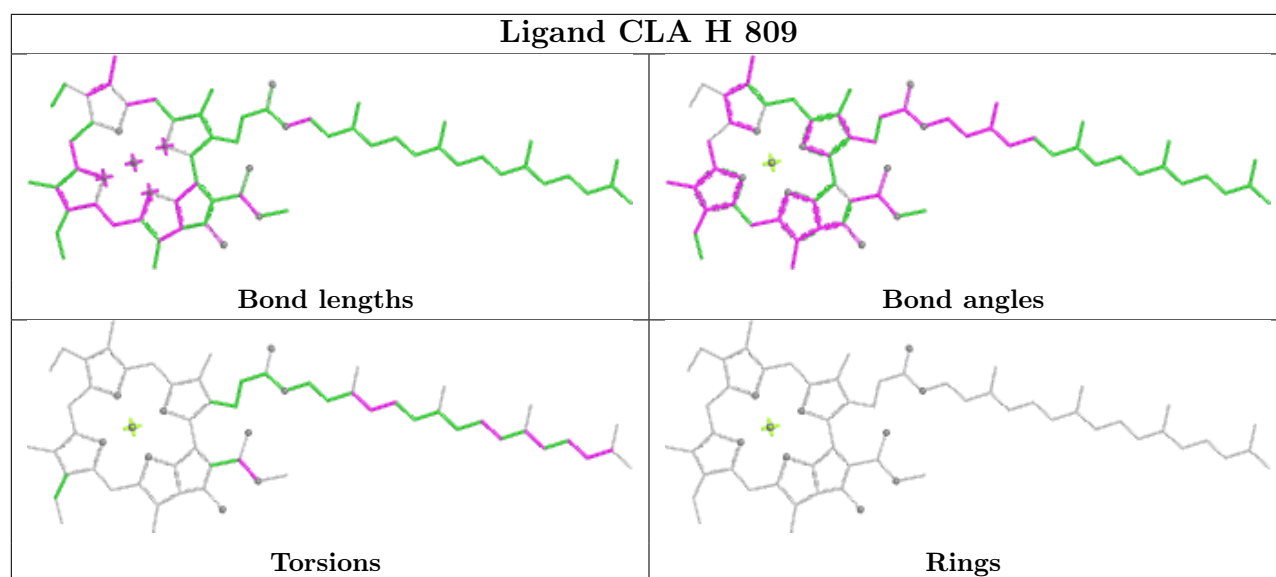


Ligand CLA G 805

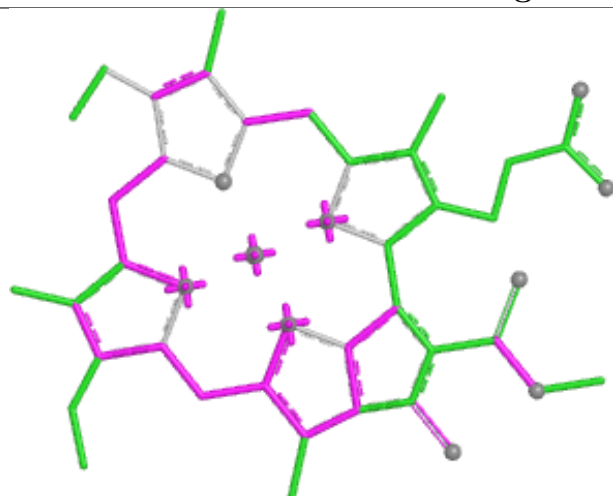


Ligand CLA I 206

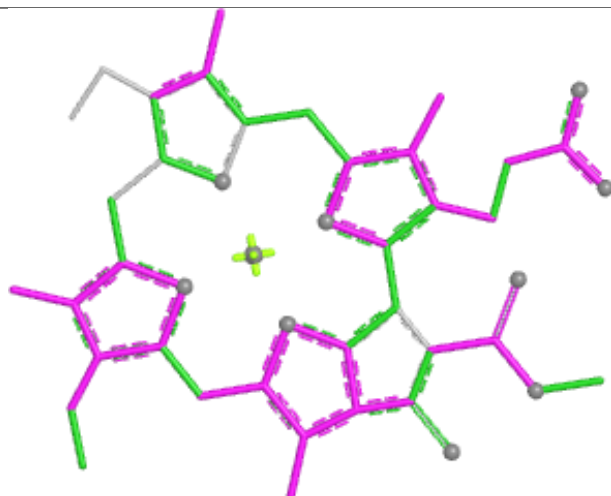




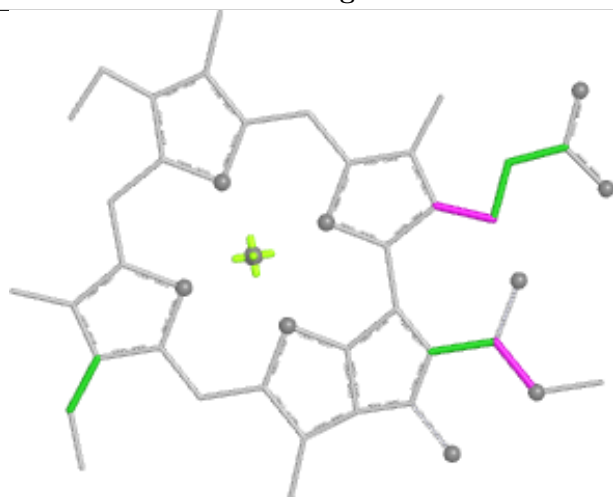
Ligand CLA B 810



Bond lengths



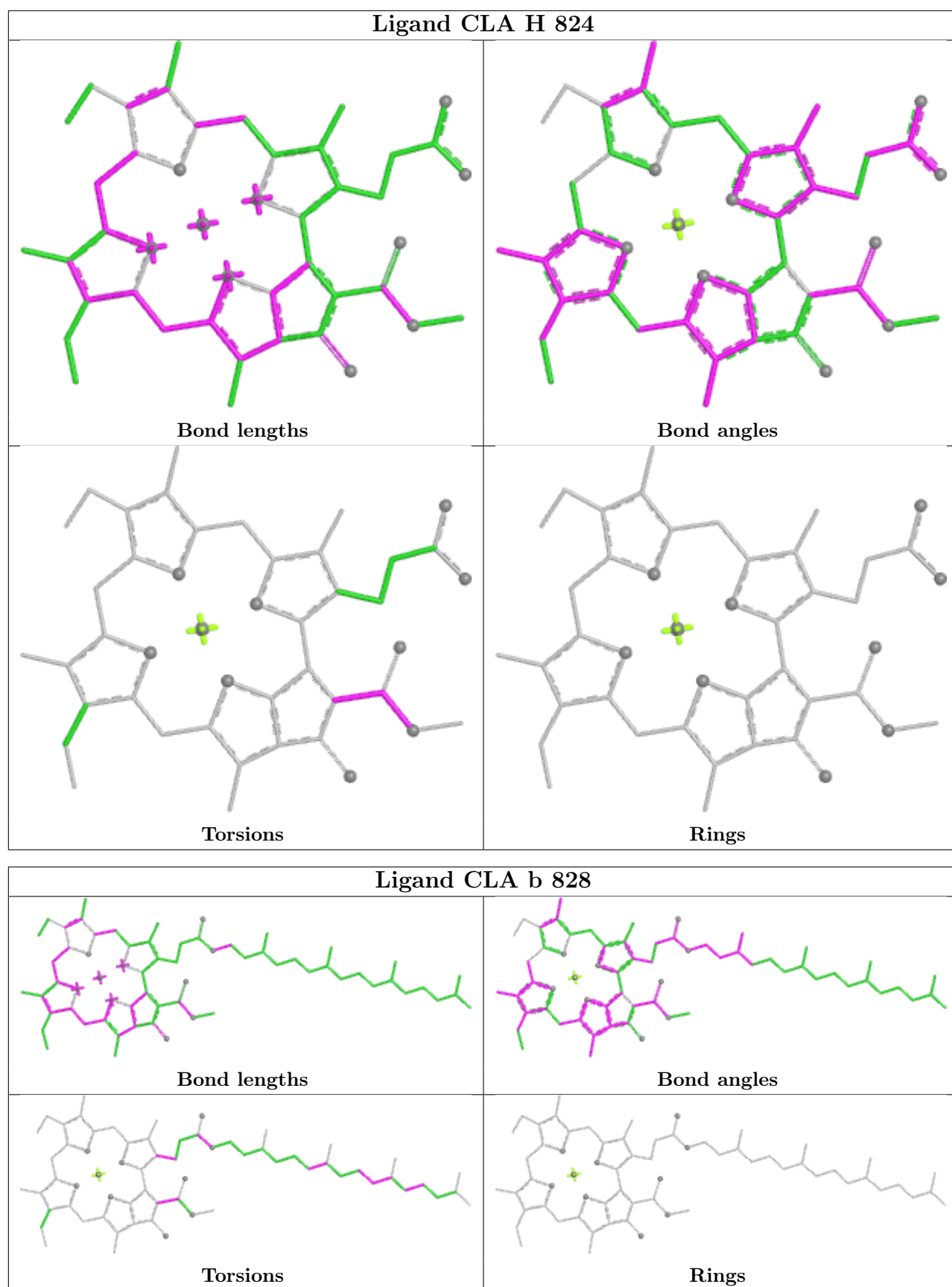
Bond angles



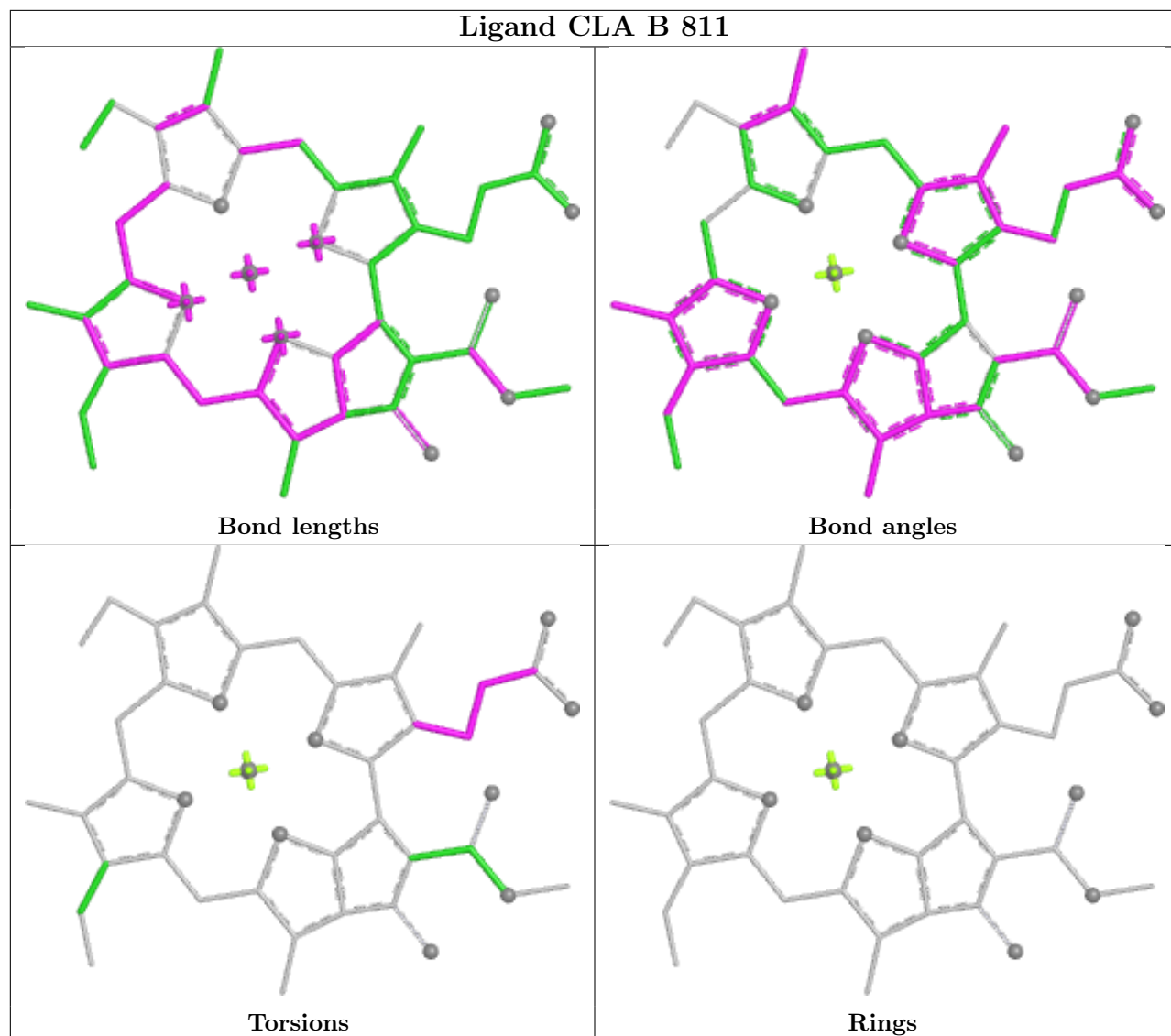
Torsions



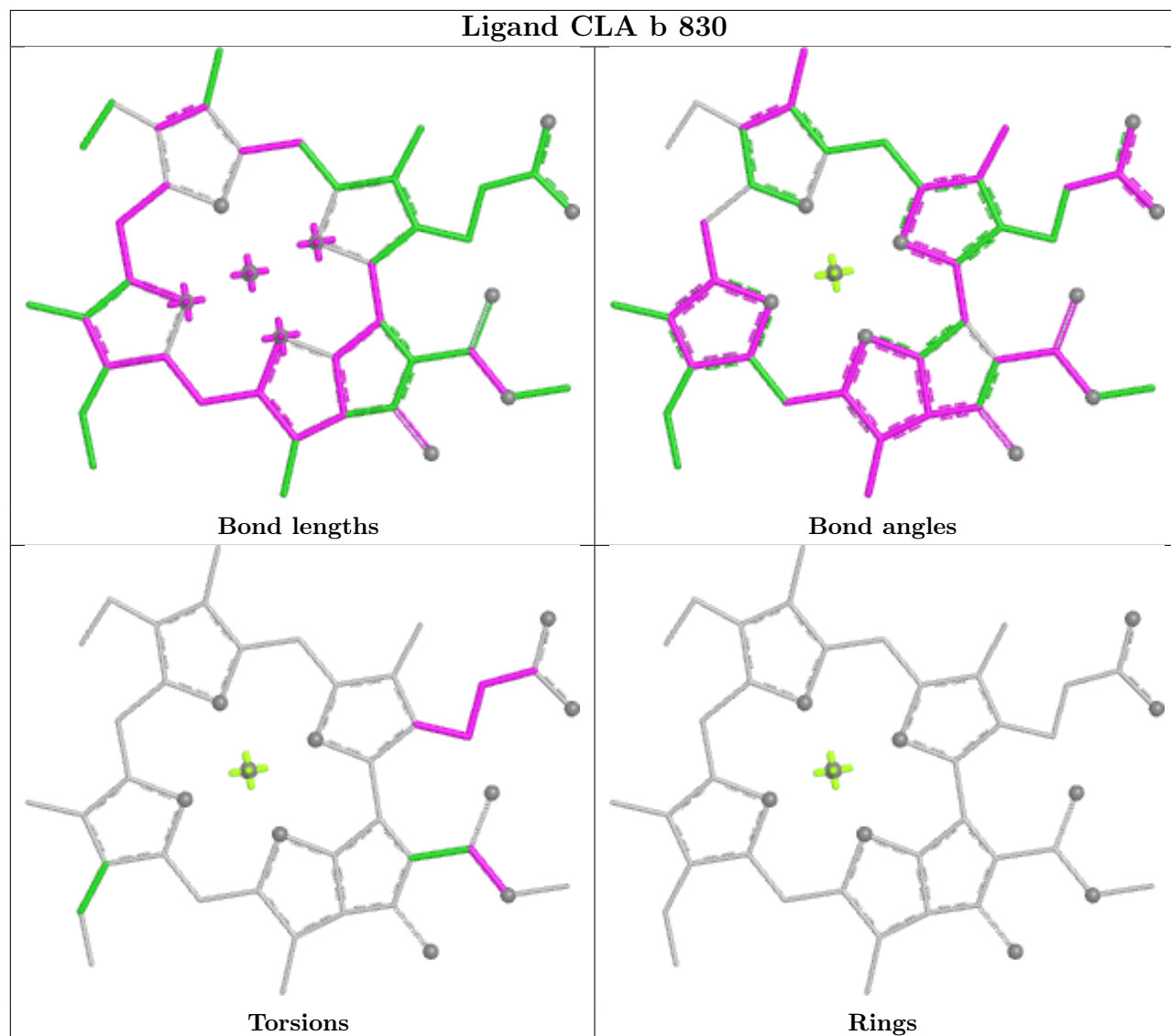
Rings

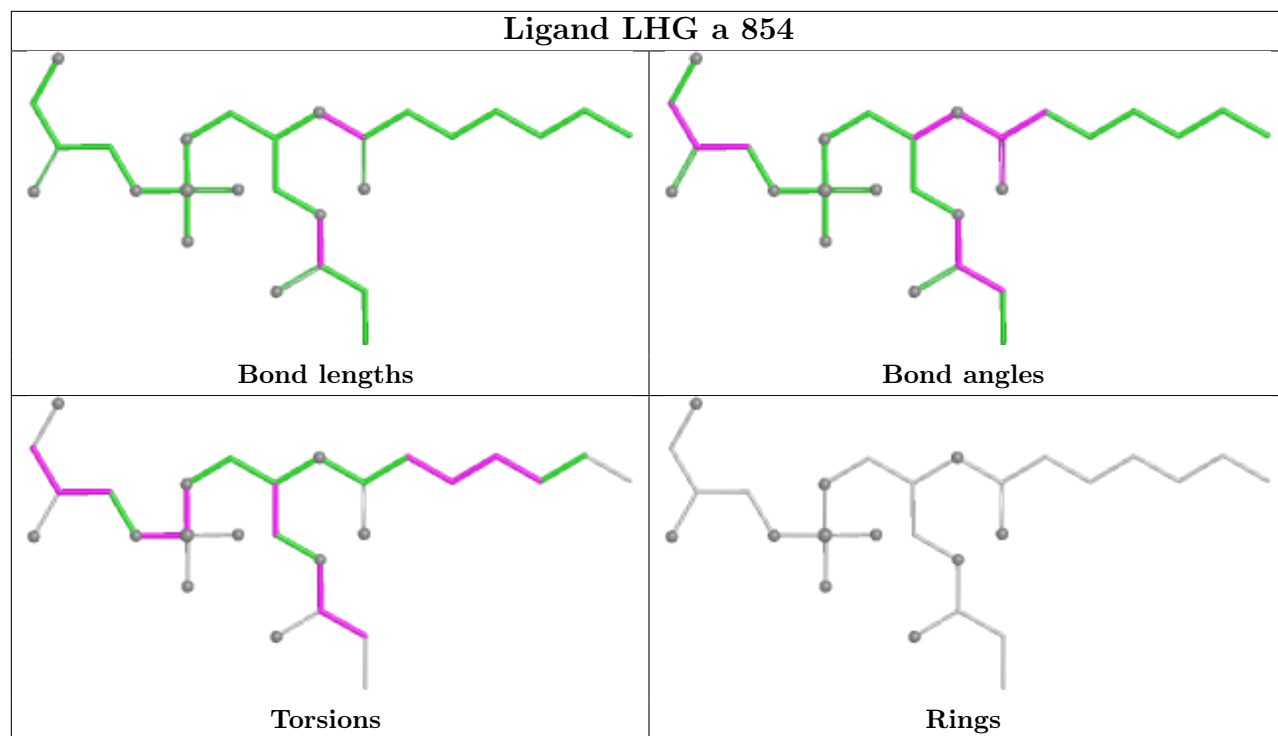


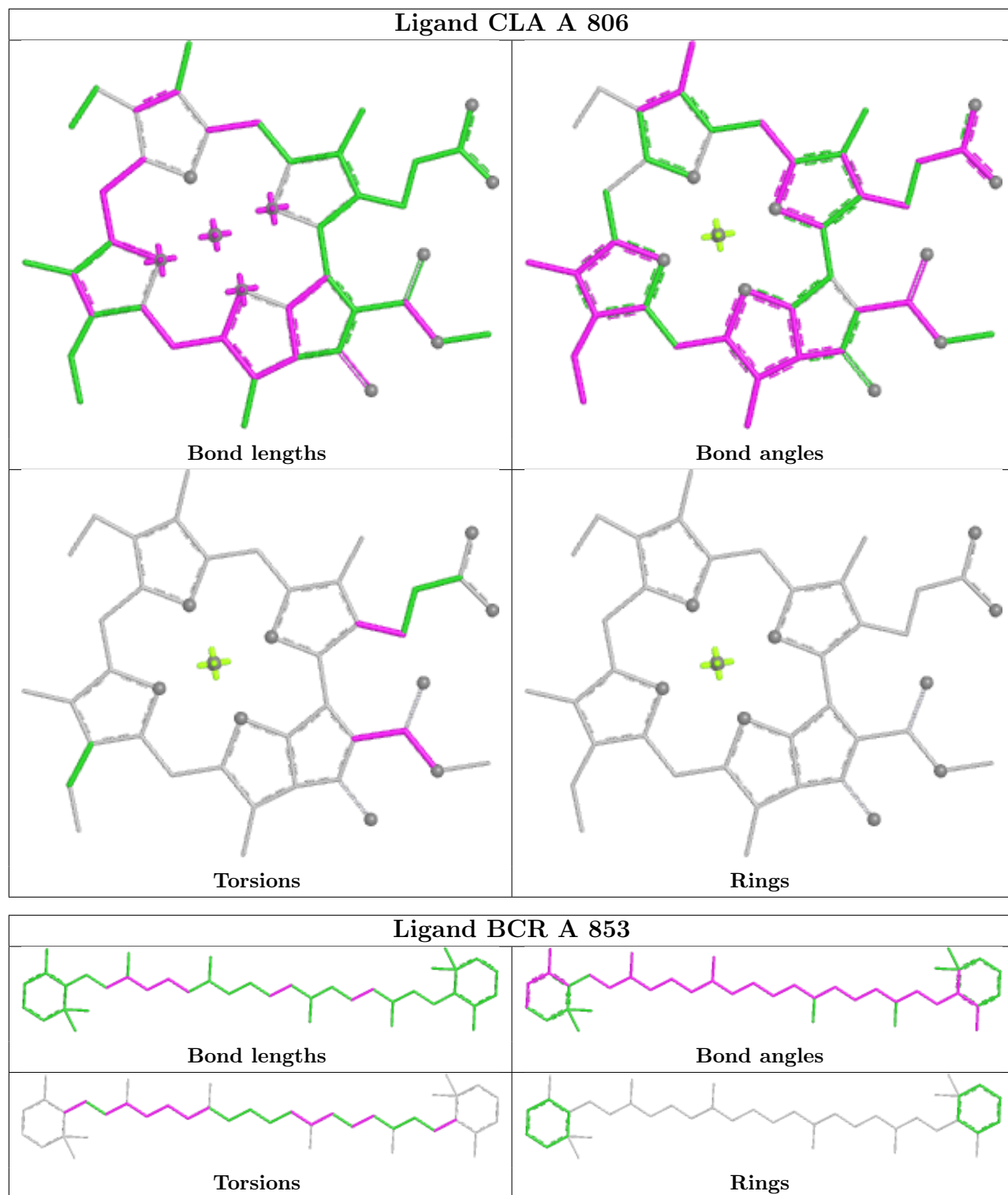
Ligand CLA B 811

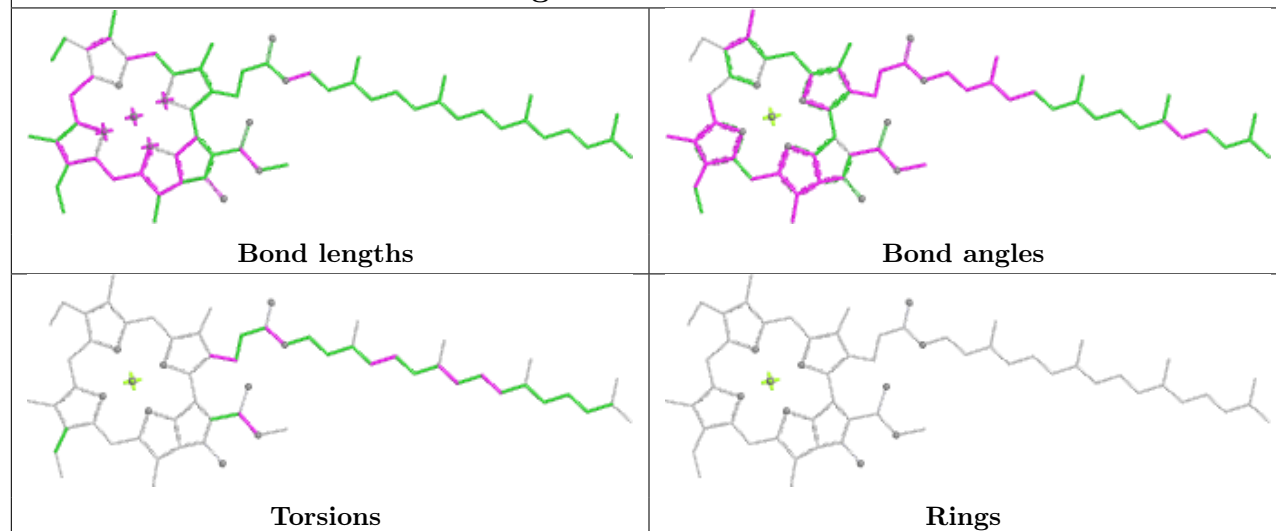
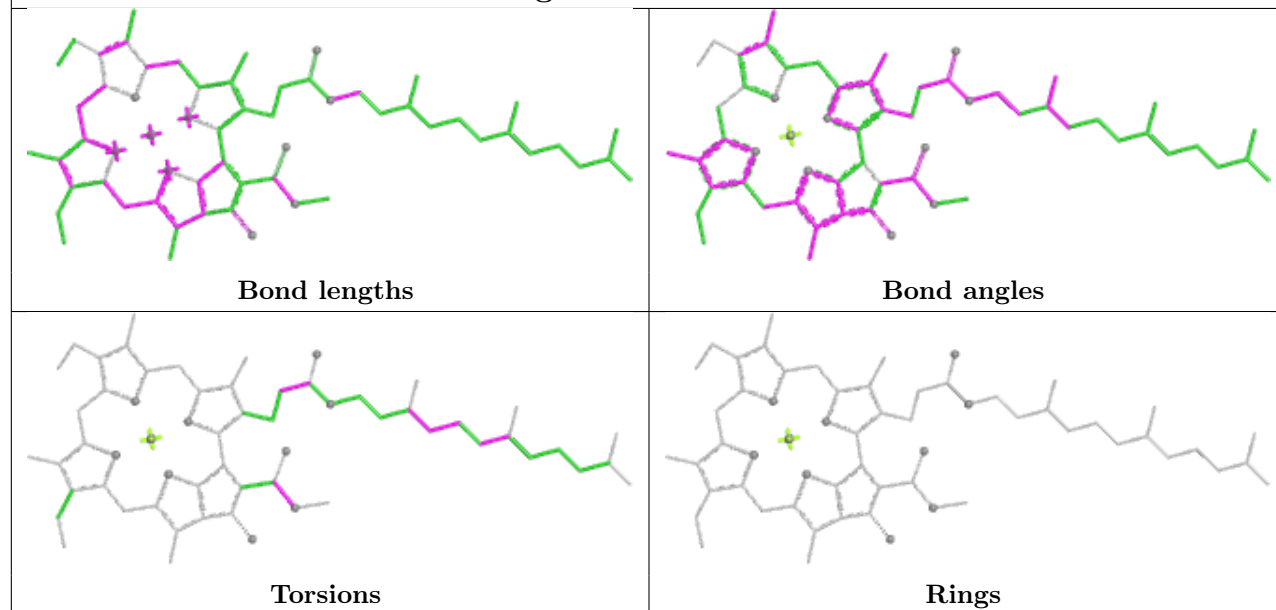


Ligand CLA b 830

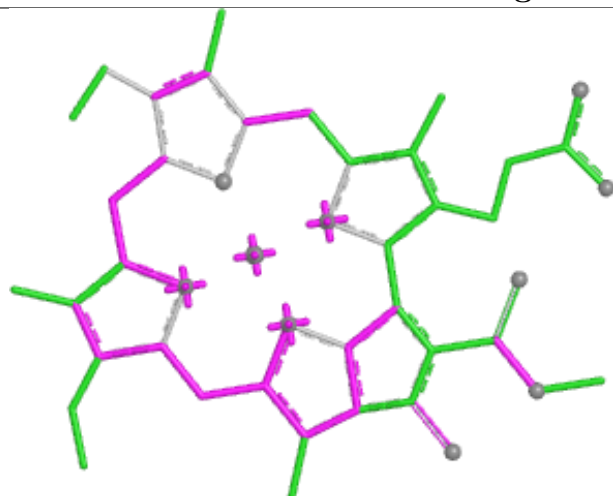




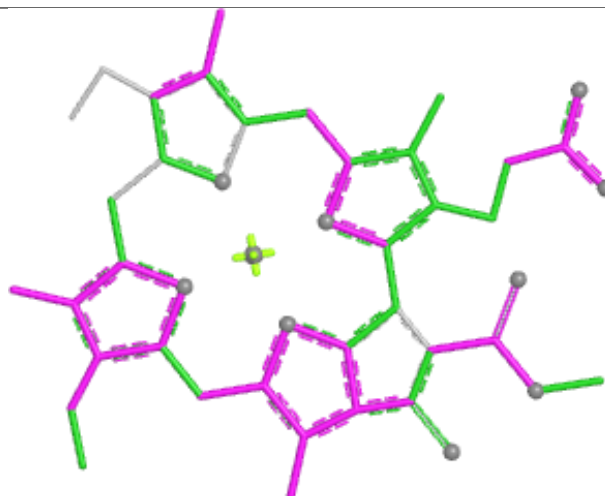


Ligand CLA A 822**Ligand CLA b 837**

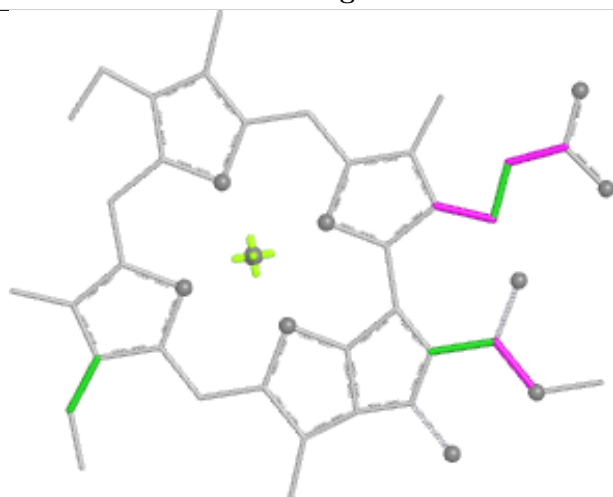
Ligand CLA B 833



Bond lengths



Bond angles

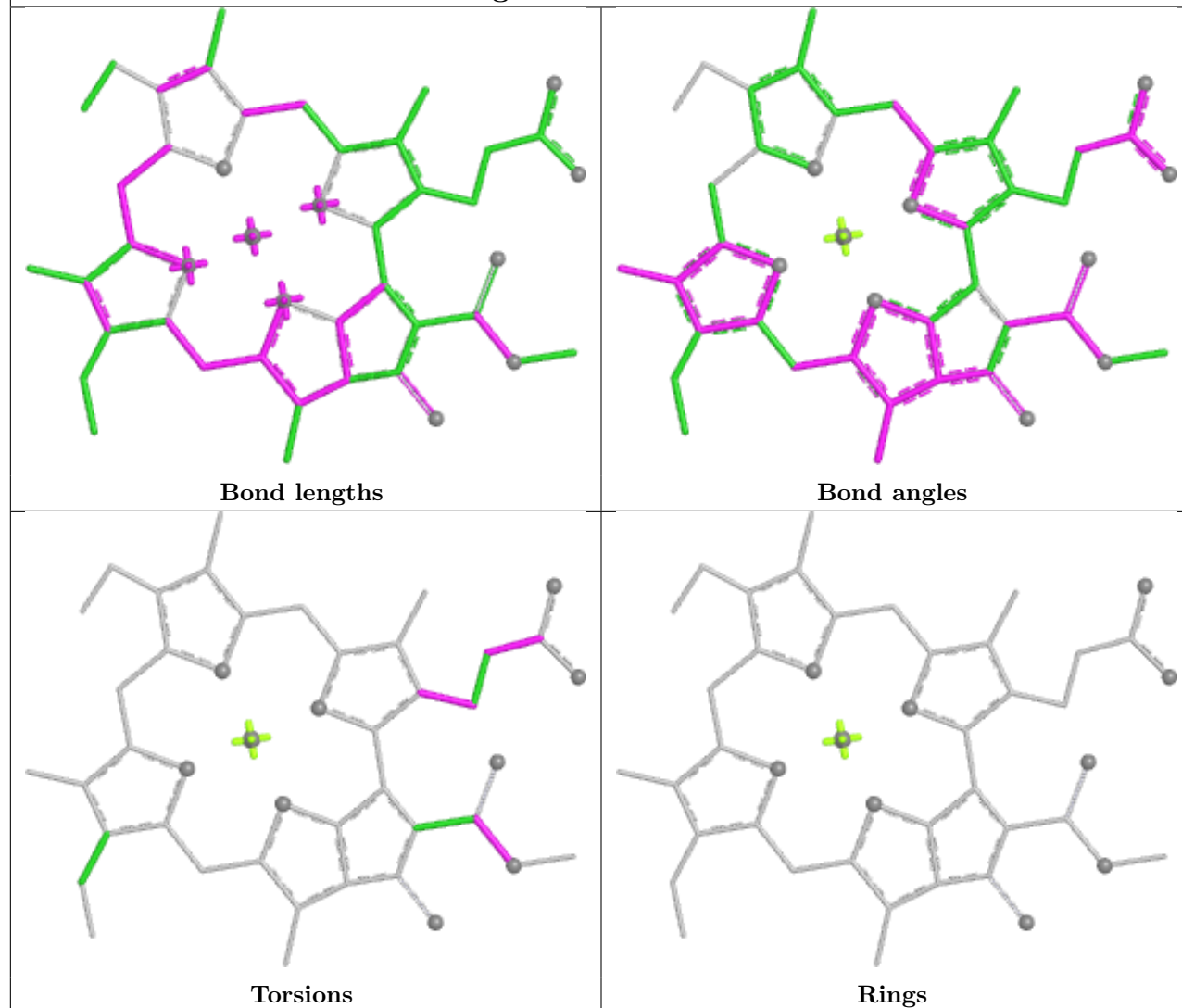


Torsions

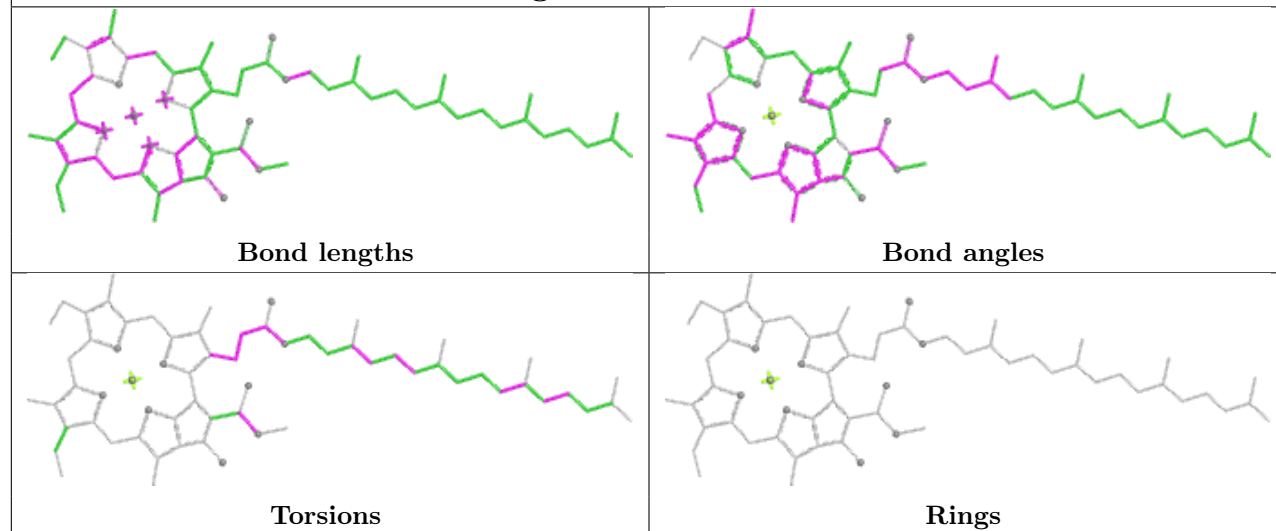


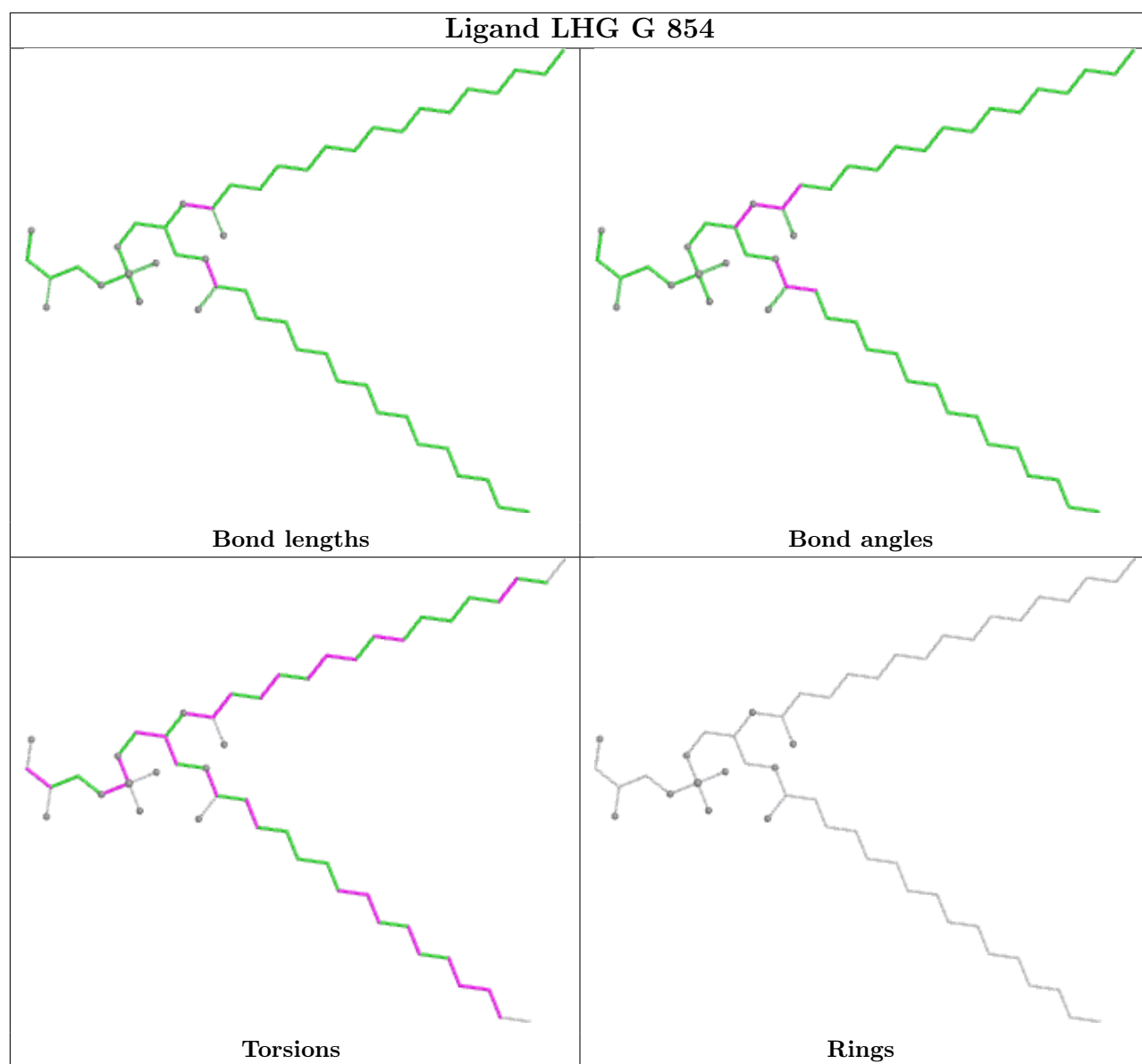
Rings

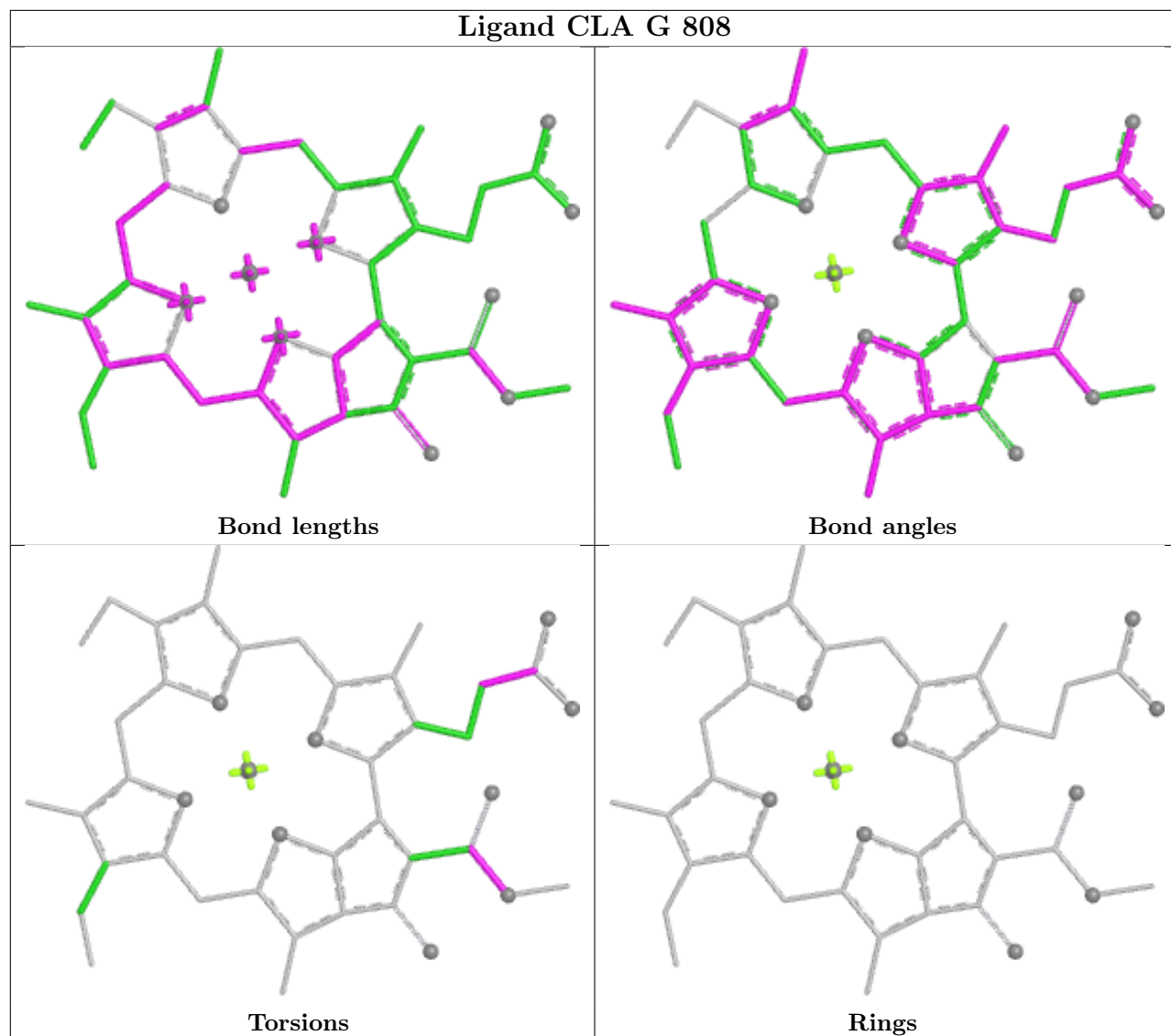
Ligand CLA A 818



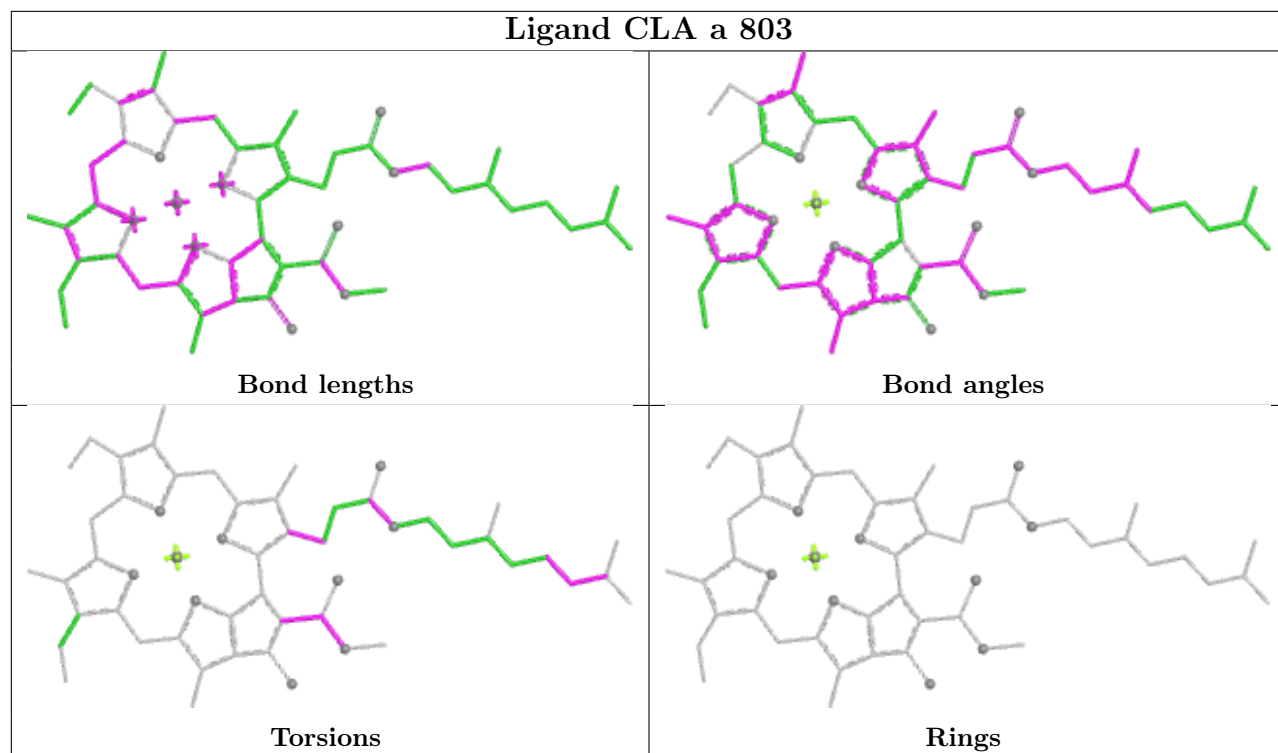
Ligand CLA H 826



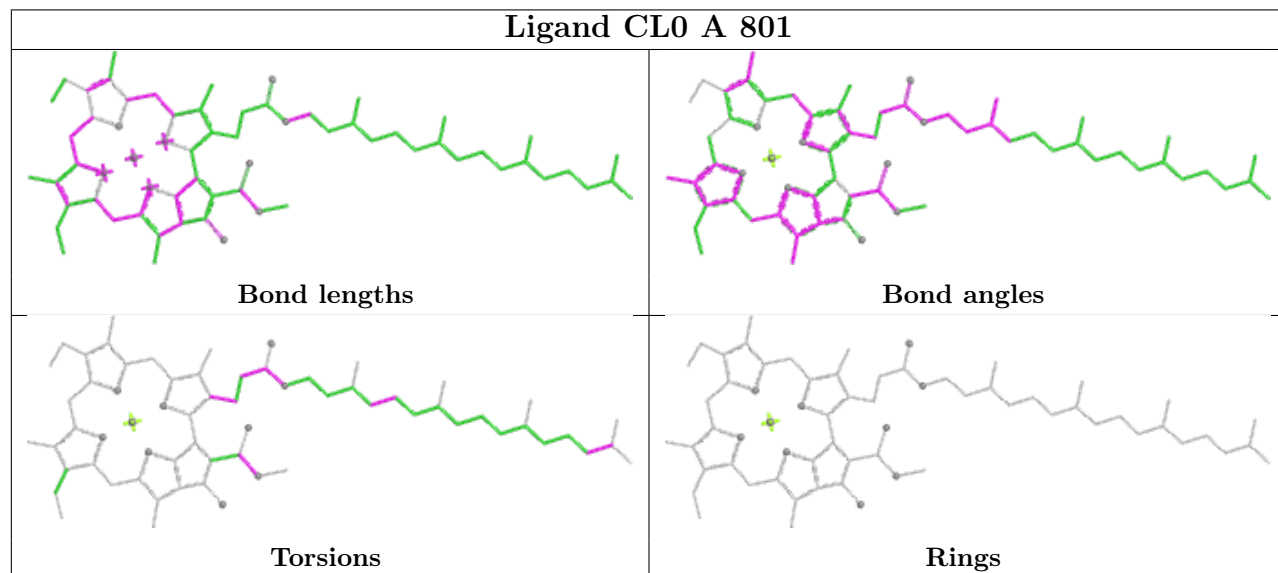


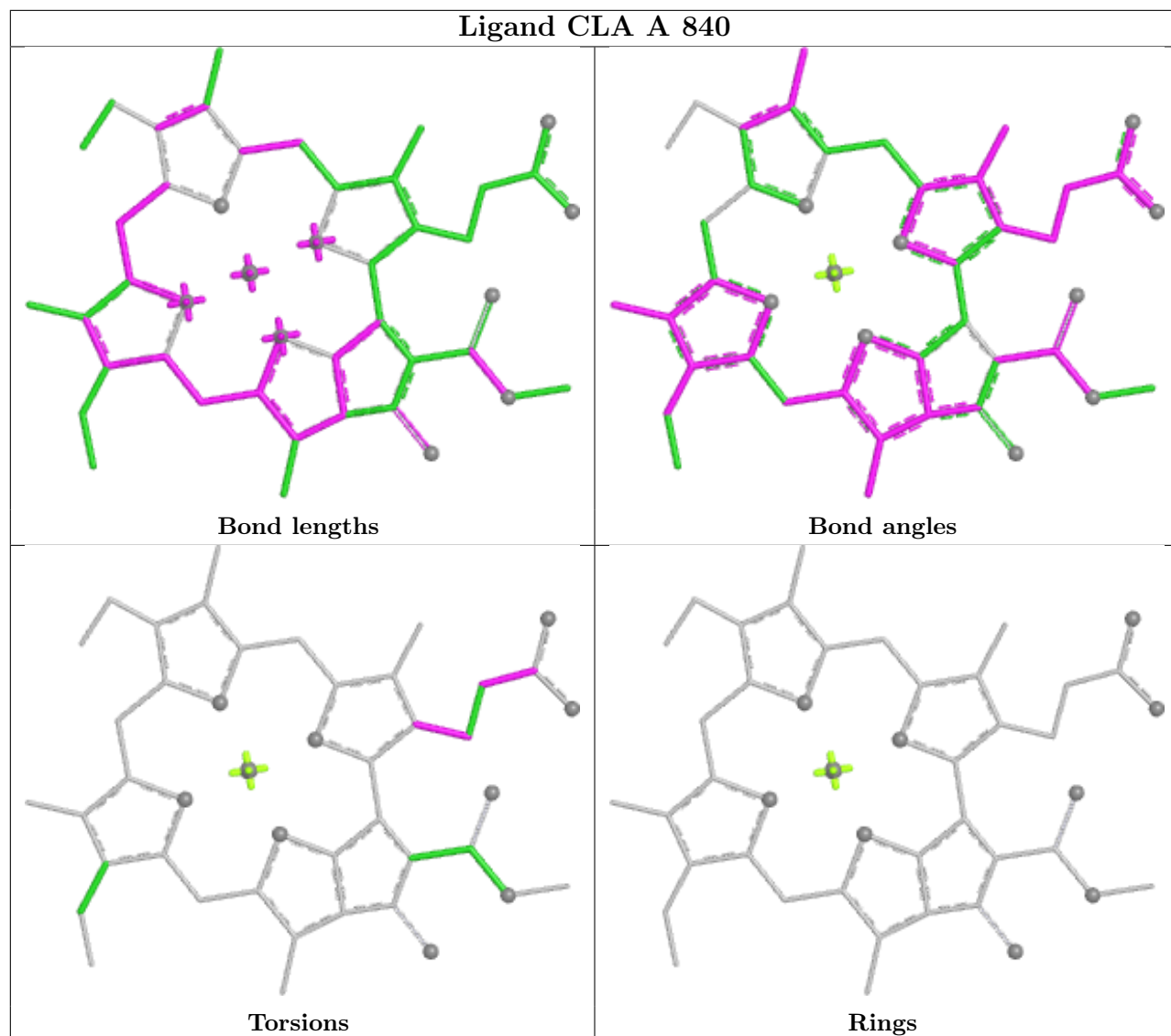


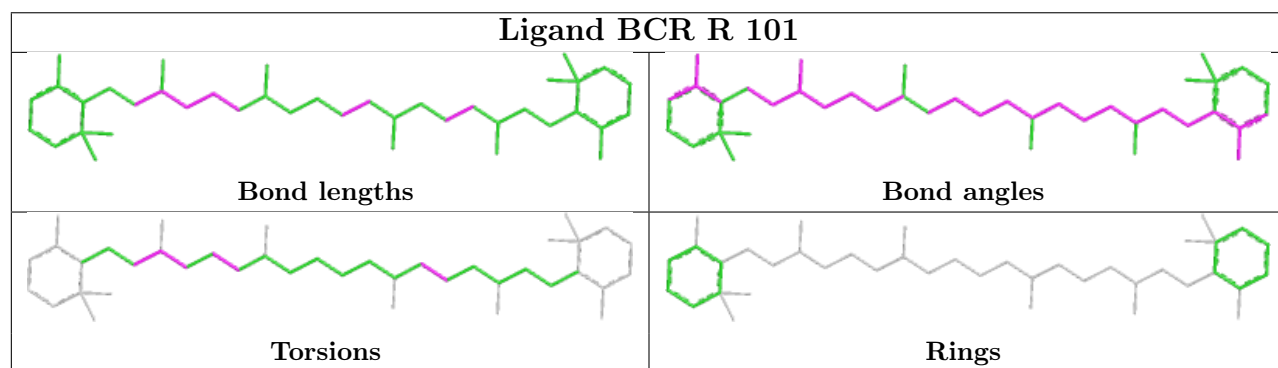
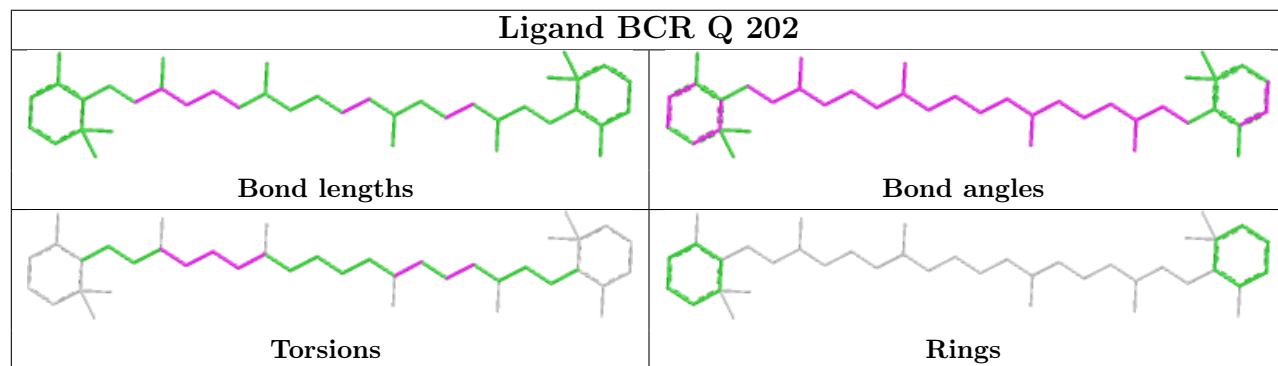
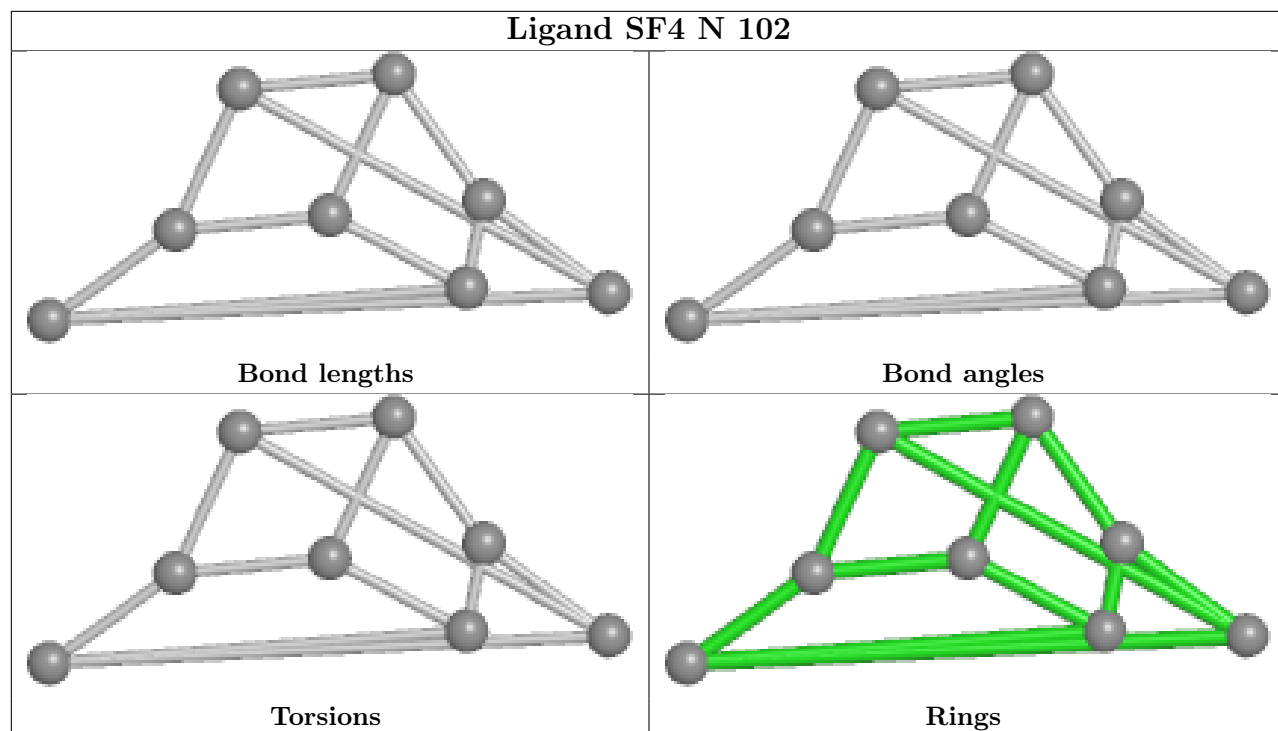
Ligand CLA a 803

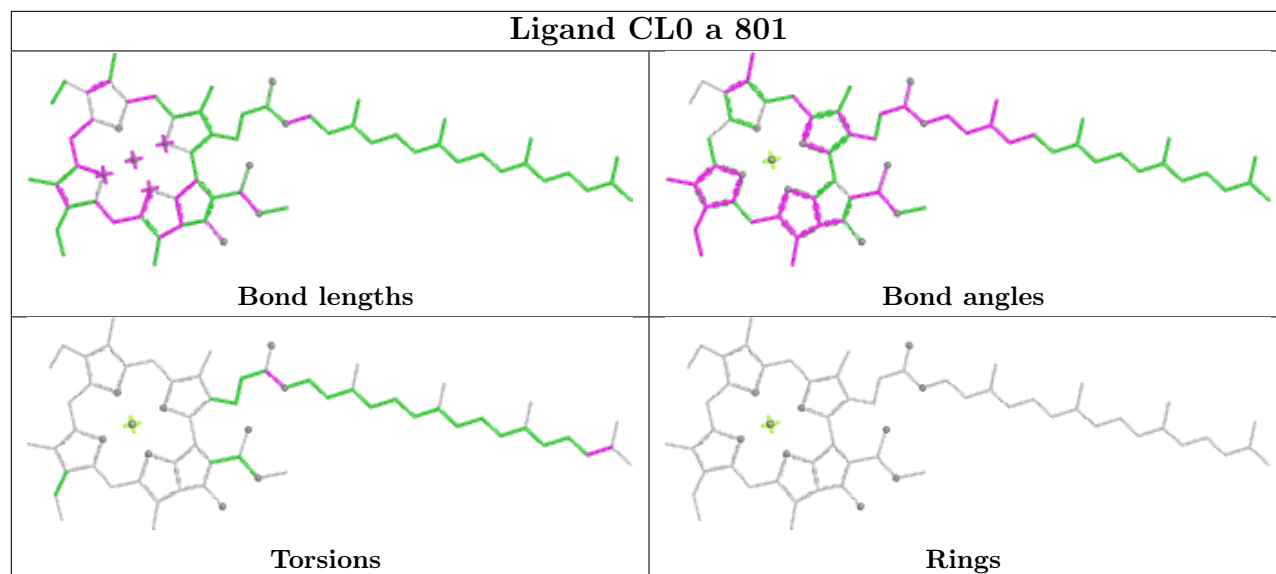
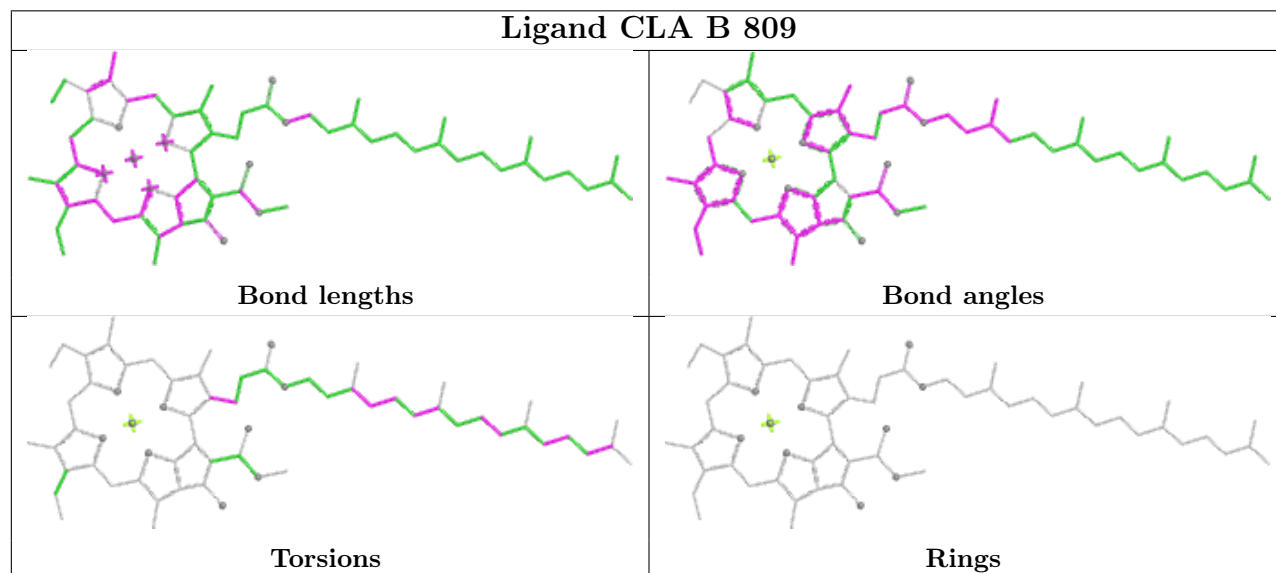


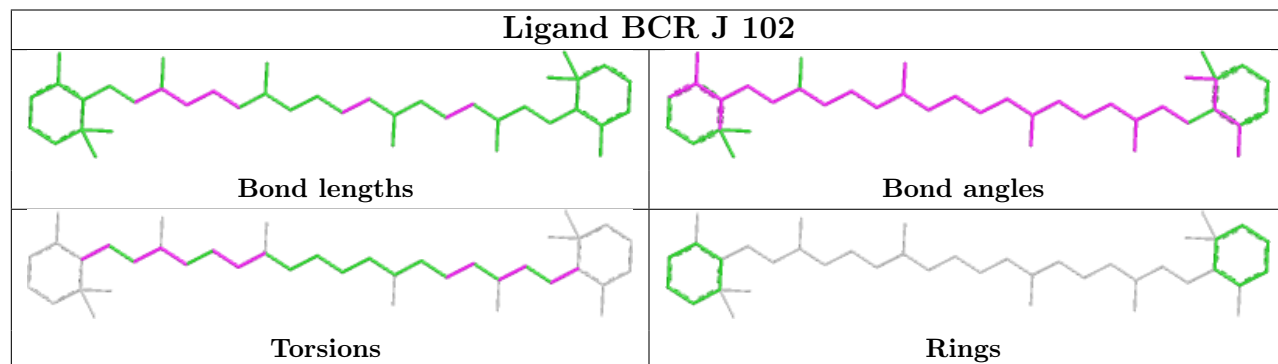
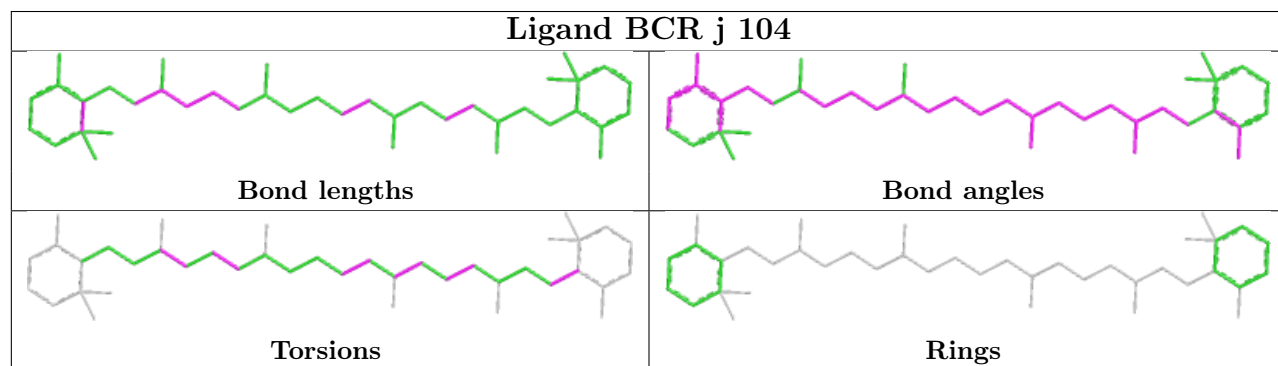
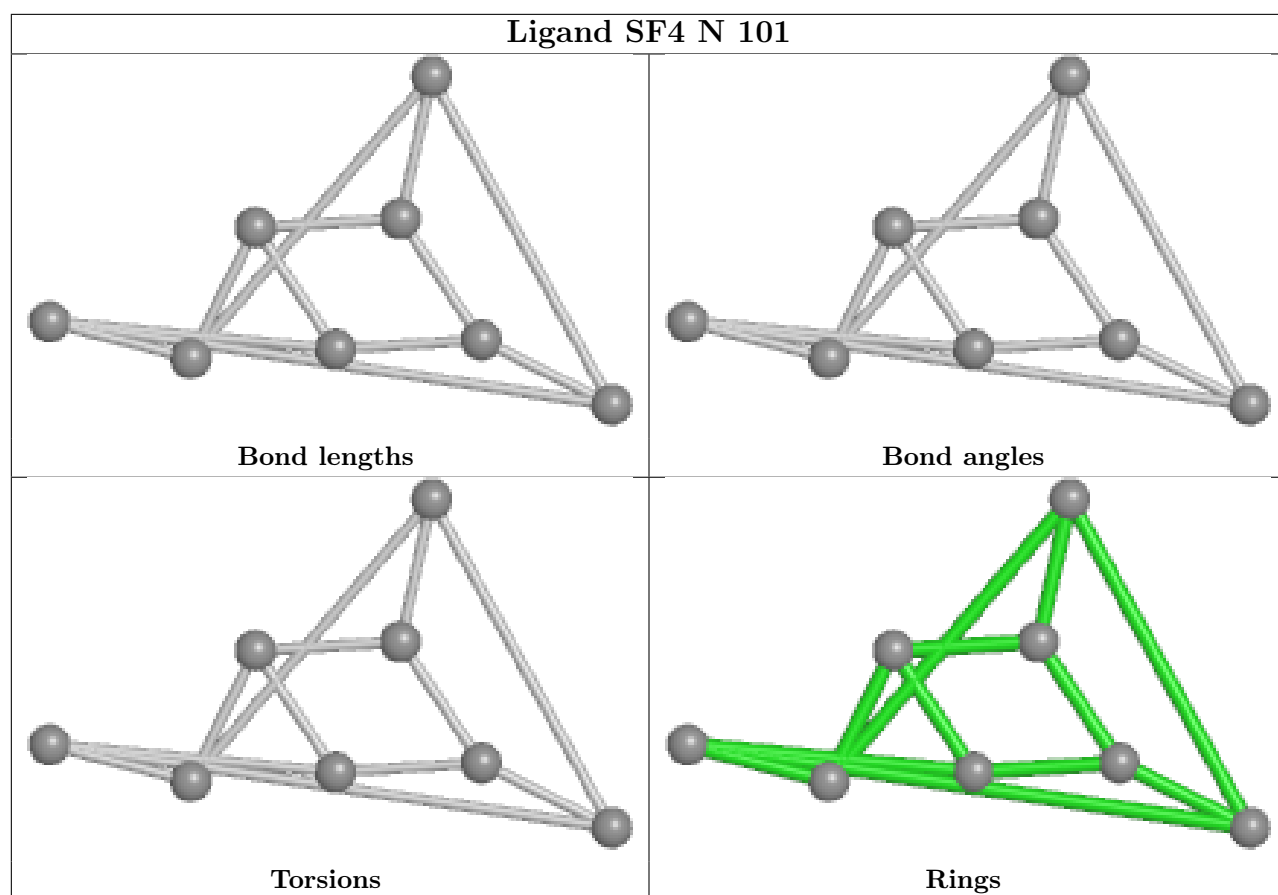
Ligand CL0 A 801



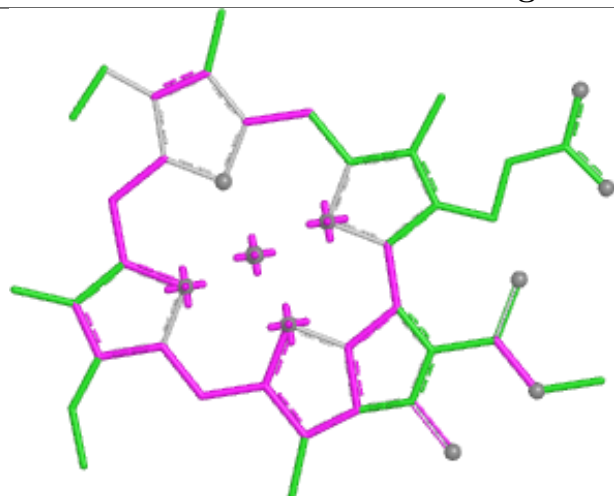




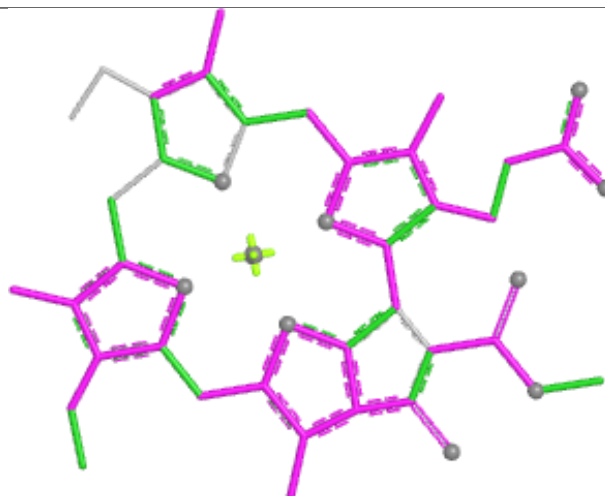
Ligand CL0 a 801**Ligand CLA B 809**



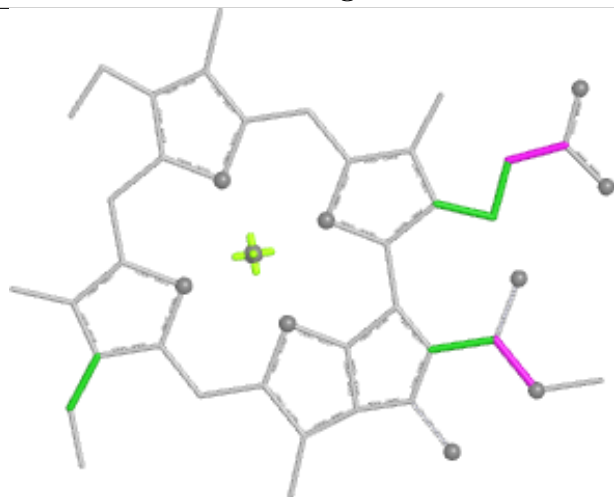
Ligand CLA J 101



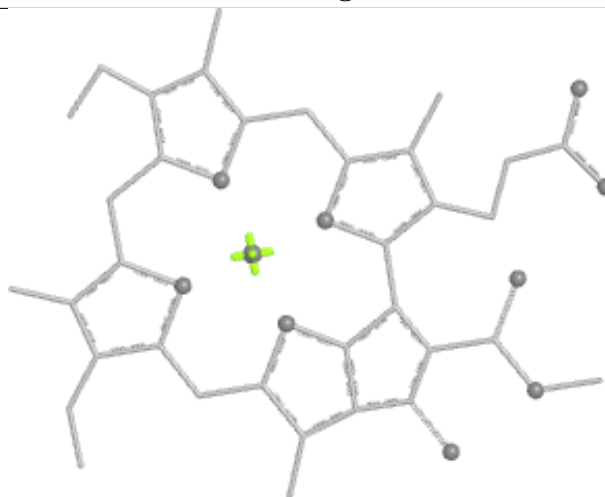
Bond lengths



Bond angles

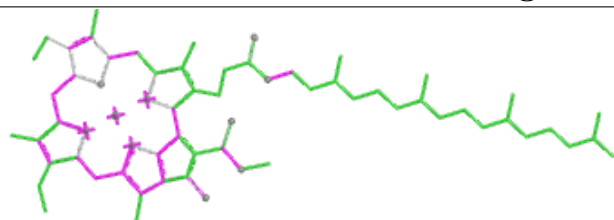


Torsions

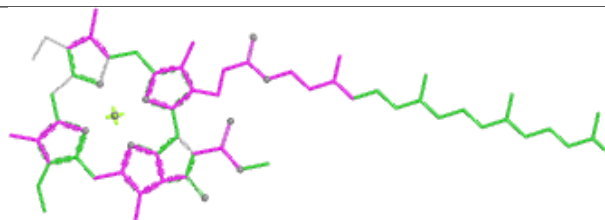


Rings

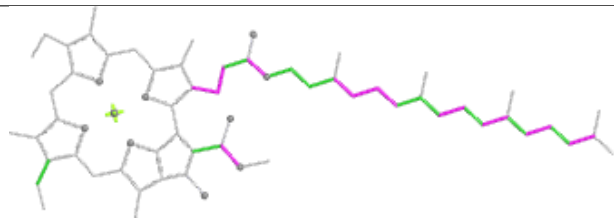
Ligand CLA a 819



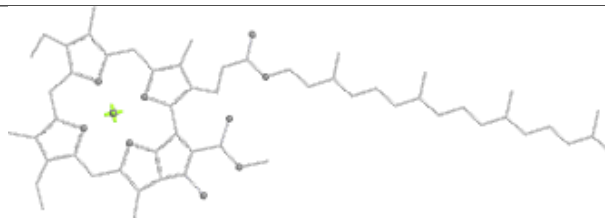
Bond lengths



Bond angles

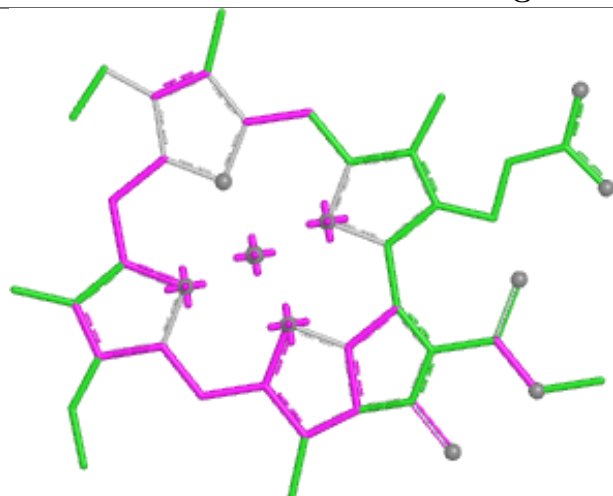


Torsions

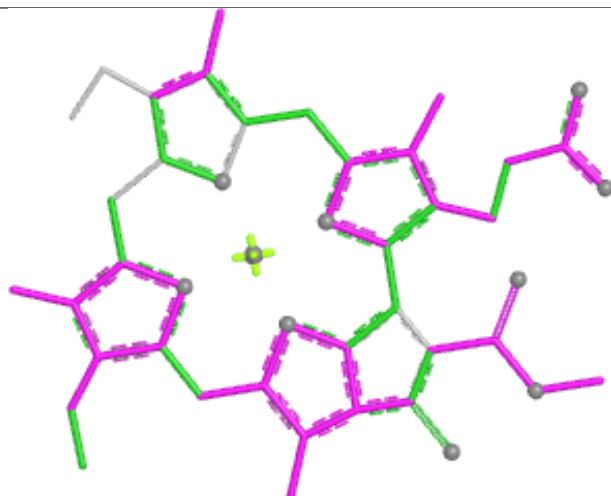


Rings

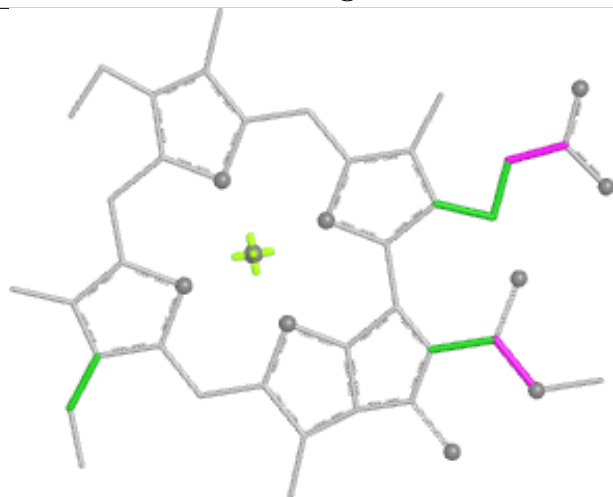
Ligand CLA A 808



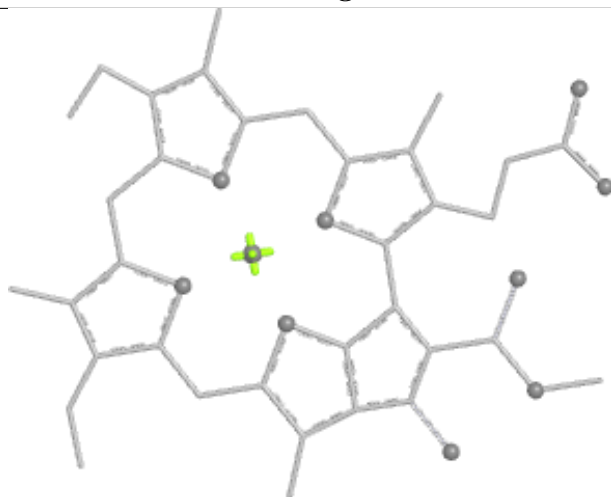
Bond lengths



Bond angles

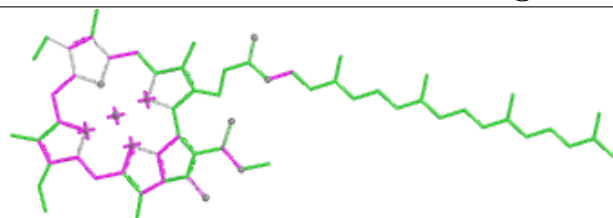


Torsions

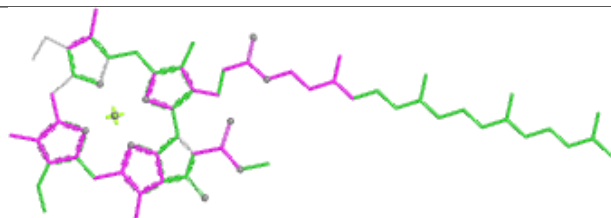


Rings

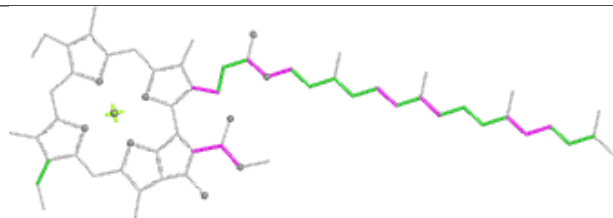
Ligand CLA A 831



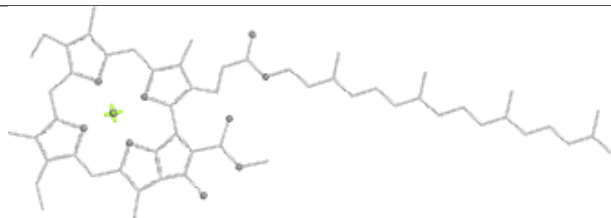
Bond lengths



Bond angles

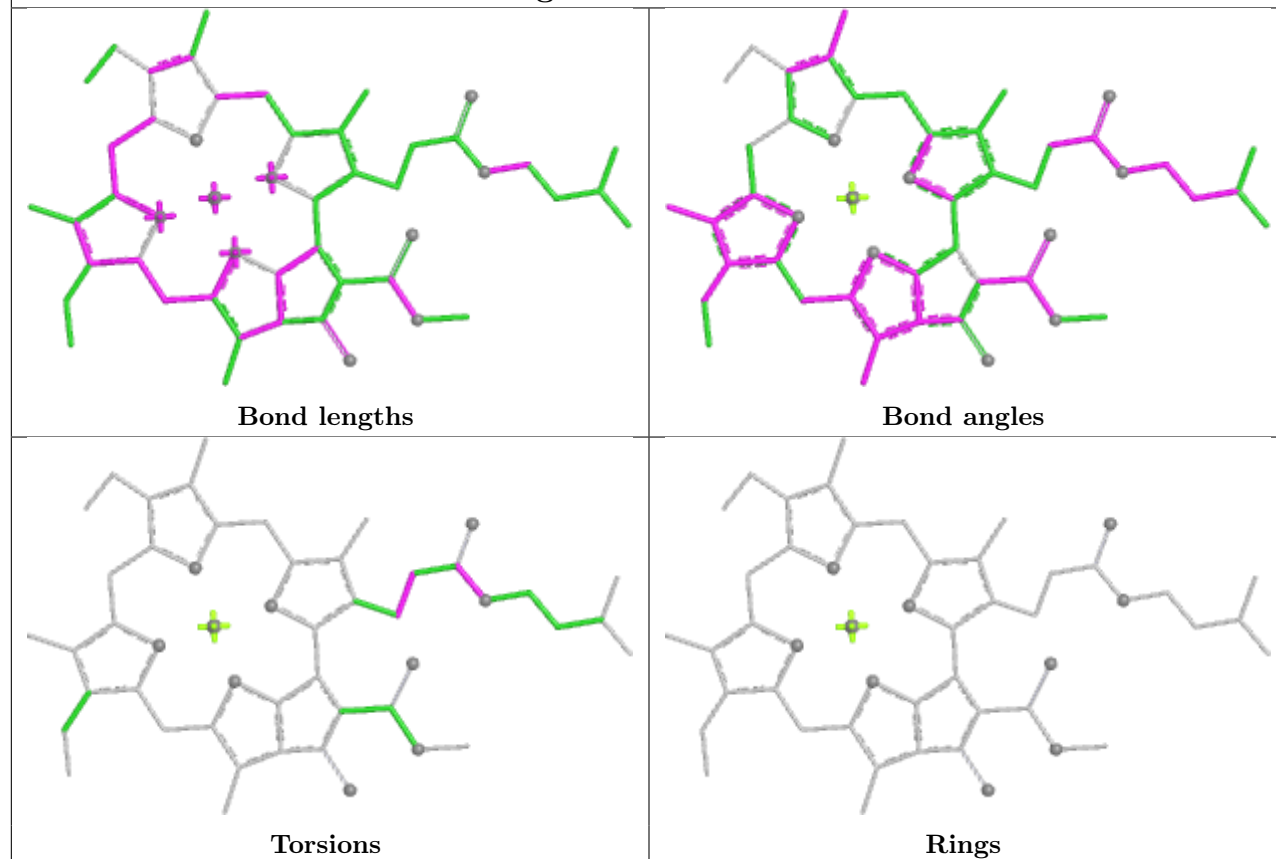


Torsions

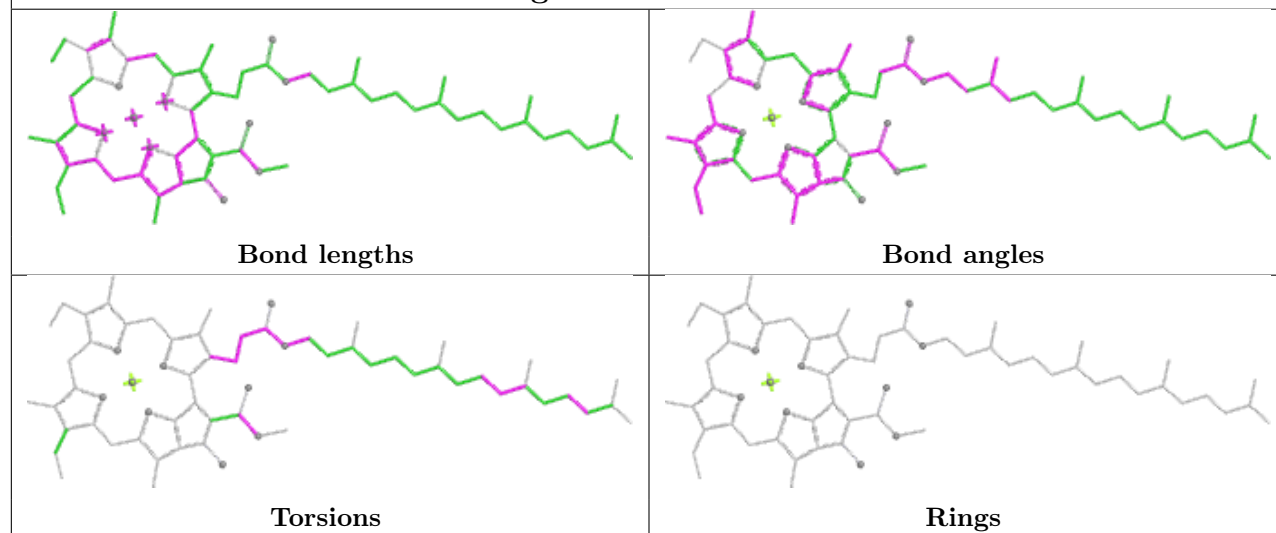


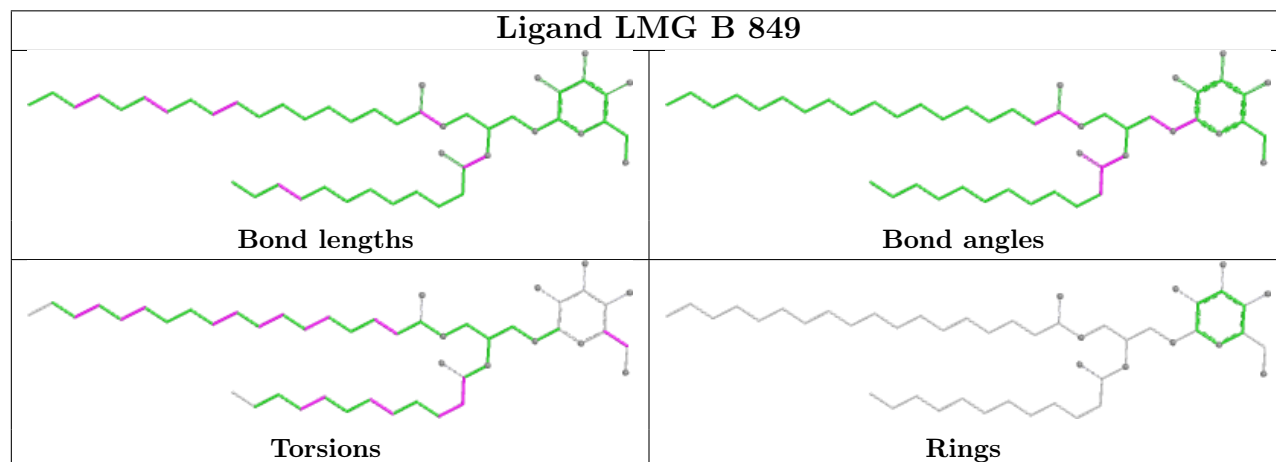
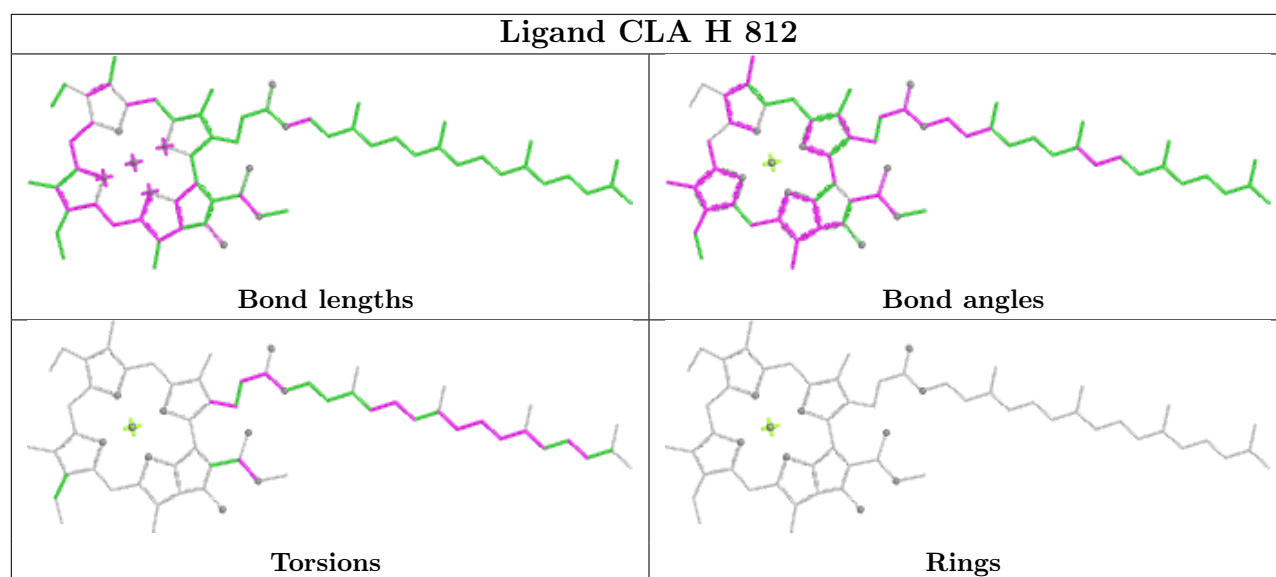
Rings

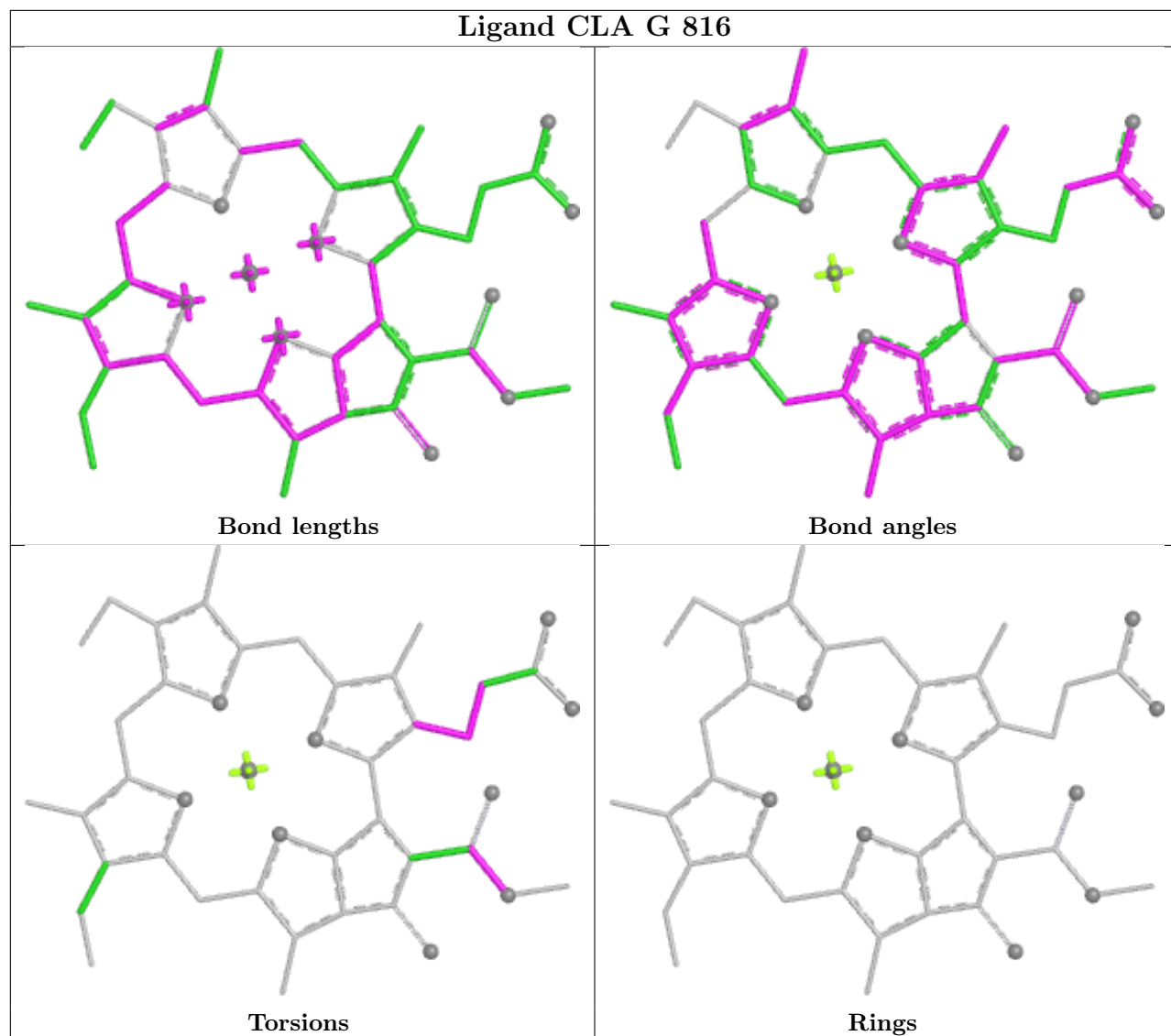
Ligand CLA a 831



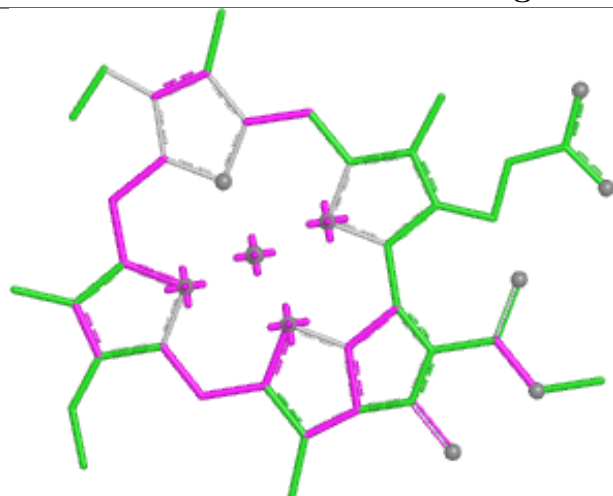
Ligand CLA G 812



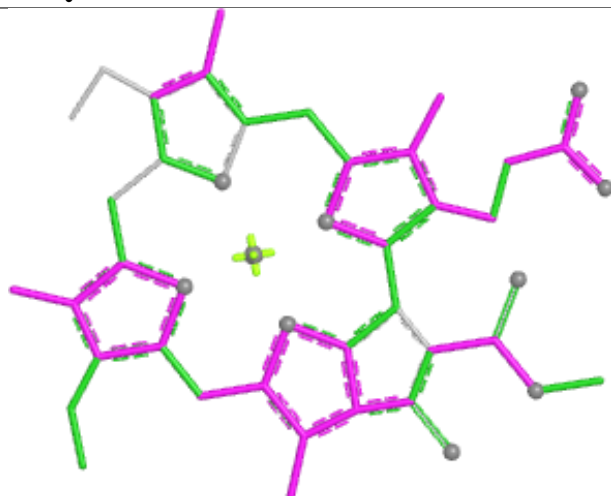




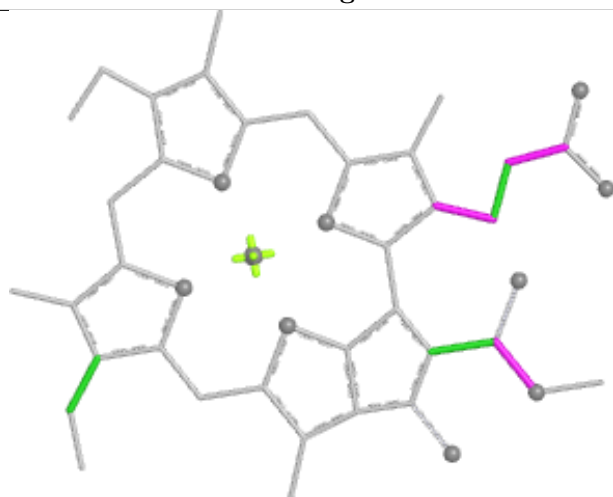
Ligand CLA Q 201



Bond lengths



Bond angles

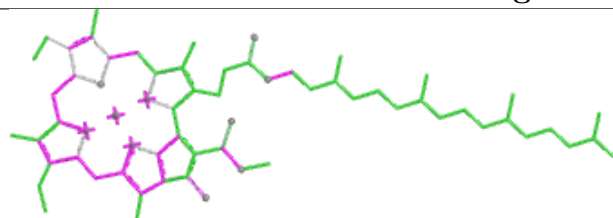


Torsions

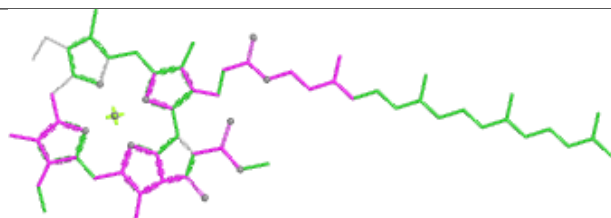


Rings

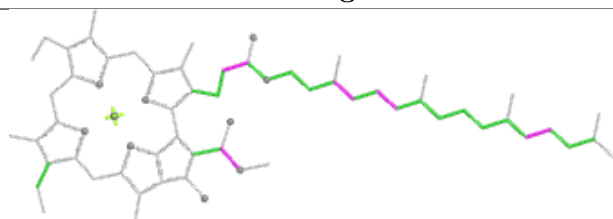
Ligand CLA H 807



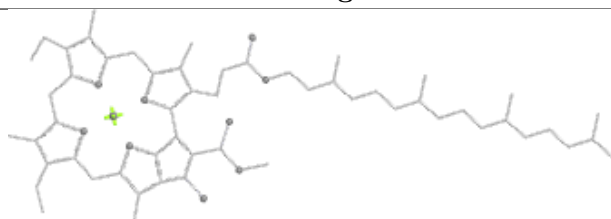
Bond lengths



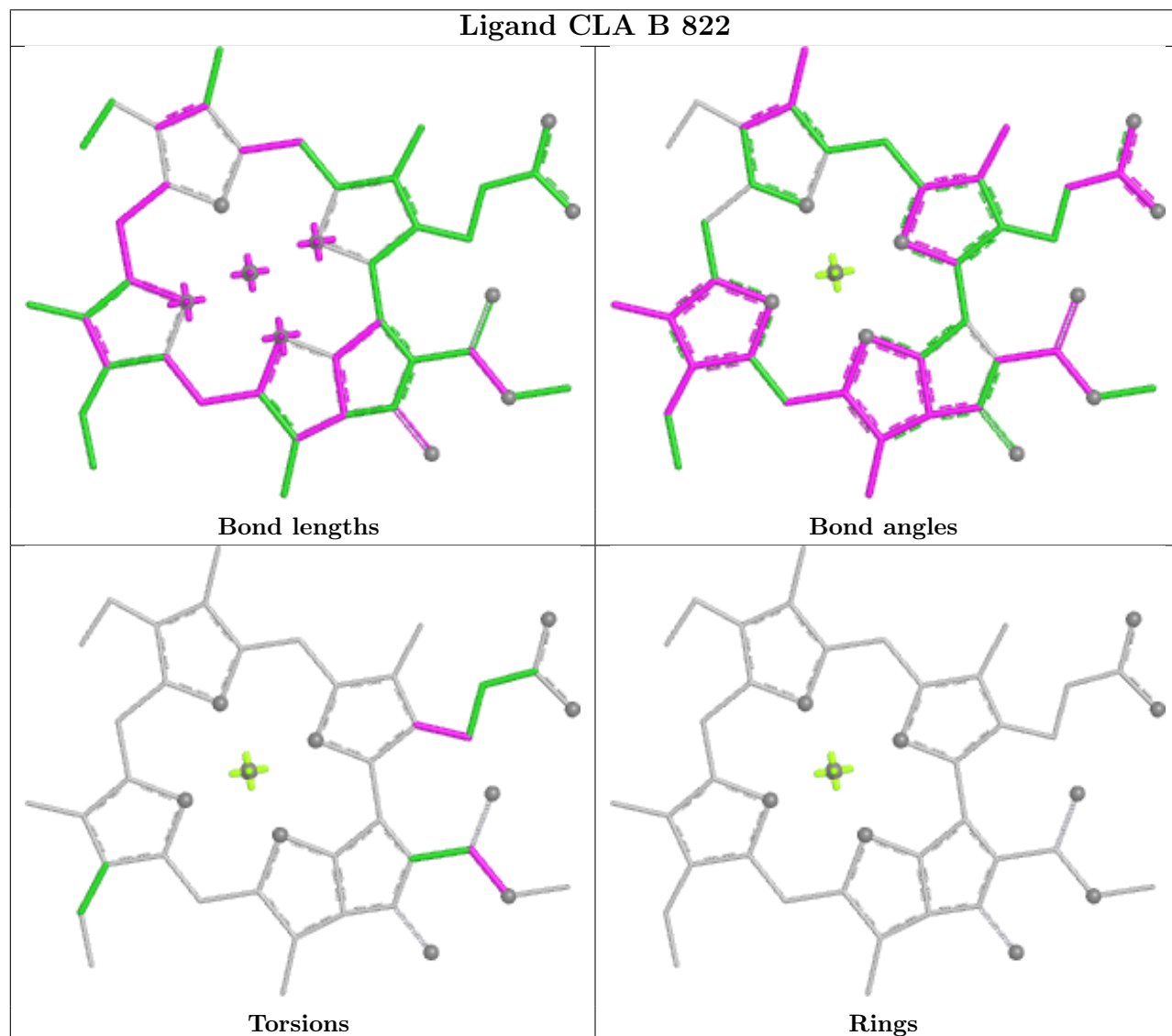
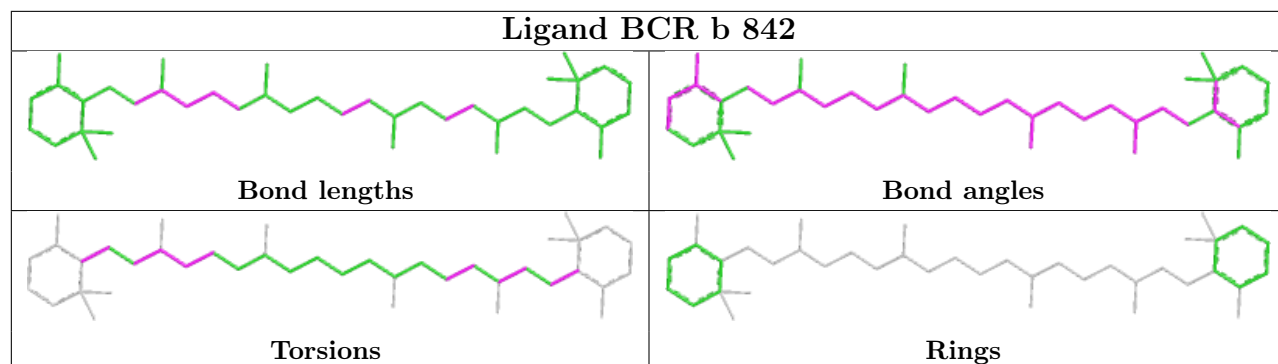
Bond angles

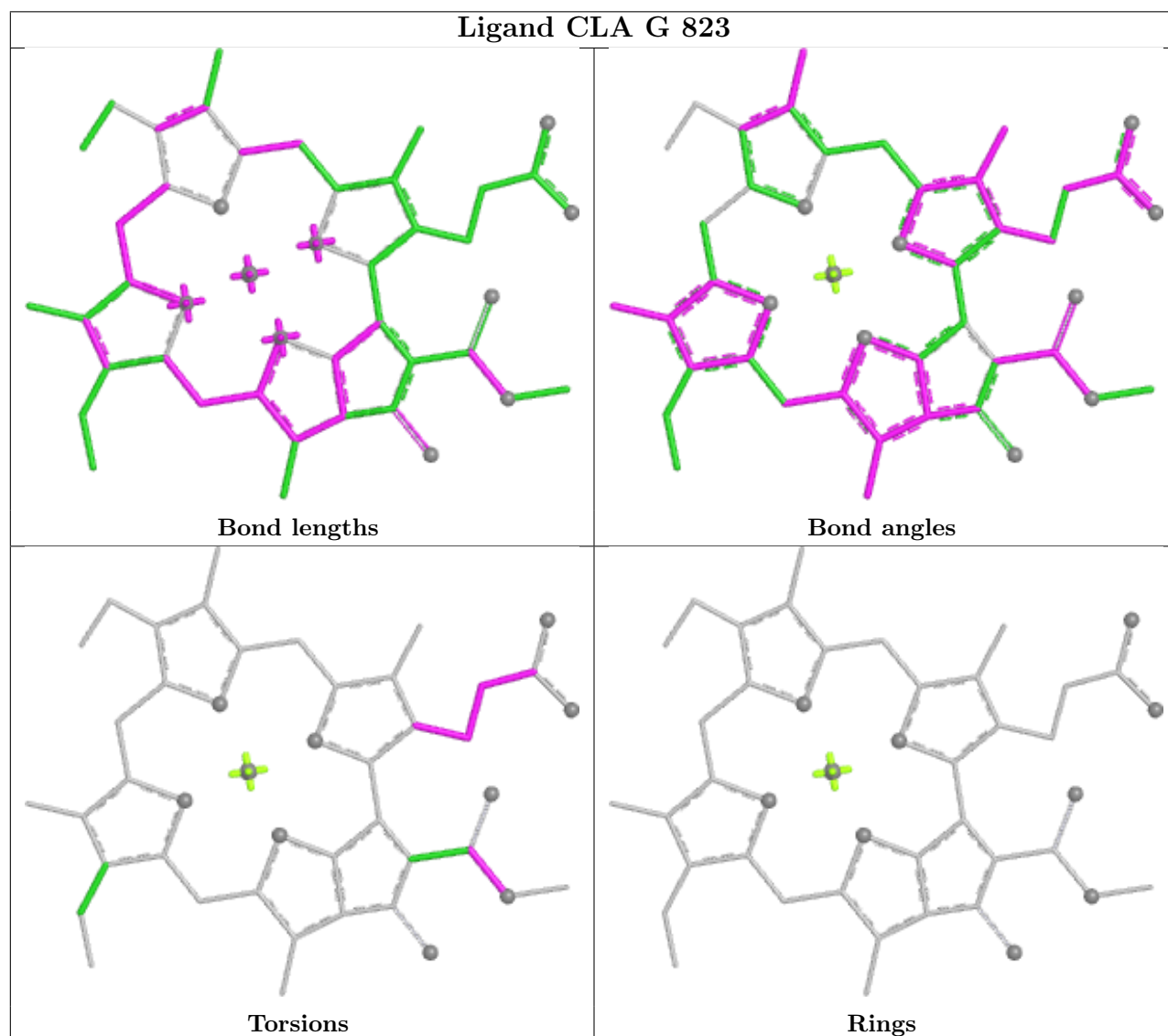
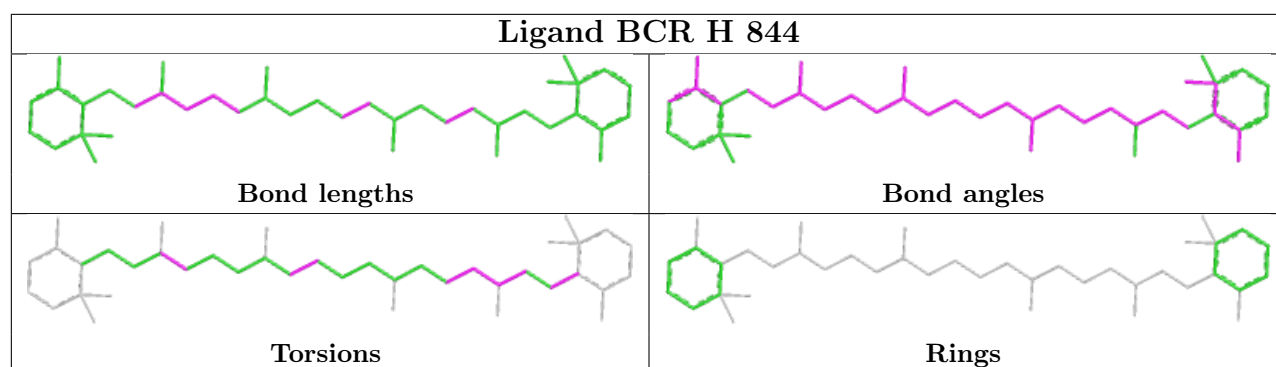


Torsions

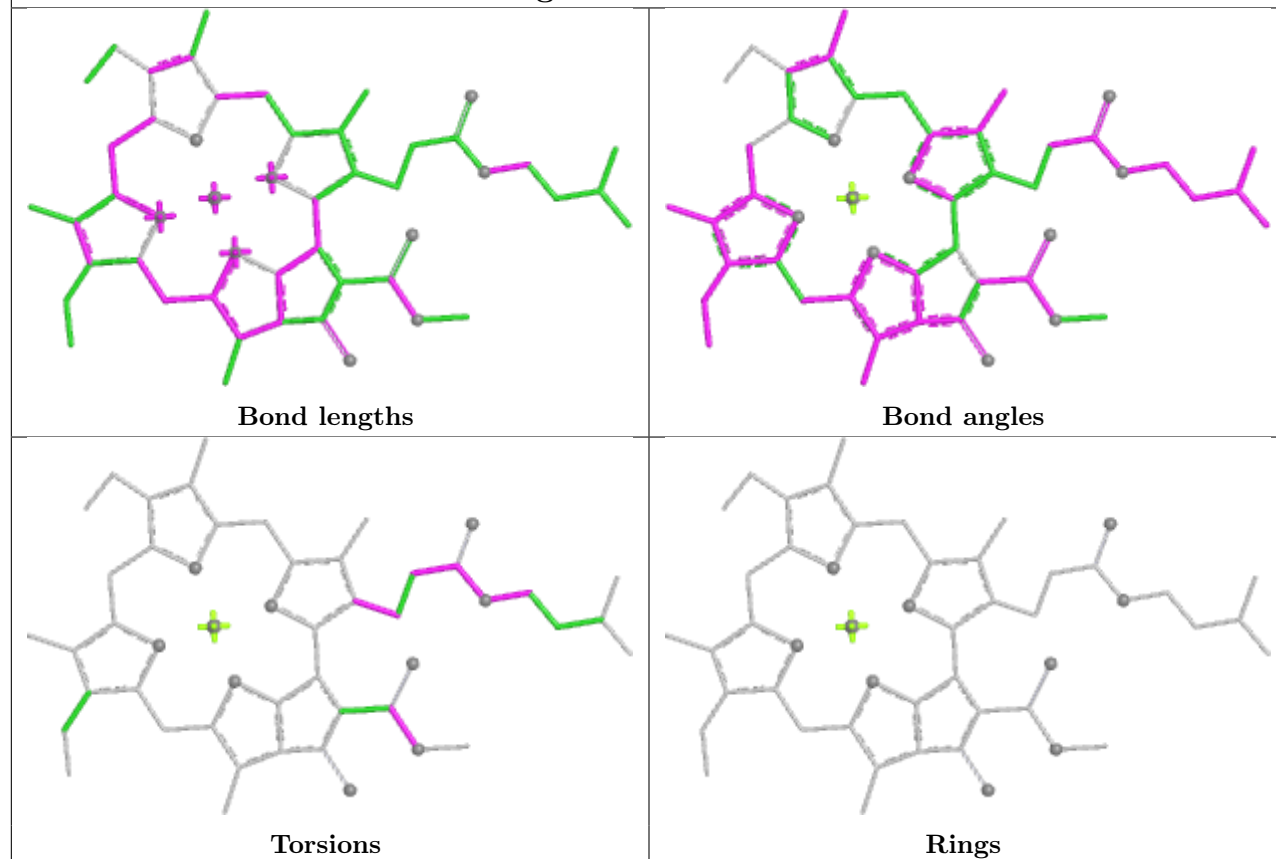


Rings

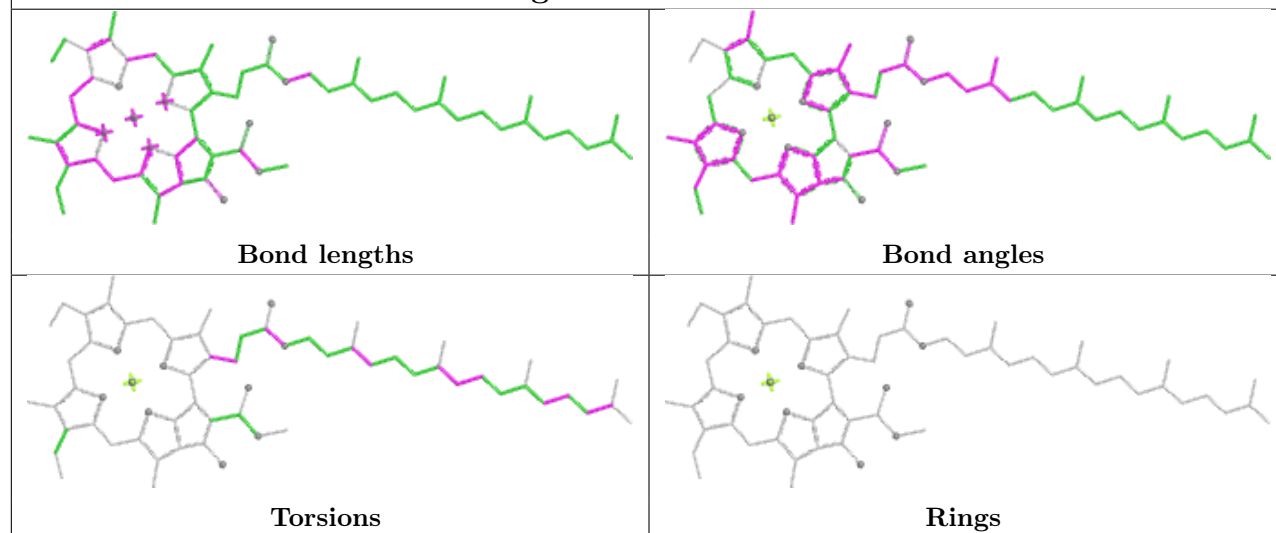




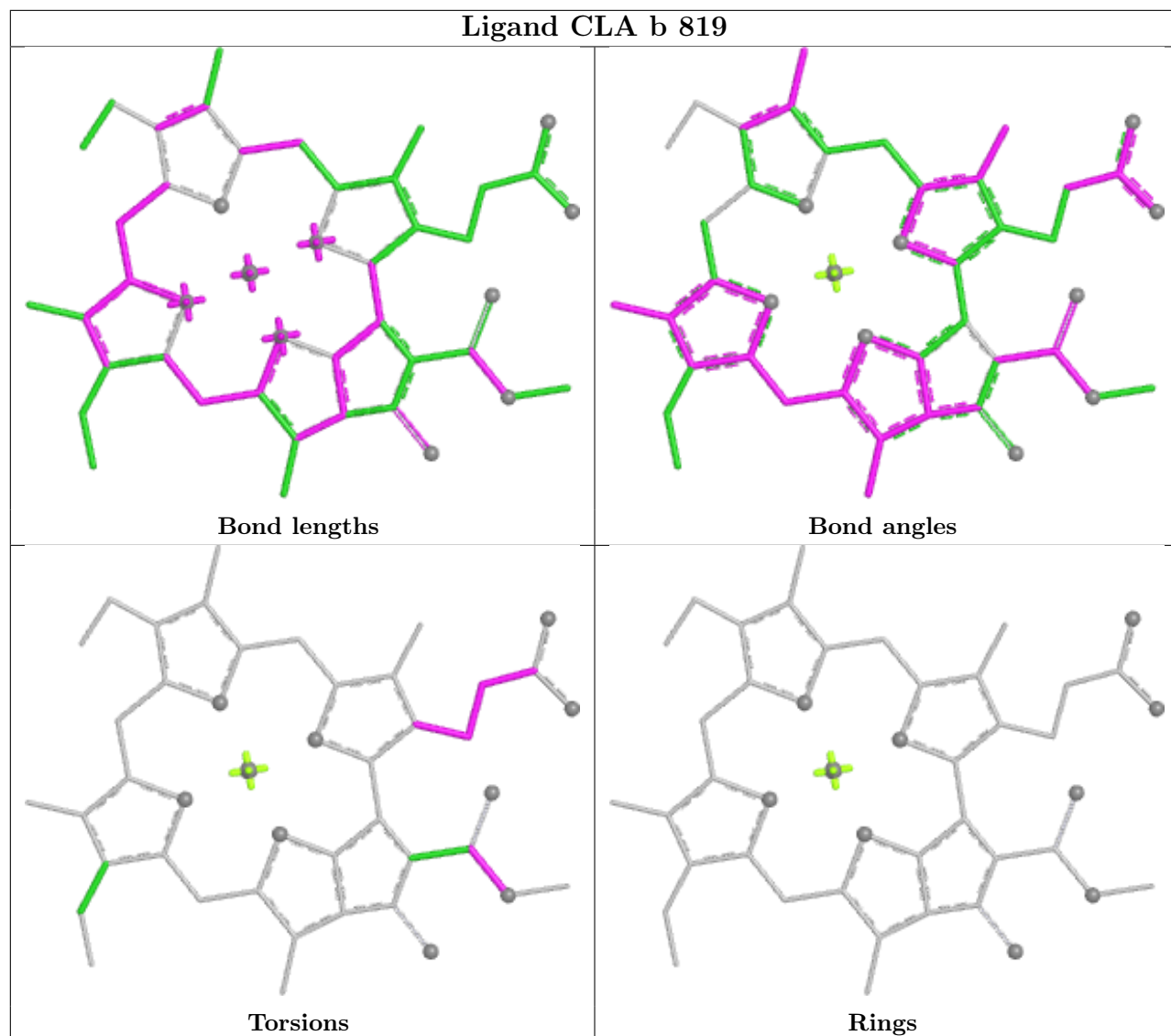
Ligand CLA a 820



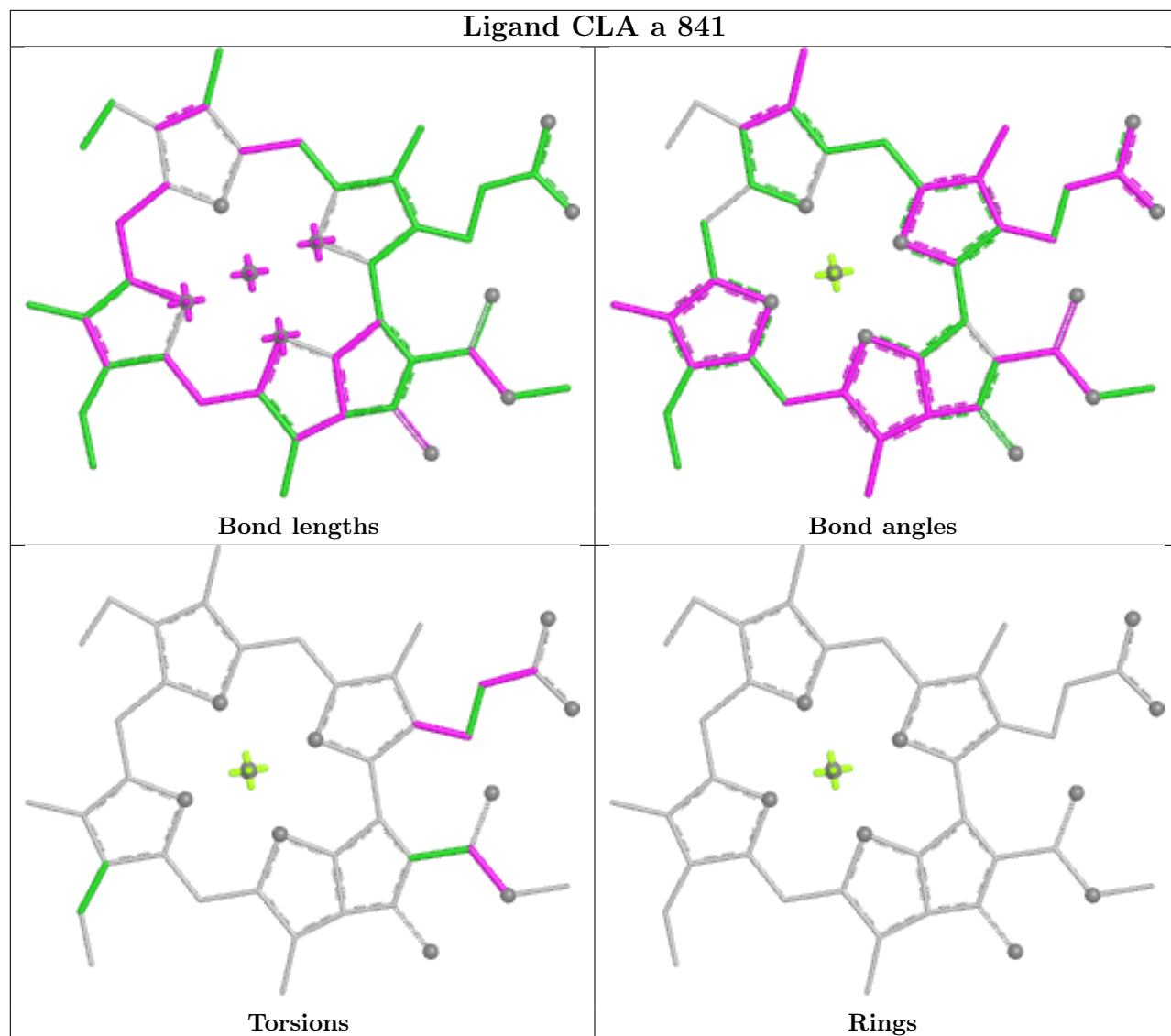
Ligand CLA U 205

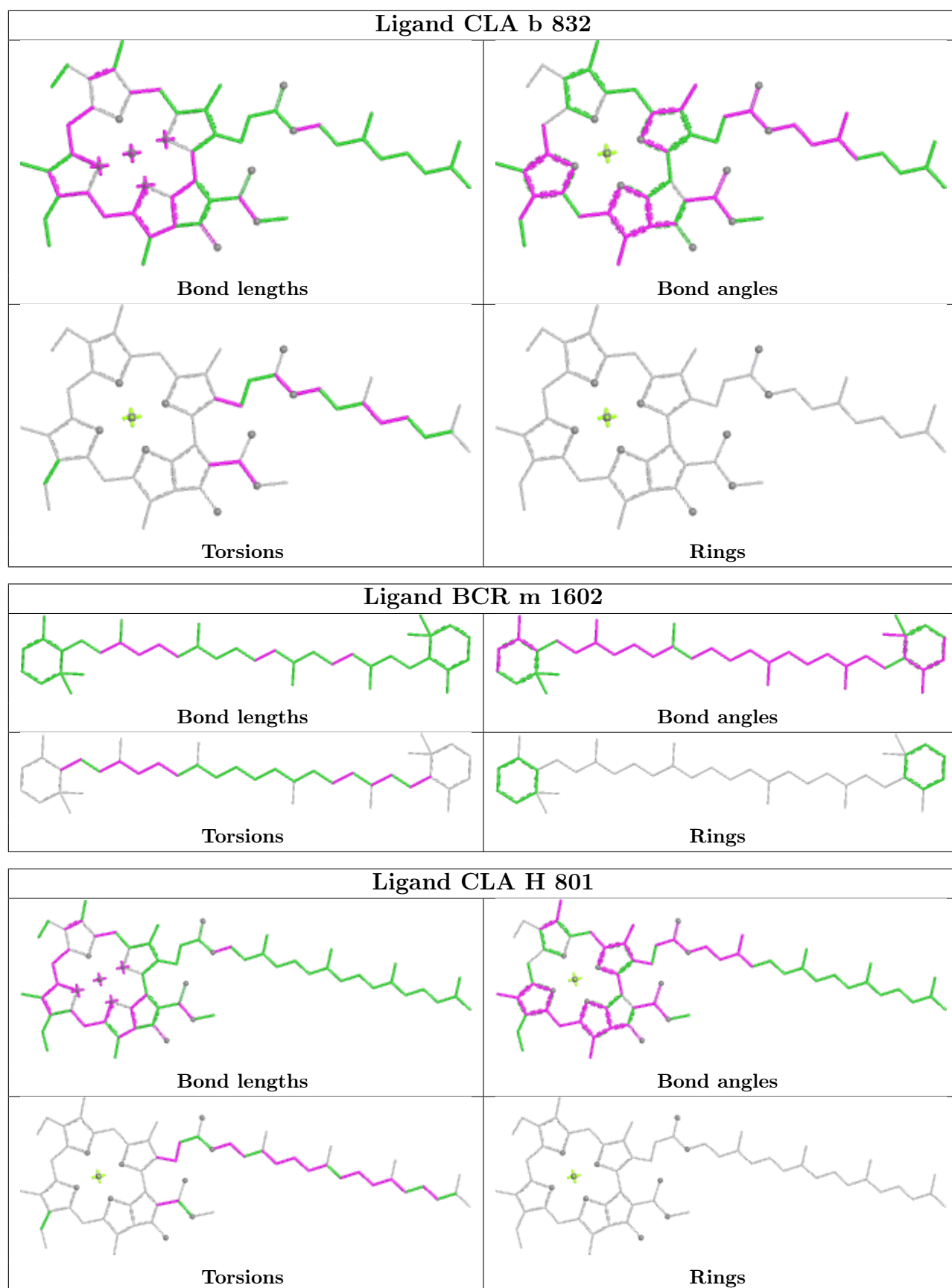


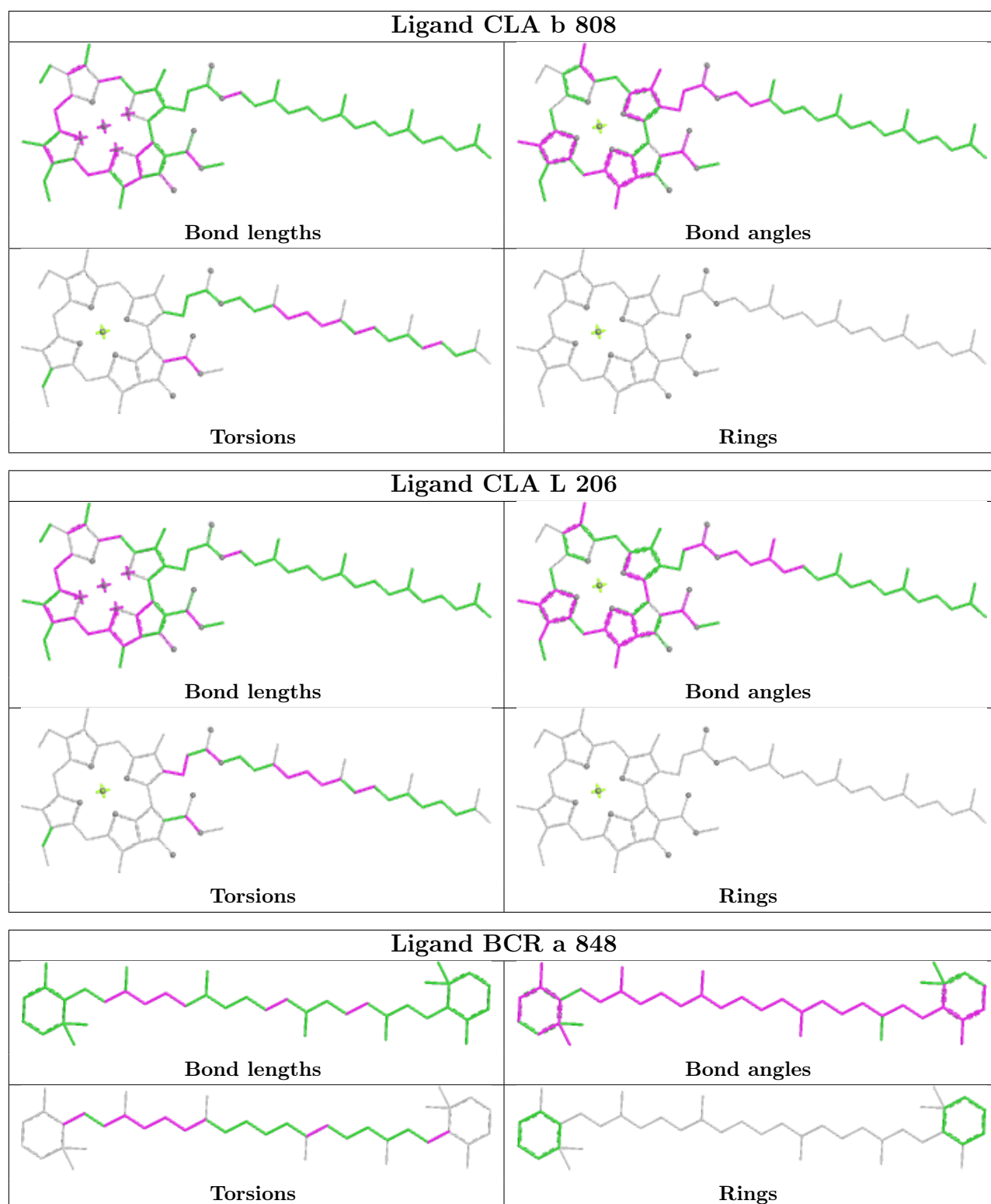
Ligand CLA b 819

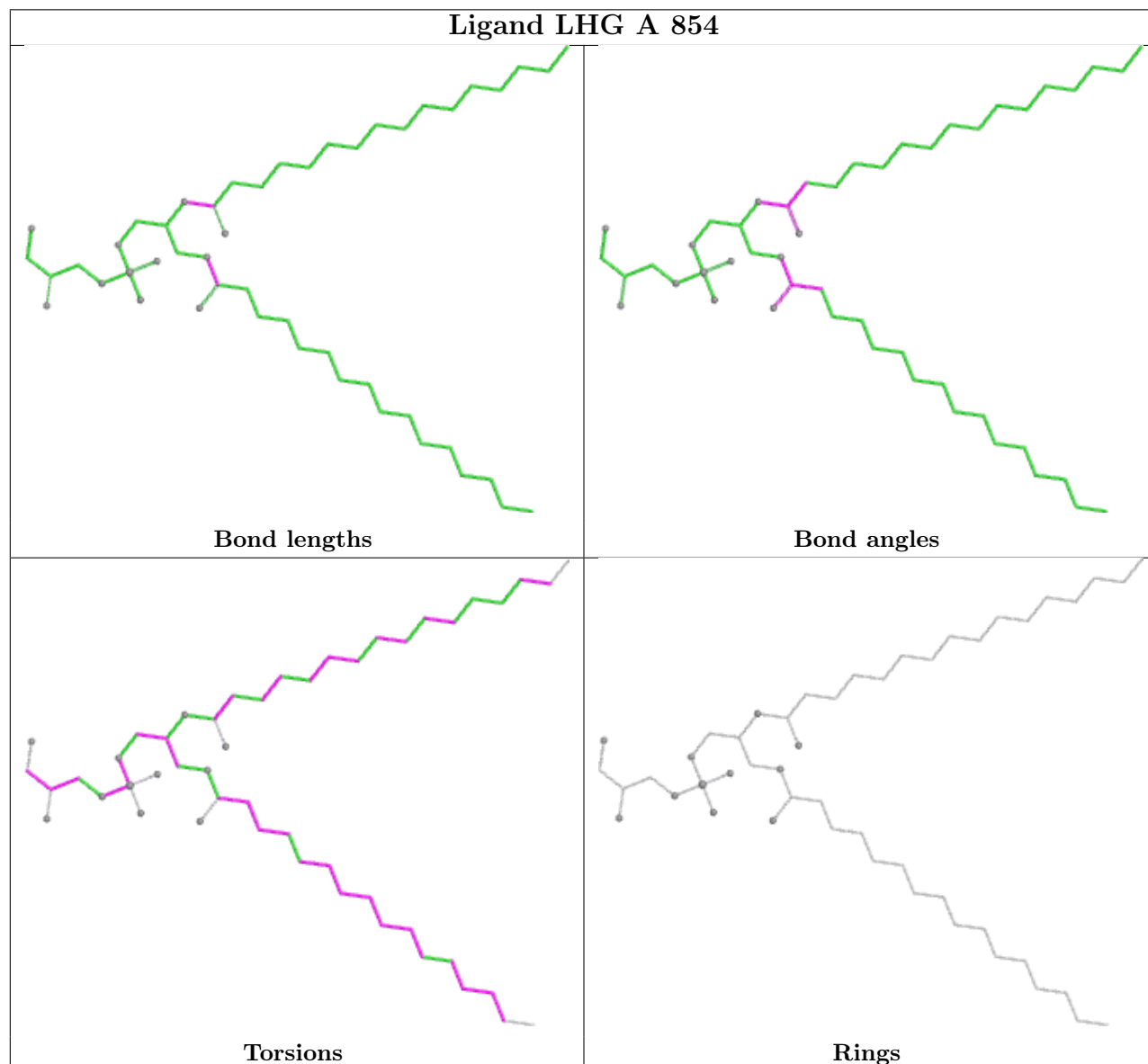
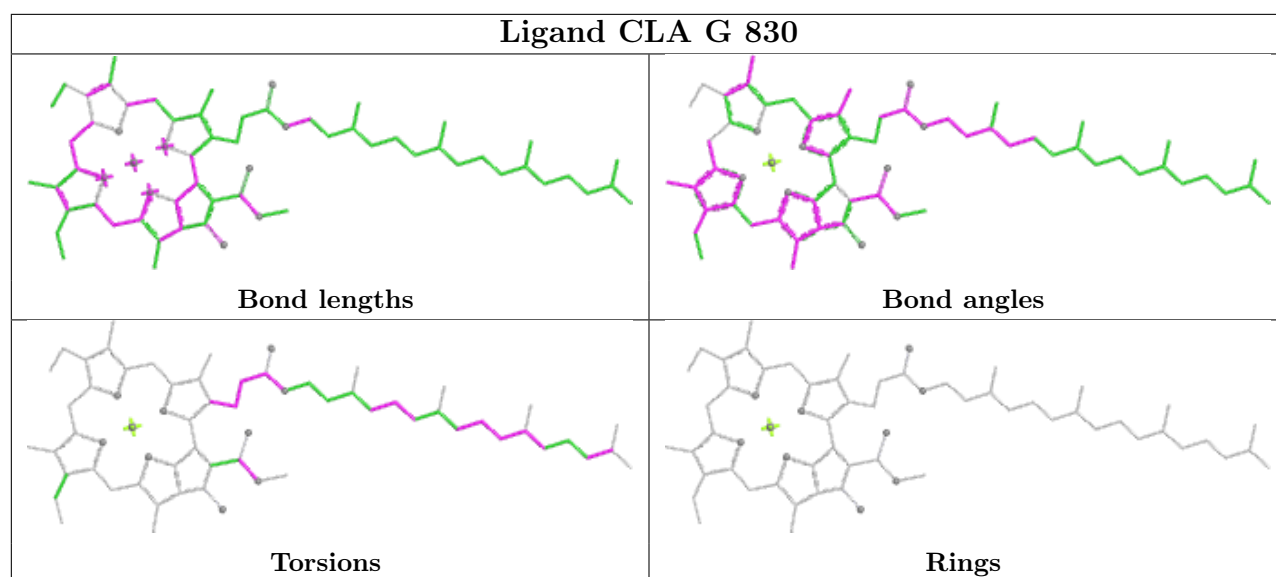


Ligand CLA a 841

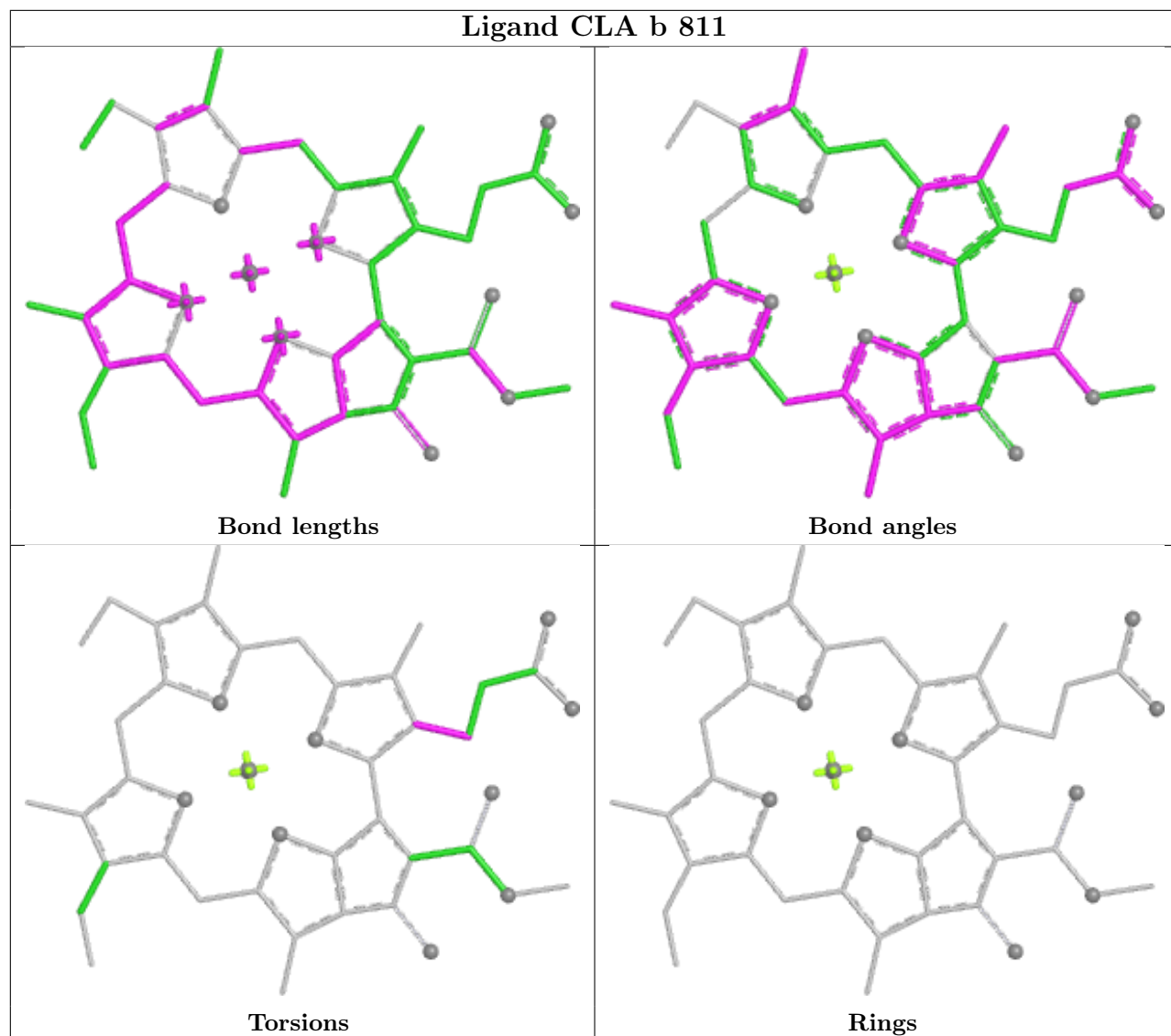




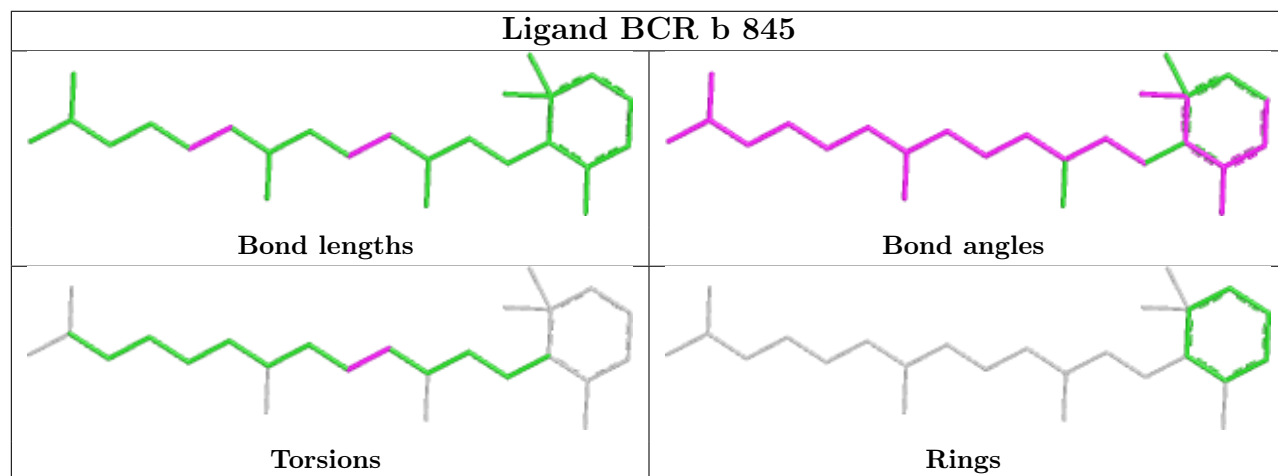


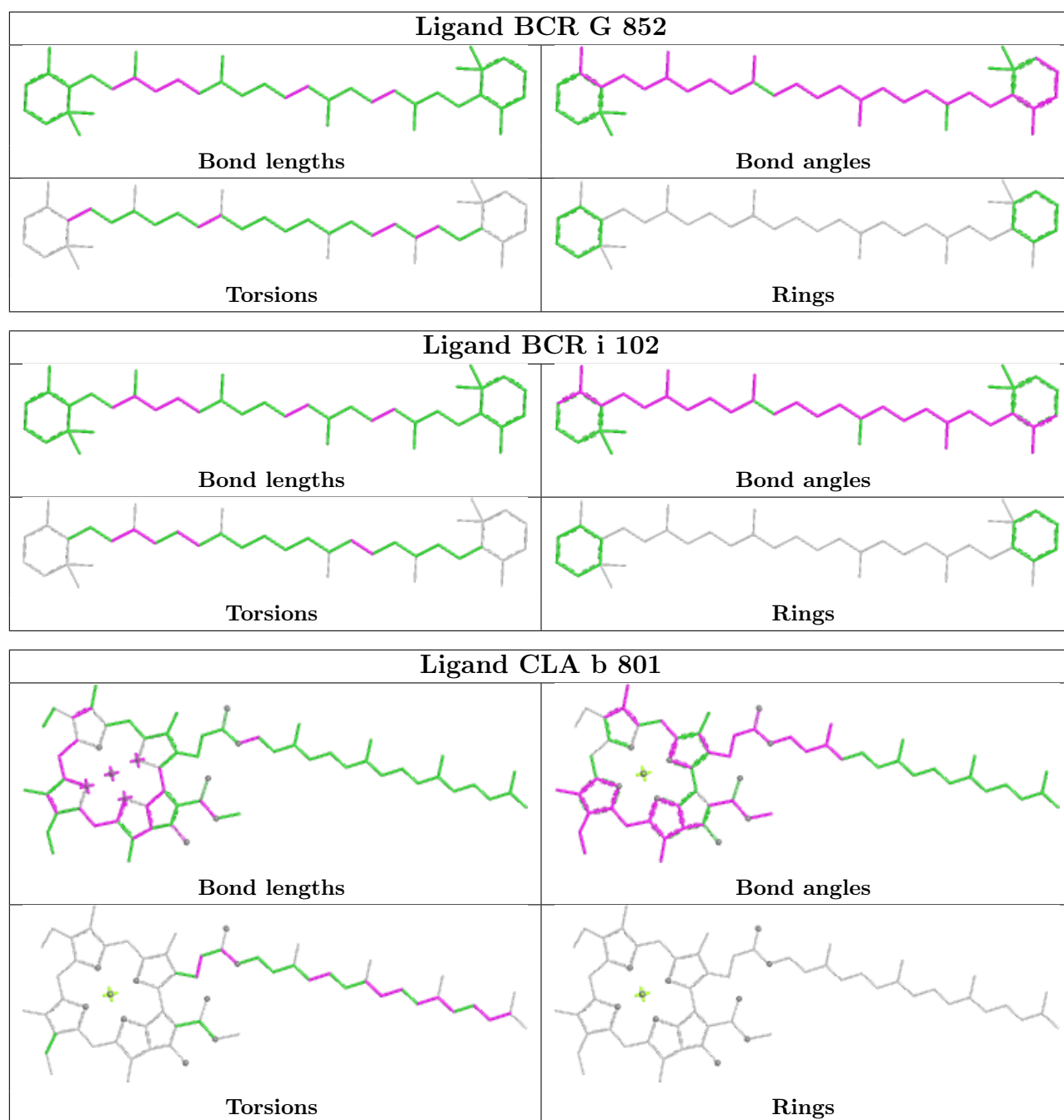


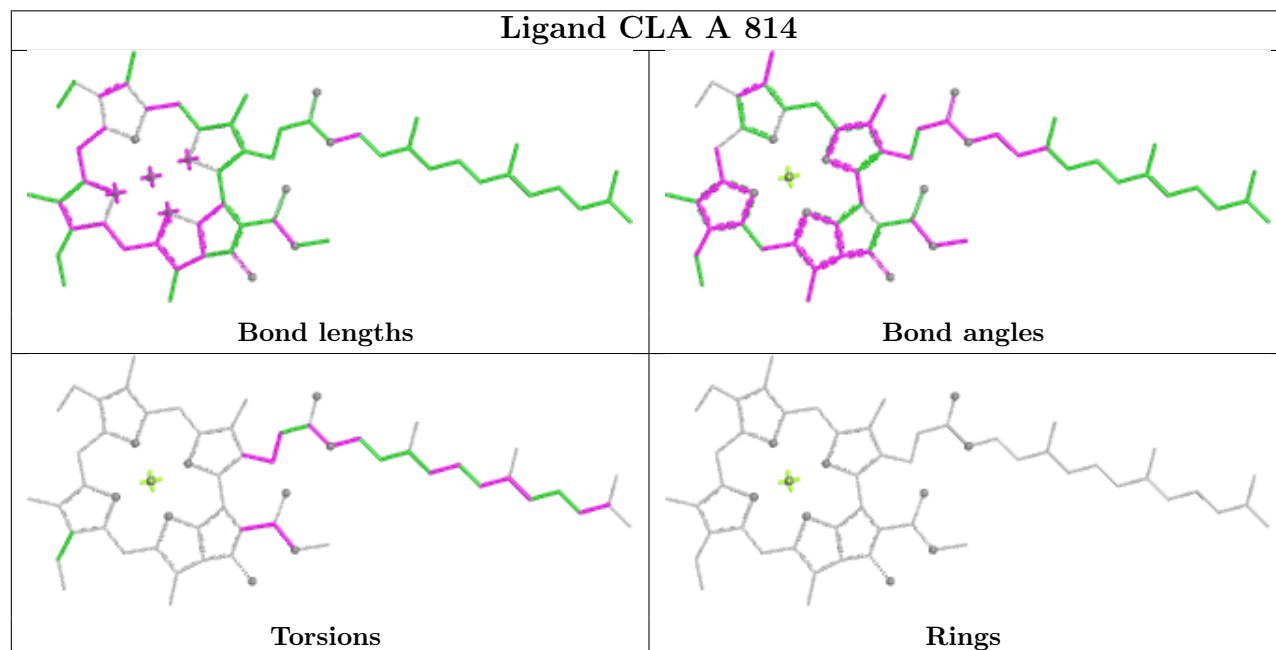
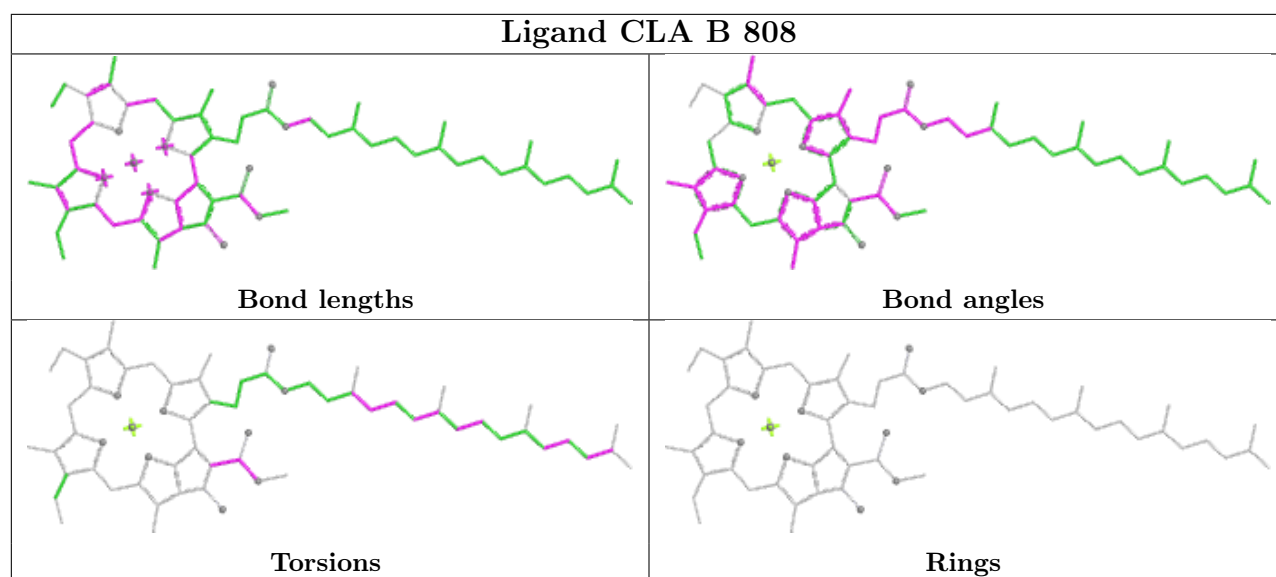
Ligand CLA b 811

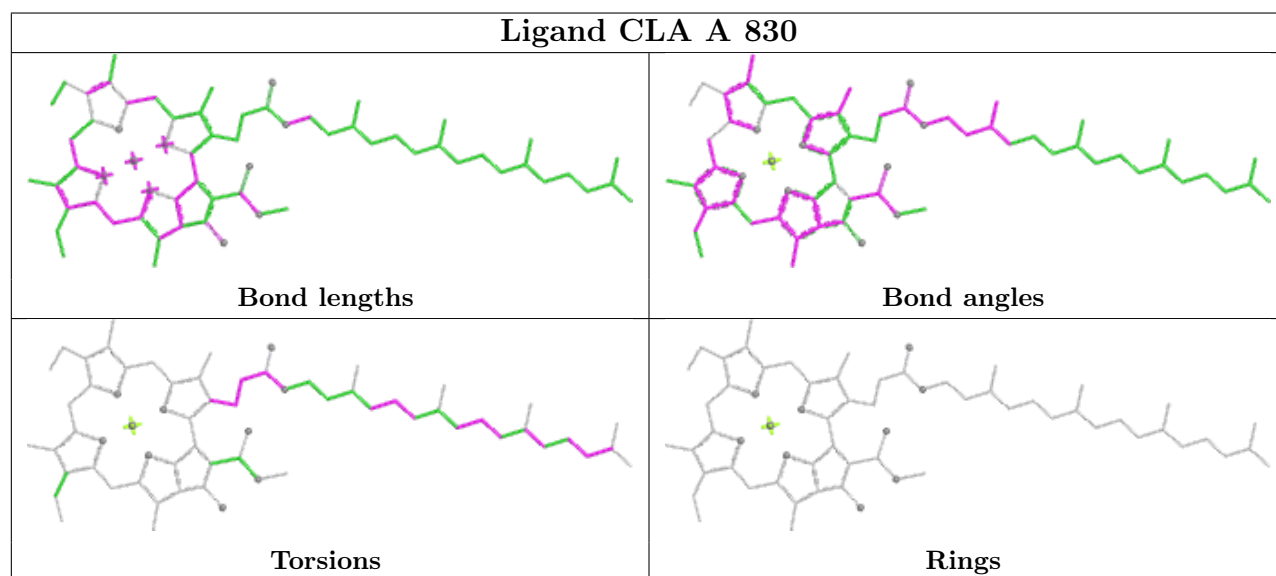
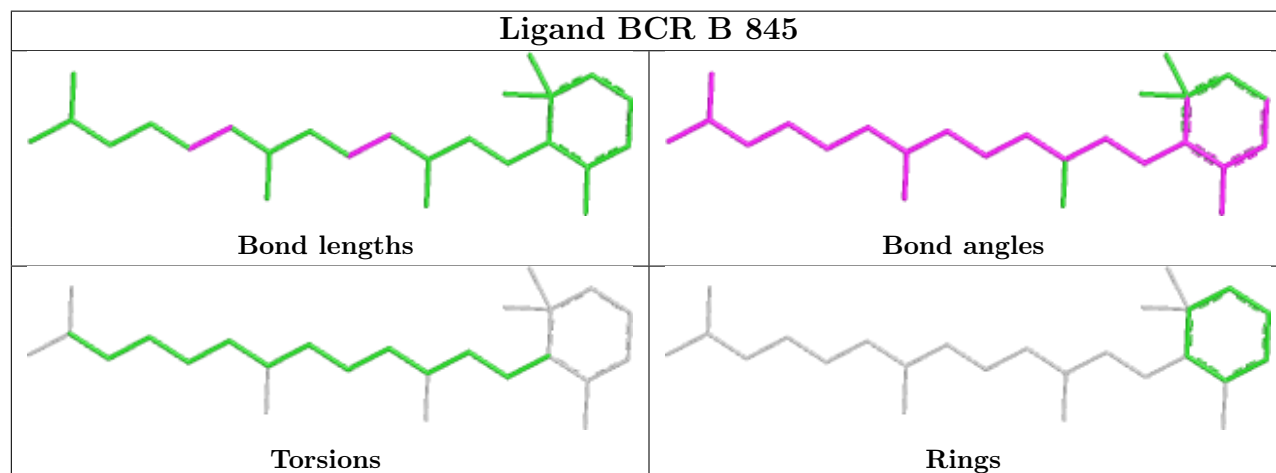
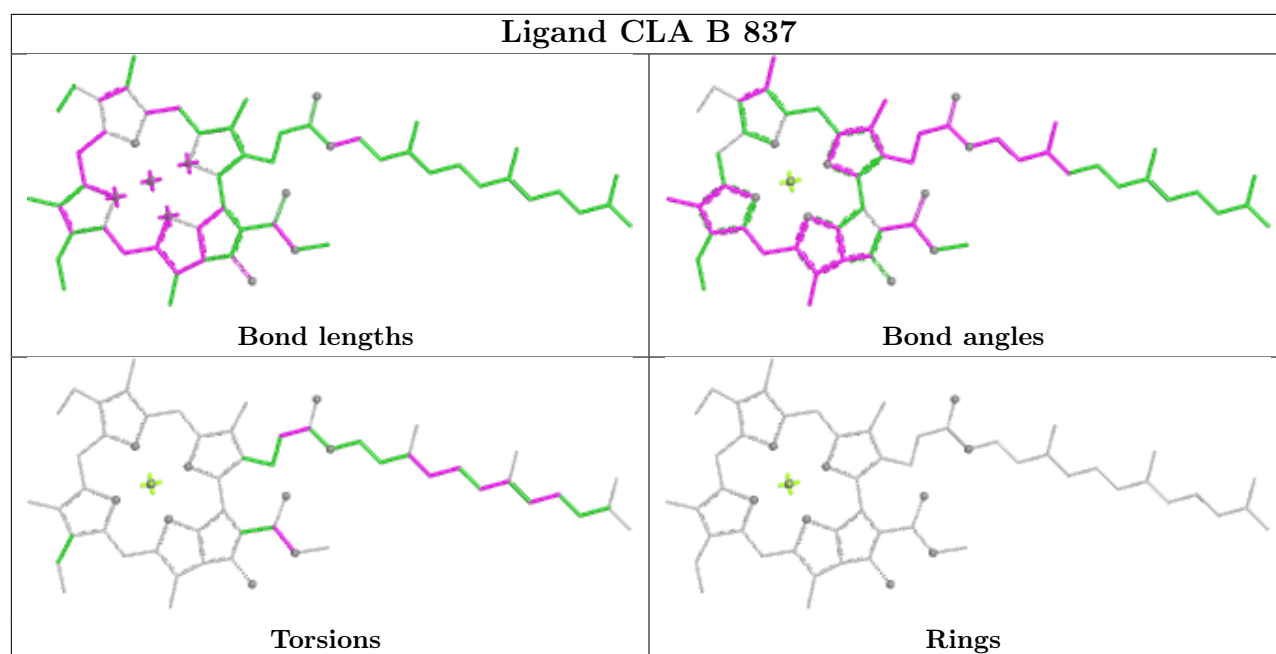


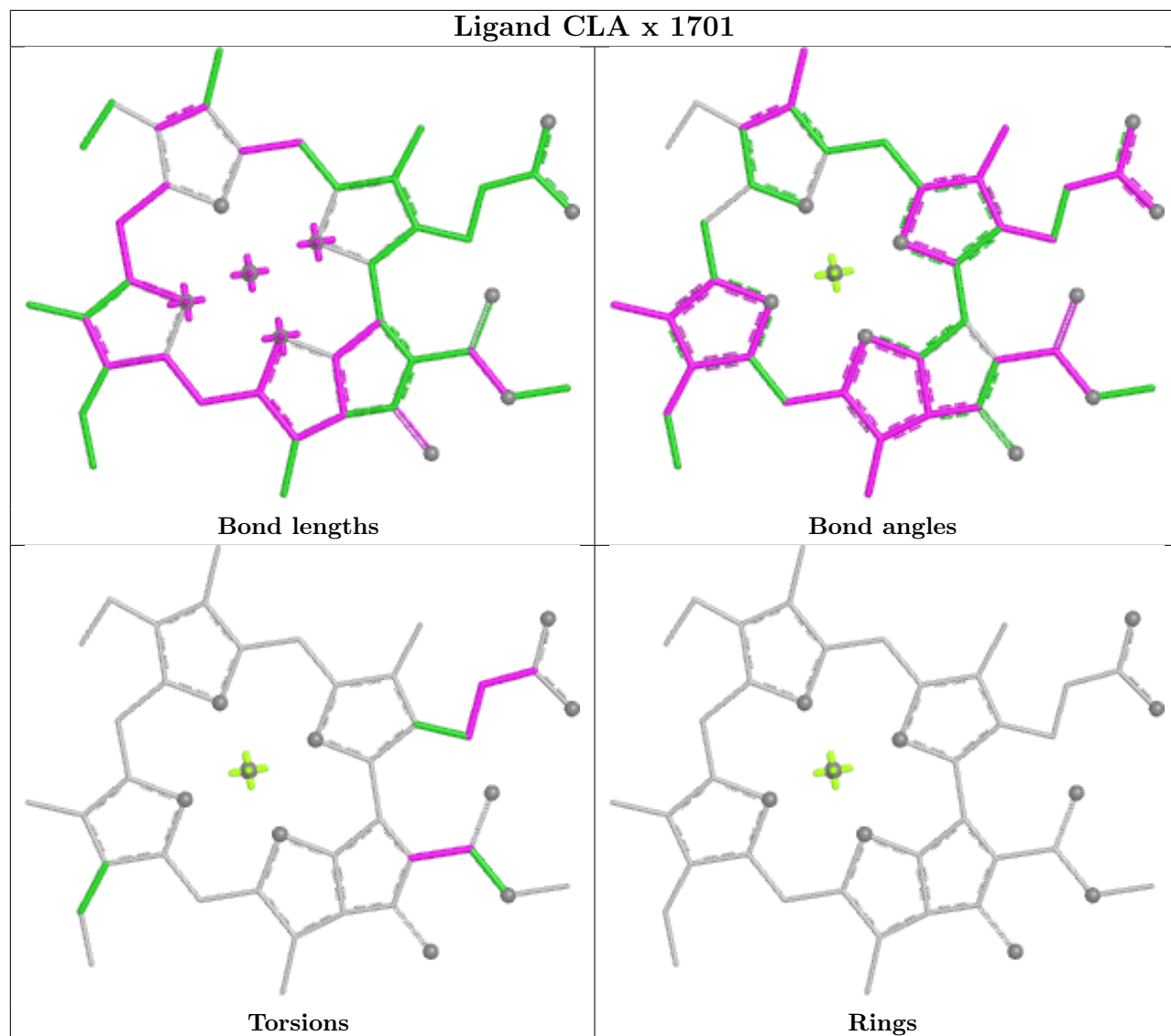
Ligand BCR b 845



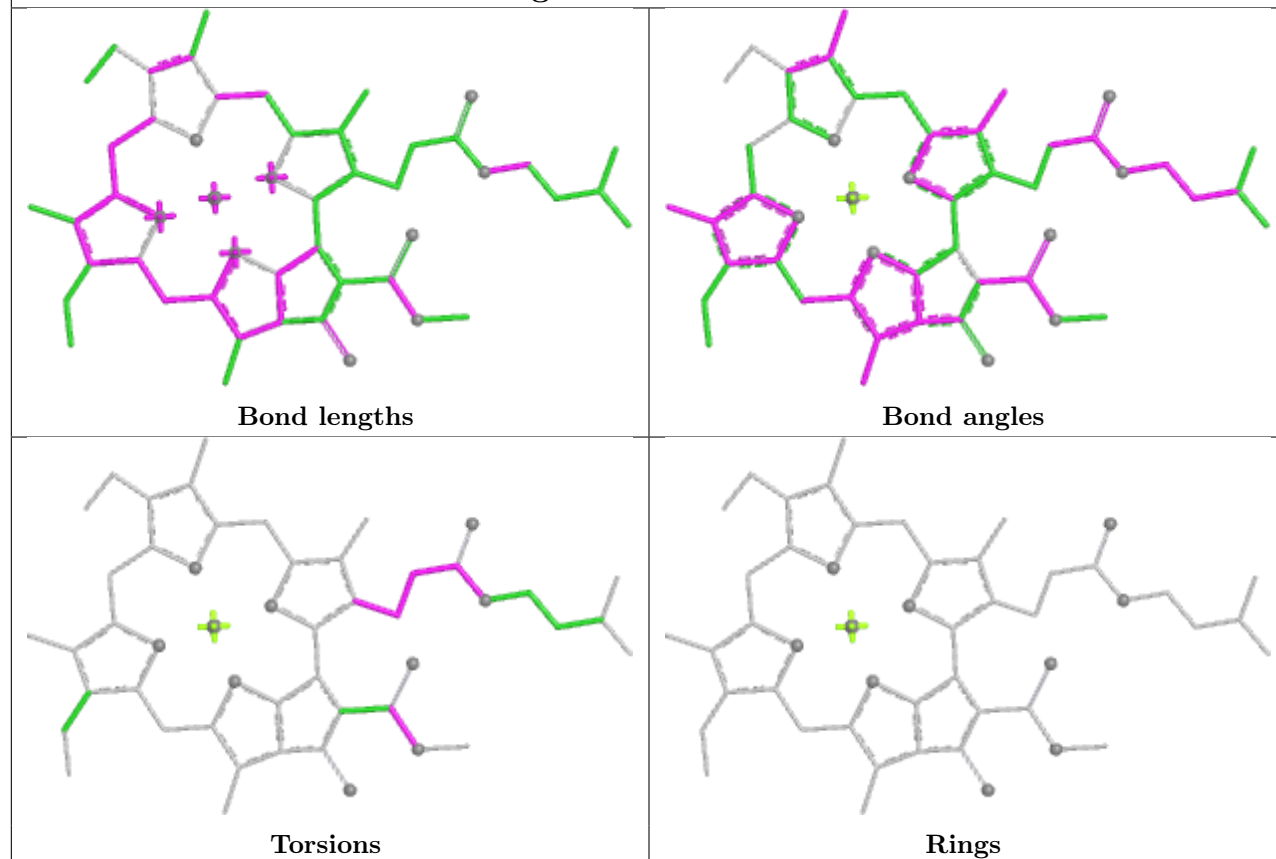




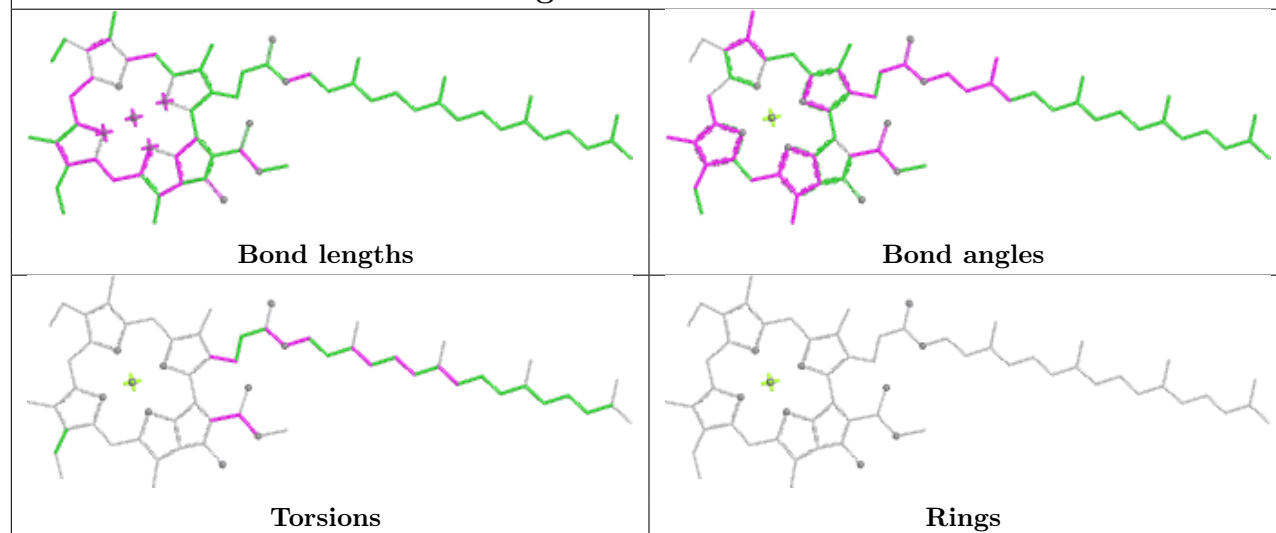




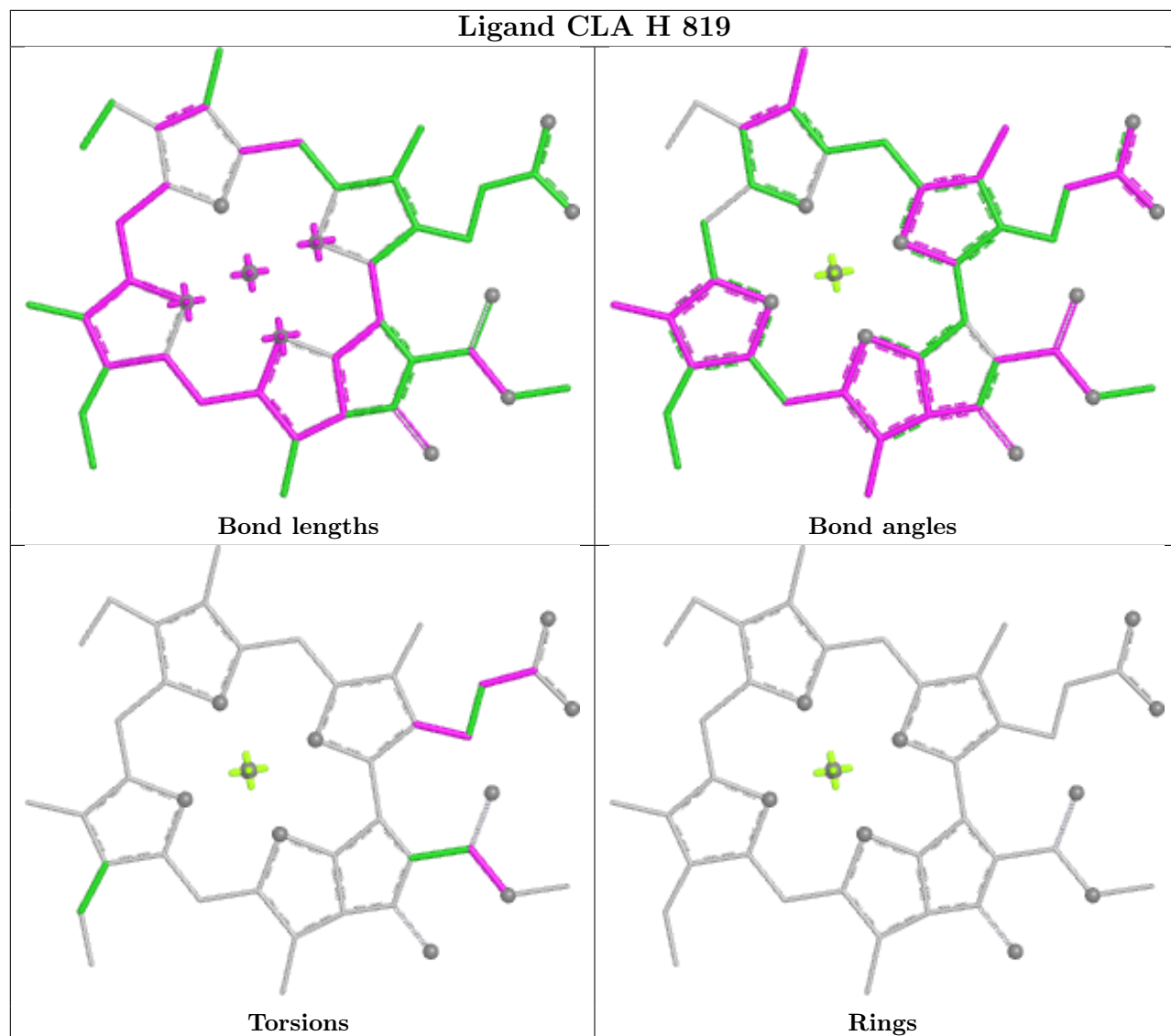
Ligand CLA A 819



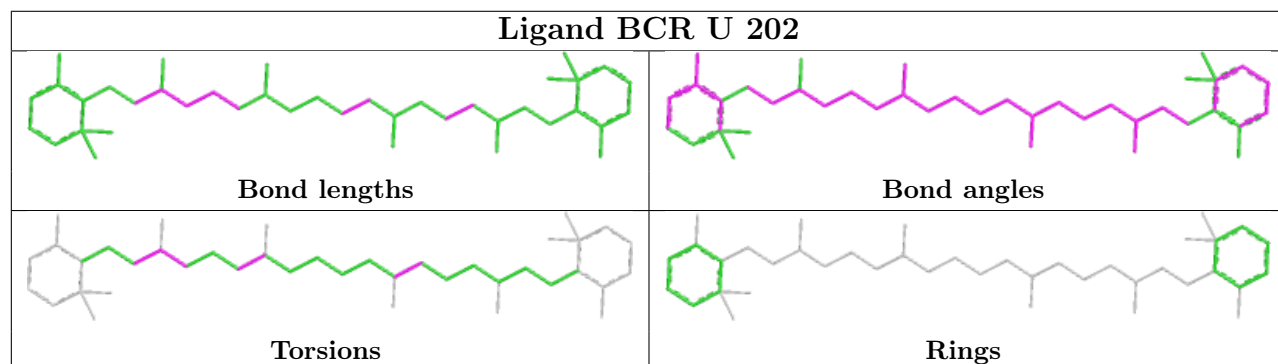
Ligand CLA a 830

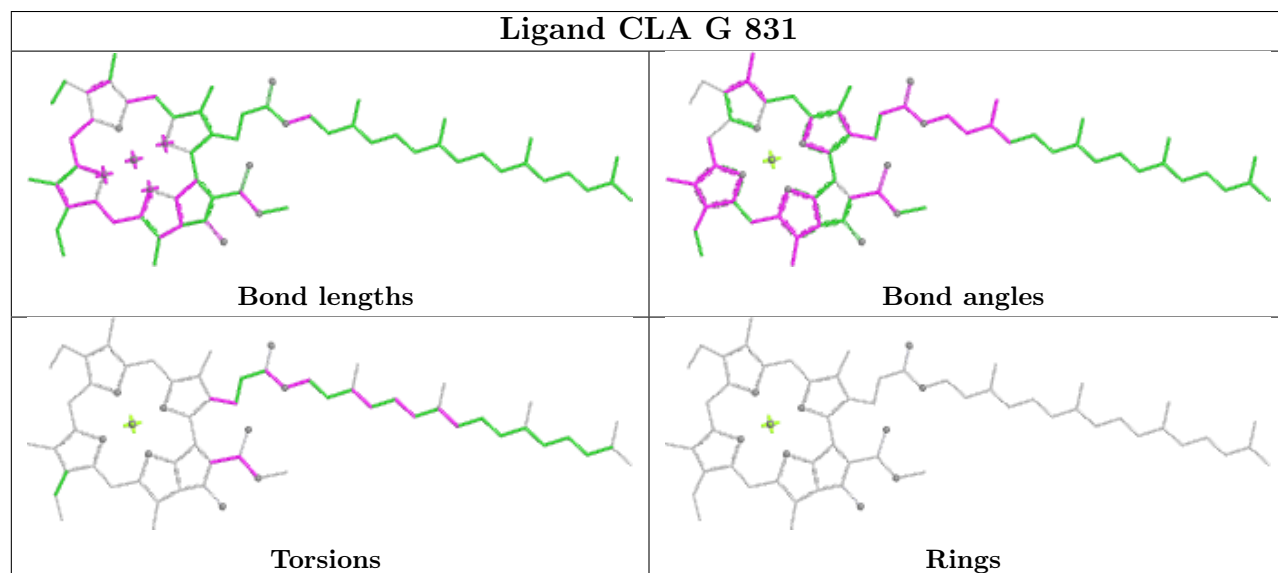
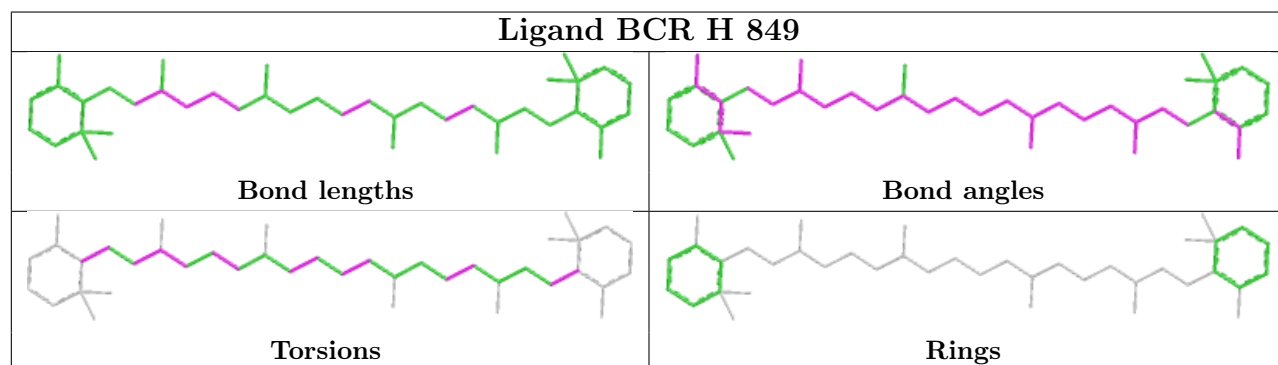
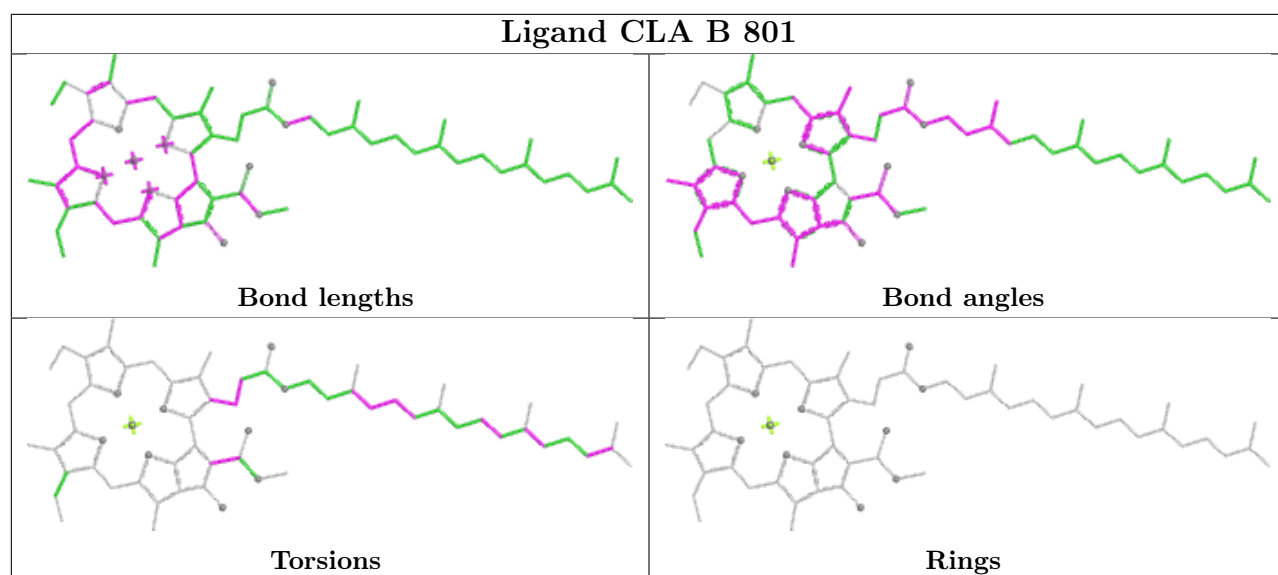


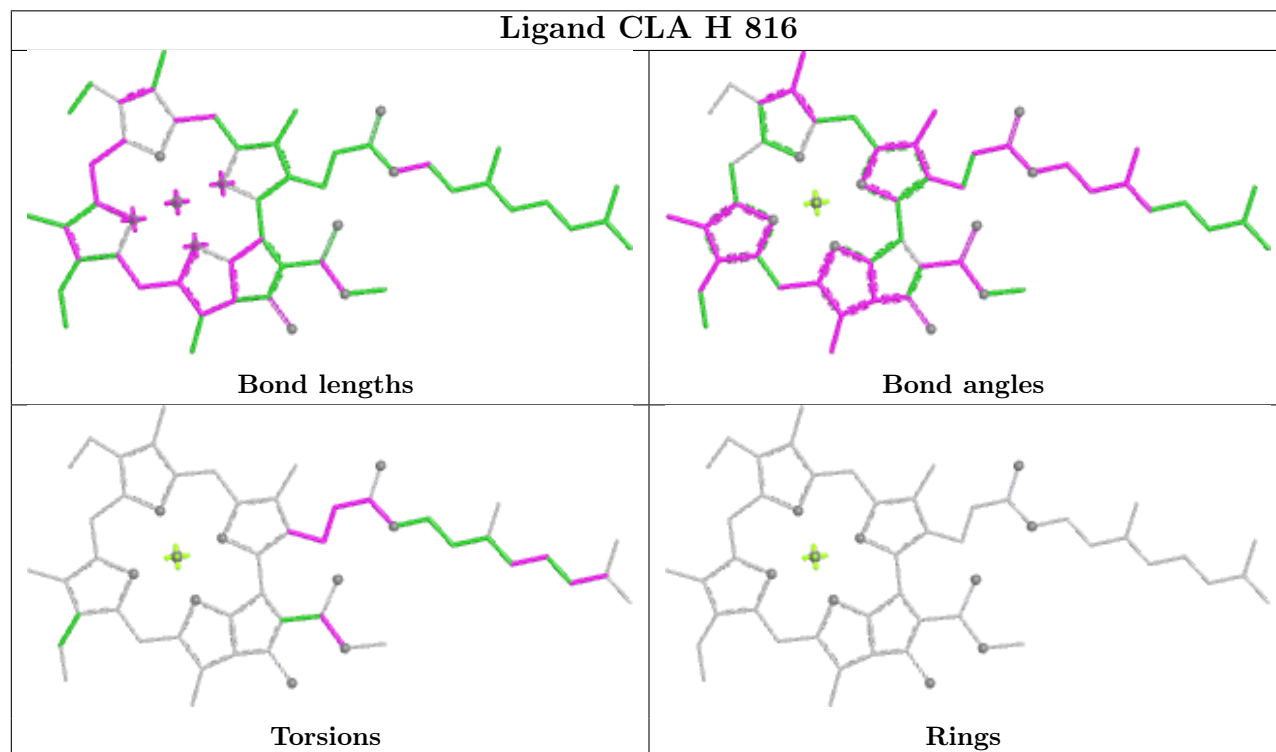
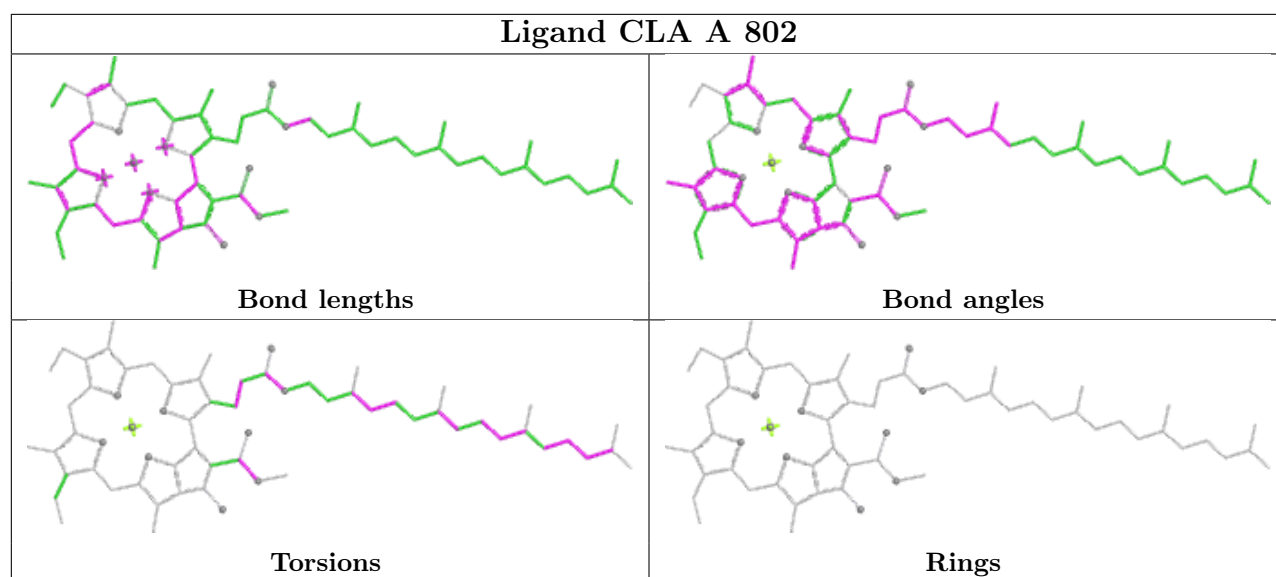
Ligand CLA H 819



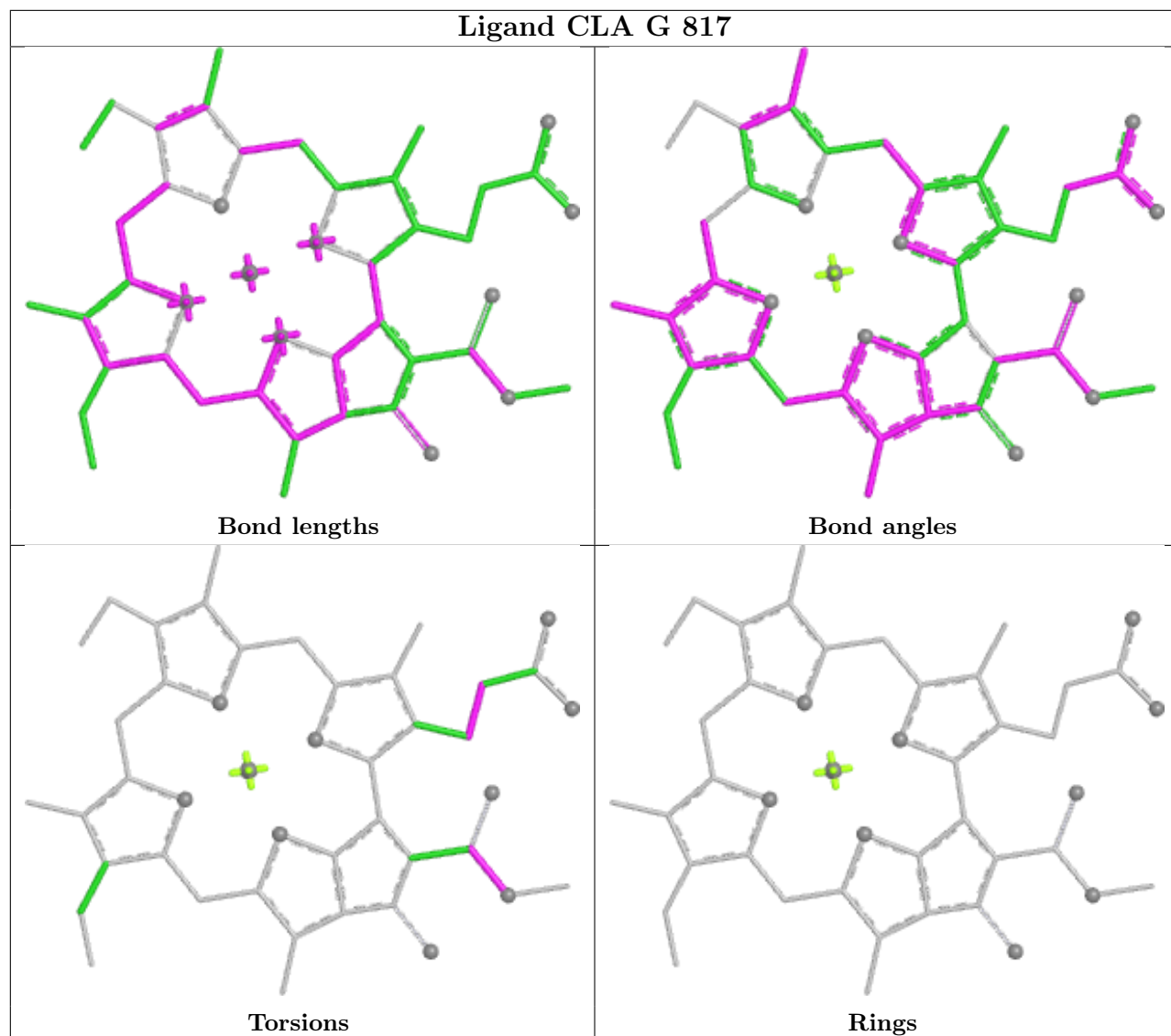
Ligand BCR U 202



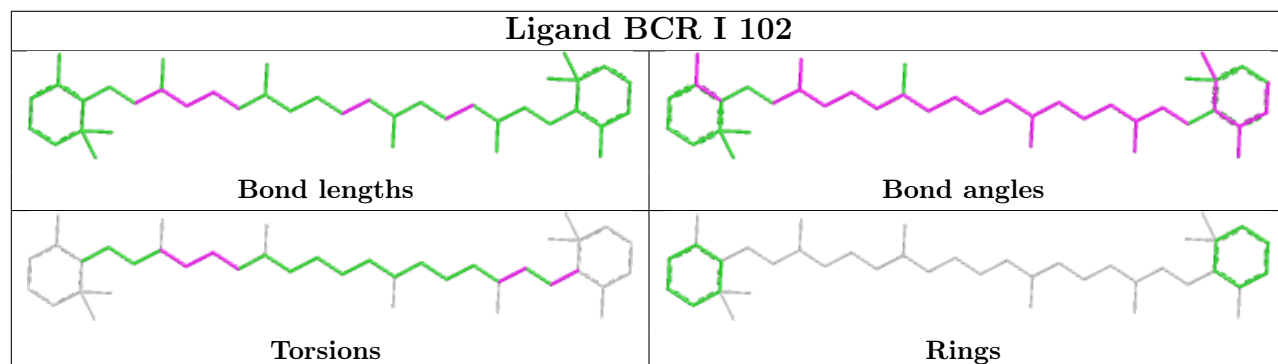




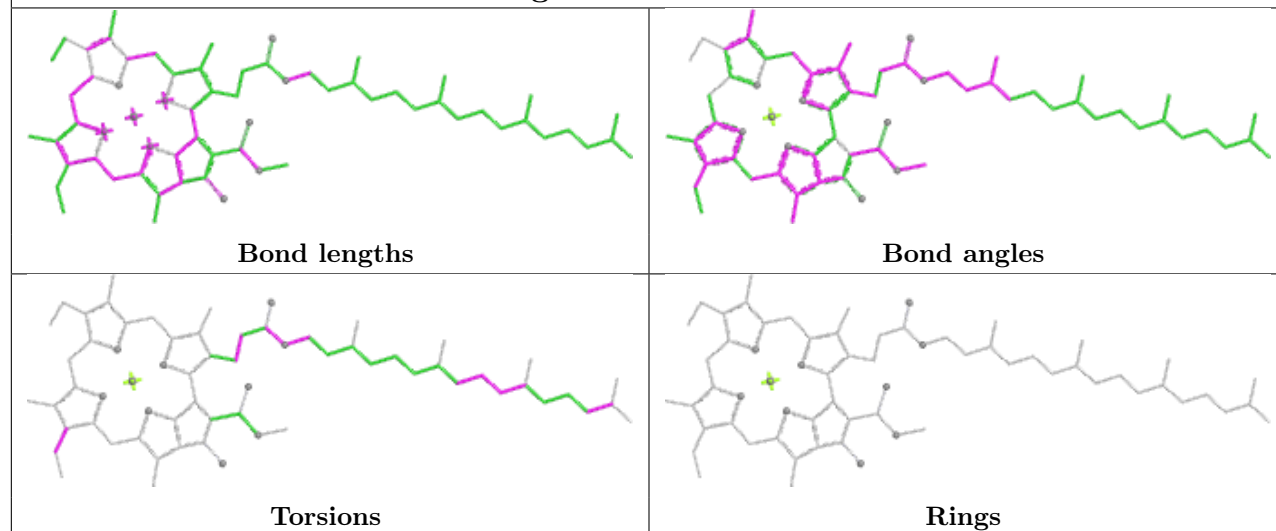
Ligand CLA G 817



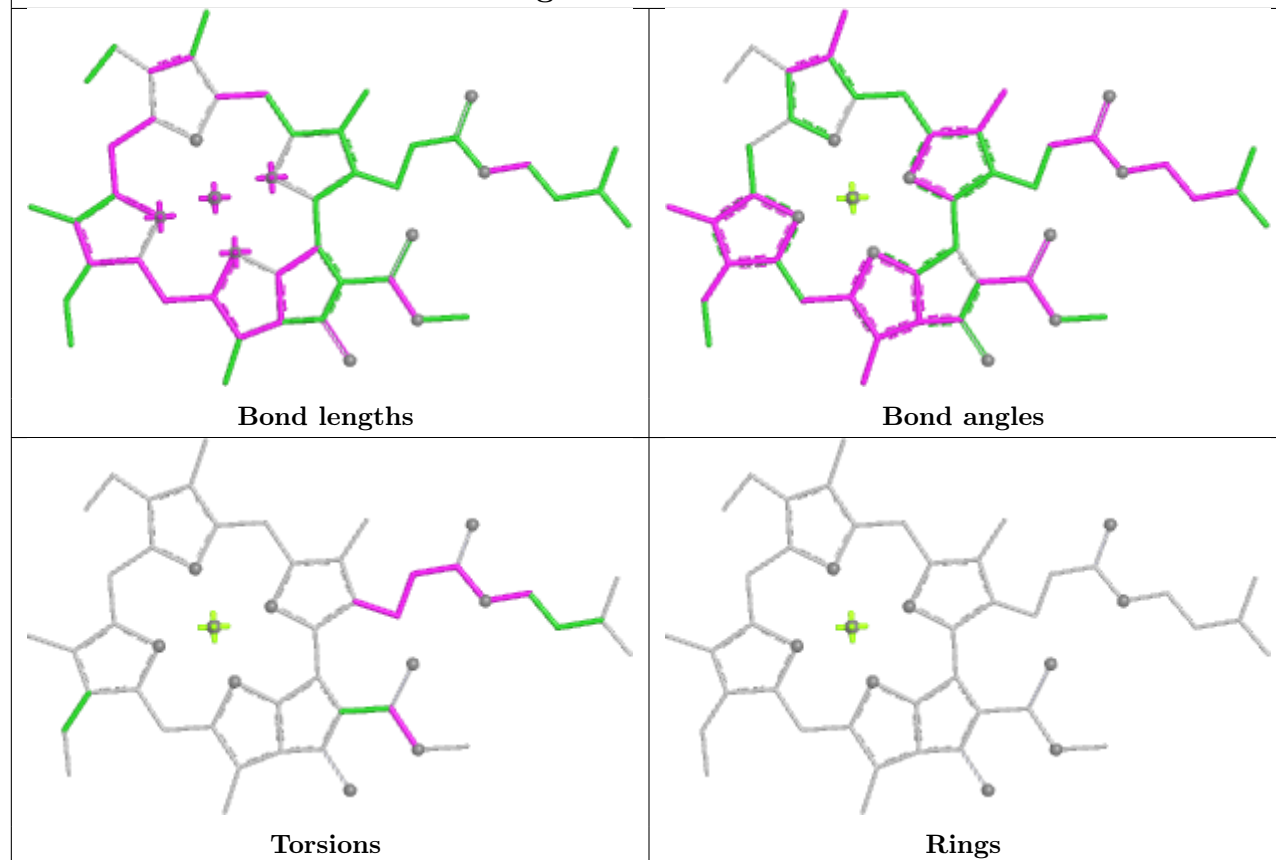
Ligand BCR I 102

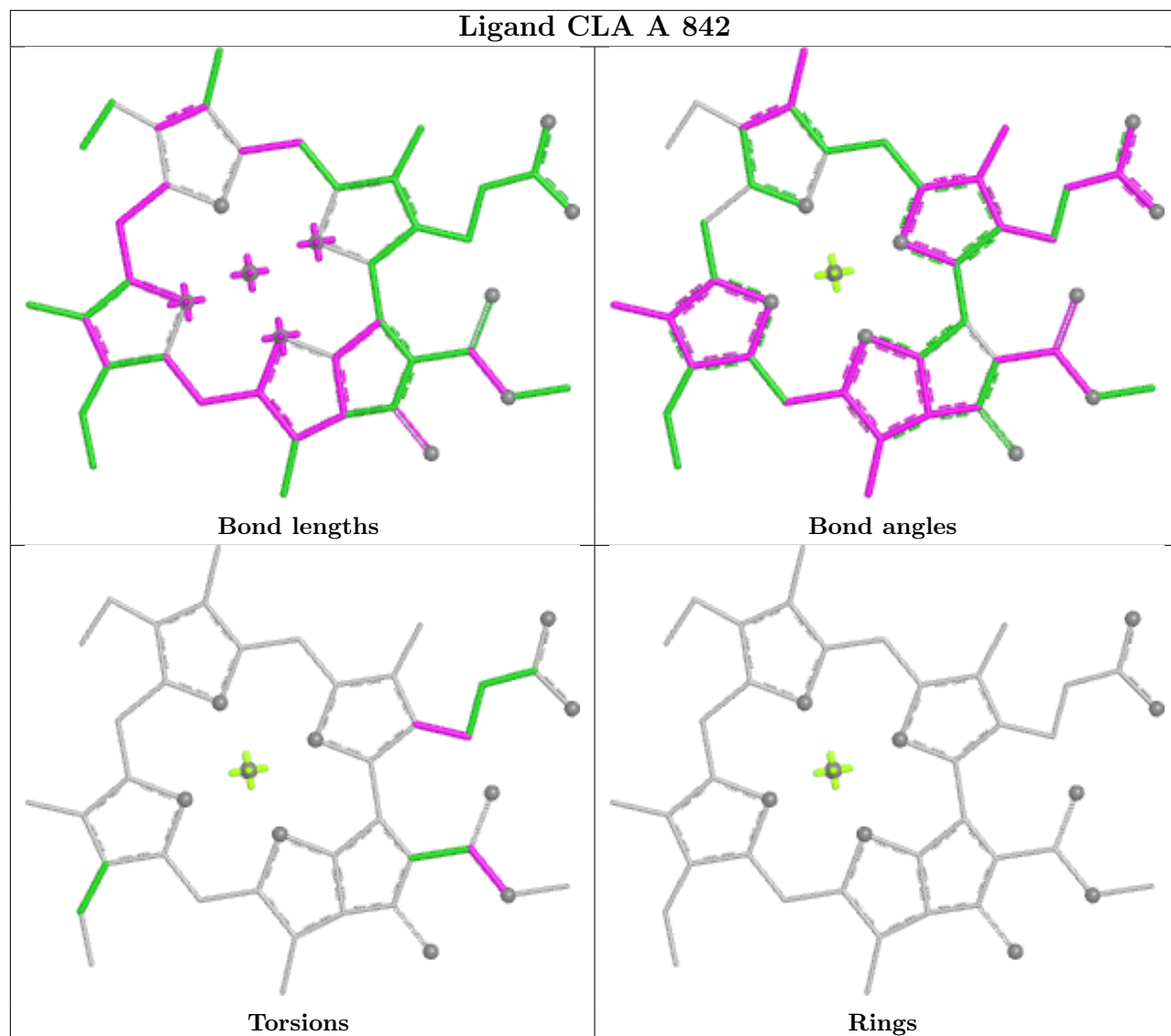


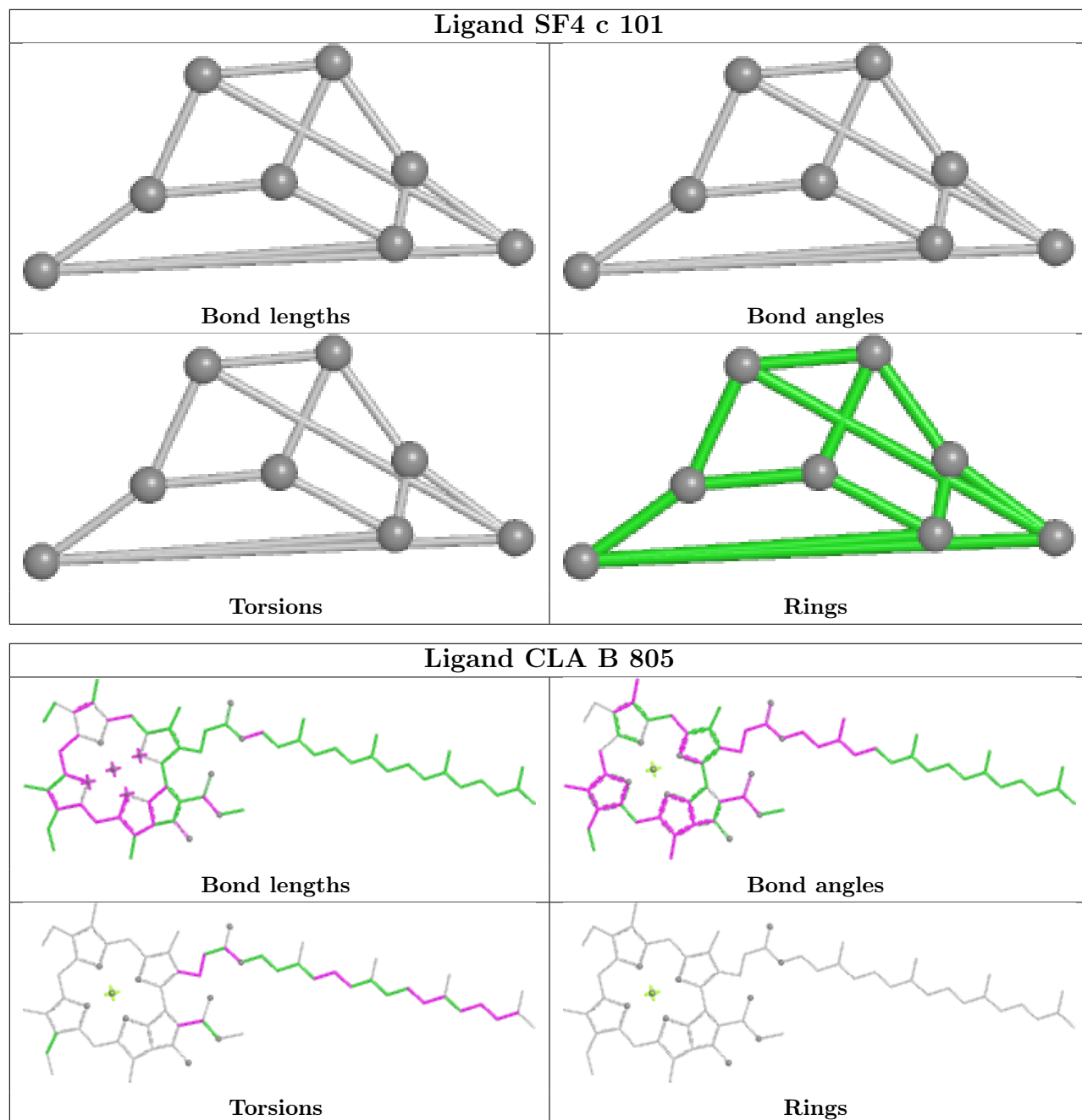
Ligand CLA H 803

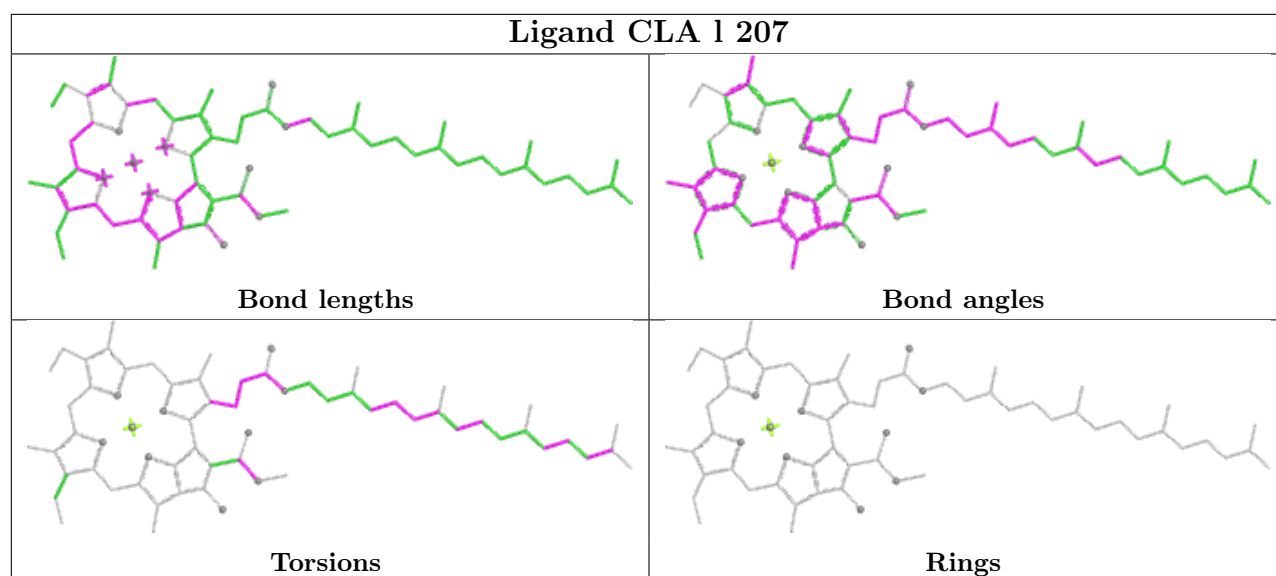
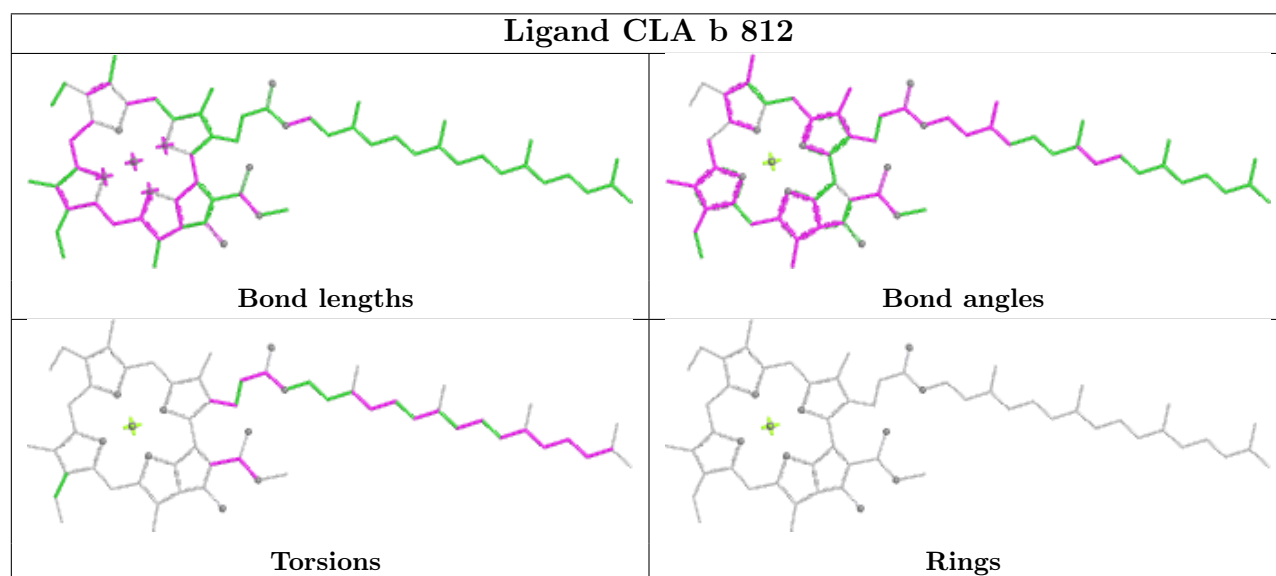
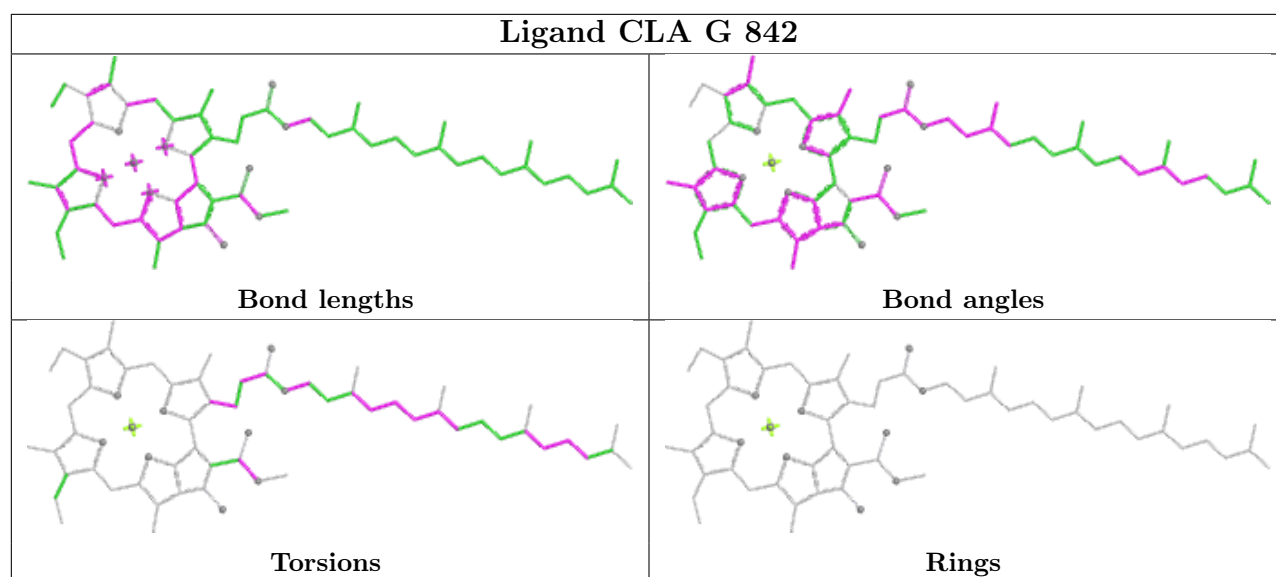


Ligand CLA a 818

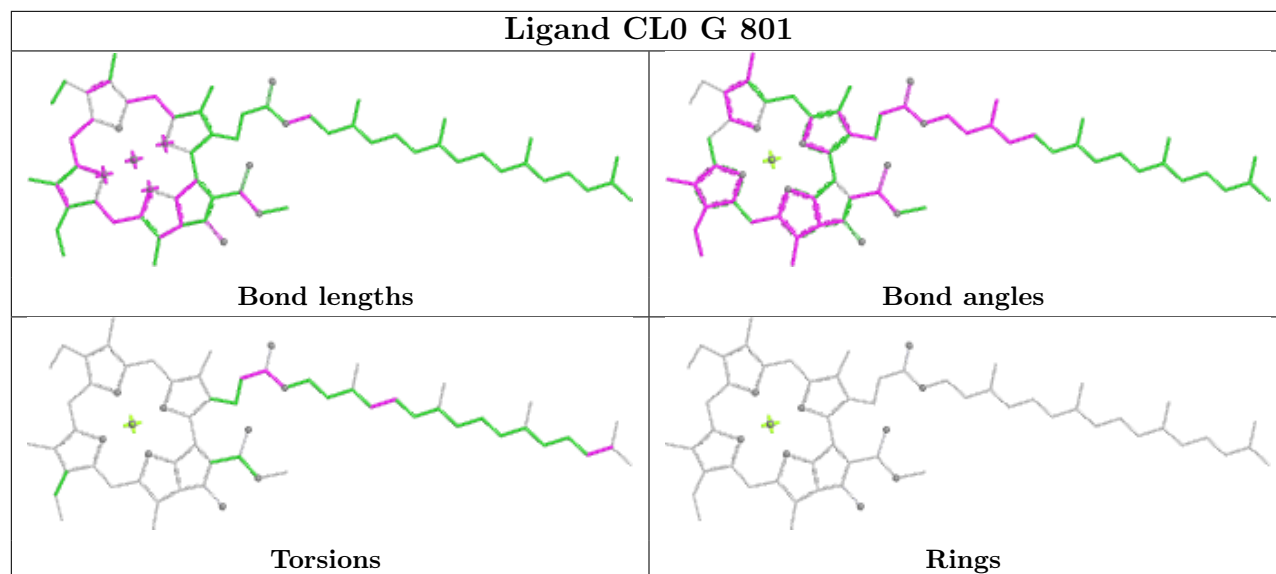




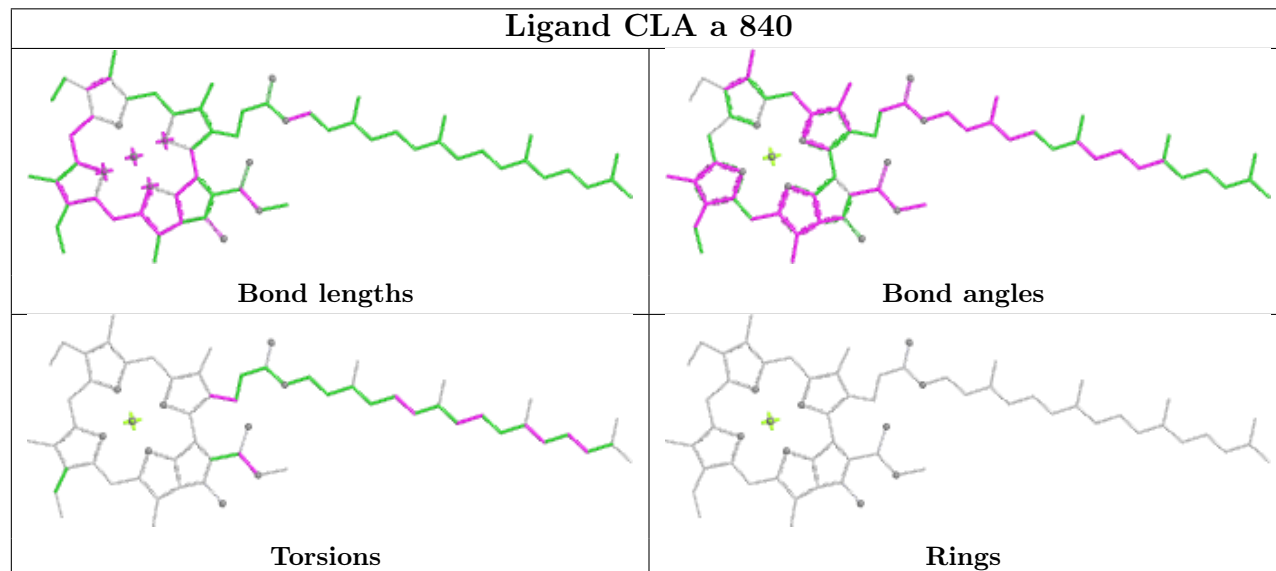




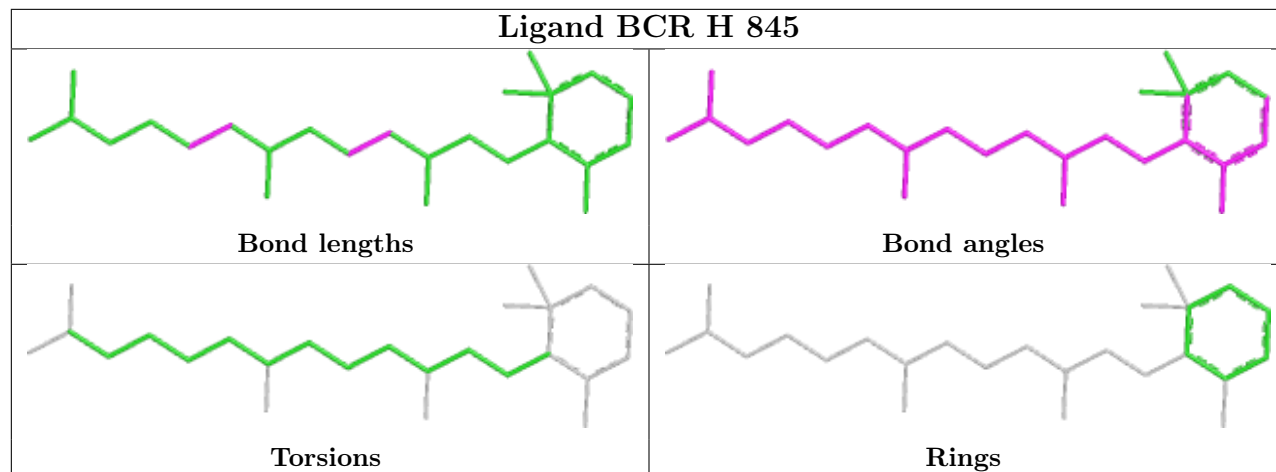
Ligand CL0 G 801

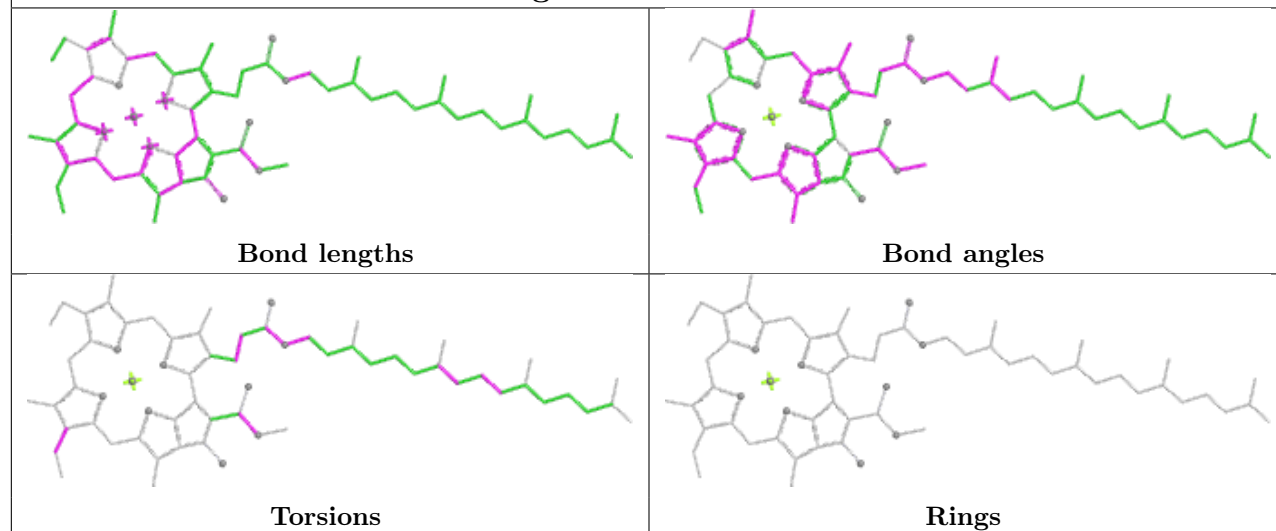
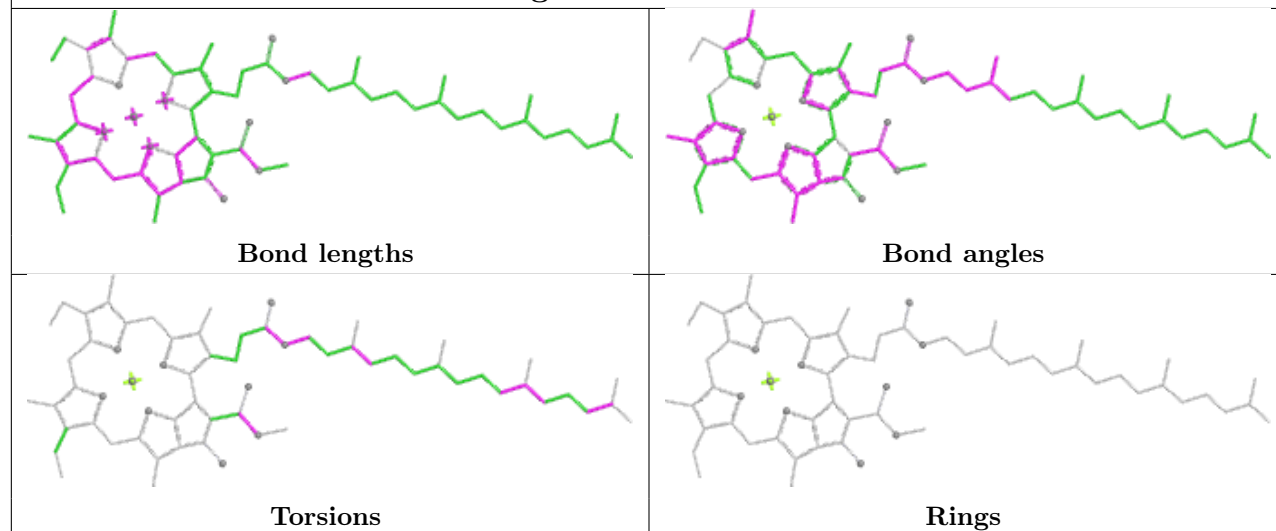


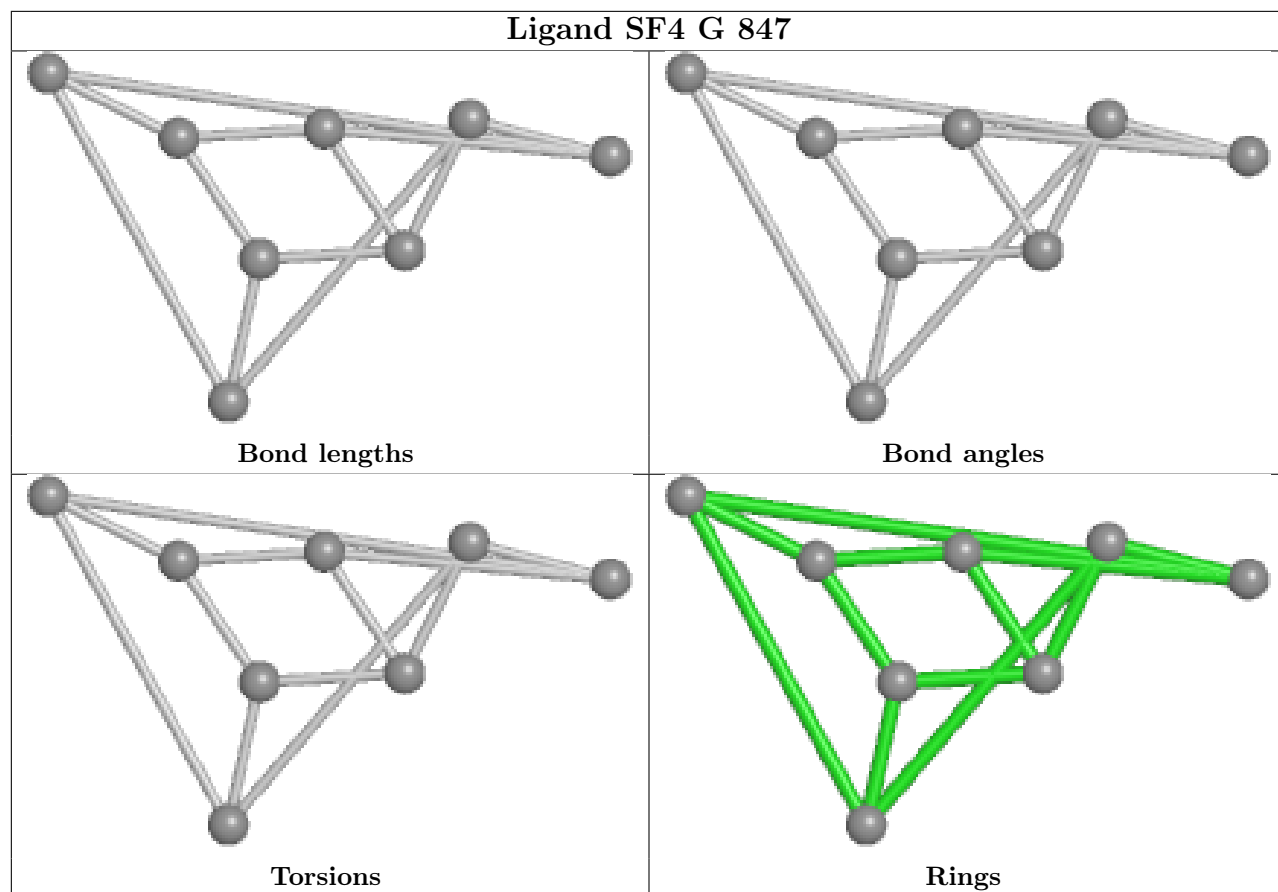
Ligand CLA a 840

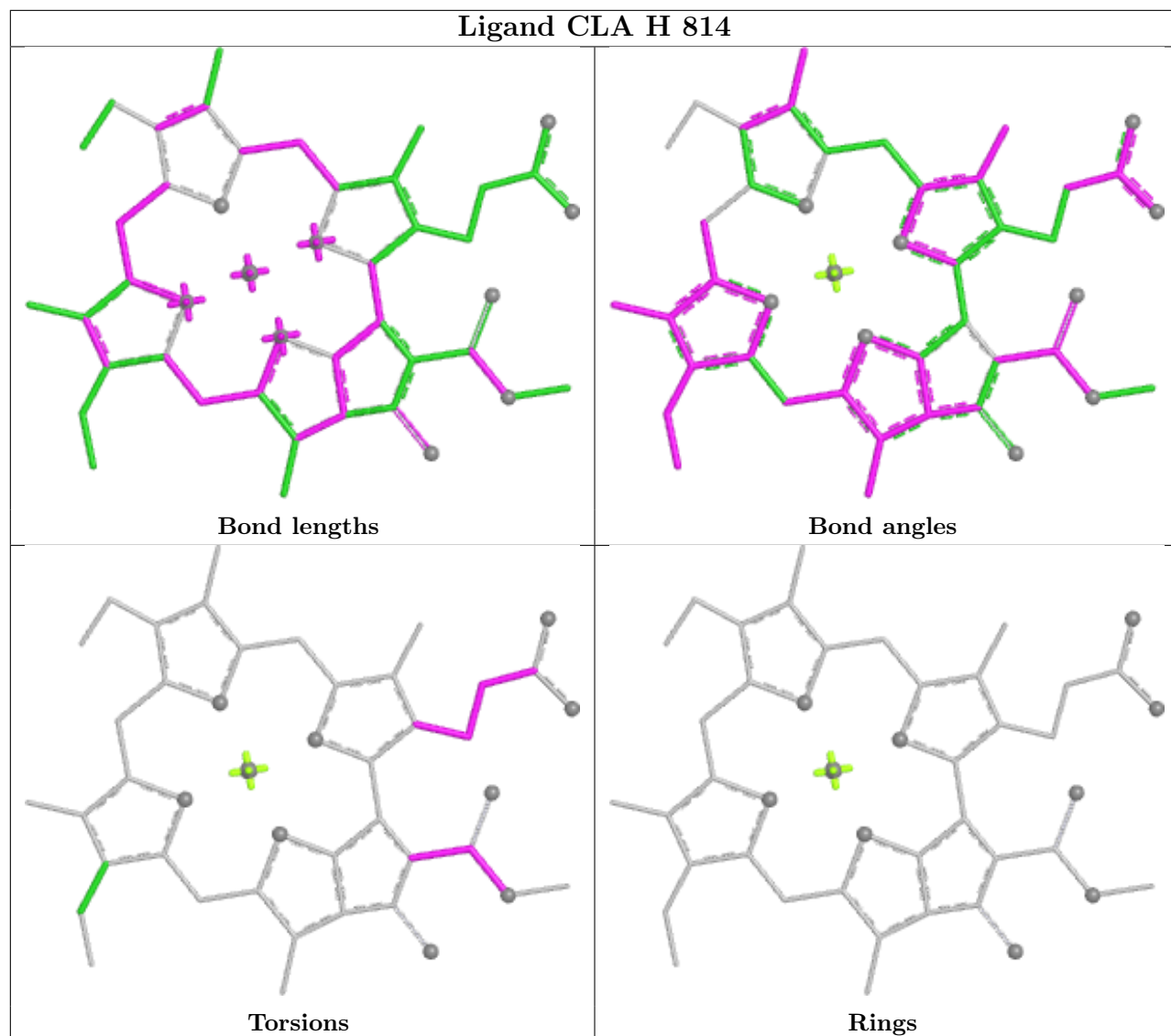


Ligand BCR H 845

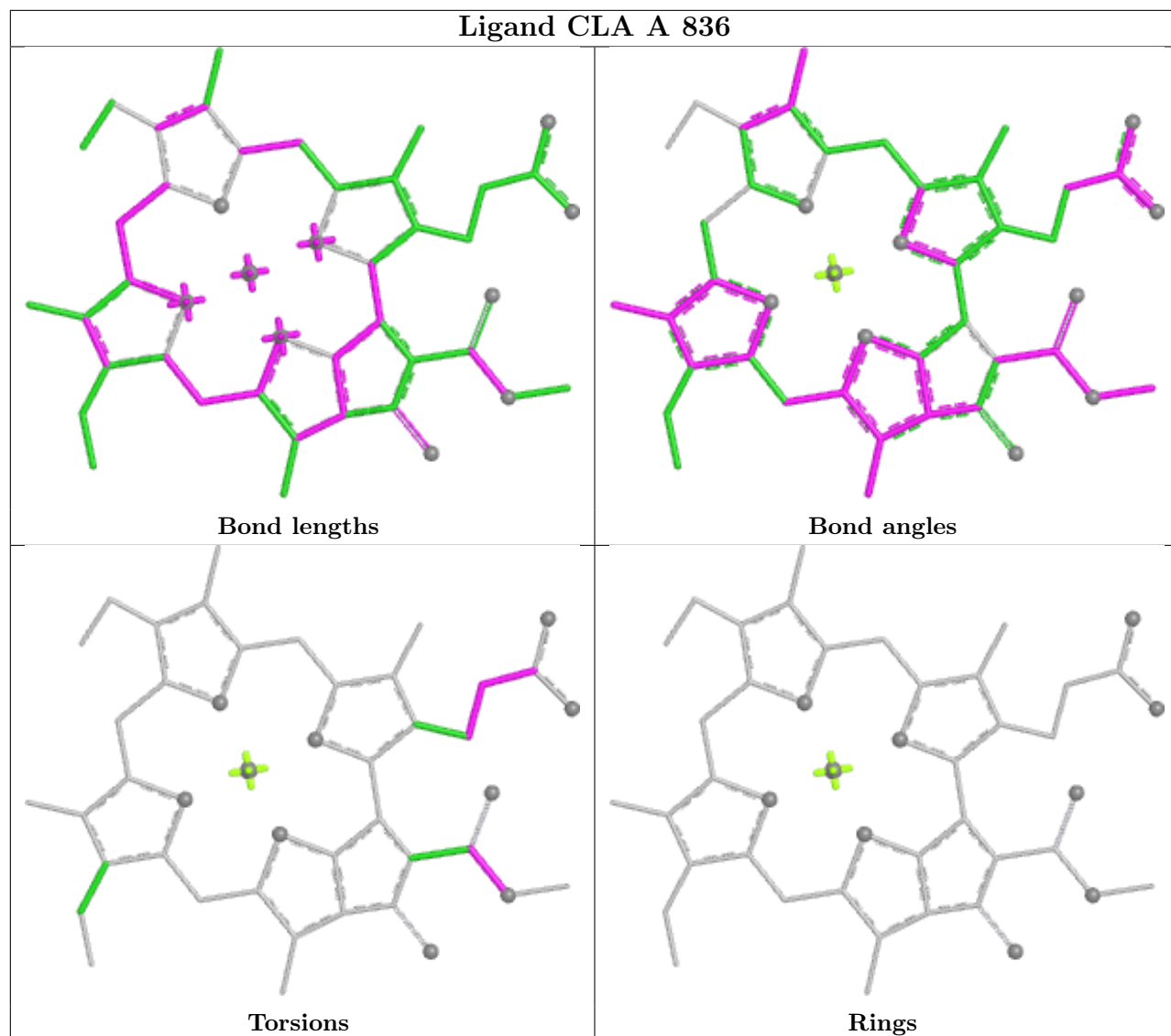


Ligand CLA B 803**Ligand CLA G 834**

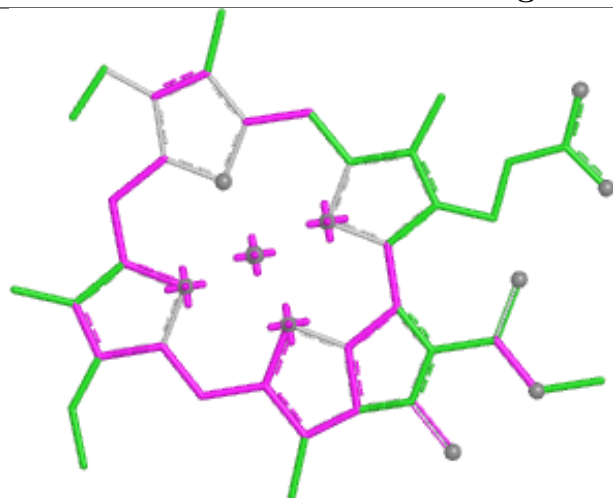




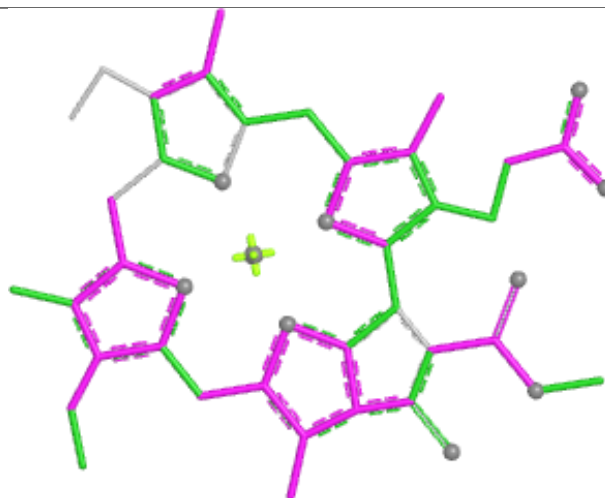
Ligand CLA A 836



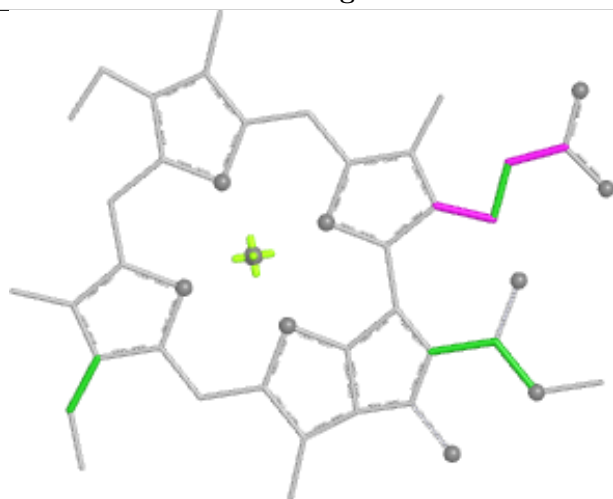
Ligand CLA b 822



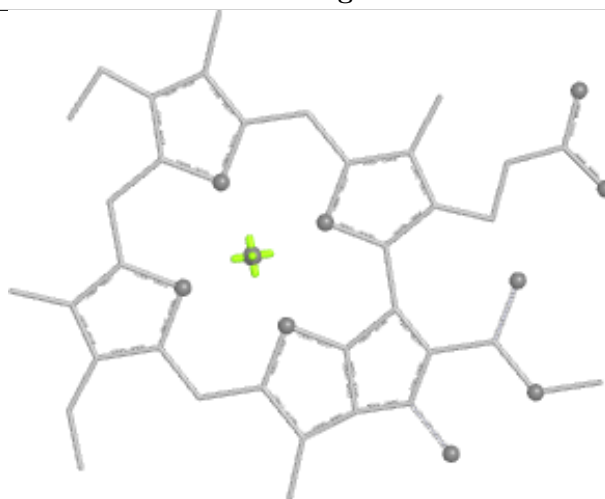
Bond lengths



Bond angles

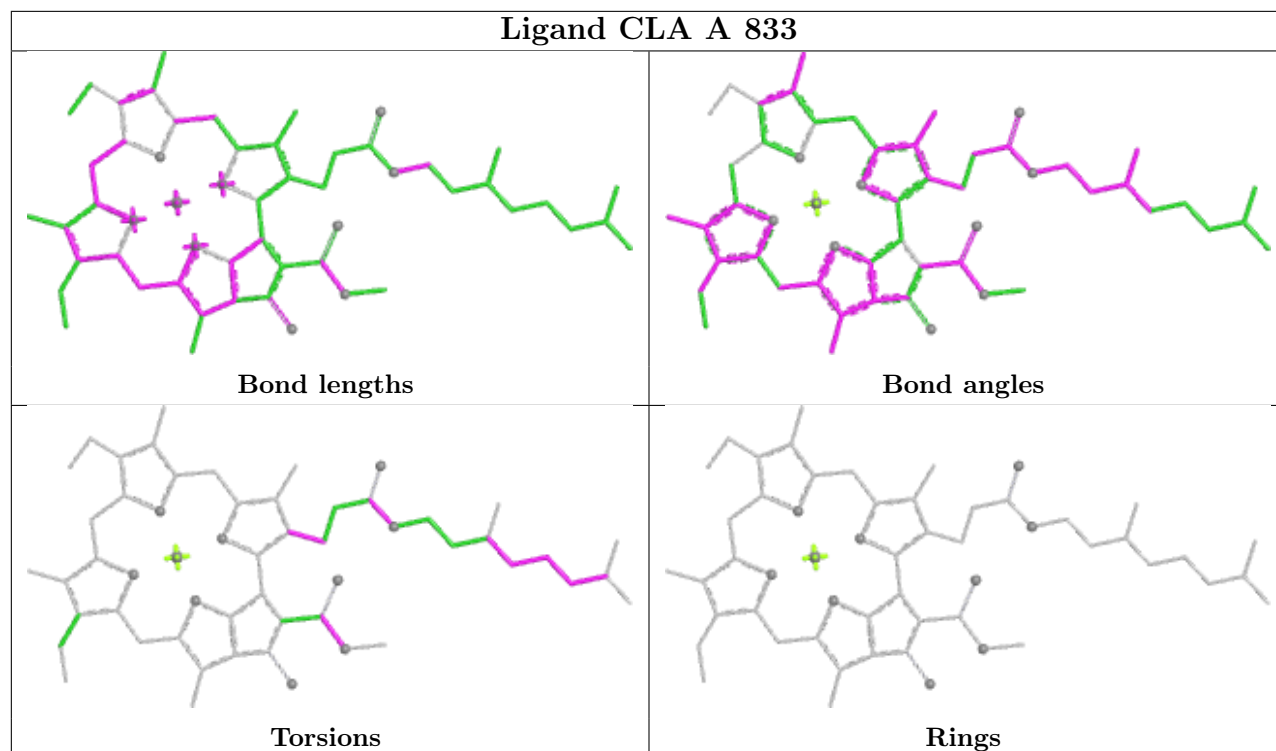


Torsions

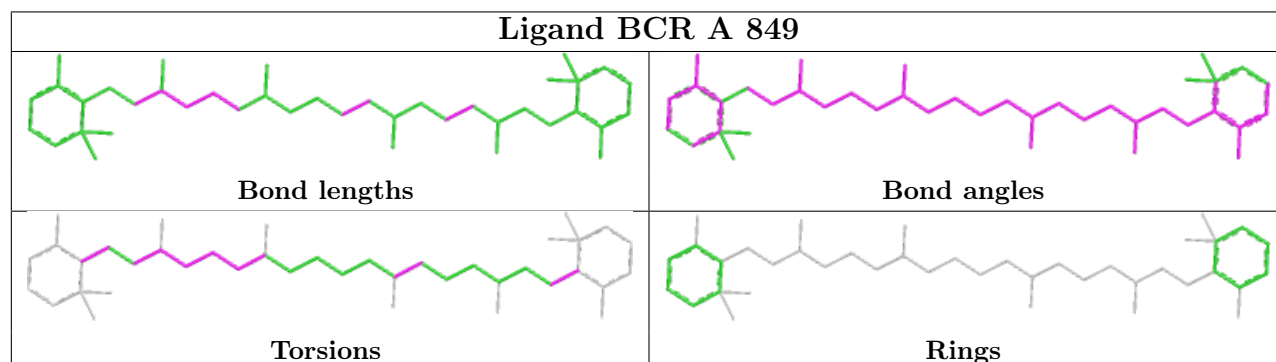


Rings

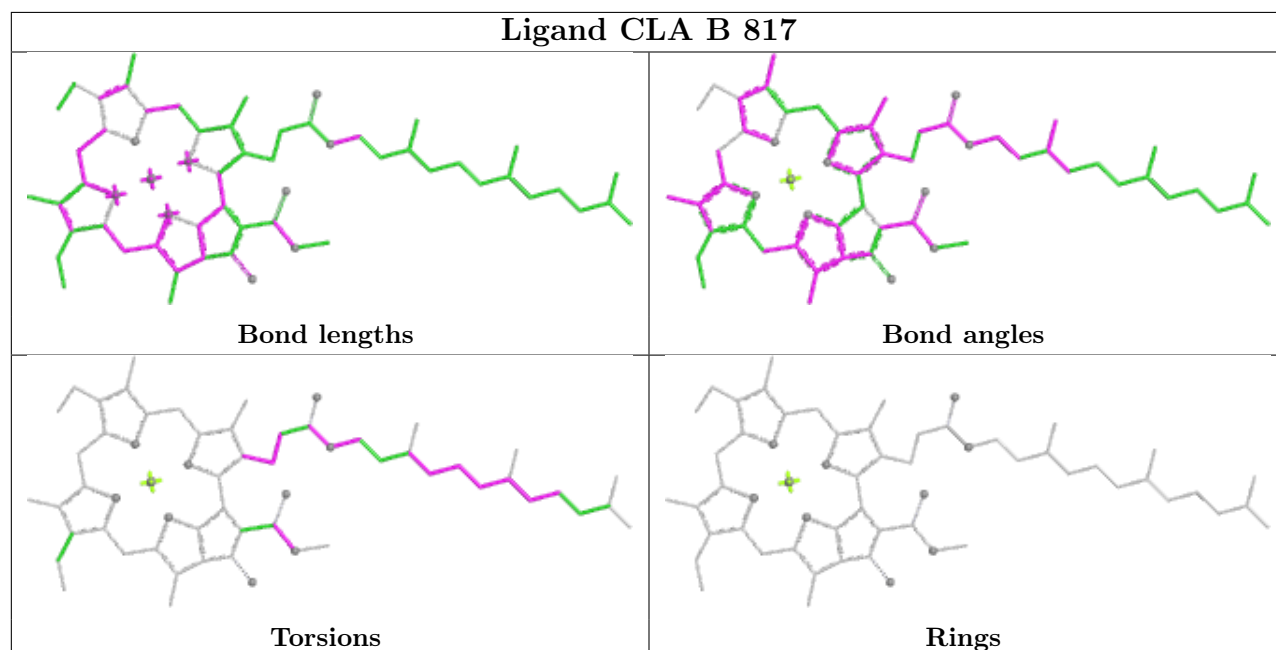
Ligand CLA A 833



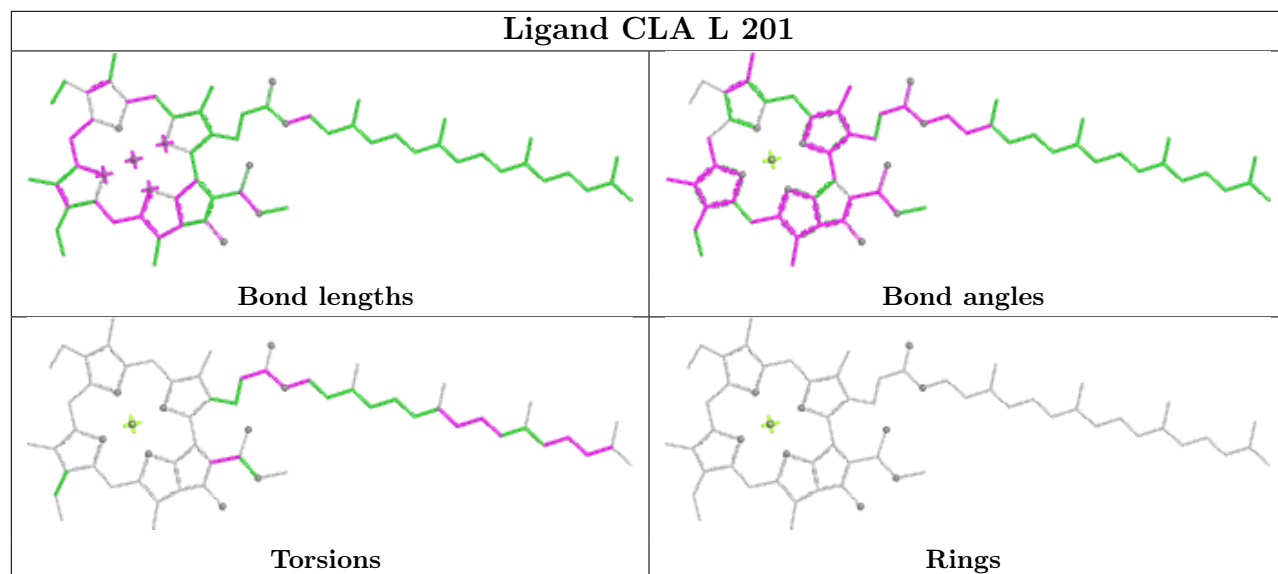
Ligand BCR A 849



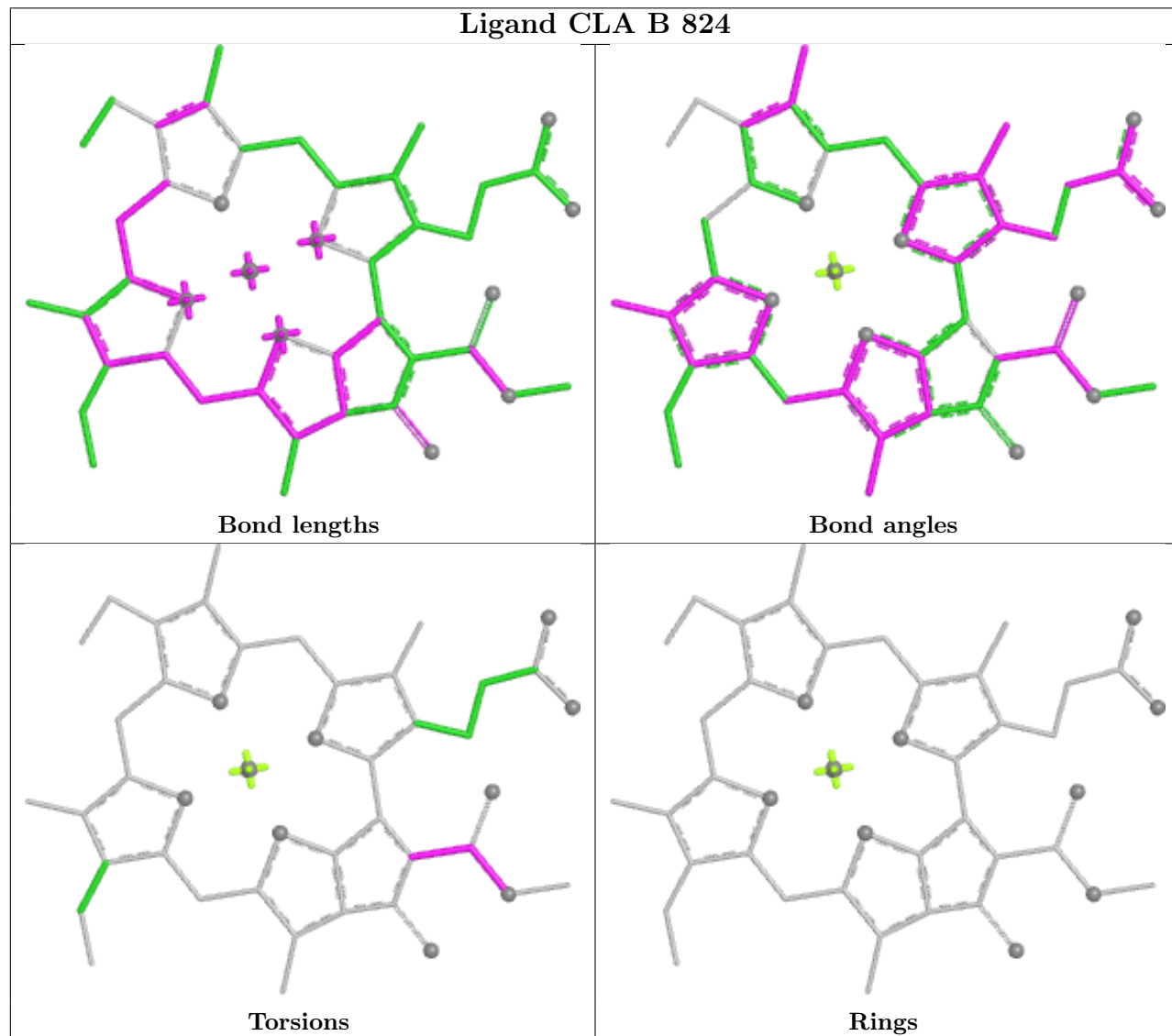
Ligand CLA B 817



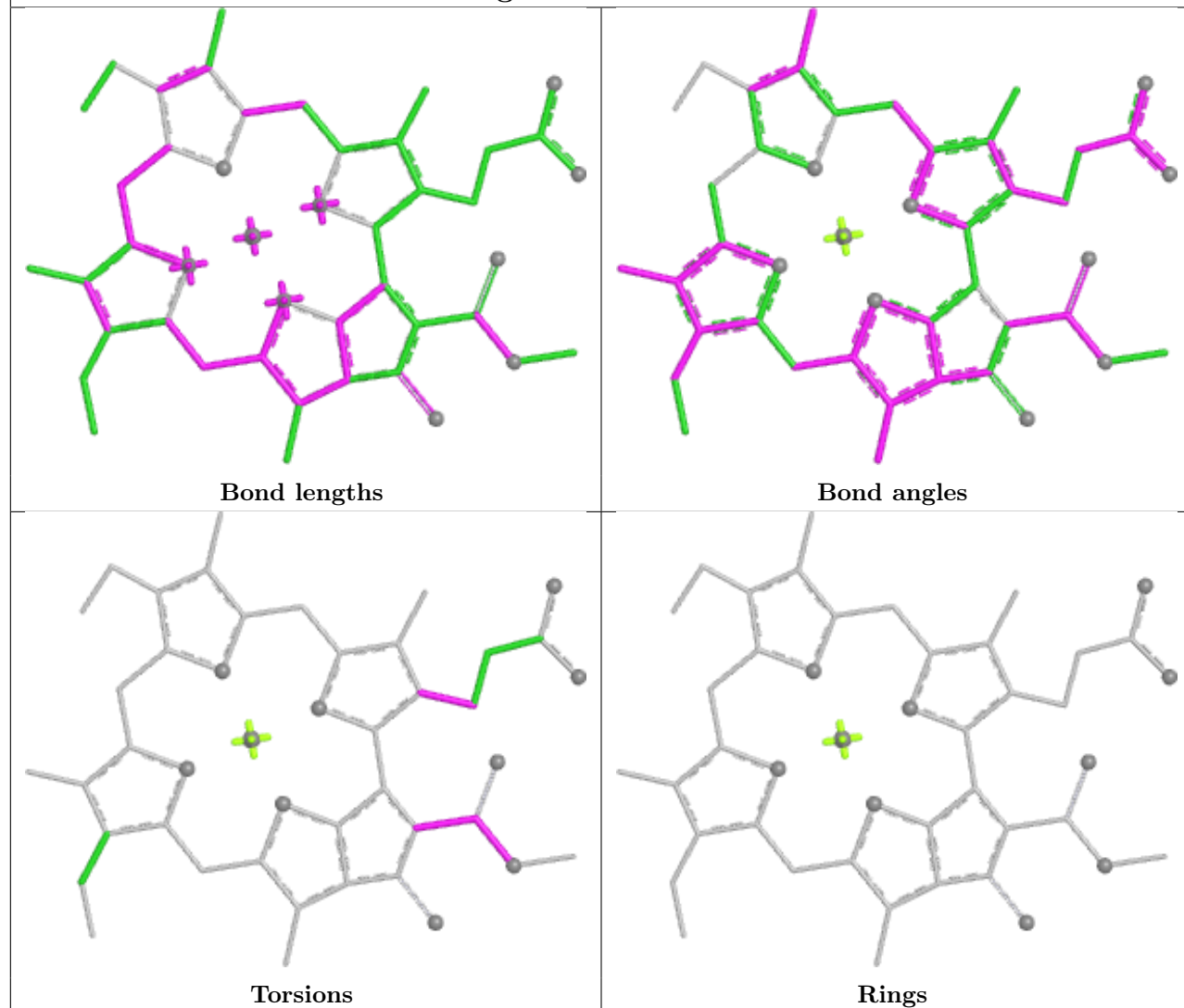
Ligand CLA L 201



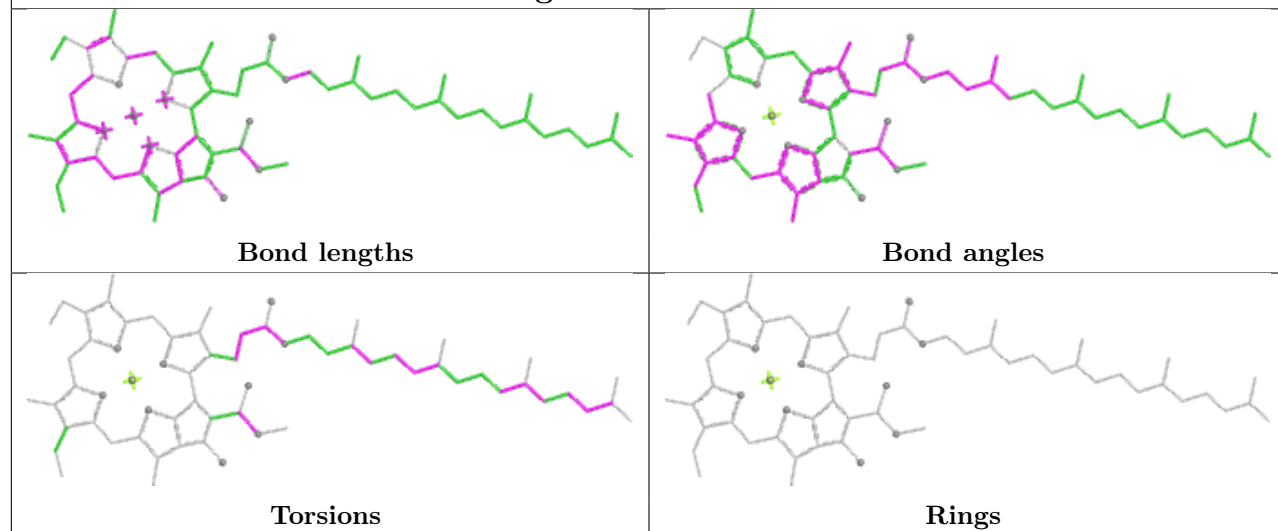
Ligand CLA B 824

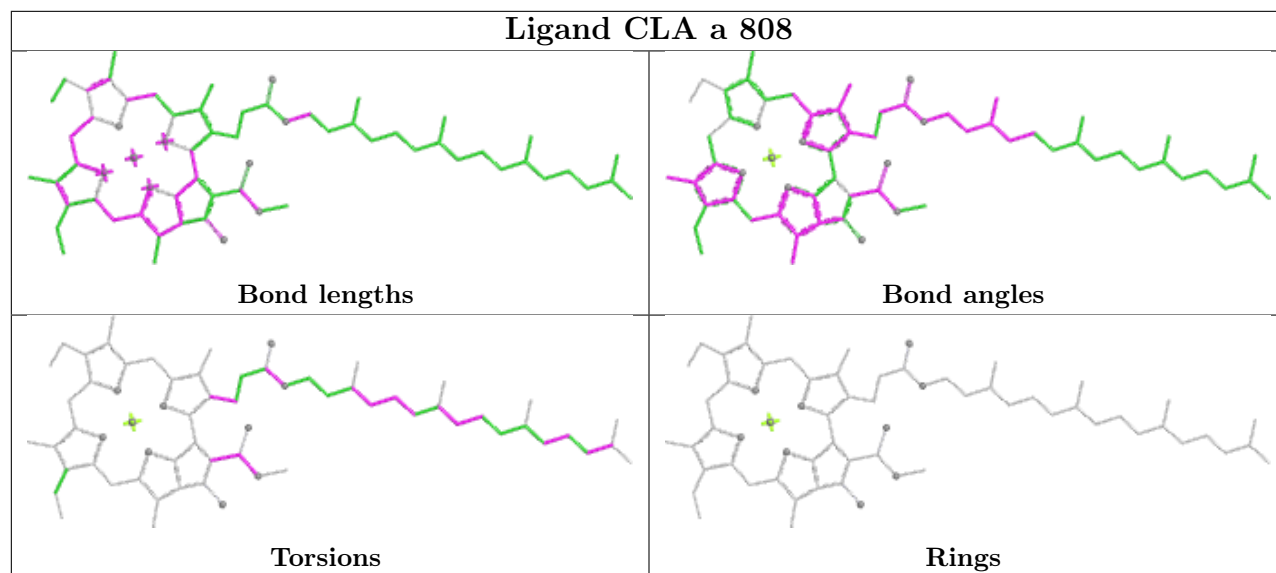
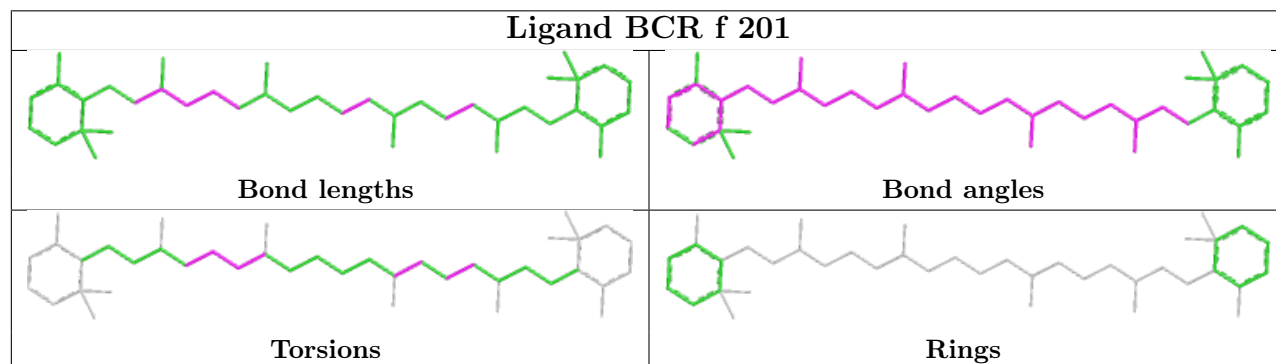
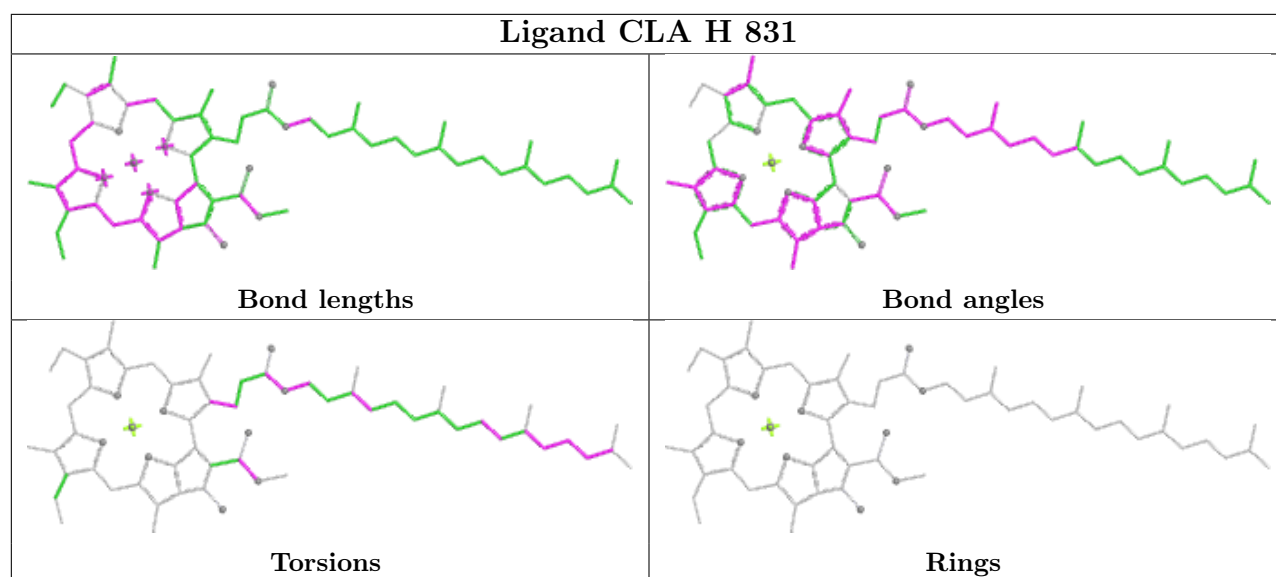


Ligand CLA a 805

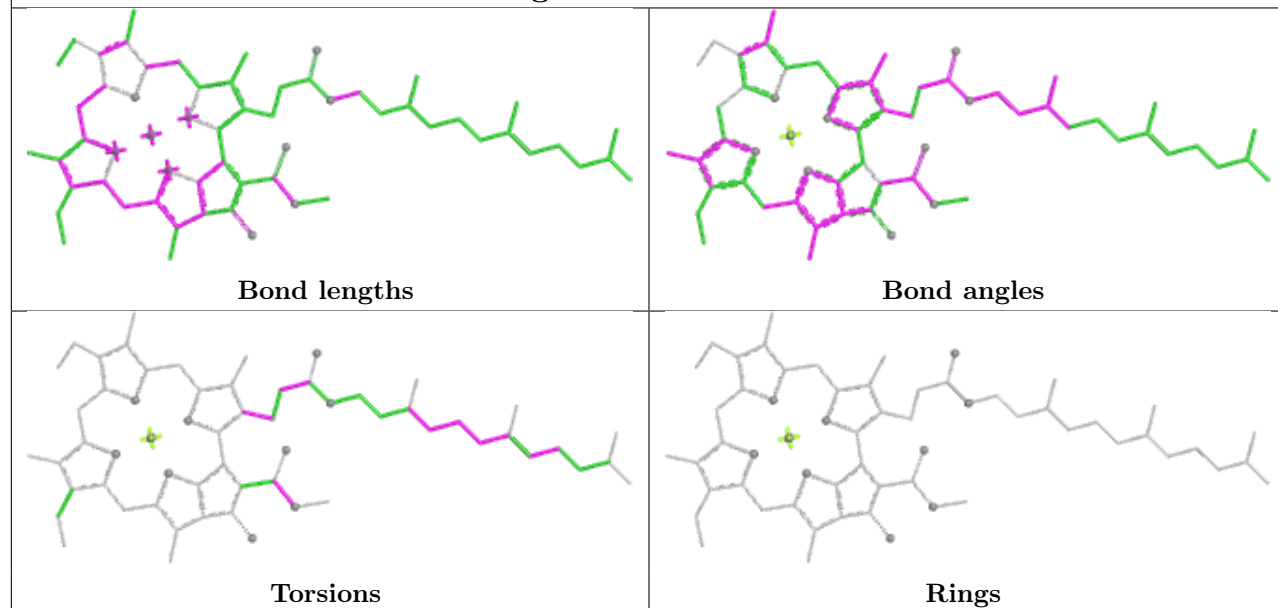


Ligand CLA b 802

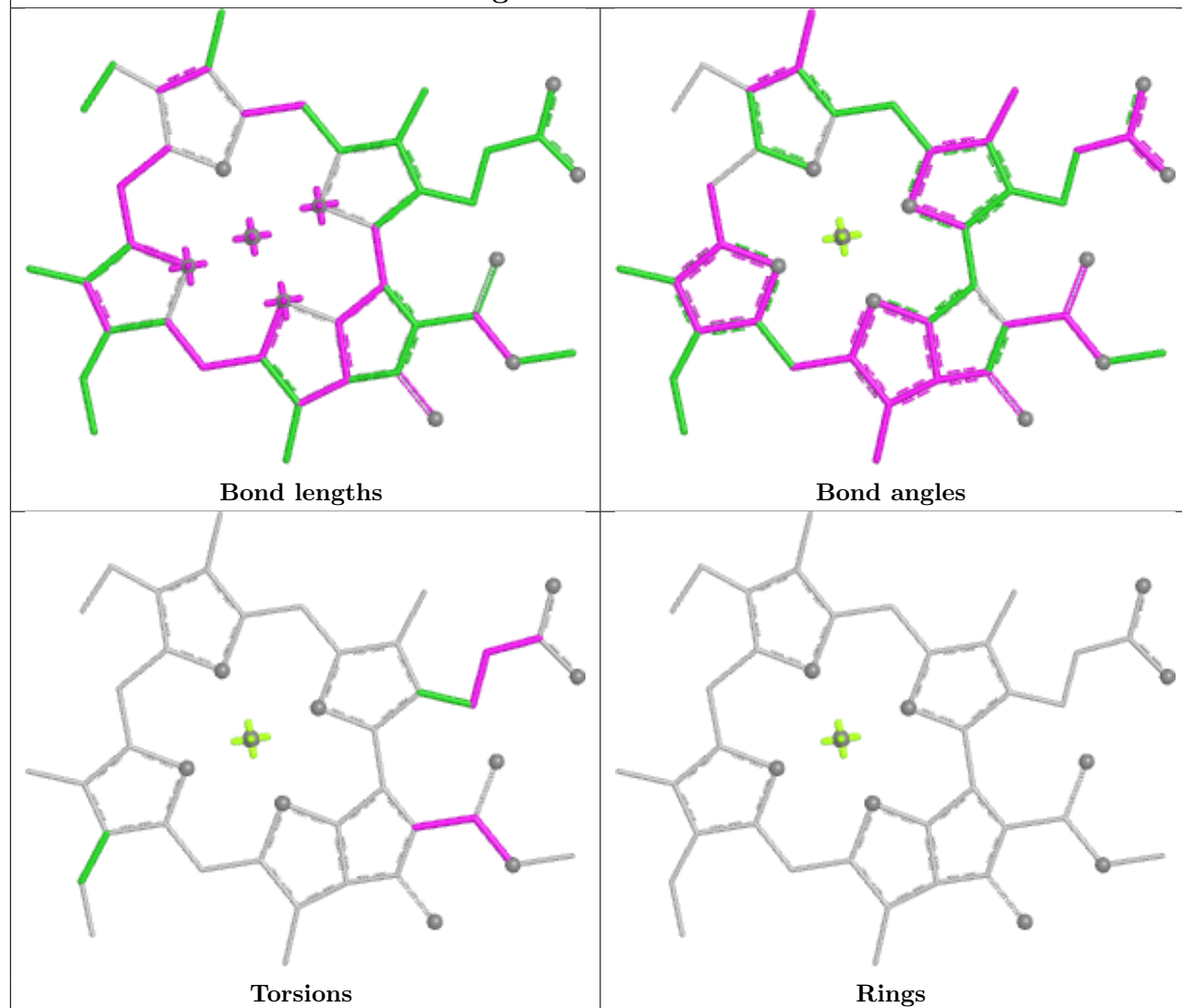




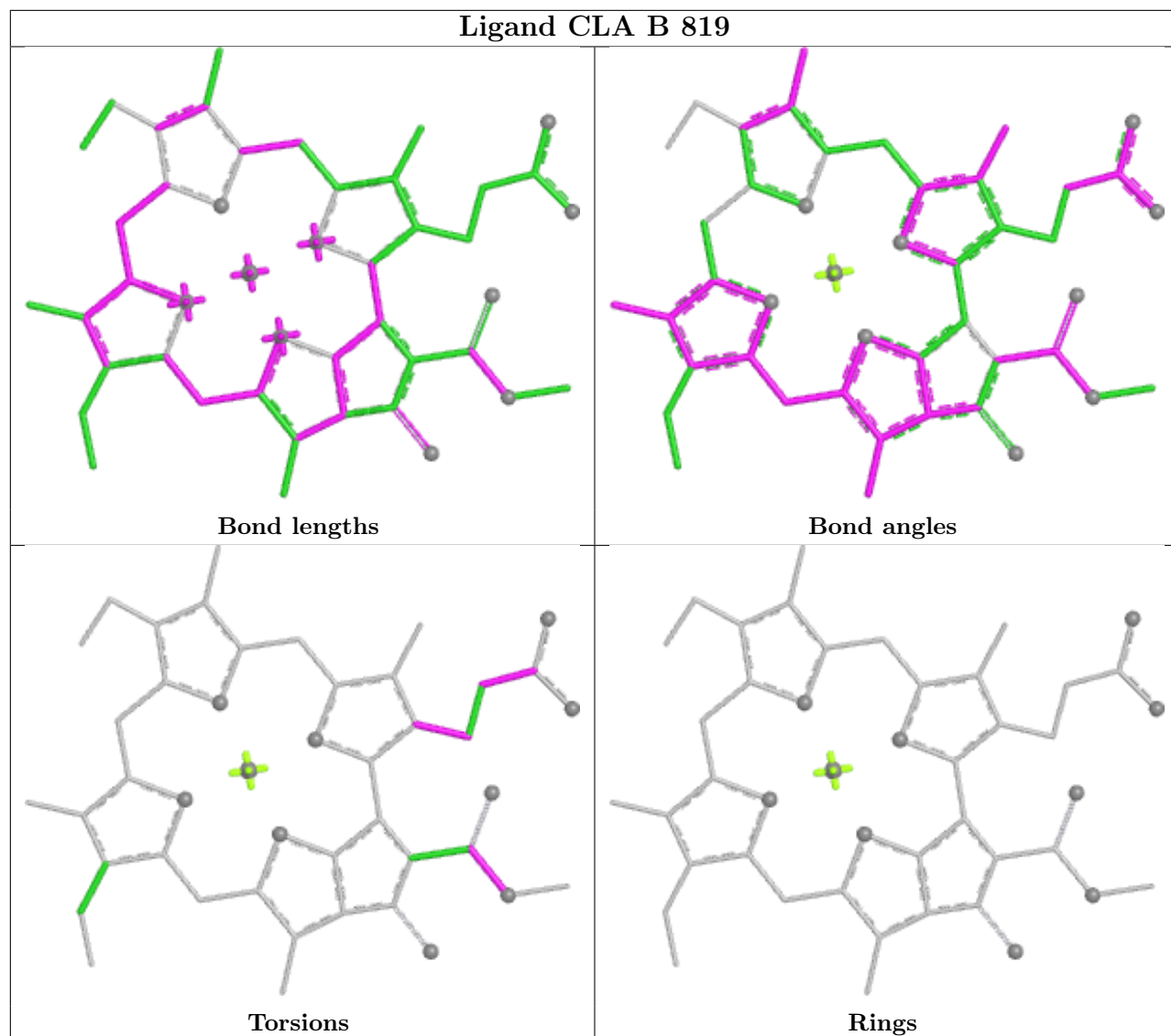
Ligand CLA H 837



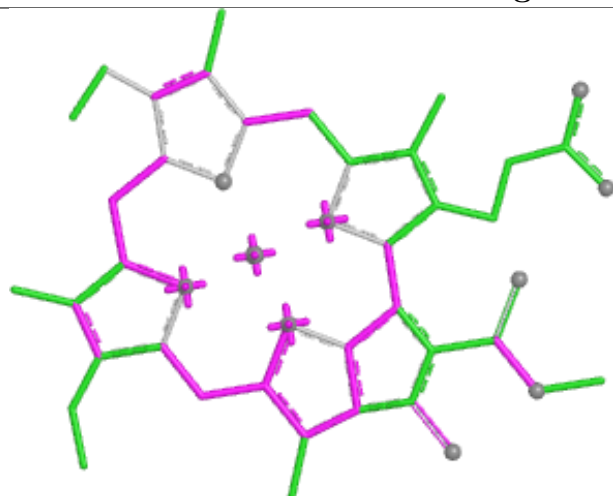
Ligand CLA B 814



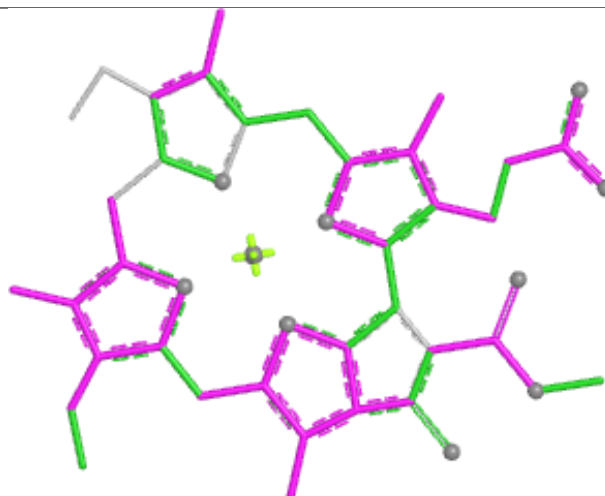
Ligand CLA B 819



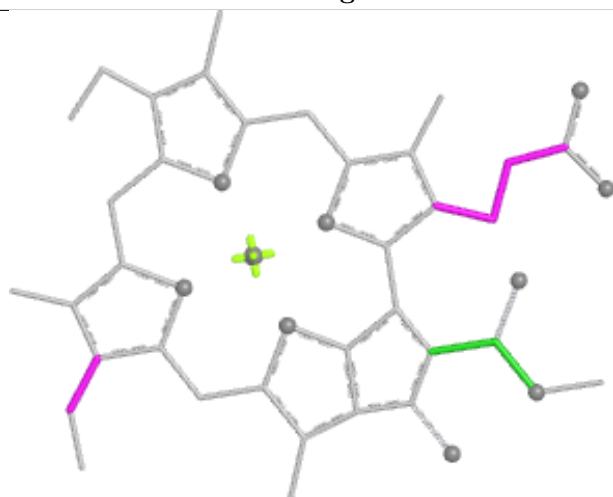
Ligand CLA A 845



Bond lengths



Bond angles

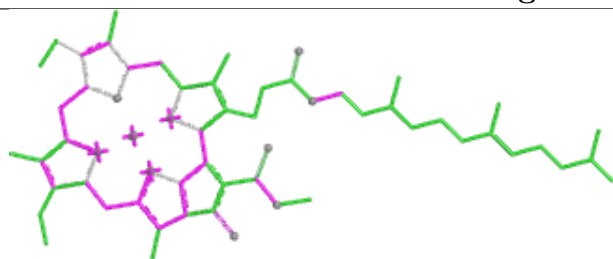


Torsions

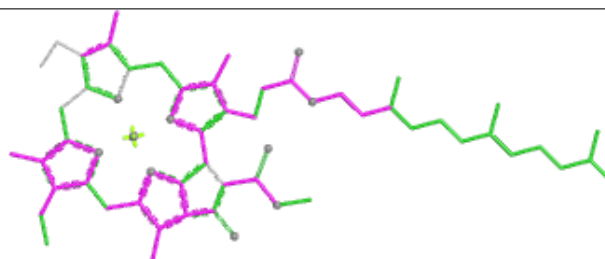


Rings

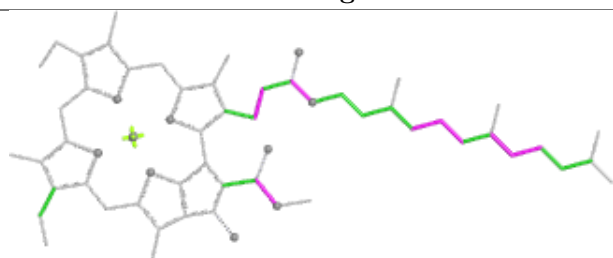
Ligand CLA a 813



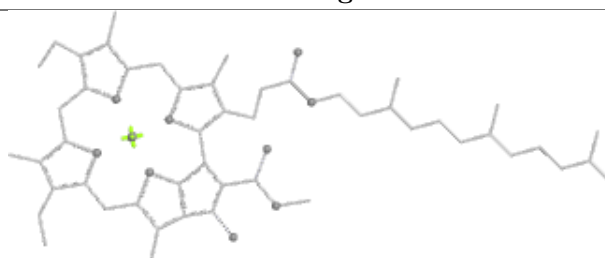
Bond lengths



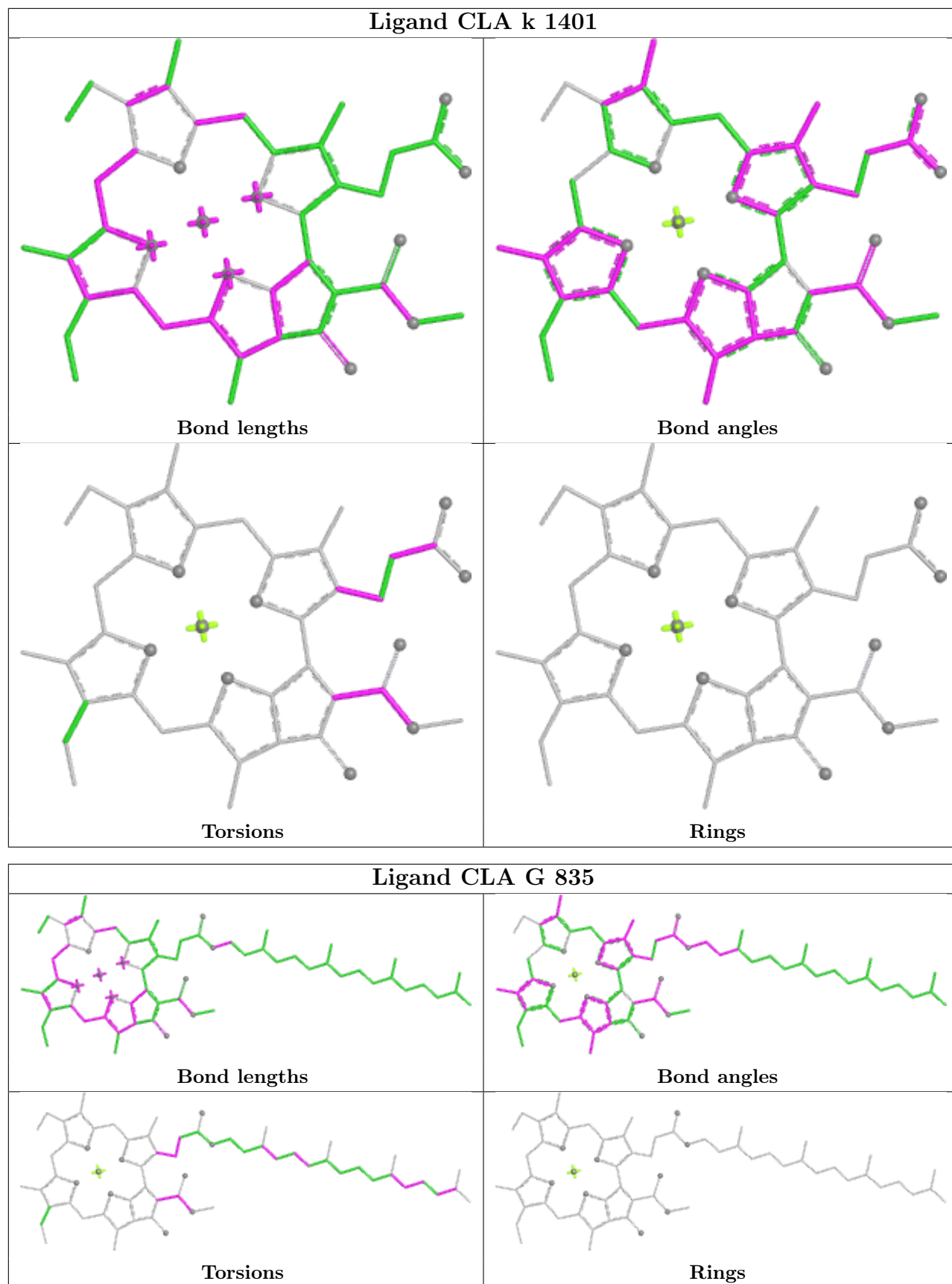
Bond angles

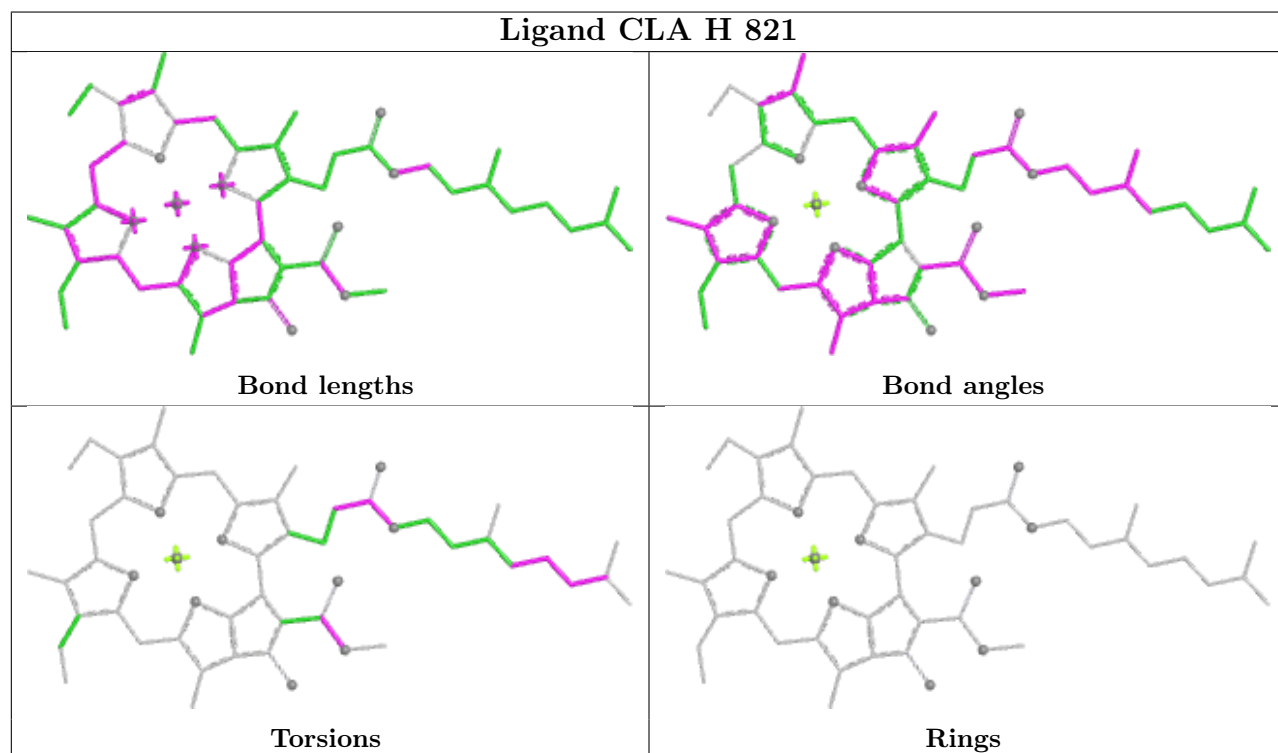
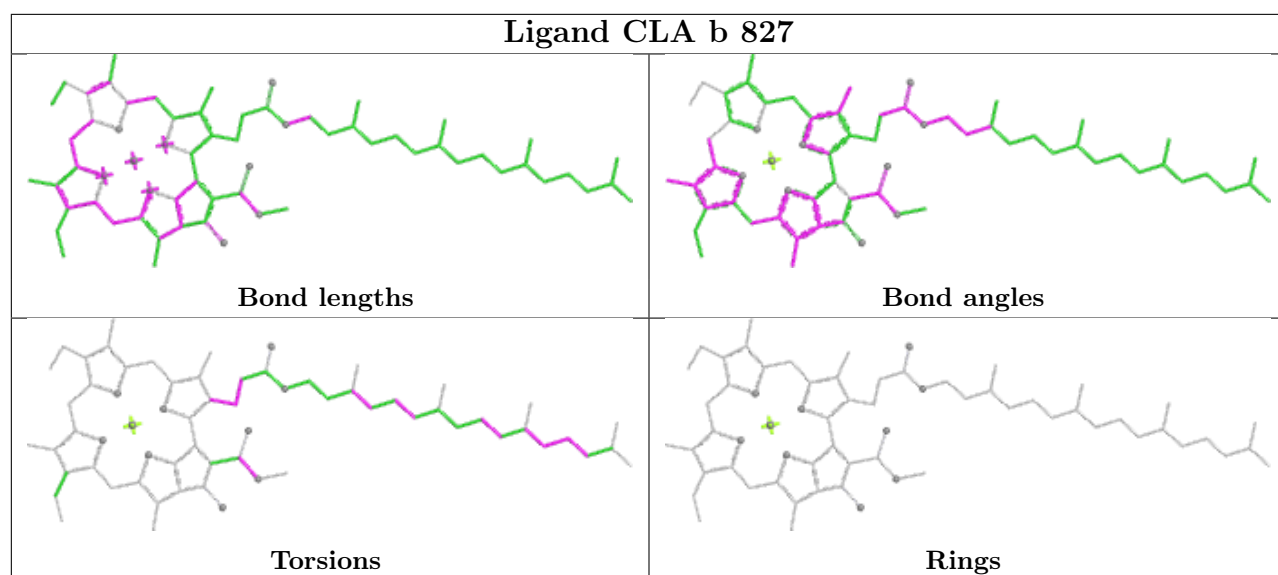


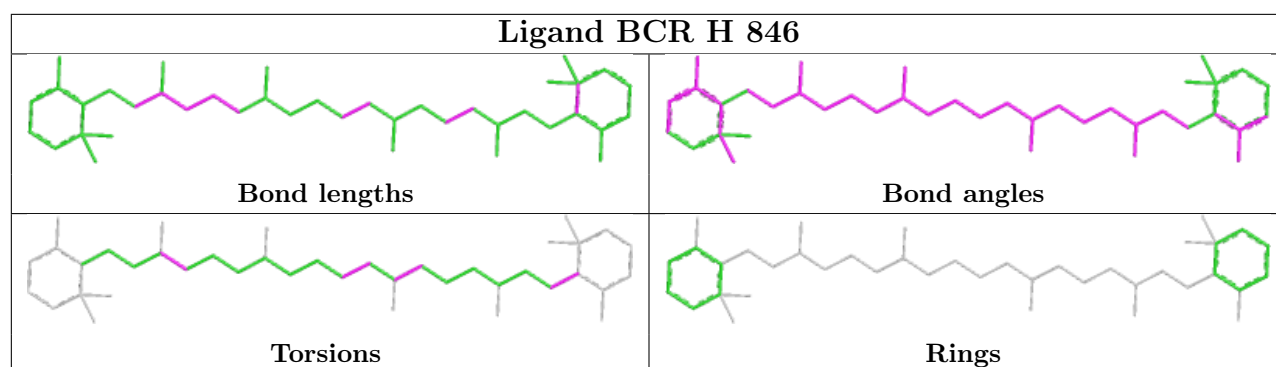
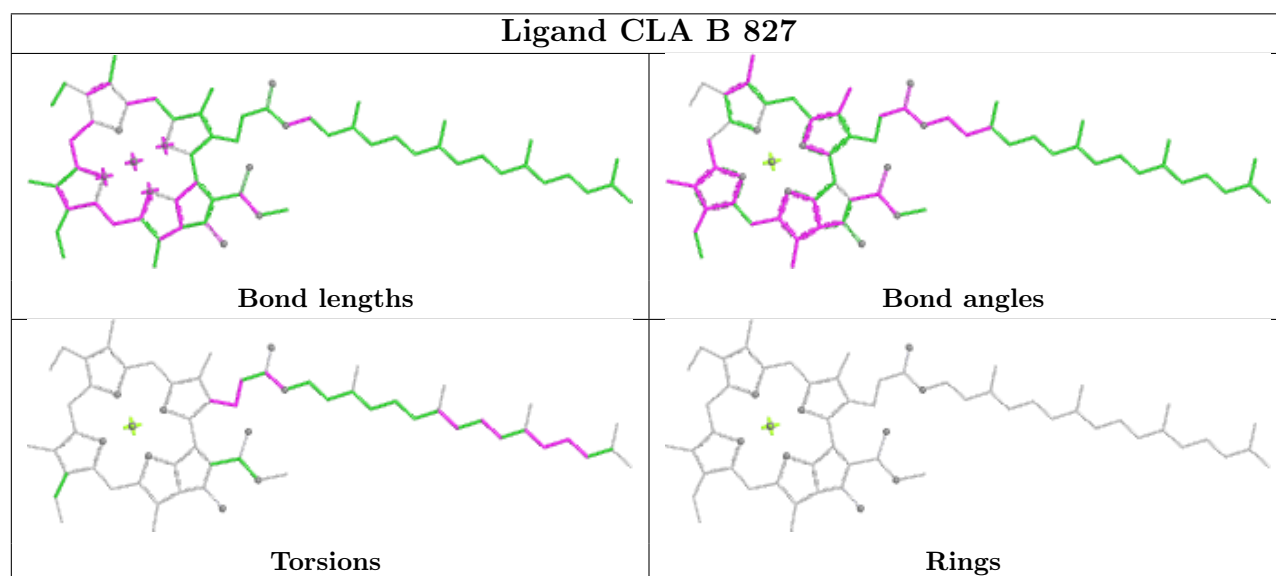
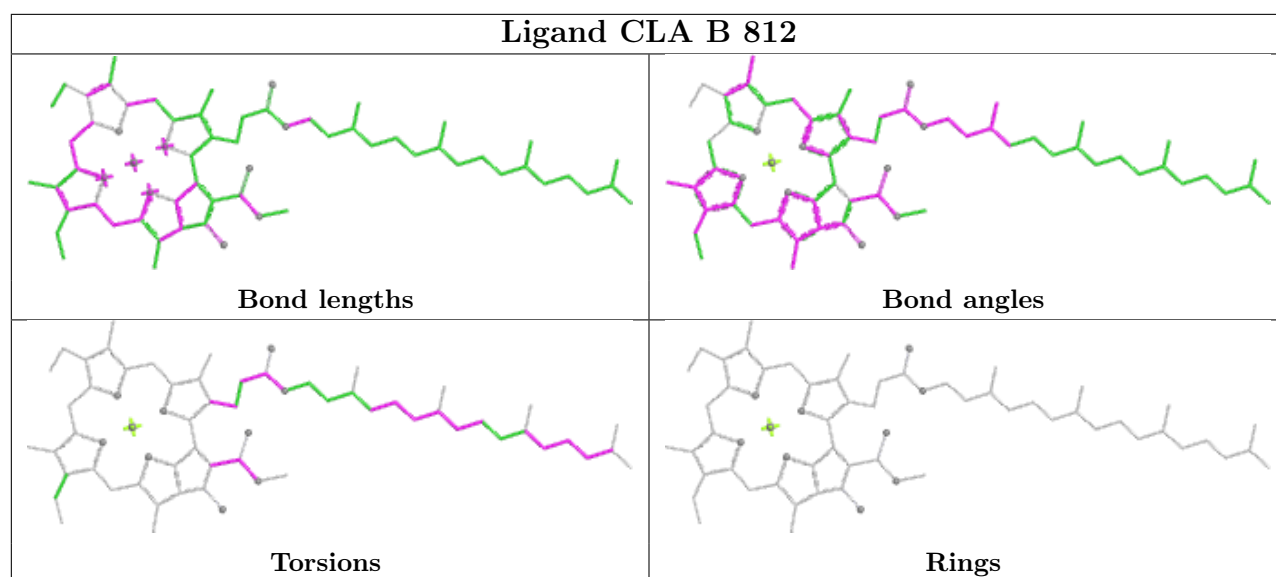
Torsions

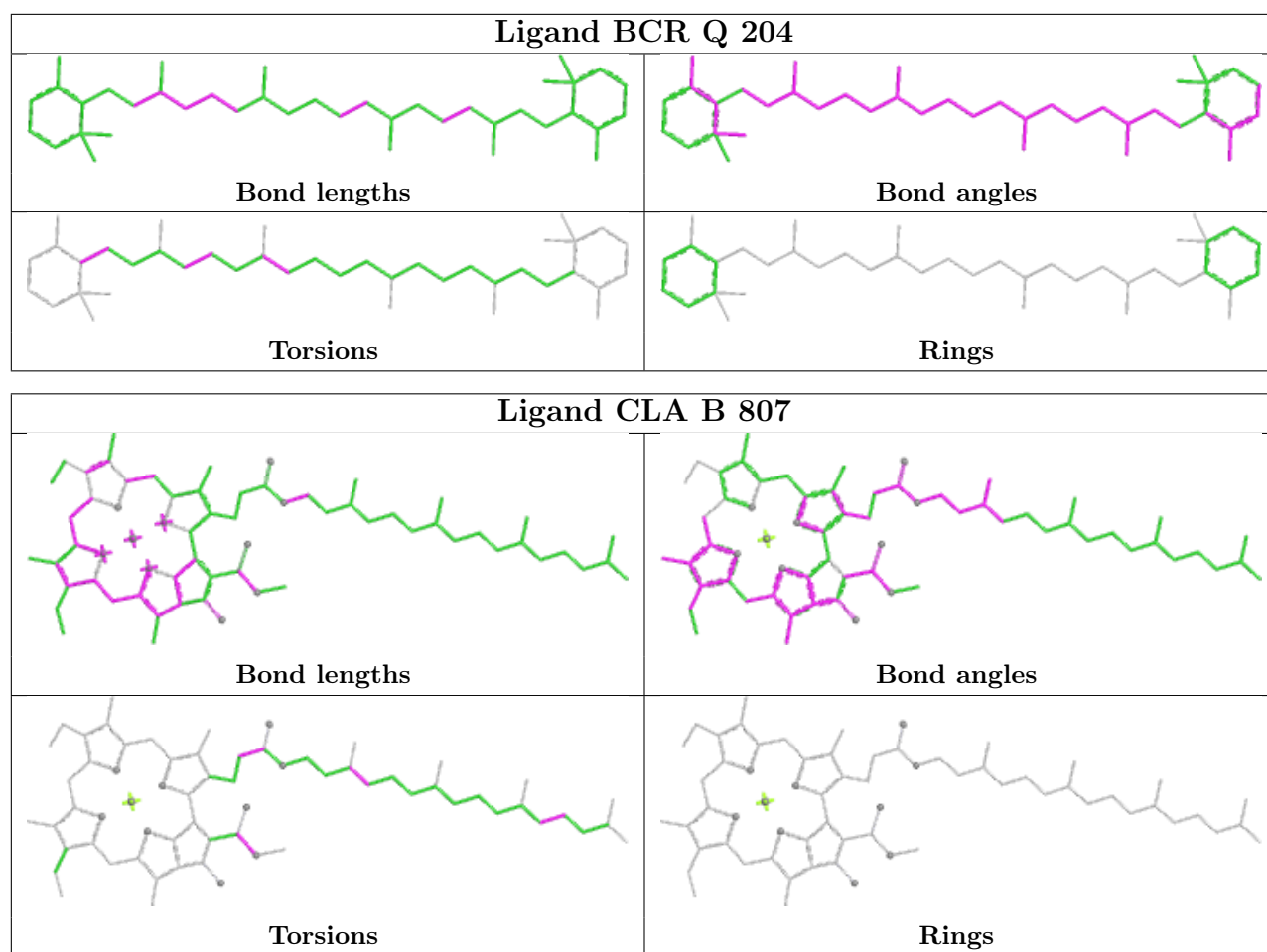


Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

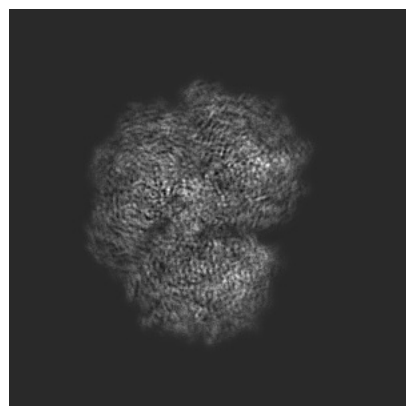
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43525. These allow visual inspection of the internal detail of the map and identification of artifacts.

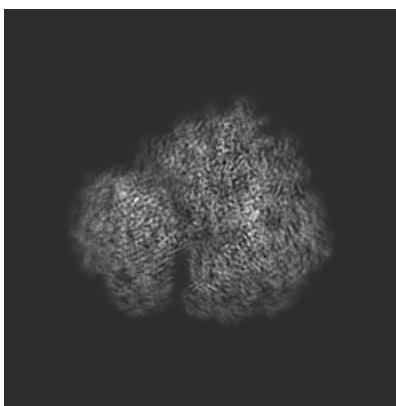
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

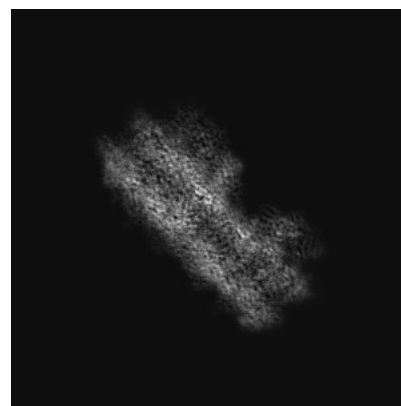
6.1.1 Primary map



X

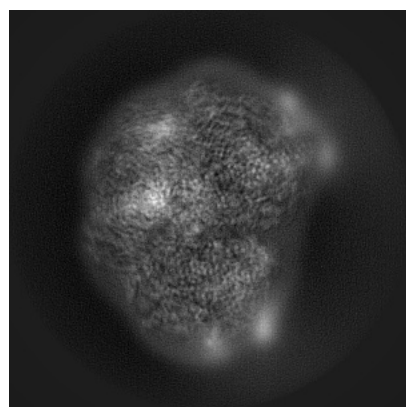


Y

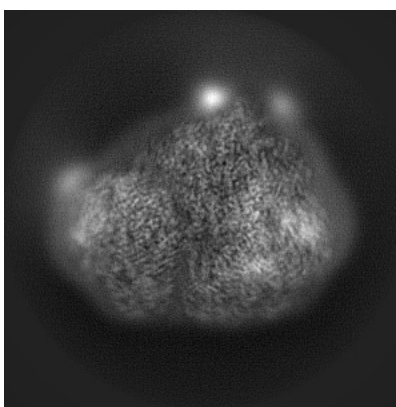


Z

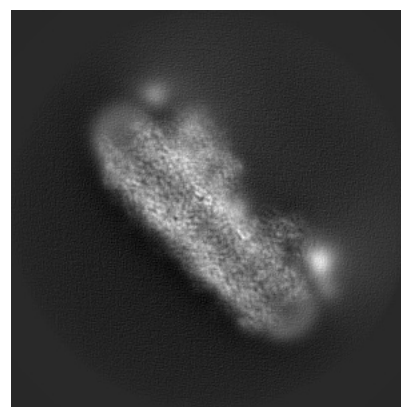
6.1.2 Raw map



X



Y

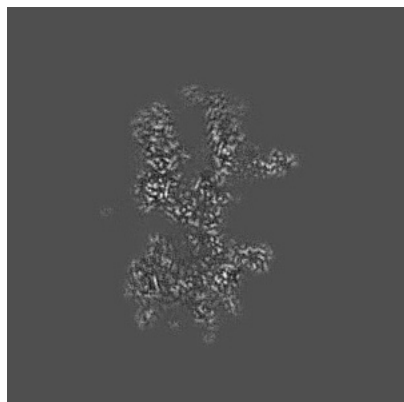


Z

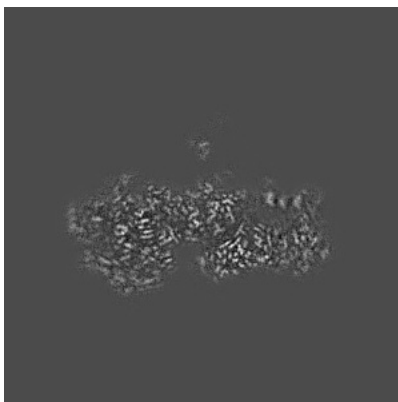
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

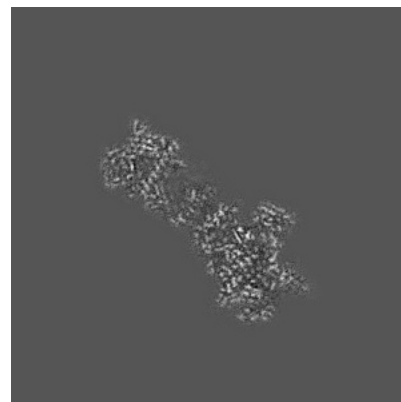
6.2.1 Primary map



X Index: 180

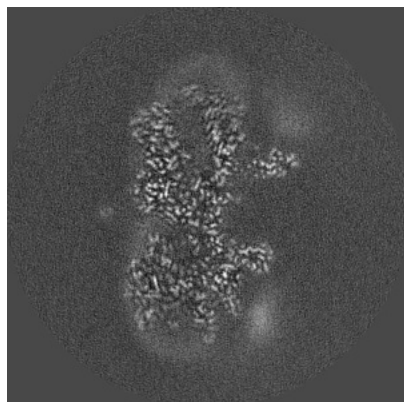


Y Index: 180

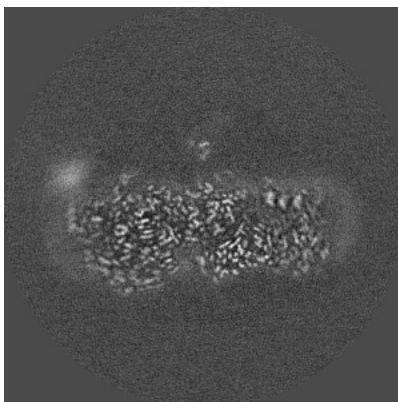


Z Index: 180

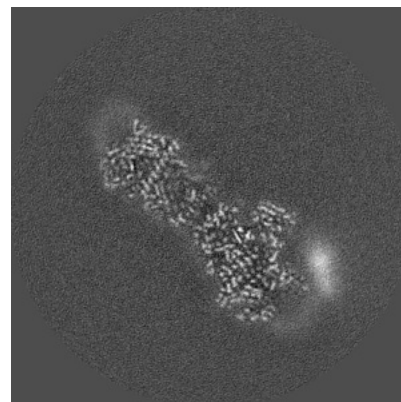
6.2.2 Raw map



X Index: 180



Y Index: 180

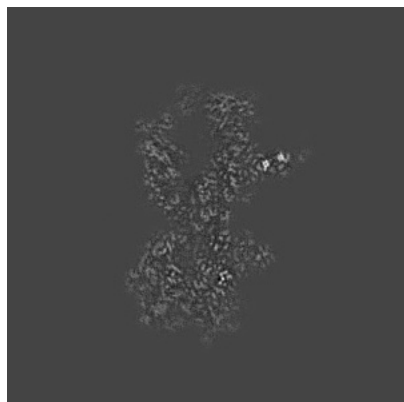


Z Index: 180

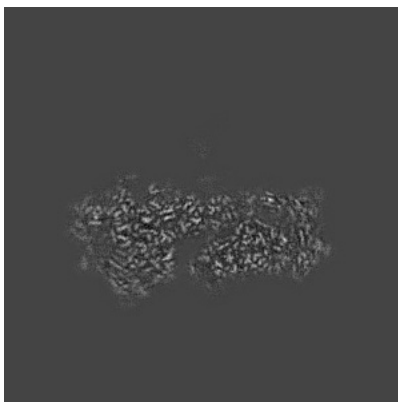
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

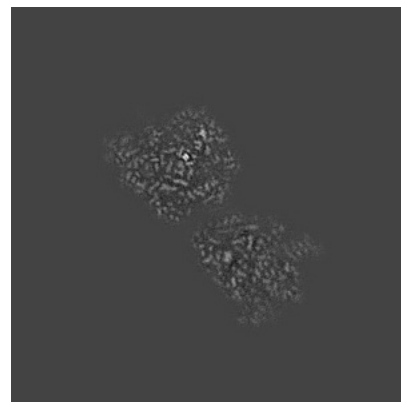
6.3.1 Primary map



X Index: 172

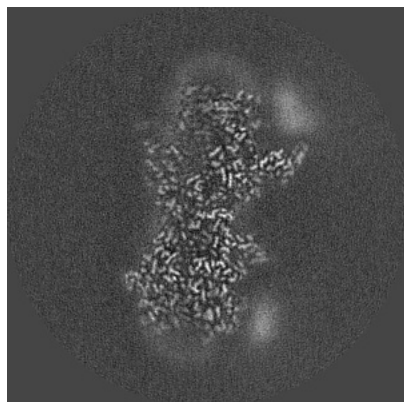


Y Index: 185

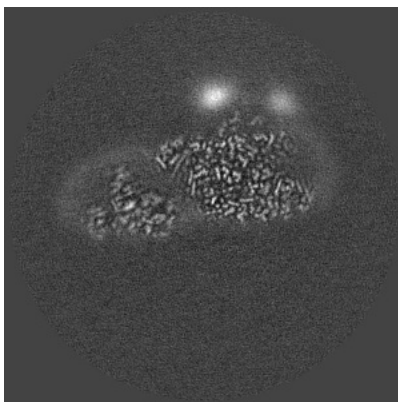


Z Index: 223

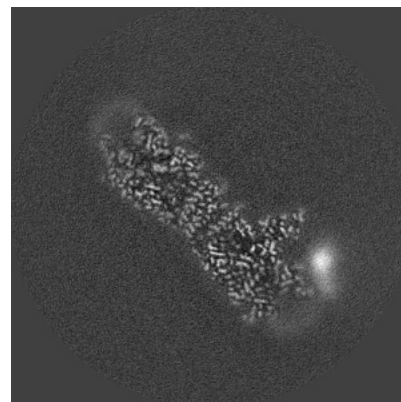
6.3.2 Raw map



X Index: 167



Y Index: 133

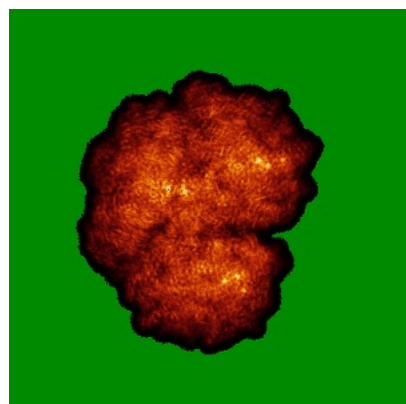


Z Index: 191

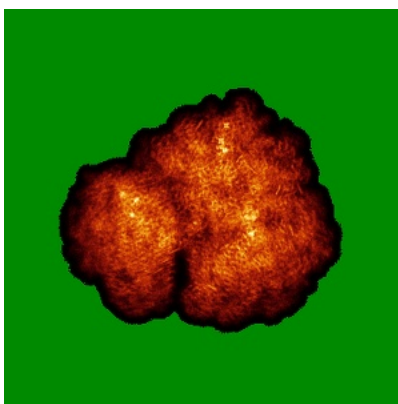
The images above show the largest variance slices of the map in three orthogonal directions.

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

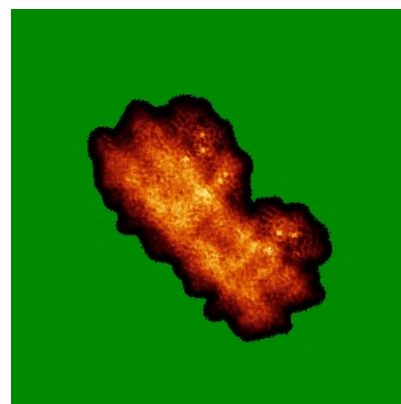
6.4.1 Primary map



X

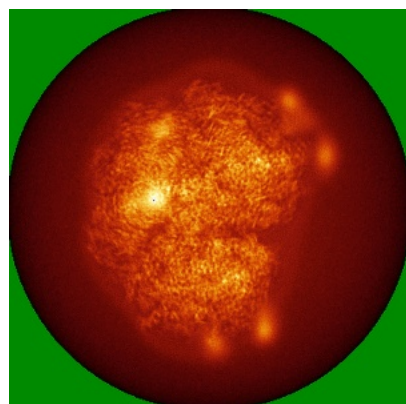


Y

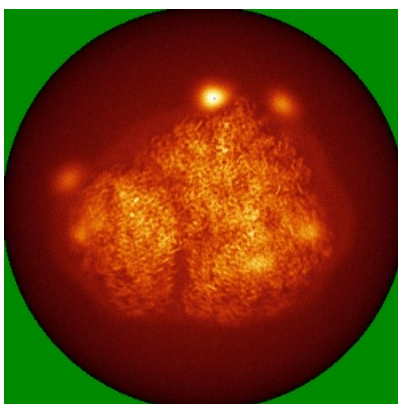


Z

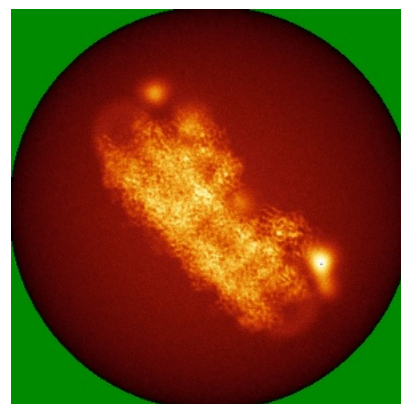
6.4.2 Raw map



X



Y

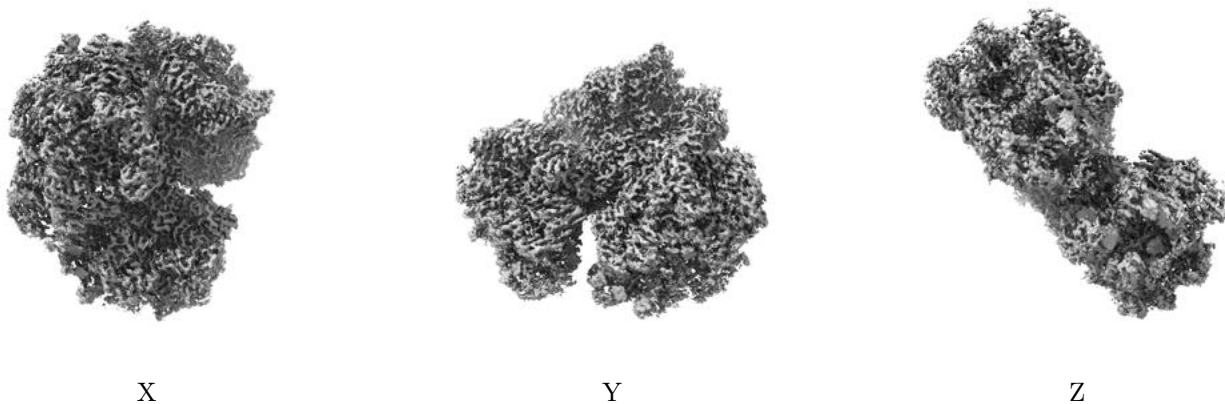


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

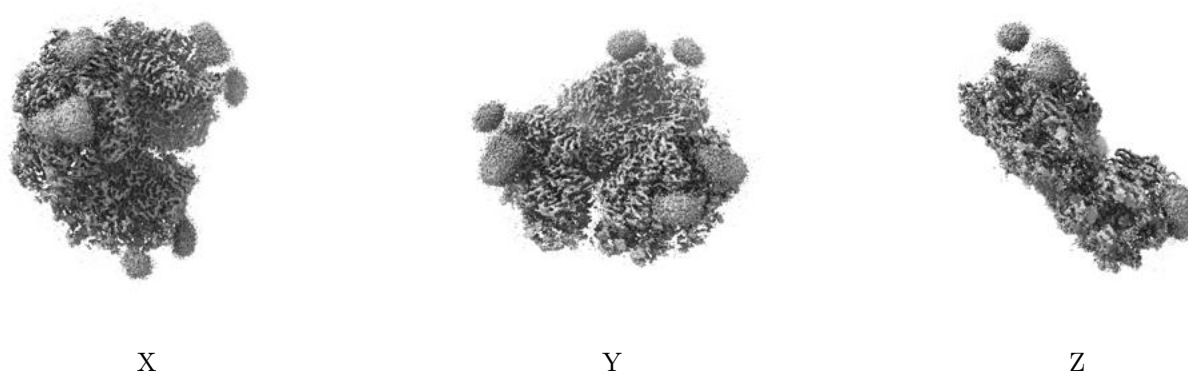
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00404. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

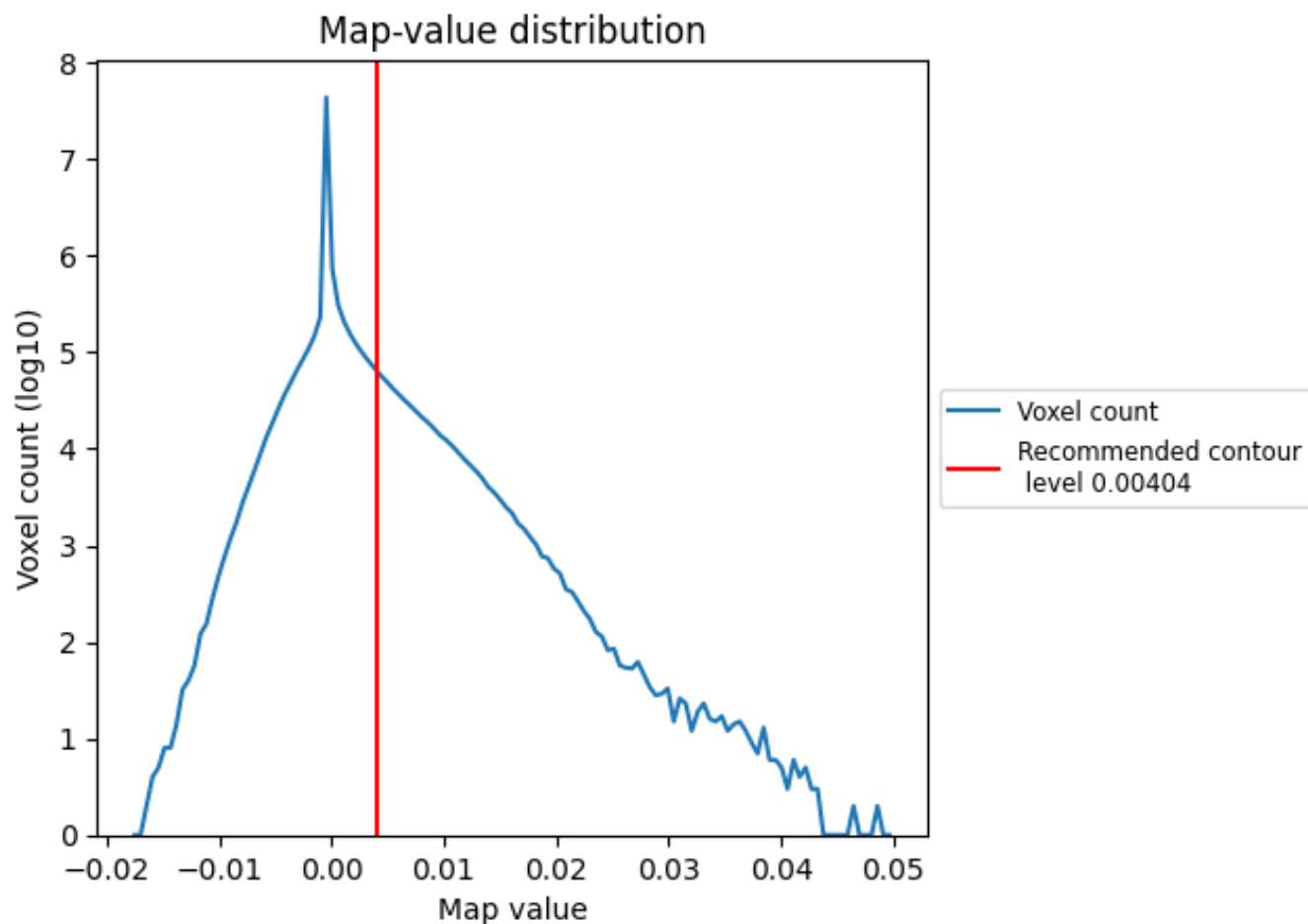
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

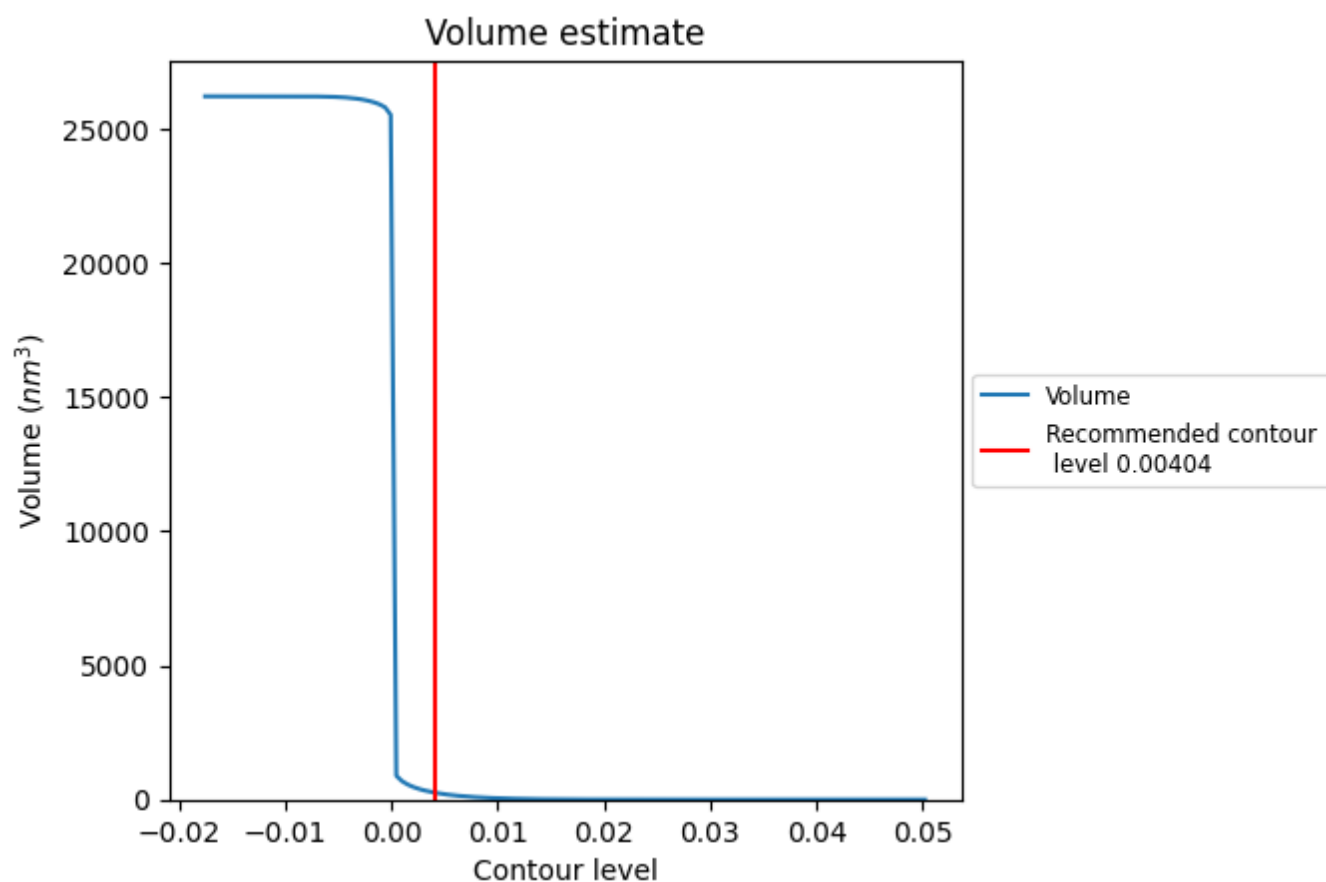
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

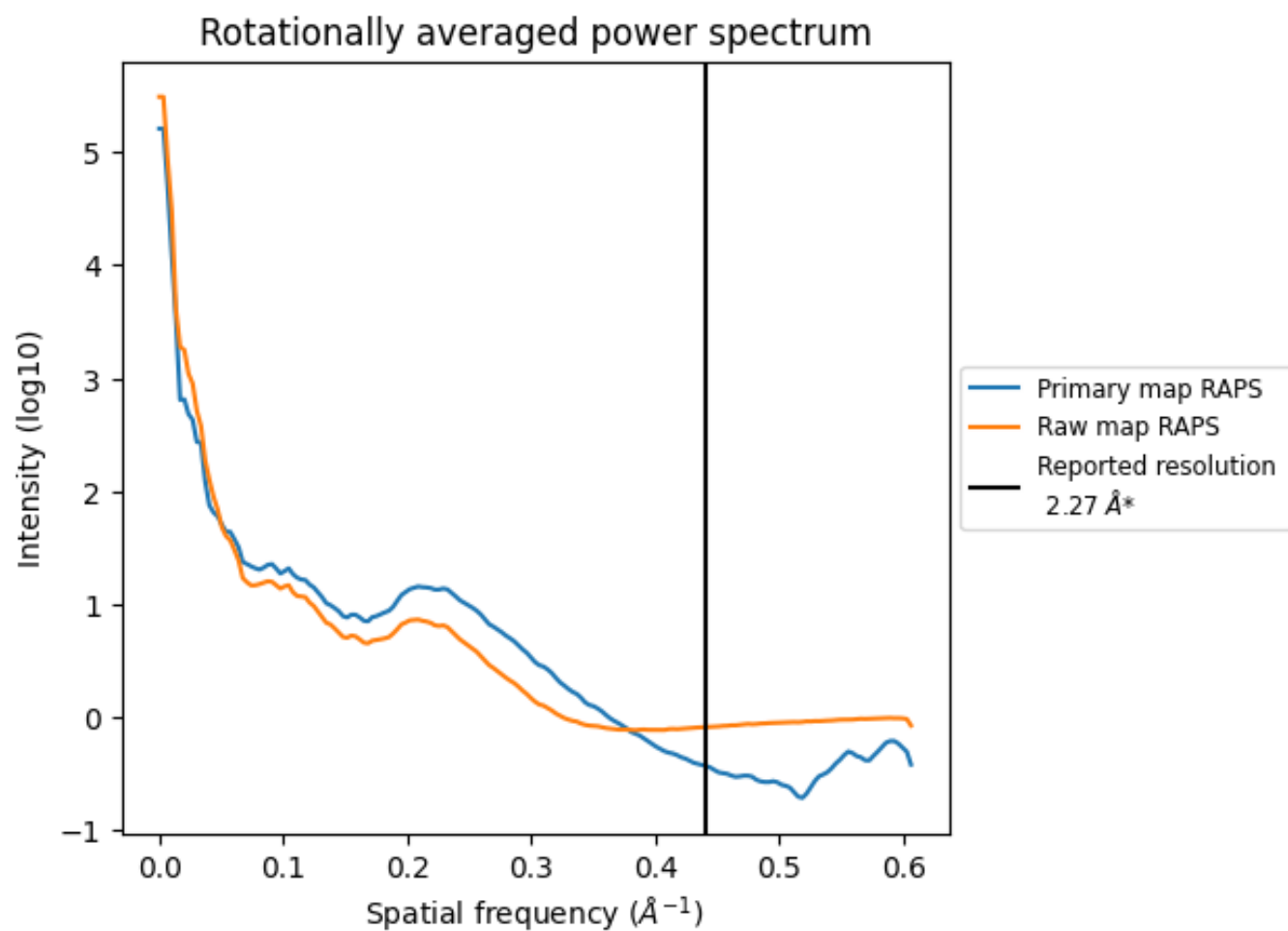
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 261 nm^3 ; this corresponds to an approximate mass of 235 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

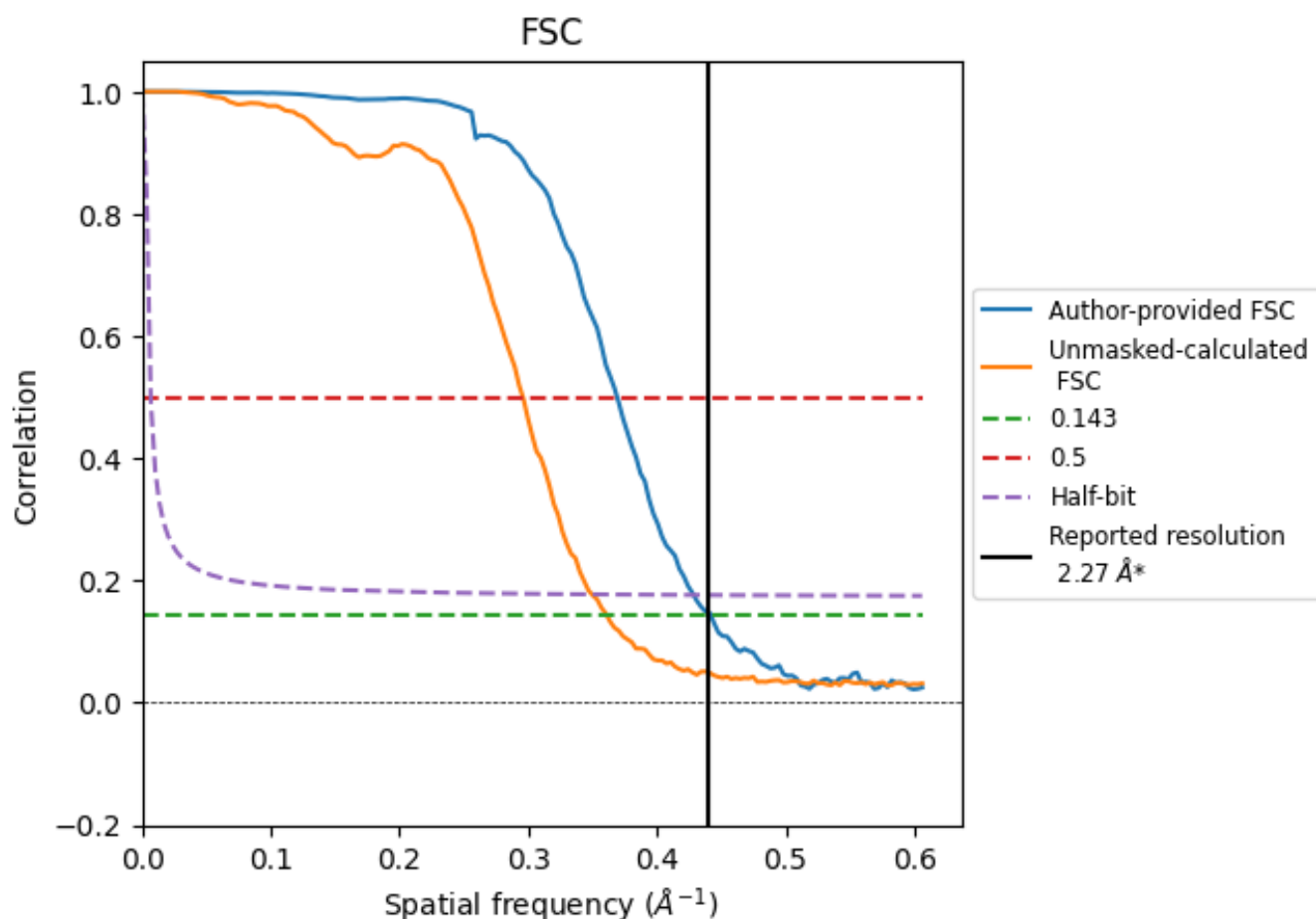


*Reported resolution corresponds to spatial frequency of 0.441 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.441 \AA^{-1}

8.2 Resolution estimates [i](#)

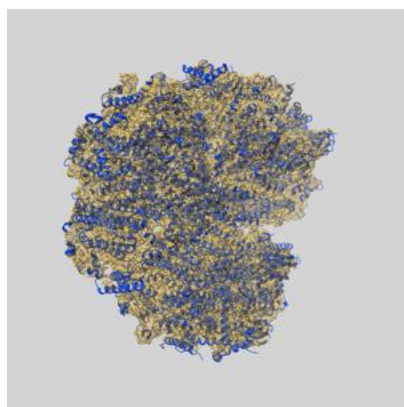
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.27	-	-
Author-provided FSC curve	2.26	2.71	2.33
Unmasked-calculated*	2.77	3.38	2.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.77 differs from the reported value 2.27 by more than 10 %

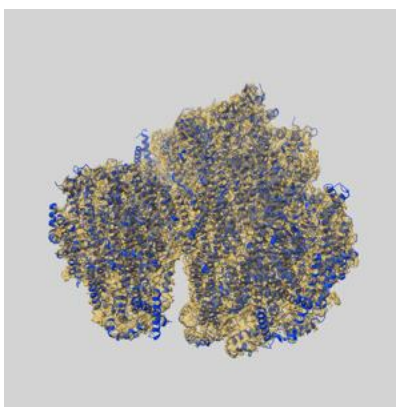
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43525 and PDB model 8VU3. Per-residue inclusion information can be found in section [3](#) on page [38](#).

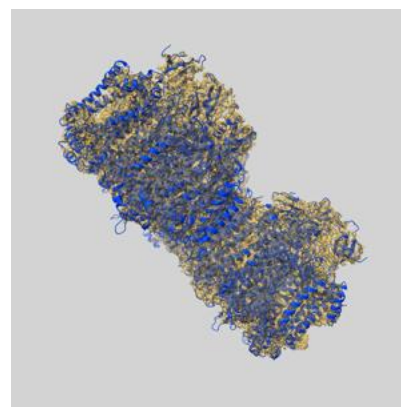
9.1 Map-model overlay [i](#)



X



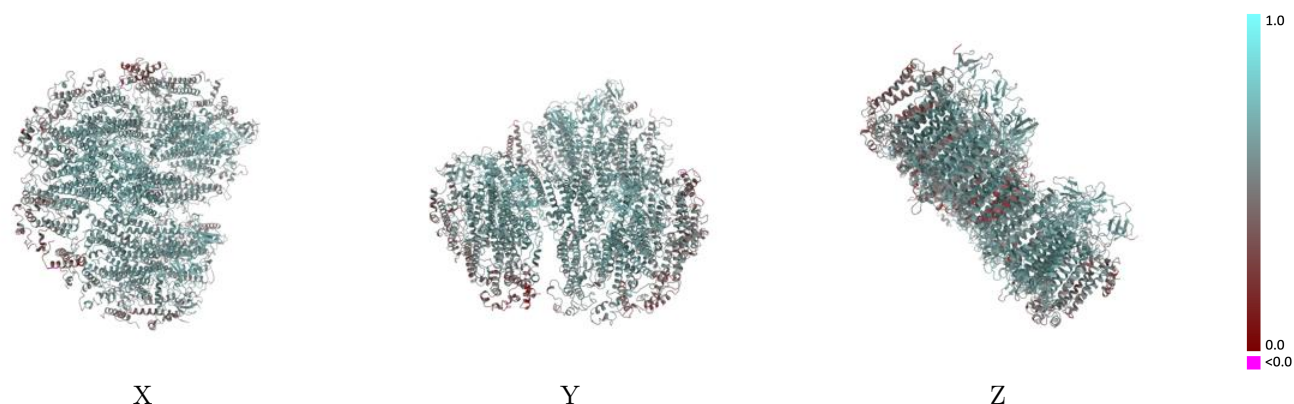
Y



Z

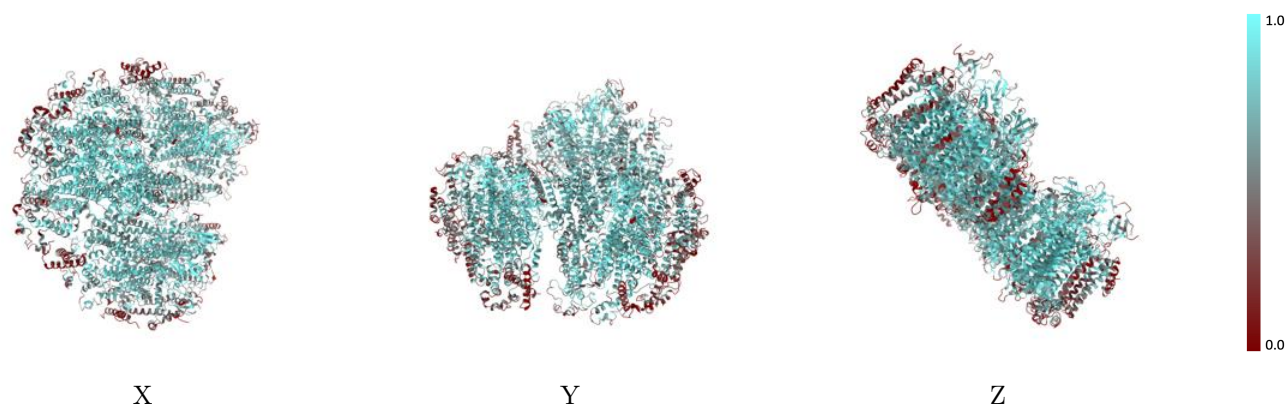
The images above show the 3D surface view of the map at the recommended contour level 0.00404 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



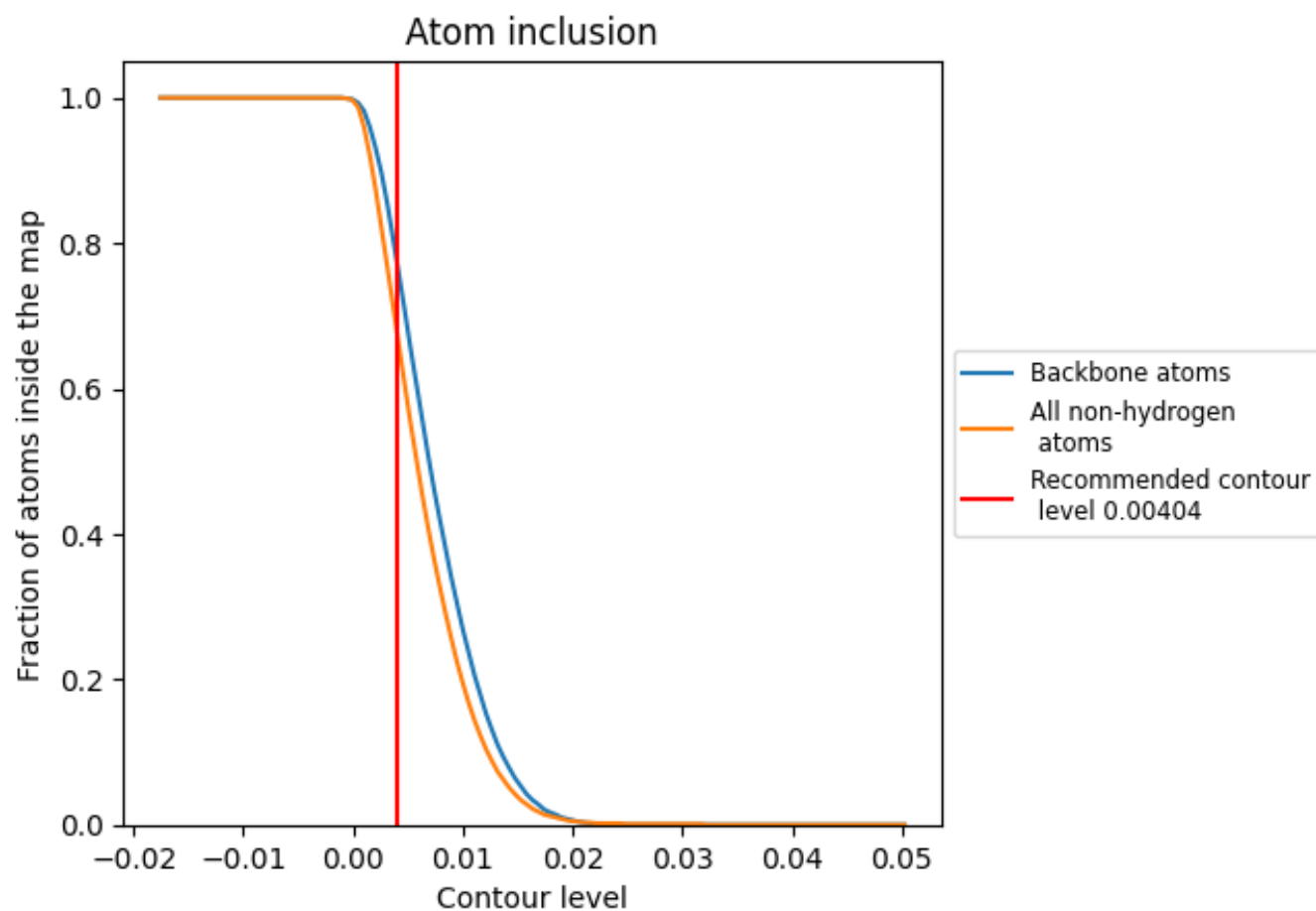
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00404).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





The table lists the average atom inclusion at the recommended contour level (0.00404) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6720	 0.5780
A	 0.6840	 0.5640
B	 0.7340	 0.6050
C	 0.8770	 0.6690
D	 0.6810	 0.6160
E	 0.5850	 0.5720
F	 0.3030	 0.4580
G	 0.7180	 0.5850
H	 0.7490	 0.6090
I	 0.7110	 0.6300
J	 0.3040	 0.4590
K	 0.1450	 0.3370
L	 0.7520	 0.6490
M	 0.4350	 0.5210
N	 0.9020	 0.6730
O	 0.7010	 0.6180
P	 0.6410	 0.5910
Q	 0.4090	 0.4840
R	 0.7590	 0.6360
S	 0.3500	 0.4650
T	 0.1470	 0.3150
U	 0.7410	 0.6430
V	 0.4640	 0.5230
W	 0.2430	 0.4390
X	 0.2020	 0.4370
a	 0.6820	 0.5690
b	 0.7270	 0.5930
c	 0.8880	 0.6710
d	 0.6740	 0.6020
e	 0.5640	 0.5570
f	 0.3000	 0.4390
i	 0.7160	 0.6300
j	 0.2980	 0.4320
k	 0.1380	 0.3200
l	 0.7440	 0.6410



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
m	 0.4040	 0.5130
x	 0.1900	 0.4080