



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:38 PM EST

PDB ID : 7LX0  
EMDB ID : EMD-23563  
Title : Quantitative assessment of chlorophyll types in cryo-EM maps of photosystem I acclimated to far-red light  
Authors : Gisriel, C.J.; Wang, J.  
Deposited on : 2021-03-02  
Resolution : 2.96 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

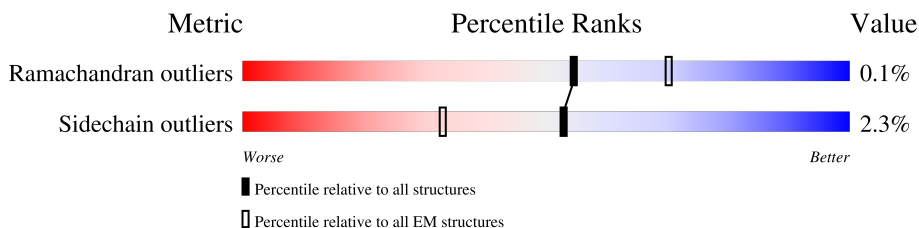
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.96 Å.

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



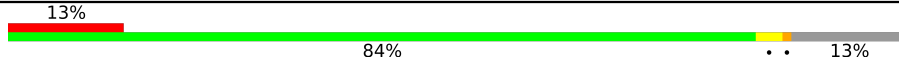

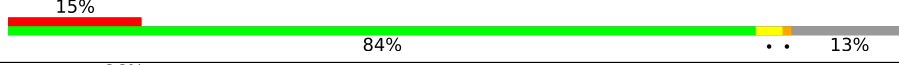

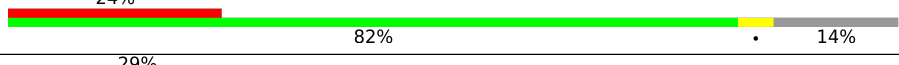
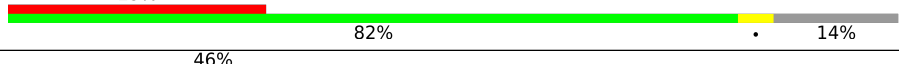


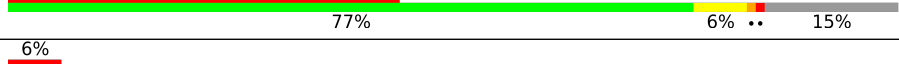


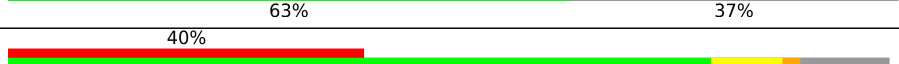
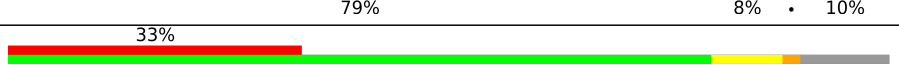
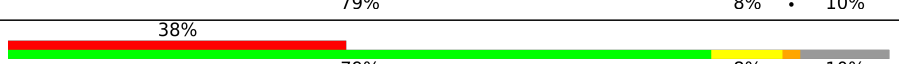

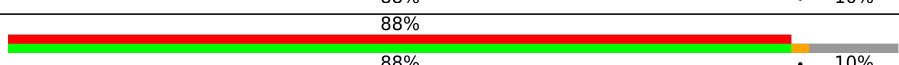

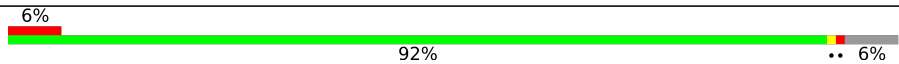
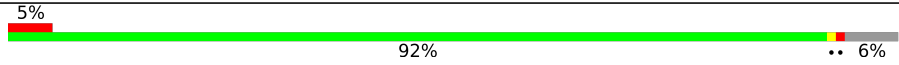
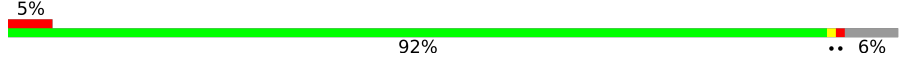
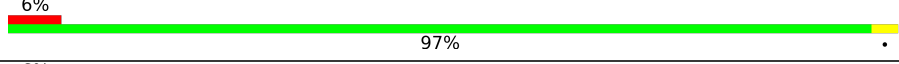
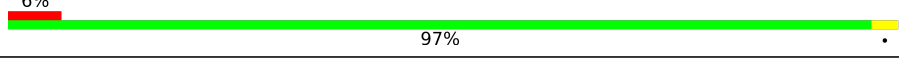
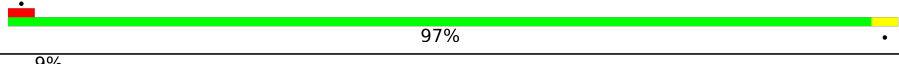


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	788	 6% 94% 5%
1	G	788	 6% 94% 5%
1	a	788	 6% 94% 5%
2	B	741	 1% 99%
2	H	741	 1% 99%
2	b	741	 1% 99%
3	C	81	 1% 93% 5%
3	N	81	 1% 93% 5%
3	c	81	 1% 93% 6%

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Mol	Chain	Length	Quality of chain
4	D	159	
4	O	159	
4	d	159	
5	E	72	
5	P	72	
5	e	72	
6	F	159	
6	Q	159	
6	f	159	
7	I	67	
7	R	67	
7	i	67	
8	J	48	
8	S	48	
8	j	48	
9	K	49	
9	T	49	
9	k	49	
10	L	174	
10	U	174	
10	l	174	
11	M	31	
11	V	31	
11	m	31	
12	W	101	

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Mol	Chain	Length	Quality of chain
12	X	101	
12	x	101	

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	1011	X	-	-	-
13	CL0	G	1011	X	-	-	-
13	CL0	a	1011	X	-	-	-
14	CLA	A	1012	X	-	-	-
14	CLA	A	1013	X	-	-	-
14	CLA	A	1101	X	-	-	-
14	CLA	A	1102	X	-	-	-
14	CLA	A	1103	X	-	-	-
14	CLA	A	1104	X	-	-	-
14	CLA	A	1105	X	-	-	-
14	CLA	A	1106	X	-	-	-
14	CLA	A	1107	X	-	-	-
14	CLA	A	1108	X	-	-	-
14	CLA	A	1109	X	-	-	-
14	CLA	A	1110	X	-	-	-
14	CLA	A	1111	X	-	-	-
14	CLA	A	1112	X	-	-	-
14	CLA	A	1113	X	-	-	-
14	CLA	A	1114	X	-	-	-
14	CLA	A	1115	X	-	-	-
14	CLA	A	1116	X	-	-	-
14	CLA	A	1117	X	-	-	-
14	CLA	A	1118	X	-	-	-
14	CLA	A	1119	X	-	-	-
14	CLA	A	1120	X	-	-	-
14	CLA	A	1122	X	-	-	-
14	CLA	A	1123	X	-	-	-
14	CLA	A	1124	X	-	-	-
14	CLA	A	1125	X	-	-	-
14	CLA	A	1126	X	-	-	-
14	CLA	A	1127	X	-	-	-
14	CLA	A	1128	X	-	-	-
14	CLA	A	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	1130	X	-	-	-
14	CLA	A	1131	X	-	-	-
14	CLA	A	1132	X	-	-	-
14	CLA	A	1133	X	-	-	-
14	CLA	A	1134	X	-	-	-
14	CLA	A	1135	X	-	-	-
14	CLA	A	1136	X	-	-	-
14	CLA	A	1137	X	-	-	-
14	CLA	A	1138	X	-	-	-
14	CLA	A	1139	X	-	-	-
14	CLA	A	1140	X	-	-	-
14	CLA	B	1021	X	-	-	-
14	CLA	B	1022	X	-	-	-
14	CLA	B	1023	X	-	-	-
14	CLA	B	1201	X	-	-	-
14	CLA	B	1202	X	-	-	-
14	CLA	B	1203	X	-	-	-
14	CLA	B	1204	X	-	-	-
14	CLA	B	1205	X	-	-	-
14	CLA	B	1206	X	-	-	-
14	CLA	B	1208	X	-	-	-
14	CLA	B	1209	X	-	-	-
14	CLA	B	1210	X	-	-	-
14	CLA	B	1211	X	-	-	-
14	CLA	B	1212	X	-	-	-
14	CLA	B	1213	X	-	-	-
14	CLA	B	1214	X	-	-	-
14	CLA	B	1215	X	-	-	-
14	CLA	B	1216	X	-	-	-
14	CLA	B	1217	X	-	-	-
14	CLA	B	1218	X	-	-	-
14	CLA	B	1219	X	-	-	-
14	CLA	B	1220	X	-	-	-
14	CLA	B	1221	X	-	-	-
14	CLA	B	1222	X	-	-	-
14	CLA	B	1223	X	-	-	-
14	CLA	B	1224	X	-	-	-
14	CLA	B	1225	X	-	-	-
14	CLA	B	1226	X	-	-	-
14	CLA	B	1227	X	-	-	-
14	CLA	B	1228	X	-	-	-
14	CLA	B	1229	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	1231	X	-	-	-
14	CLA	B	1232	X	-	-	-
14	CLA	B	1233	X	-	-	-
14	CLA	B	1234	X	-	-	-
14	CLA	B	1235	X	-	-	-
14	CLA	B	1236	X	-	-	-
14	CLA	B	1239	X	-	-	-
14	CLA	G	1012	X	-	-	-
14	CLA	G	1013	X	-	-	-
14	CLA	G	1101	X	-	-	-
14	CLA	G	1102	X	-	-	-
14	CLA	G	1103	X	-	-	-
14	CLA	G	1104	X	-	-	-
14	CLA	G	1105	X	-	-	-
14	CLA	G	1106	X	-	-	-
14	CLA	G	1107	X	-	-	-
14	CLA	G	1108	X	-	-	-
14	CLA	G	1109	X	-	-	-
14	CLA	G	1110	X	-	-	-
14	CLA	G	1111	X	-	-	-
14	CLA	G	1112	X	-	-	-
14	CLA	G	1113	X	-	-	-
14	CLA	G	1114	X	-	-	-
14	CLA	G	1115	X	-	-	-
14	CLA	G	1116	X	-	-	-
14	CLA	G	1117	X	-	-	-
14	CLA	G	1118	X	-	-	-
14	CLA	G	1119	X	-	-	-
14	CLA	G	1120	X	-	-	-
14	CLA	G	1122	X	-	-	-
14	CLA	G	1123	X	-	-	-
14	CLA	G	1124	X	-	-	-
14	CLA	G	1125	X	-	-	-
14	CLA	G	1126	X	-	-	-
14	CLA	G	1127	X	-	-	-
14	CLA	G	1128	X	-	-	-
14	CLA	G	1129	X	-	-	-
14	CLA	G	1130	X	-	-	-
14	CLA	G	1131	X	-	-	-
14	CLA	G	1132	X	-	-	-
14	CLA	G	1133	X	-	-	-
14	CLA	G	1134	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	G	1135	X	-	-	-
14	CLA	G	1136	X	-	-	-
14	CLA	G	1137	X	-	-	-
14	CLA	G	1138	X	-	-	-
14	CLA	G	1139	X	-	-	-
14	CLA	G	1140	X	-	-	-
14	CLA	H	1021	X	-	-	-
14	CLA	H	1022	X	-	-	-
14	CLA	H	1023	X	-	-	-
14	CLA	H	1201	X	-	-	-
14	CLA	H	1202	X	-	-	-
14	CLA	H	1203	X	-	-	-
14	CLA	H	1204	X	-	-	-
14	CLA	H	1205	X	-	-	-
14	CLA	H	1206	X	-	-	-
14	CLA	H	1208	X	-	-	-
14	CLA	H	1209	X	-	-	-
14	CLA	H	1210	X	-	-	-
14	CLA	H	1211	X	-	-	-
14	CLA	H	1212	X	-	-	-
14	CLA	H	1213	X	-	-	-
14	CLA	H	1214	X	-	-	-
14	CLA	H	1215	X	-	-	-
14	CLA	H	1216	X	-	-	-
14	CLA	H	1217	X	-	-	-
14	CLA	H	1218	X	-	-	-
14	CLA	H	1219	X	-	-	-
14	CLA	H	1220	X	-	-	-
14	CLA	H	1221	X	-	-	-
14	CLA	H	1222	X	-	-	-
14	CLA	H	1223	X	-	-	-
14	CLA	H	1224	X	-	-	-
14	CLA	H	1225	X	-	-	-
14	CLA	H	1226	X	-	-	-
14	CLA	H	1227	X	-	-	-
14	CLA	H	1228	X	-	-	-
14	CLA	H	1229	X	-	-	-
14	CLA	H	1231	X	-	-	-
14	CLA	H	1232	X	-	-	-
14	CLA	H	1233	X	-	-	-
14	CLA	H	1234	X	-	-	-
14	CLA	H	1235	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	H	1236	X	-	-	-
14	CLA	H	1239	X	-	-	-
14	CLA	K	1401	X	-	-	-
14	CLA	L	1501	X	-	-	-
14	CLA	L	1502	X	-	-	-
14	CLA	L	1503	X	-	-	-
14	CLA	T	1401	X	-	-	-
14	CLA	U	1501	X	-	-	-
14	CLA	U	1502	X	-	-	-
14	CLA	U	1503	X	-	-	-
14	CLA	W	1701	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	a	1012	X	-	-	-
14	CLA	a	1013	X	-	-	-
14	CLA	a	1101	X	-	-	-
14	CLA	a	1102	X	-	-	-
14	CLA	a	1103	X	-	-	-
14	CLA	a	1104	X	-	-	-
14	CLA	a	1105	X	-	-	-
14	CLA	a	1106	X	-	-	-
14	CLA	a	1107	X	-	-	-
14	CLA	a	1108	X	-	-	-
14	CLA	a	1109	X	-	-	-
14	CLA	a	1110	X	-	-	-
14	CLA	a	1111	X	-	-	-
14	CLA	a	1112	X	-	-	-
14	CLA	a	1113	X	-	-	-
14	CLA	a	1114	X	-	-	-
14	CLA	a	1115	X	-	-	-
14	CLA	a	1116	X	-	-	-
14	CLA	a	1117	X	-	-	-
14	CLA	a	1118	X	-	-	-
14	CLA	a	1119	X	-	-	-
14	CLA	a	1120	X	-	-	-
14	CLA	a	1122	X	-	-	-
14	CLA	a	1123	X	-	-	-
14	CLA	a	1124	X	-	-	-
14	CLA	a	1125	X	-	-	-
14	CLA	a	1126	X	-	-	-
14	CLA	a	1127	X	-	-	-
14	CLA	a	1128	X	-	-	-
14	CLA	a	1129	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	1130	X	-	-	-
14	CLA	a	1131	X	-	-	-
14	CLA	a	1132	X	-	-	-
14	CLA	a	1133	X	-	-	-
14	CLA	a	1134	X	-	-	-
14	CLA	a	1135	X	-	-	-
14	CLA	a	1136	X	-	-	-
14	CLA	a	1137	X	-	-	-
14	CLA	a	1138	X	-	-	-
14	CLA	a	1139	X	-	-	-
14	CLA	a	1140	X	-	-	-
14	CLA	b	1021	X	-	-	-
14	CLA	b	1022	X	-	-	-
14	CLA	b	1023	X	-	-	-
14	CLA	b	1201	X	-	-	-
14	CLA	b	1202	X	-	-	-
14	CLA	b	1203	X	-	-	-
14	CLA	b	1204	X	-	-	-
14	CLA	b	1205	X	-	-	-
14	CLA	b	1206	X	-	-	-
14	CLA	b	1208	X	-	-	-
14	CLA	b	1209	X	-	-	-
14	CLA	b	1210	X	-	-	-
14	CLA	b	1211	X	-	-	-
14	CLA	b	1212	X	-	-	-
14	CLA	b	1213	X	-	-	-
14	CLA	b	1214	X	-	-	-
14	CLA	b	1215	X	-	-	-
14	CLA	b	1216	X	-	-	-
14	CLA	b	1217	X	-	-	-
14	CLA	b	1218	X	-	-	-
14	CLA	b	1219	X	-	-	-
14	CLA	b	1220	X	-	-	-
14	CLA	b	1221	X	-	-	-
14	CLA	b	1222	X	-	-	-
14	CLA	b	1223	X	-	-	-
14	CLA	b	1224	X	-	-	-
14	CLA	b	1225	X	-	-	-
14	CLA	b	1226	X	-	-	-
14	CLA	b	1227	X	-	-	-
14	CLA	b	1228	X	-	-	-
14	CLA	b	1229	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	1231	X	-	-	-
14	CLA	b	1232	X	-	-	-
14	CLA	b	1233	X	-	-	-
14	CLA	b	1234	X	-	-	-
14	CLA	b	1235	X	-	-	-
14	CLA	b	1236	X	-	-	-
14	CLA	b	1239	X	-	-	-
14	CLA	k	1401	X	-	-	-
14	CLA	l	1501	X	-	-	-
14	CLA	l	1502	X	-	-	-
14	CLA	l	1503	X	-	-	-
14	CLA	x	1701	X	-	-	-

## 2 Entry composition i

There are 22 unique types of molecules in this entry. The entry contains 72462 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
			Total	C	N	O	S		
1	G	751	Total	C	N	O	S	0	0
			5931	3892	1013	993	33		
1	a	751	Total	C	N	O	S	0	0
			5931	3892	1013	993	33		
1	A	751	Total	C	N	O	S	0	0
			5931	3892	1013	993	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	739	Total	C	N	O	S	0	0
			5913	3896	997	1002	18		
2	b	739	Total	C	N	O	S	0	0
			5913	3896	997	1002	18		
2	B	739	Total	C	N	O	S	0	0
			5913	3896	997	1002	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	N	80	Total	C	N	O	S	0	0
			601	367	105	118	11		
3	c	80	Total	C	N	O	S	0	0
			601	367	105	118	11		
3	C	80	Total	C	N	O	S	0	0
			601	367	105	118	11		

- Molecule 4 is a protein called Photosystem I protein PsuD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	O	139	Total	C	N	O	S	0	0
			1092	694	192	203	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	139	Total	C	N	O	S	0	0
			1092	694	192	203	3		
4	D	139	Total	C	N	O	S	0	0
			1092	694	192	203	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	62	Total	C	N	O	0	0
			497	313	88	96		
5	e	62	Total	C	N	O	0	0
			497	313	88	96		
5	E	62	Total	C	N	O	0	0
			497	313	88	96		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	135	Total	C	N	O	S	0	0
			1060	694	167	192	7		
6	f	135	Total	C	N	O	S	0	0
			1060	694	167	192	7		
6	F	135	Total	C	N	O	S	0	0
			1060	694	167	192	7		

- Molecule 7 is a protein called photosystem I subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	42	Total	C	N	O	S	0	0
			350	246	48	54	2		
7	i	42	Total	C	N	O	S	0	0
			350	246	48	54	2		
7	I	42	Total	C	N	O	S	0	0
			350	246	48	54	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	-	initiating methionine	UNP A0A2N6MR25
i	1	MET	-	initiating methionine	UNP A0A2N6MR25
I	1	MET	-	initiating methionine	UNP A0A2N6MR25

- Molecule 8 is a protein called Photosystem I reaction centre subunit IX / PsaJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	S	43	Total	C	N	O	0	0
			344	238	51	55		
8	j	43	Total	C	N	O	0	0
			344	238	51	55		
8	J	43	Total	C	N	O	0	0
			344	238	51	55		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	44	Total	C	N	O	S	0	0
			253	161	46	45	1		
9	k	44	Total	C	N	O	S	0	0
			253	161	46	45	1		
9	K	44	Total	C	N	O	S	0	0
			253	161	46	45	1		

- Molecule 10 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	163	Total	C	N	O	S	0	0
			1227	792	207	223	5		
10	l	163	Total	C	N	O	S	0	0
			1227	792	207	223	5		
10	L	163	Total	C	N	O	S	0	0
			1227	792	207	223	5		

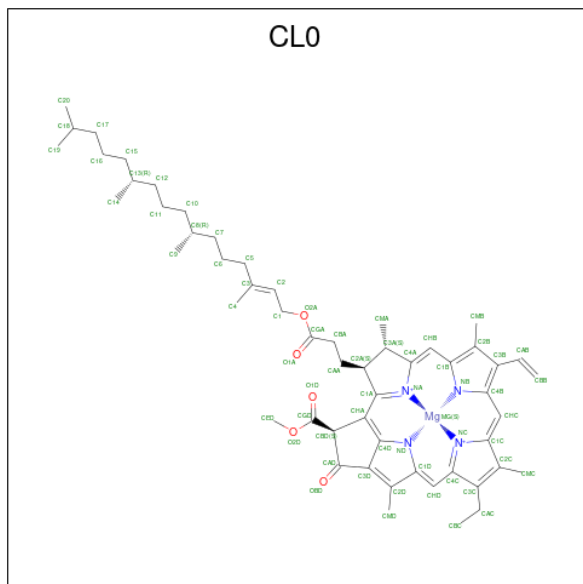
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	31	Total	C	N	O	S	0	0
			245	164	37	43	1		
11	m	31	Total	C	N	O	S	0	0
			245	164	37	43	1		
11	M	31	Total	C	N	O	S	0	0
			245	164	37	43	1		

- Molecule 12 is a protein called Photosystem one PsaX.

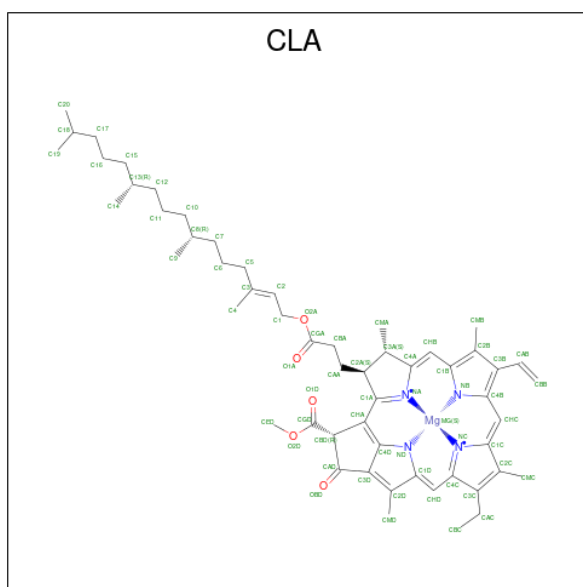
Mol	Chain	Residues	Atoms				AltConf	Trace
12	W	29	Total	C	N	O	0	0
			246	172	36	38		
12	x	29	Total	C	N	O	0	0
			246	172	36	38		
12	X	29	Total	C	N	O	0	0
			246	172	36	38		

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



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

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



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
14	G	1	2315	1905	41	164	205	0
14	G	1	2315	1905	41	164	205	0
14	G	1	2315	1905	41	164	205	0
14	G	1	2315	1905	41	164	205	0
14	G	1	2315	1905	41	164	205	0
14	G	1	2315	1905	41	164	205	0
14	G	1	2315	1905	41	164	205	0
14	G	1	2315	1905	41	164	205	0
14	G	1	2315	1905	41	164	205	0
14	G	1	2315	1905	41	164	205	0
14	G	1	2315	1905	41	164	205	0
14	G	1	2315	1905	41	164	205	0
14	G	1	2315	1905	41	164	205	0
14	G	1	2315	1905	41	164	205	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	G	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	H	1	Total 2220	C 1840	Mg 38	N 152	O 190	0

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Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total	C	Mg	N	O	0
			2220	1840	38	152	190	
14	H	1	Total	C	Mg	N	O	0
			2220	1840	38	152	190	
14	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	U	1	Total	C	Mg	N	O	0
			190	160	3	12	15	
14	U	1	Total	C	Mg	N	O	0
			190	160	3	12	15	
14	U	1	Total	C	Mg	N	O	0
			190	160	3	12	15	
14	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	a	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	a	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	a	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	a	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	a	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	a	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	a	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	a	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	a	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	a	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	a	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	a	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	a	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	a	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	a	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	a	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	a	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	a	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	b	1	Total 2220	C 1840	Mg 38	N 152	O 190	0

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			2220	1840	38	152	190	
14	b	1	Total	C	Mg	N	O	0
			2220	1840	38	152	190	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			190	160	3	12	15	
14	l	1	Total	C	Mg	N	O	0
			190	160	3	12	15	
14	l	1	Total	C	Mg	N	O	0
			190	160	3	12	15	
14	x	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	A	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	A	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	A	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	A	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	A	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	A	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	A	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	A	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	A	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	A	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	A	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	
14	A	1	Total	C	Mg	N	O	0
			2315	1905	41	164	205	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	A	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	A	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	A	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	A	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	A	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	A	1	Total 2315	C 1905	Mg 41	N 164	O 205	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0
14	B	1	Total 2220	C 1840	Mg 38	N 152	O 190	0

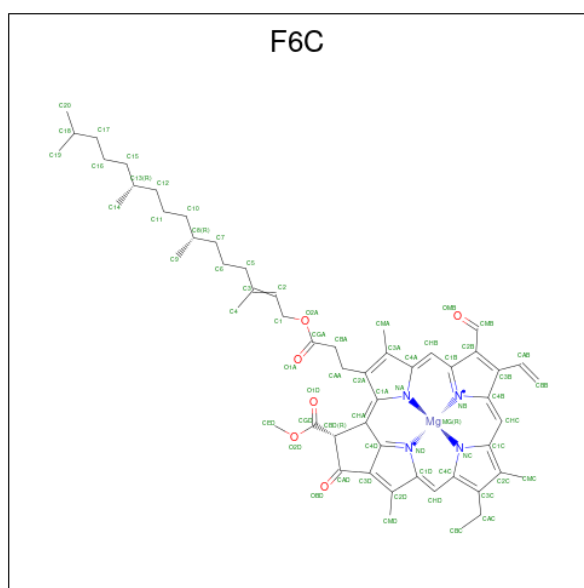
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	B	1	Total	C	Mg	N	O	0
			2220	1840	38	152	190	
14	B	1	Total	C	Mg	N	O	0
			2220	1840	38	152	190	
14	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			190	160	3	12	15	
14	L	1	Total	C	Mg	N	O	0
			190	160	3	12	15	
14	L	1	Total	C	Mg	N	O	0
			190	160	3	12	15	
14	X	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 15 is Chlorophyll F (three-letter code: F6C) (formula:  $C_{55}H_{68}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



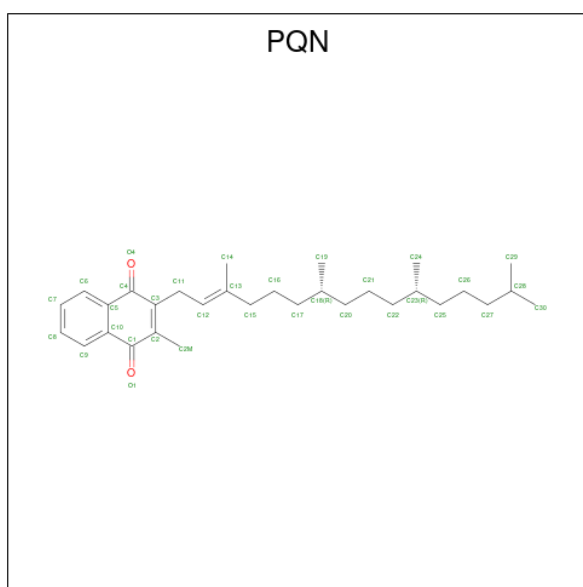
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			244	200	4	16	24	
15	H	1	Total	C	Mg	N	O	0
			244	200	4	16	24	
15	H	1	Total	C	Mg	N	O	0
			244	200	4	16	24	

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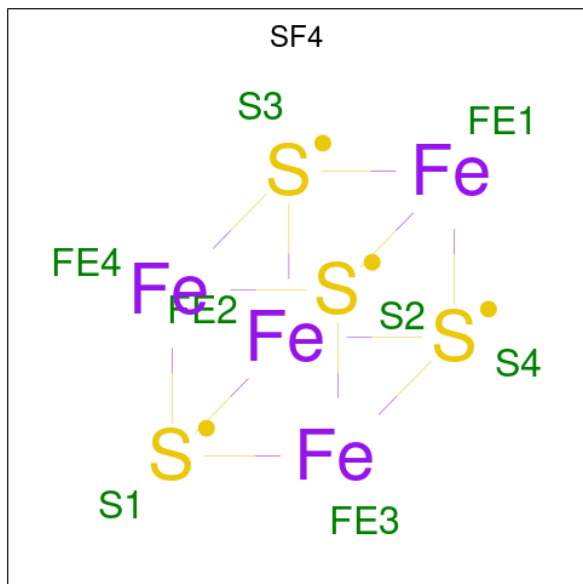
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	H	1	Total 244	C 200	Mg 4	N 16	O 24	0
15	a	1	Total 46	C 35	Mg 1	N 4	O 6	0
15	b	1	Total 244	C 200	Mg 4	N 16	O 24	0
15	b	1	Total 244	C 200	Mg 4	N 16	O 24	0
15	b	1	Total 244	C 200	Mg 4	N 16	O 24	0
15	b	1	Total 244	C 200	Mg 4	N 16	O 24	0
15	A	1	Total 46	C 35	Mg 1	N 4	O 6	0
15	B	1	Total 244	C 200	Mg 4	N 16	O 24	0
15	B	1	Total 244	C 200	Mg 4	N 16	O 24	0
15	B	1	Total 244	C 200	Mg 4	N 16	O 24	0
15	B	1	Total 244	C 200	Mg 4	N 16	O 24	0

- Molecule 16 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



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

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



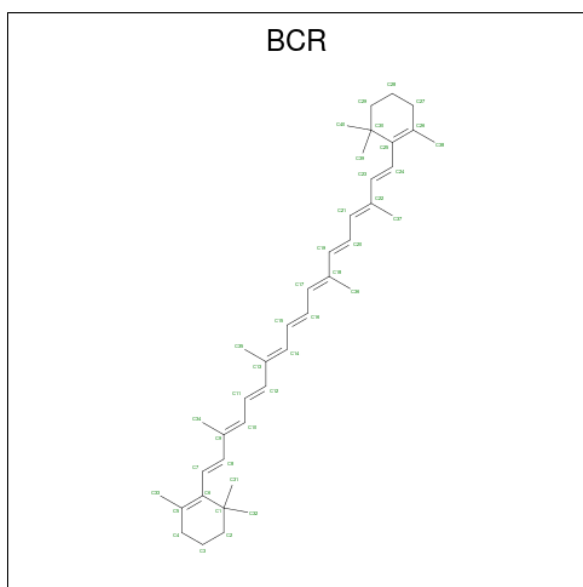
Mol	Chain	Residues	Atoms			AltConf
17	G	1	Total	Fe	S	0
			8	4	4	
17	N	1	Total	Fe	S	0
			16	8	8	
17	N	1	Total	Fe	S	0
			16	8	8	
17	a	1	Total	Fe	S	0
			8	4	4	
17	c	1	Total	Fe	S	0
			16	8	8	
17	c	1	Total	Fe	S	0
			16	8	8	

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

- Molecule 18 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		AltConf
18	G	1	Total	C	0
			240	240	
18	G	1	Total	C	0
			240	240	
18	G	1	Total	C	0
			240	240	
18	G	1	Total	C	0
			240	240	
18	G	1	Total	C	0
			240	240	
18	H	1	Total	C	0
			360	360	
18	H	1	Total	C	0
			360	360	

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Mol	Chain	Residues	Atoms		AltConf
18	H	1	Total 360	C 360	0
18	H	1	Total 360	C 360	0
18	H	1	Total 360	C 360	0
18	H	1	Total 360	C 360	0
18	H	1	Total 360	C 360	0
18	H	1	Total 360	C 360	0
18	H	1	Total 360	C 360	0
18	R	1	Total 80	C 80	0
18	R	1	Total 80	C 80	0
18	U	1	Total 80	C 80	0
18	U	1	Total 80	C 80	0
18	V	1	Total 40	C 40	0
18	a	1	Total 240	C 240	0
18	a	1	Total 240	C 240	0
18	a	1	Total 240	C 240	0
18	a	1	Total 240	C 240	0
18	a	1	Total 240	C 240	0
18	a	1	Total 240	C 240	0
18	b	1	Total 360	C 360	0
18	b	1	Total 360	C 360	0
18	b	1	Total 360	C 360	0

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Mol	Chain	Residues	Atoms		AltConf
18	b	1	Total 360	C 360	0
18	b	1	Total 360	C 360	0
18	b	1	Total 360	C 360	0
18	b	1	Total 360	C 360	0
18	b	1	Total 360	C 360	0
18	b	1	Total 360	C 360	0
18	i	1	Total 80	C 80	0
18	i	1	Total 80	C 80	0
18	l	1	Total 80	C 80	0
18	l	1	Total 80	C 80	0
18	m	1	Total 40	C 40	0
18	A	1	Total 240	C 240	0
18	A	1	Total 240	C 240	0
18	A	1	Total 240	C 240	0
18	A	1	Total 240	C 240	0
18	A	1	Total 240	C 240	0
18	A	1	Total 240	C 240	0
18	B	1	Total 360	C 360	0
18	B	1	Total 360	C 360	0
18	B	1	Total 360	C 360	0
18	B	1	Total 360	C 360	0

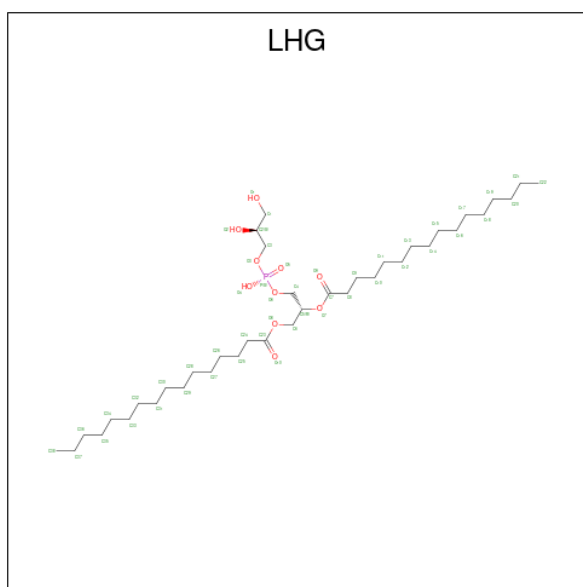
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Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	C	0
			360	360	
18	B	1	Total	C	0
			360	360	
18	B	1	Total	C	0
			360	360	
18	B	1	Total	C	0
			360	360	
18	B	1	Total	C	0
			360	360	
18	I	1	Total	C	0
			80	80	
18	I	1	Total	C	0
			80	80	
18	L	1	Total	C	0
			80	80	
18	L	1	Total	C	0
			80	80	
18	M	1	Total	C	0
			40	40	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



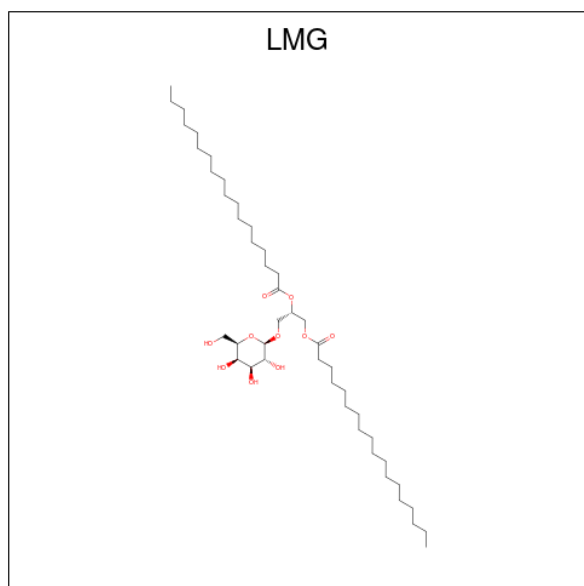
Mol	Chain	Residues	Atoms				AltConf
19	G	1	Total	C	O	P	0
			42	31	10	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	H	1	Total 44	C 33	O 10	P 1	0
19	a	1	Total 42	C 31	O 10	P 1	0
19	b	1	Total 44	C 33	O 10	P 1	0
19	A	1	Total 42	C 31	O 10	P 1	0
19	B	1	Total 44	C 33	O 10	P 1	0

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



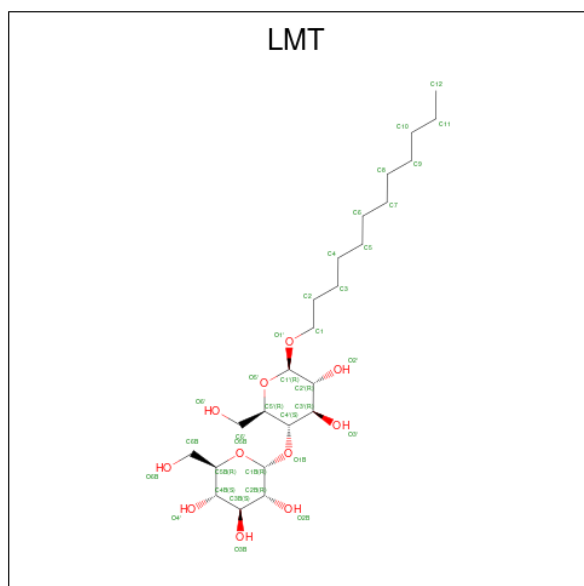
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	G	1	Total 46	C 36	O 10	0
20	H	1	Total 46	C 36	O 10	0
20	R	1	Total 37	C 27	O 10	0
20	U	1	Total 50	C 40	O 10	0
20	a	1	Total 46	C 36	O 10	0
20	b	1	Total 46	C 36	O 10	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	i	1	37	27	10	0
20	l	1	50	40	10	0
20	A	1	46	36	10	0
20	B	1	46	36	10	0
20	I	1	37	27	10	0
20	L	1	50	40	10	0

- Molecule 21 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	G	1	59	37	22	0
21	G	1	59	37	22	0
21	a	1	59	37	22	0
21	a	1	59	37	22	0
21	A	1	59	37	22	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	A	1	59	37	22	0

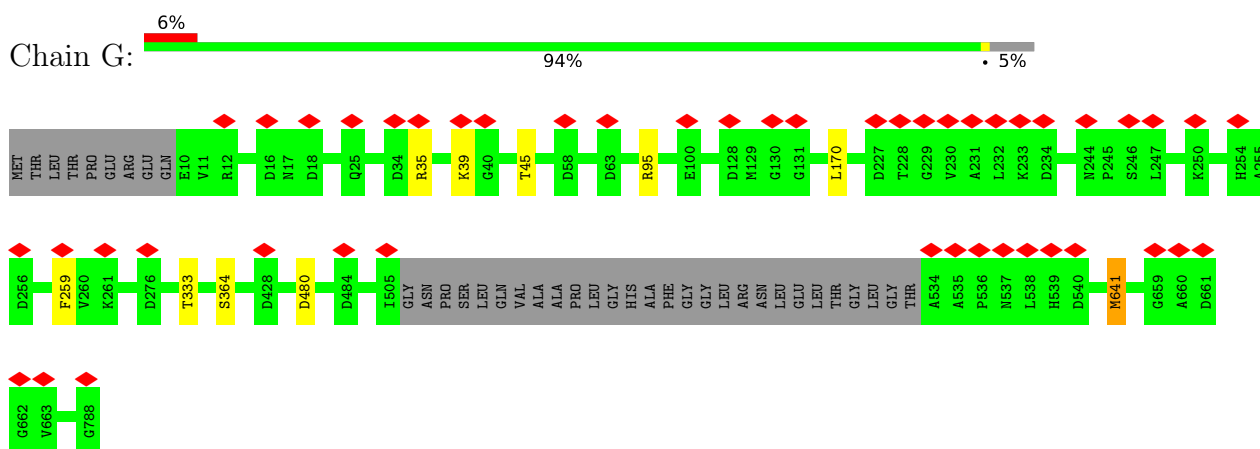
- Molecule 22 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
22	U	1	Total 1	Ca 1	0
22	1	1	Total 1	Ca 1	0
22	L	1	Total 1	Ca 1	0

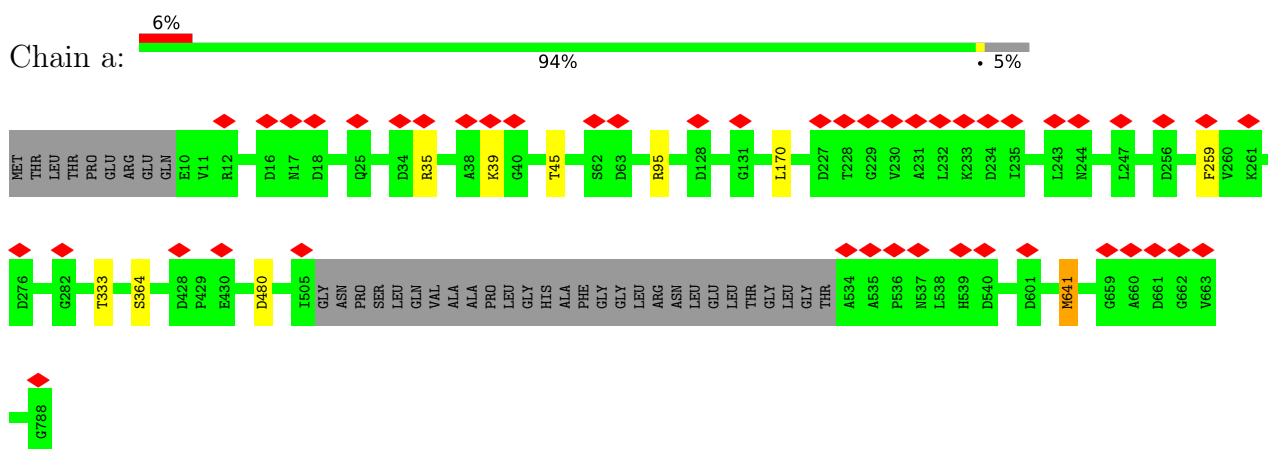
### 3 Residue-property plots [i](#)

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

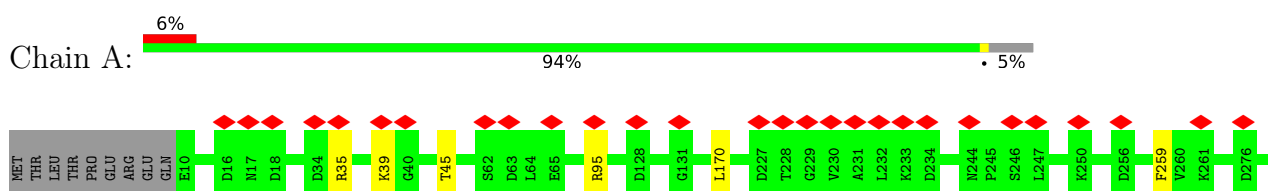
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

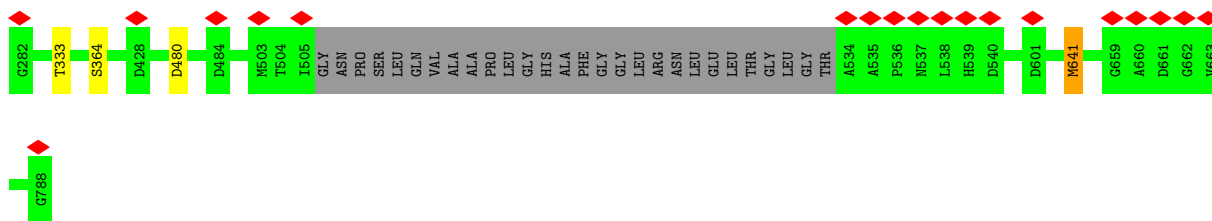


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



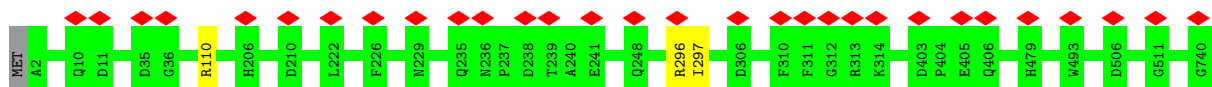
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





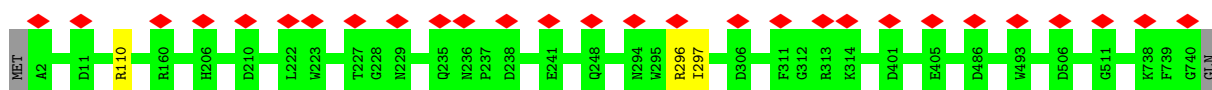
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain H: 99%



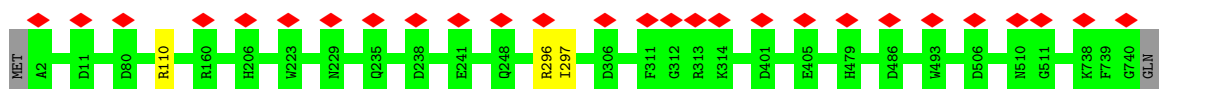
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 99%



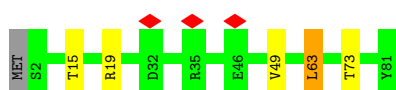
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 99%



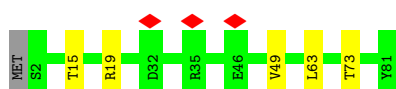
- Molecule 3: Photosystem I iron-sulfur center

Chain N: 93% 5% ..



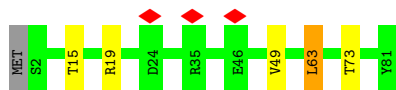
- Molecule 3: Photosystem I iron-sulfur center

Chain c: 93% 6% .

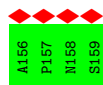
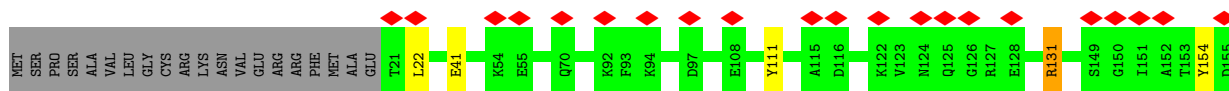
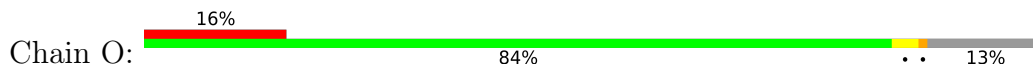


- Molecule 3: Photosystem I iron-sulfur center

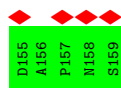
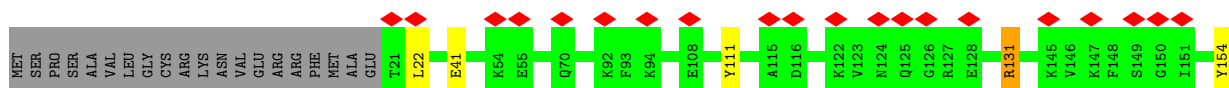
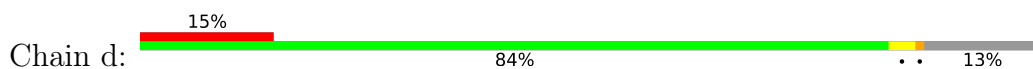
Chain C: 93% 5% ..



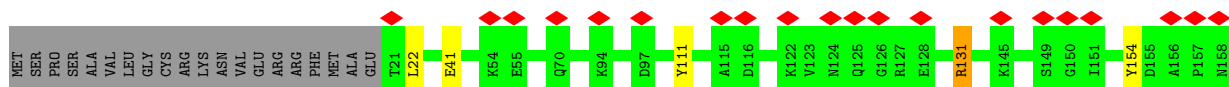
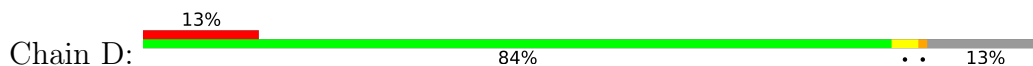
• Molecule 4: Photosystem I protein PsaD



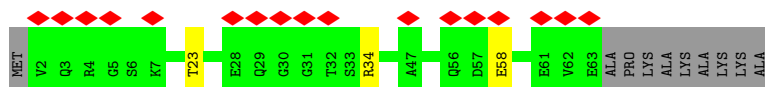
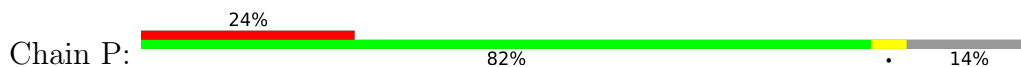
• Molecule 4: Photosystem I protein PsaD



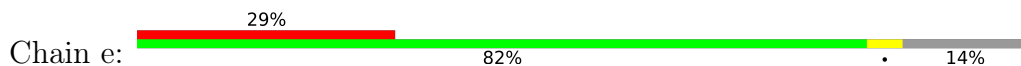
• Molecule 4: Photosystem I protein PsaD

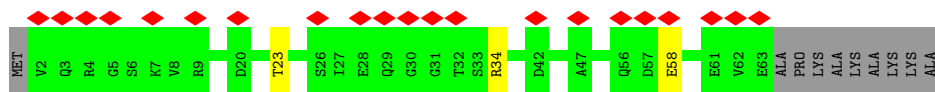


• Molecule 5: Photosystem I reaction center subunit IV

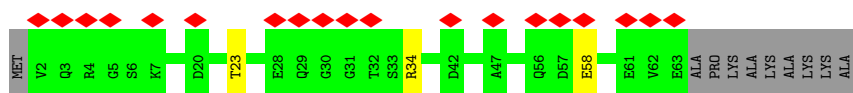
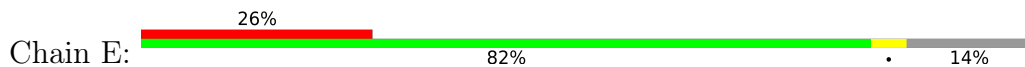


• Molecule 5: Photosystem I reaction center subunit IV

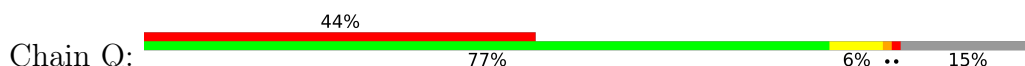




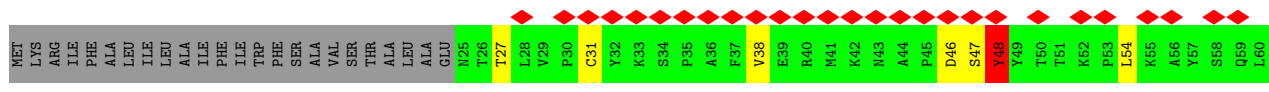
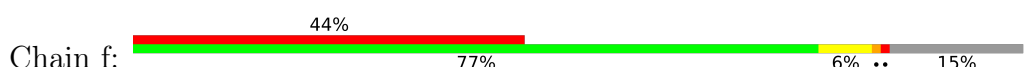
• Molecule 5: Photosystem I reaction center subunit IV



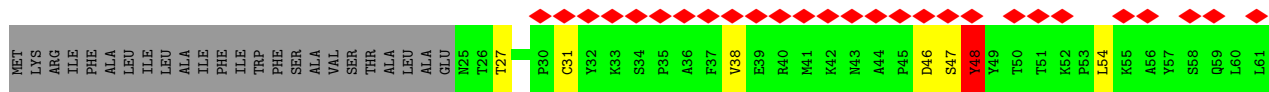
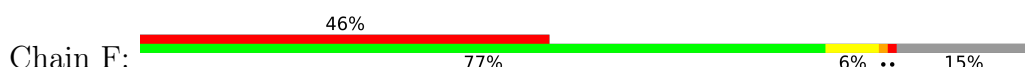
• Molecule 6: Photosystem I reaction center protein PsaF subunit III



• Molecule 6: Photosystem I reaction center protein PsaF subunit III



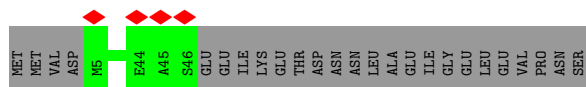
• Molecule 6: Photosystem I reaction center protein PsaF subunit III



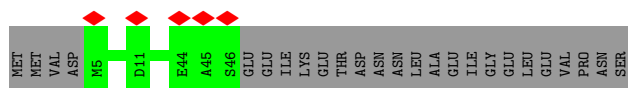
• Molecule 7: photosystem I subunit VIII



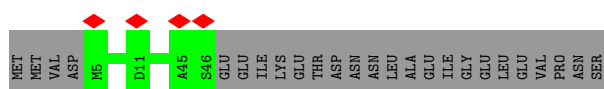




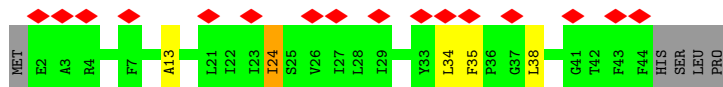
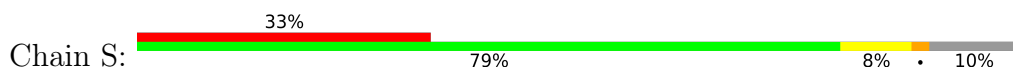
• Molecule 7: photosystem I subunit VIII



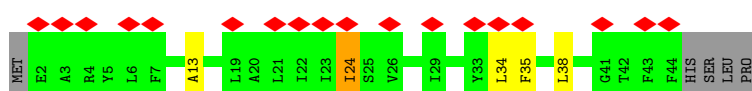
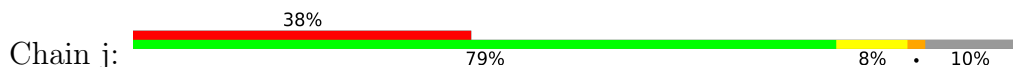
• Molecule 7: photosystem I subunit VIII



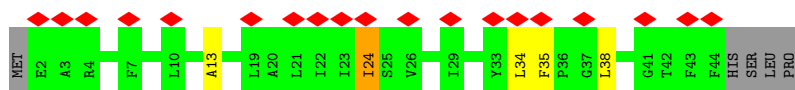
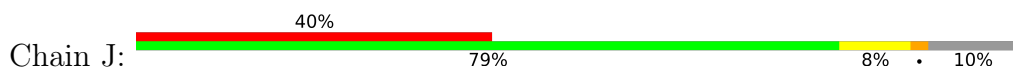
• Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



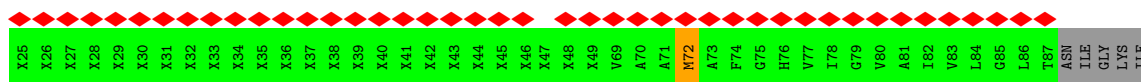
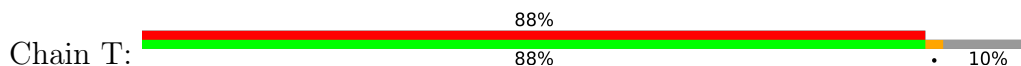
• Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



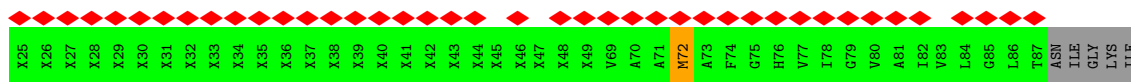
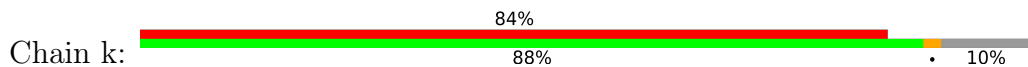
• Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



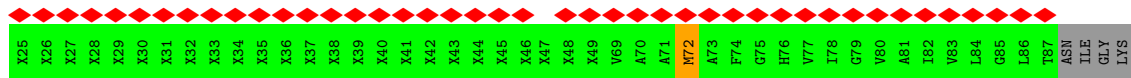
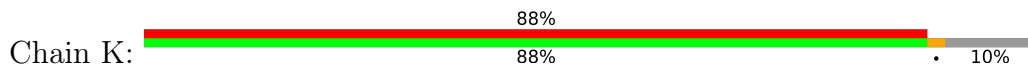
• Molecule 9: Photosystem I reaction center subunit PsaK



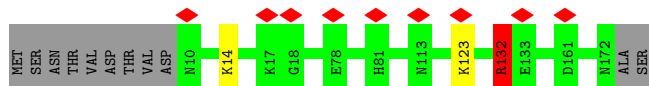
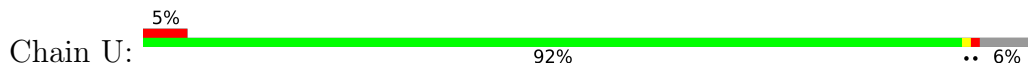
• Molecule 9: Photosystem I reaction center subunit PsaK



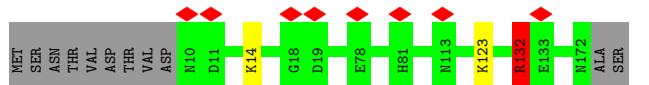
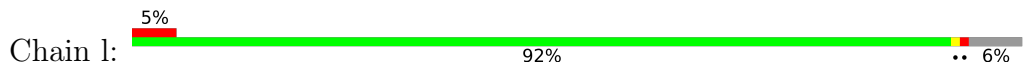
• Molecule 9: Photosystem I reaction center subunit PsaK



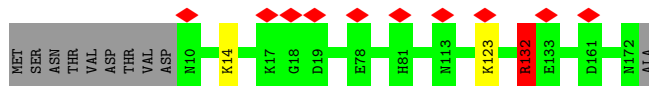
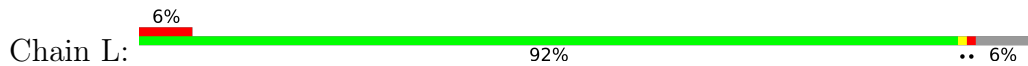
• Molecule 10: PSI subunit V



• Molecule 10: PSI subunit V



• Molecule 10: PSI subunit V



• Molecule 11: Photosystem I reaction center subunit XII



• Molecule 11: Photosystem I reaction center subunit XII





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	201104	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 ( $e^-/\text{\AA}^2$ )	57.328	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.324	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	381.6013, 381.6013, 381.6013	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49063, 1.49063, 1.49063	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, CA, CL0, PQN, F6C, BCR, SF4, LHG, LMT, 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	0.54	0/6138	0.55	1/8362 (0.0%)
1	G	0.54	0/6138	0.55	1/8362 (0.0%)
1	a	0.54	0/6138	0.55	1/8362 (0.0%)
2	B	0.57	0/6135	0.54	0/8385
2	H	0.57	0/6135	0.54	0/8385
2	b	0.57	0/6135	0.54	0/8385
3	C	0.62	0/611	0.77	1/828 (0.1%)
3	N	0.62	0/611	0.77	1/828 (0.1%)
3	c	0.62	0/611	0.77	1/828 (0.1%)
4	D	0.49	0/1116	0.64	1/1505 (0.1%)
4	O	0.49	0/1116	0.64	1/1505 (0.1%)
4	d	0.49	0/1116	0.64	1/1505 (0.1%)
5	E	0.48	0/506	0.59	0/686
5	P	0.48	0/506	0.59	0/686
5	e	0.48	0/506	0.59	0/686
6	F	0.45	0/1084	0.74	2/1470 (0.1%)
6	Q	0.45	0/1084	0.74	2/1470 (0.1%)
6	f	0.45	0/1084	0.74	2/1470 (0.1%)
7	I	0.59	0/365	0.72	0/502
7	R	0.59	0/365	0.72	0/502
7	i	0.59	0/365	0.72	0/502
8	J	0.37	0/353	0.78	1/482 (0.2%)
8	S	0.36	0/353	0.78	1/482 (0.2%)
8	j	0.37	0/353	0.78	1/482 (0.2%)
9	K	0.31	0/129	1.21	3/175 (1.7%)
9	T	0.31	0/129	1.21	3/175 (1.7%)
9	k	0.31	0/129	1.21	3/175 (1.7%)
10	L	0.56	0/1255	0.84	5/1702 (0.3%)
10	U	0.56	0/1255	0.84	5/1702 (0.3%)
10	l	0.56	0/1255	0.84	5/1702 (0.3%)
11	M	0.45	0/250	0.64	0/340
11	V	0.45	0/250	0.64	0/340

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	m	0.45	0/250	0.64	0/340
12	W	0.40	0/256	0.47	0/350
12	X	0.40	0/256	0.47	0/350
12	x	0.39	0/256	0.47	0/350
All	All	0.54	0/54594	0.61	42/74361 (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
1	G	0	1
1	a	0	1
6	F	0	2
6	Q	0	2
6	f	0	2
8	J	0	1
8	S	0	1
8	j	0	1
10	L	0	1
10	U	0	1
10	l	0	1
All	All	0	15

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	132	ARG	CG-CD-NE	12.77	138.61	111.80
10	L	132	ARG	CG-CD-NE	12.75	138.57	111.80
10	l	132	ARG	CG-CD-NE	12.74	138.55	111.80
10	l	132	ARG	NE-CZ-NH2	-12.23	114.18	120.30
10	L	132	ARG	NE-CZ-NH2	-12.18	114.21	120.30
10	U	132	ARG	NE-CZ-NH2	-12.09	114.26	120.30
10	l	132	ARG	CD-NE-CZ	10.08	137.72	123.60
10	L	132	ARG	CD-NE-CZ	10.07	137.70	123.60
10	U	132	ARG	CD-NE-CZ	10.06	137.68	123.60
10	L	132	ARG	NE-CZ-NH1	9.67	125.14	120.30
10	l	132	ARG	NE-CZ-NH1	9.65	125.12	120.30
10	U	132	ARG	NE-CZ-NH1	9.59	125.10	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	72	MET	CB-CG-SD	9.47	140.81	112.40
9	T	72	MET	CB-CG-SD	9.47	140.80	112.40
9	k	72	MET	CB-CG-SD	9.46	140.80	112.40
9	K	72	MET	CA-CB-CG	8.20	127.24	113.30
9	k	72	MET	CA-CB-CG	8.19	127.23	113.30
9	T	72	MET	CA-CB-CG	8.18	127.21	113.30
10	l	132	ARG	CB-CG-CD	7.74	131.73	111.60
10	U	132	ARG	CB-CG-CD	7.74	131.71	111.60
10	L	132	ARG	CB-CG-CD	7.73	131.70	111.60
6	f	31	CYS	CA-CB-SG	7.66	127.80	114.00
6	Q	31	CYS	CA-CB-SG	7.64	127.76	114.00
6	F	31	CYS	CA-CB-SG	7.64	127.75	114.00
4	O	131	ARG	NE-CZ-NH1	7.06	123.83	120.30
4	d	131	ARG	NE-CZ-NH1	7.05	123.83	120.30
4	D	131	ARG	NE-CZ-NH1	6.97	123.79	120.30
6	Q	115	LYS	CB-CG-CD	6.77	129.21	111.60
6	F	115	LYS	CB-CG-CD	6.77	129.20	111.60
6	f	115	LYS	CB-CG-CD	6.77	129.20	111.60
9	k	72	MET	CG-SD-CE	6.74	110.97	100.20
9	K	72	MET	CG-SD-CE	6.73	110.97	100.20
9	T	72	MET	CG-SD-CE	6.72	110.96	100.20
3	c	19	ARG	NE-CZ-NH1	6.42	123.51	120.30
3	C	19	ARG	NE-CZ-NH1	6.41	123.51	120.30
3	N	19	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	a	641	MET	CB-CG-SD	6.25	131.15	112.40
1	G	641	MET	CB-CG-SD	6.25	131.15	112.40
1	A	641	MET	CB-CG-SD	6.24	131.11	112.40
8	j	24	ILE	CG1-CB-CG2	-5.80	98.63	111.40
8	S	24	ILE	CG1-CB-CG2	-5.79	98.66	111.40
8	J	24	ILE	CG1-CB-CG2	-5.78	98.68	111.40

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	THR	Peptide
6	F	47	SER	Peptide
6	F	48	TYR	Peptide
1	G	333	THR	Peptide
8	J	35	PHE	Peptide
10	L	132	ARG	Peptide
6	Q	47	SER	Peptide

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Mol	Chain	Res	Type	Group
6	Q	48	TYR	Peptide
8	S	35	PHE	Peptide
10	U	132	ARG	Peptide
1	a	333	THR	Peptide
6	f	47	SER	Peptide
6	f	48	TYR	Peptide
8	j	35	PHE	Peptide
10	l	132	ARG	Peptide

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
1	G	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
1	a	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
2	B	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	H	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	b	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
3	C	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	12	41
3	N	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	12	41
3	c	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
4	D	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
4	O	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
4	d	137/159 (86%)	129 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
5	P	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
5	e	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
6	F	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	19	53
6	Q	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	19	53
6	f	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	19	53
7	I	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
7	R	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
7	i	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
8	J	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	6	26
8	S	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	6	26
8	j	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	6	26
9	K	17/49 (35%)	17 (100%)	0	0	100	100
9	T	17/49 (35%)	17 (100%)	0	0	100	100
9	k	17/49 (35%)	17 (100%)	0	0	100	100
10	L	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
10	U	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
10	l	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	V	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	W	27/101 (27%)	27 (100%)	0	0	100	100
12	X	27/101 (27%)	27 (100%)	0	0	100	100
12	x	27/101 (27%)	27 (100%)	0	0	100	100
All	All	6621/7410 (89%)	6240 (94%)	373 (6%)	8 (0%)	54	83

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	Q	48	TYR
6	f	48	TYR
6	F	48	TYR
3	N	63	LEU
8	S	13	ALA

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Mol	Chain	Res	Type
8	j	13	ALA
3	C	63	LEU
8	J	13	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	613/641 (96%)	604 (98%)	9 (2%)	65 85
1	G	613/641 (96%)	604 (98%)	9 (2%)	65 85
1	a	613/641 (96%)	604 (98%)	9 (2%)	65 85
2	B	595/597 (100%)	592 (100%)	3 (0%)	88 95
2	H	595/597 (100%)	592 (100%)	3 (0%)	88 95
2	b	595/597 (100%)	592 (100%)	3 (0%)	88 95
3	C	68/69 (99%)	64 (94%)	4 (6%)	19 50
3	N	68/69 (99%)	64 (94%)	4 (6%)	19 50
3	c	68/69 (99%)	64 (94%)	4 (6%)	19 50
4	D	115/132 (87%)	110 (96%)	5 (4%)	29 62
4	O	115/132 (87%)	110 (96%)	5 (4%)	29 62
4	d	115/132 (87%)	110 (96%)	5 (4%)	29 62
5	E	54/60 (90%)	51 (94%)	3 (6%)	21 53
5	P	54/60 (90%)	51 (94%)	3 (6%)	21 53
5	e	54/60 (90%)	51 (94%)	3 (6%)	21 53
6	F	115/134 (86%)	105 (91%)	10 (9%)	10 33
6	Q	115/134 (86%)	105 (91%)	10 (9%)	10 33
6	f	115/134 (86%)	105 (91%)	10 (9%)	10 33
7	I	37/60 (62%)	37 (100%)	0	100 100
7	R	37/60 (62%)	37 (100%)	0	100 100
7	i	37/60 (62%)	37 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	36/42 (86%)	33 (92%)	3 (8%)	11	35
8	S	36/42 (86%)	33 (92%)	3 (8%)	11	35
8	j	36/42 (86%)	33 (92%)	3 (8%)	11	35
9	K	12/16 (75%)	11 (92%)	1 (8%)	11	35
9	T	12/16 (75%)	11 (92%)	1 (8%)	11	35
9	k	12/16 (75%)	11 (92%)	1 (8%)	11	35
10	L	128/138 (93%)	125 (98%)	3 (2%)	50	78
10	U	128/138 (93%)	125 (98%)	3 (2%)	50	78
10	l	128/138 (93%)	125 (98%)	3 (2%)	50	78
11	M	26/26 (100%)	25 (96%)	1 (4%)	33	66
11	V	26/26 (100%)	25 (96%)	1 (4%)	33	66
11	m	26/26 (100%)	25 (96%)	1 (4%)	33	66
12	W	24/84 (29%)	24 (100%)	0	100	100
12	X	24/84 (29%)	24 (100%)	0	100	100
12	x	24/84 (29%)	24 (100%)	0	100	100
All	All	5469/5997 (91%)	5343 (98%)	126 (2%)	53	78

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	35	ARG
1	G	39	LYS
1	G	45	THR
1	G	95	ARG
1	G	170	LEU
1	G	259	PHE
1	G	364	SER
1	G	480	ASP
1	G	641	MET
2	H	110	ARG
2	H	296	ARG
2	H	297	ILE
3	N	15	THR
3	N	49	VAL
3	N	63	LEU
3	N	73	THR
4	O	22	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	O	41	GLU
4	O	111	TYR
4	O	131	ARG
4	O	154	TYR
5	P	23	THR
5	P	34	ARG
5	P	58	GLU
6	Q	27	THR
6	Q	38	VAL
6	Q	46	ASP
6	Q	48	TYR
6	Q	54	LEU
6	Q	62	CYS
6	Q	108	LYS
6	Q	115	LYS
6	Q	146	GLU
6	Q	153	GLU
8	S	24	ILE
8	S	34	LEU
8	S	38	LEU
9	T	72	MET
10	U	14	LYS
10	U	123	LYS
10	U	132	ARG
11	V	31	LYS
1	a	35	ARG
1	a	39	LYS
1	a	45	THR
1	a	95	ARG
1	a	170	LEU
1	a	259	PHE
1	a	364	SER
1	a	480	ASP
1	a	641	MET
2	b	110	ARG
2	b	296	ARG
2	b	297	ILE
3	c	15	THR
3	c	49	VAL
3	c	63	LEU
3	c	73	THR
4	d	22	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	d	41	GLU
4	d	111	TYR
4	d	131	ARG
4	d	154	TYR
5	e	23	THR
5	e	34	ARG
5	e	58	GLU
6	f	27	THR
6	f	38	VAL
6	f	46	ASP
6	f	48	TYR
6	f	54	LEU
6	f	62	CYS
6	f	108	LYS
6	f	115	LYS
6	f	146	GLU
6	f	153	GLU
8	j	24	ILE
8	j	34	LEU
8	j	38	LEU
9	k	72	MET
10	l	14	LYS
10	l	123	LYS
10	l	132	ARG
11	m	31	LYS
1	A	35	ARG
1	A	39	LYS
1	A	45	THR
1	A	95	ARG
1	A	170	LEU
1	A	259	PHE
1	A	364	SER
1	A	480	ASP
1	A	641	MET
2	B	110	ARG
2	B	296	ARG
2	B	297	ILE
3	C	15	THR
3	C	49	VAL
3	C	63	LEU
3	C	73	THR
4	D	22	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	41	GLU
4	D	111	TYR
4	D	131	ARG
4	D	154	TYR
5	E	23	THR
5	E	34	ARG
5	E	58	GLU
6	F	27	THR
6	F	38	VAL
6	F	46	ASP
6	F	48	TYR
6	F	54	LEU
6	F	62	CYS
6	F	108	LYS
6	F	115	LYS
6	F	146	GLU
6	F	153	GLU
8	J	24	ILE
8	J	34	LEU
8	J	38	LEU
9	K	72	MET
10	L	14	LYS
10	L	123	LYS
10	L	132	ARG
11	M	31	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	105	ASN
1	G	144	GLN
1	G	193	GLN
1	G	273	HIS
1	G	299	HIS
1	G	366	ASN
1	G	379	HIS
1	G	490	GLN
1	G	604	ASN
1	G	731	GLN
1	G	751	GLN
2	H	34	HIS
2	H	53	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	158	GLN
2	H	235	GLN
2	H	332	ASN
2	H	444	ASN
2	H	610	GLN
2	H	634	ASN
2	H	691	GLN
5	P	19	GLN
6	Q	104	GLN
10	U	41	ASN
1	a	105	ASN
1	a	144	GLN
1	a	193	GLN
1	a	273	HIS
1	a	299	HIS
1	a	366	ASN
1	a	379	HIS
1	a	490	GLN
1	a	539	HIS
1	a	604	ASN
1	a	731	GLN
1	a	751	GLN
2	b	34	HIS
2	b	53	HIS
2	b	111	ASN
2	b	158	GLN
2	b	235	GLN
2	b	332	ASN
2	b	444	ASN
2	b	610	GLN
2	b	634	ASN
2	b	691	GLN
5	e	19	GLN
10	l	41	ASN
1	A	105	ASN
1	A	144	GLN
1	A	193	GLN
1	A	273	HIS
1	A	299	HIS
1	A	366	ASN
1	A	379	HIS
1	A	490	GLN

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Mol	Chain	Res	Type
1	A	539	HIS
1	A	604	ASN
1	A	731	GLN
1	A	751	GLN
2	B	34	HIS
2	B	53	HIS
2	B	111	ASN
2	B	158	GLN
2	B	235	GLN
2	B	332	ASN
2	B	444	ASN
2	B	610	GLN
2	B	634	ASN
2	B	691	GLN
5	E	19	GLN
10	L	41	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

Of 372 ligands modelled in this entry, 3 are monoatomic - leaving 369 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	SF4	N	3003	3	0,12,12	-	-	-		
18	BCR	L	4019	-	41,41,41	2.98	7 (17%)	56,56,56	7.02	29 (51%)
14	CLA	U	1501	10	65,73,73	2.19	19 (29%)	76,113,113	2.52	24 (31%)
14	CLA	U	1503	-	65,73,73	2.20	18 (27%)	76,113,113	2.60	25 (32%)
18	BCR	B	4014	-	41,41,41	3.05	7 (17%)	56,56,56	6.44	24 (42%)
18	BCR	H	4004	-	41,41,41	2.85	7 (17%)	56,56,56	6.49	25 (44%)
14	CLA	G	1109	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	25 (32%)
14	CLA	b	1239	-	65,73,73	2.22	18 (27%)	76,113,113	2.71	32 (42%)
14	CLA	H	1022	-	65,73,73	2.16	18 (27%)	76,113,113	2.63	26 (34%)
18	BCR	b	4013	-	41,41,41	2.81	6 (14%)	56,56,56	6.71	22 (39%)
18	BCR	b	4005	-	41,41,41	2.99	7 (17%)	56,56,56	6.59	24 (42%)
18	BCR	I	4020	-	41,41,41	3.22	10 (24%)	56,56,56	6.75	23 (41%)
14	CLA	a	1103	-	60,68,73	2.25	19 (31%)	70,107,113	2.72	25 (35%)
18	BCR	b	4016	-	41,41,41	2.97	6 (14%)	56,56,56	6.64	20 (35%)
14	CLA	H	1204	-	65,73,73	2.21	17 (26%)	76,113,113	2.54	27 (35%)
16	PQN	A	2001	-	34,34,34	1.44	2 (5%)	42,45,45	1.25	5 (11%)
14	CLA	G	1124	-	55,63,73	2.37	18 (32%)	64,101,113	2.88	24 (37%)
14	CLA	A	1129	-	50,58,73	2.49	19 (38%)	58,95,113	2.88	23 (39%)
14	CLA	B	1217	-	55,63,73	2.35	18 (32%)	64,101,113	2.82	22 (34%)
20	LMG	i	5006	-	37,37,55	1.11	3 (8%)	45,45,63	1.20	3 (6%)
20	LMG	A	5005	-	46,46,55	1.29	5 (10%)	54,54,63	1.09	2 (3%)
13	CL0	G	1011	-	65,73,73	2.17	20 (30%)	76,113,113	2.61	23 (30%)
14	CLA	H	1221	-	65,73,73	2.18	19 (29%)	76,113,113	2.54	24 (31%)
14	CLA	l	1503	-	65,73,73	2.20	19 (29%)	76,113,113	2.59	25 (32%)
14	CLA	H	1209	-	45,53,73	2.51	18 (40%)	52,89,113	2.98	21 (40%)
14	CLA	b	1236	-	45,53,73	2.47	17 (37%)	52,89,113	2.92	19 (36%)
14	CLA	U	1502	-	60,68,73	2.23	18 (30%)	70,107,113	2.75	23 (32%)
14	CLA	H	1217	-	55,63,73	2.35	18 (32%)	64,101,113	2.81	22 (34%)
14	CLA	a	1118	-	55,63,73	2.38	18 (32%)	64,101,113	2.79	27 (42%)
14	CLA	G	1115	-	65,73,73	2.21	18 (27%)	76,113,113	2.72	26 (34%)
15	F6C	b	1237	-	69,74,74	2.67	24 (34%)	70,114,114	3.21	27 (38%)
14	CLA	A	1135	-	60,68,73	2.28	18 (30%)	70,107,113	2.68	24 (34%)
14	CLA	a	1119	-	65,73,73	2.21	19 (29%)	76,113,113	2.63	24 (31%)
14	CLA	A	1117	-	65,73,73	2.17	18 (27%)	76,113,113	2.63	27 (35%)
14	CLA	a	1116	-	55,63,73	2.39	18 (32%)	64,101,113	2.80	27 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	F6C	A	1121	-	49,54,74	3.14	23 (46%)	46,90,114	3.85	28 (60%)
14	CLA	G	1130	-	55,63,73	2.40	18 (32%)	64,101,113	2.75	25 (39%)
14	CLA	A	1138	-	60,68,73	2.31	18 (30%)	70,107,113	2.59	23 (32%)
20	LMG	l	5007	-	50,50,55	1.34	7 (14%)	58,58,63	1.09	2 (3%)
14	CLA	G	1101	-	45,53,73	2.45	17 (37%)	52,89,113	2.94	20 (38%)
14	CLA	a	1013	-	60,68,73	2.28	18 (30%)	70,107,113	2.77	24 (34%)
14	CLA	A	1125	-	65,73,73	2.16	19 (29%)	76,113,113	2.67	22 (28%)
14	CLA	G	1123	-	60,68,73	2.31	19 (31%)	70,107,113	2.65	25 (35%)
14	CLA	l	1501	10	65,73,73	2.19	19 (29%)	76,113,113	2.52	24 (31%)
14	CLA	G	1113	-	45,53,73	2.49	17 (37%)	52,89,113	2.89	22 (42%)
14	CLA	b	1226	-	65,73,73	2.24	19 (29%)	76,113,113	2.52	23 (30%)
20	LMG	B	5002	-	46,46,55	1.25	5 (10%)	54,54,63	1.26	4 (7%)
14	CLA	B	1213	-	65,73,73	2.20	18 (27%)	76,113,113	2.62	23 (30%)
14	CLA	A	1119	-	65,73,73	2.21	19 (29%)	76,113,113	2.62	24 (31%)
14	CLA	B	1225	-	65,73,73	2.24	19 (29%)	76,113,113	2.49	21 (27%)
21	LMT	a	6001	-	32,32,36	1.27	6 (18%)	43,43,47	1.05	2 (4%)
14	CLA	A	1128	-	60,68,73	2.32	19 (31%)	70,107,113	2.71	23 (32%)
14	CLA	A	1118	-	55,63,73	2.38	18 (32%)	64,101,113	2.78	27 (42%)
14	CLA	a	1109	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	25 (32%)
14	CLA	A	1114	-	45,53,73	2.54	19 (42%)	52,89,113	2.87	20 (38%)
14	CLA	G	1140	-	65,73,73	2.18	18 (27%)	76,113,113	2.52	24 (31%)
14	CLA	b	1216	-	65,73,73	2.18	18 (27%)	76,113,113	2.50	24 (31%)
14	CLA	B	1231	2	55,63,73	2.38	18 (32%)	64,101,113	2.76	22 (34%)
14	CLA	A	1137	-	50,58,73	2.50	19 (38%)	58,95,113	3.04	25 (43%)
18	BCR	B	4016	-	41,41,41	2.97	6 (14%)	56,56,56	6.64	20 (35%)
14	CLA	B	1224	-	65,73,73	2.20	19 (29%)	76,113,113	2.57	22 (28%)
14	CLA	a	1124	-	55,63,73	2.37	18 (32%)	64,101,113	2.87	24 (37%)
14	CLA	G	1012	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	26 (34%)
14	CLA	H	1023	-	65,73,73	2.19	19 (29%)	76,113,113	2.74	26 (34%)
14	CLA	b	1206	2	45,53,73	2.52	16 (35%)	52,89,113	2.79	20 (38%)
14	CLA	A	1109	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	25 (32%)
14	CLA	B	1021	-	65,73,73	2.17	20 (30%)	76,113,113	2.55	25 (32%)
14	CLA	G	1125	-	65,73,73	2.16	20 (30%)	76,113,113	2.67	22 (28%)
18	BCR	A	4001	-	41,41,41	2.95	6 (14%)	56,56,56	6.60	23 (41%)
14	CLA	a	1131	-	60,68,73	2.28	18 (30%)	70,107,113	2.65	21 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	F6C	B	1237	-	69,74,74	2.68	23 (33%)	70,114,114	3.22	27 (38%)
16	PQN	B	2002	-	34,34,34	1.47	2 (5%)	42,45,45	1.26	2 (4%)
18	BCR	i	4018	-	41,41,41	3.05	8 (19%)	56,56,56	6.57	24 (42%)
14	CLA	H	1224	-	65,73,73	2.19	18 (27%)	76,113,113	2.56	22 (28%)
18	BCR	H	4005	-	41,41,41	2.99	7 (17%)	56,56,56	6.59	24 (42%)
14	CLA	H	1205	-	65,73,73	2.16	18 (27%)	76,113,113	2.60	23 (30%)
14	CLA	a	1139	-	45,53,73	2.50	17 (37%)	52,89,113	2.85	22 (42%)
18	BCR	H	4010	-	41,41,41	3.11	7 (17%)	56,56,56	6.68	21 (37%)
13	CL0	a	1011	-	65,73,73	2.16	20 (30%)	76,113,113	2.61	23 (30%)
14	CLA	b	1213	-	65,73,73	2.20	18 (27%)	76,113,113	2.62	23 (30%)
14	CLA	k	1401	-	45,53,73	2.55	19 (42%)	52,89,113	2.94	21 (40%)
14	CLA	b	1211	-	65,73,73	2.20	20 (30%)	76,113,113	2.64	23 (30%)
14	CLA	B	1212	-	45,53,73	2.49	17 (37%)	52,89,113	2.89	19 (36%)
14	CLA	b	1021	-	65,73,73	2.17	20 (30%)	76,113,113	2.55	25 (32%)
18	BCR	G	4003	-	41,41,41	2.89	6 (14%)	56,56,56	6.55	22 (39%)
14	CLA	B	1218	-	45,53,73	2.59	18 (40%)	52,89,113	2.83	18 (34%)
14	CLA	X	1701	-	55,63,73	2.39	18 (32%)	64,101,113	2.78	23 (35%)
14	CLA	G	1132	-	65,73,73	2.17	17 (26%)	76,113,113	2.69	24 (31%)
18	BCR	a	4002	-	41,41,41	3.05	7 (17%)	56,56,56	6.29	28 (50%)
14	CLA	H	1208	-	65,73,73	2.20	18 (27%)	76,113,113	2.56	22 (28%)
18	BCR	G	4001	-	41,41,41	2.95	6 (14%)	56,56,56	6.60	23 (41%)
18	BCR	G	4011	-	41,41,41	3.03	8 (19%)	56,56,56	6.53	27 (48%)
14	CLA	a	1123	-	60,68,73	2.31	19 (31%)	70,107,113	2.64	25 (35%)
14	CLA	b	1201	-	55,63,73	2.39	17 (30%)	64,101,113	2.86	23 (35%)
14	CLA	B	1219	-	45,53,73	2.53	19 (42%)	52,89,113	2.86	21 (40%)
20	LMG	a	5005	-	46,46,55	1.30	5 (10%)	54,54,63	1.09	2 (3%)
20	LMG	H	5002	-	46,46,55	1.26	5 (10%)	54,54,63	1.25	4 (7%)
14	CLA	B	1202	-	60,68,73	2.19	19 (31%)	70,107,113	2.69	24 (34%)
14	CLA	H	1239	-	65,73,73	2.22	18 (27%)	76,113,113	2.71	32 (42%)
14	CLA	A	1122	-	55,63,73	2.36	18 (32%)	64,101,113	2.77	26 (40%)
20	LMG	R	5006	-	37,37,55	1.12	3 (8%)	45,45,63	1.20	3 (6%)
14	CLA	b	1222	-	65,73,73	2.22	19 (29%)	76,113,113	2.65	27 (35%)
14	CLA	A	1106	-	60,68,73	2.27	19 (31%)	70,107,113	2.78	24 (34%)
18	BCR	b	4006	-	41,41,41	2.87	6 (14%)	56,56,56	6.61	21 (37%)
21	LMT	G	6002	-	29,29,36	1.40	6 (20%)	40,40,47	1.16	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	A	1139	-	45,53,73	2.49	17 (37%)	52,89,113	2.85	22 (42%)
20	LMG	L	5007	-	50,50,55	1.34	7 (14%)	58,58,63	1.09	2 (3%)
14	CLA	b	1215	-	60,68,73	2.24	18 (30%)	70,107,113	2.60	21 (30%)
14	CLA	a	1125	-	65,73,73	2.17	20 (30%)	76,113,113	2.68	22 (28%)
14	CLA	G	1103	-	60,68,73	2.25	19 (31%)	70,107,113	2.72	24 (34%)
14	CLA	A	1101	-	45,53,73	2.45	17 (37%)	52,89,113	2.94	20 (38%)
14	CLA	L	1501	10	65,73,73	2.19	19 (29%)	76,113,113	2.52	23 (30%)
14	CLA	B	1210	-	65,73,73	2.21	19 (29%)	76,113,113	2.76	26 (34%)
18	BCR	b	4004	-	41,41,41	2.85	7 (17%)	56,56,56	6.49	25 (44%)
18	BCR	L	4022	-	41,41,41	3.10	9 (21%)	56,56,56	6.48	23 (41%)
21	LMT	A	6001	-	32,32,36	1.28	6 (18%)	43,43,47	1.05	2 (4%)
14	CLA	H	1218	-	45,53,73	2.58	18 (40%)	52,89,113	2.83	18 (34%)
14	CLA	A	1136	-	65,73,73	2.17	18 (27%)	76,113,113	2.59	22 (28%)
18	BCR	B	4006	-	41,41,41	2.86	6 (14%)	56,56,56	6.61	21 (37%)
14	CLA	B	1211	-	65,73,73	2.20	19 (29%)	76,113,113	2.64	23 (30%)
17	SF4	C	3002	3	0,12,12	-	-	-	-	-
18	BCR	U	4022	-	41,41,41	3.09	9 (21%)	56,56,56	6.48	23 (41%)
14	CLA	H	1219	-	45,53,73	2.53	19 (42%)	52,89,113	2.85	21 (40%)
14	CLA	B	1220	-	55,63,73	2.38	18 (32%)	64,101,113	2.92	25 (39%)
14	CLA	B	1232	-	45,53,73	2.54	18 (40%)	52,89,113	2.86	20 (38%)
14	CLA	G	1137	-	50,58,73	2.50	19 (38%)	58,95,113	3.04	25 (43%)
18	BCR	A	4002	-	41,41,41	3.06	7 (17%)	56,56,56	6.30	28 (50%)
14	CLA	H	1226	-	65,73,73	2.24	19 (29%)	76,113,113	2.52	23 (30%)
17	SF4	C	3003	3	0,12,12	-	-	-	-	-
18	BCR	R	4018	-	41,41,41	3.05	8 (19%)	56,56,56	6.57	24 (42%)
14	CLA	a	1138	-	60,68,73	2.31	18 (30%)	70,107,113	2.58	23 (32%)
18	BCR	a	4011	-	41,41,41	3.03	8 (19%)	56,56,56	6.53	27 (48%)
16	PQN	a	2001	-	34,34,34	1.43	2 (5%)	42,45,45	1.25	5 (11%)
14	CLA	b	1235	-	60,68,73	2.29	18 (30%)	70,107,113	2.67	22 (31%)
14	CLA	b	1221	-	65,73,73	2.18	19 (29%)	76,113,113	2.54	24 (31%)
18	BCR	M	4021	-	41,41,41	2.98	7 (17%)	56,56,56	6.66	19 (33%)
14	CLA	b	1209	-	45,53,73	2.51	18 (40%)	52,89,113	2.97	21 (40%)
14	CLA	B	1239	-	65,73,73	2.21	18 (27%)	76,113,113	2.71	31 (40%)
14	CLA	A	1124	-	55,63,73	2.37	18 (32%)	64,101,113	2.88	24 (37%)
14	CLA	a	1110	-	45,53,73	2.50	17 (37%)	52,89,113	2.87	20 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	b	1217	-	55,63,73	2.35	18 (32%)	64,101,113	2.81	22 (34%)
14	CLA	G	1105	-	45,53,73	2.54	18 (40%)	52,89,113	2.94	21 (40%)
14	CLA	H	1212	-	45,53,73	2.49	17 (37%)	52,89,113	2.90	19 (36%)
14	CLA	A	1116	-	55,63,73	2.39	18 (32%)	64,101,113	2.81	27 (42%)
14	CLA	B	1223	-	65,73,73	2.18	19 (29%)	76,113,113	2.66	27 (35%)
18	BCR	A	4003	-	41,41,41	2.89	6 (14%)	56,56,56	6.55	22 (39%)
14	CLA	G	1128	-	60,68,73	2.31	19 (31%)	70,107,113	2.71	23 (32%)
14	CLA	b	1227	-	45,53,73	2.57	19 (42%)	52,89,113	2.81	22 (42%)
14	CLA	G	1133	-	60,68,73	2.30	18 (30%)	70,107,113	2.77	25 (35%)
18	BCR	H	4017	-	41,41,41	3.03	9 (21%)	56,56,56	6.74	20 (35%)
14	CLA	H	1201	-	55,63,73	2.38	18 (32%)	64,101,113	2.88	23 (35%)
18	BCR	H	4016	-	41,41,41	2.98	6 (14%)	56,56,56	6.64	20 (35%)
17	SF4	a	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	A	1130	-	55,63,73	2.41	18 (32%)	64,101,113	2.75	25 (39%)
15	F6C	a	1121	-	49,54,74	3.14	23 (46%)	46,90,114	3.85	28 (60%)
18	BCR	m	4021	-	41,41,41	2.98	7 (17%)	56,56,56	6.65	19 (33%)
14	CLA	B	1234	-	65,73,73	2.14	19 (29%)	76,113,113	2.57	22 (28%)
18	BCR	R	4020	-	41,41,41	3.22	10 (24%)	56,56,56	6.75	22 (39%)
14	CLA	H	1213	-	65,73,73	2.20	18 (27%)	76,113,113	2.62	23 (30%)
14	CLA	B	1022	-	65,73,73	2.15	19 (29%)	76,113,113	2.63	26 (34%)
15	F6C	H	1207	-	69,74,74	2.73	24 (34%)	70,114,114	3.44	28 (40%)
14	CLA	H	1220	-	55,63,73	2.38	18 (32%)	64,101,113	2.92	26 (40%)
18	BCR	B	4010	-	41,41,41	3.12	7 (17%)	56,56,56	6.68	21 (37%)
18	BCR	B	4005	-	41,41,41	2.99	7 (17%)	56,56,56	6.59	24 (42%)
14	CLA	b	1023	-	65,73,73	2.18	19 (29%)	76,113,113	2.74	25 (32%)
17	SF4	c	3002	3	0,12,12	-	-	-	-	-
14	CLA	G	1139	-	45,53,73	2.50	17 (37%)	52,89,113	2.84	22 (42%)
14	CLA	T	1401	-	45,53,73	2.55	19 (42%)	52,89,113	2.95	21 (40%)
14	CLA	A	1108	-	45,53,73	2.55	18 (40%)	52,89,113	2.87	21 (40%)
14	CLA	H	1206	2	45,53,73	2.52	16 (35%)	52,89,113	2.79	19 (36%)
14	CLA	b	1228	-	55,63,73	2.39	20 (36%)	64,101,113	2.81	26 (40%)
14	CLA	A	1140	-	65,73,73	2.17	18 (27%)	76,113,113	2.52	23 (30%)
14	CLA	B	1216	-	65,73,73	2.18	18 (27%)	76,113,113	2.50	25 (32%)
14	CLA	a	1101	-	45,53,73	2.45	17 (37%)	52,89,113	2.95	20 (38%)
14	CLA	a	1107	1	45,53,73	2.50	17 (37%)	52,89,113	2.81	21 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	A	1123	-	60,68,73	2.31	19 (31%)	70,107,113	2.65	25 (35%)
14	CLA	H	1229	-	60,68,73	2.29	19 (31%)	70,107,113	2.73	24 (34%)
14	CLA	b	1224	-	65,73,73	2.19	19 (29%)	76,113,113	2.56	22 (28%)
20	LMG	G	5005	-	46,46,55	1.29	5 (10%)	54,54,63	1.09	2 (3%)
15	F6C	B	1230	-	49,54,74	3.15	26 (53%)	46,90,114	3.82	25 (54%)
18	BCR	H	4006	-	41,41,41	2.87	6 (14%)	56,56,56	6.61	21 (37%)
14	CLA	H	1234	-	65,73,73	2.15	19 (29%)	76,113,113	2.58	22 (28%)
18	BCR	B	4013	-	41,41,41	2.80	6 (14%)	56,56,56	6.71	22 (39%)
14	CLA	H	1232	-	45,53,73	2.53	18 (40%)	52,89,113	2.86	20 (38%)
14	CLA	B	1214	-	65,73,73	2.20	20 (30%)	76,113,113	2.55	26 (34%)
18	BCR	H	4014	-	41,41,41	3.05	7 (17%)	56,56,56	6.43	24 (42%)
18	BCR	G	4007	-	41,41,41	3.13	9 (21%)	56,56,56	6.55	24 (42%)
14	CLA	W	1701	-	55,63,73	2.39	18 (32%)	64,101,113	2.78	23 (35%)
18	BCR	H	4009	-	41,41,41	2.96	7 (17%)	56,56,56	6.43	23 (41%)
18	BCR	U	4019	-	41,41,41	2.98	7 (17%)	56,56,56	7.03	29 (51%)
14	CLA	H	1235	-	60,68,73	2.29	18 (30%)	70,107,113	2.68	22 (31%)
18	BCR	l	4019	-	41,41,41	2.99	7 (17%)	56,56,56	7.03	29 (51%)
14	CLA	b	1208	-	65,73,73	2.20	18 (27%)	76,113,113	2.56	23 (30%)
14	CLA	b	1229	-	60,68,73	2.29	19 (31%)	70,107,113	2.74	24 (34%)
14	CLA	G	1134	-	45,53,73	2.61	19 (42%)	52,89,113	2.93	21 (40%)
18	BCR	a	4003	-	41,41,41	2.89	6 (14%)	56,56,56	6.55	22 (39%)
14	CLA	x	1701	-	55,63,73	2.39	18 (32%)	64,101,113	2.77	23 (35%)
19	LHG	B	5004	-	43,43,48	0.96	2 (4%)	46,49,54	1.12	3 (6%)
14	CLA	A	1105	-	45,53,73	2.55	18 (40%)	52,89,113	2.95	21 (40%)
14	CLA	A	1102	-	60,68,73	2.30	18 (30%)	70,107,113	2.69	23 (32%)
14	CLA	G	1108	-	45,53,73	2.55	18 (40%)	52,89,113	2.86	21 (40%)
19	LHG	a	5001	-	41,41,48	0.99	2 (4%)	44,47,54	1.10	3 (6%)
18	BCR	G	4002	-	41,41,41	3.05	7 (17%)	56,56,56	6.30	28 (50%)
14	CLA	A	1111	-	60,68,73	2.27	19 (31%)	70,107,113	4.78	27 (38%)
14	CLA	a	1130	-	55,63,73	2.40	18 (32%)	64,101,113	2.75	25 (39%)
18	BCR	V	4021	-	41,41,41	2.99	7 (17%)	56,56,56	6.66	19 (33%)
14	CLA	A	1131	-	60,68,73	2.28	17 (28%)	70,107,113	2.66	21 (30%)
14	CLA	a	1104	-	65,73,73	2.15	19 (29%)	76,113,113	2.76	26 (34%)
14	CLA	G	1126	-	60,68,73	2.30	19 (31%)	70,107,113	2.62	25 (35%)
14	CLA	B	1204	-	65,73,73	2.21	18 (27%)	76,113,113	2.53	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	B	1226	-	65,73,73	2.23	19 (29%)	76,113,113	2.52	23 (30%)
14	CLA	A	1110	-	45,53,73	2.50	17 (37%)	52,89,113	2.87	20 (38%)
14	CLA	B	1203	-	65,73,73	2.16	19 (29%)	76,113,113	2.66	21 (27%)
15	F6C	b	1230	-	49,54,74	3.15	26 (53%)	46,90,114	3.82	25 (54%)
14	CLA	b	1218	-	45,53,73	2.58	18 (40%)	52,89,113	2.82	18 (34%)
14	CLA	A	1115	-	65,73,73	2.21	18 (27%)	76,113,113	2.72	26 (34%)
14	CLA	b	1231	2	55,63,73	2.38	18 (32%)	64,101,113	2.76	22 (34%)
14	CLA	B	1205	-	65,73,73	2.16	18 (27%)	76,113,113	2.60	22 (28%)
14	CLA	G	1111	-	60,68,73	2.27	19 (31%)	70,107,113	4.78	27 (38%)
14	CLA	B	1215	-	60,68,73	2.24	18 (30%)	70,107,113	2.60	21 (30%)
14	CLA	H	1227	-	45,53,73	2.57	19 (42%)	52,89,113	2.81	22 (42%)
14	CLA	a	1117	-	65,73,73	2.17	18 (27%)	76,113,113	2.62	27 (35%)
14	CLA	A	1133	-	60,68,73	2.30	18 (30%)	70,107,113	2.77	25 (35%)
14	CLA	H	1203	-	65,73,73	2.16	19 (29%)	76,113,113	2.66	21 (27%)
18	BCR	b	4014	-	41,41,41	3.05	8 (19%)	56,56,56	6.44	24 (42%)
17	SF4	c	3003	3	0,12,12	-	-	-	-	-
14	CLA	G	1112	-	55,63,73	2.39	18 (32%)	64,101,113	2.78	24 (37%)
14	CLA	B	1206	2	45,53,73	2.51	16 (35%)	52,89,113	2.78	19 (36%)
14	CLA	K	1401	-	45,53,73	2.56	19 (42%)	52,89,113	2.95	21 (40%)
14	CLA	a	1140	-	65,73,73	2.17	18 (27%)	76,113,113	2.53	24 (31%)
14	CLA	A	1013	-	60,68,73	2.29	18 (30%)	70,107,113	2.77	25 (35%)
14	CLA	G	1013	-	60,68,73	2.28	18 (30%)	70,107,113	2.77	24 (34%)
14	CLA	b	1234	-	65,73,73	2.15	19 (29%)	76,113,113	2.57	22 (28%)
19	LHG	H	5004	-	43,43,48	0.96	2 (4%)	46,49,54	1.12	3 (6%)
14	CLA	b	1205	-	65,73,73	2.16	18 (27%)	76,113,113	2.59	23 (30%)
14	CLA	G	1131	-	60,68,73	2.28	17 (28%)	70,107,113	2.66	22 (31%)
20	LMG	I	5006	-	37,37,55	1.11	3 (8%)	45,45,63	1.20	3 (6%)
18	BCR	G	4008	-	41,41,41	3.18	9 (21%)	56,56,56	6.46	21 (37%)
14	CLA	A	1112	-	55,63,73	2.38	18 (32%)	64,101,113	2.77	24 (37%)
14	CLA	A	1107	1	45,53,73	2.50	17 (37%)	52,89,113	2.81	21 (40%)
19	LHG	A	5001	-	41,41,48	0.99	2 (4%)	44,47,54	1.10	3 (6%)
14	CLA	a	1127	-	65,73,73	2.20	19 (29%)	76,113,113	2.60	21 (27%)
14	CLA	a	1113	-	45,53,73	2.49	17 (37%)	52,89,113	2.89	22 (42%)
14	CLA	A	1012	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	26 (34%)
14	CLA	G	1138	-	60,68,73	2.31	18 (30%)	70,107,113	2.59	23 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	BCR	b	4017	-	41,41,41	3.02	9 (21%)	56,56,56	6.73	20 (35%)
18	BCR	A	4007	-	41,41,41	3.13	9 (21%)	56,56,56	6.55	24 (42%)
17	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	B	1221	-	65,73,73	2.19	19 (29%)	76,113,113	2.55	24 (31%)
14	CLA	b	1219	-	45,53,73	2.52	18 (40%)	52,89,113	2.86	21 (40%)
14	CLA	a	1108	-	45,53,73	2.55	18 (40%)	52,89,113	2.86	21 (40%)
14	CLA	H	1202	-	60,68,73	2.19	19 (31%)	70,107,113	2.69	24 (34%)
14	CLA	B	1236	-	45,53,73	2.47	18 (40%)	52,89,113	2.93	19 (36%)
18	BCR	i	4020	-	41,41,41	3.22	10 (24%)	56,56,56	6.75	23 (41%)
14	CLA	B	1233	-	45,53,73	2.53	18 (40%)	52,89,113	2.89	20 (38%)
14	CLA	H	1216	-	65,73,73	2.18	18 (27%)	76,113,113	2.50	24 (31%)
14	CLA	H	1225	-	65,73,73	2.24	19 (29%)	76,113,113	2.48	21 (27%)
14	CLA	G	1106	-	60,68,73	2.27	18 (30%)	70,107,113	2.77	24 (34%)
14	CLA	G	1116	-	55,63,73	2.39	18 (32%)	64,101,113	2.79	27 (42%)
14	CLA	A	1127	-	65,73,73	2.20	19 (29%)	76,113,113	2.60	21 (27%)
14	CLA	G	1114	-	45,53,73	2.54	20 (44%)	52,89,113	2.86	20 (38%)
14	CLA	a	1122	-	55,63,73	2.36	18 (32%)	64,101,113	2.77	26 (40%)
14	CLA	H	1233	-	45,53,73	2.53	18 (40%)	52,89,113	2.90	19 (36%)
14	CLA	G	1107	1	45,53,73	2.50	17 (37%)	52,89,113	2.81	21 (40%)
18	BCR	l	4022	-	41,41,41	3.10	9 (21%)	56,56,56	6.49	23 (41%)
14	CLA	H	1210	-	65,73,73	2.22	20 (30%)	76,113,113	2.76	26 (34%)
14	CLA	B	1023	-	65,73,73	2.19	19 (29%)	76,113,113	2.75	26 (34%)
14	CLA	a	1112	-	55,63,73	2.39	19 (34%)	64,101,113	2.78	24 (37%)
21	LMT	a	6002	-	29,29,36	1.40	6 (20%)	40,40,47	1.16	4 (10%)
14	CLA	A	1104	-	65,73,73	2.15	19 (29%)	76,113,113	2.76	26 (34%)
14	CLA	B	1228	-	55,63,73	2.39	20 (36%)	64,101,113	2.82	26 (40%)
15	F6C	B	1207	-	69,74,74	2.73	24 (34%)	70,114,114	3.44	28 (40%)
14	CLA	G	1135	-	60,68,73	2.29	20 (33%)	70,107,113	2.68	24 (34%)
14	CLA	A	1120	-	45,53,73	2.46	17 (37%)	52,89,113	2.98	20 (38%)
14	CLA	H	1021	-	65,73,73	2.18	20 (30%)	76,113,113	2.55	25 (32%)
20	LMG	U	5007	-	50,50,55	1.34	7 (14%)	58,58,63	1.09	2 (3%)
16	PQN	b	2002	-	34,34,34	1.47	2 (5%)	42,45,45	1.26	2 (4%)
18	BCR	a	4008	-	41,41,41	3.18	9 (21%)	56,56,56	6.45	20 (35%)
14	CLA	a	1111	-	60,68,73	2.27	19 (31%)	70,107,113	4.78	27 (38%)
14	CLA	a	1012	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	26 (34%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	B	1208	-	65,73,73	2.20	18 (27%)	76,113,113	2.56	22 (28%)
15	F6C	b	1207	-	69,74,74	2.73	24 (34%)	70,114,114	3.44	28 (40%)
14	CLA	B	1222	-	65,73,73	2.22	19 (29%)	76,113,113	2.65	27 (35%)
14	CLA	A	1103	-	60,68,73	2.24	19 (31%)	70,107,113	2.72	23 (32%)
15	F6C	H	1230	-	49,54,74	3.15	26 (53%)	46,90,114	3.82	25 (54%)
14	CLA	a	1106	-	60,68,73	2.27	19 (31%)	70,107,113	2.77	24 (34%)
14	CLA	H	1231	2	55,63,73	2.38	18 (32%)	64,101,113	2.76	23 (35%)
18	BCR	H	4013	-	41,41,41	2.81	6 (14%)	56,56,56	6.71	22 (39%)
13	CL0	A	1011	-	65,73,73	2.16	20 (30%)	76,113,113	2.60	22 (28%)
14	CLA	a	1114	-	45,53,73	2.54	20 (44%)	52,89,113	2.87	20 (38%)
14	CLA	b	1212	-	45,53,73	2.49	17 (37%)	52,89,113	2.90	19 (36%)
18	BCR	A	4011	-	41,41,41	3.02	8 (19%)	56,56,56	6.53	27 (48%)
14	CLA	a	1105	-	45,53,73	2.54	18 (40%)	52,89,113	2.94	21 (40%)
14	CLA	a	1115	-	65,73,73	2.20	18 (27%)	76,113,113	2.72	26 (34%)
14	CLA	G	1102	-	60,68,73	2.30	18 (30%)	70,107,113	2.68	23 (32%)
14	CLA	G	1120	-	45,53,73	2.47	17 (37%)	52,89,113	2.99	20 (38%)
14	CLA	b	1214	-	65,73,73	2.21	20 (30%)	76,113,113	2.55	26 (34%)
14	CLA	a	1133	-	60,68,73	2.30	19 (31%)	70,107,113	2.77	25 (35%)
14	CLA	G	1117	-	65,73,73	2.18	18 (27%)	76,113,113	2.63	27 (35%)
18	BCR	a	4007	-	41,41,41	3.13	8 (19%)	56,56,56	6.56	24 (42%)
14	CLA	a	1102	-	60,68,73	2.30	18 (30%)	70,107,113	2.69	23 (32%)
14	CLA	B	1201	-	55,63,73	2.38	18 (32%)	64,101,113	2.87	23 (35%)
14	CLA	H	1236	-	45,53,73	2.48	18 (40%)	52,89,113	2.93	19 (36%)
20	LMG	b	5002	-	46,46,55	1.25	5 (10%)	54,54,63	1.25	4 (7%)
15	F6C	b	1238	-	69,74,74	2.70	23 (33%)	70,114,114	3.26	29 (41%)
14	CLA	b	1233	-	45,53,73	2.53	18 (40%)	52,89,113	2.89	18 (34%)
16	PQN	G	2001	-	34,34,34	1.44	2 (5%)	42,45,45	1.25	5 (11%)
15	F6C	H	1237	-	69,74,74	2.68	23 (33%)	70,114,114	3.22	27 (38%)
14	CLA	B	1229	-	60,68,73	2.29	19 (31%)	70,107,113	2.73	24 (34%)
14	CLA	G	1136	-	65,73,73	2.17	18 (27%)	76,113,113	2.58	22 (28%)
14	CLA	a	1137	-	50,58,73	2.50	19 (38%)	58,95,113	3.05	25 (43%)
14	CLA	A	1113	-	45,53,73	2.49	17 (37%)	52,89,113	2.89	23 (44%)
14	CLA	A	1134	-	45,53,73	2.62	19 (42%)	52,89,113	2.93	21 (40%)
14	CLA	G	1129	-	50,58,73	2.50	19 (38%)	58,95,113	2.89	23 (39%)
17	SF4	N	3002	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	a	1135	-	60,68,73	2.29	20 (33%)	70,107,113	2.68	24 (34%)
14	CLA	L	1503	-	65,73,73	2.20	18 (27%)	76,113,113	2.60	24 (31%)
14	CLA	b	1203	-	65,73,73	2.16	20 (30%)	76,113,113	2.66	21 (27%)
14	CLA	G	1119	-	65,73,73	2.20	19 (29%)	76,113,113	2.62	24 (31%)
18	BCR	B	4009	-	41,41,41	2.96	7 (17%)	56,56,56	6.43	23 (41%)
14	CLA	a	1126	-	60,68,73	2.30	19 (31%)	70,107,113	2.61	25 (35%)
15	F6C	B	1238	-	69,74,74	2.71	23 (33%)	70,114,114	3.26	29 (41%)
14	CLA	G	1127	-	65,73,73	2.20	19 (29%)	76,113,113	2.59	22 (28%)
19	LHG	b	5004	-	43,43,48	0.97	2 (4%)	46,49,54	1.12	3 (6%)
21	LMT	G	6001	-	32,32,36	1.28	6 (18%)	43,43,47	1.05	2 (4%)
14	CLA	a	1128	-	60,68,73	2.32	19 (31%)	70,107,113	2.72	23 (32%)
14	CLA	b	1204	-	65,73,73	2.21	18 (27%)	76,113,113	2.54	27 (35%)
14	CLA	b	1220	-	55,63,73	2.38	17 (30%)	64,101,113	2.92	26 (40%)
14	CLA	b	1232	-	45,53,73	2.53	18 (40%)	52,89,113	2.86	20 (38%)
19	LHG	G	5001	-	41,41,48	0.99	2 (4%)	44,47,54	1.10	3 (6%)
16	PQN	H	2002	-	34,34,34	1.48	2 (5%)	42,45,45	1.26	2 (4%)
18	BCR	b	4009	-	41,41,41	2.96	7 (17%)	56,56,56	6.43	22 (39%)
15	F6C	H	1238	-	69,74,74	2.70	23 (33%)	70,114,114	3.26	29 (41%)
14	CLA	a	1120	-	45,53,73	2.47	17 (37%)	52,89,113	2.99	20 (38%)
14	CLA	G	1122	-	55,63,73	2.37	18 (32%)	64,101,113	2.77	26 (40%)
14	CLA	A	1126	-	60,68,73	2.30	19 (31%)	70,107,113	2.62	25 (35%)
18	BCR	B	4017	-	41,41,41	3.03	8 (19%)	56,56,56	6.74	20 (35%)
21	LMT	A	6002	-	29,29,36	1.40	6 (20%)	40,40,47	1.16	4 (10%)
14	CLA	G	1118	-	55,63,73	2.38	18 (32%)	64,101,113	2.78	27 (42%)
14	CLA	G	1110	-	45,53,73	2.51	17 (37%)	52,89,113	2.88	20 (38%)
14	CLA	L	1502	-	60,68,73	2.23	18 (30%)	70,107,113	2.75	23 (32%)
14	CLA	G	1104	-	65,73,73	2.14	19 (29%)	76,113,113	2.76	25 (32%)
14	CLA	B	1235	-	60,68,73	2.30	18 (30%)	70,107,113	2.68	22 (31%)
14	CLA	b	1202	-	60,68,73	2.19	18 (30%)	70,107,113	2.69	24 (34%)
18	BCR	A	4008	-	41,41,41	3.18	9 (21%)	56,56,56	6.45	21 (37%)
14	CLA	B	1209	-	45,53,73	2.51	18 (40%)	52,89,113	2.97	21 (40%)
14	CLA	b	1225	-	65,73,73	2.24	19 (29%)	76,113,113	2.48	21 (27%)
14	CLA	a	1134	-	45,53,73	2.61	19 (42%)	52,89,113	2.93	21 (40%)
14	CLA	H	1223	-	65,73,73	2.18	19 (29%)	76,113,113	2.67	26 (34%)
14	CLA	H	1211	-	65,73,73	2.20	20 (30%)	76,113,113	2.65	22 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	F6C	G	1121	-	49,54,74	3.13	23 (46%)	46,90,114	3.86	28 (60%)
18	BCR	B	4004	-	41,41,41	2.85	7 (17%)	56,56,56	6.49	25 (44%)
14	CLA	H	1214	-	65,73,73	2.21	20 (30%)	76,113,113	2.55	27 (35%)
17	SF4	G	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	B	1227	-	45,53,73	2.57	19 (42%)	52,89,113	2.81	23 (44%)
14	CLA	a	1129	-	50,58,73	2.50	19 (38%)	58,95,113	2.89	23 (39%)
14	CLA	b	1022	-	65,73,73	2.15	18 (27%)	76,113,113	2.62	26 (34%)
14	CLA	H	1228	-	55,63,73	2.39	20 (36%)	64,101,113	2.83	26 (40%)
14	CLA	b	1210	-	65,73,73	2.22	20 (30%)	76,113,113	2.76	26 (34%)
18	BCR	I	4018	-	41,41,41	3.05	8 (19%)	56,56,56	6.57	24 (42%)
14	CLA	A	1132	-	65,73,73	2.16	17 (26%)	76,113,113	2.69	24 (31%)
14	CLA	b	1223	-	65,73,73	2.17	19 (29%)	76,113,113	2.65	26 (34%)
14	CLA	H	1222	-	65,73,73	2.21	19 (29%)	76,113,113	2.64	27 (35%)
14	CLA	a	1132	-	65,73,73	2.16	17 (26%)	76,113,113	2.69	24 (31%)
18	BCR	a	4001	-	41,41,41	2.95	6 (14%)	56,56,56	6.60	24 (42%)
14	CLA	a	1136	-	65,73,73	2.17	18 (27%)	76,113,113	2.58	22 (28%)
14	CLA	l	1502	-	60,68,73	2.23	18 (30%)	70,107,113	2.74	23 (32%)
18	BCR	b	4010	-	41,41,41	3.11	7 (17%)	56,56,56	6.68	21 (37%)
14	CLA	H	1215	-	60,68,73	2.24	18 (30%)	70,107,113	2.59	21 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	L	4019	-	-	12/29/63/63	0/2/2/2
17	SF4	N	3003	3	-	-	0/6/5/5
14	CLA	U	1501	10	1/1/15/20	14/37/115/115	-
14	CLA	U	1503	-	1/1/15/20	14/37/115/115	-
18	BCR	B	4014	-	-	7/29/63/63	0/2/2/2
18	BCR	H	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	G	1109	-	1/1/15/20	19/37/115/115	-
14	CLA	b	1239	-	1/1/15/20	20/37/115/115	-
14	CLA	H	1022	-	1/1/15/20	19/37/115/115	-
18	BCR	b	4013	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	b	4005	-	-	6/29/63/63	0/2/2/2
18	BCR	I	4020	-	-	13/29/63/63	0/2/2/2
14	CLA	a	1103	-	1/1/14/20	15/31/109/115	-
18	BCR	b	4016	-	-	12/29/63/63	0/2/2/2
14	CLA	H	1204	-	1/1/15/20	16/37/115/115	-
16	PQN	A	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	G	1124	-	1/1/13/20	9/25/103/115	-
14	CLA	A	1129	-	1/1/12/20	6/19/97/115	-
14	CLA	B	1217	-	1/1/13/20	13/25/103/115	-
20	LMG	i	5006	-	-	10/32/52/70	0/1/1/1
20	LMG	A	5005	-	-	19/41/61/70	0/1/1/1
13	CL0	G	1011	-	3/3/20/25	11/37/135/135	-
14	CLA	H	1221	-	1/1/15/20	12/37/115/115	-
14	CLA	l	1503	-	1/1/15/20	14/37/115/115	-
14	CLA	H	1209	-	1/1/11/20	3/13/91/115	-
14	CLA	b	1236	-	1/1/11/20	3/13/91/115	-
14	CLA	U	1502	-	1/1/14/20	13/31/109/115	-
14	CLA	H	1217	-	1/1/13/20	13/25/103/115	-
14	CLA	a	1118	-	1/1/13/20	11/25/103/115	-
14	CLA	G	1115	-	1/1/15/20	20/37/115/115	-
15	F6C	b	1237	-	-	21/41/97/97	-
14	CLA	A	1135	-	1/1/14/20	12/31/109/115	-
14	CLA	a	1119	-	1/1/15/20	11/37/115/115	-
14	CLA	A	1117	-	1/1/15/20	19/37/115/115	-
14	CLA	a	1116	-	1/1/13/20	10/25/103/115	-
15	F6C	A	1121	-	-	9/17/73/97	-
14	CLA	G	1130	-	1/1/13/20	9/25/103/115	-
14	CLA	A	1138	-	1/1/14/20	20/31/109/115	-
20	LMG	l	5007	-	-	15/45/65/70	0/1/1/1
14	CLA	G	1101	-	1/1/11/20	6/13/91/115	-
14	CLA	a	1013	-	1/1/14/20	13/31/109/115	-
14	CLA	A	1125	-	1/1/15/20	19/37/115/115	-
14	CLA	G	1123	-	1/1/14/20	14/31/109/115	-
14	CLA	l	1501	10	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1113	-	1/1/11/20	8/13/91/115	-
14	CLA	b	1226	-	1/1/15/20	12/37/115/115	-
20	LMG	B	5002	-	-	13/41/61/70	0/1/1/1
14	CLA	B	1213	-	1/1/15/20	17/37/115/115	-
14	CLA	A	1119	-	1/1/15/20	11/37/115/115	-
14	CLA	B	1225	-	1/1/15/20	18/37/115/115	-
21	LMT	a	6001	-	-	7/17/57/61	0/2/2/2
14	CLA	A	1128	-	1/1/14/20	15/31/109/115	-
14	CLA	A	1118	-	1/1/13/20	11/25/103/115	-
14	CLA	a	1109	-	1/1/15/20	19/37/115/115	-
14	CLA	A	1114	-	1/1/11/20	9/13/91/115	-
14	CLA	G	1140	-	1/1/15/20	21/37/115/115	-
14	CLA	b	1216	-	1/1/15/20	21/37/115/115	-
14	CLA	B	1231	2	1/1/13/20	5/25/103/115	-
14	CLA	A	1137	-	1/1/12/20	5/19/97/115	-
18	BCR	B	4016	-	-	12/29/63/63	0/2/2/2
14	CLA	B	1224	-	1/1/15/20	17/37/115/115	-
14	CLA	a	1124	-	1/1/13/20	9/25/103/115	-
14	CLA	G	1012	-	1/1/15/20	10/37/115/115	-
14	CLA	H	1023	-	1/1/15/20	15/37/115/115	-
14	CLA	b	1206	2	1/1/11/20	7/13/91/115	-
14	CLA	A	1109	-	1/1/15/20	19/37/115/115	-
14	CLA	B	1021	-	1/1/15/20	22/37/115/115	-
14	CLA	G	1125	-	1/1/15/20	19/37/115/115	-
18	BCR	A	4001	-	-	14/29/63/63	0/2/2/2
14	CLA	a	1131	-	1/1/14/20	12/31/109/115	-
15	F6C	B	1237	-	-	21/41/97/97	-
16	PQN	B	2002	-	-	12/23/43/43	0/2/2/2
18	BCR	i	4018	-	-	8/29/63/63	0/2/2/2
14	CLA	H	1224	-	1/1/15/20	17/37/115/115	-
18	BCR	H	4005	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1205	-	1/1/15/20	10/37/115/115	-
14	CLA	a	1139	-	1/1/11/20	3/13/91/115	-
18	BCR	H	4010	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CL0	a	1011	-	3/3/20/25	11/37/135/135	-
14	CLA	b	1213	-	1/1/15/20	17/37/115/115	-
14	CLA	k	1401	-	1/1/11/20	7/13/91/115	-
14	CLA	b	1211	-	1/1/15/20	20/37/115/115	-
14	CLA	B	1212	-	1/1/11/20	4/13/91/115	-
14	CLA	b	1021	-	1/1/15/20	22/37/115/115	-
18	BCR	G	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	B	1218	-	1/1/11/20	6/13/91/115	-
14	CLA	X	1701	-	1/1/13/20	11/25/103/115	-
14	CLA	G	1132	-	1/1/15/20	12/37/115/115	-
18	BCR	a	4002	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1208	-	1/1/15/20	16/37/115/115	-
18	BCR	G	4001	-	-	14/29/63/63	0/2/2/2
18	BCR	G	4011	-	-	17/29/63/63	0/2/2/2
14	CLA	a	1123	-	1/1/14/20	14/31/109/115	-
14	CLA	b	1201	-	1/1/13/20	7/25/103/115	-
14	CLA	B	1219	-	1/1/11/20	4/13/91/115	-
20	LMG	a	5005	-	-	19/41/61/70	0/1/1/1
20	LMG	H	5002	-	-	13/41/61/70	0/1/1/1
14	CLA	B	1202	-	1/1/14/20	13/31/109/115	-
14	CLA	H	1239	-	1/1/15/20	20/37/115/115	-
14	CLA	A	1122	-	1/1/13/20	13/25/103/115	-
20	LMG	R	5006	-	-	10/32/52/70	0/1/1/1
14	CLA	b	1222	-	1/1/15/20	17/37/115/115	-
14	CLA	A	1106	-	1/1/14/20	13/31/109/115	-
18	BCR	b	4006	-	-	10/29/63/63	0/2/2/2
21	LMT	G	6002	-	-	7/14/54/61	0/2/2/2
14	CLA	A	1139	-	1/1/11/20	3/13/91/115	-
20	LMG	L	5007	-	-	15/45/65/70	0/1/1/1
14	CLA	b	1215	-	1/1/14/20	18/31/109/115	-
14	CLA	a	1125	-	1/1/15/20	19/37/115/115	-
14	CLA	G	1103	-	1/1/14/20	15/31/109/115	-
14	CLA	A	1101	-	1/1/11/20	6/13/91/115	-
14	CLA	L	1501	10	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	1210	-	1/1/15/20	19/37/115/115	-
18	BCR	b	4004	-	-	7/29/63/63	0/2/2/2
18	BCR	L	4022	-	-	6/29/63/63	0/2/2/2
21	LMT	A	6001	-	-	7/17/57/61	0/2/2/2
14	CLA	H	1218	-	1/1/11/20	6/13/91/115	-
14	CLA	A	1136	-	1/1/15/20	17/37/115/115	-
18	BCR	B	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	B	1211	-	1/1/15/20	20/37/115/115	-
18	BCR	U	4022	-	-	6/29/63/63	0/2/2/2
17	SF4	C	3002	3	-	-	0/6/5/5
14	CLA	H	1219	-	1/1/11/20	4/13/91/115	-
14	CLA	B	1220	-	1/1/13/20	12/25/103/115	-
14	CLA	B	1232	-	1/1/11/20	2/13/91/115	-
14	CLA	G	1137	-	1/1/12/20	5/19/97/115	-
18	BCR	A	4002	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1226	-	1/1/15/20	12/37/115/115	-
18	BCR	R	4018	-	-	8/29/63/63	0/2/2/2
17	SF4	C	3003	3	-	-	0/6/5/5
14	CLA	a	1138	-	1/1/14/20	20/31/109/115	-
18	BCR	a	4011	-	-	17/29/63/63	0/2/2/2
16	PQN	a	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	b	1235	-	1/1/14/20	14/31/109/115	-
14	CLA	b	1221	-	1/1/15/20	12/37/115/115	-
18	BCR	M	4021	-	-	18/29/63/63	0/2/2/2
14	CLA	b	1209	-	1/1/11/20	3/13/91/115	-
14	CLA	B	1239	-	1/1/15/20	20/37/115/115	-
14	CLA	A	1124	-	1/1/13/20	9/25/103/115	-
14	CLA	a	1110	-	1/1/11/20	5/13/91/115	-
14	CLA	b	1217	-	1/1/13/20	13/25/103/115	-
14	CLA	G	1105	-	1/1/11/20	4/13/91/115	-
14	CLA	H	1212	-	1/1/11/20	4/13/91/115	-
14	CLA	A	1116	-	1/1/13/20	10/25/103/115	-
14	CLA	B	1223	-	1/1/15/20	18/37/115/115	-
18	BCR	A	4003	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1128	-	1/1/14/20	15/31/109/115	-
14	CLA	b	1227	-	1/1/11/20	5/13/91/115	-
14	CLA	G	1133	-	1/1/14/20	9/31/109/115	-
18	BCR	H	4017	-	-	15/29/63/63	0/2/2/2
14	CLA	H	1201	-	1/1/13/20	7/25/103/115	-
18	BCR	H	4016	-	-	12/29/63/63	0/2/2/2
17	SF4	a	3001	2,1	-	-	0/6/5/5
14	CLA	A	1130	-	1/1/13/20	9/25/103/115	-
15	F6C	a	1121	-	-	9/17/73/97	-
18	BCR	m	4021	-	-	18/29/63/63	0/2/2/2
14	CLA	B	1234	-	1/1/15/20	16/37/115/115	-
18	BCR	R	4020	-	-	13/29/63/63	0/2/2/2
14	CLA	H	1213	-	1/1/15/20	17/37/115/115	-
14	CLA	B	1022	-	1/1/15/20	19/37/115/115	-
15	F6C	H	1207	-	-	20/41/97/97	-
14	CLA	H	1220	-	1/1/13/20	12/25/103/115	-
18	BCR	B	4010	-	-	10/29/63/63	0/2/2/2
18	BCR	B	4005	-	-	6/29/63/63	0/2/2/2
14	CLA	b	1023	-	1/1/15/20	15/37/115/115	-
17	SF4	c	3002	3	-	-	0/6/5/5
14	CLA	G	1139	-	1/1/11/20	3/13/91/115	-
14	CLA	T	1401	-	1/1/11/20	7/13/91/115	-
14	CLA	A	1108	-	1/1/11/20	6/13/91/115	-
14	CLA	H	1206	2	1/1/11/20	7/13/91/115	-
14	CLA	b	1228	-	1/1/13/20	16/25/103/115	-
14	CLA	A	1140	-	1/1/15/20	21/37/115/115	-
14	CLA	B	1216	-	1/1/15/20	21/37/115/115	-
14	CLA	a	1101	-	1/1/11/20	6/13/91/115	-
14	CLA	a	1107	1	1/1/11/20	3/13/91/115	-
14	CLA	A	1123	-	1/1/14/20	14/31/109/115	-
14	CLA	H	1229	-	1/1/14/20	14/31/109/115	-
14	CLA	b	1224	-	1/1/15/20	17/37/115/115	-
20	LMG	G	5005	-	-	19/41/61/70	0/1/1/1
15	F6C	B	1230	-	-	8/17/73/97	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	H	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	H	1234	-	1/1/15/20	16/37/115/115	-
18	BCR	B	4013	-	-	11/29/63/63	0/2/2/2
14	CLA	H	1232	-	1/1/11/20	2/13/91/115	-
14	CLA	B	1214	-	1/1/15/20	15/37/115/115	-
18	BCR	H	4014	-	-	7/29/63/63	0/2/2/2
18	BCR	G	4007	-	-	12/29/63/63	0/2/2/2
14	CLA	W	1701	-	1/1/13/20	11/25/103/115	-
18	BCR	H	4009	-	-	9/29/63/63	0/2/2/2
18	BCR	U	4019	-	-	12/29/63/63	0/2/2/2
14	CLA	H	1235	-	1/1/14/20	14/31/109/115	-
18	BCR	l	4019	-	-	12/29/63/63	0/2/2/2
14	CLA	b	1208	-	1/1/15/20	16/37/115/115	-
14	CLA	b	1229	-	1/1/14/20	14/31/109/115	-
14	CLA	G	1134	-	1/1/11/20	8/13/91/115	-
18	BCR	a	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	x	1701	-	1/1/13/20	11/25/103/115	-
19	LHG	B	5004	-	-	25/48/48/53	-
14	CLA	A	1105	-	1/1/11/20	4/13/91/115	-
14	CLA	A	1102	-	1/1/14/20	16/31/109/115	-
14	CLA	G	1108	-	1/1/11/20	6/13/91/115	-
19	LHG	a	5001	-	-	23/46/46/53	-
18	BCR	G	4002	-	-	6/29/63/63	0/2/2/2
14	CLA	A	1111	-	1/1/14/20	15/31/109/115	-
14	CLA	a	1130	-	1/1/13/20	9/25/103/115	-
18	BCR	V	4021	-	-	18/29/63/63	0/2/2/2
14	CLA	A	1131	-	1/1/14/20	12/31/109/115	-
14	CLA	a	1104	-	1/1/15/20	10/37/115/115	-
14	CLA	G	1126	-	1/1/14/20	21/31/109/115	-
14	CLA	B	1204	-	1/1/15/20	16/37/115/115	-
14	CLA	B	1226	-	1/1/15/20	12/37/115/115	-
14	CLA	A	1110	-	1/1/11/20	5/13/91/115	-
14	CLA	B	1203	-	1/1/15/20	16/37/115/115	-
15	F6C	b	1230	-	-	8/17/73/97	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	1218	-	1/1/11/20	6/13/91/115	-
14	CLA	A	1115	-	1/1/15/20	20/37/115/115	-
14	CLA	b	1231	2	1/1/13/20	5/25/103/115	-
14	CLA	B	1205	-	1/1/15/20	10/37/115/115	-
14	CLA	G	1111	-	1/1/14/20	15/31/109/115	-
14	CLA	B	1215	-	1/1/14/20	18/31/109/115	-
14	CLA	H	1227	-	1/1/11/20	5/13/91/115	-
14	CLA	a	1117	-	1/1/15/20	19/37/115/115	-
14	CLA	A	1133	-	1/1/14/20	9/31/109/115	-
14	CLA	H	1203	-	1/1/15/20	16/37/115/115	-
18	BCR	b	4014	-	-	7/29/63/63	0/2/2/2
17	SF4	c	3003	3	-	-	0/6/5/5
14	CLA	G	1112	-	1/1/13/20	13/25/103/115	-
14	CLA	B	1206	2	1/1/11/20	7/13/91/115	-
14	CLA	K	1401	-	1/1/11/20	7/13/91/115	-
14	CLA	a	1140	-	1/1/15/20	21/37/115/115	-
14	CLA	A	1013	-	1/1/14/20	13/31/109/115	-
14	CLA	G	1013	-	1/1/14/20	13/31/109/115	-
14	CLA	b	1234	-	1/1/15/20	16/37/115/115	-
19	LHG	H	5004	-	-	25/48/48/53	-
14	CLA	b	1205	-	1/1/15/20	10/37/115/115	-
14	CLA	G	1131	-	1/1/14/20	12/31/109/115	-
20	LMG	I	5006	-	-	10/32/52/70	0/1/1/1
18	BCR	G	4008	-	-	12/29/63/63	0/2/2/2
14	CLA	A	1112	-	1/1/13/20	13/25/103/115	-
14	CLA	A	1107	1	1/1/11/20	3/13/91/115	-
19	LHG	A	5001	-	-	23/46/46/53	-
14	CLA	a	1127	-	1/1/15/20	15/37/115/115	-
14	CLA	a	1113	-	1/1/11/20	8/13/91/115	-
14	CLA	A	1012	-	1/1/15/20	10/37/115/115	-
14	CLA	G	1138	-	1/1/14/20	20/31/109/115	-
18	BCR	b	4017	-	-	15/29/63/63	0/2/2/2
18	BCR	A	4007	-	-	12/29/63/63	0/2/2/2
17	SF4	A	3001	2,1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	1221	-	1/1/15/20	12/37/115/115	-
14	CLA	b	1219	-	1/1/11/20	4/13/91/115	-
14	CLA	a	1108	-	1/1/11/20	6/13/91/115	-
14	CLA	H	1202	-	1/1/14/20	13/31/109/115	-
14	CLA	B	1236	-	1/1/11/20	3/13/91/115	-
18	BCR	i	4020	-	-	13/29/63/63	0/2/2/2
14	CLA	B	1233	-	1/1/11/20	7/13/91/115	-
14	CLA	H	1216	-	1/1/15/20	21/37/115/115	-
14	CLA	H	1225	-	1/1/15/20	18/37/115/115	-
14	CLA	G	1106	-	1/1/14/20	13/31/109/115	-
14	CLA	G	1116	-	1/1/13/20	10/25/103/115	-
14	CLA	A	1127	-	1/1/15/20	15/37/115/115	-
14	CLA	G	1114	-	1/1/11/20	9/13/91/115	-
14	CLA	a	1122	-	1/1/13/20	13/25/103/115	-
14	CLA	H	1233	-	1/1/11/20	7/13/91/115	-
14	CLA	G	1107	1	1/1/11/20	3/13/91/115	-
18	BCR	l	4022	-	-	6/29/63/63	0/2/2/2
14	CLA	H	1210	-	1/1/15/20	19/37/115/115	-
14	CLA	B	1023	-	1/1/15/20	15/37/115/115	-
14	CLA	a	1112	-	1/1/13/20	13/25/103/115	-
21	LMT	a	6002	-	-	7/14/54/61	0/2/2/2
14	CLA	A	1104	-	1/1/15/20	10/37/115/115	-
14	CLA	B	1228	-	1/1/13/20	16/25/103/115	-
15	F6C	B	1207	-	-	20/41/97/97	-
14	CLA	G	1135	-	1/1/14/20	13/31/109/115	-
14	CLA	A	1120	-	1/1/11/20	7/13/91/115	-
14	CLA	H	1021	-	1/1/15/20	22/37/115/115	-
20	LMG	U	5007	-	-	15/45/65/70	0/1/1/1
16	PQN	b	2002	-	-	12/23/43/43	0/2/2/2
18	BCR	a	4008	-	-	12/29/63/63	0/2/2/2
14	CLA	a	1111	-	1/1/14/20	15/31/109/115	-
14	CLA	a	1012	-	1/1/15/20	10/37/115/115	-
14	CLA	B	1208	-	1/1/15/20	16/37/115/115	-
15	F6C	b	1207	-	-	20/41/97/97	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	1222	-	1/1/15/20	17/37/115/115	-
14	CLA	A	1103	-	1/1/14/20	15/31/109/115	-
15	F6C	H	1230	-	-	8/17/73/97	-
14	CLA	a	1106	-	1/1/14/20	13/31/109/115	-
14	CLA	H	1231	2	1/1/13/20	5/25/103/115	-
18	BCR	H	4013	-	-	11/29/63/63	0/2/2/2
13	CL0	A	1011	-	3/3/20/25	11/37/135/135	-
14	CLA	a	1114	-	1/1/11/20	9/13/91/115	-
14	CLA	b	1212	-	1/1/11/20	4/13/91/115	-
18	BCR	A	4011	-	-	17/29/63/63	0/2/2/2
14	CLA	a	1105	-	1/1/11/20	4/13/91/115	-
14	CLA	a	1115	-	1/1/15/20	20/37/115/115	-
14	CLA	G	1102	-	1/1/14/20	16/31/109/115	-
14	CLA	G	1120	-	1/1/11/20	7/13/91/115	-
14	CLA	b	1214	-	1/1/15/20	15/37/115/115	-
14	CLA	a	1133	-	1/1/14/20	9/31/109/115	-
14	CLA	G	1117	-	1/1/15/20	19/37/115/115	-
18	BCR	a	4007	-	-	12/29/63/63	0/2/2/2
14	CLA	a	1102	-	1/1/14/20	16/31/109/115	-
14	CLA	B	1201	-	1/1/13/20	7/25/103/115	-
14	CLA	H	1236	-	1/1/11/20	3/13/91/115	-
20	LMG	b	5002	-	-	13/41/61/70	0/1/1/1
15	F6C	b	1238	-	-	16/41/97/97	-
14	CLA	b	1233	-	1/1/11/20	7/13/91/115	-
16	PQN	G	2001	-	-	9/23/43/43	0/2/2/2
15	F6C	H	1237	-	-	21/41/97/97	-
14	CLA	B	1229	-	1/1/14/20	14/31/109/115	-
14	CLA	G	1136	-	1/1/15/20	17/37/115/115	-
14	CLA	a	1137	-	1/1/12/20	5/19/97/115	-
14	CLA	A	1113	-	1/1/11/20	8/13/91/115	-
14	CLA	A	1134	-	1/1/11/20	8/13/91/115	-
14	CLA	G	1129	-	1/1/12/20	6/19/97/115	-
17	SF4	N	3002	3	-	-	0/6/5/5
14	CLA	a	1135	-	1/1/14/20	12/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	L	1503	-	1/1/15/20	14/37/115/115	-
14	CLA	b	1203	-	1/1/15/20	16/37/115/115	-
14	CLA	G	1119	-	1/1/15/20	11/37/115/115	-
18	BCR	B	4009	-	-	9/29/63/63	0/2/2/2
14	CLA	a	1126	-	1/1/14/20	21/31/109/115	-
15	F6C	B	1238	-	-	16/41/97/97	-
14	CLA	G	1127	-	1/1/15/20	15/37/115/115	-
19	LHG	b	5004	-	-	25/48/48/53	-
21	LMT	G	6001	-	-	7/17/57/61	0/2/2/2
14	CLA	a	1128	-	1/1/14/20	15/31/109/115	-
14	CLA	b	1204	-	1/1/15/20	16/37/115/115	-
14	CLA	b	1220	-	1/1/13/20	12/25/103/115	-
14	CLA	b	1232	-	1/1/11/20	2/13/91/115	-
19	LHG	G	5001	-	-	23/46/46/53	-
16	PQN	H	2002	-	-	12/23/43/43	0/2/2/2
18	BCR	b	4009	-	-	9/29/63/63	0/2/2/2
15	F6C	H	1238	-	-	16/41/97/97	-
14	CLA	a	1120	-	1/1/11/20	7/13/91/115	-
14	CLA	G	1122	-	1/1/13/20	13/25/103/115	-
14	CLA	A	1126	-	1/1/14/20	21/31/109/115	-
18	BCR	B	4017	-	-	15/29/63/63	0/2/2/2
21	LMT	A	6002	-	-	7/14/54/61	0/2/2/2
14	CLA	G	1118	-	1/1/13/20	11/25/103/115	-
14	CLA	G	1110	-	1/1/11/20	5/13/91/115	-
14	CLA	L	1502	-	1/1/14/20	13/31/109/115	-
14	CLA	G	1104	-	1/1/15/20	10/37/115/115	-
14	CLA	B	1235	-	1/1/14/20	14/31/109/115	-
14	CLA	b	1202	-	1/1/14/20	13/31/109/115	-
18	BCR	A	4008	-	-	12/29/63/63	0/2/2/2
14	CLA	B	1209	-	1/1/11/20	3/13/91/115	-
14	CLA	b	1225	-	1/1/15/20	18/37/115/115	-
14	CLA	a	1134	-	1/1/11/20	8/13/91/115	-
14	CLA	H	1223	-	1/1/15/20	18/37/115/115	-
14	CLA	H	1211	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	F6C	G	1121	-	-	9/17/73/97	-
18	BCR	B	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	H	1214	-	1/1/15/20	15/37/115/115	-
17	SF4	G	3001	2,1	-	-	0/6/5/5
14	CLA	B	1227	-	1/1/11/20	5/13/91/115	-
14	CLA	a	1129	-	1/1/12/20	6/19/97/115	-
14	CLA	b	1022	-	1/1/15/20	19/37/115/115	-
14	CLA	H	1228	-	1/1/13/20	16/25/103/115	-
14	CLA	b	1210	-	1/1/15/20	19/37/115/115	-
18	BCR	I	4018	-	-	8/29/63/63	0/2/2/2
14	CLA	A	1132	-	1/1/15/20	12/37/115/115	-
14	CLA	b	1223	-	1/1/15/20	18/37/115/115	-
14	CLA	H	1222	-	1/1/15/20	17/37/115/115	-
14	CLA	a	1132	-	1/1/15/20	12/37/115/115	-
18	BCR	a	4001	-	-	14/29/63/63	0/2/2/2
14	CLA	a	1136	-	1/1/15/20	17/37/115/115	-
14	CLA	l	1502	-	1/1/14/20	13/31/109/115	-
18	BCR	b	4010	-	-	10/29/63/63	0/2/2/2
14	CLA	H	1215	-	1/1/14/20	19/31/109/115	-

All (5605) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	4002	BCR	C10-C9	-9.91	1.22	1.35
18	G	4002	BCR	C10-C9	-9.90	1.22	1.35
18	a	4002	BCR	C10-C9	-9.85	1.22	1.35
18	A	4007	BCR	C10-C9	-9.09	1.23	1.35
18	G	4008	BCR	C10-C9	-9.08	1.23	1.35
18	a	4008	BCR	C10-C9	-9.07	1.23	1.35
18	A	4008	BCR	C10-C9	-9.07	1.23	1.35
18	a	4007	BCR	C10-C9	-9.06	1.23	1.35
18	G	4007	BCR	C10-C9	-8.98	1.23	1.35
18	R	4020	BCR	C10-C9	-8.93	1.23	1.35
18	I	4020	BCR	C10-C9	-8.92	1.24	1.35
18	i	4020	BCR	C10-C9	-8.90	1.24	1.35
18	I	4020	BCR	C8-C9	-8.88	1.26	1.45
18	V	4021	BCR	C8-C9	-8.88	1.26	1.45
15	A	1121	F6C	MG-NA	8.88	2.23	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	i	4020	BCR	C8-C9	-8.87	1.26	1.45
18	M	4021	BCR	C8-C9	-8.87	1.26	1.45
18	m	4021	BCR	C8-C9	-8.86	1.26	1.45
15	G	1121	F6C	MG-NA	8.85	2.23	2.05
15	a	1121	F6C	MG-NA	8.84	2.23	2.05
18	R	4020	BCR	C8-C9	-8.83	1.27	1.45
18	L	4022	BCR	C8-C9	-8.79	1.27	1.45
18	I	4018	BCR	C8-C9	-8.79	1.27	1.45
18	G	4007	BCR	C8-C9	-8.79	1.27	1.45
18	l	4022	BCR	C8-C9	-8.78	1.27	1.45
18	B	4010	BCR	C10-C9	-8.78	1.24	1.35
18	b	4010	BCR	C10-C9	-8.77	1.24	1.35
18	A	4007	BCR	C8-C9	-8.76	1.27	1.45
18	A	4008	BCR	C8-C9	-8.76	1.27	1.45
18	U	4022	BCR	C8-C9	-8.76	1.27	1.45
18	i	4018	BCR	C8-C9	-8.76	1.27	1.45
18	G	4011	BCR	C8-C9	-8.75	1.27	1.45
18	H	4010	BCR	C10-C9	-8.75	1.24	1.35
18	a	4007	BCR	C8-C9	-8.75	1.27	1.45
18	R	4018	BCR	C8-C9	-8.75	1.27	1.45
18	a	4008	BCR	C8-C9	-8.74	1.27	1.45
18	a	4011	BCR	C8-C9	-8.73	1.27	1.45
18	b	4010	BCR	C8-C9	-8.73	1.27	1.45
18	B	4010	BCR	C8-C9	-8.73	1.27	1.45
18	b	4016	BCR	C8-C9	-8.71	1.27	1.45
15	H	1207	F6C	MG-NA	8.71	2.23	2.05
18	B	4016	BCR	C8-C9	-8.71	1.27	1.45
15	B	1207	F6C	MG-NA	8.71	2.23	2.05
18	G	4008	BCR	C8-C9	-8.70	1.27	1.45
18	A	4011	BCR	C8-C9	-8.70	1.27	1.45
18	H	4016	BCR	C8-C9	-8.69	1.27	1.45
18	H	4010	BCR	C8-C9	-8.69	1.27	1.45
18	B	4010	BCR	C11-C10	-8.69	1.16	1.43
15	b	1207	F6C	MG-NA	8.69	2.23	2.05
18	A	4008	BCR	C11-C10	-8.69	1.16	1.43
18	G	4008	BCR	C11-C10	-8.68	1.16	1.43
18	a	4008	BCR	C11-C10	-8.68	1.16	1.43
15	H	1230	F6C	MG-NA	8.67	2.23	2.05
15	b	1230	F6C	MG-NA	8.66	2.23	2.05
18	H	4010	BCR	C11-C10	-8.66	1.16	1.43
15	B	1238	F6C	MG-NA	8.65	2.22	2.05
18	b	4010	BCR	C11-C10	-8.64	1.16	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	1238	F6C	MG-NA	8.64	2.22	2.05
15	B	1230	F6C	MG-NA	8.64	2.22	2.05
18	i	4020	BCR	C11-C10	-8.61	1.16	1.43
15	H	1238	F6C	MG-NA	8.60	2.22	2.05
18	a	4007	BCR	C11-C10	-8.59	1.16	1.43
18	G	4007	BCR	C11-C10	-8.59	1.16	1.43
18	A	4007	BCR	C11-C10	-8.57	1.16	1.43
18	B	4017	BCR	C8-C9	-8.57	1.27	1.45
18	I	4020	BCR	C11-C10	-8.57	1.16	1.43
18	R	4020	BCR	C11-C10	-8.56	1.16	1.43
18	a	4001	BCR	C8-C9	-8.56	1.27	1.45
18	b	4017	BCR	C8-C9	-8.55	1.27	1.45
18	B	4014	BCR	C10-C9	-8.55	1.24	1.35
18	G	4001	BCR	C8-C9	-8.55	1.27	1.45
18	A	4001	BCR	C8-C9	-8.55	1.27	1.45
18	b	4014	BCR	C8-C9	-8.55	1.27	1.45
18	B	4014	BCR	C8-C9	-8.54	1.27	1.45
18	H	4017	BCR	C8-C9	-8.54	1.27	1.45
18	L	4019	BCR	C8-C9	-8.54	1.27	1.45
18	H	4014	BCR	C10-C9	-8.53	1.24	1.35
18	H	4014	BCR	C8-C9	-8.53	1.27	1.45
18	l	4019	BCR	C8-C9	-8.52	1.27	1.45
18	a	4002	BCR	C8-C9	-8.52	1.27	1.45
18	A	4002	BCR	C8-C9	-8.51	1.27	1.45
18	b	4014	BCR	C10-C9	-8.51	1.24	1.35
18	U	4019	BCR	C8-C9	-8.49	1.27	1.45
18	G	4002	BCR	C8-C9	-8.49	1.27	1.45
18	l	4022	BCR	C11-C10	-8.47	1.17	1.43
18	L	4022	BCR	C11-C10	-8.46	1.17	1.43
18	b	4014	BCR	C11-C10	-8.46	1.17	1.43
18	b	4009	BCR	C8-C9	-8.46	1.27	1.45
18	U	4022	BCR	C11-C10	-8.45	1.17	1.43
18	B	4009	BCR	C8-C9	-8.45	1.27	1.45
18	H	4014	BCR	C11-C10	-8.45	1.17	1.43
18	H	4009	BCR	C8-C9	-8.44	1.27	1.45
18	B	4014	BCR	C11-C10	-8.43	1.17	1.43
18	H	4016	BCR	C10-C9	-8.41	1.24	1.35
18	I	4018	BCR	C11-C10	-8.39	1.17	1.43
18	b	4006	BCR	C8-C9	-8.38	1.27	1.45
18	b	4016	BCR	C10-C9	-8.38	1.24	1.35
18	R	4018	BCR	C11-C10	-8.38	1.17	1.43
18	i	4018	BCR	C11-C10	-8.37	1.17	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	4021	BCR	C11-C10	-8.37	1.17	1.43
18	a	4003	BCR	C8-C9	-8.37	1.28	1.45
18	B	4005	BCR	C11-C10	-8.36	1.17	1.43
18	B	4016	BCR	C10-C9	-8.35	1.24	1.35
18	G	4011	BCR	C11-C10	-8.35	1.17	1.43
18	B	4009	BCR	C11-C10	-8.34	1.17	1.43
18	H	4004	BCR	C8-C9	-8.34	1.28	1.45
18	A	4003	BCR	C8-C9	-8.34	1.28	1.45
18	b	4009	BCR	C11-C10	-8.34	1.17	1.43
18	H	4009	BCR	C11-C10	-8.34	1.17	1.43
18	B	4006	BCR	C8-C9	-8.34	1.28	1.45
18	H	4006	BCR	C8-C9	-8.33	1.28	1.45
18	H	4005	BCR	C11-C10	-8.33	1.17	1.43
18	m	4021	BCR	C11-C10	-8.33	1.17	1.43
18	M	4021	BCR	C11-C10	-8.33	1.17	1.43
18	b	4005	BCR	C11-C10	-8.32	1.17	1.43
18	B	4017	BCR	C11-C10	-8.32	1.17	1.43
18	G	4003	BCR	C8-C9	-8.32	1.28	1.45
18	H	4017	BCR	C11-C10	-8.31	1.17	1.43
18	a	4011	BCR	C11-C10	-8.31	1.17	1.43
18	U	4022	BCR	C10-C9	-8.31	1.24	1.35
18	l	4019	BCR	C11-C10	-8.31	1.17	1.43
18	A	4011	BCR	C11-C10	-8.31	1.17	1.43
18	b	4004	BCR	C8-C9	-8.31	1.28	1.45
18	m	4021	BCR	C10-C9	-8.30	1.24	1.35
18	U	4019	BCR	C11-C10	-8.30	1.17	1.43
18	l	4022	BCR	C10-C9	-8.30	1.24	1.35
18	B	4005	BCR	C8-C9	-8.29	1.28	1.45
18	G	4001	BCR	C11-C10	-8.28	1.17	1.43
18	L	4022	BCR	C10-C9	-8.28	1.24	1.35
18	L	4019	BCR	C11-C10	-8.28	1.17	1.43
18	b	4017	BCR	C11-C10	-8.28	1.17	1.43
18	a	4001	BCR	C11-C10	-8.28	1.17	1.43
18	b	4005	BCR	C8-C9	-8.28	1.28	1.45
18	B	4004	BCR	C8-C9	-8.27	1.28	1.45
18	M	4021	BCR	C10-C9	-8.27	1.24	1.35
15	b	1230	F6C	C1A-CHA	8.27	1.50	1.35
18	A	4001	BCR	C11-C10	-8.26	1.17	1.43
18	H	4005	BCR	C8-C9	-8.26	1.28	1.45
18	H	4013	BCR	C8-C9	-8.26	1.28	1.45
18	V	4021	BCR	C10-C9	-8.26	1.24	1.35
15	B	1230	F6C	C1A-CHA	8.25	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1237	F6C	MG-NA	8.25	2.22	2.05
18	a	4011	BCR	C10-C9	-8.24	1.24	1.35
15	H	1230	F6C	C1A-CHA	8.24	1.50	1.35
18	A	4001	BCR	C10-C9	-8.24	1.24	1.35
15	b	1207	F6C	C1A-CHA	8.24	1.50	1.35
18	B	4017	BCR	C10-C9	-8.23	1.24	1.35
18	B	4013	BCR	C8-C9	-8.23	1.28	1.45
15	H	1207	F6C	C1A-CHA	8.23	1.50	1.35
18	b	4013	BCR	C8-C9	-8.23	1.28	1.45
15	B	1207	F6C	C1A-CHA	8.22	1.50	1.35
15	H	1237	F6C	MG-NA	8.22	2.22	2.05
15	b	1237	F6C	MG-NA	8.21	2.22	2.05
18	H	4017	BCR	C10-C9	-8.21	1.24	1.35
18	b	4017	BCR	C10-C9	-8.21	1.24	1.35
18	A	4011	BCR	C10-C9	-8.20	1.24	1.35
18	B	4016	BCR	C11-C10	-8.20	1.18	1.43
18	a	4001	BCR	C10-C9	-8.19	1.24	1.35
18	G	4001	BCR	C10-C9	-8.19	1.24	1.35
18	b	4016	BCR	C11-C10	-8.19	1.18	1.43
18	H	4016	BCR	C11-C10	-8.18	1.18	1.43
18	H	4005	BCR	C10-C9	-8.18	1.24	1.35
18	G	4011	BCR	C10-C9	-8.18	1.24	1.35
18	l	4019	BCR	C10-C9	-8.17	1.24	1.35
18	b	4006	BCR	C11-C10	-8.15	1.18	1.43
18	H	4006	BCR	C11-C10	-8.15	1.18	1.43
18	B	4005	BCR	C10-C9	-8.14	1.25	1.35
18	b	4005	BCR	C10-C9	-8.14	1.25	1.35
18	L	4019	BCR	C10-C9	-8.14	1.25	1.35
18	U	4019	BCR	C10-C9	-8.14	1.25	1.35
18	B	4006	BCR	C11-C10	-8.13	1.18	1.43
18	a	4003	BCR	C11-C10	-8.11	1.18	1.43
15	A	1121	F6C	C1A-CHA	8.11	1.50	1.35
18	A	4003	BCR	C11-C10	-8.10	1.18	1.43
18	G	4003	BCR	C11-C10	-8.10	1.18	1.43
15	a	1121	F6C	C1A-CHA	8.09	1.50	1.35
18	R	4020	BCR	C20-C21	-8.08	1.18	1.43
18	I	4020	BCR	C20-C21	-8.08	1.18	1.43
15	G	1121	F6C	C1A-CHA	8.07	1.50	1.35
18	i	4020	BCR	C20-C21	-8.07	1.18	1.43
18	B	4013	BCR	C11-C10	-8.06	1.18	1.43
18	A	4002	BCR	C11-C10	-8.06	1.18	1.43
18	a	4002	BCR	C11-C10	-8.06	1.18	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	4002	BCR	C11-C10	-8.05	1.18	1.43
18	b	4013	BCR	C11-C10	-8.05	1.18	1.43
18	H	4013	BCR	C11-C10	-8.03	1.18	1.43
18	H	4004	BCR	C11-C10	-8.02	1.18	1.43
18	b	4004	BCR	C11-C10	-8.02	1.18	1.43
15	H	1237	F6C	C1A-CHA	8.02	1.50	1.35
18	B	4004	BCR	C11-C10	-8.01	1.18	1.43
18	U	4022	BCR	C20-C21	-8.00	1.18	1.43
15	B	1237	F6C	C1A-CHA	8.00	1.50	1.35
18	G	4008	BCR	C20-C21	-8.00	1.18	1.43
18	A	4008	BCR	C20-C21	-8.00	1.18	1.43
18	a	4008	BCR	C20-C21	-7.99	1.18	1.43
18	l	4022	BCR	C20-C21	-7.98	1.18	1.43
18	i	4018	BCR	C10-C9	-7.97	1.25	1.35
18	L	4022	BCR	C20-C21	-7.97	1.18	1.43
15	b	1237	F6C	C1A-CHA	7.97	1.50	1.35
18	R	4018	BCR	C10-C9	-7.95	1.25	1.35
18	R	4020	BCR	C16-C17	-7.95	1.18	1.43
18	I	4020	BCR	C16-C17	-7.94	1.18	1.43
18	A	4011	BCR	C20-C21	-7.94	1.18	1.43
18	a	4011	BCR	C20-C21	-7.94	1.18	1.43
18	G	4011	BCR	C20-C21	-7.93	1.18	1.43
18	i	4020	BCR	C16-C17	-7.93	1.18	1.43
18	H	4010	BCR	C16-C17	-7.89	1.19	1.43
18	b	4010	BCR	C16-C17	-7.87	1.19	1.43
18	a	4008	BCR	C16-C17	-7.87	1.19	1.43
18	I	4018	BCR	C10-C9	-7.87	1.25	1.35
18	l	4022	BCR	C16-C17	-7.86	1.19	1.43
18	L	4022	BCR	C16-C17	-7.86	1.19	1.43
18	A	4008	BCR	C16-C17	-7.86	1.19	1.43
18	B	4010	BCR	C16-C17	-7.85	1.19	1.43
18	G	4008	BCR	C16-C17	-7.85	1.19	1.43
18	H	4009	BCR	C10-C9	-7.84	1.25	1.35
18	U	4022	BCR	C16-C17	-7.83	1.19	1.43
18	I	4018	BCR	C20-C21	-7.81	1.19	1.43
18	i	4018	BCR	C20-C21	-7.81	1.19	1.43
15	B	1238	F6C	C1A-CHA	7.81	1.50	1.35
18	R	4018	BCR	C20-C21	-7.81	1.19	1.43
18	b	4009	BCR	C10-C9	-7.79	1.25	1.35
18	B	4009	BCR	C10-C9	-7.78	1.25	1.35
15	H	1238	F6C	C1A-CHA	7.78	1.49	1.35
15	b	1238	F6C	C1A-CHA	7.77	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	4003	BCR	C10-C9	-7.77	1.25	1.35
18	A	4003	BCR	C10-C9	-7.77	1.25	1.35
18	B	4014	BCR	C16-C17	-7.75	1.19	1.43
18	B	4017	BCR	C20-C21	-7.74	1.19	1.43
18	U	4019	BCR	C20-C21	-7.73	1.19	1.43
18	l	4019	BCR	C20-C21	-7.73	1.19	1.43
18	H	4017	BCR	C20-C21	-7.73	1.19	1.43
18	H	4014	BCR	C16-C17	-7.73	1.19	1.43
18	b	4017	BCR	C20-C21	-7.73	1.19	1.43
18	B	4010	BCR	C20-C21	-7.73	1.19	1.43
18	L	4019	BCR	C20-C21	-7.72	1.19	1.43
18	b	4009	BCR	C20-C21	-7.72	1.19	1.43
18	b	4014	BCR	C16-C17	-7.72	1.19	1.43
18	H	4010	BCR	C20-C21	-7.71	1.19	1.43
18	G	4007	BCR	C16-C17	-7.71	1.19	1.43
18	a	4007	BCR	C16-C17	-7.71	1.19	1.43
18	b	4010	BCR	C20-C21	-7.70	1.19	1.43
18	H	4006	BCR	C10-C9	-7.70	1.25	1.35
18	B	4009	BCR	C20-C21	-7.70	1.19	1.43
18	H	4014	BCR	C20-C21	-7.70	1.19	1.43
18	a	4003	BCR	C10-C9	-7.70	1.25	1.35
18	b	4014	BCR	C20-C21	-7.70	1.19	1.43
18	B	4014	BCR	C20-C21	-7.69	1.19	1.43
18	H	4009	BCR	C20-C21	-7.69	1.19	1.43
18	A	4007	BCR	C16-C17	-7.69	1.19	1.43
18	G	4007	BCR	C20-C21	-7.69	1.19	1.43
18	b	4017	BCR	C16-C17	-7.68	1.19	1.43
18	b	4005	BCR	C20-C21	-7.67	1.19	1.43
18	b	4006	BCR	C10-C9	-7.67	1.25	1.35
18	a	4007	BCR	C20-C21	-7.67	1.19	1.43
18	H	4017	BCR	C16-C17	-7.66	1.19	1.43
18	A	4007	BCR	C20-C21	-7.66	1.19	1.43
18	I	4018	BCR	C16-C17	-7.66	1.19	1.43
18	H	4005	BCR	C20-C21	-7.65	1.19	1.43
18	B	4017	BCR	C16-C17	-7.65	1.19	1.43
18	B	4006	BCR	C10-C9	-7.64	1.25	1.35
18	B	4005	BCR	C20-C21	-7.64	1.19	1.43
18	b	4016	BCR	C20-C21	-7.63	1.19	1.43
15	B	1238	F6C	C1A-NA	-7.62	1.27	1.37
18	G	4002	BCR	C20-C21	-7.62	1.19	1.43
18	a	4002	BCR	C20-C21	-7.62	1.19	1.43
18	R	4018	BCR	C16-C17	-7.62	1.19	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	4002	BCR	C20-C21	-7.62	1.19	1.43
18	i	4018	BCR	C16-C17	-7.61	1.19	1.43
18	H	4016	BCR	C16-C17	-7.61	1.19	1.43
18	H	4016	BCR	C20-C21	-7.60	1.19	1.43
18	B	4016	BCR	C20-C21	-7.60	1.19	1.43
18	B	4016	BCR	C16-C17	-7.59	1.19	1.43
15	b	1238	F6C	C1A-NA	-7.59	1.27	1.37
15	H	1238	F6C	C1A-NA	-7.58	1.27	1.37
18	b	4016	BCR	C16-C17	-7.58	1.20	1.43
18	G	4003	BCR	C20-C21	-7.58	1.20	1.43
18	b	4005	BCR	C16-C17	-7.58	1.20	1.43
18	V	4021	BCR	C20-C21	-7.57	1.20	1.43
18	H	4009	BCR	C16-C17	-7.57	1.20	1.43
18	A	4003	BCR	C20-C21	-7.57	1.20	1.43
18	B	4009	BCR	C16-C17	-7.57	1.20	1.43
18	L	4019	BCR	C16-C17	-7.56	1.20	1.43
18	U	4019	BCR	C16-C17	-7.56	1.20	1.43
18	B	4005	BCR	C16-C17	-7.56	1.20	1.43
18	a	4003	BCR	C20-C21	-7.56	1.20	1.43
18	l	4019	BCR	C16-C17	-7.55	1.20	1.43
18	M	4021	BCR	C20-C21	-7.55	1.20	1.43
18	G	4011	BCR	C16-C17	-7.55	1.20	1.43
18	H	4005	BCR	C16-C17	-7.55	1.20	1.43
18	m	4021	BCR	C20-C21	-7.54	1.20	1.43
18	a	4011	BCR	C16-C17	-7.54	1.20	1.43
18	A	4011	BCR	C16-C17	-7.53	1.20	1.43
14	K	1401	CLA	MG-NA	7.53	2.24	2.06
18	b	4009	BCR	C16-C17	-7.53	1.20	1.43
18	H	4004	BCR	C20-C21	-7.52	1.20	1.43
15	B	1207	F6C	C1A-NA	-7.52	1.27	1.37
18	b	4004	BCR	C20-C21	-7.51	1.20	1.43
14	T	1401	CLA	MG-NA	7.51	2.24	2.06
18	B	4004	BCR	C20-C21	-7.51	1.20	1.43
18	H	4006	BCR	C20-C21	-7.50	1.20	1.43
18	b	4006	BCR	C20-C21	-7.50	1.20	1.43
18	b	4013	BCR	C10-C9	-7.50	1.25	1.35
15	H	1207	F6C	C1A-NA	-7.50	1.27	1.37
15	B	1237	F6C	C1A-NA	-7.49	1.27	1.37
14	k	1401	CLA	MG-NA	7.49	2.24	2.06
18	B	4006	BCR	C20-C21	-7.48	1.20	1.43
18	H	4013	BCR	C10-C9	-7.48	1.25	1.35
14	a	1123	CLA	MG-NA	7.47	2.24	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1134	CLA	MG-NA	7.47	2.24	2.06
18	b	4004	BCR	C10-C9	-7.47	1.25	1.35
18	G	4001	BCR	C20-C21	-7.46	1.20	1.43
18	B	4004	BCR	C10-C9	-7.46	1.25	1.35
14	A	1123	CLA	MG-NA	7.46	2.24	2.06
14	A	1134	CLA	MG-NA	7.46	2.24	2.06
18	A	4001	BCR	C20-C21	-7.45	1.20	1.43
15	b	1207	F6C	C1A-NA	-7.45	1.27	1.37
18	A	4002	BCR	C16-C17	-7.45	1.20	1.43
18	a	4001	BCR	C20-C21	-7.45	1.20	1.43
14	b	1214	CLA	MG-NA	7.45	2.24	2.06
18	G	4002	BCR	C16-C17	-7.44	1.20	1.43
18	A	4003	BCR	C16-C17	-7.44	1.20	1.43
18	B	4013	BCR	C10-C9	-7.44	1.25	1.35
14	a	1134	CLA	MG-NA	7.44	2.23	2.06
18	a	4002	BCR	C16-C17	-7.44	1.20	1.43
15	H	1237	F6C	C1A-NA	-7.43	1.27	1.37
14	G	1123	CLA	MG-NA	7.43	2.23	2.06
18	a	4003	BCR	C16-C17	-7.43	1.20	1.43
18	G	4003	BCR	C16-C17	-7.43	1.20	1.43
18	H	4004	BCR	C10-C9	-7.42	1.25	1.35
15	b	1237	F6C	C1A-NA	-7.42	1.27	1.37
14	H	1214	CLA	MG-NA	7.41	2.23	2.06
18	H	4006	BCR	C16-C17	-7.41	1.20	1.43
18	M	4021	BCR	C16-C17	-7.41	1.20	1.43
18	b	4006	BCR	C16-C17	-7.40	1.20	1.43
14	H	1239	CLA	MG-NA	7.40	2.23	2.06
18	V	4021	BCR	C16-C17	-7.40	1.20	1.43
14	b	1232	CLA	MG-NA	7.40	2.23	2.06
18	B	4004	BCR	C16-C17	-7.40	1.20	1.43
14	B	1214	CLA	MG-NA	7.39	2.23	2.06
18	B	4006	BCR	C16-C17	-7.39	1.20	1.43
14	H	1232	CLA	MG-NA	7.39	2.23	2.06
18	A	4001	BCR	C16-C17	-7.38	1.20	1.43
14	B	1232	CLA	MG-NA	7.38	2.23	2.06
18	m	4021	BCR	C16-C17	-7.37	1.20	1.43
18	G	4001	BCR	C16-C17	-7.37	1.20	1.43
14	b	1239	CLA	MG-NA	7.37	2.23	2.06
18	b	4004	BCR	C16-C17	-7.37	1.20	1.43
18	H	4004	BCR	C16-C17	-7.37	1.20	1.43
18	a	4001	BCR	C16-C17	-7.36	1.20	1.43
18	b	4013	BCR	C20-C21	-7.36	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1233	CLA	MG-NA	7.36	2.23	2.06
14	B	1239	CLA	MG-NA	7.36	2.23	2.06
14	b	1218	CLA	MG-NA	7.35	2.23	2.06
14	H	1213	CLA	MG-NA	7.34	2.23	2.06
14	H	1233	CLA	MG-NA	7.34	2.23	2.06
14	B	1233	CLA	MG-NA	7.34	2.23	2.06
18	H	4013	BCR	C16-C17	-7.34	1.20	1.43
15	b	1230	F6C	C1A-NA	-7.33	1.27	1.37
14	B	1213	CLA	MG-NA	7.33	2.23	2.06
18	B	4013	BCR	C20-C21	-7.33	1.20	1.43
14	b	1213	CLA	MG-NA	7.32	2.23	2.06
15	H	1230	F6C	C1A-NA	-7.32	1.27	1.37
14	G	1140	CLA	MG-NA	7.32	2.23	2.06
14	B	1219	CLA	MG-NA	7.32	2.23	2.06
18	b	4013	BCR	C16-C17	-7.32	1.20	1.43
14	H	1218	CLA	MG-NA	7.31	2.23	2.06
18	H	4013	BCR	C20-C21	-7.31	1.20	1.43
15	B	1230	F6C	C1A-NA	-7.31	1.27	1.37
14	X	1701	CLA	MG-NA	7.30	2.23	2.06
18	B	4013	BCR	C16-C17	-7.29	1.20	1.43
14	x	1701	CLA	MG-NA	7.29	2.23	2.06
14	W	1701	CLA	MG-NA	7.29	2.23	2.06
14	b	1219	CLA	MG-NA	7.28	2.23	2.06
14	H	1219	CLA	MG-NA	7.28	2.23	2.06
14	B	1218	CLA	MG-NA	7.28	2.23	2.06
14	H	1209	CLA	MG-NA	7.28	2.23	2.06
15	a	1121	F6C	C1A-NA	-7.27	1.27	1.37
15	A	1121	F6C	C1A-NA	-7.26	1.27	1.37
14	a	1139	CLA	MG-NA	7.25	2.23	2.06
14	B	1209	CLA	MG-NA	7.25	2.23	2.06
14	A	1140	CLA	MG-NA	7.25	2.23	2.06
14	H	1223	CLA	MG-NA	7.24	2.23	2.06
14	a	1135	CLA	MG-NA	7.24	2.23	2.06
15	G	1121	F6C	C1A-NA	-7.24	1.27	1.37
14	G	1139	CLA	MG-NA	7.24	2.23	2.06
14	A	1135	CLA	MG-NA	7.24	2.23	2.06
14	B	1223	CLA	MG-NA	7.24	2.23	2.06
14	a	1127	CLA	MG-NA	7.24	2.23	2.06
14	a	1140	CLA	MG-NA	7.24	2.23	2.06
14	b	1223	CLA	MG-NA	7.24	2.23	2.06
14	b	1209	CLA	MG-NA	7.24	2.23	2.06
14	G	1135	CLA	MG-NA	7.23	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1139	CLA	MG-NA	7.23	2.23	2.06
14	G	1113	CLA	MG-NA	7.23	2.23	2.06
14	A	1127	CLA	MG-NA	7.23	2.23	2.06
14	b	1217	CLA	MG-NA	7.22	2.23	2.06
14	G	1127	CLA	MG-NA	7.22	2.23	2.06
14	B	1217	CLA	MG-NA	7.22	2.23	2.06
14	G	1114	CLA	MG-NA	7.21	2.23	2.06
14	b	1229	CLA	MG-NA	7.21	2.23	2.06
14	a	1113	CLA	MG-NA	7.21	2.23	2.06
14	B	1224	CLA	MG-NA	7.21	2.23	2.06
14	B	1229	CLA	MG-NA	7.20	2.23	2.06
14	H	1217	CLA	MG-NA	7.20	2.23	2.06
14	H	1229	CLA	MG-NA	7.20	2.23	2.06
15	H	1230	F6C	C2A-C3A	7.20	1.52	1.36
14	H	1227	CLA	MG-NA	7.19	2.23	2.06
14	G	1110	CLA	MG-NA	7.19	2.23	2.06
14	H	1224	CLA	MG-NA	7.19	2.23	2.06
14	H	1022	CLA	MG-NA	7.19	2.23	2.06
14	b	1022	CLA	MG-NA	7.19	2.23	2.06
14	b	1224	CLA	MG-NA	7.18	2.23	2.06
14	A	1113	CLA	MG-NA	7.18	2.23	2.06
14	a	1118	CLA	MG-NA	7.18	2.23	2.06
14	b	1227	CLA	MG-NA	7.18	2.23	2.06
14	A	1118	CLA	MG-NA	7.18	2.23	2.06
15	H	1207	F6C	C2A-C3A	7.18	1.52	1.36
15	B	1207	F6C	C2A-C3A	7.18	1.52	1.36
14	B	1022	CLA	MG-NA	7.17	2.23	2.06
14	B	1227	CLA	MG-NA	7.17	2.23	2.06
14	H	1212	CLA	MG-NA	7.17	2.23	2.06
14	G	1118	CLA	MG-NA	7.17	2.23	2.06
14	G	1131	CLA	MG-NA	7.16	2.23	2.06
14	a	1115	CLA	MG-NA	7.16	2.23	2.06
14	A	1131	CLA	MG-NA	7.16	2.23	2.06
14	G	1115	CLA	MG-NA	7.16	2.23	2.06
14	a	1110	CLA	MG-NA	7.16	2.23	2.06
14	a	1131	CLA	MG-NA	7.16	2.23	2.06
14	a	1111	CLA	MG-NA	7.16	2.23	2.06
14	A	1110	CLA	MG-NA	7.16	2.23	2.06
14	b	1210	CLA	MG-NA	7.15	2.23	2.06
14	H	1210	CLA	MG-NA	7.15	2.23	2.06
15	b	1207	F6C	C2A-C3A	7.15	1.51	1.36
14	a	1114	CLA	MG-NA	7.15	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1012	CLA	MG-NA	7.15	2.23	2.06
14	A	1111	CLA	MG-NA	7.15	2.23	2.06
15	B	1230	F6C	C2A-C3A	7.15	1.51	1.36
14	A	1115	CLA	MG-NA	7.14	2.23	2.06
14	b	1231	CLA	MG-NA	7.14	2.23	2.06
14	A	1114	CLA	MG-NA	7.14	2.23	2.06
14	B	1235	CLA	MG-NA	7.14	2.23	2.06
15	b	1230	F6C	C2A-C3A	7.14	1.51	1.36
14	G	1111	CLA	MG-NA	7.14	2.23	2.06
14	B	1210	CLA	MG-NA	7.14	2.23	2.06
14	G	1112	CLA	MG-NA	7.14	2.23	2.06
14	b	1212	CLA	MG-NA	7.14	2.23	2.06
14	G	1138	CLA	MG-NA	7.14	2.23	2.06
14	a	1112	CLA	MG-NA	7.14	2.23	2.06
14	B	1212	CLA	MG-NA	7.13	2.23	2.06
14	B	1234	CLA	MG-NA	7.13	2.23	2.06
14	B	1225	CLA	MG-NA	7.13	2.23	2.06
14	G	1137	CLA	MG-NA	7.13	2.23	2.06
14	H	1234	CLA	MG-NA	7.13	2.23	2.06
14	A	1105	CLA	MG-NA	7.13	2.23	2.06
14	B	1231	CLA	MG-NA	7.12	2.23	2.06
14	a	1105	CLA	MG-NA	7.12	2.23	2.06
14	A	1138	CLA	MG-NA	7.12	2.23	2.06
14	G	1120	CLA	MG-NA	7.12	2.23	2.06
14	A	1129	CLA	MG-NA	7.12	2.23	2.06
14	a	1120	CLA	MG-NA	7.11	2.23	2.06
14	a	1138	CLA	MG-NA	7.11	2.23	2.06
14	b	1234	CLA	MG-NA	7.11	2.23	2.06
14	G	1105	CLA	MG-NA	7.11	2.23	2.06
14	A	1116	CLA	MG-NA	7.11	2.23	2.06
14	a	1129	CLA	MG-NA	7.11	2.23	2.06
14	a	1012	CLA	MG-NA	7.11	2.23	2.06
14	A	1137	CLA	MG-NA	7.11	2.23	2.06
14	A	1120	CLA	MG-NA	7.11	2.23	2.06
14	A	1107	CLA	MG-NA	7.11	2.23	2.06
14	G	1129	CLA	MG-NA	7.10	2.23	2.06
14	a	1137	CLA	MG-NA	7.10	2.23	2.06
14	b	1225	CLA	MG-NA	7.10	2.23	2.06
14	H	1231	CLA	MG-NA	7.10	2.23	2.06
14	A	1130	CLA	MG-NA	7.10	2.23	2.06
14	a	1107	CLA	MG-NA	7.10	2.23	2.06
14	a	1122	CLA	MG-NA	7.10	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	2002	PQN	C3-C2	7.09	1.48	1.35
14	G	1107	CLA	MG-NA	7.09	2.23	2.06
14	G	1133	CLA	MG-NA	7.09	2.23	2.06
14	A	1112	CLA	MG-NA	7.09	2.23	2.06
16	b	2002	PQN	C3-C2	7.09	1.48	1.35
14	H	1225	CLA	MG-NA	7.09	2.23	2.06
14	b	1235	CLA	MG-NA	7.09	2.23	2.06
14	H	1235	CLA	MG-NA	7.09	2.23	2.06
14	A	1122	CLA	MG-NA	7.09	2.23	2.06
14	L	1501	CLA	MG-NA	7.09	2.23	2.06
14	l	1501	CLA	MG-NA	7.09	2.23	2.06
14	B	1228	CLA	MG-NA	7.09	2.23	2.06
14	A	1101	CLA	MG-NA	7.09	2.23	2.06
14	U	1501	CLA	MG-NA	7.08	2.23	2.06
14	b	1228	CLA	MG-NA	7.08	2.23	2.06
14	G	1130	CLA	MG-NA	7.08	2.23	2.06
14	A	1012	CLA	MG-NA	7.08	2.23	2.06
14	G	1122	CLA	MG-NA	7.08	2.23	2.06
14	A	1133	CLA	MG-NA	7.08	2.23	2.06
16	B	2002	PQN	C3-C2	7.07	1.48	1.35
14	a	1116	CLA	MG-NA	7.07	2.23	2.06
14	a	1130	CLA	MG-NA	7.07	2.23	2.06
14	G	1101	CLA	MG-NA	7.06	2.23	2.06
16	A	2001	PQN	C3-C2	7.06	1.48	1.35
14	G	1116	CLA	MG-NA	7.06	2.23	2.06
14	H	1228	CLA	MG-NA	7.06	2.23	2.06
14	a	1133	CLA	MG-NA	7.06	2.23	2.06
14	a	1101	CLA	MG-NA	7.06	2.23	2.06
14	a	1102	CLA	MG-NA	7.05	2.23	2.06
15	A	1121	F6C	C2A-C3A	7.05	1.51	1.36
14	H	1204	CLA	MG-NA	7.05	2.23	2.06
15	G	1121	F6C	C2A-C3A	7.04	1.51	1.36
14	G	1102	CLA	MG-NA	7.04	2.23	2.06
14	A	1102	CLA	MG-NA	7.03	2.23	2.06
14	G	1109	CLA	MG-NA	7.03	2.23	2.06
16	G	2001	PQN	C3-C2	7.03	1.48	1.35
14	a	1132	CLA	MG-NA	7.02	2.23	2.06
14	B	1204	CLA	MG-NA	7.02	2.22	2.06
14	G	1132	CLA	MG-NA	7.02	2.22	2.06
14	A	1109	CLA	MG-NA	7.01	2.22	2.06
16	a	2001	PQN	C3-C2	7.01	1.48	1.35
14	b	1215	CLA	MG-NA	7.01	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1204	CLA	MG-NA	7.01	2.22	2.06
15	a	1121	F6C	C2A-C3A	7.01	1.51	1.36
14	a	1109	CLA	MG-NA	7.01	2.22	2.06
14	B	1215	CLA	MG-NA	7.00	2.22	2.06
14	b	1220	CLA	MG-NA	7.00	2.22	2.06
14	B	1208	CLA	MG-NA	7.00	2.22	2.06
14	H	1215	CLA	MG-NA	7.00	2.22	2.06
14	H	1208	CLA	MG-NA	7.00	2.22	2.06
14	b	1236	CLA	MG-NA	7.00	2.22	2.06
14	A	1132	CLA	MG-NA	7.00	2.22	2.06
14	H	1236	CLA	MG-NA	6.99	2.22	2.06
14	b	1208	CLA	MG-NA	6.99	2.22	2.06
14	G	1108	CLA	MG-NA	6.99	2.22	2.06
14	B	1216	CLA	MG-NA	6.99	2.22	2.06
14	B	1236	CLA	MG-NA	6.99	2.22	2.06
14	B	1220	CLA	MG-NA	6.99	2.22	2.06
14	H	1216	CLA	MG-NA	6.98	2.22	2.06
14	b	1216	CLA	MG-NA	6.98	2.22	2.06
14	B	1211	CLA	MG-NA	6.97	2.22	2.06
14	A	1128	CLA	MG-NA	6.97	2.22	2.06
14	B	1222	CLA	MG-NA	6.97	2.22	2.06
14	a	1136	CLA	MG-NA	6.97	2.22	2.06
14	b	1211	CLA	MG-NA	6.97	2.22	2.06
14	H	1220	CLA	MG-NA	6.97	2.22	2.06
14	A	1108	CLA	MG-NA	6.96	2.22	2.06
14	H	1203	CLA	MG-NA	6.96	2.22	2.06
14	a	1128	CLA	MG-NA	6.95	2.22	2.06
14	A	1136	CLA	MG-NA	6.95	2.22	2.06
14	G	1136	CLA	MG-NA	6.95	2.22	2.06
14	a	1108	CLA	MG-NA	6.95	2.22	2.06
14	B	1203	CLA	MG-NA	6.95	2.22	2.06
14	H	1211	CLA	MG-NA	6.95	2.22	2.06
14	B	1221	CLA	MG-NA	6.95	2.22	2.06
14	H	1221	CLA	MG-NA	6.94	2.22	2.06
14	H	1222	CLA	MG-NA	6.94	2.22	2.06
14	b	1221	CLA	MG-NA	6.93	2.22	2.06
14	b	1222	CLA	MG-NA	6.93	2.22	2.06
14	G	1128	CLA	MG-NA	6.93	2.22	2.06
14	b	1203	CLA	MG-NA	6.93	2.22	2.06
14	G	1117	CLA	MG-NA	6.92	2.22	2.06
14	A	1106	CLA	MG-NA	6.92	2.22	2.06
14	A	1117	CLA	MG-NA	6.91	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1106	CLA	MG-NA	6.90	2.22	2.06
14	a	1117	CLA	MG-NA	6.90	2.22	2.06
14	b	1226	CLA	MG-NA	6.90	2.22	2.06
14	H	1226	CLA	MG-NA	6.90	2.22	2.06
14	G	1106	CLA	MG-NA	6.90	2.22	2.06
14	l	1503	CLA	MG-NA	6.89	2.22	2.06
14	A	1125	CLA	MG-NA	6.88	2.22	2.06
14	a	1125	CLA	MG-NA	6.88	2.22	2.06
14	A	1126	CLA	MG-NA	6.87	2.22	2.06
14	G	1126	CLA	MG-NA	6.87	2.22	2.06
14	U	1503	CLA	MG-NA	6.87	2.22	2.06
14	B	1226	CLA	MG-NA	6.87	2.22	2.06
14	G	1125	CLA	MG-NA	6.86	2.22	2.06
14	a	1124	CLA	MG-NA	6.86	2.22	2.06
14	A	1124	CLA	MG-NA	6.86	2.22	2.06
14	L	1503	CLA	MG-NA	6.86	2.22	2.06
14	a	1126	CLA	MG-NA	6.86	2.22	2.06
14	H	1201	CLA	MG-NA	6.85	2.22	2.06
14	H	1202	CLA	MG-NA	6.83	2.22	2.06
14	B	1201	CLA	MG-NA	6.83	2.22	2.06
14	b	1201	CLA	MG-NA	6.83	2.22	2.06
15	b	1238	F6C	C2A-C3A	6.83	1.51	1.36
14	B	1202	CLA	MG-NA	6.83	2.22	2.06
14	H	1206	CLA	MG-NA	6.83	2.22	2.06
14	G	1124	CLA	MG-NA	6.82	2.22	2.06
14	b	1206	CLA	MG-NA	6.82	2.22	2.06
14	H	1205	CLA	MG-NA	6.82	2.22	2.06
14	B	1206	CLA	MG-NA	6.82	2.22	2.06
14	B	1205	CLA	MG-NA	6.81	2.22	2.06
14	b	1205	CLA	MG-NA	6.81	2.22	2.06
14	l	1502	CLA	MG-NA	6.81	2.22	2.06
14	L	1502	CLA	MG-NA	6.81	2.22	2.06
15	H	1238	F6C	C2A-C3A	6.81	1.51	1.36
14	b	1202	CLA	MG-NA	6.80	2.22	2.06
15	B	1238	F6C	C2A-C3A	6.80	1.51	1.36
14	U	1502	CLA	MG-NA	6.79	2.22	2.06
15	B	1237	F6C	C2A-C3A	6.79	1.51	1.36
13	G	1011	CL0	MG-NA	6.79	2.22	2.06
15	H	1237	F6C	C2A-C3A	6.79	1.51	1.36
15	b	1237	F6C	C2A-C3A	6.78	1.51	1.36
13	A	1011	CL0	MG-NA	6.76	2.22	2.06
14	G	1104	CLA	MG-NA	6.75	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	1011	CL0	MG-NA	6.74	2.22	2.06
14	a	1104	CLA	MG-NA	6.73	2.22	2.06
14	A	1104	CLA	MG-NA	6.70	2.22	2.06
14	A	1013	CLA	MG-NA	6.63	2.22	2.06
14	a	1013	CLA	MG-NA	6.63	2.22	2.06
14	b	1021	CLA	MG-NA	6.63	2.22	2.06
14	G	1013	CLA	MG-NA	6.62	2.22	2.06
14	H	1021	CLA	MG-NA	6.62	2.22	2.06
14	a	1119	CLA	MG-NA	6.62	2.22	2.06
14	G	1119	CLA	MG-NA	6.62	2.22	2.06
14	A	1119	CLA	MG-NA	6.62	2.22	2.06
14	B	1023	CLA	MG-NA	6.62	2.22	2.06
14	G	1103	CLA	MG-NA	6.61	2.22	2.06
14	B	1021	CLA	MG-NA	6.61	2.22	2.06
14	a	1103	CLA	MG-NA	6.60	2.22	2.06
14	A	1103	CLA	MG-NA	6.60	2.21	2.06
14	H	1023	CLA	MG-NA	6.58	2.21	2.06
14	b	1023	CLA	MG-NA	6.57	2.21	2.06
15	H	1207	F6C	C4A-NA	-5.47	1.31	1.37
15	b	1207	F6C	C4A-NA	-5.47	1.31	1.37
15	B	1207	F6C	C4A-NA	-5.45	1.31	1.37
15	B	1238	F6C	C4A-NA	-5.41	1.31	1.37
15	b	1238	F6C	C4A-NA	-5.36	1.31	1.37
15	B	1237	F6C	C4A-NA	-5.35	1.31	1.37
15	A	1121	F6C	C4A-NA	-5.35	1.31	1.37
15	a	1121	F6C	C4A-NA	-5.34	1.31	1.37
15	H	1237	F6C	C4A-NA	-5.33	1.31	1.37
15	H	1238	F6C	C4A-NA	-5.31	1.31	1.37
14	H	1215	CLA	O2A-C1	5.30	1.61	1.46
14	B	1215	CLA	O2A-C1	5.29	1.61	1.46
15	G	1121	F6C	C4A-NA	-5.29	1.31	1.37
15	b	1237	F6C	C4A-NA	-5.28	1.31	1.37
14	b	1215	CLA	O2A-C1	5.26	1.61	1.46
14	b	1225	CLA	O2A-C1	5.25	1.60	1.46
14	H	1225	CLA	O2A-C1	5.24	1.60	1.46
14	B	1225	CLA	O2A-C1	5.21	1.60	1.46
14	G	1116	CLA	O2A-C1	5.21	1.60	1.46
14	G	1123	CLA	O2A-C1	5.21	1.60	1.46
14	a	1123	CLA	O2A-C1	5.20	1.60	1.46
14	a	1116	CLA	O2A-C1	5.20	1.60	1.46
14	A	1123	CLA	O2A-C1	5.19	1.60	1.46
14	A	1118	CLA	O2A-C1	5.19	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1116	CLA	O2A-C1	5.18	1.60	1.46
14	H	1213	CLA	O2A-C1	5.18	1.60	1.46
14	B	1213	CLA	O2A-C1	5.17	1.60	1.46
14	a	1118	CLA	O2A-C1	5.17	1.60	1.46
14	b	1213	CLA	O2A-C1	5.17	1.60	1.46
15	B	1238	F6C	O2A-C1	5.16	1.60	1.46
14	G	1118	CLA	O2A-C1	5.15	1.60	1.46
14	G	1133	CLA	O2A-C1	5.15	1.60	1.46
14	a	1133	CLA	O2A-C1	5.15	1.60	1.46
14	a	1109	CLA	O2A-C1	5.15	1.60	1.46
15	H	1238	F6C	O2A-C1	5.15	1.60	1.46
14	A	1133	CLA	O2A-C1	5.15	1.60	1.46
15	b	1238	F6C	O2A-C1	5.15	1.60	1.46
14	A	1130	CLA	C3D-C4D	-5.14	1.32	1.44
14	A	1109	CLA	O2A-C1	5.14	1.60	1.46
14	A	1130	CLA	O2A-C1	5.14	1.60	1.46
14	H	1208	CLA	O2A-C1	5.14	1.60	1.46
14	G	1109	CLA	O2A-C1	5.14	1.60	1.46
14	G	1130	CLA	C3D-C4D	-5.14	1.32	1.44
14	a	1130	CLA	O2A-C1	5.14	1.60	1.46
14	G	1130	CLA	O2A-C1	5.14	1.60	1.46
14	k	1401	CLA	O2D-CGD	5.12	1.45	1.33
14	H	1217	CLA	O2A-C1	5.12	1.60	1.46
14	B	1021	CLA	C1D-ND	-5.12	1.31	1.37
14	A	1140	CLA	O2A-C1	5.11	1.60	1.46
14	a	1130	CLA	C3D-C4D	-5.11	1.32	1.44
14	B	1208	CLA	O2A-C1	5.11	1.60	1.46
14	b	1217	CLA	O2A-C1	5.11	1.60	1.46
14	x	1701	CLA	O2A-C1	5.11	1.60	1.46
14	K	1401	CLA	O2D-CGD	5.11	1.45	1.33
14	T	1401	CLA	O2D-CGD	5.11	1.45	1.33
14	b	1228	CLA	O2A-C1	5.11	1.60	1.46
14	b	1208	CLA	O2A-C1	5.11	1.60	1.46
14	b	1021	CLA	C1D-ND	-5.10	1.31	1.37
14	B	1211	CLA	O2A-C1	5.10	1.60	1.46
14	b	1211	CLA	O2A-C1	5.10	1.60	1.46
14	X	1701	CLA	O2A-C1	5.09	1.60	1.46
14	H	1228	CLA	O2A-C1	5.09	1.60	1.46
14	U	1503	CLA	O2A-C1	5.09	1.60	1.46
15	H	1207	F6C	O2A-C1	5.09	1.60	1.46
14	b	1239	CLA	C3C-C2C	5.09	1.47	1.36
14	B	1228	CLA	O2A-C1	5.08	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1217	CLA	O2A-C1	5.08	1.60	1.46
14	H	1211	CLA	O2A-C1	5.08	1.60	1.46
14	H	1021	CLA	C1D-ND	-5.08	1.31	1.37
14	l	1503	CLA	O2A-C1	5.07	1.60	1.46
15	b	1207	F6C	O2A-C1	5.07	1.60	1.46
15	B	1207	F6C	O2A-C1	5.07	1.60	1.46
14	A	1013	CLA	CHC-C1C	5.07	1.48	1.35
14	L	1503	CLA	O2A-C1	5.07	1.60	1.46
14	H	1239	CLA	C3C-C2C	5.07	1.47	1.36
14	b	1233	CLA	O2D-CGD	5.07	1.45	1.33
14	B	1220	CLA	O2D-CGD	5.07	1.45	1.33
14	G	1140	CLA	O2A-C1	5.06	1.60	1.46
14	H	1220	CLA	O2D-CGD	5.06	1.45	1.33
14	a	1140	CLA	O2A-C1	5.06	1.60	1.46
14	H	1233	CLA	O2D-CGD	5.06	1.45	1.33
14	G	1013	CLA	CHC-C1C	5.06	1.47	1.35
14	a	1125	CLA	O2A-C1	5.06	1.60	1.46
14	G	1119	CLA	O2A-C1	5.06	1.60	1.46
14	W	1701	CLA	O2A-C1	5.06	1.60	1.46
14	a	1013	CLA	CHC-C1C	5.06	1.47	1.35
14	A	1138	CLA	O2D-CGD	5.06	1.45	1.33
14	A	1125	CLA	O2A-C1	5.06	1.60	1.46
14	G	1122	CLA	O2A-C1	5.05	1.60	1.46
14	G	1138	CLA	O2D-CGD	5.05	1.45	1.33
14	B	1216	CLA	O2D-CGD	5.05	1.45	1.33
14	a	1119	CLA	O2A-C1	5.04	1.60	1.46
14	B	1239	CLA	C3C-C2C	5.04	1.47	1.36
14	H	1218	CLA	O2D-CGD	5.04	1.45	1.33
14	B	1221	CLA	O2A-C1	5.04	1.60	1.46
14	b	1220	CLA	O2D-CGD	5.04	1.45	1.33
14	A	1137	CLA	O2A-C1	5.04	1.60	1.46
14	B	1218	CLA	O2D-CGD	5.04	1.45	1.33
14	b	1216	CLA	O2D-CGD	5.04	1.45	1.33
14	b	1221	CLA	O2A-C1	5.04	1.60	1.46
14	G	1125	CLA	O2A-C1	5.04	1.60	1.46
14	G	1012	CLA	C3D-C4D	-5.04	1.32	1.44
14	A	1119	CLA	O2A-C1	5.03	1.60	1.46
14	a	1129	CLA	O2A-C1	5.03	1.60	1.46
14	G	1125	CLA	C3D-C4D	-5.03	1.32	1.44
14	B	1233	CLA	O2D-CGD	5.03	1.45	1.33
14	G	1112	CLA	O2A-C1	5.03	1.60	1.46
14	G	1115	CLA	O2A-C1	5.03	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1221	CLA	O2A-C1	5.02	1.60	1.46
14	b	1218	CLA	O2D-CGD	5.02	1.45	1.33
14	A	1013	CLA	C1D-ND	-5.02	1.31	1.37
14	A	1122	CLA	O2A-C1	5.02	1.60	1.46
14	a	1012	CLA	C3D-C4D	-5.02	1.32	1.44
14	a	1125	CLA	C3D-C4D	-5.02	1.32	1.44
14	b	1231	CLA	O2A-C1	5.02	1.60	1.46
14	A	1129	CLA	O2A-C1	5.02	1.60	1.46
14	a	1138	CLA	O2D-CGD	5.01	1.45	1.33
14	H	1216	CLA	O2D-CGD	5.01	1.45	1.33
14	H	1229	CLA	O2A-C1	5.01	1.60	1.46
14	B	1231	CLA	O2A-C1	5.01	1.60	1.46
14	H	1201	CLA	O2A-C1	5.01	1.60	1.46
14	B	1227	CLA	O2D-CGD	5.01	1.45	1.33
14	A	1112	CLA	O2A-C1	5.01	1.60	1.46
14	a	1137	CLA	O2A-C1	5.01	1.60	1.46
14	A	1138	CLA	O2A-C1	5.01	1.60	1.46
14	a	1112	CLA	O2A-C1	5.01	1.60	1.46
14	A	1012	CLA	C3D-C4D	-5.01	1.32	1.44
14	a	1122	CLA	O2A-C1	5.01	1.60	1.46
14	B	1201	CLA	O2A-C1	5.01	1.60	1.46
14	b	1201	CLA	O2A-C1	5.00	1.60	1.46
14	G	1138	CLA	O2A-C1	5.00	1.60	1.46
14	A	1134	CLA	CHC-C1C	5.00	1.47	1.35
14	a	1102	CLA	O2A-C1	5.00	1.60	1.46
14	G	1129	CLA	O2A-C1	5.00	1.60	1.46
14	a	1134	CLA	CHC-C1C	5.00	1.47	1.35
14	H	1219	CLA	CHC-C1C	5.00	1.47	1.35
14	H	1231	CLA	O2A-C1	5.00	1.60	1.46
14	B	1234	CLA	O2A-C1	5.00	1.60	1.46
14	G	1137	CLA	O2A-C1	5.00	1.60	1.46
14	b	1234	CLA	CHC-C1C	5.00	1.47	1.35
14	H	1234	CLA	CHC-C1C	5.00	1.47	1.35
14	G	1102	CLA	O2A-C1	4.99	1.60	1.46
14	b	1219	CLA	CHC-C1C	4.99	1.47	1.35
14	a	1115	CLA	O2A-C1	4.99	1.60	1.46
14	b	1234	CLA	O2A-C1	4.99	1.60	1.46
14	b	1229	CLA	O2A-C1	4.99	1.60	1.46
14	a	1138	CLA	O2A-C1	4.99	1.60	1.46
14	A	1115	CLA	O2A-C1	4.99	1.60	1.46
14	B	1219	CLA	CHC-C1C	4.99	1.47	1.35
14	B	1234	CLA	CHC-C1C	4.99	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1125	CLA	C3D-C4D	-4.99	1.32	1.44
14	A	1102	CLA	O2A-C1	4.99	1.60	1.46
14	H	1227	CLA	O2D-CGD	4.98	1.45	1.33
14	H	1234	CLA	O2A-C1	4.98	1.60	1.46
14	b	1227	CLA	O2D-CGD	4.98	1.45	1.33
14	A	1128	CLA	O2A-C1	4.98	1.60	1.46
14	H	1218	CLA	C3B-C2B	4.98	1.47	1.40
14	B	1022	CLA	O2A-C1	4.97	1.60	1.46
14	a	1013	CLA	C1D-ND	-4.97	1.31	1.37
14	H	1229	CLA	CHC-C1C	4.97	1.47	1.35
14	G	1104	CLA	O2A-C1	4.97	1.60	1.46
14	B	1218	CLA	C3B-C2B	4.97	1.47	1.40
14	b	1229	CLA	CHC-C1C	4.97	1.47	1.35
14	A	1132	CLA	O2A-C1	4.97	1.60	1.46
14	b	1022	CLA	O2A-C1	4.97	1.60	1.46
14	A	1013	CLA	O2A-C1	4.97	1.60	1.46
14	a	1103	CLA	C3D-C4D	-4.97	1.33	1.44
14	H	1022	CLA	O2A-C1	4.96	1.60	1.46
14	a	1013	CLA	O2A-C1	4.96	1.60	1.46
14	G	1114	CLA	O2D-CGD	4.96	1.45	1.33
14	A	1114	CLA	O2D-CGD	4.96	1.45	1.33
14	G	1134	CLA	CHC-C1C	4.96	1.47	1.35
14	B	1229	CLA	O2A-C1	4.96	1.60	1.46
14	b	1202	CLA	O2A-C1	4.96	1.60	1.46
14	b	1214	CLA	O2A-C1	4.96	1.60	1.46
14	a	1129	CLA	C3D-C4D	-4.95	1.33	1.44
14	a	1114	CLA	O2D-CGD	4.95	1.45	1.33
14	G	1103	CLA	C3D-C4D	-4.95	1.33	1.44
14	B	1203	CLA	C3D-C4D	-4.95	1.33	1.44
14	B	1204	CLA	C1D-ND	-4.95	1.31	1.37
14	H	1202	CLA	O2A-C1	4.95	1.60	1.46
14	G	1013	CLA	O2A-C1	4.95	1.60	1.46
14	A	1104	CLA	O2A-C1	4.95	1.60	1.46
14	A	1126	CLA	C3D-C4D	-4.95	1.33	1.44
14	G	1103	CLA	O2A-C1	4.95	1.60	1.46
14	H	1203	CLA	C3D-C4D	-4.95	1.33	1.44
14	G	1132	CLA	O2A-C1	4.94	1.60	1.46
14	B	1229	CLA	CHC-C1C	4.94	1.47	1.35
14	B	1214	CLA	O2A-C1	4.94	1.60	1.46
14	A	1103	CLA	O2A-C1	4.94	1.60	1.46
14	a	1137	CLA	C3D-C4D	-4.94	1.33	1.44
14	b	1203	CLA	C3D-C4D	-4.94	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1131	CLA	O2A-C1	4.94	1.60	1.46
14	G	1013	CLA	C1D-ND	-4.94	1.31	1.37
15	B	1230	F6C	C4A-NA	-4.94	1.31	1.37
14	A	1137	CLA	C3D-C4D	-4.94	1.33	1.44
14	A	1103	CLA	C3D-C4D	-4.94	1.33	1.44
14	G	1126	CLA	C3D-C4D	-4.94	1.33	1.44
14	L	1502	CLA	O2A-C1	4.93	1.60	1.46
14	b	1204	CLA	C1D-ND	-4.93	1.31	1.37
14	G	1128	CLA	O2A-C1	4.93	1.60	1.46
14	G	1137	CLA	C3D-C4D	-4.93	1.33	1.44
14	H	1214	CLA	O2A-C1	4.93	1.60	1.46
14	a	1128	CLA	O2A-C1	4.93	1.60	1.46
14	H	1204	CLA	C1D-ND	-4.93	1.31	1.37
14	B	1220	CLA	O2A-C1	4.93	1.60	1.46
14	a	1104	CLA	O2A-C1	4.93	1.60	1.46
14	a	1132	CLA	O2A-C1	4.93	1.60	1.46
14	U	1502	CLA	O2A-C1	4.93	1.60	1.46
14	G	1129	CLA	C3D-C4D	-4.93	1.33	1.44
14	B	1218	CLA	CHC-C1C	4.93	1.47	1.35
14	B	1202	CLA	O2A-C1	4.93	1.60	1.46
14	X	1701	CLA	CHC-C1C	4.93	1.47	1.35
14	H	1226	CLA	O2A-C1	4.93	1.60	1.46
14	a	1103	CLA	O2A-C1	4.92	1.60	1.46
14	H	1022	CLA	CHC-C1C	4.92	1.47	1.35
14	B	1022	CLA	CHC-C1C	4.92	1.47	1.35
14	B	1226	CLA	O2A-C1	4.92	1.60	1.46
14	b	1220	CLA	O2A-C1	4.92	1.60	1.46
14	A	1126	CLA	O2A-C1	4.92	1.60	1.46
14	G	1126	CLA	O2A-C1	4.92	1.60	1.46
14	H	1202	CLA	C3D-C4D	-4.92	1.33	1.44
15	a	1121	F6C	O2D-CGD	4.92	1.45	1.33
14	G	1110	CLA	CHC-C1C	4.92	1.47	1.35
14	a	1119	CLA	O2D-CGD	4.92	1.45	1.33
14	H	1220	CLA	O2A-C1	4.92	1.60	1.46
14	b	1218	CLA	CHC-C1C	4.92	1.47	1.35
14	b	1226	CLA	O2A-C1	4.92	1.60	1.46
14	l	1502	CLA	O2A-C1	4.92	1.60	1.46
14	a	1108	CLA	O2D-CGD	4.92	1.45	1.33
14	a	1126	CLA	C3D-C4D	-4.92	1.33	1.44
15	H	1230	F6C	O2D-CGD	4.92	1.45	1.33
14	b	1218	CLA	C3B-C2B	4.92	1.47	1.40
14	A	1108	CLA	O2D-CGD	4.92	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	1121	F6C	O2D-CGD	4.92	1.45	1.33
14	L	1501	CLA	O2D-CGD	4.91	1.45	1.33
15	b	1230	F6C	C4A-NA	-4.91	1.31	1.37
14	l	1501	CLA	O2D-CGD	4.91	1.45	1.33
14	A	1012	CLA	O2A-C1	4.91	1.60	1.46
14	b	1239	CLA	O2D-CGD	4.91	1.45	1.33
14	A	1131	CLA	O2A-C1	4.91	1.60	1.46
14	a	1126	CLA	O2A-C1	4.91	1.60	1.46
14	b	1216	CLA	O2A-C1	4.91	1.60	1.46
14	H	1219	CLA	O2D-CGD	4.91	1.45	1.33
15	b	1230	F6C	O2D-CGD	4.91	1.45	1.33
14	H	1239	CLA	O2D-CGD	4.91	1.45	1.33
14	a	1012	CLA	O2A-C1	4.91	1.60	1.46
14	b	1202	CLA	C3D-C4D	-4.91	1.33	1.44
14	a	1131	CLA	O2A-C1	4.91	1.60	1.46
14	H	1218	CLA	CHC-C1C	4.91	1.47	1.35
14	H	1216	CLA	O2A-C1	4.91	1.60	1.46
14	B	1216	CLA	O2A-C1	4.91	1.60	1.46
14	x	1701	CLA	CHC-C1C	4.90	1.47	1.35
14	W	1701	CLA	CHC-C1C	4.90	1.47	1.35
14	U	1501	CLA	O2D-CGD	4.90	1.45	1.33
15	H	1230	F6C	C4A-NA	-4.90	1.31	1.37
14	H	1214	CLA	O2D-CGD	4.90	1.45	1.33
15	B	1230	F6C	O2D-CGD	4.90	1.45	1.33
14	b	1219	CLA	O2D-CGD	4.90	1.45	1.33
14	B	1214	CLA	O2D-CGD	4.90	1.45	1.33
14	A	1111	CLA	O2A-C1	4.89	1.59	1.46
14	a	1110	CLA	CHC-C1C	4.89	1.47	1.35
14	a	1139	CLA	CHC-C1C	4.89	1.47	1.35
14	b	1204	CLA	C3D-C4D	-4.89	1.33	1.44
14	b	1214	CLA	O2D-CGD	4.89	1.45	1.33
14	G	1116	CLA	CHC-C1C	4.89	1.47	1.35
14	G	1108	CLA	O2D-CGD	4.89	1.45	1.33
14	B	1219	CLA	O2D-CGD	4.89	1.45	1.33
13	A	1011	CL0	C1D-ND	-4.89	1.31	1.37
15	A	1121	F6C	O2D-CGD	4.89	1.45	1.33
14	b	1022	CLA	CHC-C1C	4.89	1.47	1.35
14	G	1012	CLA	O2A-C1	4.89	1.59	1.46
14	H	1204	CLA	C3D-C4D	-4.89	1.33	1.44
14	G	1111	CLA	O2A-C1	4.89	1.59	1.46
14	a	1111	CLA	O2A-C1	4.89	1.59	1.46
13	A	1011	CL0	O2A-C1	4.89	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1235	CLA	O2A-C1	4.89	1.59	1.46
14	a	1135	CLA	C3D-C4D	-4.89	1.33	1.44
14	G	1119	CLA	O2D-CGD	4.88	1.45	1.33
14	T	1401	CLA	CHC-C1C	4.88	1.47	1.35
14	K	1401	CLA	CHC-C1C	4.88	1.47	1.35
14	A	1135	CLA	C3D-C4D	-4.88	1.33	1.44
15	B	1237	F6C	O2D-CGD	4.88	1.45	1.33
14	A	1129	CLA	C3D-C4D	-4.88	1.33	1.44
14	B	1224	CLA	O2A-C1	4.88	1.59	1.46
14	B	1202	CLA	C3D-C4D	-4.88	1.33	1.44
14	b	1235	CLA	O2A-C1	4.88	1.59	1.46
14	A	1119	CLA	O2D-CGD	4.88	1.45	1.33
13	G	1011	CL0	O2A-C1	4.87	1.59	1.46
14	G	1120	CLA	O2D-CGD	4.87	1.45	1.33
14	a	1120	CLA	O2D-CGD	4.87	1.45	1.33
14	A	1139	CLA	CHC-C1C	4.87	1.47	1.35
14	A	1110	CLA	CHC-C1C	4.87	1.47	1.35
15	B	1238	F6C	CHC-C4B	4.87	1.47	1.35
15	H	1237	F6C	O2D-CGD	4.87	1.45	1.33
14	B	1204	CLA	C3D-C4D	-4.87	1.33	1.44
13	a	1011	CL0	O2A-C1	4.87	1.59	1.46
14	B	1239	CLA	O2D-CGD	4.87	1.45	1.33
14	H	1224	CLA	O2A-C1	4.87	1.59	1.46
14	x	1701	CLA	C3B-C2B	4.87	1.47	1.40
14	A	1126	CLA	CHC-C1C	4.86	1.47	1.35
14	B	1212	CLA	CHC-C1C	4.86	1.47	1.35
14	B	1206	CLA	C3D-C4D	-4.86	1.33	1.44
14	k	1401	CLA	CHC-C1C	4.86	1.47	1.35
14	A	1104	CLA	O2D-CGD	4.86	1.45	1.33
14	A	1116	CLA	CHC-C1C	4.86	1.47	1.35
15	H	1238	F6C	CHC-C4B	4.86	1.47	1.35
15	b	1237	F6C	O2D-CGD	4.86	1.45	1.33
14	B	1204	CLA	O2A-C1	4.86	1.59	1.46
14	a	1117	CLA	O2A-C1	4.86	1.59	1.46
14	G	1139	CLA	CHC-C1C	4.86	1.47	1.35
14	B	1213	CLA	CHC-C1C	4.86	1.47	1.35
14	A	1117	CLA	O2A-C1	4.86	1.59	1.46
14	H	1214	CLA	C3D-C4D	-4.86	1.33	1.44
14	G	1135	CLA	C3D-C4D	-4.86	1.33	1.44
14	A	1136	CLA	O2A-C1	4.86	1.59	1.46
14	G	1126	CLA	CHC-C1C	4.86	1.47	1.35
14	B	1214	CLA	C3D-C4D	-4.86	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1117	CLA	O2A-C1	4.86	1.59	1.46
14	H	1204	CLA	O2A-C1	4.86	1.59	1.46
14	b	1204	CLA	O2A-C1	4.86	1.59	1.46
14	a	1116	CLA	CHC-C1C	4.86	1.47	1.35
14	a	1126	CLA	CHC-C1C	4.85	1.47	1.35
14	H	1235	CLA	O2A-C1	4.85	1.59	1.46
14	a	1136	CLA	O2A-C1	4.85	1.59	1.46
14	a	1124	CLA	CHC-C1C	4.85	1.47	1.35
14	G	1104	CLA	O2D-CGD	4.85	1.45	1.33
14	G	1124	CLA	CHC-C1C	4.85	1.47	1.35
14	H	1235	CLA	C3D-C4D	-4.85	1.33	1.44
14	b	1206	CLA	C3D-C4D	-4.85	1.33	1.44
14	G	1136	CLA	O2A-C1	4.85	1.59	1.46
15	H	1237	F6C	O2A-C1	4.85	1.59	1.46
14	H	1206	CLA	C3D-C4D	-4.85	1.33	1.44
14	A	1124	CLA	CHC-C1C	4.85	1.47	1.35
14	B	1227	CLA	C3D-C4D	-4.85	1.33	1.44
14	b	1234	CLA	C3D-C4D	-4.84	1.33	1.44
14	B	1203	CLA	O2A-C1	4.84	1.59	1.46
14	A	1113	CLA	CHC-C1C	4.84	1.47	1.35
14	b	1224	CLA	O2A-C1	4.84	1.59	1.46
14	B	1222	CLA	CHC-C1C	4.84	1.47	1.35
15	B	1237	F6C	O2A-C1	4.84	1.59	1.46
14	b	1226	CLA	C3D-C4D	-4.84	1.33	1.44
14	H	1226	CLA	C3D-C4D	-4.84	1.33	1.44
14	G	1102	CLA	CHC-C1C	4.84	1.47	1.35
14	B	1225	CLA	O2D-CGD	4.84	1.45	1.33
14	A	1134	CLA	C3B-C2B	4.84	1.47	1.40
14	H	1222	CLA	CHC-C1C	4.84	1.47	1.35
14	A	1120	CLA	O2D-CGD	4.84	1.45	1.33
14	H	1022	CLA	C3D-C4D	-4.84	1.33	1.44
14	b	1213	CLA	CHC-C1C	4.84	1.47	1.35
14	b	1210	CLA	O2A-C1	4.84	1.59	1.46
14	a	1138	CLA	C3D-C4D	-4.84	1.33	1.44
15	b	1238	F6C	CHC-C4B	4.84	1.47	1.35
14	B	1226	CLA	C3D-C4D	-4.84	1.33	1.44
14	a	1115	CLA	O2D-CGD	4.84	1.45	1.33
14	H	1223	CLA	O2A-C1	4.84	1.59	1.46
14	a	1134	CLA	O2D-CGD	4.84	1.45	1.33
14	b	1227	CLA	C3D-C4D	-4.84	1.33	1.44
14	G	1135	CLA	O2A-C1	4.84	1.59	1.46
14	b	1212	CLA	CHC-C1C	4.84	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1124	CLA	O2A-C1	4.84	1.59	1.46
14	b	1203	CLA	O2A-C1	4.84	1.59	1.46
14	b	1223	CLA	O2A-C1	4.84	1.59	1.46
14	H	1212	CLA	CHC-C1C	4.84	1.47	1.35
14	b	1225	CLA	O2D-CGD	4.84	1.45	1.33
13	G	1011	CL0	C1D-ND	-4.84	1.31	1.37
14	B	1224	CLA	C3D-C4D	-4.83	1.33	1.44
14	b	1235	CLA	C3D-C4D	-4.83	1.33	1.44
14	a	1113	CLA	CHC-C1C	4.83	1.47	1.35
14	H	1213	CLA	CHC-C1C	4.83	1.47	1.35
14	G	1134	CLA	O2D-CGD	4.83	1.45	1.33
14	B	1222	CLA	O2A-C1	4.83	1.59	1.46
14	H	1210	CLA	O2A-C1	4.83	1.59	1.46
14	a	1135	CLA	O2A-C1	4.83	1.59	1.46
14	W	1701	CLA	C3B-C2B	4.83	1.47	1.40
14	H	1224	CLA	C3D-C4D	-4.83	1.33	1.44
14	A	1134	CLA	O2D-CGD	4.83	1.45	1.33
14	A	1102	CLA	CHC-C1C	4.83	1.47	1.35
14	B	1211	CLA	CHC-C1C	4.83	1.47	1.35
14	a	1136	CLA	C3D-C4D	-4.83	1.33	1.44
14	G	1140	CLA	C3D-C4D	-4.83	1.33	1.44
14	b	1214	CLA	C3D-C4D	-4.83	1.33	1.44
14	A	1124	CLA	O2A-C1	4.83	1.59	1.46
14	A	1123	CLA	O2D-CGD	4.83	1.45	1.33
14	a	1104	CLA	O2D-CGD	4.83	1.45	1.33
14	B	1235	CLA	C3D-C4D	-4.83	1.33	1.44
14	G	1113	CLA	CHC-C1C	4.83	1.47	1.35
14	H	1234	CLA	C3D-C4D	-4.83	1.33	1.44
14	B	1223	CLA	O2A-C1	4.83	1.59	1.46
14	H	1203	CLA	O2A-C1	4.83	1.59	1.46
14	G	1138	CLA	C3D-C4D	-4.83	1.33	1.44
14	B	1227	CLA	CHC-C1C	4.83	1.47	1.35
14	A	1138	CLA	CHC-C1C	4.82	1.47	1.35
14	a	1124	CLA	O2A-C1	4.82	1.59	1.46
14	B	1234	CLA	C3D-C4D	-4.82	1.33	1.44
14	A	1125	CLA	O2D-CGD	4.82	1.45	1.33
14	b	1222	CLA	CHC-C1C	4.82	1.47	1.35
14	B	1232	CLA	CHC-C1C	4.82	1.47	1.35
14	a	1140	CLA	C3D-C4D	-4.82	1.33	1.44
14	G	1129	CLA	CHC-C1C	4.82	1.47	1.35
14	A	1136	CLA	C3D-C4D	-4.82	1.33	1.44
13	a	1011	CL0	C1D-ND	-4.82	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1217	CLA	O2D-CGD	4.82	1.45	1.33
14	G	1131	CLA	C3D-C4D	-4.82	1.33	1.44
14	H	1227	CLA	C3D-C4D	-4.82	1.33	1.44
14	b	1211	CLA	CHC-C1C	4.82	1.47	1.35
15	b	1237	F6C	O2A-C1	4.82	1.59	1.46
14	b	1232	CLA	CHC-C1C	4.82	1.47	1.35
14	G	1123	CLA	O2D-CGD	4.81	1.44	1.33
14	G	1115	CLA	O2D-CGD	4.81	1.44	1.33
14	L	1501	CLA	O2A-C1	4.81	1.59	1.46
14	b	1224	CLA	C3D-C4D	-4.81	1.33	1.44
14	A	1138	CLA	C3D-C4D	-4.81	1.33	1.44
14	G	1125	CLA	O2D-CGD	4.81	1.44	1.33
14	a	1120	CLA	CHC-C1C	4.81	1.47	1.35
14	b	1205	CLA	C1D-ND	-4.81	1.31	1.37
14	a	1105	CLA	O2D-CGD	4.81	1.44	1.33
14	a	1102	CLA	CHC-C1C	4.81	1.47	1.35
14	a	1115	CLA	CHC-C1C	4.81	1.47	1.35
14	H	1211	CLA	CHC-C1C	4.81	1.47	1.35
14	a	1123	CLA	O2D-CGD	4.81	1.44	1.33
14	A	1115	CLA	O2D-CGD	4.81	1.44	1.33
14	b	1236	CLA	C3D-C4D	-4.81	1.33	1.44
14	X	1701	CLA	C3B-C2B	4.81	1.47	1.40
14	A	1105	CLA	O2D-CGD	4.81	1.44	1.33
14	B	1217	CLA	O2D-CGD	4.81	1.44	1.33
14	B	1210	CLA	O2A-C1	4.81	1.59	1.46
14	A	1115	CLA	CHC-C1C	4.80	1.47	1.35
14	B	1223	CLA	C3D-C4D	-4.80	1.33	1.44
14	G	1105	CLA	O2D-CGD	4.80	1.44	1.33
14	G	1136	CLA	C3D-C4D	-4.80	1.33	1.44
14	H	1217	CLA	O2D-CGD	4.80	1.44	1.33
14	A	1135	CLA	O2A-C1	4.80	1.59	1.46
14	b	1022	CLA	C3D-C4D	-4.80	1.33	1.44
14	B	1236	CLA	C3D-C4D	-4.80	1.33	1.44
14	b	1217	CLA	CHC-C1C	4.80	1.47	1.35
14	b	1201	CLA	C3D-C4D	-4.80	1.33	1.44
14	B	1022	CLA	C3D-C4D	-4.80	1.33	1.44
14	B	1233	CLA	CHC-C1C	4.80	1.47	1.35
14	a	1125	CLA	O2D-CGD	4.80	1.44	1.33
14	a	1124	CLA	C3D-C4D	-4.80	1.33	1.44
14	B	1225	CLA	C3D-C4D	-4.80	1.33	1.44
14	A	1131	CLA	C3D-C4D	-4.80	1.33	1.44
14	b	1227	CLA	CHC-C1C	4.80	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1228	CLA	O2D-CGD	4.80	1.44	1.33
14	b	1223	CLA	C3D-C4D	-4.80	1.33	1.44
14	G	1120	CLA	CHC-C1C	4.80	1.47	1.35
14	H	1233	CLA	CHC-C1C	4.80	1.47	1.35
14	l	1501	CLA	O2A-C1	4.79	1.59	1.46
14	B	1205	CLA	O2A-C1	4.79	1.59	1.46
14	G	1115	CLA	CHC-C1C	4.79	1.47	1.35
14	A	1106	CLA	CHC-C1C	4.79	1.47	1.35
14	G	1101	CLA	CHC-C1C	4.79	1.47	1.35
14	G	1138	CLA	CHC-C1C	4.79	1.47	1.35
14	H	1225	CLA	C3D-C4D	-4.79	1.33	1.44
14	G	1107	CLA	O2D-CGD	4.79	1.44	1.33
14	a	1129	CLA	CHC-C1C	4.79	1.47	1.35
14	H	1232	CLA	CHC-C1C	4.79	1.47	1.35
14	b	1225	CLA	C3D-C4D	-4.79	1.33	1.44
14	H	1227	CLA	CHC-C1C	4.79	1.47	1.35
14	A	1111	CLA	CHC-C1C	4.79	1.47	1.35
14	H	1236	CLA	C3D-C4D	-4.79	1.33	1.44
14	B	1209	CLA	CHC-C1C	4.79	1.47	1.35
14	H	1201	CLA	C3D-C4D	-4.79	1.33	1.44
14	H	1223	CLA	C3D-C4D	-4.79	1.33	1.44
13	G	1011	CL0	C3D-C4D	-4.79	1.33	1.44
14	a	1138	CLA	CHC-C1C	4.79	1.47	1.35
14	G	1111	CLA	CHC-C1C	4.79	1.47	1.35
14	B	1210	CLA	C3D-C4D	-4.79	1.33	1.44
14	A	1120	CLA	CHC-C1C	4.79	1.47	1.35
14	a	1134	CLA	C3B-C2B	4.79	1.47	1.40
14	H	1222	CLA	O2A-C1	4.79	1.59	1.46
14	H	1225	CLA	O2D-CGD	4.79	1.44	1.33
14	H	1205	CLA	C1D-ND	-4.79	1.31	1.37
14	B	1221	CLA	CHC-C1C	4.79	1.47	1.35
14	a	1128	CLA	C3D-C4D	-4.79	1.33	1.44
14	H	1239	CLA	O2A-C1	4.78	1.59	1.46
14	b	1239	CLA	O2A-C1	4.78	1.59	1.46
14	H	1217	CLA	CHC-C1C	4.78	1.47	1.35
14	A	1124	CLA	C3D-C4D	-4.78	1.33	1.44
14	B	1201	CLA	C3D-C4D	-4.78	1.33	1.44
14	H	1209	CLA	CHC-C1C	4.78	1.47	1.35
14	H	1211	CLA	C3D-C4D	-4.78	1.33	1.44
14	a	1131	CLA	C3D-C4D	-4.78	1.33	1.44
14	b	1233	CLA	CHC-C1C	4.78	1.47	1.35
14	A	1115	CLA	C3B-C2B	4.78	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1217	CLA	CHC-C1C	4.78	1.47	1.35
14	A	1140	CLA	C3D-C4D	-4.78	1.33	1.44
14	B	1239	CLA	O2A-C1	4.78	1.59	1.46
14	H	1223	CLA	CHC-C1C	4.78	1.47	1.35
14	A	1108	CLA	CHC-C1C	4.78	1.47	1.35
14	G	1106	CLA	CHC-C1C	4.78	1.47	1.35
14	G	1128	CLA	C3D-C4D	-4.78	1.33	1.44
14	a	1130	CLA	O2D-CGD	4.78	1.44	1.33
14	U	1501	CLA	O2A-C1	4.78	1.59	1.46
14	B	1205	CLA	C1D-ND	-4.78	1.31	1.37
14	G	1109	CLA	O2D-CGD	4.78	1.44	1.33
14	H	1202	CLA	CHC-C1C	4.78	1.47	1.35
14	A	1129	CLA	CHC-C1C	4.78	1.47	1.35
14	b	1205	CLA	O2A-C1	4.78	1.59	1.46
14	H	1205	CLA	O2A-C1	4.78	1.59	1.46
14	B	1202	CLA	CHC-C1C	4.77	1.47	1.35
14	a	1114	CLA	CHD-C1D	4.77	1.47	1.38
14	G	1113	CLA	O2D-CGD	4.77	1.44	1.33
14	a	1111	CLA	CHC-C1C	4.77	1.47	1.35
14	A	1126	CLA	O2D-CGD	4.77	1.44	1.33
14	b	1222	CLA	O2A-C1	4.77	1.59	1.46
14	H	1221	CLA	CHC-C1C	4.77	1.47	1.35
14	b	1209	CLA	CHC-C1C	4.77	1.47	1.35
14	b	1223	CLA	CHC-C1C	4.77	1.47	1.35
14	b	1202	CLA	CHC-C1C	4.77	1.47	1.35
14	a	1101	CLA	CHC-C1C	4.77	1.47	1.35
14	A	1101	CLA	CHC-C1C	4.77	1.47	1.35
14	G	1124	CLA	C3D-C4D	-4.77	1.33	1.44
14	H	1228	CLA	O2D-CGD	4.77	1.44	1.33
14	U	1503	CLA	O2D-CGD	4.77	1.44	1.33
14	G	1127	CLA	O2D-CGD	4.77	1.44	1.33
14	a	1106	CLA	C3B-C2B	4.77	1.47	1.40
14	G	1102	CLA	C3D-C4D	-4.77	1.33	1.44
14	A	1128	CLA	C3D-C4D	-4.76	1.33	1.44
14	A	1130	CLA	O2D-CGD	4.76	1.44	1.33
14	H	1023	CLA	C1D-ND	-4.76	1.31	1.37
14	a	1107	CLA	O2D-CGD	4.76	1.44	1.33
14	b	1221	CLA	CHC-C1C	4.76	1.47	1.35
14	a	1108	CLA	CHC-C1C	4.76	1.47	1.35
14	A	1136	CLA	O2D-CGD	4.76	1.44	1.33
14	B	1208	CLA	O2D-CGD	4.76	1.44	1.33
14	a	1130	CLA	CHC-C1C	4.76	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1102	CLA	C3D-C4D	-4.76	1.33	1.44
14	G	1108	CLA	CHC-C1C	4.76	1.47	1.35
14	A	1132	CLA	CHC-C1C	4.76	1.47	1.35
14	a	1106	CLA	CHC-C1C	4.76	1.47	1.35
14	B	1223	CLA	CHC-C1C	4.76	1.47	1.35
14	H	1208	CLA	CHC-C1C	4.76	1.47	1.35
14	A	1114	CLA	CHD-C1D	4.76	1.47	1.38
14	a	1113	CLA	O2D-CGD	4.76	1.44	1.33
14	B	1209	CLA	O2D-CGD	4.76	1.44	1.33
14	b	1210	CLA	C3D-C4D	-4.76	1.33	1.44
14	B	1235	CLA	CHC-C1C	4.76	1.47	1.35
14	a	1116	CLA	O2D-CGD	4.76	1.44	1.33
14	b	1228	CLA	O2D-CGD	4.76	1.44	1.33
14	H	1210	CLA	CHC-C1C	4.75	1.47	1.35
14	H	1021	CLA	O2A-C1	4.75	1.59	1.46
14	L	1503	CLA	O2D-CGD	4.75	1.44	1.33
14	G	1136	CLA	CHC-C1C	4.75	1.47	1.35
14	b	1235	CLA	CHC-C1C	4.75	1.47	1.35
14	H	1239	CLA	C3D-C4D	-4.75	1.33	1.44
14	a	1126	CLA	O2D-CGD	4.75	1.44	1.33
14	a	1112	CLA	CHC-C1C	4.75	1.47	1.35
14	H	1216	CLA	CHC-C1C	4.75	1.47	1.35
14	a	1127	CLA	O2D-CGD	4.75	1.44	1.33
14	b	1208	CLA	O2D-CGD	4.75	1.44	1.33
14	a	1117	CLA	O2D-CGD	4.75	1.44	1.33
14	A	1113	CLA	O2D-CGD	4.75	1.44	1.33
14	A	1116	CLA	O2D-CGD	4.75	1.44	1.33
14	A	1107	CLA	O2D-CGD	4.75	1.44	1.33
14	A	1109	CLA	O2D-CGD	4.75	1.44	1.33
14	B	1216	CLA	CHC-C1C	4.75	1.47	1.35
14	B	1222	CLA	C3B-C2B	4.75	1.47	1.40
14	B	1239	CLA	C3D-C4D	-4.75	1.33	1.44
14	X	1701	CLA	O2D-CGD	4.75	1.44	1.33
14	a	1109	CLA	CHC-C1C	4.75	1.47	1.35
14	G	1130	CLA	CHC-C1C	4.75	1.47	1.35
14	H	1235	CLA	CHC-C1C	4.75	1.47	1.35
14	b	1214	CLA	CHC-C1C	4.75	1.47	1.35
14	a	1109	CLA	O2D-CGD	4.75	1.44	1.33
14	b	1216	CLA	CHC-C1C	4.75	1.47	1.35
14	G	1136	CLA	O2D-CGD	4.75	1.44	1.33
14	b	1239	CLA	C3D-C4D	-4.75	1.33	1.44
14	B	1232	CLA	O2D-CGD	4.74	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1109	CLA	CHC-C1C	4.74	1.47	1.35
14	H	1210	CLA	C3D-C4D	-4.74	1.33	1.44
14	a	1139	CLA	C3D-C4D	-4.74	1.33	1.44
14	G	1105	CLA	CHC-C1C	4.74	1.47	1.35
14	G	1134	CLA	C3B-C2B	4.74	1.46	1.40
14	L	1501	CLA	C3D-C4D	-4.74	1.33	1.44
14	a	1132	CLA	CHC-C1C	4.74	1.47	1.35
13	a	1011	CL0	C3D-C4D	-4.74	1.33	1.44
14	H	1021	CLA	C3D-C4D	-4.74	1.33	1.44
14	a	1102	CLA	C3D-C4D	-4.74	1.33	1.44
14	b	1225	CLA	CHC-C1C	4.74	1.47	1.35
14	H	1208	CLA	O2D-CGD	4.74	1.44	1.33
14	l	1503	CLA	O2D-CGD	4.74	1.44	1.33
14	b	1021	CLA	O2A-C1	4.74	1.59	1.46
14	A	1140	CLA	CHC-C1C	4.74	1.47	1.35
14	G	1115	CLA	C3B-C2B	4.74	1.46	1.40
14	H	1023	CLA	O2A-C1	4.74	1.59	1.46
14	b	1211	CLA	C3D-C4D	-4.74	1.33	1.44
14	H	1225	CLA	CHC-C1C	4.74	1.47	1.35
14	b	1209	CLA	O2D-CGD	4.74	1.44	1.33
13	A	1011	CL0	C3D-C4D	-4.74	1.33	1.44
14	G	1116	CLA	O2D-CGD	4.74	1.44	1.33
14	B	1211	CLA	C3D-C4D	-4.74	1.33	1.44
14	A	1117	CLA	O2D-CGD	4.74	1.44	1.33
14	A	1130	CLA	CHC-C1C	4.73	1.47	1.35
14	G	1130	CLA	O2D-CGD	4.73	1.44	1.33
14	b	1203	CLA	O2D-CGD	4.73	1.44	1.33
15	a	1121	F6C	CHC-C4B	4.73	1.47	1.35
14	G	1126	CLA	O2D-CGD	4.73	1.44	1.33
14	B	1211	CLA	O2D-CGD	4.73	1.44	1.33
14	A	1133	CLA	O2D-CGD	4.73	1.44	1.33
14	B	1021	CLA	O2A-C1	4.73	1.59	1.46
14	a	1136	CLA	O2D-CGD	4.73	1.44	1.33
14	l	1501	CLA	C3D-C4D	-4.73	1.33	1.44
15	G	1121	F6C	CHC-C4B	4.73	1.47	1.35
14	H	1221	CLA	C3D-C4D	-4.73	1.33	1.44
14	a	1140	CLA	CHC-C1C	4.73	1.47	1.35
14	b	1221	CLA	C3D-C4D	-4.73	1.33	1.44
14	B	1203	CLA	O2D-CGD	4.73	1.44	1.33
14	B	1023	CLA	C1D-ND	-4.73	1.32	1.37
14	A	1109	CLA	CHC-C1C	4.73	1.47	1.35
14	U	1501	CLA	C3D-C4D	-4.73	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1133	CLA	O2D-CGD	4.73	1.44	1.33
14	H	1214	CLA	CHC-C1C	4.73	1.47	1.35
15	A	1121	F6C	CHC-C4B	4.73	1.47	1.35
14	a	1136	CLA	CHC-C1C	4.73	1.47	1.35
14	H	1221	CLA	O2D-CGD	4.73	1.44	1.33
14	b	1211	CLA	O2D-CGD	4.72	1.44	1.33
14	H	1232	CLA	O2D-CGD	4.72	1.44	1.33
14	W	1701	CLA	O2D-CGD	4.72	1.44	1.33
14	H	1201	CLA	CHC-C1C	4.72	1.47	1.35
14	a	1119	CLA	C3D-C4D	-4.72	1.33	1.44
14	b	1222	CLA	C3D-C4D	-4.72	1.33	1.44
14	b	1205	CLA	C3D-C4D	-4.72	1.33	1.44
14	a	1139	CLA	O2D-CGD	4.72	1.44	1.33
14	H	1203	CLA	O2D-CGD	4.72	1.44	1.33
14	b	1221	CLA	O2D-CGD	4.72	1.44	1.33
14	G	1106	CLA	C3B-C2B	4.72	1.46	1.40
14	G	1137	CLA	C3B-C2B	4.72	1.46	1.40
14	G	1139	CLA	C3D-C4D	-4.72	1.33	1.44
14	b	1023	CLA	O2A-C1	4.72	1.59	1.46
14	G	1112	CLA	CHC-C1C	4.72	1.47	1.35
14	b	1201	CLA	CHC-C1C	4.71	1.47	1.35
14	a	1115	CLA	C3B-C2B	4.71	1.46	1.40
14	H	1204	CLA	O2D-CGD	4.71	1.44	1.33
14	G	1118	CLA	C3D-C4D	-4.71	1.33	1.44
14	A	1127	CLA	O2D-CGD	4.71	1.44	1.33
14	B	1021	CLA	C3D-C4D	-4.71	1.33	1.44
14	L	1502	CLA	CHC-C1C	4.71	1.47	1.35
14	b	1208	CLA	CHC-C1C	4.71	1.47	1.35
14	b	1210	CLA	CHC-C1C	4.71	1.47	1.35
14	B	1023	CLA	O2A-C1	4.71	1.59	1.46
14	B	1221	CLA	O2D-CGD	4.71	1.44	1.33
14	B	1221	CLA	C3D-C4D	-4.71	1.33	1.44
14	x	1701	CLA	O2D-CGD	4.71	1.44	1.33
14	b	1021	CLA	C3D-C4D	-4.71	1.33	1.44
14	H	1209	CLA	O2D-CGD	4.71	1.44	1.33
14	A	1106	CLA	C3B-C2B	4.71	1.46	1.40
14	b	1203	CLA	CHC-C1C	4.71	1.47	1.35
14	A	1136	CLA	CHC-C1C	4.71	1.47	1.35
14	a	1118	CLA	C3D-C4D	-4.71	1.33	1.44
14	a	1105	CLA	CHC-C1C	4.71	1.47	1.35
14	A	1107	CLA	CHC-C1C	4.71	1.47	1.35
14	G	1140	CLA	CHC-C1C	4.71	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1123	CLA	CHC-C1C	4.71	1.47	1.35
14	a	1132	CLA	C3D-C4D	-4.71	1.33	1.44
14	G	1117	CLA	O2D-CGD	4.70	1.44	1.33
14	G	1106	CLA	O2A-C1	4.70	1.59	1.46
14	B	1225	CLA	CHC-C1C	4.70	1.47	1.35
14	G	1139	CLA	O2D-CGD	4.70	1.44	1.33
14	H	1211	CLA	O2D-CGD	4.70	1.44	1.33
14	B	1208	CLA	CHC-C1C	4.70	1.47	1.35
14	B	1223	CLA	C3B-C2B	4.70	1.46	1.40
14	H	1213	CLA	O2D-CGD	4.70	1.44	1.33
14	a	1134	CLA	C3C-C2C	4.70	1.46	1.36
14	A	1112	CLA	CHC-C1C	4.70	1.47	1.35
14	A	1106	CLA	O2A-C1	4.70	1.59	1.46
14	B	1210	CLA	CHC-C1C	4.70	1.47	1.35
14	B	1213	CLA	O2D-CGD	4.70	1.44	1.33
14	A	1104	CLA	C3D-C4D	-4.70	1.33	1.44
14	G	1132	CLA	C3D-C4D	-4.70	1.33	1.44
14	A	1132	CLA	C3D-C4D	-4.70	1.33	1.44
14	G	1133	CLA	O2D-CGD	4.70	1.44	1.33
14	A	1139	CLA	C3D-C4D	-4.70	1.33	1.44
14	A	1105	CLA	CHC-C1C	4.70	1.47	1.35
14	G	1132	CLA	CHC-C1C	4.70	1.47	1.35
14	G	1114	CLA	CHD-C1D	4.70	1.47	1.38
14	a	1122	CLA	O2D-CGD	4.70	1.44	1.33
14	H	1228	CLA	C3D-C4D	-4.70	1.33	1.44
14	H	1236	CLA	O2D-CGD	4.70	1.44	1.33
14	B	1023	CLA	O2D-CGD	4.70	1.44	1.33
14	U	1503	CLA	CHC-C1C	4.70	1.47	1.35
14	a	1106	CLA	O2A-C1	4.69	1.59	1.46
14	H	1203	CLA	CHC-C1C	4.69	1.47	1.35
14	l	1503	CLA	C3D-C4D	-4.69	1.33	1.44
14	b	1222	CLA	C3B-C2B	4.69	1.46	1.40
14	B	1228	CLA	C3D-C4D	-4.69	1.33	1.44
14	H	1205	CLA	C3D-C4D	-4.69	1.33	1.44
14	A	1112	CLA	O2D-CGD	4.69	1.44	1.33
15	H	1238	F6C	O2D-CGD	4.69	1.44	1.33
14	G	1013	CLA	O2D-CGD	4.69	1.44	1.33
14	A	1106	CLA	O2D-CGD	4.69	1.44	1.33
14	H	1236	CLA	CHC-C1C	4.69	1.47	1.35
14	B	1201	CLA	CHC-C1C	4.69	1.47	1.35
14	B	1214	CLA	CHC-C1C	4.69	1.47	1.35
14	A	1119	CLA	C3D-C4D	-4.69	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1134	CLA	CHD-C1D	4.69	1.47	1.38
14	H	1222	CLA	C3B-C2B	4.69	1.46	1.40
14	G	1112	CLA	O2D-CGD	4.69	1.44	1.33
14	b	1236	CLA	O2D-CGD	4.69	1.44	1.33
14	a	1110	CLA	O2D-CGD	4.69	1.44	1.33
14	b	1232	CLA	O2D-CGD	4.69	1.44	1.33
14	G	1107	CLA	CHC-C1C	4.69	1.47	1.35
14	U	1502	CLA	CHC-C1C	4.69	1.47	1.35
14	G	1111	CLA	C3D-C4D	-4.69	1.33	1.44
14	b	1204	CLA	O2D-CGD	4.69	1.44	1.33
14	b	1023	CLA	C1D-ND	-4.69	1.32	1.37
14	H	1231	CLA	CHC-C1C	4.68	1.47	1.35
14	B	1203	CLA	CHC-C1C	4.68	1.47	1.35
14	G	1116	CLA	C3D-C4D	-4.68	1.33	1.44
15	b	1238	F6C	O2D-CGD	4.68	1.44	1.33
14	G	1128	CLA	C1D-ND	-4.68	1.32	1.37
14	B	1231	CLA	CHC-C1C	4.68	1.47	1.35
14	G	1119	CLA	C3D-C4D	-4.68	1.33	1.44
14	A	1013	CLA	O2D-CGD	4.68	1.44	1.33
14	B	1222	CLA	C3D-C4D	-4.68	1.33	1.44
14	U	1503	CLA	C3D-C4D	-4.68	1.33	1.44
14	l	1502	CLA	CHC-C1C	4.68	1.47	1.35
14	l	1503	CLA	CHC-C1C	4.68	1.47	1.35
14	G	1123	CLA	CHC-C1C	4.68	1.47	1.35
14	G	1104	CLA	C3D-C4D	-4.68	1.33	1.44
14	H	1023	CLA	O2D-CGD	4.68	1.44	1.33
14	a	1127	CLA	O2A-C1	4.67	1.59	1.46
14	L	1503	CLA	C3D-C4D	-4.67	1.33	1.44
14	G	1104	CLA	CHC-C1C	4.67	1.47	1.35
14	H	1204	CLA	CHC-C1C	4.67	1.47	1.35
14	b	1236	CLA	CHC-C1C	4.67	1.47	1.35
14	a	1112	CLA	O2D-CGD	4.67	1.44	1.33
14	b	1231	CLA	CHC-C1C	4.67	1.47	1.35
14	A	1111	CLA	C3D-C4D	-4.67	1.33	1.44
14	L	1503	CLA	CHC-C1C	4.67	1.47	1.35
14	b	1023	CLA	O2D-CGD	4.67	1.44	1.33
14	A	1110	CLA	O2D-CGD	4.67	1.44	1.33
14	A	1139	CLA	O2D-CGD	4.67	1.44	1.33
14	G	1127	CLA	O2A-C1	4.67	1.59	1.46
14	B	1204	CLA	O2D-CGD	4.67	1.44	1.33
14	B	1205	CLA	C3D-C4D	-4.67	1.33	1.44
14	B	1218	CLA	C1D-ND	-4.67	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1127	CLA	O2A-C1	4.67	1.59	1.46
14	H	1226	CLA	O2D-CGD	4.67	1.44	1.33
14	G	1122	CLA	O2D-CGD	4.67	1.44	1.33
14	a	1123	CLA	CHC-C1C	4.67	1.46	1.35
14	A	1106	CLA	C3D-C4D	-4.67	1.33	1.44
14	G	1107	CLA	C3D-C4D	-4.67	1.33	1.44
14	G	1140	CLA	O2D-CGD	4.67	1.44	1.33
14	G	1102	CLA	O2D-CGD	4.67	1.44	1.33
14	a	1113	CLA	C3D-C4D	-4.67	1.33	1.44
14	a	1104	CLA	CHC-C1C	4.67	1.46	1.35
14	A	1122	CLA	O2D-CGD	4.67	1.44	1.33
14	A	1140	CLA	O2D-CGD	4.67	1.44	1.33
15	B	1238	F6C	O2D-CGD	4.67	1.44	1.33
14	b	1229	CLA	C3D-C4D	-4.67	1.33	1.44
14	A	1118	CLA	C3D-C4D	-4.66	1.33	1.44
14	G	1106	CLA	O2D-CGD	4.66	1.44	1.33
14	B	1236	CLA	O2D-CGD	4.66	1.44	1.33
14	G	1134	CLA	C3C-C2C	4.66	1.46	1.36
14	a	1107	CLA	C3D-C4D	-4.66	1.33	1.44
14	G	1110	CLA	O2D-CGD	4.66	1.44	1.33
14	a	1111	CLA	C3D-C4D	-4.66	1.33	1.44
14	b	1226	CLA	C1D-ND	-4.66	1.32	1.37
14	a	1127	CLA	C3D-C4D	-4.66	1.33	1.44
14	H	1222	CLA	C3D-C4D	-4.66	1.33	1.44
14	a	1123	CLA	C3D-C4D	-4.66	1.33	1.44
14	a	1106	CLA	O2D-CGD	4.66	1.44	1.33
14	H	1215	CLA	C3D-C4D	-4.66	1.33	1.44
14	A	1104	CLA	CHC-C1C	4.66	1.46	1.35
14	a	1104	CLA	C3D-C4D	-4.66	1.33	1.44
14	B	1224	CLA	CHC-C1C	4.66	1.46	1.35
14	a	1013	CLA	O2D-CGD	4.66	1.44	1.33
14	b	1228	CLA	C3D-C4D	-4.66	1.33	1.44
14	a	1107	CLA	CHC-C1C	4.66	1.46	1.35
14	b	1213	CLA	O2D-CGD	4.65	1.44	1.33
14	b	1231	CLA	O2D-CGD	4.65	1.44	1.33
14	b	1224	CLA	CHC-C1C	4.65	1.46	1.35
14	B	1226	CLA	O2D-CGD	4.65	1.44	1.33
14	H	1224	CLA	CHC-C1C	4.65	1.46	1.35
14	G	1106	CLA	C3D-C4D	-4.65	1.33	1.44
14	a	1140	CLA	O2D-CGD	4.65	1.44	1.33
14	H	1023	CLA	C3D-C4D	-4.65	1.33	1.44
14	A	1137	CLA	C3B-C2B	4.65	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1218	CLA	C1D-ND	-4.65	1.32	1.37
14	b	1204	CLA	CHC-C1C	4.65	1.46	1.35
14	a	1134	CLA	CHD-C1D	4.65	1.47	1.38
14	B	1236	CLA	CHC-C1C	4.65	1.46	1.35
14	a	1109	CLA	C3D-C4D	-4.65	1.33	1.44
14	b	1223	CLA	C3B-C2B	4.65	1.46	1.40
14	G	1118	CLA	O2D-CGD	4.65	1.44	1.33
14	A	1123	CLA	C3D-C4D	-4.65	1.33	1.44
14	b	1218	CLA	C1D-ND	-4.65	1.32	1.37
14	H	1228	CLA	CHC-C1C	4.65	1.46	1.35
15	b	1207	F6C	CHC-C4B	4.65	1.46	1.35
14	A	1118	CLA	O2D-CGD	4.65	1.44	1.33
14	b	1216	CLA	C3D-C4D	-4.65	1.33	1.44
14	B	1205	CLA	CHC-C1C	4.64	1.46	1.35
14	B	1231	CLA	O2D-CGD	4.64	1.44	1.33
14	A	1113	CLA	C3D-C4D	-4.64	1.33	1.44
14	B	1204	CLA	CHC-C1C	4.64	1.46	1.35
14	a	1106	CLA	C3D-C4D	-4.64	1.33	1.44
14	b	1208	CLA	C3D-C4D	-4.64	1.33	1.44
14	H	1205	CLA	CHC-C1C	4.64	1.46	1.35
14	H	1229	CLA	C3D-C4D	-4.64	1.33	1.44
14	a	1105	CLA	C3D-C4D	-4.64	1.33	1.44
14	A	1107	CLA	C3D-C4D	-4.64	1.33	1.44
14	G	1122	CLA	C3D-C4D	-4.64	1.33	1.44
14	G	1134	CLA	CHD-C1D	4.64	1.47	1.38
14	b	1226	CLA	O2D-CGD	4.64	1.44	1.33
15	b	1230	F6C	CHC-C4B	4.64	1.46	1.35
14	a	1116	CLA	C3D-C4D	-4.64	1.33	1.44
14	a	1118	CLA	O2D-CGD	4.64	1.44	1.33
14	A	1128	CLA	C1D-ND	-4.64	1.32	1.37
14	a	1102	CLA	O2D-CGD	4.64	1.44	1.33
14	b	1228	CLA	CHC-C1C	4.64	1.46	1.35
14	G	1113	CLA	C3D-C4D	-4.64	1.33	1.44
14	a	1114	CLA	CHC-C1C	4.64	1.46	1.35
14	a	1102	CLA	C3B-C2B	4.64	1.46	1.40
14	l	1502	CLA	C3D-C4D	-4.64	1.33	1.44
14	B	1228	CLA	CHC-C1C	4.64	1.46	1.35
15	G	1121	F6C	CHD-C1D	4.64	1.46	1.35
14	a	1137	CLA	C3B-C2B	4.64	1.46	1.40
14	B	1229	CLA	C3D-C4D	-4.64	1.33	1.44
14	G	1117	CLA	C3D-C4D	-4.63	1.33	1.44
14	a	1122	CLA	C3D-C4D	-4.63	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1226	CLA	C1D-ND	-4.63	1.32	1.37
14	a	1128	CLA	C1D-ND	-4.63	1.32	1.37
14	B	1235	CLA	O2D-CGD	4.63	1.44	1.33
14	a	1118	CLA	CHC-C1C	4.63	1.46	1.35
14	A	1116	CLA	C3D-C4D	-4.63	1.33	1.44
14	H	1231	CLA	O2D-CGD	4.63	1.44	1.33
14	G	1123	CLA	C3D-C4D	-4.63	1.33	1.44
14	b	1205	CLA	CHC-C1C	4.63	1.46	1.35
14	a	1117	CLA	C3D-C4D	-4.63	1.33	1.44
14	B	1215	CLA	C3D-C4D	-4.63	1.33	1.44
14	H	1208	CLA	C3D-C4D	-4.63	1.33	1.44
14	A	1105	CLA	C3D-C4D	-4.63	1.33	1.44
14	G	1133	CLA	C3D-C4D	-4.63	1.33	1.44
14	A	1114	CLA	CHC-C1C	4.63	1.46	1.35
14	B	1229	CLA	C3B-C2B	4.63	1.46	1.40
14	A	1134	CLA	C3C-C2C	4.63	1.46	1.36
14	H	1223	CLA	C3B-C2B	4.63	1.46	1.40
14	H	1229	CLA	C3B-C2B	4.63	1.46	1.40
14	b	1235	CLA	O2D-CGD	4.63	1.44	1.33
13	A	1011	CL0	O2D-CGD	4.62	1.44	1.33
15	H	1230	F6C	CHC-C4B	4.62	1.46	1.35
14	G	1127	CLA	CHC-C1C	4.62	1.46	1.35
14	b	1215	CLA	C3D-C4D	-4.62	1.33	1.44
15	A	1121	F6C	CHD-C1D	4.62	1.46	1.35
13	a	1011	CL0	O2D-CGD	4.62	1.44	1.33
14	G	1127	CLA	C3D-C4D	-4.62	1.33	1.44
14	b	1212	CLA	O2D-CGD	4.62	1.44	1.33
14	B	1208	CLA	C3D-C4D	-4.62	1.33	1.44
14	G	1110	CLA	C3D-C4D	-4.62	1.33	1.44
14	A	1127	CLA	C3D-C4D	-4.62	1.33	1.44
14	A	1127	CLA	CHC-C1C	4.62	1.46	1.35
14	a	1127	CLA	CHC-C1C	4.62	1.46	1.35
14	b	1224	CLA	O2D-CGD	4.62	1.44	1.33
14	A	1118	CLA	CHC-C1C	4.62	1.46	1.35
14	B	1224	CLA	C1D-ND	-4.62	1.32	1.37
14	A	1102	CLA	C3B-C2B	4.62	1.46	1.40
14	G	1114	CLA	CHC-C1C	4.62	1.46	1.35
14	G	1114	CLA	C3D-C4D	-4.61	1.33	1.44
15	B	1230	F6C	CHC-C4B	4.61	1.46	1.35
14	a	1108	CLA	C3D-C4D	-4.61	1.33	1.44
14	B	1222	CLA	O2D-CGD	4.61	1.44	1.33
14	H	1224	CLA	O2D-CGD	4.61	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1122	CLA	C3D-C4D	-4.61	1.33	1.44
13	G	1011	CL0	O2D-CGD	4.61	1.44	1.33
14	G	1118	CLA	CHC-C1C	4.61	1.46	1.35
14	G	1109	CLA	C3D-C4D	-4.61	1.33	1.44
14	G	1112	CLA	C3D-C4D	-4.61	1.33	1.44
14	A	1108	CLA	C3D-C4D	-4.61	1.33	1.44
14	A	1110	CLA	C3D-C4D	-4.61	1.33	1.44
14	b	1229	CLA	C3B-C2B	4.61	1.46	1.40
15	B	1207	F6C	CHC-C4B	4.61	1.46	1.35
14	b	1201	CLA	O2D-CGD	4.61	1.44	1.33
14	H	1216	CLA	C3D-C4D	-4.61	1.33	1.44
15	H	1207	F6C	CHC-C4B	4.60	1.46	1.35
14	H	1235	CLA	O2D-CGD	4.60	1.44	1.33
14	G	1105	CLA	C3D-C4D	-4.60	1.33	1.44
14	A	1102	CLA	O2D-CGD	4.60	1.44	1.33
14	B	1231	CLA	C3D-C4D	-4.60	1.33	1.44
14	A	1105	CLA	C3B-C2B	4.60	1.46	1.40
14	b	1215	CLA	O2D-CGD	4.60	1.44	1.33
14	A	1133	CLA	C3D-C4D	-4.60	1.33	1.44
14	B	1023	CLA	C3D-C4D	-4.60	1.33	1.44
14	A	1117	CLA	C3D-C4D	-4.60	1.33	1.44
14	b	1215	CLA	CHC-C1C	4.60	1.46	1.35
14	B	1216	CLA	C3D-C4D	-4.60	1.33	1.44
14	G	1131	CLA	CHC-C1C	4.60	1.46	1.35
14	G	1102	CLA	C3B-C2B	4.60	1.46	1.40
14	H	1222	CLA	O2D-CGD	4.60	1.44	1.33
14	a	1110	CLA	C3D-C4D	-4.60	1.33	1.44
14	U	1502	CLA	C3D-C4D	-4.60	1.33	1.44
14	B	1229	CLA	O2D-CGD	4.60	1.44	1.33
14	A	1109	CLA	C3D-C4D	-4.60	1.33	1.44
14	b	1229	CLA	O2D-CGD	4.60	1.44	1.33
14	A	1103	CLA	CHC-C1C	4.60	1.46	1.35
14	G	1122	CLA	CHC-C1C	4.60	1.46	1.35
14	H	1215	CLA	CHC-C1C	4.60	1.46	1.35
15	H	1237	F6C	CHC-C4B	4.59	1.46	1.35
15	a	1121	F6C	CHD-C1D	4.59	1.46	1.35
14	b	1023	CLA	C3D-C4D	-4.59	1.33	1.44
14	B	1201	CLA	O2D-CGD	4.59	1.44	1.33
14	B	1224	CLA	O2D-CGD	4.59	1.44	1.33
14	H	1229	CLA	O2D-CGD	4.59	1.44	1.33
14	B	1215	CLA	O2D-CGD	4.59	1.44	1.33
14	H	1231	CLA	C3D-C4D	-4.59	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1137	CLA	CHC-C1C	4.59	1.46	1.35
14	b	1231	CLA	C3D-C4D	-4.59	1.33	1.44
14	b	1220	CLA	C3D-C4D	-4.59	1.33	1.44
14	G	1103	CLA	CHC-C1C	4.59	1.46	1.35
15	b	1237	F6C	CHC-C4B	4.59	1.46	1.35
14	a	1103	CLA	CHC-C1C	4.59	1.46	1.35
14	A	1114	CLA	C3D-C4D	-4.58	1.33	1.44
14	a	1131	CLA	CHC-C1C	4.58	1.46	1.35
14	L	1502	CLA	C3D-C4D	-4.58	1.33	1.44
14	A	1131	CLA	CHC-C1C	4.58	1.46	1.35
14	B	1217	CLA	C3D-C4D	-4.58	1.33	1.44
14	B	1212	CLA	O2D-CGD	4.58	1.44	1.33
14	H	1211	CLA	C3B-C2B	4.58	1.46	1.40
14	G	1137	CLA	CHC-C1C	4.58	1.46	1.35
14	B	1215	CLA	CHC-C1C	4.58	1.46	1.35
14	a	1114	CLA	C3D-C4D	-4.58	1.33	1.44
14	B	1206	CLA	O2D-CGD	4.58	1.44	1.33
14	b	1211	CLA	C3B-C2B	4.58	1.46	1.40
14	a	1133	CLA	CHC-C1C	4.58	1.46	1.35
14	b	1222	CLA	O2D-CGD	4.58	1.44	1.33
14	B	1220	CLA	C3D-C4D	-4.58	1.33	1.44
14	H	1215	CLA	O2D-CGD	4.58	1.44	1.33
14	A	1127	CLA	C1D-ND	-4.58	1.32	1.37
14	A	1112	CLA	C3D-C4D	-4.58	1.33	1.44
14	H	1212	CLA	O2D-CGD	4.58	1.44	1.33
14	B	1210	CLA	C3B-C2B	4.58	1.46	1.40
14	G	1108	CLA	C3D-C4D	-4.58	1.33	1.44
15	B	1237	F6C	CHC-C4B	4.57	1.46	1.35
14	a	1127	CLA	C1D-ND	-4.57	1.32	1.37
14	H	1224	CLA	C1D-ND	-4.57	1.32	1.37
14	B	1213	CLA	C3D-C4D	-4.57	1.33	1.44
14	a	1133	CLA	C3D-C4D	-4.57	1.33	1.44
14	G	1101	CLA	O2D-CGD	4.57	1.44	1.33
14	H	1220	CLA	C3D-C4D	-4.57	1.33	1.44
14	a	1115	CLA	C3D-C4D	-4.57	1.33	1.44
14	b	1224	CLA	C1D-ND	-4.57	1.32	1.37
14	b	1217	CLA	C3D-C4D	-4.57	1.33	1.44
14	A	1137	CLA	CHC-C1C	4.57	1.46	1.35
14	G	1114	CLA	C3C-C2C	4.57	1.46	1.36
14	H	1217	CLA	C3D-C4D	-4.57	1.33	1.44
14	A	1122	CLA	CHC-C1C	4.56	1.46	1.35
14	G	1115	CLA	C3D-C4D	-4.56	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1213	CLA	C3D-C4D	-4.56	1.33	1.44
14	B	1232	CLA	C3D-C4D	-4.56	1.33	1.44
14	b	1213	CLA	C3D-C4D	-4.56	1.33	1.44
14	A	1108	CLA	C3B-C2B	4.56	1.46	1.40
14	A	1115	CLA	C3D-C4D	-4.56	1.33	1.44
14	A	1101	CLA	O2D-CGD	4.56	1.44	1.33
14	B	1211	CLA	C3B-C2B	4.55	1.46	1.40
14	G	1105	CLA	C3B-C2B	4.55	1.46	1.40
14	a	1105	CLA	C3B-C2B	4.55	1.46	1.40
14	a	1122	CLA	CHC-C1C	4.55	1.46	1.35
14	l	1501	CLA	CHC-C1C	4.55	1.46	1.35
14	b	1232	CLA	C3D-C4D	-4.55	1.33	1.44
14	G	1127	CLA	C1D-ND	-4.55	1.32	1.37
14	a	1114	CLA	C3C-C2C	4.55	1.46	1.36
14	H	1206	CLA	O2D-CGD	4.55	1.44	1.33
14	a	1101	CLA	O2D-CGD	4.55	1.44	1.33
14	B	1209	CLA	C3D-C4D	-4.55	1.33	1.44
14	b	1206	CLA	O2D-CGD	4.55	1.44	1.33
14	H	1201	CLA	O2D-CGD	4.55	1.44	1.33
14	U	1501	CLA	C3B-C2B	4.55	1.46	1.40
14	U	1502	CLA	O2D-CGD	4.55	1.44	1.33
14	A	1114	CLA	C3C-C2C	4.55	1.46	1.36
14	H	1232	CLA	C3D-C4D	-4.54	1.33	1.44
14	l	1502	CLA	O2D-CGD	4.54	1.44	1.33
14	A	1133	CLA	CHC-C1C	4.54	1.46	1.35
14	a	1119	CLA	C3C-C2C	4.54	1.46	1.36
14	G	1135	CLA	CHC-C1C	4.54	1.46	1.35
14	G	1129	CLA	O2D-CGD	4.54	1.44	1.33
14	L	1501	CLA	CHC-C1C	4.54	1.46	1.35
14	b	1223	CLA	O2D-CGD	4.54	1.44	1.33
14	b	1220	CLA	CHC-C1C	4.54	1.46	1.35
14	G	1120	CLA	C3D-C4D	-4.54	1.33	1.44
14	H	1223	CLA	O2D-CGD	4.53	1.44	1.33
14	b	1209	CLA	C3D-C4D	-4.53	1.33	1.44
14	G	1133	CLA	CHC-C1C	4.53	1.46	1.35
14	H	1209	CLA	C3D-C4D	-4.53	1.33	1.44
14	B	1021	CLA	CHC-C1C	4.53	1.46	1.35
14	U	1501	CLA	CHC-C1C	4.53	1.46	1.35
14	G	1103	CLA	O2D-CGD	4.53	1.44	1.33
14	b	1021	CLA	CHC-C1C	4.53	1.46	1.35
14	l	1501	CLA	C3B-C2B	4.53	1.46	1.40
14	L	1501	CLA	C3B-C2B	4.53	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1205	CLA	O2D-CGD	4.53	1.44	1.33
14	b	1227	CLA	CHD-C1D	4.53	1.47	1.38
14	G	1108	CLA	C3B-C2B	4.53	1.46	1.40
14	A	1130	CLA	C3B-C2B	4.53	1.46	1.40
14	A	1103	CLA	O2D-CGD	4.53	1.44	1.33
14	B	1235	CLA	C3B-C2B	4.53	1.46	1.40
14	a	1112	CLA	C3D-C4D	-4.53	1.34	1.44
14	b	1205	CLA	O2D-CGD	4.52	1.44	1.33
14	B	1223	CLA	O2D-CGD	4.52	1.44	1.33
14	A	1101	CLA	C3D-C4D	-4.52	1.34	1.44
14	G	1123	CLA	C3B-C2B	4.52	1.46	1.40
14	H	1210	CLA	C3B-C2B	4.52	1.46	1.40
14	A	1129	CLA	O2D-CGD	4.52	1.44	1.33
14	H	1021	CLA	CHC-C1C	4.52	1.46	1.35
14	a	1101	CLA	C3D-C4D	-4.52	1.34	1.44
14	A	1123	CLA	C3B-C2B	4.52	1.46	1.40
14	a	1103	CLA	O2D-CGD	4.52	1.44	1.33
14	A	1135	CLA	CHC-C1C	4.52	1.46	1.35
14	A	1119	CLA	C3C-C2C	4.52	1.46	1.36
14	a	1135	CLA	CHC-C1C	4.52	1.46	1.35
14	B	1226	CLA	C1D-ND	-4.52	1.32	1.37
14	a	1104	CLA	C3B-C2B	4.52	1.46	1.40
14	L	1502	CLA	O2D-CGD	4.52	1.44	1.33
14	B	1225	CLA	C1D-ND	-4.51	1.32	1.37
14	G	1131	CLA	O2D-CGD	4.51	1.44	1.33
14	H	1220	CLA	CHC-C1C	4.51	1.46	1.35
14	b	1201	CLA	C3B-C2B	4.51	1.46	1.40
14	A	1131	CLA	O2D-CGD	4.51	1.44	1.33
14	a	1129	CLA	O2D-CGD	4.51	1.44	1.33
14	x	1701	CLA	C3D-C4D	-4.51	1.34	1.44
14	H	1233	CLA	CHD-C1D	4.51	1.47	1.38
14	b	1202	CLA	O2D-CGD	4.51	1.44	1.33
14	a	1108	CLA	C3B-C2B	4.50	1.46	1.40
14	a	1123	CLA	C3B-C2B	4.50	1.46	1.40
14	H	1225	CLA	C1D-ND	-4.50	1.32	1.37
14	B	1205	CLA	O2D-CGD	4.50	1.44	1.33
14	a	1120	CLA	C3D-C4D	-4.50	1.34	1.44
14	G	1119	CLA	C3C-C2C	4.50	1.46	1.36
14	A	1125	CLA	CHC-C1C	4.50	1.46	1.35
14	B	1202	CLA	O2D-CGD	4.50	1.44	1.33
14	a	1130	CLA	C3B-C2B	4.50	1.46	1.40
14	G	1012	CLA	CHC-C1C	4.50	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	5005	LMG	O8-C28	4.50	1.46	1.33
14	A	1120	CLA	C3D-C4D	-4.50	1.34	1.44
14	G	1101	CLA	C3D-C4D	-4.50	1.34	1.44
14	H	1202	CLA	O2D-CGD	4.50	1.44	1.33
14	a	1131	CLA	O2D-CGD	4.49	1.44	1.33
14	b	1233	CLA	CHD-C1D	4.49	1.47	1.38
14	B	1220	CLA	CHC-C1C	4.49	1.46	1.35
14	a	1012	CLA	CHC-C1C	4.49	1.46	1.35
14	A	1013	CLA	C3D-C4D	-4.49	1.34	1.44
14	b	1210	CLA	C3B-C2B	4.49	1.46	1.40
14	H	1227	CLA	CHD-C1D	4.49	1.47	1.38
14	B	1214	CLA	CHD-C1D	4.49	1.47	1.38
14	K	1401	CLA	CHD-C1D	4.49	1.47	1.38
14	b	1214	CLA	CHD-C1D	4.49	1.47	1.38
20	G	5005	LMG	O8-C28	4.49	1.46	1.33
14	a	1135	CLA	O2D-CGD	4.49	1.44	1.33
14	W	1701	CLA	C3D-C4D	-4.48	1.34	1.44
14	a	1125	CLA	CHC-C1C	4.48	1.46	1.35
14	a	1119	CLA	CHD-C1D	4.48	1.47	1.38
14	G	1127	CLA	C3B-C2B	4.48	1.46	1.40
14	A	1012	CLA	CHC-C1C	4.48	1.46	1.35
14	G	1135	CLA	O2D-CGD	4.48	1.44	1.33
14	B	1201	CLA	C3B-C2B	4.48	1.46	1.40
14	B	1225	CLA	C3B-C2B	4.48	1.46	1.40
14	b	1021	CLA	O2D-CGD	4.48	1.44	1.33
14	G	1125	CLA	CHC-C1C	4.48	1.46	1.35
14	A	1135	CLA	O2D-CGD	4.48	1.44	1.33
14	H	1208	CLA	C3B-C2B	4.48	1.46	1.40
14	b	1225	CLA	C3B-C2B	4.48	1.46	1.40
14	G	1119	CLA	CHD-C1D	4.48	1.47	1.38
14	b	1225	CLA	C1D-ND	-4.48	1.32	1.37
14	X	1701	CLA	C3D-C4D	-4.48	1.34	1.44
14	A	1119	CLA	CHD-C1D	4.47	1.47	1.38
20	A	5005	LMG	O8-C28	4.47	1.46	1.33
14	H	1201	CLA	C3B-C2B	4.47	1.46	1.40
14	B	1227	CLA	CHD-C1D	4.47	1.47	1.38
14	H	1021	CLA	O2D-CGD	4.47	1.44	1.33
15	H	1238	F6C	C3D-C4D	-4.47	1.32	1.43
14	B	1021	CLA	O2D-CGD	4.46	1.44	1.33
14	B	1233	CLA	CHD-C1D	4.46	1.47	1.38
14	G	1130	CLA	C3B-C2B	4.46	1.46	1.40
14	A	1127	CLA	C3B-C2B	4.46	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1013	CLA	C3D-C4D	-4.46	1.34	1.44
14	T	1401	CLA	CHD-C1D	4.46	1.47	1.38
15	H	1207	F6C	CHD-C1D	4.46	1.46	1.35
14	b	1235	CLA	C3B-C2B	4.46	1.46	1.40
14	b	1023	CLA	CHC-C1C	4.46	1.46	1.35
15	B	1238	F6C	C3D-C4D	-4.46	1.32	1.43
14	k	1401	CLA	C3B-C2B	4.46	1.46	1.40
14	B	1023	CLA	CHC-C1C	4.46	1.46	1.35
14	H	1214	CLA	CHD-C1D	4.45	1.47	1.38
14	a	1013	CLA	C3D-C4D	-4.45	1.34	1.44
14	H	1233	CLA	C3D-C4D	-4.45	1.34	1.44
14	b	1023	CLA	C1C-NC	-4.45	1.31	1.37
13	a	1011	CL0	CHC-C1C	4.45	1.46	1.35
15	b	1238	F6C	C3D-C4D	-4.44	1.32	1.43
14	b	1233	CLA	C3D-C4D	-4.44	1.34	1.44
14	b	1227	CLA	C3C-C2C	4.44	1.46	1.36
14	G	1104	CLA	C3B-C2B	4.44	1.46	1.40
14	H	1235	CLA	C3B-C2B	4.44	1.46	1.40
14	a	1112	CLA	C3B-C2B	4.44	1.46	1.40
14	T	1401	CLA	C3B-C2B	4.44	1.46	1.40
14	H	1227	CLA	C3C-C2C	4.44	1.46	1.36
14	A	1132	CLA	C3C-C2C	4.44	1.46	1.36
14	B	1223	CLA	C3C-C2C	4.44	1.46	1.36
14	a	1127	CLA	C3B-C2B	4.44	1.46	1.40
14	B	1233	CLA	C3C-C2C	4.44	1.46	1.36
14	B	1219	CLA	C3D-C4D	-4.44	1.34	1.44
14	H	1226	CLA	CHC-C1C	4.43	1.46	1.35
14	H	1225	CLA	C3B-C2B	4.43	1.46	1.40
14	B	1216	CLA	CHD-C1D	4.43	1.47	1.38
14	b	1216	CLA	CHD-C1D	4.43	1.47	1.38
14	H	1216	CLA	CHD-C1D	4.43	1.47	1.38
14	H	1023	CLA	CHC-C1C	4.43	1.46	1.35
14	H	1219	CLA	C3D-C4D	-4.43	1.34	1.44
14	A	1117	CLA	CHC-C1C	4.43	1.46	1.35
14	b	1226	CLA	CHC-C1C	4.43	1.46	1.35
14	A	1128	CLA	O2D-CGD	4.43	1.44	1.33
13	A	1011	CL0	CHC-C1C	4.43	1.46	1.35
14	A	1111	CLA	C3B-C2B	4.43	1.46	1.40
14	a	1122	CLA	CHD-C1D	4.43	1.47	1.38
14	H	1233	CLA	C3C-C2C	4.43	1.46	1.36
14	B	1226	CLA	CHC-C1C	4.43	1.46	1.35
14	a	1132	CLA	C3C-C2C	4.43	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1117	CLA	CHD-C1D	4.42	1.47	1.38
14	H	1221	CLA	C3B-C2B	4.42	1.46	1.40
14	K	1401	CLA	C3B-C2B	4.42	1.46	1.40
14	B	1233	CLA	C3D-C4D	-4.42	1.34	1.44
14	a	1128	CLA	O2D-CGD	4.42	1.44	1.33
14	A	1104	CLA	C3B-C2B	4.42	1.46	1.40
14	k	1401	CLA	CHD-C1D	4.42	1.47	1.38
14	A	1126	CLA	C1D-ND	-4.42	1.32	1.37
14	G	1132	CLA	C3C-C2C	4.42	1.46	1.36
14	G	1126	CLA	C1D-ND	-4.42	1.32	1.37
14	T	1401	CLA	C3C-C2C	4.42	1.46	1.36
14	G	1111	CLA	C3B-C2B	4.42	1.46	1.40
14	b	1221	CLA	C3B-C2B	4.42	1.46	1.40
14	b	1228	CLA	C3B-C2B	4.42	1.46	1.40
14	B	1208	CLA	C3B-C2B	4.42	1.46	1.40
14	G	1112	CLA	CHD-C1D	4.42	1.47	1.38
14	A	1122	CLA	CHD-C1D	4.42	1.47	1.38
14	H	1209	CLA	CHD-C1D	4.42	1.47	1.38
15	b	1207	F6C	CHD-C1D	4.42	1.46	1.35
14	H	1212	CLA	C3B-C2B	4.42	1.46	1.40
14	H	1229	CLA	C3C-C2C	4.41	1.46	1.36
14	b	1210	CLA	CHD-C1D	4.41	1.47	1.38
14	b	1219	CLA	C3D-C4D	-4.41	1.34	1.44
14	H	1223	CLA	C3C-C2C	4.41	1.46	1.36
14	B	1216	CLA	C3C-C2C	4.41	1.46	1.36
13	G	1011	CL0	CHC-C1C	4.41	1.46	1.35
14	b	1223	CLA	C3C-C2C	4.40	1.46	1.36
14	G	1117	CLA	CHC-C1C	4.40	1.46	1.35
14	U	1503	CLA	C3C-C2C	4.40	1.46	1.36
14	a	1112	CLA	CHD-C1D	4.40	1.46	1.38
15	B	1207	F6C	CHD-C1D	4.40	1.46	1.35
14	B	1221	CLA	C3B-C2B	4.40	1.46	1.40
14	b	1233	CLA	C3C-C2C	4.40	1.46	1.36
14	B	1227	CLA	C3C-C2C	4.40	1.46	1.36
14	a	1117	CLA	CHC-C1C	4.40	1.46	1.35
14	l	1503	CLA	C3C-C2C	4.40	1.46	1.36
14	G	1122	CLA	CHD-C1D	4.40	1.46	1.38
14	a	1138	CLA	C3B-C2B	4.40	1.46	1.40
14	A	1112	CLA	C3B-C2B	4.40	1.46	1.40
14	B	1212	CLA	C3B-C2B	4.40	1.46	1.40
14	B	1222	CLA	C3C-C2C	4.40	1.46	1.36
14	H	1210	CLA	CHD-C1D	4.39	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1234	CLA	O2D-CGD	4.39	1.43	1.33
14	H	1222	CLA	C3C-C2C	4.39	1.46	1.36
14	a	1117	CLA	CHD-C1D	4.39	1.46	1.38
14	b	1212	CLA	C3B-C2B	4.39	1.46	1.40
14	A	1131	CLA	CHD-C1D	4.39	1.46	1.38
14	B	1210	CLA	CHD-C1D	4.39	1.46	1.38
14	G	1124	CLA	C3C-C2C	4.39	1.46	1.36
14	b	1216	CLA	C3C-C2C	4.39	1.46	1.36
14	B	1218	CLA	C3D-C4D	-4.39	1.34	1.44
14	H	1023	CLA	C1C-NC	-4.38	1.31	1.37
14	G	1131	CLA	CHD-C1D	4.38	1.46	1.38
14	a	1131	CLA	CHD-C1D	4.38	1.46	1.38
14	b	1226	CLA	C3C-C2C	4.38	1.46	1.36
14	G	1137	CLA	O2D-CGD	4.38	1.43	1.33
14	a	1135	CLA	C3B-C2B	4.38	1.46	1.40
14	B	1209	CLA	C3C-C2C	4.38	1.46	1.36
14	G	1135	CLA	C3B-C2B	4.38	1.46	1.40
14	b	1208	CLA	C3B-C2B	4.38	1.46	1.40
14	a	1126	CLA	C1D-ND	-4.38	1.32	1.37
14	A	1112	CLA	CHD-C1D	4.38	1.46	1.38
14	B	1228	CLA	C3B-C2B	4.38	1.46	1.40
14	a	1116	CLA	C3C-C2C	4.38	1.46	1.36
14	G	1128	CLA	O2D-CGD	4.38	1.43	1.33
14	B	1023	CLA	C1C-NC	-4.38	1.31	1.37
14	H	1226	CLA	C3C-C2C	4.38	1.46	1.36
14	b	1229	CLA	C3C-C2C	4.38	1.46	1.36
14	G	1124	CLA	O2D-CGD	4.38	1.43	1.33
14	a	1128	CLA	CHC-C1C	4.37	1.46	1.35
14	A	1128	CLA	CHC-C1C	4.37	1.46	1.35
14	a	1137	CLA	O2D-CGD	4.37	1.43	1.33
14	K	1401	CLA	C3C-C2C	4.37	1.46	1.36
14	B	1229	CLA	C3C-C2C	4.37	1.46	1.36
14	B	1209	CLA	CHD-C1D	4.37	1.46	1.38
14	k	1401	CLA	C3C-C2C	4.37	1.46	1.36
14	l	1502	CLA	C1D-ND	-4.37	1.32	1.37
14	b	1222	CLA	C3C-C2C	4.37	1.46	1.36
14	G	1112	CLA	C3C-C2C	4.37	1.46	1.36
14	G	1128	CLA	CHC-C1C	4.37	1.46	1.35
14	b	1234	CLA	O2D-CGD	4.37	1.43	1.33
14	H	1239	CLA	CHC-C1C	4.37	1.46	1.35
14	b	1239	CLA	CHC-C1C	4.37	1.46	1.35
14	b	1209	CLA	C3C-C2C	4.37	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1235	CLA	CHD-C1D	4.36	1.46	1.38
14	a	1124	CLA	O2D-CGD	4.36	1.43	1.33
14	A	1128	CLA	C3C-C2C	4.36	1.46	1.36
14	H	1216	CLA	C3C-C2C	4.36	1.46	1.36
14	a	1111	CLA	C3B-C2B	4.36	1.46	1.40
14	G	1105	CLA	CHD-C1D	4.36	1.46	1.38
14	A	1117	CLA	CHD-C1D	4.36	1.46	1.38
14	a	1119	CLA	CHC-C1C	4.36	1.46	1.35
14	H	1234	CLA	O2D-CGD	4.36	1.43	1.33
14	G	1132	CLA	O2D-CGD	4.36	1.43	1.33
14	H	1218	CLA	C3D-C4D	-4.36	1.34	1.44
14	G	1112	CLA	C3B-C2B	4.36	1.46	1.40
14	A	1138	CLA	C3B-C2B	4.36	1.46	1.40
14	A	1119	CLA	CHC-C1C	4.36	1.46	1.35
20	L	5007	LMG	O8-C28	4.36	1.46	1.33
14	B	1239	CLA	CHC-C1C	4.35	1.46	1.35
14	B	1235	CLA	CHD-C1D	4.35	1.46	1.38
14	A	1137	CLA	O2D-CGD	4.35	1.43	1.33
14	B	1232	CLA	C3B-C2B	4.35	1.46	1.40
14	A	1105	CLA	CHD-C1D	4.35	1.46	1.38
14	A	1124	CLA	C3C-C2C	4.35	1.46	1.36
14	L	1503	CLA	C3C-C2C	4.35	1.46	1.36
20	U	5007	LMG	O8-C28	4.35	1.46	1.33
14	a	1124	CLA	C3C-C2C	4.35	1.46	1.36
14	H	1219	CLA	CHD-C1D	4.35	1.46	1.38
14	b	1209	CLA	CHD-C1D	4.35	1.46	1.38
14	H	1206	CLA	CHC-C1C	4.35	1.46	1.35
14	a	1112	CLA	C3C-C2C	4.35	1.46	1.36
14	B	1219	CLA	CHD-C1D	4.35	1.46	1.38
14	U	1502	CLA	C1D-ND	-4.35	1.32	1.37
14	H	1235	CLA	CHD-C1D	4.35	1.46	1.38
14	B	1213	CLA	C3B-C2B	4.35	1.46	1.40
14	B	1220	CLA	C3B-C2B	4.35	1.46	1.40
20	l	5007	LMG	O8-C28	4.35	1.46	1.33
14	H	1209	CLA	C3C-C2C	4.35	1.46	1.36
14	L	1502	CLA	C1D-ND	-4.35	1.32	1.37
14	A	1112	CLA	C3C-C2C	4.34	1.46	1.36
14	A	1116	CLA	C3C-C2C	4.34	1.46	1.36
14	A	1132	CLA	O2D-CGD	4.34	1.43	1.33
14	A	1135	CLA	C3B-C2B	4.34	1.46	1.40
14	a	1132	CLA	O2D-CGD	4.34	1.43	1.33
14	B	1228	CLA	C3C-C2C	4.34	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1124	CLA	O2D-CGD	4.34	1.43	1.33
14	a	1125	CLA	C1C-NC	-4.34	1.31	1.37
14	b	1218	CLA	C3D-C4D	-4.34	1.34	1.44
14	a	1128	CLA	C3C-C2C	4.34	1.45	1.36
14	b	1219	CLA	CHD-C1D	4.33	1.46	1.38
14	B	1206	CLA	CHC-C1C	4.33	1.46	1.35
14	G	1116	CLA	C3C-C2C	4.33	1.45	1.36
14	H	1021	CLA	C3B-C2B	4.33	1.46	1.40
14	A	1134	CLA	C3D-C4D	-4.33	1.34	1.44
14	b	1213	CLA	C3B-C2B	4.33	1.46	1.40
19	G	5001	LHG	O8-C23	4.33	1.46	1.33
14	b	1228	CLA	C3C-C2C	4.33	1.45	1.36
14	H	1228	CLA	C3B-C2B	4.33	1.46	1.40
14	H	1220	CLA	C3B-C2B	4.33	1.46	1.40
14	a	1105	CLA	CHD-C1D	4.32	1.46	1.38
14	H	1213	CLA	C3B-C2B	4.32	1.46	1.40
14	a	1125	CLA	C3B-C2B	4.32	1.46	1.40
14	G	1128	CLA	C3C-C2C	4.32	1.45	1.36
14	B	1021	CLA	C3B-C2B	4.32	1.46	1.40
14	B	1232	CLA	CHD-C1D	4.32	1.46	1.38
14	b	1206	CLA	CHC-C1C	4.32	1.46	1.35
14	B	1226	CLA	C3C-C2C	4.32	1.45	1.36
14	G	1110	CLA	C3C-C2C	4.32	1.45	1.36
14	a	1138	CLA	CHD-C1D	4.32	1.46	1.38
14	B	1206	CLA	C1D-ND	-4.32	1.32	1.37
14	b	1206	CLA	C1D-ND	-4.32	1.32	1.37
14	H	1232	CLA	CHD-C1D	4.32	1.46	1.38
14	H	1228	CLA	C3C-C2C	4.32	1.45	1.36
14	G	1138	CLA	C3B-C2B	4.32	1.46	1.40
14	H	1212	CLA	C3D-C4D	-4.32	1.34	1.44
14	b	1232	CLA	CHD-C1D	4.32	1.46	1.38
14	G	1125	CLA	C1C-NC	-4.32	1.31	1.37
14	A	1125	CLA	C1C-NC	-4.31	1.31	1.37
15	b	1230	F6C	CHD-C1D	4.31	1.46	1.35
14	H	1206	CLA	C1D-ND	-4.31	1.32	1.37
14	G	1119	CLA	CHC-C1C	4.31	1.46	1.35
14	B	1212	CLA	C3D-C4D	-4.31	1.34	1.44
15	H	1230	F6C	CHD-C1D	4.31	1.46	1.35
14	b	1201	CLA	CHD-C1D	4.31	1.46	1.38
14	a	1102	CLA	C3C-C2C	4.31	1.45	1.36
14	b	1219	CLA	C3C-C2C	4.31	1.45	1.36
14	G	1138	CLA	CHD-C1D	4.31	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1212	CLA	C3D-C4D	-4.31	1.34	1.44
14	H	1232	CLA	C3C-C2C	4.31	1.45	1.36
14	H	1210	CLA	O2D-CGD	4.31	1.43	1.33
14	b	1210	CLA	O2D-CGD	4.31	1.43	1.33
14	B	1219	CLA	C3C-C2C	4.30	1.45	1.36
19	A	5001	LHG	O8-C23	4.30	1.45	1.33
14	a	1109	CLA	C3B-C2B	4.30	1.46	1.40
14	A	1102	CLA	C3C-C2C	4.30	1.45	1.36
15	B	1230	F6C	CHD-C1D	4.30	1.46	1.35
14	G	1134	CLA	C3D-C4D	-4.30	1.34	1.44
14	B	1222	CLA	C1D-ND	-4.30	1.32	1.37
14	a	1110	CLA	C3C-C2C	4.30	1.45	1.36
14	A	1138	CLA	CHD-C1D	4.29	1.46	1.38
14	B	1235	CLA	C3C-C2C	4.29	1.45	1.36
14	b	1212	CLA	C3C-C2C	4.29	1.45	1.36
14	H	1219	CLA	C3C-C2C	4.29	1.45	1.36
14	b	1232	CLA	C3B-C2B	4.29	1.46	1.40
14	b	1217	CLA	C3C-C2C	4.29	1.45	1.36
14	H	1201	CLA	CHD-C1D	4.29	1.46	1.38
14	b	1220	CLA	C3B-C2B	4.29	1.46	1.40
14	a	1134	CLA	C3D-C4D	-4.29	1.34	1.44
14	a	1133	CLA	CHD-C1D	4.29	1.46	1.38
14	a	1108	CLA	CHD-C1D	4.29	1.46	1.38
14	A	1108	CLA	CHD-C1D	4.28	1.46	1.38
14	A	1125	CLA	C3B-C2B	4.28	1.46	1.40
14	b	1235	CLA	C3C-C2C	4.28	1.45	1.36
14	A	1110	CLA	C3C-C2C	4.28	1.45	1.36
19	a	5001	LHG	O8-C23	4.28	1.45	1.33
14	G	1108	CLA	CHD-C1D	4.28	1.46	1.38
14	H	1232	CLA	C3B-C2B	4.28	1.46	1.40
14	H	1215	CLA	CHD-C1D	4.28	1.46	1.38
14	B	1232	CLA	C3C-C2C	4.28	1.45	1.36
14	G	1129	CLA	C3C-C2C	4.28	1.45	1.36
14	A	1133	CLA	CHD-C1D	4.28	1.46	1.38
14	B	1201	CLA	CHD-C1D	4.27	1.46	1.38
15	H	1237	F6C	CHD-C1D	4.27	1.45	1.35
14	G	1125	CLA	C3B-C2B	4.27	1.46	1.40
14	A	1136	CLA	CHD-C1D	4.27	1.46	1.38
15	H	1207	F6C	O2D-CGD	4.27	1.43	1.33
14	G	1102	CLA	C3C-C2C	4.27	1.45	1.36
14	A	1133	CLA	C3C-C2C	4.27	1.45	1.36
14	B	1210	CLA	O2D-CGD	4.27	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1108	CLA	C3C-C2C	4.27	1.45	1.36
15	b	1207	F6C	O2D-CGD	4.27	1.43	1.33
14	A	1111	CLA	O2D-CGD	4.27	1.43	1.33
14	H	1212	CLA	C3C-C2C	4.27	1.45	1.36
14	G	1109	CLA	C3B-C2B	4.27	1.46	1.40
14	b	1021	CLA	C3B-C2B	4.27	1.46	1.40
14	H	1022	CLA	C1D-ND	-4.27	1.32	1.37
15	b	1237	F6C	CHD-C1D	4.27	1.45	1.35
14	G	1133	CLA	C3B-C2B	4.26	1.46	1.40
14	G	1133	CLA	C3C-C2C	4.26	1.45	1.36
14	a	1133	CLA	C3C-C2C	4.26	1.45	1.36
14	B	1236	CLA	C3C-C2C	4.26	1.45	1.36
14	H	1235	CLA	C3C-C2C	4.26	1.45	1.36
14	A	1136	CLA	C3C-C2C	4.26	1.45	1.36
14	G	1133	CLA	CHD-C1D	4.26	1.46	1.38
14	A	1102	CLA	CHD-C1D	4.26	1.46	1.38
14	a	1108	CLA	C3C-C2C	4.26	1.45	1.36
14	H	1226	CLA	CHD-C1D	4.26	1.46	1.38
14	G	1136	CLA	CHD-C1D	4.26	1.46	1.38
14	B	1217	CLA	C3C-C2C	4.26	1.45	1.36
15	B	1237	F6C	CHD-C1D	4.26	1.45	1.35
14	b	1236	CLA	C3C-C2C	4.26	1.45	1.36
14	A	1118	CLA	C3C-C2C	4.26	1.45	1.36
14	G	1132	CLA	CHD-C1D	4.25	1.46	1.38
14	G	1111	CLA	O2D-CGD	4.25	1.43	1.33
14	b	1214	CLA	C3C-C2C	4.25	1.45	1.36
14	b	1232	CLA	C3C-C2C	4.25	1.45	1.36
14	A	1130	CLA	C3C-C2C	4.25	1.45	1.36
14	A	1129	CLA	C1D-ND	-4.25	1.32	1.37
14	a	1133	CLA	C3B-C2B	4.25	1.46	1.40
14	a	1136	CLA	CHD-C1D	4.25	1.46	1.38
14	B	1226	CLA	CHD-C1D	4.25	1.46	1.38
14	H	1211	CLA	CHD-C1D	4.25	1.46	1.38
14	A	1129	CLA	C3C-C2C	4.24	1.45	1.36
14	A	1133	CLA	C3B-C2B	4.24	1.46	1.40
14	a	1111	CLA	O2D-CGD	4.24	1.43	1.33
14	b	1222	CLA	C1D-ND	-4.24	1.32	1.37
14	H	1214	CLA	C3C-C2C	4.24	1.45	1.36
14	b	1215	CLA	CHD-C1D	4.24	1.46	1.38
14	H	1217	CLA	C3C-C2C	4.24	1.45	1.36
14	H	1229	CLA	CHD-C1D	4.24	1.46	1.38
14	G	1102	CLA	CHD-C1D	4.24	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1207	F6C	O2D-CGD	4.24	1.43	1.33
15	H	1207	F6C	C3D-C4D	-4.24	1.33	1.43
14	G	1118	CLA	C3C-C2C	4.24	1.45	1.36
14	a	1130	CLA	C3C-C2C	4.24	1.45	1.36
14	A	1108	CLA	C3C-C2C	4.24	1.45	1.36
14	B	1218	CLA	C3C-C2C	4.24	1.45	1.36
14	b	1211	CLA	CHD-C1D	4.24	1.46	1.38
14	a	1129	CLA	C1D-ND	-4.24	1.32	1.37
14	a	1132	CLA	CHD-C1D	4.24	1.46	1.38
14	B	1208	CLA	C3C-C2C	4.24	1.45	1.36
14	B	1212	CLA	C3C-C2C	4.23	1.45	1.36
14	a	1118	CLA	CHD-C1D	4.23	1.46	1.38
14	G	1136	CLA	C3C-C2C	4.23	1.45	1.36
14	H	1236	CLA	C3C-C2C	4.23	1.45	1.36
14	a	1129	CLA	C3C-C2C	4.23	1.45	1.36
14	G	1138	CLA	C3C-C2C	4.23	1.45	1.36
14	A	1118	CLA	CHD-C1D	4.23	1.46	1.38
20	H	5002	LMG	O8-C28	4.23	1.45	1.33
14	A	1012	CLA	C1D-ND	-4.23	1.32	1.37
14	K	1401	CLA	C3D-C4D	-4.23	1.34	1.44
14	B	1229	CLA	CHD-C1D	4.23	1.46	1.38
14	G	1109	CLA	C3C-C2C	4.23	1.45	1.36
14	G	1103	CLA	C3B-C2B	4.22	1.46	1.40
14	T	1401	CLA	C3D-C4D	-4.22	1.34	1.44
14	B	1214	CLA	C3C-C2C	4.22	1.45	1.36
14	A	1109	CLA	C3B-C2B	4.22	1.46	1.40
14	a	1102	CLA	CHD-C1D	4.22	1.46	1.38
14	A	1105	CLA	C3C-C2C	4.22	1.45	1.36
14	l	1501	CLA	C3C-C2C	4.22	1.45	1.36
14	U	1501	CLA	C3C-C2C	4.22	1.45	1.36
14	H	1211	CLA	C3C-C2C	4.22	1.45	1.36
14	a	1109	CLA	CHD-C1D	4.22	1.46	1.38
15	b	1207	F6C	C3D-C4D	-4.22	1.33	1.43
14	G	1130	CLA	C3C-C2C	4.22	1.45	1.36
13	A	1011	CL0	C3C-C2C	4.22	1.45	1.36
14	A	1109	CLA	C3C-C2C	4.22	1.45	1.36
14	b	1229	CLA	CHD-C1D	4.22	1.46	1.38
14	a	1136	CLA	C3C-C2C	4.22	1.45	1.36
14	b	1208	CLA	C3C-C2C	4.22	1.45	1.36
14	b	1202	CLA	C1D-ND	-4.21	1.32	1.37
14	G	1106	CLA	C3C-C2C	4.21	1.45	1.36
14	k	1401	CLA	C3D-C4D	-4.21	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1109	CLA	C3C-C2C	4.21	1.45	1.36
14	a	1107	CLA	C3C-C2C	4.21	1.45	1.36
14	G	1105	CLA	C3C-C2C	4.21	1.45	1.36
14	L	1501	CLA	C3C-C2C	4.21	1.45	1.36
14	b	1218	CLA	C3C-C2C	4.21	1.45	1.36
14	A	1109	CLA	CHD-C1D	4.21	1.46	1.38
14	b	1208	CLA	CHD-C1D	4.21	1.46	1.38
14	H	1208	CLA	C3C-C2C	4.21	1.45	1.36
14	B	1202	CLA	C1D-ND	-4.21	1.32	1.37
14	H	1201	CLA	C3C-C2C	4.21	1.45	1.36
14	A	1132	CLA	CHD-C1D	4.21	1.46	1.38
14	H	1208	CLA	CHD-C1D	4.21	1.46	1.38
13	G	1011	CL0	C3C-C2C	4.21	1.45	1.36
14	a	1137	CLA	C1D-ND	-4.20	1.32	1.37
14	b	1239	CLA	C1D-ND	-4.20	1.32	1.37
14	G	1118	CLA	CHD-C1D	4.20	1.46	1.38
14	B	1211	CLA	CHD-C1D	4.20	1.46	1.38
14	G	1129	CLA	C1D-ND	-4.20	1.32	1.37
14	a	1118	CLA	C3C-C2C	4.20	1.45	1.36
14	B	1217	CLA	C3B-C2B	4.20	1.46	1.40
14	B	1022	CLA	C1D-ND	-4.20	1.32	1.37
14	H	1218	CLA	C3C-C2C	4.20	1.45	1.36
20	i	5006	LMG	O8-C28	4.20	1.45	1.33
15	B	1207	F6C	C3D-C4D	-4.20	1.33	1.43
20	R	5006	LMG	O8-C28	4.20	1.45	1.33
14	b	1022	CLA	C1D-ND	-4.20	1.32	1.37
14	B	1215	CLA	CHD-C1D	4.20	1.46	1.38
14	G	1126	CLA	C3C-C2C	4.20	1.45	1.36
14	a	1105	CLA	C3C-C2C	4.20	1.45	1.36
14	A	1107	CLA	C3C-C2C	4.20	1.45	1.36
14	b	1211	CLA	C3C-C2C	4.20	1.45	1.36
14	G	1117	CLA	C3B-C2B	4.20	1.46	1.40
14	G	1107	CLA	C3C-C2C	4.20	1.45	1.36
14	b	1236	CLA	C1D-ND	-4.19	1.32	1.37
14	H	1217	CLA	C3B-C2B	4.19	1.46	1.40
13	a	1011	CL0	C3C-C2C	4.19	1.45	1.36
14	a	1138	CLA	C3C-C2C	4.19	1.45	1.36
14	A	1138	CLA	C3C-C2C	4.19	1.45	1.36
19	b	5004	LHG	O8-C23	4.19	1.45	1.33
14	B	1208	CLA	CHD-C1D	4.19	1.46	1.38
15	H	1237	F6C	C3D-C4D	-4.19	1.33	1.43
14	B	1201	CLA	C3C-C2C	4.19	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1226	CLA	CHD-C1D	4.19	1.46	1.38
14	A	1115	CLA	C3C-C2C	4.19	1.45	1.36
20	B	5002	LMG	O8-C28	4.19	1.45	1.33
14	b	1217	CLA	C3B-C2B	4.19	1.46	1.40
14	A	1124	CLA	C1D-ND	-4.19	1.32	1.37
14	G	1113	CLA	C3B-C2B	4.19	1.46	1.40
14	a	1103	CLA	CHD-C1D	4.19	1.46	1.38
14	G	1109	CLA	CHD-C1D	4.18	1.46	1.38
14	A	1127	CLA	C3C-C2C	4.18	1.45	1.36
14	b	1231	CLA	C3B-C2B	4.18	1.46	1.40
20	b	5002	LMG	O8-C28	4.18	1.45	1.33
14	A	1126	CLA	C3C-C2C	4.18	1.45	1.36
20	U	5007	LMG	O7-C10	4.18	1.46	1.34
14	G	1115	CLA	C3C-C2C	4.18	1.45	1.36
14	a	1115	CLA	C3C-C2C	4.18	1.45	1.36
14	H	1231	CLA	C3B-C2B	4.17	1.46	1.40
19	B	5004	LHG	O8-C23	4.17	1.45	1.33
14	a	1135	CLA	C3C-C2C	4.17	1.45	1.36
14	a	1126	CLA	C3C-C2C	4.17	1.45	1.36
14	G	1135	CLA	C3C-C2C	4.17	1.45	1.36
14	A	1113	CLA	C3C-C2C	4.17	1.45	1.36
14	A	1130	CLA	C1D-ND	-4.17	1.32	1.37
15	b	1237	F6C	C3D-C4D	-4.17	1.33	1.43
14	H	1213	CLA	C3C-C2C	4.17	1.45	1.36
20	I	5006	LMG	O8-C28	4.17	1.45	1.33
14	a	1106	CLA	C3C-C2C	4.17	1.45	1.36
14	H	1222	CLA	C1D-ND	-4.17	1.32	1.37
14	A	1103	CLA	C3B-C2B	4.17	1.46	1.40
14	U	1502	CLA	C3C-C2C	4.17	1.45	1.36
14	B	1234	CLA	C3C-C2C	4.17	1.45	1.36
14	b	1201	CLA	C3C-C2C	4.17	1.45	1.36
14	A	1106	CLA	C3C-C2C	4.17	1.45	1.36
14	G	1103	CLA	CHD-C1D	4.17	1.46	1.38
14	H	1213	CLA	CHD-C1D	4.17	1.46	1.38
14	G	1127	CLA	C3C-C2C	4.17	1.45	1.36
14	G	1117	CLA	C3C-C2C	4.17	1.45	1.36
14	G	1113	CLA	CHD-C1D	4.16	1.46	1.38
14	A	1104	CLA	C3C-C2C	4.16	1.45	1.36
14	a	1131	CLA	C1D-ND	-4.16	1.32	1.37
14	A	1103	CLA	CHD-C1D	4.16	1.46	1.38
14	L	1502	CLA	C3C-C2C	4.16	1.45	1.36
14	a	1103	CLA	C3B-C2B	4.16	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	l	5007	LMG	O7-C10	4.16	1.46	1.34
14	b	1022	CLA	O2D-CGD	4.16	1.43	1.33
14	G	1124	CLA	C1D-ND	-4.16	1.32	1.37
14	b	1234	CLA	C1D-ND	-4.16	1.32	1.37
14	H	1228	CLA	CHD-C1D	4.16	1.46	1.38
14	A	1131	CLA	C1D-ND	-4.16	1.32	1.37
14	L	1501	CLA	C1D-ND	-4.16	1.32	1.37
14	U	1501	CLA	C1D-ND	-4.16	1.32	1.37
14	B	1236	CLA	C1D-ND	-4.16	1.32	1.37
14	l	1502	CLA	C3C-C2C	4.16	1.45	1.36
14	a	1101	CLA	C3C-C2C	4.16	1.45	1.36
14	H	1022	CLA	O2D-CGD	4.16	1.43	1.33
20	a	5005	LMG	O7-C10	4.16	1.46	1.34
14	A	1117	CLA	C3C-C2C	4.16	1.45	1.36
14	B	1211	CLA	C3C-C2C	4.16	1.45	1.36
15	B	1238	F6C	CHD-C1D	4.16	1.45	1.35
20	A	5005	LMG	O7-C10	4.15	1.46	1.34
19	H	5004	LHG	O8-C23	4.15	1.45	1.33
20	L	5007	LMG	O7-C10	4.15	1.46	1.34
14	G	1113	CLA	C3C-C2C	4.15	1.45	1.36
14	a	1117	CLA	C3C-C2C	4.15	1.45	1.36
15	H	1238	F6C	CHD-C1D	4.15	1.45	1.35
14	B	1213	CLA	CHD-C1D	4.15	1.46	1.38
20	G	5005	LMG	O7-C10	4.15	1.46	1.34
14	a	1120	CLA	C3C-C2C	4.15	1.45	1.36
14	b	1213	CLA	CHD-C1D	4.15	1.46	1.38
14	b	1204	CLA	C3C-C2C	4.15	1.45	1.36
14	A	1135	CLA	C3C-C2C	4.15	1.45	1.36
14	G	1102	CLA	C1D-ND	-4.15	1.32	1.37
14	B	1220	CLA	C3C-C2C	4.15	1.45	1.36
14	G	1131	CLA	C1D-ND	-4.15	1.32	1.37
14	B	1022	CLA	O2D-CGD	4.15	1.43	1.33
14	b	1203	CLA	C3B-C2B	4.15	1.46	1.40
15	B	1237	F6C	C3D-C4D	-4.15	1.33	1.43
14	b	1234	CLA	C3C-C2C	4.15	1.45	1.36
14	B	1228	CLA	CHD-C1D	4.14	1.46	1.38
15	b	1238	F6C	CHD-C1D	4.14	1.45	1.35
14	a	1104	CLA	C3C-C2C	4.14	1.45	1.36
14	G	1137	CLA	C1D-ND	-4.14	1.32	1.37
14	H	1203	CLA	C3B-C2B	4.14	1.46	1.40
14	A	1117	CLA	C3B-C2B	4.14	1.46	1.40
14	a	1113	CLA	C3C-C2C	4.14	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1127	CLA	C3C-C2C	4.14	1.45	1.36
14	a	1113	CLA	CHD-C1D	4.14	1.46	1.38
14	G	1130	CLA	C1D-ND	-4.14	1.32	1.37
14	H	1202	CLA	C1D-ND	-4.14	1.32	1.37
14	B	1239	CLA	C1D-ND	-4.14	1.32	1.37
14	A	1131	CLA	C3C-C2C	4.14	1.45	1.36
14	B	1203	CLA	C3B-C2B	4.14	1.46	1.40
14	A	1113	CLA	C3B-C2B	4.14	1.46	1.40
14	A	1101	CLA	C3C-C2C	4.14	1.45	1.36
14	B	1213	CLA	C3C-C2C	4.14	1.45	1.36
14	B	1206	CLA	CHD-C1D	4.14	1.46	1.38
14	b	1213	CLA	C3C-C2C	4.14	1.45	1.36
14	H	1236	CLA	C1D-ND	-4.14	1.32	1.37
14	G	1013	CLA	C3B-C2B	4.14	1.46	1.40
14	a	1113	CLA	C3B-C2B	4.14	1.46	1.40
14	H	1220	CLA	C3C-C2C	4.14	1.45	1.36
14	l	1501	CLA	C1D-ND	-4.14	1.32	1.37
14	a	1013	CLA	C3B-C2B	4.14	1.46	1.40
14	A	1013	CLA	C3B-C2B	4.13	1.46	1.40
14	b	1220	CLA	C3C-C2C	4.13	1.45	1.36
14	H	1234	CLA	C3C-C2C	4.13	1.45	1.36
14	G	1107	CLA	CHD-C1D	4.13	1.46	1.38
14	A	1122	CLA	C3B-C2B	4.13	1.46	1.40
14	G	1111	CLA	CHD-C1D	4.13	1.46	1.38
14	H	1231	CLA	CHD-C1D	4.13	1.46	1.38
14	A	1107	CLA	CHD-C1D	4.13	1.46	1.38
14	A	1111	CLA	CHD-C1D	4.13	1.46	1.38
14	G	1131	CLA	C3C-C2C	4.13	1.45	1.36
14	A	1120	CLA	C3C-C2C	4.13	1.45	1.36
14	a	1130	CLA	C1D-ND	-4.13	1.32	1.37
14	H	1224	CLA	C3C-C2C	4.13	1.45	1.36
14	H	1239	CLA	C1D-ND	-4.13	1.32	1.37
14	b	1228	CLA	CHD-C1D	4.13	1.46	1.38
14	B	1231	CLA	C3B-C2B	4.13	1.46	1.40
14	G	1104	CLA	C3C-C2C	4.13	1.45	1.36
14	B	1221	CLA	C1D-ND	-4.13	1.32	1.37
14	H	1234	CLA	C1D-ND	-4.13	1.32	1.37
14	b	1231	CLA	CHD-C1D	4.13	1.46	1.38
14	G	1012	CLA	O2D-CGD	4.13	1.43	1.33
14	G	1012	CLA	C1D-ND	-4.13	1.32	1.37
14	G	1101	CLA	C3C-C2C	4.12	1.45	1.36
14	W	1701	CLA	C3C-C2C	4.12	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1101	CLA	CHD-C1D	4.12	1.46	1.38
14	a	1012	CLA	C1D-ND	-4.12	1.32	1.37
14	a	1124	CLA	C1D-ND	-4.12	1.32	1.37
14	A	1012	CLA	C3C-C2C	4.12	1.45	1.36
14	B	1224	CLA	C3C-C2C	4.12	1.45	1.36
14	a	1117	CLA	C3B-C2B	4.12	1.46	1.40
14	A	1113	CLA	CHD-C1D	4.12	1.46	1.38
14	a	1140	CLA	C3C-C2C	4.12	1.45	1.36
14	a	1012	CLA	C3C-C2C	4.12	1.45	1.36
14	B	1204	CLA	C3C-C2C	4.12	1.45	1.36
14	H	1206	CLA	CHD-C1D	4.12	1.46	1.38
14	a	1111	CLA	CHD-C1D	4.12	1.46	1.38
14	A	1123	CLA	CHD-C1D	4.12	1.46	1.38
14	a	1107	CLA	CHD-C1D	4.11	1.46	1.38
14	x	1701	CLA	C3C-C2C	4.11	1.45	1.36
14	b	1239	CLA	CHD-C1D	4.11	1.46	1.38
14	G	1012	CLA	C3C-C2C	4.11	1.45	1.36
14	A	1102	CLA	C1D-ND	-4.11	1.32	1.37
14	H	1204	CLA	C3C-C2C	4.11	1.45	1.36
14	b	1206	CLA	CHD-C1D	4.11	1.46	1.38
14	G	1139	CLA	C3C-C2C	4.11	1.45	1.36
14	G	1140	CLA	C3C-C2C	4.11	1.45	1.36
14	G	1122	CLA	C3B-C2B	4.11	1.46	1.40
14	X	1701	CLA	C3C-C2C	4.11	1.45	1.36
14	a	1122	CLA	C3B-C2B	4.11	1.46	1.40
14	a	1102	CLA	C1D-ND	-4.11	1.32	1.37
14	A	1012	CLA	CHD-C1D	4.11	1.46	1.38
14	A	1012	CLA	O2D-CGD	4.11	1.43	1.33
14	a	1101	CLA	CHD-C1D	4.10	1.46	1.38
14	L	1502	CLA	CHD-C1D	4.10	1.46	1.38
14	B	1225	CLA	C3C-C2C	4.10	1.45	1.36
14	G	1130	CLA	CHD-C1D	4.10	1.46	1.38
14	a	1012	CLA	CHD-C1D	4.10	1.46	1.38
14	b	1221	CLA	C1D-ND	-4.10	1.32	1.37
14	B	1234	CLA	C1D-ND	-4.10	1.32	1.37
14	B	1231	CLA	C3C-C2C	4.09	1.45	1.36
18	a	4008	BCR	C11-C12	-4.09	1.24	1.34
14	G	1135	CLA	CHD-C1D	4.09	1.46	1.38
14	a	1012	CLA	O2D-CGD	4.09	1.43	1.33
14	a	1131	CLA	C3C-C2C	4.09	1.45	1.36
14	A	1139	CLA	C3C-C2C	4.09	1.45	1.36
14	a	1139	CLA	C3C-C2C	4.09	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1239	CLA	CHD-C1D	4.09	1.46	1.38
14	A	1101	CLA	CHD-C1D	4.09	1.46	1.38
14	a	1116	CLA	CHD-C1D	4.09	1.46	1.38
15	a	1121	F6C	C3D-C4D	-4.09	1.33	1.43
14	G	1120	CLA	C3B-C2B	4.08	1.46	1.40
14	U	1502	CLA	CHD-C1D	4.08	1.46	1.38
14	B	1231	CLA	CHD-C1D	4.08	1.46	1.38
14	A	1115	CLA	CHD-C1D	4.08	1.46	1.38
14	G	1012	CLA	CHD-C1D	4.08	1.46	1.38
14	a	1116	CLA	C1D-ND	-4.08	1.32	1.37
14	b	1231	CLA	C3C-C2C	4.08	1.45	1.36
14	b	1224	CLA	C3C-C2C	4.08	1.45	1.36
14	a	1130	CLA	CHD-C1D	4.08	1.46	1.38
14	a	1137	CLA	CHD-C1D	4.08	1.46	1.38
15	G	1121	F6C	C3D-C4D	-4.08	1.33	1.43
18	G	4008	BCR	C11-C12	-4.08	1.24	1.34
14	a	1135	CLA	C1D-ND	-4.08	1.32	1.37
14	A	1120	CLA	C3B-C2B	4.07	1.46	1.40
16	G	2001	PQN	C10-C5	4.07	1.47	1.40
14	G	1123	CLA	C3C-C2C	4.07	1.45	1.36
14	G	1123	CLA	C1D-ND	-4.07	1.32	1.37
14	G	1123	CLA	CHD-C1D	4.07	1.46	1.38
14	A	1137	CLA	C1D-ND	-4.07	1.32	1.37
14	A	1123	CLA	C3C-C2C	4.07	1.45	1.36
14	L	1503	CLA	CHD-C1D	4.07	1.46	1.38
14	b	1203	CLA	C1D-ND	-4.07	1.32	1.37
14	A	1123	CLA	C1D-ND	-4.07	1.32	1.37
14	H	1221	CLA	C1D-ND	-4.07	1.32	1.37
15	A	1121	F6C	C3D-C4D	-4.07	1.33	1.43
14	G	1110	CLA	CHD-C1D	4.07	1.46	1.38
14	B	1205	CLA	C3B-C2B	4.07	1.46	1.40
14	U	1503	CLA	CHD-C1D	4.07	1.46	1.38
14	G	1120	CLA	C3C-C2C	4.07	1.45	1.36
14	b	1225	CLA	C3C-C2C	4.07	1.45	1.36
14	a	1128	CLA	CHD-C1D	4.07	1.46	1.38
14	A	1130	CLA	CHD-C1D	4.07	1.46	1.38
14	a	1129	CLA	CHD-C1D	4.07	1.46	1.38
14	a	1135	CLA	CHD-C1D	4.07	1.46	1.38
14	H	1203	CLA	C1D-ND	-4.06	1.32	1.37
14	l	1502	CLA	CHD-C1D	4.06	1.46	1.38
14	A	1110	CLA	CHD-C1D	4.06	1.46	1.38
14	a	1115	CLA	CHD-C1D	4.06	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1220	CLA	CHD-C1D	4.06	1.46	1.38
14	b	1205	CLA	C3C-C2C	4.06	1.45	1.36
14	G	1128	CLA	CHD-C1D	4.06	1.46	1.38
14	G	1115	CLA	CHD-C1D	4.06	1.46	1.38
14	G	1126	CLA	CHD-C1D	4.06	1.46	1.38
14	A	1135	CLA	CHD-C1D	4.06	1.46	1.38
14	a	1123	CLA	C3C-C2C	4.06	1.45	1.36
14	A	1140	CLA	C3C-C2C	4.06	1.45	1.36
14	B	1205	CLA	C3C-C2C	4.05	1.45	1.36
14	A	1116	CLA	CHD-C1D	4.05	1.46	1.38
14	B	1203	CLA	C1D-ND	-4.05	1.32	1.37
14	H	1205	CLA	C3C-C2C	4.05	1.45	1.36
14	G	1116	CLA	CHD-C1D	4.05	1.46	1.38
14	B	1239	CLA	CHD-C1D	4.05	1.46	1.38
14	a	1123	CLA	CHD-C1D	4.05	1.46	1.38
14	A	1128	CLA	CHD-C1D	4.05	1.46	1.38
14	H	1225	CLA	C3C-C2C	4.05	1.45	1.36
15	B	1230	F6C	C3D-C4D	-4.04	1.33	1.43
18	b	4010	BCR	C11-C12	-4.04	1.24	1.34
14	G	1135	CLA	C1D-ND	-4.04	1.32	1.37
14	G	1140	CLA	C1D-ND	-4.04	1.32	1.37
14	a	1120	CLA	C3B-C2B	4.04	1.46	1.40
14	A	1137	CLA	C3C-C2C	4.04	1.45	1.36
14	A	1136	CLA	C1D-ND	-4.04	1.32	1.37
14	H	1231	CLA	C3C-C2C	4.04	1.45	1.36
14	b	1227	CLA	C3B-C2B	4.04	1.46	1.40
18	A	4008	BCR	C11-C12	-4.04	1.24	1.34
14	a	1110	CLA	CHD-C1D	4.04	1.46	1.38
14	A	1126	CLA	CHD-C1D	4.03	1.46	1.38
20	R	5006	LMG	O7-C10	4.03	1.45	1.34
14	H	1215	CLA	C1D-ND	-4.03	1.32	1.37
14	a	1123	CLA	C1D-ND	-4.03	1.32	1.37
16	A	2001	PQN	C10-C5	4.03	1.47	1.40
14	l	1503	CLA	CHD-C1D	4.03	1.46	1.38
14	G	1137	CLA	C3C-C2C	4.03	1.45	1.36
14	a	1104	CLA	C1D-ND	-4.02	1.32	1.37
14	a	1140	CLA	CHD-C1D	4.02	1.46	1.38
14	A	1140	CLA	C1D-ND	-4.02	1.32	1.37
14	H	1220	CLA	CHD-C1D	4.02	1.46	1.38
14	b	1215	CLA	C1D-ND	-4.02	1.32	1.37
18	H	4010	BCR	C11-C12	-4.02	1.24	1.34
14	H	1227	CLA	C3B-C2B	4.02	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	1503	CLA	C1D-ND	-4.02	1.32	1.37
14	a	1111	CLA	C3C-C2C	4.02	1.45	1.36
14	B	1220	CLA	CHD-C1D	4.02	1.46	1.38
14	A	1114	CLA	CHD-C4C	4.02	1.48	1.39
14	B	1217	CLA	CHD-C1D	4.02	1.46	1.38
14	B	1221	CLA	CHD-C1D	4.02	1.46	1.38
14	a	1125	CLA	C1D-ND	-4.01	1.32	1.37
14	H	1206	CLA	C3C-C2C	4.01	1.45	1.36
14	a	1013	CLA	C3C-C2C	4.01	1.45	1.36
14	G	1140	CLA	CHD-C1D	4.01	1.46	1.38
18	B	4010	BCR	C11-C12	-4.01	1.24	1.34
14	A	1137	CLA	CHD-C1D	4.01	1.46	1.38
14	a	1124	CLA	C3B-C2B	4.01	1.45	1.40
14	A	1104	CLA	C1D-ND	-4.01	1.32	1.37
15	b	1230	F6C	C3D-C4D	-4.01	1.33	1.43
14	H	1205	CLA	C3B-C2B	4.01	1.45	1.40
14	a	1126	CLA	CHD-C1D	4.01	1.46	1.38
14	H	1212	CLA	C1D-ND	-4.01	1.32	1.37
14	A	1116	CLA	C1D-ND	-4.01	1.32	1.37
14	G	1114	CLA	CHD-C4C	4.01	1.48	1.39
14	H	1022	CLA	C3C-C2C	4.01	1.45	1.36
14	a	1137	CLA	C3C-C2C	4.00	1.45	1.36
14	b	1022	CLA	C3C-C2C	4.00	1.45	1.36
14	b	1206	CLA	C3C-C2C	4.00	1.45	1.36
14	A	1124	CLA	C3B-C2B	4.00	1.45	1.40
14	G	1129	CLA	CHD-C1D	4.00	1.46	1.38
14	a	1114	CLA	CHD-C4C	4.00	1.48	1.39
14	A	1129	CLA	CHD-C1D	4.00	1.46	1.38
14	G	1013	CLA	C3C-C2C	4.00	1.45	1.36
14	b	1235	CLA	C1D-ND	-4.00	1.32	1.37
20	I	5006	LMG	O7-C10	4.00	1.45	1.34
16	a	2001	PQN	C10-C5	4.00	1.47	1.40
14	B	1227	CLA	C3B-C2B	4.00	1.45	1.40
14	A	1140	CLA	CHD-C1D	4.00	1.46	1.38
14	A	1013	CLA	C3C-C2C	4.00	1.45	1.36
14	B	1225	CLA	CHD-C1D	3.99	1.46	1.38
14	A	1111	CLA	C3C-C2C	3.99	1.45	1.36
18	R	4020	BCR	C11-C12	-3.99	1.24	1.34
15	H	1230	F6C	C3D-C4D	-3.99	1.34	1.43
14	U	1503	CLA	C3B-C2B	3.99	1.45	1.40
14	G	1124	CLA	CHD-C1D	3.99	1.46	1.38
14	A	1125	CLA	C1D-ND	-3.99	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1140	CLA	C1D-ND	-3.98	1.32	1.37
14	b	1208	CLA	C1D-ND	-3.98	1.32	1.37
14	A	1120	CLA	C1D-ND	-3.98	1.32	1.37
20	i	5006	LMG	O7-C10	3.98	1.45	1.34
14	b	1225	CLA	CHD-C1D	3.98	1.46	1.38
14	G	1120	CLA	C1D-ND	-3.98	1.32	1.37
14	G	1125	CLA	C1D-ND	-3.98	1.32	1.37
14	a	1136	CLA	C1D-ND	-3.98	1.32	1.37
14	H	1217	CLA	CHD-C1D	3.98	1.46	1.38
14	A	1118	CLA	C3B-C2B	3.98	1.45	1.40
14	H	1215	CLA	C3C-C2C	3.98	1.45	1.36
14	G	1116	CLA	C1D-ND	-3.98	1.32	1.37
14	l	1503	CLA	C1D-ND	-3.98	1.32	1.37
14	U	1503	CLA	C1D-ND	-3.98	1.32	1.37
14	G	1137	CLA	CHD-C1D	3.98	1.46	1.38
14	B	1235	CLA	C1D-ND	-3.98	1.32	1.37
14	A	1124	CLA	CHD-C1D	3.98	1.46	1.38
14	B	1212	CLA	C1D-ND	-3.98	1.32	1.37
14	B	1206	CLA	C3C-C2C	3.98	1.45	1.36
14	A	1135	CLA	C1D-ND	-3.98	1.32	1.37
14	H	1225	CLA	CHD-C1D	3.98	1.46	1.38
14	H	1221	CLA	C3C-C2C	3.97	1.45	1.36
18	I	4020	BCR	C11-C12	-3.97	1.24	1.34
14	G	1124	CLA	C3B-C2B	3.97	1.45	1.40
14	G	1136	CLA	C1D-ND	-3.97	1.32	1.37
14	L	1503	CLA	C3B-C2B	3.97	1.45	1.40
14	b	1212	CLA	C1D-ND	-3.97	1.32	1.37
14	G	1111	CLA	C3C-C2C	3.97	1.45	1.36
14	H	1220	CLA	C1D-ND	-3.97	1.32	1.37
14	b	1217	CLA	CHD-C1D	3.97	1.46	1.38
14	b	1215	CLA	C3C-C2C	3.97	1.45	1.36
14	a	1118	CLA	C3B-C2B	3.97	1.45	1.40
14	B	1022	CLA	C3C-C2C	3.97	1.45	1.36
14	l	1503	CLA	C3B-C2B	3.97	1.45	1.40
14	H	1235	CLA	C1D-ND	-3.96	1.32	1.37
14	b	1209	CLA	C3B-C2B	3.96	1.45	1.40
14	a	1120	CLA	C1D-ND	-3.96	1.32	1.37
14	a	1133	CLA	C1D-ND	-3.96	1.32	1.37
14	G	1104	CLA	C1D-ND	-3.95	1.32	1.37
14	b	1205	CLA	C3B-C2B	3.95	1.45	1.40
14	B	1220	CLA	C1D-ND	-3.95	1.32	1.37
14	B	1224	CLA	C3B-C2B	3.95	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	5004	LHG	O7-C7	3.95	1.45	1.34
14	G	1139	CLA	CHD-C1D	3.95	1.46	1.38
19	b	5004	LHG	O7-C7	3.95	1.45	1.34
14	b	1221	CLA	CHD-C1D	3.95	1.46	1.38
14	A	1139	CLA	CHD-C1D	3.95	1.46	1.38
14	b	1221	CLA	C3C-C2C	3.95	1.45	1.36
14	B	1215	CLA	C3C-C2C	3.95	1.45	1.36
14	a	1138	CLA	C1D-ND	-3.95	1.32	1.37
14	B	1215	CLA	C1D-ND	-3.94	1.32	1.37
14	B	1221	CLA	C3C-C2C	3.94	1.45	1.36
14	a	1134	CLA	CHD-C4C	3.94	1.48	1.39
18	i	4020	BCR	C11-C12	-3.94	1.24	1.34
14	a	1129	CLA	C3B-C2B	3.94	1.45	1.40
14	a	1124	CLA	CHD-C1D	3.94	1.46	1.38
14	b	1220	CLA	C1D-ND	-3.93	1.32	1.37
16	H	2002	PQN	C10-C5	3.93	1.47	1.40
14	H	1204	CLA	CHD-C4C	3.93	1.48	1.39
14	H	1208	CLA	C1D-ND	-3.93	1.33	1.37
14	G	1118	CLA	C3B-C2B	3.93	1.45	1.40
14	G	1119	CLA	C3B-C2B	3.93	1.45	1.40
14	A	1107	CLA	C3B-C2B	3.93	1.45	1.40
14	H	1221	CLA	CHD-C1D	3.93	1.46	1.38
14	b	1210	CLA	C1D-ND	-3.93	1.33	1.37
14	B	1208	CLA	C1D-ND	-3.93	1.33	1.37
14	H	1224	CLA	C3B-C2B	3.93	1.45	1.40
14	H	1203	CLA	C3C-C2C	3.93	1.45	1.36
14	x	1701	CLA	CHD-C1D	3.93	1.46	1.38
14	G	1134	CLA	CHD-C4C	3.92	1.48	1.39
14	G	1106	CLA	C1D-ND	-3.92	1.33	1.37
14	a	1103	CLA	C1D-ND	-3.92	1.33	1.37
14	b	1203	CLA	C3C-C2C	3.92	1.45	1.36
14	B	1209	CLA	C3B-C2B	3.92	1.45	1.40
18	A	4007	BCR	C11-C12	-3.92	1.24	1.34
19	H	5004	LHG	O7-C7	3.92	1.45	1.34
14	b	1224	CLA	C3B-C2B	3.92	1.45	1.40
14	X	1701	CLA	CHD-C1D	3.92	1.46	1.38
14	B	1203	CLA	C3C-C2C	3.91	1.45	1.36
14	b	1204	CLA	CHD-C1D	3.91	1.46	1.38
14	b	1236	CLA	CHD-C1D	3.91	1.46	1.38
14	G	1106	CLA	CHD-C1D	3.91	1.46	1.38
14	A	1134	CLA	CHD-C4C	3.91	1.48	1.39
14	A	1110	CLA	C1D-ND	-3.90	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1231	CLA	C1D-ND	-3.90	1.33	1.37
14	G	1129	CLA	C3B-C2B	3.90	1.45	1.40
14	H	1209	CLA	C3B-C2B	3.90	1.45	1.40
14	G	1110	CLA	C3B-C2B	3.90	1.45	1.40
14	B	1021	CLA	C3C-C2C	3.90	1.45	1.36
14	G	1110	CLA	C1D-ND	-3.90	1.33	1.37
14	B	1236	CLA	CHD-C1D	3.90	1.46	1.38
18	G	4007	BCR	C11-C12	-3.90	1.24	1.34
14	b	1227	CLA	CHD-C4C	3.90	1.48	1.39
14	W	1701	CLA	CHD-C1D	3.90	1.46	1.38
14	A	1106	CLA	CHD-C1D	3.90	1.46	1.38
14	H	1210	CLA	C1D-ND	-3.90	1.33	1.37
14	A	1129	CLA	C3B-C2B	3.90	1.45	1.40
14	G	1103	CLA	C1D-ND	-3.90	1.33	1.37
18	a	4007	BCR	C11-C12	-3.90	1.24	1.34
14	B	1202	CLA	C3C-C2C	3.89	1.45	1.36
14	G	1138	CLA	C1D-ND	-3.89	1.33	1.37
14	B	1231	CLA	C1D-ND	-3.89	1.33	1.37
14	H	1021	CLA	C3C-C2C	3.89	1.45	1.36
14	H	1236	CLA	CHD-C1D	3.89	1.45	1.38
14	A	1119	CLA	C3B-C2B	3.89	1.45	1.40
14	a	1110	CLA	C1D-ND	-3.89	1.33	1.37
14	a	1139	CLA	CHD-C1D	3.89	1.45	1.38
14	B	1227	CLA	CHD-C4C	3.89	1.48	1.39
14	A	1106	CLA	C1D-ND	-3.89	1.33	1.37
14	H	1227	CLA	CHD-C4C	3.89	1.48	1.39
14	A	1133	CLA	C1D-ND	-3.88	1.33	1.37
14	a	1106	CLA	C1D-ND	-3.88	1.33	1.37
14	A	1110	CLA	C3B-C2B	3.88	1.45	1.40
14	a	1128	CLA	MG-ND	-3.88	1.98	2.05
14	G	1132	CLA	C1D-ND	-3.88	1.33	1.37
16	b	2002	PQN	C10-C5	3.88	1.47	1.40
14	b	1202	CLA	C3C-C2C	3.88	1.45	1.36
14	H	1023	CLA	C3C-C2C	3.88	1.45	1.36
14	A	1128	CLA	MG-ND	-3.88	1.98	2.05
14	G	1103	CLA	C3C-C2C	3.88	1.45	1.36
14	a	1103	CLA	C3C-C2C	3.88	1.45	1.36
14	B	1023	CLA	C3C-C2C	3.88	1.45	1.36
14	b	1210	CLA	C3C-C2C	3.88	1.45	1.36
14	A	1118	CLA	C1D-ND	-3.88	1.33	1.37
14	b	1204	CLA	CHD-C4C	3.88	1.48	1.39
14	A	1138	CLA	C1D-ND	-3.87	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1122	CLA	C3C-C2C	3.87	1.44	1.36
16	B	2002	PQN	C10-C5	3.87	1.47	1.40
14	b	1231	CLA	C1D-ND	-3.87	1.33	1.37
14	a	1116	CLA	C3B-C2B	3.87	1.45	1.40
14	b	1021	CLA	C3C-C2C	3.87	1.44	1.36
14	A	1103	CLA	C3C-C2C	3.87	1.44	1.36
14	a	1110	CLA	C3B-C2B	3.87	1.45	1.40
14	a	1106	CLA	CHD-C1D	3.87	1.45	1.38
14	B	1210	CLA	C3C-C2C	3.87	1.44	1.36
14	a	1119	CLA	C3B-C2B	3.87	1.45	1.40
14	B	1204	CLA	CHD-C1D	3.86	1.45	1.38
14	A	1116	CLA	C3B-C2B	3.86	1.45	1.40
14	B	1204	CLA	CHD-C4C	3.86	1.48	1.39
14	G	1139	CLA	C3B-C2B	3.86	1.45	1.40
14	b	1227	CLA	C1D-ND	-3.86	1.33	1.37
14	B	1214	CLA	C1D-ND	-3.86	1.33	1.37
14	a	1107	CLA	C3B-C2B	3.86	1.45	1.40
14	B	1219	CLA	CHD-C4C	3.86	1.48	1.39
14	A	1115	CLA	C1D-ND	-3.86	1.33	1.37
14	a	1139	CLA	C3B-C2B	3.86	1.45	1.40
14	G	1118	CLA	C1D-ND	-3.86	1.33	1.37
14	G	1115	CLA	C1D-ND	-3.86	1.33	1.37
14	A	1132	CLA	C1D-ND	-3.86	1.33	1.37
14	b	1023	CLA	C3C-C2C	3.86	1.44	1.36
14	B	1214	CLA	CHD-C4C	3.86	1.48	1.39
18	R	4018	BCR	C11-C12	-3.85	1.24	1.34
14	H	1202	CLA	C3C-C2C	3.85	1.44	1.36
14	B	1227	CLA	C1D-ND	-3.85	1.33	1.37
14	b	1201	CLA	C1D-ND	-3.85	1.33	1.37
14	H	1210	CLA	C3C-C2C	3.85	1.44	1.36
14	H	1201	CLA	C1D-ND	-3.85	1.33	1.37
14	H	1227	CLA	C1D-ND	-3.85	1.33	1.37
14	H	1204	CLA	CHD-C1D	3.85	1.45	1.38
14	G	1116	CLA	C3B-C2B	3.85	1.45	1.40
14	b	1214	CLA	CHD-C4C	3.85	1.48	1.39
14	a	1132	CLA	C1D-ND	-3.85	1.33	1.37
14	G	1139	CLA	C1D-ND	-3.85	1.33	1.37
14	a	1131	CLA	CHD-C4C	3.85	1.48	1.39
14	G	1134	CLA	OBD-CAD	3.85	1.29	1.22
14	G	1128	CLA	MG-ND	-3.85	1.98	2.05
18	I	4018	BCR	C11-C12	-3.85	1.24	1.34
14	G	1126	CLA	C3B-C2B	3.85	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	i	4018	BCR	C11-C12	-3.85	1.24	1.34
14	A	1103	CLA	C1D-ND	-3.85	1.33	1.37
14	G	1107	CLA	C3B-C2B	3.85	1.45	1.40
14	A	1119	CLA	CHD-C4C	3.85	1.48	1.39
14	H	1233	CLA	CHD-C4C	3.84	1.48	1.39
14	H	1228	CLA	CHD-C4C	3.84	1.48	1.39
14	a	1107	CLA	C1D-ND	-3.84	1.33	1.37
14	A	1139	CLA	C3B-C2B	3.84	1.45	1.40
14	a	1119	CLA	C1C-NC	-3.84	1.32	1.37
14	G	1131	CLA	CHD-C4C	3.84	1.48	1.39
14	G	1133	CLA	C1D-ND	-3.84	1.33	1.37
14	b	1219	CLA	CHD-C4C	3.84	1.48	1.39
14	B	1201	CLA	C1D-ND	-3.84	1.33	1.37
14	a	1118	CLA	C1D-ND	-3.84	1.33	1.37
14	H	1223	CLA	CHD-C1D	3.83	1.45	1.38
14	B	1210	CLA	C1D-ND	-3.83	1.33	1.37
14	b	1228	CLA	C1D-ND	-3.83	1.33	1.37
14	A	1119	CLA	C1C-NC	-3.83	1.32	1.37
14	a	1122	CLA	C1D-ND	-3.83	1.33	1.37
14	a	1119	CLA	CHD-C4C	3.83	1.48	1.39
14	U	1501	CLA	CHD-C1D	3.83	1.45	1.38
14	H	1219	CLA	CHD-C4C	3.83	1.48	1.39
14	b	1226	CLA	C3B-C2B	3.83	1.45	1.40
14	a	1115	CLA	C1D-ND	-3.83	1.33	1.37
14	a	1139	CLA	C1D-ND	-3.83	1.33	1.37
14	H	1214	CLA	CHD-C4C	3.83	1.48	1.39
14	l	1501	CLA	CHD-C1D	3.82	1.45	1.38
14	T	1401	CLA	CHD-C4C	3.82	1.48	1.39
14	G	1119	CLA	CHD-C4C	3.82	1.48	1.39
14	B	1205	CLA	CHD-C1D	3.82	1.45	1.38
14	a	1109	CLA	C1D-ND	-3.82	1.33	1.37
15	H	1238	F6C	C1D-ND	-3.82	1.32	1.37
14	A	1140	CLA	C3B-C2B	3.82	1.45	1.40
14	B	1228	CLA	CHD-C4C	3.82	1.47	1.39
14	L	1501	CLA	CHD-C1D	3.82	1.45	1.38
14	H	1228	CLA	C1D-ND	-3.82	1.33	1.37
14	k	1401	CLA	CHD-C4C	3.82	1.47	1.39
14	A	1107	CLA	C1D-ND	-3.81	1.33	1.37
14	K	1401	CLA	CHD-C4C	3.81	1.47	1.39
14	G	1107	CLA	C1D-ND	-3.81	1.33	1.37
14	A	1131	CLA	CHD-C4C	3.81	1.47	1.39
14	B	1228	CLA	C1D-ND	-3.81	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1228	CLA	CHD-C4C	3.81	1.47	1.39
14	G	1105	CLA	C1D-ND	-3.81	1.33	1.37
14	B	1233	CLA	CHD-C4C	3.81	1.47	1.39
14	G	1140	CLA	C3B-C2B	3.81	1.45	1.40
14	A	1122	CLA	C1D-ND	-3.81	1.33	1.37
15	B	1238	F6C	C1D-ND	-3.81	1.32	1.37
15	b	1238	F6C	C1D-ND	-3.81	1.32	1.37
14	A	1101	CLA	C3B-C2B	3.81	1.45	1.40
14	H	1222	CLA	CHD-C1D	3.80	1.45	1.38
14	H	1205	CLA	CHD-C1D	3.80	1.45	1.38
14	b	1233	CLA	CHD-C4C	3.80	1.47	1.39
14	A	1109	CLA	C1D-ND	-3.80	1.33	1.37
14	b	1205	CLA	CHD-C1D	3.80	1.45	1.38
14	B	1212	CLA	CHD-C1D	3.80	1.45	1.38
14	b	1209	CLA	CHD-C4C	3.80	1.47	1.39
14	G	1101	CLA	C3B-C2B	3.80	1.45	1.40
14	a	1101	CLA	C3B-C2B	3.80	1.45	1.40
14	b	1214	CLA	C1D-ND	-3.80	1.33	1.37
14	B	1223	CLA	CHD-C1D	3.79	1.45	1.38
14	A	1122	CLA	C3C-C2C	3.79	1.44	1.36
14	B	1206	CLA	C3B-C2B	3.79	1.45	1.40
14	b	1222	CLA	CHD-C1D	3.79	1.45	1.38
14	a	1140	CLA	C3B-C2B	3.79	1.45	1.40
14	A	1105	CLA	C1D-ND	-3.79	1.33	1.37
14	a	1122	CLA	C3C-C2C	3.79	1.44	1.36
14	A	1126	CLA	C3B-C2B	3.78	1.45	1.40
14	H	1209	CLA	CHD-C4C	3.78	1.47	1.39
14	A	1139	CLA	C1D-ND	-3.78	1.33	1.37
14	b	1206	CLA	C3B-C2B	3.78	1.45	1.40
14	B	1201	CLA	CHD-C4C	3.78	1.47	1.39
14	A	1127	CLA	CHD-C1D	3.78	1.45	1.38
14	H	1214	CLA	C1D-ND	-3.78	1.33	1.37
14	b	1201	CLA	CHD-C4C	3.78	1.47	1.39
14	H	1022	CLA	CHD-C1D	3.78	1.45	1.38
14	b	1223	CLA	CHD-C1D	3.78	1.45	1.38
14	H	1201	CLA	CHD-C4C	3.78	1.47	1.39
14	B	1209	CLA	CHD-C4C	3.78	1.47	1.39
14	H	1233	CLA	C3B-C2B	3.78	1.45	1.40
14	B	1022	CLA	CHD-C1D	3.78	1.45	1.38
14	a	1105	CLA	C1D-ND	-3.78	1.33	1.37
14	A	1138	CLA	CHD-C4C	3.78	1.47	1.39
13	G	1011	CL0	CHD-C1D	3.78	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1134	CLA	OBD-CAD	3.78	1.29	1.22
14	B	1224	CLA	CHD-C1D	3.77	1.45	1.38
14	G	1122	CLA	C1D-ND	-3.77	1.33	1.37
14	G	1108	CLA	CHD-C4C	3.77	1.47	1.39
14	a	1134	CLA	OBD-CAD	3.77	1.29	1.22
14	H	1206	CLA	C3B-C2B	3.77	1.45	1.40
14	a	1126	CLA	C3B-C2B	3.77	1.45	1.40
14	b	1212	CLA	CHD-C1D	3.77	1.45	1.38
14	b	1233	CLA	C3B-C2B	3.77	1.45	1.40
14	G	1109	CLA	C1D-ND	-3.77	1.33	1.37
18	H	4014	BCR	C11-C12	-3.77	1.24	1.34
14	B	1222	CLA	CHD-C1D	3.77	1.45	1.38
14	a	1127	CLA	CHD-C1D	3.76	1.45	1.38
19	G	5001	LHG	O7-C7	3.76	1.44	1.34
14	b	1224	CLA	CHD-C1D	3.76	1.45	1.38
14	B	1226	CLA	C3B-C2B	3.76	1.45	1.40
14	H	1212	CLA	CHD-C1D	3.75	1.45	1.38
14	G	1119	CLA	C1C-NC	-3.75	1.32	1.37
14	G	1117	CLA	C1D-ND	-3.75	1.33	1.37
14	A	1108	CLA	CHD-C4C	3.75	1.47	1.39
14	G	1138	CLA	CHD-C4C	3.75	1.47	1.39
14	a	1128	CLA	C3B-C2B	3.75	1.45	1.40
14	a	1138	CLA	CHD-C4C	3.75	1.47	1.39
14	A	1105	CLA	CHD-C4C	3.75	1.47	1.39
19	a	5001	LHG	O7-C7	3.75	1.44	1.34
14	l	1502	CLA	CHD-C4C	3.74	1.47	1.39
14	H	1226	CLA	C3B-C2B	3.74	1.45	1.40
14	G	1115	CLA	CHD-C4C	3.74	1.47	1.39
14	a	1105	CLA	CHD-C4C	3.74	1.47	1.39
14	H	1223	CLA	C1D-ND	-3.74	1.33	1.37
14	B	1233	CLA	C3B-C2B	3.74	1.45	1.40
18	L	4022	BCR	C11-C12	-3.74	1.24	1.34
18	b	4017	BCR	C11-C12	-3.74	1.24	1.34
14	G	1127	CLA	CHD-C1D	3.74	1.45	1.38
14	b	1022	CLA	CHD-C1D	3.74	1.45	1.38
18	B	4014	BCR	C11-C12	-3.74	1.24	1.34
18	H	4017	BCR	C11-C12	-3.74	1.24	1.34
14	G	1118	CLA	CHD-C4C	3.73	1.47	1.39
14	G	1112	CLA	CHD-C4C	3.73	1.47	1.39
14	a	1108	CLA	CHD-C4C	3.73	1.47	1.39
14	B	1235	CLA	CHD-C4C	3.73	1.47	1.39
13	a	1011	CL0	CHD-C1D	3.73	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1226	CLA	CHD-C4C	3.73	1.47	1.39
14	b	1235	CLA	CHD-C4C	3.73	1.47	1.39
19	A	5001	LHG	O7-C7	3.73	1.44	1.34
14	b	1216	CLA	CHD-C4C	3.73	1.47	1.39
14	A	1111	CLA	C1D-ND	-3.73	1.33	1.37
14	G	1114	CLA	C3B-C2B	3.73	1.45	1.40
14	a	1118	CLA	CHD-C4C	3.72	1.47	1.39
14	B	1023	CLA	C3B-C2B	3.72	1.45	1.40
14	b	1223	CLA	C1D-ND	-3.72	1.33	1.37
14	A	1128	CLA	C3B-C2B	3.72	1.45	1.40
18	l	4022	BCR	C11-C12	-3.72	1.25	1.34
14	G	1111	CLA	C1D-ND	-3.72	1.33	1.37
14	H	1224	CLA	CHD-C1D	3.72	1.45	1.38
18	b	4014	BCR	C11-C12	-3.72	1.25	1.34
14	H	1216	CLA	CHD-C4C	3.72	1.47	1.39
14	L	1502	CLA	CHD-C4C	3.72	1.47	1.39
14	a	1012	CLA	MG-ND	-3.72	1.98	2.05
13	A	1011	CL0	CHD-C1D	3.72	1.45	1.38
14	B	1232	CLA	CHD-C4C	3.72	1.47	1.39
14	H	1235	CLA	CHD-C4C	3.71	1.47	1.39
14	G	1109	CLA	CHD-C4C	3.71	1.47	1.39
14	A	1112	CLA	CHD-C4C	3.71	1.47	1.39
14	G	1128	CLA	C3B-C2B	3.71	1.45	1.40
18	B	4017	BCR	C11-C12	-3.71	1.25	1.34
14	A	1109	CLA	CHD-C4C	3.71	1.47	1.39
14	H	1219	CLA	C3B-C2B	3.71	1.45	1.40
14	H	1232	CLA	CHD-C4C	3.71	1.47	1.39
14	A	1122	CLA	CHD-C4C	3.71	1.47	1.39
18	U	4022	BCR	C11-C12	-3.71	1.25	1.34
14	G	1108	CLA	C1D-ND	-3.71	1.33	1.37
14	a	1109	CLA	CHD-C4C	3.71	1.47	1.39
14	B	1216	CLA	CHD-C4C	3.71	1.47	1.39
14	A	1117	CLA	C1D-ND	-3.71	1.33	1.37
14	B	1223	CLA	C1D-ND	-3.71	1.33	1.37
14	G	1122	CLA	CHD-C4C	3.70	1.47	1.39
14	H	1215	CLA	CHD-C4C	3.70	1.47	1.39
14	a	1112	CLA	CHD-C4C	3.70	1.47	1.39
14	W	1701	CLA	C1D-ND	-3.70	1.33	1.37
14	B	1210	CLA	CHD-C4C	3.70	1.47	1.39
14	U	1502	CLA	CHD-C4C	3.70	1.47	1.39
14	a	1122	CLA	CHD-C4C	3.70	1.47	1.39
14	G	1105	CLA	CHD-C4C	3.70	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1115	CLA	CHD-C4C	3.70	1.47	1.39
14	H	1226	CLA	CHD-C4C	3.70	1.47	1.39
14	A	1136	CLA	CHD-C4C	3.70	1.47	1.39
14	X	1701	CLA	C1D-ND	-3.70	1.33	1.37
14	G	1120	CLA	CHD-C1D	3.70	1.45	1.38
14	B	1218	CLA	CHD-C1D	3.70	1.45	1.38
14	B	1211	CLA	C1D-ND	-3.70	1.33	1.37
14	A	1013	CLA	C1B-NB	-3.69	1.31	1.35
14	a	1108	CLA	C1D-ND	-3.69	1.33	1.37
14	a	1114	CLA	C3B-C2B	3.69	1.45	1.40
14	H	1211	CLA	C1D-ND	-3.69	1.33	1.37
14	a	1124	CLA	CHD-C4C	3.69	1.47	1.39
14	a	1111	CLA	C1D-ND	-3.69	1.33	1.37
14	A	1115	CLA	CHD-C4C	3.69	1.47	1.39
18	b	4005	BCR	C11-C12	-3.69	1.25	1.34
14	a	1120	CLA	CHD-C1D	3.69	1.45	1.38
14	b	1215	CLA	CHD-C4C	3.69	1.47	1.39
14	A	1118	CLA	CHD-C4C	3.69	1.47	1.39
14	A	1120	CLA	CHD-C1D	3.69	1.45	1.38
14	a	1136	CLA	CHD-C4C	3.69	1.47	1.39
14	b	1210	CLA	CHD-C4C	3.69	1.47	1.39
14	H	1206	CLA	C1C-NC	-3.69	1.32	1.37
14	b	1232	CLA	CHD-C4C	3.69	1.47	1.39
14	B	1215	CLA	CHD-C4C	3.69	1.47	1.39
14	G	1124	CLA	CHD-C4C	3.69	1.47	1.39
14	B	1226	CLA	CHD-C4C	3.68	1.47	1.39
14	H	1218	CLA	CHD-C1D	3.68	1.45	1.38
14	B	1021	CLA	MG-ND	-3.68	1.98	2.05
14	H	1224	CLA	MG-ND	-3.68	1.98	2.05
18	B	4005	BCR	C11-C12	-3.68	1.25	1.34
14	H	1023	CLA	CHD-C1D	3.68	1.45	1.38
18	M	4021	BCR	C11-C12	-3.68	1.25	1.34
14	G	1012	CLA	MG-ND	-3.68	1.98	2.05
14	H	1023	CLA	C3B-C2B	3.68	1.45	1.40
14	a	1117	CLA	CHD-C4C	3.67	1.47	1.39
14	A	1114	CLA	C3B-C2B	3.67	1.45	1.40
14	b	1218	CLA	CHD-C1D	3.67	1.45	1.38
14	A	1124	CLA	CHD-C4C	3.67	1.47	1.39
14	b	1224	CLA	MG-ND	-3.67	1.98	2.05
14	a	1117	CLA	C1D-ND	-3.67	1.33	1.37
14	H	1210	CLA	CHD-C4C	3.67	1.47	1.39
14	A	1117	CLA	CHD-C4C	3.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1012	CLA	MG-ND	-3.67	1.98	2.05
14	A	1116	CLA	CHD-C4C	3.67	1.47	1.39
14	H	1021	CLA	MG-ND	-3.67	1.98	2.05
14	b	1211	CLA	C1D-ND	-3.67	1.33	1.37
14	b	1226	CLA	MG-ND	-3.67	1.98	2.05
14	G	1125	CLA	MG-ND	-3.67	1.98	2.05
14	B	1229	CLA	CHD-C4C	3.67	1.47	1.39
14	b	1021	CLA	MG-ND	-3.67	1.98	2.05
14	x	1701	CLA	C1D-ND	-3.67	1.33	1.37
18	A	4011	BCR	C11-C12	-3.67	1.25	1.34
14	G	1136	CLA	CHD-C4C	3.67	1.47	1.39
18	H	4005	BCR	C11-C12	-3.66	1.25	1.34
14	b	1023	CLA	CHD-C1D	3.66	1.45	1.38
14	A	1125	CLA	C3C-C2C	3.66	1.44	1.36
14	H	1203	CLA	CHD-C1D	3.66	1.45	1.38
20	H	5002	LMG	O7-C10	3.66	1.44	1.34
14	b	1216	CLA	C1D-ND	-3.66	1.33	1.37
14	b	1229	CLA	CHD-C4C	3.66	1.47	1.39
14	H	1202	CLA	CHD-C1D	3.66	1.45	1.38
18	a	4001	BCR	C11-C12	-3.66	1.25	1.34
14	B	1226	CLA	MG-ND	-3.66	1.98	2.05
14	a	1125	CLA	C3C-C2C	3.66	1.44	1.36
14	G	1133	CLA	CHD-C4C	3.66	1.47	1.39
14	a	1126	CLA	CHD-C4C	3.66	1.47	1.39
14	A	1108	CLA	C1D-ND	-3.66	1.33	1.37
14	B	1023	CLA	CHD-C1D	3.65	1.45	1.38
14	H	1229	CLA	CHD-C4C	3.65	1.47	1.39
14	B	1213	CLA	CHD-C4C	3.65	1.47	1.39
14	B	1202	CLA	CHD-C1D	3.65	1.45	1.38
14	G	1117	CLA	CHD-C4C	3.65	1.47	1.39
14	b	1206	CLA	MG-ND	-3.65	1.98	2.05
14	b	1204	CLA	MG-ND	-3.65	1.98	2.05
14	G	1104	CLA	CHD-C1D	3.65	1.45	1.38
14	a	1132	CLA	CHD-C4C	3.65	1.47	1.39
20	B	5002	LMG	O7-C10	3.65	1.44	1.34
18	m	4021	BCR	C11-C12	-3.65	1.25	1.34
18	G	4001	BCR	C11-C12	-3.65	1.25	1.34
14	A	1125	CLA	MG-ND	-3.65	1.98	2.05
14	B	1224	CLA	MG-ND	-3.65	1.98	2.05
14	H	1216	CLA	C1D-ND	-3.65	1.33	1.37
14	a	1133	CLA	CHD-C4C	3.65	1.47	1.39
14	A	1132	CLA	CHD-C4C	3.65	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1208	CLA	CHD-C4C	3.65	1.47	1.39
14	a	1125	CLA	MG-ND	-3.65	1.98	2.05
14	b	1023	CLA	C3B-C2B	3.64	1.45	1.40
14	G	1102	CLA	CHD-C4C	3.64	1.47	1.39
18	a	4011	BCR	C11-C12	-3.64	1.25	1.34
14	b	1206	CLA	C1C-NC	-3.64	1.32	1.37
14	A	1102	CLA	CHD-C4C	3.64	1.47	1.39
14	B	1219	CLA	C3B-C2B	3.64	1.45	1.40
14	B	1206	CLA	C1C-NC	-3.64	1.32	1.37
14	a	1101	CLA	CHD-C4C	3.64	1.47	1.39
14	b	1202	CLA	CHD-C1D	3.64	1.45	1.38
14	H	1208	CLA	CHD-C4C	3.64	1.47	1.39
18	A	4001	BCR	C11-C12	-3.64	1.25	1.34
14	B	1204	CLA	C3B-C2B	3.64	1.45	1.40
14	A	1104	CLA	CHD-C1D	3.64	1.45	1.38
14	a	1102	CLA	CHD-C4C	3.64	1.47	1.39
20	b	5002	LMG	O7-C10	3.64	1.44	1.34
14	G	1116	CLA	CHD-C4C	3.64	1.47	1.39
14	H	1239	CLA	CHD-C4C	3.64	1.47	1.39
14	b	1219	CLA	C3B-C2B	3.64	1.45	1.40
14	G	1101	CLA	CHD-C4C	3.63	1.47	1.39
14	H	1204	CLA	MG-ND	-3.63	1.98	2.05
14	G	1132	CLA	CHD-C4C	3.63	1.47	1.39
14	G	1125	CLA	C3C-C2C	3.63	1.44	1.36
14	A	1133	CLA	CHD-C4C	3.63	1.47	1.39
18	L	4019	BCR	C11-C12	-3.63	1.25	1.34
14	b	1213	CLA	CHD-C4C	3.63	1.47	1.39
14	A	1101	CLA	CHD-C4C	3.62	1.47	1.39
14	B	1204	CLA	MG-ND	-3.62	1.98	2.05
14	b	1203	CLA	CHD-C1D	3.62	1.45	1.38
14	a	1116	CLA	CHD-C4C	3.62	1.47	1.39
14	b	1023	CLA	MG-ND	-3.62	1.98	2.05
14	H	1226	CLA	MG-ND	-3.62	1.98	2.05
14	a	1104	CLA	CHD-C1D	3.62	1.45	1.38
14	A	1111	CLA	CHD-C4C	3.62	1.47	1.39
14	G	1111	CLA	CHD-C4C	3.62	1.47	1.39
18	V	4021	BCR	C11-C12	-3.62	1.25	1.34
14	a	1131	CLA	C3B-C2B	3.62	1.45	1.40
14	b	1234	CLA	C3B-C2B	3.62	1.45	1.40
18	G	4011	BCR	C11-C12	-3.62	1.25	1.34
14	G	1108	CLA	OBD-CAD	3.62	1.28	1.22
14	b	1208	CLA	CHD-C4C	3.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1239	CLA	CHD-C4C	3.62	1.47	1.39
14	A	1131	CLA	C3B-C2B	3.62	1.45	1.40
14	b	1211	CLA	CHD-C4C	3.62	1.47	1.39
14	B	1211	CLA	CHD-C4C	3.62	1.47	1.39
14	b	1204	CLA	C3B-C2B	3.61	1.45	1.40
14	a	1111	CLA	CHD-C4C	3.61	1.47	1.39
14	B	1239	CLA	CHD-C4C	3.61	1.47	1.39
14	G	1131	CLA	C3B-C2B	3.61	1.45	1.40
14	H	1229	CLA	C1D-ND	-3.61	1.33	1.37
18	l	4019	BCR	C11-C12	-3.61	1.25	1.34
18	U	4019	BCR	C11-C12	-3.61	1.25	1.34
14	H	1206	CLA	CHD-C4C	3.60	1.47	1.39
14	H	1234	CLA	C3B-C2B	3.60	1.45	1.40
14	W	1701	CLA	CHD-C4C	3.60	1.47	1.39
14	A	1126	CLA	CHD-C4C	3.60	1.47	1.39
14	a	1013	CLA	C1B-NB	-3.60	1.32	1.35
14	B	1203	CLA	CHD-C1D	3.60	1.45	1.38
14	G	1126	CLA	CHD-C4C	3.59	1.47	1.39
15	b	1237	F6C	C1D-ND	-3.59	1.32	1.37
14	H	1231	CLA	CHD-C4C	3.59	1.47	1.39
14	a	1119	CLA	C1D-ND	-3.59	1.33	1.37
14	b	1206	CLA	CHD-C4C	3.59	1.47	1.39
14	b	1210	CLA	OBD-CAD	3.59	1.28	1.22
14	H	1213	CLA	CHD-C4C	3.59	1.47	1.39
14	H	1206	CLA	MG-ND	-3.59	1.98	2.05
14	b	1229	CLA	C1D-ND	-3.59	1.33	1.37
14	H	1023	CLA	MG-ND	-3.59	1.98	2.05
14	H	1226	CLA	C1C-NC	-3.59	1.32	1.37
14	B	1023	CLA	MG-ND	-3.59	1.98	2.05
14	H	1213	CLA	C1D-ND	-3.59	1.33	1.37
14	B	1219	CLA	C1D-ND	-3.58	1.33	1.37
14	H	1211	CLA	CHD-C4C	3.58	1.47	1.39
14	a	1108	CLA	OBD-CAD	3.58	1.28	1.22
14	b	1213	CLA	C1D-ND	-3.58	1.33	1.37
14	B	1213	CLA	C1D-ND	-3.58	1.33	1.37
14	B	1216	CLA	C1D-ND	-3.58	1.33	1.37
14	X	1701	CLA	CHD-C4C	3.58	1.47	1.39
14	K	1401	CLA	OBD-CAD	3.58	1.28	1.22
14	B	1218	CLA	MG-ND	-3.58	1.98	2.05
14	B	1210	CLA	OBD-CAD	3.58	1.28	1.22
14	G	1122	CLA	C1C-NC	-3.58	1.32	1.37
14	b	1205	CLA	C1C-NC	-3.58	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1108	CLA	OBD-CAD	3.58	1.28	1.22
14	b	1218	CLA	MG-ND	-3.58	1.98	2.05
14	G	1114	CLA	OBD-CAD	3.57	1.28	1.22
14	b	1231	CLA	CHD-C4C	3.57	1.47	1.39
15	B	1230	F6C	CHB-C1B	3.57	1.47	1.39
14	A	1114	CLA	OBD-CAD	3.57	1.28	1.22
14	A	1110	CLA	CHD-C4C	3.57	1.47	1.39
14	B	1229	CLA	C1D-ND	-3.57	1.33	1.37
15	b	1230	F6C	CHB-C1B	3.57	1.47	1.39
14	b	1231	CLA	OBD-CAD	3.57	1.28	1.22
14	B	1022	CLA	MG-ND	-3.57	1.98	2.05
14	H	1220	CLA	CHD-C4C	3.57	1.47	1.39
14	H	1231	CLA	OBD-CAD	3.57	1.28	1.22
14	B	1206	CLA	MG-ND	-3.57	1.98	2.05
15	H	1237	F6C	C1D-ND	-3.57	1.32	1.37
14	H	1225	CLA	MG-ND	-3.57	1.98	2.05
14	H	1218	CLA	MG-ND	-3.57	1.98	2.05
14	x	1701	CLA	CHD-C4C	3.56	1.47	1.39
14	H	1204	CLA	C3B-C2B	3.56	1.45	1.40
14	A	1128	CLA	C1C-NC	-3.56	1.32	1.37
14	T	1401	CLA	OBD-CAD	3.56	1.28	1.22
14	B	1206	CLA	CHD-C4C	3.56	1.47	1.39
14	G	1113	CLA	C1D-ND	-3.56	1.33	1.37
14	U	1503	CLA	CHD-C4C	3.56	1.47	1.39
14	G	1117	CLA	C1C-NC	-3.56	1.32	1.37
14	A	1117	CLA	C1C-NC	-3.56	1.32	1.37
14	H	1217	CLA	CHD-C4C	3.56	1.47	1.39
14	b	1217	CLA	CHD-C4C	3.56	1.47	1.39
14	B	1217	CLA	CHD-C4C	3.56	1.47	1.39
14	H	1022	CLA	MG-ND	-3.56	1.98	2.05
14	A	1119	CLA	C1D-ND	-3.55	1.33	1.37
14	b	1220	CLA	CHD-C4C	3.55	1.47	1.39
14	b	1233	CLA	OBD-CAD	3.55	1.28	1.22
14	B	1231	CLA	OBD-CAD	3.55	1.28	1.22
14	B	1231	CLA	CHD-C4C	3.55	1.47	1.39
14	G	1128	CLA	C1C-NC	-3.55	1.32	1.37
14	a	1114	CLA	OBD-CAD	3.55	1.28	1.22
14	G	1103	CLA	CHD-C4C	3.55	1.47	1.39
15	H	1230	F6C	CHB-C1B	3.55	1.47	1.39
14	B	1236	CLA	CHD-C4C	3.55	1.47	1.39
14	b	1226	CLA	C1C-NC	-3.55	1.32	1.37
14	a	1135	CLA	CHD-C4C	3.55	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1113	CLA	CHD-C4C	3.55	1.47	1.39
14	a	1117	CLA	C1C-NC	-3.55	1.32	1.37
14	L	1503	CLA	CHD-C4C	3.54	1.47	1.39
14	l	1503	CLA	CHD-C4C	3.54	1.47	1.39
14	B	1233	CLA	OBD-CAD	3.54	1.28	1.22
14	B	1021	CLA	CHD-C1D	3.54	1.45	1.38
14	B	1220	CLA	CHD-C4C	3.54	1.47	1.39
14	k	1401	CLA	OBD-CAD	3.54	1.28	1.22
14	G	1129	CLA	CHD-C4C	3.54	1.47	1.39
14	A	1103	CLA	C1C-NC	-3.54	1.32	1.37
14	G	1135	CLA	CHD-C4C	3.54	1.47	1.39
14	b	1225	CLA	MG-ND	-3.54	1.98	2.05
14	G	1119	CLA	C1D-ND	-3.54	1.33	1.37
14	a	1103	CLA	C1C-NC	-3.54	1.32	1.37
14	H	1217	CLA	C1D-ND	-3.54	1.33	1.37
14	a	1110	CLA	CHD-C4C	3.53	1.47	1.39
14	G	1113	CLA	CHD-C4C	3.53	1.47	1.39
14	a	1122	CLA	C1C-NC	-3.53	1.32	1.37
14	H	1205	CLA	C1C-NC	-3.53	1.32	1.37
14	G	1110	CLA	CHD-C4C	3.53	1.47	1.39
18	H	4016	BCR	C11-C12	-3.53	1.25	1.34
14	a	1113	CLA	C1D-ND	-3.53	1.33	1.37
14	b	1022	CLA	MG-ND	-3.53	1.98	2.05
14	a	1128	CLA	C1C-NC	-3.53	1.32	1.37
15	B	1237	F6C	C1D-ND	-3.53	1.32	1.37
14	G	1012	CLA	CHD-C4C	3.53	1.47	1.39
14	B	1205	CLA	C1C-NC	-3.53	1.32	1.37
14	H	1219	CLA	C1D-ND	-3.53	1.33	1.37
14	A	1130	CLA	CHD-C4C	3.52	1.47	1.39
14	B	1239	CLA	C1C-NC	-3.52	1.32	1.37
14	H	1210	CLA	OBD-CAD	3.52	1.28	1.22
14	B	1219	CLA	OBD-CAD	3.52	1.28	1.22
14	B	1225	CLA	MG-ND	-3.52	1.98	2.05
14	H	1233	CLA	OBD-CAD	3.52	1.28	1.22
14	a	1112	CLA	C1D-ND	-3.52	1.33	1.37
14	H	1219	CLA	OBD-CAD	3.52	1.28	1.22
14	a	1113	CLA	CHD-C4C	3.52	1.47	1.39
14	H	1222	CLA	CHD-C4C	3.52	1.47	1.39
14	a	1103	CLA	CHD-C4C	3.52	1.47	1.39
14	a	1130	CLA	CHD-C4C	3.52	1.47	1.39
14	H	1236	CLA	CHD-C4C	3.52	1.47	1.39
14	B	1221	CLA	MG-ND	-3.52	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1226	CLA	C1C-NC	-3.52	1.32	1.37
14	B	1217	CLA	C1D-ND	-3.52	1.33	1.37
14	A	1122	CLA	C1C-NC	-3.51	1.32	1.37
14	G	1124	CLA	C1C-NC	-3.51	1.32	1.37
14	a	1012	CLA	CHD-C4C	3.51	1.47	1.39
14	A	1106	CLA	CHD-C4C	3.51	1.47	1.39
14	G	1103	CLA	C1C-NC	-3.51	1.32	1.37
14	H	1021	CLA	CHD-C1D	3.51	1.45	1.38
14	b	1236	CLA	CHD-C4C	3.51	1.47	1.39
14	H	1239	CLA	C1C-NC	-3.51	1.32	1.37
14	a	1129	CLA	CHD-C4C	3.51	1.47	1.39
14	b	1222	CLA	CHD-C4C	3.51	1.47	1.39
14	A	1135	CLA	CHD-C4C	3.51	1.47	1.39
14	B	1234	CLA	C3B-C2B	3.51	1.45	1.40
14	B	1222	CLA	CHD-C4C	3.51	1.47	1.39
14	b	1219	CLA	C1D-ND	-3.51	1.33	1.37
14	A	1103	CLA	CHD-C4C	3.51	1.47	1.39
14	H	1210	CLA	C1C-NC	-3.51	1.32	1.37
14	A	1012	CLA	CHD-C4C	3.51	1.47	1.39
14	a	1132	CLA	OBD-CAD	3.50	1.28	1.22
14	G	1137	CLA	CHD-C4C	3.50	1.47	1.39
14	b	1236	CLA	C3B-C2B	3.50	1.45	1.40
18	B	4016	BCR	C11-C12	-3.50	1.25	1.34
14	b	1210	CLA	C1C-NC	-3.50	1.32	1.37
14	A	1105	CLA	OBD-CAD	3.50	1.28	1.22
14	b	1217	CLA	C1D-ND	-3.50	1.33	1.37
14	b	1221	CLA	MG-ND	-3.50	1.98	2.05
14	G	1106	CLA	CHD-C4C	3.50	1.47	1.39
14	G	1013	CLA	C1B-NB	-3.50	1.32	1.35
14	b	1219	CLA	OBD-CAD	3.50	1.28	1.22
14	H	1221	CLA	MG-ND	-3.50	1.98	2.05
14	H	1234	CLA	CHD-C1D	3.49	1.45	1.38
14	b	1234	CLA	CHD-C1D	3.49	1.45	1.38
14	A	1129	CLA	CHD-C4C	3.49	1.47	1.39
14	a	1107	CLA	CHD-C4C	3.49	1.47	1.39
14	G	1130	CLA	CHD-C4C	3.49	1.47	1.39
14	B	1234	CLA	CHD-C1D	3.49	1.45	1.38
18	b	4016	BCR	C11-C12	-3.49	1.25	1.34
14	b	1232	CLA	OBD-CAD	3.49	1.28	1.22
14	A	1113	CLA	C1D-ND	-3.49	1.33	1.37
14	A	1124	CLA	C1C-NC	-3.49	1.32	1.37
14	G	1107	CLA	CHD-C4C	3.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1021	CLA	CHD-C1D	3.49	1.45	1.38
14	G	1105	CLA	OBD-CAD	3.49	1.28	1.22
14	B	1021	CLA	C1C-NC	-3.48	1.32	1.37
14	a	1106	CLA	CHD-C4C	3.48	1.47	1.39
15	B	1230	F6C	OBD-CAD	3.48	1.28	1.22
14	B	1205	CLA	MG-ND	-3.48	1.98	2.05
14	a	1124	CLA	C1C-NC	-3.48	1.32	1.37
14	b	1239	CLA	C1C-NC	-3.48	1.32	1.37
14	a	1137	CLA	CHD-C4C	3.48	1.47	1.39
14	A	1137	CLA	CHD-C4C	3.48	1.47	1.39
14	G	1101	CLA	C1D-ND	-3.48	1.33	1.37
14	A	1101	CLA	C1D-ND	-3.47	1.33	1.37
14	b	1216	CLA	OBD-CAD	3.47	1.28	1.22
14	a	1101	CLA	C1D-ND	-3.47	1.33	1.37
14	a	1105	CLA	OBD-CAD	3.47	1.28	1.22
14	a	1130	CLA	MG-ND	-3.47	1.98	2.05
14	b	1021	CLA	C1C-NC	-3.47	1.32	1.37
14	B	1216	CLA	OBD-CAD	3.47	1.28	1.22
14	a	1125	CLA	CHD-C1D	3.47	1.45	1.38
14	H	1236	CLA	C3B-C2B	3.47	1.45	1.40
13	G	1011	CL0	C1C-NC	-3.46	1.32	1.37
14	G	1132	CLA	OBD-CAD	3.46	1.28	1.22
14	A	1104	CLA	CHD-C4C	3.46	1.47	1.39
14	B	1236	CLA	C3B-C2B	3.46	1.45	1.40
14	B	1210	CLA	C1C-NC	-3.46	1.32	1.37
14	G	1125	CLA	CHD-C1D	3.46	1.45	1.38
14	H	1205	CLA	MG-ND	-3.46	1.98	2.05
14	a	1115	CLA	OBD-CAD	3.46	1.28	1.22
14	A	1107	CLA	CHD-C4C	3.46	1.47	1.39
14	G	1130	CLA	MG-ND	-3.46	1.98	2.05
14	H	1021	CLA	C1C-NC	-3.46	1.32	1.37
14	H	1232	CLA	OBD-CAD	3.45	1.28	1.22
14	A	1126	CLA	MG-ND	-3.45	1.98	2.05
14	A	1112	CLA	OBD-CAD	3.45	1.28	1.22
14	a	1132	CLA	C3B-C2B	3.45	1.45	1.40
13	a	1011	CL0	MG-ND	-3.45	1.98	2.05
14	A	1137	CLA	MG-ND	-3.45	1.98	2.05
13	G	1011	CL0	MG-ND	-3.45	1.98	2.05
14	A	1130	CLA	MG-ND	-3.45	1.98	2.05
13	a	1011	CL0	C1C-NC	-3.45	1.32	1.37
14	A	1132	CLA	OBD-CAD	3.45	1.28	1.22
14	a	1123	CLA	MG-ND	-3.45	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1133	CLA	OBD-CAD	3.45	1.28	1.22
14	H	1216	CLA	OBD-CAD	3.45	1.28	1.22
14	A	1112	CLA	C1D-ND	-3.44	1.33	1.37
14	G	1132	CLA	C3B-C2B	3.44	1.45	1.40
18	H	4006	BCR	C11-C12	-3.44	1.25	1.34
18	b	4006	BCR	C11-C12	-3.44	1.25	1.34
14	G	1123	CLA	MG-ND	-3.44	1.99	2.05
15	H	1230	F6C	OBD-CAD	3.44	1.28	1.22
14	A	1132	CLA	C3B-C2B	3.44	1.45	1.40
14	B	1232	CLA	OBD-CAD	3.44	1.28	1.22
14	a	1112	CLA	OBD-CAD	3.44	1.28	1.22
14	B	1209	CLA	C1D-ND	-3.44	1.33	1.37
14	H	1220	CLA	C1C-NC	-3.44	1.32	1.37
14	G	1112	CLA	OBD-CAD	3.44	1.28	1.22
14	A	1125	CLA	CHD-C1D	3.44	1.45	1.38
14	B	1227	CLA	OBD-CAD	3.44	1.28	1.22
18	B	4006	BCR	C11-C12	-3.44	1.25	1.34
14	G	1112	CLA	C1D-ND	-3.44	1.33	1.37
14	H	1209	CLA	C1D-ND	-3.44	1.33	1.37
14	H	1232	CLA	C1D-ND	-3.44	1.33	1.37
14	G	1133	CLA	OBD-CAD	3.44	1.28	1.22
14	G	1126	CLA	MG-ND	-3.44	1.99	2.05
14	a	1120	CLA	CHD-C4C	3.44	1.47	1.39
14	a	1126	CLA	MG-ND	-3.43	1.99	2.05
14	A	1120	CLA	CHD-C4C	3.43	1.47	1.39
18	A	4003	BCR	C11-C12	-3.43	1.25	1.34
14	G	1127	CLA	MG-ND	-3.43	1.99	2.05
14	H	1223	CLA	MG-ND	-3.43	1.99	2.05
14	a	1133	CLA	OBD-CAD	3.43	1.28	1.22
14	A	1115	CLA	OBD-CAD	3.43	1.28	1.22
14	a	1013	CLA	OBD-CAD	3.43	1.28	1.22
14	B	1218	CLA	OBD-CAD	3.43	1.28	1.22
18	B	4009	BCR	C11-C12	-3.43	1.25	1.34
14	A	1123	CLA	MG-ND	-3.43	1.99	2.05
15	b	1230	F6C	OBD-CAD	3.43	1.28	1.22
14	B	1220	CLA	OBD-CAD	3.43	1.28	1.22
14	b	1205	CLA	MG-ND	-3.43	1.99	2.05
14	H	1236	CLA	C1C-NC	-3.43	1.32	1.37
14	L	1502	CLA	C3B-C2B	3.43	1.45	1.40
14	B	1223	CLA	MG-ND	-3.43	1.99	2.05
18	b	4009	BCR	C11-C12	-3.42	1.25	1.34
14	A	1139	CLA	C1C-NC	-3.42	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1226	CLA	OBD-CAD	3.42	1.28	1.22
14	G	1136	CLA	C3B-C2B	3.42	1.45	1.40
13	A	1011	CL0	MG-ND	-3.42	1.99	2.05
14	A	1127	CLA	MG-ND	-3.42	1.99	2.05
18	H	4009	BCR	C11-C12	-3.42	1.25	1.34
14	b	1218	CLA	OBD-CAD	3.42	1.28	1.22
14	G	1120	CLA	CHD-C4C	3.42	1.47	1.39
14	G	1123	CLA	CHD-C4C	3.42	1.47	1.39
14	H	1023	CLA	CHD-C4C	3.42	1.47	1.39
14	H	1227	CLA	OBD-CAD	3.42	1.28	1.22
13	A	1011	CL0	C1C-NC	-3.42	1.32	1.37
14	G	1104	CLA	CHD-C4C	3.42	1.47	1.39
18	a	4003	BCR	C11-C12	-3.42	1.25	1.34
14	b	1220	CLA	C1C-NC	-3.42	1.32	1.37
14	G	1129	CLA	MG-ND	-3.42	1.99	2.05
14	a	1127	CLA	MG-ND	-3.42	1.99	2.05
14	a	1104	CLA	CHD-C4C	3.41	1.47	1.39
14	b	1227	CLA	OBD-CAD	3.41	1.28	1.22
14	G	1115	CLA	OBD-CAD	3.41	1.28	1.22
14	H	1218	CLA	OBD-CAD	3.41	1.28	1.22
14	A	1013	CLA	OBD-CAD	3.41	1.28	1.22
14	a	1129	CLA	MG-ND	-3.41	1.99	2.05
14	A	1129	CLA	MG-ND	-3.41	1.99	2.05
14	B	1023	CLA	CHD-C4C	3.41	1.47	1.39
14	A	1135	CLA	MG-ND	-3.41	1.99	2.05
14	b	1209	CLA	C1D-ND	-3.40	1.33	1.37
14	H	1216	CLA	C3B-C2B	3.40	1.45	1.40
14	b	1023	CLA	CHD-C4C	3.40	1.47	1.39
14	G	1013	CLA	OBD-CAD	3.40	1.28	1.22
14	H	1226	CLA	OBD-CAD	3.40	1.28	1.22
14	a	1139	CLA	C1C-NC	-3.40	1.32	1.37
14	a	1102	CLA	MG-ND	-3.40	1.99	2.05
14	A	1013	CLA	CHD-C1D	3.40	1.45	1.38
18	G	4003	BCR	C11-C12	-3.40	1.25	1.34
14	A	1136	CLA	C3B-C2B	3.40	1.45	1.40
14	b	1212	CLA	CHD-C4C	3.40	1.47	1.39
14	H	1213	CLA	OBD-CAD	3.39	1.28	1.22
14	G	1137	CLA	C1C-NC	-3.39	1.32	1.37
14	a	1013	CLA	CHD-C1D	3.39	1.45	1.38
14	H	1228	CLA	OBD-CAD	3.39	1.28	1.22
14	a	1137	CLA	MG-ND	-3.39	1.99	2.05
14	H	1212	CLA	CHD-C4C	3.39	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1107	CLA	MG-ND	-3.39	1.99	2.05
14	L	1501	CLA	CHD-C4C	3.39	1.47	1.39
14	H	1221	CLA	CHD-C4C	3.39	1.47	1.39
14	a	1128	CLA	CHD-C4C	3.39	1.47	1.39
14	G	1118	CLA	OBD-CAD	3.38	1.28	1.22
14	A	1128	CLA	C1B-NB	-3.38	1.32	1.35
14	B	1232	CLA	C1D-ND	-3.38	1.33	1.37
14	A	1128	CLA	CHD-C4C	3.38	1.47	1.39
14	b	1232	CLA	C1D-ND	-3.38	1.33	1.37
14	l	1501	CLA	CHD-C4C	3.38	1.46	1.39
14	b	1220	CLA	OBD-CAD	3.38	1.28	1.22
13	a	1011	CL0	CHD-C4C	3.38	1.46	1.39
14	A	1137	CLA	C1C-NC	-3.38	1.32	1.37
14	a	1123	CLA	CHD-C4C	3.38	1.46	1.39
14	G	1137	CLA	MG-ND	-3.38	1.99	2.05
14	b	1228	CLA	OBD-CAD	3.37	1.28	1.22
14	A	1131	CLA	MG-ND	-3.37	1.99	2.05
14	b	1201	CLA	C1C-NC	-3.37	1.32	1.37
14	U	1502	CLA	C3B-C2B	3.37	1.45	1.40
14	G	1111	CLA	OBD-CAD	3.37	1.28	1.22
14	G	1128	CLA	CHD-C4C	3.37	1.46	1.39
14	a	1128	CLA	C1B-NB	-3.37	1.32	1.35
14	G	1135	CLA	MG-ND	-3.37	1.99	2.05
14	W	1701	CLA	OBD-CAD	3.37	1.28	1.22
14	G	1013	CLA	CHD-C1D	3.37	1.44	1.38
14	a	1102	CLA	OBD-CAD	3.37	1.28	1.22
14	G	1107	CLA	MG-ND	-3.37	1.99	2.05
14	B	1221	CLA	CHD-C4C	3.37	1.46	1.39
14	B	1226	CLA	OBD-CAD	3.37	1.28	1.22
14	b	1213	CLA	OBD-CAD	3.37	1.28	1.22
14	A	1123	CLA	CHD-C4C	3.36	1.46	1.39
14	H	1229	CLA	OBD-CAD	3.36	1.28	1.22
14	G	1102	CLA	MG-ND	-3.36	1.99	2.05
14	G	1139	CLA	C1C-NC	-3.36	1.32	1.37
14	L	1503	CLA	C1C-NC	-3.36	1.32	1.37
14	a	1111	CLA	OBD-CAD	3.36	1.28	1.22
13	A	1011	CL0	CHD-C4C	3.36	1.46	1.39
14	A	1102	CLA	MG-ND	-3.36	1.99	2.05
14	a	1135	CLA	OBD-CAD	3.36	1.28	1.22
14	a	1101	CLA	OBD-CAD	3.36	1.28	1.22
14	A	1102	CLA	OBD-CAD	3.36	1.28	1.22
14	a	1136	CLA	C3B-C2B	3.36	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1107	CLA	MG-ND	-3.36	1.99	2.05
14	B	1215	CLA	MG-ND	-3.36	1.99	2.05
14	A	1140	CLA	CHD-C4C	3.36	1.46	1.39
14	A	1101	CLA	OBD-CAD	3.36	1.28	1.22
14	H	1224	CLA	CHD-C4C	3.36	1.46	1.39
14	b	1221	CLA	CHD-C4C	3.36	1.46	1.39
14	B	1208	CLA	OBD-CAD	3.36	1.28	1.22
14	G	1102	CLA	OBD-CAD	3.36	1.28	1.22
14	b	1225	CLA	C1C-NC	-3.36	1.32	1.37
14	B	1220	CLA	C1C-NC	-3.36	1.32	1.37
14	B	1212	CLA	CHD-C4C	3.35	1.46	1.39
14	b	1216	CLA	C3B-C2B	3.35	1.45	1.40
14	U	1501	CLA	CHD-C4C	3.35	1.46	1.39
14	H	1215	CLA	MG-ND	-3.35	1.99	2.05
14	b	1215	CLA	MG-ND	-3.35	1.99	2.05
14	H	1220	CLA	OBD-CAD	3.35	1.28	1.22
13	G	1011	CL0	CHD-C4C	3.35	1.46	1.39
14	H	1239	CLA	C3B-C2B	3.35	1.45	1.40
14	a	1118	CLA	MG-ND	-3.35	1.99	2.05
14	a	1135	CLA	MG-ND	-3.35	1.99	2.05
13	G	1011	CL0	C3B-C2B	3.35	1.45	1.40
14	l	1503	CLA	C1C-NC	-3.35	1.32	1.37
14	a	1118	CLA	OBD-CAD	3.35	1.28	1.22
14	G	1131	CLA	MG-ND	-3.35	1.99	2.05
14	b	1223	CLA	MG-ND	-3.35	1.99	2.05
14	A	1130	CLA	C1C-NC	-3.35	1.32	1.37
14	A	1118	CLA	OBD-CAD	3.35	1.28	1.22
14	b	1233	CLA	C1D-ND	-3.35	1.33	1.37
14	A	1111	CLA	OBD-CAD	3.35	1.28	1.22
14	a	1114	CLA	C1D-ND	-3.34	1.33	1.37
14	b	1224	CLA	CHD-C4C	3.34	1.46	1.39
14	B	1239	CLA	C3B-C2B	3.34	1.45	1.40
14	a	1140	CLA	CHD-C4C	3.34	1.46	1.39
14	B	1223	CLA	CHD-C4C	3.34	1.46	1.39
14	H	1223	CLA	CHD-C4C	3.34	1.46	1.39
14	b	1202	CLA	CHD-C4C	3.34	1.46	1.39
14	G	1110	CLA	OBD-CAD	3.34	1.28	1.22
14	B	1224	CLA	CHD-C4C	3.34	1.46	1.39
14	l	1502	CLA	C3B-C2B	3.34	1.45	1.40
14	G	1101	CLA	OBD-CAD	3.34	1.28	1.22
14	b	1229	CLA	OBD-CAD	3.34	1.28	1.22
14	a	1137	CLA	C1C-NC	-3.34	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1119	CLA	OBD-CAD	3.34	1.28	1.22
14	b	1214	CLA	MG-ND	-3.34	1.99	2.05
14	H	1201	CLA	C1C-NC	-3.34	1.32	1.37
14	B	1201	CLA	OBD-CAD	3.33	1.28	1.22
14	a	1131	CLA	MG-ND	-3.33	1.99	2.05
14	L	1501	CLA	MG-ND	-3.33	1.99	2.05
14	b	1223	CLA	CHD-C4C	3.33	1.46	1.39
14	b	1228	CLA	C1C-NC	-3.33	1.32	1.37
14	G	1116	CLA	OBD-CAD	3.33	1.28	1.22
14	H	1228	CLA	C1C-NC	-3.33	1.32	1.37
14	B	1228	CLA	C1C-NC	-3.33	1.32	1.37
14	G	1140	CLA	CHD-C4C	3.33	1.46	1.39
20	U	5007	LMG	C19-C18	-3.33	1.32	1.51
14	G	1135	CLA	OBD-CAD	3.33	1.28	1.22
14	B	1216	CLA	C3B-C2B	3.33	1.45	1.40
14	A	1119	CLA	OBD-CAD	3.33	1.28	1.22
14	A	1135	CLA	OBD-CAD	3.33	1.28	1.22
14	H	1239	CLA	MG-ND	-3.33	1.99	2.05
14	B	1209	CLA	OBD-CAD	3.33	1.28	1.22
14	A	1126	CLA	C1C-NC	-3.33	1.32	1.37
14	H	1202	CLA	CHD-C4C	3.33	1.46	1.39
14	H	1209	CLA	OBD-CAD	3.33	1.28	1.22
14	a	1110	CLA	OBD-CAD	3.32	1.28	1.22
14	B	1215	CLA	OBD-CAD	3.32	1.28	1.22
14	A	1118	CLA	MG-ND	-3.32	1.99	2.05
14	b	1236	CLA	C1C-NC	-3.32	1.32	1.37
14	A	1116	CLA	OBD-CAD	3.32	1.28	1.22
14	B	1229	CLA	OBD-CAD	3.32	1.28	1.22
14	a	1130	CLA	C1C-NC	-3.32	1.32	1.37
14	B	1236	CLA	C1C-NC	-3.32	1.32	1.37
14	H	1201	CLA	OBD-CAD	3.32	1.28	1.22
14	X	1701	CLA	OBD-CAD	3.32	1.28	1.22
14	H	1225	CLA	C1C-NC	-3.32	1.32	1.37
14	a	1126	CLA	C1C-NC	-3.32	1.32	1.37
14	G	1118	CLA	MG-ND	-3.32	1.99	2.05
14	l	1501	CLA	MG-ND	-3.32	1.99	2.05
14	b	1209	CLA	OBD-CAD	3.32	1.28	1.22
14	A	1103	CLA	MG-ND	-3.32	1.99	2.05
14	A	1140	CLA	MG-ND	-3.32	1.99	2.05
20	A	5005	LMG	C40-C39	-3.32	1.32	1.51
14	U	1503	CLA	C1C-NC	-3.32	1.32	1.37
20	U	5007	LMG	C40-C39	-3.32	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1022	CLA	C3B-C2B	3.32	1.45	1.40
14	a	1139	CLA	CHD-C4C	3.32	1.46	1.39
14	B	1202	CLA	CHD-C4C	3.32	1.46	1.39
20	l	5007	LMG	C40-C39	-3.32	1.33	1.51
20	L	5007	LMG	C19-C18	-3.31	1.33	1.51
20	a	5005	LMG	C40-C39	-3.31	1.33	1.51
20	L	5007	LMG	C40-C39	-3.31	1.33	1.51
18	H	4013	BCR	C11-C12	-3.31	1.26	1.34
14	H	1214	CLA	MG-ND	-3.31	1.99	2.05
14	B	1239	CLA	MG-ND	-3.31	1.99	2.05
14	B	1222	CLA	C1C-NC	-3.31	1.32	1.37
14	x	1701	CLA	OBD-CAD	3.31	1.28	1.22
14	H	1208	CLA	OBD-CAD	3.31	1.28	1.22
14	a	1116	CLA	OBD-CAD	3.31	1.28	1.22
20	b	5002	LMG	C22-C21	-3.31	1.33	1.51
14	a	1111	CLA	C1C-NC	-3.31	1.32	1.37
15	b	1207	F6C	C1C-NC	-3.31	1.32	1.35
14	A	1139	CLA	CHD-C4C	3.31	1.46	1.39
15	b	1237	F6C	CHB-C1B	3.31	1.46	1.39
14	H	1215	CLA	OBD-CAD	3.31	1.28	1.22
15	H	1237	F6C	CHB-C1B	3.31	1.46	1.39
14	b	1223	CLA	C1C-NC	-3.31	1.32	1.37
14	H	1203	CLA	MG-ND	-3.31	1.99	2.05
14	B	1228	CLA	OBD-CAD	3.31	1.28	1.22
20	G	5005	LMG	C40-C39	-3.31	1.33	1.51
14	b	1239	CLA	C3B-C2B	3.30	1.45	1.40
20	l	5007	LMG	C19-C18	-3.30	1.33	1.51
14	b	1201	CLA	OBD-CAD	3.30	1.28	1.22
14	b	1202	CLA	C3B-C2B	3.30	1.45	1.40
14	a	1013	CLA	CHD-C4C	3.30	1.46	1.39
14	b	1225	CLA	CHD-C4C	3.30	1.46	1.39
20	B	5002	LMG	C22-C21	-3.30	1.33	1.51
14	a	1140	CLA	MG-ND	-3.30	1.99	2.05
14	b	1208	CLA	OBD-CAD	3.30	1.28	1.22
14	A	1110	CLA	OBD-CAD	3.30	1.28	1.22
14	B	1224	CLA	OBD-CAD	3.30	1.28	1.22
14	a	1117	CLA	OBD-CAD	3.30	1.28	1.22
14	B	1223	CLA	C1C-NC	-3.30	1.32	1.37
18	b	4013	BCR	C11-C12	-3.30	1.26	1.34
14	H	1204	CLA	C1C-NC	-3.30	1.32	1.37
14	b	1215	CLA	OBD-CAD	3.30	1.28	1.22
14	G	1120	CLA	OBD-CAD	3.30	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1127	CLA	OBD-CAD	3.30	1.28	1.22
14	A	1126	CLA	OBD-CAD	3.30	1.28	1.22
14	B	1213	CLA	OBD-CAD	3.30	1.28	1.22
14	A	1117	CLA	OBD-CAD	3.30	1.28	1.22
14	B	1023	CLA	OBD-CAD	3.30	1.28	1.22
14	H	1221	CLA	C1C-NC	-3.30	1.32	1.37
14	B	1225	CLA	C1C-NC	-3.30	1.32	1.37
14	G	1124	CLA	OBD-CAD	3.30	1.28	1.22
14	B	1239	CLA	OBD-CAD	3.30	1.28	1.22
15	B	1237	F6C	CHB-C1B	3.30	1.46	1.39
14	G	1119	CLA	OBD-CAD	3.30	1.28	1.22
14	U	1501	CLA	MG-ND	-3.30	1.99	2.05
14	G	1126	CLA	C1C-NC	-3.30	1.32	1.37
14	A	1120	CLA	OBD-CAD	3.29	1.28	1.22
14	G	1117	CLA	OBD-CAD	3.29	1.28	1.22
14	a	1120	CLA	OBD-CAD	3.29	1.28	1.22
14	L	1501	CLA	OBD-CAD	3.29	1.28	1.22
14	G	1114	CLA	C1D-ND	-3.29	1.33	1.37
14	A	1111	CLA	C1C-NC	-3.29	1.32	1.37
14	A	1124	CLA	OBD-CAD	3.29	1.28	1.22
14	G	1140	CLA	C1C-NC	-3.29	1.32	1.37
14	G	1128	CLA	C1B-NB	-3.29	1.32	1.35
20	H	5002	LMG	C22-C21	-3.29	1.33	1.51
18	B	4013	BCR	C11-C12	-3.29	1.26	1.34
14	a	1103	CLA	MG-ND	-3.29	1.99	2.05
14	H	1233	CLA	C1D-ND	-3.29	1.33	1.37
14	G	1139	CLA	CHD-C4C	3.29	1.46	1.39
14	G	1013	CLA	CHD-C4C	3.29	1.46	1.39
14	A	1013	CLA	CHD-C4C	3.29	1.46	1.39
14	a	1117	CLA	MG-ND	-3.29	1.99	2.05
14	b	1203	CLA	C1C-NC	-3.29	1.32	1.37
14	B	1221	CLA	C1C-NC	-3.29	1.32	1.37
14	b	1023	CLA	OBD-CAD	3.29	1.28	1.22
14	A	1116	CLA	MG-ND	-3.29	1.99	2.05
14	H	1227	CLA	MG-ND	-3.29	1.99	2.05
14	G	1131	CLA	C1C-NC	-3.29	1.32	1.37
14	b	1227	CLA	MG-ND	-3.28	1.99	2.05
15	b	1230	F6C	C1C-NC	-3.28	1.32	1.35
14	A	1131	CLA	C1C-NC	-3.28	1.32	1.37
14	B	1233	CLA	C1D-ND	-3.28	1.33	1.37
14	B	1201	CLA	C1C-NC	-3.28	1.32	1.37
13	a	1011	CL0	C3B-C2B	3.28	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1011	CL0	C3B-C2B	3.28	1.44	1.40
20	B	5002	LMG	C37-C36	-3.28	1.33	1.51
14	G	1119	CLA	MG-ND	-3.28	1.99	2.05
14	H	1222	CLA	C1C-NC	-3.28	1.32	1.37
14	A	1140	CLA	C1C-NC	-3.28	1.32	1.37
14	G	1116	CLA	MG-ND	-3.28	1.99	2.05
14	A	1119	CLA	MG-ND	-3.28	1.99	2.05
14	A	1139	CLA	OBD-CAD	3.28	1.28	1.22
14	B	1203	CLA	CHD-C4C	3.28	1.46	1.39
15	G	1121	F6C	OBD-CAD	3.28	1.28	1.22
15	A	1121	F6C	OBD-CAD	3.28	1.28	1.22
14	a	1136	CLA	C1C-NC	-3.28	1.32	1.37
14	A	1114	CLA	C1D-ND	-3.28	1.33	1.37
14	B	1205	CLA	CHD-C4C	3.28	1.46	1.39
14	A	1135	CLA	C1C-NC	-3.28	1.32	1.37
14	L	1501	CLA	C1C-NC	-3.28	1.32	1.37
14	A	1127	CLA	OBD-CAD	3.28	1.28	1.22
14	a	1124	CLA	OBD-CAD	3.28	1.28	1.22
14	b	1222	CLA	MG-ND	-3.28	1.99	2.05
14	B	1203	CLA	C1C-NC	-3.28	1.32	1.37
14	H	1236	CLA	OBD-CAD	3.28	1.28	1.22
14	l	1501	CLA	C1C-NC	-3.28	1.32	1.37
14	H	1022	CLA	C3B-C2B	3.28	1.44	1.40
14	B	1227	CLA	MG-ND	-3.28	1.99	2.05
14	B	1202	CLA	C3B-C2B	3.27	1.44	1.40
14	a	1126	CLA	OBD-CAD	3.27	1.28	1.22
14	G	1130	CLA	C1C-NC	-3.27	1.32	1.37
20	l	5007	LMG	C37-C36	-3.27	1.33	1.51
14	U	1501	CLA	OBD-CAD	3.27	1.28	1.22
20	U	5007	LMG	C37-C36	-3.27	1.33	1.51
15	a	1121	F6C	OBD-CAD	3.27	1.28	1.22
14	b	1224	CLA	OBD-CAD	3.27	1.28	1.22
14	H	1222	CLA	MG-ND	-3.27	1.99	2.05
20	b	5002	LMG	C37-C36	-3.27	1.33	1.51
14	B	1222	CLA	MG-ND	-3.27	1.99	2.05
14	H	1023	CLA	OBD-CAD	3.27	1.28	1.22
14	L	1503	CLA	OBD-CAD	3.27	1.28	1.22
14	G	1140	CLA	MG-ND	-3.27	1.99	2.05
14	b	1239	CLA	OBD-CAD	3.27	1.28	1.22
14	G	1111	CLA	C1C-NC	-3.27	1.32	1.37
14	b	1221	CLA	C1C-NC	-3.27	1.32	1.37
14	B	1204	CLA	C1C-NC	-3.27	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1122	CLA	OBD-CAD	3.27	1.28	1.22
14	B	1203	CLA	MG-ND	-3.27	1.99	2.05
14	H	1224	CLA	OBD-CAD	3.27	1.28	1.22
14	b	1212	CLA	OBD-CAD	3.27	1.28	1.22
14	B	1211	CLA	OBD-CAD	3.27	1.28	1.22
20	L	5007	LMG	C37-C36	-3.27	1.33	1.51
14	G	1117	CLA	MG-ND	-3.27	1.99	2.05
14	b	1203	CLA	MG-ND	-3.27	1.99	2.05
14	a	1122	CLA	OBD-CAD	3.27	1.28	1.22
14	G	1103	CLA	MG-ND	-3.27	1.99	2.05
14	A	1117	CLA	MG-ND	-3.27	1.99	2.05
14	a	1119	CLA	MG-ND	-3.26	1.99	2.05
20	G	5005	LMG	C43-C42	-3.26	1.33	1.51
14	H	1223	CLA	C1C-NC	-3.26	1.32	1.37
14	A	1136	CLA	C1C-NC	-3.26	1.32	1.37
14	G	1106	CLA	C1C-NC	-3.26	1.32	1.37
14	b	1204	CLA	C1C-NC	-3.26	1.32	1.37
15	B	1230	F6C	C1C-NC	-3.26	1.32	1.35
20	A	5005	LMG	C43-C42	-3.26	1.33	1.51
14	H	1234	CLA	CHD-C4C	3.26	1.46	1.39
14	G	1126	CLA	OBD-CAD	3.26	1.28	1.22
14	A	1113	CLA	C1C-NC	-3.26	1.32	1.37
14	H	1225	CLA	CHD-C4C	3.26	1.46	1.39
14	B	1225	CLA	CHD-C4C	3.26	1.46	1.39
14	G	1104	CLA	OBD-CAD	3.26	1.28	1.22
14	B	1212	CLA	OBD-CAD	3.26	1.28	1.22
14	B	1022	CLA	C3B-C2B	3.26	1.44	1.40
14	a	1116	CLA	MG-ND	-3.26	1.99	2.05
14	l	1503	CLA	OBD-CAD	3.26	1.28	1.22
14	G	1136	CLA	C1C-NC	-3.26	1.32	1.37
14	H	1203	CLA	C1C-NC	-3.26	1.32	1.37
14	A	1109	CLA	OBD-CAD	3.26	1.28	1.22
20	H	5002	LMG	C37-C36	-3.26	1.33	1.51
14	a	1106	CLA	OBD-CAD	3.26	1.28	1.22
14	H	1205	CLA	CHD-C4C	3.26	1.46	1.39
14	b	1203	CLA	CHD-C4C	3.26	1.46	1.39
14	a	1106	CLA	C1C-NC	-3.26	1.32	1.37
14	H	1202	CLA	C3B-C2B	3.26	1.44	1.40
14	H	1234	CLA	C1C-NC	-3.26	1.32	1.37
14	B	1214	CLA	MG-ND	-3.26	1.99	2.05
14	b	1234	CLA	CHD-C4C	3.26	1.46	1.39
18	B	4004	BCR	C11-C12	-3.26	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	4004	BCR	C11-C12	-3.26	1.26	1.34
18	b	4004	BCR	C11-C12	-3.26	1.26	1.34
14	H	1211	CLA	OBD-CAD	3.26	1.28	1.22
14	b	1239	CLA	MG-ND	-3.26	1.99	2.05
14	a	1104	CLA	OBD-CAD	3.25	1.28	1.22
14	a	1139	CLA	OBD-CAD	3.25	1.28	1.22
14	a	1112	CLA	C1C-NC	-3.25	1.32	1.37
14	a	1135	CLA	C1C-NC	-3.25	1.32	1.37
14	H	1239	CLA	OBD-CAD	3.25	1.28	1.22
20	a	5005	LMG	C43-C42	-3.25	1.33	1.51
15	A	1121	F6C	C1D-ND	-3.25	1.33	1.37
14	G	1139	CLA	OBD-CAD	3.25	1.28	1.22
14	G	1112	CLA	C1C-NC	-3.25	1.33	1.37
14	l	1501	CLA	OBD-CAD	3.25	1.28	1.22
14	a	1131	CLA	C1C-NC	-3.25	1.33	1.37
14	U	1501	CLA	C1C-NC	-3.25	1.33	1.37
15	H	1230	F6C	C1C-NC	-3.25	1.32	1.35
14	H	1212	CLA	OBD-CAD	3.24	1.28	1.22
14	A	1106	CLA	OBD-CAD	3.24	1.28	1.22
14	b	1222	CLA	C1C-NC	-3.24	1.33	1.37
15	B	1207	F6C	C1C-NC	-3.24	1.32	1.35
14	U	1503	CLA	OBD-CAD	3.24	1.28	1.22
14	G	1108	CLA	C1C-NC	-3.24	1.33	1.37
14	a	1108	CLA	C1C-NC	-3.24	1.33	1.37
14	B	1234	CLA	CHD-C4C	3.24	1.46	1.39
14	B	1201	CLA	MG-ND	-3.24	1.99	2.05
14	H	1224	CLA	C1C-NC	-3.24	1.33	1.37
14	H	1203	CLA	CHD-C4C	3.24	1.46	1.39
14	G	1109	CLA	OBD-CAD	3.24	1.28	1.22
20	b	5002	LMG	C19-C18	-3.24	1.33	1.51
14	b	1205	CLA	CHD-C4C	3.24	1.46	1.39
14	b	1201	CLA	MG-ND	-3.23	1.99	2.05
20	B	5002	LMG	C19-C18	-3.23	1.33	1.51
14	G	1127	CLA	OBD-CAD	3.23	1.28	1.22
14	b	1202	CLA	MG-ND	-3.23	1.99	2.05
14	G	1135	CLA	C1C-NC	-3.23	1.33	1.37
14	A	1106	CLA	C1C-NC	-3.23	1.33	1.37
14	a	1127	CLA	CHD-C4C	3.23	1.46	1.39
14	G	1106	CLA	OBD-CAD	3.23	1.28	1.22
14	B	1236	CLA	OBD-CAD	3.23	1.28	1.22
14	b	1234	CLA	C1C-NC	-3.23	1.33	1.37
14	G	1127	CLA	CHD-C4C	3.23	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1113	CLA	C1C-NC	-3.23	1.33	1.37
15	H	1207	F6C	C1C-NC	-3.23	1.32	1.35
14	H	1201	CLA	MG-ND	-3.23	1.99	2.05
20	H	5002	LMG	C19-C18	-3.23	1.33	1.51
14	a	1109	CLA	OBD-CAD	3.23	1.28	1.22
14	b	1211	CLA	OBD-CAD	3.22	1.28	1.22
14	b	1236	CLA	OBD-CAD	3.22	1.28	1.22
14	G	1122	CLA	OBD-CAD	3.22	1.28	1.22
14	G	1013	CLA	MG-ND	-3.22	1.99	2.05
14	H	1202	CLA	MG-ND	-3.22	1.99	2.05
14	a	1104	CLA	C1C-NC	-3.22	1.33	1.37
15	a	1121	F6C	CHB-C1B	3.22	1.46	1.39
14	A	1138	CLA	OBD-CAD	3.22	1.28	1.22
14	H	1211	CLA	C1C-NC	-3.22	1.33	1.37
14	a	1013	CLA	MG-ND	-3.22	1.99	2.05
14	G	1132	CLA	C1C-NC	-3.22	1.33	1.37
14	a	1012	CLA	C1C-NC	-3.22	1.33	1.37
14	a	1140	CLA	C1C-NC	-3.22	1.33	1.37
15	H	1207	F6C	C1D-ND	-3.22	1.33	1.37
14	a	1115	CLA	MG-ND	-3.22	1.99	2.05
14	A	1132	CLA	C1C-NC	-3.21	1.33	1.37
14	H	1202	CLA	OBD-CAD	3.21	1.28	1.22
14	A	1133	CLA	MG-ND	-3.21	1.99	2.05
14	b	1208	CLA	MG-ND	-3.21	1.99	2.05
14	a	1138	CLA	OBD-CAD	3.21	1.28	1.22
14	G	1133	CLA	MG-ND	-3.21	1.99	2.05
14	B	1234	CLA	C1C-NC	-3.21	1.33	1.37
14	b	1214	CLA	OBD-CAD	3.21	1.28	1.22
14	A	1112	CLA	C1C-NC	-3.21	1.33	1.37
14	l	1502	CLA	C1C-NC	-3.21	1.33	1.37
15	b	1207	F6C	C1D-ND	-3.21	1.33	1.37
14	A	1104	CLA	C1C-NC	-3.21	1.33	1.37
14	A	1108	CLA	C1C-NC	-3.21	1.33	1.37
18	a	4002	BCR	C11-C12	-3.21	1.26	1.34
15	G	1121	F6C	CHB-C1B	3.20	1.46	1.39
14	A	1104	CLA	OBD-CAD	3.20	1.28	1.22
14	H	1208	CLA	MG-ND	-3.20	1.99	2.05
14	b	1232	CLA	MG-ND	-3.20	1.99	2.05
14	A	1127	CLA	CHD-C4C	3.20	1.46	1.39
14	b	1211	CLA	C1C-NC	-3.20	1.33	1.37
14	b	1224	CLA	C1C-NC	-3.20	1.33	1.37
14	a	1107	CLA	OBD-CAD	3.20	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1121	F6C	CHB-C1B	3.20	1.46	1.39
14	B	1202	CLA	MG-ND	-3.20	1.99	2.05
14	H	1218	CLA	CHD-C4C	3.19	1.46	1.39
15	a	1121	F6C	C1D-ND	-3.19	1.33	1.37
14	A	1013	CLA	MG-ND	-3.19	1.99	2.05
14	A	1123	CLA	OBD-CAD	3.19	1.28	1.22
14	H	1234	CLA	MG-ND	-3.19	1.99	2.05
14	G	1123	CLA	OBD-CAD	3.19	1.28	1.22
14	B	1202	CLA	OBD-CAD	3.19	1.28	1.22
14	a	1133	CLA	MG-ND	-3.19	1.99	2.05
14	G	1107	CLA	OBD-CAD	3.19	1.28	1.22
14	L	1502	CLA	C1C-NC	-3.19	1.33	1.37
15	B	1207	F6C	C1D-ND	-3.19	1.33	1.37
14	H	1225	CLA	C1B-NB	-3.19	1.32	1.35
14	G	1012	CLA	C1C-NC	-3.19	1.33	1.37
14	G	1012	CLA	OBD-CAD	3.19	1.28	1.22
15	B	1238	F6C	OBD-CAD	3.19	1.28	1.22
14	G	1115	CLA	MG-ND	-3.19	1.99	2.05
14	b	1234	CLA	MG-ND	-3.19	1.99	2.05
18	G	4002	BCR	C11-C12	-3.19	1.26	1.34
14	G	1109	CLA	C1C-NC	-3.18	1.33	1.37
14	B	1225	CLA	C1B-NB	-3.18	1.32	1.35
14	B	1217	CLA	OBD-CAD	3.18	1.28	1.22
15	G	1121	F6C	C1D-ND	-3.18	1.33	1.37
14	G	1113	CLA	C1C-NC	-3.18	1.33	1.37
14	G	1138	CLA	MG-ND	-3.18	1.99	2.05
14	B	1211	CLA	C1C-NC	-3.18	1.33	1.37
14	b	1202	CLA	OBD-CAD	3.18	1.28	1.22
14	A	1012	CLA	OBD-CAD	3.18	1.28	1.22
14	A	1115	CLA	MG-ND	-3.18	1.99	2.05
14	B	1218	CLA	CHD-C4C	3.18	1.46	1.39
14	A	1138	CLA	MG-ND	-3.18	1.99	2.05
14	B	1234	CLA	MG-ND	-3.18	1.99	2.05
14	x	1701	CLA	MG-ND	-3.17	1.99	2.05
20	G	5005	LMG	C37-C36	-3.17	1.33	1.51
14	a	1131	CLA	OBD-CAD	3.17	1.27	1.22
14	A	1131	CLA	OBD-CAD	3.17	1.27	1.22
14	W	1701	CLA	MG-ND	-3.17	1.99	2.05
20	A	5005	LMG	C37-C36	-3.17	1.33	1.51
14	B	1224	CLA	C1C-NC	-3.17	1.33	1.37
14	a	1132	CLA	C1C-NC	-3.17	1.33	1.37
14	B	1214	CLA	OBD-CAD	3.17	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	X	1701	CLA	MG-ND	-3.17	1.99	2.05
14	H	1022	CLA	CHD-C4C	3.17	1.46	1.39
14	a	1139	CLA	MG-ND	-3.17	1.99	2.05
15	H	1207	F6C	MG-ND	-3.17	1.98	2.06
15	b	1207	F6C	MG-ND	-3.17	1.98	2.06
14	U	1503	CLA	MG-ND	-3.17	1.99	2.05
14	B	1208	CLA	MG-ND	-3.17	1.99	2.05
15	B	1207	F6C	MG-ND	-3.17	1.98	2.06
14	H	1214	CLA	OBD-CAD	3.17	1.27	1.22
14	b	1231	CLA	C1C-NC	-3.16	1.33	1.37
14	A	1012	CLA	C1C-NC	-3.16	1.33	1.37
14	b	1218	CLA	CHD-C4C	3.16	1.46	1.39
20	a	5005	LMG	C37-C36	-3.16	1.33	1.51
14	A	1107	CLA	OBD-CAD	3.16	1.27	1.22
14	G	1139	CLA	MG-ND	-3.16	1.99	2.05
14	G	1131	CLA	OBD-CAD	3.16	1.27	1.22
14	B	1232	CLA	MG-ND	-3.16	1.99	2.05
14	G	1104	CLA	C1C-NC	-3.16	1.33	1.37
14	b	1022	CLA	CHD-C4C	3.16	1.46	1.39
14	U	1502	CLA	C1C-NC	-3.16	1.33	1.37
14	a	1012	CLA	OBD-CAD	3.16	1.27	1.22
14	H	1232	CLA	MG-ND	-3.16	1.99	2.05
14	G	1129	CLA	OBD-CAD	3.16	1.27	1.22
14	b	1217	CLA	OBD-CAD	3.16	1.27	1.22
14	B	1022	CLA	CHD-C4C	3.15	1.46	1.39
14	H	1021	CLA	OBD-CAD	3.15	1.27	1.22
15	B	1237	F6C	OBD-CAD	3.15	1.27	1.22
14	A	1105	CLA	C1C-NC	-3.15	1.33	1.37
18	A	4002	BCR	C11-C12	-3.15	1.26	1.34
14	b	1213	CLA	MG-ND	-3.15	1.99	2.05
14	G	1112	CLA	MG-ND	-3.15	1.99	2.05
14	G	1138	CLA	OBD-CAD	3.15	1.27	1.22
14	A	1112	CLA	MG-ND	-3.15	1.99	2.05
14	H	1213	CLA	MG-ND	-3.15	1.99	2.05
14	B	1021	CLA	OBD-CAD	3.14	1.27	1.22
14	A	1107	CLA	C1C-NC	-3.14	1.33	1.37
14	B	1212	CLA	C1C-NC	-3.14	1.33	1.37
14	H	1225	CLA	OBD-CAD	3.14	1.27	1.22
14	B	1202	CLA	C1C-NC	-3.14	1.33	1.37
15	H	1238	F6C	OBD-CAD	3.14	1.27	1.22
14	B	1226	CLA	C1B-NB	-3.14	1.32	1.35
14	a	1105	CLA	C1C-NC	-3.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1215	CLA	C1C-NC	-3.14	1.33	1.37
14	b	1225	CLA	OBD-CAD	3.14	1.27	1.22
14	b	1215	CLA	C1C-NC	-3.14	1.33	1.37
14	A	1139	CLA	MG-ND	-3.14	1.99	2.05
14	b	1225	CLA	C1B-NB	-3.14	1.32	1.35
14	B	1213	CLA	MG-ND	-3.14	1.99	2.05
14	b	1204	CLA	OBD-CAD	3.14	1.27	1.22
14	H	1217	CLA	OBD-CAD	3.14	1.27	1.22
14	B	1225	CLA	OBD-CAD	3.14	1.27	1.22
15	b	1238	F6C	OBD-CAD	3.13	1.27	1.22
15	b	1237	F6C	OBD-CAD	3.13	1.27	1.22
14	G	1140	CLA	OBD-CAD	3.13	1.27	1.22
14	H	1216	CLA	C1C-NC	-3.13	1.33	1.37
14	a	1136	CLA	OBD-CAD	3.13	1.27	1.22
14	G	1108	CLA	MG-ND	-3.13	1.99	2.05
14	b	1222	CLA	OBD-CAD	3.13	1.27	1.22
14	A	1140	CLA	OBD-CAD	3.13	1.27	1.22
14	G	1105	CLA	C1C-NC	-3.13	1.33	1.37
14	B	1204	CLA	OBD-CAD	3.13	1.27	1.22
14	a	1112	CLA	MG-ND	-3.13	1.99	2.05
15	H	1237	F6C	OBD-CAD	3.13	1.27	1.22
14	a	1123	CLA	OBD-CAD	3.13	1.27	1.22
14	a	1129	CLA	OBD-CAD	3.13	1.27	1.22
14	l	1503	CLA	MG-ND	-3.13	1.99	2.05
14	B	1231	CLA	C1C-NC	-3.13	1.33	1.37
14	H	1231	CLA	MG-ND	-3.13	1.99	2.05
14	A	1108	CLA	MG-ND	-3.13	1.99	2.05
14	B	1235	CLA	MG-ND	-3.13	1.99	2.05
14	b	1226	CLA	C1B-NB	-3.12	1.32	1.35
14	H	1222	CLA	OBD-CAD	3.12	1.27	1.22
14	a	1113	CLA	OBD-CAD	3.12	1.27	1.22
14	A	1113	CLA	OBD-CAD	3.12	1.27	1.22
14	A	1129	CLA	OBD-CAD	3.12	1.27	1.22
14	a	1140	CLA	OBD-CAD	3.12	1.27	1.22
14	a	1128	CLA	OBD-CAD	3.12	1.27	1.22
14	L	1503	CLA	MG-ND	-3.12	1.99	2.05
14	B	1231	CLA	MG-ND	-3.12	1.99	2.05
14	a	1109	CLA	C1C-NC	-3.12	1.33	1.37
14	H	1212	CLA	C1C-NC	-3.12	1.33	1.37
14	H	1235	CLA	MG-ND	-3.12	1.99	2.05
14	B	1216	CLA	C1C-NC	-3.12	1.33	1.37
14	H	1231	CLA	C1C-NC	-3.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1220	CLA	MG-ND	-3.12	1.99	2.05
14	b	1212	CLA	C1C-NC	-3.12	1.33	1.37
14	b	1235	CLA	MG-ND	-3.11	1.99	2.05
14	H	1202	CLA	C1C-NC	-3.11	1.33	1.37
14	G	1109	CLA	MG-ND	-3.11	1.99	2.05
14	B	1228	CLA	MG-ND	-3.11	1.99	2.05
14	b	1216	CLA	C1C-NC	-3.11	1.33	1.37
14	G	1107	CLA	C1C-NC	-3.11	1.33	1.37
14	H	1228	CLA	MG-ND	-3.11	1.99	2.05
15	H	1237	F6C	C4B-NB	-3.11	1.33	1.37
14	b	1021	CLA	OBD-CAD	3.11	1.27	1.22
14	b	1231	CLA	MG-ND	-3.11	1.99	2.05
14	H	1218	CLA	C3D-C2D	3.11	1.47	1.39
14	H	1215	CLA	C1C-NC	-3.11	1.33	1.37
14	G	1127	CLA	C1C-NC	-3.11	1.33	1.37
14	b	1208	CLA	C1C-NC	-3.11	1.33	1.37
14	G	1128	CLA	OBD-CAD	3.10	1.27	1.22
14	A	1128	CLA	OBD-CAD	3.10	1.27	1.22
14	a	1138	CLA	MG-ND	-3.10	1.99	2.05
14	b	1228	CLA	MG-ND	-3.10	1.99	2.05
14	A	1109	CLA	C1C-NC	-3.10	1.33	1.37
14	a	1109	CLA	MG-ND	-3.10	1.99	2.05
14	H	1226	CLA	C1B-NB	-3.10	1.32	1.35
14	b	1212	CLA	MG-ND	-3.10	1.99	2.05
14	B	1220	CLA	MG-ND	-3.10	1.99	2.05
14	a	1120	CLA	C1C-NC	-3.10	1.33	1.37
14	G	1136	CLA	MG-ND	-3.09	1.99	2.05
14	a	1108	CLA	MG-ND	-3.09	1.99	2.05
14	A	1110	CLA	MG-ND	-3.09	1.99	2.05
14	B	1218	CLA	C3D-C2D	3.09	1.47	1.39
14	G	1118	CLA	C1C-NC	-3.09	1.33	1.37
14	B	1212	CLA	MG-ND	-3.09	1.99	2.05
14	G	1013	CLA	C1C-NC	-3.09	1.33	1.37
14	a	1013	CLA	C1C-NC	-3.09	1.33	1.37
14	G	1122	CLA	MG-ND	-3.09	1.99	2.05
14	A	1122	CLA	MG-ND	-3.09	1.99	2.05
14	B	1213	CLA	C1C-NC	-3.09	1.33	1.37
14	H	1213	CLA	C1C-NC	-3.09	1.33	1.37
14	G	1110	CLA	MG-ND	-3.09	1.99	2.05
14	G	1113	CLA	OBD-CAD	3.09	1.27	1.22
14	G	1136	CLA	OBD-CAD	3.09	1.27	1.22
14	b	1202	CLA	C1C-NC	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1220	CLA	MG-ND	-3.09	1.99	2.05
14	a	1107	CLA	C1C-NC	-3.09	1.33	1.37
14	G	1101	CLA	C1C-NC	-3.08	1.33	1.37
14	G	1129	CLA	C1C-NC	-3.08	1.33	1.37
14	K	1401	CLA	C1D-ND	-3.08	1.34	1.37
15	b	1237	F6C	C4B-NB	-3.08	1.33	1.37
14	A	1109	CLA	MG-ND	-3.08	1.99	2.05
14	b	1218	CLA	C3D-C2D	3.08	1.47	1.39
14	A	1113	CLA	MG-ND	-3.08	1.99	2.05
14	H	1212	CLA	MG-ND	-3.07	1.99	2.05
14	B	1208	CLA	C1C-NC	-3.07	1.33	1.37
14	a	1122	CLA	MG-ND	-3.07	1.99	2.05
14	b	1213	CLA	C1C-NC	-3.07	1.33	1.37
14	B	1229	CLA	C1C-NC	-3.07	1.33	1.37
15	H	1230	F6C	C1D-ND	-3.07	1.33	1.37
14	H	1208	CLA	C1C-NC	-3.07	1.33	1.37
14	H	1236	CLA	MG-ND	-3.07	1.99	2.05
14	H	1022	CLA	C1C-NC	-3.07	1.33	1.37
15	B	1237	F6C	C3B-C2B	3.07	1.46	1.39
14	H	1204	CLA	OBD-CAD	3.07	1.27	1.22
14	H	1022	CLA	OBD-CAD	3.07	1.27	1.22
15	b	1238	F6C	MG-ND	-3.07	1.99	2.06
14	B	1217	CLA	MG-ND	-3.07	1.99	2.05
14	B	1236	CLA	MG-ND	-3.07	1.99	2.05
15	H	1237	F6C	C3B-C2B	3.07	1.46	1.39
14	G	1111	CLA	MG-ND	-3.06	1.99	2.05
14	a	1110	CLA	MG-ND	-3.06	1.99	2.05
14	T	1401	CLA	C1D-ND	-3.06	1.34	1.37
14	A	1138	CLA	C1C-NC	-3.06	1.33	1.37
14	A	1129	CLA	C1C-NC	-3.06	1.33	1.37
15	H	1238	F6C	MG-ND	-3.06	1.99	2.06
14	b	1229	CLA	C1C-NC	-3.06	1.33	1.37
15	b	1230	F6C	C1D-ND	-3.06	1.33	1.37
14	H	1217	CLA	MG-ND	-3.06	1.99	2.05
15	B	1237	F6C	C4B-NB	-3.06	1.33	1.37
14	a	1134	CLA	C1D-ND	-3.06	1.34	1.37
14	a	1113	CLA	MG-ND	-3.06	1.99	2.05
14	a	1127	CLA	C1C-NC	-3.06	1.33	1.37
14	A	1118	CLA	C1C-NC	-3.06	1.33	1.37
14	H	1229	CLA	C1C-NC	-3.06	1.33	1.37
14	A	1101	CLA	C1C-NC	-3.06	1.33	1.37
14	G	1106	CLA	MG-ND	-3.05	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1124	CLA	MG-ND	-3.05	1.99	2.05
14	A	1106	CLA	MG-ND	-3.05	1.99	2.05
15	B	1238	F6C	CHB-C1B	3.05	1.46	1.39
14	a	1101	CLA	C1C-NC	-3.05	1.33	1.37
14	A	1013	CLA	C1C-NC	-3.05	1.33	1.37
14	B	1222	CLA	OBD-CAD	3.05	1.27	1.22
15	b	1207	F6C	OBD-CAD	3.05	1.27	1.22
14	a	1118	CLA	C1C-NC	-3.05	1.33	1.37
14	a	1106	CLA	MG-ND	-3.05	1.99	2.05
14	a	1136	CLA	MG-ND	-3.05	1.99	2.05
15	b	1238	F6C	CHB-C1B	3.05	1.46	1.39
14	a	1120	CLA	MG-ND	-3.05	1.99	2.05
14	a	1138	CLA	C1C-NC	-3.04	1.33	1.37
15	B	1230	F6C	C1D-ND	-3.04	1.33	1.37
14	G	1124	CLA	MG-ND	-3.04	1.99	2.05
14	A	1111	CLA	MG-ND	-3.04	1.99	2.05
15	H	1238	F6C	CHB-C1B	3.04	1.46	1.39
14	G	1120	CLA	C1C-NC	-3.04	1.33	1.37
14	A	1120	CLA	MG-ND	-3.04	1.99	2.05
14	A	1120	CLA	C1C-NC	-3.04	1.33	1.37
14	k	1401	CLA	C1D-ND	-3.04	1.34	1.37
14	B	1235	CLA	C1C-NC	-3.04	1.33	1.37
14	G	1115	CLA	C1C-NC	-3.04	1.33	1.37
15	B	1207	F6C	OBD-CAD	3.04	1.27	1.22
14	b	1022	CLA	OBD-CAD	3.04	1.27	1.22
14	G	1133	CLA	C1C-NC	-3.04	1.33	1.37
15	B	1238	F6C	MG-ND	-3.04	1.99	2.06
14	G	1120	CLA	MG-ND	-3.04	1.99	2.05
14	a	1129	CLA	C1C-NC	-3.04	1.33	1.37
15	H	1207	F6C	OBD-CAD	3.04	1.27	1.22
14	B	1226	CLA	C3D-C2D	3.04	1.47	1.39
14	A	1132	CLA	MG-ND	-3.03	1.99	2.05
14	A	1115	CLA	C1C-NC	-3.03	1.33	1.37
14	b	1226	CLA	C3D-C2D	3.03	1.47	1.39
14	A	1136	CLA	MG-ND	-3.03	1.99	2.05
14	A	1124	CLA	MG-ND	-3.03	1.99	2.05
14	B	1022	CLA	C1C-NC	-3.03	1.33	1.37
14	G	1132	CLA	MG-ND	-3.03	1.99	2.05
14	a	1134	CLA	MG-NC	3.03	2.13	2.06
14	G	1113	CLA	MG-ND	-3.03	1.99	2.05
14	a	1105	CLA	MG-ND	-3.03	1.99	2.05
14	H	1226	CLA	C3D-C2D	3.03	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1136	CLA	OBD-CAD	3.03	1.27	1.22
14	a	1132	CLA	MG-ND	-3.02	1.99	2.05
14	B	1216	CLA	MG-ND	-3.02	1.99	2.05
14	G	1110	CLA	C1C-NC	-3.02	1.33	1.37
14	G	1138	CLA	C1C-NC	-3.02	1.33	1.37
14	H	1235	CLA	C1C-NC	-3.02	1.33	1.37
14	a	1133	CLA	C1C-NC	-3.02	1.33	1.37
14	a	1111	CLA	MG-ND	-3.02	1.99	2.05
14	G	1134	CLA	MG-NC	3.02	2.13	2.06
14	a	1119	CLA	C3D-C2D	3.02	1.47	1.39
14	b	1021	CLA	CHD-C4C	3.02	1.46	1.39
14	A	1127	CLA	C1C-NC	-3.02	1.33	1.37
14	b	1236	CLA	MG-ND	-3.02	1.99	2.05
14	A	1134	CLA	MG-NC	3.02	2.13	2.06
14	k	1401	CLA	MG-NC	3.01	2.13	2.06
14	a	1114	CLA	MG-ND	-3.01	1.99	2.05
15	b	1237	F6C	C3B-C2B	3.01	1.46	1.39
14	A	1119	CLA	C3D-C2D	3.01	1.47	1.39
15	H	1207	F6C	CHB-C4A	-3.01	1.32	1.38
14	b	1217	CLA	MG-ND	-3.01	1.99	2.05
14	B	1210	CLA	MG-ND	-3.01	1.99	2.05
14	b	1210	CLA	MG-ND	-3.01	1.99	2.05
14	H	1216	CLA	MG-ND	-3.01	1.99	2.05
14	A	1105	CLA	MG-ND	-3.01	1.99	2.05
14	H	1210	CLA	MG-ND	-3.01	1.99	2.05
14	b	1235	CLA	C1C-NC	-3.01	1.33	1.37
14	b	1022	CLA	C1C-NC	-3.01	1.33	1.37
14	B	1022	CLA	OBD-CAD	3.01	1.27	1.22
14	a	1115	CLA	C1C-NC	-3.01	1.33	1.37
15	b	1230	F6C	C3B-C2B	3.00	1.46	1.39
14	b	1216	CLA	MG-ND	-3.00	1.99	2.05
14	b	1205	CLA	OBD-CAD	3.00	1.27	1.22
14	a	1123	CLA	MG-NC	3.00	2.13	2.06
14	G	1123	CLA	MG-NC	3.00	2.13	2.06
15	b	1207	F6C	CHB-C4A	-3.00	1.32	1.38
15	H	1230	F6C	C3B-C2B	3.00	1.46	1.39
14	A	1114	CLA	MG-ND	-2.99	1.99	2.05
14	G	1103	CLA	OBD-CAD	2.99	1.27	1.22
14	H	1209	CLA	MG-ND	-2.99	1.99	2.05
15	B	1207	F6C	CHB-C4A	-2.99	1.32	1.38
14	a	1110	CLA	C1C-NC	-2.99	1.33	1.37
14	B	1209	CLA	MG-ND	-2.99	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1209	CLA	MG-ND	-2.99	1.99	2.05
14	G	1105	CLA	MG-ND	-2.99	1.99	2.05
14	H	1211	CLA	MG-ND	-2.99	1.99	2.05
14	A	1012	CLA	C3D-C2D	2.99	1.47	1.39
14	G	1114	CLA	MG-ND	-2.99	1.99	2.05
14	G	1012	CLA	C3D-C2D	2.99	1.47	1.39
15	B	1230	F6C	C3B-C2B	2.98	1.46	1.39
14	A	1134	CLA	C3D-C2D	2.98	1.47	1.39
14	A	1134	CLA	C1D-ND	-2.98	1.34	1.37
14	A	1123	CLA	MG-NC	2.98	2.13	2.06
14	A	1110	CLA	C1C-NC	-2.98	1.33	1.37
14	U	1502	CLA	MG-ND	-2.98	1.99	2.05
14	K	1401	CLA	MG-NC	2.98	2.13	2.06
14	l	1502	CLA	MG-ND	-2.97	1.99	2.05
14	L	1502	CLA	MG-ND	-2.97	1.99	2.05
14	a	1012	CLA	C3D-C2D	2.97	1.47	1.39
14	A	1133	CLA	C1C-NC	-2.97	1.33	1.37
14	G	1119	CLA	C3D-C2D	2.97	1.47	1.39
14	B	1021	CLA	CHD-C4C	2.97	1.46	1.39
14	T	1401	CLA	MG-NC	2.97	2.13	2.06
14	L	1502	CLA	OBD-CAD	2.97	1.27	1.22
14	H	1021	CLA	CHD-C4C	2.97	1.46	1.39
14	a	1134	CLA	C3D-C2D	2.97	1.47	1.39
14	B	1205	CLA	OBD-CAD	2.97	1.27	1.22
14	H	1206	CLA	C3D-C2D	2.96	1.47	1.39
14	G	1134	CLA	C3D-C2D	2.96	1.47	1.39
14	H	1205	CLA	OBD-CAD	2.96	1.27	1.22
14	H	1227	CLA	C1C-NC	-2.96	1.33	1.37
14	b	1211	CLA	MG-ND	-2.96	1.99	2.05
14	b	1206	CLA	C3D-C2D	2.95	1.47	1.39
14	G	1134	CLA	C1D-ND	-2.95	1.34	1.37
15	B	1238	F6C	C4B-NB	-2.95	1.33	1.37
14	b	1219	CLA	MG-ND	-2.95	1.99	2.05
14	U	1501	CLA	C3D-C2D	2.95	1.47	1.39
14	X	1701	CLA	C1C-NC	-2.95	1.33	1.37
14	H	1219	CLA	MG-ND	-2.94	2.00	2.05
14	L	1501	CLA	C3D-C2D	2.94	1.47	1.39
14	b	1221	CLA	OBD-CAD	2.94	1.27	1.22
14	b	1022	CLA	MG-NC	2.94	2.13	2.06
14	B	1218	CLA	MG-NC	2.94	2.13	2.06
14	a	1103	CLA	OBD-CAD	2.94	1.27	1.22
14	H	1233	CLA	C3D-C2D	2.94	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1022	CLA	MG-NC	2.94	2.13	2.06
14	l	1501	CLA	C3D-C2D	2.93	1.47	1.39
14	B	1211	CLA	MG-ND	-2.93	2.00	2.05
14	A	1103	CLA	OBD-CAD	2.93	1.27	1.22
14	B	1206	CLA	C1B-NB	-2.93	1.32	1.35
15	H	1237	F6C	MG-ND	-2.92	1.99	2.06
14	B	1219	CLA	MG-ND	-2.92	2.00	2.05
14	B	1206	CLA	C3D-C2D	2.92	1.47	1.39
15	B	1237	F6C	MG-ND	-2.92	1.99	2.06
14	B	1233	CLA	C3D-C2D	2.92	1.47	1.39
14	B	1227	CLA	C1C-NC	-2.92	1.33	1.37
14	U	1502	CLA	OBD-CAD	2.92	1.27	1.22
14	l	1502	CLA	OBD-CAD	2.92	1.27	1.22
14	b	1218	CLA	MG-NC	2.91	2.13	2.06
14	b	1206	CLA	C1B-NB	-2.91	1.32	1.35
14	b	1233	CLA	C3D-C2D	2.91	1.47	1.39
14	B	1221	CLA	OBD-CAD	2.91	1.27	1.22
14	B	1209	CLA	C1C-NC	-2.91	1.33	1.37
14	W	1701	CLA	C1C-NC	-2.91	1.33	1.37
14	b	1216	CLA	C3D-C2D	2.90	1.47	1.39
14	H	1206	CLA	C1B-NB	-2.90	1.32	1.35
14	H	1221	CLA	OBD-CAD	2.90	1.27	1.22
15	H	1238	F6C	C4B-NB	-2.90	1.33	1.37
14	B	1215	CLA	C3D-C2D	2.90	1.47	1.39
14	H	1217	CLA	MG-NC	2.90	2.13	2.06
14	x	1701	CLA	C1C-NC	-2.90	1.33	1.37
14	b	1235	CLA	OBD-CAD	2.90	1.27	1.22
14	H	1216	CLA	C3D-C2D	2.90	1.47	1.39
14	H	1022	CLA	MG-NC	2.90	2.13	2.06
14	G	1120	CLA	C3D-C2D	2.89	1.47	1.39
14	B	1216	CLA	C3D-C2D	2.89	1.47	1.39
15	b	1238	F6C	C4B-NB	-2.89	1.33	1.37
14	b	1209	CLA	C1C-NC	-2.89	1.33	1.37
14	H	1209	CLA	C1C-NC	-2.89	1.33	1.37
14	b	1227	CLA	C1C-NC	-2.89	1.33	1.37
14	k	1401	CLA	C3D-C2D	2.89	1.47	1.39
14	H	1218	CLA	MG-NC	2.88	2.13	2.06
14	B	1214	CLA	C3D-C2D	2.88	1.47	1.39
14	b	1212	CLA	C3D-C2D	2.88	1.47	1.39
14	A	1123	CLA	C1C-NC	-2.88	1.33	1.37
21	A	6001	LMT	O3'-C3'	-2.88	1.36	1.43
14	H	1212	CLA	C3D-C2D	2.88	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1207	F6C	C4B-NB	-2.88	1.33	1.37
14	H	1235	CLA	C3D-C2D	2.88	1.47	1.39
14	H	1235	CLA	OBD-CAD	2.88	1.27	1.22
14	b	1215	CLA	C3D-C2D	2.87	1.47	1.39
14	X	1701	CLA	MG-NC	2.87	2.13	2.06
14	A	1138	CLA	C3D-C2D	2.87	1.47	1.39
14	G	1112	CLA	C3D-C2D	2.87	1.47	1.39
14	B	1212	CLA	C3D-C2D	2.87	1.47	1.39
15	b	1237	F6C	MG-ND	-2.87	1.99	2.06
14	K	1401	CLA	C3D-C2D	2.87	1.46	1.39
14	G	1138	CLA	C3D-C2D	2.86	1.46	1.39
14	B	1235	CLA	OBD-CAD	2.86	1.27	1.22
14	b	1217	CLA	MG-NC	2.86	2.13	2.06
14	a	1120	CLA	C3D-C2D	2.86	1.46	1.39
14	a	1138	CLA	C3D-C2D	2.86	1.46	1.39
14	H	1215	CLA	C3D-C2D	2.86	1.46	1.39
14	A	1120	CLA	C3D-C2D	2.86	1.46	1.39
14	H	1214	CLA	C3D-C2D	2.86	1.46	1.39
14	T	1401	CLA	C3D-C2D	2.86	1.46	1.39
14	W	1701	CLA	MG-NC	2.86	2.13	2.06
21	a	6001	LMT	O3'-C3'	-2.86	1.36	1.43
14	B	1233	CLA	MG-NC	2.86	2.13	2.06
14	H	1232	CLA	MG-NC	2.86	2.13	2.06
15	b	1238	F6C	C3B-C2B	2.85	1.46	1.39
14	b	1235	CLA	C3D-C2D	2.85	1.46	1.39
14	B	1232	CLA	MG-NC	2.85	2.13	2.06
14	a	1123	CLA	C1C-NC	-2.85	1.33	1.37
15	b	1207	F6C	C4B-NB	-2.85	1.33	1.37
14	A	1112	CLA	C3D-C2D	2.85	1.46	1.39
14	G	1128	CLA	C3D-C2D	2.85	1.46	1.39
14	H	1228	CLA	C3D-C2D	2.85	1.46	1.39
14	x	1701	CLA	MG-NC	2.85	2.13	2.06
14	b	1214	CLA	C3D-C2D	2.85	1.46	1.39
14	A	1118	CLA	MG-NC	2.85	2.13	2.06
14	B	1217	CLA	MG-NC	2.85	2.13	2.06
14	G	1118	CLA	MG-NC	2.84	2.13	2.06
14	B	1235	CLA	C3D-C2D	2.84	1.46	1.39
14	a	1128	CLA	C3D-C2D	2.84	1.46	1.39
15	B	1238	F6C	C3B-C2B	2.84	1.45	1.39
14	a	1101	CLA	MG-ND	-2.84	2.00	2.05
14	B	1208	CLA	C3D-C2D	2.84	1.46	1.39
21	G	6002	LMT	O3B-C3B	-2.84	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1227	CLA	MG-NC	2.84	2.13	2.06
14	b	1233	CLA	MG-NC	2.84	2.13	2.06
14	b	1232	CLA	MG-NC	2.84	2.13	2.06
14	b	1214	CLA	C1C-NC	-2.84	1.33	1.37
14	B	1233	CLA	MG-ND	-2.83	2.00	2.05
14	b	1219	CLA	MG-NC	2.83	2.13	2.06
14	A	1128	CLA	C3D-C2D	2.83	1.46	1.39
15	H	1207	F6C	C4B-NB	-2.83	1.33	1.37
14	B	1219	CLA	MG-NC	2.83	2.13	2.06
14	b	1208	CLA	C3D-C2D	2.83	1.46	1.39
21	A	6002	LMT	O3'-C3'	-2.83	1.36	1.43
14	B	1218	CLA	C1C-NC	-2.83	1.33	1.37
14	G	1101	CLA	MG-ND	-2.83	2.00	2.05
14	B	1228	CLA	C3D-C2D	2.83	1.46	1.39
21	G	6001	LMT	O3'-C3'	-2.83	1.36	1.43
21	a	6002	LMT	O3'-C3'	-2.83	1.36	1.43
14	H	1219	CLA	C3D-C2D	2.83	1.46	1.39
14	H	1234	CLA	OBD-CAD	2.83	1.27	1.22
14	A	1107	CLA	MG-NC	2.83	2.13	2.06
14	B	1214	CLA	MG-NC	2.83	2.13	2.06
21	a	6002	LMT	O3B-C3B	-2.83	1.36	1.43
14	B	1214	CLA	C3B-C2B	2.83	1.44	1.40
15	H	1238	F6C	C3B-C2B	2.83	1.45	1.39
14	H	1219	CLA	MG-NC	2.83	2.13	2.06
14	H	1233	CLA	MG-NC	2.83	2.13	2.06
14	a	1125	CLA	OBD-CAD	2.82	1.27	1.22
14	B	1221	CLA	C3D-C2D	2.82	1.46	1.39
14	G	1102	CLA	C1C-NC	-2.82	1.33	1.37
14	a	1114	CLA	C3D-C2D	2.82	1.46	1.39
14	H	1233	CLA	MG-ND	-2.82	2.00	2.05
14	a	1108	CLA	C3D-C2D	2.82	1.46	1.39
14	b	1214	CLA	C3B-C2B	2.82	1.44	1.40
14	a	1112	CLA	C3D-C2D	2.82	1.46	1.39
14	B	1219	CLA	C3D-C2D	2.82	1.46	1.39
21	G	6002	LMT	O3'-C3'	-2.82	1.36	1.43
14	b	1227	CLA	MG-NC	2.82	2.13	2.06
14	G	1123	CLA	C1C-NC	-2.82	1.33	1.37
14	H	1214	CLA	C3B-C2B	2.82	1.44	1.40
15	B	1238	F6C	CHB-C4A	-2.82	1.32	1.38
14	a	1125	CLA	CHD-C4C	2.82	1.45	1.39
14	b	1228	CLA	C3D-C2D	2.82	1.46	1.39
14	a	1137	CLA	OBD-CAD	2.82	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1237	F6C	C1C-NC	-2.82	1.32	1.35
15	H	1207	F6C	CHB-C1B	2.81	1.45	1.39
15	H	1238	F6C	CHB-C4A	-2.81	1.32	1.38
14	B	1223	CLA	OBD-CAD	2.81	1.27	1.22
14	A	1101	CLA	MG-ND	-2.81	2.00	2.05
14	U	1502	CLA	C3D-C2D	2.81	1.46	1.39
14	B	1227	CLA	MG-NC	2.81	2.13	2.06
14	a	1107	CLA	MG-NC	2.81	2.12	2.06
14	G	1117	CLA	C3D-C2D	2.81	1.46	1.39
14	H	1214	CLA	C1C-NC	-2.81	1.33	1.37
14	A	1117	CLA	C3D-C2D	2.81	1.46	1.39
15	b	1238	F6C	CHB-C4A	-2.81	1.32	1.38
14	H	1208	CLA	C3D-C2D	2.81	1.46	1.39
14	H	1218	CLA	C1C-NC	-2.81	1.33	1.37
14	b	1221	CLA	C3D-C2D	2.81	1.46	1.39
14	A	1114	CLA	C3D-C2D	2.81	1.46	1.39
14	a	1118	CLA	MG-NC	2.81	2.12	2.06
14	H	1217	CLA	C1C-NC	-2.81	1.33	1.37
14	A	1125	CLA	CHD-C4C	2.81	1.45	1.39
14	B	1214	CLA	C1C-NC	-2.81	1.33	1.37
14	H	1220	CLA	C3D-C2D	2.81	1.46	1.39
15	H	1207	F6C	C3B-C2B	2.80	1.45	1.39
14	a	1116	CLA	C1C-NC	-2.80	1.33	1.37
14	H	1214	CLA	MG-NC	2.80	2.12	2.06
14	a	1114	CLA	C1C-NC	-2.80	1.33	1.37
15	G	1121	F6C	C3D-C2D	2.80	1.46	1.39
14	B	1232	CLA	C1C-NC	-2.80	1.33	1.37
13	a	1011	CL0	OBD-CAD	2.80	1.27	1.22
14	L	1502	CLA	C3D-C2D	2.80	1.46	1.39
14	K	1401	CLA	C4D-CHA	2.80	1.48	1.38
15	B	1207	F6C	C3B-C2B	2.80	1.45	1.39
21	A	6002	LMT	O3B-C3B	-2.80	1.36	1.43
14	A	1114	CLA	C1C-NC	-2.80	1.33	1.37
15	b	1207	F6C	CHB-C1B	2.80	1.45	1.39
14	H	1221	CLA	C3D-C2D	2.80	1.46	1.39
14	b	1234	CLA	OBD-CAD	2.80	1.27	1.22
14	l	1502	CLA	C3D-C2D	2.80	1.46	1.39
14	G	1114	CLA	C3D-C2D	2.80	1.46	1.39
14	b	1219	CLA	C3D-C2D	2.80	1.46	1.39
14	a	1102	CLA	C1C-NC	-2.80	1.33	1.37
15	b	1207	F6C	C3B-C2B	2.80	1.45	1.39
14	G	1104	CLA	MG-ND	-2.79	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1218	CLA	C1C-NC	-2.79	1.33	1.37
14	A	1108	CLA	C3D-C2D	2.79	1.46	1.39
14	A	1134	CLA	MG-ND	-2.79	2.00	2.05
13	A	1011	CL0	OBD-CAD	2.79	1.27	1.22
14	A	1137	CLA	OBD-CAD	2.79	1.27	1.22
14	G	1108	CLA	C3D-C2D	2.79	1.46	1.39
14	b	1233	CLA	MG-ND	-2.79	2.00	2.05
14	k	1401	CLA	C4D-CHA	2.79	1.48	1.38
13	G	1011	CL0	OBD-CAD	2.79	1.27	1.22
14	A	1116	CLA	C1C-NC	-2.79	1.33	1.37
14	G	1127	CLA	MG-NC	2.79	2.12	2.06
15	B	1207	F6C	CHB-C1B	2.79	1.45	1.39
14	G	1134	CLA	MG-ND	-2.79	2.00	2.05
14	b	1214	CLA	MG-NC	2.79	2.12	2.06
15	H	1230	F6C	C4B-NB	-2.78	1.33	1.37
14	A	1104	CLA	MG-ND	-2.78	2.00	2.05
15	G	1121	F6C	MG-ND	-2.78	1.99	2.06
14	a	1134	CLA	C4D-CHA	2.78	1.48	1.38
14	G	1125	CLA	CHD-C4C	2.78	1.45	1.39
14	G	1134	CLA	C4D-CHA	2.78	1.48	1.38
14	a	1013	CLA	C3D-C2D	2.78	1.46	1.39
14	B	1217	CLA	C1C-NC	-2.78	1.33	1.37
14	a	1117	CLA	C3D-C2D	2.78	1.46	1.39
15	a	1121	F6C	C3D-C2D	2.78	1.46	1.39
14	A	1134	CLA	C4D-CHA	2.78	1.48	1.38
14	b	1223	CLA	OBD-CAD	2.78	1.27	1.22
14	b	1217	CLA	C1C-NC	-2.78	1.33	1.37
14	B	1234	CLA	OBD-CAD	2.78	1.27	1.22
14	b	1220	CLA	C3D-C2D	2.78	1.46	1.39
15	A	1121	F6C	MG-ND	-2.78	1.99	2.06
14	G	1013	CLA	C3D-C2D	2.78	1.46	1.39
14	a	1104	CLA	MG-ND	-2.78	2.00	2.05
14	T	1401	CLA	C4D-CHA	2.78	1.48	1.38
18	i	4018	BCR	C30-C25	-2.77	1.50	1.53
15	a	1121	F6C	MG-ND	-2.77	1.99	2.06
14	G	1116	CLA	C1C-NC	-2.77	1.33	1.37
14	G	1137	CLA	OBD-CAD	2.77	1.27	1.22
14	B	1220	CLA	C3D-C2D	2.77	1.46	1.39
14	G	1114	CLA	C1C-NC	-2.77	1.33	1.37
14	G	1107	CLA	MG-NC	2.77	2.12	2.06
18	b	4005	BCR	C30-C25	-2.77	1.50	1.53
14	G	1125	CLA	OBD-CAD	2.77	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1012	CLA	C3B-C2B	2.77	1.44	1.40
14	a	1105	CLA	C3D-C2D	2.77	1.46	1.39
15	b	1237	F6C	C1C-NC	-2.77	1.32	1.35
15	B	1230	F6C	C4B-NB	-2.77	1.33	1.37
14	A	1113	CLA	C3D-C2D	2.77	1.46	1.39
14	H	1223	CLA	OBD-CAD	2.77	1.27	1.22
14	A	1013	CLA	C3D-C2D	2.77	1.46	1.39
15	B	1237	F6C	C3D-C2D	2.77	1.46	1.39
14	A	1125	CLA	OBD-CAD	2.77	1.27	1.22
14	H	1232	CLA	C1C-NC	-2.76	1.33	1.37
14	A	1105	CLA	C3D-C2D	2.76	1.46	1.39
14	B	1231	CLA	C3D-C2D	2.76	1.46	1.39
14	G	1105	CLA	C3D-C2D	2.76	1.46	1.39
14	a	1140	CLA	C3D-C2D	2.76	1.46	1.39
15	H	1237	F6C	C1C-NC	-2.76	1.32	1.35
14	a	1134	CLA	MG-ND	-2.76	2.00	2.05
14	B	1215	CLA	C3B-C2B	2.76	1.44	1.40
14	a	1113	CLA	C3D-C2D	2.76	1.46	1.39
14	H	1215	CLA	C3B-C2B	2.76	1.44	1.40
14	A	1133	CLA	C3D-C2D	2.76	1.46	1.39
15	A	1121	F6C	C3D-C2D	2.76	1.46	1.39
14	A	1102	CLA	C1C-NC	-2.76	1.33	1.37
14	G	1114	CLA	C4D-CHA	2.76	1.48	1.38
14	A	1140	CLA	C3D-C2D	2.76	1.46	1.39
15	H	1237	F6C	C3D-C2D	2.76	1.46	1.39
14	a	1114	CLA	C4D-CHA	2.76	1.48	1.38
14	A	1118	CLA	C3D-C2D	2.75	1.46	1.39
14	b	1232	CLA	C1C-NC	-2.75	1.33	1.37
14	A	1114	CLA	C4D-CHA	2.75	1.48	1.38
14	b	1022	CLA	C3D-C2D	2.75	1.46	1.39
14	a	1117	CLA	C4D-CHA	2.75	1.48	1.38
14	G	1113	CLA	C3D-C2D	2.75	1.46	1.39
14	a	1118	CLA	C3D-C2D	2.75	1.46	1.39
14	a	1012	CLA	C3B-C2B	2.75	1.44	1.40
15	b	1230	F6C	C4B-NB	-2.75	1.33	1.37
15	b	1237	F6C	C3D-C2D	2.75	1.46	1.39
18	i	4020	BCR	C21-C22	-2.75	1.32	1.35
14	G	1117	CLA	C4D-CHA	2.75	1.48	1.38
14	G	1140	CLA	C3D-C2D	2.75	1.46	1.39
14	A	1117	CLA	C4D-CHA	2.75	1.48	1.38
14	b	1203	CLA	C1B-NB	-2.75	1.32	1.35
14	G	1133	CLA	C3D-C2D	2.75	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1231	CLA	C3D-C2D	2.75	1.46	1.39
14	A	1012	CLA	C3B-C2B	2.74	1.44	1.40
18	B	4005	BCR	C30-C25	-2.74	1.50	1.53
14	A	1136	CLA	C3D-C2D	2.74	1.46	1.39
14	A	1127	CLA	MG-NC	2.74	2.12	2.06
14	b	1215	CLA	C3B-C2B	2.74	1.44	1.40
14	a	1106	CLA	C3D-C2D	2.74	1.46	1.39
21	A	6002	LMT	O4'-C4B	-2.74	1.36	1.43
14	G	1102	CLA	MG-NC	2.74	2.12	2.06
14	G	1118	CLA	C3D-C2D	2.74	1.46	1.39
14	A	1106	CLA	C3D-C2D	2.74	1.46	1.39
14	a	1133	CLA	C3D-C2D	2.74	1.46	1.39
14	a	1127	CLA	MG-NC	2.74	2.12	2.06
14	H	1231	CLA	C3D-C2D	2.74	1.46	1.39
18	R	4020	BCR	C21-C22	-2.73	1.32	1.35
21	a	6002	LMT	O4'-C4B	-2.73	1.36	1.43
15	b	1230	F6C	C3D-C2D	2.73	1.46	1.39
14	T	1401	CLA	MG-ND	-2.73	2.00	2.05
21	G	6002	LMT	O4'-C4B	-2.73	1.36	1.43
14	b	1209	CLA	C3D-C2D	2.73	1.46	1.39
14	a	1102	CLA	MG-NC	2.73	2.12	2.06
14	a	1116	CLA	MG-NC	2.73	2.12	2.06
14	H	1211	CLA	C3D-C2D	2.73	1.46	1.39
14	A	1102	CLA	MG-NC	2.73	2.12	2.06
15	G	1121	F6C	C3B-C2B	2.73	1.45	1.39
14	H	1209	CLA	C3D-C2D	2.73	1.46	1.39
14	b	1210	CLA	C3D-C2D	2.73	1.46	1.39
14	H	1022	CLA	C3D-C2D	2.72	1.46	1.39
14	b	1206	CLA	OBD-CAD	2.72	1.27	1.22
14	U	1503	CLA	C3D-C2D	2.72	1.46	1.39
14	B	1022	CLA	C3D-C2D	2.72	1.46	1.39
15	B	1230	F6C	C3D-C2D	2.72	1.46	1.39
14	H	1203	CLA	C1B-NB	-2.72	1.32	1.35
14	H	1215	CLA	C4D-CHA	2.72	1.48	1.38
14	b	1233	CLA	C1C-NC	-2.72	1.33	1.37
14	B	1210	CLA	C3D-C2D	2.72	1.46	1.39
14	G	1116	CLA	MG-NC	2.72	2.12	2.06
14	G	1111	CLA	C3D-C2D	2.72	1.46	1.39
18	I	4018	BCR	C30-C25	-2.72	1.50	1.53
14	G	1106	CLA	C3D-C2D	2.72	1.46	1.39
14	b	1229	CLA	MG-ND	-2.72	2.00	2.05
15	a	1121	F6C	C3B-C2B	2.72	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	4018	BCR	C30-C25	-2.72	1.50	1.53
14	G	1138	CLA	C4D-CHA	2.71	1.48	1.38
15	A	1121	F6C	C3B-C2B	2.71	1.45	1.39
14	B	1203	CLA	C1B-NB	-2.71	1.32	1.35
14	B	1209	CLA	C3D-C2D	2.71	1.46	1.39
14	B	1211	CLA	C3D-C2D	2.71	1.46	1.39
20	L	5007	LMG	C43-C42	-2.71	1.32	1.51
14	a	1136	CLA	C3D-C2D	2.71	1.46	1.39
14	A	1116	CLA	C3D-C2D	2.71	1.46	1.39
14	H	1239	CLA	C3D-C2D	2.71	1.46	1.39
14	H	1023	CLA	C3D-C2D	2.71	1.46	1.39
14	H	1206	CLA	OBD-CAD	2.71	1.27	1.22
14	b	1213	CLA	MG-NC	2.71	2.12	2.06
14	A	1139	CLA	MG-NC	2.71	2.12	2.06
14	G	1115	CLA	C3D-C2D	2.71	1.46	1.39
14	H	1233	CLA	C1C-NC	-2.71	1.33	1.37
14	A	1012	CLA	MG-NC	2.71	2.12	2.06
14	H	1205	CLA	C3D-C2D	2.71	1.46	1.39
14	H	1210	CLA	C3D-C2D	2.71	1.46	1.39
14	G	1136	CLA	C3D-C2D	2.71	1.46	1.39
14	b	1215	CLA	C4D-CHA	2.71	1.48	1.38
20	U	5007	LMG	C43-C42	-2.71	1.32	1.51
14	L	1503	CLA	C3D-C2D	2.71	1.46	1.39
20	l	5007	LMG	C43-C42	-2.71	1.32	1.51
14	H	1222	CLA	MG-NC	2.71	2.12	2.06
14	k	1401	CLA	MG-ND	-2.71	2.00	2.05
14	B	1232	CLA	C3D-C2D	2.71	1.46	1.39
14	K	1401	CLA	MG-ND	-2.71	2.00	2.05
14	b	1211	CLA	C3D-C2D	2.70	1.46	1.39
18	H	4005	BCR	C30-C25	-2.70	1.50	1.53
14	B	1215	CLA	C4D-CHA	2.70	1.48	1.38
14	A	1115	CLA	C3D-C2D	2.70	1.46	1.39
14	B	1219	CLA	C1C-NC	-2.70	1.33	1.37
14	B	1233	CLA	C1C-NC	-2.70	1.33	1.37
14	a	1111	CLA	C3D-C2D	2.70	1.46	1.39
14	b	1201	CLA	C3D-C2D	2.70	1.46	1.39
14	B	1229	CLA	MG-ND	-2.70	2.00	2.05
15	B	1230	F6C	MG-ND	-2.70	1.99	2.06
18	I	4020	BCR	C21-C22	-2.70	1.32	1.35
14	B	1239	CLA	C3D-C2D	2.70	1.46	1.39
14	B	1213	CLA	MG-NC	2.70	2.12	2.06
14	A	1138	CLA	C4D-CHA	2.70	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1201	CLA	C3D-C2D	2.70	1.46	1.39
14	b	1232	CLA	C3D-C2D	2.70	1.46	1.39
14	H	1224	CLA	MG-NC	2.70	2.12	2.06
14	b	1239	CLA	C3D-C2D	2.70	1.46	1.39
15	H	1230	F6C	C3D-C2D	2.70	1.46	1.39
14	G	1127	CLA	C3D-C2D	2.70	1.46	1.39
14	H	1213	CLA	C4D-CHA	2.70	1.48	1.38
15	b	1230	F6C	MG-ND	-2.70	1.99	2.06
14	H	1231	CLA	MG-NC	2.70	2.12	2.06
14	b	1222	CLA	C3D-C2D	2.70	1.46	1.39
14	B	1229	CLA	C3D-C2D	2.70	1.46	1.39
14	A	1115	CLA	MG-NC	2.70	2.12	2.06
14	l	1503	CLA	C3D-C2D	2.70	1.46	1.39
14	B	1213	CLA	C3D-C2D	2.70	1.46	1.39
14	l	1501	CLA	MG-NC	2.69	2.12	2.06
14	H	1201	CLA	C3D-C2D	2.69	1.46	1.39
14	H	1213	CLA	C3D-C2D	2.69	1.46	1.39
14	H	1219	CLA	C1C-NC	-2.69	1.33	1.37
14	b	1213	CLA	C3D-C2D	2.69	1.46	1.39
14	a	1138	CLA	C4D-CHA	2.69	1.48	1.38
14	a	1116	CLA	C3D-C2D	2.69	1.46	1.39
14	a	1115	CLA	C3D-C2D	2.69	1.46	1.39
14	B	1213	CLA	C4D-CHA	2.69	1.48	1.38
14	b	1217	CLA	C3D-C2D	2.69	1.46	1.39
14	B	1219	CLA	C4D-CHA	2.69	1.48	1.38
14	b	1229	CLA	C3D-C2D	2.69	1.46	1.39
14	b	1231	CLA	MG-NC	2.69	2.12	2.06
14	B	1217	CLA	C3D-C2D	2.69	1.46	1.39
14	H	1217	CLA	C3D-C2D	2.69	1.46	1.39
14	A	1116	CLA	MG-NC	2.69	2.12	2.06
15	H	1230	F6C	MG-ND	-2.69	1.99	2.06
14	b	1213	CLA	C4D-CHA	2.69	1.47	1.38
14	H	1229	CLA	MG-ND	-2.69	2.00	2.05
14	a	1127	CLA	C3D-C2D	2.69	1.46	1.39
14	G	1116	CLA	C3D-C2D	2.68	1.46	1.39
14	b	1224	CLA	MG-NC	2.68	2.12	2.06
14	A	1140	CLA	MG-NC	2.68	2.12	2.06
14	B	1232	CLA	C4D-CHA	2.68	1.47	1.38
15	A	1121	F6C	CHB-C4A	-2.68	1.33	1.38
14	a	1140	CLA	MG-NC	2.68	2.12	2.06
14	B	1224	CLA	MG-NC	2.68	2.12	2.06
14	G	1131	CLA	C3D-C2D	2.68	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1131	CLA	C3D-C2D	2.68	1.46	1.39
15	A	1121	F6C	C3C-C2C	2.68	1.45	1.37
14	X	1701	CLA	C3D-C2D	2.68	1.46	1.39
15	G	1121	F6C	C3C-C2C	2.68	1.45	1.37
14	H	1213	CLA	MG-NC	2.68	2.12	2.06
15	B	1238	F6C	C3C-C2C	2.68	1.45	1.37
14	b	1222	CLA	MG-NC	2.68	2.12	2.06
14	b	1224	CLA	C3D-C2D	2.68	1.46	1.39
14	G	1101	CLA	C3D-C2D	2.68	1.46	1.39
14	A	1127	CLA	C3D-C2D	2.68	1.46	1.39
14	a	1012	CLA	MG-NC	2.68	2.12	2.06
14	a	1130	CLA	C1B-NB	-2.68	1.32	1.35
14	A	1101	CLA	C3D-C2D	2.68	1.46	1.39
15	H	1238	F6C	C3C-C2C	2.68	1.45	1.37
14	B	1206	CLA	OBD-CAD	2.68	1.27	1.22
14	U	1501	CLA	MG-NC	2.68	2.12	2.06
14	G	1139	CLA	MG-NC	2.68	2.12	2.06
14	B	1023	CLA	C3D-C2D	2.68	1.46	1.39
14	L	1501	CLA	MG-NC	2.68	2.12	2.06
14	b	1219	CLA	C4D-CHA	2.68	1.47	1.38
14	B	1224	CLA	C3D-C2D	2.68	1.46	1.39
14	b	1232	CLA	C4D-CHA	2.68	1.47	1.38
14	a	1135	CLA	MG-NC	2.68	2.12	2.06
15	a	1121	F6C	CHB-C4A	-2.68	1.33	1.38
14	H	1232	CLA	C3D-C2D	2.67	1.46	1.39
14	b	1205	CLA	C3D-C2D	2.67	1.46	1.39
14	A	1130	CLA	C1B-NB	-2.67	1.32	1.35
14	G	1140	CLA	MG-NC	2.67	2.12	2.06
14	x	1701	CLA	C3D-C2D	2.67	1.46	1.39
14	a	1101	CLA	C3D-C2D	2.67	1.46	1.39
14	b	1023	CLA	C1B-NB	-2.67	1.32	1.35
14	H	1232	CLA	C4D-CHA	2.67	1.47	1.38
14	b	1023	CLA	C3D-C2D	2.67	1.46	1.39
14	G	1129	CLA	MG-NC	2.67	2.12	2.06
14	G	1112	CLA	C4D-CHA	2.67	1.47	1.38
14	B	1231	CLA	MG-NC	2.67	2.12	2.06
14	l	1501	CLA	C4D-CHA	2.67	1.47	1.38
14	H	1229	CLA	C3D-C2D	2.67	1.46	1.39
14	A	1135	CLA	MG-NC	2.67	2.12	2.06
14	B	1222	CLA	MG-NC	2.67	2.12	2.06
14	H	1222	CLA	C3D-C2D	2.66	1.46	1.39
14	a	1123	CLA	C3D-C2D	2.66	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1219	CLA	C4D-CHA	2.66	1.47	1.38
14	H	1235	CLA	MG-NC	2.66	2.12	2.06
14	B	1222	CLA	C3D-C2D	2.66	1.46	1.39
14	W	1701	CLA	C3D-C2D	2.66	1.46	1.39
14	X	1701	CLA	C4D-CHA	2.66	1.47	1.38
14	U	1501	CLA	C4D-CHA	2.66	1.47	1.38
14	G	1109	CLA	MG-NC	2.66	2.12	2.06
15	G	1121	F6C	CHB-C4A	-2.66	1.33	1.38
14	b	1223	CLA	MG-NC	2.66	2.12	2.06
14	G	1130	CLA	C1B-NB	-2.66	1.32	1.35
15	a	1121	F6C	C3C-C2C	2.66	1.45	1.37
14	a	1122	CLA	C3D-C2D	2.66	1.46	1.39
14	G	1123	CLA	C3D-C2D	2.66	1.46	1.39
14	B	1205	CLA	C3D-C2D	2.66	1.46	1.39
15	b	1238	F6C	C3C-C2C	2.66	1.45	1.37
14	G	1102	CLA	C3D-C2D	2.66	1.46	1.39
14	H	1212	CLA	C4D-CHA	2.66	1.47	1.38
14	L	1501	CLA	C4D-CHA	2.66	1.47	1.38
14	H	1224	CLA	C3D-C2D	2.66	1.46	1.39
14	A	1111	CLA	C3D-C2D	2.66	1.46	1.39
14	G	1135	CLA	MG-NC	2.66	2.12	2.06
14	A	1109	CLA	C3D-C2D	2.66	1.46	1.39
14	G	1115	CLA	MG-NC	2.66	2.12	2.06
14	b	1235	CLA	MG-NC	2.66	2.12	2.06
14	W	1701	CLA	C4D-CHA	2.65	1.47	1.38
14	a	1137	CLA	C3D-C2D	2.65	1.46	1.39
14	x	1701	CLA	C4D-CHA	2.65	1.47	1.38
14	A	1112	CLA	C4D-CHA	2.65	1.47	1.38
14	a	1139	CLA	MG-NC	2.65	2.12	2.06
14	B	1212	CLA	C4D-CHA	2.65	1.47	1.38
18	a	4008	BCR	C14-C13	-2.65	1.32	1.35
14	a	1112	CLA	C4D-CHA	2.65	1.47	1.38
14	a	1131	CLA	C3D-C2D	2.65	1.46	1.39
14	a	1115	CLA	MG-NC	2.65	2.12	2.06
14	B	1223	CLA	MG-NC	2.65	2.12	2.06
14	a	1109	CLA	MG-NC	2.65	2.12	2.06
14	G	1107	CLA	C3D-C2D	2.64	1.46	1.39
14	a	1102	CLA	C3D-C2D	2.64	1.46	1.39
14	G	1135	CLA	C1B-NB	-2.64	1.32	1.35
14	a	1107	CLA	C3D-C2D	2.64	1.46	1.39
14	A	1108	CLA	C4D-CHA	2.64	1.47	1.38
14	H	1223	CLA	MG-NC	2.64	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1219	CLA	C1C-NC	-2.64	1.33	1.37
14	b	1221	CLA	MG-NC	2.64	2.12	2.06
14	A	1122	CLA	C3D-C2D	2.64	1.46	1.39
14	B	1235	CLA	MG-NC	2.64	2.12	2.06
14	H	1233	CLA	C4D-CHA	2.64	1.47	1.38
14	b	1212	CLA	C4D-CHA	2.64	1.47	1.38
14	G	1109	CLA	C3D-C2D	2.64	1.46	1.39
14	a	1122	CLA	C4D-CHA	2.64	1.47	1.38
14	A	1122	CLA	C4D-CHA	2.64	1.47	1.38
14	G	1137	CLA	C3D-C2D	2.64	1.46	1.39
14	A	1102	CLA	C4D-CHA	2.64	1.47	1.38
14	B	1233	CLA	C4D-CHA	2.63	1.47	1.38
14	H	1023	CLA	C4B-NB	-2.63	1.32	1.35
14	G	1122	CLA	C4D-CHA	2.63	1.47	1.38
18	G	4008	BCR	C14-C13	-2.63	1.32	1.35
14	G	1012	CLA	MG-NC	2.63	2.12	2.06
14	A	1107	CLA	C3D-C2D	2.63	1.46	1.39
14	a	1115	CLA	C4D-CHA	2.63	1.47	1.38
14	A	1115	CLA	C4D-CHA	2.63	1.47	1.38
14	a	1108	CLA	C4D-CHA	2.63	1.47	1.38
14	G	1122	CLA	C3D-C2D	2.63	1.46	1.39
14	A	1137	CLA	C3D-C2D	2.63	1.46	1.39
18	A	4008	BCR	C14-C13	-2.63	1.32	1.35
14	a	1130	CLA	C3D-C2D	2.63	1.46	1.39
14	H	1203	CLA	OBD-CAD	2.63	1.27	1.22
14	G	1130	CLA	C3D-C2D	2.63	1.46	1.39
14	A	1102	CLA	C3D-C2D	2.63	1.46	1.39
14	a	1129	CLA	MG-NC	2.63	2.12	2.06
14	A	1114	CLA	MG-NC	2.63	2.12	2.06
15	B	1237	F6C	C3C-C2C	2.63	1.45	1.37
14	G	1110	CLA	C3D-C2D	2.63	1.46	1.39
14	a	1109	CLA	C3D-C2D	2.63	1.46	1.39
14	b	1233	CLA	C4D-CHA	2.63	1.47	1.38
14	A	1123	CLA	C3D-C2D	2.63	1.46	1.39
14	a	1110	CLA	C3D-C2D	2.63	1.46	1.39
14	A	1109	CLA	MG-NC	2.63	2.12	2.06
13	G	1011	CL0	C3D-C2D	2.63	1.46	1.39
14	B	1210	CLA	MG-NC	2.63	2.12	2.06
14	a	1113	CLA	MG-NC	2.62	2.12	2.06
14	b	1208	CLA	MG-NC	2.62	2.12	2.06
14	B	1217	CLA	C4D-CHA	2.62	1.47	1.38
14	a	1102	CLA	C4D-CHA	2.62	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1123	CLA	C4D-CHA	2.62	1.47	1.38
14	H	1204	CLA	C3D-C2D	2.62	1.46	1.39
14	H	1220	CLA	C4D-CHA	2.62	1.47	1.38
14	b	1212	CLA	MG-NC	2.62	2.12	2.06
13	a	1011	CL0	C3D-C2D	2.62	1.46	1.39
14	B	1203	CLA	OBD-CAD	2.62	1.27	1.22
14	A	1123	CLA	C4D-CHA	2.62	1.47	1.38
14	A	1113	CLA	MG-NC	2.62	2.12	2.06
14	A	1130	CLA	C3D-C2D	2.62	1.46	1.39
14	G	1115	CLA	C4D-CHA	2.62	1.47	1.38
14	b	1210	CLA	MG-NC	2.62	2.12	2.06
14	b	1204	CLA	C3D-C2D	2.62	1.46	1.39
14	B	1216	CLA	C4D-CHA	2.62	1.47	1.38
14	G	1123	CLA	C4D-CHA	2.62	1.47	1.38
14	H	1217	CLA	C4D-CHA	2.62	1.47	1.38
14	b	1220	CLA	C4D-CHA	2.62	1.47	1.38
14	H	1221	CLA	MG-NC	2.62	2.12	2.06
14	G	1126	CLA	C3D-C2D	2.62	1.46	1.39
14	b	1204	CLA	C1B-NB	-2.61	1.32	1.35
14	b	1209	CLA	MG-NC	2.61	2.12	2.06
21	G	6001	LMT	O2'-C2'	-2.61	1.36	1.43
14	G	1113	CLA	C4D-CHA	2.61	1.47	1.38
14	G	1133	CLA	MG-NC	2.61	2.12	2.06
14	G	1108	CLA	C4D-CHA	2.61	1.47	1.38
14	b	1203	CLA	OBD-CAD	2.61	1.27	1.22
14	H	1223	CLA	C4D-CHA	2.61	1.47	1.38
18	a	4007	BCR	C1-C6	-2.61	1.50	1.53
14	G	1111	CLA	C4D-CHA	2.61	1.47	1.38
14	b	1217	CLA	C4D-CHA	2.61	1.47	1.38
14	a	1114	CLA	MG-NC	2.61	2.12	2.06
14	a	1110	CLA	MG-NC	2.61	2.12	2.06
14	H	1201	CLA	C4D-CHA	2.61	1.47	1.38
14	H	1216	CLA	C4D-CHA	2.61	1.47	1.38
14	A	1110	CLA	MG-NC	2.61	2.12	2.06
14	B	1221	CLA	MG-NC	2.61	2.12	2.06
15	B	1207	F6C	C3D-C2D	2.61	1.46	1.39
14	G	1110	CLA	MG-NC	2.61	2.12	2.06
14	a	1133	CLA	MG-NC	2.60	2.12	2.06
14	A	1113	CLA	C4D-CHA	2.60	1.47	1.38
15	b	1207	F6C	C3D-C2D	2.60	1.46	1.39
14	G	1133	CLA	C4D-CHA	2.60	1.47	1.38
14	A	1129	CLA	MG-NC	2.60	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1208	CLA	MG-NC	2.60	2.12	2.06
14	H	1220	CLA	MG-NC	2.60	2.12	2.06
13	A	1011	CL0	C3D-C2D	2.60	1.46	1.39
14	b	1216	CLA	C4D-CHA	2.60	1.47	1.38
14	B	1201	CLA	C4D-CHA	2.60	1.47	1.38
14	B	1220	CLA	C4D-CHA	2.60	1.47	1.38
14	B	1023	CLA	C1B-NB	-2.60	1.32	1.35
14	G	1102	CLA	C4D-CHA	2.60	1.47	1.38
14	G	1116	CLA	C4D-CHA	2.60	1.47	1.38
14	H	1212	CLA	MG-NC	2.60	2.12	2.06
14	a	1133	CLA	C4D-CHA	2.60	1.47	1.38
14	A	1133	CLA	C4D-CHA	2.60	1.47	1.38
15	H	1207	F6C	C3D-C2D	2.60	1.46	1.39
14	a	1135	CLA	C1B-NB	-2.60	1.32	1.35
14	a	1126	CLA	C3D-C2D	2.60	1.46	1.39
14	A	1111	CLA	C4D-CHA	2.60	1.47	1.38
14	G	1125	CLA	C3D-C2D	2.60	1.46	1.39
21	a	6002	LMT	O2'-C2'	-2.60	1.36	1.43
14	a	1125	CLA	C3D-C2D	2.60	1.46	1.39
14	H	1231	CLA	C4D-CHA	2.60	1.47	1.38
21	G	6002	LMT	O2'-C2'	-2.60	1.36	1.43
14	G	1107	CLA	C4D-CHA	2.60	1.47	1.38
14	A	1136	CLA	C4D-CHA	2.60	1.47	1.38
14	A	1126	CLA	C3D-C2D	2.60	1.46	1.39
14	b	1231	CLA	C4D-CHA	2.60	1.47	1.38
21	A	6001	LMT	O2'-C2'	-2.60	1.36	1.43
14	B	1218	CLA	C4D-CHA	2.59	1.47	1.38
14	a	1111	CLA	C4D-CHA	2.59	1.47	1.38
14	G	1113	CLA	MG-NC	2.59	2.12	2.06
14	H	1204	CLA	C1B-NB	-2.59	1.32	1.35
14	b	1023	CLA	C4B-NB	-2.59	1.32	1.35
14	a	1101	CLA	C4D-CHA	2.59	1.47	1.38
14	b	1201	CLA	C4D-CHA	2.59	1.47	1.38
14	G	1128	CLA	C4D-CHA	2.59	1.47	1.38
14	A	1133	CLA	MG-NC	2.59	2.12	2.06
14	G	1136	CLA	C4D-CHA	2.59	1.47	1.38
14	A	1110	CLA	C3D-C2D	2.59	1.46	1.39
14	A	1125	CLA	C3D-C2D	2.59	1.46	1.39
14	b	1223	CLA	C4D-CHA	2.59	1.47	1.38
14	A	1107	CLA	C4D-CHA	2.59	1.47	1.38
14	B	1204	CLA	C3D-C2D	2.59	1.46	1.39
14	H	1208	CLA	C4D-CHA	2.59	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1136	CLA	C4D-CHA	2.59	1.47	1.38
14	a	1107	CLA	C4D-CHA	2.59	1.47	1.38
14	H	1208	CLA	MG-NC	2.59	2.12	2.06
14	B	1220	CLA	MG-NC	2.59	2.12	2.06
14	G	1132	CLA	MG-NC	2.59	2.12	2.06
14	H	1209	CLA	MG-NC	2.59	2.12	2.06
18	G	4007	BCR	C1-C6	-2.59	1.50	1.53
14	a	1113	CLA	C4D-CHA	2.59	1.47	1.38
14	B	1223	CLA	C4D-CHA	2.59	1.47	1.38
15	H	1237	F6C	C3C-C2C	2.59	1.45	1.37
14	H	1023	CLA	C1B-NB	-2.59	1.32	1.35
14	H	1210	CLA	MG-NC	2.59	2.12	2.06
14	H	1218	CLA	C4D-CHA	2.59	1.47	1.38
14	b	1218	CLA	C4D-CHA	2.59	1.47	1.38
14	G	1101	CLA	C4D-CHA	2.59	1.47	1.38
14	B	1225	CLA	C3D-C2D	2.58	1.46	1.39
15	b	1207	F6C	C1A-C2A	2.58	1.51	1.45
14	B	1212	CLA	MG-NC	2.58	2.12	2.06
14	H	1235	CLA	C4D-CHA	2.58	1.47	1.38
14	a	1128	CLA	C4D-CHA	2.58	1.47	1.38
14	A	1135	CLA	C1B-NB	-2.58	1.32	1.35
15	b	1237	F6C	C3C-C2C	2.58	1.45	1.37
18	i	4020	BCR	C14-C13	-2.58	1.32	1.35
21	A	6002	LMT	O2'-C2'	-2.58	1.36	1.43
14	H	1214	CLA	C4D-CHA	2.58	1.47	1.38
14	a	1119	CLA	C4D-CHA	2.58	1.47	1.38
14	A	1101	CLA	C4D-CHA	2.58	1.47	1.38
14	B	1209	CLA	C4D-CHA	2.58	1.47	1.38
14	G	1114	CLA	MG-NC	2.58	2.12	2.06
15	B	1207	F6C	C1A-C2A	2.58	1.51	1.45
14	a	1137	CLA	MG-NC	2.58	2.12	2.06
14	B	1235	CLA	C4D-CHA	2.58	1.47	1.38
20	U	5007	LMG	C22-C21	-2.58	1.33	1.51
14	b	1201	CLA	MG-NC	2.58	2.12	2.06
14	H	1206	CLA	C4D-CHA	2.58	1.47	1.38
14	b	1209	CLA	C4D-CHA	2.58	1.47	1.38
21	a	6001	LMT	O2'-C2'	-2.58	1.36	1.43
14	A	1119	CLA	C4D-CHA	2.58	1.47	1.38
14	a	1116	CLA	C4D-CHA	2.58	1.47	1.38
14	A	1116	CLA	C4D-CHA	2.58	1.47	1.38
14	b	1214	CLA	C4D-CHA	2.57	1.47	1.38
14	A	1132	CLA	MG-NC	2.57	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1221	CLA	C4D-CHA	2.57	1.47	1.38
14	B	1023	CLA	C4B-NB	-2.57	1.32	1.35
14	a	1132	CLA	C4D-CHA	2.57	1.47	1.38
14	A	1127	CLA	C4D-CHA	2.57	1.47	1.38
14	H	1201	CLA	MG-NC	2.57	2.12	2.06
20	L	5007	LMG	C22-C21	-2.57	1.33	1.51
14	B	1209	CLA	MG-NC	2.57	2.12	2.06
14	G	1131	CLA	C4D-CHA	2.57	1.47	1.38
14	H	1021	CLA	C3D-C2D	2.57	1.46	1.39
14	B	1214	CLA	C4D-CHA	2.57	1.47	1.38
14	a	1138	CLA	MG-NC	2.57	2.12	2.06
21	G	6001	LMT	O2B-C2B	-2.57	1.36	1.43
14	B	1234	CLA	C3D-C2D	2.57	1.46	1.39
14	H	1239	CLA	C4D-CHA	2.57	1.47	1.38
14	a	1101	CLA	MG-NC	2.57	2.12	2.06
14	B	1201	CLA	MG-NC	2.57	2.12	2.06
14	A	1112	CLA	MG-NC	2.57	2.12	2.06
20	l	5007	LMG	C22-C21	-2.57	1.33	1.51
14	B	1208	CLA	C4D-CHA	2.57	1.47	1.38
14	B	1239	CLA	MG-NC	2.57	2.12	2.06
13	a	1011	CL0	C1B-NB	-2.57	1.32	1.35
14	B	1210	CLA	C4D-CHA	2.57	1.47	1.38
14	a	1109	CLA	C4D-CHA	2.57	1.47	1.38
14	b	1208	CLA	C4D-CHA	2.57	1.47	1.38
14	G	1124	CLA	C3D-C2D	2.57	1.46	1.39
14	G	1105	CLA	C4D-CHA	2.57	1.47	1.38
14	b	1234	CLA	C3D-C2D	2.57	1.46	1.39
14	H	1234	CLA	C3D-C2D	2.56	1.46	1.39
14	A	1106	CLA	C4D-CHA	2.56	1.47	1.38
14	A	1128	CLA	C4D-CHA	2.56	1.47	1.38
14	a	1105	CLA	C4D-CHA	2.56	1.47	1.38
14	b	1210	CLA	C4D-CHA	2.56	1.47	1.38
14	B	1204	CLA	C1B-NB	-2.56	1.32	1.35
14	a	1127	CLA	C4D-CHA	2.56	1.47	1.38
14	B	1221	CLA	C4D-CHA	2.56	1.47	1.38
18	I	4020	BCR	C14-C13	-2.56	1.32	1.35
14	B	1231	CLA	C4D-CHA	2.56	1.47	1.38
14	G	1132	CLA	C3D-C2D	2.56	1.46	1.39
14	G	1127	CLA	C4D-CHA	2.56	1.47	1.38
14	H	1209	CLA	C4D-CHA	2.56	1.47	1.38
14	k	1401	CLA	C1C-NC	-2.56	1.34	1.37
14	G	1119	CLA	C4D-CHA	2.56	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1216	CLA	MG-NC	2.56	2.12	2.06
18	R	4020	BCR	C14-C13	-2.56	1.32	1.35
18	A	4007	BCR	C1-C6	-2.56	1.50	1.53
14	b	1220	CLA	MG-NC	2.56	2.12	2.06
14	B	1206	CLA	C4D-CHA	2.56	1.47	1.38
14	G	1132	CLA	C4D-CHA	2.56	1.47	1.38
14	H	1221	CLA	C4D-CHA	2.56	1.47	1.38
14	A	1137	CLA	MG-NC	2.56	2.12	2.06
14	G	1106	CLA	C4D-CHA	2.56	1.47	1.38
14	A	1119	CLA	C1B-NB	-2.56	1.32	1.35
14	A	1105	CLA	C4D-CHA	2.56	1.47	1.38
14	A	1132	CLA	C3D-C2D	2.56	1.46	1.39
14	H	1225	CLA	C3D-C2D	2.56	1.46	1.39
14	H	1210	CLA	C4D-CHA	2.56	1.47	1.38
14	G	1120	CLA	C4D-CHA	2.55	1.47	1.38
14	A	1120	CLA	C4D-CHA	2.55	1.47	1.38
14	H	1236	CLA	C3D-C2D	2.55	1.46	1.39
15	H	1207	F6C	C1A-C2A	2.55	1.51	1.45
14	a	1132	CLA	MG-NC	2.55	2.12	2.06
14	H	1205	CLA	C4D-CHA	2.55	1.47	1.38
14	K	1401	CLA	C1C-NC	-2.55	1.34	1.37
14	H	1216	CLA	MG-NC	2.55	2.12	2.06
14	a	1131	CLA	MG-NC	2.55	2.12	2.06
14	b	1206	CLA	C4D-CHA	2.55	1.47	1.38
14	H	1203	CLA	C4D-CHA	2.55	1.47	1.38
14	H	1234	CLA	C4D-CHA	2.55	1.47	1.38
14	G	1101	CLA	MG-NC	2.55	2.12	2.06
14	G	1106	CLA	MG-NC	2.55	2.12	2.06
14	G	1138	CLA	MG-NC	2.55	2.12	2.06
14	A	1132	CLA	C4D-CHA	2.55	1.47	1.38
14	b	1236	CLA	C3D-C2D	2.55	1.46	1.39
14	a	1120	CLA	C4D-CHA	2.55	1.47	1.38
14	b	1022	CLA	C4D-CHA	2.55	1.47	1.38
14	H	1239	CLA	MG-NC	2.55	2.12	2.06
14	A	1131	CLA	C4D-CHA	2.55	1.47	1.38
14	A	1131	CLA	MG-NC	2.55	2.12	2.06
14	a	1112	CLA	MG-NC	2.55	2.12	2.06
14	b	1235	CLA	C4D-CHA	2.55	1.47	1.38
14	H	1227	CLA	C4D-CHA	2.55	1.47	1.38
14	U	1502	CLA	MG-NC	2.55	2.12	2.06
14	a	1111	CLA	MG-NC	2.55	2.12	2.06
14	A	1109	CLA	C4D-CHA	2.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1203	CLA	C4D-CHA	2.54	1.47	1.38
14	A	1138	CLA	MG-NC	2.54	2.12	2.06
14	a	1131	CLA	C4D-CHA	2.54	1.47	1.38
14	a	1132	CLA	C3D-C2D	2.54	1.46	1.39
21	A	6001	LMT	O2B-C2B	-2.54	1.37	1.43
14	H	1228	CLA	MG-NC	2.54	2.12	2.06
14	a	1124	CLA	C3D-C2D	2.54	1.46	1.39
14	b	1203	CLA	C4D-CHA	2.54	1.47	1.38
14	B	1236	CLA	C3D-C2D	2.54	1.46	1.39
14	B	1227	CLA	C4D-CHA	2.54	1.47	1.38
14	a	1106	CLA	C4D-CHA	2.54	1.47	1.38
14	G	1112	CLA	MG-NC	2.54	2.12	2.06
14	a	1012	CLA	C4D-CHA	2.54	1.47	1.38
14	b	1234	CLA	C4D-CHA	2.54	1.47	1.38
14	B	1216	CLA	MG-NC	2.54	2.12	2.06
14	B	1022	CLA	C4D-CHA	2.54	1.47	1.38
14	a	1140	CLA	C4D-CHA	2.54	1.47	1.38
14	b	1021	CLA	C3D-C2D	2.54	1.46	1.39
14	b	1239	CLA	C4D-CHA	2.54	1.47	1.38
14	b	1225	CLA	C3D-C2D	2.54	1.46	1.39
14	G	1109	CLA	C4D-CHA	2.54	1.47	1.38
14	H	1022	CLA	C4D-CHA	2.54	1.47	1.38
14	B	1234	CLA	C4D-CHA	2.54	1.47	1.38
14	b	1228	CLA	MG-NC	2.53	2.12	2.06
14	b	1205	CLA	C4D-CHA	2.53	1.47	1.38
14	B	1228	CLA	MG-NC	2.53	2.12	2.06
14	B	1205	CLA	C4D-CHA	2.53	1.47	1.38
14	b	1226	CLA	C4D-CHA	2.53	1.47	1.38
14	l	1502	CLA	MG-NC	2.53	2.12	2.06
14	b	1227	CLA	C4D-CHA	2.53	1.47	1.38
14	A	1101	CLA	MG-NC	2.53	2.12	2.06
14	G	1111	CLA	MG-NC	2.53	2.12	2.06
14	a	1120	CLA	MG-NC	2.53	2.12	2.06
14	H	1225	CLA	C4D-CHA	2.53	1.47	1.38
14	G	1137	CLA	MG-NC	2.53	2.12	2.06
14	b	1222	CLA	C4D-CHA	2.53	1.47	1.38
14	A	1124	CLA	C3D-C2D	2.53	1.46	1.39
14	a	1103	CLA	C3D-C2D	2.53	1.46	1.39
21	G	6001	LMT	O3B-C3B	-2.53	1.37	1.43
14	A	1139	CLA	C4B-CHC	2.53	1.48	1.41
14	G	1118	CLA	C4D-CHA	2.53	1.47	1.38
14	G	1131	CLA	MG-NC	2.53	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1110	CLA	C4D-CHA	2.53	1.47	1.38
14	G	1110	CLA	C4D-CHA	2.53	1.47	1.38
14	B	1021	CLA	C3D-C2D	2.53	1.46	1.39
14	l	1503	CLA	MG-NC	2.52	2.12	2.06
14	T	1401	CLA	C1C-NC	-2.52	1.34	1.37
14	A	1111	CLA	MG-NC	2.52	2.12	2.06
14	A	1120	CLA	MG-NC	2.52	2.12	2.06
21	a	6001	LMT	O2B-C2B	-2.52	1.37	1.43
14	b	1225	CLA	C4D-CHA	2.52	1.47	1.38
14	G	1140	CLA	C4D-CHA	2.52	1.47	1.38
14	b	1239	CLA	MG-NC	2.52	2.12	2.06
14	G	1105	CLA	MG-NC	2.52	2.12	2.06
14	B	1211	CLA	MG-NC	2.52	2.12	2.06
14	H	1226	CLA	C4D-CHA	2.52	1.47	1.38
15	b	1230	F6C	C3C-C2C	2.52	1.45	1.37
18	i	4020	BCR	C17-C18	-2.52	1.32	1.35
14	L	1502	CLA	MG-NC	2.52	2.12	2.06
14	H	1234	CLA	MG-NC	2.52	2.12	2.06
14	A	1118	CLA	C4D-CHA	2.52	1.47	1.38
14	a	1106	CLA	MG-NC	2.52	2.12	2.06
14	L	1503	CLA	MG-NC	2.52	2.12	2.06
14	a	1118	CLA	C4D-CHA	2.52	1.47	1.38
14	a	1130	CLA	C4D-CHA	2.52	1.47	1.38
14	a	1139	CLA	C4B-CHC	2.52	1.48	1.41
14	b	1211	CLA	MG-NC	2.52	2.12	2.06
14	A	1137	CLA	C4D-CHA	2.52	1.47	1.38
14	B	1225	CLA	C4D-CHA	2.52	1.47	1.38
14	G	1119	CLA	C1B-NB	-2.52	1.33	1.35
14	a	1136	CLA	MG-NC	2.52	2.12	2.06
14	B	1226	CLA	C4D-CHA	2.52	1.47	1.38
14	A	1103	CLA	C3D-C2D	2.52	1.46	1.39
14	B	1239	CLA	C4D-CHA	2.51	1.47	1.38
21	a	6001	LMT	O3B-C3B	-2.51	1.37	1.43
14	a	1122	CLA	MG-NC	2.51	2.12	2.06
14	a	1110	CLA	C4D-CHA	2.51	1.47	1.38
21	A	6001	LMT	O3B-C3B	-2.51	1.37	1.43
14	A	1122	CLA	MG-NC	2.51	2.12	2.06
14	G	1103	CLA	C3D-C2D	2.51	1.46	1.39
14	b	1234	CLA	MG-NC	2.51	2.12	2.06
14	b	1211	CLA	C4D-CHA	2.51	1.47	1.38
14	a	1119	CLA	C1B-NB	-2.51	1.33	1.35
14	B	1234	CLA	MG-NC	2.51	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1140	CLA	C4D-CHA	2.51	1.47	1.38
14	B	1211	CLA	C4D-CHA	2.51	1.47	1.38
14	a	1137	CLA	C4D-CHA	2.51	1.47	1.38
14	A	1126	CLA	C4D-CHA	2.51	1.47	1.38
14	H	1225	CLA	MG-NC	2.51	2.12	2.06
15	H	1230	F6C	C3C-C2C	2.51	1.45	1.37
14	G	1124	CLA	C1B-NB	-2.51	1.33	1.35
14	H	1211	CLA	C4D-CHA	2.51	1.47	1.38
14	A	1106	CLA	MG-NC	2.51	2.12	2.06
14	U	1503	CLA	MG-NC	2.51	2.12	2.06
14	G	1140	CLA	C4B-CHC	2.51	1.48	1.41
14	B	1202	CLA	C3D-C2D	2.51	1.46	1.39
18	I	4020	BCR	C17-C18	-2.50	1.32	1.35
14	B	1202	CLA	C4D-CHA	2.50	1.47	1.38
14	H	1211	CLA	MG-NC	2.50	2.12	2.06
14	A	1012	CLA	C4D-CHA	2.50	1.47	1.38
14	B	1222	CLA	C4D-CHA	2.50	1.47	1.38
14	G	1122	CLA	MG-NC	2.50	2.12	2.06
14	G	1126	CLA	C4D-CHA	2.50	1.47	1.38
14	B	1225	CLA	MG-NC	2.50	2.12	2.06
14	b	1202	CLA	C3D-C2D	2.50	1.45	1.39
18	L	4022	BCR	C21-C22	-2.50	1.32	1.35
14	H	1218	CLA	C4B-CHC	2.50	1.47	1.41
14	b	1226	CLA	MG-NC	2.50	2.12	2.06
14	G	1125	CLA	C4D-CHA	2.50	1.47	1.38
14	A	1136	CLA	MG-NC	2.50	2.12	2.06
14	K	1401	CLA	C4B-CHC	2.50	1.47	1.41
14	A	1130	CLA	C4D-CHA	2.50	1.47	1.38
14	b	1202	CLA	C4D-CHA	2.50	1.47	1.38
14	G	1012	CLA	C4D-CHA	2.50	1.47	1.38
14	G	1137	CLA	C4D-CHA	2.50	1.47	1.38
14	a	1134	CLA	C1D-C2D	2.50	1.50	1.45
14	G	1120	CLA	MG-NC	2.49	2.12	2.06
14	G	1128	CLA	MG-NC	2.49	2.12	2.06
14	G	1130	CLA	C4D-CHA	2.49	1.47	1.38
14	a	1108	CLA	MG-NC	2.49	2.12	2.06
14	A	1108	CLA	MG-NC	2.49	2.12	2.06
14	H	1222	CLA	C4D-CHA	2.49	1.47	1.38
14	a	1126	CLA	C4D-CHA	2.49	1.47	1.38
14	B	1227	CLA	C3D-C2D	2.49	1.45	1.39
15	B	1230	F6C	C3C-C2C	2.49	1.45	1.37
14	U	1503	CLA	C4D-CHA	2.49	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1139	CLA	C4D-CHA	2.49	1.47	1.38
14	b	1222	CLA	C1B-NB	-2.49	1.33	1.35
14	B	1224	CLA	C4D-CHA	2.49	1.47	1.38
14	A	1105	CLA	MG-NC	2.49	2.12	2.06
14	G	1104	CLA	C3D-C2D	2.49	1.45	1.39
14	B	1218	CLA	C4B-CHC	2.49	1.47	1.41
14	H	1202	CLA	C4D-CHA	2.49	1.47	1.38
14	A	1139	CLA	C4D-CHA	2.49	1.47	1.38
14	T	1401	CLA	C4B-CHC	2.49	1.47	1.41
14	H	1202	CLA	C3D-C2D	2.49	1.45	1.39
14	b	1225	CLA	MG-NC	2.49	2.12	2.06
14	B	1226	CLA	MG-NC	2.49	2.12	2.06
18	U	4022	BCR	C17-C18	-2.49	1.32	1.35
14	G	1134	CLA	C1D-C2D	2.49	1.50	1.45
14	A	1134	CLA	C1C-NC	-2.49	1.34	1.37
14	H	1226	CLA	MG-NC	2.48	2.12	2.06
15	B	1207	F6C	C3C-C2C	2.48	1.45	1.37
14	L	1503	CLA	C4D-CHA	2.48	1.47	1.38
14	G	1136	CLA	MG-NC	2.48	2.12	2.06
14	a	1140	CLA	C4B-CHC	2.48	1.47	1.41
14	G	1139	CLA	C4D-CHA	2.48	1.47	1.38
14	b	1224	CLA	C4D-CHA	2.48	1.47	1.38
14	a	1105	CLA	MG-NC	2.48	2.12	2.06
18	a	4011	BCR	C21-C22	-2.48	1.32	1.35
14	a	1134	CLA	C1C-NC	-2.48	1.34	1.37
14	k	1401	CLA	C4B-CHC	2.48	1.47	1.41
14	a	1129	CLA	C4D-CHA	2.48	1.47	1.38
14	a	1128	CLA	MG-NC	2.48	2.12	2.06
14	a	1125	CLA	C4D-CHA	2.47	1.47	1.38
14	G	1139	CLA	C4B-CHC	2.47	1.47	1.41
14	B	1223	CLA	C3D-C2D	2.47	1.45	1.39
14	a	1103	CLA	C4D-CHA	2.47	1.47	1.38
13	G	1011	CL0	C1B-NB	-2.47	1.33	1.35
14	l	1503	CLA	C4D-CHA	2.47	1.47	1.38
14	A	1124	CLA	C4D-CHA	2.47	1.47	1.38
14	A	1140	CLA	C4B-CHC	2.47	1.47	1.41
14	B	1229	CLA	MG-NC	2.47	2.12	2.06
18	R	4020	BCR	C17-C18	-2.47	1.32	1.35
14	A	1128	CLA	MG-NC	2.47	2.12	2.06
18	L	4022	BCR	C17-C18	-2.47	1.32	1.35
14	b	1218	CLA	C4B-CHC	2.47	1.47	1.41
14	G	1134	CLA	C1C-NC	-2.47	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1224	CLA	C4D-CHA	2.47	1.47	1.38
14	a	1124	CLA	C4D-CHA	2.47	1.47	1.38
14	B	1236	CLA	C4D-CHA	2.47	1.47	1.38
15	H	1207	F6C	C3C-C2C	2.47	1.45	1.37
14	G	1124	CLA	C4D-CHA	2.47	1.47	1.38
14	G	1129	CLA	C4D-CHA	2.47	1.47	1.38
14	H	1214	CLA	C1B-NB	-2.47	1.33	1.35
14	A	1103	CLA	MG-NC	2.47	2.12	2.06
13	a	1011	CL0	C4D-CHA	2.46	1.47	1.38
18	U	4022	BCR	C21-C22	-2.46	1.32	1.35
14	A	1113	CLA	C4B-CHC	2.46	1.47	1.41
14	b	1236	CLA	C4D-CHA	2.46	1.47	1.38
14	H	1236	CLA	C4D-CHA	2.46	1.47	1.38
14	A	1139	CLA	C3D-C2D	2.46	1.45	1.39
15	b	1207	F6C	C3C-C2C	2.46	1.45	1.37
14	A	1104	CLA	C4D-CHA	2.46	1.47	1.38
14	A	1125	CLA	C4D-CHA	2.46	1.47	1.38
14	b	1203	CLA	C3D-C2D	2.46	1.45	1.39
14	H	1227	CLA	C3D-C2D	2.46	1.45	1.39
14	a	1126	CLA	MG-NC	2.46	2.12	2.06
14	A	1104	CLA	C3D-C2D	2.46	1.45	1.39
14	A	1134	CLA	C1D-C2D	2.46	1.50	1.45
14	G	1108	CLA	MG-NC	2.46	2.12	2.06
14	H	1236	CLA	MG-NC	2.46	2.12	2.06
14	G	1129	CLA	C3D-C2D	2.46	1.45	1.39
14	a	1139	CLA	C3D-C2D	2.46	1.45	1.39
14	A	1124	CLA	C1B-NB	-2.46	1.33	1.35
14	B	1220	CLA	C1B-CHB	2.46	1.47	1.41
14	a	1134	CLA	C4B-CHC	2.46	1.47	1.41
14	A	1134	CLA	C4B-CHC	2.46	1.47	1.41
14	a	1103	CLA	MG-NC	2.46	2.12	2.06
14	H	1203	CLA	C3D-C2D	2.45	1.45	1.39
14	b	1220	CLA	C1B-CHB	2.45	1.47	1.41
14	a	1129	CLA	C3D-C2D	2.45	1.45	1.39
14	b	1229	CLA	MG-NC	2.45	2.12	2.06
14	A	1126	CLA	MG-NC	2.45	2.12	2.06
14	a	1104	CLA	C3D-C2D	2.45	1.45	1.39
14	H	1222	CLA	C1B-NB	-2.45	1.33	1.35
14	B	1229	CLA	C4B-CHC	2.45	1.47	1.41
14	b	1229	CLA	C4D-CHA	2.45	1.47	1.38
14	B	1203	CLA	C3D-C2D	2.45	1.45	1.39
14	A	1129	CLA	C4D-CHA	2.45	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1215	CLA	MG-NC	2.45	2.12	2.06
14	G	1134	CLA	C4B-CHC	2.45	1.47	1.41
14	B	1023	CLA	C4D-CHA	2.45	1.47	1.38
14	G	1110	CLA	C4B-CHC	2.45	1.47	1.41
15	a	1121	F6C	C4C-CHD	2.45	1.47	1.41
14	G	1125	CLA	C4B-NB	-2.45	1.33	1.35
14	G	1103	CLA	C4D-CHA	2.45	1.47	1.38
18	B	4017	BCR	C30-C25	-2.45	1.50	1.53
14	H	1229	CLA	MG-NC	2.45	2.12	2.06
14	B	1229	CLA	C4D-CHA	2.45	1.47	1.38
14	b	1215	CLA	C1B-NB	-2.45	1.33	1.35
14	x	1701	CLA	C4B-CHC	2.45	1.47	1.41
15	A	1121	F6C	C4C-CHD	2.45	1.47	1.41
14	B	1234	CLA	C4B-CHC	2.45	1.47	1.41
14	H	1229	CLA	C4D-CHA	2.44	1.47	1.38
14	H	1229	CLA	C4B-CHC	2.44	1.47	1.41
18	B	4010	BCR	C17-C18	-2.44	1.32	1.35
14	a	1125	CLA	C4B-NB	-2.44	1.33	1.35
14	H	1220	CLA	C1B-CHB	2.44	1.47	1.41
14	a	1110	CLA	C4B-CHC	2.44	1.47	1.41
14	A	1110	CLA	C4B-CHC	2.44	1.47	1.41
13	G	1011	CL0	C4D-CHA	2.44	1.47	1.38
13	A	1011	CL0	C1B-NB	-2.44	1.33	1.35
14	b	1214	CLA	C1B-NB	-2.44	1.33	1.35
14	G	1139	CLA	C3D-C2D	2.44	1.45	1.39
18	l	4022	BCR	C21-C22	-2.44	1.32	1.35
14	A	1129	CLA	C3D-C2D	2.44	1.45	1.39
14	b	1021	CLA	C1B-NB	-2.44	1.33	1.35
14	b	1223	CLA	C3D-C2D	2.44	1.45	1.39
14	H	1234	CLA	C4B-CHC	2.44	1.47	1.41
14	b	1023	CLA	C4D-CHA	2.44	1.47	1.38
14	B	1228	CLA	C4D-CHA	2.44	1.47	1.38
14	H	1223	CLA	C3D-C2D	2.44	1.45	1.39
18	l	4022	BCR	C17-C18	-2.44	1.32	1.35
14	b	1234	CLA	C4B-CHC	2.44	1.47	1.41
14	G	1104	CLA	C4D-CHA	2.44	1.47	1.38
14	G	1113	CLA	C4B-CHC	2.44	1.47	1.41
14	a	1113	CLA	C4B-CHC	2.44	1.47	1.41
14	b	1229	CLA	C4B-CHC	2.44	1.47	1.41
14	a	1104	CLA	C4D-CHA	2.44	1.47	1.38
14	H	1215	CLA	MG-NC	2.43	2.12	2.06
14	b	1227	CLA	C3D-C2D	2.43	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	W	1701	CLA	C4B-CHC	2.43	1.47	1.41
14	A	1103	CLA	C4D-CHA	2.43	1.47	1.38
14	a	1129	CLA	C1B-NB	-2.43	1.33	1.35
14	X	1701	CLA	C4B-CHC	2.43	1.47	1.41
14	H	1228	CLA	C4D-CHA	2.43	1.47	1.38
14	G	1126	CLA	MG-NC	2.43	2.12	2.06
13	A	1011	CL0	C4D-CHA	2.43	1.47	1.38
18	A	4008	BCR	C21-C22	-2.43	1.32	1.35
14	H	1023	CLA	C4D-CHA	2.43	1.47	1.38
14	a	1124	CLA	C1B-NB	-2.43	1.33	1.35
14	G	1103	CLA	MG-NC	2.43	2.12	2.06
14	H	1236	CLA	C4B-CHC	2.42	1.47	1.41
21	a	6002	LMT	O2B-C2B	-2.42	1.37	1.43
14	H	1216	CLA	C4B-CHC	2.42	1.47	1.41
15	G	1121	F6C	C4C-CHD	2.42	1.47	1.41
14	b	1236	CLA	MG-NC	2.42	2.12	2.06
14	B	1236	CLA	MG-NC	2.42	2.12	2.06
14	B	1222	CLA	C1B-NB	-2.42	1.33	1.35
14	b	1228	CLA	C4D-CHA	2.42	1.47	1.38
15	A	1121	F6C	C1D-C2D	2.42	1.49	1.44
14	G	1136	CLA	C1B-NB	-2.42	1.33	1.35
18	H	4017	BCR	C30-C25	-2.41	1.50	1.53
14	a	1130	CLA	OBD-CAD	2.41	1.26	1.22
14	a	1135	CLA	C4D-CHA	2.41	1.47	1.38
15	a	1121	F6C	C1D-C2D	2.41	1.49	1.44
14	G	1135	CLA	C4D-CHA	2.41	1.47	1.38
14	B	1216	CLA	C4B-CHC	2.41	1.47	1.41
14	b	1215	CLA	MG-NC	2.41	2.12	2.06
15	G	1121	F6C	C1D-C2D	2.41	1.49	1.44
14	B	1236	CLA	C4B-CHC	2.41	1.47	1.41
14	G	1013	CLA	C4D-CHA	2.40	1.46	1.38
14	b	1216	CLA	C4B-CHC	2.40	1.47	1.41
14	b	1236	CLA	C4B-CHC	2.40	1.47	1.41
14	H	1021	CLA	C4D-CHA	2.40	1.46	1.38
14	a	1127	CLA	C1B-NB	-2.40	1.33	1.35
14	b	1233	CLA	C4B-CHC	2.40	1.47	1.41
14	A	1013	CLA	C4D-CHA	2.40	1.46	1.38
18	G	4011	BCR	C21-C22	-2.40	1.32	1.35
18	a	4008	BCR	C21-C22	-2.40	1.32	1.35
14	B	1233	CLA	C4B-CHC	2.40	1.47	1.41
14	A	1117	CLA	MG-NC	2.40	2.12	2.06
14	A	1130	CLA	OBD-CAD	2.40	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1205	CLA	MG-NC	2.40	2.12	2.06
14	a	1013	CLA	C4D-CHA	2.40	1.46	1.38
14	B	1205	CLA	MG-NC	2.39	2.12	2.06
14	b	1209	CLA	C4B-CHC	2.39	1.47	1.41
14	G	1117	CLA	MG-NC	2.39	2.12	2.06
14	B	1219	CLA	C4B-CHC	2.39	1.47	1.41
15	a	1121	F6C	C4B-NB	-2.39	1.34	1.37
14	l	1502	CLA	C4D-CHA	2.39	1.46	1.38
14	H	1217	CLA	C4B-CHC	2.39	1.47	1.41
14	B	1021	CLA	C4D-CHA	2.39	1.46	1.38
14	A	1135	CLA	C4D-CHA	2.39	1.46	1.38
18	H	4010	BCR	C17-C18	-2.39	1.32	1.35
14	A	1101	CLA	C4B-CHC	2.39	1.47	1.41
14	b	1021	CLA	C4D-CHA	2.38	1.46	1.38
14	H	1209	CLA	C4B-CHC	2.38	1.47	1.41
15	A	1121	F6C	C4B-NB	-2.38	1.34	1.37
18	a	4002	BCR	C14-C13	-2.38	1.32	1.35
14	b	1204	CLA	MG-NC	2.38	2.11	2.06
14	L	1502	CLA	C4D-CHA	2.38	1.46	1.38
14	G	1013	CLA	C4B-CHC	2.38	1.47	1.41
14	H	1233	CLA	C4B-CHC	2.38	1.47	1.41
14	a	1117	CLA	MG-NC	2.38	2.11	2.06
14	b	1202	CLA	MG-NC	2.38	2.11	2.06
21	A	6002	LMT	O2B-C2B	-2.37	1.37	1.43
15	G	1121	F6C	C4B-NB	-2.37	1.34	1.37
14	U	1502	CLA	C4D-CHA	2.37	1.46	1.38
14	A	1116	CLA	C4B-CHC	2.37	1.47	1.41
14	B	1221	CLA	C1B-NB	-2.37	1.33	1.35
14	A	1013	CLA	C4B-CHC	2.37	1.47	1.41
14	B	1204	CLA	MG-NC	2.37	2.11	2.06
14	A	1129	CLA	C1B-NB	-2.37	1.33	1.35
14	H	1205	CLA	MG-NC	2.37	2.11	2.06
14	B	1217	CLA	C4B-CHC	2.37	1.47	1.41
18	b	4010	BCR	C17-C18	-2.37	1.32	1.35
14	G	1130	CLA	OBD-CAD	2.37	1.26	1.22
18	G	4008	BCR	C21-C22	-2.37	1.32	1.35
14	B	1209	CLA	C4B-CHC	2.37	1.47	1.41
14	H	1217	CLA	C1B-CHB	2.37	1.47	1.41
18	A	4011	BCR	C21-C22	-2.37	1.32	1.35
14	b	1213	CLA	C4B-CHC	2.37	1.47	1.41
14	H	1213	CLA	C4B-CHC	2.37	1.47	1.41
14	H	1219	CLA	C4B-CHC	2.37	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1116	CLA	C4B-CHC	2.37	1.47	1.41
21	G	6002	LMT	O2B-C2B	-2.36	1.37	1.43
14	G	1125	CLA	MG-NC	2.36	2.11	2.06
14	B	1202	CLA	MG-NC	2.36	2.11	2.06
14	B	1218	CLA	C1B-CHB	2.36	1.47	1.41
14	b	1219	CLA	C4B-CHC	2.36	1.47	1.41
14	b	1203	CLA	MG-NC	2.36	2.11	2.06
14	a	1013	CLA	C4B-CHC	2.36	1.47	1.41
14	k	1401	CLA	C1B-CHB	2.36	1.47	1.41
14	G	1116	CLA	C4B-CHC	2.36	1.47	1.41
21	G	6001	LMT	O1'-C1'	-2.36	1.36	1.40
14	B	1203	CLA	MG-NC	2.36	2.11	2.06
14	B	1217	CLA	C1B-CHB	2.36	1.47	1.41
14	b	1217	CLA	C1B-CHB	2.36	1.47	1.41
15	b	1207	F6C	CMB-C2B	2.36	1.50	1.45
14	B	1214	CLA	C1B-NB	-2.36	1.33	1.35
14	b	1223	CLA	C4B-CHC	2.36	1.47	1.41
14	G	1127	CLA	C1B-NB	-2.36	1.33	1.35
14	a	1123	CLA	C1B-NB	-2.36	1.33	1.35
15	B	1238	F6C	C1C-CHC	2.36	1.47	1.41
14	B	1231	CLA	C4B-CHC	2.36	1.47	1.41
14	a	1136	CLA	C1B-NB	-2.36	1.33	1.35
14	H	1202	CLA	MG-NC	2.35	2.11	2.06
14	A	1130	CLA	MG-NC	2.35	2.11	2.06
14	H	1204	CLA	MG-NC	2.35	2.11	2.06
15	b	1230	F6C	CMB-C2B	2.35	1.50	1.45
14	H	1204	CLA	C4D-CHA	2.35	1.46	1.38
14	K	1401	CLA	C1D-C2D	2.35	1.50	1.45
14	G	1130	CLA	MG-NC	2.35	2.11	2.06
14	G	1101	CLA	C4B-CHC	2.35	1.47	1.41
14	b	1217	CLA	C4B-CHC	2.35	1.47	1.41
14	G	1124	CLA	MG-NC	2.35	2.11	2.06
14	H	1231	CLA	C4B-CHC	2.35	1.47	1.41
14	H	1203	CLA	MG-NC	2.35	2.11	2.06
14	K	1401	CLA	C1B-CHB	2.35	1.47	1.41
18	b	4017	BCR	C30-C25	-2.35	1.50	1.53
14	a	1130	CLA	MG-NC	2.35	2.11	2.06
14	H	1221	CLA	C1B-NB	-2.35	1.33	1.35
14	A	1125	CLA	MG-NC	2.35	2.11	2.06
14	H	1223	CLA	C4B-CHC	2.34	1.47	1.41
14	a	1125	CLA	MG-NC	2.34	2.11	2.06
14	b	1204	CLA	C4D-CHA	2.34	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1223	CLA	C4B-CHC	2.34	1.47	1.41
14	a	1101	CLA	C4B-CHC	2.34	1.47	1.41
14	A	1125	CLA	C4B-NB	-2.34	1.33	1.35
14	B	1021	CLA	C1B-NB	-2.34	1.33	1.35
14	B	1213	CLA	C4B-CHC	2.34	1.47	1.41
18	A	4002	BCR	C14-C13	-2.34	1.32	1.35
14	B	1204	CLA	C4D-CHA	2.34	1.46	1.38
14	b	1231	CLA	C4B-CHC	2.34	1.47	1.41
15	B	1207	F6C	CMB-C2B	2.33	1.50	1.45
14	T	1401	CLA	C1B-CHB	2.33	1.47	1.41
14	A	1118	CLA	C4B-CHC	2.33	1.47	1.41
14	b	1218	CLA	C1B-CHB	2.33	1.47	1.41
14	A	1124	CLA	MG-NC	2.33	2.11	2.06
15	B	1230	F6C	CMB-C2B	2.33	1.50	1.45
18	A	4011	BCR	C1-C6	-2.33	1.50	1.53
14	a	1124	CLA	MG-NC	2.33	2.11	2.06
14	B	1022	CLA	C4B-CHC	2.33	1.47	1.41
15	b	1238	F6C	C1C-CHC	2.33	1.47	1.41
21	a	6001	LMT	O1'-C1'	-2.33	1.36	1.40
14	x	1701	CLA	C1B-CHB	2.33	1.47	1.41
14	b	1239	CLA	C1B-CHB	2.32	1.47	1.41
14	b	1222	CLA	C4B-CHC	2.32	1.47	1.41
14	H	1021	CLA	C1B-NB	-2.32	1.33	1.35
18	G	4011	BCR	C1-C6	-2.32	1.50	1.53
14	H	1222	CLA	C4B-CHC	2.32	1.47	1.41
14	A	1139	CLA	C1B-CHB	2.32	1.47	1.41
14	X	1701	CLA	C1B-CHB	2.32	1.47	1.41
14	a	1117	CLA	C1B-NB	-2.32	1.33	1.35
14	a	1126	CLA	C4B-NB	-2.32	1.33	1.35
14	A	1127	CLA	C1B-NB	-2.32	1.33	1.35
14	H	1022	CLA	C4B-CHC	2.32	1.47	1.41
14	a	1139	CLA	C1B-CHB	2.32	1.47	1.41
14	H	1205	CLA	C1B-NB	-2.32	1.33	1.35
15	b	1238	F6C	C3D-C2D	2.32	1.45	1.39
15	H	1238	F6C	C1C-CHC	2.32	1.47	1.41
15	H	1207	F6C	CMB-C2B	2.32	1.50	1.45
14	A	1124	CLA	C4B-CHC	2.32	1.47	1.41
14	G	1123	CLA	C1B-NB	-2.32	1.33	1.35
14	b	1022	CLA	C4B-CHC	2.32	1.47	1.41
14	B	1239	CLA	C1B-CHB	2.32	1.47	1.41
14	H	1218	CLA	C1B-CHB	2.31	1.47	1.41
14	B	1023	CLA	C4C-C3C	2.31	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1134	CLA	C1B-CHB	2.31	1.47	1.41
14	W	1701	CLA	C1B-CHB	2.31	1.47	1.41
14	k	1401	CLA	C1D-C2D	2.31	1.49	1.45
18	G	4002	BCR	C14-C13	-2.31	1.32	1.35
14	A	1136	CLA	C1B-NB	-2.31	1.33	1.35
15	B	1238	F6C	C3D-C2D	2.31	1.45	1.39
21	A	6001	LMT	O1'-C1'	-2.31	1.36	1.40
14	G	1115	CLA	C4B-CHC	2.31	1.47	1.41
18	a	4011	BCR	C1-C6	-2.31	1.50	1.53
14	H	1239	CLA	C1B-CHB	2.31	1.47	1.41
14	H	1023	CLA	C4C-C3C	2.31	1.49	1.45
15	H	1230	F6C	CMB-C2B	2.31	1.50	1.45
14	G	1120	CLA	C1B-CHB	2.31	1.47	1.41
14	a	1120	CLA	C1B-CHB	2.31	1.47	1.41
14	a	1118	CLA	C4B-CHC	2.31	1.47	1.41
14	H	1215	CLA	C1B-NB	-2.30	1.33	1.35
14	A	1123	CLA	C1B-NB	-2.30	1.33	1.35
14	a	1106	CLA	C4B-CHC	2.30	1.47	1.41
14	B	1222	CLA	C4B-CHC	2.30	1.47	1.41
15	B	1238	F6C	C1C-NC	-2.30	1.33	1.35
14	G	1124	CLA	C4B-CHC	2.30	1.47	1.41
14	A	1134	CLA	C1B-CHB	2.30	1.47	1.41
14	b	1208	CLA	C4B-CHC	2.30	1.47	1.41
14	G	1139	CLA	C1B-CHB	2.30	1.47	1.41
14	G	1118	CLA	C4B-CHC	2.30	1.47	1.41
15	B	1230	F6C	C1A-C2A	2.30	1.50	1.45
14	a	1124	CLA	C4B-CHC	2.30	1.47	1.41
14	A	1120	CLA	C1B-CHB	2.30	1.47	1.41
15	H	1238	F6C	C3D-C2D	2.30	1.45	1.39
14	B	1215	CLA	C1B-NB	-2.30	1.33	1.35
14	A	1115	CLA	C4B-CHC	2.30	1.47	1.41
18	G	4008	BCR	C17-C18	-2.30	1.32	1.35
14	A	1102	CLA	C4B-CHC	2.30	1.47	1.41
14	B	1208	CLA	C4B-CHC	2.30	1.47	1.41
14	a	1102	CLA	C4B-CHC	2.30	1.47	1.41
14	A	1106	CLA	C4B-CHC	2.30	1.47	1.41
14	L	1502	CLA	C4B-CHC	2.29	1.47	1.41
14	G	1106	CLA	C4B-CHC	2.29	1.47	1.41
14	G	1132	CLA	C4B-CHC	2.29	1.47	1.41
14	B	1233	CLA	C1B-CHB	2.29	1.47	1.41
14	b	1224	CLA	C1B-NB	-2.29	1.33	1.35
14	G	1102	CLA	C4B-CHC	2.29	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1115	CLA	C4B-CHC	2.29	1.47	1.41
14	H	1208	CLA	C4B-CHC	2.29	1.47	1.41
15	H	1230	F6C	C1A-C2A	2.29	1.50	1.45
14	T	1401	CLA	C1D-C2D	2.29	1.49	1.45
14	b	1211	CLA	C4B-CHC	2.29	1.47	1.41
14	b	1233	CLA	C1B-CHB	2.29	1.47	1.41
14	b	1023	CLA	C4C-C3C	2.28	1.49	1.45
14	H	1235	CLA	C4B-CHC	2.28	1.47	1.41
14	B	1211	CLA	C4B-CHC	2.28	1.47	1.41
14	G	1123	CLA	C1B-CHB	2.28	1.47	1.41
14	H	1202	CLA	C4B-CHC	2.28	1.47	1.41
14	A	1107	CLA	C1B-CHB	2.28	1.47	1.41
18	G	4007	BCR	C14-C13	-2.28	1.32	1.35
14	a	1123	CLA	C1B-CHB	2.28	1.47	1.41
18	a	4007	BCR	C14-C13	-2.28	1.32	1.35
14	B	1233	CLA	C1D-C2D	2.28	1.49	1.45
14	l	1502	CLA	C4B-CHC	2.28	1.47	1.41
14	a	1134	CLA	C1B-CHB	2.27	1.47	1.41
14	U	1502	CLA	C4B-CHC	2.27	1.47	1.41
14	b	1232	CLA	C4B-CHC	2.27	1.47	1.41
14	A	1111	CLA	C4B-CHC	2.27	1.47	1.41
14	a	1138	CLA	C4B-CHC	2.27	1.47	1.41
14	G	1114	CLA	C1D-C2D	2.27	1.49	1.45
14	H	1211	CLA	C4B-CHC	2.27	1.47	1.41
14	B	1231	CLA	C1B-CHB	2.27	1.47	1.41
15	B	1230	F6C	CHB-C4A	-2.27	1.34	1.38
14	b	1202	CLA	C4B-CHC	2.27	1.47	1.41
14	G	1129	CLA	C1B-NB	-2.27	1.33	1.35
14	a	1132	CLA	C4B-CHC	2.27	1.47	1.41
15	H	1238	F6C	C1C-NC	-2.27	1.33	1.35
14	H	1232	CLA	C4B-CHC	2.27	1.47	1.41
15	H	1207	F6C	C4D-CHA	2.27	1.48	1.42
14	G	1138	CLA	C4B-CHC	2.27	1.47	1.41
14	b	1235	CLA	C4B-CHC	2.27	1.47	1.41
14	A	1138	CLA	C4B-CHC	2.27	1.47	1.41
15	G	1121	F6C	C1A-C2A	2.27	1.50	1.45
14	H	1231	CLA	C1B-CHB	2.27	1.47	1.41
14	B	1235	CLA	C4B-CHC	2.27	1.47	1.41
14	A	1132	CLA	C4B-CHC	2.27	1.47	1.41
18	l	4019	BCR	C21-C22	-2.27	1.32	1.35
14	G	1107	CLA	C1B-CHB	2.27	1.47	1.41
14	a	1104	CLA	C1B-NB	-2.26	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1120	CLA	C4B-CHC	2.26	1.47	1.41
14	A	1128	CLA	CMB-C2B	-2.26	1.46	1.51
14	a	1111	CLA	C4B-CHC	2.26	1.47	1.41
14	l	1503	CLA	C1B-CHB	2.26	1.47	1.41
14	A	1110	CLA	C1B-CHB	2.26	1.47	1.41
14	U	1501	CLA	C1B-NB	-2.26	1.33	1.35
14	B	1219	CLA	C4C-C3C	2.26	1.48	1.45
14	H	1233	CLA	C1B-CHB	2.26	1.47	1.41
14	A	1133	CLA	C1B-CHB	2.26	1.47	1.41
14	G	1137	CLA	C4B-NB	-2.26	1.33	1.35
14	a	1107	CLA	C1B-CHB	2.26	1.47	1.41
14	a	1134	CLA	C4C-C3C	2.26	1.48	1.45
14	b	1221	CLA	C1B-NB	-2.26	1.33	1.35
15	b	1230	F6C	CHB-C4A	-2.26	1.34	1.38
15	a	1121	F6C	C1A-C2A	2.26	1.50	1.45
14	b	1206	CLA	MG-NC	2.25	2.11	2.06
14	B	1205	CLA	C1B-NB	-2.25	1.33	1.35
14	A	1123	CLA	C1B-CHB	2.25	1.47	1.41
14	H	1206	CLA	MG-NC	2.25	2.11	2.06
14	G	1108	CLA	C4B-CHC	2.25	1.47	1.41
14	B	1232	CLA	C4B-CHC	2.25	1.47	1.41
14	A	1134	CLA	C4C-C3C	2.25	1.48	1.45
14	b	1212	CLA	C4B-CHC	2.25	1.47	1.41
14	a	1119	CLA	MG-NC	2.25	2.11	2.06
14	b	1219	CLA	C4C-C3C	2.25	1.48	1.45
14	A	1108	CLA	C4B-CHC	2.25	1.47	1.41
14	a	1120	CLA	C4B-CHC	2.25	1.47	1.41
14	A	1120	CLA	C4B-CHC	2.25	1.47	1.41
14	b	1234	CLA	C1B-NB	-2.25	1.33	1.35
14	A	1127	CLA	C1B-CHB	2.25	1.47	1.41
14	b	1231	CLA	C1B-CHB	2.25	1.47	1.41
14	B	1202	CLA	C4B-CHC	2.25	1.47	1.41
14	G	1134	CLA	C4C-C3C	2.25	1.48	1.45
14	H	1219	CLA	C4C-C3C	2.25	1.48	1.45
14	B	1206	CLA	MG-NC	2.25	2.11	2.06
14	A	1126	CLA	C1B-NB	-2.25	1.33	1.35
15	b	1237	F6C	CHB-C4A	-2.25	1.34	1.38
14	A	1114	CLA	C1D-C2D	2.24	1.49	1.45
14	a	1114	CLA	C1D-C2D	2.24	1.49	1.45
14	G	1111	CLA	C4B-CHC	2.24	1.47	1.41
15	B	1207	F6C	C4C-CHD	2.24	1.47	1.41
15	b	1230	F6C	C1A-C2A	2.24	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1140	CLA	C1B-CHB	2.24	1.47	1.41
14	L	1503	CLA	C1B-CHB	2.24	1.47	1.41
15	b	1238	F6C	C1C-NC	-2.24	1.33	1.35
14	a	1127	CLA	C1B-CHB	2.24	1.47	1.41
14	G	1126	CLA	C1B-NB	-2.24	1.33	1.35
14	A	1104	CLA	C1B-NB	-2.24	1.33	1.35
14	G	1140	CLA	C1B-CHB	2.24	1.47	1.41
14	G	1136	CLA	C4B-CHC	2.24	1.47	1.41
14	H	1212	CLA	C1B-CHB	2.24	1.47	1.41
18	A	4008	BCR	C17-C18	-2.24	1.32	1.35
14	A	1136	CLA	C4B-CHC	2.24	1.47	1.41
14	B	1021	CLA	C1B-CHB	2.24	1.47	1.41
15	B	1207	F6C	C4D-CHA	2.24	1.48	1.42
18	H	4004	BCR	C30-C25	-2.23	1.50	1.53
14	l	1501	CLA	C1B-NB	-2.23	1.33	1.35
14	L	1501	CLA	C1B-NB	-2.23	1.33	1.35
14	a	1110	CLA	C1B-CHB	2.23	1.47	1.41
14	b	1021	CLA	C1B-CHB	2.23	1.47	1.41
14	H	1224	CLA	C1B-NB	-2.23	1.33	1.35
14	a	1136	CLA	C4B-CHC	2.23	1.47	1.41
15	b	1207	F6C	C4D-CHA	2.23	1.48	1.42
15	A	1121	F6C	C1A-C2A	2.23	1.50	1.45
14	H	1212	CLA	C4B-CHC	2.23	1.47	1.41
14	U	1503	CLA	C1B-CHB	2.23	1.47	1.41
14	A	1140	CLA	C1B-CHB	2.23	1.47	1.41
15	b	1207	F6C	C4C-CHD	2.23	1.47	1.41
15	H	1230	F6C	CHB-C4A	-2.23	1.34	1.38
14	b	1225	CLA	C4B-CHC	2.23	1.47	1.41
14	G	1133	CLA	C1B-CHB	2.23	1.47	1.41
14	b	1212	CLA	C1B-CHB	2.23	1.47	1.41
15	b	1237	F6C	CMB-C2B	2.23	1.49	1.45
14	B	1212	CLA	C4B-CHC	2.22	1.47	1.41
14	G	1117	CLA	C1B-NB	-2.22	1.33	1.35
14	A	1115	CLA	C1B-CHB	2.22	1.47	1.41
14	b	1227	CLA	C4B-CHC	2.22	1.47	1.41
14	a	1128	CLA	CMB-C2B	-2.22	1.47	1.51
14	B	1224	CLA	C1B-NB	-2.22	1.33	1.35
14	B	1227	CLA	C4B-CHC	2.22	1.47	1.41
14	G	1110	CLA	C1B-CHB	2.22	1.47	1.41
14	H	1021	CLA	C1B-CHB	2.22	1.47	1.41
14	H	1225	CLA	C4B-CHC	2.22	1.47	1.41
14	a	1108	CLA	C4B-CHC	2.22	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1237	F6C	CHB-C4A	-2.22	1.34	1.38
14	A	1119	CLA	MG-NC	2.22	2.11	2.06
14	a	1133	CLA	C1B-CHB	2.22	1.47	1.41
14	A	1104	CLA	C1B-CHB	2.22	1.47	1.41
14	A	1117	CLA	C1B-NB	-2.22	1.33	1.35
18	B	4004	BCR	C30-C25	-2.22	1.50	1.53
14	G	1128	CLA	CMB-C2B	-2.22	1.47	1.51
14	a	1107	CLA	C4B-CHC	2.22	1.47	1.41
15	H	1207	F6C	C4C-CHD	2.22	1.47	1.41
14	G	1125	CLA	C1B-NB	-2.21	1.33	1.35
14	a	1137	CLA	C4B-NB	-2.21	1.33	1.35
14	b	1210	CLA	C4B-CHC	2.21	1.47	1.41
14	G	1119	CLA	MG-NC	2.21	2.11	2.06
14	A	1104	CLA	C4B-CHC	2.21	1.47	1.41
18	b	4004	BCR	C30-C25	-2.21	1.50	1.53
14	G	1107	CLA	C4B-CHC	2.21	1.47	1.41
14	G	1127	CLA	C1B-CHB	2.21	1.47	1.41
21	A	6002	LMT	O1'-C1'	-2.21	1.36	1.40
14	H	1227	CLA	C4B-CHC	2.21	1.47	1.41
14	a	1101	CLA	C1B-CHB	2.21	1.47	1.41
14	a	1104	CLA	C4B-CHC	2.21	1.47	1.41
14	a	1125	CLA	C1B-CHB	2.21	1.47	1.41
14	H	1233	CLA	C1D-C2D	2.21	1.49	1.45
14	U	1501	CLA	C1B-CHB	2.21	1.47	1.41
18	a	4008	BCR	C17-C18	-2.21	1.32	1.35
14	B	1225	CLA	C4B-CHC	2.21	1.47	1.41
14	a	1123	CLA	C4B-CHC	2.21	1.47	1.41
14	B	1212	CLA	C1B-CHB	2.21	1.47	1.41
21	G	6002	LMT	O1'-C1'	-2.21	1.36	1.40
14	G	1104	CLA	C4B-CHC	2.21	1.47	1.41
14	H	1210	CLA	C4B-CHC	2.21	1.47	1.41
14	H	1208	CLA	C1B-CHB	2.21	1.47	1.41
14	G	1115	CLA	C1B-CHB	2.20	1.47	1.41
14	G	1123	CLA	C4B-CHC	2.20	1.47	1.41
14	a	1109	CLA	C1B-CHB	2.20	1.47	1.41
14	G	1125	CLA	C1B-CHB	2.20	1.47	1.41
18	L	4019	BCR	C21-C22	-2.20	1.32	1.35
14	A	1125	CLA	C1B-CHB	2.20	1.47	1.41
14	a	1125	CLA	C1B-NB	-2.20	1.33	1.35
14	L	1503	CLA	C4B-CHC	2.20	1.47	1.41
14	L	1501	CLA	C1B-CHB	2.20	1.47	1.41
15	B	1237	F6C	CMB-C2B	2.20	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	4007	BCR	C14-C13	-2.20	1.32	1.35
14	a	1104	CLA	C1B-CHB	2.20	1.47	1.41
14	b	1233	CLA	C1D-C2D	2.20	1.49	1.45
14	a	1103	CLA	C1B-NB	-2.20	1.33	1.35
14	b	1224	CLA	C4B-CHC	2.19	1.47	1.41
14	B	1210	CLA	C4B-CHC	2.19	1.47	1.41
13	G	1011	CL0	C4B-CHC	2.19	1.47	1.41
14	G	1104	CLA	C1B-CHB	2.19	1.47	1.41
14	B	1234	CLA	C1B-NB	-2.19	1.33	1.35
14	A	1127	CLA	C4B-CHC	2.19	1.47	1.41
13	G	1011	CL0	C3A-C2A	-2.19	1.48	1.54
14	H	1223	CLA	C1B-NB	-2.19	1.33	1.35
14	a	1130	CLA	C4B-CHC	2.19	1.47	1.41
14	A	1119	CLA	C4C-C3C	2.19	1.48	1.45
14	G	1130	CLA	C4B-CHC	2.19	1.47	1.41
14	a	1126	CLA	C4B-CHC	2.19	1.47	1.41
15	a	1121	F6C	C1C-CHC	2.19	1.47	1.41
14	H	1228	CLA	C1B-CHB	2.19	1.47	1.41
14	A	1126	CLA	C4B-NB	-2.19	1.33	1.35
14	a	1118	CLA	C1B-CHB	2.19	1.47	1.41
14	A	1126	CLA	C4B-CHC	2.19	1.47	1.41
14	b	1227	CLA	C1B-CHB	2.19	1.47	1.41
15	b	1230	F6C	C1C-CHC	2.19	1.47	1.41
14	b	1211	CLA	C1B-CHB	2.19	1.47	1.41
14	H	1234	CLA	C1B-NB	-2.18	1.33	1.35
13	A	1011	CL0	C4B-CHC	2.18	1.47	1.41
14	b	1221	CLA	C4B-CHC	2.18	1.47	1.41
14	B	1228	CLA	C1B-CHB	2.18	1.47	1.41
15	G	1121	F6C	C1C-CHC	2.18	1.47	1.41
14	G	1109	CLA	C4B-CHC	2.18	1.47	1.41
14	b	1208	CLA	C1B-CHB	2.18	1.47	1.41
13	a	1011	CL0	C4B-CHC	2.18	1.47	1.41
14	A	1107	CLA	C4B-CHC	2.18	1.47	1.41
14	A	1129	CLA	C4B-CHC	2.18	1.47	1.41
14	U	1503	CLA	C4B-CHC	2.18	1.47	1.41
15	H	1237	F6C	C4C-CHD	2.18	1.47	1.41
14	A	1137	CLA	C4B-NB	-2.18	1.33	1.35
14	b	1023	CLA	MG-NC	2.18	2.11	2.06
14	a	1109	CLA	C4B-CHC	2.18	1.47	1.41
14	b	1228	CLA	C1B-CHB	2.18	1.47	1.41
15	b	1237	F6C	C4C-CHD	2.18	1.47	1.41
14	H	1211	CLA	C1B-CHB	2.18	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1115	CLA	C1B-CHB	2.18	1.47	1.41
14	a	1131	CLA	C4B-CHC	2.18	1.47	1.41
14	b	1232	CLA	C1B-CHB	2.18	1.47	1.41
14	B	1227	CLA	C1B-CHB	2.18	1.47	1.41
14	a	1127	CLA	C4B-CHC	2.18	1.47	1.41
14	H	1221	CLA	C4B-CHC	2.18	1.47	1.41
14	G	1127	CLA	C4B-CHC	2.18	1.47	1.41
14	A	1109	CLA	C1B-CHB	2.18	1.47	1.41
14	A	1109	CLA	C4B-CHC	2.18	1.47	1.41
14	B	1201	CLA	C4B-CHC	2.18	1.47	1.41
14	G	1109	CLA	C1B-CHB	2.18	1.47	1.41
14	b	1205	CLA	C1B-NB	-2.17	1.33	1.35
15	H	1237	F6C	CMB-C2B	2.17	1.49	1.45
14	G	1126	CLA	C4B-CHC	2.17	1.47	1.41
14	A	1130	CLA	C4B-CHC	2.17	1.47	1.41
14	B	1208	CLA	C1B-CHB	2.17	1.47	1.41
14	A	1101	CLA	C1B-CHB	2.17	1.47	1.41
15	B	1238	F6C	CMB-C2B	2.17	1.49	1.45
14	H	1227	CLA	C1B-CHB	2.17	1.47	1.41
14	G	1112	CLA	C4B-CHC	2.17	1.47	1.41
14	H	1210	CLA	C1B-NB	-2.17	1.33	1.35
13	a	1011	CL0	C3A-C2A	-2.17	1.48	1.54
14	l	1501	CLA	C1B-CHB	2.17	1.47	1.41
14	H	1224	CLA	C4B-CHC	2.17	1.47	1.41
13	a	1011	CL0	MG-NC	2.17	2.11	2.06
15	b	1238	F6C	CMB-C2B	2.17	1.49	1.45
14	B	1221	CLA	C4B-CHC	2.17	1.47	1.41
14	G	1131	CLA	C4B-CHC	2.17	1.47	1.41
14	l	1503	CLA	C4B-CHC	2.17	1.47	1.41
14	A	1135	CLA	C1B-CHB	2.17	1.47	1.41
14	H	1232	CLA	C1B-CHB	2.17	1.47	1.41
14	a	1135	CLA	C1B-CHB	2.17	1.47	1.41
14	a	1129	CLA	C1B-CHB	2.17	1.47	1.41
15	A	1121	F6C	C1C-CHC	2.17	1.47	1.41
18	U	4019	BCR	C21-C22	-2.17	1.32	1.35
14	A	1131	CLA	C4B-CHC	2.17	1.47	1.41
15	H	1237	F6C	CHB-C4A	-2.16	1.34	1.38
14	G	1104	CLA	C1B-NB	-2.16	1.33	1.35
14	B	1224	CLA	C4B-CHC	2.16	1.47	1.41
14	H	1022	CLA	C1B-NB	-2.16	1.33	1.35
14	A	1103	CLA	C1B-NB	-2.16	1.33	1.35
14	A	1125	CLA	C1B-NB	-2.16	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1209	CLA	C1D-C2D	2.16	1.49	1.45
13	A	1011	CL0	C3A-C2A	-2.16	1.48	1.54
14	B	1214	CLA	C4B-CHC	2.16	1.47	1.41
14	a	1126	CLA	C1B-NB	-2.16	1.33	1.35
18	b	4014	BCR	C14-C13	-2.16	1.32	1.35
14	B	1022	CLA	C1B-NB	-2.16	1.33	1.35
14	G	1105	CLA	C1B-CHB	2.16	1.47	1.41
14	G	1129	CLA	C4B-CHC	2.16	1.47	1.41
14	H	1023	CLA	MG-NC	2.16	2.11	2.06
14	A	1114	CLA	C1B-NB	-2.16	1.33	1.35
14	A	1129	CLA	C1B-CHB	2.16	1.47	1.41
14	G	1101	CLA	C1B-CHB	2.16	1.47	1.41
14	A	1108	CLA	C1B-CHB	2.16	1.47	1.41
14	a	1129	CLA	C4B-CHC	2.16	1.47	1.41
14	B	1232	CLA	C1B-CHB	2.16	1.47	1.41
14	B	1211	CLA	C1B-CHB	2.16	1.47	1.41
14	G	1119	CLA	C4C-C3C	2.16	1.48	1.45
14	A	1118	CLA	C1B-CHB	2.15	1.47	1.41
15	B	1237	F6C	C4C-CHD	2.15	1.47	1.41
14	A	1123	CLA	C4B-CHC	2.15	1.47	1.41
14	G	1118	CLA	C1B-CHB	2.15	1.47	1.41
13	A	1011	CL0	MG-NC	2.15	2.11	2.06
14	G	1135	CLA	C1B-CHB	2.15	1.47	1.41
14	a	1112	CLA	C4B-CHC	2.15	1.47	1.41
14	a	1108	CLA	C1B-CHB	2.15	1.47	1.41
15	H	1238	F6C	CMB-C2B	2.15	1.49	1.45
14	B	1229	CLA	C1B-CHB	2.15	1.47	1.41
14	H	1214	CLA	C4B-CHC	2.15	1.47	1.41
14	A	1112	CLA	C4B-CHC	2.15	1.47	1.41
15	B	1230	F6C	C1C-CHC	2.15	1.47	1.41
14	A	1128	CLA	C1B-CHB	2.15	1.47	1.41
14	b	1201	CLA	C4B-CHC	2.15	1.47	1.41
14	H	1209	CLA	C1D-C2D	2.15	1.49	1.45
21	a	6002	LMT	O1'-C1'	-2.15	1.36	1.40
14	H	1201	CLA	C4B-CHC	2.15	1.47	1.41
14	b	1228	CLA	C1D-C2D	2.15	1.49	1.45
14	a	1119	CLA	C4C-C3C	2.15	1.48	1.45
14	a	1128	CLA	C1B-CHB	2.14	1.47	1.41
15	H	1230	F6C	C1C-CHC	2.14	1.47	1.41
14	B	1227	CLA	C1B-NB	-2.14	1.33	1.35
14	a	1105	CLA	C1B-CHB	2.14	1.47	1.41
14	G	1013	CLA	MG-NC	2.14	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1215	CLA	C4B-CHC	2.14	1.46	1.41
18	b	4009	BCR	C30-C25	-2.14	1.50	1.53
14	b	1239	CLA	C4B-CHC	2.14	1.46	1.41
14	H	1229	CLA	C1B-CHB	2.14	1.46	1.41
15	a	1121	F6C	C1C-NC	-2.14	1.33	1.35
14	A	1135	CLA	C3D-C2D	2.14	1.45	1.39
14	H	1202	CLA	C1B-CHB	2.14	1.46	1.41
14	G	1108	CLA	C1B-CHB	2.14	1.46	1.41
14	A	1114	CLA	C4B-CHC	2.14	1.46	1.41
14	a	1013	CLA	MG-NC	2.14	2.11	2.06
14	G	1012	CLA	C1B-NB	-2.14	1.33	1.35
14	G	1106	CLA	C1B-CHB	2.14	1.46	1.41
14	G	1135	CLA	C3D-C2D	2.14	1.44	1.39
14	a	1106	CLA	C1B-CHB	2.14	1.46	1.41
14	G	1113	CLA	C1B-CHB	2.14	1.46	1.41
14	H	1239	CLA	C4B-CHC	2.14	1.46	1.41
14	A	1113	CLA	C1B-CHB	2.13	1.46	1.41
14	a	1135	CLA	C3D-C2D	2.13	1.44	1.39
18	A	4007	BCR	C17-C18	-2.13	1.33	1.35
14	A	1133	CLA	C4B-CHC	2.13	1.46	1.41
14	b	1214	CLA	C4B-CHC	2.13	1.46	1.41
13	G	1011	CL0	MG-NC	2.13	2.11	2.06
14	G	1129	CLA	C1B-CHB	2.13	1.46	1.41
14	A	1105	CLA	C1B-CHB	2.13	1.46	1.41
14	T	1401	CLA	C4C-C3C	2.13	1.48	1.45
14	A	1122	CLA	C1B-CHB	2.13	1.46	1.41
14	B	1209	CLA	C1D-C2D	2.13	1.49	1.45
14	a	1103	CLA	C1B-CHB	2.13	1.46	1.41
15	b	1230	F6C	C4C-CHD	2.13	1.46	1.41
14	a	1114	CLA	C1B-NB	-2.13	1.33	1.35
14	b	1022	CLA	C1B-NB	-2.13	1.33	1.35
18	H	4014	BCR	C14-C13	-2.13	1.33	1.35
14	B	1236	CLA	C1B-CHB	2.13	1.46	1.41
14	A	1114	CLA	C4C-C3C	2.13	1.48	1.45
14	B	1239	CLA	C4B-CHC	2.12	1.46	1.41
15	B	1230	F6C	C2B-C1B	2.12	1.49	1.44
14	a	1114	CLA	C4C-C3C	2.12	1.48	1.45
14	b	1222	CLA	C1B-CHB	2.12	1.46	1.41
15	H	1230	F6C	C2B-C1B	2.12	1.49	1.44
14	G	1122	CLA	C1B-CHB	2.12	1.46	1.41
14	b	1229	CLA	C1B-CHB	2.12	1.46	1.41
14	G	1103	CLA	C1B-CHB	2.12	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1102	CLA	C1B-NB	-2.12	1.33	1.35
14	A	1012	CLA	C1B-NB	-2.12	1.33	1.35
14	A	1111	CLA	C1B-NB	-2.12	1.33	1.35
14	H	1221	CLA	C1B-CHB	2.12	1.46	1.41
18	B	4009	BCR	C30-C25	-2.12	1.50	1.53
14	G	1133	CLA	C4B-CHC	2.12	1.46	1.41
15	H	1230	F6C	C1D-C2D	2.12	1.48	1.44
14	l	1502	CLA	C1D-C2D	2.12	1.49	1.45
14	B	1228	CLA	C1D-C2D	2.12	1.49	1.45
14	A	1013	CLA	MG-NC	2.12	2.11	2.06
14	b	1215	CLA	C4B-CHC	2.12	1.46	1.41
14	H	1215	CLA	C4B-CHC	2.12	1.46	1.41
14	A	1103	CLA	C1B-CHB	2.12	1.46	1.41
14	k	1401	CLA	C4C-C3C	2.12	1.48	1.45
14	a	1114	CLA	C4B-CHC	2.12	1.46	1.41
14	B	1023	CLA	MG-NC	2.12	2.11	2.06
14	a	1012	CLA	C1B-NB	-2.12	1.33	1.35
14	U	1502	CLA	C1D-C2D	2.12	1.49	1.45
14	b	1214	CLA	C1B-CHB	2.12	1.46	1.41
14	A	1137	CLA	C4B-CHC	2.12	1.46	1.41
14	G	1114	CLA	C4C-C3C	2.12	1.48	1.45
15	B	1230	F6C	C1D-C2D	2.12	1.48	1.44
14	G	1128	CLA	C1B-CHB	2.12	1.46	1.41
15	H	1230	F6C	C4C-CHD	2.11	1.46	1.41
15	b	1230	F6C	C2B-C1B	2.11	1.49	1.44
14	a	1122	CLA	C1B-CHB	2.11	1.46	1.41
14	b	1223	CLA	C1B-CHB	2.11	1.46	1.41
14	H	1222	CLA	C1B-CHB	2.11	1.46	1.41
14	H	1228	CLA	C1D-C2D	2.11	1.49	1.45
14	B	1221	CLA	C1B-CHB	2.11	1.46	1.41
18	B	4014	BCR	C14-C13	-2.11	1.33	1.35
15	b	1230	F6C	C1D-C2D	2.11	1.48	1.44
14	b	1223	CLA	C1B-NB	-2.11	1.33	1.35
14	L	1502	CLA	C1D-C2D	2.11	1.49	1.45
14	A	1106	CLA	C1B-CHB	2.11	1.46	1.41
14	a	1012	CLA	C4B-NB	-2.11	1.33	1.35
14	a	1133	CLA	C4B-CHC	2.11	1.46	1.41
14	G	1126	CLA	C4B-NB	-2.11	1.33	1.35
14	a	1108	CLA	C1D-C2D	2.11	1.49	1.45
14	K	1401	CLA	C4C-C3C	2.11	1.48	1.45
14	B	1205	CLA	C4B-CHC	2.11	1.46	1.41
14	B	1235	CLA	C1B-CHB	2.11	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1223	CLA	C1B-NB	-2.11	1.33	1.35
14	b	1235	CLA	C1B-CHB	2.11	1.46	1.41
14	G	1114	CLA	C4B-CHC	2.11	1.46	1.41
14	G	1103	CLA	C1B-NB	-2.10	1.33	1.35
14	b	1202	CLA	C1B-CHB	2.10	1.46	1.41
14	b	1205	CLA	C4B-CHC	2.10	1.46	1.41
18	H	4009	BCR	C30-C25	-2.10	1.50	1.53
14	H	1236	CLA	C1B-CHB	2.10	1.46	1.41
14	A	1105	CLA	C4B-CHC	2.10	1.46	1.41
15	B	1230	F6C	C4C-CHD	2.10	1.46	1.41
14	B	1209	CLA	C1B-CHB	2.10	1.46	1.41
14	a	1113	CLA	C1B-CHB	2.10	1.46	1.41
14	G	1114	CLA	C1B-NB	-2.10	1.33	1.35
14	b	1211	CLA	C1B-NB	-2.10	1.33	1.35
14	b	1234	CLA	C1B-CHB	2.10	1.46	1.41
14	b	1236	CLA	C1B-CHB	2.10	1.46	1.41
18	R	4018	BCR	C21-C22	-2.10	1.33	1.35
14	H	1214	CLA	C1B-CHB	2.10	1.46	1.41
14	b	1214	CLA	C1D-C2D	2.10	1.49	1.45
15	H	1238	F6C	C4C-CHD	2.10	1.46	1.41
14	b	1221	CLA	C1B-CHB	2.10	1.46	1.41
14	A	1108	CLA	C1D-C2D	2.10	1.49	1.45
14	b	1219	CLA	C1D-C2D	2.10	1.49	1.45
14	H	1216	CLA	C1D-C2D	2.09	1.49	1.45
14	H	1235	CLA	C1B-CHB	2.09	1.46	1.41
14	B	1225	CLA	C1B-CHB	2.09	1.46	1.41
14	H	1213	CLA	C1B-CHB	2.09	1.46	1.41
14	A	1104	CLA	MG-NC	2.09	2.11	2.06
14	b	1213	CLA	C1B-CHB	2.09	1.46	1.41
14	b	1218	CLA	C1B-NB	-2.09	1.33	1.35
13	a	1011	CL0	C1B-CHB	2.09	1.46	1.41
14	G	1137	CLA	C4B-CHC	2.09	1.46	1.41
14	a	1105	CLA	C4B-CHC	2.09	1.46	1.41
14	B	1218	CLA	C1B-NB	-2.09	1.33	1.35
14	H	1205	CLA	C4B-CHC	2.09	1.46	1.41
14	G	1111	CLA	C1B-NB	-2.09	1.33	1.35
18	m	4021	BCR	C1-C6	-2.09	1.50	1.53
14	b	1209	CLA	C1B-CHB	2.09	1.46	1.41
14	a	1104	CLA	MG-NC	2.09	2.11	2.06
14	G	1108	CLA	C1D-C2D	2.09	1.49	1.45
15	b	1230	F6C	C4A-C3A	2.09	1.49	1.45
18	I	4018	BCR	C21-C22	-2.09	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1210	CLA	C1B-NB	-2.09	1.33	1.35
14	B	1021	CLA	MG-NC	2.09	2.11	2.06
14	B	1202	CLA	C1B-CHB	2.09	1.46	1.41
14	H	1223	CLA	C1B-CHB	2.09	1.46	1.41
14	H	1218	CLA	C1B-NB	-2.09	1.33	1.35
14	H	1227	CLA	C1B-NB	-2.09	1.33	1.35
15	G	1121	F6C	C1C-NC	-2.09	1.33	1.35
14	B	1228	CLA	C4B-CHC	2.08	1.46	1.41
18	L	4022	BCR	C14-C13	-2.08	1.33	1.35
14	B	1223	CLA	C1B-CHB	2.08	1.46	1.41
14	a	1111	CLA	C1B-NB	-2.08	1.33	1.35
14	b	1228	CLA	C4B-CHC	2.08	1.46	1.41
14	l	1501	CLA	C4B-CHC	2.08	1.46	1.41
14	b	1203	CLA	C4B-NB	-2.08	1.33	1.35
14	H	1234	CLA	C1B-CHB	2.08	1.46	1.41
18	i	4018	BCR	C21-C22	-2.08	1.33	1.35
14	H	1236	CLA	C1B-NB	-2.08	1.33	1.35
14	b	1227	CLA	C1B-NB	-2.08	1.33	1.35
14	A	1012	CLA	C4B-NB	-2.08	1.33	1.35
14	U	1501	CLA	C4B-CHC	2.07	1.46	1.41
14	H	1225	CLA	C1B-CHB	2.07	1.46	1.41
14	B	1214	CLA	C1D-C2D	2.07	1.49	1.45
14	G	1105	CLA	C4B-CHC	2.07	1.46	1.41
14	a	1137	CLA	C4B-CHC	2.07	1.46	1.41
14	a	1138	CLA	C1B-NB	-2.07	1.33	1.35
14	L	1501	CLA	C4B-CHC	2.07	1.46	1.41
14	B	1236	CLA	C1B-NB	-2.07	1.33	1.35
14	B	1234	CLA	C1B-CHB	2.07	1.46	1.41
18	M	4021	BCR	C1-C6	-2.07	1.50	1.53
14	a	1111	CLA	C1B-CHB	2.07	1.46	1.41
14	H	1228	CLA	C4B-CHC	2.07	1.46	1.41
14	G	1104	CLA	MG-NC	2.07	2.11	2.06
18	V	4021	BCR	C1-C6	-2.07	1.50	1.53
13	A	1011	CL0	C1B-CHB	2.07	1.46	1.41
14	H	1209	CLA	C1B-CHB	2.07	1.46	1.41
14	B	1213	CLA	C1B-CHB	2.07	1.46	1.41
14	B	1222	CLA	C1B-CHB	2.07	1.46	1.41
14	A	1106	CLA	C1B-NB	-2.07	1.33	1.35
18	l	4022	BCR	C14-C13	-2.06	1.33	1.35
14	G	1105	CLA	C1D-C2D	2.06	1.49	1.45
14	A	1119	CLA	C1D-C2D	2.06	1.49	1.45
14	b	1226	CLA	CMB-C2B	-2.06	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1203	CLA	C4B-CHC	2.06	1.46	1.41
14	B	1214	CLA	C1B-CHB	2.06	1.46	1.41
14	B	1219	CLA	C1D-C2D	2.06	1.49	1.45
14	a	1116	CLA	C1B-CHB	2.06	1.46	1.41
14	b	1021	CLA	C4B-CHC	2.06	1.46	1.41
14	b	1203	CLA	C4B-CHC	2.06	1.46	1.41
14	a	1119	CLA	C1D-C2D	2.06	1.49	1.45
15	b	1238	F6C	C4C-CHD	2.06	1.46	1.41
15	A	1121	F6C	C1C-NC	-2.06	1.33	1.35
14	H	1021	CLA	C4B-CHC	2.06	1.46	1.41
14	H	1210	CLA	C1B-CHB	2.06	1.46	1.41
18	U	4022	BCR	C14-C13	-2.06	1.33	1.35
14	H	1219	CLA	C1D-C2D	2.06	1.49	1.45
15	B	1230	F6C	C4A-C3A	2.06	1.49	1.45
14	B	1203	CLA	C1B-CHB	2.06	1.46	1.41
14	a	1105	CLA	C1D-C2D	2.06	1.49	1.45
14	H	1021	CLA	MG-NC	2.06	2.11	2.06
14	b	1021	CLA	MG-NC	2.05	2.11	2.06
15	b	1237	F6C	C1D-C2D	2.05	1.48	1.44
14	b	1021	CLA	C3A-C2A	-2.05	1.48	1.54
14	G	1102	CLA	C1B-NB	-2.05	1.33	1.35
14	b	1232	CLA	C1B-NB	-2.05	1.33	1.35
14	a	1117	CLA	C1B-CHB	2.05	1.46	1.41
14	b	1203	CLA	C1B-CHB	2.05	1.46	1.41
14	A	1102	CLA	C1B-NB	-2.05	1.33	1.35
13	G	1011	CL0	C1B-CHB	2.05	1.46	1.41
14	A	1103	CLA	C4B-CHC	2.05	1.46	1.41
14	H	1021	CLA	C3A-C2A	-2.05	1.48	1.54
14	A	1111	CLA	C1B-CHB	2.05	1.46	1.41
15	B	1238	F6C	C4C-CHD	2.05	1.46	1.41
14	A	1138	CLA	C1B-NB	-2.05	1.33	1.35
14	A	1116	CLA	C1B-CHB	2.05	1.46	1.41
18	G	4007	BCR	C17-C18	-2.05	1.33	1.35
14	B	1228	CLA	C4C-C3C	2.05	1.48	1.45
14	G	1138	CLA	C1B-NB	-2.05	1.33	1.35
15	B	1237	F6C	C1D-C2D	2.05	1.48	1.44
21	A	6001	LMT	O4'-C4B	-2.05	1.38	1.43
21	G	6001	LMT	O4'-C4B	-2.05	1.38	1.43
14	G	1103	CLA	C4B-CHC	2.05	1.46	1.41
14	a	1112	CLA	C1B-CHB	2.05	1.46	1.41
14	B	1210	CLA	C1B-CHB	2.05	1.46	1.41
18	B	4017	BCR	C14-C13	-2.04	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1112	CLA	C1B-CHB	2.04	1.46	1.41
14	A	1117	CLA	C1B-CHB	2.04	1.46	1.41
14	B	1232	CLA	C1B-NB	-2.04	1.33	1.35
14	H	1214	CLA	C1D-C2D	2.04	1.49	1.45
14	a	1103	CLA	C4B-CHC	2.04	1.46	1.41
14	b	1210	CLA	C1B-CHB	2.04	1.46	1.41
18	b	4017	BCR	C21-C22	-2.04	1.33	1.35
15	H	1230	F6C	C4A-C3A	2.04	1.49	1.45
14	B	1210	CLA	C1B-NB	-2.04	1.33	1.35
14	B	1226	CLA	CMB-C2B	-2.04	1.47	1.51
21	a	6001	LMT	O4'-C4B	-2.04	1.38	1.43
14	B	1021	CLA	C3A-C2A	-2.04	1.48	1.54
14	b	1216	CLA	C1D-C2D	2.04	1.49	1.45
14	H	1211	CLA	C1B-NB	-2.04	1.33	1.35
14	l	1503	CLA	C1B-NB	-2.04	1.33	1.35
14	G	1111	CLA	C1B-CHB	2.04	1.46	1.41
14	B	1211	CLA	C1D-C2D	2.04	1.49	1.45
14	G	1012	CLA	C4B-NB	-2.04	1.33	1.35
14	b	1228	CLA	C4C-C3C	2.04	1.48	1.45
14	H	1210	CLA	C1D-C2D	2.04	1.49	1.45
14	b	1225	CLA	C1B-CHB	2.04	1.46	1.41
14	B	1021	CLA	C4B-CHC	2.04	1.46	1.41
14	H	1226	CLA	CMB-C2B	-2.04	1.47	1.51
15	H	1237	F6C	C1D-C2D	2.04	1.48	1.44
14	B	1203	CLA	C4B-CHC	2.03	1.46	1.41
14	B	1229	CLA	C1D-C2D	2.03	1.49	1.45
18	R	4020	BCR	C30-C25	-2.03	1.51	1.53
14	G	1116	CLA	C1B-CHB	2.03	1.46	1.41
14	G	1117	CLA	C1B-CHB	2.03	1.46	1.41
14	B	1204	CLA	C4B-CHC	2.03	1.46	1.41
14	a	1137	CLA	C1B-CHB	2.03	1.46	1.41
14	A	1105	CLA	C1D-C2D	2.03	1.49	1.45
14	H	1211	CLA	C1D-C2D	2.03	1.49	1.45
14	b	1210	CLA	C1D-C2D	2.03	1.49	1.45
18	i	4020	BCR	C30-C25	-2.03	1.51	1.53
14	H	1226	CLA	C1B-CHB	2.03	1.46	1.41
14	b	1227	CLA	C4C-C3C	2.02	1.48	1.45
14	a	1135	CLA	C4B-NB	-2.02	1.33	1.35
14	G	1119	CLA	C1D-C2D	2.02	1.49	1.45
14	H	1219	CLA	C1B-CHB	2.02	1.46	1.41
14	H	1229	CLA	C1D-C2D	2.02	1.49	1.45
20	i	5006	LMG	C37-C36	-2.02	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	I	4020	BCR	C30-C25	-2.02	1.51	1.53
14	B	1219	CLA	C1B-CHB	2.02	1.46	1.41
14	a	1106	CLA	C1B-NB	-2.02	1.33	1.35
18	H	4017	BCR	C21-C22	-2.02	1.33	1.35
14	B	1216	CLA	C1D-C2D	2.02	1.49	1.45
14	b	1226	CLA	C1B-CHB	2.02	1.46	1.41
14	A	1112	CLA	C1B-CHB	2.02	1.46	1.41
14	b	1211	CLA	C1D-C2D	2.02	1.49	1.45
14	b	1224	CLA	C1B-CHB	2.02	1.46	1.41
14	A	1137	CLA	C1B-CHB	2.02	1.46	1.41
14	H	1203	CLA	C1B-CHB	2.02	1.46	1.41
14	a	1114	CLA	C1B-CHB	2.02	1.46	1.41
14	B	1202	CLA	C1B-NB	-2.02	1.33	1.35
18	b	4017	BCR	C14-C13	-2.02	1.33	1.35
14	G	1137	CLA	C1B-CHB	2.02	1.46	1.41
14	a	1135	CLA	C4B-CHC	2.02	1.46	1.41
14	B	1227	CLA	C4C-C3C	2.01	1.48	1.45
14	H	1201	CLA	C1B-CHB	2.01	1.46	1.41
14	G	1125	CLA	C4B-CHC	2.01	1.46	1.41
20	I	5006	LMG	C37-C36	-2.01	1.33	1.49
14	G	1135	CLA	C4B-CHC	2.01	1.46	1.41
14	a	1133	CLA	C1D-C2D	2.01	1.49	1.45
14	B	1226	CLA	C1B-CHB	2.01	1.46	1.41
20	R	5006	LMG	C37-C36	-2.01	1.33	1.49
14	H	1227	CLA	C4C-C3C	2.01	1.48	1.45
14	B	1201	CLA	C1B-CHB	2.01	1.46	1.41
14	b	1204	CLA	C4B-CHC	2.01	1.46	1.41
14	G	1114	CLA	C1B-CHB	2.01	1.46	1.41
14	H	1202	CLA	C1B-NB	-2.01	1.33	1.35
14	a	1131	CLA	C1B-NB	-2.01	1.33	1.35
18	H	4017	BCR	C14-C13	-2.01	1.33	1.35
14	a	1122	CLA	C4B-CHC	2.01	1.46	1.41
14	A	1122	CLA	C4B-CHC	2.01	1.46	1.41
14	B	1224	CLA	C1B-CHB	2.00	1.46	1.41
14	H	1220	CLA	C4B-CHC	2.00	1.46	1.41
14	G	1122	CLA	C4B-CHC	2.00	1.46	1.41
14	B	1220	CLA	C4B-CHC	2.00	1.46	1.41
14	G	1135	CLA	C4B-NB	-2.00	1.33	1.35
18	b	4014	BCR	C1-C6	-2.00	1.51	1.53
14	H	1228	CLA	C4C-C3C	2.00	1.48	1.45
14	b	1229	CLA	C1D-C2D	2.00	1.49	1.45
14	B	1022	CLA	C1B-CHB	2.00	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	1237	F6C	C1C-CHC	2.00	1.46	1.41
14	H	1232	CLA	C1B-NB	-2.00	1.33	1.35
14	a	1125	CLA	C4B-CHC	2.00	1.46	1.41
14	a	1112	CLA	C1D-C2D	2.00	1.49	1.45

All (7829) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	H	4010	BCR	C16-C17-C18	25.75	164.06	127.31
18	b	4010	BCR	C16-C17-C18	25.71	164.00	127.31
18	B	4010	BCR	C16-C17-C18	25.69	163.97	127.31
18	H	4017	BCR	C20-C21-C22	24.30	161.99	127.31
18	B	4017	BCR	C20-C21-C22	24.30	161.99	127.31
18	U	4019	BCR	C16-C17-C18	24.29	161.98	127.31
18	l	4019	BCR	C16-C17-C18	24.29	161.98	127.31
18	L	4019	BCR	C16-C17-C18	24.28	161.96	127.31
18	b	4017	BCR	C20-C21-C22	24.23	161.89	127.31
18	R	4020	BCR	C20-C21-C22	24.14	161.76	127.31
18	i	4020	BCR	C20-C21-C22	24.14	161.75	127.31
18	I	4020	BCR	C20-C21-C22	24.11	161.71	127.31
18	B	4016	BCR	C16-C17-C18	23.32	160.60	127.31
18	b	4016	BCR	C16-C17-C18	23.30	160.57	127.31
18	H	4016	BCR	C16-C17-C18	23.26	160.51	127.31
18	I	4018	BCR	C16-C17-C18	22.84	159.90	127.31
18	i	4018	BCR	C16-C17-C18	22.80	159.86	127.31
18	R	4018	BCR	C16-C17-C18	22.76	159.80	127.31
18	b	4013	BCR	C16-C17-C18	22.59	159.55	127.31
18	H	4013	BCR	C16-C17-C18	22.58	159.54	127.31
18	B	4013	BCR	C16-C17-C18	22.55	159.50	127.31
18	a	4007	BCR	C20-C21-C22	22.52	159.45	127.31
18	G	4007	BCR	C20-C21-C22	22.50	159.42	127.31
18	A	4007	BCR	C20-C21-C22	22.50	159.42	127.31
18	A	4001	BCR	C20-C21-C22	22.23	159.04	127.31
18	G	4001	BCR	C20-C21-C22	22.21	159.01	127.31
18	a	4001	BCR	C20-C21-C22	22.20	158.99	127.31
18	B	4006	BCR	C20-C21-C22	22.18	158.97	127.31
18	b	4006	BCR	C20-C21-C22	22.13	158.89	127.31
18	H	4006	BCR	C20-C21-C22	22.12	158.88	127.31
18	b	4016	BCR	C20-C21-C22	21.98	158.68	127.31
18	B	4016	BCR	C20-C21-C22	21.97	158.67	127.31
18	H	4016	BCR	C20-C21-C22	21.96	158.65	127.31
18	A	4003	BCR	C20-C21-C22	21.88	158.53	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	4003	BCR	C20-C21-C22	21.86	158.50	127.31
18	a	4003	BCR	C20-C21-C22	21.83	158.46	127.31
18	M	4021	BCR	C20-C21-C22	21.80	158.42	127.31
18	V	4021	BCR	C20-C21-C22	21.79	158.40	127.31
18	m	4021	BCR	C20-C21-C22	21.75	158.35	127.31
18	A	4001	BCR	C16-C17-C18	21.72	158.31	127.31
18	G	4001	BCR	C16-C17-C18	21.70	158.28	127.31
18	G	4008	BCR	C20-C21-C22	21.69	158.26	127.31
18	a	4008	BCR	C20-C21-C22	21.68	158.25	127.31
18	A	4008	BCR	C20-C21-C22	21.66	158.22	127.31
18	a	4001	BCR	C16-C17-C18	21.65	158.21	127.31
18	A	4002	BCR	C15-C16-C17	21.59	167.71	123.47
18	G	4002	BCR	C15-C16-C17	21.58	167.69	123.47
18	a	4002	BCR	C15-C16-C17	21.58	167.69	123.47
18	B	4013	BCR	C20-C21-C22	21.58	158.11	127.31
18	H	4013	BCR	C20-C21-C22	21.57	158.09	127.31
18	b	4013	BCR	C20-C21-C22	21.57	158.09	127.31
18	H	4014	BCR	C15-C16-C17	21.56	167.63	123.47
18	b	4014	BCR	C15-C16-C17	21.55	167.62	123.47
18	B	4014	BCR	C15-C16-C17	21.54	167.60	123.47
18	B	4009	BCR	C16-C17-C18	21.49	157.98	127.31
18	b	4010	BCR	C20-C21-C22	21.47	157.95	127.31
18	b	4009	BCR	C16-C17-C18	21.47	157.95	127.31
18	H	4010	BCR	C20-C21-C22	21.44	157.91	127.31
18	B	4010	BCR	C20-C21-C22	21.44	157.91	127.31
18	H	4009	BCR	C16-C17-C18	21.43	157.90	127.31
18	I	4020	BCR	C16-C17-C18	21.42	157.88	127.31
18	i	4020	BCR	C16-C17-C18	21.42	157.88	127.31
18	R	4020	BCR	C16-C17-C18	21.41	157.86	127.31
18	V	4021	BCR	C16-C17-C18	21.14	157.49	127.31
18	M	4021	BCR	C16-C17-C18	21.13	157.46	127.31
18	m	4021	BCR	C16-C17-C18	21.12	157.45	127.31
14	a	1111	CLA	C4-C3-C5	-21.04	79.87	115.27
14	A	1111	CLA	C4-C3-C5	-21.04	79.87	115.27
18	G	4002	BCR	C20-C21-C22	21.04	157.34	127.31
18	a	4002	BCR	C20-C21-C22	21.02	157.31	127.31
14	G	1111	CLA	C4-C3-C5	-21.02	79.91	115.27
18	A	4002	BCR	C20-C21-C22	21.01	157.29	127.31
18	U	4019	BCR	C20-C21-C22	21.01	157.29	127.31
18	l	4019	BCR	C20-C21-C22	21.00	157.27	127.31
18	H	4005	BCR	C16-C17-C18	20.98	157.26	127.31
18	L	4019	BCR	C20-C21-C22	20.98	157.25	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	4005	BCR	C16-C17-C18	20.97	157.23	127.31
18	B	4005	BCR	C16-C17-C18	20.97	157.23	127.31
18	B	4014	BCR	C20-C21-C22	20.89	157.13	127.31
18	b	4014	BCR	C20-C21-C22	20.88	157.11	127.31
18	H	4014	BCR	C20-C21-C22	20.86	157.08	127.31
18	b	4006	BCR	C16-C17-C18	20.70	156.86	127.31
18	H	4006	BCR	C16-C17-C18	20.70	156.85	127.31
18	H	4009	BCR	C20-C21-C22	20.68	156.83	127.31
18	B	4009	BCR	C20-C21-C22	20.67	156.81	127.31
18	b	4009	BCR	C20-C21-C22	20.66	156.80	127.31
18	a	4011	BCR	C16-C17-C18	20.65	156.78	127.31
18	A	4011	BCR	C16-C17-C18	20.65	156.78	127.31
18	B	4006	BCR	C16-C17-C18	20.64	156.77	127.31
18	G	4011	BCR	C16-C17-C18	20.62	156.73	127.31
18	a	4007	BCR	C16-C17-C18	20.57	156.66	127.31
18	H	4005	BCR	C15-C16-C17	20.55	165.57	123.47
18	G	4007	BCR	C16-C17-C18	20.54	156.62	127.31
18	A	4007	BCR	C16-C17-C18	20.54	156.62	127.31
18	b	4005	BCR	C15-C16-C17	20.54	165.54	123.47
18	B	4005	BCR	C15-C16-C17	20.53	165.53	123.47
18	b	4017	BCR	C16-C17-C18	20.52	156.59	127.31
18	B	4017	BCR	C16-C17-C18	20.49	156.56	127.31
18	G	4008	BCR	C15-C16-C17	20.47	165.41	123.47
18	A	4008	BCR	C15-C16-C17	20.47	165.40	123.47
18	H	4017	BCR	C16-C17-C18	20.46	156.51	127.31
18	G	4003	BCR	C16-C17-C18	20.43	156.47	127.31
18	a	4008	BCR	C15-C16-C17	20.42	165.31	123.47
18	A	4003	BCR	C16-C17-C18	20.41	156.44	127.31
18	a	4003	BCR	C16-C17-C18	20.41	156.44	127.31
18	b	4005	BCR	C20-C21-C22	20.39	156.40	127.31
18	B	4005	BCR	C20-C21-C22	20.38	156.40	127.31
18	l	4022	BCR	C15-C16-C17	20.37	165.20	123.47
18	H	4005	BCR	C20-C21-C22	20.35	156.36	127.31
18	L	4022	BCR	C15-C16-C17	20.34	165.14	123.47
18	U	4022	BCR	C15-C16-C17	20.32	165.11	123.47
18	B	4004	BCR	C15-C16-C17	20.32	165.10	123.47
18	b	4004	BCR	C15-C16-C17	20.31	165.09	123.47
18	H	4004	BCR	C15-C16-C17	20.31	165.08	123.47
18	L	4022	BCR	C20-C21-C22	20.26	156.22	127.31
18	l	4022	BCR	C20-C21-C22	20.26	156.22	127.31
18	U	4022	BCR	C20-C21-C22	20.22	156.17	127.31
18	G	4003	BCR	C15-C16-C17	20.10	164.65	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	4003	BCR	C15-C16-C17	20.10	164.65	123.47
18	A	4003	BCR	C15-C16-C17	20.10	164.64	123.47
18	R	4018	BCR	C20-C21-C22	20.05	155.92	127.31
18	i	4018	BCR	C20-C21-C22	20.04	155.90	127.31
18	I	4020	BCR	C15-C16-C17	20.03	164.51	123.47
18	i	4020	BCR	C15-C16-C17	20.02	164.49	123.47
18	R	4020	BCR	C15-C16-C17	20.00	164.44	123.47
18	I	4018	BCR	C20-C21-C22	19.99	155.84	127.31
18	L	4019	BCR	C15-C16-C17	19.79	164.01	123.47
18	l	4019	BCR	C15-C16-C17	19.79	164.00	123.47
18	U	4019	BCR	C15-C16-C17	19.78	163.99	123.47
18	H	4006	BCR	C15-C16-C17	19.75	163.93	123.47
18	b	4006	BCR	C15-C16-C17	19.75	163.93	123.47
18	a	4011	BCR	C15-C16-C17	19.74	163.92	123.47
18	A	4011	BCR	C15-C16-C17	19.74	163.91	123.47
18	B	4006	BCR	C15-C16-C17	19.73	163.89	123.47
18	G	4011	BCR	C15-C16-C17	19.73	163.89	123.47
18	M	4021	BCR	C15-C16-C17	19.64	163.70	123.47
18	V	4021	BCR	C15-C16-C17	19.62	163.67	123.47
18	m	4021	BCR	C15-C16-C17	19.61	163.65	123.47
18	l	4022	BCR	C16-C17-C18	19.56	155.22	127.31
18	B	4017	BCR	C15-C16-C17	19.56	163.54	123.47
18	b	4009	BCR	C15-C16-C17	19.55	163.53	123.47
18	B	4009	BCR	C15-C16-C17	19.55	163.53	123.47
18	H	4009	BCR	C15-C16-C17	19.54	163.50	123.47
18	b	4017	BCR	C15-C16-C17	19.54	163.50	123.47
18	H	4017	BCR	C15-C16-C17	19.54	163.49	123.47
18	L	4022	BCR	C16-C17-C18	19.51	155.15	127.31
18	U	4022	BCR	C16-C17-C18	19.50	155.14	127.31
18	G	4011	BCR	C20-C21-C22	19.46	155.09	127.31
18	a	4011	BCR	C20-C21-C22	19.45	155.06	127.31
18	A	4011	BCR	C20-C21-C22	19.44	155.06	127.31
18	A	4007	BCR	C15-C16-C17	19.25	162.91	123.47
18	G	4007	BCR	C15-C16-C17	19.25	162.90	123.47
18	a	4007	BCR	C15-C16-C17	19.25	162.90	123.47
14	G	1111	CLA	C5-C3-C2	19.17	159.91	121.12
14	a	1111	CLA	C5-C3-C2	19.17	159.91	121.12
14	A	1111	CLA	C5-C3-C2	19.15	159.87	121.12
18	H	4004	BCR	C20-C21-C22	19.08	154.54	127.31
18	B	4004	BCR	C20-C21-C22	19.07	154.53	127.31
18	b	4004	BCR	C20-C21-C22	19.07	154.53	127.31
18	G	4008	BCR	C16-C17-C18	19.03	154.47	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	4008	BCR	C16-C17-C18	19.00	154.42	127.31
18	B	4004	BCR	C16-C17-C18	18.98	154.40	127.31
18	H	4004	BCR	C16-C17-C18	18.95	154.35	127.31
18	b	4004	BCR	C16-C17-C18	18.95	154.35	127.31
18	a	4008	BCR	C16-C17-C18	18.94	154.35	127.31
18	I	4018	BCR	C15-C16-C17	18.31	160.99	123.47
18	R	4018	BCR	C15-C16-C17	18.29	160.94	123.47
18	i	4018	BCR	C15-C16-C17	18.27	160.91	123.47
18	b	4014	BCR	C16-C17-C18	18.27	153.39	127.31
18	H	4014	BCR	C16-C17-C18	18.26	153.38	127.31
18	B	4014	BCR	C16-C17-C18	18.26	153.37	127.31
18	A	4001	BCR	C15-C16-C17	18.17	160.70	123.47
18	a	4001	BCR	C15-C16-C17	18.15	160.66	123.47
18	G	4001	BCR	C15-C16-C17	18.14	160.64	123.47
18	b	4013	BCR	C15-C16-C17	17.78	159.90	123.47
18	H	4013	BCR	C15-C16-C17	17.77	159.87	123.47
18	B	4013	BCR	C15-C16-C17	17.74	159.81	123.47
18	V	4021	BCR	C10-C11-C12	17.59	178.11	123.22
18	H	4016	BCR	C15-C16-C17	17.58	159.49	123.47
18	M	4021	BCR	C10-C11-C12	17.57	178.06	123.22
18	m	4021	BCR	C10-C11-C12	17.57	178.04	123.22
18	b	4016	BCR	C15-C16-C17	17.56	159.44	123.47
18	B	4016	BCR	C15-C16-C17	17.55	159.43	123.47
18	B	4010	BCR	C10-C11-C12	17.45	177.69	123.22
18	G	4003	BCR	C10-C11-C12	17.45	177.67	123.22
18	H	4010	BCR	C10-C11-C12	17.45	177.66	123.22
18	a	4003	BCR	C10-C11-C12	17.44	177.65	123.22
18	A	4003	BCR	C10-C11-C12	17.43	177.62	123.22
18	b	4010	BCR	C10-C11-C12	17.43	177.60	123.22
18	A	4001	BCR	C10-C11-C12	17.42	177.58	123.22
18	G	4001	BCR	C10-C11-C12	17.40	177.52	123.22
18	a	4001	BCR	C10-C11-C12	17.40	177.52	123.22
18	a	4007	BCR	C10-C11-C12	17.36	177.38	123.22
18	A	4007	BCR	C10-C11-C12	17.35	177.37	123.22
18	G	4007	BCR	C10-C11-C12	17.33	177.29	123.22
18	U	4022	BCR	C10-C11-C12	17.32	177.26	123.22
18	l	4022	BCR	C10-C11-C12	17.31	177.24	123.22
18	L	4022	BCR	C10-C11-C12	17.31	177.24	123.22
18	R	4018	BCR	C10-C11-C12	17.28	177.14	123.22
18	H	4016	BCR	C10-C11-C12	17.27	177.10	123.22
18	b	4016	BCR	C10-C11-C12	17.26	177.08	123.22
18	B	4016	BCR	C10-C11-C12	17.26	177.08	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	i	4018	BCR	C10-C11-C12	17.26	177.07	123.22
18	H	4004	BCR	C10-C11-C12	17.25	177.05	123.22
18	b	4004	BCR	C10-C11-C12	17.25	177.05	123.22
18	B	4004	BCR	C10-C11-C12	17.24	177.03	123.22
18	I	4018	BCR	C10-C11-C12	17.24	177.02	123.22
18	A	4008	BCR	C10-C11-C12	17.17	176.81	123.22
18	a	4008	BCR	C10-C11-C12	17.17	176.79	123.22
18	G	4008	BCR	C10-C11-C12	17.16	176.78	123.22
18	U	4019	BCR	C10-C11-C12	17.15	176.73	123.22
18	l	4019	BCR	C10-C11-C12	17.14	176.72	123.22
18	L	4019	BCR	C10-C11-C12	17.12	176.65	123.22
18	B	4017	BCR	C10-C11-C12	17.11	176.60	123.22
18	H	4017	BCR	C10-C11-C12	17.10	176.57	123.22
18	b	4017	BCR	C10-C11-C12	17.10	176.57	123.22
18	A	4002	BCR	C16-C17-C18	17.01	151.59	127.31
14	A	1111	CLA	C4-C3-C2	-17.01	80.04	123.68
14	G	1111	CLA	C4-C3-C2	-17.01	80.04	123.68
18	G	4002	BCR	C16-C17-C18	17.00	151.57	127.31
14	a	1111	CLA	C4-C3-C2	-17.00	80.07	123.68
18	b	4014	BCR	C10-C11-C12	16.99	176.23	123.22
18	B	4014	BCR	C10-C11-C12	16.99	176.23	123.22
18	H	4014	BCR	C10-C11-C12	16.99	176.23	123.22
18	a	4002	BCR	C16-C17-C18	16.98	151.55	127.31
18	H	4009	BCR	C10-C11-C12	16.94	176.08	123.22
18	B	4009	BCR	C10-C11-C12	16.93	176.06	123.22
18	b	4009	BCR	C10-C11-C12	16.93	176.04	123.22
18	R	4020	BCR	C10-C11-C12	16.88	175.90	123.22
18	B	4005	BCR	C10-C11-C12	16.88	175.88	123.22
18	i	4020	BCR	C10-C11-C12	16.87	175.88	123.22
18	I	4020	BCR	C10-C11-C12	16.87	175.86	123.22
18	H	4005	BCR	C10-C11-C12	16.86	175.83	123.22
18	b	4005	BCR	C10-C11-C12	16.85	175.79	123.22
18	H	4006	BCR	C10-C11-C12	16.79	175.62	123.22
18	B	4006	BCR	C10-C11-C12	16.78	175.60	123.22
18	b	4006	BCR	C10-C11-C12	16.78	175.58	123.22
18	H	4013	BCR	C10-C11-C12	16.62	175.08	123.22
18	B	4013	BCR	C10-C11-C12	16.61	175.05	123.22
18	b	4013	BCR	C10-C11-C12	16.60	175.02	123.22
18	L	4019	BCR	C16-C15-C14	16.59	157.46	123.47
18	l	4019	BCR	C16-C15-C14	16.58	157.43	123.47
18	U	4019	BCR	C16-C15-C14	16.57	157.41	123.47
18	G	4002	BCR	C10-C11-C12	16.32	174.14	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	4002	BCR	C10-C11-C12	16.32	174.14	123.22
18	A	4002	BCR	C10-C11-C12	16.31	174.10	123.22
18	G	4011	BCR	C10-C11-C12	16.08	173.40	123.22
18	A	4011	BCR	C10-C11-C12	16.07	173.38	123.22
18	a	4011	BCR	C10-C11-C12	16.07	173.36	123.22
18	H	4010	BCR	C15-C16-C17	15.85	155.94	123.47
18	B	4010	BCR	C15-C16-C17	15.82	155.88	123.47
18	b	4010	BCR	C15-C16-C17	15.80	155.85	123.47
18	V	4021	BCR	C16-C15-C14	15.26	154.73	123.47
18	M	4021	BCR	C16-C15-C14	15.24	154.69	123.47
18	m	4021	BCR	C16-C15-C14	15.24	154.69	123.47
18	G	4011	BCR	C11-C10-C9	14.78	148.41	127.31
18	a	4011	BCR	C11-C10-C9	14.78	148.40	127.31
18	A	4011	BCR	C11-C10-C9	14.74	148.35	127.31
18	i	4018	BCR	C16-C15-C14	14.64	153.46	123.47
18	R	4018	BCR	C16-C15-C14	14.64	153.46	123.47
18	I	4018	BCR	C16-C15-C14	14.59	153.36	123.47
18	B	4013	BCR	C16-C15-C14	14.55	153.29	123.47
18	H	4013	BCR	C16-C15-C14	14.52	153.22	123.47
18	b	4013	BCR	C16-C15-C14	14.51	153.21	123.47
18	G	4001	BCR	C16-C15-C14	14.46	153.10	123.47
18	a	4001	BCR	C16-C15-C14	14.45	153.07	123.47
18	A	4001	BCR	C16-C15-C14	14.44	153.05	123.47
18	H	4013	BCR	C11-C10-C9	14.37	147.82	127.31
18	b	4013	BCR	C11-C10-C9	14.35	147.79	127.31
18	B	4013	BCR	C11-C10-C9	14.35	147.79	127.31
18	B	4016	BCR	C16-C15-C14	14.33	152.84	123.47
18	b	4016	BCR	C16-C15-C14	14.32	152.81	123.47
18	H	4016	BCR	C16-C15-C14	14.32	152.81	123.47
18	B	4017	BCR	C11-C10-C9	14.27	147.68	127.31
18	H	4017	BCR	C11-C10-C9	14.27	147.68	127.31
18	b	4017	BCR	C11-C10-C9	14.23	147.62	127.31
18	b	4006	BCR	C11-C10-C9	14.13	147.48	127.31
18	H	4006	BCR	C11-C10-C9	14.13	147.48	127.31
18	B	4006	BCR	C11-C10-C9	14.13	147.47	127.31
18	H	4004	BCR	C21-C20-C19	13.98	166.85	123.22
18	b	4004	BCR	C21-C20-C19	13.98	166.85	123.22
18	B	4004	BCR	C21-C20-C19	13.97	166.81	123.22
18	B	4005	BCR	C11-C10-C9	13.45	146.51	127.31
18	U	4019	BCR	C11-C10-C9	13.44	146.49	127.31
18	H	4004	BCR	C11-C10-C9	13.44	146.49	127.31
18	l	4019	BCR	C11-C10-C9	13.44	146.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	4004	BCR	C11-C10-C9	13.43	146.48	127.31
18	H	4005	BCR	C11-C10-C9	13.43	146.47	127.31
18	B	4004	BCR	C11-C10-C9	13.41	146.45	127.31
18	b	4005	BCR	C11-C10-C9	13.40	146.43	127.31
18	L	4019	BCR	C11-C10-C9	13.40	146.43	127.31
18	L	4022	BCR	C21-C20-C19	13.33	164.82	123.22
18	l	4022	BCR	C21-C20-C19	13.33	164.81	123.22
18	U	4022	BCR	C21-C20-C19	13.31	164.76	123.22
18	H	4016	BCR	C11-C10-C9	13.29	146.28	127.31
18	B	4014	BCR	C21-C20-C19	13.26	164.60	123.22
18	b	4014	BCR	C21-C20-C19	13.26	164.59	123.22
18	B	4016	BCR	C11-C10-C9	13.26	146.23	127.31
18	b	4016	BCR	C11-C10-C9	13.26	146.23	127.31
18	H	4014	BCR	C21-C20-C19	13.24	164.53	123.22
18	I	4020	BCR	C11-C10-C9	13.20	146.15	127.31
18	b	4010	BCR	C16-C15-C14	13.19	150.48	123.47
18	G	4011	BCR	C21-C20-C19	13.18	164.35	123.22
18	A	4011	BCR	C21-C20-C19	13.18	164.35	123.22
18	R	4020	BCR	C11-C10-C9	13.18	146.12	127.31
18	i	4020	BCR	C11-C10-C9	13.18	146.12	127.31
18	B	4010	BCR	C16-C15-C14	13.18	150.46	123.47
18	H	4010	BCR	C16-C15-C14	13.16	150.44	123.47
18	a	4011	BCR	C21-C20-C19	13.16	164.30	123.22
18	B	4009	BCR	C16-C15-C14	13.16	150.43	123.47
18	H	4009	BCR	C16-C15-C14	13.16	150.43	123.47
18	b	4009	BCR	C16-C15-C14	13.15	150.42	123.47
18	b	4010	BCR	C21-C20-C19	12.93	163.58	123.22
18	B	4010	BCR	C21-C20-C19	12.92	163.53	123.22
18	H	4010	BCR	C21-C20-C19	12.92	163.52	123.22
18	a	4002	BCR	C21-C20-C19	12.91	163.50	123.22
18	G	4002	BCR	C21-C20-C19	12.90	163.49	123.22
18	A	4002	BCR	C21-C20-C19	12.90	163.49	123.22
18	B	4004	BCR	C16-C15-C14	12.90	149.91	123.47
18	b	4004	BCR	C16-C15-C14	12.89	149.89	123.47
18	G	4003	BCR	C11-C10-C9	12.89	145.71	127.31
18	H	4004	BCR	C16-C15-C14	12.89	149.88	123.47
18	A	4008	BCR	C21-C20-C19	12.87	163.39	123.22
18	a	4008	BCR	C21-C20-C19	12.87	163.39	123.22
18	G	4008	BCR	C21-C20-C19	12.87	163.38	123.22
18	A	4003	BCR	C11-C10-C9	12.86	145.67	127.31
18	a	4003	BCR	C11-C10-C9	12.85	145.65	127.31
18	l	4022	BCR	C11-C10-C9	12.85	145.64	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	U	4022	BCR	C11-C10-C9	12.84	145.64	127.31
18	L	4022	BCR	C11-C10-C9	12.83	145.62	127.31
18	b	4006	BCR	C16-C15-C14	12.76	149.61	123.47
18	B	4006	BCR	C16-C15-C14	12.76	149.61	123.47
18	H	4006	BCR	C16-C15-C14	12.75	149.59	123.47
18	A	4007	BCR	C16-C15-C14	12.68	149.45	123.47
18	G	4007	BCR	C16-C15-C14	12.67	149.44	123.47
18	b	4005	BCR	C21-C20-C19	12.67	162.76	123.22
18	H	4005	BCR	C21-C20-C19	12.67	162.76	123.22
18	a	4007	BCR	C16-C15-C14	12.66	149.41	123.47
18	B	4005	BCR	C21-C20-C19	12.66	162.71	123.22
18	B	4013	BCR	C21-C20-C19	12.61	162.56	123.22
18	b	4013	BCR	C21-C20-C19	12.60	162.53	123.22
18	H	4013	BCR	C21-C20-C19	12.59	162.51	123.22
18	i	4020	BCR	C21-C20-C19	12.57	162.45	123.22
18	R	4020	BCR	C21-C20-C19	12.56	162.42	123.22
18	I	4020	BCR	C21-C20-C19	12.56	162.41	123.22
18	H	4009	BCR	C21-C20-C19	12.48	162.15	123.22
18	G	4001	BCR	C21-C20-C19	12.48	162.15	123.22
18	A	4001	BCR	C21-C20-C19	12.47	162.14	123.22
18	B	4009	BCR	C21-C20-C19	12.47	162.13	123.22
18	A	4003	BCR	C16-C15-C14	12.46	149.00	123.47
18	a	4001	BCR	C21-C20-C19	12.46	162.10	123.22
18	B	4017	BCR	C16-C15-C14	12.45	148.99	123.47
18	b	4009	BCR	C21-C20-C19	12.45	162.07	123.22
18	a	4003	BCR	C16-C15-C14	12.45	148.98	123.47
18	H	4017	BCR	C16-C15-C14	12.45	148.97	123.47
18	b	4017	BCR	C16-C15-C14	12.44	148.97	123.47
18	G	4003	BCR	C16-C15-C14	12.44	148.95	123.47
18	M	4021	BCR	C21-C20-C19	12.43	162.00	123.22
18	G	4011	BCR	C16-C15-C14	12.42	148.91	123.47
18	a	4011	BCR	C16-C15-C14	12.41	148.90	123.47
18	V	4021	BCR	C21-C20-C19	12.40	161.93	123.22
18	A	4011	BCR	C16-C15-C14	12.40	148.88	123.47
18	b	4017	BCR	C21-C20-C19	12.40	161.92	123.22
18	m	4021	BCR	C21-C20-C19	12.40	161.92	123.22
18	H	4017	BCR	C21-C20-C19	12.39	161.90	123.22
18	B	4017	BCR	C21-C20-C19	12.39	161.90	123.22
18	H	4016	BCR	C21-C20-C19	12.39	161.88	123.22
18	B	4016	BCR	C21-C20-C19	12.39	161.88	123.22
18	b	4016	BCR	C21-C20-C19	12.38	161.86	123.22
18	B	4014	BCR	C11-C10-C9	12.26	144.81	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	V	4021	BCR	C11-C10-C9	12.25	144.79	127.31
18	b	4014	BCR	C11-C10-C9	12.24	144.78	127.31
18	H	4014	BCR	C11-C10-C9	12.23	144.76	127.31
18	M	4021	BCR	C11-C10-C9	12.22	144.75	127.31
18	m	4021	BCR	C11-C10-C9	12.22	144.75	127.31
18	a	4002	BCR	C16-C15-C14	12.19	148.44	123.47
18	G	4002	BCR	C16-C15-C14	12.17	148.41	123.47
18	A	4002	BCR	C16-C15-C14	12.17	148.40	123.47
18	a	4007	BCR	C21-C20-C19	12.15	161.14	123.22
18	A	4007	BCR	C21-C20-C19	12.15	161.14	123.22
18	G	4007	BCR	C21-C20-C19	12.15	161.13	123.22
18	B	4006	BCR	C21-C20-C19	12.10	160.99	123.22
18	b	4006	BCR	C21-C20-C19	12.08	160.92	123.22
18	H	4006	BCR	C21-C20-C19	12.07	160.89	123.22
18	L	4019	BCR	C21-C20-C19	12.07	160.88	123.22
18	l	4019	BCR	C21-C20-C19	12.06	160.84	123.22
18	U	4019	BCR	C21-C20-C19	12.05	160.84	123.22
18	a	4007	BCR	C11-C10-C9	12.04	144.50	127.31
18	A	4007	BCR	C11-C10-C9	12.03	144.47	127.31
18	G	4007	BCR	C11-C10-C9	12.01	144.44	127.31
18	l	4022	BCR	C16-C15-C14	12.00	148.06	123.47
18	U	4022	BCR	C16-C15-C14	12.00	148.05	123.47
18	L	4022	BCR	C16-C15-C14	11.98	148.02	123.47
18	a	4008	BCR	C11-C10-C9	11.97	144.39	127.31
18	G	4008	BCR	C11-C10-C9	11.93	144.34	127.31
18	I	4020	BCR	C16-C15-C14	11.92	147.90	123.47
18	i	4020	BCR	C16-C15-C14	11.92	147.88	123.47
18	A	4003	BCR	C21-C20-C19	11.91	160.38	123.22
18	A	4008	BCR	C11-C10-C9	11.91	144.30	127.31
18	R	4020	BCR	C16-C15-C14	11.90	147.86	123.47
18	a	4003	BCR	C21-C20-C19	11.90	160.35	123.22
18	G	4003	BCR	C21-C20-C19	11.90	160.34	123.22
18	A	4008	BCR	C16-C15-C14	11.86	147.78	123.47
18	G	4008	BCR	C16-C15-C14	11.85	147.75	123.47
18	a	4008	BCR	C16-C15-C14	11.85	147.75	123.47
18	A	4001	BCR	C11-C10-C9	11.72	144.03	127.31
18	a	4001	BCR	C11-C10-C9	11.71	144.03	127.31
18	G	4001	BCR	C11-C10-C9	11.71	144.02	127.31
15	H	1230	F6C	CAA-C2A-C3A	-11.68	106.13	127.88
18	R	4018	BCR	C21-C20-C19	11.67	159.64	123.22
15	b	1230	F6C	CAA-C2A-C3A	-11.67	106.15	127.88
18	i	4018	BCR	C21-C20-C19	11.66	159.60	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	I	4018	BCR	C21-C20-C19	11.65	159.56	123.22
15	B	1230	F6C	CAA-C2A-C3A	-11.64	106.19	127.88
18	B	4005	BCR	C16-C15-C14	11.52	147.06	123.47
18	H	4005	BCR	C16-C15-C14	11.51	147.05	123.47
18	b	4005	BCR	C16-C15-C14	11.50	147.03	123.47
18	B	4010	BCR	C11-C10-C9	11.43	143.63	127.31
18	b	4010	BCR	C11-C10-C9	11.41	143.59	127.31
15	H	1238	F6C	CAA-C2A-C3A	-11.39	106.67	127.88
18	H	4010	BCR	C11-C10-C9	11.38	143.56	127.31
15	b	1238	F6C	CAA-C2A-C3A	-11.38	106.69	127.88
15	B	1238	F6C	CAA-C2A-C3A	-11.36	106.73	127.88
18	B	4013	BCR	C11-C12-C13	11.16	157.76	126.42
18	H	4013	BCR	C11-C12-C13	11.16	157.75	126.42
18	b	4013	BCR	C11-C12-C13	11.15	157.72	126.42
18	H	4014	BCR	C11-C12-C13	11.08	157.56	126.42
18	B	4014	BCR	C11-C12-C13	11.08	157.55	126.42
18	b	4014	BCR	C11-C12-C13	11.08	157.54	126.42
18	A	4008	BCR	C11-C12-C13	11.06	157.49	126.42
18	a	4008	BCR	C11-C12-C13	11.05	157.46	126.42
18	H	4006	BCR	C11-C12-C13	11.04	157.42	126.42
18	G	4008	BCR	C11-C12-C13	11.03	157.41	126.42
18	B	4006	BCR	C11-C12-C13	11.03	157.39	126.42
18	b	4006	BCR	C11-C12-C13	11.02	157.38	126.42
18	H	4014	BCR	C16-C15-C14	11.02	146.04	123.47
18	b	4014	BCR	C16-C15-C14	11.00	146.01	123.47
18	B	4014	BCR	C16-C15-C14	10.98	145.97	123.47
18	B	4005	BCR	C11-C12-C13	10.93	157.12	126.42
18	H	4005	BCR	C11-C12-C13	10.93	157.11	126.42
18	b	4005	BCR	C11-C12-C13	10.92	157.10	126.42
18	G	4011	BCR	C11-C12-C13	10.92	157.08	126.42
18	A	4011	BCR	C11-C12-C13	10.90	157.03	126.42
18	a	4011	BCR	C11-C12-C13	10.88	156.99	126.42
18	i	4020	BCR	C11-C12-C13	10.84	156.87	126.42
18	R	4020	BCR	C11-C12-C13	10.84	156.86	126.42
18	I	4020	BCR	C11-C12-C13	10.82	156.81	126.42
15	B	1207	F6C	CAA-C2A-C3A	-10.71	107.93	127.88
15	H	1207	F6C	CAA-C2A-C3A	-10.71	107.93	127.88
18	H	4009	BCR	C11-C10-C9	10.71	142.59	127.31
18	b	4009	BCR	C11-C10-C9	10.71	142.59	127.31
15	b	1237	F6C	CAA-C2A-C3A	-10.70	107.94	127.88
18	H	4004	BCR	C11-C12-C13	10.70	156.48	126.42
15	H	1237	F6C	CAA-C2A-C3A	-10.70	107.95	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	4009	BCR	C11-C10-C9	10.70	142.58	127.31
15	B	1237	F6C	CAA-C2A-C3A	-10.70	107.96	127.88
18	L	4022	BCR	C11-C12-C13	10.69	156.44	126.42
15	b	1207	F6C	CAA-C2A-C3A	-10.69	107.97	127.88
18	B	4004	BCR	C11-C12-C13	10.68	156.41	126.42
18	b	4004	BCR	C11-C12-C13	10.68	156.41	126.42
18	l	4022	BCR	C11-C12-C13	10.67	156.40	126.42
18	U	4022	BCR	C11-C12-C13	10.67	156.39	126.42
18	a	4007	BCR	C11-C12-C13	10.66	156.37	126.42
18	a	4002	BCR	C11-C12-C13	10.66	156.35	126.42
18	A	4007	BCR	C11-C12-C13	10.65	156.33	126.42
18	G	4007	BCR	C11-C12-C13	10.64	156.30	126.42
18	A	4002	BCR	C11-C12-C13	10.63	156.28	126.42
18	G	4002	BCR	C11-C12-C13	10.63	156.27	126.42
18	A	4001	BCR	C11-C12-C13	10.62	156.25	126.42
18	a	4001	BCR	C11-C12-C13	10.62	156.25	126.42
18	G	4001	BCR	C11-C12-C13	10.61	156.22	126.42
18	i	4018	BCR	C11-C10-C9	10.47	142.26	127.31
18	R	4018	BCR	C11-C10-C9	10.47	142.25	127.31
18	H	4010	BCR	C11-C12-C13	10.44	155.76	126.42
18	B	4010	BCR	C11-C12-C13	10.44	155.75	126.42
18	b	4010	BCR	C11-C12-C13	10.43	155.73	126.42
18	I	4018	BCR	C11-C10-C9	10.42	142.19	127.31
15	G	1121	F6C	CAA-C2A-C3A	-10.36	108.59	127.88
15	A	1121	F6C	CAA-C2A-C3A	-10.36	108.59	127.88
15	a	1121	F6C	CAA-C2A-C3A	-10.35	108.60	127.88
18	H	4016	BCR	C11-C12-C13	10.31	155.38	126.42
18	b	4016	BCR	C11-C12-C13	10.29	155.33	126.42
18	B	4016	BCR	C11-C12-C13	10.29	155.32	126.42
18	A	4003	BCR	C11-C12-C13	10.22	155.13	126.42
18	a	4003	BCR	C11-C12-C13	10.21	155.09	126.42
18	G	4003	BCR	C11-C12-C13	10.20	155.06	126.42
18	L	4019	BCR	C11-C12-C13	10.17	154.98	126.42
18	l	4019	BCR	C11-C12-C13	10.16	154.95	126.42
18	U	4019	BCR	C11-C12-C13	10.15	154.93	126.42
18	V	4021	BCR	C11-C12-C13	9.89	154.20	126.42
18	M	4021	BCR	C11-C12-C13	9.89	154.19	126.42
18	m	4021	BCR	C11-C12-C13	9.87	154.16	126.42
18	R	4018	BCR	C11-C12-C13	9.58	153.32	126.42
18	i	4018	BCR	C11-C12-C13	9.55	153.25	126.42
18	I	4018	BCR	C11-C12-C13	9.55	153.25	126.42
18	H	4009	BCR	C11-C12-C13	9.45	152.96	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	4009	BCR	C11-C12-C13	9.45	152.96	126.42
18	B	4009	BCR	C11-C12-C13	9.44	152.94	126.42
18	B	4017	BCR	C11-C12-C13	9.09	151.96	126.42
18	H	4017	BCR	C11-C12-C13	9.09	151.95	126.42
18	b	4017	BCR	C11-C12-C13	9.08	151.93	126.42
15	B	1238	F6C	CMD-C2D-C1D	8.98	138.71	125.04
15	b	1238	F6C	CMD-C2D-C1D	8.97	138.70	125.04
15	H	1238	F6C	CMD-C2D-C1D	8.96	138.69	125.04
14	a	1135	CLA	CMD-C2D-C1D	8.96	140.51	124.71
14	A	1135	CLA	CMD-C2D-C1D	8.95	140.49	124.71
14	G	1135	CLA	CMD-C2D-C1D	8.94	140.47	124.71
15	B	1207	F6C	C1C-C2C-C3C	-8.91	100.80	107.00
15	b	1207	F6C	C1C-C2C-C3C	-8.90	100.80	107.00
15	H	1207	F6C	C1C-C2C-C3C	-8.86	100.83	107.00
18	H	4013	BCR	C20-C19-C18	8.83	151.22	126.42
18	b	4013	BCR	C20-C19-C18	8.81	151.17	126.42
18	B	4013	BCR	C20-C19-C18	8.81	151.16	126.42
15	G	1121	F6C	CMD-C2D-C1D	8.76	138.38	125.04
15	A	1121	F6C	CMD-C2D-C1D	8.74	138.35	125.04
15	a	1121	F6C	CMD-C2D-C1D	8.73	138.34	125.04
14	G	1013	CLA	C2D-C1D-ND	8.72	116.53	110.10
14	A	1013	CLA	C2D-C1D-ND	8.70	116.52	110.10
14	a	1013	CLA	C2D-C1D-ND	8.69	116.51	110.10
15	B	1207	F6C	CMD-C2D-C1D	8.68	138.26	125.04
15	b	1207	F6C	CMD-C2D-C1D	8.67	138.25	125.04
15	B	1230	F6C	C1D-ND-C4D	-8.66	102.81	106.71
15	H	1207	F6C	CMD-C2D-C1D	8.66	138.23	125.04
15	b	1230	F6C	C1D-ND-C4D	-8.65	102.82	106.71
15	H	1230	F6C	C1D-ND-C4D	-8.58	102.85	106.71
18	I	4020	BCR	C20-C19-C18	8.58	150.51	126.42
15	B	1237	F6C	CMD-C2D-C1D	8.57	138.09	125.04
15	H	1237	F6C	CMD-C2D-C1D	8.57	138.09	125.04
18	R	4020	BCR	C20-C19-C18	8.56	150.48	126.42
15	b	1237	F6C	CMD-C2D-C1D	8.56	138.07	125.04
18	i	4020	BCR	C20-C19-C18	8.55	150.44	126.42
15	G	1121	F6C	C1C-C2C-C3C	-8.51	101.08	107.00
15	A	1121	F6C	C1C-C2C-C3C	-8.49	101.09	107.00
15	a	1121	F6C	C1C-C2C-C3C	-8.48	101.10	107.00
14	B	1227	CLA	CMD-C2D-C1D	8.45	139.61	124.71
15	b	1230	F6C	CMD-C2D-C1D	8.43	137.88	125.04
14	b	1227	CLA	CMD-C2D-C1D	8.43	139.56	124.71
15	H	1230	F6C	CMD-C2D-C1D	8.42	137.87	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1230	F6C	CMD-C2D-C1D	8.42	137.86	125.04
14	H	1227	CLA	CMD-C2D-C1D	8.41	139.54	124.71
14	H	1232	CLA	CMD-C2D-C1D	8.35	139.43	124.71
14	B	1232	CLA	CMD-C2D-C1D	8.35	139.43	124.71
14	b	1232	CLA	CMD-C2D-C1D	8.34	139.41	124.71
14	H	1234	CLA	C2D-C1D-ND	8.32	116.24	110.10
14	H	1209	CLA	CMD-C2D-C1D	8.30	139.35	124.71
14	B	1234	CLA	C2D-C1D-ND	8.30	116.22	110.10
14	a	1130	CLA	CMD-C2D-C1D	8.29	139.32	124.71
18	a	4003	BCR	C20-C19-C18	8.29	149.70	126.42
14	b	1234	CLA	C2D-C1D-ND	8.29	116.21	110.10
14	B	1209	CLA	CMD-C2D-C1D	8.29	139.31	124.71
14	b	1209	CLA	CMD-C2D-C1D	8.28	139.31	124.71
18	G	4003	BCR	C20-C19-C18	8.28	149.67	126.42
14	A	1130	CLA	CMD-C2D-C1D	8.28	139.30	124.71
18	A	4003	BCR	C20-C19-C18	8.28	149.67	126.42
14	G	1130	CLA	CMD-C2D-C1D	8.27	139.29	124.71
14	G	1124	CLA	CMD-C2D-C1D	8.27	139.29	124.71
14	A	1124	CLA	CMD-C2D-C1D	8.27	139.29	124.71
14	A	1132	CLA	CMD-C2D-C1D	8.27	139.28	124.71
14	a	1114	CLA	CMD-C2D-C1D	8.27	139.28	124.71
14	G	1132	CLA	CMD-C2D-C1D	8.26	139.27	124.71
14	A	1114	CLA	CMD-C2D-C1D	8.26	139.26	124.71
14	a	1124	CLA	CMD-C2D-C1D	8.25	139.26	124.71
14	a	1132	CLA	CMD-C2D-C1D	8.25	139.25	124.71
14	B	1223	CLA	CMD-C2D-C1D	8.24	139.24	124.71
14	G	1114	CLA	CMD-C2D-C1D	8.24	139.24	124.71
14	K	1401	CLA	CMD-C2D-C1D	8.24	139.24	124.71
14	H	1223	CLA	CMD-C2D-C1D	8.23	139.22	124.71
14	k	1401	CLA	CMD-C2D-C1D	8.22	139.21	124.71
14	T	1401	CLA	CMD-C2D-C1D	8.22	139.20	124.71
14	b	1223	CLA	CMD-C2D-C1D	8.22	139.20	124.71
14	G	1139	CLA	CMD-C2D-C1D	8.21	139.18	124.71
14	G	1104	CLA	CMD-C2D-C1D	8.20	139.16	124.71
14	H	1228	CLA	CMD-C2D-C1D	8.20	139.16	124.71
14	A	1139	CLA	CMD-C2D-C1D	8.20	139.16	124.71
14	A	1131	CLA	CMD-C2D-C1D	8.19	139.16	124.71
14	H	1213	CLA	CMD-C2D-C1D	8.19	139.15	124.71
14	a	1139	CLA	CMD-C2D-C1D	8.19	139.15	124.71
14	A	1103	CLA	CMD-C2D-C1D	8.19	139.15	124.71
14	a	1116	CLA	CMD-C2D-C1D	8.19	139.15	124.71
14	a	1103	CLA	CMD-C2D-C1D	8.19	139.14	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1213	CLA	CMD-C2D-C1D	8.19	139.14	124.71
14	A	1116	CLA	CMD-C2D-C1D	8.19	139.14	124.71
14	B	1228	CLA	CMD-C2D-C1D	8.18	139.14	124.71
14	H	1203	CLA	CMD-C2D-C1D	8.18	139.12	124.71
14	G	1103	CLA	CMD-C2D-C1D	8.18	139.12	124.71
14	a	1104	CLA	CMD-C2D-C1D	8.17	139.12	124.71
14	A	1104	CLA	CMD-C2D-C1D	8.17	139.12	124.71
14	G	1131	CLA	CMD-C2D-C1D	8.17	139.11	124.71
14	b	1213	CLA	CMD-C2D-C1D	8.17	139.11	124.71
14	b	1228	CLA	CMD-C2D-C1D	8.17	139.11	124.71
14	A	1105	CLA	CMD-C2D-C1D	8.17	139.10	124.71
14	A	1109	CLA	CMD-C2D-C1D	8.16	139.10	124.71
14	A	1115	CLA	CMD-C2D-C1D	8.16	139.10	124.71
14	G	1115	CLA	CMD-C2D-C1D	8.16	139.10	124.71
14	a	1131	CLA	CMD-C2D-C1D	8.16	139.09	124.71
14	a	1105	CLA	CMD-C2D-C1D	8.16	139.09	124.71
14	b	1203	CLA	CMD-C2D-C1D	8.16	139.09	124.71
18	H	4006	BCR	C20-C19-C18	8.15	149.32	126.42
14	G	1105	CLA	CMD-C2D-C1D	8.15	139.08	124.71
14	B	1211	CLA	CMD-C2D-C1D	8.14	139.07	124.71
14	G	1109	CLA	CMD-C2D-C1D	8.14	139.06	124.71
14	a	1109	CLA	CMD-C2D-C1D	8.14	139.06	124.71
14	b	1211	CLA	CMD-C2D-C1D	8.14	139.06	124.71
18	B	4006	BCR	C20-C19-C18	8.14	149.28	126.42
18	b	4006	BCR	C20-C19-C18	8.13	149.27	126.42
14	B	1203	CLA	CMD-C2D-C1D	8.13	139.05	124.71
14	H	1211	CLA	CMD-C2D-C1D	8.13	139.04	124.71
14	a	1115	CLA	CMD-C2D-C1D	8.12	139.03	124.71
14	G	1116	CLA	CMD-C2D-C1D	8.12	139.03	124.71
14	B	1201	CLA	CMD-C2D-C1D	8.11	139.01	124.71
14	A	1133	CLA	CMD-C2D-C1D	8.10	138.99	124.71
14	H	1201	CLA	CMD-C2D-C1D	8.10	138.99	124.71
14	a	1133	CLA	CMD-C2D-C1D	8.10	138.98	124.71
14	b	1201	CLA	CMD-C2D-C1D	8.09	138.97	124.71
14	G	1133	CLA	CMD-C2D-C1D	8.09	138.96	124.71
14	B	1229	CLA	CMD-C2D-C1D	8.08	138.96	124.71
14	a	1134	CLA	CMD-C2D-C1D	8.08	138.96	124.71
14	U	1502	CLA	CMD-C2D-C1D	8.08	138.96	124.71
14	A	1134	CLA	CMD-C2D-C1D	8.08	138.95	124.71
14	A	1101	CLA	CMD-C2D-C1D	8.08	138.95	124.71
14	G	1101	CLA	CMD-C2D-C1D	8.07	138.94	124.71
14	G	1120	CLA	C2D-C1D-ND	8.07	116.05	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1101	CLA	CMD-C2D-C1D	8.07	138.94	124.71
14	G	1134	CLA	CMD-C2D-C1D	8.07	138.93	124.71
15	H	1237	F6C	C1D-ND-C4D	-8.06	103.08	106.71
14	H	1229	CLA	CMD-C2D-C1D	8.06	138.92	124.71
14	b	1229	CLA	CMD-C2D-C1D	8.06	138.92	124.71
14	b	1210	CLA	CMD-C2D-C1D	8.05	138.91	124.71
14	L	1502	CLA	CMD-C2D-C1D	8.05	138.91	124.71
14	B	1210	CLA	CMD-C2D-C1D	8.05	138.91	124.71
14	a	1120	CLA	C2D-C1D-ND	8.05	116.04	110.10
14	a	1137	CLA	CMD-C2D-C1D	8.05	138.90	124.71
14	H	1210	CLA	CMD-C2D-C1D	8.05	138.90	124.71
14	l	1502	CLA	CMD-C2D-C1D	8.04	138.88	124.71
14	A	1104	CLA	C2D-C1D-ND	8.04	116.03	110.10
14	G	1104	CLA	C2D-C1D-ND	8.03	116.02	110.10
14	G	1137	CLA	CMD-C2D-C1D	8.03	138.86	124.71
14	G	1111	CLA	CMD-C2D-C1D	8.02	138.84	124.71
14	A	1120	CLA	C2D-C1D-ND	8.01	116.01	110.10
14	G	1112	CLA	CMD-C2D-C1D	8.01	138.82	124.71
14	a	1112	CLA	CMD-C2D-C1D	8.01	138.82	124.71
14	A	1137	CLA	CMD-C2D-C1D	8.00	138.82	124.71
14	A	1136	CLA	CMD-C2D-C1D	8.00	138.81	124.71
14	A	1112	CLA	CMD-C2D-C1D	8.00	138.81	124.71
14	a	1104	CLA	C2D-C1D-ND	7.99	115.99	110.10
18	G	4002	BCR	C11-C10-C9	7.99	138.72	127.31
14	a	1111	CLA	CMD-C2D-C1D	7.99	138.80	124.71
14	B	1218	CLA	C2D-C1D-ND	7.99	115.99	110.10
14	H	1218	CLA	C2D-C1D-ND	7.98	115.99	110.10
14	G	1110	CLA	CMD-C2D-C1D	7.98	138.78	124.71
14	a	1122	CLA	CMD-C2D-C1D	7.98	138.77	124.71
14	A	1111	CLA	CMD-C2D-C1D	7.97	138.76	124.71
18	A	4002	BCR	C11-C10-C9	7.97	138.69	127.31
14	A	1122	CLA	CMD-C2D-C1D	7.97	138.76	124.71
18	a	4002	BCR	C11-C10-C9	7.97	138.68	127.31
14	G	1122	CLA	CMD-C2D-C1D	7.97	138.75	124.71
14	a	1110	CLA	CMD-C2D-C1D	7.97	138.75	124.71
14	a	1136	CLA	CMD-C2D-C1D	7.97	138.75	124.71
14	B	1233	CLA	CMD-C2D-C1D	7.96	138.75	124.71
14	A	1110	CLA	CMD-C2D-C1D	7.96	138.74	124.71
14	H	1233	CLA	CMD-C2D-C1D	7.96	138.74	124.71
18	A	4007	BCR	C20-C19-C18	7.95	148.75	126.42
14	G	1136	CLA	CMD-C2D-C1D	7.95	138.73	124.71
14	b	1212	CLA	C2D-C1D-ND	7.95	115.96	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1233	CLA	CMD-C2D-C1D	7.95	138.72	124.71
18	G	4007	BCR	C20-C19-C18	7.95	148.74	126.42
18	L	4019	BCR	C20-C19-C18	7.95	148.74	126.42
15	B	1237	F6C	C1D-ND-C4D	-7.95	103.13	106.71
14	b	1218	CLA	C2D-C1D-ND	7.95	115.96	110.10
18	a	4007	BCR	C20-C19-C18	7.94	148.72	126.42
14	B	1214	CLA	CMD-C2D-C1D	7.94	138.70	124.71
18	U	4019	BCR	C20-C19-C18	7.93	148.71	126.42
18	l	4019	BCR	C20-C19-C18	7.93	148.69	126.42
14	H	1214	CLA	CMD-C2D-C1D	7.93	138.68	124.71
14	B	1202	CLA	CMD-C2D-C1D	7.93	138.68	124.71
18	H	4017	BCR	C20-C19-C18	7.92	148.68	126.42
18	l	4019	BCR	C24-C23-C22	-7.92	114.26	126.23
14	b	1202	CLA	CMD-C2D-C1D	7.92	138.67	124.71
14	b	1214	CLA	CMD-C2D-C1D	7.92	138.67	124.71
18	b	4017	BCR	C20-C19-C18	7.92	148.66	126.42
14	H	1202	CLA	CMD-C2D-C1D	7.92	138.67	124.71
18	B	4017	BCR	C20-C19-C18	7.92	148.65	126.42
18	R	4018	BCR	C20-C19-C18	7.91	148.65	126.42
18	U	4019	BCR	C24-C23-C22	-7.91	114.28	126.23
14	A	1113	CLA	CMD-C2D-C1D	7.90	138.64	124.71
14	a	1113	CLA	CMD-C2D-C1D	7.90	138.63	124.71
15	H	1238	F6C	C1C-C2C-C3C	-7.90	101.50	107.00
14	G	1113	CLA	CMD-C2D-C1D	7.90	138.63	124.71
18	I	4018	BCR	C20-C19-C18	7.90	148.60	126.42
15	B	1238	F6C	C1C-C2C-C3C	-7.90	101.50	107.00
18	L	4019	BCR	C24-C23-C22	-7.90	114.31	126.23
18	i	4018	BCR	C20-C19-C18	7.89	148.58	126.42
14	G	1117	CLA	CMD-C2D-C1D	7.88	138.60	124.71
15	b	1237	F6C	C1D-ND-C4D	-7.87	103.17	106.71
14	A	1117	CLA	CMD-C2D-C1D	7.87	138.59	124.71
14	a	1108	CLA	CMD-C2D-C1D	7.87	138.58	124.71
14	H	1212	CLA	C2D-C1D-ND	7.87	115.90	110.10
15	B	1237	F6C	C1C-C2C-C3C	-7.87	101.52	107.00
14	b	1217	CLA	CMD-C2D-C1D	7.87	138.58	124.71
14	G	1129	CLA	CMD-C2D-C1D	7.87	138.57	124.71
14	B	1217	CLA	CMD-C2D-C1D	7.86	138.57	124.71
14	a	1129	CLA	CMD-C2D-C1D	7.86	138.57	124.71
14	a	1117	CLA	CMD-C2D-C1D	7.86	138.56	124.71
14	B	1212	CLA	C2D-C1D-ND	7.86	115.89	110.10
14	G	1108	CLA	CMD-C2D-C1D	7.85	138.55	124.71
14	H	1217	CLA	CMD-C2D-C1D	7.85	138.55	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1108	CLA	CMD-C2D-C1D	7.85	138.55	124.71
14	A	1129	CLA	CMD-C2D-C1D	7.85	138.54	124.71
15	b	1238	F6C	C1C-C2C-C3C	-7.85	101.54	107.00
15	b	1238	F6C	C1D-ND-C4D	-7.83	103.19	106.71
14	H	1219	CLA	CMD-C2D-C1D	7.83	138.51	124.71
14	a	1106	CLA	CMD-C2D-C1D	7.82	138.50	124.71
14	b	1219	CLA	CMD-C2D-C1D	7.82	138.49	124.71
14	H	1239	CLA	CMD-C2D-C1D	7.82	138.49	124.71
14	b	1239	CLA	CMD-C2D-C1D	7.82	138.49	124.71
14	H	1239	CLA	C2C-C1C-NC	7.82	117.29	109.97
15	B	1238	F6C	C1D-ND-C4D	-7.81	103.19	106.71
14	b	1239	CLA	C2C-C1C-NC	7.81	117.29	109.97
14	G	1106	CLA	CMD-C2D-C1D	7.81	138.48	124.71
14	B	1219	CLA	CMD-C2D-C1D	7.81	138.48	124.71
15	H	1238	F6C	C1D-ND-C4D	-7.81	103.20	106.71
14	A	1106	CLA	CMD-C2D-C1D	7.80	138.47	124.71
14	B	1239	CLA	C2C-C1C-NC	7.80	117.28	109.97
15	H	1237	F6C	C1C-C2C-C3C	-7.80	101.57	107.00
14	B	1239	CLA	CMD-C2D-C1D	7.79	138.44	124.71
15	b	1237	F6C	C1C-C2C-C3C	-7.78	101.58	107.00
14	B	1236	CLA	CMD-C2D-C1D	7.78	138.42	124.71
14	H	1236	CLA	CMD-C2D-C1D	7.77	138.41	124.71
14	b	1236	CLA	CMD-C2D-C1D	7.76	138.39	124.71
14	A	1102	CLA	CMD-C2D-C1D	7.76	138.39	124.71
14	a	1102	CLA	CMD-C2D-C1D	7.76	138.38	124.71
14	G	1102	CLA	CMD-C2D-C1D	7.75	138.37	124.71
14	a	1119	CLA	CMD-C2D-C1D	7.73	138.34	124.71
14	H	1023	CLA	C2D-C1D-ND	7.72	115.80	110.10
14	b	1023	CLA	C2D-C1D-ND	7.72	115.79	110.10
14	A	1119	CLA	CMD-C2D-C1D	7.71	138.31	124.71
14	A	1137	CLA	O2D-CGD-CBD	7.71	124.97	111.27
14	G	1119	CLA	CMD-C2D-C1D	7.70	138.28	124.71
14	G	1137	CLA	O2D-CGD-CBD	7.70	124.95	111.27
14	X	1701	CLA	CMD-C2D-C1D	7.70	138.28	124.71
14	b	1216	CLA	CMD-C2D-C1D	7.69	138.27	124.71
14	a	1137	CLA	O2D-CGD-CBD	7.69	124.93	111.27
14	a	1125	CLA	C2D-C1D-ND	7.68	115.77	110.10
14	x	1701	CLA	CMD-C2D-C1D	7.68	138.25	124.71
14	H	1203	CLA	C2D-C1D-ND	7.68	115.76	110.10
14	B	1023	CLA	C2D-C1D-ND	7.67	115.76	110.10
14	W	1701	CLA	CMD-C2D-C1D	7.67	138.24	124.71
14	b	1203	CLA	C2D-C1D-ND	7.67	115.76	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1216	CLA	CMD-C2D-C1D	7.67	138.23	124.71
14	A	1125	CLA	C2D-C1D-ND	7.67	115.75	110.10
14	G	1126	CLA	CMD-C2D-C1D	7.66	138.22	124.71
14	G	1125	CLA	C2D-C1D-ND	7.66	115.75	110.10
14	A	1126	CLA	CMD-C2D-C1D	7.66	138.21	124.71
14	b	1208	CLA	CMD-C2D-C1D	7.65	138.20	124.71
14	B	1216	CLA	CMD-C2D-C1D	7.65	138.20	124.71
14	B	1208	CLA	CMD-C2D-C1D	7.64	138.18	124.71
18	H	4016	BCR	C20-C19-C18	7.64	147.88	126.42
18	B	4016	BCR	C20-C19-C18	7.64	147.87	126.42
14	H	1208	CLA	CMD-C2D-C1D	7.63	138.16	124.71
18	b	4016	BCR	C20-C19-C18	7.63	147.85	126.42
14	B	1203	CLA	C2D-C1D-ND	7.62	115.72	110.10
14	a	1126	CLA	CMD-C2D-C1D	7.62	138.14	124.71
14	B	1234	CLA	CMD-C2D-C1D	7.62	138.14	124.71
14	A	1118	CLA	CMD-C2D-C1D	7.61	138.12	124.71
14	H	1234	CLA	CMD-C2D-C1D	7.61	138.12	124.71
14	a	1118	CLA	CMD-C2D-C1D	7.61	138.12	124.71
14	a	1140	CLA	CMD-C2D-C1D	7.61	138.12	124.71
14	A	1140	CLA	CMD-C2D-C1D	7.60	138.11	124.71
14	G	1118	CLA	CMD-C2D-C1D	7.60	138.11	124.71
14	G	1140	CLA	CMD-C2D-C1D	7.59	138.10	124.71
14	b	1234	CLA	CMD-C2D-C1D	7.59	138.09	124.71
14	b	1220	CLA	CMD-C2D-C1D	7.59	138.08	124.71
14	H	1231	CLA	CMD-C2D-C1D	7.58	138.07	124.71
14	B	1023	CLA	C4A-NA-C1A	7.58	110.11	106.71
14	B	1231	CLA	CMD-C2D-C1D	7.58	138.07	124.71
14	H	1220	CLA	CMD-C2D-C1D	7.58	138.06	124.71
14	U	1503	CLA	CMD-C2D-C1D	7.57	138.05	124.71
14	B	1220	CLA	CMD-C2D-C1D	7.57	138.05	124.71
14	L	1503	CLA	CMD-C2D-C1D	7.56	138.04	124.71
14	b	1231	CLA	CMD-C2D-C1D	7.56	138.04	124.71
14	H	1211	CLA	O2A-C1-C2	7.55	128.49	108.64
14	b	1211	CLA	O2A-C1-C2	7.55	128.49	108.64
14	l	1503	CLA	CMD-C2D-C1D	7.55	138.03	124.71
14	B	1211	CLA	O2A-C1-C2	7.55	128.49	108.64
14	a	1107	CLA	CMD-C2D-C1D	7.55	138.02	124.71
14	G	1107	CLA	CMD-C2D-C1D	7.55	138.02	124.71
14	B	1215	CLA	CMD-C2D-C1D	7.54	138.01	124.71
14	H	1215	CLA	CMD-C2D-C1D	7.54	138.01	124.71
14	b	1215	CLA	CMD-C2D-C1D	7.54	138.00	124.71
14	A	1107	CLA	CMD-C2D-C1D	7.54	138.00	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1235	CLA	CMD-C2D-C1D	7.53	137.99	124.71
14	B	1235	CLA	CMD-C2D-C1D	7.53	137.98	124.71
14	H	1023	CLA	C4A-NA-C1A	7.52	110.09	106.71
14	b	1235	CLA	CMD-C2D-C1D	7.52	137.97	124.71
18	m	4021	BCR	C20-C19-C18	7.52	147.55	126.42
14	A	1138	CLA	CMD-C2D-C1D	7.52	137.96	124.71
14	G	1138	CLA	CMD-C2D-C1D	7.51	137.95	124.71
18	V	4021	BCR	C20-C19-C18	7.51	147.51	126.42
18	M	4021	BCR	C20-C19-C18	7.50	147.49	126.42
14	A	1012	CLA	CMD-C2D-C1D	7.50	137.93	124.71
14	a	1138	CLA	CMD-C2D-C1D	7.50	137.93	124.71
18	l	4022	BCR	C7-C8-C9	-7.48	114.93	126.23
14	G	1012	CLA	CMD-C2D-C1D	7.47	137.89	124.71
14	A	1132	CLA	O2D-CGD-CBD	7.47	124.54	111.27
15	G	1121	F6C	C1D-ND-C4D	-7.46	103.35	106.71
14	a	1012	CLA	CMD-C2D-C1D	7.46	137.87	124.71
18	U	4022	BCR	C7-C8-C9	-7.46	114.97	126.23
18	H	4005	BCR	C20-C19-C18	7.44	147.32	126.42
14	b	1023	CLA	C4A-NA-C1A	7.44	110.05	106.71
14	H	1204	CLA	CMD-C2D-C1D	7.44	137.82	124.71
14	b	1204	CLA	CMD-C2D-C1D	7.43	137.82	124.71
18	b	4005	BCR	C20-C19-C18	7.43	147.30	126.42
18	L	4022	BCR	C7-C8-C9	-7.43	115.00	126.23
14	a	1132	CLA	O2D-CGD-CBD	7.43	124.47	111.27
14	G	1132	CLA	O2D-CGD-CBD	7.43	124.47	111.27
18	B	4005	BCR	C20-C19-C18	7.42	147.26	126.42
14	A	1119	CLA	C2C-C1C-NC	7.42	116.92	109.97
14	a	1119	CLA	C2C-C1C-NC	7.41	116.92	109.97
14	G	1106	CLA	C2D-C1D-ND	7.41	115.57	110.10
14	H	1210	CLA	O2D-CGD-CBD	7.41	124.44	111.27
14	A	1106	CLA	C2D-C1D-ND	7.41	115.56	110.10
14	B	1210	CLA	O2D-CGD-CBD	7.41	124.43	111.27
14	B	1204	CLA	CMD-C2D-C1D	7.39	137.75	124.71
15	a	1121	F6C	C1D-ND-C4D	-7.39	103.38	106.71
14	a	1106	CLA	C2D-C1D-ND	7.39	115.55	110.10
14	b	1210	CLA	O2D-CGD-CBD	7.39	124.40	111.27
14	G	1119	CLA	C2C-C1C-NC	7.37	116.88	109.97
15	A	1121	F6C	C1D-ND-C4D	-7.37	103.39	106.71
18	G	4001	BCR	C20-C19-C18	7.36	147.09	126.42
18	A	4001	BCR	C20-C19-C18	7.36	147.08	126.42
18	a	4001	BCR	C20-C19-C18	7.35	147.06	126.42
15	G	1121	F6C	CAA-C2A-C1A	-7.34	107.89	128.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1202	CLA	C2D-C1D-ND	7.34	115.52	110.10
15	a	1121	F6C	CAA-C2A-C1A	-7.33	107.93	128.11
15	A	1121	F6C	CAA-C2A-C1A	-7.33	107.94	128.11
14	B	1202	CLA	C2D-C1D-ND	7.31	115.49	110.10
14	H	1202	CLA	C2D-C1D-ND	7.31	115.49	110.10
14	U	1502	CLA	C2D-C1D-ND	7.30	115.48	110.10
14	B	1021	CLA	C2D-C1D-ND	7.30	115.48	110.10
14	H	1021	CLA	C2D-C1D-ND	7.29	115.48	110.10
14	b	1021	CLA	C2D-C1D-ND	7.28	115.47	110.10
14	L	1502	CLA	C2D-C1D-ND	7.28	115.47	110.10
14	a	1127	CLA	C2D-C1D-ND	7.27	115.46	110.10
14	A	1127	CLA	C2D-C1D-ND	7.27	115.46	110.10
14	G	1127	CLA	C2D-C1D-ND	7.25	115.45	110.10
14	l	1502	CLA	C2D-C1D-ND	7.25	115.45	110.10
14	A	1128	CLA	C2C-C1C-NC	7.25	116.76	109.97
14	H	1223	CLA	C2D-C1D-ND	7.24	115.44	110.10
14	a	1128	CLA	C2C-C1C-NC	7.23	116.74	109.97
14	G	1120	CLA	CMD-C2D-C1D	7.22	137.44	124.71
14	G	1123	CLA	CMD-C2D-C1D	7.22	137.44	124.71
14	a	1012	CLA	C2C-C1C-NC	7.21	116.73	109.97
14	a	1123	CLA	CMD-C2D-C1D	7.21	137.42	124.71
14	A	1123	CLA	CMD-C2D-C1D	7.21	137.42	124.71
14	G	1012	CLA	C2C-C1C-NC	7.20	116.71	109.97
14	a	1114	CLA	C2C-C1C-NC	7.20	116.71	109.97
14	A	1114	CLA	C2C-C1C-NC	7.20	116.71	109.97
14	G	1128	CLA	C2C-C1C-NC	7.19	116.71	109.97
14	a	1120	CLA	CMD-C2D-C1D	7.19	137.38	124.71
14	G	1114	CLA	C2C-C1C-NC	7.18	116.69	109.97
14	B	1223	CLA	C2D-C1D-ND	7.17	115.39	110.10
14	A	1120	CLA	CMD-C2D-C1D	7.17	137.35	124.71
14	L	1501	CLA	C2D-C1D-ND	7.17	115.39	110.10
14	A	1012	CLA	C2C-C1C-NC	7.16	116.68	109.97
14	H	1022	CLA	C2D-C1D-ND	7.16	115.38	110.10
14	H	1236	CLA	C2D-C1D-ND	7.16	115.38	110.10
14	B	1236	CLA	C2D-C1D-ND	7.16	115.38	110.10
14	a	1117	CLA	O2D-CGD-CBD	7.13	123.93	111.27
14	b	1223	CLA	C2D-C1D-ND	7.12	115.35	110.10
14	G	1118	CLA	C2C-C1C-NC	7.12	116.64	109.97
14	A	1118	CLA	C2C-C1C-NC	7.12	116.64	109.97
14	A	1117	CLA	O2D-CGD-CBD	7.12	123.92	111.27
14	l	1501	CLA	C2D-C1D-ND	7.12	115.35	110.10
14	G	1124	CLA	C2D-C1D-ND	7.11	115.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1022	CLA	C2D-C1D-ND	7.11	115.34	110.10
14	G	1117	CLA	O2D-CGD-CBD	7.10	123.89	111.27
14	A	1124	CLA	C2D-C1D-ND	7.10	115.33	110.10
14	a	1118	CLA	C2C-C1C-NC	7.10	116.62	109.97
14	a	1133	CLA	C2C-C1C-NC	7.10	116.62	109.97
14	G	1135	CLA	C2C-C1C-NC	7.10	116.62	109.97
14	L	1503	CLA	C2D-C1D-ND	7.09	115.33	110.10
14	a	1135	CLA	C2C-C1C-NC	7.09	116.61	109.97
14	A	1135	CLA	C2C-C1C-NC	7.09	116.61	109.97
14	U	1501	CLA	C2D-C1D-ND	7.09	115.33	110.10
14	b	1222	CLA	C2D-C1D-ND	7.08	115.33	110.10
14	X	1701	CLA	C2D-C1D-ND	7.08	115.32	110.10
14	U	1503	CLA	C2D-C1D-ND	7.08	115.32	110.10
14	B	1224	CLA	CMD-C2D-C1D	7.08	137.19	124.71
14	b	1224	CLA	CMD-C2D-C1D	7.07	137.18	124.71
14	G	1133	CLA	C2C-C1C-NC	7.07	116.59	109.97
14	A	1119	CLA	O2A-C1-C2	7.07	127.21	108.64
14	a	1119	CLA	O2A-C1-C2	7.07	127.21	108.64
18	B	4009	BCR	C20-C19-C18	7.06	146.26	126.42
14	b	1236	CLA	C2D-C1D-ND	7.06	115.31	110.10
18	H	4009	BCR	C20-C19-C18	7.06	146.24	126.42
14	A	1133	CLA	C2C-C1C-NC	7.06	116.58	109.97
14	G	1119	CLA	O2A-C1-C2	7.06	127.18	108.64
14	H	1224	CLA	CMD-C2D-C1D	7.06	137.15	124.71
14	H	1205	CLA	C2D-C1D-ND	7.05	115.30	110.10
14	A	1115	CLA	C2D-C1D-ND	7.05	115.30	110.10
14	G	1115	CLA	C2D-C1D-ND	7.05	115.30	110.10
14	b	1220	CLA	C2D-C1D-ND	7.05	115.30	110.10
14	b	1220	CLA	C2C-C1C-NC	7.05	116.58	109.97
14	H	1206	CLA	C2C-C1C-NC	7.05	116.58	109.97
14	G	1137	CLA	C2C-C1C-NC	7.05	116.58	109.97
14	H	1220	CLA	C2D-C1D-ND	7.05	115.30	110.10
14	B	1205	CLA	C2D-C1D-ND	7.05	115.30	110.10
14	H	1220	CLA	C2C-C1C-NC	7.05	116.57	109.97
18	b	4009	BCR	C20-C19-C18	7.04	146.19	126.42
14	B	1220	CLA	C2D-C1D-ND	7.04	115.29	110.10
14	a	1101	CLA	C2D-C1D-ND	7.04	115.29	110.10
14	b	1022	CLA	C2D-C1D-ND	7.04	115.29	110.10
15	b	1207	F6C	C3A-C4A-NA	7.04	115.29	110.10
14	B	1226	CLA	C2C-C1C-NC	7.03	116.56	109.97
14	W	1701	CLA	C2D-C1D-ND	7.03	115.28	110.10
14	B	1206	CLA	C2C-C1C-NC	7.02	116.55	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1101	CLA	C2D-C1D-ND	7.02	115.28	110.10
14	A	1125	CLA	CMD-C2D-C1D	7.02	137.09	124.71
14	b	1206	CLA	C2C-C1C-NC	7.02	116.54	109.97
14	b	1222	CLA	CMD-C2D-C1D	7.01	137.07	124.71
14	b	1226	CLA	C2C-C1C-NC	7.01	116.54	109.97
14	x	1701	CLA	C2D-C1D-ND	7.01	115.27	110.10
14	B	1217	CLA	C2D-C1D-ND	7.01	115.27	110.10
14	H	1222	CLA	CMD-C2D-C1D	7.01	137.07	124.71
14	H	1226	CLA	C2C-C1C-NC	7.01	116.54	109.97
14	B	1222	CLA	CMD-C2D-C1D	7.00	137.06	124.71
14	a	1125	CLA	CMD-C2D-C1D	7.00	137.06	124.71
14	a	1115	CLA	C2D-C1D-ND	7.00	115.26	110.10
14	a	1124	CLA	C2D-C1D-ND	7.00	115.26	110.10
15	B	1207	F6C	C3A-C4A-NA	7.00	115.26	110.10
14	B	1229	CLA	C2D-C1D-ND	7.00	115.26	110.10
14	b	1205	CLA	C2D-C1D-ND	6.99	115.26	110.10
14	G	1125	CLA	CMD-C2D-C1D	6.99	137.04	124.71
14	B	1222	CLA	C2D-C1D-ND	6.99	115.25	110.10
14	a	1137	CLA	C2C-C1C-NC	6.99	116.52	109.97
14	H	1222	CLA	C2D-C1D-ND	6.98	115.25	110.10
14	A	1101	CLA	C2D-C1D-ND	6.98	115.25	110.10
15	H	1207	F6C	C3A-C4A-NA	6.97	115.24	110.10
14	A	1137	CLA	C2C-C1C-NC	6.97	116.50	109.97
14	A	1013	CLA	C4A-NA-C1A	6.97	109.84	106.71
14	G	1110	CLA	C2D-C1D-ND	6.97	115.24	110.10
14	b	1214	CLA	C2C-C1C-NC	6.97	116.50	109.97
14	B	1220	CLA	C2C-C1C-NC	6.97	116.50	109.97
14	B	1226	CLA	CMD-C2D-C1D	6.96	136.97	124.71
14	a	1113	CLA	C2D-C1D-ND	6.95	115.23	110.10
14	l	1503	CLA	C2D-C1D-ND	6.95	115.23	110.10
14	b	1226	CLA	CMD-C2D-C1D	6.95	136.97	124.71
14	A	1110	CLA	C2D-C1D-ND	6.95	115.23	110.10
14	H	1226	CLA	CMD-C2D-C1D	6.95	136.96	124.71
14	B	1224	CLA	C2D-C1D-ND	6.95	115.23	110.10
14	H	1229	CLA	C2D-C1D-ND	6.95	115.22	110.10
14	H	1206	CLA	CMD-C2D-C1D	6.95	136.96	124.71
14	b	1229	CLA	C2D-C1D-ND	6.95	115.22	110.10
14	a	1013	CLA	C4A-NA-C1A	6.94	109.83	106.71
14	G	1123	CLA	C2C-C1C-NC	6.94	116.47	109.97
14	A	1123	CLA	C2C-C1C-NC	6.94	116.47	109.97
14	a	1110	CLA	C2D-C1D-ND	6.94	115.22	110.10
14	b	1206	CLA	CMD-C2D-C1D	6.93	136.93	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1214	CLA	C2C-C1C-NC	6.93	116.46	109.97
14	A	1113	CLA	C2D-C1D-ND	6.92	115.21	110.10
14	H	1217	CLA	C2D-C1D-ND	6.92	115.20	110.10
14	G	1113	CLA	C2D-C1D-ND	6.92	115.20	110.10
14	B	1206	CLA	CMD-C2D-C1D	6.92	136.90	124.71
14	b	1217	CLA	C2D-C1D-ND	6.92	115.20	110.10
14	b	1224	CLA	C2D-C1D-ND	6.92	115.20	110.10
18	b	4017	BCR	C7-C8-C9	-6.90	115.81	126.23
14	G	1111	CLA	C2D-C1D-ND	6.89	115.19	110.10
14	b	1021	CLA	C4A-NA-C1A	6.89	109.80	106.71
14	G	1013	CLA	C4A-NA-C1A	6.89	109.80	106.71
14	a	1123	CLA	C2C-C1C-NC	6.89	116.42	109.97
18	H	4017	BCR	C7-C8-C9	-6.88	115.84	126.23
14	B	1021	CLA	C4A-NA-C1A	6.88	109.80	106.71
13	G	1011	CL0	C2D-C1D-ND	6.87	115.17	110.10
14	B	1214	CLA	C2C-C1C-NC	6.87	116.41	109.97
13	a	1011	CL0	C2D-C1D-ND	6.87	115.17	110.10
14	H	1022	CLA	CMD-C2D-C1D	6.87	136.81	124.71
14	B	1022	CLA	CMD-C2D-C1D	6.86	136.80	124.71
14	l	1501	CLA	C2C-C1C-NC	6.85	116.39	109.97
14	b	1022	CLA	CMD-C2D-C1D	6.85	136.78	124.71
18	B	4017	BCR	C7-C8-C9	-6.84	115.89	126.23
14	a	1111	CLA	C2D-C1D-ND	6.84	115.15	110.10
14	H	1224	CLA	C2D-C1D-ND	6.84	115.15	110.10
14	a	1117	CLA	C2C-C1C-NC	6.84	116.38	109.97
14	H	1231	CLA	C2D-C1D-ND	6.84	115.14	110.10
14	B	1205	CLA	C4A-NA-C1A	6.84	109.78	106.71
13	A	1011	CL0	C2D-C1D-ND	6.84	115.14	110.10
14	A	1127	CLA	C2C-C1C-NC	6.83	116.37	109.97
14	K	1401	CLA	C2C-C1C-NC	6.83	116.37	109.97
14	b	1231	CLA	C2D-C1D-ND	6.83	115.14	110.10
14	A	1117	CLA	C2C-C1C-NC	6.83	116.37	109.97
14	b	1217	CLA	C2C-C1C-NC	6.82	116.36	109.97
14	L	1501	CLA	C2C-C1C-NC	6.82	116.36	109.97
14	b	1212	CLA	CMD-C2D-C1D	6.82	136.74	124.71
14	B	1227	CLA	C2C-C1C-NC	6.82	116.36	109.97
14	B	1231	CLA	C2D-C1D-ND	6.82	115.13	110.10
14	A	1111	CLA	C2D-C1D-ND	6.82	115.13	110.10
14	B	1233	CLA	C2C-C1C-NC	6.82	116.36	109.97
14	b	1205	CLA	C4A-NA-C1A	6.81	109.77	106.71
14	H	1228	CLA	C2D-C1D-ND	6.81	115.12	110.10
14	H	1233	CLA	C2C-C1C-NC	6.81	116.35	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	U	1501	CLA	C2C-C1C-NC	6.81	116.35	109.97
14	a	1127	CLA	C2C-C1C-NC	6.81	116.35	109.97
14	T	1401	CLA	C2C-C1C-NC	6.81	116.35	109.97
15	H	1207	F6C	O2D-CGD-CBD	6.80	123.35	111.27
14	B	1217	CLA	C2C-C1C-NC	6.80	116.34	109.97
14	A	1140	CLA	C2D-C1D-ND	6.79	115.11	110.10
14	b	1233	CLA	C2C-C1C-NC	6.79	116.34	109.97
13	a	1011	CL0	C2C-C1C-NC	6.79	116.33	109.97
14	G	1117	CLA	C2C-C1C-NC	6.79	116.33	109.97
14	H	1205	CLA	C4A-NA-C1A	6.79	109.76	106.71
15	b	1230	F6C	O2D-CGD-CBD	6.79	123.33	111.27
15	b	1207	F6C	O2D-CGD-CBD	6.79	123.33	111.27
15	H	1230	F6C	O2D-CGD-CBD	6.79	123.33	111.27
14	H	1227	CLA	C2C-C1C-NC	6.79	116.33	109.97
15	B	1230	F6C	O2D-CGD-CBD	6.79	123.33	111.27
15	B	1207	F6C	O2D-CGD-CBD	6.78	123.32	111.27
14	b	1227	CLA	C2C-C1C-NC	6.78	116.32	109.97
14	H	1212	CLA	CMD-C2D-C1D	6.78	136.65	124.71
14	a	1140	CLA	C2D-C1D-ND	6.77	115.09	110.10
14	H	1217	CLA	C2C-C1C-NC	6.77	116.32	109.97
14	B	1212	CLA	CMD-C2D-C1D	6.77	136.65	124.71
14	H	1023	CLA	CMD-C2D-C1D	6.77	136.64	124.71
14	G	1127	CLA	C2C-C1C-NC	6.76	116.31	109.97
14	a	1134	CLA	C2C-C1C-NC	6.76	116.31	109.97
14	B	1225	CLA	CMD-C2D-C1D	6.76	136.62	124.71
14	B	1228	CLA	C2D-C1D-ND	6.76	115.08	110.10
14	H	1021	CLA	C4A-NA-C1A	6.75	109.74	106.71
14	B	1023	CLA	CMD-C2D-C1D	6.75	136.60	124.71
14	G	1140	CLA	C2D-C1D-ND	6.74	115.07	110.10
14	A	1134	CLA	C2C-C1C-NC	6.74	116.29	109.97
14	k	1401	CLA	C2C-C1C-NC	6.74	116.29	109.97
13	A	1011	CL0	C2C-C1C-NC	6.74	116.29	109.97
14	b	1205	CLA	O2D-CGD-CBD	6.74	123.24	111.27
14	b	1023	CLA	CMD-C2D-C1D	6.73	136.58	124.71
13	G	1011	CL0	C2C-C1C-NC	6.73	116.28	109.97
14	H	1225	CLA	CMD-C2D-C1D	6.73	136.58	124.71
14	a	1112	CLA	C2C-C1C-NC	6.73	116.28	109.97
14	B	1221	CLA	CMD-C2D-C1D	6.73	136.57	124.71
14	b	1228	CLA	C2D-C1D-ND	6.72	115.06	110.10
14	b	1225	CLA	CMD-C2D-C1D	6.72	136.56	124.71
14	B	1205	CLA	O2D-CGD-CBD	6.72	123.21	111.27
14	T	1401	CLA	C2D-C1D-ND	6.71	115.05	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1213	CLA	C2D-C1D-ND	6.71	115.05	110.10
13	a	1011	CL0	CMD-C2D-C1D	6.71	136.54	124.71
14	G	1134	CLA	C2C-C1C-NC	6.70	116.25	109.97
14	H	1213	CLA	C2D-C1D-ND	6.70	115.04	110.10
14	b	1221	CLA	CMD-C2D-C1D	6.70	136.52	124.71
14	H	1205	CLA	O2D-CGD-CBD	6.70	123.17	111.27
14	k	1401	CLA	C2D-C1D-ND	6.70	115.04	110.10
13	A	1011	CL0	CMD-C2D-C1D	6.70	136.52	124.71
14	B	1228	CLA	C2C-C1C-NC	6.70	116.25	109.97
14	b	1022	CLA	O2A-C1-C2	6.70	126.23	108.64
14	K	1401	CLA	C2D-C1D-ND	6.70	115.04	110.10
14	B	1022	CLA	O2A-C1-C2	6.70	126.23	108.64
14	H	1022	CLA	O2A-C1-C2	6.69	126.23	108.64
14	H	1221	CLA	CMD-C2D-C1D	6.69	136.51	124.71
14	b	1208	CLA	C2D-C1D-ND	6.69	115.03	110.10
14	G	1112	CLA	C2C-C1C-NC	6.69	116.24	109.97
14	A	1105	CLA	C2C-C1C-NC	6.69	116.24	109.97
13	G	1011	CL0	CMD-C2D-C1D	6.69	136.50	124.71
14	G	1105	CLA	C2C-C1C-NC	6.68	116.23	109.97
14	a	1105	CLA	C2C-C1C-NC	6.68	116.23	109.97
14	A	1112	CLA	C2C-C1C-NC	6.68	116.23	109.97
15	B	1238	F6C	CAA-C2A-C1A	-6.67	109.73	128.11
14	H	1228	CLA	C2C-C1C-NC	6.67	116.22	109.97
18	b	4004	BCR	C24-C23-C22	-6.67	116.15	126.23
18	H	4004	BCR	C24-C23-C22	-6.67	116.15	126.23
14	b	1213	CLA	C2D-C1D-ND	6.67	115.02	110.10
14	G	1107	CLA	C2C-C1C-NC	6.67	116.22	109.97
14	B	1216	CLA	C2C-C1C-NC	6.67	116.22	109.97
15	H	1238	F6C	CAA-C2A-C1A	-6.67	109.75	128.11
15	b	1238	F6C	CAA-C2A-C1A	-6.66	109.76	128.11
18	B	4004	BCR	C24-C23-C22	-6.65	116.18	126.23
14	H	1219	CLA	C2D-C1D-ND	6.64	115.00	110.10
14	A	1107	CLA	C2C-C1C-NC	6.64	116.19	109.97
15	B	1207	F6C	O2A-C1-C2	6.64	126.08	108.64
14	H	1208	CLA	C2D-C1D-ND	6.64	115.00	110.10
14	B	1219	CLA	C2D-C1D-ND	6.64	115.00	110.10
15	H	1207	F6C	O2A-C1-C2	6.64	126.08	108.64
15	b	1207	F6C	O2A-C1-C2	6.64	126.08	108.64
14	b	1228	CLA	C2C-C1C-NC	6.63	116.19	109.97
14	b	1216	CLA	C2C-C1C-NC	6.63	116.18	109.97
14	H	1216	CLA	C2C-C1C-NC	6.62	116.18	109.97
14	B	1208	CLA	C2D-C1D-ND	6.62	114.98	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1219	CLA	C2D-C1D-ND	6.62	114.98	110.10
14	A	1109	CLA	C2D-C1D-ND	6.61	114.97	110.10
14	b	1236	CLA	C2C-C1C-NC	6.61	116.16	109.97
14	a	1107	CLA	C2C-C1C-NC	6.60	116.16	109.97
14	G	1103	CLA	C2C-C1C-NC	6.60	116.16	109.97
14	H	1215	CLA	C2C-C1C-NC	6.60	116.16	109.97
14	a	1109	CLA	C2D-C1D-ND	6.60	114.97	110.10
14	A	1105	CLA	C2D-C1D-ND	6.59	114.96	110.10
14	A	1128	CLA	CMD-C2D-C1D	6.59	136.33	124.71
14	G	1128	CLA	CMD-C2D-C1D	6.59	136.33	124.71
14	b	1215	CLA	C2C-C1C-NC	6.59	116.14	109.97
14	G	1105	CLA	C2D-C1D-ND	6.58	114.95	110.10
14	A	1103	CLA	C2C-C1C-NC	6.58	116.14	109.97
14	a	1129	CLA	O2D-CGD-CBD	6.58	122.96	111.27
14	B	1215	CLA	C2C-C1C-NC	6.58	116.13	109.97
14	H	1236	CLA	C2C-C1C-NC	6.58	116.13	109.97
14	a	1128	CLA	CMD-C2D-C1D	6.58	136.30	124.71
14	U	1502	CLA	CHD-C1D-ND	-6.57	118.41	124.45
14	L	1502	CLA	CHD-C1D-ND	-6.57	118.41	124.45
14	G	1109	CLA	C2D-C1D-ND	6.57	114.95	110.10
14	A	1116	CLA	C2D-C1D-ND	6.57	114.94	110.10
14	G	1129	CLA	O2D-CGD-CBD	6.57	122.94	111.27
14	a	1105	CLA	C2D-C1D-ND	6.57	114.94	110.10
14	B	1221	CLA	C2D-C1D-ND	6.57	114.94	110.10
14	A	1129	CLA	O2D-CGD-CBD	6.56	122.93	111.27
14	B	1236	CLA	C2C-C1C-NC	6.56	116.12	109.97
14	H	1204	CLA	C2D-C1D-ND	6.56	114.94	110.10
14	H	1201	CLA	C2C-C1C-NC	6.55	116.11	109.97
14	b	1215	CLA	C2D-C1D-ND	6.55	114.93	110.10
14	a	1103	CLA	C2C-C1C-NC	6.55	116.11	109.97
14	b	1204	CLA	C2D-C1D-ND	6.55	114.93	110.10
14	a	1109	CLA	C2C-C1C-NC	6.54	116.10	109.97
14	a	1116	CLA	C2D-C1D-ND	6.54	114.92	110.10
14	G	1139	CLA	C2D-C1D-ND	6.54	114.92	110.10
14	b	1204	CLA	C2C-C1C-NC	6.54	116.10	109.97
14	b	1210	CLA	C2D-C1D-ND	6.54	114.92	110.10
14	A	1139	CLA	C2D-C1D-ND	6.53	114.92	110.10
14	H	1210	CLA	C2D-C1D-ND	6.52	114.91	110.10
14	G	1109	CLA	C2C-C1C-NC	6.52	116.08	109.97
14	l	1502	CLA	CHD-C1D-ND	-6.52	118.47	124.45
14	a	1125	CLA	C4A-NA-C1A	6.51	109.64	106.71
14	B	1215	CLA	C2D-C1D-ND	6.51	114.91	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1204	CLA	C2C-C1C-NC	6.51	116.07	109.97
14	H	1223	CLA	C2C-C1C-NC	6.51	116.07	109.97
14	H	1215	CLA	C2D-C1D-ND	6.51	114.90	110.10
14	G	1131	CLA	C2C-C1C-NC	6.51	116.07	109.97
18	G	4008	BCR	C20-C19-C18	6.51	144.69	126.42
18	a	4008	BCR	C20-C19-C18	6.51	144.69	126.42
14	a	1139	CLA	C2D-C1D-ND	6.51	114.90	110.10
18	A	4008	BCR	C20-C19-C18	6.50	144.69	126.42
14	G	1132	CLA	C2D-C1D-ND	6.50	114.90	110.10
14	B	1218	CLA	C2C-C1C-NC	6.50	116.06	109.97
14	B	1232	CLA	C2C-C1C-NC	6.50	116.06	109.97
14	B	1210	CLA	C2D-C1D-ND	6.49	114.89	110.10
14	H	1204	CLA	C2C-C1C-NC	6.49	116.05	109.97
14	A	1109	CLA	C2C-C1C-NC	6.49	116.05	109.97
14	B	1201	CLA	C2C-C1C-NC	6.49	116.05	109.97
14	b	1232	CLA	C2C-C1C-NC	6.49	116.05	109.97
14	b	1201	CLA	C2C-C1C-NC	6.48	116.05	109.97
14	G	1125	CLA	C4A-NA-C1A	6.48	109.62	106.71
14	A	1132	CLA	C2D-C1D-ND	6.48	114.88	110.10
14	H	1218	CLA	C2C-C1C-NC	6.48	116.04	109.97
14	H	1232	CLA	C2C-C1C-NC	6.47	116.03	109.97
14	a	1132	CLA	C2D-C1D-ND	6.47	114.87	110.10
14	a	1106	CLA	O2D-CGD-CBD	6.47	122.76	111.27
14	A	1106	CLA	O2D-CGD-CBD	6.47	122.76	111.27
14	B	1223	CLA	C2C-C1C-NC	6.46	116.03	109.97
14	b	1221	CLA	C2D-C1D-ND	6.46	114.87	110.10
14	B	1204	CLA	C2D-C1D-ND	6.46	114.87	110.10
14	b	1223	CLA	C2C-C1C-NC	6.46	116.02	109.97
14	U	1503	CLA	C2C-C1C-NC	6.46	116.02	109.97
14	B	1231	CLA	C2C-C1C-NC	6.46	116.02	109.97
14	b	1218	CLA	C2C-C1C-NC	6.45	116.01	109.97
14	G	1123	CLA	C2D-C1D-ND	6.44	114.85	110.10
14	G	1129	CLA	C2C-C1C-NC	6.44	116.01	109.97
14	A	1131	CLA	C2C-C1C-NC	6.44	116.01	109.97
14	A	1129	CLA	C2C-C1C-NC	6.44	116.01	109.97
14	A	1125	CLA	C4A-NA-C1A	6.43	109.60	106.71
14	a	1130	CLA	C2C-C1C-NC	6.43	116.00	109.97
14	G	1116	CLA	C2D-C1D-ND	6.43	114.84	110.10
14	G	1106	CLA	O2D-CGD-CBD	6.43	122.69	111.27
14	a	1128	CLA	C2D-C1D-ND	6.43	114.84	110.10
14	H	1221	CLA	C2D-C1D-ND	6.42	114.84	110.10
14	B	1023	CLA	C2C-C1C-NC	6.42	115.99	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1235	CLA	C2C-C1C-NC	6.42	115.98	109.97
14	A	1127	CLA	CMD-C2D-C1D	6.41	136.02	124.71
14	G	1127	CLA	CMD-C2D-C1D	6.41	136.02	124.71
14	G	1115	CLA	O2D-CGD-CBD	6.41	122.66	111.27
14	a	1127	CLA	CMD-C2D-C1D	6.41	136.01	124.71
14	H	1231	CLA	C2C-C1C-NC	6.41	115.98	109.97
14	B	1235	CLA	C2C-C1C-NC	6.41	115.98	109.97
14	a	1012	CLA	C2D-C1D-ND	6.41	114.83	110.10
14	G	1128	CLA	C2D-C1D-ND	6.41	114.83	110.10
14	A	1012	CLA	C2D-C1D-ND	6.41	114.83	110.10
18	b	4010	BCR	C20-C19-C18	6.41	144.41	126.42
14	L	1501	CLA	CMD-C2D-C1D	6.40	136.00	124.71
14	a	1115	CLA	O2D-CGD-CBD	6.40	122.65	111.27
14	H	1233	CLA	C2D-C1D-ND	6.40	114.82	110.10
14	a	1133	CLA	C2D-C1D-ND	6.40	114.82	110.10
14	A	1123	CLA	C2D-C1D-ND	6.40	114.82	110.10
14	l	1501	CLA	CMD-C2D-C1D	6.40	136.00	124.71
14	L	1503	CLA	C2C-C1C-NC	6.40	115.97	109.97
14	A	1115	CLA	O2D-CGD-CBD	6.40	122.64	111.27
14	H	1209	CLA	C2D-C1D-ND	6.40	114.82	110.10
14	b	1233	CLA	C2D-C1D-ND	6.39	114.82	110.10
14	a	1129	CLA	C2C-C1C-NC	6.39	115.96	109.97
14	b	1231	CLA	C2C-C1C-NC	6.39	115.96	109.97
14	U	1501	CLA	CMD-C2D-C1D	6.39	135.98	124.71
18	B	4010	BCR	C20-C19-C18	6.39	144.38	126.42
14	A	1133	CLA	C2D-C1D-ND	6.39	114.81	110.10
14	B	1225	CLA	C2D-C1D-ND	6.39	114.81	110.10
18	H	4010	BCR	C20-C19-C18	6.39	144.37	126.42
14	H	1235	CLA	C2C-C1C-NC	6.39	115.96	109.97
14	A	1130	CLA	C2C-C1C-NC	6.39	115.96	109.97
14	l	1503	CLA	C2C-C1C-NC	6.39	115.95	109.97
14	G	1130	CLA	C2C-C1C-NC	6.38	115.95	109.97
14	a	1131	CLA	C2C-C1C-NC	6.38	115.95	109.97
14	a	1108	CLA	C2D-C1D-ND	6.38	114.80	110.10
14	A	1108	CLA	C2D-C1D-ND	6.38	114.80	110.10
14	G	1108	CLA	C2D-C1D-ND	6.38	114.80	110.10
14	b	1239	CLA	C2D-C1D-ND	6.37	114.80	110.10
14	A	1128	CLA	C2D-C1D-ND	6.37	114.80	110.10
14	a	1122	CLA	C2D-C1D-ND	6.36	114.79	110.10
14	H	1023	CLA	C2C-C1C-NC	6.36	115.93	109.97
14	b	1225	CLA	C2D-C1D-ND	6.36	114.79	110.10
14	B	1210	CLA	O2A-C1-C2	6.36	125.35	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1133	CLA	C2D-C1D-ND	6.36	114.79	110.10
14	b	1023	CLA	C2C-C1C-NC	6.36	115.93	109.97
14	H	1210	CLA	O2A-C1-C2	6.36	125.34	108.64
14	H	1201	CLA	C4A-NA-C1A	6.35	109.56	106.71
14	A	1136	CLA	C2C-C1C-NC	6.35	115.92	109.97
14	A	1122	CLA	C2D-C1D-ND	6.35	114.79	110.10
14	B	1233	CLA	C2D-C1D-ND	6.35	114.79	110.10
14	G	1122	CLA	C2C-C1C-NC	6.35	115.92	109.97
14	b	1210	CLA	O2A-C1-C2	6.35	125.33	108.64
14	a	1115	CLA	C2C-C1C-NC	6.35	115.92	109.97
14	A	1132	CLA	C2C-C1C-NC	6.35	115.92	109.97
14	A	1136	CLA	C2D-C1D-ND	6.35	114.78	110.10
14	G	1136	CLA	C2C-C1C-NC	6.34	115.92	109.97
14	b	1203	CLA	C2C-C1C-NC	6.34	115.92	109.97
14	H	1225	CLA	C2D-C1D-ND	6.34	114.78	110.10
14	A	1115	CLA	C2C-C1C-NC	6.34	115.91	109.97
14	G	1012	CLA	C2D-C1D-ND	6.34	114.78	110.10
14	H	1239	CLA	C2D-C1D-ND	6.34	114.78	110.10
14	H	1201	CLA	O2D-CGD-CBD	6.34	122.53	111.27
14	a	1123	CLA	C2D-C1D-ND	6.34	114.77	110.10
14	B	1235	CLA	C2D-C1D-ND	6.33	114.77	110.10
14	H	1208	CLA	C2C-C1C-NC	6.33	115.90	109.97
14	B	1223	CLA	O2D-CGD-CBD	6.33	122.51	111.27
14	G	1115	CLA	C2C-C1C-NC	6.33	115.90	109.97
14	a	1120	CLA	C2C-C1C-NC	6.33	115.90	109.97
14	b	1224	CLA	C2C-C1C-NC	6.33	115.90	109.97
14	H	1211	CLA	C2D-C1D-ND	6.33	114.77	110.10
14	B	1239	CLA	C2D-C1D-ND	6.32	114.76	110.10
14	b	1201	CLA	O2D-CGD-CBD	6.32	122.50	111.27
14	B	1023	CLA	CAC-C3C-C4C	6.32	133.01	124.81
14	G	1132	CLA	C2C-C1C-NC	6.32	115.89	109.97
14	B	1201	CLA	O2D-CGD-CBD	6.32	122.50	111.27
14	H	1224	CLA	C2C-C1C-NC	6.32	115.89	109.97
14	B	1209	CLA	C2D-C1D-ND	6.32	114.76	110.10
14	H	1223	CLA	O2D-CGD-CBD	6.32	122.49	111.27
14	a	1132	CLA	C2C-C1C-NC	6.31	115.89	109.97
15	H	1207	F6C	C1D-ND-C4D	-6.31	103.87	106.71
14	b	1223	CLA	O2D-CGD-CBD	6.31	122.48	111.27
14	H	1235	CLA	C2D-C1D-ND	6.31	114.75	110.10
14	G	1122	CLA	C2D-C1D-ND	6.31	114.75	110.10
14	b	1209	CLA	C2D-C1D-ND	6.31	114.75	110.10
14	A	1134	CLA	C2D-C1D-ND	6.31	114.75	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1136	CLA	C2C-C1C-NC	6.30	115.88	109.97
14	B	1224	CLA	C2C-C1C-NC	6.30	115.88	109.97
14	B	1208	CLA	C2C-C1C-NC	6.30	115.88	109.97
14	b	1235	CLA	C2D-C1D-ND	6.30	114.75	110.10
14	b	1211	CLA	C2D-C1D-ND	6.30	114.75	110.10
14	H	1220	CLA	C4A-NA-C1A	6.30	109.54	106.71
14	G	1120	CLA	C2C-C1C-NC	6.30	115.87	109.97
14	a	1139	CLA	C2C-C1C-NC	6.30	115.87	109.97
14	A	1120	CLA	C2C-C1C-NC	6.30	115.87	109.97
14	H	1023	CLA	CAC-C3C-C4C	6.29	132.98	124.81
14	G	1136	CLA	C2D-C1D-ND	6.29	114.74	110.10
14	B	1211	CLA	C2D-C1D-ND	6.29	114.74	110.10
14	A	1104	CLA	C2C-C1C-NC	6.29	115.87	109.97
14	A	1102	CLA	C2C-C1C-NC	6.29	115.86	109.97
14	B	1220	CLA	C4A-NA-C1A	6.29	109.53	106.71
14	B	1203	CLA	C2C-C1C-NC	6.29	115.86	109.97
14	b	1023	CLA	CAC-C3C-C4C	6.29	132.97	124.81
14	H	1203	CLA	C2C-C1C-NC	6.29	115.86	109.97
15	B	1207	F6C	C1D-ND-C4D	-6.29	103.88	106.71
18	b	4014	BCR	C20-C19-C18	6.28	144.06	126.42
14	H	1205	CLA	CMD-C2D-C1D	6.28	135.78	124.71
14	a	1104	CLA	C2C-C1C-NC	6.28	115.85	109.97
14	G	1102	CLA	C2C-C1C-NC	6.28	115.85	109.97
18	B	4014	BCR	C20-C19-C18	6.27	144.04	126.42
18	a	4002	BCR	C20-C19-C18	6.27	144.03	126.42
15	b	1230	F6C	C1C-C2C-C3C	-6.27	102.63	107.00
18	H	4014	BCR	C20-C19-C18	6.27	144.03	126.42
14	b	1222	CLA	O2D-CGD-CBD	6.27	122.41	111.27
14	G	1101	CLA	C2C-C1C-NC	6.27	115.84	109.97
14	B	1222	CLA	O2D-CGD-CBD	6.27	122.41	111.27
14	b	1205	CLA	CMD-C2D-C1D	6.27	135.76	124.71
14	a	1124	CLA	C2C-C1C-NC	6.27	115.84	109.97
14	G	1112	CLA	C2D-C1D-ND	6.27	114.72	110.10
14	a	1112	CLA	C2D-C1D-ND	6.27	114.72	110.10
14	H	1213	CLA	C2C-C1C-NC	6.27	115.84	109.97
18	A	4002	BCR	C20-C19-C18	6.27	144.02	126.42
15	H	1230	F6C	C1C-C2C-C3C	-6.27	102.64	107.00
15	B	1230	F6C	C1C-C2C-C3C	-6.27	102.64	107.00
14	a	1136	CLA	C2D-C1D-ND	6.27	114.72	110.10
14	b	1208	CLA	C2C-C1C-NC	6.26	115.84	109.97
14	a	1134	CLA	C2D-C1D-ND	6.26	114.72	110.10
14	b	1220	CLA	C4A-NA-C1A	6.26	109.52	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1021	CLA	CMD-C2D-C1D	6.26	135.75	124.71
14	H	1222	CLA	O2D-CGD-CBD	6.26	122.39	111.27
14	H	1210	CLA	C2C-C1C-NC	6.26	115.84	109.97
14	B	1205	CLA	CMD-C2D-C1D	6.26	135.74	124.71
18	G	4002	BCR	C20-C19-C18	6.26	143.99	126.42
14	b	1216	CLA	C2D-C1D-ND	6.25	114.71	110.10
14	G	1104	CLA	C2C-C1C-NC	6.25	115.83	109.97
14	A	1122	CLA	C2C-C1C-NC	6.25	115.83	109.97
14	b	1213	CLA	O2D-CGD-CBD	6.25	122.37	111.27
14	a	1122	CLA	C2C-C1C-NC	6.25	115.82	109.97
14	B	1021	CLA	CMD-C2D-C1D	6.25	135.72	124.71
14	b	1021	CLA	CMD-C2D-C1D	6.24	135.72	124.71
14	L	1502	CLA	O2D-CGD-CBD	6.24	122.36	111.27
14	a	1102	CLA	C2C-C1C-NC	6.24	115.82	109.97
14	a	1104	CLA	C1C-C2C-C3C	-6.24	100.39	106.96
14	G	1124	CLA	C2C-C1C-NC	6.24	115.82	109.97
14	G	1134	CLA	C2D-C1D-ND	6.24	114.70	110.10
14	G	1104	CLA	C1C-C2C-C3C	-6.24	100.40	106.96
14	B	1216	CLA	C2D-C1D-ND	6.24	114.70	110.10
14	G	1138	CLA	O2D-CGD-CBD	6.24	122.35	111.27
14	a	1138	CLA	O2D-CGD-CBD	6.24	122.35	111.27
14	b	1213	CLA	C2C-C1C-NC	6.24	115.81	109.97
14	H	1216	CLA	C2D-C1D-ND	6.23	114.70	110.10
18	R	4018	BCR	C3-C4-C5	-6.23	102.95	114.08
14	A	1101	CLA	C2C-C1C-NC	6.23	115.81	109.97
14	A	1104	CLA	C1C-C2C-C3C	-6.23	100.41	106.96
14	A	1106	CLA	C2C-C1C-NC	6.23	115.81	109.97
14	B	1213	CLA	C2C-C1C-NC	6.23	115.81	109.97
14	H	1232	CLA	C2D-C1D-ND	6.23	114.69	110.10
14	A	1139	CLA	C2C-C1C-NC	6.23	115.81	109.97
14	G	1126	CLA	C2D-C1D-ND	6.23	114.69	110.10
14	A	1138	CLA	C2C-C1C-NC	6.23	115.80	109.97
14	A	1126	CLA	C2D-C1D-ND	6.22	114.69	110.10
14	B	1232	CLA	C2D-C1D-ND	6.22	114.69	110.10
14	l	1503	CLA	C4A-NA-C1A	6.22	109.50	106.71
14	G	1106	CLA	C2C-C1C-NC	6.22	115.80	109.97
15	b	1207	F6C	C1D-ND-C4D	-6.22	103.91	106.71
14	a	1137	CLA	C2D-C1D-ND	6.22	114.69	110.10
14	l	1502	CLA	O2D-CGD-CBD	6.22	122.31	111.27
14	A	1138	CLA	O2D-CGD-CBD	6.22	122.31	111.27
14	A	1112	CLA	C2D-C1D-ND	6.21	114.68	110.10
14	G	1110	CLA	C2C-C1C-NC	6.21	115.79	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1106	CLA	C2C-C1C-NC	6.21	115.79	109.97
13	a	1011	CL0	C1C-C2C-C3C	-6.21	100.43	106.96
14	G	1130	CLA	C2D-C1D-ND	6.21	114.68	110.10
14	a	1140	CLA	C2C-C1C-NC	6.21	115.79	109.97
18	i	4018	BCR	C3-C4-C5	-6.21	102.99	114.08
14	B	1213	CLA	O2A-C1-C2	6.21	124.95	108.64
14	A	1106	CLA	C4A-NA-C1A	6.21	109.50	106.71
14	b	1232	CLA	C2D-C1D-ND	6.21	114.68	110.10
14	A	1140	CLA	C2C-C1C-NC	6.21	115.78	109.97
14	B	1213	CLA	O2D-CGD-CBD	6.20	122.29	111.27
14	G	1138	CLA	C2C-C1C-NC	6.20	115.78	109.97
14	a	1101	CLA	C2C-C1C-NC	6.20	115.78	109.97
14	a	1110	CLA	C2C-C1C-NC	6.20	115.78	109.97
14	H	1213	CLA	O2A-C1-C2	6.20	124.94	108.64
18	I	4018	BCR	C3-C4-C5	-6.20	103.00	114.08
14	H	1219	CLA	C2C-C1C-NC	6.20	115.78	109.97
14	G	1139	CLA	C2C-C1C-NC	6.20	115.78	109.97
14	a	1130	CLA	C2D-C1D-ND	6.20	114.67	110.10
14	H	1213	CLA	O2D-CGD-CBD	6.20	122.29	111.27
14	U	1502	CLA	O2D-CGD-CBD	6.20	122.29	111.27
14	B	1201	CLA	C4A-NA-C1A	6.20	109.49	106.71
14	A	1138	CLA	C2D-C1D-ND	6.20	114.67	110.10
14	b	1205	CLA	C2C-C1C-NC	6.19	115.77	109.97
14	H	1205	CLA	C2C-C1C-NC	6.19	115.77	109.97
14	b	1210	CLA	C2C-C1C-NC	6.19	115.77	109.97
14	A	1124	CLA	C2C-C1C-NC	6.19	115.77	109.97
14	b	1213	CLA	O2A-C1-C2	6.19	124.91	108.64
14	B	1205	CLA	C2C-C1C-NC	6.19	115.77	109.97
14	G	1106	CLA	C4A-NA-C1A	6.19	109.49	106.71
14	H	1206	CLA	C2D-C1D-ND	6.18	114.66	110.10
14	B	1210	CLA	C2C-C1C-NC	6.18	115.76	109.97
14	G	1140	CLA	C2C-C1C-NC	6.18	115.76	109.97
14	b	1201	CLA	C4A-NA-C1A	6.18	109.48	106.71
13	A	1011	CL0	C1C-C2C-C3C	-6.18	100.46	106.96
14	b	1219	CLA	C2C-C1C-NC	6.18	115.76	109.97
14	a	1118	CLA	C2D-C1D-ND	6.18	114.66	110.10
14	b	1206	CLA	C2D-C1D-ND	6.17	114.65	110.10
14	H	1212	CLA	C2C-C1C-NC	6.17	115.75	109.97
14	A	1130	CLA	C2D-C1D-ND	6.17	114.65	110.10
18	U	4019	BCR	C15-C14-C13	-6.17	118.51	127.31
18	L	4019	BCR	C15-C14-C13	-6.17	118.51	127.31
14	B	1212	CLA	C2C-C1C-NC	6.17	115.75	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1104	CLA	C4A-NA-C1A	6.17	109.48	106.71
14	A	1116	CLA	C2C-C1C-NC	6.17	115.75	109.97
14	G	1138	CLA	C2D-C1D-ND	6.16	114.65	110.10
14	b	1212	CLA	C2C-C1C-NC	6.16	115.75	109.97
13	G	1011	CL0	C1C-C2C-C3C	-6.16	100.48	106.96
14	a	1126	CLA	C2D-C1D-ND	6.16	114.64	110.10
14	b	1225	CLA	C2C-C1C-NC	6.16	115.74	109.97
14	B	1209	CLA	C2C-C1C-NC	6.16	115.74	109.97
14	B	1219	CLA	C2C-C1C-NC	6.16	115.74	109.97
14	G	1127	CLA	C4A-NA-C1A	6.16	109.47	106.71
18	l	4019	BCR	C15-C14-C13	-6.16	118.52	127.31
14	B	1206	CLA	C2D-C1D-ND	6.15	114.64	110.10
14	G	1116	CLA	C2C-C1C-NC	6.15	115.73	109.97
14	a	1116	CLA	C2C-C1C-NC	6.15	115.73	109.97
14	a	1119	CLA	C4A-NA-C1A	6.15	109.47	106.71
14	a	1107	CLA	C2D-C1D-ND	6.15	114.63	110.10
14	B	1222	CLA	C2C-C1C-NC	6.14	115.73	109.97
14	A	1104	CLA	C4A-NA-C1A	6.14	109.47	106.71
14	A	1110	CLA	C2C-C1C-NC	6.14	115.72	109.97
14	a	1104	CLA	C4A-NA-C1A	6.13	109.46	106.71
14	a	1138	CLA	C2C-C1C-NC	6.13	115.72	109.97
14	U	1503	CLA	C4A-NA-C1A	6.13	109.46	106.71
14	A	1137	CLA	C2D-C1D-ND	6.13	114.62	110.10
14	H	1224	CLA	O2D-CGD-CBD	6.13	122.15	111.27
14	B	1224	CLA	O2D-CGD-CBD	6.13	122.15	111.27
14	A	1118	CLA	C2D-C1D-ND	6.12	114.61	110.10
14	b	1209	CLA	C2C-C1C-NC	6.12	115.70	109.97
14	G	1107	CLA	C2D-C1D-ND	6.12	114.61	110.10
14	G	1118	CLA	C2D-C1D-ND	6.12	114.61	110.10
14	B	1221	CLA	C2C-C1C-NC	6.12	115.70	109.97
14	a	1127	CLA	C4A-NA-C1A	6.11	109.45	106.71
14	H	1211	CLA	C2C-C1C-NC	6.11	115.70	109.97
14	a	1128	CLA	O2D-CGD-CBD	6.11	122.13	111.27
14	b	1211	CLA	C2C-C1C-NC	6.11	115.70	109.97
14	G	1128	CLA	O2D-CGD-CBD	6.11	122.13	111.27
14	X	1701	CLA	C2C-C1C-NC	6.11	115.69	109.97
14	A	1127	CLA	C4A-NA-C1A	6.11	109.45	106.71
14	a	1138	CLA	C2D-C1D-ND	6.11	114.61	110.10
14	H	1225	CLA	C2C-C1C-NC	6.11	115.69	109.97
14	H	1209	CLA	C2C-C1C-NC	6.10	115.69	109.97
14	G	1137	CLA	C2D-C1D-ND	6.10	114.60	110.10
14	H	1221	CLA	C2C-C1C-NC	6.10	115.69	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1103	CLA	C2D-C1D-ND	6.10	114.60	110.10
14	b	1224	CLA	O2D-CGD-CBD	6.10	122.10	111.27
14	B	1225	CLA	C2C-C1C-NC	6.10	115.68	109.97
14	b	1222	CLA	C2C-C1C-NC	6.10	115.68	109.97
14	A	1107	CLA	C2D-C1D-ND	6.09	114.59	110.10
14	a	1106	CLA	C4A-NA-C1A	6.09	109.44	106.71
14	L	1503	CLA	C4A-NA-C1A	6.09	109.44	106.71
14	H	1222	CLA	C2C-C1C-NC	6.09	115.67	109.97
14	A	1128	CLA	O2D-CGD-CBD	6.08	122.08	111.27
14	x	1701	CLA	C2C-C1C-NC	6.08	115.67	109.97
14	G	1119	CLA	C4A-NA-C1A	6.08	109.44	106.71
14	B	1211	CLA	C2C-C1C-NC	6.07	115.66	109.97
18	B	4014	BCR	C24-C23-C22	-6.07	117.06	126.23
14	A	1103	CLA	C2D-C1D-ND	6.07	114.58	110.10
14	G	1013	CLA	CMD-C2D-C1D	6.07	135.41	124.71
14	a	1013	CLA	CMD-C2D-C1D	6.07	135.41	124.71
14	G	1135	CLA	C2D-C1D-ND	6.07	114.58	110.10
14	W	1701	CLA	C2C-C1C-NC	6.07	115.66	109.97
14	A	1013	CLA	CMD-C2D-C1D	6.07	135.41	124.71
14	A	1111	CLA	C2C-C1C-NC	6.07	115.66	109.97
14	H	1239	CLA	C1C-C2C-C3C	-6.06	100.58	106.96
14	G	1103	CLA	C2D-C1D-ND	6.06	114.57	110.10
18	b	4014	BCR	C24-C23-C22	-6.06	117.08	126.23
18	H	4005	BCR	C24-C23-C22	-6.05	117.09	126.23
14	a	1135	CLA	C2D-C1D-ND	6.05	114.56	110.10
15	B	1238	F6C	O2A-C1-C2	6.05	124.53	108.64
14	b	1221	CLA	C2C-C1C-NC	6.04	115.63	109.97
18	H	4014	BCR	C24-C23-C22	-6.04	117.10	126.23
15	b	1238	F6C	O2A-C1-C2	6.04	124.51	108.64
14	G	1111	CLA	C2C-C1C-NC	6.04	115.63	109.97
18	A	4011	BCR	C20-C19-C18	6.04	143.37	126.42
14	A	1125	CLA	O2A-C1-C2	6.03	124.49	108.64
14	G	1125	CLA	O2A-C1-C2	6.03	124.49	108.64
14	a	1125	CLA	O2A-C1-C2	6.03	124.49	108.64
18	G	4011	BCR	C7-C8-C9	-6.03	117.12	126.23
14	B	1239	CLA	C1C-C2C-C3C	-6.03	100.62	106.96
14	b	1239	CLA	C1C-C2C-C3C	-6.03	100.62	106.96
14	G	1117	CLA	C2D-C1D-ND	6.03	114.55	110.10
15	H	1238	F6C	O2A-C1-C2	6.03	124.48	108.64
14	a	1111	CLA	C2C-C1C-NC	6.03	115.62	109.97
18	A	4011	BCR	C7-C8-C9	-6.03	117.13	126.23
15	B	1230	F6C	CAA-C2A-C1A	-6.03	111.52	128.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1133	CLA	O2A-C1-C2	6.03	124.47	108.64
18	G	4011	BCR	C20-C19-C18	6.02	143.34	126.42
15	H	1230	F6C	CAA-C2A-C1A	-6.02	111.53	128.11
14	A	1119	CLA	C4A-NA-C1A	6.02	109.41	106.71
14	A	1135	CLA	C2D-C1D-ND	6.02	114.54	110.10
18	B	4005	BCR	C24-C23-C22	-6.02	117.14	126.23
18	a	4011	BCR	C20-C19-C18	6.01	143.31	126.42
15	b	1230	F6C	CAA-C2A-C1A	-6.01	111.55	128.11
14	a	1133	CLA	O2A-C1-C2	6.01	124.44	108.64
14	a	1108	CLA	C2C-C1C-NC	6.01	115.60	109.97
18	b	4005	BCR	C24-C23-C22	-6.01	117.16	126.23
14	G	1133	CLA	O2A-C1-C2	6.01	124.42	108.64
14	A	1120	CLA	C4A-NA-C1A	6.01	109.41	106.71
14	G	1124	CLA	O2A-C1-C2	6.00	124.41	108.64
14	l	1501	CLA	C4A-NA-C1A	6.00	109.41	106.71
14	A	1124	CLA	O2A-C1-C2	6.00	124.41	108.64
18	a	4011	BCR	C7-C8-C9	-6.00	117.17	126.23
14	a	1120	CLA	C4A-NA-C1A	6.00	109.40	106.71
14	B	1202	CLA	C4A-NA-C1A	6.00	109.40	106.71
14	U	1502	CLA	O2A-C1-C2	6.00	124.39	108.64
14	B	1201	CLA	C2D-C1D-ND	6.00	114.52	110.10
14	b	1201	CLA	C2D-C1D-ND	5.99	114.52	110.10
14	L	1502	CLA	O2A-C1-C2	5.99	124.39	108.64
14	a	1124	CLA	O2A-C1-C2	5.99	124.38	108.64
14	G	1120	CLA	C4A-NA-C1A	5.99	109.40	106.71
14	H	1202	CLA	C4A-NA-C1A	5.99	109.40	106.71
14	b	1202	CLA	C4A-NA-C1A	5.99	109.40	106.71
14	G	1108	CLA	C2C-C1C-NC	5.99	115.58	109.97
14	G	1124	CLA	CHD-C1D-ND	-5.99	118.95	124.45
14	l	1502	CLA	O2A-C1-C2	5.99	124.37	108.64
14	G	1109	CLA	C4A-NA-C1A	5.99	109.40	106.71
14	A	1131	CLA	CHD-C1D-ND	-5.99	118.95	124.45
14	G	1131	CLA	CHD-C1D-ND	-5.99	118.95	124.45
14	U	1501	CLA	C4A-NA-C1A	5.98	109.40	106.71
14	A	1108	CLA	C2C-C1C-NC	5.98	115.57	109.97
14	a	1131	CLA	CHD-C1D-ND	-5.98	118.96	124.45
14	b	1235	CLA	O2D-CGD-CBD	5.97	121.88	111.27
14	A	1117	CLA	C4A-NA-C1A	5.97	109.39	106.71
14	H	1201	CLA	C2D-C1D-ND	5.97	114.50	110.10
14	H	1202	CLA	O2A-CGA-O1A	-5.97	108.53	123.59
14	a	1126	CLA	C2C-C1C-NC	5.96	115.56	109.97
14	A	1117	CLA	C2D-C1D-ND	5.96	114.50	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1234	CLA	C3D-C2D-C1D	-5.96	97.69	105.83
14	b	1202	CLA	O2A-CGA-O1A	-5.96	108.55	123.59
14	G	1126	CLA	C2C-C1C-NC	5.96	115.55	109.97
14	H	1235	CLA	O2D-CGD-CBD	5.96	121.86	111.27
14	B	1202	CLA	O2A-CGA-O1A	-5.96	108.56	123.59
14	B	1221	CLA	O2A-C1-C2	5.95	124.28	108.64
14	a	1117	CLA	C2D-C1D-ND	5.95	114.49	110.10
14	B	1204	CLA	O2D-CGD-CBD	5.95	121.85	111.27
14	B	1235	CLA	O2D-CGD-CBD	5.95	121.85	111.27
14	H	1234	CLA	C3D-C2D-C1D	-5.95	97.71	105.83
14	B	1234	CLA	C3D-C2D-C1D	-5.95	97.71	105.83
14	H	1204	CLA	O2D-CGD-CBD	5.95	121.84	111.27
14	L	1501	CLA	C4A-NA-C1A	5.95	109.38	106.71
14	A	1126	CLA	C2C-C1C-NC	5.94	115.54	109.97
14	a	1125	CLA	C2C-C1C-NC	5.94	115.54	109.97
15	b	1230	F6C	C2D-C1D-ND	5.94	115.54	109.97
14	b	1221	CLA	O2A-C1-C2	5.94	124.24	108.64
14	B	1226	CLA	C2D-C1D-ND	5.94	114.48	110.10
14	A	1124	CLA	CHD-C1D-ND	-5.94	119.00	124.45
14	A	1125	CLA	C2C-C1C-NC	5.93	115.53	109.97
14	A	1131	CLA	C2D-C1D-ND	5.93	114.48	110.10
14	b	1204	CLA	O2D-CGD-CBD	5.93	121.81	111.27
14	H	1221	CLA	O2A-C1-C2	5.93	124.22	108.64
18	b	4004	BCR	C20-C19-C18	5.93	143.07	126.42
14	a	1131	CLA	O2A-C1-C2	5.93	124.22	108.64
14	G	1129	CLA	C2D-C1D-ND	5.93	114.47	110.10
14	H	1226	CLA	C2D-C1D-ND	5.93	114.47	110.10
14	a	1124	CLA	CHD-C1D-ND	-5.93	119.01	124.45
14	b	1225	CLA	O2A-C1-C2	5.92	124.20	108.64
14	G	1131	CLA	O2A-C1-C2	5.92	124.20	108.64
14	G	1117	CLA	C4A-NA-C1A	5.92	109.37	106.71
14	B	1225	CLA	O2A-C1-C2	5.92	124.19	108.64
14	a	1129	CLA	C2D-C1D-ND	5.92	114.47	110.10
14	a	1131	CLA	O2D-CGD-CBD	5.92	121.78	111.27
14	A	1131	CLA	O2A-C1-C2	5.92	124.18	108.64
14	H	1225	CLA	O2A-C1-C2	5.91	124.18	108.64
18	B	4004	BCR	C20-C19-C18	5.91	143.03	126.42
15	B	1230	F6C	C2D-C1D-ND	5.91	115.51	109.97
14	a	1114	CLA	O2D-CGD-CBD	5.91	121.77	111.27
14	A	1114	CLA	O2D-CGD-CBD	5.91	121.77	111.27
14	B	1203	CLA	C3D-C2D-C1D	-5.91	97.76	105.83
14	A	1109	CLA	C4A-NA-C1A	5.91	109.36	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1102	CLA	O2D-CGD-CBD	5.91	121.77	111.27
15	H	1230	F6C	C2D-C1D-ND	5.91	115.51	109.97
18	H	4004	BCR	C20-C19-C18	5.91	143.01	126.42
14	G	1125	CLA	C2C-C1C-NC	5.91	115.50	109.97
14	b	1226	CLA	C2D-C1D-ND	5.90	114.45	110.10
14	H	1203	CLA	C3D-C2D-C1D	-5.90	97.78	105.83
14	H	1229	CLA	C2C-C1C-NC	5.90	115.50	109.97
14	B	1021	CLA	C2C-C1C-NC	5.90	115.50	109.97
14	b	1229	CLA	C2C-C1C-NC	5.90	115.50	109.97
14	b	1203	CLA	C3D-C2D-C1D	-5.90	97.78	105.83
14	A	1131	CLA	O2D-CGD-CBD	5.89	121.74	111.27
14	G	1131	CLA	C2D-C1D-ND	5.89	114.45	110.10
14	G	1114	CLA	O2D-CGD-CBD	5.89	121.74	111.27
14	A	1129	CLA	C2D-C1D-ND	5.89	114.44	110.10
15	A	1121	F6C	C3A-C4A-NA	5.89	114.44	110.10
14	b	1021	CLA	C2C-C1C-NC	5.89	115.49	109.97
14	G	1102	CLA	O2D-CGD-CBD	5.89	121.73	111.27
14	G	1131	CLA	O2D-CGD-CBD	5.89	121.73	111.27
14	a	1102	CLA	O2D-CGD-CBD	5.88	121.72	111.27
14	B	1219	CLA	O2D-CGD-CBD	5.88	121.72	111.27
14	a	1131	CLA	C2D-C1D-ND	5.88	114.44	110.10
14	H	1021	CLA	C2C-C1C-NC	5.88	115.48	109.97
14	a	1109	CLA	C4A-NA-C1A	5.88	109.35	106.71
14	b	1219	CLA	O2D-CGD-CBD	5.86	121.69	111.27
14	a	1128	CLA	C4A-NA-C1A	5.86	109.34	106.71
14	H	1022	CLA	O2D-CGD-CBD	5.86	121.67	111.27
14	G	1126	CLA	O2D-CGD-CBD	5.85	121.66	111.27
14	b	1215	CLA	C1C-C2C-C3C	-5.85	100.81	106.96
14	B	1022	CLA	O2D-CGD-CBD	5.85	121.66	111.27
14	a	1102	CLA	C2D-C1D-ND	5.85	114.41	110.10
14	H	1215	CLA	C1C-C2C-C3C	-5.84	100.81	106.96
14	H	1219	CLA	O2D-CGD-CBD	5.84	121.65	111.27
14	a	1101	CLA	O2D-CGD-CBD	5.84	121.65	111.27
14	B	1215	CLA	C1C-C2C-C3C	-5.84	100.81	106.96
14	G	1128	CLA	C4A-NA-C1A	5.84	109.33	106.71
14	a	1126	CLA	O2D-CGD-CBD	5.84	121.65	111.27
15	G	1121	F6C	C3A-C4A-NA	5.84	114.41	110.10
14	b	1022	CLA	O2D-CGD-CBD	5.84	121.64	111.27
15	a	1121	F6C	C3A-C4A-NA	5.84	114.41	110.10
14	a	1012	CLA	C1C-C2C-C3C	-5.84	100.82	106.96
14	A	1128	CLA	C4A-NA-C1A	5.84	109.33	106.71
14	a	1118	CLA	O2D-CGD-CBD	5.84	121.64	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1114	CLA	C1C-C2C-C3C	-5.84	100.82	106.96
14	A	1012	CLA	C1C-C2C-C3C	-5.83	100.82	106.96
14	G	1140	CLA	O2D-CGD-CBD	5.83	121.63	111.27
14	A	1101	CLA	O2D-CGD-CBD	5.83	121.62	111.27
14	A	1140	CLA	O2D-CGD-CBD	5.83	121.62	111.27
14	G	1012	CLA	C1C-C2C-C3C	-5.82	100.83	106.96
14	A	1126	CLA	O2D-CGD-CBD	5.82	121.62	111.27
14	a	1140	CLA	O2D-CGD-CBD	5.82	121.62	111.27
14	A	1113	CLA	C2C-C1C-NC	5.82	115.42	109.97
14	G	1118	CLA	O2D-CGD-CBD	5.82	121.60	111.27
14	a	1117	CLA	C4A-NA-C1A	5.82	109.32	106.71
14	b	1221	CLA	C4A-NA-C1A	5.82	109.32	106.71
14	A	1102	CLA	C2D-C1D-ND	5.82	114.39	110.10
14	A	1118	CLA	O2D-CGD-CBD	5.81	121.59	111.27
14	G	1125	CLA	C3D-C2D-C1D	-5.80	97.91	105.83
14	H	1022	CLA	C2C-C1C-NC	5.80	115.41	109.97
14	H	1221	CLA	C4A-NA-C1A	5.80	109.31	106.71
14	A	1125	CLA	C3D-C2D-C1D	-5.80	97.91	105.83
14	a	1113	CLA	C2C-C1C-NC	5.80	115.41	109.97
14	G	1102	CLA	C2D-C1D-ND	5.80	114.38	110.10
14	a	1119	CLA	C2D-C1D-ND	5.80	114.38	110.10
14	B	1229	CLA	C2C-C1C-NC	5.80	115.41	109.97
14	G	1113	CLA	C2C-C1C-NC	5.80	115.40	109.97
14	G	1114	CLA	C1C-C2C-C3C	-5.80	100.86	106.96
14	G	1101	CLA	O2D-CGD-CBD	5.79	121.56	111.27
14	G	1109	CLA	O2A-C1-C2	5.79	123.86	108.64
14	A	1109	CLA	O2A-C1-C2	5.79	123.85	108.64
14	a	1114	CLA	C1C-C2C-C3C	-5.79	100.87	106.96
15	H	1237	F6C	C2D-C1D-ND	5.79	115.39	109.97
14	H	1239	CLA	O2D-CGD-CBD	5.79	121.55	111.27
14	a	1125	CLA	C3D-C2D-C1D	-5.78	97.94	105.83
14	B	1239	CLA	O2D-CGD-CBD	5.78	121.55	111.27
14	a	1109	CLA	O2A-C1-C2	5.78	123.83	108.64
14	b	1214	CLA	O2D-CGD-CBD	5.78	121.53	111.27
14	A	1104	CLA	C1D-ND-C4D	-5.77	102.23	106.33
14	G	1103	CLA	C4A-NA-C1A	5.77	109.30	106.71
14	H	1214	CLA	O2D-CGD-CBD	5.77	121.53	111.27
14	B	1221	CLA	C4A-NA-C1A	5.77	109.30	106.71
14	b	1202	CLA	C2C-C1C-NC	5.77	115.38	109.97
14	b	1239	CLA	O2D-CGD-CBD	5.77	121.52	111.27
14	A	1103	CLA	C4A-NA-C1A	5.77	109.30	106.71
14	B	1022	CLA	C2C-C1C-NC	5.77	115.37	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	1502	CLA	C2C-C1C-NC	5.76	115.37	109.97
14	G	1104	CLA	C1D-ND-C4D	-5.76	102.24	106.33
14	B	1202	CLA	C2C-C1C-NC	5.76	115.36	109.97
14	H	1228	CLA	CHD-C1D-ND	-5.75	119.17	124.45
14	B	1214	CLA	O2D-CGD-CBD	5.75	121.49	111.27
14	H	1223	CLA	C3D-C2D-C1D	-5.75	97.98	105.83
14	B	1209	CLA	O2D-CGD-CBD	5.75	121.49	111.27
14	B	1228	CLA	CHD-C1D-ND	-5.75	119.17	124.45
14	H	1209	CLA	O2D-CGD-CBD	5.75	121.48	111.27
14	G	1133	CLA	C1C-C2C-C3C	-5.75	100.91	106.96
14	G	1119	CLA	C2D-C1D-ND	5.75	114.34	110.10
14	A	1122	CLA	C4A-NA-C1A	5.75	109.29	106.71
14	a	1133	CLA	C4A-NA-C1A	5.74	109.29	106.71
14	b	1209	CLA	O2D-CGD-CBD	5.74	121.47	111.27
14	B	1236	CLA	O2D-CGD-CBD	5.74	121.47	111.27
14	G	1120	CLA	C3D-C2D-C1D	-5.74	98.00	105.83
14	H	1202	CLA	C2C-C1C-NC	5.74	115.35	109.97
14	H	1236	CLA	O2D-CGD-CBD	5.74	121.46	111.27
14	G	1104	CLA	CHD-C1D-ND	-5.74	119.18	124.45
14	H	1212	CLA	C4A-NA-C1A	5.73	109.28	106.71
14	a	1114	CLA	C2D-C1D-ND	5.73	114.33	110.10
14	b	1236	CLA	O2D-CGD-CBD	5.73	121.44	111.27
14	b	1228	CLA	CHD-C1D-ND	-5.73	119.19	124.45
14	G	1133	CLA	C4A-NA-C1A	5.73	109.28	106.71
14	A	1119	CLA	C2D-C1D-ND	5.72	114.32	110.10
13	G	1011	CL0	O2D-CGD-CBD	5.72	121.44	111.27
15	b	1237	F6C	C2D-C1D-ND	5.72	115.33	109.97
14	b	1202	CLA	O2D-CGD-CBD	5.72	121.44	111.27
14	B	1223	CLA	C3D-C2D-C1D	-5.72	98.02	105.83
15	B	1237	F6C	C2D-C1D-ND	5.72	115.33	109.97
14	U	1502	CLA	C2C-C1C-NC	5.72	115.33	109.97
18	l	4022	BCR	C20-C19-C18	5.72	142.48	126.42
14	A	1133	CLA	C4A-NA-C1A	5.72	109.28	106.71
13	A	1011	CL0	O2D-CGD-CBD	5.72	121.43	111.27
14	A	1134	CLA	O2D-CGD-CBD	5.72	121.43	111.27
14	A	1103	CLA	O2D-CGD-CBD	5.72	121.42	111.27
14	b	1217	CLA	C1C-C2C-C3C	-5.71	100.95	106.96
14	a	1103	CLA	C4A-NA-C1A	5.71	109.28	106.71
18	L	4022	BCR	C20-C19-C18	5.71	142.47	126.42
14	a	1133	CLA	C1C-C2C-C3C	-5.71	100.95	106.96
18	U	4022	BCR	C20-C19-C18	5.71	142.47	126.42
14	B	1214	CLA	C2D-C1D-ND	5.71	114.31	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1227	CLA	O2D-CGD-CBD	5.71	121.42	111.27
14	b	1022	CLA	C2C-C1C-NC	5.71	115.32	109.97
14	l	1502	CLA	C2C-C1C-NC	5.71	115.32	109.97
13	a	1011	CL0	O2D-CGD-CBD	5.71	121.41	111.27
14	a	1120	CLA	C3D-C2D-C1D	-5.71	98.04	105.83
14	B	1202	CLA	O2D-CGD-CBD	5.70	121.41	111.27
14	H	1202	CLA	O2D-CGD-CBD	5.70	121.40	111.27
14	G	1103	CLA	O2D-CGD-CBD	5.70	121.40	111.27
14	b	1223	CLA	C3D-C2D-C1D	-5.70	98.05	105.83
14	b	1227	CLA	O2D-CGD-CBD	5.70	121.40	111.27
14	A	1120	CLA	C3D-C2D-C1D	-5.70	98.05	105.83
14	a	1103	CLA	O2D-CGD-CBD	5.70	121.40	111.27
14	A	1104	CLA	CHD-C1D-ND	-5.70	119.22	124.45
14	a	1134	CLA	O2D-CGD-CBD	5.70	121.39	111.27
14	G	1134	CLA	O2D-CGD-CBD	5.70	121.39	111.27
14	B	1227	CLA	O2D-CGD-CBD	5.69	121.39	111.27
14	a	1136	CLA	O2D-CGD-CBD	5.69	121.38	111.27
14	A	1114	CLA	C2D-C1D-ND	5.69	114.30	110.10
14	A	1133	CLA	C1C-C2C-C3C	-5.69	100.98	106.96
14	B	1217	CLA	C1C-C2C-C3C	-5.68	100.98	106.96
14	b	1204	CLA	CHD-C1D-ND	-5.68	119.23	124.45
14	a	1104	CLA	CHD-C1D-ND	-5.68	119.23	124.45
14	a	1104	CLA	C1D-ND-C4D	-5.68	102.30	106.33
14	H	1217	CLA	C1C-C2C-C3C	-5.68	100.99	106.96
14	H	1214	CLA	C1C-C2C-C3C	-5.67	101.00	106.96
14	b	1214	CLA	C1C-C2C-C3C	-5.67	101.00	106.96
14	a	1102	CLA	O2A-C1-C2	5.67	123.53	108.64
14	A	1102	CLA	O2A-C1-C2	5.67	123.53	108.64
14	b	1234	CLA	C2C-C1C-NC	5.66	115.28	109.97
14	a	1111	CLA	O2D-CGD-CBD	5.66	121.33	111.27
14	G	1122	CLA	C4A-NA-C1A	5.66	109.25	106.71
14	G	1102	CLA	O2A-C1-C2	5.66	123.50	108.64
14	H	1203	CLA	O2A-C1-C2	5.66	123.50	108.64
14	B	1214	CLA	C1C-C2C-C3C	-5.66	101.01	106.96
14	H	1204	CLA	CHD-C1D-ND	-5.66	119.26	124.45
14	B	1205	CLA	O2A-CGA-O1A	-5.65	109.32	123.59
14	A	1136	CLA	O2D-CGD-CBD	5.65	121.31	111.27
14	B	1203	CLA	O2A-C1-C2	5.65	123.49	108.64
14	G	1136	CLA	O2D-CGD-CBD	5.65	121.31	111.27
14	b	1205	CLA	O2A-CGA-O1A	-5.65	109.33	123.59
14	H	1205	CLA	O2A-CGA-O1A	-5.65	109.33	123.59
14	G	1111	CLA	O2D-CGD-CBD	5.65	121.31	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1125	CLA	O2D-CGD-CBD	5.65	121.30	111.27
14	A	1125	CLA	O2D-CGD-CBD	5.64	121.30	111.27
14	b	1203	CLA	O2A-C1-C2	5.64	123.47	108.64
14	b	1214	CLA	C2D-C1D-ND	5.64	114.26	110.10
15	B	1237	F6C	C1A-C2A-C3A	-5.64	101.03	106.97
14	G	1131	CLA	C1C-C2C-C3C	-5.64	101.02	106.96
14	H	1214	CLA	C2D-C1D-ND	5.64	114.26	110.10
14	b	1212	CLA	C4A-NA-C1A	5.64	109.24	106.71
14	B	1217	CLA	C4A-NA-C1A	5.64	109.24	106.71
14	G	1114	CLA	C2D-C1D-ND	5.64	114.26	110.10
14	A	1111	CLA	O2D-CGD-CBD	5.64	121.29	111.27
15	H	1237	F6C	C1A-C2A-C3A	-5.64	101.03	106.97
14	H	1235	CLA	O2A-CGA-O1A	-5.64	109.37	123.59
14	A	1116	CLA	O2D-CGD-CBD	5.64	121.28	111.27
14	B	1234	CLA	C2C-C1C-NC	5.64	115.25	109.97
14	B	1204	CLA	CHD-C1D-ND	-5.63	119.28	124.45
14	A	1013	CLA	O2A-C1-C2	5.63	123.43	108.64
14	H	1217	CLA	C4A-NA-C1A	5.63	109.24	106.71
14	G	1013	CLA	O2A-C1-C2	5.63	123.42	108.64
14	b	1226	CLA	O2D-CGD-CBD	5.63	121.26	111.27
14	B	1222	CLA	C4A-NA-C1A	5.63	109.23	106.71
14	a	1013	CLA	O2A-C1-C2	5.62	123.42	108.64
14	a	1113	CLA	O2D-CGD-CBD	5.62	121.26	111.27
14	H	1226	CLA	O2D-CGD-CBD	5.62	121.26	111.27
14	G	1113	CLA	O2D-CGD-CBD	5.62	121.26	111.27
14	a	1125	CLA	O2D-CGD-CBD	5.62	121.25	111.27
14	B	1235	CLA	O2A-CGA-O1A	-5.62	109.41	123.59
14	B	1226	CLA	O2D-CGD-CBD	5.62	121.25	111.27
14	b	1235	CLA	O2A-CGA-O1A	-5.61	109.42	123.59
14	B	1215	CLA	CHD-C1D-ND	-5.61	119.29	124.45
15	b	1237	F6C	C1A-C2A-C3A	-5.61	101.06	106.97
14	a	1122	CLA	C4A-NA-C1A	5.61	109.23	106.71
14	B	1212	CLA	C4A-NA-C1A	5.61	109.23	106.71
14	a	1012	CLA	O2A-C1-C2	5.61	123.38	108.64
14	H	1234	CLA	C2C-C1C-NC	5.61	115.22	109.97
14	H	1215	CLA	CHD-C1D-ND	-5.60	119.31	124.45
14	a	1104	CLA	C3D-C2D-C1D	-5.60	98.19	105.83
14	G	1013	CLA	C1D-ND-C4D	-5.60	102.36	106.33
14	A	1012	CLA	O2A-C1-C2	5.60	123.36	108.64
14	A	1113	CLA	O2D-CGD-CBD	5.60	121.22	111.27
14	G	1116	CLA	O2D-CGD-CBD	5.60	121.22	111.27
14	A	1115	CLA	C4A-NA-C1A	5.60	109.22	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1137	CLA	C1C-C2C-C3C	-5.60	101.07	106.96
14	A	1116	CLA	O2A-C1-C2	5.60	123.34	108.64
14	b	1215	CLA	CHD-C1D-ND	-5.59	119.31	124.45
14	G	1012	CLA	O2A-C1-C2	5.59	123.33	108.64
18	R	4018	BCR	C7-C8-C9	-5.59	117.78	126.23
14	a	1116	CLA	O2D-CGD-CBD	5.59	121.20	111.27
14	a	1136	CLA	O2A-CGA-O1A	-5.59	109.48	123.59
14	b	1217	CLA	C4A-NA-C1A	5.59	109.22	106.71
14	A	1104	CLA	C3D-C2D-C1D	-5.59	98.20	105.83
14	A	1136	CLA	O2A-CGA-O1A	-5.59	109.49	123.59
14	G	1136	CLA	CHD-C1D-ND	-5.58	119.33	124.45
14	A	1131	CLA	C1C-C2C-C3C	-5.58	101.09	106.96
18	m	4021	BCR	C7-C8-C9	-5.58	117.81	126.23
14	G	1116	CLA	O2A-C1-C2	5.58	123.30	108.64
14	B	1226	CLA	C1C-C2C-C3C	-5.58	101.09	106.96
14	a	1116	CLA	O2A-C1-C2	5.58	123.29	108.64
14	b	1226	CLA	C1C-C2C-C3C	-5.57	101.10	106.96
14	U	1503	CLA	O2D-CGD-CBD	5.57	121.17	111.27
14	A	1136	CLA	CHD-C1D-ND	-5.57	119.33	124.45
14	G	1136	CLA	O2A-CGA-O1A	-5.57	109.53	123.59
18	M	4021	BCR	C7-C8-C9	-5.57	117.82	126.23
18	V	4021	BCR	C7-C8-C9	-5.57	117.82	126.23
14	a	1136	CLA	CHD-C1D-ND	-5.57	119.34	124.45
14	H	1221	CLA	O2D-CGD-CBD	5.57	121.16	111.27
14	G	1104	CLA	C3D-C2D-C1D	-5.57	98.23	105.83
14	b	1231	CLA	O2D-CGD-CBD	5.57	121.16	111.27
14	B	1231	CLA	O2D-CGD-CBD	5.57	121.16	111.27
14	b	1208	CLA	O2D-CGD-CBD	5.56	121.16	111.27
14	H	1226	CLA	C1C-C2C-C3C	-5.56	101.11	106.96
14	H	1231	CLA	O2D-CGD-CBD	5.56	121.15	111.27
14	A	1137	CLA	C1C-C2C-C3C	-5.56	101.11	106.96
14	L	1501	CLA	C1C-C2C-C3C	-5.56	101.11	106.96
14	B	1221	CLA	O2D-CGD-CBD	5.56	121.14	111.27
14	a	1128	CLA	C1C-C2C-C3C	-5.56	101.11	106.96
14	l	1503	CLA	O2D-CGD-CBD	5.55	121.14	111.27
18	i	4018	BCR	C7-C8-C9	-5.55	117.84	126.23
14	A	1118	CLA	C1C-C2C-C3C	-5.55	101.12	106.96
18	V	4021	BCR	C24-C23-C22	-5.55	117.85	126.23
14	G	1133	CLA	O2D-CGD-CBD	5.55	121.13	111.27
14	L	1503	CLA	O2D-CGD-CBD	5.55	121.13	111.27
14	B	1216	CLA	O2D-CGD-CBD	5.55	121.13	111.27
14	A	1013	CLA	C1D-ND-C4D	-5.55	102.39	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1216	CLA	O2D-CGD-CBD	5.55	121.13	111.27
18	M	4021	BCR	C24-C23-C22	-5.55	117.85	126.23
14	l	1501	CLA	C1C-C2C-C3C	-5.55	101.12	106.96
14	a	1013	CLA	C1D-ND-C4D	-5.54	102.40	106.33
14	A	1128	CLA	C1C-C2C-C3C	-5.54	101.13	106.96
14	H	1216	CLA	O2D-CGD-CBD	5.54	121.12	111.27
18	I	4018	BCR	C7-C8-C9	-5.54	117.86	126.23
18	H	4005	BCR	C7-C8-C9	-5.54	117.86	126.23
14	G	1105	CLA	CHD-C1D-ND	-5.54	119.36	124.45
14	A	1105	CLA	CHD-C1D-ND	-5.54	119.36	124.45
14	a	1131	CLA	C1C-C2C-C3C	-5.54	101.13	106.96
14	H	1208	CLA	O2D-CGD-CBD	5.54	121.11	111.27
14	a	1118	CLA	C1C-C2C-C3C	-5.54	101.14	106.96
14	b	1221	CLA	O2D-CGD-CBD	5.54	121.11	111.27
14	G	1115	CLA	C4A-NA-C1A	5.54	109.19	106.71
14	G	1128	CLA	C1C-C2C-C3C	-5.53	101.14	106.96
14	b	1236	CLA	C1C-C2C-C3C	-5.53	101.14	106.96
18	b	4005	BCR	C7-C8-C9	-5.53	117.88	126.23
14	G	1118	CLA	C1C-C2C-C3C	-5.53	101.14	106.96
18	H	4010	BCR	C24-C23-C22	-5.53	117.88	126.23
18	b	4010	BCR	C24-C23-C22	-5.53	117.88	126.23
14	H	1236	CLA	C1C-C2C-C3C	-5.53	101.15	106.96
14	a	1105	CLA	CHD-C1D-ND	-5.52	119.38	124.45
14	X	1701	CLA	O2A-C1-C2	5.52	123.15	108.64
14	U	1501	CLA	C1C-C2C-C3C	-5.52	101.15	106.96
14	b	1203	CLA	C1C-C2C-C3C	-5.52	101.15	106.96
14	a	1112	CLA	C4A-NA-C1A	5.52	109.19	106.71
14	a	1133	CLA	O2D-CGD-CBD	5.52	121.08	111.27
14	A	1133	CLA	O2D-CGD-CBD	5.52	121.08	111.27
14	a	1137	CLA	C1C-C2C-C3C	-5.52	101.15	106.96
14	x	1701	CLA	O2A-C1-C2	5.52	123.14	108.64
14	B	1236	CLA	C1C-C2C-C3C	-5.52	101.16	106.96
18	B	4010	BCR	C24-C23-C22	-5.51	117.91	126.23
14	W	1701	CLA	O2A-C1-C2	5.51	123.12	108.64
14	B	1208	CLA	O2D-CGD-CBD	5.51	121.06	111.27
14	a	1105	CLA	O2D-CGD-CBD	5.51	121.05	111.27
14	b	1233	CLA	C1C-C2C-C3C	-5.50	101.17	106.96
18	m	4021	BCR	C24-C23-C22	-5.50	117.92	126.23
14	H	1202	CLA	C3D-C2D-C1D	-5.50	98.32	105.83
14	B	1202	CLA	C3D-C2D-C1D	-5.50	98.33	105.83
14	a	1130	CLA	C1C-C2C-C3C	-5.50	101.17	106.96
15	b	1207	F6C	O2A-CGA-O1A	-5.50	109.72	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	4005	BCR	C7-C8-C9	-5.50	117.93	126.23
14	A	1105	CLA	O2D-CGD-CBD	5.50	121.03	111.27
14	a	1115	CLA	C4A-NA-C1A	5.50	109.18	106.71
14	G	1112	CLA	O2D-CGD-CBD	5.49	121.03	111.27
14	b	1218	CLA	C4A-NA-C1A	5.49	109.18	106.71
14	b	1202	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
14	a	1108	CLA	C4A-NA-C1A	5.49	109.17	106.71
14	H	1203	CLA	C1C-C2C-C3C	-5.49	101.19	106.96
14	B	1233	CLA	C1C-C2C-C3C	-5.49	101.19	106.96
14	B	1203	CLA	C1C-C2C-C3C	-5.49	101.19	106.96
14	b	1212	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
14	A	1130	CLA	C1C-C2C-C3C	-5.48	101.19	106.96
15	B	1207	F6C	O2A-CGA-O1A	-5.48	109.76	123.59
14	G	1105	CLA	O2D-CGD-CBD	5.48	121.00	111.27
14	H	1233	CLA	C1C-C2C-C3C	-5.48	101.20	106.96
14	A	1108	CLA	C4A-NA-C1A	5.48	109.17	106.71
15	H	1237	F6C	CAA-C2A-C1A	-5.48	113.03	128.11
15	H	1207	F6C	O2A-CGA-O1A	-5.48	109.77	123.59
14	H	1212	CLA	C3D-C2D-C1D	-5.47	98.36	105.83
14	G	1112	CLA	C4A-NA-C1A	5.47	109.17	106.71
14	a	1106	CLA	C3D-C2D-C1D	-5.47	98.36	105.83
14	A	1106	CLA	C3D-C2D-C1D	-5.47	98.36	105.83
15	b	1237	F6C	CAA-C2A-C1A	-5.47	113.05	128.11
14	a	1112	CLA	O2D-CGD-CBD	5.47	120.98	111.27
14	A	1112	CLA	O2D-CGD-CBD	5.47	120.98	111.27
14	a	1012	CLA	CHD-C1D-ND	-5.47	119.43	124.45
14	T	1401	CLA	O2D-CGD-CBD	5.47	120.98	111.27
14	A	1130	CLA	C3D-C2D-C1D	-5.46	98.37	105.83
14	k	1401	CLA	O2D-CGD-CBD	5.46	120.98	111.27
14	A	1112	CLA	C4A-NA-C1A	5.46	109.16	106.71
15	B	1237	F6C	CAA-C2A-C1A	-5.46	113.07	128.11
14	B	1212	CLA	C3D-C2D-C1D	-5.46	98.38	105.83
14	H	1228	CLA	C4A-NA-C1A	5.46	109.16	106.71
14	a	1132	CLA	C1C-C2C-C3C	-5.46	101.22	106.96
14	G	1106	CLA	C3D-C2D-C1D	-5.46	98.38	105.83
14	H	1212	CLA	O2D-CGD-CBD	5.46	120.96	111.27
14	H	1218	CLA	C4A-NA-C1A	5.46	109.16	106.71
14	H	1222	CLA	C4A-NA-C1A	5.46	109.16	106.71
14	A	1135	CLA	C4A-NA-C1A	5.46	109.16	106.71
14	U	1502	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
14	K	1401	CLA	O2D-CGD-CBD	5.45	120.95	111.27
14	b	1229	CLA	CHD-C1D-ND	-5.45	119.44	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1218	CLA	C4A-NA-C1A	5.45	109.16	106.71
14	H	1023	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
18	H	4009	BCR	C24-C23-C22	-5.44	118.01	126.23
14	G	1130	CLA	C1C-C2C-C3C	-5.44	101.24	106.96
14	A	1132	CLA	C1C-C2C-C3C	-5.44	101.24	106.96
14	H	1220	CLA	O2A-C1-C2	5.44	122.93	108.64
14	G	1132	CLA	C1C-C2C-C3C	-5.44	101.24	106.96
18	L	4019	BCR	C3-C4-C5	-5.44	104.37	114.08
14	l	1502	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
14	L	1502	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
14	a	1130	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
14	B	1229	CLA	CHD-C1D-ND	-5.43	119.46	124.45
14	G	1012	CLA	CHD-C1D-ND	-5.43	119.46	124.45
14	G	1130	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
14	b	1220	CLA	O2A-C1-C2	5.43	122.91	108.64
14	B	1218	CLA	O2D-CGD-CBD	5.43	120.92	111.27
14	a	1120	CLA	C1C-C2C-C3C	-5.43	101.25	106.96
14	G	1115	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
14	U	1501	CLA	O2D-CGD-CBD	5.43	120.92	111.27
14	l	1501	CLA	O2D-CGD-CBD	5.43	120.91	111.27
18	U	4019	BCR	C3-C4-C5	-5.43	104.39	114.08
14	A	1115	CLA	C3D-C2D-C1D	-5.43	98.43	105.83
14	b	1231	CLA	C4A-NA-C1A	5.43	109.14	106.71
14	b	1212	CLA	O2D-CGD-CBD	5.42	120.90	111.27
14	b	1218	CLA	O2D-CGD-CBD	5.42	120.90	111.27
14	H	1218	CLA	O2D-CGD-CBD	5.42	120.90	111.27
14	L	1501	CLA	O2D-CGD-CBD	5.42	120.90	111.27
14	K	1401	CLA	C1C-C2C-C3C	-5.42	101.26	106.96
14	B	1228	CLA	C4A-NA-C1A	5.42	109.14	106.71
14	B	1220	CLA	O2A-C1-C2	5.42	122.87	108.64
14	H	1201	CLA	O2A-CGA-O1A	-5.41	109.93	123.59
14	G	1113	CLA	C3D-C2D-C1D	-5.41	98.44	105.83
18	b	4009	BCR	C24-C23-C22	-5.41	118.06	126.23
14	H	1228	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
15	A	1121	F6C	O2D-CGD-CBD	5.41	120.88	111.27
14	a	1136	CLA	C4A-NA-C1A	5.41	109.14	106.71
14	a	1135	CLA	C4A-NA-C1A	5.41	109.14	106.71
14	a	1126	CLA	O2A-CGA-O1A	-5.41	109.95	123.59
14	B	1212	CLA	O2D-CGD-CBD	5.41	120.88	111.27
15	G	1121	F6C	O2D-CGD-CBD	5.40	120.87	111.27
14	H	1236	CLA	CHD-C1D-ND	-5.40	119.49	124.45
14	b	1228	CLA	C4A-NA-C1A	5.40	109.14	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1023	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
14	A	1126	CLA	O2A-CGA-O1A	-5.40	109.96	123.59
14	a	1113	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
14	A	1120	CLA	C1C-C2C-C3C	-5.40	101.28	106.96
14	B	1023	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
14	G	1108	CLA	C4A-NA-C1A	5.40	109.13	106.71
14	b	1239	CLA	C4A-NA-C1A	5.40	109.13	106.71
14	B	1201	CLA	O2A-CGA-O1A	-5.40	109.96	123.59
18	l	4019	BCR	C3-C4-C5	-5.40	104.44	114.08
14	a	1120	CLA	O2D-CGD-CBD	5.40	120.86	111.27
14	A	1113	CLA	C3D-C2D-C1D	-5.40	98.47	105.83
14	A	1115	CLA	CHD-C1D-ND	-5.40	119.50	124.45
14	H	1229	CLA	CHD-C1D-ND	-5.39	119.50	124.45
14	A	1012	CLA	CHD-C1D-ND	-5.39	119.50	124.45
14	b	1222	CLA	O2A-C1-C2	5.39	122.81	108.64
14	G	1126	CLA	C4A-NA-C1A	5.39	109.13	106.71
14	A	1122	CLA	O2D-CGD-CBD	5.39	120.85	111.27
14	G	1126	CLA	O2A-CGA-O1A	-5.39	109.99	123.59
14	G	1132	CLA	CHD-C1D-ND	-5.39	119.50	124.45
14	a	1115	CLA	CHD-C1D-ND	-5.39	119.50	124.45
14	A	1116	CLA	CHD-C1D-ND	-5.39	119.50	124.45
14	G	1123	CLA	O2D-CGD-CBD	5.39	120.84	111.27
18	B	4009	BCR	C24-C23-C22	-5.39	118.09	126.23
14	a	1116	CLA	CHD-C1D-ND	-5.39	119.50	124.45
14	G	1118	CLA	O2A-C1-C2	5.38	122.78	108.64
14	A	1120	CLA	O2D-CGD-CBD	5.38	120.83	111.27
15	a	1121	F6C	O2D-CGD-CBD	5.38	120.83	111.27
15	b	1238	F6C	C1A-C2A-C3A	-5.38	101.30	106.97
14	b	1201	CLA	O2A-CGA-O1A	-5.38	110.01	123.59
14	a	1134	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
14	A	1013	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
14	H	1222	CLA	O2A-C1-C2	5.38	122.77	108.64
14	T	1401	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
14	A	1107	CLA	O2D-CGD-CBD	5.38	120.83	111.27
14	B	1228	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
14	A	1127	CLA	C1C-C2C-C3C	-5.38	101.30	106.96
15	A	1121	F6C	C1A-C2A-C3A	-5.38	101.31	106.97
14	B	1222	CLA	O2A-C1-C2	5.38	122.76	108.64
14	a	1127	CLA	C1C-C2C-C3C	-5.37	101.31	106.96
14	H	1229	CLA	O2D-CGD-CBD	5.37	120.82	111.27
14	a	1122	CLA	O2D-CGD-CBD	5.37	120.82	111.27
14	G	1116	CLA	CHD-C1D-ND	-5.37	119.52	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1120	CLA	O2D-CGD-CBD	5.37	120.82	111.27
14	H	1228	CLA	O2D-CGD-CBD	5.37	120.81	111.27
14	a	1115	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
14	a	1107	CLA	O2D-CGD-CBD	5.37	120.81	111.27
14	A	1116	CLA	C1C-C2C-C3C	-5.37	101.31	106.96
14	A	1012	CLA	C3D-C2D-C1D	-5.36	98.51	105.83
14	a	1116	CLA	C1C-C2C-C3C	-5.36	101.32	106.96
14	G	1134	CLA	C1C-C2C-C3C	-5.36	101.32	106.96
14	G	1109	CLA	C1C-C2C-C3C	-5.36	101.32	106.96
14	G	1013	CLA	C3D-C2D-C1D	-5.36	98.51	105.83
14	B	1235	CLA	CHD-C1D-ND	-5.36	119.53	124.45
14	G	1111	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
14	a	1123	CLA	O2D-CGD-CBD	5.36	120.79	111.27
14	B	1236	CLA	CHD-C1D-ND	-5.36	119.53	124.45
14	b	1228	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
14	A	1118	CLA	O2A-C1-C2	5.36	122.71	108.64
14	G	1122	CLA	O2D-CGD-CBD	5.36	120.79	111.27
14	a	1118	CLA	O2A-C1-C2	5.36	122.71	108.64
18	B	4010	BCR	C15-C14-C13	-5.36	119.67	127.31
14	b	1229	CLA	O2D-CGD-CBD	5.36	120.78	111.27
14	H	1229	CLA	C1C-C2C-C3C	-5.36	101.33	106.96
14	k	1401	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
14	a	1102	CLA	O2A-CGA-O1A	-5.35	110.08	123.59
14	G	1120	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
14	H	1234	CLA	C1D-ND-C4D	-5.35	102.53	106.33
14	a	1132	CLA	CHD-C1D-ND	-5.35	119.53	124.45
14	b	1229	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
15	B	1238	F6C	C1A-C2A-C3A	-5.35	101.33	106.97
14	A	1110	CLA	O2D-CGD-CBD	5.35	120.78	111.27
14	G	1135	CLA	C4A-NA-C1A	5.35	109.11	106.71
14	B	1239	CLA	C4A-NA-C1A	5.35	109.11	106.71
18	H	4010	BCR	C15-C14-C13	-5.35	119.67	127.31
14	B	1229	CLA	O2D-CGD-CBD	5.35	120.78	111.27
14	a	1012	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
14	A	1124	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
15	a	1121	F6C	C1A-C2A-C3A	-5.35	101.34	106.97
14	G	1107	CLA	O2D-CGD-CBD	5.35	120.77	111.27
14	b	1222	CLA	C4A-NA-C1A	5.35	109.11	106.71
14	A	1136	CLA	C4A-NA-C1A	5.35	109.11	106.71
14	G	1116	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
14	H	1223	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
18	b	4010	BCR	C15-C14-C13	-5.35	119.68	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1123	CLA	O2D-CGD-CBD	5.35	120.77	111.27
14	H	1227	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
14	a	1109	CLA	C1C-C2C-C3C	-5.35	101.33	106.96
14	A	1134	CLA	C1C-C2C-C3C	-5.35	101.34	106.96
15	H	1207	F6C	O2D-CGD-O1D	-5.34	113.39	123.84
14	A	1013	CLA	CMB-C2B-C3B	5.34	134.67	124.68
14	H	1216	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
15	b	1207	F6C	O2D-CGD-O1D	-5.34	113.39	123.84
14	G	1110	CLA	O2D-CGD-CBD	5.34	120.76	111.27
14	B	1223	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
14	b	1228	CLA	O2D-CGD-CBD	5.34	120.76	111.27
14	B	1228	CLA	O2D-CGD-CBD	5.34	120.76	111.27
14	G	1130	CLA	CHD-C1D-ND	-5.34	119.55	124.45
14	A	1132	CLA	CHD-C1D-ND	-5.34	119.55	124.45
15	H	1238	F6C	C1A-C2A-C3A	-5.34	101.35	106.97
14	a	1111	CLA	C3D-C2D-C1D	-5.34	98.55	105.83
14	A	1111	CLA	C3D-C2D-C1D	-5.34	98.55	105.83
14	G	1102	CLA	O2A-CGA-O1A	-5.34	110.12	123.59
14	a	1013	CLA	C3D-C2D-C1D	-5.34	98.55	105.83
14	B	1216	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
15	G	1121	F6C	C1A-C2A-C3A	-5.33	101.35	106.97
14	B	1226	CLA	CHD-C1D-ND	-5.33	119.55	124.45
14	G	1013	CLA	CMB-C2B-C3B	5.33	134.66	124.68
14	G	1115	CLA	CHD-C1D-ND	-5.33	119.55	124.45
14	G	1105	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
14	G	1127	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
14	H	1239	CLA	C4A-NA-C1A	5.33	109.10	106.71
14	A	1126	CLA	C4A-NA-C1A	5.33	109.10	106.71
14	B	1231	CLA	C4A-NA-C1A	5.33	109.10	106.71
14	a	1110	CLA	O2D-CGD-CBD	5.33	120.74	111.27
14	b	1204	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
18	b	4016	BCR	C15-C14-C13	-5.33	119.70	127.31
14	B	1229	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
14	H	1209	CLA	CHD-C1D-ND	-5.33	119.56	124.45
14	b	1211	CLA	C1C-C2C-C3C	-5.33	101.35	106.96
14	B	1225	CLA	O2D-CGD-CBD	5.33	120.74	111.27
14	A	1107	CLA	C4A-NA-C1A	5.33	109.10	106.71
14	B	1213	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
14	b	1213	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
14	H	1022	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
14	a	1013	CLA	CMB-C2B-C3B	5.32	134.64	124.68
14	A	1102	CLA	O2A-CGA-O1A	-5.32	110.16	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1209	CLA	CHD-C1D-ND	-5.32	119.56	124.45
14	B	1217	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
14	H	1235	CLA	CHD-C1D-ND	-5.32	119.56	124.45
14	H	1213	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
14	H	1225	CLA	O2D-CGD-CBD	5.32	120.72	111.27
14	G	1012	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
15	B	1207	F6C	O2D-CGD-O1D	-5.32	113.44	123.84
14	B	1227	CLA	C1C-C2C-C3C	-5.32	101.37	106.96
14	G	1135	CLA	C1C-C2C-C3C	-5.32	101.37	106.96
14	b	1223	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
18	B	4016	BCR	C15-C14-C13	-5.31	119.72	127.31
14	b	1225	CLA	O2D-CGD-CBD	5.31	120.71	111.27
14	G	1124	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
14	A	1109	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
14	a	1124	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
14	B	1022	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
14	b	1022	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
14	A	1105	CLA	C1C-C2C-C3C	-5.31	101.37	106.96
14	B	1218	CLA	C1C-C2C-C3C	-5.31	101.38	106.96
14	x	1701	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
14	b	1220	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
14	G	1123	CLA	C1C-C2C-C3C	-5.30	101.38	106.96
14	b	1236	CLA	CHD-C1D-ND	-5.30	119.58	124.45
14	H	1209	CLA	CAA-C2A-C3A	-5.30	98.26	112.78
14	B	1234	CLA	C1D-ND-C4D	-5.30	102.57	106.33
14	b	1209	CLA	CHD-C1D-ND	-5.30	119.58	124.45
14	b	1235	CLA	CHD-C1D-ND	-5.30	119.58	124.45
14	G	1127	CLA	O2A-CGA-O1A	-5.30	110.21	123.59
14	b	1227	CLA	C1C-C2C-C3C	-5.30	101.38	106.96
14	H	1217	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
14	b	1220	CLA	O2D-CGD-CBD	5.30	120.68	111.27
14	a	1130	CLA	CHD-C1D-ND	-5.30	119.58	124.45
14	b	1217	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
14	H	1231	CLA	C4A-NA-C1A	5.30	109.09	106.71
14	L	1503	CLA	O2A-C1-C2	5.30	122.55	108.64
14	a	1105	CLA	C1C-C2C-C3C	-5.30	101.39	106.96
14	b	1216	CLA	C1C-C2C-C3C	-5.30	101.39	106.96
14	L	1501	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
14	B	1209	CLA	CAA-C2A-C3A	-5.29	98.28	112.78
14	a	1135	CLA	C1C-C2C-C3C	-5.29	101.39	106.96
14	l	1501	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
14	b	1209	CLA	CAA-C2A-C3A	-5.29	98.29	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1108	CLA	CHD-C1D-ND	-5.29	119.59	124.45
18	H	4016	BCR	C15-C14-C13	-5.29	119.76	127.31
14	B	1209	CLA	C1C-C2C-C3C	-5.29	101.39	106.96
14	H	1211	CLA	C1C-C2C-C3C	-5.29	101.40	106.96
14	b	1215	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
14	b	1234	CLA	C1D-ND-C4D	-5.29	102.58	106.33
14	H	1226	CLA	CHD-C1D-ND	-5.29	119.59	124.45
14	B	1220	CLA	O2D-CGD-CBD	5.29	120.67	111.27
15	B	1237	F6C	O2D-CGD-CBD	5.29	120.66	111.27
14	A	1123	CLA	C1C-C2C-C3C	-5.29	101.40	106.96
14	X	1701	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
14	A	1136	CLA	C1C-C2C-C3C	-5.28	101.40	106.96
14	H	1220	CLA	O2D-CGD-CBD	5.28	120.65	111.27
14	a	1136	CLA	C1C-C2C-C3C	-5.28	101.40	106.96
14	U	1503	CLA	O2A-C1-C2	5.28	122.52	108.64
14	a	1126	CLA	C4A-NA-C1A	5.28	109.08	106.71
14	A	1127	CLA	O2A-CGA-O1A	-5.28	110.27	123.59
14	l	1503	CLA	O2A-C1-C2	5.28	122.51	108.64
14	b	1209	CLA	C1C-C2C-C3C	-5.28	101.41	106.96
14	B	1204	CLA	C1C-C2C-C3C	-5.28	101.41	106.96
14	a	1101	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
14	a	1013	CLA	O2D-CGD-CBD	5.28	120.65	111.27
14	A	1101	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
14	B	1215	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
14	a	1104	CLA	O2A-CGA-O1A	-5.28	110.27	123.59
14	H	1201	CLA	C1C-C2C-C3C	-5.28	101.41	106.96
14	G	1128	CLA	O2A-C1-C2	5.28	122.50	108.64
14	A	1104	CLA	O2A-CGA-O1A	-5.27	110.28	123.59
14	a	1128	CLA	O2A-C1-C2	5.27	122.50	108.64
15	H	1237	F6C	O2D-CGD-CBD	5.27	120.64	111.27
14	a	1132	CLA	O2A-C1-C2	5.27	122.50	108.64
13	a	1011	CL0	O2A-CGA-O1A	-5.27	110.28	123.59
14	G	1107	CLA	C4A-NA-C1A	5.27	109.08	106.71
14	H	1220	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
14	a	1127	CLA	O2A-CGA-O1A	-5.27	110.29	123.59
14	H	1204	CLA	C1C-C2C-C3C	-5.27	101.41	106.96
14	G	1136	CLA	C4A-NA-C1A	5.27	109.08	106.71
14	A	1132	CLA	O2A-C1-C2	5.27	122.49	108.64
14	G	1108	CLA	CHD-C1D-ND	-5.27	119.61	124.45
14	A	1135	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
14	b	1214	CLA	O2A-C1-C2	5.27	122.48	108.64
14	B	1220	CLA	C3D-C2D-C1D	-5.27	98.64	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1224	CLA	O2A-C1-C2	5.27	122.48	108.64
14	a	1123	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
14	b	1218	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
14	B	1021	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
14	B	1235	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
14	B	1210	CLA	CHD-C1D-ND	-5.27	119.61	124.45
14	G	1136	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
14	B	1211	CLA	C1C-C2C-C3C	-5.27	101.42	106.96
14	A	1013	CLA	O2D-CGD-CBD	5.26	120.62	111.27
14	B	1224	CLA	O2A-C1-C2	5.26	122.47	108.64
14	H	1218	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
14	U	1501	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
14	H	1215	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
14	B	1229	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
14	W	1701	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
14	G	1102	CLA	C1C-C2C-C3C	-5.26	101.42	106.96
14	H	1210	CLA	CHD-C1D-ND	-5.26	119.62	124.45
14	b	1226	CLA	CHD-C1D-ND	-5.26	119.62	124.45
14	A	1104	CLA	O2D-CGD-CBD	5.26	120.62	111.27
14	G	1132	CLA	O2A-C1-C2	5.26	122.46	108.64
14	a	1104	CLA	O2D-CGD-CBD	5.26	120.61	111.27
14	G	1104	CLA	O2A-CGA-O1A	-5.26	110.32	123.59
14	A	1102	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
14	b	1231	CLA	C1C-C2C-C3C	-5.26	101.43	106.96
14	H	1229	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
13	A	1011	CL0	O2A-CGA-O1A	-5.26	110.32	123.59
18	R	4020	BCR	C24-C23-C22	-5.26	118.29	126.23
18	I	4020	BCR	C24-C23-C22	-5.26	118.29	126.23
14	b	1208	CLA	CHD-C1D-ND	-5.26	119.62	124.45
14	G	1104	CLA	O2D-CGD-CBD	5.26	120.61	111.27
14	G	1101	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
14	H	1214	CLA	O2A-C1-C2	5.25	122.44	108.64
14	G	1138	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
14	H	1217	CLA	O2A-C1-C2	5.25	122.44	108.64
14	A	1128	CLA	O2A-C1-C2	5.25	122.44	108.64
14	B	1217	CLA	O2A-C1-C2	5.25	122.44	108.64
14	H	1211	CLA	CHD-C1D-ND	-5.25	119.63	124.45
14	H	1023	CLA	O2A-C1-C2	5.25	122.43	108.64
14	b	1224	CLA	O2A-C1-C2	5.25	122.43	108.64
15	b	1237	F6C	O2D-CGD-CBD	5.25	120.60	111.27
14	B	1214	CLA	O2A-C1-C2	5.25	122.43	108.64
14	a	1102	CLA	C1C-C2C-C3C	-5.25	101.44	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1231	CLA	C1C-C2C-C3C	-5.25	101.44	106.96
14	b	1210	CLA	CHD-C1D-ND	-5.24	119.64	124.45
14	G	1013	CLA	O2D-CGD-CBD	5.24	120.58	111.27
14	b	1217	CLA	O2A-C1-C2	5.24	122.41	108.64
14	A	1130	CLA	CHD-C1D-ND	-5.24	119.64	124.45
14	A	1124	CLA	O2D-CGD-CBD	5.24	120.58	111.27
14	l	1502	CLA	C1C-C2C-C3C	-5.24	101.45	106.96
18	i	4020	BCR	C24-C23-C22	-5.24	118.32	126.23
14	b	1201	CLA	C1C-C2C-C3C	-5.24	101.45	106.96
14	a	1124	CLA	O2D-CGD-CBD	5.24	120.57	111.27
14	H	1235	CLA	C1C-C2C-C3C	-5.24	101.45	106.96
13	G	1011	CL0	O2A-CGA-O1A	-5.24	110.38	123.59
14	H	1231	CLA	C1C-C2C-C3C	-5.23	101.45	106.96
14	B	1232	CLA	C1C-C2C-C3C	-5.23	101.45	106.96
14	a	1103	CLA	O2A-C1-C2	5.23	122.39	108.64
14	A	1112	CLA	O2A-CGA-O1A	-5.23	110.39	123.59
14	H	1209	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
14	A	1138	CLA	C4A-NA-C1A	5.23	109.06	106.71
14	G	1124	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
14	G	1111	CLA	O2A-C1-C2	5.23	122.38	108.64
14	b	1235	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
14	a	1111	CLA	O2A-C1-C2	5.23	122.38	108.64
14	G	1110	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
18	H	4014	BCR	C7-C8-C9	-5.23	118.34	126.23
14	B	1201	CLA	CHD-C1D-ND	-5.23	119.65	124.45
14	B	1023	CLA	O2A-C1-C2	5.23	122.37	108.64
14	b	1229	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
14	A	1138	CLA	C1C-C2C-C3C	-5.23	101.46	106.96
14	a	1133	CLA	O2A-CGA-O1A	-5.22	110.41	123.59
14	a	1107	CLA	C4A-NA-C1A	5.22	109.05	106.71
14	a	1125	CLA	O2A-CGA-O1A	-5.22	110.41	123.59
14	H	1208	CLA	CHD-C1D-ND	-5.22	119.66	124.45
14	b	1206	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
14	B	1201	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
14	H	1211	CLA	C4A-NA-C1A	5.22	109.05	106.71
14	A	1140	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
14	A	1107	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
14	A	1103	CLA	O2A-C1-C2	5.22	122.35	108.64
14	A	1133	CLA	O2A-CGA-O1A	-5.22	110.42	123.59
14	H	1231	CLA	O2A-C1-C2	5.22	122.35	108.64
14	G	1106	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
14	A	1110	CLA	C3D-C2D-C1D	-5.22	98.71	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	i	4018	BCR	C24-C23-C22	-5.22	118.35	126.23
18	I	4018	BCR	C24-C23-C22	-5.22	118.35	126.23
14	a	1108	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
14	A	1111	CLA	O2A-C1-C2	5.22	122.34	108.64
14	U	1502	CLA	C1C-C2C-C3C	-5.22	101.47	106.96
18	B	4014	BCR	C7-C8-C9	-5.22	118.35	126.23
14	G	1112	CLA	O2A-CGA-O1A	-5.22	110.43	123.59
14	H	1201	CLA	CHD-C1D-ND	-5.22	119.66	124.45
14	G	1125	CLA	O2A-CGA-O1A	-5.22	110.43	123.59
14	B	1215	CLA	O2D-CGD-CBD	5.22	120.53	111.27
14	a	1108	CLA	CHD-C1D-ND	-5.21	119.66	124.45
14	B	1233	CLA	O2D-CGD-CBD	5.21	120.53	111.27
14	b	1023	CLA	O2A-C1-C2	5.21	122.33	108.64
14	b	1211	CLA	CHD-C1D-ND	-5.21	119.67	124.45
14	L	1502	CLA	C1C-C2C-C3C	-5.21	101.48	106.96
14	a	1112	CLA	O2A-CGA-O1A	-5.21	110.44	123.59
14	a	1124	CLA	C1C-C2C-C3C	-5.21	101.48	106.96
14	H	1021	CLA	C1C-C2C-C3C	-5.21	101.48	106.96
14	B	1211	CLA	CHD-C1D-ND	-5.21	119.67	124.45
14	b	1233	CLA	O2D-CGD-CBD	5.21	120.52	111.27
14	b	1021	CLA	C1C-C2C-C3C	-5.21	101.48	106.96
14	A	1106	CLA	C1C-C2C-C3C	-5.21	101.48	106.96
14	H	1233	CLA	O2D-CGD-CBD	5.21	120.52	111.27
14	G	1109	CLA	CHD-C1D-ND	-5.20	119.67	124.45
14	G	1129	CLA	C1C-C2C-C3C	-5.20	101.48	106.96
14	H	1210	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	K	1401	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	H	1206	CLA	C1C-C2C-C3C	-5.20	101.49	106.96
14	G	1103	CLA	O2A-C1-C2	5.20	122.31	108.64
14	G	1124	CLA	O2D-CGD-CBD	5.20	120.51	111.27
14	b	1215	CLA	O2D-CGD-CBD	5.20	120.51	111.27
18	R	4018	BCR	C24-C23-C22	-5.20	118.38	126.23
14	a	1140	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	H	1208	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	a	1110	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	b	1231	CLA	O2A-C1-C2	5.20	122.30	108.64
14	B	1208	CLA	CHD-C1D-ND	-5.20	119.68	124.45
14	A	1127	CLA	O2D-CGD-CBD	5.20	120.50	111.27
14	b	1210	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
14	A	1108	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
14	B	1217	CLA	O2A-CGA-O1A	-5.20	110.48	123.59
14	a	1109	CLA	CHD-C1D-ND	-5.20	119.68	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1109	CLA	CHD-C1D-ND	-5.20	119.68	124.45
14	b	1217	CLA	O2A-CGA-O1A	-5.20	110.48	123.59
14	G	1140	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
14	a	1116	CLA	C3D-C2D-C1D	-5.19	98.74	105.83
14	b	1201	CLA	CHD-C1D-ND	-5.19	119.68	124.45
14	b	1022	CLA	C4A-NA-C1A	5.19	109.04	106.71
14	a	1106	CLA	C1C-C2C-C3C	-5.19	101.50	106.96
14	B	1211	CLA	C4A-NA-C1A	5.19	109.04	106.71
15	H	1238	F6C	O2D-CGD-CBD	5.19	120.49	111.27
14	B	1231	CLA	O2A-C1-C2	5.19	122.28	108.64
18	l	4022	BCR	C24-C23-C22	-5.19	118.39	126.23
14	H	1215	CLA	O2D-CGD-CBD	5.19	120.49	111.27
14	A	1134	CLA	CHD-C1D-ND	-5.19	119.69	124.45
14	A	1112	CLA	C1C-C2C-C3C	-5.19	101.50	106.96
14	A	1129	CLA	C1C-C2C-C3C	-5.19	101.50	106.96
18	b	4014	BCR	C7-C8-C9	-5.19	118.39	126.23
14	H	1217	CLA	O2A-CGA-O1A	-5.19	110.50	123.59
14	b	1208	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
14	A	1125	CLA	O2A-CGA-O1A	-5.19	110.50	123.59
14	B	1236	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
14	G	1138	CLA	C4A-NA-C1A	5.19	109.04	106.71
14	B	1208	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	a	1112	CLA	C1C-C2C-C3C	-5.18	101.51	106.96
14	B	1206	CLA	C1C-C2C-C3C	-5.18	101.51	106.96
14	a	1138	CLA	C1C-C2C-C3C	-5.18	101.51	106.96
14	A	1116	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
18	G	4008	BCR	C24-C23-C22	-5.18	118.41	126.23
14	G	1134	CLA	CHD-C1D-ND	-5.18	119.69	124.45
14	L	1503	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	G	1133	CLA	O2A-CGA-O1A	-5.18	110.52	123.59
15	H	1207	F6C	C2D-C1D-ND	5.18	114.83	109.97
14	B	1210	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	U	1503	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
18	a	4008	BCR	C24-C23-C22	-5.18	118.41	126.23
14	H	1229	CLA	O2A-CGA-O1A	-5.18	110.52	123.59
18	L	4022	BCR	C24-C23-C22	-5.18	118.41	126.23
14	G	1107	CLA	C1C-C2C-C3C	-5.18	101.51	106.96
14	G	1108	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
18	U	4022	BCR	C24-C23-C22	-5.18	118.41	126.23
14	G	1112	CLA	CHD-C1D-ND	-5.18	119.70	124.45
14	A	1105	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
14	a	1129	CLA	C1C-C2C-C3C	-5.17	101.52	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1101	CLA	C4A-NA-C1A	5.17	109.03	106.71
14	A	1124	CLA	C1C-C2C-C3C	-5.17	101.52	106.96
14	B	1234	CLA	O2A-C1-C2	5.17	122.23	108.64
14	G	1112	CLA	C1C-C2C-C3C	-5.17	101.52	106.96
14	k	1401	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
14	b	1021	CLA	O2D-CGD-CBD	5.17	120.46	111.27
14	b	1211	CLA	C4A-NA-C1A	5.17	109.03	106.71
14	b	1229	CLA	O2A-CGA-O1A	-5.17	110.54	123.59
14	a	1105	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
14	H	1236	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
14	a	1107	CLA	C1C-C2C-C3C	-5.17	101.52	106.96
14	a	1112	CLA	CHD-C1D-ND	-5.17	119.70	124.45
14	b	1232	CLA	C1C-C2C-C3C	-5.17	101.52	106.96
14	G	1105	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
15	B	1207	F6C	C2D-C1D-ND	5.17	114.81	109.97
14	B	1224	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
14	A	1133	CLA	CHD-C1D-ND	-5.17	119.71	124.45
14	b	1236	CLA	C3D-C2D-C1D	-5.16	98.78	105.83
14	G	1116	CLA	C3D-C2D-C1D	-5.16	98.78	105.83
14	G	1108	CLA	O2D-CGD-CBD	5.16	120.44	111.27
14	a	1127	CLA	O2D-CGD-CBD	5.16	120.44	111.27
14	B	1234	CLA	O2D-CGD-CBD	5.16	120.44	111.27
14	b	1226	CLA	C4A-NA-C1A	5.16	109.03	106.71
14	b	1234	CLA	O2A-C1-C2	5.16	122.20	108.64
14	B	1229	CLA	O2A-CGA-O1A	-5.16	110.57	123.59
14	G	1112	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	a	1103	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	b	1234	CLA	O2D-CGD-CBD	5.16	120.44	111.27
14	H	1234	CLA	O2A-C1-C2	5.16	122.19	108.64
14	a	1137	CLA	C4A-NA-C1A	5.16	109.02	106.71
14	a	1138	CLA	C4A-NA-C1A	5.16	109.02	106.71
14	T	1401	CLA	C3D-C2D-C1D	-5.16	98.80	105.83
14	H	1021	CLA	O2D-CGD-CBD	5.15	120.43	111.27
14	H	1232	CLA	C1C-C2C-C3C	-5.15	101.54	106.96
14	H	1213	CLA	C4A-NA-C1A	5.15	109.02	106.71
14	A	1110	CLA	CHD-C1D-ND	-5.15	119.72	124.45
14	B	1208	CLA	O2A-C1-C2	5.15	122.17	108.64
14	B	1205	CLA	C1C-C2C-C3C	-5.15	101.54	106.96
14	G	1127	CLA	O2D-CGD-CBD	5.15	120.42	111.27
14	B	1021	CLA	O2D-CGD-CBD	5.15	120.42	111.27
14	b	1205	CLA	C1C-C2C-C3C	-5.15	101.55	106.96
14	A	1137	CLA	CHD-C1D-ND	-5.15	119.72	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1238	F6C	O2D-CGD-CBD	5.15	120.41	111.27
14	B	1022	CLA	C4A-NA-C1A	5.14	109.02	106.71
14	H	1234	CLA	O2D-CGD-CBD	5.14	120.41	111.27
14	A	1108	CLA	O2D-CGD-CBD	5.14	120.41	111.27
15	b	1238	F6C	O2D-CGD-CBD	5.14	120.41	111.27
14	l	1503	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
14	H	1224	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
14	a	1122	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
14	B	1236	CLA	C1D-ND-C4D	-5.14	102.68	106.33
15	b	1207	F6C	C2D-C1D-ND	5.14	114.79	109.97
14	G	1128	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
14	a	1137	CLA	CHD-C1D-ND	-5.14	119.73	124.45
18	A	4008	BCR	C24-C23-C22	-5.14	118.47	126.23
14	T	1401	CLA	CHD-C1D-ND	-5.14	119.73	124.45
14	H	1022	CLA	O2A-CGA-O1A	-5.14	110.62	123.59
15	b	1237	F6C	O2A-C1-C2	5.14	122.14	108.64
14	H	1205	CLA	C1C-C2C-C3C	-5.14	101.56	106.96
14	a	1109	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
14	A	1112	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
14	H	1236	CLA	C1D-ND-C4D	-5.14	102.69	106.33
14	H	1208	CLA	O2A-C1-C2	5.14	122.13	108.64
14	G	1130	CLA	O2D-CGD-CBD	5.13	120.39	111.27
14	b	1208	CLA	O2A-C1-C2	5.13	122.12	108.64
14	a	1110	CLA	CHD-C1D-ND	-5.13	119.74	124.45
14	k	1401	CLA	CHD-C1D-ND	-5.13	119.74	124.45
14	G	1132	CLA	C4A-NA-C1A	5.13	109.01	106.71
14	a	1133	CLA	CHD-C1D-ND	-5.13	119.74	124.45
14	b	1224	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
15	B	1237	F6C	O2A-C1-C2	5.13	122.12	108.64
14	H	1220	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
14	G	1110	CLA	CHD-C1D-ND	-5.13	119.74	124.45
14	b	1208	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
14	G	1133	CLA	CHD-C1D-ND	-5.13	119.74	124.45
14	G	1109	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
14	A	1123	CLA	O2A-C1-C2	5.13	122.11	108.64
14	B	1232	CLA	C3D-C2D-C1D	-5.13	98.84	105.83
14	a	1112	CLA	C3D-C2D-C1D	-5.13	98.84	105.83
18	G	4001	BCR	C7-C8-C9	-5.13	118.49	126.23
14	H	1208	CLA	C1C-C2C-C3C	-5.13	101.57	106.96
14	b	1022	CLA	O2A-CGA-O1A	-5.13	110.66	123.59
14	a	1128	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	a	1123	CLA	O2A-C1-C2	5.12	122.10	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1109	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	H	1232	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	b	1208	CLA	O2A-CGA-O1A	-5.12	110.67	123.59
14	G	1115	CLA	O2A-C1-C2	5.12	122.09	108.64
14	B	1228	CLA	O2A-C1-C2	5.12	122.09	108.64
14	A	1122	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	G	1137	CLA	C4A-NA-C1A	5.12	109.01	106.71
15	H	1237	F6C	O2A-C1-C2	5.12	122.09	108.64
14	b	1228	CLA	O2A-C1-C2	5.12	122.09	108.64
14	A	1128	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
18	a	4001	BCR	C7-C8-C9	-5.12	118.50	126.23
14	a	1108	CLA	O2D-CGD-CBD	5.12	120.36	111.27
14	G	1103	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
15	G	1121	F6C	C2D-C1D-ND	5.12	114.77	109.97
14	b	1220	CLA	C1C-C2C-C3C	-5.12	101.58	106.96
14	G	1122	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
14	b	1219	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
14	A	1103	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
14	B	1233	CLA	O2A-CGA-O1A	-5.11	110.55	123.30
14	A	1112	CLA	CHD-C1D-ND	-5.11	119.75	124.45
14	A	1122	CLA	CHD-C1D-ND	-5.11	119.75	124.45
14	B	1208	CLA	C1C-C2C-C3C	-5.11	101.58	106.96
18	B	4006	BCR	C7-C8-C9	-5.11	118.51	126.23
14	a	1134	CLA	CHD-C1D-ND	-5.11	119.76	124.45
14	a	1133	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
14	a	1130	CLA	O2D-CGD-CBD	5.11	120.35	111.27
14	A	1139	CLA	O2D-CGD-CBD	5.11	120.35	111.27
14	B	1220	CLA	C1C-C2C-C3C	-5.11	101.58	106.96
14	H	1233	CLA	O2A-CGA-O1A	-5.11	110.56	123.30
14	H	1219	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
14	B	1208	CLA	O2A-CGA-O1A	-5.11	110.70	123.59
14	G	1133	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
14	B	1235	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
15	H	1207	F6C	C3D-C2D-C1D	-5.11	98.44	105.83
14	G	1123	CLA	O2A-C1-C2	5.11	122.05	108.64
14	a	1115	CLA	O2A-C1-C2	5.11	122.05	108.64
14	A	1115	CLA	O2A-C1-C2	5.10	122.05	108.64
14	H	1203	CLA	O2D-CGD-CBD	5.10	120.33	111.27
14	G	1132	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	B	1206	CLA	CHD-C1D-ND	-5.10	119.77	124.45
14	H	1208	CLA	O2A-CGA-O1A	-5.10	110.72	123.59
14	B	1229	CLA	C1D-ND-C4D	-5.10	102.71	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1115	CLA	C1C-C2C-C3C	-5.10	101.60	106.96
14	a	1137	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	H	1228	CLA	O2A-C1-C2	5.10	122.03	108.64
14	B	1203	CLA	C4A-NA-C1A	5.10	109.00	106.71
14	a	1122	CLA	CHD-C1D-ND	-5.10	119.77	124.45
14	A	1130	CLA	O2D-CGD-CBD	5.10	120.33	111.27
14	B	1219	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	G	1137	CLA	CHD-C1D-ND	-5.10	119.77	124.45
14	G	1117	CLA	C1C-C2C-C3C	-5.10	101.60	106.96
14	b	1233	CLA	O2A-CGA-O1A	-5.10	110.60	123.30
14	b	1229	CLA	C1D-ND-C4D	-5.10	102.72	106.33
14	B	1203	CLA	O2D-CGD-CBD	5.09	120.32	111.27
18	H	4006	BCR	C7-C8-C9	-5.09	118.54	126.23
18	A	4001	BCR	C7-C8-C9	-5.09	118.54	126.23
14	B	1022	CLA	O2A-CGA-O1A	-5.09	110.74	123.59
14	H	1219	CLA	CHD-C1D-ND	-5.09	119.77	124.45
15	H	1230	F6C	C1A-C2A-C3A	-5.09	101.61	106.97
14	A	1117	CLA	C1C-C2C-C3C	-5.09	101.60	106.96
14	G	1101	CLA	C4A-NA-C1A	5.09	109.00	106.71
14	H	1234	CLA	O2A-CGA-O1A	-5.09	110.75	123.59
14	A	1136	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
14	b	1232	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
14	b	1234	CLA	O2A-CGA-O1A	-5.09	110.75	123.59
14	G	1122	CLA	CHD-C1D-ND	-5.09	119.78	124.45
15	b	1207	F6C	C3D-C2D-C1D	-5.09	98.46	105.83
14	G	1110	CLA	C1C-C2C-C3C	-5.09	101.61	106.96
14	b	1212	CLA	C1C-C2C-C3C	-5.09	101.61	106.96
14	A	1133	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
14	a	1139	CLA	O2D-CGD-CBD	5.09	120.31	111.27
14	b	1235	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
14	B	1234	CLA	O2A-CGA-O1A	-5.09	110.76	123.59
14	a	1117	CLA	C1C-C2C-C3C	-5.08	101.61	106.96
14	G	1139	CLA	O2D-CGD-CBD	5.08	120.30	111.27
14	H	1206	CLA	CHD-C1D-ND	-5.08	119.78	124.45
14	b	1203	CLA	O2D-CGD-CBD	5.08	120.30	111.27
15	B	1237	F6C	C4A-NA-C1A	5.08	109.95	106.33
14	H	1216	CLA	O2A-C1-C2	5.08	121.99	108.64
18	b	4006	BCR	C7-C8-C9	-5.08	118.56	126.23
14	H	1203	CLA	C4A-NA-C1A	5.08	108.99	106.71
14	B	1216	CLA	O2A-C1-C2	5.08	121.99	108.64
14	A	1132	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
14	G	1117	CLA	C3D-C2D-C1D	-5.08	98.90	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1216	CLA	O2A-C1-C2	5.08	121.98	108.64
14	A	1134	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
13	a	1011	CL0	C4A-NA-C1A	5.08	108.99	106.71
14	G	1115	CLA	C1C-C2C-C3C	-5.08	101.62	106.96
14	a	1101	CLA	C4A-NA-C1A	5.08	108.99	106.71
15	b	1238	F6C	C3A-C4A-NA	5.08	113.84	110.10
14	H	1235	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	B	1216	CLA	CHD-C1D-ND	-5.07	119.79	124.45
14	B	1206	CLA	O2A-CGA-O1A	-5.07	110.65	123.30
14	H	1209	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
13	G	1011	CL0	C4A-NA-C1A	5.07	108.99	106.71
15	B	1207	F6C	C3D-C2D-C1D	-5.07	98.48	105.83
14	a	1134	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	b	1219	CLA	CHD-C1D-ND	-5.07	119.79	124.45
14	a	1132	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	G	1134	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	G	1137	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	B	1219	CLA	CHD-C1D-ND	-5.07	119.80	124.45
15	B	1230	F6C	C3D-C2D-C1D	-5.07	98.49	105.83
15	B	1230	F6C	C1A-C2A-C3A	-5.07	101.63	106.97
14	H	1022	CLA	C4A-NA-C1A	5.07	108.98	106.71
14	K	1401	CLA	CHD-C1D-ND	-5.07	119.80	124.45
14	A	1110	CLA	C1C-C2C-C3C	-5.07	101.63	106.96
15	b	1230	F6C	C3D-C2D-C1D	-5.07	98.49	105.83
14	G	1101	CLA	CHD-C1D-ND	-5.07	119.80	124.45
15	A	1121	F6C	C2D-C1D-ND	5.07	114.72	109.97
14	X	1701	CLA	C4A-NA-C1A	5.06	108.98	106.71
14	A	1117	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
14	a	1101	CLA	O2A-CGA-O1A	-5.06	110.68	123.30
14	H	1212	CLA	C1C-C2C-C3C	-5.06	101.63	106.96
14	b	1209	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
14	b	1206	CLA	O2A-CGA-O1A	-5.06	110.68	123.30
14	a	1103	CLA	C1C-C2C-C3C	-5.06	101.64	106.96
14	a	1132	CLA	C4A-NA-C1A	5.06	108.98	106.71
14	b	1203	CLA	C4A-NA-C1A	5.06	108.98	106.71
14	a	1120	CLA	C1D-ND-C4D	-5.06	102.74	106.33
15	H	1238	F6C	C3A-C4A-NA	5.06	113.83	110.10
14	a	1110	CLA	C1C-C2C-C3C	-5.06	101.64	106.96
14	A	1102	CLA	C4A-NA-C1A	5.06	108.98	106.71
14	a	1101	CLA	CHD-C1D-ND	-5.06	119.81	124.45
14	H	1206	CLA	O2A-CGA-O1A	-5.06	110.70	123.30
14	B	1233	CLA	C3D-C2D-C1D	-5.05	98.93	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1238	F6C	C3A-C4A-NA	5.05	113.83	110.10
14	a	1115	CLA	C1C-C2C-C3C	-5.05	101.64	106.96
14	G	1101	CLA	O2A-CGA-O1A	-5.05	110.70	123.30
14	A	1137	CLA	C3D-C2D-C1D	-5.05	98.93	105.83
15	H	1230	F6C	C3D-C2D-C1D	-5.05	98.51	105.83
14	b	1233	CLA	CHD-C1D-ND	-5.05	119.81	124.45
14	B	1214	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
14	A	1103	CLA	C1C-C2C-C3C	-5.05	101.65	106.96
14	a	1137	CLA	O2A-CGA-O1A	-5.05	110.85	123.59
18	B	4004	BCR	C7-C8-C9	-5.05	118.61	126.23
14	B	1236	CLA	C4A-NA-C1A	5.05	108.97	106.71
14	a	1138	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
14	b	1206	CLA	C3D-C2D-C1D	-5.05	98.95	105.83
14	G	1137	CLA	O2A-CGA-O1A	-5.04	110.86	123.59
14	b	1023	CLA	O2A-CGA-O1A	-5.04	110.86	123.59
14	G	1120	CLA	C1D-ND-C4D	-5.04	102.75	106.33
14	B	1226	CLA	C4A-NA-C1A	5.04	108.97	106.71
14	b	1023	CLA	O2D-CGD-CBD	5.04	120.23	111.27
14	b	1206	CLA	CHD-C1D-ND	-5.04	119.82	124.45
14	A	1101	CLA	O2A-CGA-O1A	-5.04	110.73	123.30
15	a	1121	F6C	C2D-C1D-ND	5.04	114.69	109.97
14	H	1206	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
14	a	1136	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
18	b	4004	BCR	C7-C8-C9	-5.04	118.62	126.23
14	a	1117	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
14	A	1138	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
14	b	1222	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
14	B	1231	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
14	B	1209	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
14	H	1233	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
14	G	1101	CLA	C1C-C2C-C3C	-5.03	101.66	106.96
14	G	1138	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
14	B	1218	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
14	A	1137	CLA	O2A-CGA-O1A	-5.03	110.89	123.59
14	a	1139	CLA	C1C-C2C-C3C	-5.03	101.67	106.96
14	H	1229	CLA	C1D-ND-C4D	-5.03	102.76	106.33
14	B	1023	CLA	O2D-CGD-CBD	5.03	120.21	111.27
14	H	1226	CLA	C4A-NA-C1A	5.03	108.97	106.71
14	a	1102	CLA	C4A-NA-C1A	5.03	108.97	106.71
15	b	1230	F6C	C1A-C2A-C3A	-5.03	101.67	106.97
14	b	1231	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
14	B	1206	CLA	C3D-C2D-C1D	-5.03	98.97	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1233	CLA	CHD-C1D-ND	-5.03	119.84	124.45
14	b	1214	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
14	H	1220	CLA	CHD-C1D-ND	-5.02	119.84	124.45
14	b	1213	CLA	C1C-C2C-C3C	-5.02	101.67	106.96
14	H	1216	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
14	b	1236	CLA	C1D-ND-C4D	-5.02	102.77	106.33
14	H	1023	CLA	O2D-CGD-CBD	5.02	120.19	111.27
14	G	1127	CLA	O2A-C1-C2	5.02	121.83	108.64
18	H	4004	BCR	C7-C8-C9	-5.02	118.65	126.23
14	b	1233	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
14	G	1103	CLA	C1C-C2C-C3C	-5.02	101.68	106.96
14	H	1209	CLA	O2A-CGA-O1A	-5.02	110.79	123.30
14	B	1209	CLA	O2A-CGA-O1A	-5.02	110.79	123.30
14	B	1204	CLA	O2A-CGA-O1A	-5.02	110.93	123.59
14	B	1023	CLA	O2A-CGA-O1A	-5.02	110.93	123.59
14	A	1127	CLA	O2A-C1-C2	5.02	121.82	108.64
14	b	1225	CLA	C1C-C2C-C3C	-5.02	101.68	106.96
14	G	1102	CLA	C4A-NA-C1A	5.02	108.96	106.71
15	H	1237	F6C	C3D-C2D-C1D	-5.02	98.57	105.83
14	b	1216	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	a	1119	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	H	1023	CLA	O2A-CGA-O1A	-5.01	110.94	123.59
14	B	1213	CLA	C4A-NA-C1A	5.01	108.96	106.71
14	H	1211	CLA	O2D-CGD-CBD	5.01	120.18	111.27
14	G	1136	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
15	b	1207	F6C	CAA-C2A-C1A	-5.01	114.30	128.11
14	H	1214	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
13	A	1011	CL0	C4A-NA-C1A	5.01	108.96	106.71
14	b	1213	CLA	C4A-NA-C1A	5.01	108.96	106.71
14	A	1101	CLA	C1C-C2C-C3C	-5.01	101.69	106.96
14	B	1212	CLA	C1C-C2C-C3C	-5.01	101.69	106.96
14	B	1220	CLA	CHD-C1D-ND	-5.01	119.85	124.45
14	A	1132	CLA	O2A-CGA-O1A	-5.01	110.95	123.59
14	A	1132	CLA	C4A-NA-C1A	5.01	108.96	106.71
14	A	1101	CLA	CHD-C1D-ND	-5.01	119.85	124.45
15	B	1207	F6C	CAA-C2A-C1A	-5.01	114.32	128.11
14	G	1129	CLA	O2A-CGA-O1A	-5.01	110.95	123.59
14	b	1204	CLA	O2A-CGA-O1A	-5.01	110.95	123.59
14	H	1213	CLA	C1C-C2C-C3C	-5.01	101.69	106.96
14	a	1132	CLA	O2A-CGA-O1A	-5.01	110.95	123.59
14	b	1209	CLA	O2A-CGA-O1A	-5.01	110.82	123.30
14	A	1131	CLA	C3D-C2D-C1D	-5.01	99.00	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1231	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
14	A	1137	CLA	C4A-NA-C1A	5.00	108.96	106.71
14	G	1139	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
14	A	1120	CLA	C1D-ND-C4D	-5.00	102.78	106.33
14	G	1132	CLA	O2A-CGA-O1A	-5.00	110.96	123.59
14	B	1222	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
14	A	1139	CLA	C1C-C2C-C3C	-5.00	101.70	106.96
14	a	1127	CLA	O2A-C1-C2	5.00	121.78	108.64
14	b	1236	CLA	C4A-NA-C1A	5.00	108.95	106.71
14	H	1204	CLA	O2A-CGA-O1A	-5.00	110.97	123.59
14	a	1101	CLA	C1C-C2C-C3C	-5.00	101.70	106.96
14	b	1220	CLA	CHD-C1D-ND	-5.00	119.86	124.45
15	H	1207	F6C	CAA-C2A-C1A	-5.00	114.34	128.11
14	H	1218	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
14	B	1215	CLA	C4A-NA-C1A	5.00	108.95	106.71
14	H	1225	CLA	C1C-C2C-C3C	-5.00	101.70	106.96
14	A	1012	CLA	O2A-CGA-O1A	-5.00	110.98	123.59
14	a	1127	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
14	G	1127	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
14	a	1113	CLA	O2A-CGA-O1A	-4.99	110.85	123.30
14	B	1225	CLA	C1C-C2C-C3C	-4.99	101.71	106.96
14	B	1213	CLA	CHD-C1D-ND	-4.99	119.86	124.45
14	H	1211	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
14	G	1131	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
14	A	1107	CLA	O2A-CGA-O1A	-4.99	110.86	123.30
14	G	1120	CLA	CHD-C1D-ND	-4.99	119.87	124.45
14	H	1213	CLA	CHD-C1D-ND	-4.99	119.87	124.45
14	a	1107	CLA	O2A-CGA-O1A	-4.99	110.86	123.30
14	A	1119	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
14	G	1139	CLA	C1C-C2C-C3C	-4.99	101.71	106.96
15	b	1237	F6C	C3D-C2D-C1D	-4.99	98.61	105.83
14	A	1103	CLA	CHD-C1D-ND	-4.99	119.87	124.45
14	H	1216	CLA	CHD-C1D-ND	-4.99	119.87	124.45
14	a	1012	CLA	O2A-CGA-O1A	-4.99	111.00	123.59
14	G	1012	CLA	O2A-CGA-O1A	-4.99	111.00	123.59
14	b	1216	CLA	CHD-C1D-ND	-4.99	119.87	124.45
14	b	1239	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
14	a	1120	CLA	CHD-C1D-ND	-4.99	119.87	124.45
14	a	1129	CLA	O2A-CGA-O1A	-4.99	111.01	123.59
14	B	1211	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
14	B	1226	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
14	b	1239	CLA	CHD-C1D-ND	-4.98	119.88	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1233	CLA	C4A-NA-C1A	4.98	108.95	106.71
14	A	1139	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
14	G	1113	CLA	O2A-CGA-O1A	-4.98	110.88	123.30
14	a	1131	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
14	H	1222	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	a	1139	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	H	1239	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	H	1226	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	b	1211	CLA	O2D-CGD-CBD	4.98	120.11	111.27
14	A	1129	CLA	O2A-CGA-O1A	-4.98	111.03	123.59
14	b	1213	CLA	CHD-C1D-ND	-4.98	119.88	124.45
15	B	1237	F6C	C3D-C2D-C1D	-4.98	98.63	105.83
14	b	1226	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	W	1701	CLA	C4A-NA-C1A	4.98	108.94	106.71
14	U	1503	CLA	C1C-C2C-C3C	-4.98	101.73	106.96
14	A	1127	CLA	C3D-C2D-C1D	-4.97	99.04	105.83
14	G	1126	CLA	CHD-C1D-ND	-4.97	119.88	124.45
14	A	1120	CLA	CHD-C1D-ND	-4.97	119.88	124.45
14	B	1211	CLA	O2D-CGD-CBD	4.97	120.10	111.27
14	b	1218	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
14	G	1107	CLA	O2A-CGA-O1A	-4.97	110.91	123.30
14	B	1239	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
14	A	1108	CLA	O2A-CGA-O1A	-4.97	110.91	123.30
14	a	1117	CLA	CHD-C1D-ND	-4.97	119.89	124.45
14	b	1206	CLA	O2D-CGD-CBD	4.97	120.10	111.27
14	B	1239	CLA	CHD-C1D-ND	-4.97	119.89	124.45
14	G	1108	CLA	O2A-CGA-O1A	-4.97	110.92	123.30
14	H	1206	CLA	O2D-CGD-CBD	4.97	120.10	111.27
14	G	1103	CLA	CHD-C1D-ND	-4.97	119.89	124.45
14	G	1117	CLA	CHD-C1D-ND	-4.97	119.89	124.45
14	a	1103	CLA	CHD-C1D-ND	-4.97	119.89	124.45
14	A	1113	CLA	O2A-CGA-O1A	-4.97	110.92	123.30
14	B	1206	CLA	O2D-CGD-CBD	4.97	120.09	111.27
14	B	1205	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
18	I	4018	BCR	C15-C14-C13	-4.97	120.22	127.31
14	H	1226	CLA	O2A-CGA-O1A	-4.97	111.06	123.59
14	b	1211	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
14	b	1226	CLA	O2A-CGA-O1A	-4.97	111.06	123.59
14	H	1205	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
14	b	1205	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
14	a	1140	CLA	C1C-C2C-C3C	-4.96	101.74	106.96
14	H	1236	CLA	C4A-NA-C1A	4.96	108.94	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1221	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
14	A	1114	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
14	G	1123	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
14	a	1139	CLA	O2A-CGA-O1A	-4.96	110.94	123.30
14	B	1233	CLA	CHD-C1D-ND	-4.96	119.90	124.45
14	X	1701	CLA	O2D-CGD-CBD	4.96	120.08	111.27
14	B	1213	CLA	C1C-C2C-C3C	-4.96	101.74	106.96
14	B	1208	CLA	C4A-NA-C1A	4.96	108.94	106.71
14	H	1239	CLA	CHD-C1D-ND	-4.96	119.90	124.45
14	A	1126	CLA	CHD-C1D-ND	-4.96	119.90	124.45
14	a	1126	CLA	CHD-C1D-ND	-4.96	119.90	124.45
14	G	1114	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
14	B	1216	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
14	B	1226	CLA	O2A-CGA-O1A	-4.95	111.09	123.59
14	b	1206	CLA	C4A-NA-C1A	4.95	108.93	106.71
14	G	1119	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
14	A	1115	CLA	O2A-CGA-O1A	-4.95	111.10	123.59
14	b	1202	CLA	CHD-C1D-ND	-4.95	119.91	124.45
14	b	1201	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
14	G	1139	CLA	O2A-CGA-O1A	-4.95	110.97	123.30
14	a	1108	CLA	O2A-CGA-O1A	-4.95	110.97	123.30
14	l	1503	CLA	C1C-C2C-C3C	-4.95	101.75	106.96
15	H	1237	F6C	C4A-NA-C1A	4.95	109.85	106.33
14	G	1118	CLA	O2A-CGA-O1A	-4.95	111.11	123.59
14	a	1114	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
14	x	1701	CLA	O2D-CGD-CBD	4.94	120.05	111.27
15	b	1237	F6C	C4A-NA-C1A	4.94	109.85	106.33
14	a	1123	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
14	W	1701	CLA	O2D-CGD-CBD	4.94	120.05	111.27
14	H	1202	CLA	CHD-C1D-ND	-4.94	119.91	124.45
14	G	1140	CLA	C1C-C2C-C3C	-4.94	101.76	106.96
14	A	1123	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
14	H	1202	CLA	O2A-CGA-CBA	4.94	127.41	111.91
14	a	1115	CLA	O2A-CGA-O1A	-4.94	111.13	123.59
14	B	1201	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
14	A	1140	CLA	C1C-C2C-C3C	-4.94	101.77	106.96
14	a	1123	CLA	C4A-NA-C1A	4.94	108.93	106.71
14	b	1202	CLA	O2A-CGA-CBA	4.94	127.40	111.91
14	A	1139	CLA	O2A-CGA-O1A	-4.94	111.00	123.30
14	a	1122	CLA	O2A-C1-C2	4.94	121.61	108.64
14	A	1117	CLA	CHD-C1D-ND	-4.93	119.92	124.45
14	B	1227	CLA	C2D-C1D-ND	4.93	113.74	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1215	CLA	C4A-NA-C1A	4.93	108.92	106.71
14	G	1134	CLA	O2A-CGA-O1A	-4.93	111.01	123.30
14	G	1115	CLA	O2A-CGA-O1A	-4.93	111.15	123.59
14	H	1221	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
14	A	1118	CLA	O2A-CGA-O1A	-4.93	111.15	123.59
14	A	1123	CLA	O2A-CGA-O1A	-4.93	111.16	123.59
14	a	1101	CLA	C1D-ND-C4D	-4.93	102.84	106.33
14	a	1122	CLA	O2A-CGA-O1A	-4.93	111.16	123.59
14	B	1202	CLA	CHD-C1D-ND	-4.93	119.93	124.45
14	H	1201	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
14	A	1122	CLA	O2A-C1-C2	4.92	121.58	108.64
14	A	1128	CLA	O2A-CGA-O1A	-4.92	111.17	123.59
14	a	1134	CLA	O2A-CGA-O1A	-4.92	111.03	123.30
14	H	1224	CLA	C1C-C2C-C3C	-4.92	101.78	106.96
14	a	1128	CLA	O2A-CGA-O1A	-4.92	111.17	123.59
14	b	1221	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
14	B	1202	CLA	O2A-CGA-CBA	4.92	127.35	111.91
14	G	1128	CLA	O2A-CGA-O1A	-4.92	111.18	123.59
14	b	1233	CLA	C4A-NA-C1A	4.92	108.92	106.71
14	A	1134	CLA	O2A-CGA-O1A	-4.92	111.04	123.30
14	x	1701	CLA	C4A-NA-C1A	4.92	108.92	106.71
14	L	1503	CLA	C1D-ND-C4D	-4.92	102.84	106.33
14	a	1118	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
14	G	1122	CLA	O2A-CGA-O1A	-4.91	111.19	123.59
14	G	1012	CLA	O2D-CGD-CBD	4.91	120.00	111.27
14	B	1224	CLA	C1C-C2C-C3C	-4.91	101.79	106.96
14	A	1138	CLA	CHD-C1D-ND	-4.91	119.94	124.45
14	a	1118	CLA	O2A-CGA-O1A	-4.91	111.19	123.59
18	R	4018	BCR	C15-C14-C13	-4.91	120.30	127.31
14	A	1119	CLA	C1C-C2C-C3C	-4.91	101.79	106.96
14	L	1503	CLA	C1C-C2C-C3C	-4.91	101.79	106.96
14	A	1118	CLA	C4A-NA-C1A	4.91	108.91	106.71
18	i	4018	BCR	C15-C14-C13	-4.91	120.30	127.31
14	G	1124	CLA	C1D-ND-C4D	-4.91	102.85	106.33
14	a	1119	CLA	C1C-C2C-C3C	-4.91	101.80	106.96
15	B	1207	F6C	C1-C2-C3	-4.91	117.56	126.04
14	G	1118	CLA	C4A-NA-C1A	4.91	108.91	106.71
14	a	1123	CLA	O2A-CGA-O1A	-4.91	111.21	123.59
14	G	1122	CLA	O2A-C1-C2	4.90	121.53	108.64
14	H	1234	CLA	C4A-NA-C1A	4.90	108.91	106.71
14	b	1203	CLA	CHD-C1D-ND	-4.90	119.95	124.45
14	B	1225	CLA	O2A-CGA-O1A	-4.90	111.22	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1236	CLA	O2A-CGA-O1A	-4.90	111.08	123.30
14	B	1224	CLA	O2A-CGA-O1A	-4.90	111.22	123.59
14	B	1214	CLA	CHD-C1D-ND	-4.90	119.95	124.45
14	A	1122	CLA	O2A-CGA-O1A	-4.90	111.23	123.59
14	X	1701	CLA	O2A-CGA-O1A	-4.90	111.23	123.59
14	U	1503	CLA	C1D-ND-C4D	-4.90	102.86	106.33
14	H	1221	CLA	O2A-CGA-O1A	-4.90	111.23	123.59
14	A	1124	CLA	C1D-ND-C4D	-4.90	102.86	106.33
14	a	1113	CLA	CHD-C1D-ND	-4.90	119.95	124.45
14	G	1123	CLA	O2A-CGA-O1A	-4.89	111.24	123.59
14	G	1101	CLA	C1D-ND-C4D	-4.89	102.86	106.33
14	b	1236	CLA	O2A-CGA-O1A	-4.89	111.10	123.30
14	G	1118	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
14	A	1118	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
14	A	1012	CLA	O2D-CGD-CBD	4.89	119.96	111.27
14	B	1236	CLA	O2A-CGA-O1A	-4.89	111.11	123.30
14	b	1224	CLA	O2A-CGA-O1A	-4.89	111.25	123.59
14	a	1012	CLA	O2D-CGD-CBD	4.89	119.96	111.27
15	b	1207	F6C	C1-C2-C3	-4.89	117.58	126.04
14	b	1227	CLA	C2D-C1D-ND	4.89	113.71	110.10
14	H	1203	CLA	CHD-C1D-ND	-4.89	119.96	124.45
14	H	1214	CLA	CHD-C1D-ND	-4.89	119.96	124.45
14	H	1224	CLA	O2A-CGA-O1A	-4.89	111.26	123.59
14	B	1221	CLA	O2A-CGA-O1A	-4.89	111.26	123.59
14	B	1222	CLA	O2A-CGA-O1A	-4.89	111.26	123.59
14	G	1104	CLA	O2A-C1-C2	4.89	121.48	108.64
14	A	1104	CLA	O2A-C1-C2	4.89	121.48	108.64
14	H	1225	CLA	O2A-CGA-O1A	-4.89	111.26	123.59
14	b	1225	CLA	O2A-CGA-O1A	-4.89	111.26	123.59
14	b	1221	CLA	O2A-CGA-O1A	-4.89	111.26	123.59
14	H	1215	CLA	C4A-NA-C1A	4.88	108.90	106.71
14	H	1233	CLA	C4A-NA-C1A	4.88	108.90	106.71
14	H	1201	CLA	O2A-C1-C2	4.88	121.47	108.64
14	H	1222	CLA	O2A-CGA-O1A	-4.88	111.27	123.59
14	a	1135	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
14	b	1201	CLA	O2A-C1-C2	4.88	121.47	108.64
14	G	1135	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
14	x	1701	CLA	O2A-CGA-O1A	-4.88	111.28	123.59
14	B	1201	CLA	O2A-C1-C2	4.88	121.45	108.64
14	b	1234	CLA	C4A-NA-C1A	4.88	108.90	106.71
14	a	1104	CLA	O2A-C1-C2	4.88	121.45	108.64
15	H	1230	F6C	O2A-CGA-O1A	-4.88	111.14	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1206	CLA	C4A-NA-C1A	4.88	108.90	106.71
14	H	1208	CLA	C4A-NA-C1A	4.88	108.90	106.71
14	A	1130	CLA	CMB-C2B-C3B	4.87	133.80	124.68
14	a	1114	CLA	CHD-C1D-ND	-4.87	119.97	124.45
14	A	1114	CLA	CHD-C1D-ND	-4.87	119.97	124.45
14	W	1701	CLA	O2A-CGA-O1A	-4.87	111.29	123.59
14	b	1222	CLA	O2A-CGA-O1A	-4.87	111.30	123.59
14	b	1224	CLA	C1C-C2C-C3C	-4.87	101.83	106.96
14	B	1214	CLA	O2A-CGA-O1A	-4.87	111.30	123.59
14	G	1105	CLA	C4A-NA-C1A	4.87	108.90	106.71
14	G	1123	CLA	C4A-NA-C1A	4.87	108.90	106.71
14	G	1138	CLA	CHD-C1D-ND	-4.87	119.98	124.45
14	H	1214	CLA	O2A-CGA-O1A	-4.87	111.30	123.59
15	H	1207	F6C	C1-C2-C3	-4.87	117.62	126.04
14	a	1140	CLA	CHD-C1D-ND	-4.87	119.98	124.45
14	b	1217	CLA	O2D-CGD-CBD	4.87	119.92	111.27
14	a	1124	CLA	C1D-ND-C4D	-4.87	102.88	106.33
14	G	1140	CLA	C4A-NA-C1A	4.87	108.89	106.71
15	B	1230	F6C	O2A-CGA-O1A	-4.87	111.17	123.30
14	G	1130	CLA	CMB-C2B-C3B	4.87	133.78	124.68
14	B	1235	CLA	C4A-NA-C1A	4.87	108.89	106.71
14	b	1212	CLA	C1D-ND-C4D	-4.87	102.88	106.33
14	A	1140	CLA	CHD-C1D-ND	-4.87	119.98	124.45
14	A	1135	CLA	C3D-C2D-C1D	-4.86	99.19	105.83
14	b	1228	CLA	O2A-CGA-O1A	-4.86	111.32	123.59
14	A	1106	CLA	C1D-ND-C4D	-4.86	102.88	106.33
14	b	1214	CLA	O2A-CGA-O1A	-4.86	111.32	123.59
14	A	1114	CLA	O2A-CGA-O1A	-4.86	111.18	123.30
15	b	1238	F6C	C2D-C1D-ND	4.86	114.53	109.97
14	A	1126	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
14	G	1140	CLA	CHD-C1D-ND	-4.86	119.99	124.45
14	a	1114	CLA	O2A-CGA-O1A	-4.86	111.18	123.30
14	B	1206	CLA	C4A-NA-C1A	4.86	108.89	106.71
14	A	1113	CLA	CHD-C1D-ND	-4.86	119.99	124.45
14	G	1106	CLA	C1D-ND-C4D	-4.86	102.88	106.33
14	H	1227	CLA	C2D-C1D-ND	4.86	113.69	110.10
14	G	1013	CLA	CHD-C1D-ND	-4.86	119.99	124.45
14	G	1140	CLA	O2A-CGA-O1A	-4.86	111.33	123.59
14	a	1109	CLA	O2D-CGD-CBD	4.86	119.90	111.27
14	A	1109	CLA	O2D-CGD-CBD	4.86	119.90	111.27
14	B	1217	CLA	O2D-CGD-CBD	4.86	119.90	111.27
14	B	1203	CLA	CHD-C1D-ND	-4.86	119.99	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1129	CLA	O2A-C1-C2	4.86	121.40	108.64
14	b	1214	CLA	CHD-C1D-ND	-4.86	119.99	124.45
14	B	1218	CLA	O2A-CGA-O1A	-4.86	111.20	123.30
15	B	1238	F6C	C2D-C1D-ND	4.85	114.52	109.97
14	a	1140	CLA	O2A-CGA-O1A	-4.85	111.34	123.59
14	A	1101	CLA	C1D-ND-C4D	-4.85	102.89	106.33
14	G	1114	CLA	CHD-C1D-ND	-4.85	119.99	124.45
14	G	1119	CLA	CHD-C1D-ND	-4.85	119.99	124.45
15	b	1230	F6C	O2A-CGA-O1A	-4.85	111.20	123.30
14	G	1114	CLA	O2A-CGA-O1A	-4.85	111.20	123.30
14	B	1228	CLA	O2A-CGA-O1A	-4.85	111.35	123.59
14	G	1134	CLA	C4A-NA-C1A	4.85	108.89	106.71
14	A	1117	CLA	O2A-C1-C2	4.85	121.38	108.64
14	A	1111	CLA	O2A-CGA-O1A	-4.85	111.36	123.59
14	a	1117	CLA	O2A-C1-C2	4.85	121.38	108.64
14	k	1401	CLA	O2A-CGA-O1A	-4.85	111.22	123.30
14	H	1217	CLA	O2D-CGD-CBD	4.85	119.88	111.27
14	G	1119	CLA	C1C-C2C-C3C	-4.84	101.86	106.96
14	a	1130	CLA	CMB-C2B-C3B	4.84	133.74	124.68
14	a	1105	CLA	O2A-CGA-O1A	-4.84	111.22	123.30
14	G	1109	CLA	O2D-CGD-CBD	4.84	119.88	111.27
14	G	1126	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
13	G	1011	CL0	CHD-C1D-ND	-4.84	120.00	124.45
14	A	1140	CLA	O2A-CGA-O1A	-4.84	111.37	123.59
14	A	1108	CLA	C1C-C2C-C3C	-4.84	101.87	106.96
14	b	1208	CLA	C4A-NA-C1A	4.84	108.88	106.71
14	H	1212	CLA	O2A-CGA-O1A	-4.84	111.24	123.30
14	H	1228	CLA	O2A-CGA-O1A	-4.84	111.38	123.59
14	H	1218	CLA	O2A-CGA-O1A	-4.84	111.24	123.30
14	b	1232	CLA	CHD-C1D-ND	-4.84	120.01	124.45
14	B	1223	CLA	O2A-C1-C2	4.84	121.35	108.64
14	a	1111	CLA	O2A-CGA-O1A	-4.84	111.38	123.59
14	B	1212	CLA	O2A-CGA-O1A	-4.84	111.24	123.30
14	A	1105	CLA	O2A-CGA-O1A	-4.84	111.24	123.30
14	a	1129	CLA	O2A-C1-C2	4.84	121.35	108.64
14	K	1401	CLA	O2A-CGA-O1A	-4.84	111.25	123.30
14	A	1129	CLA	O2A-C1-C2	4.84	121.34	108.64
14	T	1401	CLA	C4A-NA-C1A	4.84	108.88	106.71
14	K	1401	CLA	C4A-NA-C1A	4.84	108.88	106.71
14	H	1235	CLA	C4A-NA-C1A	4.83	108.88	106.71
14	a	1108	CLA	C1C-C2C-C3C	-4.83	101.88	106.96
14	a	1013	CLA	CHD-C1D-ND	-4.83	120.01	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1110	CLA	O2A-CGA-O1A	-4.83	111.26	123.30
14	G	1105	CLA	O2A-CGA-O1A	-4.83	111.26	123.30
14	B	1228	CLA	C1C-C2C-C3C	-4.83	101.88	106.96
14	A	1013	CLA	CHD-C1D-ND	-4.83	120.02	124.45
14	a	1111	CLA	CHD-C1D-ND	-4.83	120.02	124.45
14	G	1117	CLA	O2A-C1-C2	4.83	121.33	108.64
14	G	1111	CLA	O2A-CGA-O1A	-4.83	111.41	123.59
14	b	1218	CLA	O2A-CGA-O1A	-4.83	111.27	123.30
14	T	1401	CLA	O2A-CGA-O1A	-4.83	111.27	123.30
14	H	1232	CLA	O2A-CGA-O1A	-4.83	111.27	123.30
14	H	1228	CLA	C1C-C2C-C3C	-4.83	101.88	106.96
14	a	1138	CLA	CHD-C1D-ND	-4.82	120.02	124.45
14	A	1111	CLA	CHD-C1D-ND	-4.82	120.02	124.45
14	b	1223	CLA	O2A-C1-C2	4.82	121.31	108.64
14	l	1503	CLA	C1D-ND-C4D	-4.82	102.91	106.33
14	a	1118	CLA	C4A-NA-C1A	4.82	108.87	106.71
14	A	1123	CLA	C4A-NA-C1A	4.82	108.87	106.71
15	H	1238	F6C	C2D-C1D-ND	4.82	114.49	109.97
14	a	1126	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
14	a	1102	CLA	CHD-C1D-ND	-4.82	120.03	124.45
14	b	1212	CLA	O2A-CGA-O1A	-4.82	111.29	123.30
14	H	1232	CLA	CHD-C1D-ND	-4.82	120.03	124.45
14	B	1234	CLA	C4A-NA-C1A	4.82	108.87	106.71
14	H	1223	CLA	O2A-C1-C2	4.82	121.29	108.64
14	a	1105	CLA	C4A-NA-C1A	4.81	108.87	106.71
14	a	1106	CLA	C1D-ND-C4D	-4.81	102.92	106.33
14	G	1108	CLA	C1C-C2C-C3C	-4.81	101.90	106.96
14	B	1219	CLA	O2A-CGA-O1A	-4.81	111.31	123.30
14	B	1232	CLA	O2A-CGA-O1A	-4.81	111.31	123.30
14	A	1105	CLA	C4A-NA-C1A	4.81	108.87	106.71
14	b	1219	CLA	O2A-CGA-O1A	-4.81	111.31	123.30
14	a	1119	CLA	CHD-C1D-ND	-4.81	120.03	124.45
15	H	1230	F6C	C3A-C4A-NA	4.81	113.65	110.10
14	A	1125	CLA	OBD-CAD-C3D	-4.81	116.95	128.52
14	H	1232	CLA	C4A-NA-C1A	4.80	108.86	106.71
14	A	1134	CLA	C4A-NA-C1A	4.80	108.86	106.71
14	B	1232	CLA	CHD-C1D-ND	-4.80	120.04	124.45
14	a	1125	CLA	OBD-CAD-C3D	-4.80	116.96	128.52
14	B	1224	CLA	C4A-NA-C1A	4.80	108.86	106.71
14	B	1219	CLA	C1C-C2C-C3C	-4.80	101.91	106.96
14	G	1110	CLA	C1D-ND-C4D	-4.80	102.93	106.33
18	b	4013	BCR	C24-C23-C22	-4.80	118.98	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1131	CLA	O2A-CGA-O1A	-4.80	111.49	123.59
14	b	1228	CLA	C1C-C2C-C3C	-4.80	101.91	106.96
14	A	1112	CLA	O2A-C1-C2	4.80	121.24	108.64
18	H	4013	BCR	C24-C23-C22	-4.79	118.99	126.23
14	G	1111	CLA	CHD-C1D-ND	-4.79	120.05	124.45
14	G	1112	CLA	O2A-C1-C2	4.79	121.23	108.64
14	A	1131	CLA	O2A-CGA-O1A	-4.79	111.49	123.59
14	G	1113	CLA	CHD-C1D-ND	-4.79	120.05	124.45
14	b	1213	CLA	O2A-CGA-O1A	-4.79	111.50	123.59
14	A	1110	CLA	C1D-ND-C4D	-4.79	102.93	106.33
14	a	1131	CLA	O2A-CGA-O1A	-4.79	111.50	123.59
14	G	1124	CLA	O2A-CGA-O1A	-4.79	111.50	123.59
15	B	1230	F6C	C3A-C4A-NA	4.79	113.63	110.10
14	G	1110	CLA	O2A-CGA-O1A	-4.79	111.36	123.30
14	b	1232	CLA	O2A-CGA-O1A	-4.79	111.36	123.30
14	b	1235	CLA	C4A-NA-C1A	4.79	108.86	106.71
14	A	1110	CLA	O2A-CGA-O1A	-4.79	111.36	123.30
14	H	1219	CLA	O2A-CGA-O1A	-4.79	111.37	123.30
14	l	1501	CLA	O2A-CGA-O1A	-4.79	111.51	123.59
13	A	1011	CL0	CHD-C1D-ND	-4.79	120.06	124.45
14	A	1106	CLA	CHD-C1D-ND	-4.79	120.06	124.45
14	B	1212	CLA	C1D-ND-C4D	-4.78	102.94	106.33
14	b	1231	CLA	CHD-C1D-ND	-4.78	120.06	124.45
14	G	1125	CLA	OBD-CAD-C3D	-4.78	117.01	128.52
14	l	1502	CLA	C1D-ND-C4D	-4.78	102.94	106.33
14	A	1116	CLA	O2A-CGA-O1A	-4.78	111.52	123.59
14	a	1112	CLA	O2A-C1-C2	4.78	121.20	108.64
13	a	1011	CL0	CHD-C1D-ND	-4.78	120.06	124.45
14	A	1102	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
18	V	4021	BCR	C33-C5-C6	-4.78	119.16	124.53
14	H	1224	CLA	C4A-NA-C1A	4.78	108.85	106.71
14	G	1107	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
14	H	1212	CLA	C1D-ND-C4D	-4.78	102.94	106.33
14	G	1102	CLA	CHD-C1D-ND	-4.78	120.06	124.45
14	B	1217	CLA	CHD-C1D-ND	-4.78	120.06	124.45
14	A	1124	CLA	O2A-CGA-O1A	-4.78	111.54	123.59
14	H	1219	CLA	C1C-C2C-C3C	-4.78	101.94	106.96
14	b	1219	CLA	C1C-C2C-C3C	-4.77	101.94	106.96
14	a	1110	CLA	C1D-ND-C4D	-4.77	102.94	106.33
14	H	1213	CLA	O2A-CGA-O1A	-4.77	111.55	123.59
14	H	1231	CLA	CHD-C1D-ND	-4.77	120.07	124.45
14	B	1213	CLA	O2A-CGA-O1A	-4.77	111.55	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1223	CLA	O2A-CGA-O1A	-4.77	111.55	123.59
14	b	1223	CLA	O2A-CGA-O1A	-4.77	111.55	123.59
14	a	1102	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
14	a	1116	CLA	O2A-CGA-O1A	-4.77	111.55	123.59
14	B	1231	CLA	CHD-C1D-ND	-4.77	120.07	124.45
14	a	1134	CLA	C4A-NA-C1A	4.77	108.85	106.71
14	H	1223	CLA	O2A-CGA-O1A	-4.77	111.56	123.59
14	b	1227	CLA	O2A-CGA-O1A	-4.77	111.42	123.30
14	a	1124	CLA	O2A-CGA-O1A	-4.77	111.56	123.59
14	G	1013	CLA	O2A-CGA-O1A	-4.77	111.56	123.59
14	H	1227	CLA	O2A-CGA-O1A	-4.77	111.42	123.30
14	G	1106	CLA	CHD-C1D-ND	-4.77	120.08	124.45
14	a	1106	CLA	CHD-C1D-ND	-4.77	120.08	124.45
14	A	1102	CLA	CHD-C1D-ND	-4.77	120.08	124.45
18	M	4021	BCR	C33-C5-C6	-4.76	119.18	124.53
15	G	1121	F6C	O2A-CGA-O1A	-4.76	111.43	123.30
14	U	1502	CLA	C1D-ND-C4D	-4.76	102.95	106.33
14	U	1501	CLA	O2A-CGA-O1A	-4.76	111.57	123.59
14	A	1119	CLA	CHD-C1D-ND	-4.76	120.08	124.45
15	b	1230	F6C	C3A-C4A-NA	4.76	113.61	110.10
15	A	1121	F6C	O2A-CGA-O1A	-4.76	111.43	123.30
14	a	1136	CLA	O2A-CGA-CBA	4.76	126.85	111.91
15	B	1238	F6C	O2A-CGA-O1A	-4.76	111.58	123.59
14	A	1013	CLA	O2A-CGA-O1A	-4.76	111.58	123.59
14	H	1021	CLA	C1D-ND-C4D	-4.76	102.95	106.33
14	G	1102	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
14	a	1140	CLA	C4A-NA-C1A	4.76	108.84	106.71
18	B	4013	BCR	C24-C23-C22	-4.76	119.05	126.23
14	H	1202	CLA	C1D-ND-C4D	-4.76	102.96	106.33
14	A	1140	CLA	C4A-NA-C1A	4.76	108.84	106.71
14	a	1013	CLA	O2A-CGA-O1A	-4.75	111.59	123.59
14	b	1232	CLA	C4A-NA-C1A	4.75	108.84	106.71
14	B	1232	CLA	C4A-NA-C1A	4.75	108.84	106.71
14	G	1116	CLA	O2A-CGA-O1A	-4.75	111.60	123.59
14	L	1502	CLA	C1D-ND-C4D	-4.75	102.96	106.33
14	L	1501	CLA	O2A-CGA-O1A	-4.75	111.60	123.59
15	a	1121	F6C	O2A-CGA-O1A	-4.75	111.46	123.30
14	b	1202	CLA	C1D-ND-C4D	-4.75	102.96	106.33
14	a	1107	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
14	H	1222	CLA	C1C-C2C-C3C	-4.74	101.97	106.96
14	B	1227	CLA	O2A-CGA-O1A	-4.74	111.48	123.30
14	b	1021	CLA	C3D-C2D-C1D	-4.74	99.36	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1107	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
15	H	1238	F6C	O2A-CGA-O1A	-4.74	111.62	123.59
14	H	1204	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
15	b	1238	F6C	O2A-CGA-O1A	-4.74	111.63	123.59
14	b	1204	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
14	H	1021	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
18	A	4002	BCR	C24-C23-C22	-4.74	119.08	126.23
14	b	1225	CLA	CMB-C2B-C3B	4.74	133.54	124.68
14	A	1136	CLA	O2A-CGA-CBA	4.74	126.77	111.91
14	B	1225	CLA	C4A-NA-C1A	4.74	108.83	106.71
14	B	1021	CLA	C1D-ND-C4D	-4.74	102.97	106.33
14	B	1234	CLA	CHD-C1D-ND	-4.73	120.10	124.45
14	B	1222	CLA	C1C-C2C-C3C	-4.73	101.98	106.96
14	G	1136	CLA	O2A-CGA-CBA	4.73	126.77	111.91
14	b	1210	CLA	O2A-CGA-O1A	-4.73	111.65	123.59
14	b	1021	CLA	O2A-CGA-O1A	-4.73	111.65	123.59
14	B	1210	CLA	O2A-CGA-O1A	-4.73	111.66	123.59
18	G	4002	BCR	C24-C23-C22	-4.73	119.09	126.23
14	b	1224	CLA	C4A-NA-C1A	4.73	108.83	106.71
14	B	1204	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
18	a	4002	BCR	C24-C23-C22	-4.72	119.10	126.23
14	k	1401	CLA	C4A-NA-C1A	4.72	108.83	106.71
18	m	4021	BCR	C33-C5-C6	-4.72	119.22	124.53
18	b	4010	BCR	C7-C8-C9	-4.72	119.10	126.23
14	B	1021	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
14	b	1021	CLA	C1D-ND-C4D	-4.72	102.98	106.33
14	H	1210	CLA	O2A-CGA-O1A	-4.72	111.68	123.59
14	H	1234	CLA	CHD-C1D-ND	-4.72	120.12	124.45
14	H	1225	CLA	C4A-NA-C1A	4.72	108.83	106.71
14	a	1124	CLA	C4A-NA-C1A	4.71	108.83	106.71
14	G	1135	CLA	CHD-C1D-ND	-4.71	120.12	124.45
18	H	4010	BCR	C7-C8-C9	-4.71	119.11	126.23
14	H	1021	CLA	O2A-CGA-O1A	-4.71	111.70	123.59
14	B	1021	CLA	O2A-CGA-O1A	-4.71	111.70	123.59
14	b	1222	CLA	C1C-C2C-C3C	-4.71	102.00	106.96
18	A	4007	BCR	C24-C23-C22	-4.71	119.12	126.23
14	b	1217	CLA	CHD-C1D-ND	-4.71	120.13	124.45
14	H	1231	CLA	C1D-ND-C4D	-4.70	102.99	106.33
14	a	1137	CLA	O2A-C1-C2	4.70	121.00	108.64
14	H	1225	CLA	CMB-C2B-C3B	4.70	133.48	124.68
18	G	4007	BCR	C24-C23-C22	-4.70	119.13	126.23
18	a	4007	BCR	C24-C23-C22	-4.70	119.13	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1217	CLA	CHD-C1D-ND	-4.70	120.14	124.45
18	b	4009	BCR	C15-C14-C13	-4.70	120.60	127.31
14	b	1231	CLA	O2A-CGA-O1A	-4.70	111.73	123.59
14	G	1137	CLA	O2A-C1-C2	4.70	120.98	108.64
14	B	1231	CLA	O2A-CGA-O1A	-4.69	111.74	123.59
14	L	1503	CLA	CHD-C1D-ND	-4.69	120.14	124.45
14	A	1137	CLA	O2A-C1-C2	4.69	120.97	108.64
14	A	1135	CLA	CHD-C1D-ND	-4.69	120.14	124.45
14	B	1202	CLA	C1D-ND-C4D	-4.69	103.00	106.33
13	G	1011	CL0	C1D-ND-C4D	-4.69	103.00	106.33
14	B	1225	CLA	CMB-C2B-C3B	4.69	133.45	124.68
14	B	1217	CLA	C1D-ND-C4D	-4.69	103.00	106.33
14	A	1124	CLA	C4A-NA-C1A	4.69	108.81	106.71
18	H	4009	BCR	C15-C14-C13	-4.69	120.62	127.31
14	H	1231	CLA	O2A-CGA-O1A	-4.68	111.77	123.59
15	G	1121	F6C	C3D-C2D-C1D	-4.68	99.05	105.83
13	G	1011	CL0	C3D-C2D-C1D	-4.68	99.44	105.83
14	G	1126	CLA	C1C-C2C-C3C	-4.68	102.04	106.96
13	a	1011	CL0	C1D-ND-C4D	-4.68	103.01	106.33
14	A	1120	CLA	O2A-CGA-O1A	-4.68	111.64	123.30
14	b	1234	CLA	CHD-C1D-ND	-4.68	120.16	124.45
13	A	1011	CL0	C3D-C2D-C1D	-4.67	99.45	105.83
14	G	1120	CLA	O2A-CGA-O1A	-4.67	111.66	123.30
14	b	1231	CLA	C1D-ND-C4D	-4.67	103.02	106.33
14	U	1503	CLA	CHD-C1D-ND	-4.67	120.16	124.45
14	a	1120	CLA	O2A-CGA-O1A	-4.67	111.66	123.30
14	a	1126	CLA	C1C-C2C-C3C	-4.67	102.05	106.96
14	G	1124	CLA	C4A-NA-C1A	4.67	108.80	106.71
18	B	4010	BCR	C7-C8-C9	-4.67	119.18	126.23
14	H	1203	CLA	C1D-ND-C4D	-4.67	103.02	106.33
13	a	1011	CL0	C3D-C2D-C1D	-4.66	99.47	105.83
14	B	1227	CLA	CHD-C1D-ND	-4.66	120.17	124.45
14	b	1203	CLA	C1D-ND-C4D	-4.66	103.03	106.33
14	H	1022	CLA	C1C-C2C-C3C	-4.66	102.06	106.96
14	B	1022	CLA	C1C-C2C-C3C	-4.66	102.06	106.96
18	B	4009	BCR	C15-C14-C13	-4.66	120.67	127.31
14	H	1218	CLA	CMD-C2D-C1D	4.66	132.92	124.71
14	B	1218	CLA	CMD-C2D-C1D	4.65	132.91	124.71
14	A	1126	CLA	C1C-C2C-C3C	-4.65	102.07	106.96
14	b	1203	CLA	O2A-CGA-O1A	-4.65	111.86	123.59
14	a	1135	CLA	CHD-C1D-ND	-4.65	120.18	124.45
18	B	4017	BCR	C24-C23-C22	-4.64	119.22	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1239	CLA	O2A-C1-C2	4.64	120.83	108.64
14	b	1023	CLA	CHD-C1D-ND	-4.64	120.19	124.45
14	b	1218	CLA	CMD-C2D-C1D	4.64	132.89	124.71
14	B	1239	CLA	O2A-C1-C2	4.64	120.82	108.64
14	B	1224	CLA	CHD-C1D-ND	-4.64	120.19	124.45
15	A	1121	F6C	C3D-C2D-C1D	-4.64	99.12	105.83
15	a	1121	F6C	C3D-C2D-C1D	-4.63	99.12	105.83
14	H	1203	CLA	O2A-CGA-O1A	-4.63	111.90	123.59
14	a	1126	CLA	O2A-C1-C2	4.63	120.81	108.64
14	B	1203	CLA	O2A-CGA-O1A	-4.63	111.90	123.59
14	B	1231	CLA	C1D-ND-C4D	-4.63	103.05	106.33
14	G	1126	CLA	O2A-C1-C2	4.63	120.80	108.64
15	B	1207	F6C	C4A-C3A-C2A	-4.63	100.18	106.94
14	B	1220	CLA	C1D-ND-C4D	-4.63	103.05	106.33
14	a	1139	CLA	C1D-ND-C4D	-4.63	103.05	106.33
18	b	4017	BCR	C24-C23-C22	-4.62	119.25	126.23
14	H	1239	CLA	O2A-C1-C2	4.62	120.79	108.64
14	A	1139	CLA	C1D-ND-C4D	-4.62	103.05	106.33
14	H	1227	CLA	CHD-C1D-ND	-4.62	120.20	124.45
14	G	1122	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
14	b	1220	CLA	C1D-ND-C4D	-4.62	103.05	106.33
14	H	1216	CLA	C4A-NA-C1A	4.62	108.78	106.71
14	a	1013	CLA	C2C-C1C-NC	4.62	114.30	109.97
14	B	1222	CLA	O2A-CGA-CBA	4.62	126.40	111.91
14	A	1113	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
14	a	1129	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
14	b	1226	CLA	CMB-C2B-C3B	4.62	133.31	124.68
20	i	5006	LMG	O7-C10-C11	4.62	121.45	111.50
14	G	1129	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
18	A	4003	BCR	C24-C23-C22	-4.61	119.26	126.23
14	b	1227	CLA	CHD-C1D-ND	-4.61	120.21	124.45
14	A	1126	CLA	O2A-C1-C2	4.61	120.76	108.64
14	B	1226	CLA	CMB-C2B-C3B	4.61	133.31	124.68
15	b	1207	F6C	C4A-C3A-C2A	-4.61	100.21	106.94
14	b	1222	CLA	O2A-CGA-CBA	4.61	126.38	111.91
14	A	1111	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
20	R	5006	LMG	O7-C10-C11	4.61	121.43	111.50
18	H	4017	BCR	C24-C23-C22	-4.61	119.27	126.23
14	a	1118	CLA	CHD-C1D-ND	-4.61	120.22	124.45
14	l	1503	CLA	CHD-C1D-ND	-4.61	120.22	124.45
14	H	1226	CLA	CMB-C2B-C3B	4.61	133.30	124.68
14	A	1119	CLA	O2D-CGD-CBD	4.61	119.45	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1222	CLA	O2A-CGA-CBA	4.61	126.36	111.91
14	G	1111	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
14	B	1203	CLA	C1D-ND-C4D	-4.61	103.06	106.33
15	H	1207	F6C	C4A-C3A-C2A	-4.61	100.21	106.94
14	G	1013	CLA	C2C-C1C-NC	4.60	114.29	109.97
14	B	1239	CLA	O2A-CGA-O1A	-4.60	111.97	123.59
14	b	1225	CLA	C4A-NA-C1A	4.60	108.78	106.71
14	b	1220	CLA	O2A-CGA-O1A	-4.60	111.97	123.59
14	G	1128	CLA	CMB-C2B-C3B	4.60	133.29	124.68
20	I	5006	LMG	O7-C10-C11	4.60	121.42	111.50
14	H	1239	CLA	O2A-CGA-O1A	-4.60	111.98	123.59
14	B	1220	CLA	O2A-CGA-O1A	-4.60	111.98	123.59
14	a	1113	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
14	b	1224	CLA	CHD-C1D-ND	-4.60	120.23	124.45
14	L	1502	CLA	C4A-NA-C1A	4.60	108.77	106.71
18	G	4002	BCR	C34-C9-C10	-4.60	116.48	122.92
14	G	1135	CLA	O2D-CGD-CBD	4.60	119.44	111.27
14	T	1401	CLA	C1D-ND-C4D	-4.60	103.07	106.33
18	a	4002	BCR	C34-C9-C10	-4.59	116.49	122.92
14	a	1128	CLA	CMB-C2B-C3B	4.59	133.27	124.68
14	U	1502	CLA	C4A-NA-C1A	4.59	108.77	106.71
14	H	1220	CLA	O2A-CGA-O1A	-4.59	112.00	123.59
14	A	1013	CLA	C2C-C1C-NC	4.59	114.27	109.97
14	b	1217	CLA	C1D-ND-C4D	-4.59	103.07	106.33
14	A	1128	CLA	CMB-C2B-C3B	4.59	133.27	124.68
14	G	1139	CLA	C1D-ND-C4D	-4.59	103.08	106.33
14	b	1022	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
14	a	1119	CLA	O2D-CGD-CBD	4.59	119.42	111.27
14	A	1135	CLA	O2D-CGD-CBD	4.59	119.42	111.27
14	H	1211	CLA	C1D-ND-C4D	-4.59	103.08	106.33
14	H	1226	CLA	O2A-C1-C2	4.59	120.69	108.64
14	G	1106	CLA	O2A-CGA-O1A	-4.59	112.02	123.59
14	B	1225	CLA	C3D-C2D-C1D	-4.58	99.57	105.83
14	b	1239	CLA	O2A-CGA-O1A	-4.58	112.03	123.59
14	G	1119	CLA	O2D-CGD-CBD	4.58	119.41	111.27
14	X	1701	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
14	l	1502	CLA	C4A-NA-C1A	4.58	108.77	106.71
14	B	1219	CLA	C4A-NA-C1A	4.58	108.77	106.71
13	A	1011	CL0	C1D-ND-C4D	-4.58	103.08	106.33
14	H	1217	CLA	C1D-ND-C4D	-4.58	103.08	106.33
14	a	1135	CLA	O2D-CGD-CBD	4.58	119.41	111.27
14	G	1113	CLA	C1C-C2C-C3C	-4.58	102.14	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	4002	BCR	C34-C9-C10	-4.58	116.51	122.92
14	b	1222	CLA	C1D-ND-C4D	-4.58	103.08	106.33
14	b	1219	CLA	C4A-NA-C1A	4.58	108.76	106.71
14	a	1111	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
14	H	1023	CLA	CHD-C1D-ND	-4.57	120.25	124.45
14	b	1216	CLA	C4A-NA-C1A	4.57	108.76	106.71
14	A	1118	CLA	CHD-C1D-ND	-4.57	120.25	124.45
14	H	1219	CLA	C4A-NA-C1A	4.57	108.76	106.71
14	G	1113	CLA	C4A-NA-C1A	4.57	108.76	106.71
14	b	1226	CLA	O2A-C1-C2	4.57	120.63	108.64
18	B	4005	BCR	C33-C5-C6	-4.56	119.40	124.53
14	B	1023	CLA	CHD-C1D-ND	-4.56	120.26	124.45
14	A	1129	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
14	k	1401	CLA	C1D-ND-C4D	-4.56	103.09	106.33
14	a	1113	CLA	C4A-NA-C1A	4.56	108.76	106.71
14	B	1223	CLA	C4A-NA-C1A	4.56	108.76	106.71
14	a	1106	CLA	O2A-CGA-O1A	-4.56	112.08	123.59
14	B	1212	CLA	CHD-C1D-ND	-4.56	120.26	124.45
14	B	1226	CLA	O2A-C1-C2	4.56	120.62	108.64
14	A	1106	CLA	O2A-CGA-O1A	-4.56	112.08	123.59
14	a	1122	CLA	C1C-C2C-C3C	-4.56	102.17	106.96
14	H	1220	CLA	C1D-ND-C4D	-4.56	103.10	106.33
15	b	1207	F6C	O2A-CGA-CBA	4.55	126.20	111.91
14	b	1212	CLA	CHD-C1D-ND	-4.55	120.27	124.45
14	B	1218	CLA	C1D-ND-C4D	-4.55	103.10	106.33
15	H	1207	F6C	O2A-CGA-CBA	4.55	126.19	111.91
14	b	1225	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
14	H	1224	CLA	CHD-C1D-ND	-4.55	120.28	124.45
18	a	4003	BCR	C24-C23-C22	-4.55	119.36	126.23
14	H	1218	CLA	C1D-ND-C4D	-4.55	103.11	106.33
18	G	4003	BCR	C24-C23-C22	-4.55	119.37	126.23
14	b	1211	CLA	C1D-ND-C4D	-4.55	103.11	106.33
14	U	1502	CLA	O2A-CGA-O1A	-4.55	112.12	123.59
14	H	1223	CLA	C4A-NA-C1A	4.54	108.75	106.71
15	B	1207	F6C	O2A-CGA-CBA	4.54	126.17	111.91
14	H	1225	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
14	K	1401	CLA	C1D-ND-C4D	-4.54	103.11	106.33
14	L	1502	CLA	O2A-CGA-O1A	-4.54	112.13	123.59
14	G	1109	CLA	O2A-CGA-O1A	-4.54	112.13	123.59
14	H	1212	CLA	CHD-C1D-ND	-4.53	120.29	124.45
14	A	1109	CLA	O2A-CGA-O1A	-4.53	112.15	123.59
14	x	1701	CLA	C1C-C2C-C3C	-4.53	102.19	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	l	1502	CLA	O2A-CGA-O1A	-4.53	112.16	123.59
14	a	1109	CLA	O2A-CGA-O1A	-4.53	112.16	123.59
14	b	1222	CLA	CHD-C1D-ND	-4.53	120.30	124.45
14	a	1109	CLA	C1D-ND-C4D	-4.52	103.12	106.33
14	A	1102	CLA	CMB-C2B-C3B	4.52	133.14	124.68
14	a	1135	CLA	O2A-CGA-O1A	-4.52	112.17	123.59
14	G	1118	CLA	CHD-C1D-ND	-4.52	120.30	124.45
14	H	1215	CLA	O2A-CGA-CBA	4.52	126.10	111.91
14	b	1023	CLA	C1D-ND-C4D	-4.52	103.12	106.33
14	b	1202	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
14	A	1122	CLA	C1C-C2C-C3C	-4.52	102.20	106.96
14	b	1215	CLA	O2A-CGA-CBA	4.52	126.09	111.91
14	B	1215	CLA	O2A-CGA-CBA	4.52	126.09	111.91
14	A	1130	CLA	O2A-CGA-O1A	-4.52	112.19	123.59
18	b	4005	BCR	C33-C5-C6	-4.52	119.46	124.53
14	A	1129	CLA	CHD-C1D-ND	-4.52	120.30	124.45
18	H	4005	BCR	C33-C5-C6	-4.52	119.46	124.53
14	B	1202	CLA	C1C-C2C-C3C	-4.52	102.21	106.96
14	a	1107	CLA	CHD-C1D-ND	-4.51	120.31	124.45
14	A	1135	CLA	O2A-CGA-O1A	-4.51	112.21	123.59
14	b	1210	CLA	CAC-C3C-C4C	4.51	130.66	124.81
14	W	1701	CLA	C1C-C2C-C3C	-4.51	102.22	106.96
14	a	1128	CLA	CHD-C1D-ND	-4.51	120.31	124.45
14	G	1111	CLA	C1D-ND-C4D	-4.51	103.13	106.33
14	a	1132	CLA	C1D-ND-C4D	-4.51	103.13	106.33
14	A	1132	CLA	C1D-ND-C4D	-4.51	103.13	106.33
14	G	1135	CLA	O2A-CGA-O1A	-4.51	112.21	123.59
14	a	1102	CLA	CMB-C2B-C3B	4.51	133.11	124.68
14	b	1218	CLA	C1D-ND-C4D	-4.51	103.13	106.33
14	B	1211	CLA	C1D-ND-C4D	-4.51	103.13	106.33
18	U	4022	BCR	C33-C5-C6	-4.51	119.47	124.53
14	a	1115	CLA	C1D-ND-C4D	-4.50	103.14	106.33
14	H	1202	CLA	C1C-C2C-C3C	-4.50	102.22	106.96
14	B	1228	CLA	C1D-ND-C4D	-4.50	103.14	106.33
14	G	1103	CLA	O2A-CGA-O1A	-4.50	112.23	123.59
14	a	1130	CLA	O2A-CGA-O1A	-4.50	112.23	123.59
14	G	1130	CLA	O2A-CGA-O1A	-4.50	112.23	123.59
14	G	1102	CLA	CMB-C2B-C3B	4.50	133.10	124.68
14	H	1204	CLA	C1D-ND-C4D	-4.50	103.14	106.33
14	G	1140	CLA	O2A-C1-C2	4.50	120.45	108.64
14	B	1216	CLA	C4A-NA-C1A	4.50	108.73	106.71
14	a	1102	CLA	O2A-CGA-CBA	4.49	126.01	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1114	CLA	C4A-NA-C1A	4.49	108.73	106.71
14	a	1140	CLA	O2A-C1-C2	4.49	120.44	108.64
14	H	1222	CLA	C1D-ND-C4D	-4.49	103.14	106.33
14	H	1228	CLA	C1D-ND-C4D	-4.49	103.14	106.33
14	A	1140	CLA	O2A-C1-C2	4.49	120.44	108.64
14	A	1107	CLA	CHD-C1D-ND	-4.49	120.33	124.45
14	B	1210	CLA	CAC-C3C-C4C	4.49	130.64	124.81
14	G	1129	CLA	CHD-C1D-ND	-4.49	120.33	124.45
14	B	1221	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
14	G	1102	CLA	O2A-CGA-CBA	4.49	125.99	111.91
14	a	1129	CLA	CHD-C1D-ND	-4.49	120.33	124.45
14	b	1215	CLA	O2A-C1-C2	4.49	120.42	108.64
14	G	1107	CLA	CHD-C1D-ND	-4.48	120.33	124.45
14	A	1103	CLA	O2A-CGA-O1A	-4.48	112.28	123.59
14	H	1210	CLA	CAC-C3C-C4C	4.48	130.63	124.81
13	a	1011	CL0	O2A-C1-C2	4.48	120.42	108.64
14	A	1112	CLA	O2A-CGA-CBA	4.48	125.97	111.91
14	a	1103	CLA	O2A-CGA-O1A	-4.48	112.29	123.59
14	G	1112	CLA	O2A-CGA-CBA	4.48	125.96	111.91
14	a	1112	CLA	O2A-CGA-CBA	4.48	125.96	111.91
14	H	1221	CLA	C1C-C2C-C3C	-4.48	102.25	106.96
14	A	1109	CLA	C1D-ND-C4D	-4.48	103.16	106.33
14	A	1102	CLA	O2A-CGA-CBA	4.48	125.95	111.91
14	A	1111	CLA	C4A-NA-C1A	4.48	108.72	106.71
14	a	1113	CLA	C1D-ND-C4D	-4.48	103.16	106.33
13	A	1011	CL0	O2A-C1-C2	4.47	120.39	108.64
18	l	4022	BCR	C33-C5-C6	-4.47	119.50	124.53
14	H	1222	CLA	CHD-C1D-ND	-4.47	120.34	124.45
14	A	1113	CLA	C1D-ND-C4D	-4.47	103.16	106.33
14	H	1215	CLA	O2A-C1-C2	4.47	120.38	108.64
14	B	1215	CLA	O2A-C1-C2	4.47	120.38	108.64
14	G	1115	CLA	C1D-ND-C4D	-4.47	103.16	106.33
14	b	1204	CLA	C1D-ND-C4D	-4.47	103.16	106.33
14	G	1132	CLA	C1D-ND-C4D	-4.46	103.16	106.33
13	G	1011	CL0	O2A-C1-C2	4.46	120.36	108.64
14	B	1222	CLA	CHD-C1D-ND	-4.46	120.35	124.45
14	G	1109	CLA	C1D-ND-C4D	-4.46	103.17	106.33
18	L	4022	BCR	C33-C5-C6	-4.46	119.52	124.53
14	a	1127	CLA	C1D-ND-C4D	-4.46	103.17	106.33
14	A	1127	CLA	C1D-ND-C4D	-4.46	103.17	106.33
14	G	1111	CLA	C4A-NA-C1A	4.46	108.71	106.71
14	G	1111	CLA	C1-C2-C3	-4.45	118.34	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1111	CLA	C1-C2-C3	-4.45	118.35	126.04
14	a	1105	CLA	C1D-ND-C4D	-4.45	103.17	106.33
14	X	1701	CLA	CHD-C1D-ND	-4.45	120.36	124.45
14	A	1111	CLA	C1-C2-C3	-4.45	118.35	126.04
14	A	1128	CLA	CHD-C1D-ND	-4.45	120.37	124.45
14	H	1209	CLA	C1D-ND-C4D	-4.45	103.17	106.33
14	a	1111	CLA	C1D-ND-C4D	-4.45	103.17	106.33
14	A	1115	CLA	C1D-ND-C4D	-4.45	103.17	106.33
14	b	1223	CLA	C4A-NA-C1A	4.45	108.70	106.71
14	A	1116	CLA	C4A-NA-C1A	4.44	108.70	106.71
14	B	1023	CLA	C1D-ND-C4D	-4.44	103.18	106.33
14	B	1222	CLA	C1D-ND-C4D	-4.44	103.18	106.33
14	b	1221	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
14	H	1023	CLA	C1D-ND-C4D	-4.44	103.18	106.33
14	A	1111	CLA	C1D-ND-C4D	-4.44	103.18	106.33
14	B	1210	CLA	C1D-ND-C4D	-4.44	103.18	106.33
14	G	1127	CLA	C1D-ND-C4D	-4.44	103.18	106.33
14	b	1228	CLA	C1D-ND-C4D	-4.44	103.18	106.33
14	x	1701	CLA	CHD-C1D-ND	-4.44	120.38	124.45
14	A	1105	CLA	C1D-ND-C4D	-4.43	103.19	106.33
14	H	1210	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
15	b	1207	F6C	C4-C3-C5	4.43	122.72	115.27
14	G	1113	CLA	C1D-ND-C4D	-4.43	103.19	106.33
14	a	1111	CLA	C4A-NA-C1A	4.42	108.69	106.71
18	H	4004	BCR	C3-C4-C5	-4.42	106.18	114.08
14	A	1113	CLA	C4A-NA-C1A	4.42	108.69	106.71
14	G	1128	CLA	CHD-C1D-ND	-4.42	120.39	124.45
14	W	1701	CLA	CHD-C1D-ND	-4.42	120.39	124.45
14	G	1105	CLA	C1D-ND-C4D	-4.41	103.20	106.33
14	H	1233	CLA	C1D-ND-C4D	-4.41	103.20	106.33
14	a	1119	CLA	C1-C2-C3	-4.41	118.42	126.04
18	b	4004	BCR	C3-C4-C5	-4.41	106.20	114.08
15	B	1207	F6C	C4-C3-C5	4.41	122.69	115.27
14	B	1204	CLA	C1D-ND-C4D	-4.41	103.20	106.33
14	B	1209	CLA	C1D-ND-C4D	-4.41	103.20	106.33
15	b	1237	F6C	O2A-CGA-O1A	-4.41	112.46	123.59
14	A	1114	CLA	C4A-NA-C1A	4.41	108.69	106.71
15	H	1237	F6C	O2A-CGA-O1A	-4.41	112.47	123.59
15	B	1237	F6C	O2A-CGA-O1A	-4.41	112.47	123.59
15	H	1207	F6C	C4-C3-C5	4.40	122.68	115.27
14	a	1114	CLA	C4A-NA-C1A	4.40	108.69	106.71
14	a	1139	CLA	CHD-C1D-ND	-4.40	120.41	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1119	CLA	C1-C2-C3	-4.40	118.43	126.04
14	b	1210	CLA	C1D-ND-C4D	-4.40	103.21	106.33
18	B	4004	BCR	C3-C4-C5	-4.40	106.22	114.08
14	H	1219	CLA	C1D-ND-C4D	-4.40	103.21	106.33
14	b	1219	CLA	C1D-ND-C4D	-4.40	103.21	106.33
14	a	1013	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
14	X	1701	CLA	C1D-ND-C4D	-4.39	103.21	106.33
14	A	1139	CLA	CHD-C1D-ND	-4.39	120.42	124.45
14	B	1219	CLA	C1D-ND-C4D	-4.39	103.22	106.33
14	H	1210	CLA	C1D-ND-C4D	-4.39	103.22	106.33
14	B	1210	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
14	b	1209	CLA	C1D-ND-C4D	-4.38	103.22	106.33
14	G	1139	CLA	CHD-C1D-ND	-4.38	120.42	124.45
14	l	1503	CLA	O2A-CGA-O1A	-4.38	112.53	123.59
14	A	1133	CLA	O2A-CGA-CBA	4.38	125.66	111.91
14	A	1119	CLA	C1-C2-C3	-4.38	118.46	126.04
14	a	1133	CLA	O2A-CGA-CBA	4.38	125.66	111.91
14	b	1233	CLA	C1D-ND-C4D	-4.38	103.22	106.33
14	L	1503	CLA	O2A-CGA-O1A	-4.38	112.55	123.59
14	G	1013	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
14	b	1210	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
14	G	1133	CLA	O2A-CGA-CBA	4.37	125.63	111.91
14	b	1232	CLA	O2D-CGD-CBD	4.37	119.04	111.27
14	U	1503	CLA	O2A-CGA-O1A	-4.37	112.56	123.59
14	W	1701	CLA	C1D-ND-C4D	-4.37	103.23	106.33
14	a	1116	CLA	C4A-NA-C1A	4.37	108.67	106.71
18	a	4008	BCR	C7-C8-C9	-4.37	119.64	126.23
14	G	1129	CLA	C4A-NA-C1A	4.37	108.67	106.71
14	B	1232	CLA	O2D-CGD-CBD	4.37	119.03	111.27
18	G	4008	BCR	C7-C8-C9	-4.36	119.64	126.23
18	A	4011	BCR	C24-C23-C22	-4.36	119.64	126.23
14	G	1116	CLA	C4A-NA-C1A	4.36	108.67	106.71
14	A	1013	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
14	B	1234	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
14	b	1229	CLA	C4A-NA-C1A	4.36	108.67	106.71
14	A	1131	CLA	C4A-NA-C1A	4.36	108.67	106.71
14	G	1125	CLA	C1D-ND-C4D	-4.36	103.24	106.33
14	a	1135	CLA	C1D-ND-C4D	-4.36	103.24	106.33
14	a	1140	CLA	C1D-ND-C4D	-4.36	103.24	106.33
14	b	1234	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
14	G	1135	CLA	C1D-ND-C4D	-4.35	103.25	106.33
14	A	1134	CLA	C1D-ND-C4D	-4.35	103.25	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1135	CLA	C1D-ND-C4D	-4.34	103.25	106.33
14	H	1232	CLA	O2D-CGD-CBD	4.34	118.98	111.27
14	B	1229	CLA	O2A-CGA-CBA	4.34	125.53	111.91
15	a	1121	F6C	CMA-C3A-C4A	-4.34	117.06	124.71
14	b	1211	CLA	C1-C2-C3	-4.34	118.53	126.04
14	H	1229	CLA	O2A-CGA-CBA	4.34	125.53	111.91
18	G	4003	BCR	C7-C8-C9	-4.34	119.68	126.23
18	G	4011	BCR	C24-C23-C22	-4.34	119.68	126.23
14	H	1223	CLA	CHD-C1D-ND	-4.34	120.47	124.45
14	B	1233	CLA	C1D-ND-C4D	-4.34	103.25	106.33
14	H	1234	CLA	C1C-C2C-C3C	-4.33	102.40	106.96
14	a	1125	CLA	C1D-ND-C4D	-4.33	103.26	106.33
14	a	1129	CLA	C4A-NA-C1A	4.33	108.65	106.71
14	G	1110	CLA	C4A-NA-C1A	4.33	108.65	106.71
14	x	1701	CLA	C1D-ND-C4D	-4.33	103.26	106.33
18	a	4003	BCR	C7-C8-C9	-4.32	119.70	126.23
18	A	4008	BCR	C7-C8-C9	-4.32	119.70	126.23
15	H	1207	F6C	C1A-C2A-C3A	-4.32	102.42	106.97
14	H	1211	CLA	C1-C2-C3	-4.32	118.57	126.04
18	m	4021	BCR	C15-C14-C13	-4.32	121.14	127.31
14	b	1229	CLA	O2A-CGA-CBA	4.32	125.46	111.91
18	G	4002	BCR	C19-C18-C17	4.32	125.57	118.94
18	a	4002	BCR	C19-C18-C17	4.32	125.57	118.94
18	A	4002	BCR	C19-C18-C17	4.32	125.56	118.94
18	a	4011	BCR	C24-C23-C22	-4.32	119.71	126.23
14	G	1131	CLA	C4A-NA-C1A	4.32	108.65	106.71
14	G	1136	CLA	C1D-ND-C4D	-4.31	103.27	106.33
18	A	4001	BCR	C28-C27-C26	-4.31	106.38	114.08
18	V	4021	BCR	C15-C14-C13	-4.31	121.16	127.31
20	B	5002	LMG	O7-C10-C11	4.31	120.78	111.50
15	G	1121	F6C	CMA-C3A-C4A	-4.31	117.12	124.71
15	B	1230	F6C	C4A-NA-C1A	4.31	109.39	106.33
18	G	4001	BCR	C28-C27-C26	-4.31	106.39	114.08
15	A	1121	F6C	CMA-C3A-C4A	-4.30	117.13	124.71
14	L	1501	CLA	CHD-C1D-ND	-4.30	120.50	124.45
18	a	4001	BCR	C28-C27-C26	-4.30	106.39	114.08
20	b	5002	LMG	O7-C10-C11	4.30	120.77	111.50
14	G	1140	CLA	C1D-ND-C4D	-4.30	103.28	106.33
14	l	1501	CLA	CHD-C1D-ND	-4.30	120.50	124.45
14	B	1223	CLA	CHD-C1D-ND	-4.30	120.50	124.45
18	A	4003	BCR	C7-C8-C9	-4.30	119.74	126.23
14	b	1223	CLA	CHD-C1D-ND	-4.30	120.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	1207	F6C	C1A-C2A-C3A	-4.30	102.44	106.97
15	B	1207	F6C	C1A-C2A-C3A	-4.30	102.45	106.97
14	a	1131	CLA	C4A-NA-C1A	4.29	108.64	106.71
14	B	1211	CLA	C1-C2-C3	-4.29	118.62	126.04
14	U	1501	CLA	CHD-C1D-ND	-4.29	120.51	124.45
14	A	1130	CLA	O2A-C1-C2	4.29	119.91	108.64
14	A	1140	CLA	C1D-ND-C4D	-4.29	103.29	106.33
15	H	1230	F6C	C4A-NA-C1A	4.29	109.38	106.33
14	a	1110	CLA	C4A-NA-C1A	4.29	108.63	106.71
14	b	1226	CLA	O2A-CGA-CBA	4.29	125.36	111.91
18	M	4021	BCR	C15-C14-C13	-4.29	121.19	127.31
20	H	5002	LMG	O7-C10-C11	4.29	120.74	111.50
14	G	1134	CLA	C1D-ND-C4D	-4.28	103.29	106.33
14	B	1229	CLA	C4A-NA-C1A	4.28	108.63	106.71
15	b	1230	F6C	C4A-NA-C1A	4.28	109.38	106.33
14	b	1234	CLA	O2A-CGA-CBA	4.28	125.35	111.91
14	G	1130	CLA	O2A-C1-C2	4.28	119.89	108.64
14	a	1130	CLA	O2A-C1-C2	4.28	119.88	108.64
14	b	1216	CLA	O2A-CGA-O1A	-4.28	112.79	123.59
14	a	1119	CLA	O2A-CGA-O1A	-4.28	112.79	123.59
18	I	4018	BCR	C4-C5-C6	-4.28	116.52	122.73
14	B	1216	CLA	O2A-CGA-O1A	-4.28	112.80	123.59
14	H	1022	CLA	C1D-ND-C4D	-4.28	103.30	106.33
14	H	1234	CLA	O2A-CGA-CBA	4.28	125.33	111.91
14	G	1125	CLA	C1-C2-C3	-4.28	118.65	126.04
14	A	1127	CLA	C1-C2-C3	-4.28	118.65	126.04
14	A	1125	CLA	C1D-ND-C4D	-4.28	103.30	106.33
14	H	1226	CLA	O2A-CGA-CBA	4.28	125.32	111.91
14	a	1127	CLA	C1-C2-C3	-4.27	118.65	126.04
14	B	1226	CLA	O2A-CGA-CBA	4.27	125.32	111.91
14	A	1119	CLA	O2A-CGA-O1A	-4.27	112.81	123.59
14	b	1225	CLA	C1D-ND-C4D	-4.27	103.30	106.33
14	H	1216	CLA	O2A-CGA-O1A	-4.27	112.82	123.59
18	i	4018	BCR	C4-C5-C6	-4.27	116.54	122.73
14	G	1127	CLA	C1-C2-C3	-4.26	118.67	126.04
14	G	1119	CLA	O2A-CGA-O1A	-4.26	112.83	123.59
18	R	4018	BCR	C4-C5-C6	-4.26	116.54	122.73
14	a	1125	CLA	C1-C2-C3	-4.26	118.67	126.04
15	B	1207	F6C	CMA-C3A-C4A	-4.26	117.20	124.71
14	B	1022	CLA	C1D-ND-C4D	-4.26	103.31	106.33
15	H	1207	F6C	CMA-C3A-C4A	-4.26	117.20	124.71
14	B	1229	CLA	CMB-C2B-C3B	4.26	132.64	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1205	CLA	O2A-CGA-CBA	4.26	125.26	111.91
14	A	1125	CLA	C1-C2-C3	-4.25	118.68	126.04
14	H	1229	CLA	CMB-C2B-C3B	4.25	132.64	124.68
14	B	1234	CLA	O2A-CGA-CBA	4.25	125.25	111.91
18	H	4017	BCR	C38-C26-C25	-4.25	119.75	124.53
14	b	1229	CLA	CMB-C2B-C3B	4.25	132.63	124.68
15	b	1207	F6C	CMA-C3A-C4A	-4.25	117.22	124.71
14	H	1205	CLA	O2A-CGA-CBA	4.25	125.24	111.91
14	A	1110	CLA	C4A-NA-C1A	4.25	108.62	106.71
14	G	1108	CLA	CMB-C2B-C3B	4.24	132.62	124.68
14	A	1136	CLA	C1D-ND-C4D	-4.24	103.32	106.33
14	B	1223	CLA	CMB-C2B-C3B	4.24	132.62	124.68
14	B	1229	CLA	CAA-C2A-C3A	-4.24	101.16	112.78
14	a	1129	CLA	C1D-ND-C4D	-4.24	103.32	106.33
14	b	1205	CLA	O2A-CGA-CBA	4.24	125.22	111.91
14	A	1108	CLA	CMB-C2B-C3B	4.24	132.61	124.68
14	B	1235	CLA	O2A-CGA-CBA	4.24	125.21	111.91
14	G	1012	CLA	O2A-CGA-CBA	4.24	125.20	111.91
14	G	1125	CLA	O2A-CGA-CBA	4.24	125.20	111.91
14	a	1134	CLA	C1D-ND-C4D	-4.24	103.33	106.33
14	a	1136	CLA	C1D-ND-C4D	-4.24	103.33	106.33
14	b	1223	CLA	CMB-C2B-C3B	4.24	132.60	124.68
14	H	1223	CLA	C1D-ND-C4D	-4.23	103.33	106.33
14	A	1129	CLA	C4A-NA-C1A	4.23	108.61	106.71
14	H	1229	CLA	CAA-C2A-C3A	-4.23	101.19	112.78
16	b	2002	PQN	C14-C13-C15	4.23	122.39	115.27
14	b	1229	CLA	CAA-C2A-C3A	-4.23	101.19	112.78
14	A	1012	CLA	O2A-CGA-CBA	4.23	125.19	111.91
14	B	1021	CLA	CHD-C1D-ND	-4.23	120.57	124.45
14	H	1235	CLA	O2A-CGA-CBA	4.23	125.18	111.91
14	b	1208	CLA	C1D-ND-C4D	-4.23	103.33	106.33
14	a	1108	CLA	CMB-C2B-C3B	4.23	132.59	124.68
14	a	1136	CLA	O2A-C1-C2	4.23	119.75	108.64
18	H	4017	BCR	C3-C4-C5	-4.23	106.53	114.08
14	G	1136	CLA	O2A-C1-C2	4.23	119.75	108.64
14	H	1225	CLA	C1D-ND-C4D	-4.23	103.33	106.33
16	B	2002	PQN	C14-C13-C15	4.23	122.38	115.27
14	H	1223	CLA	CMB-C2B-C3B	4.23	132.59	124.68
14	b	1021	CLA	CHD-C1D-ND	-4.23	120.57	124.45
14	G	1129	CLA	C1D-ND-C4D	-4.22	103.33	106.33
14	H	1021	CLA	CHD-C1D-ND	-4.22	120.57	124.45
14	H	1229	CLA	C4A-NA-C1A	4.22	108.61	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	4017	BCR	C38-C26-C25	-4.22	119.79	124.53
14	H	1220	CLA	C1-C2-C3	-4.22	118.75	126.04
14	a	1012	CLA	O2A-CGA-CBA	4.22	125.15	111.91
16	H	2002	PQN	C14-C13-C15	4.22	122.37	115.27
14	a	1138	CLA	O2A-CGA-O1A	-4.22	112.95	123.59
14	A	1136	CLA	O2A-C1-C2	4.22	119.71	108.64
14	a	1125	CLA	O2A-CGA-CBA	4.22	125.14	111.91
14	B	1213	CLA	C1D-ND-C4D	-4.21	103.34	106.33
14	B	1220	CLA	C1-C2-C3	-4.21	118.76	126.04
14	G	1138	CLA	CMB-C2B-C3B	4.21	132.56	124.68
18	B	4017	BCR	C3-C4-C5	-4.21	106.56	114.08
14	b	1208	CLA	O2A-CGA-CBA	4.21	125.13	111.91
14	b	1235	CLA	O2A-CGA-CBA	4.21	125.12	111.91
14	A	1125	CLA	O2A-CGA-CBA	4.21	125.12	111.91
14	B	1216	CLA	C1D-ND-C4D	-4.21	103.34	106.33
14	b	1220	CLA	C1-C2-C3	-4.21	118.77	126.04
18	H	4005	BCR	C34-C9-C10	-4.21	117.03	122.92
14	H	1213	CLA	C1D-ND-C4D	-4.21	103.35	106.33
14	A	1132	CLA	O2D-CGD-O1D	-4.21	115.61	123.84
18	b	4017	BCR	C3-C4-C5	-4.20	106.57	114.08
14	B	1208	CLA	O2A-CGA-CBA	4.20	125.10	111.91
18	B	4017	BCR	C38-C26-C25	-4.20	119.81	124.53
14	G	1132	CLA	O2D-CGD-O1D	-4.20	115.62	123.84
14	H	1208	CLA	C1D-ND-C4D	-4.20	103.35	106.33
14	B	1223	CLA	C1D-ND-C4D	-4.20	103.35	106.33
14	a	1138	CLA	CMB-C2B-C3B	4.20	132.53	124.68
14	A	1138	CLA	O2A-CGA-O1A	-4.20	113.00	123.59
14	a	1132	CLA	O2D-CGD-O1D	-4.20	115.63	123.84
14	B	1227	CLA	C3D-C2D-C1D	-4.20	100.11	105.83
14	H	1208	CLA	O2A-CGA-CBA	4.19	125.07	111.91
14	A	1138	CLA	CMB-C2B-C3B	4.19	132.52	124.68
14	A	1139	CLA	C4A-NA-C1A	4.19	108.59	106.71
14	A	1126	CLA	C1D-ND-C4D	-4.19	103.36	106.33
14	B	1225	CLA	C1D-ND-C4D	-4.19	103.36	106.33
14	B	1022	CLA	CHD-C1D-ND	-4.18	120.61	124.45
14	G	1126	CLA	C1D-ND-C4D	-4.18	103.36	106.33
14	B	1203	CLA	CAA-C2A-C3A	-4.18	101.33	112.78
14	a	1128	CLA	O2A-CGA-CBA	4.18	125.02	111.91
14	b	1210	CLA	C4A-NA-C1A	4.17	108.58	106.71
14	b	1227	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
14	B	1208	CLA	C1D-ND-C4D	-4.17	103.37	106.33
14	A	1128	CLA	O2A-CGA-CBA	4.17	124.99	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1138	CLA	O2A-CGA-O1A	-4.17	113.07	123.59
14	H	1022	CLA	CHD-C1D-ND	-4.17	120.62	124.45
14	b	1223	CLA	C1D-ND-C4D	-4.17	103.37	106.33
14	b	1023	CLA	O2A-CGA-CBA	4.17	124.99	111.91
14	H	1235	CLA	C1D-ND-C4D	-4.17	103.38	106.33
14	b	1213	CLA	C1D-ND-C4D	-4.17	103.38	106.33
18	b	4005	BCR	C34-C9-C10	-4.17	117.09	122.92
15	b	1238	F6C	C3D-C2D-C1D	-4.16	99.80	105.83
14	A	1129	CLA	C1D-ND-C4D	-4.16	103.38	106.33
15	B	1238	F6C	C3D-C2D-C1D	-4.16	99.80	105.83
14	H	1203	CLA	CAA-C2A-C3A	-4.16	101.39	112.78
14	B	1210	CLA	C4A-NA-C1A	4.16	108.58	106.71
14	A	1117	CLA	O2A-CGA-O1A	-4.16	113.10	123.59
15	H	1238	F6C	C3D-C2D-C1D	-4.15	99.81	105.83
14	b	1022	CLA	C1D-ND-C4D	-4.15	103.38	106.33
14	B	1023	CLA	O2A-CGA-CBA	4.15	124.94	111.91
14	G	1115	CLA	CMB-C2B-C3B	4.15	132.45	124.68
14	H	1227	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
14	b	1203	CLA	CAA-C2A-C3A	-4.15	101.41	112.78
14	B	1235	CLA	C1D-ND-C4D	-4.15	103.39	106.33
14	G	1117	CLA	O2A-CGA-O1A	-4.15	113.12	123.59
18	L	4019	BCR	C38-C26-C25	-4.15	119.87	124.53
14	a	1115	CLA	CMB-C2B-C3B	4.15	132.44	124.68
14	b	1216	CLA	C1D-ND-C4D	-4.15	103.39	106.33
14	L	1501	CLA	C1D-ND-C4D	-4.15	103.39	106.33
14	b	1217	CLA	O2A-CGA-CBA	4.15	124.92	111.91
14	H	1023	CLA	O2A-CGA-CBA	4.15	124.92	111.91
18	G	4011	BCR	C38-C26-C25	-4.14	119.87	124.53
14	H	1217	CLA	O2A-CGA-CBA	4.14	124.91	111.91
14	G	1128	CLA	O2A-CGA-CBA	4.14	124.91	111.91
18	B	4005	BCR	C34-C9-C10	-4.14	117.12	122.92
14	H	1225	CLA	O2A-CGA-CBA	4.14	124.91	111.91
14	a	1117	CLA	O2A-CGA-O1A	-4.14	113.14	123.59
18	B	4005	BCR	C38-C26-C25	-4.14	119.88	124.53
14	B	1225	CLA	O2A-CGA-CBA	4.14	124.90	111.91
14	a	1126	CLA	C1D-ND-C4D	-4.14	103.39	106.33
18	H	4005	BCR	C38-C26-C25	-4.14	119.88	124.53
14	B	1217	CLA	O2A-CGA-CBA	4.14	124.89	111.91
18	B	4010	BCR	C36-C18-C17	-4.14	117.13	122.92
14	A	1115	CLA	CMB-C2B-C3B	4.13	132.41	124.68
14	H	1210	CLA	C4A-NA-C1A	4.13	108.56	106.71
18	A	4011	BCR	C38-C26-C25	-4.13	119.89	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1225	CLA	O2A-CGA-CBA	4.13	124.87	111.91
14	b	1022	CLA	CHD-C1D-ND	-4.13	120.66	124.45
14	G	1122	CLA	O2A-CGA-CBA	4.13	124.86	111.91
18	a	4011	BCR	C38-C26-C25	-4.13	119.89	124.53
18	l	4019	BCR	C38-C26-C25	-4.12	119.90	124.53
14	b	1203	CLA	O2A-CGA-CBA	4.12	124.84	111.91
15	B	1207	F6C	C4A-NA-C1A	4.12	109.26	106.33
14	b	1235	CLA	C1D-ND-C4D	-4.12	103.41	106.33
14	H	1216	CLA	C1D-ND-C4D	-4.12	103.41	106.33
14	A	1108	CLA	C1D-ND-C4D	-4.12	103.41	106.33
18	U	4019	BCR	C38-C26-C25	-4.12	119.90	124.53
18	b	4010	BCR	C36-C18-C17	-4.12	117.16	122.92
15	H	1207	F6C	C4A-NA-C1A	4.12	109.26	106.33
18	G	4011	BCR	C3-C4-C5	-4.12	106.73	114.08
14	a	1139	CLA	C4A-NA-C1A	4.11	108.56	106.71
18	I	4018	BCR	C38-C26-C25	-4.11	119.91	124.53
18	a	4011	BCR	C3-C4-C5	-4.11	106.74	114.08
14	A	1122	CLA	O2A-CGA-CBA	4.11	124.81	111.91
18	H	4010	BCR	C36-C18-C17	-4.11	117.17	122.92
14	l	1501	CLA	C1D-ND-C4D	-4.11	103.42	106.33
14	a	1122	CLA	O2A-CGA-CBA	4.11	124.81	111.91
18	A	4011	BCR	C3-C4-C5	-4.11	106.74	114.08
14	A	1131	CLA	O2A-CGA-CBA	4.11	124.80	111.91
14	H	1205	CLA	CHD-C1D-ND	-4.11	120.68	124.45
14	B	1205	CLA	CHD-C1D-ND	-4.11	120.68	124.45
14	B	1203	CLA	O2A-CGA-CBA	4.11	124.80	111.91
14	a	1134	CLA	CMB-C2B-C3B	4.11	132.36	124.68
14	A	1013	CLA	O2A-CGA-CBA	4.11	124.79	111.91
14	b	1224	CLA	C1D-ND-C4D	-4.10	103.42	106.33
14	B	1211	CLA	C1-O2A-CGA	4.10	127.20	116.44
14	H	1203	CLA	O2A-CGA-CBA	4.10	124.78	111.91
14	G	1131	CLA	O2A-CGA-CBA	4.10	124.78	111.91
14	H	1211	CLA	C1-O2A-CGA	4.10	127.19	116.44
14	a	1137	CLA	O2A-CGA-CBA	4.10	124.76	111.91
14	a	1013	CLA	O2A-CGA-CBA	4.10	124.76	111.91
14	b	1210	CLA	CMB-C2B-C3B	4.09	132.34	124.68
14	b	1210	CLA	C1-C2-C3	-4.09	118.96	126.04
14	G	1134	CLA	CMB-C2B-C3B	4.09	132.34	124.68
14	a	1131	CLA	O2A-CGA-CBA	4.09	124.75	111.91
14	B	1210	CLA	CMB-C2B-C3B	4.09	132.33	124.68
14	a	1132	CLA	O2A-CGA-CBA	4.09	124.75	111.91
14	H	1210	CLA	C1-C2-C3	-4.09	118.97	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1211	CLA	C1-O2A-CGA	4.09	127.17	116.44
14	H	1210	CLA	CMB-C2B-C3B	4.09	132.33	124.68
14	G	1013	CLA	O2A-CGA-CBA	4.09	124.74	111.91
14	G	1133	CLA	C1D-ND-C4D	-4.09	103.43	106.33
14	A	1116	CLA	C1D-ND-C4D	-4.09	103.43	106.33
14	B	1224	CLA	C1D-ND-C4D	-4.09	103.43	106.33
14	H	1205	CLA	C1D-ND-C4D	-4.09	103.43	106.33
18	B	4013	BCR	C7-C8-C9	-4.08	120.06	126.23
14	H	1201	CLA	O2A-CGA-CBA	4.08	124.72	111.91
14	B	1210	CLA	C1-C2-C3	-4.08	118.98	126.04
14	H	1235	CLA	CMB-C2B-C3B	4.08	132.31	124.68
14	b	1218	CLA	CMB-C2B-C3B	4.08	132.31	124.68
14	G	1137	CLA	O2A-CGA-CBA	4.08	124.71	111.91
14	H	1218	CLA	CMB-C2B-C3B	4.08	132.31	124.68
14	A	1134	CLA	CMB-C2B-C3B	4.08	132.31	124.68
14	G	1132	CLA	O2A-CGA-CBA	4.08	124.71	111.91
14	U	1501	CLA	C1D-ND-C4D	-4.08	103.44	106.33
14	b	1205	CLA	CHD-C1D-ND	-4.08	120.71	124.45
14	B	1218	CLA	CMB-C2B-C3B	4.08	132.30	124.68
15	b	1207	F6C	C4A-NA-C1A	4.08	109.23	106.33
18	H	4013	BCR	C7-C8-C9	-4.07	120.08	126.23
14	a	1104	CLA	O2A-CGA-CBA	4.07	124.69	111.91
14	b	1213	CLA	O2A-CGA-CBA	4.07	124.69	111.91
14	b	1235	CLA	CMB-C2B-C3B	4.07	132.30	124.68
14	B	1205	CLA	C1D-ND-C4D	-4.07	103.44	106.33
14	B	1201	CLA	O2A-CGA-CBA	4.07	124.69	111.91
18	b	4005	BCR	C38-C26-C25	-4.07	119.96	124.53
14	A	1104	CLA	O2A-CGA-CBA	4.07	124.68	111.91
14	B	1213	CLA	O2A-CGA-CBA	4.07	124.68	111.91
14	A	1133	CLA	C1D-ND-C4D	-4.07	103.44	106.33
14	B	1235	CLA	CMB-C2B-C3B	4.07	132.29	124.68
14	G	1104	CLA	O2A-CGA-CBA	4.07	124.67	111.91
14	A	1132	CLA	O2A-CGA-CBA	4.07	124.67	111.91
14	A	1137	CLA	O2A-CGA-CBA	4.07	124.67	111.91
18	b	4013	BCR	C7-C8-C9	-4.06	120.09	126.23
14	G	1139	CLA	C4A-NA-C1A	4.06	108.53	106.71
14	a	1129	CLA	O2A-CGA-CBA	4.06	124.65	111.91
18	B	4014	BCR	C33-C5-C6	-4.06	119.97	124.53
14	b	1201	CLA	O2A-CGA-CBA	4.06	124.64	111.91
18	H	4009	BCR	C38-C26-C25	-4.06	119.97	124.53
18	b	4014	BCR	C33-C5-C6	-4.06	119.97	124.53
14	G	1108	CLA	C1D-ND-C4D	-4.05	103.45	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1224	CLA	C1D-ND-C4D	-4.05	103.46	106.33
15	H	1237	F6C	C1-C2-C3	-4.05	119.03	126.04
14	b	1222	CLA	CMB-C2B-C3B	4.05	132.26	124.68
14	G	1122	CLA	C1D-ND-C4D	-4.05	103.46	106.33
14	A	1122	CLA	C1D-ND-C4D	-4.05	103.46	106.33
14	H	1214	CLA	O2A-CGA-CBA	4.05	124.62	111.91
14	a	1108	CLA	C1D-ND-C4D	-4.05	103.46	106.33
14	G	1129	CLA	O2A-CGA-CBA	4.05	124.62	111.91
15	B	1237	F6C	C1-C2-C3	-4.05	119.04	126.04
18	R	4018	BCR	C38-C26-C25	-4.05	119.98	124.53
18	A	4011	BCR	C33-C5-C6	-4.05	119.98	124.53
14	H	1213	CLA	O2A-CGA-CBA	4.05	124.61	111.91
18	H	4014	BCR	C33-C5-C6	-4.05	119.98	124.53
14	A	1129	CLA	O2A-CGA-CBA	4.04	124.60	111.91
14	H	1222	CLA	CMB-C2B-C3B	4.04	132.25	124.68
14	B	1222	CLA	CMB-C2B-C3B	4.04	132.24	124.68
14	a	1122	CLA	C1D-ND-C4D	-4.04	103.46	106.33
18	b	4010	BCR	C3-C4-C5	-4.04	106.86	114.08
14	B	1214	CLA	O2A-CGA-CBA	4.04	124.59	111.91
18	B	4009	BCR	C38-C26-C25	-4.04	119.99	124.53
14	b	1239	CLA	CAC-C3C-C2C	4.04	134.44	127.53
14	H	1022	CLA	O2A-CGA-CBA	4.04	124.58	111.91
14	b	1205	CLA	C1D-ND-C4D	-4.04	103.47	106.33
14	A	1137	CLA	O2D-CGD-O1D	-4.04	115.94	123.84
15	b	1237	F6C	CMA-C3A-C4A	-4.04	117.60	124.71
14	b	1214	CLA	O2A-CGA-CBA	4.04	124.57	111.91
14	B	1201	CLA	CMB-C2B-C3B	4.04	132.23	124.68
14	B	1239	CLA	CAC-C3C-C2C	4.04	134.43	127.53
14	G	1116	CLA	C1D-ND-C4D	-4.03	103.47	106.33
15	B	1237	F6C	CMA-C3A-C4A	-4.03	117.60	124.71
14	H	1239	CLA	CAC-C3C-C2C	4.03	134.43	127.53
15	b	1237	F6C	C1-C2-C3	-4.03	119.07	126.04
18	B	4010	BCR	C3-C4-C5	-4.03	106.87	114.08
18	b	4009	BCR	C38-C26-C25	-4.03	120.00	124.53
14	A	1123	CLA	CHD-C1D-ND	-4.03	120.75	124.45
14	G	1103	CLA	C1D-ND-C4D	-4.03	103.47	106.33
14	b	1022	CLA	O2A-CGA-CBA	4.03	124.54	111.91
14	a	1103	CLA	C1D-ND-C4D	-4.02	103.48	106.33
14	B	1221	CLA	C1D-ND-C4D	-4.02	103.48	106.33
14	B	1022	CLA	O2A-CGA-CBA	4.02	124.54	111.91
14	A	1103	CLA	C1D-ND-C4D	-4.02	103.48	106.33
14	a	1109	CLA	O2A-CGA-CBA	4.02	124.53	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1109	CLA	O2A-CGA-CBA	4.02	124.53	111.91
14	a	1133	CLA	C1D-ND-C4D	-4.02	103.48	106.33
18	a	4011	BCR	C33-C5-C6	-4.02	120.01	124.53
14	A	1109	CLA	O2A-CGA-CBA	4.02	124.53	111.91
14	H	1228	CLA	O2A-CGA-CBA	4.02	124.52	111.91
18	i	4018	BCR	C38-C26-C25	-4.02	120.02	124.53
15	H	1237	F6C	CMA-C3A-C4A	-4.02	117.63	124.71
14	a	1137	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
14	H	1201	CLA	CMB-C2B-C3B	4.02	132.19	124.68
18	G	4011	BCR	C33-C5-C6	-4.02	120.02	124.53
14	G	1123	CLA	CHD-C1D-ND	-4.01	120.77	124.45
14	G	1137	CLA	O2D-CGD-O1D	-4.01	115.99	123.84
14	a	1118	CLA	C1D-ND-C4D	-4.01	103.49	106.33
14	B	1228	CLA	O2A-CGA-CBA	4.01	124.49	111.91
14	b	1228	CLA	O2A-CGA-CBA	4.01	124.48	111.91
14	b	1232	CLA	C1D-ND-C4D	-4.01	103.49	106.33
14	H	1239	CLA	C1-C2-C3	-4.00	119.12	126.04
14	b	1201	CLA	CMB-C2B-C3B	4.00	132.17	124.68
18	H	4010	BCR	C3-C4-C5	-4.00	106.93	114.08
14	a	1116	CLA	C1D-ND-C4D	-4.00	103.49	106.33
14	G	1135	CLA	O2A-C1-C2	3.99	119.13	108.64
14	a	1137	CLA	CMB-C2B-C3B	3.99	132.15	124.68
14	a	1135	CLA	O2A-C1-C2	3.99	119.12	108.64
14	A	1137	CLA	CMB-C2B-C3B	3.99	132.14	124.68
14	a	1123	CLA	CHD-C1D-ND	-3.99	120.79	124.45
14	a	1107	CLA	C1D-ND-C4D	-3.99	103.50	106.33
14	A	1135	CLA	O2A-C1-C2	3.98	119.11	108.64
14	B	1232	CLA	C1D-ND-C4D	-3.98	103.50	106.33
14	G	1137	CLA	CMB-C2B-C3B	3.98	132.13	124.68
14	a	1111	CLA	CMB-C2B-C3B	3.98	132.13	124.68
14	A	1111	CLA	CMB-C2B-C3B	3.98	132.13	124.68
14	A	1111	CLA	O2A-CGA-CBA	3.98	124.39	111.91
14	A	1103	CLA	CAA-C2A-C3A	-3.98	101.88	112.78
14	a	1103	CLA	CAA-C2A-C3A	-3.98	101.89	112.78
14	b	1239	CLA	C1-C2-C3	-3.98	119.16	126.04
14	B	1239	CLA	C1-C2-C3	-3.98	119.16	126.04
14	A	1137	CLA	C1D-ND-C4D	-3.98	103.51	106.33
13	G	1011	CL0	O2A-CGA-CBA	3.97	124.38	111.91
14	A	1106	CLA	O2A-C1-C2	3.97	119.08	108.64
14	a	1127	CLA	CHD-C1D-ND	-3.97	120.80	124.45
14	G	1118	CLA	C1D-ND-C4D	-3.97	103.51	106.33
13	a	1011	CL0	O2A-CGA-CBA	3.97	124.37	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1106	CLA	O2A-C1-C2	3.97	119.07	108.64
14	G	1111	CLA	O2A-CGA-CBA	3.97	124.36	111.91
14	G	1106	CLA	O2A-C1-C2	3.97	119.06	108.64
14	b	1221	CLA	C1D-ND-C4D	-3.97	103.52	106.33
14	A	1140	CLA	O2A-CGA-CBA	3.97	124.35	111.91
14	G	1103	CLA	CAA-C2A-C3A	-3.96	101.92	112.78
14	a	1140	CLA	O2A-CGA-CBA	3.96	124.34	111.91
14	H	1232	CLA	C1D-ND-C4D	-3.96	103.52	106.33
14	G	1140	CLA	O2A-CGA-CBA	3.96	124.33	111.91
13	A	1011	CL0	O2A-CGA-CBA	3.96	124.33	111.91
14	G	1107	CLA	C1D-ND-C4D	-3.96	103.52	106.33
18	A	4003	BCR	C28-C27-C26	-3.95	107.02	114.08
14	G	1111	CLA	CMB-C2B-C3B	3.95	132.08	124.68
14	a	1111	CLA	O2A-CGA-CBA	3.95	124.31	111.91
14	X	1701	CLA	O2A-CGA-CBA	3.95	124.31	111.91
14	H	1206	CLA	CMB-C2B-C3B	3.95	132.06	124.68
14	H	1210	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
14	x	1701	CLA	O2A-CGA-CBA	3.95	124.29	111.91
14	b	1214	CLA	C4A-NA-C1A	3.95	108.48	106.71
14	A	1107	CLA	C1D-ND-C4D	-3.95	103.53	106.33
14	G	1112	CLA	C1D-ND-C4D	-3.94	103.53	106.33
14	A	1106	CLA	CMB-C2B-C3B	3.94	132.06	124.68
14	b	1210	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
14	B	1221	CLA	CHD-C1D-ND	-3.94	120.83	124.45
14	a	1137	CLA	C1D-ND-C4D	-3.94	103.54	106.33
14	W	1701	CLA	O2A-CGA-CBA	3.94	124.26	111.91
14	A	1127	CLA	O2A-CGA-CBA	3.94	124.26	111.91
14	b	1221	CLA	CHD-C1D-ND	-3.93	120.84	124.45
14	H	1221	CLA	C1D-ND-C4D	-3.93	103.54	106.33
14	H	1239	CLA	C1D-ND-C4D	-3.93	103.54	106.33
14	A	1117	CLA	CMB-C2B-C3B	3.93	132.04	124.68
14	A	1127	CLA	CHD-C1D-ND	-3.93	120.84	124.45
14	a	1133	CLA	C1-C2-C3	-3.93	119.24	126.04
14	G	1106	CLA	CMB-C2B-C3B	3.93	132.03	124.68
14	B	1211	CLA	CMB-C2B-C3B	3.93	132.03	124.68
14	G	1118	CLA	O2A-CGA-CBA	3.93	124.25	111.91
14	G	1127	CLA	O2A-CGA-CBA	3.93	124.24	111.91
18	a	4003	BCR	C28-C27-C26	-3.93	107.07	114.08
14	b	1206	CLA	CMB-C2B-C3B	3.93	132.02	124.68
14	B	1206	CLA	CMB-C2B-C3B	3.92	132.02	124.68
18	G	4003	BCR	C28-C27-C26	-3.92	107.07	114.08
14	A	1118	CLA	O2A-CGA-CBA	3.92	124.22	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1133	CLA	C1-C2-C3	-3.92	119.26	126.04
14	A	1123	CLA	O2A-CGA-CBA	3.92	124.21	111.91
14	G	1123	CLA	C1D-ND-C4D	-3.92	103.55	106.33
14	G	1127	CLA	CHD-C1D-ND	-3.92	120.85	124.45
14	a	1127	CLA	O2A-CGA-CBA	3.92	124.20	111.91
18	G	4007	BCR	C38-C26-C25	-3.92	120.13	124.53
14	a	1106	CLA	CMB-C2B-C3B	3.92	132.00	124.68
14	A	1133	CLA	C1-C2-C3	-3.91	119.27	126.04
14	B	1239	CLA	C1D-ND-C4D	-3.91	103.55	106.33
14	A	1123	CLA	C1D-ND-C4D	-3.91	103.56	106.33
14	H	1227	CLA	C4A-NA-C1A	3.91	108.46	106.71
14	H	1224	CLA	O2A-CGA-CBA	3.91	124.18	111.91
14	a	1118	CLA	O2A-CGA-CBA	3.91	124.18	111.91
14	b	1224	CLA	O2A-CGA-CBA	3.91	124.17	111.91
15	H	1207	F6C	CHB-C4A-C3A	-3.91	117.28	125.48
14	A	1118	CLA	C1D-ND-C4D	-3.91	103.56	106.33
14	B	1224	CLA	O2A-CGA-CBA	3.91	124.17	111.91
15	B	1207	F6C	CHB-C4A-C3A	-3.91	117.29	125.48
14	B	1211	CLA	O2A-CGA-O1A	-3.91	113.73	123.59
14	A	1103	CLA	C1-C2-C3	-3.90	119.29	126.04
14	a	1117	CLA	CMB-C2B-C3B	3.90	131.98	124.68
14	G	1123	CLA	O2A-CGA-CBA	3.90	124.16	111.91
14	G	1117	CLA	CMB-C2B-C3B	3.90	131.98	124.68
14	B	1210	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
14	l	1502	CLA	C1-C2-C3	-3.90	119.29	126.04
14	L	1502	CLA	C1-C2-C3	-3.90	119.29	126.04
14	H	1221	CLA	CHD-C1D-ND	-3.90	120.87	124.45
14	b	1211	CLA	CMB-C2B-C3B	3.90	131.98	124.68
14	H	1211	CLA	O2A-CGA-O1A	-3.90	113.75	123.59
14	G	1103	CLA	C1-C2-C3	-3.90	119.30	126.04
14	H	1211	CLA	CMB-C2B-C3B	3.90	131.97	124.68
14	b	1239	CLA	C1D-ND-C4D	-3.90	103.57	106.33
14	G	1103	CLA	O2A-CGA-CBA	3.90	124.14	111.91
14	b	1211	CLA	O2A-CGA-O1A	-3.90	113.76	123.59
14	U	1502	CLA	C1-C2-C3	-3.89	119.31	126.04
18	b	4013	BCR	C33-C5-C6	-3.89	120.16	124.53
18	a	4007	BCR	C38-C26-C25	-3.89	120.16	124.53
18	A	4007	BCR	C38-C26-C25	-3.89	120.16	124.53
15	b	1207	F6C	CHB-C4A-C3A	-3.89	117.32	125.48
14	H	1209	CLA	C4A-NA-C1A	3.89	108.45	106.71
14	a	1123	CLA	O2A-CGA-CBA	3.89	124.11	111.91
15	b	1230	F6C	C4A-C3A-C2A	-3.88	101.27	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1103	CLA	O2A-CGA-CBA	3.88	124.10	111.91
14	G	1129	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
14	A	1103	CLA	O2A-CGA-CBA	3.88	124.08	111.91
14	b	1229	CLA	C4-C3-C5	3.87	121.79	115.27
14	a	1129	CLA	O2D-CGD-O1D	-3.87	116.26	123.84
18	B	4013	BCR	C33-C5-C6	-3.87	120.18	124.53
18	A	4002	BCR	C8-C9-C10	3.87	124.88	118.94
14	b	1227	CLA	C4A-NA-C1A	3.87	108.45	106.71
14	B	1227	CLA	C4A-NA-C1A	3.87	108.45	106.71
14	G	1135	CLA	CMB-C2B-C3B	3.87	131.92	124.68
14	a	1112	CLA	C1D-ND-C4D	-3.87	103.59	106.33
14	G	1012	CLA	C4A-NA-C1A	3.87	108.44	106.71
14	b	1215	CLA	O2A-CGA-O1A	-3.87	113.84	123.59
18	H	4013	BCR	C33-C5-C6	-3.86	120.19	124.53
14	a	1124	CLA	C1-C2-C3	-3.86	119.36	126.04
14	H	1229	CLA	C4-C3-C5	3.86	121.77	115.27
18	G	4002	BCR	C8-C9-C10	3.86	124.87	118.94
14	A	1135	CLA	CMB-C2B-C3B	3.86	131.90	124.68
15	H	1230	F6C	C4A-C3A-C2A	-3.86	101.30	106.94
14	a	1103	CLA	C1-C2-C3	-3.86	119.37	126.04
14	H	1215	CLA	O2A-CGA-O1A	-3.86	113.85	123.59
18	I	4020	BCR	C38-C26-C25	-3.86	120.19	124.53
14	a	1123	CLA	C1D-ND-C4D	-3.86	103.59	106.33
14	G	1137	CLA	C1D-ND-C4D	-3.86	103.59	106.33
14	A	1112	CLA	C1D-ND-C4D	-3.86	103.59	106.33
14	H	1214	CLA	C4A-NA-C1A	3.86	108.44	106.71
15	a	1121	F6C	C4A-C3A-C2A	-3.86	101.31	106.94
15	B	1230	F6C	C4A-C3A-C2A	-3.86	101.31	106.94
14	A	1124	CLA	C1-C2-C3	-3.86	119.37	126.04
14	A	1129	CLA	O2D-CGD-O1D	-3.86	116.30	123.84
15	A	1121	F6C	C4A-C3A-C2A	-3.86	101.31	106.94
14	U	1501	CLA	CMB-C2B-C3B	3.86	131.89	124.68
18	G	4011	BCR	C34-C9-C10	-3.85	117.52	122.92
14	a	1012	CLA	C4A-NA-C1A	3.85	108.44	106.71
14	B	1215	CLA	O2A-CGA-O1A	-3.85	113.87	123.59
18	a	4001	BCR	C15-C14-C13	-3.85	121.82	127.31
14	l	1501	CLA	CMB-C2B-C3B	3.85	131.87	124.68
15	G	1121	F6C	C4A-C3A-C2A	-3.85	101.32	106.94
18	A	4002	BCR	C36-C18-C17	-3.85	117.54	122.92
18	G	4008	BCR	C15-C14-C13	-3.84	121.82	127.31
14	a	1115	CLA	O2A-CGA-CBA	3.84	123.97	111.91
14	a	1135	CLA	CMB-C2B-C3B	3.84	131.87	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1115	CLA	O2A-CGA-CBA	3.84	123.96	111.91
14	G	1124	CLA	C1-C2-C3	-3.84	119.40	126.04
14	B	1229	CLA	C4-C3-C5	3.84	121.73	115.27
14	a	1112	CLA	CMB-C2B-C3B	3.84	131.86	124.68
14	L	1501	CLA	CMB-C2B-C3B	3.84	131.86	124.68
18	a	4011	BCR	C34-C9-C10	-3.84	117.55	122.92
18	A	4008	BCR	C15-C14-C13	-3.84	121.83	127.31
18	R	4020	BCR	C38-C26-C25	-3.84	120.22	124.53
14	G	1115	CLA	O2A-CGA-CBA	3.84	123.94	111.91
19	A	5001	LHG	O7-C7-C8	3.83	119.76	111.50
18	a	4002	BCR	C8-C9-C10	3.83	124.82	118.94
14	b	1201	CLA	C1D-ND-C4D	-3.83	103.61	106.33
14	B	1201	CLA	C1D-ND-C4D	-3.83	103.61	106.33
18	A	4011	BCR	C34-C9-C10	-3.83	117.56	122.92
14	H	1201	CLA	C1D-ND-C4D	-3.83	103.61	106.33
18	G	4002	BCR	C36-C18-C17	-3.83	117.56	122.92
14	A	1112	CLA	CMB-C2B-C3B	3.83	131.84	124.68
14	B	1214	CLA	C4A-NA-C1A	3.83	108.43	106.71
18	G	4001	BCR	C15-C14-C13	-3.83	121.85	127.31
19	a	5001	LHG	O7-C7-C8	3.82	119.74	111.50
14	B	1220	CLA	CMA-C3A-C4A	3.81	122.03	111.77
14	B	1209	CLA	C4A-NA-C1A	3.81	108.42	106.71
18	i	4020	BCR	C38-C26-C25	-3.81	120.25	124.53
18	a	4008	BCR	C15-C14-C13	-3.81	121.87	127.31
14	b	1220	CLA	CMA-C3A-C4A	3.81	122.02	111.77
14	B	1221	CLA	CMB-C2B-C3B	3.81	131.81	124.68
14	G	1126	CLA	O2A-CGA-CBA	3.81	123.86	111.91
19	G	5001	LHG	O7-C7-C8	3.81	119.70	111.50
14	A	1126	CLA	O2A-CGA-CBA	3.81	123.85	111.91
14	H	1221	CLA	O2A-CGA-CBA	3.80	123.85	111.91
18	a	4002	BCR	C36-C18-C17	-3.80	117.59	122.92
14	a	1126	CLA	O2A-CGA-CBA	3.80	123.85	111.91
14	A	1128	CLA	C1-C2-C3	-3.80	119.47	126.04
18	A	4001	BCR	C15-C14-C13	-3.80	121.88	127.31
14	b	1221	CLA	O2A-CGA-CBA	3.80	123.84	111.91
14	G	1112	CLA	CMB-C2B-C3B	3.80	131.79	124.68
14	b	1221	CLA	CMB-C2B-C3B	3.80	131.79	124.68
14	H	1220	CLA	CMA-C3A-C4A	3.80	121.99	111.77
18	B	4006	BCR	C24-C23-C22	-3.80	120.49	126.23
14	H	1204	CLA	C4A-NA-C1A	3.80	108.42	106.71
14	A	1012	CLA	C4A-NA-C1A	3.80	108.42	106.71
14	a	1125	CLA	C3C-C4C-NC	3.80	114.83	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1221	CLA	O2A-CGA-CBA	3.80	123.83	111.91
15	B	1238	F6C	C4A-C3A-C2A	-3.80	101.39	106.94
14	B	1204	CLA	C4A-NA-C1A	3.80	108.41	106.71
14	A	1138	CLA	C1D-ND-C4D	-3.80	103.64	106.33
15	H	1238	F6C	C4A-C3A-C2A	-3.79	101.40	106.94
14	H	1221	CLA	CMB-C2B-C3B	3.79	131.77	124.68
14	G	1138	CLA	C1D-ND-C4D	-3.79	103.64	106.33
19	H	5004	LHG	O7-C7-C8	3.79	119.67	111.50
14	b	1215	CLA	C1D-ND-C4D	-3.79	103.64	106.33
14	A	1130	CLA	C4A-NA-C1A	3.79	108.41	106.71
14	A	1125	CLA	C3C-C4C-NC	3.79	114.82	110.57
15	b	1238	F6C	C4A-C3A-C2A	-3.79	101.41	106.94
18	H	4013	BCR	C38-C26-C25	-3.79	120.28	124.53
14	b	1209	CLA	C4A-NA-C1A	3.79	108.41	106.71
14	B	1225	CLA	CHD-C1D-ND	-3.78	120.98	124.45
14	b	1208	CLA	CMB-C2B-C3B	3.78	131.75	124.68
14	A	1127	CLA	CMB-C2B-C3B	3.78	131.75	124.68
18	b	4006	BCR	C24-C23-C22	-3.78	120.52	126.23
18	b	4013	BCR	C15-C14-C13	-3.78	121.92	127.31
14	G	1128	CLA	C1-C2-C3	-3.78	119.51	126.04
14	B	1208	CLA	CMB-C2B-C3B	3.78	131.75	124.68
14	a	1127	CLA	CMB-C2B-C3B	3.78	131.74	124.68
14	b	1223	CLA	O2A-CGA-CBA	3.77	123.75	111.91
14	U	1501	CLA	O2A-C1-C2	3.77	118.56	108.64
14	l	1501	CLA	O2A-C1-C2	3.77	118.56	108.64
19	b	5004	LHG	O7-C7-C8	3.77	119.63	111.50
19	B	5004	LHG	O7-C7-C8	3.77	119.63	111.50
14	L	1501	CLA	O2A-C1-C2	3.77	118.54	108.64
18	H	4006	BCR	C24-C23-C22	-3.77	120.54	126.23
14	G	1127	CLA	CMB-C2B-C3B	3.77	131.73	124.68
14	G	1123	CLA	CMB-C2B-C3B	3.77	131.73	124.68
14	H	1223	CLA	O2A-CGA-CBA	3.77	123.73	111.91
18	H	4013	BCR	C15-C14-C13	-3.77	121.94	127.31
14	G	1125	CLA	C3C-C4C-NC	3.76	114.79	110.57
14	b	1224	CLA	C1-C2-C3	-3.76	119.53	126.04
14	B	1223	CLA	O2A-CGA-CBA	3.76	123.71	111.91
14	a	1140	CLA	C4-C3-C5	3.76	121.59	115.27
14	G	1140	CLA	C4-C3-C5	3.76	121.59	115.27
14	b	1227	CLA	C1D-ND-C4D	-3.76	103.67	106.33
14	b	1204	CLA	C4A-NA-C1A	3.75	108.39	106.71
14	A	1117	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
18	B	4013	BCR	C38-C26-C25	-3.75	120.31	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1123	CLA	CMB-C2B-C3B	3.75	131.70	124.68
14	a	1123	CLA	CMB-C2B-C3B	3.75	131.70	124.68
14	a	1128	CLA	C1-C2-C3	-3.75	119.55	126.04
14	a	1117	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
20	G	5005	LMG	O7-C10-C11	3.75	119.58	111.50
14	A	1140	CLA	C4-C3-C5	3.75	121.58	115.27
14	H	1208	CLA	CMB-C2B-C3B	3.75	131.69	124.68
20	L	5007	LMG	O7-C10-C11	3.75	119.57	111.50
14	H	1215	CLA	C1D-ND-C4D	-3.74	103.67	106.33
14	B	1215	CLA	C1D-ND-C4D	-3.74	103.68	106.33
20	A	5005	LMG	O7-C10-C11	3.74	119.56	111.50
18	A	4002	BCR	C38-C26-C25	-3.74	120.33	124.53
13	A	1011	CL0	C1-C2-C3	-3.74	119.58	126.04
13	a	1011	CL0	C1-C2-C3	-3.74	119.58	126.04
14	B	1224	CLA	C1-C2-C3	-3.74	119.58	126.04
14	H	1224	CLA	C1-C2-C3	-3.74	119.58	126.04
14	l	1503	CLA	O2A-CGA-CBA	3.74	123.63	111.91
14	A	1116	CLA	O2A-CGA-CBA	3.74	123.63	111.91
14	H	1227	CLA	C1D-ND-C4D	-3.73	103.68	106.33
14	H	1220	CLA	O2A-CGA-CBA	3.73	123.62	111.91
14	B	1220	CLA	O2A-CGA-CBA	3.73	123.62	111.91
14	b	1225	CLA	CHD-C1D-ND	-3.73	121.03	124.45
18	b	4013	BCR	C38-C26-C25	-3.73	120.34	124.53
14	H	1225	CLA	CHD-C1D-ND	-3.73	121.03	124.45
14	a	1130	CLA	C4A-NA-C1A	3.73	108.38	106.71
14	G	1117	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
14	B	1227	CLA	C1D-ND-C4D	-3.73	103.69	106.33
18	b	4006	BCR	C33-C5-C6	-3.73	120.34	124.53
14	L	1503	CLA	O2A-CGA-CBA	3.73	123.60	111.91
14	H	1239	CLA	O2A-CGA-CBA	3.73	123.60	111.91
20	l	5007	LMG	O7-C10-C11	3.73	119.53	111.50
14	G	1116	CLA	O2A-CGA-CBA	3.72	123.60	111.91
20	a	5005	LMG	O7-C10-C11	3.72	119.53	111.50
18	G	4002	BCR	C38-C26-C25	-3.72	120.35	124.53
18	a	4008	BCR	C34-C9-C10	-3.72	117.71	122.92
18	B	4013	BCR	C15-C14-C13	-3.72	122.00	127.31
13	G	1011	CL0	C1-C2-C3	-3.72	119.61	126.04
14	A	1115	CLA	C1-C2-C3	-3.72	119.61	126.04
14	a	1115	CLA	C1-C2-C3	-3.72	119.61	126.04
14	b	1220	CLA	O2A-CGA-CBA	3.72	123.57	111.91
20	U	5007	LMG	O7-C10-C11	3.72	119.51	111.50
14	a	1116	CLA	O2A-CGA-CBA	3.71	123.57	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1022	CLA	CMC-C2C-C1C	3.71	130.70	125.04
14	b	1239	CLA	O2A-CGA-CBA	3.71	123.56	111.91
15	b	1238	F6C	O2A-CGA-CBA	3.71	123.56	111.91
15	B	1238	F6C	O2A-CGA-CBA	3.71	123.56	111.91
14	B	1231	CLA	O2A-CGA-CBA	3.71	123.56	111.91
14	b	1231	CLA	O2A-CGA-CBA	3.71	123.56	111.91
14	b	1205	CLA	O2A-C1-C2	3.71	118.39	108.64
15	H	1238	F6C	O2A-CGA-CBA	3.71	123.56	111.91
18	H	4006	BCR	C33-C5-C6	-3.71	120.36	124.53
14	U	1503	CLA	O2A-CGA-CBA	3.71	123.55	111.91
18	b	4017	BCR	C15-C14-C13	-3.71	122.02	127.31
14	B	1239	CLA	O2A-CGA-CBA	3.71	123.55	111.91
18	a	4002	BCR	C38-C26-C25	-3.71	120.36	124.53
18	H	4004	BCR	C38-C26-C25	-3.71	120.37	124.53
18	B	4006	BCR	C33-C5-C6	-3.71	120.37	124.53
18	A	4008	BCR	C34-C9-C10	-3.71	117.73	122.92
14	H	1231	CLA	O2A-CGA-CBA	3.71	123.53	111.91
14	G	1115	CLA	C1-C2-C3	-3.70	119.64	126.04
14	B	1205	CLA	O2A-C1-C2	3.70	118.37	108.64
14	X	1701	CLA	CMB-C2B-C3B	3.70	131.61	124.68
14	B	1022	CLA	CMC-C2C-C1C	3.70	130.68	125.04
14	H	1205	CLA	O2A-C1-C2	3.70	118.36	108.64
18	B	4017	BCR	C15-C14-C13	-3.70	122.03	127.31
18	H	4017	BCR	C15-C14-C13	-3.70	122.03	127.31
14	x	1701	CLA	CMB-C2B-C3B	3.70	131.60	124.68
18	B	4016	BCR	C33-C5-C6	-3.70	120.38	124.53
14	a	1114	CLA	C1D-ND-C4D	-3.69	103.71	106.33
14	a	1138	CLA	C1D-ND-C4D	-3.69	103.71	106.33
14	W	1701	CLA	CMB-C2B-C3B	3.69	131.59	124.68
18	A	4011	BCR	C33-C5-C4	3.69	120.71	113.62
14	b	1022	CLA	CMC-C2C-C1C	3.69	130.66	125.04
14	G	1124	CLA	CMB-C2B-C3B	3.69	131.58	124.68
18	b	4016	BCR	C33-C5-C6	-3.69	120.39	124.53
14	a	1012	CLA	C1D-ND-C4D	-3.68	103.72	106.33
14	a	1102	CLA	C1D-ND-C4D	-3.68	103.72	106.33
14	b	1203	CLA	C1-C2-C3	-3.68	119.67	126.04
18	A	4007	BCR	C33-C5-C6	-3.68	120.40	124.53
18	H	4016	BCR	C33-C5-C6	-3.68	120.40	124.53
18	b	4004	BCR	C38-C26-C25	-3.68	120.40	124.53
14	A	1124	CLA	CMB-C2B-C3B	3.68	131.55	124.68
18	G	4008	BCR	C34-C9-C10	-3.67	117.78	122.92
18	a	4007	BCR	C33-C5-C6	-3.67	120.41	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	1237	F6C	C4-C3-C5	3.67	121.44	115.27
14	A	1102	CLA	C1D-ND-C4D	-3.67	103.73	106.33
14	H	1235	CLA	O2A-C1-C2	3.67	118.27	108.64
14	G	1130	CLA	C4A-NA-C1A	3.67	108.35	106.71
14	G	1130	CLA	C1D-ND-C4D	-3.66	103.73	106.33
18	a	4011	BCR	C33-C5-C4	3.66	120.65	113.62
14	a	1124	CLA	CMB-C2B-C3B	3.66	131.53	124.68
15	B	1237	F6C	C4-C3-C5	3.66	121.42	115.27
15	H	1238	F6C	C1-C2-C3	-3.65	119.72	126.04
15	B	1238	F6C	C1-C2-C3	-3.65	119.72	126.04
14	b	1022	CLA	C4-C3-C5	3.65	121.42	115.27
14	W	1701	CLA	C1-C2-C3	-3.65	119.73	126.04
14	x	1701	CLA	C1-C2-C3	-3.65	119.73	126.04
14	B	1235	CLA	O2A-C1-C2	3.65	118.23	108.64
14	H	1232	CLA	CMB-C2B-C3B	3.65	131.51	124.68
18	G	4011	BCR	C33-C5-C4	3.65	120.63	113.62
15	b	1238	F6C	C1-C2-C3	-3.65	119.73	126.04
14	B	1204	CLA	O2A-C1-C2	3.65	118.22	108.64
14	B	1022	CLA	C4-C3-C5	3.65	121.41	115.27
14	a	1130	CLA	C1D-ND-C4D	-3.65	103.74	106.33
14	b	1235	CLA	O2A-C1-C2	3.65	118.22	108.64
14	G	1114	CLA	C1D-ND-C4D	-3.65	103.74	106.33
14	A	1114	CLA	C1D-ND-C4D	-3.65	103.74	106.33
15	b	1237	F6C	C4-C3-C5	3.65	121.40	115.27
14	H	1022	CLA	C4-C3-C5	3.64	121.40	115.27
14	B	1232	CLA	CMB-C2B-C3B	3.64	131.49	124.68
18	B	4004	BCR	C38-C26-C25	-3.64	120.44	124.53
14	b	1232	CLA	CMB-C2B-C3B	3.64	131.49	124.68
14	A	1132	CLA	C1-C2-C3	-3.64	119.75	126.04
14	B	1203	CLA	C1-C2-C3	-3.64	119.75	126.04
14	B	1202	CLA	O2A-C1-C2	3.64	118.19	108.64
14	X	1701	CLA	C1-C2-C3	-3.64	119.75	126.04
18	b	4016	BCR	C24-C23-C22	-3.63	120.74	126.23
18	B	4016	BCR	C24-C23-C22	-3.63	120.74	126.23
14	H	1204	CLA	O2A-C1-C2	3.63	118.19	108.64
18	G	4007	BCR	C33-C5-C6	-3.63	120.45	124.53
14	H	1202	CLA	O2A-C1-C2	3.63	118.19	108.64
14	b	1204	CLA	O2A-C1-C2	3.63	118.19	108.64
14	b	1202	CLA	O2A-C1-C2	3.63	118.18	108.64
14	G	1132	CLA	C1-C2-C3	-3.63	119.76	126.04
18	H	4016	BCR	C24-C23-C22	-3.63	120.75	126.23
14	G	1131	CLA	C1D-ND-C4D	-3.63	103.76	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	H	4004	BCR	C38-C26-C27	3.62	120.58	113.62
18	B	4004	BCR	C19-C18-C17	3.62	124.50	118.94
14	H	1203	CLA	C1-C2-C3	-3.62	119.78	126.04
14	B	1021	CLA	CAA-C2A-C3A	-3.62	102.87	112.78
14	b	1021	CLA	CAA-C2A-C3A	-3.62	102.87	112.78
18	b	4004	BCR	C19-C18-C17	3.62	124.49	118.94
15	H	1237	F6C	C3A-C4A-NA	3.62	112.77	110.10
16	a	2001	PQN	C14-C13-C15	3.62	121.35	115.27
14	H	1021	CLA	CAA-C2A-C3A	-3.62	102.88	112.78
18	H	4005	BCR	C38-C26-C27	3.61	120.56	113.62
14	A	1105	CLA	CMB-C2B-C3B	3.61	131.43	124.68
14	G	1102	CLA	C1D-ND-C4D	-3.61	103.77	106.33
14	A	1131	CLA	C1D-ND-C4D	-3.61	103.77	106.33
14	B	1022	CLA	C3C-C4C-NC	3.61	114.62	110.57
14	a	1105	CLA	CMB-C2B-C3B	3.61	131.43	124.68
14	H	1222	CLA	CAA-CBA-CGA	-3.61	102.71	113.25
14	G	1105	CLA	CMB-C2B-C3B	3.61	131.43	124.68
14	b	1022	CLA	C3C-C4C-NC	3.61	114.61	110.57
18	B	4005	BCR	C38-C26-C27	3.60	120.54	113.62
14	B	1222	CLA	CAA-CBA-CGA	-3.60	102.72	113.25
14	H	1218	CLA	C3C-C4C-NC	3.60	114.61	110.57
14	b	1214	CLA	C1-C2-C3	-3.60	119.81	126.04
14	B	1228	CLA	CMB-C2B-C3B	3.60	131.42	124.68
14	b	1205	CLA	CMB-C2B-C3B	3.60	131.42	124.68
14	B	1202	CLA	C4-C3-C5	3.60	121.33	115.27
14	H	1214	CLA	C1-C2-C3	-3.60	119.82	126.04
14	b	1222	CLA	CAA-CBA-CGA	-3.60	102.74	113.25
14	b	1202	CLA	C4-C3-C5	3.60	121.32	115.27
14	a	1132	CLA	C1-C2-C3	-3.60	119.82	126.04
14	a	1131	CLA	C1D-ND-C4D	-3.60	103.78	106.33
18	b	4004	BCR	C38-C26-C27	3.60	120.53	113.62
14	H	1202	CLA	C4-C3-C5	3.60	121.32	115.27
14	B	1204	CLA	O2A-CGA-CBA	3.60	123.19	111.91
14	H	1204	CLA	O2A-CGA-CBA	3.60	123.19	111.91
14	A	1103	CLA	O2D-CGD-O1D	-3.60	116.81	123.84
14	H	1223	CLA	C1-C2-C3	-3.59	119.83	126.04
14	B	1214	CLA	C1-C2-C3	-3.59	119.83	126.04
16	A	2001	PQN	C14-C13-C15	3.59	121.32	115.27
14	a	1103	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
14	B	1218	CLA	C3C-C4C-NC	3.59	114.60	110.57
14	b	1204	CLA	O2A-CGA-CBA	3.59	123.18	111.91
16	G	2001	PQN	C14-C13-C15	3.59	121.31	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1223	CLA	C1-C2-C3	-3.59	119.84	126.04
14	H	1205	CLA	CMB-C2B-C3B	3.59	131.39	124.68
14	G	1103	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
18	H	4004	BCR	C19-C18-C17	3.58	124.44	118.94
14	G	1012	CLA	C1D-ND-C4D	-3.58	103.79	106.33
14	B	1223	CLA	C1-C2-C3	-3.58	119.85	126.04
14	H	1022	CLA	C3C-C4C-NC	3.58	114.59	110.57
15	B	1237	F6C	CHB-C4A-NA	3.58	127.74	124.45
14	A	1130	CLA	C1D-ND-C4D	-3.58	103.79	106.33
18	b	4009	BCR	C7-C8-C9	-3.58	120.83	126.23
18	B	4004	BCR	C38-C26-C27	3.58	120.49	113.62
14	b	1228	CLA	CMB-C2B-C3B	3.58	131.37	124.68
18	b	4005	BCR	C38-C26-C27	3.57	120.48	113.62
14	b	1218	CLA	C3C-C4C-NC	3.57	114.58	110.57
14	B	1205	CLA	CMB-C2B-C3B	3.57	131.36	124.68
14	G	1104	CLA	C1-C2-C3	-3.57	119.87	126.04
18	H	4009	BCR	C7-C8-C9	-3.57	120.84	126.23
15	b	1237	F6C	C3A-C4A-NA	3.57	112.73	110.10
14	G	1106	CLA	O2A-CGA-CBA	3.56	123.09	111.91
14	H	1228	CLA	CMB-C2B-C3B	3.56	131.35	124.68
14	a	1119	CLA	C1D-ND-C4D	-3.56	103.80	106.33
14	A	1104	CLA	C1-C2-C3	-3.56	119.88	126.04
18	A	4007	BCR	C31-C1-C6	-3.56	104.52	110.30
14	G	1119	CLA	C1D-ND-C4D	-3.56	103.81	106.33
14	G	1124	CLA	O2A-CGA-CBA	3.56	123.08	111.91
14	a	1104	CLA	C1-C2-C3	-3.56	119.89	126.04
14	A	1126	CLA	CMB-C2B-C3B	3.56	131.33	124.68
14	a	1124	CLA	O2A-CGA-CBA	3.55	123.06	111.91
18	a	4007	BCR	C31-C1-C6	-3.55	104.54	110.30
18	B	4009	BCR	C7-C8-C9	-3.55	120.87	126.23
14	A	1124	CLA	O2A-CGA-CBA	3.55	123.05	111.91
14	a	1106	CLA	O2A-CGA-CBA	3.55	123.04	111.91
14	B	1219	CLA	CAC-C3C-C4C	3.55	129.41	124.81
14	G	1102	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
14	A	1106	CLA	O2A-CGA-CBA	3.54	123.03	111.91
14	A	1012	CLA	C1D-ND-C4D	-3.54	103.82	106.33
14	a	1138	CLA	CED-O2D-CGD	3.54	123.95	115.94
14	b	1219	CLA	CAC-C3C-C4C	3.54	129.40	124.81
14	a	1119	CLA	CMB-C2B-C3B	3.53	131.29	124.68
14	a	1126	CLA	CMB-C2B-C3B	3.53	131.29	124.68
18	G	4007	BCR	C31-C1-C6	-3.53	104.57	110.30
14	G	1126	CLA	CMB-C2B-C3B	3.53	131.28	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1119	CLA	CMB-C2B-C3B	3.53	131.28	124.68
14	l	1501	CLA	O2A-CGA-CBA	3.53	122.98	111.91
15	b	1237	F6C	CHB-C4A-NA	3.53	127.69	124.45
15	H	1237	F6C	O2A-CGA-CBA	3.53	122.97	111.91
15	B	1238	F6C	C4A-NA-C1A	3.53	108.84	106.33
15	B	1237	F6C	O2A-CGA-CBA	3.53	122.97	111.91
14	U	1501	CLA	O2A-CGA-CBA	3.52	122.97	111.91
14	H	1219	CLA	CAC-C3C-C4C	3.52	129.38	124.81
15	b	1237	F6C	O2A-CGA-CBA	3.52	122.96	111.91
14	A	1138	CLA	CED-O2D-CGD	3.52	123.90	115.94
15	B	1237	F6C	C3A-C4A-NA	3.52	112.70	110.10
14	A	1102	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
14	L	1501	CLA	O2A-CGA-CBA	3.51	122.94	111.91
14	G	1138	CLA	CED-O2D-CGD	3.51	123.88	115.94
18	U	4022	BCR	C33-C5-C4	3.51	120.36	113.62
14	a	1102	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
14	B	1201	CLA	C1-C2-C3	-3.51	119.97	126.04
15	H	1237	F6C	CHB-C4A-NA	3.51	127.68	124.45
18	B	4006	BCR	C34-C9-C10	-3.51	118.01	122.92
13	a	1011	CL0	CAA-C2A-C3A	-3.51	103.18	112.78
18	U	4019	BCR	C30-C25-C24	3.50	125.69	115.78
18	H	4006	BCR	C34-C9-C10	-3.50	118.02	122.92
18	l	4019	BCR	C30-C25-C24	3.50	125.68	115.78
14	H	1201	CLA	C1-C2-C3	-3.50	119.99	126.04
14	B	1231	CLA	C1-C2-C3	-3.50	119.99	126.04
18	l	4022	BCR	C33-C5-C4	3.50	120.33	113.62
14	A	1130	CLA	O2A-CGA-CBA	3.50	122.88	111.91
18	L	4022	BCR	C33-C5-C4	3.50	120.33	113.62
13	G	1011	CL0	CAA-C2A-C3A	-3.50	103.20	112.78
13	A	1011	CL0	CAA-C2A-C3A	-3.50	103.20	112.78
14	G	1119	CLA	CMB-C2B-C3B	3.49	131.22	124.68
18	b	4006	BCR	C34-C9-C10	-3.49	118.03	122.92
18	R	4020	BCR	C7-C8-C9	-3.49	120.96	126.23
14	A	1119	CLA	C1D-ND-C4D	-3.49	103.86	106.33
14	b	1201	CLA	C1-C2-C3	-3.49	120.01	126.04
14	G	1116	CLA	CMB-C2B-C3B	3.49	131.20	124.68
18	L	4019	BCR	C30-C25-C24	3.49	125.64	115.78
14	G	1130	CLA	O2A-CGA-CBA	3.48	122.84	111.91
14	b	1231	CLA	C1-C2-C3	-3.48	120.02	126.04
18	B	4014	BCR	C34-C9-C10	-3.48	118.05	122.92
14	H	1231	CLA	C1-C2-C3	-3.48	120.02	126.04
14	a	1116	CLA	CMB-C2B-C3B	3.48	131.19	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1130	CLA	O2A-CGA-CBA	3.48	122.83	111.91
14	B	1021	CLA	O2A-CGA-CBA	3.48	122.82	111.91
18	I	4020	BCR	C7-C8-C9	-3.48	120.98	126.23
14	B	1224	CLA	CMB-C2B-C3B	3.48	131.18	124.68
14	A	1116	CLA	CMB-C2B-C3B	3.47	131.18	124.68
18	H	4014	BCR	C34-C9-C10	-3.47	118.06	122.92
14	H	1021	CLA	O2A-CGA-CBA	3.47	122.81	111.91
14	b	1021	CLA	O2A-CGA-CBA	3.47	122.80	111.91
14	B	1213	CLA	CMB-C2B-C3B	3.47	131.17	124.68
14	B	1217	CLA	C1-C2-C3	-3.47	120.05	126.04
18	b	4004	BCR	C36-C18-C17	-3.47	118.07	122.92
14	H	1023	CLA	C1-C2-C3	-3.47	120.05	126.04
14	b	1217	CLA	C1-C2-C3	-3.47	120.05	126.04
14	G	1133	CLA	CMB-C2B-C3B	3.46	131.16	124.68
14	a	1133	CLA	CMB-C2B-C3B	3.46	131.15	124.68
14	H	1213	CLA	CMB-C2B-C3B	3.46	131.15	124.68
18	i	4020	BCR	C7-C8-C9	-3.46	121.01	126.23
14	b	1224	CLA	CMB-C2B-C3B	3.46	131.15	124.68
14	b	1213	CLA	CMB-C2B-C3B	3.45	131.14	124.68
18	H	4004	BCR	C36-C18-C17	-3.45	118.08	122.92
18	B	4013	BCR	C28-C27-C26	-3.45	107.91	114.08
14	A	1135	CLA	O2A-CGA-CBA	3.45	122.74	111.91
18	B	4004	BCR	C36-C18-C17	-3.45	118.09	122.92
14	H	1224	CLA	CMB-C2B-C3B	3.45	131.14	124.68
18	b	4013	BCR	C28-C27-C26	-3.45	107.91	114.08
14	b	1023	CLA	C1-C2-C3	-3.45	120.08	126.04
14	a	1135	CLA	O2A-CGA-CBA	3.45	122.73	111.91
14	H	1217	CLA	C1-C2-C3	-3.45	120.08	126.04
14	B	1023	CLA	C1-C2-C3	-3.45	120.08	126.04
18	b	4014	BCR	C34-C9-C10	-3.45	118.10	122.92
14	a	1117	CLA	C1D-ND-C4D	-3.44	103.89	106.33
14	A	1133	CLA	CMB-C2B-C3B	3.44	131.12	124.68
18	A	4001	BCR	C36-C18-C17	-3.44	118.10	122.92
15	b	1238	F6C	C4A-NA-C1A	3.44	108.78	106.33
15	H	1238	F6C	C4A-NA-C1A	3.44	108.78	106.33
14	H	1212	CLA	CMB-C2B-C3B	3.44	131.11	124.68
14	G	1135	CLA	O2A-CGA-CBA	3.43	122.69	111.91
14	G	1117	CLA	C1D-ND-C4D	-3.43	103.90	106.33
18	b	4017	BCR	C34-C9-C10	-3.43	118.11	122.92
14	L	1502	CLA	O2A-CGA-CBA	3.43	122.68	111.91
18	B	4016	BCR	C7-C8-C9	-3.43	121.05	126.23
18	H	4013	BCR	C28-C27-C26	-3.43	107.95	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1214	CLA	C1D-ND-C4D	-3.43	103.90	106.33
13	G	1011	CL0	O2D-CGD-O1D	-3.43	117.13	123.84
14	U	1502	CLA	O2A-CGA-CBA	3.43	122.67	111.91
14	B	1231	CLA	CMC-C2C-C1C	3.43	130.26	125.04
18	H	4017	BCR	C34-C9-C10	-3.43	118.12	122.92
13	A	1011	CL0	O2D-CGD-O1D	-3.43	117.14	123.84
18	b	4016	BCR	C7-C8-C9	-3.43	121.06	126.23
18	A	4002	BCR	C28-C27-C26	-3.42	107.96	114.08
14	b	1201	CLA	C4-C3-C5	3.42	121.03	115.27
14	l	1502	CLA	O2A-CGA-CBA	3.42	122.65	111.91
15	b	1238	F6C	CMA-C3A-C4A	-3.42	118.68	124.71
18	a	4002	BCR	C28-C27-C26	-3.42	107.97	114.08
14	B	1214	CLA	C1D-ND-C4D	-3.42	103.90	106.33
18	L	4022	BCR	C15-C14-C13	-3.42	122.43	127.31
14	B	1201	CLA	C4-C3-C5	3.42	121.02	115.27
15	H	1238	F6C	CMA-C3A-C4A	-3.42	118.69	124.71
14	a	1116	CLA	C1-C2-C3	-3.42	120.13	126.04
14	b	1216	CLA	C1-C2-C3	-3.42	120.14	126.04
18	H	4016	BCR	C7-C8-C9	-3.41	121.08	126.23
14	b	1212	CLA	CMB-C2B-C3B	3.41	131.06	124.68
14	b	1231	CLA	CMC-C2C-C1C	3.41	130.24	125.04
14	H	1201	CLA	C4-C3-C5	3.41	121.01	115.27
14	H	1214	CLA	C1D-ND-C4D	-3.41	103.91	106.33
15	B	1238	F6C	CMA-C3A-C4A	-3.41	118.70	124.71
14	A	1111	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
14	A	1125	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
14	B	1023	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
18	I	4018	BCR	C38-C26-C27	3.41	120.16	113.62
18	A	4007	BCR	C3-C4-C5	-3.41	107.99	114.08
13	a	1011	CL0	O2D-CGD-O1D	-3.41	117.18	123.84
18	l	4022	BCR	C15-C14-C13	-3.40	122.45	127.31
18	B	4017	BCR	C34-C9-C10	-3.40	118.15	122.92
18	i	4018	BCR	C38-C26-C27	3.40	120.15	113.62
14	A	1117	CLA	O2A-CGA-CBA	3.40	122.57	111.91
14	a	1117	CLA	O2A-CGA-CBA	3.40	122.57	111.91
14	G	1111	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
14	G	1117	CLA	O2A-CGA-CBA	3.40	122.57	111.91
18	G	4002	BCR	C28-C27-C26	-3.40	108.01	114.08
14	B	1216	CLA	C1-C2-C3	-3.39	120.17	126.04
14	a	1111	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
18	b	4017	BCR	C33-C5-C6	-3.39	120.72	124.53
14	H	1231	CLA	CMC-C2C-C1C	3.39	130.20	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1216	CLA	C1-C2-C3	-3.39	120.18	126.04
14	b	1206	CLA	C1D-ND-C4D	-3.39	103.93	106.33
14	G	1116	CLA	C1-C2-C3	-3.39	120.18	126.04
18	G	4007	BCR	C3-C4-C5	-3.39	108.03	114.08
18	G	4001	BCR	C36-C18-C17	-3.39	118.18	122.92
14	G	1012	CLA	C1-C2-C3	-3.39	120.18	126.04
14	B	1233	CLA	O2A-CGA-CBA	3.39	124.92	114.03
14	A	1119	CLA	CMC-C2C-C3C	3.39	135.31	126.12
14	a	1119	CLA	CMC-C2C-C3C	3.39	135.31	126.12
15	G	1121	F6C	C4A-NA-C1A	3.39	108.74	106.33
18	a	4001	BCR	C36-C18-C17	-3.39	118.18	122.92
14	a	1129	CLA	C1-C2-C3	-3.39	121.27	126.75
18	a	4007	BCR	C3-C4-C5	-3.39	108.03	114.08
18	H	4017	BCR	C33-C5-C6	-3.39	120.73	124.53
18	R	4018	BCR	C38-C26-C27	3.39	120.12	113.62
14	b	1023	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
14	H	1023	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
18	a	4001	BCR	C3-C4-C5	-3.38	108.04	114.08
18	A	4001	BCR	C3-C4-C5	-3.38	108.04	114.08
14	b	1233	CLA	O2A-CGA-CBA	3.38	124.89	114.03
14	H	1233	CLA	O2A-CGA-CBA	3.38	124.89	114.03
14	B	1212	CLA	CMB-C2B-C3B	3.38	131.00	124.68
14	b	1223	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
14	A	1012	CLA	C1-C2-C3	-3.38	120.20	126.04
18	G	4001	BCR	C3-C4-C5	-3.38	108.05	114.08
14	b	1210	CLA	O2A-CGA-CBA	3.38	122.51	111.91
14	B	1216	CLA	C4-C3-C5	3.38	120.95	115.27
14	B	1223	CLA	O2D-CGD-O1D	-3.38	117.24	123.84
14	A	1116	CLA	C1-C2-C3	-3.37	120.21	126.04
18	U	4022	BCR	C15-C14-C13	-3.37	122.49	127.31
14	H	1206	CLA	C1D-ND-C4D	-3.37	103.94	106.33
14	G	1013	CLA	C1-C2-C3	-3.37	120.21	126.04
14	B	1210	CLA	O2A-CGA-CBA	3.37	122.49	111.91
14	a	1012	CLA	C1-C2-C3	-3.37	120.21	126.04
14	B	1206	CLA	C1D-ND-C4D	-3.37	103.94	106.33
14	G	1119	CLA	CMC-C2C-C3C	3.37	135.27	126.12
14	a	1137	CLA	C1-C2-C3	-3.37	121.30	126.75
14	A	1117	CLA	C1D-ND-C4D	-3.37	103.94	106.33
14	b	1021	CLA	C6-C5-C3	-3.37	104.62	113.45
14	A	1122	CLA	C4-C3-C5	3.37	120.94	115.27
14	H	1234	CLA	C1-C2-C3	-3.37	120.22	126.04
14	a	1113	CLA	CMB-C2B-C3B	3.37	130.98	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1021	CLA	C6-C5-C3	-3.36	104.63	113.45
14	b	1021	CLA	CMB-C2B-C3B	3.36	130.97	124.68
14	G	1137	CLA	C1-C2-C3	-3.36	121.31	126.75
14	H	1210	CLA	O2A-CGA-CBA	3.36	122.46	111.91
14	H	1021	CLA	C6-C5-C3	-3.36	104.64	113.45
14	b	1205	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
14	H	1216	CLA	C4-C3-C5	3.36	120.92	115.27
14	A	1137	CLA	C1-C2-C3	-3.36	121.31	126.75
14	a	1013	CLA	C1-C2-C3	-3.36	120.23	126.04
14	B	1205	CLA	O2D-CGD-O1D	-3.36	117.28	123.84
18	B	4017	BCR	C33-C5-C6	-3.36	120.76	124.53
14	H	1223	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
14	H	1205	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
14	b	1234	CLA	C1-C2-C3	-3.35	120.24	126.04
14	W	1701	CLA	C4-C3-C5	3.35	120.91	115.27
14	a	1101	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
14	H	1021	CLA	CMB-C2B-C3B	3.35	130.95	124.68
14	a	1125	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
14	A	1113	CLA	CMB-C2B-C3B	3.35	130.95	124.68
14	G	1125	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
14	B	1021	CLA	CMB-C2B-C3B	3.35	130.95	124.68
14	G	1113	CLA	CMB-C2B-C3B	3.35	130.94	124.68
14	B	1209	CLA	O2A-CGA-CBA	3.35	124.79	114.03
14	A	1013	CLA	C1-C2-C3	-3.35	120.25	126.04
14	B	1203	CLA	CMB-C2B-C3B	3.35	130.94	124.68
14	A	1129	CLA	C1-C2-C3	-3.35	121.34	126.75
14	G	1122	CLA	C4-C3-C5	3.34	120.90	115.27
14	G	1129	CLA	C1-C2-C3	-3.34	121.34	126.75
14	H	1209	CLA	O2A-CGA-CBA	3.34	124.77	114.03
14	a	1122	CLA	C4-C3-C5	3.34	120.89	115.27
14	G	1013	CLA	CMC-C2C-C1C	3.34	130.13	125.04
18	G	4002	BCR	C38-C26-C27	3.34	120.03	113.62
18	a	4002	BCR	C33-C5-C6	-3.34	120.78	124.53
18	G	4002	BCR	C33-C5-C6	-3.34	120.78	124.53
14	B	1234	CLA	C1-C2-C3	-3.34	120.27	126.04
14	b	1216	CLA	C4-C3-C5	3.33	120.88	115.27
14	a	1013	CLA	CMC-C2C-C1C	3.33	130.11	125.04
18	G	4001	BCR	C24-C23-C22	-3.33	121.20	126.23
14	A	1101	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
14	x	1701	CLA	C4-C3-C5	3.33	120.87	115.27
18	A	4002	BCR	C38-C26-C27	3.33	120.01	113.62
15	a	1121	F6C	C4A-NA-C1A	3.33	108.70	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1125	CLA	CMB-C2B-C3B	3.33	130.91	124.68
14	X	1701	CLA	C4-C3-C5	3.33	120.86	115.27
14	b	1209	CLA	O2A-CGA-CBA	3.32	124.70	114.03
14	B	1224	CLA	O1D-CGD-CBD	-3.32	117.69	124.48
14	G	1128	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
14	H	1203	CLA	CMB-C2B-C3B	3.32	130.88	124.68
18	a	4002	BCR	C38-C26-C27	3.32	119.99	113.62
14	G	1101	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
18	a	4001	BCR	C24-C23-C22	-3.32	121.22	126.23
14	H	1224	CLA	O1D-CGD-CBD	-3.32	117.70	124.48
14	b	1203	CLA	CMB-C2B-C3B	3.31	130.88	124.68
18	A	4002	BCR	C33-C5-C6	-3.31	120.81	124.53
14	b	1239	CLA	C3C-C4C-NC	3.31	114.29	110.57
14	G	1135	CLA	C4D-C3D-CAD	3.31	112.00	108.10
15	A	1121	F6C	C4A-NA-C1A	3.31	108.69	106.33
14	A	1013	CLA	CMC-C2C-C1C	3.31	130.08	125.04
18	A	4001	BCR	C24-C23-C22	-3.31	121.24	126.23
14	a	1103	CLA	CMB-C2B-C3B	3.31	130.86	124.68
14	A	1125	CLA	CMB-C2B-C3B	3.30	130.86	124.68
18	b	4010	BCR	C34-C9-C10	-3.30	118.30	122.92
14	a	1119	CLA	C1-O2A-CGA	3.30	125.10	116.44
14	B	1022	CLA	OBD-CAD-C3D	-3.30	120.58	128.52
14	b	1224	CLA	O1D-CGD-CBD	-3.30	117.74	124.48
14	A	1103	CLA	CMB-C2B-C3B	3.30	130.85	124.68
14	H	1239	CLA	C3C-C4C-NC	3.30	114.27	110.57
14	a	1135	CLA	C4D-C3D-CAD	3.30	111.98	108.10
14	a	1125	CLA	CMB-C2B-C3B	3.29	130.84	124.68
18	B	4010	BCR	C34-C9-C10	-3.29	118.31	122.92
14	B	1223	CLA	C3C-C4C-NC	3.29	114.26	110.57
14	G	1103	CLA	CMB-C2B-C3B	3.29	130.84	124.68
18	G	4007	BCR	C34-C9-C8	3.29	123.26	118.08
18	A	4007	BCR	C34-C9-C8	3.29	123.26	118.08
14	A	1119	CLA	C1-O2A-CGA	3.29	125.07	116.44
14	H	1223	CLA	C3C-C4C-NC	3.29	114.26	110.57
14	G	1119	CLA	C1-O2A-CGA	3.29	125.07	116.44
14	b	1022	CLA	OBD-CAD-C3D	-3.29	120.61	128.52
18	a	4007	BCR	C34-C9-C8	3.28	123.25	118.08
14	A	1128	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
15	H	1207	F6C	CHB-C4A-NA	3.28	127.47	124.45
14	G	1138	CLA	O2A-C1-C2	3.28	117.25	108.64
14	G	1117	CLA	C1-C2-C3	-3.28	120.37	126.04
18	H	4010	BCR	C34-C9-C10	-3.27	118.34	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1209	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
14	A	1135	CLA	C4D-C3D-CAD	3.27	111.95	108.10
14	B	1209	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
18	B	4010	BCR	C19-C18-C17	3.27	123.96	118.94
14	a	1138	CLA	O2A-C1-C2	3.27	117.23	108.64
14	a	1128	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
14	H	1022	CLA	OBD-CAD-C3D	-3.27	120.65	128.52
14	b	1021	CLA	O2A-C1-C2	3.27	117.22	108.64
14	B	1023	CLA	CMB-C2B-C3B	3.26	130.79	124.68
14	A	1107	CLA	O2A-CGA-CBA	3.26	124.52	114.03
14	b	1209	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
14	b	1023	CLA	CMB-C2B-C3B	3.26	130.78	124.68
14	B	1239	CLA	C3C-C4C-NC	3.26	114.23	110.57
14	H	1021	CLA	O2A-C1-C2	3.26	117.20	108.64
14	a	1125	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
14	B	1021	CLA	O2A-C1-C2	3.26	117.20	108.64
14	a	1107	CLA	O2A-CGA-CBA	3.26	124.50	114.03
14	H	1023	CLA	CMB-C2B-C3B	3.26	130.78	124.68
14	A	1138	CLA	O2A-C1-C2	3.26	117.19	108.64
14	G	1107	CLA	O2A-CGA-CBA	3.26	124.49	114.03
15	B	1207	F6C	CHB-C4A-NA	3.26	127.45	124.45
14	A	1117	CLA	C1-C2-C3	-3.26	120.41	126.04
14	a	1117	CLA	C1-C2-C3	-3.25	120.41	126.04
14	G	1123	CLA	CMA-C3A-C4A	3.25	120.52	111.77
14	a	1123	CLA	CMA-C3A-C4A	3.25	120.51	111.77
18	b	4010	BCR	C19-C18-C17	3.25	123.93	118.94
14	a	1102	CLA	C1-C2-C3	-3.25	120.43	126.04
18	a	4007	BCR	C15-C14-C13	-3.25	122.68	127.31
14	l	1503	CLA	C1-C2-C3	-3.25	120.43	126.04
14	L	1503	CLA	C1-C2-C3	-3.24	120.43	126.04
14	U	1503	CLA	C1-C2-C3	-3.24	120.43	126.04
14	G	1131	CLA	C1-C2-C3	-3.24	120.43	126.04
14	A	1129	CLA	CMB-C2B-C3B	3.24	130.74	124.68
14	G	1129	CLA	CMB-C2B-C3B	3.24	130.74	124.68
14	A	1123	CLA	CMA-C3A-C4A	3.24	120.48	111.77
14	b	1227	CLA	O2A-CGA-CBA	3.24	124.43	114.03
14	a	1129	CLA	CMB-C2B-C3B	3.24	130.73	124.68
14	G	1102	CLA	C1-C2-C3	-3.24	120.45	126.04
14	B	1206	CLA	O2A-CGA-CBA	3.24	124.42	114.03
14	b	1223	CLA	C3C-C4C-NC	3.23	114.20	110.57
14	G	1125	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
14	G	1104	CLA	CMB-C2B-C3B	3.23	130.72	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1122	CLA	CAC-C3C-C4C	3.23	129.00	124.81
14	b	1206	CLA	O2A-CGA-CBA	3.23	124.40	114.03
18	H	4010	BCR	C19-C18-C17	3.23	123.89	118.94
14	A	1102	CLA	C1-C2-C3	-3.23	120.47	126.04
18	A	4007	BCR	C15-C14-C13	-3.22	122.71	127.31
14	A	1109	CLA	CMB-C2B-C3B	3.22	130.71	124.68
14	H	1227	CLA	O2A-CGA-CBA	3.22	124.38	114.03
14	A	1104	CLA	CMB-C2B-C3B	3.22	130.71	124.68
14	A	1125	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
14	A	1131	CLA	C1-C2-C3	-3.22	120.47	126.04
14	a	1127	CLA	C3C-C4C-NC	3.22	114.18	110.57
18	R	4020	BCR	C15-C14-C13	-3.22	122.72	127.31
14	H	1206	CLA	O2A-CGA-CBA	3.22	124.37	114.03
14	H	1208	CLA	C1-C2-C3	-3.22	120.48	126.04
18	B	4006	BCR	C3-C4-C5	-3.22	108.33	114.08
14	a	1109	CLA	CMB-C2B-C3B	3.21	130.69	124.68
14	B	1227	CLA	O2A-CGA-CBA	3.21	124.36	114.03
14	G	1114	CLA	O2A-CGA-CBA	3.21	124.36	114.03
14	A	1114	CLA	O2A-CGA-CBA	3.21	124.35	114.03
14	b	1235	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
18	I	4020	BCR	C15-C14-C13	-3.21	122.73	127.31
18	G	4007	BCR	C15-C14-C13	-3.21	122.73	127.31
18	H	4006	BCR	C3-C4-C5	-3.21	108.35	114.08
14	K	1401	CLA	O2A-CGA-CBA	3.21	124.34	114.03
14	k	1401	CLA	O2A-CGA-CBA	3.21	124.34	114.03
14	a	1104	CLA	CMB-C2B-C3B	3.21	130.68	124.68
14	a	1131	CLA	C1-C2-C3	-3.21	120.50	126.04
14	a	1114	CLA	O2A-CGA-CBA	3.21	124.34	114.03
15	H	1230	F6C	O2A-CGA-CBA	3.21	124.34	114.03
14	H	1232	CLA	O2A-CGA-CBA	3.21	124.33	114.03
18	b	4006	BCR	C3-C4-C5	-3.21	108.35	114.08
14	H	1215	CLA	C4-C3-C5	3.20	120.66	115.27
14	B	1232	CLA	O2A-CGA-CBA	3.20	124.33	114.03
14	T	1401	CLA	O2A-CGA-CBA	3.20	124.31	114.03
14	b	1208	CLA	C1-C2-C3	-3.20	120.51	126.04
14	a	1108	CLA	O2A-CGA-CBA	3.20	124.31	114.03
14	B	1215	CLA	C4-C3-C5	3.20	120.65	115.27
14	G	1108	CLA	O2A-CGA-CBA	3.20	124.30	114.03
18	i	4020	BCR	C15-C14-C13	-3.20	122.75	127.31
14	H	1235	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
14	G	1127	CLA	C3C-C4C-NC	3.19	114.15	110.57
15	B	1230	F6C	O2A-CGA-CBA	3.19	124.29	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1138	CLA	O2A-CGA-CBA	3.19	121.93	111.91
14	U	1503	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
14	b	1232	CLA	O2A-CGA-CBA	3.19	124.29	114.03
14	G	1109	CLA	CMB-C2B-C3B	3.19	130.65	124.68
14	B	1235	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
14	a	1138	CLA	O2A-CGA-CBA	3.19	121.92	111.91
14	a	1122	CLA	CMB-C2B-C3B	3.19	130.65	124.68
14	a	1124	CLA	CAA-C2A-C3A	-3.19	104.04	112.78
14	G	1120	CLA	O2A-CGA-CBA	3.19	124.28	114.03
15	b	1230	F6C	O2A-CGA-CBA	3.19	124.28	114.03
20	a	5005	LMG	O8-C28-C29	3.19	121.92	111.91
18	G	4008	BCR	C33-C5-C6	-3.19	120.94	124.53
14	B	1022	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
14	A	1108	CLA	O2A-CGA-CBA	3.19	124.28	114.03
14	a	1109	CLA	C4-C3-C5	3.19	120.64	115.27
14	A	1124	CLA	CAA-C2A-C3A	-3.19	104.05	112.78
15	a	1121	F6C	CHB-C4A-C3A	-3.19	118.79	125.48
20	A	5005	LMG	O8-C28-C29	3.19	121.91	111.91
18	A	4008	BCR	C33-C5-C6	-3.19	120.95	124.53
14	H	1022	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
14	B	1227	CLA	CMD-C2D-C3D	-3.19	120.28	127.61
15	b	1207	F6C	CHB-C4A-NA	3.19	127.38	124.45
14	G	1138	CLA	O2A-CGA-CBA	3.19	121.91	111.91
14	A	1120	CLA	O2A-CGA-CBA	3.19	124.26	114.03
14	b	1215	CLA	C4-C3-C5	3.19	120.63	115.27
15	A	1121	F6C	CHB-C4A-C3A	-3.18	118.80	125.48
14	a	1120	CLA	O2A-CGA-CBA	3.18	124.26	114.03
14	B	1234	CLA	C3C-C4C-NC	3.18	114.14	110.57
14	B	1212	CLA	O2A-CGA-CBA	3.18	124.25	114.03
20	G	5005	LMG	O8-C28-C29	3.18	121.89	111.91
14	B	1222	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
18	a	4003	BCR	C27-C26-C25	-3.18	118.11	122.73
14	H	1236	CLA	O2A-CGA-CBA	3.18	124.25	114.03
14	G	1124	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
14	H	1227	CLA	CMD-C2D-C3D	-3.18	120.30	127.61
18	B	4014	BCR	C36-C18-C17	-3.18	118.47	122.92
14	b	1227	CLA	CMD-C2D-C3D	-3.18	120.30	127.61
14	B	1208	CLA	C1-C2-C3	-3.18	120.55	126.04
14	A	1127	CLA	C3C-C4C-NC	3.18	114.14	110.57
14	A	1122	CLA	CMB-C2B-C3B	3.18	130.62	124.68
18	G	4008	BCR	C35-C13-C12	3.18	123.08	118.08
14	A	1122	CLA	CAC-C3C-C4C	3.18	128.93	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	l	1503	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
14	G	1138	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
14	H	1222	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
14	A	1130	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
14	G	1122	CLA	CMB-C2B-C3B	3.18	130.62	124.68
14	A	1115	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
14	H	1212	CLA	O2A-CGA-CBA	3.17	124.23	114.03
14	G	1130	CLA	CAA-C2A-C3A	-3.17	104.09	112.78
14	b	1236	CLA	O2A-CGA-CBA	3.17	124.23	114.03
14	b	1022	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
14	A	1135	CLA	CMD-C2D-C3D	-3.17	120.32	127.61
14	b	1212	CLA	O2A-CGA-CBA	3.17	124.22	114.03
14	G	1101	CLA	O2A-CGA-CBA	3.17	124.22	114.03
14	H	1234	CLA	C3C-C4C-NC	3.17	114.13	110.57
18	A	4003	BCR	C3-C4-C5	-3.17	108.42	114.08
18	a	4003	BCR	C3-C4-C5	-3.17	108.42	114.08
18	B	4004	BCR	C37-C22-C21	-3.17	118.48	122.92
14	a	1135	CLA	CMD-C2D-C3D	-3.17	120.33	127.61
15	G	1121	F6C	CHB-C4A-C3A	-3.17	118.83	125.48
14	H	1021	CLA	C1-C2-C3	-3.17	120.56	126.04
18	b	4014	BCR	C36-C18-C17	-3.17	118.49	122.92
14	G	1109	CLA	C4-C3-C5	3.17	120.60	115.27
14	a	1115	CLA	CAA-C2A-C3A	-3.17	104.11	112.78
14	A	1110	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
14	B	1236	CLA	O2A-CGA-CBA	3.17	124.20	114.03
14	a	1110	CLA	O2A-CGA-CBA	3.16	124.20	114.03
14	a	1130	CLA	CAA-C2A-C3A	-3.16	104.11	112.78
18	G	4003	BCR	C3-C4-C5	-3.16	108.43	114.08
14	a	1122	CLA	CAC-C3C-C4C	3.16	128.91	124.81
14	a	1113	CLA	O2A-CGA-CBA	3.16	124.19	114.03
18	A	4008	BCR	C35-C13-C12	3.16	123.06	118.08
14	A	1109	CLA	C4-C3-C5	3.16	120.59	115.27
14	L	1503	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
18	a	4008	BCR	C35-C13-C12	3.16	123.06	118.08
14	b	1222	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
18	b	4004	BCR	C37-C22-C21	-3.16	118.50	122.92
14	b	1226	CLA	C4-C3-C5	3.16	120.58	115.27
14	G	1115	CLA	CAA-C2A-C3A	-3.15	104.14	112.78
14	b	1021	CLA	C1-C2-C3	-3.15	120.59	126.04
14	a	1136	CLA	C4-C3-C5	3.15	120.58	115.27
14	G	1135	CLA	CMD-C2D-C3D	-3.15	120.36	127.61
18	H	4014	BCR	C36-C18-C17	-3.15	118.51	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	4003	BCR	C27-C26-C25	-3.15	118.15	122.73
14	a	1101	CLA	O2A-CGA-CBA	3.15	124.16	114.03
14	A	1113	CLA	O2A-CGA-CBA	3.15	124.16	114.03
14	a	1140	CLA	CMC-C2C-C1C	3.15	129.84	125.04
14	G	1113	CLA	O2A-CGA-CBA	3.15	124.15	114.03
18	a	4008	BCR	C33-C5-C6	-3.15	120.99	124.53
15	B	1207	F6C	C4-C3-C2	-3.15	115.60	123.68
14	a	1110	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
14	G	1110	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
14	b	1229	CLA	O2A-C1-C2	3.15	116.91	108.64
14	G	1110	CLA	O2A-CGA-CBA	3.15	124.14	114.03
18	G	4003	BCR	C27-C26-C25	-3.15	118.16	122.73
14	a	1138	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
14	A	1101	CLA	O2A-CGA-CBA	3.14	124.13	114.03
14	a	1130	CLA	OBD-CAD-C3D	-3.14	120.95	128.52
14	U	1502	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
14	A	1138	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
14	A	1110	CLA	O2A-CGA-CBA	3.14	124.13	114.03
14	G	1140	CLA	CMC-C2C-C1C	3.14	129.83	125.04
14	A	1140	CLA	CMC-C2C-C1C	3.14	129.83	125.04
14	B	1021	CLA	C1-C2-C3	-3.14	120.61	126.04
14	H	1226	CLA	C4-C3-C5	3.14	120.56	115.27
14	B	1229	CLA	O2A-C1-C2	3.14	116.89	108.64
14	B	1226	CLA	C4-C3-C5	3.14	120.56	115.27
14	b	1234	CLA	C3C-C4C-NC	3.14	114.09	110.57
14	l	1502	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
19	a	5001	LHG	O8-C23-C24	3.14	121.76	111.91
18	H	4004	BCR	C37-C22-C21	-3.14	118.52	122.92
15	b	1207	F6C	C4-C3-C2	-3.14	115.62	123.68
14	x	1701	CLA	CAC-C3C-C4C	3.14	128.88	124.81
15	a	1121	F6C	O2A-CGA-CBA	3.14	124.11	114.03
14	W	1701	CLA	CAC-C3C-C4C	3.14	128.88	124.81
19	A	5001	LHG	O8-C23-C24	3.14	121.75	111.91
14	H	1229	CLA	O2A-C1-C2	3.14	116.88	108.64
14	L	1502	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
14	G	1123	CLA	C3C-C4C-NC	3.13	114.09	110.57
14	a	1105	CLA	O2A-CGA-CBA	3.13	124.10	114.03
15	G	1121	F6C	O2A-CGA-CBA	3.13	124.09	114.03
14	B	1220	CLA	CAA-C2A-C3A	-3.13	104.21	112.78
14	A	1136	CLA	C4-C3-C5	3.13	120.53	115.27
13	A	1011	CL0	CBC-CAC-C3C	-3.13	103.81	112.43
14	a	1139	CLA	O2A-CGA-CBA	3.13	124.08	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	4003	BCR	C33-C5-C6	-3.13	121.02	124.53
14	G	1130	CLA	OBD-CAD-C3D	-3.13	121.00	128.52
14	H	1235	CLA	C1-O2A-CGA	3.13	124.65	116.44
19	G	5001	LHG	O8-C23-C24	3.13	121.72	111.91
14	H	1220	CLA	CAA-C2A-C3A	-3.13	104.22	112.78
15	H	1207	F6C	C4-C3-C2	-3.12	115.66	123.68
14	A	1139	CLA	O2A-CGA-CBA	3.12	124.06	114.03
20	H	5002	LMG	C8-O7-C10	-3.12	110.11	117.79
14	B	1235	CLA	C1-O2A-CGA	3.12	124.63	116.44
14	A	1105	CLA	O2A-CGA-CBA	3.12	124.06	114.03
14	G	1139	CLA	O2A-CGA-CBA	3.12	124.06	114.03
14	a	1128	CLA	C1D-ND-C4D	-3.12	104.12	106.33
14	A	1130	CLA	OBD-CAD-C3D	-3.12	121.01	128.52
14	B	1216	CLA	O2A-CGA-CBA	3.12	121.69	111.91
14	U	1502	CLA	CMC-C2C-C1C	3.12	129.79	125.04
14	b	1220	CLA	CAA-C2A-C3A	-3.12	104.24	112.78
14	G	1105	CLA	O2A-CGA-CBA	3.12	124.05	114.03
14	b	1216	CLA	O2A-CGA-CBA	3.12	121.69	111.91
14	H	1225	CLA	C1-C2-C3	-3.12	120.65	126.04
13	G	1011	CL0	CBC-CAC-C3C	-3.11	103.84	112.43
18	G	4011	BCR	C28-C27-C26	-3.11	108.52	114.08
18	G	4003	BCR	C33-C5-C6	-3.11	121.03	124.53
14	G	1136	CLA	C4-C3-C5	3.11	120.51	115.27
15	A	1121	F6C	O2A-CGA-CBA	3.11	124.03	114.03
15	H	1238	F6C	C3D-C4D-ND	3.11	114.72	110.17
14	b	1235	CLA	C1-O2A-CGA	3.11	124.61	116.44
14	X	1701	CLA	CAC-C3C-C4C	3.11	128.84	124.81
18	A	4003	BCR	C33-C5-C6	-3.11	121.04	124.53
14	a	1123	CLA	C3C-C4C-NC	3.11	114.06	110.57
14	a	1134	CLA	O2A-CGA-CBA	3.11	124.01	114.03
14	G	1134	CLA	O2A-CGA-CBA	3.11	124.01	114.03
15	H	1237	F6C	CHD-C1D-ND	-3.10	119.49	124.20
18	a	4011	BCR	C28-C27-C26	-3.10	108.54	114.08
14	A	1134	CLA	O2A-CGA-CBA	3.10	124.00	114.03
14	H	1216	CLA	O2A-CGA-CBA	3.10	121.64	111.91
13	a	1011	CL0	CBC-CAC-C3C	-3.10	103.88	112.43
14	A	1123	CLA	C3C-C4C-NC	3.10	114.05	110.57
14	H	1222	CLA	CAA-C2A-C3A	-3.10	104.29	112.78
14	L	1502	CLA	CMC-C2C-C1C	3.10	129.76	125.04
14	l	1502	CLA	CMC-C2C-C1C	3.10	129.76	125.04
14	B	1222	CLA	CAA-C2A-C3A	-3.10	104.30	112.78
15	b	1238	F6C	C3D-C4D-ND	3.10	114.69	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1222	CLA	CAA-C2A-C3A	-3.10	104.30	112.78
18	A	4011	BCR	C28-C27-C26	-3.09	108.56	114.08
15	B	1238	F6C	C3D-C4D-ND	3.09	114.69	110.17
20	B	5002	LMG	C8-O7-C10	-3.09	110.19	117.79
14	a	1106	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
14	H	1227	CLA	CMB-C2B-C3B	3.09	130.45	124.68
14	b	1225	CLA	C1-C2-C3	-3.08	120.71	126.04
15	H	1237	F6C	C4A-C3A-C2A	-3.08	102.44	106.94
20	b	5002	LMG	C8-O7-C10	-3.08	110.20	117.79
15	B	1237	F6C	C4A-C3A-C2A	-3.08	102.44	106.94
18	U	4019	BCR	C37-C22-C21	-3.08	118.61	122.92
15	b	1237	F6C	C4A-C3A-C2A	-3.08	102.44	106.94
18	m	4021	BCR	C19-C18-C17	3.08	123.67	118.94
14	b	1222	CLA	C3C-C4C-NC	3.08	114.03	110.57
14	a	1128	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
14	H	1023	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
15	B	1237	F6C	CHD-C1D-ND	-3.07	119.54	124.20
15	b	1237	F6C	CHD-C1D-ND	-3.07	119.54	124.20
14	B	1239	CLA	CMC-C2C-C3C	3.07	134.46	126.12
14	B	1227	CLA	CMB-C2B-C3B	3.07	130.42	124.68
14	B	1023	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
18	V	4021	BCR	C19-C18-C17	3.07	123.65	118.94
14	A	1106	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
14	B	1225	CLA	C1-C2-C3	-3.07	120.73	126.04
14	B	1221	CLA	CAA-C2A-C3A	-3.07	104.38	112.78
14	H	1222	CLA	C3C-C4C-NC	3.07	114.01	110.57
14	B	1222	CLA	C3C-C4C-NC	3.07	114.01	110.57
18	M	4021	BCR	C19-C18-C17	3.07	123.65	118.94
18	U	4019	BCR	C33-C5-C4	3.07	119.51	113.62
14	b	1023	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
14	A	1119	CLA	CHC-C1C-C2C	-3.07	118.24	126.72
14	b	1239	CLA	CMC-C2C-C3C	3.06	134.44	126.12
14	a	1140	CLA	C3C-C4C-NC	3.06	114.01	110.57
14	H	1204	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
14	H	1239	CLA	CMC-C2C-C3C	3.06	134.43	126.12
18	l	4022	BCR	C3-C4-C5	-3.06	108.61	114.08
14	G	1128	CLA	C1D-ND-C4D	-3.06	104.16	106.33
14	H	1221	CLA	CAA-C2A-C3A	-3.06	104.41	112.78
14	a	1118	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
14	A	1128	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
14	b	1212	CLA	C3C-C4C-NC	3.05	114.00	110.57
15	B	1207	F6C	OMB-CMB-C2B	-3.05	118.78	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1227	CLA	CMB-C2B-C3B	3.05	130.39	124.68
18	U	4022	BCR	C3-C4-C5	-3.05	108.62	114.08
14	a	1119	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
18	L	4019	BCR	C37-C22-C21	-3.05	118.65	122.92
14	b	1221	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
15	b	1207	F6C	OMB-CMB-C2B	-3.05	118.79	125.69
14	b	1202	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
14	G	1119	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
14	A	1118	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
14	a	1128	CLA	C4-C3-C5	3.05	120.40	115.27
14	B	1218	CLA	O2A-CGA-CBA	3.05	123.83	114.03
18	L	4022	BCR	C3-C4-C5	-3.05	108.64	114.08
14	G	1012	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
18	L	4019	BCR	C33-C5-C4	3.05	119.47	113.62
14	G	1128	CLA	C4-C3-C5	3.04	120.39	115.27
14	G	1106	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
14	H	1212	CLA	C3C-C4C-NC	3.04	113.98	110.57
14	B	1212	CLA	C3C-C4C-NC	3.04	113.98	110.57
14	a	1106	CLA	C4-C3-C5	3.04	120.39	115.27
14	k	1401	CLA	CMA-C3A-C4A	3.04	119.95	111.77
14	a	1139	CLA	C3C-C4C-NC	3.04	113.98	110.57
14	K	1401	CLA	CMA-C3A-C4A	3.04	119.95	111.77
14	b	1218	CLA	O2A-CGA-CBA	3.04	123.80	114.03
14	G	1128	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
14	H	1218	CLA	O2A-CGA-CBA	3.04	123.80	114.03
18	i	4020	BCR	C3-C4-C5	-3.04	108.65	114.08
14	G	1132	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
15	H	1207	F6C	OMB-CMB-C2B	-3.04	118.82	125.69
14	G	1118	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
14	T	1401	CLA	CMA-C3A-C4A	3.04	119.94	111.77
18	l	4019	BCR	C37-C22-C21	-3.04	118.67	122.92
14	A	1126	CLA	CAA-C2A-C3A	-3.04	104.47	112.78
14	A	1132	CLA	CAA-C2A-C3A	-3.03	104.47	112.78
14	G	1113	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
14	a	1132	CLA	CAA-C2A-C3A	-3.03	104.48	112.78
14	B	1204	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
14	G	1139	CLA	C3C-C4C-NC	3.03	113.97	110.57
14	G	1140	CLA	C3C-C4C-NC	3.03	113.97	110.57
14	b	1219	CLA	O2A-CGA-CBA	3.03	123.76	114.03
18	l	4019	BCR	C33-C5-C4	3.03	119.43	113.62
14	B	1219	CLA	O2A-CGA-CBA	3.03	123.76	114.03
14	G	1106	CLA	C4-C3-C5	3.03	120.36	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1128	CLA	C4-C3-C5	3.03	120.36	115.27
15	b	1230	F6C	O1D-CGD-CBD	-3.02	118.30	124.48
14	a	1012	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
14	A	1139	CLA	C3C-C4C-NC	3.02	113.96	110.57
14	G	1124	CLA	CAA-C2A-C1A	-3.02	102.07	111.97
14	A	1140	CLA	C3C-C4C-NC	3.02	113.96	110.57
14	G	1126	CLA	CAA-C2A-C3A	-3.02	104.51	112.78
14	H	1202	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
14	a	1116	CLA	CMC-C2C-C1C	3.02	129.63	125.04
14	a	1126	CLA	CAA-C2A-C3A	-3.02	104.51	112.78
14	B	1202	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
14	A	1126	CLA	C1-C2-C3	-3.02	120.82	126.04
14	A	1124	CLA	CAA-C2A-C1A	-3.02	102.09	111.97
18	I	4020	BCR	C3-C4-C5	-3.02	108.69	114.08
14	b	1204	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
14	B	1218	CLA	CMC-C2C-C1C	3.02	129.63	125.04
14	G	1126	CLA	C1-C2-C3	-3.01	120.83	126.04
15	H	1230	F6C	O1D-CGD-CBD	-3.01	118.32	124.48
14	H	1219	CLA	O2A-CGA-CBA	3.01	123.71	114.03
14	A	1012	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
14	A	1106	CLA	C4-C3-C5	3.01	120.34	115.27
14	H	1228	CLA	C1-C2-C3	-3.01	120.84	126.04
18	I	4018	BCR	C33-C5-C4	3.01	119.40	113.62
14	A	1128	CLA	C1D-ND-C4D	-3.01	104.20	106.33
14	b	1217	CLA	CMC-C2C-C1C	3.01	129.62	125.04
14	A	1115	CLA	CMC-C2C-C1C	3.01	129.62	125.04
14	a	1124	CLA	CAA-C2A-C1A	-3.01	102.13	111.97
14	a	1109	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
14	b	1210	CLA	CAA-C2A-C3A	-3.01	104.55	112.78
14	B	1205	CLA	C3C-C4C-NC	3.00	113.94	110.57
14	G	1109	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
14	H	1210	CLA	CAA-C2A-C3A	-3.00	104.55	112.78
14	b	1203	CLA	CMC-C2C-C1C	3.00	129.61	125.04
18	R	4020	BCR	C3-C4-C5	-3.00	108.72	114.08
15	B	1230	F6C	O1D-CGD-CBD	-3.00	118.34	124.48
14	B	1224	CLA	C3C-C4C-NC	3.00	113.94	110.57
14	A	1116	CLA	CMC-C2C-C1C	3.00	129.61	125.04
14	B	1210	CLA	CAA-C2A-C3A	-3.00	104.57	112.78
14	a	1126	CLA	C1-C2-C3	-3.00	120.86	126.04
14	B	1217	CLA	CMC-C2C-C1C	3.00	129.60	125.04
18	R	4018	BCR	C33-C5-C4	3.00	119.37	113.62
14	H	1023	CLA	C4-C3-C5	2.99	120.31	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	4001	BCR	C38-C26-C25	-2.99	121.17	124.53
14	G	1116	CLA	CMC-C2C-C1C	2.99	129.59	125.04
14	B	1023	CLA	CAA-C2A-C3A	-2.99	104.59	112.78
14	a	1136	CLA	CMA-C3A-C4A	2.99	119.80	111.77
18	i	4018	BCR	C33-C5-C4	2.99	119.35	113.62
14	a	1115	CLA	CMC-C2C-C1C	2.99	129.59	125.04
14	G	1115	CLA	CMC-C2C-C1C	2.99	129.59	125.04
14	H	1205	CLA	C3C-C4C-NC	2.99	113.92	110.57
14	A	1109	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
14	H	1217	CLA	CMC-C2C-C1C	2.98	129.58	125.04
14	b	1218	CLA	CMC-C2C-C1C	2.98	129.58	125.04
14	a	1113	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
14	A	1113	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
14	B	1210	CLA	C4-C3-C5	2.98	120.28	115.27
14	H	1210	CLA	C4-C3-C5	2.98	120.28	115.27
14	G	1125	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
14	G	1136	CLA	CMA-C3A-C4A	2.98	119.78	111.77
14	b	1228	CLA	C1-C2-C3	-2.98	120.89	126.04
14	B	1023	CLA	C4-C3-C5	2.98	120.28	115.27
14	H	1023	CLA	CAA-C2A-C3A	-2.97	104.63	112.78
14	A	1125	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
14	B	1217	CLA	C3C-C4C-NC	2.97	113.91	110.57
14	A	1136	CLA	CMA-C3A-C4A	2.97	119.76	111.77
14	B	1221	CLA	C3C-C4C-NC	2.97	113.90	110.57
18	B	4005	BCR	C37-C22-C21	-2.97	118.76	122.92
14	b	1023	CLA	CAA-C2A-C3A	-2.97	104.64	112.78
14	b	1023	CLA	C4-C3-C5	2.97	120.27	115.27
14	B	1228	CLA	C1-C2-C3	-2.97	120.90	126.04
14	A	1114	CLA	CMB-C2B-C3B	2.97	130.24	124.68
14	a	1125	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
14	b	1204	CLA	C1-C2-C3	-2.97	120.91	126.04
14	H	1203	CLA	CMC-C2C-C1C	2.97	129.56	125.04
14	B	1228	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
14	H	1224	CLA	C3C-C4C-NC	2.97	113.90	110.57
14	b	1217	CLA	C3C-C4C-NC	2.97	113.90	110.57
14	H	1229	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
14	B	1203	CLA	CMC-C2C-C1C	2.97	129.56	125.04
14	G	1114	CLA	CMB-C2B-C3B	2.96	130.22	124.68
14	a	1114	CLA	CMB-C2B-C3B	2.96	130.22	124.68
14	H	1218	CLA	CMC-C2C-C1C	2.96	129.55	125.04
14	b	1224	CLA	C3C-C4C-NC	2.96	113.89	110.57
14	a	1111	CLA	CAC-C3C-C4C	2.96	128.65	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1222	CLA	C1-C2-C3	-2.96	120.92	126.04
14	H	1213	CLA	CMC-C2C-C1C	2.96	129.55	125.04
14	b	1229	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
14	B	1201	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
14	H	1228	CLA	CAA-C2A-C3A	-2.96	104.68	112.78
14	b	1221	CLA	C1-C2-C3	-2.96	120.93	126.04
20	B	5002	LMG	O8-C28-C29	2.96	121.19	111.91
14	H	1211	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
14	B	1215	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
14	H	1221	CLA	C3C-C4C-NC	2.96	113.89	110.57
14	A	1115	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
14	b	1228	CLA	CAA-C2A-C3A	-2.96	104.69	112.78
14	a	1136	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
14	U	1501	CLA	C3C-C4C-NC	2.95	113.89	110.57
14	B	1229	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
18	U	4019	BCR	C4-C5-C6	-2.95	118.44	122.73
14	H	1204	CLA	C1-C2-C3	-2.95	120.94	126.04
18	b	4006	BCR	C38-C26-C25	-2.95	121.21	124.53
14	a	1115	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
14	B	1221	CLA	C1-C2-C3	-2.95	120.94	126.04
18	G	4001	BCR	C38-C26-C25	-2.95	121.21	124.53
15	B	1238	F6C	OMB-CMB-C2B	-2.95	119.02	125.69
14	G	1115	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
14	a	1131	CLA	CMB-C2B-C3B	2.95	130.20	124.68
14	b	1210	CLA	C4-C3-C5	2.95	120.23	115.27
20	H	5002	LMG	O8-C28-C29	2.95	121.16	111.91
18	b	4005	BCR	C37-C22-C21	-2.95	118.79	122.92
14	b	1201	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
14	B	1211	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
14	l	1501	CLA	C3C-C4C-NC	2.95	113.88	110.57
14	H	1222	CLA	C1-C2-C3	-2.95	120.95	126.04
15	G	1121	F6C	CHD-C1D-ND	-2.94	119.73	124.20
14	H	1221	CLA	C1-C2-C3	-2.94	120.95	126.04
14	X	1701	CLA	CMC-C2C-C1C	2.94	129.52	125.04
14	B	1204	CLA	C1-C2-C3	-2.94	120.95	126.04
14	B	1226	CLA	C1D-ND-C4D	-2.94	104.25	106.33
14	A	1111	CLA	CAC-C3C-C4C	2.94	128.62	124.81
14	G	1135	CLA	C4-C3-C5	2.94	120.22	115.27
14	A	1135	CLA	C4-C3-C5	2.94	120.22	115.27
14	A	1113	CLA	CMA-C3A-C4A	2.94	119.67	111.77
18	H	4013	BCR	C34-C9-C10	-2.94	118.81	122.92
15	b	1238	F6C	OMB-CMB-C2B	-2.94	119.04	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	W	1701	CLA	CMC-C2C-C1C	2.94	129.51	125.04
14	A	1136	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
14	b	1205	CLA	C3C-C4C-NC	2.94	113.87	110.57
14	G	1131	CLA	CMB-C2B-C3B	2.94	130.18	124.68
14	H	1201	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
14	G	1131	CLA	CMC-C2C-C1C	2.94	129.51	125.04
14	b	1216	CLA	CED-O2D-CGD	2.94	122.58	115.94
14	H	1217	CLA	C3C-C4C-NC	2.94	113.86	110.57
15	H	1238	F6C	OMB-CMB-C2B	-2.94	119.05	125.69
14	L	1501	CLA	C3C-C4C-NC	2.94	113.86	110.57
14	b	1211	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
14	G	1113	CLA	CMA-C3A-C4A	2.93	119.66	111.77
14	b	1222	CLA	C1-C2-C3	-2.93	120.97	126.04
14	a	1118	CLA	C4-C3-C5	2.93	120.20	115.27
14	G	1118	CLA	C4-C3-C5	2.93	120.20	115.27
20	b	5002	LMG	O8-C28-C29	2.93	121.10	111.91
14	b	1215	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
14	x	1701	CLA	CMC-C2C-C1C	2.93	129.50	125.04
14	a	1135	CLA	C4-C3-C5	2.93	120.20	115.27
14	G	1136	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
14	b	1221	CLA	C3C-C4C-NC	2.93	113.86	110.57
14	a	1105	CLA	CAA-C2A-C3A	-2.93	104.76	112.78
14	A	1106	CLA	C1-C2-C3	-2.93	120.98	126.04
18	l	4019	BCR	C4-C5-C6	-2.93	118.48	122.73
18	L	4019	BCR	C4-C5-C6	-2.93	118.48	122.73
14	a	1131	CLA	CMC-C2C-C1C	2.93	129.50	125.04
14	b	1213	CLA	CMC-C2C-C1C	2.93	129.49	125.04
18	A	4001	BCR	C38-C26-C25	-2.92	121.24	124.53
14	b	1220	CLA	CMB-C2B-C3B	2.92	130.15	124.68
14	H	1216	CLA	CED-O2D-CGD	2.92	122.55	115.94
18	H	4005	BCR	C37-C22-C21	-2.92	118.83	122.92
15	H	1237	F6C	C3D-C4D-ND	2.92	114.44	110.17
14	A	1131	CLA	CMC-C2C-C1C	2.92	129.49	125.04
18	B	4013	BCR	C34-C9-C10	-2.92	118.83	122.92
14	a	1113	CLA	CMA-C3A-C4A	2.92	119.62	111.77
14	A	1105	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
18	B	4006	BCR	C38-C26-C25	-2.92	121.25	124.53
14	H	1220	CLA	CMB-C2B-C3B	2.92	130.14	124.68
14	G	1105	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
15	B	1230	F6C	C3D-C4D-ND	2.92	114.44	110.17
15	B	1237	F6C	C3D-C4D-ND	2.92	114.44	110.17
14	G	1140	CLA	O2D-CGD-O1D	-2.92	118.13	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1140	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
14	A	1118	CLA	C4-C3-C5	2.92	120.18	115.27
18	b	4013	BCR	C34-C9-C10	-2.91	118.84	122.92
14	G	1138	CLA	CMC-C2C-C1C	2.91	129.48	125.04
15	H	1237	F6C	CMA-C3A-C2A	-2.91	118.21	126.12
14	G	1111	CLA	CAC-C3C-C4C	2.91	128.59	124.81
14	a	1106	CLA	C1-C2-C3	-2.91	121.01	126.04
14	a	1130	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
14	B	1213	CLA	CMC-C2C-C1C	2.91	129.47	125.04
15	b	1230	F6C	C3D-C4D-ND	2.91	114.42	110.17
14	a	1140	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
14	a	1119	CLA	O2A-CGA-CBA	2.91	121.03	111.91
14	a	1012	CLA	CMC-C2C-C1C	2.91	129.47	125.04
14	b	1239	CLA	C4-C3-C5	2.91	120.16	115.27
14	H	1215	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
14	G	1106	CLA	C1-C2-C3	-2.90	121.02	126.04
14	b	1213	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
14	H	1226	CLA	C1D-ND-C4D	-2.90	104.27	106.33
14	H	1213	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
14	A	1119	CLA	O2A-CGA-CBA	2.90	121.02	111.91
15	B	1237	F6C	CMA-C3A-C2A	-2.90	118.24	126.12
14	b	1021	CLA	C3C-C4C-NC	2.90	113.83	110.57
14	H	1239	CLA	C4-C3-C5	2.90	120.15	115.27
14	A	1131	CLA	CMB-C2B-C3B	2.90	130.10	124.68
14	B	1213	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
14	b	1211	CLA	O2A-CGA-CBA	2.90	121.01	111.91
14	H	1222	CLA	C4-C3-C5	2.90	120.15	115.27
14	B	1239	CLA	C4-C3-C5	2.90	120.15	115.27
14	a	1109	CLA	CMA-C3A-C4A	2.90	119.56	111.77
14	K	1401	CLA	CMC-C2C-C1C	2.90	129.45	125.04
14	B	1222	CLA	C4-C3-C5	2.90	120.15	115.27
14	B	1226	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
14	G	1130	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
14	A	1130	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
15	G	1121	F6C	C3D-C4D-ND	2.90	114.41	110.17
18	b	4009	BCR	C33-C5-C6	-2.90	121.27	124.53
14	B	1216	CLA	CED-O2D-CGD	2.90	122.49	115.94
14	W	1701	CLA	C3C-C4C-NC	2.90	113.82	110.57
18	L	4019	BCR	C38-C26-C27	2.90	119.18	113.62
14	x	1701	CLA	C3C-C4C-NC	2.90	113.82	110.57
15	b	1237	F6C	CMA-C3A-C2A	-2.90	118.26	126.12
18	i	4018	BCR	C37-C22-C21	-2.89	118.87	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	1121	F6C	CHD-C1D-ND	-2.89	119.81	124.20
14	b	1021	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
14	G	1119	CLA	O2A-CGA-CBA	2.89	120.99	111.91
14	B	1220	CLA	CMB-C2B-C3B	2.89	130.09	124.68
15	a	1121	F6C	C3D-C4D-ND	2.89	114.40	110.17
18	H	4006	BCR	C38-C26-C25	-2.89	121.28	124.53
14	G	1012	CLA	CMC-C2C-C1C	2.89	129.44	125.04
15	A	1121	F6C	CHD-C1D-ND	-2.89	119.82	124.20
15	H	1230	F6C	C3D-C4D-ND	2.89	114.39	110.17
14	A	1138	CLA	CMC-C2C-C1C	2.89	129.44	125.04
18	G	4007	BCR	C34-C9-C10	-2.89	118.88	122.92
14	A	1135	CLA	C1-C2-C3	-2.89	121.05	126.04
18	I	4019	BCR	C38-C26-C27	2.89	119.16	113.62
14	H	1211	CLA	O2A-CGA-CBA	2.89	120.96	111.91
14	T	1401	CLA	CMC-C2C-C1C	2.88	129.43	125.04
14	G	1107	CLA	C3C-C4C-NC	2.88	113.81	110.57
18	U	4019	BCR	C38-C26-C27	2.88	119.16	113.62
14	H	1226	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
14	a	1138	CLA	CMC-C2C-C1C	2.88	129.43	125.04
14	A	1012	CLA	CMC-C2C-C1C	2.88	129.43	125.04
14	B	1219	CLA	O1D-CGD-CBD	-2.88	118.59	124.48
14	B	1211	CLA	O2A-CGA-CBA	2.88	120.95	111.91
18	a	4001	BCR	C34-C9-C10	-2.88	118.89	122.92
14	G	1109	CLA	CMA-C3A-C4A	2.88	119.51	111.77
14	a	1128	CLA	C3C-C4C-NC	2.88	113.80	110.57
14	A	1109	CLA	CMA-C3A-C4A	2.88	119.51	111.77
14	H	1204	CLA	C3D-C4D-ND	2.88	114.89	110.24
18	A	4001	BCR	C34-C9-C10	-2.88	118.89	122.92
14	b	1219	CLA	O1D-CGD-CBD	-2.88	118.60	124.48
14	B	1021	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
14	H	1219	CLA	O1D-CGD-CBD	-2.88	118.60	124.48
18	R	4018	BCR	C37-C22-C21	-2.88	118.89	122.92
14	X	1701	CLA	C3C-C4C-NC	2.87	113.80	110.57
14	H	1221	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
14	H	1225	CLA	C3C-C4C-NC	2.87	113.79	110.57
14	b	1222	CLA	C4-C3-C5	2.87	120.11	115.27
14	B	1221	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
14	G	1135	CLA	C1-C2-C3	-2.87	121.08	126.04
18	G	4001	BCR	C34-C9-C10	-2.87	118.90	122.92
18	B	4009	BCR	C33-C5-C6	-2.87	121.31	124.53
14	H	1021	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
14	A	1128	CLA	C3C-C4C-NC	2.87	113.79	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	1237	F6C	C3D-C4D-ND	2.87	114.36	110.17
14	B	1225	CLA	C3C-C4C-NC	2.87	113.78	110.57
18	I	4018	BCR	C37-C22-C21	-2.87	118.91	122.92
14	b	1226	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
18	b	4004	BCR	C2-C1-C6	2.86	114.89	110.48
14	k	1401	CLA	CMC-C2C-C1C	2.86	129.40	125.04
18	b	4016	BCR	C30-C25-C26	-2.86	118.58	122.61
14	B	1021	CLA	C3C-C4C-NC	2.86	113.78	110.57
14	B	1204	CLA	C3D-C4D-ND	2.86	114.87	110.24
14	b	1021	CLA	C4-C3-C5	2.86	120.08	115.27
14	B	1021	CLA	C4-C3-C5	2.86	120.08	115.27
14	H	1021	CLA	C3C-C4C-NC	2.86	113.78	110.57
15	A	1121	F6C	C3D-C4D-ND	2.86	114.35	110.17
14	a	1120	CLA	OBD-CAD-C3D	-2.86	121.64	128.52
18	B	4016	BCR	C30-C25-C26	-2.86	118.59	122.61
14	a	1013	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
18	H	4009	BCR	C33-C5-C6	-2.86	121.32	124.53
14	b	1225	CLA	C3C-C4C-NC	2.86	113.77	110.57
14	b	1221	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
14	H	1021	CLA	C4-C3-C5	2.85	120.07	115.27
14	A	1012	CLA	CAA-C2A-C3A	-2.85	104.96	112.78
14	b	1209	CLA	CMC-C2C-C1C	2.85	129.38	125.04
14	b	1215	CLA	CMC-C2C-C1C	2.85	129.38	125.04
18	B	4004	BCR	C2-C1-C6	2.85	114.87	110.48
14	b	1226	CLA	C1D-ND-C4D	-2.85	104.31	106.33
14	b	1204	CLA	C3D-C4D-ND	2.85	114.85	110.24
14	A	1013	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
14	a	1135	CLA	C1-C2-C3	-2.85	121.11	126.04
14	a	1125	CLA	CHD-C1D-ND	-2.85	121.83	124.45
14	a	1012	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
14	b	1233	CLA	CMA-C3A-C4A	2.85	119.44	111.77
14	G	1012	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
18	A	4007	BCR	C34-C9-C10	-2.85	118.93	122.92
14	a	1107	CLA	C3C-C4C-NC	2.85	113.77	110.57
14	B	1233	CLA	CMA-C3A-C4A	2.85	119.43	111.77
14	B	1209	CLA	CMC-C2C-C1C	2.85	129.38	125.04
14	H	1218	CLA	CMA-C3A-C4A	2.85	119.42	111.77
18	a	4007	BCR	C34-C9-C10	-2.85	118.94	122.92
14	B	1218	CLA	CMA-C3A-C4A	2.85	119.42	111.77
14	A	1125	CLA	CHD-C1D-ND	-2.85	121.84	124.45
14	H	1236	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
14	a	1012	CLA	C6-C5-C3	-2.84	106.00	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1235	CLA	CAA-C2A-C3A	-2.84	104.99	112.78
14	H	1235	CLA	CAA-C2A-C3A	-2.84	104.99	112.78
18	H	4016	BCR	C30-C25-C26	-2.84	118.61	122.61
14	H	1215	CLA	CMC-C2C-C1C	2.84	129.37	125.04
14	H	1233	CLA	CMA-C3A-C4A	2.84	119.41	111.77
14	b	1236	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
14	a	1114	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
14	B	1236	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
14	G	1125	CLA	CHD-C1D-ND	-2.84	121.84	124.45
14	G	1013	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
14	A	1013	CLA	C3C-C4C-NC	2.84	113.75	110.57
14	A	1120	CLA	OBD-CAD-C3D	-2.84	121.69	128.52
14	B	1227	CLA	C4D-C3D-CAD	2.84	111.44	108.10
14	b	1218	CLA	CMA-C3A-C4A	2.84	119.40	111.77
14	H	1226	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
14	a	1122	CLA	C1-C2-C3	-2.84	121.14	126.04
14	A	1115	CLA	C4-C3-C5	2.83	120.04	115.27
18	H	4004	BCR	C2-C1-C6	2.83	114.84	110.48
14	b	1226	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
15	B	1238	F6C	CMA-C3A-C2A	-2.83	118.42	126.12
14	G	1120	CLA	OBD-CAD-C3D	-2.83	121.70	128.52
16	b	2002	PQN	C11-C12-C13	-2.83	122.08	126.79
14	A	1012	CLA	C6-C5-C3	-2.83	106.03	113.45
14	a	1105	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
16	B	2002	PQN	C11-C12-C13	-2.83	122.08	126.79
14	A	1123	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
21	A	6002	LMT	C1'-O5'-C5'	-2.83	108.14	113.69
14	A	1105	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
14	a	1115	CLA	C4-C3-C5	2.83	120.03	115.27
18	B	4009	BCR	C37-C22-C21	-2.83	118.96	122.92
14	G	1119	CLA	CED-O2D-CGD	2.83	122.33	115.94
14	G	1122	CLA	C1-C2-C3	-2.83	121.15	126.04
15	H	1237	F6C	CHB-C4A-C3A	-2.83	119.55	125.48
21	G	6002	LMT	C1'-O5'-C5'	-2.83	108.14	113.69
15	b	1238	F6C	CMA-C3A-C2A	-2.83	118.44	126.12
14	G	1012	CLA	C6-C5-C3	-2.83	106.04	113.45
14	H	1209	CLA	CMC-C2C-C1C	2.83	129.34	125.04
18	H	4009	BCR	C37-C22-C21	-2.83	118.97	122.92
15	H	1238	F6C	CMA-C3A-C2A	-2.83	118.45	126.12
14	A	1106	CLA	C3C-C4C-NC	2.82	113.74	110.57
14	A	1132	CLA	CMB-C2B-C3B	2.82	129.96	124.68
14	H	1227	CLA	C4D-C3D-CAD	2.82	111.42	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1237	F6C	CHB-C4A-C3A	-2.82	119.56	125.48
14	G	1115	CLA	C4-C3-C5	2.82	120.02	115.27
14	G	1128	CLA	C3C-C4C-NC	2.82	113.74	110.57
14	a	1013	CLA	C3C-C4C-NC	2.82	113.74	110.57
14	a	1129	CLA	C3C-C4C-NC	2.82	113.74	110.57
14	a	1132	CLA	CMB-C2B-C3B	2.82	129.96	124.68
18	b	4009	BCR	C37-C22-C21	-2.82	118.97	122.92
14	H	1204	CLA	CMB-C2B-C3B	2.82	129.95	124.68
18	b	4005	BCR	C28-C27-C26	-2.82	109.04	114.08
14	A	1114	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
14	a	1136	CLA	CMB-C2B-C3B	2.82	129.95	124.68
14	G	1114	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
14	A	1107	CLA	C3C-C4C-NC	2.82	113.73	110.57
14	G	1123	CLA	C1-C2-C3	-2.82	121.17	126.04
14	b	1218	CLA	CHD-C1D-ND	-2.82	121.86	124.45
14	G	1132	CLA	CMB-C2B-C3B	2.82	129.95	124.68
16	H	2002	PQN	C11-C12-C13	-2.82	122.10	126.79
14	A	1122	CLA	C1-C2-C3	-2.82	121.17	126.04
14	b	1229	CLA	C3D-C4D-ND	2.82	114.79	110.24
15	b	1237	F6C	CHB-C4A-C3A	-2.82	119.57	125.48
15	B	1230	F6C	O2D-CGD-O1D	-2.82	118.33	123.84
14	b	1235	CLA	CAA-C2A-C3A	-2.82	105.07	112.78
14	H	1231	CLA	C3C-C4C-NC	2.82	113.73	110.57
14	a	1103	CLA	C4-C3-C5	2.81	120.00	115.27
14	G	1123	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
14	B	1226	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
14	b	1204	CLA	C6-C5-C3	-2.81	106.08	113.45
14	A	1119	CLA	CED-O2D-CGD	2.81	122.29	115.94
14	H	1222	CLA	CAA-C2A-C1A	-2.81	102.77	111.97
14	b	1222	CLA	CAA-C2A-C1A	-2.81	102.77	111.97
14	A	1136	CLA	CMB-C2B-C3B	2.81	129.93	124.68
21	a	6002	LMT	C1'-O5'-C5'	-2.81	108.17	113.69
14	a	1123	CLA	C1-C2-C3	-2.81	121.19	126.04
14	G	1103	CLA	C4-C3-C5	2.81	120.00	115.27
14	A	1118	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
14	G	1105	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
14	B	1215	CLA	CMC-C2C-C1C	2.81	129.31	125.04
18	l	4022	BCR	C37-C22-C21	-2.81	118.99	122.92
14	B	1204	CLA	C6-C5-C3	-2.81	106.09	113.45
14	G	1136	CLA	CMB-C2B-C3B	2.81	129.93	124.68
14	a	1106	CLA	C3C-C4C-NC	2.81	113.72	110.57
14	b	1202	CLA	C3C-C4C-NC	2.81	113.72	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	4008	BCR	C34-C9-C8	2.81	122.50	118.08
14	B	1202	CLA	C3C-C4C-NC	2.81	113.72	110.57
14	H	1214	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
15	H	1230	F6C	O2D-CGD-O1D	-2.80	118.35	123.84
19	H	5004	LHG	O8-C23-C24	2.80	120.71	111.91
14	H	1204	CLA	C6-C5-C3	-2.80	106.10	113.45
14	a	1109	CLA	C4D-C3D-CAD	2.80	111.40	108.10
14	a	1139	CLA	C4D-C3D-CAD	2.80	111.40	108.10
14	B	1210	CLA	C1-O2A-CGA	2.80	123.80	116.44
14	A	1126	CLA	C4-C3-C5	2.80	119.99	115.27
14	a	1122	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
18	a	4008	BCR	C34-C9-C8	2.80	122.49	118.08
14	a	1119	CLA	CED-O2D-CGD	2.80	122.28	115.94
14	G	1106	CLA	C3C-C4C-NC	2.80	113.71	110.57
14	a	1126	CLA	C4-C3-C5	2.80	119.98	115.27
14	B	1229	CLA	C3D-C4D-ND	2.80	114.77	110.24
14	b	1227	CLA	C4D-C3D-CAD	2.80	111.40	108.10
14	G	1126	CLA	C4-C3-C5	2.80	119.98	115.27
14	a	1138	CLA	C4-C3-C5	2.80	119.98	115.27
19	B	5004	LHG	O8-C23-C24	2.80	120.69	111.91
20	l	5007	LMG	O8-C28-C29	2.80	120.69	111.91
14	B	1222	CLA	CAA-C2A-C1A	-2.80	102.80	111.97
14	G	1118	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
14	b	1214	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
14	A	1138	CLA	C4-C3-C5	2.80	119.98	115.27
20	U	5007	LMG	O8-C28-C29	2.80	120.69	111.91
15	b	1230	F6C	O2D-CGD-O1D	-2.80	118.37	123.84
14	A	1103	CLA	C4-C3-C5	2.80	119.98	115.27
14	G	1129	CLA	C3C-C4C-NC	2.80	113.71	110.57
18	G	4008	BCR	C34-C9-C8	2.80	122.48	118.08
14	A	1122	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
14	a	1118	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
19	b	5004	LHG	O8-C23-C24	2.80	120.68	111.91
14	a	1123	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
14	A	1110	CLA	CMB-C2B-C3B	2.80	129.91	124.68
14	B	1209	CLA	CMB-C2B-C3B	2.79	129.91	124.68
14	b	1204	CLA	CMB-C2B-C3B	2.79	129.91	124.68
14	G	1138	CLA	C4-C3-C5	2.79	119.97	115.27
14	b	1210	CLA	C1-O2A-CGA	2.79	123.77	116.44
14	A	1129	CLA	C3C-C4C-NC	2.79	113.70	110.57
14	b	1232	CLA	CMA-C3A-C4A	2.79	119.28	111.77
14	B	1205	CLA	CAA-C2A-C3A	-2.79	105.14	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1202	CLA	C3C-C4C-NC	2.79	113.70	110.57
14	B	1204	CLA	CMB-C2B-C3B	2.79	129.90	124.68
14	A	1134	CLA	CMA-C3A-C4A	2.79	119.27	111.77
14	H	1205	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
20	L	5007	LMG	O8-C28-C29	2.79	120.66	111.91
18	H	4005	BCR	C28-C27-C26	-2.79	109.10	114.08
14	l	1502	CLA	C3D-C4D-ND	2.79	114.75	110.24
18	B	4005	BCR	C28-C27-C26	-2.79	109.10	114.08
14	a	1110	CLA	CMB-C2B-C3B	2.78	129.89	124.68
14	B	1214	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
14	H	1210	CLA	C1-O2A-CGA	2.78	123.74	116.44
14	B	1232	CLA	CMA-C3A-C4A	2.78	119.25	111.77
18	L	4022	BCR	C37-C22-C21	-2.78	119.03	122.92
14	b	1231	CLA	C3C-C4C-NC	2.78	113.69	110.57
14	B	1231	CLA	C3C-C4C-NC	2.78	113.69	110.57
14	A	1139	CLA	C4D-C3D-CAD	2.78	111.37	108.10
14	H	1232	CLA	CMA-C3A-C4A	2.78	119.24	111.77
14	B	1213	CLA	C3C-C4C-NC	2.78	113.69	110.57
15	H	1237	F6C	CMC-C2C-C3C	2.78	130.18	124.94
18	U	4022	BCR	C37-C22-C21	-2.78	119.03	122.92
14	H	1224	CLA	CMC-C2C-C1C	2.78	129.27	125.04
14	H	1217	CLA	C4-C3-C5	2.78	119.94	115.27
14	b	1213	CLA	C3C-C4C-NC	2.78	113.68	110.57
14	b	1205	CLA	CAA-C2A-C3A	-2.77	105.18	112.78
14	B	1231	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
14	G	1110	CLA	CMB-C2B-C3B	2.77	129.87	124.68
18	b	4010	BCR	C34-C9-C8	2.77	122.44	118.08
14	A	1127	CLA	CMC-C2C-C1C	2.77	129.26	125.04
14	A	1123	CLA	C1-C2-C3	-2.77	121.25	126.04
14	a	1134	CLA	CMA-C3A-C4A	2.77	119.22	111.77
14	H	1209	CLA	CMB-C2B-C3B	2.77	129.86	124.68
14	H	1239	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
14	A	1012	CLA	C4-C3-C5	2.77	119.93	115.27
14	B	1224	CLA	CMC-C2C-C1C	2.77	129.25	125.04
14	A	1120	CLA	C3C-C4C-NC	2.77	113.67	110.57
14	B	1236	CLA	C3D-C4D-ND	2.77	114.71	110.24
14	G	1134	CLA	CMA-C3A-C4A	2.77	119.20	111.77
14	B	1218	CLA	CHD-C1D-ND	-2.77	121.91	124.45
14	H	1236	CLA	C3D-C4D-ND	2.76	114.71	110.24
14	H	1229	CLA	C3D-C4D-ND	2.76	114.71	110.24
15	b	1237	F6C	CMC-C2C-C3C	2.76	130.15	124.94
14	U	1503	CLA	C3C-C4C-NC	2.76	113.67	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1239	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
18	b	4014	BCR	C28-C27-C26	-2.76	109.14	114.08
14	A	1109	CLA	C4D-C3D-CAD	2.76	111.35	108.10
14	a	1127	CLA	CMC-C2C-C1C	2.76	129.24	125.04
18	H	4009	BCR	C3-C4-C5	-2.76	109.15	114.08
14	G	1122	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
18	U	4019	BCR	C24-C25-C26	-2.76	114.78	121.46
14	G	1139	CLA	C4D-C3D-CAD	2.76	111.35	108.10
14	H	1218	CLA	CHD-C1D-ND	-2.76	121.92	124.45
18	l	4019	BCR	C24-C25-C26	-2.76	114.78	121.46
18	H	4010	BCR	C38-C26-C25	-2.76	121.43	124.53
20	R	5006	LMG	C8-O7-C10	-2.76	111.00	117.79
14	b	1231	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
14	H	1221	CLA	C4-C3-C5	2.76	119.91	115.27
14	b	1220	CLA	C4-C3-C5	2.76	119.91	115.27
14	G	1135	CLA	C3C-C4C-NC	2.76	113.66	110.57
14	G	1106	CLA	CMC-C2C-C1C	2.76	129.24	125.04
14	B	1235	CLA	CMC-C2C-C1C	2.76	129.24	125.04
14	a	1120	CLA	C3C-C4C-NC	2.76	113.66	110.57
18	B	4010	BCR	C38-C26-C25	-2.75	121.44	124.53
14	a	1110	CLA	CMC-C2C-C1C	2.75	129.23	125.04
14	A	1116	CLA	C3C-C4C-NC	2.75	113.66	110.57
18	H	4014	BCR	C28-C27-C26	-2.75	109.16	114.08
15	B	1238	F6C	CHB-C4A-C3A	-2.75	119.71	125.48
14	b	1236	CLA	C3D-C4D-ND	2.75	114.69	110.24
20	I	5006	LMG	C8-O7-C10	-2.75	111.02	117.79
14	B	1239	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
14	G	1012	CLA	C4-C3-C5	2.75	119.90	115.27
14	H	1213	CLA	C3C-C4C-NC	2.75	113.65	110.57
14	H	1211	CLA	C3D-C4D-ND	2.75	114.68	110.24
14	G	1013	CLA	C3C-C4C-NC	2.75	113.65	110.57
15	B	1237	F6C	CMC-C2C-C3C	2.75	130.12	124.94
14	b	1217	CLA	C4-C3-C5	2.75	119.89	115.27
14	U	1502	CLA	C3D-C4D-ND	2.75	114.68	110.24
14	A	1102	CLA	CMC-C2C-C1C	2.75	129.22	125.04
18	B	4006	BCR	C28-C27-C26	-2.75	109.17	114.08
14	L	1502	CLA	C3D-C4D-ND	2.75	114.68	110.24
14	a	1135	CLA	C3C-C4C-NC	2.75	113.65	110.57
20	i	5006	LMG	C8-O7-C10	-2.75	111.03	117.79
18	A	4011	BCR	C31-C1-C6	-2.75	105.85	110.30
14	G	1116	CLA	C3C-C4C-NC	2.74	113.65	110.57
14	b	1023	CLA	O2D-CGD-O1D	-2.74	118.47	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	1503	CLA	C3D-C4D-ND	2.74	114.68	110.24
14	a	1120	CLA	CMC-C2C-C1C	2.74	129.22	125.04
14	a	1012	CLA	C4-C3-C5	2.74	119.89	115.27
14	b	1209	CLA	CMB-C2B-C3B	2.74	129.81	124.68
14	b	1224	CLA	CMC-C2C-C1C	2.74	129.22	125.04
14	B	1023	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
14	b	1221	CLA	C4-C3-C5	2.74	119.89	115.27
14	H	1220	CLA	C4-C3-C5	2.74	119.88	115.27
18	b	4009	BCR	C3-C4-C5	-2.74	109.18	114.08
18	B	4014	BCR	C28-C27-C26	-2.74	109.18	114.08
18	L	4019	BCR	C24-C25-C26	-2.74	114.82	121.46
14	l	1503	CLA	C3C-C4C-NC	2.74	113.64	110.57
14	L	1503	CLA	C4-C3-C5	2.74	119.88	115.27
15	b	1238	F6C	CHB-C4A-C3A	-2.74	119.73	125.48
18	H	4010	BCR	C34-C9-C8	2.74	122.39	118.08
18	H	4006	BCR	C28-C27-C26	-2.74	109.19	114.08
15	A	1121	F6C	CMA-C3A-C2A	-2.74	118.68	126.12
14	U	1503	CLA	C3D-C4D-ND	2.74	114.67	110.24
14	G	1102	CLA	CMC-C2C-C1C	2.74	129.21	125.04
14	G	1110	CLA	CMC-C2C-C1C	2.74	129.21	125.04
18	H	4010	BCR	C33-C5-C6	-2.74	121.45	124.53
14	L	1503	CLA	C3C-C4C-NC	2.74	113.64	110.57
14	b	1235	CLA	CMC-C2C-C1C	2.74	129.21	125.04
14	B	1217	CLA	C4-C3-C5	2.74	119.88	115.27
14	a	1102	CLA	CMC-C2C-C1C	2.74	129.21	125.04
14	G	1120	CLA	C3C-C4C-NC	2.73	113.64	110.57
18	a	4011	BCR	C31-C1-C6	-2.73	105.86	110.30
14	a	1106	CLA	CMC-C2C-C1C	2.73	129.20	125.04
14	b	1208	CLA	CMC-C2C-C1C	2.73	129.20	125.04
18	B	4010	BCR	C33-C5-C6	-2.73	121.46	124.53
14	H	1231	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
15	G	1121	F6C	CMA-C3A-C2A	-2.73	118.70	126.12
14	A	1113	CLA	C3C-C4C-NC	2.73	113.64	110.57
14	B	1233	CLA	CMC-C2C-C1C	2.73	129.20	125.04
18	B	4009	BCR	C3-C4-C5	-2.73	109.20	114.08
14	G	1109	CLA	C4D-C3D-CAD	2.73	111.31	108.10
14	H	1208	CLA	CMC-C2C-C1C	2.73	129.20	125.04
14	A	1106	CLA	CMC-C2C-C1C	2.73	129.20	125.04
14	a	1116	CLA	C3C-C4C-NC	2.73	113.63	110.57
14	G	1127	CLA	CMC-C2C-C1C	2.73	129.20	125.04
18	b	4004	BCR	C15-C14-C13	-2.73	123.42	127.31
14	B	1211	CLA	C4-C3-C5	2.73	119.86	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	4005	BCR	C40-C30-C25	-2.73	105.87	110.30
14	B	1208	CLA	CMC-C2C-C1C	2.73	129.19	125.04
14	U	1503	CLA	C4-C3-C5	2.73	119.86	115.27
14	H	1231	CLA	CMB-C2B-C3B	2.73	129.78	124.68
18	b	4006	BCR	C28-C27-C26	-2.73	109.21	114.08
14	A	1109	CLA	C1-C2-C3	-2.73	121.33	126.04
18	H	4009	BCR	C38-C26-C27	2.73	118.85	113.62
16	G	2001	PQN	C11-C12-C13	-2.73	122.25	126.79
14	H	1235	CLA	CMC-C2C-C1C	2.73	129.19	125.04
15	H	1238	F6C	CHB-C4A-C3A	-2.73	119.76	125.48
18	H	4005	BCR	C40-C30-C25	-2.73	105.88	110.30
14	G	1013	CLA	C3D-C4D-ND	2.73	114.65	110.24
18	b	4010	BCR	C38-C26-C25	-2.72	121.47	124.53
14	a	1109	CLA	C1-C2-C3	-2.72	121.33	126.04
14	l	1503	CLA	C4-C3-C5	2.72	119.85	115.27
14	H	1201	CLA	CMC-C2C-C1C	2.72	129.19	125.04
14	a	1125	CLA	CAC-C3C-C4C	2.72	128.34	124.81
18	b	4010	BCR	C33-C5-C6	-2.72	121.47	124.53
14	B	1231	CLA	CMB-C2B-C3B	2.72	129.77	124.68
14	B	1221	CLA	C4-C3-C5	2.72	119.85	115.27
14	A	1125	CLA	CAC-C3C-C4C	2.72	128.34	124.81
14	b	1231	CLA	CMB-C2B-C3B	2.72	129.77	124.68
18	i	4018	BCR	C23-C24-C25	-2.72	119.56	127.20
18	B	4010	BCR	C34-C9-C8	2.72	122.36	118.08
14	b	1211	CLA	C4-C3-C5	2.72	119.85	115.27
18	G	4011	BCR	C31-C1-C6	-2.72	105.89	110.30
14	G	1133	CLA	CMC-C2C-C1C	2.72	129.18	125.04
14	A	1110	CLA	CMC-C2C-C1C	2.72	129.18	125.04
14	H	1023	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
18	H	4004	BCR	C15-C14-C13	-2.72	123.43	127.31
18	R	4018	BCR	C23-C24-C25	-2.72	119.57	127.20
18	A	4002	BCR	C3-C4-C5	-2.72	109.22	114.08
14	G	1129	CLA	CAA-C2A-C3A	-2.72	105.34	112.78
18	I	4020	BCR	C34-C9-C8	2.72	122.36	118.08
18	a	4007	BCR	C7-C8-C9	-2.72	122.13	126.23
14	b	1233	CLA	CMC-C2C-C1C	2.72	129.18	125.04
14	B	1021	CLA	CMC-C2C-C1C	2.72	129.18	125.04
14	B	1211	CLA	C3D-C4D-ND	2.72	114.63	110.24
18	b	4005	BCR	C40-C30-C25	-2.72	105.89	110.30
14	G	1113	CLA	C3C-C4C-NC	2.72	113.62	110.57
18	I	4018	BCR	C23-C24-C25	-2.71	119.58	127.20
18	A	4007	BCR	C7-C8-C9	-2.71	122.13	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1124	CLA	C3D-C4D-ND	2.71	114.63	110.24
14	b	1211	CLA	C3D-C4D-ND	2.71	114.63	110.24
14	H	1228	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
14	B	1220	CLA	C4-C3-C5	2.71	119.84	115.27
15	a	1121	F6C	CMA-C3A-C2A	-2.71	118.75	126.12
14	H	1233	CLA	CMC-C2C-C1C	2.71	129.17	125.04
14	a	1133	CLA	CMC-C2C-C1C	2.71	129.17	125.04
14	A	1120	CLA	CMC-C2C-C1C	2.71	129.17	125.04
14	B	1232	CLA	C4D-C3D-CAD	2.71	111.29	108.10
14	l	1503	CLA	C3D-C4D-ND	2.71	114.62	110.24
14	B	1228	CLA	C3D-C4D-ND	2.71	114.62	110.24
14	a	1124	CLA	C3D-C4D-ND	2.71	114.62	110.24
14	a	1013	CLA	C3D-C4D-ND	2.71	114.62	110.24
14	B	1213	CLA	C4-C3-C5	2.71	119.83	115.27
18	G	4002	BCR	C3-C4-C5	-2.71	109.24	114.08
14	H	1211	CLA	C4-C3-C5	2.71	119.83	115.27
18	i	4020	BCR	C34-C9-C8	2.71	122.34	118.08
14	B	1225	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
14	b	1219	CLA	CMC-C2C-C1C	2.70	129.16	125.04
14	G	1109	CLA	C1-C2-C3	-2.70	121.37	126.04
14	G	1125	CLA	CAC-C3C-C4C	2.70	128.32	124.81
14	H	1214	CLA	CMC-C2C-C1C	2.70	129.15	125.04
14	G	1123	CLA	CMC-C2C-C1C	2.70	129.15	125.04
14	A	1123	CLA	CMC-C2C-C1C	2.70	129.15	125.04
14	B	1236	CLA	C3C-C4C-NC	2.70	113.60	110.57
18	b	4006	BCR	C36-C18-C17	-2.70	119.14	122.92
14	G	1104	CLA	C3D-C4D-ND	2.70	114.61	110.24
14	A	1013	CLA	C3D-C4D-ND	2.70	114.61	110.24
18	B	4009	BCR	C38-C26-C27	2.70	118.80	113.62
18	a	4002	BCR	C3-C4-C5	-2.70	109.26	114.08
18	R	4020	BCR	C34-C9-C8	2.70	122.33	118.08
14	H	1219	CLA	CMC-C2C-C1C	2.70	129.15	125.04
14	a	1129	CLA	CAA-C2A-C3A	-2.70	105.39	112.78
13	G	1011	CL0	C3D-C4D-ND	2.70	114.60	110.24
14	H	1218	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
14	B	1228	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
15	H	1237	F6C	O2D-CGD-O1D	-2.70	118.56	123.84
15	B	1237	F6C	O2D-CGD-O1D	-2.70	118.56	123.84
14	H	1213	CLA	C4-C3-C5	2.70	119.81	115.27
14	a	1127	CLA	C4-C3-C5	2.70	119.81	115.27
14	b	1021	CLA	CMC-C2C-C1C	2.70	129.15	125.04
14	H	1221	CLA	CMA-C3A-C4A	2.70	119.02	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1124	CLA	C3D-C4D-ND	2.70	114.60	110.24
19	B	5004	LHG	C5-O7-C7	-2.70	111.15	117.79
16	A	2001	PQN	C11-C12-C13	-2.70	122.30	126.79
18	b	4009	BCR	C38-C26-C27	2.70	118.80	113.62
14	b	1214	CLA	CMC-C2C-C1C	2.70	129.15	125.04
14	a	1111	CLA	CAA-C2A-C3A	-2.70	105.39	112.78
14	b	1213	CLA	C4-C3-C5	2.70	119.81	115.27
14	H	1220	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
14	G	1127	CLA	C4-C3-C5	2.70	119.81	115.27
14	H	1021	CLA	CMC-C2C-C1C	2.69	129.14	125.04
14	b	1232	CLA	C4D-C3D-CAD	2.69	111.27	108.10
14	A	1111	CLA	C3C-C4C-NC	2.69	113.59	110.57
14	G	1139	CLA	CMC-C2C-C1C	2.69	129.14	125.04
14	A	1129	CLA	CAA-C2A-C3A	-2.69	105.40	112.78
13	a	1011	CL0	C3D-C4D-ND	2.69	114.59	110.24
14	A	1104	CLA	C3D-C4D-ND	2.69	114.59	110.24
14	B	1221	CLA	CMA-C3A-C4A	2.69	119.01	111.77
14	b	1229	CLA	CMC-C2C-C1C	2.69	129.14	125.04
16	a	2001	PQN	C11-C12-C13	-2.69	122.31	126.79
14	b	1218	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
14	A	1131	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
14	H	1229	CLA	CMC-C2C-C1C	2.69	129.14	125.04
14	b	1220	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
14	a	1113	CLA	C3C-C4C-NC	2.69	113.59	110.57
14	B	1219	CLA	CMC-C2C-C1C	2.69	129.14	125.04
14	B	1220	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
14	b	1221	CLA	CMA-C3A-C4A	2.69	119.00	111.77
14	b	1201	CLA	CMC-C2C-C1C	2.69	129.13	125.04
14	a	1126	CLA	C3C-C4C-NC	2.69	113.59	110.57
14	A	1108	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
14	a	1012	CLA	OBD-CAD-C3D	-2.69	122.05	128.52
14	A	1012	CLA	OBD-CAD-C3D	-2.69	122.05	128.52
14	G	1012	CLA	OBD-CAD-C3D	-2.69	122.05	128.52
14	G	1120	CLA	CMC-C2C-C1C	2.69	129.13	125.04
14	B	1022	CLA	C1-C2-C3	-2.69	121.40	126.04
14	B	1226	CLA	C1-C2-C3	-2.69	121.40	126.04
14	B	1218	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
14	B	1201	CLA	CMC-C2C-C1C	2.68	129.13	125.04
18	B	4004	BCR	C15-C14-C13	-2.68	123.48	127.31
14	B	1203	CLA	C3C-C4C-NC	2.68	113.58	110.57
14	H	1022	CLA	C1-C2-C3	-2.68	121.41	126.04
14	A	1127	CLA	C4-C3-C5	2.68	119.78	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1131	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
14	b	1022	CLA	C1-C2-C3	-2.68	121.41	126.04
14	a	1139	CLA	CMC-C2C-C1C	2.68	129.12	125.04
14	A	1135	CLA	C3C-C4C-NC	2.68	113.58	110.57
15	b	1237	F6C	O2D-CGD-O1D	-2.68	118.60	123.84
18	b	4004	BCR	C33-C5-C6	-2.68	121.52	124.53
19	b	5004	LHG	C5-O7-C7	-2.68	111.19	117.79
14	G	1133	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
14	G	1126	CLA	C3C-C4C-NC	2.68	113.57	110.57
18	G	4011	BCR	C1-C6-C5	-2.68	118.84	122.61
14	b	1228	CLA	C3D-C4D-ND	2.68	114.57	110.24
14	b	1228	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
14	a	1111	CLA	CMC-C2C-C1C	2.68	129.12	125.04
18	H	4006	BCR	C36-C18-C17	-2.68	119.17	122.92
14	B	1214	CLA	CMC-C2C-C1C	2.68	129.11	125.04
14	a	1131	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
14	G	1111	CLA	CAA-C2A-C3A	-2.68	105.45	112.78
14	H	1228	CLA	C3D-C4D-ND	2.68	114.56	110.24
14	b	1236	CLA	C3C-C4C-NC	2.68	113.57	110.57
14	b	1225	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
14	A	1133	CLA	CMC-C2C-C1C	2.67	129.11	125.04
14	A	1111	CLA	CAA-C2A-C3A	-2.67	105.45	112.78
14	A	1139	CLA	CMC-C2C-C1C	2.67	129.11	125.04
14	H	1235	CLA	C3D-C4D-ND	2.67	114.56	110.24
18	G	4007	BCR	C7-C8-C9	-2.67	122.19	126.23
14	b	1226	CLA	C1-C2-C3	-2.67	121.42	126.04
14	G	1108	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
14	A	1126	CLA	C3C-C4C-NC	2.67	113.57	110.57
14	a	1108	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
14	G	1118	CLA	C4D-C3D-CAD	2.67	111.25	108.10
19	H	5004	LHG	C5-O7-C7	-2.67	111.21	117.79
18	G	4002	BCR	C37-C22-C21	-2.67	119.18	122.92
14	H	1021	CLA	C3D-C4D-ND	2.67	114.56	110.24
18	b	4013	BCR	C3-C4-C5	-2.67	109.31	114.08
18	B	4013	BCR	C3-C4-C5	-2.67	109.31	114.08
14	T	1401	CLA	C3C-C4C-NC	2.67	113.57	110.57
18	b	4013	BCR	C37-C22-C21	-2.67	119.18	122.92
13	A	1011	CL0	CMC-C2C-C1C	2.67	129.10	125.04
14	H	1210	CLA	CMC-C2C-C1C	2.67	129.10	125.04
14	A	1111	CLA	CMC-C2C-C1C	2.67	129.10	125.04
14	a	1123	CLA	CMC-C2C-C1C	2.67	129.10	125.04
14	a	1129	CLA	C4D-C3D-CAD	2.67	111.24	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1105	CLA	C3D-C4D-ND	2.67	114.55	110.24
14	b	1235	CLA	CMA-C3A-C4A	2.67	118.94	111.77
18	B	4013	BCR	C37-C22-C21	-2.67	119.19	122.92
15	b	1207	F6C	C1-O2A-CGA	2.67	123.44	116.44
15	B	1238	F6C	CMD-C2D-C3D	-2.67	121.48	127.61
14	H	1226	CLA	C1-C2-C3	-2.66	121.44	126.04
15	B	1230	F6C	CMC-C2C-C3C	2.66	129.97	124.94
13	a	1011	CL0	CMC-C2C-C1C	2.66	129.10	125.04
18	A	4002	BCR	C37-C22-C21	-2.66	119.19	122.92
14	B	1229	CLA	CMC-C2C-C1C	2.66	129.09	125.04
14	G	1012	CLA	C3C-C4C-NC	2.66	113.56	110.57
14	H	1232	CLA	C4D-C3D-CAD	2.66	111.23	108.10
18	H	4013	BCR	C3-C4-C5	-2.66	109.33	114.08
14	A	1110	CLA	C3C-C4C-NC	2.66	113.56	110.57
14	H	1228	CLA	CAC-C3C-C4C	2.66	128.26	124.81
14	G	1111	CLA	CMC-C2C-C1C	2.66	129.09	125.04
15	H	1238	F6C	CMD-C2D-C3D	-2.66	121.50	127.61
15	b	1238	F6C	CMD-C2D-C3D	-2.66	121.50	127.61
14	a	1104	CLA	C3D-C4D-ND	2.66	114.54	110.24
14	H	1235	CLA	CMA-C3A-C4A	2.66	118.92	111.77
15	H	1230	F6C	CHB-C4A-C3A	-2.66	119.91	125.48
13	G	1011	CL0	CMC-C2C-C1C	2.66	129.09	125.04
15	B	1207	F6C	C1-O2A-CGA	2.66	123.41	116.44
18	H	4004	BCR	C33-C5-C6	-2.66	121.55	124.53
14	B	1210	CLA	CMC-C2C-C1C	2.66	129.08	125.04
18	H	4013	BCR	C37-C22-C21	-2.65	119.20	122.92
14	B	1235	CLA	CMA-C3A-C4A	2.65	118.91	111.77
18	B	4004	BCR	C33-C5-C6	-2.65	121.55	124.53
14	b	1210	CLA	CMC-C2C-C1C	2.65	129.08	125.04
18	G	4008	BCR	C36-C18-C17	-2.65	119.21	122.92
14	H	1220	CLA	C3C-C4C-NC	2.65	113.55	110.57
14	b	1208	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
14	B	1217	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
14	G	1137	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
14	a	1135	CLA	CAC-C3C-C4C	2.65	128.25	124.81
14	H	1225	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
14	G	1136	CLA	C3D-C4D-ND	2.65	114.53	110.24
18	B	4006	BCR	C36-C18-C17	-2.65	119.21	122.92
14	b	1220	CLA	C3C-C4C-NC	2.65	113.54	110.57
15	H	1207	F6C	C1-O2A-CGA	2.65	123.40	116.44
15	G	1121	F6C	CMC-C2C-C3C	2.65	129.94	124.94
15	a	1121	F6C	CMC-C2C-C3C	2.65	129.94	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	1230	F6C	CMC-C2C-C3C	2.65	129.94	124.94
14	H	1203	CLA	C3C-C4C-NC	2.65	113.54	110.57
14	H	1221	CLA	CAC-C3C-C4C	2.65	128.25	124.81
14	a	1118	CLA	C4D-C3D-CAD	2.65	111.22	108.10
14	G	1110	CLA	C3D-C4D-ND	2.65	114.52	110.24
18	A	4008	BCR	C36-C18-C17	-2.65	119.21	122.92
14	G	1110	CLA	C3C-C4C-NC	2.65	113.54	110.57
14	G	1115	CLA	C3C-C4C-NC	2.65	113.54	110.57
14	b	1023	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
18	a	4011	BCR	C1-C6-C5	-2.65	118.89	122.61
14	H	1211	CLA	CMC-C2C-C1C	2.65	129.07	125.04
14	H	1227	CLA	C3D-C4D-ND	2.65	114.52	110.24
14	B	1210	CLA	C3D-C4D-ND	2.65	114.52	110.24
14	B	1235	CLA	C3D-C4D-ND	2.65	114.52	110.24
15	B	1238	F6C	CHD-C1D-ND	-2.65	120.19	124.20
18	a	4002	BCR	C37-C22-C21	-2.65	119.22	122.92
14	H	1232	CLA	CMC-C2C-C1C	2.64	129.07	125.04
14	b	1203	CLA	C3C-C4C-NC	2.64	113.54	110.57
15	B	1230	F6C	CHB-C4A-C3A	-2.64	119.93	125.48
14	A	1118	CLA	C4D-C3D-CAD	2.64	111.21	108.10
14	b	1223	CLA	C4-C3-C5	2.64	119.72	115.27
14	a	1118	CLA	C3C-C4C-NC	2.64	113.54	110.57
14	H	1208	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
14	G	1135	CLA	CAC-C3C-C4C	2.64	128.24	124.81
14	b	1228	CLA	CAC-C3C-C4C	2.64	128.24	124.81
15	b	1238	F6C	CHD-C1D-ND	-2.64	120.19	124.20
15	b	1230	F6C	CHB-C4A-C3A	-2.64	119.94	125.48
14	A	1133	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
14	a	1012	CLA	C3C-C4C-NC	2.64	113.53	110.57
14	H	1236	CLA	C3C-C4C-NC	2.64	113.53	110.57
14	a	1137	CLA	O1D-CGD-CBD	-2.64	119.08	124.48
13	A	1011	CL0	C3D-C4D-ND	2.64	114.51	110.24
14	b	1211	CLA	CMC-C2C-C1C	2.64	129.06	125.04
14	a	1111	CLA	C3C-C4C-NC	2.64	113.53	110.57
14	b	1217	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
14	A	1117	CLA	CMA-C3A-C4A	2.64	118.87	111.77
14	A	1118	CLA	CMC-C2C-C1C	2.64	129.06	125.04
18	A	4011	BCR	C1-C6-C5	-2.64	118.90	122.61
15	A	1121	F6C	CMC-C2C-C3C	2.64	129.92	124.94
18	i	4020	BCR	C37-C22-C21	-2.64	119.23	122.92
15	H	1230	F6C	CMC-C2C-C3C	2.64	129.92	124.94
14	G	1105	CLA	C3D-C4D-ND	2.64	114.51	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	I	4020	BCR	C37-C22-C21	-2.64	119.23	122.92
14	G	1111	CLA	C3C-C4C-NC	2.64	113.53	110.57
14	a	1133	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
14	H	1023	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
14	A	1012	CLA	C3C-C4C-NC	2.64	113.53	110.57
14	A	1137	CLA	O1D-CGD-CBD	-2.64	119.09	124.48
14	B	1232	CLA	CMC-C2C-C1C	2.64	129.06	125.04
14	H	1021	CLA	CBC-CAC-C3C	-2.64	105.16	112.43
14	B	1023	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
14	H	1233	CLA	C3D-C4D-ND	2.64	114.50	110.24
14	a	1110	CLA	C3D-C4D-ND	2.64	114.50	110.24
14	A	1105	CLA	C3D-C4D-ND	2.64	114.50	110.24
14	K	1401	CLA	C3C-C4C-NC	2.64	113.53	110.57
14	G	1117	CLA	CMA-C3A-C4A	2.64	118.86	111.77
14	b	1235	CLA	C3D-C4D-ND	2.64	114.50	110.24
14	T	1401	CLA	CMB-C2B-C3B	2.63	129.61	124.68
14	B	1205	CLA	C4-C3-C5	2.63	119.70	115.27
14	G	1118	CLA	CMC-C2C-C1C	2.63	129.05	125.04
14	B	1228	CLA	CAC-C3C-C4C	2.63	128.23	124.81
14	K	1401	CLA	CMB-C2B-C3B	2.63	129.60	124.68
14	b	1232	CLA	CMC-C2C-C1C	2.63	129.05	125.04
14	B	1202	CLA	CMC-C2C-C1C	2.63	129.05	125.04
14	H	1220	CLA	CAC-C3C-C4C	2.63	128.23	124.81
14	a	1115	CLA	C3C-C4C-NC	2.63	113.52	110.57
18	I	4020	BCR	C35-C13-C12	2.63	122.22	118.08
14	b	1021	CLA	CBC-CAC-C3C	-2.63	105.17	112.43
14	B	1208	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
14	G	1129	CLA	C4D-C3D-CAD	2.63	111.20	108.10
14	H	1023	CLA	CHB-C4A-NA	2.63	128.15	124.51
14	H	1217	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
14	G	1136	CLA	C1-C2-C3	-2.63	121.50	126.04
14	a	1134	CLA	C3C-C4C-NC	2.63	113.52	110.57
14	a	1136	CLA	C3D-C4D-ND	2.63	114.49	110.24
14	b	1021	CLA	C3D-C4D-ND	2.63	114.49	110.24
14	B	1216	CLA	C3D-C4D-ND	2.63	114.49	110.24
14	A	1136	CLA	C1-C2-C3	-2.63	121.50	126.04
14	H	1223	CLA	C4-C3-C5	2.63	119.69	115.27
14	a	1117	CLA	CMA-C3A-C4A	2.63	118.83	111.77
14	a	1110	CLA	C3C-C4C-NC	2.63	113.52	110.57
14	a	1136	CLA	C1-C2-C3	-2.63	121.50	126.04
14	b	1227	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
14	H	1229	CLA	CMA-C3A-C4A	2.63	118.83	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1136	CLA	C3D-C4D-ND	2.62	114.48	110.24
14	B	1221	CLA	CAC-C3C-C4C	2.62	128.22	124.81
14	G	1120	CLA	CMB-C2B-C3B	2.62	129.59	124.68
14	a	1120	CLA	CMB-C2B-C3B	2.62	129.59	124.68
14	A	1115	CLA	C3C-C4C-NC	2.62	113.51	110.57
14	b	1205	CLA	C4-C3-C5	2.62	119.68	115.27
14	B	1021	CLA	CBC-CAC-C3C	-2.62	105.20	112.43
14	a	1118	CLA	CMC-C2C-C1C	2.62	129.03	125.04
14	A	1139	CLA	CAA-C2A-C3A	-2.62	105.60	112.78
14	B	1229	CLA	CMA-C3A-C4A	2.62	118.82	111.77
14	b	1214	CLA	CMA-C3A-C4A	2.62	118.82	111.77
18	R	4020	BCR	C37-C22-C21	-2.62	119.25	122.92
14	H	1227	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
14	B	1021	CLA	C3D-C4D-ND	2.62	114.48	110.24
14	k	1401	CLA	C3C-C4C-NC	2.62	113.51	110.57
14	H	1239	CLA	CAA-CBA-CGA	-2.62	105.59	113.25
14	b	1214	CLA	CAA-CBA-CGA	-2.62	105.59	113.25
14	b	1210	CLA	C3D-C4D-ND	2.62	114.48	110.24
18	R	4020	BCR	C35-C13-C12	2.62	122.20	118.08
14	B	1227	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
14	H	1205	CLA	C4-C3-C5	2.62	119.67	115.27
14	a	1139	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
14	B	1214	CLA	CAA-CBA-CGA	-2.62	105.61	113.25
18	a	4008	BCR	C36-C18-C17	-2.62	119.26	122.92
14	B	1220	CLA	C3C-C4C-NC	2.62	113.51	110.57
14	b	1221	CLA	CAC-C3C-C4C	2.62	128.21	124.81
14	b	1227	CLA	C3D-C4D-ND	2.62	114.47	110.24
14	A	1110	CLA	C3D-C4D-ND	2.62	114.47	110.24
18	A	4003	BCR	C36-C18-C17	-2.62	119.26	122.92
14	b	1239	CLA	CAA-CBA-CGA	-2.62	105.61	113.25
14	B	1214	CLA	CMA-C3A-C4A	2.62	118.80	111.77
14	k	1401	CLA	CMB-C2B-C3B	2.61	129.57	124.68
14	A	1112	CLA	C4-C3-C5	2.61	119.67	115.27
15	A	1121	F6C	OMB-CMB-C2B	-2.61	119.78	125.69
14	B	1023	CLA	CHB-C4A-NA	2.61	128.12	124.51
14	H	1214	CLA	CMA-C3A-C4A	2.61	118.79	111.77
14	b	1205	CLA	CMC-C2C-C1C	2.61	129.02	125.04
14	B	1239	CLA	CAA-CBA-CGA	-2.61	105.62	113.25
18	i	4020	BCR	C35-C13-C12	2.61	122.19	118.08
14	b	1220	CLA	CAC-C3C-C4C	2.61	128.20	124.81
14	B	1223	CLA	C4-C3-C5	2.61	119.66	115.27
14	A	1105	CLA	CAC-C3C-C4C	2.61	128.20	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1208	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
14	H	1208	CLA	C4-C3-C5	2.61	119.66	115.27
14	H	1231	CLA	C3D-C4D-ND	2.61	114.46	110.24
14	b	1220	CLA	C3D-C4D-ND	2.61	114.46	110.24
14	b	1233	CLA	C3D-C4D-ND	2.61	114.46	110.24
14	H	1208	CLA	C3C-C4C-NC	2.61	113.50	110.57
14	G	1139	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
14	B	1220	CLA	C3D-C4D-ND	2.61	114.46	110.24
13	a	1011	CL0	C4-C3-C5	2.61	119.66	115.27
14	B	1233	CLA	C3D-C4D-ND	2.61	114.45	110.24
14	b	1231	CLA	C3D-C4D-ND	2.61	114.45	110.24
14	b	1233	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
18	G	4011	BCR	C37-C22-C21	-2.61	119.27	122.92
14	B	1206	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
14	a	1113	CLA	OBD-CAD-C3D	-2.61	122.25	128.52
14	b	1216	CLA	C3D-C4D-ND	2.60	114.45	110.24
14	l	1501	CLA	C1-C2-C3	-2.60	121.54	126.04
14	a	1129	CLA	C3D-C4D-ND	2.60	114.45	110.24
14	b	1229	CLA	CMA-C3A-C4A	2.60	118.77	111.77
14	a	1101	CLA	C3D-C4D-ND	2.60	114.45	110.24
14	B	1208	CLA	CAA-C2A-C3A	-2.60	105.65	112.78
15	b	1207	F6C	CMC-C2C-C3C	2.60	129.85	124.94
14	B	1220	CLA	CAC-C3C-C4C	2.60	128.19	124.81
14	b	1208	CLA	C4-C3-C5	2.60	119.65	115.27
14	H	1206	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
14	b	1208	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
18	I	4020	BCR	C31-C1-C6	-2.60	106.08	110.30
14	B	1205	CLA	CMC-C2C-C1C	2.60	129.00	125.04
14	A	1129	CLA	C4D-C3D-CAD	2.60	111.16	108.10
14	L	1501	CLA	CMC-C2C-C1C	2.60	129.00	125.04
18	l	4022	BCR	C19-C18-C17	2.60	122.93	118.94
14	G	1134	CLA	C3C-C4C-NC	2.60	113.49	110.57
15	H	1207	F6C	CMC-C2C-C3C	2.60	129.84	124.94
14	b	1206	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
14	B	1211	CLA	CMC-C2C-C1C	2.60	129.00	125.04
14	A	1135	CLA	CAC-C3C-C4C	2.60	128.18	124.81
14	a	1114	CLA	CMD-C2D-C3D	-2.60	121.64	127.61
14	G	1126	CLA	C3D-C4D-ND	2.60	114.44	110.24
14	a	1112	CLA	C4-C3-C5	2.60	119.64	115.27
14	H	1216	CLA	C3D-C4D-ND	2.60	114.44	110.24
14	H	1214	CLA	CAA-CBA-CGA	-2.60	105.66	113.25
15	G	1121	F6C	OMB-CMB-C2B	-2.60	119.81	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	4014	BCR	C37-C22-C21	-2.60	119.28	122.92
14	G	1112	CLA	C4-C3-C5	2.60	119.64	115.27
15	H	1238	F6C	CHD-C1D-ND	-2.60	120.26	124.20
18	R	4020	BCR	C31-C1-C6	-2.60	106.09	110.30
14	H	1210	CLA	C3D-C4D-ND	2.60	114.44	110.24
14	a	1013	CLA	C4-C3-C5	2.60	119.64	115.27
14	B	1227	CLA	C3D-C4D-ND	2.60	114.44	110.24
14	A	1132	CLA	C3D-C4D-ND	2.59	114.43	110.24
14	l	1501	CLA	CMC-C2C-C1C	2.59	128.99	125.04
18	U	4022	BCR	C19-C18-C17	2.59	122.92	118.94
14	b	1235	CLA	C4-C3-C5	2.59	119.63	115.27
18	a	4003	BCR	C36-C18-C17	-2.59	119.29	122.92
18	a	4003	BCR	C38-C26-C27	2.59	118.60	113.62
14	A	1120	CLA	CMB-C2B-C3B	2.59	129.53	124.68
14	b	1202	CLA	CMC-C2C-C1C	2.59	128.99	125.04
18	G	4003	BCR	C36-C18-C17	-2.59	119.29	122.92
13	A	1011	CL0	C4-C3-C5	2.59	119.63	115.27
18	a	4003	BCR	C34-C9-C10	-2.59	119.29	122.92
14	A	1013	CLA	C4-C3-C5	2.59	119.63	115.27
14	b	1216	CLA	CMB-C2B-C3B	2.59	129.53	124.68
14	H	1220	CLA	C3D-C4D-ND	2.59	114.43	110.24
14	U	1503	CLA	CBA-CAA-C2A	-2.59	106.22	113.86
14	A	1101	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
14	b	1023	CLA	CHB-C4A-NA	2.59	128.09	124.51
14	H	1233	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
13	G	1011	CL0	C4-C3-C5	2.59	119.63	115.27
14	A	1118	CLA	C3C-C4C-NC	2.59	113.47	110.57
14	b	1209	CLA	C3D-C4D-ND	2.59	114.43	110.24
18	G	4003	BCR	C34-C9-C10	-2.59	119.30	122.92
14	G	1118	CLA	C3C-C4C-NC	2.59	113.47	110.57
14	A	1101	CLA	C3D-C4D-ND	2.59	114.42	110.24
14	A	1126	CLA	C3D-C4D-ND	2.59	114.42	110.24
15	B	1207	F6C	CMC-C2C-C3C	2.59	129.82	124.94
14	H	1236	CLA	CMC-C2C-C1C	2.59	128.98	125.04
18	b	4014	BCR	C33-C5-C4	2.59	118.59	113.62
14	B	1208	CLA	C4-C3-C5	2.59	119.62	115.27
14	A	1102	CLA	C1-O2A-CGA	2.59	123.23	116.44
14	A	1113	CLA	OBD-CAD-C3D	-2.59	122.30	128.52
14	G	1101	CLA	C3D-C4D-ND	2.59	114.42	110.24
18	A	4003	BCR	C38-C26-C27	2.59	118.58	113.62
14	a	1104	CLA	CAA-C2A-C3A	-2.59	105.70	112.78
18	H	4014	BCR	C33-C5-C4	2.59	118.58	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1130	CLA	C4-C3-C5	2.59	119.62	115.27
18	G	4003	BCR	C38-C26-C27	2.59	118.58	113.62
14	a	1123	CLA	C4-C3-C5	2.58	119.62	115.27
14	B	1233	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
14	B	1235	CLA	C4-C3-C5	2.58	119.62	115.27
14	a	1101	CLA	CAA-C2A-C3A	-2.58	105.70	112.78
14	H	1216	CLA	CMB-C2B-C3B	2.58	129.51	124.68
14	B	1216	CLA	CMB-C2B-C3B	2.58	129.51	124.68
14	G	1123	CLA	C4-C3-C5	2.58	119.62	115.27
14	G	1113	CLA	OBD-CAD-C3D	-2.58	122.30	128.52
14	H	1202	CLA	CMC-C2C-C1C	2.58	128.97	125.04
14	a	1109	CLA	C3D-C4D-ND	2.58	114.41	110.24
14	H	1235	CLA	C4-C3-C5	2.58	119.61	115.27
14	a	1132	CLA	C3D-C4D-ND	2.58	114.41	110.24
18	b	4014	BCR	C37-C22-C21	-2.58	119.31	122.92
14	A	1114	CLA	CMD-C2D-C3D	-2.58	121.68	127.61
15	a	1121	F6C	OMB-CMB-C2B	-2.58	119.85	125.69
14	L	1501	CLA	C1-C2-C3	-2.58	121.58	126.04
14	B	1209	CLA	C3D-C4D-ND	2.58	114.41	110.24
14	X	1701	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
14	A	1104	CLA	CAA-C2A-C3A	-2.58	105.71	112.78
14	l	1503	CLA	CBA-CAA-C2A	-2.58	106.25	113.86
15	b	1238	F6C	CHA-C1A-C2A	-2.58	122.84	129.84
14	W	1701	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
18	U	4019	BCR	C8-C7-C6	-2.58	119.96	127.20
14	b	1229	CLA	C4D-C3D-CAD	2.58	111.14	108.10
14	G	1101	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
14	a	1137	CLA	C3C-C4C-NC	2.58	113.46	110.57
14	B	1231	CLA	C3D-C4D-ND	2.58	114.41	110.24
14	b	1236	CLA	CMC-C2C-C1C	2.58	128.97	125.04
14	B	1208	CLA	C3C-C4C-NC	2.58	113.46	110.57
18	b	4016	BCR	C35-C13-C14	-2.58	119.31	122.92
14	A	1123	CLA	C4-C3-C5	2.58	119.61	115.27
14	G	1129	CLA	C3D-C4D-ND	2.58	114.41	110.24
14	A	1134	CLA	C3D-C4D-ND	2.58	114.41	110.24
14	G	1105	CLA	CAC-C3C-C4C	2.58	128.15	124.81
14	a	1105	CLA	CAC-C3C-C4C	2.58	128.15	124.81
14	B	1219	CLA	CMB-C2B-C3B	2.58	129.50	124.68
18	L	4019	BCR	C8-C7-C6	-2.58	119.96	127.20
14	A	1134	CLA	C3C-C4C-NC	2.58	113.46	110.57
14	H	1205	CLA	CMC-C2C-C1C	2.58	128.96	125.04
14	G	1104	CLA	CAA-C2A-C3A	-2.58	105.72	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1238	F6C	CHA-C1A-C2A	-2.58	122.85	129.84
18	l	4019	BCR	C8-C7-C6	-2.58	119.97	127.20
18	A	4003	BCR	C37-C22-C21	-2.58	119.31	122.92
14	A	1109	CLA	C3D-C4D-ND	2.58	114.40	110.24
14	G	1114	CLA	CMD-C2D-C3D	-2.58	121.69	127.61
18	A	4003	BCR	C34-C9-C10	-2.57	119.32	122.92
18	B	4016	BCR	C35-C13-C14	-2.57	119.32	122.92
14	L	1503	CLA	CBA-CAA-C2A	-2.57	106.27	113.86
14	B	1236	CLA	CMC-C2C-C1C	2.57	128.96	125.04
14	l	1502	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
14	B	1224	CLA	C4-C3-C5	2.57	119.60	115.27
14	G	1102	CLA	C1-O2A-CGA	2.57	123.19	116.44
14	a	1139	CLA	C3D-C4D-ND	2.57	114.40	110.24
18	B	4014	BCR	C33-C5-C4	2.57	118.56	113.62
14	A	1106	CLA	CMA-C3A-C4A	2.57	118.68	111.77
14	U	1501	CLA	C1-C2-C3	-2.57	121.60	126.04
14	G	1120	CLA	CMA-C3A-C4A	2.57	118.68	111.77
18	H	4014	BCR	C37-C22-C21	-2.57	119.32	122.92
14	G	1112	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
14	L	1502	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
18	L	4022	BCR	C19-C18-C17	2.57	122.89	118.94
14	a	1126	CLA	C3D-C4D-ND	2.57	114.39	110.24
14	b	1232	CLA	CMD-C2D-C3D	-2.57	121.70	127.61
14	H	1209	CLA	C3D-C4D-ND	2.57	114.39	110.24
14	A	1120	CLA	CMA-C3A-C4A	2.57	118.68	111.77
14	G	1134	CLA	C3D-C4D-ND	2.57	114.39	110.24
15	H	1238	F6C	CHA-C1A-C2A	-2.57	122.87	129.84
14	a	1127	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	H	1232	CLA	C3C-C4C-NC	2.57	113.45	110.57
18	G	4003	BCR	C37-C22-C21	-2.57	119.33	122.92
14	G	1013	CLA	C4-C3-C5	2.57	119.59	115.27
14	A	1134	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	B	1234	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
14	B	1214	CLA	C4-C3-C5	2.57	119.59	115.27
14	a	1106	CLA	CMA-C3A-C4A	2.57	118.67	111.77
20	I	5006	LMG	O8-C28-C29	2.57	119.96	111.91
14	a	1120	CLA	CMA-C3A-C4A	2.57	118.67	111.77
18	b	4010	BCR	C28-C27-C26	-2.56	109.50	114.08
14	A	1107	CLA	CMC-C2C-C1C	2.56	128.94	125.04
14	a	1130	CLA	C4-C3-C5	2.56	119.58	115.27
14	a	1102	CLA	C1-O2A-CGA	2.56	123.17	116.44
14	b	1205	CLA	OBD-CAD-C3D	-2.56	122.35	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	U	1502	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
20	i	5006	LMG	O8-C28-C29	2.56	119.95	111.91
15	b	1230	F6C	CHD-C1D-ND	-2.56	120.32	124.20
14	b	1208	CLA	C3C-C4C-NC	2.56	113.44	110.57
14	b	1224	CLA	C4-C3-C5	2.56	119.58	115.27
15	B	1230	F6C	CHD-C1D-ND	-2.56	120.32	124.20
14	H	1232	CLA	CMD-C2D-C3D	-2.56	121.73	127.61
14	B	1209	CLA	CMD-C2D-C3D	-2.56	121.73	127.61
14	U	1501	CLA	CMC-C2C-C1C	2.56	128.94	125.04
14	b	1213	CLA	CAC-C3C-C4C	2.56	128.13	124.81
14	x	1701	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
14	a	1120	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
14	b	1234	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
18	B	4010	BCR	C28-C27-C26	-2.56	109.51	114.08
14	G	1130	CLA	C4-C3-C5	2.56	119.57	115.27
14	G	1137	CLA	C3C-C4C-NC	2.56	113.44	110.57
18	a	4011	BCR	C37-C22-C21	-2.55	119.34	122.92
14	G	1106	CLA	CMA-C3A-C4A	2.55	118.64	111.77
18	i	4020	BCR	C31-C1-C6	-2.55	106.16	110.30
14	B	1232	CLA	CMD-C2D-C3D	-2.55	121.74	127.61
14	A	1139	CLA	C3D-C4D-ND	2.55	114.37	110.24
14	b	1204	CLA	CAC-C3C-C4C	2.55	128.12	124.81
15	a	1121	F6C	CHB-C4A-NA	2.55	126.80	124.45
14	A	1120	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
14	A	1137	CLA	C3C-C4C-NC	2.55	113.44	110.57
14	B	1232	CLA	C3C-C4C-NC	2.55	113.44	110.57
14	B	1235	CLA	C3C-C4C-NC	2.55	113.44	110.57
14	G	1107	CLA	CMC-C2C-C1C	2.55	128.93	125.04
14	G	1132	CLA	C3D-C4D-ND	2.55	114.37	110.24
14	U	1503	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
14	G	1134	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
18	a	4003	BCR	C37-C22-C21	-2.55	119.35	122.92
18	A	4011	BCR	C37-C22-C21	-2.55	119.35	122.92
14	b	1232	CLA	C3C-C4C-NC	2.55	113.43	110.57
18	a	4011	BCR	C38-C26-C27	2.55	118.52	113.62
14	H	1209	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
14	G	1115	CLA	O1D-CGD-CBD	-2.55	119.27	124.48
14	H	1233	CLA	C3C-C4C-NC	2.55	113.43	110.57
14	H	1219	CLA	CMB-C2B-C3B	2.55	129.45	124.68
14	A	1129	CLA	C3D-C4D-ND	2.55	114.36	110.24
14	L	1503	CLA	CAA-C2A-C3A	-2.55	105.80	112.78
18	A	4002	BCR	C15-C14-C13	-2.55	123.67	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1205	CLA	OBD-CAD-C3D	-2.55	122.39	128.52
14	H	1214	CLA	C4-C3-C5	2.55	119.56	115.27
14	A	1101	CLA	CMC-C2C-C1C	2.55	128.92	125.04
18	G	4011	BCR	C38-C26-C27	2.55	118.51	113.62
14	k	1401	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
14	a	1134	CLA	C3D-C4D-ND	2.55	114.36	110.24
14	T	1401	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
18	A	4003	BCR	C33-C5-C4	2.55	118.51	113.62
14	B	1205	CLA	OBD-CAD-C3D	-2.55	122.39	128.52
14	b	1212	CLA	CMC-C2C-C1C	2.55	128.91	125.04
20	R	5006	LMG	O8-C28-C29	2.54	119.89	111.91
14	b	1214	CLA	OBD-CAD-C3D	-2.54	122.40	128.52
18	H	4010	BCR	C28-C27-C26	-2.54	109.53	114.08
14	H	1212	CLA	CMC-C2C-C1C	2.54	128.91	125.04
14	A	1127	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
14	b	1209	CLA	CMD-C2D-C3D	-2.54	121.76	127.61
15	H	1230	F6C	CHD-C1D-ND	-2.54	120.34	124.20
14	G	1109	CLA	C3D-C4D-ND	2.54	114.35	110.24
18	G	4002	BCR	C7-C8-C9	-2.54	122.39	126.23
14	a	1115	CLA	O1D-CGD-CBD	-2.54	119.28	124.48
14	B	1233	CLA	C3C-C4C-NC	2.54	113.42	110.57
14	b	1225	CLA	CMC-C2C-C1C	2.54	128.91	125.04
14	b	1219	CLA	CMB-C2B-C3B	2.54	129.43	124.68
14	G	1120	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
14	B	1213	CLA	CAC-C3C-C4C	2.54	128.11	124.81
14	A	1116	CLA	C4-C3-C5	2.54	119.54	115.27
14	H	1234	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
14	H	1204	CLA	CAC-C3C-C4C	2.54	128.10	124.81
14	A	1112	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
18	G	4003	BCR	C33-C5-C4	2.54	118.49	113.62
18	H	4016	BCR	C35-C13-C14	-2.54	119.37	122.92
18	a	4003	BCR	C33-C5-C4	2.54	118.49	113.62
14	a	1134	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
14	H	1220	CLA	CED-O2D-CGD	2.54	121.67	115.94
14	A	1106	CLA	C3D-C4D-ND	2.53	114.34	110.24
14	b	1214	CLA	C4-C3-C5	2.53	119.53	115.27
14	k	1401	CLA	C3D-C4D-ND	2.53	114.34	110.24
18	A	4011	BCR	C38-C26-C27	2.53	118.48	113.62
14	B	1225	CLA	CMC-C2C-C1C	2.53	128.90	125.04
14	A	1115	CLA	O1D-CGD-CBD	-2.53	119.30	124.48
14	a	1134	CLA	CMC-C2C-C1C	2.53	128.90	125.04
14	B	1216	CLA	O2D-CGD-O1D	-2.53	118.89	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	l	1503	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
14	a	1107	CLA	CMC-C2C-C1C	2.53	128.90	125.04
14	a	1115	CLA	CBA-CAA-C2A	2.53	121.33	113.86
14	H	1213	CLA	CAC-C3C-C4C	2.53	128.09	124.81
14	B	1214	CLA	OBD-CAD-C3D	-2.53	122.43	128.52
18	B	4005	BCR	C33-C5-C4	2.53	118.48	113.62
18	H	4004	BCR	C27-C26-C25	-2.53	119.06	122.73
14	b	1212	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
14	G	1101	CLA	CMC-C2C-C1C	2.53	128.89	125.04
14	a	1126	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
14	a	1112	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
14	K	1401	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
14	B	1204	CLA	CAC-C3C-C4C	2.53	128.09	124.81
18	H	4005	BCR	C33-C5-C4	2.53	118.47	113.62
14	H	1224	CLA	C4-C3-C5	2.53	119.52	115.27
14	a	1101	CLA	CMC-C2C-C1C	2.53	128.89	125.04
18	A	4002	BCR	C7-C8-C9	-2.53	122.42	126.23
14	G	1105	CLA	CMC-C2C-C1C	2.53	128.89	125.04
14	H	1214	CLA	OBD-CAD-C3D	-2.53	122.44	128.52
18	a	4008	BCR	C28-C27-C26	-2.53	109.57	114.08
14	l	1503	CLA	CMB-C2B-C3B	2.52	129.40	124.68
14	G	1138	CLA	CAC-C3C-C4C	2.52	128.09	124.81
14	A	1138	CLA	CAC-C3C-C4C	2.52	128.09	124.81
14	G	1134	CLA	CMC-C2C-C1C	2.52	128.88	125.04
14	A	1139	CLA	CMD-C2D-C3D	-2.52	121.81	127.61
14	l	1501	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
14	G	1106	CLA	C3D-C4D-ND	2.52	114.32	110.24
14	K	1401	CLA	C3D-C4D-ND	2.52	114.32	110.24
14	a	1139	CLA	CMD-C2D-C3D	-2.52	121.81	127.61
14	G	1116	CLA	C4-C3-C5	2.52	119.51	115.27
14	a	1116	CLA	C4-C3-C5	2.52	119.51	115.27
14	G	1139	CLA	C3D-C4D-ND	2.52	114.32	110.24
21	G	6002	LMT	O5B-C5B-C4B	2.52	114.27	109.69
14	L	1502	CLA	C4-C3-C5	2.52	119.51	115.27
14	b	1220	CLA	CED-O2D-CGD	2.52	121.64	115.94
18	B	4004	BCR	C27-C26-C25	-2.52	119.07	122.73
14	B	1212	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
14	T	1401	CLA	C3D-C4D-ND	2.52	114.31	110.24
18	U	4022	BCR	C35-C13-C12	2.52	122.05	118.08
18	G	4002	BCR	C15-C14-C13	-2.52	123.71	127.31
14	A	1132	CLA	CMD-C2D-C3D	-2.52	121.82	127.61
14	H	1212	CLA	O2D-CGD-O1D	-2.52	118.91	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	6002	LMT	O5B-C5B-C4B	2.52	114.27	109.69
14	G	1139	CLA	CMD-C2D-C3D	-2.52	121.82	127.61
14	G	1127	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
18	b	4005	BCR	C33-C5-C4	2.52	118.45	113.62
14	l	1502	CLA	C4-C3-C5	2.52	119.51	115.27
18	G	4008	BCR	C28-C27-C26	-2.52	109.58	114.08
14	G	1115	CLA	CBA-CAA-C2A	2.52	121.30	113.86
14	A	1105	CLA	CMC-C2C-C1C	2.52	128.87	125.04
14	B	1229	CLA	C4D-C3D-CAD	2.52	111.06	108.10
14	H	1234	CLA	C4-C3-C5	2.52	119.51	115.27
18	b	4004	BCR	C27-C26-C25	-2.52	119.08	122.73
14	a	1124	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
14	B	1210	CLA	C3C-C4C-NC	2.52	113.39	110.57
14	a	1119	CLA	C3D-C4D-ND	2.51	114.31	110.24
14	A	1126	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
14	B	1234	CLA	C4-C3-C5	2.51	119.50	115.27
14	G	1102	CLA	C3C-C4C-NC	2.51	113.39	110.57
14	A	1102	CLA	C3C-C4C-NC	2.51	113.39	110.57
14	B	1212	CLA	CMC-C2C-C1C	2.51	128.87	125.04
14	G	1126	CLA	O1D-CGD-CBD	-2.51	119.34	124.48
15	b	1230	F6C	CMA-C3A-C4A	-2.51	120.29	124.71
18	A	4008	BCR	C28-C27-C26	-2.51	109.59	114.08
14	a	1132	CLA	CMD-C2D-C3D	-2.51	121.84	127.61
14	a	1104	CLA	C4-C3-C5	2.51	119.49	115.27
14	H	1216	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
14	b	1216	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
14	b	1235	CLA	C3C-C4C-NC	2.51	113.38	110.57
14	A	1131	CLA	CMD-C2D-C3D	-2.51	121.84	127.61
18	B	4013	BCR	C33-C5-C4	2.51	118.43	113.62
18	a	4002	BCR	C15-C14-C13	-2.51	123.73	127.31
14	A	1115	CLA	CBA-CAA-C2A	2.51	121.27	113.86
14	G	1106	CLA	CAA-C2A-C1A	-2.51	103.76	111.97
14	U	1502	CLA	C4-C3-C5	2.51	119.49	115.27
14	b	1234	CLA	C4-C3-C5	2.51	119.49	115.27
18	R	4020	BCR	C33-C5-C6	-2.51	121.71	124.53
14	U	1501	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
14	A	1124	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
14	U	1502	CLA	CMB-C2B-C3B	2.51	129.37	124.68
14	A	1114	CLA	CHC-C1C-C2C	-2.51	119.79	126.72
14	A	1116	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
14	A	1129	CLA	CMD-C2D-C3D	-2.51	121.85	127.61
14	a	1117	CLA	CAA-C2A-C1A	-2.51	103.76	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1102	CLA	C3C-C4C-NC	2.51	113.38	110.57
14	L	1501	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
15	G	1121	F6C	CHB-C4A-NA	2.50	126.76	124.45
14	B	1210	CLA	O1D-CGD-CBD	-2.50	119.36	124.48
14	A	1119	CLA	C3D-C4D-ND	2.50	114.29	110.24
14	a	1101	CLA	CMA-C3A-C4A	2.50	118.50	111.77
14	A	1133	CLA	C4D-C3D-CAD	2.50	111.05	108.10
14	G	1117	CLA	CAA-C2A-C1A	-2.50	103.77	111.97
14	b	1219	CLA	C3D-C4D-ND	2.50	114.29	110.24
15	H	1230	F6C	CMA-C3A-C4A	-2.50	120.30	124.71
14	b	1208	CLA	C3D-C4D-ND	2.50	114.29	110.24
14	G	1132	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
14	b	1223	CLA	C6-C5-C3	-2.50	106.89	113.45
14	H	1225	CLA	C3D-C4D-ND	2.50	114.28	110.24
14	H	1224	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
15	A	1121	F6C	CHB-C4A-NA	2.50	126.75	124.45
14	l	1502	CLA	CMB-C2B-C3B	2.50	129.36	124.68
14	H	1235	CLA	C3C-C4C-NC	2.50	113.38	110.57
15	B	1237	F6C	CHA-C1A-C2A	-2.50	123.06	129.84
14	b	1225	CLA	C3D-C4D-ND	2.50	114.28	110.24
14	B	1219	CLA	C3D-C4D-ND	2.50	114.28	110.24
18	A	4002	BCR	C30-C25-C26	-2.50	119.09	122.61
14	B	1224	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
14	H	1208	CLA	C3D-C4D-ND	2.50	114.28	110.24
18	l	4022	BCR	C35-C13-C12	2.50	122.01	118.08
14	L	1502	CLA	CMB-C2B-C3B	2.50	129.35	124.68
14	G	1124	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
14	b	1219	CLA	C3C-C4C-NC	2.50	113.37	110.57
15	b	1238	F6C	C6-C7-C8	-2.50	107.84	115.92
14	U	1503	CLA	CMB-C2B-C3B	2.50	129.35	124.68
14	A	1117	CLA	CAA-C2A-C1A	-2.50	103.79	111.97
14	a	1138	CLA	CAC-C3C-C4C	2.50	128.05	124.81
14	B	1208	CLA	C3D-C4D-ND	2.50	114.28	110.24
14	b	1210	CLA	C3C-C4C-NC	2.50	113.37	110.57
14	a	1131	CLA	CMD-C2D-C3D	-2.50	121.87	127.61
14	G	1131	CLA	CMD-C2D-C3D	-2.50	121.87	127.61
14	H	1201	CLA	O1D-CGD-CBD	-2.50	119.38	124.48
14	H	1225	CLA	CMC-C2C-C1C	2.50	128.84	125.04
14	A	1134	CLA	CMC-C2C-C1C	2.50	128.84	125.04
14	a	1106	CLA	C3D-C4D-ND	2.50	114.28	110.24
14	A	1108	CLA	C3D-C4D-ND	2.50	114.28	110.24
14	b	1233	CLA	C3C-C4C-NC	2.49	113.37	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1224	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
14	a	1106	CLA	CAA-C2A-C1A	-2.49	103.80	111.97
14	A	1106	CLA	CAA-C2A-C1A	-2.49	103.80	111.97
14	A	1113	CLA	CMC-C2C-C1C	2.49	128.84	125.04
14	a	1119	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
21	a	6002	LMT	O5B-C5B-C4B	2.49	114.22	109.69
14	a	1105	CLA	CMC-C2C-C1C	2.49	128.84	125.04
14	H	1231	CLA	C4-C3-C5	2.49	119.47	115.27
18	a	4008	BCR	C23-C24-C25	-2.49	120.20	127.20
18	a	4002	BCR	C7-C8-C9	-2.49	122.47	126.23
14	H	1223	CLA	C6-C5-C3	-2.49	106.92	113.45
14	b	1211	CLA	CMD-C2D-C3D	-2.49	121.88	127.61
14	G	1119	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
14	H	1229	CLA	C4D-C3D-CAD	2.49	111.03	108.10
15	H	1238	F6C	C6-C7-C8	-2.49	107.87	115.92
18	i	4020	BCR	C33-C5-C6	-2.49	121.73	124.53
14	a	1114	CLA	CHC-C1C-C2C	-2.49	119.84	126.72
18	b	4013	BCR	C33-C5-C4	2.49	118.40	113.62
14	G	1129	CLA	CMD-C2D-C3D	-2.49	121.89	127.61
14	G	1114	CLA	CHC-C1C-C2C	-2.49	119.84	126.72
14	L	1503	CLA	CMB-C2B-C3B	2.49	129.33	124.68
14	G	1103	CLA	CAC-C3C-C4C	2.49	128.04	124.81
14	B	1223	CLA	C6-C5-C3	-2.49	106.93	113.45
14	A	1101	CLA	CMA-C3A-C4A	2.49	118.46	111.77
14	G	1119	CLA	C3D-C4D-ND	2.49	114.26	110.24
18	B	4005	BCR	C31-C1-C6	-2.49	106.27	110.30
14	A	1118	CLA	CMB-C2B-C3B	2.49	129.33	124.68
15	B	1238	F6C	C6-C7-C8	-2.49	107.88	115.92
14	G	1104	CLA	C4-C3-C5	2.49	119.45	115.27
14	H	1219	CLA	C3D-C4D-ND	2.49	114.26	110.24
14	G	1126	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
14	H	1223	CLA	CMC-C2C-C1C	2.49	128.82	125.04
14	B	1220	CLA	CED-O2D-CGD	2.49	121.56	115.94
14	G	1101	CLA	CMA-C3A-C4A	2.49	118.45	111.77
18	H	4013	BCR	C33-C5-C4	2.49	118.39	113.62
14	A	1104	CLA	C4-C3-C5	2.49	119.45	115.27
14	B	1201	CLA	CMD-C2D-C3D	-2.49	121.90	127.61
14	A	1106	CLA	O1D-CGD-CBD	-2.49	119.40	124.48
14	G	1116	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
15	A	1121	F6C	O2D-CGD-O1D	-2.48	118.98	123.84
18	I	4020	BCR	C33-C5-C6	-2.48	121.74	124.53
14	A	1140	CLA	C1-C2-C3	-2.48	121.75	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1129	CLA	CMD-C2D-C3D	-2.48	121.90	127.61
14	B	1211	CLA	CMD-C2D-C3D	-2.48	121.90	127.61
14	a	1103	CLA	CAC-C3C-C4C	2.48	128.03	124.81
14	H	1201	CLA	CMD-C2D-C3D	-2.48	121.90	127.61
14	B	1219	CLA	C3C-C4C-NC	2.48	113.35	110.57
18	G	4008	BCR	C23-C24-C25	-2.48	120.23	127.20
15	a	1121	F6C	O2D-CGD-O1D	-2.48	118.99	123.84
14	a	1140	CLA	C1-C2-C3	-2.48	121.75	126.04
14	H	1210	CLA	C3C-C4C-NC	2.48	113.35	110.57
14	G	1120	CLA	C3D-C4D-ND	2.48	114.25	110.24
15	b	1237	F6C	CHA-C1A-C2A	-2.48	123.11	129.84
15	B	1230	F6C	CMA-C3A-C4A	-2.48	120.34	124.71
14	G	1118	CLA	C3D-C4D-ND	2.48	114.25	110.24
14	a	1120	CLA	C3D-C4D-ND	2.48	114.25	110.24
15	a	1121	F6C	CBC-CAC-C3C	-2.48	105.95	112.27
14	b	1223	CLA	CMC-C2C-C1C	2.48	128.81	125.04
14	b	1231	CLA	C4-C3-C5	2.48	119.44	115.27
14	a	1113	CLA	CMC-C2C-C1C	2.48	128.81	125.04
14	a	1140	CLA	CMB-C2B-C3B	2.48	129.31	124.68
18	b	4014	BCR	C19-C18-C17	2.48	122.74	118.94
14	B	1223	CLA	CMC-C2C-C1C	2.48	128.81	125.04
14	G	1106	CLA	O1D-CGD-CBD	-2.48	119.42	124.48
14	a	1133	CLA	C3C-C4C-NC	2.48	113.35	110.57
14	G	1113	CLA	CMC-C2C-C1C	2.48	128.81	125.04
14	G	1103	CLA	C3D-C4D-ND	2.48	114.24	110.24
14	G	1101	CLA	C3C-C4C-NC	2.48	113.35	110.57
15	H	1237	F6C	CHA-C1A-C2A	-2.48	123.13	129.84
14	B	1225	CLA	C3D-C4D-ND	2.47	114.24	110.24
18	G	4002	BCR	C30-C25-C26	-2.47	119.13	122.61
14	b	1229	CLA	CAA-C2A-C1A	-2.47	103.87	111.97
14	b	1022	CLA	CAA-C2A-C3A	-2.47	106.00	112.78
14	A	1119	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
14	G	1111	CLA	C3D-C4D-ND	2.47	114.24	110.24
14	a	1103	CLA	C3D-C4D-ND	2.47	114.24	110.24
18	H	4005	BCR	C31-C1-C6	-2.47	106.29	110.30
14	b	1201	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
14	a	1116	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
14	A	1103	CLA	CAC-C3C-C4C	2.47	128.02	124.81
14	a	1108	CLA	C3D-C4D-ND	2.47	114.24	110.24
14	a	1118	CLA	C1-C2-C3	-2.47	121.77	126.04
14	A	1133	CLA	C3C-C4C-NC	2.47	113.34	110.57
14	a	1118	CLA	C3D-C4D-ND	2.47	114.23	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1106	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
18	H	4014	BCR	C19-C18-C17	2.47	122.73	118.94
14	a	1140	CLA	C3D-C4D-ND	2.47	114.23	110.24
14	A	1120	CLA	C3D-C4D-ND	2.47	114.23	110.24
14	H	1211	CLA	CMD-C2D-C3D	-2.47	121.93	127.61
14	G	1140	CLA	CMB-C2B-C3B	2.47	129.30	124.68
14	A	1140	CLA	CMB-C2B-C3B	2.47	129.30	124.68
14	G	1140	CLA	C1-C2-C3	-2.47	121.77	126.04
14	A	1106	CLA	C4D-C3D-CAD	2.47	111.00	108.10
14	a	1132	CLA	C3C-C4C-NC	2.47	113.34	110.57
18	l	4022	BCR	C36-C18-C17	-2.47	119.47	122.92
14	G	1013	CLA	CMB-C2B-C1B	-2.47	124.67	128.46
18	L	4022	BCR	C35-C13-C12	2.47	121.96	118.08
18	A	4008	BCR	C23-C24-C25	-2.47	120.27	127.20
18	b	4005	BCR	C31-C1-C6	-2.47	106.30	110.30
14	B	1022	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
15	A	1121	F6C	CBC-CAC-C3C	-2.47	105.98	112.27
15	G	1121	F6C	O2D-CGD-O1D	-2.47	119.02	123.84
14	G	1133	CLA	C3D-C4D-ND	2.47	114.23	110.24
14	H	1210	CLA	O1D-CGD-CBD	-2.47	119.44	124.48
18	a	4011	BCR	C35-C13-C12	2.47	121.96	118.08
14	A	1133	CLA	C3D-C4D-ND	2.47	114.23	110.24
14	H	1229	CLA	CAA-C2A-C1A	-2.47	103.90	111.97
14	B	1229	CLA	CAA-C2A-C1A	-2.47	103.90	111.97
18	B	4014	BCR	C19-C18-C17	2.46	122.72	118.94
14	G	1118	CLA	C1-C2-C3	-2.46	121.78	126.04
14	H	1219	CLA	C3C-C4C-NC	2.46	113.33	110.57
14	a	1126	CLA	O1D-CGD-CBD	-2.46	119.44	124.48
14	a	1130	CLA	CMC-C2C-C1C	2.46	128.79	125.04
14	A	1126	CLA	O1D-CGD-CBD	-2.46	119.44	124.48
14	A	1118	CLA	C1-C2-C3	-2.46	121.78	126.04
14	B	1201	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
14	G	1133	CLA	C4D-C3D-CAD	2.46	111.00	108.10
14	G	1118	CLA	CMB-C2B-C3B	2.46	129.28	124.68
14	b	1227	CLA	CMA-C3A-C4A	2.46	118.39	111.77
18	a	4002	BCR	C30-C25-C26	-2.46	119.15	122.61
14	B	1231	CLA	C4-C3-C5	2.46	119.41	115.27
14	G	1129	CLA	CMC-C2C-C1C	2.46	128.79	125.04
14	b	1201	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
14	H	1233	CLA	C4D-C3D-CAD	2.46	111.00	108.10
14	G	1133	CLA	C3C-C4C-NC	2.46	113.33	110.57
14	H	1022	CLA	CAA-C2A-C3A	-2.46	106.04	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1012	CLA	C3D-C4D-ND	2.46	114.22	110.24
14	A	1101	CLA	C3C-C4C-NC	2.46	113.33	110.57
18	A	4011	BCR	C35-C13-C12	2.46	121.95	118.08
18	U	4022	BCR	C36-C18-C17	-2.46	119.48	122.92
14	b	1202	CLA	CAC-C3C-C4C	2.46	128.00	124.81
14	b	1204	CLA	C1-O2A-CGA	2.46	122.89	116.44
14	H	1227	CLA	CMA-C3A-C4A	2.46	118.38	111.77
18	A	4011	BCR	C24-C25-C26	-2.46	115.51	121.46
14	H	1206	CLA	CHC-C1C-C2C	-2.46	119.93	126.72
14	a	1104	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
14	B	1021	CLA	CAA-CBA-CGA	-2.46	106.08	113.25
18	A	4011	BCR	C30-C25-C24	2.46	122.73	115.78
15	G	1121	F6C	CBC-CAC-C3C	-2.46	106.01	112.27
18	a	4011	BCR	C30-C25-C24	2.46	122.72	115.78
18	a	4011	BCR	C24-C25-C26	-2.46	115.52	121.46
14	b	1210	CLA	O1D-CGD-CBD	-2.45	119.46	124.48
14	a	1118	CLA	CMB-C2B-C3B	2.45	129.27	124.68
14	A	1137	CLA	C3D-C4D-ND	2.45	114.21	110.24
18	G	4011	BCR	C30-C25-C24	2.45	122.72	115.78
14	B	1203	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
14	a	1101	CLA	C3C-C4C-NC	2.45	113.32	110.57
14	A	1132	CLA	C3C-C4C-NC	2.45	113.32	110.57
14	A	1104	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
14	A	1118	CLA	C3D-C4D-ND	2.45	114.20	110.24
14	G	1108	CLA	C3D-C4D-ND	2.45	114.20	110.24
14	a	1137	CLA	CAA-CBA-CGA	-2.45	106.09	113.25
18	G	4011	BCR	C35-C13-C12	2.45	121.94	118.08
14	b	1213	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
14	b	1222	CLA	C3D-C4D-ND	2.45	114.20	110.24
18	G	4011	BCR	C24-C25-C26	-2.45	115.53	121.46
14	H	1021	CLA	CAA-CBA-CGA	-2.45	106.10	113.25
21	a	6001	LMT	O5'-C5'-C4'	2.45	114.92	109.75
18	G	4007	BCR	C23-C24-C25	-2.45	120.33	127.20
14	T	1401	CLA	CAC-C3C-C4C	2.45	127.99	124.81
14	H	1204	CLA	C1-O2A-CGA	2.45	122.87	116.44
14	B	1206	CLA	CHC-C1C-C2C	-2.45	119.95	126.72
14	A	1103	CLA	C3D-C4D-ND	2.45	114.20	110.24
14	B	1234	CLA	CMB-C2B-C3B	2.45	129.26	124.68
15	B	1207	F6C	CHD-C1D-ND	-2.45	120.49	124.20
14	a	1013	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
14	G	1132	CLA	C3C-C4C-NC	2.45	113.31	110.57
14	A	1013	CLA	CMB-C2B-C1B	-2.45	124.70	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1021	CLA	CAA-CBA-CGA	-2.45	106.11	113.25
14	G	1137	CLA	CMC-C2C-C1C	2.45	128.76	125.04
14	b	1206	CLA	CHC-C1C-C2C	-2.45	119.96	126.72
14	B	1213	CLA	CMA-C3A-C4A	2.44	118.34	111.77
14	G	1137	CLA	CAA-CBA-CGA	-2.44	106.11	113.25
14	A	1129	CLA	CMC-C2C-C1C	2.44	128.76	125.04
14	B	1227	CLA	CMA-C3A-C4A	2.44	118.34	111.77
14	b	1223	CLA	OBD-CAD-C3D	-2.44	122.64	128.52
14	H	1223	CLA	OBD-CAD-C3D	-2.44	122.64	128.52
14	a	1135	CLA	C3D-C4D-ND	2.44	114.19	110.24
14	B	1204	CLA	C1-O2A-CGA	2.44	122.85	116.44
14	b	1216	CLA	C3C-C4C-NC	2.44	113.31	110.57
14	A	1137	CLA	CMC-C2C-C1C	2.44	128.76	125.04
14	B	1202	CLA	CAC-C3C-C4C	2.44	127.98	124.81
14	G	1132	CLA	CMA-C3A-C4A	2.44	118.33	111.77
15	H	1207	F6C	CHD-C1D-ND	-2.44	120.50	124.20
14	H	1202	CLA	CAC-C3C-C4C	2.44	127.98	124.81
14	A	1103	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
18	M	4021	BCR	C37-C22-C21	-2.44	119.50	122.92
14	b	1205	CLA	O1D-CGD-CBD	-2.44	119.49	124.48
14	G	1104	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
14	k	1401	CLA	CAC-C3C-C4C	2.44	127.98	124.81
14	H	1213	CLA	CMA-C3A-C4A	2.44	118.33	111.77
14	b	1213	CLA	CMA-C3A-C4A	2.44	118.33	111.77
14	T	1401	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
14	b	1204	CLA	C6-C7-C8	-2.44	108.04	115.92
18	A	4007	BCR	C23-C24-C25	-2.44	120.36	127.20
14	b	1227	CLA	CAC-C3C-C4C	2.44	127.97	124.81
14	a	1137	CLA	C3D-C4D-ND	2.44	114.18	110.24
14	a	1133	CLA	C3D-C4D-ND	2.44	114.18	110.24
14	a	1132	CLA	CMA-C3A-C4A	2.44	118.32	111.77
14	A	1132	CLA	CMA-C3A-C4A	2.44	118.32	111.77
14	b	1233	CLA	C4D-C3D-CAD	2.44	110.97	108.10
14	a	1101	CLA	CMB-C2B-C3B	2.44	129.24	124.68
18	A	4002	BCR	C23-C24-C25	-2.44	120.36	127.20
14	H	1216	CLA	C3C-C4C-NC	2.44	113.30	110.57
14	A	1130	CLA	C3C-C4C-NC	2.44	113.30	110.57
14	B	1216	CLA	C3C-C4C-NC	2.44	113.30	110.57
18	G	4002	BCR	C23-C24-C25	-2.43	120.36	127.20
14	H	1203	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
14	A	1137	CLA	CAA-CBA-CGA	-2.43	106.14	113.25
14	B	1201	CLA	C3C-C4C-NC	2.43	113.30	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1204	CLA	C6-C7-C8	-2.43	108.06	115.92
18	a	4002	BCR	C23-C24-C25	-2.43	120.37	127.20
14	G	1108	CLA	C3C-C4C-NC	2.43	113.30	110.57
14	H	1234	CLA	CMB-C2B-C3B	2.43	129.23	124.68
14	G	1140	CLA	C3D-C4D-ND	2.43	114.17	110.24
14	k	1401	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
14	a	1133	CLA	C4D-C3D-CAD	2.43	110.96	108.10
21	G	6001	LMT	O5'-C5'-C4'	2.43	114.88	109.75
14	B	1205	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
14	G	1106	CLA	C4D-C3D-CAD	2.43	110.96	108.10
14	G	1103	CLA	CMD-C2D-C3D	-2.43	122.03	127.61
14	b	1217	CLA	CMA-C3A-C4A	2.43	118.30	111.77
14	K	1401	CLA	CMD-C2D-C3D	-2.43	122.03	127.61
14	G	1130	CLA	C3C-C4C-NC	2.43	113.29	110.57
14	a	1111	CLA	C3D-C4D-ND	2.43	114.17	110.24
14	K	1401	CLA	CAC-C3C-C4C	2.43	127.96	124.81
14	G	1136	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
14	B	1204	CLA	C6-C7-C8	-2.43	108.07	115.92
18	L	4022	BCR	C36-C18-C17	-2.43	119.52	122.92
14	a	1130	CLA	C3C-C4C-NC	2.43	113.29	110.57
14	A	1136	CLA	CAA-C2A-C3A	-2.43	106.14	112.78
18	a	4007	BCR	C23-C24-C25	-2.43	120.39	127.20
14	a	1117	CLA	O1D-CGD-CBD	-2.43	119.52	124.48
14	G	1131	CLA	C3D-C4D-ND	2.42	114.16	110.24
14	G	1117	CLA	O1D-CGD-CBD	-2.42	119.52	124.48
14	G	1130	CLA	CMC-C2C-C1C	2.42	128.73	125.04
15	b	1207	F6C	CHD-C1D-ND	-2.42	120.53	124.20
18	G	4003	BCR	C30-C25-C26	-2.42	119.20	122.61
14	G	1113	CLA	C4D-C3D-CAD	2.42	110.95	108.10
21	A	6001	LMT	O5'-C5'-C4'	2.42	114.86	109.75
14	b	1234	CLA	CMB-C2B-C3B	2.42	129.21	124.68
18	b	4009	BCR	C33-C5-C4	2.42	118.27	113.62
14	A	1140	CLA	C3D-C4D-ND	2.42	114.16	110.24
14	B	1217	CLA	C3D-C4D-ND	2.42	114.16	110.24
14	G	1135	CLA	C3D-C4D-ND	2.42	114.16	110.24
14	b	1204	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
14	H	1217	CLA	C3D-C4D-ND	2.42	114.16	110.24
14	b	1204	CLA	CMC-C2C-C1C	2.42	128.73	125.04
14	A	1135	CLA	C3D-C4D-ND	2.42	114.15	110.24
14	a	1115	CLA	C3D-C4D-ND	2.42	114.15	110.24
14	H	1204	CLA	C4D-C3D-CAD	2.42	110.95	108.10
18	V	4021	BCR	C37-C22-C21	-2.42	119.53	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1221	CLA	C3D-C4D-ND	2.42	114.15	110.24
14	B	1233	CLA	C4D-C3D-CAD	2.42	110.95	108.10
14	H	1205	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
14	B	1213	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
14	H	1204	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
14	A	1130	CLA	CMC-C2C-C1C	2.42	128.72	125.04
14	A	1117	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
14	A	1109	CLA	CMD-C2D-C3D	-2.42	122.06	127.61
14	A	1101	CLA	CMB-C2B-C3B	2.42	129.20	124.68
14	G	1116	CLA	C3D-C4D-ND	2.41	114.14	110.24
14	H	1201	CLA	C3C-C4C-NC	2.41	113.28	110.57
14	G	1116	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
14	G	1012	CLA	C3D-C4D-ND	2.41	114.14	110.24
14	H	1222	CLA	C3D-C4D-ND	2.41	114.14	110.24
14	B	1217	CLA	CMA-C3A-C4A	2.41	118.26	111.77
14	A	1105	CLA	C3C-C4C-NC	2.41	113.28	110.57
14	A	1123	CLA	C1-O2A-CGA	2.41	122.77	116.44
14	b	1203	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
14	H	1213	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
14	a	1103	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
14	B	1204	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
14	a	1136	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
14	a	1129	CLA	CMC-C2C-C1C	2.41	128.71	125.04
14	A	1111	CLA	C3D-C4D-ND	2.41	114.14	110.24
14	G	1101	CLA	CMB-C2B-C3B	2.41	129.19	124.68
14	b	1209	CLA	C4D-C3D-CAD	2.41	110.94	108.10
14	B	1223	CLA	OBD-CAD-C3D	-2.41	122.72	128.52
14	a	1106	CLA	C4D-C3D-CAD	2.41	110.94	108.10
14	b	1217	CLA	C3D-C4D-ND	2.41	114.13	110.24
14	A	1108	CLA	C3C-C4C-NC	2.41	113.27	110.57
14	A	1136	CLA	C3C-C4C-NC	2.41	113.27	110.57
14	B	1203	CLA	C4-C3-C5	2.41	119.32	115.27
14	a	1123	CLA	C4D-C3D-CAD	2.41	110.93	108.10
14	a	1105	CLA	C3C-C4C-NC	2.41	113.27	110.57
14	b	1227	CLA	C3C-C4C-NC	2.41	113.27	110.57
14	H	1201	CLA	C3D-C4D-ND	2.41	114.13	110.24
14	G	1123	CLA	C1-O2A-CGA	2.41	122.76	116.44
14	H	1217	CLA	CMA-C3A-C4A	2.41	118.24	111.77
14	a	1137	CLA	CMC-C2C-C1C	2.41	128.70	125.04
14	B	1222	CLA	C3D-C4D-ND	2.41	114.13	110.24
18	a	4003	BCR	C30-C25-C26	-2.40	119.23	122.61
14	H	1227	CLA	CAC-C3C-C4C	2.40	127.93	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1116	CLA	C3D-C4D-ND	2.40	114.13	110.24
18	b	4016	BCR	C34-C9-C10	-2.40	119.56	122.92
18	m	4021	BCR	C37-C22-C21	-2.40	119.56	122.92
18	A	4003	BCR	C30-C25-C26	-2.40	119.23	122.61
18	G	4002	BCR	C30-C25-C24	2.40	122.58	115.78
14	H	1203	CLA	C4-C3-C5	2.40	119.31	115.27
18	A	4001	BCR	C19-C18-C17	2.40	122.63	118.94
14	G	1137	CLA	C3D-C4D-ND	2.40	114.12	110.24
14	a	1126	CLA	CMC-C2C-C1C	2.40	128.70	125.04
14	A	1139	CLA	CMA-C3A-C4A	2.40	118.23	111.77
14	A	1122	CLA	C3D-C4D-ND	2.40	114.12	110.24
14	a	1123	CLA	C1-O2A-CGA	2.40	122.74	116.44
14	a	1122	CLA	C3D-C4D-ND	2.40	114.12	110.24
14	G	1137	CLA	C5-C3-C4	2.40	119.90	114.60
14	b	1201	CLA	C3D-C4D-ND	2.40	114.12	110.24
14	G	1110	CLA	C4D-C3D-CAD	2.40	110.92	108.10
14	b	1212	CLA	C3D-C4D-ND	2.40	114.12	110.24
14	G	1122	CLA	C3D-C4D-ND	2.40	114.12	110.24
14	A	1117	CLA	CHC-C1C-C2C	-2.40	120.09	126.72
14	b	1221	CLA	C3D-C4D-ND	2.40	114.11	110.24
14	A	1012	CLA	C3D-C4D-ND	2.40	114.11	110.24
14	G	1117	CLA	CHC-C1C-C2C	-2.40	120.09	126.72
18	B	4009	BCR	C33-C5-C4	2.40	118.22	113.62
18	U	4019	BCR	C34-C9-C8	2.40	121.85	118.08
18	L	4019	BCR	C34-C9-C8	2.40	121.85	118.08
14	G	1109	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
18	H	4016	BCR	C34-C9-C10	-2.40	119.57	122.92
14	H	1205	CLA	C4D-C3D-CAD	2.40	110.92	108.10
14	a	1110	CLA	C4D-C3D-CAD	2.40	110.92	108.10
14	A	1116	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
14	A	1116	CLA	CAA-C2A-C3A	-2.39	106.22	112.78
18	A	4002	BCR	C30-C25-C24	2.39	122.55	115.78
14	G	1127	CLA	CMA-C3A-C4A	2.39	118.21	111.77
18	A	4007	BCR	C38-C26-C27	2.39	118.22	113.62
14	H	1221	CLA	C3D-C4D-ND	2.39	114.11	110.24
14	b	1214	CLA	C3D-C4D-ND	2.39	114.11	110.24
14	A	1113	CLA	C4D-C3D-CAD	2.39	110.92	108.10
14	A	1132	CLA	C4D-C3D-CAD	2.39	110.92	108.10
18	b	4016	BCR	C27-C26-C25	-2.39	119.26	122.73
14	a	1116	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
18	H	4016	BCR	C27-C26-C25	-2.39	119.26	122.73
14	a	1109	CLA	CMD-C2D-C3D	-2.39	122.11	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1227	CLA	CAC-C3C-C4C	2.39	127.91	124.81
14	G	1105	CLA	C3C-C4C-NC	2.39	113.25	110.57
14	a	1116	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
14	A	1131	CLA	C3D-C4D-ND	2.39	114.11	110.24
14	b	1022	CLA	CMB-C2B-C3B	2.39	129.15	124.68
14	a	1117	CLA	CHC-C1C-C2C	-2.39	120.11	126.72
14	G	1139	CLA	CMA-C3A-C4A	2.39	118.20	111.77
14	A	1133	CLA	CMD-C2D-C3D	-2.39	122.12	127.61
14	a	1138	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
18	B	4016	BCR	C34-C9-C10	-2.39	119.58	122.92
14	a	1137	CLA	C5-C3-C4	2.39	119.88	114.60
14	G	1115	CLA	C3D-C4D-ND	2.39	114.10	110.24
15	H	1230	F6C	CHA-C1A-C2A	-2.39	123.36	129.84
15	B	1230	F6C	CHA-C1A-C2A	-2.39	123.36	129.84
14	a	1131	CLA	C3D-C4D-ND	2.39	114.10	110.24
14	G	1126	CLA	CMC-C2C-C1C	2.39	128.68	125.04
14	A	1107	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
18	H	4009	BCR	C33-C5-C4	2.39	118.20	113.62
14	A	1110	CLA	C4D-C3D-CAD	2.39	110.91	108.10
14	G	1124	CLA	CMD-C2D-C3D	-2.39	122.12	127.61
14	B	1201	CLA	C3D-C4D-ND	2.39	114.10	110.24
14	A	1105	CLA	CMD-C2D-C3D	-2.39	122.13	127.61
14	B	1212	CLA	C3D-C4D-ND	2.39	114.10	110.24
14	a	1107	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
14	a	1119	CLA	CHB-C4A-NA	2.38	127.81	124.51
18	a	4002	BCR	C30-C25-C24	2.38	122.53	115.78
14	b	1231	CLA	CAC-C3C-C4C	2.38	127.90	124.81
14	a	1113	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
14	a	1127	CLA	CMA-C3A-C4A	2.38	118.18	111.77
14	G	1107	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
18	a	4007	BCR	C38-C26-C27	2.38	118.19	113.62
14	a	1131	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
14	a	1013	CLA	CHB-C4A-NA	2.38	127.81	124.51
14	A	1013	CLA	CHB-C4A-NA	2.38	127.81	124.51
14	a	1134	CLA	CMD-C2D-C3D	-2.38	122.13	127.61
14	H	1212	CLA	C3D-C4D-ND	2.38	114.09	110.24
14	G	1127	CLA	C3D-C4D-ND	2.38	114.09	110.24
14	B	1204	CLA	CMC-C2C-C1C	2.38	128.66	125.04
14	A	1138	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
18	b	4009	BCR	C34-C9-C10	-2.38	119.59	122.92
14	B	1204	CLA	C4D-C3D-CAD	2.38	110.90	108.10
14	G	1105	CLA	CMD-C2D-C3D	-2.38	122.14	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1105	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
14	A	1119	CLA	CHB-C4A-NA	2.38	127.80	124.51
14	G	1132	CLA	C4D-C3D-CAD	2.38	110.90	108.10
14	A	1115	CLA	C3D-C4D-ND	2.38	114.09	110.24
14	b	1203	CLA	C4-C3-C5	2.38	119.27	115.27
14	A	1113	CLA	C3D-C4D-ND	2.38	114.08	110.24
18	B	4016	BCR	C27-C26-C25	-2.38	119.28	122.73
15	b	1230	F6C	CHA-C1A-C2A	-2.38	123.39	129.84
18	H	4009	BCR	C34-C9-C10	-2.38	119.59	122.92
14	A	1105	CLA	CMA-C3A-C4A	2.38	118.16	111.77
14	H	1204	CLA	CMC-C2C-C1C	2.38	128.66	125.04
14	A	1113	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
14	A	1134	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
14	G	1113	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
18	G	4001	BCR	C19-C18-C17	2.38	122.59	118.94
14	B	1228	CLA	C4-C3-C5	2.38	119.27	115.27
14	G	1113	CLA	C3D-C4D-ND	2.38	114.08	110.24
14	a	1113	CLA	C4D-C3D-CAD	2.38	110.90	108.10
14	A	1127	CLA	CMA-C3A-C4A	2.38	118.16	111.77
14	A	1137	CLA	C5-C3-C4	2.38	119.85	114.60
14	G	1104	CLA	C4D-C3D-CAD	2.37	110.89	108.10
18	b	4006	BCR	C15-C14-C13	-2.37	123.92	127.31
14	B	1023	CLA	C3C-C4C-NC	2.37	113.23	110.57
18	a	4007	BCR	C8-C7-C6	-2.37	120.53	127.20
14	a	1130	CLA	C1-O2A-CGA	2.37	122.67	116.44
14	A	1104	CLA	C4D-C3D-CAD	2.37	110.89	108.10
14	B	1209	CLA	C4D-C3D-CAD	2.37	110.89	108.10
18	B	4009	BCR	C36-C18-C17	-2.37	119.60	122.92
14	G	1112	CLA	C3D-C4D-ND	2.37	114.08	110.24
14	H	1209	CLA	C4D-C3D-CAD	2.37	110.89	108.10
14	G	1130	CLA	C1-O2A-CGA	2.37	122.67	116.44
14	a	1139	CLA	CMA-C3A-C4A	2.37	118.15	111.77
14	B	1214	CLA	C3D-C4D-ND	2.37	114.08	110.24
18	A	4007	BCR	C8-C7-C6	-2.37	120.54	127.20
18	B	4006	BCR	C15-C14-C13	-2.37	123.92	127.31
14	a	1124	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
14	a	1133	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
14	G	1134	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
14	b	1228	CLA	C4-C3-C5	2.37	119.26	115.27
14	G	1138	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
14	G	1123	CLA	C4D-C3D-CAD	2.37	110.89	108.10
14	H	1234	CLA	C4C-C3C-C2C	-2.37	103.44	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1218	CLA	C3D-C4D-ND	2.37	114.07	110.24
14	b	1201	CLA	C3C-C4C-NC	2.37	113.23	110.57
14	b	1023	CLA	C3D-C4D-ND	2.37	114.07	110.24
14	A	1130	CLA	C1-O2A-CGA	2.37	122.66	116.44
14	H	1220	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
18	l	4019	BCR	C34-C9-C8	2.37	121.81	118.08
14	G	1107	CLA	C3D-C4D-ND	2.37	114.07	110.24
14	G	1105	CLA	CMA-C3A-C4A	2.37	118.14	111.77
21	G	6001	LMT	O5'-C5'-C6'	2.37	112.32	106.44
14	H	1228	CLA	C4-C3-C5	2.37	119.25	115.27
21	a	6001	LMT	O5'-C5'-C6'	2.37	112.32	106.44
14	H	1239	CLA	C3D-C4D-ND	2.37	114.07	110.24
14	A	1127	CLA	C3D-C4D-ND	2.37	114.06	110.24
18	G	4007	BCR	C38-C26-C27	2.37	118.16	113.62
18	A	4011	BCR	C4-C5-C6	-2.37	119.30	122.73
18	B	4009	BCR	C34-C9-C10	-2.37	119.61	122.92
14	B	1220	CLA	CAA-CBA-CGA	-2.37	106.34	113.25
18	H	4006	BCR	C15-C14-C13	-2.37	123.93	127.31
14	G	1119	CLA	CHB-C4A-NA	2.37	127.78	124.51
14	H	1234	CLA	C3D-C4D-ND	2.36	114.06	110.24
14	A	1109	CLA	C3C-C4C-NC	2.36	113.22	110.57
21	A	6001	LMT	O5'-C5'-C6'	2.36	112.31	106.44
14	G	1133	CLA	CMD-C2D-C3D	-2.36	122.17	127.61
14	b	1204	CLA	C4D-C3D-CAD	2.36	110.88	108.10
14	G	1013	CLA	CHB-C4A-NA	2.36	127.78	124.51
14	A	1107	CLA	C3D-C4D-ND	2.36	114.06	110.24
14	G	1112	CLA	C3C-C4C-NC	2.36	113.22	110.57
18	G	4002	BCR	C33-C5-C4	2.36	118.16	113.62
14	B	1234	CLA	C4C-C3C-C2C	-2.36	103.45	106.90
18	H	4005	BCR	C23-C24-C25	-2.36	120.57	127.20
14	a	1127	CLA	C3D-C4D-ND	2.36	114.06	110.24
18	a	4001	BCR	C33-C5-C6	-2.36	121.88	124.53
14	B	1022	CLA	CMB-C2B-C3B	2.36	129.10	124.68
14	A	1124	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
14	a	1102	CLA	C4-C3-C5	2.36	119.24	115.27
18	a	4001	BCR	C19-C18-C17	2.36	122.56	118.94
18	a	4002	BCR	C33-C5-C4	2.36	118.15	113.62
14	H	1022	CLA	CMB-C2B-C3B	2.36	129.09	124.68
18	G	4007	BCR	C8-C7-C6	-2.36	120.58	127.20
14	a	1108	CLA	C3C-C4C-NC	2.36	113.22	110.57
14	B	1023	CLA	C3D-C4D-ND	2.36	114.05	110.24
18	H	4014	BCR	C35-C13-C12	2.36	121.79	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	1122	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
14	b	1205	CLA	C4D-C3D-CAD	2.36	110.88	108.10
14	G	1116	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
14	H	1239	CLA	C4D-C3D-CAD	2.36	110.88	108.10
14	a	1105	CLA	CMA-C3A-C4A	2.36	118.11	111.77
14	H	1231	CLA	CAC-C3C-C4C	2.36	127.87	124.81
14	H	1023	CLA	C3C-C4C-NC	2.36	113.22	110.57
14	A	1126	CLA	CMC-C2C-C1C	2.36	128.63	125.04
14	A	1123	CLA	C4D-C3D-CAD	2.36	110.87	108.10
14	B	1231	CLA	CAC-C3C-C4C	2.36	127.87	124.81
14	B	1218	CLA	C3D-C4D-ND	2.36	114.05	110.24
14	a	1107	CLA	C3D-C4D-ND	2.36	114.05	110.24
18	B	4014	BCR	C35-C13-C12	2.36	121.79	118.08
14	A	1122	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
14	b	1022	CLA	C4D-C3D-CAD	2.35	110.87	108.10
14	A	1102	CLA	C3D-C4D-ND	2.35	114.05	110.24
14	b	1220	CLA	CAA-CBA-CGA	-2.35	106.37	113.25
14	b	1224	CLA	C3D-C4D-ND	2.35	114.05	110.24
18	b	4009	BCR	C36-C18-C17	-2.35	119.63	122.92
14	A	1102	CLA	C4-C3-C5	2.35	119.23	115.27
14	B	1227	CLA	C3C-C4C-NC	2.35	113.21	110.57
14	b	1234	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
14	G	1120	CLA	C4D-C3D-CAD	2.35	110.87	108.10
18	b	4006	BCR	C33-C5-C4	2.35	118.13	113.62
18	A	4002	BCR	C33-C5-C4	2.35	118.13	113.62
14	a	1113	CLA	C3D-C4D-ND	2.35	114.04	110.24
18	b	4014	BCR	C35-C13-C12	2.35	121.78	118.08
18	R	4018	BCR	C31-C1-C6	-2.35	106.48	110.30
14	b	1229	CLA	C3C-C4C-NC	2.35	113.21	110.57
14	G	1131	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
14	a	1116	CLA	C3D-C4D-ND	2.35	114.04	110.24
14	G	1138	CLA	C3D-C4D-ND	2.35	114.04	110.24
14	a	1102	CLA	C3D-C4D-ND	2.35	114.04	110.24
15	A	1121	F6C	CHA-C1A-C2A	-2.35	123.47	129.84
14	a	1114	CLA	C3D-C4D-ND	2.35	114.04	110.24
14	b	1239	CLA	C4D-C3D-CAD	2.35	110.86	108.10
19	G	5001	LHG	C5-O7-C7	-2.35	112.01	117.79
14	H	1202	CLA	C3D-C4D-ND	2.35	114.04	110.24
14	H	1214	CLA	C3D-C4D-ND	2.35	114.04	110.24
18	b	4017	BCR	C33-C5-C4	2.35	118.13	113.62
14	H	1227	CLA	C3C-C4C-NC	2.35	113.20	110.57
19	A	5001	LHG	C5-O7-C7	-2.35	112.01	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	a	1121	F6C	CHA-C1A-C2A	-2.35	123.47	129.84
18	a	4011	BCR	C4-C5-C6	-2.35	119.32	122.73
18	b	4005	BCR	C23-C24-C25	-2.35	120.61	127.20
18	G	4001	BCR	C33-C5-C6	-2.35	121.89	124.53
14	A	1131	CLA	C4-C3-C5	2.35	119.22	115.27
14	H	1205	CLA	C3D-C4D-ND	2.35	114.03	110.24
14	A	1131	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
14	B	1239	CLA	CAC-C3C-C4C	-2.35	121.77	124.81
18	B	4017	BCR	C33-C5-C4	2.35	118.12	113.62
14	H	1023	CLA	C3D-C4D-ND	2.35	114.03	110.24
19	a	5001	LHG	C5-O7-C7	-2.35	112.02	117.79
18	I	4018	BCR	C31-C1-C6	-2.34	106.50	110.30
18	G	4002	BCR	C8-C7-C6	-2.34	120.62	127.20
14	b	1215	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
14	H	1201	CLA	C4D-C3D-CAD	2.34	110.86	108.10
14	a	1132	CLA	C4D-C3D-CAD	2.34	110.86	108.10
14	G	1136	CLA	C3C-C4C-NC	2.34	113.20	110.57
14	H	1022	CLA	C4D-C3D-CAD	2.34	110.86	108.10
14	a	1109	CLA	C3C-C4C-NC	2.34	113.20	110.57
14	G	1122	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
14	U	1501	CLA	C3D-C4D-ND	2.34	114.03	110.24
14	G	1137	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
14	B	1239	CLA	C4D-C3D-CAD	2.34	110.86	108.10
18	B	4014	BCR	C15-C14-C13	-2.34	123.97	127.31
14	H	1217	CLA	CMB-C2B-C3B	2.34	129.06	124.68
14	B	1205	CLA	C4D-C3D-CAD	2.34	110.86	108.10
14	B	1239	CLA	C3D-C4D-ND	2.34	114.02	110.24
14	a	1137	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
18	H	4017	BCR	C33-C5-C4	2.34	118.11	113.62
15	G	1121	F6C	CHA-C1A-C2A	-2.34	123.49	129.84
14	b	1218	CLA	C3D-C4D-ND	2.34	114.02	110.24
14	A	1138	CLA	C3D-C4D-ND	2.34	114.02	110.24
14	B	1224	CLA	C3D-C4D-ND	2.34	114.02	110.24
14	B	1217	CLA	CMB-C2B-C3B	2.34	129.06	124.68
14	H	1239	CLA	CAC-C3C-C4C	-2.34	121.77	124.81
14	B	1022	CLA	C4D-C3D-CAD	2.34	110.85	108.10
14	B	1202	CLA	C3D-C4D-ND	2.34	114.02	110.24
14	L	1501	CLA	C3D-C4D-ND	2.34	114.02	110.24
18	i	4018	BCR	C31-C1-C6	-2.34	106.51	110.30
14	a	1108	CLA	CMC-C2C-C1C	2.34	128.60	125.04
14	b	1202	CLA	C3D-C4D-ND	2.34	114.02	110.24
14	a	1131	CLA	C4-C3-C5	2.34	119.20	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1107	CLA	CMB-C2B-C3B	2.34	129.05	124.68
14	H	1224	CLA	C3D-C4D-ND	2.34	114.02	110.24
14	A	1120	CLA	C4D-C3D-CAD	2.34	110.85	108.10
18	B	4006	BCR	C33-C5-C4	2.34	118.10	113.62
14	B	1215	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
14	A	1132	CLA	CMC-C2C-C1C	2.34	128.59	125.04
14	A	1107	CLA	CMB-C2B-C3B	2.33	129.05	124.68
14	H	1206	CLA	C3C-C4C-NC	2.33	113.19	110.57
14	G	1132	CLA	CMC-C2C-C1C	2.33	128.59	125.04
18	G	4011	BCR	C4-C5-C6	-2.33	119.34	122.73
14	B	1221	CLA	CMC-C2C-C1C	2.33	128.59	125.04
14	b	1234	CLA	C3D-C4D-ND	2.33	114.01	110.24
14	l	1501	CLA	C3D-C4D-ND	2.33	114.01	110.24
18	B	4005	BCR	C23-C24-C25	-2.33	120.65	127.20
14	A	1137	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
14	a	1107	CLA	CMB-C2B-C3B	2.33	129.04	124.68
14	H	1215	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
18	G	4007	BCR	C29-C30-C25	-2.33	106.89	110.48
14	b	1023	CLA	C3C-C4C-NC	2.33	113.19	110.57
14	G	1131	CLA	C4-C3-C5	2.33	119.19	115.27
14	G	1109	CLA	C3C-C4C-NC	2.33	113.19	110.57
14	G	1139	CLA	CMB-C2B-C3B	2.33	129.04	124.68
18	H	4006	BCR	C33-C5-C4	2.33	118.09	113.62
14	a	1138	CLA	C3D-C4D-ND	2.33	114.01	110.24
14	a	1139	CLA	CMB-C2B-C3B	2.33	129.04	124.68
14	G	1102	CLA	C4-C3-C5	2.33	119.19	115.27
18	H	4017	BCR	C23-C24-C25	-2.33	120.66	127.20
14	a	1115	CLA	C4D-C3D-CAD	2.33	110.84	108.10
14	b	1239	CLA	C3D-C4D-ND	2.33	114.00	110.24
14	A	1112	CLA	C3D-C4D-ND	2.33	114.00	110.24
14	a	1120	CLA	C4D-C3D-CAD	2.33	110.84	108.10
14	G	1102	CLA	C3D-C4D-ND	2.33	114.00	110.24
18	b	4017	BCR	C36-C18-C17	-2.33	119.66	122.92
14	a	1136	CLA	C3C-C4C-NC	2.33	113.18	110.57
14	b	1239	CLA	CAC-C3C-C4C	-2.33	121.79	124.81
14	B	1234	CLA	C3D-C4D-ND	2.33	114.00	110.24
14	a	1134	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
18	b	4004	BCR	C33-C5-C4	2.33	118.08	113.62
18	b	4017	BCR	C23-C24-C25	-2.33	120.67	127.20
14	a	1130	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
18	H	4009	BCR	C36-C18-C17	-2.32	119.67	122.92
14	b	1215	CLA	C3D-C4D-ND	2.32	114.00	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1214	CLA	C4D-C3D-CAD	2.32	110.83	108.10
18	H	4004	BCR	C33-C5-C4	2.32	118.08	113.62
18	a	4007	BCR	C29-C30-C25	-2.32	106.90	110.48
14	b	1215	CLA	C1-O2A-CGA	2.32	122.54	116.44
14	G	1114	CLA	C3D-C4D-ND	2.32	114.00	110.24
18	B	4017	BCR	C23-C24-C25	-2.32	120.68	127.20
14	H	1215	CLA	C1-O2A-CGA	2.32	122.54	116.44
14	B	1229	CLA	C3C-C4C-NC	2.32	113.18	110.57
18	a	4002	BCR	C8-C7-C6	-2.32	120.68	127.20
14	b	1217	CLA	CMB-C2B-C3B	2.32	129.02	124.68
14	H	1228	CLA	CHC-C1C-C2C	-2.32	120.30	126.72
14	G	1108	CLA	CMC-C2C-C1C	2.32	128.57	125.04
14	H	1221	CLA	CMC-C2C-C1C	2.32	128.57	125.04
14	H	1213	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
14	b	1232	CLA	C3D-C4D-ND	2.32	113.99	110.24
14	G	1124	CLA	C3C-C4C-NC	2.32	113.17	110.57
14	H	1228	CLA	C3C-C4C-NC	2.32	113.17	110.57
14	b	1205	CLA	C3D-C4D-ND	2.32	113.99	110.24
14	b	1228	CLA	CHC-C1C-C2C	-2.32	120.31	126.72
14	a	1140	CLA	C4D-C3D-CAD	2.32	110.83	108.10
14	G	1136	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
14	G	1130	CLA	CMD-C2D-C3D	-2.32	122.29	127.61
14	B	1228	CLA	CHC-C1C-C2C	-2.32	120.32	126.72
14	b	1206	CLA	C3D-C4D-ND	2.31	113.98	110.24
14	b	1201	CLA	C4D-C3D-CAD	2.31	110.82	108.10
14	a	1136	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
14	B	1215	CLA	C1-O2A-CGA	2.31	122.51	116.44
18	H	4014	BCR	C15-C14-C13	-2.31	124.01	127.31
18	B	4017	BCR	C36-C18-C17	-2.31	119.68	122.92
15	H	1238	F6C	O2D-CGD-O1D	-2.31	119.32	123.84
18	B	4004	BCR	C33-C5-C4	2.31	118.06	113.62
14	H	1214	CLA	C6-C5-C3	-2.31	107.39	113.45
14	A	1134	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
14	B	1211	CLA	C3C-C4C-NC	2.31	113.16	110.57
14	B	1213	CLA	C4D-C3D-CAD	2.31	110.82	108.10
14	G	1102	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
14	a	1102	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
14	b	1233	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
18	A	4001	BCR	C33-C5-C6	-2.31	121.93	124.53
14	H	1233	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
14	B	1213	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
20	B	5002	LMG	O7-C10-O9	-2.31	118.12	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	4002	BCR	C8-C7-C6	-2.31	120.71	127.20
14	A	1114	CLA	C3D-C4D-ND	2.31	113.97	110.24
14	H	1229	CLA	C3C-C4C-NC	2.31	113.16	110.57
20	b	5002	LMG	O7-C10-O9	-2.31	118.12	123.70
14	A	1104	CLA	CMC-C2C-C1C	2.31	128.56	125.04
14	H	1226	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
14	b	1226	CLA	CHC-C1C-C2C	-2.31	120.33	126.72
14	a	1112	CLA	C3D-C4D-ND	2.31	113.97	110.24
14	a	1104	CLA	C4D-C3D-CAD	2.31	110.82	108.10
14	H	1206	CLA	C3D-C4D-ND	2.31	113.97	110.24
14	A	1136	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
14	A	1108	CLA	CMC-C2C-C1C	2.31	128.55	125.04
14	A	1102	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
14	G	1134	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
14	b	1213	CLA	C4D-C3D-CAD	2.31	110.82	108.10
14	a	1132	CLA	CMC-C2C-C1C	2.31	128.55	125.04
14	A	1115	CLA	C4D-C3D-CAD	2.31	110.81	108.10
14	B	1205	CLA	C3D-C4D-ND	2.31	113.97	110.24
14	b	1228	CLA	C3C-C4C-NC	2.30	113.16	110.57
14	b	1214	CLA	C6-C5-C3	-2.30	107.41	113.45
14	G	1012	CLA	C11-C12-C13	-2.30	108.47	115.92
14	A	1012	CLA	C11-C12-C13	-2.30	108.47	115.92
14	H	1211	CLA	C3C-C4C-NC	2.30	113.15	110.57
14	B	1209	CLA	C3C-C4C-NC	2.30	113.15	110.57
14	A	1107	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
14	b	1206	CLA	C3C-C4C-NC	2.30	113.15	110.57
14	B	1233	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
14	B	1214	CLA	C6-C5-C3	-2.30	107.42	113.45
14	B	1232	CLA	C3D-C4D-ND	2.30	113.96	110.24
14	H	1021	CLA	CHD-C4C-C3C	-2.30	121.46	124.84
14	a	1012	CLA	C11-C12-C13	-2.30	108.48	115.92
14	A	1116	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
14	G	1103	CLA	C3C-C4C-NC	2.30	113.15	110.57
14	a	1112	CLA	C3C-C4C-NC	2.30	113.15	110.57
14	A	1108	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
14	G	1108	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
14	A	1139	CLA	CMB-C2B-C3B	2.30	128.98	124.68
14	a	1104	CLA	CMC-C2C-C1C	2.30	128.54	125.04
14	B	1228	CLA	C3C-C4C-NC	2.30	113.15	110.57
18	A	4007	BCR	C29-C30-C25	-2.30	106.94	110.48
14	H	1214	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
14	A	1130	CLA	CMD-C2D-C3D	-2.30	122.33	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1125	CLA	C4D-C3D-CAD	2.30	110.81	108.10
14	a	1107	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
14	b	1231	CLA	C4D-C3D-CAD	2.30	110.80	108.10
14	B	1215	CLA	C3D-C4D-ND	2.30	113.95	110.24
14	b	1213	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
14	B	1210	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
14	b	1209	CLA	CAA-CBA-CGA	-2.30	106.41	112.51
14	B	1209	CLA	CAA-CBA-CGA	-2.30	106.41	112.51
14	B	1022	CLA	C3D-C4D-ND	2.30	113.95	110.24
14	a	1123	CLA	C3D-C4D-ND	2.30	113.95	110.24
14	G	1126	CLA	C4D-C3D-CAD	2.30	110.80	108.10
14	G	1109	CLA	C1-O2A-CGA	2.29	122.46	116.44
14	a	1116	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
14	B	1206	CLA	C3D-C4D-ND	2.29	113.95	110.24
14	B	1206	CLA	C3C-C4C-NC	2.29	113.14	110.57
18	U	4022	BCR	C28-C27-C26	-2.29	109.98	114.08
14	B	1021	CLA	CHD-C4C-C3C	-2.29	121.47	124.84
14	A	1140	CLA	C4D-C3D-CAD	2.29	110.80	108.10
14	B	1201	CLA	C4D-C3D-CAD	2.29	110.80	108.10
14	H	1215	CLA	C3D-C4D-ND	2.29	113.95	110.24
14	b	1022	CLA	C3D-C4D-ND	2.29	113.95	110.24
18	a	4011	BCR	C8-C9-C10	2.29	122.46	118.94
14	a	1112	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
18	R	4018	BCR	C2-C1-C6	2.29	114.01	110.48
14	b	1209	CLA	C3C-C4C-NC	2.29	113.14	110.57
18	A	4011	BCR	C8-C9-C10	2.29	122.46	118.94
14	B	1226	CLA	CHC-C1C-C2C	-2.29	120.39	126.72
18	H	4017	BCR	C36-C18-C17	-2.29	119.72	122.92
14	a	1124	CLA	C3C-C4C-NC	2.29	113.14	110.57
14	G	1116	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
14	G	1123	CLA	C3D-C4D-ND	2.29	113.94	110.24
14	A	1122	CLA	CMA-C3A-C4A	2.29	117.93	111.77
14	a	1118	CLA	OBD-CAD-C3D	-2.29	123.01	128.52
18	b	4014	BCR	C15-C14-C13	-2.29	124.04	127.31
14	H	1209	CLA	CAA-CBA-CGA	-2.29	106.43	112.51
14	G	1122	CLA	CMA-C3A-C4A	2.29	117.92	111.77
14	G	1128	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
14	b	1211	CLA	C3C-C4C-NC	2.29	113.14	110.57
14	b	1221	CLA	CMC-C2C-C1C	2.29	128.52	125.04
18	l	4022	BCR	C38-C26-C25	-2.29	121.96	124.53
14	a	1109	CLA	C1-O2A-CGA	2.29	122.44	116.44
14	b	1021	CLA	CHD-C4C-C3C	-2.29	121.48	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1210	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
14	b	1214	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
14	G	1140	CLA	C4D-C3D-CAD	2.29	110.79	108.10
18	I	4018	BCR	C2-C1-C6	2.29	114.00	110.48
14	A	1118	CLA	OBD-CAD-C3D	-2.29	123.02	128.52
14	B	1239	CLA	C11-C10-C8	-2.29	108.53	115.92
18	b	4006	BCR	C38-C26-C27	2.29	118.01	113.62
14	H	1209	CLA	C3C-C4C-NC	2.29	113.14	110.57
14	b	1226	CLA	C3C-C4C-NC	2.29	113.14	110.57
14	G	1123	CLA	CAC-C3C-C4C	2.29	127.78	124.81
14	G	1109	CLA	CMC-C2C-C1C	2.29	128.52	125.04
14	G	1115	CLA	C4D-C3D-CAD	2.29	110.79	108.10
14	H	1213	CLA	C4D-C3D-CAD	2.29	110.79	108.10
14	a	1126	CLA	C4D-C3D-CAD	2.29	110.79	108.10
14	a	1109	CLA	CMC-C2C-C1C	2.28	128.52	125.04
14	G	1135	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
18	H	4013	BCR	C38-C26-C27	2.28	118.00	113.62
18	a	4007	BCR	C33-C5-C4	2.28	118.00	113.62
14	B	1214	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
14	b	1236	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
14	H	1214	CLA	C4D-C3D-CAD	2.28	110.79	108.10
14	b	1225	CLA	CMB-C2B-C1B	-2.28	124.95	128.46
14	A	1123	CLA	C3D-C4D-ND	2.28	113.93	110.24
14	x	1701	CLA	C4D-C3D-CAD	2.28	110.79	108.10
14	A	1123	CLA	CAC-C3C-C4C	2.28	127.77	124.81
14	A	1132	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
14	A	1112	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
14	H	1231	CLA	C4D-C3D-CAD	2.28	110.78	108.10
14	A	1128	CLA	CHC-C1C-C2C	-2.28	120.41	126.72
14	H	1022	CLA	C3D-C4D-ND	2.28	113.93	110.24
14	G	1107	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
14	a	1124	CLA	CMA-C3A-C4A	2.28	117.90	111.77
14	A	1135	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
14	H	1226	CLA	C3D-C4D-ND	2.28	113.92	110.24
14	B	1228	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
14	a	1133	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
14	B	1236	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
14	b	1228	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
14	A	1124	CLA	C3C-C4C-NC	2.28	113.13	110.57
14	G	1128	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
14	a	1122	CLA	CMA-C3A-C4A	2.28	117.90	111.77
14	A	1109	CLA	C1-O2A-CGA	2.28	122.42	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1222	CLA	C4C-C3C-C2C	-2.28	103.58	106.90
20	H	5002	LMG	O7-C10-O9	-2.28	118.20	123.70
14	H	1210	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
18	L	4022	BCR	C28-C27-C26	-2.28	110.01	114.08
15	b	1238	F6C	O2D-CGD-O1D	-2.28	119.39	123.84
14	G	1117	CLA	CAC-C3C-C4C	2.28	127.76	124.81
14	A	1128	CLA	CAA-C2A-C3A	-2.28	106.55	112.78
14	W	1701	CLA	CMA-C3A-C4A	2.27	117.89	111.77
14	b	1229	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
14	W	1701	CLA	C4D-C3D-CAD	2.27	110.78	108.10
14	A	1124	CLA	CMA-C3A-C4A	2.27	117.88	111.77
18	i	4018	BCR	C2-C1-C6	2.27	113.98	110.48
14	H	1232	CLA	C3D-C4D-ND	2.27	113.92	110.24
14	B	1223	CLA	C4D-C3D-CAD	2.27	110.78	108.10
14	a	1108	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
14	H	1236	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
14	B	1231	CLA	C4D-C3D-CAD	2.27	110.77	108.10
14	G	1112	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
14	H	1239	CLA	C11-C10-C8	-2.27	108.58	115.92
14	a	1123	CLA	CAC-C3C-C4C	2.27	127.76	124.81
14	b	1214	CLA	C4D-C3D-CAD	2.27	110.77	108.10
18	B	4006	BCR	C38-C26-C27	2.27	117.98	113.62
14	G	1124	CLA	CMA-C3A-C4A	2.27	117.88	111.77
14	H	1213	CLA	C3D-C4D-ND	2.27	113.91	110.24
14	a	1118	CLA	C1-O2A-CGA	2.27	122.40	116.44
14	B	1229	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
14	B	1226	CLA	C3D-C4D-ND	2.27	113.91	110.24
16	G	2001	PQN	C21-C22-C23	-2.27	108.58	115.92
14	a	1135	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
14	G	1118	CLA	C1-O2A-CGA	2.27	122.40	116.44
14	X	1701	CLA	C4D-C3D-CAD	2.27	110.77	108.10
14	G	1122	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
14	H	1226	CLA	C3C-C4C-NC	2.27	113.11	110.57
14	b	1239	CLA	C11-C10-C8	-2.27	108.59	115.92
14	b	1222	CLA	C4C-C3C-C2C	-2.27	103.59	106.90
14	H	1228	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
18	G	4011	BCR	C8-C9-C10	2.27	122.42	118.94
14	G	1122	CLA	C3C-C4C-NC	2.27	113.11	110.57
14	A	1122	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
14	G	1118	CLA	OBD-CAD-C3D	-2.27	123.06	128.52
14	G	1101	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
14	A	1109	CLA	CMC-C2C-C1C	2.27	128.49	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	x	1701	CLA	CMA-C3A-C4A	2.27	117.86	111.77
14	a	1128	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
18	G	4007	BCR	C33-C5-C4	2.27	117.97	113.62
16	a	2001	PQN	C21-C22-C23	-2.27	108.60	115.92
16	A	2001	PQN	C21-C22-C23	-2.26	108.60	115.92
14	A	1112	CLA	C3C-C4C-NC	2.26	113.11	110.57
14	G	1104	CLA	CMC-C2C-C1C	2.26	128.49	125.04
18	B	4013	BCR	C38-C26-C27	2.26	117.96	113.62
15	B	1238	F6C	O2D-CGD-O1D	-2.26	119.41	123.84
14	G	1119	CLA	C4C-C3C-C2C	-2.26	103.60	106.90
14	A	1117	CLA	CAC-C3C-C4C	2.26	127.75	124.81
18	L	4022	BCR	C38-C26-C25	-2.26	121.99	124.53
14	a	1128	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
18	B	4004	BCR	C28-C27-C26	-2.26	110.04	114.08
14	A	1122	CLA	C3C-C4C-NC	2.26	113.11	110.57
14	a	1122	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
15	H	1238	F6C	CMC-C2C-C3C	2.26	129.20	124.94
14	b	1214	CLA	CAC-C3C-C4C	2.26	127.74	124.81
18	l	4022	BCR	C28-C27-C26	-2.26	110.04	114.08
14	B	1213	CLA	C3D-C4D-ND	2.26	113.89	110.24
18	A	4007	BCR	C33-C5-C4	2.26	117.96	113.62
14	G	1133	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
18	b	4005	BCR	C36-C18-C17	-2.26	119.76	122.92
14	A	1133	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
14	H	1222	CLA	C4C-C3C-C2C	-2.26	103.61	106.90
18	b	4014	BCR	C39-C30-C25	-2.26	106.64	110.30
18	b	4004	BCR	C28-C27-C26	-2.26	110.05	114.08
14	H	1225	CLA	CMB-C2B-C1B	-2.26	125.00	128.46
14	A	1101	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
18	b	4013	BCR	C38-C26-C27	2.26	117.95	113.62
14	a	1132	CLA	O1D-CGD-CBD	-2.26	119.87	124.48
14	a	1103	CLA	C3C-C4C-NC	2.26	113.10	110.57
14	b	1220	CLA	CHC-C1C-C2C	-2.26	120.48	126.72
14	H	1229	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
14	b	1226	CLA	C3D-C4D-ND	2.26	113.89	110.24
14	b	1223	CLA	C4D-C3D-CAD	2.26	110.75	108.10
14	A	1118	CLA	C1-O2A-CGA	2.25	122.36	116.44
14	H	1227	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
18	a	4003	BCR	C15-C14-C13	-2.25	124.09	127.31
14	b	1213	CLA	C3D-C4D-ND	2.25	113.88	110.24
18	G	4003	BCR	C15-C14-C13	-2.25	124.09	127.31
14	A	1126	CLA	C4D-C3D-CAD	2.25	110.75	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	V	4021	BCR	C38-C26-C25	-2.25	122.00	124.53
14	a	1101	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
14	X	1701	CLA	CMA-C3A-C4A	2.25	117.82	111.77
18	B	4005	BCR	C36-C18-C17	-2.25	119.77	122.92
14	A	1112	CLA	CAA-CBA-CGA	-2.25	106.68	113.25
18	B	4014	BCR	C39-C30-C25	-2.25	106.65	110.30
18	H	4014	BCR	C39-C30-C25	-2.25	106.65	110.30
14	a	1119	CLA	C4C-C3C-C2C	-2.25	103.62	106.90
14	a	1115	CLA	CAC-C3C-C4C	2.25	127.73	124.81
14	H	1220	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
18	U	4022	BCR	C38-C26-C25	-2.25	122.00	124.53
14	A	1119	CLA	C4C-C3C-C2C	-2.25	103.62	106.90
14	G	1132	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
14	A	1110	CLA	CMA-C3A-C4A	2.25	117.81	111.77
14	a	1116	CLA	CHD-C4C-C3C	-2.25	121.54	124.84
15	b	1238	F6C	CMC-C2C-C3C	2.25	129.18	124.94
14	H	1223	CLA	C4D-C3D-CAD	2.25	110.74	108.10
14	A	1118	CLA	CAC-C3C-C4C	2.25	127.72	124.81
14	G	1119	CLA	C3B-C4B-NB	2.25	112.11	109.21
14	G	1118	CLA	CAC-C3C-C4C	2.25	127.72	124.81
14	A	1119	CLA	C3B-C4B-NB	2.25	112.11	109.21
14	B	1225	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
14	b	1214	CLA	C3C-C4C-NC	2.25	113.09	110.57
14	a	1125	CLA	C4D-C3D-CAD	2.24	110.74	108.10
14	G	1110	CLA	CMA-C3A-C4A	2.24	117.80	111.77
14	G	1111	CLA	C4D-C3D-CAD	2.24	110.74	108.10
14	B	1227	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
14	a	1135	CLA	CMC-C2C-C1C	2.24	128.46	125.04
18	A	4001	BCR	C2-C1-C6	2.24	113.93	110.48
14	G	1115	CLA	CAC-C3C-C4C	2.24	127.72	124.81
14	a	1129	CLA	CMA-C3A-C4A	2.24	117.80	111.77
14	b	1227	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
14	a	1117	CLA	CAC-C3C-C4C	2.24	127.72	124.81
14	B	1209	CLA	CMA-C3A-C4A	2.24	117.80	111.77
14	A	1114	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
18	H	4004	BCR	C28-C27-C26	-2.24	110.08	114.08
14	A	1115	CLA	CAC-C3C-C4C	2.24	127.72	124.81
14	A	1135	CLA	CMC-C2C-C1C	2.24	128.45	125.04
18	H	4006	BCR	C38-C26-C27	2.24	117.92	113.62
15	H	1237	F6C	CAA-CBA-CGA	-2.24	106.92	113.43
14	G	1112	CLA	CAA-CBA-CGA	-2.24	106.71	113.25
14	A	1136	CLA	CMC-C2C-C1C	2.24	128.45	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1129	CLA	CMA-C3A-C4A	2.24	117.79	111.77
14	a	1118	CLA	CAC-C3C-C4C	2.24	127.72	124.81
18	G	4001	BCR	C2-C1-C6	2.24	113.93	110.48
18	L	4019	BCR	C30-C25-C26	-2.24	119.46	122.61
14	G	1129	CLA	CMA-C3A-C4A	2.24	117.79	111.77
15	B	1238	F6C	CMC-C2C-C3C	2.24	129.16	124.94
14	G	1107	CLA	C4D-C3D-CAD	2.24	110.73	108.10
14	a	1115	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
14	A	1116	CLA	CHD-C4C-C3C	-2.24	121.55	124.84
14	A	1140	CLA	CMA-C3A-C4A	2.24	117.78	111.77
14	G	1106	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
14	H	1239	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
14	B	1220	CLA	CHC-C1C-C2C	-2.24	120.54	126.72
14	k	1401	CLA	C4D-C3D-CAD	2.24	110.73	108.10
18	U	4019	BCR	C30-C25-C26	-2.24	119.47	122.61
18	l	4019	BCR	C30-C25-C26	-2.24	119.47	122.61
14	A	1115	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
14	H	1215	CLA	CMB-C2B-C3B	2.24	128.86	124.68
14	b	1206	CLA	CAA-C2A-C3A	-2.24	106.66	112.78
14	a	1130	CLA	C3D-C4D-ND	2.23	113.85	110.24
15	B	1237	F6C	CAA-CBA-CGA	-2.23	106.94	113.43
18	U	4019	BCR	C34-C9-C10	-2.23	119.80	122.92
14	H	1224	CLA	CHD-C4C-C3C	-2.23	121.56	124.84
13	G	1011	CL0	C3C-C4C-NC	2.23	113.08	110.57
14	a	1117	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
14	L	1502	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
14	A	1125	CLA	C4D-C3D-CAD	2.23	110.73	108.10
14	G	1135	CLA	CMC-C2C-C1C	2.23	128.44	125.04
14	a	1136	CLA	CMC-C2C-C1C	2.23	128.44	125.04
14	B	1214	CLA	C3C-C4C-NC	2.23	113.07	110.57
14	G	1115	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
15	b	1237	F6C	CAA-CBA-CGA	-2.23	106.94	113.43
18	H	4005	BCR	C36-C18-C17	-2.23	119.80	122.92
18	a	4001	BCR	C2-C1-C6	2.23	113.92	110.48
14	H	1222	CLA	CAC-C3C-C4C	2.23	127.70	124.81
14	a	1112	CLA	CAA-CBA-CGA	-2.23	106.74	113.25
14	b	1239	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
14	a	1122	CLA	C3C-C4C-NC	2.23	113.07	110.57
14	a	1106	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
18	M	4021	BCR	C38-C26-C25	-2.23	122.03	124.53
14	B	1215	CLA	CMB-C2B-C3B	2.23	128.84	124.68
14	A	1117	CLA	CMD-C2D-C3D	-2.23	122.49	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	4019	BCR	C40-C30-C25	2.23	113.91	110.30
14	b	1209	CLA	CMA-C3A-C4A	2.23	117.76	111.77
14	G	1116	CLA	CHD-C4C-C3C	-2.23	121.57	124.84
14	b	1222	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
14	G	1103	CLA	CHC-C1C-C2C	-2.23	120.56	126.72
14	a	1103	CLA	CHC-C1C-C2C	-2.23	120.56	126.72
14	b	1022	CLA	C4C-C3C-C2C	-2.23	103.65	106.90
14	a	1140	CLA	CMA-C3A-C4A	2.23	117.75	111.77
14	a	1119	CLA	C3B-C4B-NB	2.23	112.09	109.21
14	G	1117	CLA	CMD-C2D-C3D	-2.23	122.50	127.61
14	G	1114	CLA	O1D-CGD-CBD	-2.22	119.93	124.48
14	b	1216	CLA	O1D-CGD-CBD	-2.22	119.93	124.48
14	H	1206	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
18	L	4019	BCR	C34-C9-C10	-2.22	119.81	122.92
14	B	1214	CLA	CAC-C3C-C4C	2.22	127.69	124.81
18	A	4003	BCR	C15-C14-C13	-2.22	124.14	127.31
14	G	1117	CLA	C3B-C4B-NB	2.22	112.08	109.21
15	H	1230	F6C	CMA-C3A-C2A	-2.22	120.08	126.12
14	b	1210	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
14	b	1215	CLA	CMB-C2B-C3B	2.22	128.84	124.68
14	a	1114	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
14	b	1224	CLA	CHD-C4C-C3C	-2.22	121.58	124.84
14	A	1107	CLA	C4D-C3D-CAD	2.22	110.71	108.10
14	A	1103	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
14	b	1206	CLA	CMC-C2C-C3C	2.22	132.15	126.12
14	a	1110	CLA	CMA-C3A-C4A	2.22	117.74	111.77
14	a	1107	CLA	C4D-C3D-CAD	2.22	110.71	108.10
14	H	1216	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
14	a	1110	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
14	W	1701	CLA	C3D-C4D-ND	2.22	113.83	110.24
14	G	1136	CLA	CMC-C2C-C1C	2.22	128.42	125.04
14	G	1124	CLA	C4D-C3D-CAD	2.22	110.71	108.10
18	B	4016	BCR	C8-C7-C6	-2.22	120.97	127.20
14	A	1103	CLA	C3C-C4C-NC	2.22	113.06	110.57
18	A	4011	BCR	C15-C14-C13	-2.22	124.14	127.31
14	B	1239	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
14	B	1210	CLA	C4C-C3C-C2C	-2.22	103.67	106.90
14	A	1106	CLA	CAA-C2A-C3A	-2.22	106.71	112.78
14	G	1140	CLA	CMA-C3A-C4A	2.22	117.73	111.77
14	U	1503	CLA	CMA-C3A-C4A	2.22	117.73	111.77
14	G	1130	CLA	C3D-C4D-ND	2.22	113.82	110.24
14	B	1226	CLA	C3C-C4C-NC	2.22	113.06	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	4016	BCR	C8-C7-C6	-2.22	120.98	127.20
14	l	1503	CLA	CMA-C3A-C4A	2.22	117.73	111.77
14	H	1209	CLA	CMA-C3A-C4A	2.21	117.72	111.77
14	A	1139	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
14	B	1224	CLA	CHD-C4C-C3C	-2.21	121.59	124.84
14	a	1138	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
14	a	1114	CLA	CAC-C3C-C4C	2.21	127.68	124.81
14	G	1110	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
14	a	1125	CLA	CHD-C4C-C3C	-2.21	121.59	124.84
14	L	1503	CLA	CMA-C3A-C4A	2.21	117.72	111.77
14	B	1023	CLA	CMC-C2C-C3C	2.21	132.12	126.12
14	a	1125	CLA	C1D-CHD-C4C	-2.21	121.29	126.06
13	A	1011	CL0	C3C-C4C-NC	2.21	113.05	110.57
14	B	1222	CLA	CAC-C3C-C4C	2.21	127.68	124.81
18	m	4021	BCR	C38-C26-C25	-2.21	122.05	124.53
14	H	1211	CLA	C4D-C3D-CAD	2.21	110.70	108.10
18	A	4007	BCR	C35-C13-C12	2.21	121.56	118.08
14	X	1701	CLA	C3D-C4D-ND	2.21	113.81	110.24
14	B	1206	CLA	CMC-C2C-C3C	2.21	132.12	126.12
18	a	4011	BCR	C15-C14-C13	-2.21	124.16	127.31
14	G	1114	CLA	CAC-C3C-C4C	2.21	127.68	124.81
15	A	1121	F6C	CMD-C2D-C3D	-2.21	122.53	127.61
14	G	1125	CLA	C1D-CHD-C4C	-2.21	121.29	126.06
18	U	4019	BCR	C40-C30-C25	2.21	113.88	110.30
18	H	4016	BCR	C8-C7-C6	-2.21	121.00	127.20
14	A	1134	CLA	C4D-C3D-CAD	2.21	110.70	108.10
14	K	1401	CLA	C4D-C3D-CAD	2.21	110.70	108.10
14	B	1212	CLA	CMA-C3A-C4A	2.21	117.70	111.77
14	G	1139	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
14	A	1117	CLA	C3B-C4B-NB	2.21	112.06	109.21
18	U	4019	BCR	C33-C5-C6	-2.21	122.05	124.53
18	L	4019	BCR	C33-C5-C6	-2.21	122.05	124.53
15	a	1121	F6C	CMD-C2D-C3D	-2.21	122.54	127.61
14	l	1502	CLA	O1D-CGD-CBD	-2.20	119.97	124.48
14	B	1206	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
14	b	1222	CLA	C4D-C3D-CAD	2.20	110.69	108.10
14	b	1212	CLA	CMA-C3A-C4A	2.20	117.69	111.77
13	a	1011	CL0	C3C-C4C-NC	2.20	113.04	110.57
14	H	1023	CLA	CMC-C2C-C3C	2.20	132.10	126.12
14	B	1216	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
18	l	4019	BCR	C34-C9-C10	-2.20	119.84	122.92
14	G	1129	CLA	C5-C3-C4	2.20	119.47	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	1230	F6C	CMA-C3A-C2A	-2.20	120.14	126.12
14	H	1222	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
14	B	1222	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
14	A	1110	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
14	T	1401	CLA	C4D-C3D-CAD	2.20	110.69	108.10
14	A	1138	CLA	C3C-C4C-NC	2.20	113.04	110.57
14	A	1125	CLA	CHD-C4C-C3C	-2.20	121.60	124.84
14	G	1128	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
14	b	1234	CLA	CMC-C2C-C1C	2.20	128.39	125.04
14	b	1221	CLA	C4C-C3C-C2C	-2.20	103.69	106.90
14	H	1221	CLA	C4C-C3C-C2C	-2.20	103.69	106.90
14	G	1125	CLA	CHD-C4C-C3C	-2.20	121.61	124.84
14	a	1124	CLA	C4D-C3D-CAD	2.20	110.69	108.10
18	G	4007	BCR	C35-C13-C12	2.20	121.54	118.08
14	H	1206	CLA	CMC-C2C-C3C	2.20	132.09	126.12
14	G	1112	CLA	C1-C2-C3	-2.20	122.24	126.04
14	a	1112	CLA	C1-C2-C3	-2.20	122.24	126.04
14	b	1023	CLA	CMC-C2C-C3C	2.20	132.09	126.12
14	A	1125	CLA	C1D-CHD-C4C	-2.20	121.31	126.06
18	B	4016	BCR	C3-C4-C5	-2.20	110.15	114.08
14	H	1214	CLA	CAC-C3C-C4C	2.20	127.66	124.81
18	B	4005	BCR	C30-C25-C26	-2.20	119.52	122.61
14	G	1126	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
14	B	1239	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
14	G	1102	CLA	C4D-C3D-CAD	2.20	110.68	108.10
14	H	1022	CLA	C4C-C3C-C2C	-2.19	103.70	106.90
14	x	1701	CLA	C3D-C4D-ND	2.19	113.79	110.24
14	a	1138	CLA	CHB-C4A-NA	2.19	127.55	124.51
14	A	1138	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
14	H	1212	CLA	CMA-C3A-C4A	2.19	117.67	111.77
14	b	1222	CLA	CAC-C3C-C4C	2.19	127.66	124.81
14	A	1102	CLA	C4D-C3D-CAD	2.19	110.68	108.10
14	B	1211	CLA	C4D-C3D-CAD	2.19	110.68	108.10
15	G	1121	F6C	CMD-C2D-C3D	-2.19	122.57	127.61
14	H	1214	CLA	C3C-C4C-NC	2.19	113.03	110.57
14	B	1221	CLA	C4C-C3C-C2C	-2.19	103.70	106.90
18	H	4016	BCR	C3-C4-C5	-2.19	110.16	114.08
18	H	4005	BCR	C30-C25-C26	-2.19	119.53	122.61
14	B	1022	CLA	C4C-C3C-C2C	-2.19	103.70	106.90
18	l	4019	BCR	C40-C30-C25	2.19	113.85	110.30
14	H	1201	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
14	A	1107	CLA	O1D-CGD-CBD	-2.19	120.00	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	1230	F6C	CMA-C3A-C2A	-2.19	120.17	126.12
15	G	1121	F6C	CAA-CBA-CGA	-2.19	108.89	113.60
14	H	1022	CLA	C6-C7-C8	-2.19	108.84	115.92
18	U	4019	BCR	C7-C8-C9	-2.19	122.93	126.23
14	U	1502	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
14	a	1111	CLA	C4D-C3D-CAD	2.19	110.67	108.10
18	b	4005	BCR	C27-C26-C25	-2.19	119.56	122.73
14	a	1107	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
14	a	1139	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
14	B	1234	CLA	CAC-C3C-C4C	2.18	127.64	124.81
18	b	4016	BCR	C37-C22-C21	-2.18	119.86	122.92
14	B	1022	CLA	C6-C7-C8	-2.18	108.86	115.92
14	A	1114	CLA	CAC-C3C-C4C	2.18	127.64	124.81
18	a	4007	BCR	C35-C13-C12	2.18	121.52	118.08
15	H	1207	F6C	C3D-C4D-ND	2.18	113.36	110.17
14	G	1138	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
18	H	4005	BCR	C27-C26-C25	-2.18	119.56	122.73
14	H	1210	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
14	A	1126	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
15	A	1121	F6C	CAA-CBA-CGA	-2.18	108.91	113.60
14	A	1130	CLA	C3D-C4D-ND	2.18	113.77	110.24
18	L	4019	BCR	C7-C8-C9	-2.18	122.94	126.23
15	B	1207	F6C	C3D-C4D-ND	2.18	113.36	110.17
14	H	1239	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
14	H	1239	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
14	H	1234	CLA	CMC-C2C-C1C	2.18	128.36	125.04
14	b	1216	CLA	C1-O2A-CGA	2.18	122.17	116.44
14	H	1206	CLA	CAC-C3C-C4C	2.18	127.64	124.81
14	a	1114	CLA	C4D-C3D-CAD	2.18	110.67	108.10
15	B	1238	F6C	CHB-C4A-NA	2.18	126.46	124.45
14	G	1117	CLA	C4-C3-C5	2.18	118.94	115.27
14	G	1138	CLA	CHB-C4A-NA	2.18	127.52	124.51
14	A	1124	CLA	C4D-C3D-CAD	2.18	110.66	108.10
14	G	1104	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
14	a	1126	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
14	B	1201	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
14	a	1129	CLA	C5-C3-C4	2.18	119.41	114.60
18	l	4019	BCR	C33-C5-C6	-2.18	122.08	124.53
14	A	1138	CLA	CHB-C4A-NA	2.18	127.52	124.51
14	B	1216	CLA	C1-O2A-CGA	2.18	122.15	116.44
18	b	4016	BCR	C3-C4-C5	-2.18	110.19	114.08
18	G	4011	BCR	C15-C14-C13	-2.17	124.21	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1239	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
14	b	1206	CLA	CAC-C3C-C4C	2.17	127.63	124.81
14	H	1235	CLA	C4-C3-C2	-2.17	118.10	123.68
14	A	1111	CLA	C4D-C3D-CAD	2.17	110.66	108.10
14	a	1107	CLA	CAC-C3C-C4C	2.17	127.63	124.81
14	b	1239	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
18	l	4019	BCR	C7-C8-C9	-2.17	122.95	126.23
14	G	1138	CLA	C3C-C4C-NC	2.17	113.01	110.57
14	b	1239	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
14	a	1117	CLA	C3B-C4B-NB	2.17	112.02	109.21
18	R	4018	BCR	C1-C6-C5	-2.17	119.55	122.61
14	a	1102	CLA	C4D-C3D-CAD	2.17	110.66	108.10
14	a	1139	CLA	CAC-C3C-C4C	2.17	127.63	124.81
14	A	1112	CLA	C1-C2-C3	-2.17	122.29	126.04
14	G	1112	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
14	A	1129	CLA	C5-C3-C4	2.17	119.40	114.60
14	A	1139	CLA	CAC-C3C-C4C	2.17	127.63	124.81
14	a	1112	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
18	B	4005	BCR	C27-C26-C25	-2.17	119.58	122.73
14	G	1112	CLA	C4D-C3D-CAD	2.17	110.65	108.10
18	b	4005	BCR	C30-C25-C26	-2.17	119.56	122.61
14	a	1107	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
14	a	1105	CLA	C4D-C3D-CAD	2.17	110.65	108.10
14	a	1128	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
15	b	1207	F6C	C3D-C4D-ND	2.17	113.34	110.17
14	G	1107	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
14	b	1022	CLA	C6-C7-C8	-2.17	108.91	115.92
14	G	1134	CLA	C4D-C3D-CAD	2.17	110.65	108.10
14	B	1222	CLA	C4D-C3D-CAD	2.17	110.65	108.10
14	H	1219	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
14	b	1201	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
15	a	1121	F6C	CAA-CBA-CGA	-2.17	108.94	113.60
14	a	1134	CLA	C4D-C3D-CAD	2.17	110.65	108.10
14	G	1139	CLA	CAC-C3C-C4C	2.17	127.62	124.81
14	H	1216	CLA	C1-O2A-CGA	2.17	122.12	116.44
14	G	1107	CLA	CAC-C3C-C4C	2.16	127.62	124.81
14	A	1128	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
14	b	1211	CLA	C4D-C3D-CAD	2.16	110.65	108.10
14	H	1234	CLA	CBA-CAA-C2A	-2.16	107.48	113.86
14	G	1111	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
14	b	1234	CLA	CBA-CAA-C2A	-2.16	107.48	113.86
14	b	1239	CLA	C4C-C3C-C2C	-2.16	103.75	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	1212	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
14	G	1119	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
18	H	4016	BCR	C37-C22-C21	-2.16	119.90	122.92
14	A	1107	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
14	A	1112	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
14	B	1225	CLA	C4D-C3D-CAD	2.16	110.64	108.10
14	b	1212	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
14	H	1022	CLA	CHA-C1A-NA	-2.16	121.45	126.40
14	B	1219	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
14	B	1234	CLA	CMC-C2C-C1C	2.16	128.33	125.04
14	H	1212	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
14	a	1138	CLA	C3C-C4C-NC	2.16	112.99	110.57
14	A	1104	CLA	C3C-C4C-NC	2.16	112.99	110.57
14	a	1117	CLA	C4-C3-C5	2.16	118.90	115.27
14	b	1239	CLA	CMB-C2B-C3B	2.16	128.71	124.68
14	b	1239	CLA	C6-C5-C3	-2.16	107.80	113.45
14	a	1101	CLA	C4D-C3D-CAD	2.16	110.64	108.10
14	a	1111	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
14	A	1122	CLA	C1-O2A-CGA	2.16	122.10	116.44
14	A	1107	CLA	CAC-C3C-C4C	2.16	127.61	124.81
14	G	1102	CLA	CHB-C4A-NA	2.16	127.49	124.51
14	b	1235	CLA	C4-C3-C2	-2.16	118.15	123.68
14	b	1219	CLA	CMD-C2D-C3D	-2.16	122.66	127.61
15	H	1230	F6C	CHB-C4A-NA	2.16	126.44	124.45
15	b	1230	F6C	CHB-C4A-NA	2.16	126.44	124.45
14	U	1502	CLA	CMD-C2D-C3D	-2.16	122.66	127.61
14	A	1101	CLA	C4D-C3D-CAD	2.16	110.64	108.10
14	H	1222	CLA	C4-C3-C2	-2.15	118.15	123.68
14	B	1234	CLA	CBA-CAA-C2A	-2.15	107.51	113.86
14	B	1222	CLA	C4-C3-C2	-2.15	118.16	123.68
14	H	1215	CLA	CMA-C3A-C4A	2.15	117.56	111.77
14	B	1239	CLA	CMB-C2B-C3B	2.15	128.70	124.68
18	L	4022	BCR	C31-C1-C6	-2.15	106.81	110.30
18	B	4016	BCR	C37-C22-C21	-2.15	119.91	122.92
14	B	1235	CLA	C4-C3-C2	-2.15	118.16	123.68
14	b	1022	CLA	CHD-C4C-C3C	-2.15	121.68	124.84
18	M	4021	BCR	C36-C18-C17	-2.15	119.91	122.92
14	B	1215	CLA	CMA-C3A-C4A	2.15	117.55	111.77
14	A	1105	CLA	C4D-C3D-CAD	2.15	110.63	108.10
14	H	1202	CLA	CHB-C4A-NA	2.15	127.48	124.51
14	G	1107	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
14	a	1117	CLA	C3D-C4D-ND	2.15	113.71	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	4010	BCR	C37-C22-C21	-2.15	119.91	122.92
18	A	4001	BCR	C37-C22-C21	-2.15	119.91	122.92
18	a	4001	BCR	C34-C9-C8	2.15	121.46	118.08
14	G	1114	CLA	C4D-C3D-CAD	2.15	110.63	108.10
18	b	4014	BCR	C29-C28-C27	-2.15	106.58	111.38
14	a	1119	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
14	A	1119	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
14	A	1114	CLA	C4D-C3D-CAD	2.15	110.63	108.10
18	l	4022	BCR	C31-C1-C6	-2.15	106.82	110.30
14	G	1105	CLA	C4D-C3D-CAD	2.15	110.63	108.10
14	B	1022	CLA	CHD-C4C-C3C	-2.15	121.69	124.84
18	G	4002	BCR	C27-C26-C25	-2.15	119.61	122.73
14	B	1022	CLA	CHA-C1A-NA	-2.15	121.48	126.40
14	G	1122	CLA	C1-O2A-CGA	2.15	122.07	116.44
14	A	1104	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
14	L	1502	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
14	G	1104	CLA	C3C-C4C-NC	2.15	112.98	110.57
14	a	1122	CLA	C1-O2A-CGA	2.15	122.07	116.44
14	G	1108	CLA	CMD-C2D-C3D	-2.14	122.68	127.61
14	a	1104	CLA	C3C-C4C-NC	2.14	112.98	110.57
14	H	1234	CLA	CAC-C3C-C4C	2.14	127.59	124.81
14	a	1124	CLA	C4-C3-C5	2.14	118.88	115.27
14	H	1204	CLA	C3C-C4C-NC	2.14	112.97	110.57
14	b	1214	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
13	G	1011	CL0	CHB-C4A-NA	2.14	127.48	124.51
14	b	1224	CLA	CMA-C3A-C4A	2.14	117.53	111.77
18	I	4020	BCR	C23-C24-C25	-2.14	121.19	127.20
13	a	1011	CL0	CHB-C4A-NA	2.14	127.47	124.51
14	G	1124	CLA	CMC-C2C-C1C	2.14	128.30	125.04
14	A	1126	CLA	CAC-C3C-C4C	2.14	127.59	124.81
14	B	1220	CLA	C3B-C4B-NB	2.14	111.98	109.21
14	A	1111	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
18	H	4014	BCR	C29-C28-C27	-2.14	106.59	111.38
14	G	1117	CLA	C3D-C4D-ND	2.14	113.70	110.24
14	a	1102	CLA	CHB-C4A-NA	2.14	127.47	124.51
14	H	1220	CLA	C3B-C4B-NB	2.14	111.98	109.21
18	R	4020	BCR	C23-C24-C25	-2.14	121.19	127.20
14	G	1124	CLA	C4-C3-C5	2.14	118.87	115.27
14	B	1214	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
14	G	1122	CLA	CMC-C2C-C1C	2.14	128.30	125.04
18	B	4014	BCR	C29-C28-C27	-2.14	106.59	111.38
14	H	1239	CLA	C4C-C3C-C2C	-2.14	103.78	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1215	CLA	CMA-C3A-C4A	2.14	117.52	111.77
14	b	1222	CLA	C4-C3-C2	-2.14	118.19	123.68
14	H	1022	CLA	CHD-C4C-C3C	-2.14	121.69	124.84
14	B	1224	CLA	CMA-C3A-C4A	2.14	117.52	111.77
18	I	4018	BCR	C1-C6-C5	-2.14	119.60	122.61
14	a	1104	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
15	G	1121	F6C	O1D-CGD-CBD	-2.14	120.11	124.48
14	H	1239	CLA	C6-C5-C3	-2.14	107.85	113.45
14	B	1239	CLA	C6-C5-C3	-2.14	107.85	113.45
15	B	1230	F6C	CHB-C4A-NA	2.14	126.42	124.45
18	V	4021	BCR	C36-C18-C17	-2.14	119.93	122.92
14	H	1227	CLA	CMC-C2C-C1C	2.14	128.29	125.04
14	L	1502	CLA	CAC-C3C-C4C	2.14	127.58	124.81
14	G	1101	CLA	C4D-C3D-CAD	2.14	110.61	108.10
14	B	1239	CLA	C4C-C3C-C2C	-2.14	103.78	106.90
18	G	4001	BCR	C34-C9-C8	2.14	121.44	118.08
18	m	4021	BCR	C36-C18-C17	-2.14	119.93	122.92
14	B	1228	CLA	C4D-C3D-CAD	2.14	110.61	108.10
14	H	1214	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
15	b	1238	F6C	CHB-C4A-NA	2.13	126.42	124.45
14	H	1224	CLA	CMA-C3A-C4A	2.13	117.51	111.77
14	a	1108	CLA	CMD-C2D-C3D	-2.13	122.70	127.61
14	H	1239	CLA	CMB-C2B-C3B	2.13	128.67	124.68
14	H	1222	CLA	C4D-C3D-CAD	2.13	110.61	108.10
14	a	1012	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
14	B	1219	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
18	b	4006	BCR	C23-C24-C25	-2.13	121.21	127.20
16	a	2001	PQN	C16-C17-C18	-2.13	109.02	115.92
18	a	4001	BCR	C37-C22-C21	-2.13	119.94	122.92
18	i	4020	BCR	C23-C24-C25	-2.13	121.21	127.20
14	H	1212	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
14	G	1135	CLA	CHC-C1C-C2C	-2.13	120.82	126.72
14	G	1127	CLA	CAC-C3C-C4C	2.13	127.58	124.81
14	L	1501	CLA	C16-C15-C13	-2.13	109.03	115.92
14	H	1222	CLA	CMC-C2C-C1C	2.13	128.28	125.04
14	b	1022	CLA	CHA-C1A-NA	-2.13	121.52	126.40
14	A	1108	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
14	a	1112	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
14	L	1503	CLA	C4D-C3D-CAD	2.13	110.61	108.10
14	l	1502	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
14	b	1202	CLA	CHB-C4A-NA	2.13	127.46	124.51
14	B	1202	CLA	CHB-C4A-NA	2.13	127.46	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	4006	BCR	C23-C24-C25	-2.13	121.22	127.20
14	B	1222	CLA	CMC-C2C-C1C	2.13	128.28	125.04
14	A	1012	CLA	CAA-CBA-CGA	-2.13	107.03	113.25
18	G	4001	BCR	C37-C22-C21	-2.13	119.94	122.92
14	A	1112	CLA	C4D-C3D-CAD	2.13	110.60	108.10
14	a	1118	CLA	CMA-C3A-C4A	2.13	117.49	111.77
14	H	1202	CLA	C1-C2-C3	-2.13	122.36	126.04
13	A	1011	CL0	CHB-C4A-NA	2.13	127.45	124.51
14	G	1126	CLA	CAC-C3C-C4C	2.13	127.57	124.81
14	A	1116	CLA	CBA-CAA-C2A	2.13	120.14	113.86
14	a	1135	CLA	CHC-C1C-C2C	-2.13	120.84	126.72
14	A	1118	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
14	a	1139	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
15	A	1121	F6C	O1D-CGD-CBD	-2.13	120.13	124.48
18	a	4002	BCR	C27-C26-C25	-2.13	119.64	122.73
14	A	1117	CLA	C3D-C4D-ND	2.12	113.67	110.24
14	a	1124	CLA	CMC-C2C-C1C	2.12	128.27	125.04
14	a	1126	CLA	CAC-C3C-C4C	2.12	127.57	124.81
14	G	1108	CLA	CMA-C3A-C4A	2.12	117.48	111.77
14	a	1109	CLA	C6-C7-C8	-2.12	109.06	115.92
14	B	1216	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
14	B	1206	CLA	CAC-C3C-C4C	2.12	127.56	124.81
14	B	1202	CLA	C1-C2-C3	-2.12	122.37	126.04
14	b	1219	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
14	G	1130	CLA	C4D-C3D-CAD	2.12	110.60	108.10
14	a	1108	CLA	C4D-C3D-CAD	2.12	110.60	108.10
16	G	2001	PQN	C16-C17-C18	-2.12	109.06	115.92
14	U	1501	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
14	G	1117	CLA	C4D-C3D-CAD	2.12	110.60	108.10
14	H	1217	CLA	C4D-C3D-CAD	2.12	110.60	108.10
14	A	1112	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
14	A	1124	CLA	C4-C3-C5	2.12	118.84	115.27
14	B	1223	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
14	H	1225	CLA	C4D-C3D-CAD	2.12	110.59	108.10
14	B	1219	CLA	C4D-C3D-CAD	2.12	110.59	108.10
14	b	1234	CLA	CAC-C3C-C4C	2.12	127.56	124.81
14	A	1118	CLA	CMA-C3A-C4A	2.12	117.47	111.77
14	G	1118	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
14	H	1221	CLA	C1-O2A-CGA	2.12	122.00	116.44
14	A	1116	CLA	C1-O2A-CGA	2.12	122.00	116.44
14	A	1139	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
18	H	4004	BCR	C34-C9-C10	-2.12	119.95	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1131	CLA	C3C-C4C-NC	2.12	112.95	110.57
14	b	1204	CLA	C3C-C4C-NC	2.12	112.95	110.57
14	A	1132	CLA	C4-C3-C5	2.12	118.84	115.27
18	A	4001	BCR	C34-C9-C8	2.12	121.42	118.08
16	A	2001	PQN	C16-C17-C18	-2.12	109.07	115.92
14	G	1118	CLA	CMA-C3A-C4A	2.12	117.47	111.77
14	a	1108	CLA	CMA-C3A-C4A	2.12	117.47	111.77
14	b	1219	CLA	CMA-C3A-C4A	2.12	117.47	111.77
14	A	1108	CLA	C4D-C3D-CAD	2.12	110.59	108.10
14	U	1501	CLA	C16-C15-C13	-2.12	109.08	115.92
18	A	4002	BCR	C27-C26-C25	-2.12	119.66	122.73
14	K	1401	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
14	b	1227	CLA	CMC-C2C-C1C	2.12	128.26	125.04
14	H	1202	CLA	C4D-C3D-CAD	2.12	110.59	108.10
14	L	1501	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
14	b	1216	CLA	CMD-C2D-C3D	-2.12	122.75	127.61
15	H	1238	F6C	CHB-C4A-NA	2.12	126.40	124.45
14	l	1502	CLA	CAC-C3C-C4C	2.12	127.56	124.81
14	b	1222	CLA	CMC-C2C-C1C	2.12	128.26	125.04
14	W	1701	CLA	C4C-C3C-C2C	-2.12	103.81	106.90
14	A	1104	CLA	CHB-C4A-NA	2.12	127.44	124.51
15	B	1238	F6C	O1D-CGD-CBD	-2.12	120.16	124.48
14	B	1226	CLA	CMC-C2C-C3C	2.12	131.86	126.12
14	G	1013	CLA	C6-C5-C3	-2.12	107.91	113.45
14	G	1012	CLA	CAA-CBA-CGA	-2.11	107.07	113.25
14	G	1112	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
14	b	1202	CLA	C1-C2-C3	-2.11	122.39	126.04
14	b	1228	CLA	CMA-C3A-C4A	2.11	117.46	111.77
14	B	1202	CLA	C4D-C3D-CAD	2.11	110.59	108.10
14	a	1013	CLA	C6-C5-C3	-2.11	107.91	113.45
14	x	1701	CLA	C4C-C3C-C2C	-2.11	103.82	106.90
14	A	1124	CLA	CMC-C2C-C1C	2.11	128.26	125.04
14	b	1223	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
14	U	1503	CLA	C4D-C3D-CAD	2.11	110.59	108.10
18	U	4022	BCR	C31-C1-C6	-2.11	106.87	110.30
14	T	1401	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
14	G	1116	CLA	CBA-CAA-C2A	2.11	120.10	113.86
14	A	1110	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
14	H	1226	CLA	CMC-C2C-C3C	2.11	131.85	126.12
14	a	1118	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
14	A	1117	CLA	C4-C3-C5	2.11	118.82	115.27
14	a	1116	CLA	CBA-CAA-C2A	2.11	120.10	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1228	CLA	CMA-C3A-C4A	2.11	117.45	111.77
14	A	1135	CLA	CHC-C1C-C2C	-2.11	120.88	126.72
14	b	1221	CLA	C1-O2A-CGA	2.11	121.98	116.44
14	H	1219	CLA	CMA-C3A-C4A	2.11	117.45	111.77
14	B	1219	CLA	CMA-C3A-C4A	2.11	117.45	111.77
18	L	4019	BCR	C32-C1-C6	-2.11	106.88	110.30
14	k	1401	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
14	b	1229	CLA	CAA-CBA-CGA	-2.11	107.09	113.25
14	G	1132	CLA	C4-C3-C5	2.11	118.82	115.27
14	a	1116	CLA	C1-O2A-CGA	2.11	121.98	116.44
18	i	4018	BCR	C1-C6-C5	-2.11	119.64	122.61
14	B	1228	CLA	CMA-C3A-C4A	2.11	117.44	111.77
14	b	1202	CLA	C4D-C3D-CAD	2.11	110.58	108.10
18	H	4006	BCR	C23-C24-C25	-2.11	121.28	127.20
18	H	4010	BCR	C37-C22-C21	-2.11	119.97	122.92
14	l	1501	CLA	C16-C15-C13	-2.11	109.11	115.92
14	B	1204	CLA	C3C-C4C-NC	2.11	112.94	110.57
14	b	1225	CLA	C4D-C3D-CAD	2.11	110.58	108.10
15	H	1238	F6C	O1D-CGD-CBD	-2.11	120.17	124.48
14	a	1132	CLA	C4-C3-C5	2.11	118.81	115.27
18	B	4010	BCR	C37-C22-C21	-2.11	119.97	122.92
15	a	1121	F6C	O1D-CGD-CBD	-2.11	120.17	124.48
14	A	1108	CLA	CMA-C3A-C4A	2.11	117.43	111.77
14	A	1012	CLA	CHA-C1A-NA	-2.11	121.58	126.40
14	a	1104	CLA	CHB-C4A-NA	2.11	127.42	124.51
14	A	1102	CLA	CHB-C4A-NA	2.11	127.42	124.51
14	G	1116	CLA	C4D-C3D-CAD	2.10	110.58	108.10
14	l	1501	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
14	H	1219	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
14	U	1501	CLA	C4-C3-C5	2.10	118.81	115.27
14	A	1109	CLA	C6-C7-C8	-2.10	109.12	115.92
14	b	1226	CLA	CMC-C2C-C3C	2.10	131.83	126.12
14	G	1139	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
14	l	1501	CLA	C4-C3-C5	2.10	118.81	115.27
14	a	1013	CLA	C4D-C3D-CAD	2.10	110.57	108.10
14	b	1208	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
14	a	1127	CLA	CAC-C3C-C4C	2.10	127.54	124.81
14	A	1127	CLA	CAC-C3C-C4C	2.10	127.54	124.81
14	A	1013	CLA	C6-C5-C3	-2.10	107.94	113.45
18	U	4019	BCR	C32-C1-C6	-2.10	106.89	110.30
18	A	4008	BCR	C38-C26-C27	2.10	117.65	113.62
14	b	1220	CLA	C3B-C4B-NB	2.10	111.93	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1228	CLA	C4D-C3D-CAD	2.10	110.57	108.10
14	H	1227	CLA	CHC-C1C-C2C	-2.10	120.91	126.72
15	b	1238	F6C	O1D-CGD-CBD	-2.10	120.19	124.48
14	G	1012	CLA	CHA-C1A-NA	-2.10	121.59	126.40
14	A	1130	CLA	C4D-C3D-CAD	2.10	110.57	108.10
14	B	1221	CLA	C1-O2A-CGA	2.10	121.95	116.44
14	a	1131	CLA	C3C-C4C-NC	2.10	112.92	110.57
13	a	1011	CL0	C1-O2A-CGA	2.10	121.95	116.44
14	a	1112	CLA	C4D-C3D-CAD	2.10	110.57	108.10
14	B	1227	CLA	CMC-C2C-C1C	2.10	128.23	125.04
14	H	1216	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
14	A	1013	CLA	C4D-C3D-CAD	2.10	110.57	108.10
14	H	1219	CLA	C4D-C3D-CAD	2.10	110.57	108.10
18	H	4009	BCR	C23-C24-C25	-2.10	121.32	127.20
18	b	4009	BCR	C23-C24-C25	-2.10	121.32	127.20
14	a	1110	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
14	H	1223	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
14	G	1116	CLA	C1-O2A-CGA	2.09	121.94	116.44
14	G	1013	CLA	C4D-C3D-CAD	2.09	110.56	108.10
14	a	1128	CLA	CMC-C2C-C3C	2.09	131.80	126.12
14	a	1111	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
18	l	4019	BCR	C32-C1-C6	-2.09	106.91	110.30
14	G	1110	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
14	b	1212	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
14	a	1133	CLA	CAC-C3C-C4C	2.09	127.52	124.81
14	A	1123	CLA	C4-C3-C2	-2.09	118.31	123.68
18	a	4008	BCR	C38-C26-C27	2.09	117.63	113.62
13	G	1011	CL0	C1-O2A-CGA	2.09	121.93	116.44
14	B	1227	CLA	CHC-C1C-C2C	-2.09	120.94	126.72
14	G	1012	CLA	C11-C10-C8	-2.09	109.16	115.92
14	G	1109	CLA	C6-C7-C8	-2.09	109.16	115.92
18	b	4013	BCR	C35-C13-C12	2.09	121.37	118.08
14	A	1116	CLA	CMA-C3A-C4A	2.09	117.39	111.77
14	a	1130	CLA	C4D-C3D-CAD	2.09	110.56	108.10
16	G	2001	PQN	C12-C11-C3	-2.09	106.41	112.05
14	A	1104	CLA	C7-C6-C5	-2.09	107.68	113.36
14	b	1219	CLA	C4D-C3D-CAD	2.09	110.56	108.10
14	A	1117	CLA	C4D-C3D-CAD	2.09	110.56	108.10
14	B	1212	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
18	R	4020	BCR	C28-C29-C30	-2.09	107.14	114.60
14	G	1108	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
14	A	1111	CLA	C4C-C3C-C2C	-2.09	103.86	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	H	1236	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
14	H	1208	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
14	A	1122	CLA	CMC-C2C-C1C	2.09	128.22	125.04
14	b	1227	CLA	CHC-C1C-C2C	-2.09	120.95	126.72
14	H	1229	CLA	CAA-CBA-CGA	-2.09	107.16	113.25
14	L	1503	CLA	C4C-C3C-C2C	-2.09	103.86	106.90
14	a	1117	CLA	C4D-C3D-CAD	2.09	110.56	108.10
14	A	1126	CLA	C4C-C3C-C2C	-2.09	103.86	106.90
14	G	1133	CLA	CAC-C3C-C4C	2.09	127.52	124.81
14	A	1128	CLA	CMC-C2C-C3C	2.09	131.78	126.12
18	G	4008	BCR	C38-C26-C27	2.09	117.62	113.62
14	a	1126	CLA	C4C-C3C-C2C	-2.09	103.86	106.90
14	l	1503	CLA	C4C-C3C-C2C	-2.09	103.86	106.90
14	L	1502	CLA	C3C-C4C-NC	2.08	112.91	110.57
14	l	1503	CLA	C4D-C3D-CAD	2.08	110.55	108.10
14	B	1217	CLA	C4D-C3D-CAD	2.08	110.55	108.10
14	H	1204	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
14	B	1208	CLA	CAC-C3C-C4C	2.08	127.51	124.81
14	b	1217	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
14	H	1239	CLA	CMA-C3A-C4A	2.08	117.37	111.77
14	b	1204	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
14	H	1223	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
18	B	4009	BCR	C23-C24-C25	-2.08	121.35	127.20
14	G	1137	CLA	CAC-C3C-C4C	2.08	127.51	124.81
14	A	1133	CLA	CAC-C3C-C4C	2.08	127.51	124.81
14	a	1116	CLA	CMA-C3A-C4A	2.08	117.37	111.77
14	b	1236	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
18	A	4001	BCR	C23-C24-C25	-2.08	121.36	127.20
18	I	4020	BCR	C28-C29-C30	-2.08	107.16	114.60
14	H	1208	CLA	CAC-C3C-C4C	2.08	127.51	124.81
14	G	1128	CLA	CMC-C2C-C3C	2.08	131.76	126.12
14	H	1203	CLA	C3D-C4D-ND	2.08	113.60	110.24
16	A	2001	PQN	C12-C11-C3	-2.08	106.44	112.05
14	B	1218	CLA	CHD-C4C-C3C	-2.08	121.78	124.84
14	B	1236	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
14	B	1216	CLA	CMC-C2C-C1C	2.08	128.21	125.04
14	a	1140	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
14	a	1012	CLA	CHA-C1A-NA	-2.08	121.64	126.40
18	i	4020	BCR	C28-C29-C30	-2.08	107.17	114.60
14	G	1104	CLA	C7-C6-C5	-2.08	107.71	113.36
14	X	1701	CLA	C4C-C3C-C2C	-2.08	103.87	106.90
14	G	1117	CLA	CMC-C2C-C3C	2.08	131.76	126.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	U	1502	CLA	CAC-C3C-C4C	2.08	127.51	124.81
18	b	4013	BCR	C36-C18-C17	-2.08	120.01	122.92
14	G	1116	CLA	CMA-C3A-C4A	2.08	117.36	111.77
14	A	1012	CLA	C11-C10-C8	-2.08	109.20	115.92
14	G	1140	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
14	b	1203	CLA	C3D-C4D-ND	2.08	113.60	110.24
15	H	1230	F6C	CAA-CBA-CGA	-2.08	109.13	113.60
18	G	4001	BCR	C23-C24-C25	-2.08	121.37	127.20
14	b	1239	CLA	CMA-C3A-C4A	2.08	117.35	111.77
14	B	1204	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
14	H	1239	CLA	C11-C12-C13	-2.08	109.21	115.92
14	H	1232	CLA	CAC-C3C-C4C	2.08	127.50	124.81
14	U	1503	CLA	C4C-C3C-C2C	-2.08	103.87	106.90
14	G	1104	CLA	CHB-C4A-NA	2.07	127.38	124.51
14	b	1239	CLA	C11-C12-C13	-2.07	109.21	115.92
14	L	1501	CLA	C4-C3-C5	2.07	118.76	115.27
14	a	1117	CLA	CMC-C2C-C3C	2.07	131.75	126.12
21	a	6002	LMT	O5B-C5B-C6B	2.07	111.59	106.44
14	B	1236	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
14	A	1140	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
13	A	1011	CL0	C1-O2A-CGA	2.07	121.88	116.44
14	a	1133	CLA	C1-O2A-CGA	2.07	121.88	116.44
18	a	4001	BCR	C23-C24-C25	-2.07	121.38	127.20
14	a	1134	CLA	CAC-C3C-C4C	2.07	127.50	124.81
14	B	1239	CLA	C11-C12-C13	-2.07	109.22	115.92
14	a	1111	CLA	CAA-CBA-CGA	-2.07	107.20	113.25
14	a	1108	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
14	a	1133	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
14	B	1208	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
14	B	1223	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
14	G	1123	CLA	C4-C3-C2	-2.07	118.36	123.68
21	A	6002	LMT	O5B-C5B-C6B	2.07	111.59	106.44
14	a	1104	CLA	C7-C6-C5	-2.07	107.73	113.36
18	b	4004	BCR	C34-C9-C10	-2.07	120.02	122.92
18	I	4018	BCR	C28-C27-C26	-2.07	110.38	114.08
14	H	1217	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
14	b	1228	CLA	C4D-C3D-CAD	2.07	110.54	108.10
14	A	1116	CLA	C4D-C3D-CAD	2.07	110.54	108.10
14	a	1137	CLA	CAC-C3C-C4C	2.07	127.50	124.81
18	b	4004	BCR	C31-C1-C6	-2.07	106.94	110.30
14	a	1122	CLA	CMC-C2C-C1C	2.07	128.19	125.04
14	a	1012	CLA	C11-C10-C8	-2.07	109.23	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1133	CLA	C1-O2A-CGA	2.07	121.88	116.44
14	B	1210	CLA	CMA-C3A-C4A	2.07	117.34	111.77
14	b	1204	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
14	a	1123	CLA	C4-C3-C2	-2.07	118.37	123.68
14	b	1208	CLA	CAC-C3C-C4C	2.07	127.50	124.81
14	A	1108	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
18	H	4013	BCR	C36-C18-C17	-2.07	120.03	122.92
14	A	1133	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
16	a	2001	PQN	C12-C11-C3	-2.07	106.47	112.05
14	G	1122	CLA	CHC-C1C-C2C	-2.07	121.00	126.72
18	L	4022	BCR	C34-C9-C10	-2.07	120.03	122.92
14	G	1133	CLA	C1-O2A-CGA	2.07	121.87	116.44
14	A	1012	CLA	C1-O2A-CGA	2.07	121.87	116.44
14	H	1228	CLA	CMC-C2C-C3C	2.07	131.73	126.12
14	B	1229	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
14	B	1239	CLA	CMA-C3A-C4A	2.07	117.33	111.77
18	B	4013	BCR	C35-C13-C12	2.07	121.33	118.08
15	H	1207	F6C	CHB-C1B-C2B	-2.07	120.68	125.13
15	b	1207	F6C	CHB-C1B-C2B	-2.07	120.68	125.13
14	G	1108	CLA	C4D-C3D-CAD	2.07	110.53	108.10
14	A	1117	CLA	CMC-C2C-C3C	2.07	131.73	126.12
18	H	4013	BCR	C35-C13-C12	2.07	121.33	118.08
14	G	1012	CLA	C1-O2A-CGA	2.07	121.87	116.44
14	b	1216	CLA	CMC-C2C-C1C	2.07	128.19	125.04
14	H	1236	CLA	O1D-CGD-CBD	-2.07	120.26	124.48
14	A	1131	CLA	C3C-C4C-NC	2.07	112.89	110.57
18	U	4022	BCR	C34-C9-C10	-2.07	120.03	122.92
14	b	1228	CLA	C4C-C3C-C2C	-2.07	103.89	106.90
15	b	1230	F6C	CAA-CBA-CGA	-2.07	109.16	113.60
14	A	1137	CLA	CAC-C3C-C4C	2.07	127.49	124.81
18	H	4004	BCR	C31-C1-C6	-2.07	106.95	110.30
18	B	4013	BCR	C36-C18-C17	-2.07	120.03	122.92
14	G	1126	CLA	C4C-C3C-C2C	-2.07	103.89	106.90
14	B	1217	CLA	CMD-C2D-C3D	-2.06	122.86	127.61
18	l	4022	BCR	C34-C9-C10	-2.06	120.03	122.92
14	b	1217	CLA	C4D-C3D-CAD	2.06	110.53	108.10
15	B	1207	F6C	CHB-C1B-C2B	-2.06	120.69	125.13
14	H	1210	CLA	CMA-C3A-C4A	2.06	117.32	111.77
14	b	1202	CLA	C4-C3-C2	-2.06	118.38	123.68
18	I	4018	BCR	C30-C25-C26	-2.06	119.71	122.61
14	b	1236	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
14	B	1023	CLA	CHD-C4C-NC	-2.06	120.96	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1133	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
14	B	1204	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
14	b	1023	CLA	CHD-C4C-NC	-2.06	120.96	124.20
14	b	1223	CLA	C6-C7-C8	-2.06	109.26	115.92
18	i	4018	BCR	C28-C27-C26	-2.06	110.40	114.08
14	B	1202	CLA	C4-C3-C2	-2.06	118.39	123.68
14	H	1218	CLA	CHD-C4C-C3C	-2.06	121.81	124.84
14	b	1218	CLA	CHD-C4C-C3C	-2.06	121.81	124.84
14	A	1137	CLA	CHC-C1C-C2C	-2.06	121.02	126.72
21	G	6002	LMT	O1'-C1'-C2'	2.06	111.52	108.30
14	b	1210	CLA	CMA-C3A-C4A	2.06	117.31	111.77
14	b	1236	CLA	CMB-C2B-C3B	2.06	128.53	124.68
18	H	4014	BCR	C3-C4-C5	-2.06	110.40	114.08
21	G	6002	LMT	O5B-C5B-C6B	2.06	111.56	106.44
18	B	4004	BCR	C34-C9-C10	-2.06	120.04	122.92
18	I	4020	BCR	C40-C30-C25	-2.06	106.96	110.30
18	B	4009	BCR	C35-C13-C14	-2.06	120.04	122.92
18	i	4020	BCR	C40-C30-C25	-2.06	106.96	110.30
14	A	1111	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
18	R	4018	BCR	C28-C27-C26	-2.06	110.40	114.08
14	A	1113	CLA	C4C-C3C-C2C	-2.06	103.90	106.90
14	B	1228	CLA	C4C-C3C-C2C	-2.06	103.90	106.90
13	G	1011	CL0	C4D-C3D-CAD	2.06	110.52	108.10
15	B	1230	F6C	CAA-CBA-CGA	-2.06	109.18	113.60
14	b	1223	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
14	H	1202	CLA	C4-C3-C2	-2.06	118.41	123.68
14	a	1012	CLA	C1-O2A-CGA	2.06	121.84	116.44
14	G	1111	CLA	CAA-CBA-CGA	-2.05	107.25	113.25
18	I	4020	BCR	C34-C9-C10	-2.05	120.05	122.92
14	l	1502	CLA	C3C-C4C-NC	2.05	112.88	110.57
18	R	4018	BCR	C30-C25-C26	-2.05	119.72	122.61
14	G	1131	CLA	C4D-C3D-CAD	2.05	110.52	108.10
14	G	1109	CLA	OBD-CAD-C3D	-2.05	123.58	128.52
14	H	1216	CLA	CMC-C2C-C1C	2.05	128.17	125.04
14	H	1223	CLA	C6-C7-C8	-2.05	109.28	115.92
21	A	6002	LMT	O1'-C1'-C2'	2.05	111.51	108.30
14	G	1134	CLA	CAC-C3C-C4C	2.05	127.47	124.81
14	G	1133	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
14	A	1113	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
14	a	1118	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
14	a	1013	CLA	CBC-CAC-C3C	-2.05	106.78	112.43
14	B	1203	CLA	C3D-C4D-ND	2.05	113.56	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	U	4019	BCR	C2-C1-C6	2.05	113.64	110.48
14	a	1116	CLA	C4D-C3D-CAD	2.05	110.51	108.10
18	b	4017	BCR	C35-C13-C12	2.05	121.31	118.08
14	H	1023	CLA	CHD-C4C-NC	-2.05	120.97	124.20
14	b	1203	CLA	CHA-C4D-ND	2.05	136.79	132.50
14	A	1109	CLA	OBD-CAD-C3D	-2.05	123.59	128.52
14	B	1228	CLA	CMC-C2C-C3C	2.05	131.68	126.12
14	A	1130	CLA	CHA-C4D-ND	2.05	136.79	132.50
14	b	1232	CLA	CHA-C1A-NA	-2.05	121.70	126.40
18	H	4017	BCR	C35-C13-C12	2.05	121.31	118.08
14	U	1502	CLA	C3C-C4C-NC	2.05	112.87	110.57
14	G	1137	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
14	a	1130	CLA	CHA-C4D-ND	2.05	136.78	132.50
18	R	4020	BCR	C40-C30-C25	-2.05	106.98	110.30
18	b	4014	BCR	C3-C4-C5	-2.05	110.42	114.08
14	A	1118	CLA	CHC-C1C-C2C	-2.05	121.06	126.72
14	a	1113	CLA	CMD-C2D-C3D	-2.05	122.91	127.61
14	b	1204	CLA	OBD-CAD-C3D	-2.05	123.59	128.52
18	m	4021	BCR	C34-C9-C10	-2.05	120.06	122.92
14	a	1133	CLA	CHC-C1C-C2C	-2.05	121.06	126.72
14	G	1140	CLA	OBD-CAD-C3D	-2.05	123.60	128.52
14	B	1204	CLA	OBD-CAD-C3D	-2.05	123.60	128.52
14	A	1117	CLA	C3C-C4C-NC	2.05	112.86	110.57
18	i	4020	BCR	C34-C9-C10	-2.05	120.06	122.92
14	H	1228	CLA	C4C-C3C-C2C	-2.05	103.92	106.90
14	H	1223	CLA	CHA-C4D-ND	2.05	136.78	132.50
14	G	1118	CLA	CHC-C1C-C2C	-2.05	121.06	126.72
14	G	1130	CLA	CHA-C1A-NA	-2.04	121.72	126.40
14	B	1203	CLA	CHA-C4D-ND	2.04	136.78	132.50
14	B	1223	CLA	C6-C7-C8	-2.04	109.31	115.92
14	B	1232	CLA	CAC-C3C-C4C	2.04	127.46	124.81
14	a	1122	CLA	C4D-C3D-CAD	2.04	110.50	108.10
18	B	4014	BCR	C3-C4-C5	-2.04	110.43	114.08
14	a	1120	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
14	b	1228	CLA	CMC-C2C-C3C	2.04	131.66	126.12
14	G	1135	CLA	CHA-C4D-ND	2.04	136.77	132.50
14	G	1111	CLA	C4C-C3C-C2C	-2.04	103.92	106.90
14	G	1113	CLA	C4C-C3C-C2C	-2.04	103.92	106.90
14	a	1140	CLA	OBD-CAD-C3D	-2.04	123.61	128.52
14	b	1223	CLA	CHA-C4D-ND	2.04	136.77	132.50
14	H	1204	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
18	V	4021	BCR	C34-C9-C10	-2.04	120.06	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	1140	CLA	OBD-CAD-C3D	-2.04	123.61	128.52
14	G	1122	CLA	C4D-C3D-CAD	2.04	110.50	108.10
14	H	1236	CLA	CMB-C2B-C3B	2.04	128.50	124.68
14	G	1013	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
14	G	1120	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
14	a	1130	CLA	CHA-C1A-NA	-2.04	121.73	126.40
14	U	1501	CLA	CMA-C3A-C4A	2.04	117.25	111.77
14	G	1113	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
14	G	1112	CLA	CMA-C3A-C4A	2.04	117.25	111.77
18	U	4019	BCR	C29-C30-C25	-2.04	107.34	110.48
14	G	1130	CLA	CHA-C4D-ND	2.04	136.76	132.50
14	H	1220	CLA	C4D-C3D-CAD	2.04	110.50	108.10
14	A	1134	CLA	CAC-C3C-C4C	2.04	127.45	124.81
14	H	1232	CLA	CHA-C1A-NA	-2.04	121.73	126.40
14	B	1232	CLA	CHA-C1A-NA	-2.04	121.73	126.40
14	a	1122	CLA	CHC-C1C-C2C	-2.04	121.09	126.72
14	H	1231	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
14	H	1203	CLA	CHA-C4D-ND	2.04	136.76	132.50
14	A	1122	CLA	C4D-C3D-CAD	2.04	110.50	108.10
14	A	1120	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
14	G	1104	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
14	H	1226	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
14	b	1208	CLA	C4D-C3D-CAD	2.03	110.49	108.10
14	A	1013	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
21	a	6002	LMT	O1'-C1'-C2'	2.03	111.48	108.30
14	a	1112	CLA	CMA-C3A-C4A	2.03	117.24	111.77
14	B	1236	CLA	CMB-C2B-C3B	2.03	128.48	124.68
14	B	1226	CLA	CMA-C3A-C4A	2.03	117.24	111.77
14	b	1232	CLA	CAC-C3C-C4C	2.03	127.45	124.81
14	A	1133	CLA	CHC-C1C-C2C	-2.03	121.10	126.72
14	B	1215	CLA	C11-C10-C8	-2.03	109.35	115.92
14	l	1501	CLA	CMA-C3A-C4A	2.03	117.23	111.77
18	H	4014	BCR	C34-C9-C8	2.03	121.28	118.08
18	H	4009	BCR	C35-C13-C14	-2.03	120.08	122.92
14	b	1215	CLA	C11-C10-C8	-2.03	109.36	115.92
14	A	1013	CLA	CHD-C4C-C3C	-2.03	121.86	124.84
18	l	4019	BCR	C29-C30-C25	-2.03	107.36	110.48
14	A	1122	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
14	B	1226	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
14	A	1114	CLA	CMC-C2C-C3C	2.03	131.62	126.12
18	l	4019	BCR	C2-C1-C6	2.03	113.60	110.48
18	L	4019	BCR	C2-C1-C6	2.03	113.60	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	4019	BCR	C29-C30-C25	-2.03	107.36	110.48
14	G	1114	CLA	CMC-C2C-C3C	2.03	131.62	126.12
14	A	1112	CLA	CMA-C3A-C4A	2.03	117.22	111.77
18	i	4018	BCR	C30-C25-C26	-2.03	119.76	122.61
14	B	1223	CLA	CHA-C4D-ND	2.03	136.74	132.50
14	A	1104	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
14	a	1137	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
18	M	4021	BCR	C34-C9-C10	-2.03	120.08	122.92
14	A	1135	CLA	CHA-C4D-ND	2.03	136.74	132.50
14	G	1103	CLA	CMC-C2C-C1C	2.03	128.12	125.04
14	B	1202	CLA	C4C-C3C-C2C	-2.03	103.94	106.90
18	G	4008	BCR	C19-C18-C17	2.03	122.05	118.94
14	B	1021	CLA	C11-C10-C8	-2.02	109.37	115.92
14	a	1103	CLA	CMC-C2C-C1C	2.02	128.12	125.04
14	A	1115	CLA	CMA-C3A-C4A	2.02	117.21	111.77
18	B	4017	BCR	C35-C13-C12	2.02	121.27	118.08
14	B	1223	CLA	CHD-C4C-C3C	-2.02	121.86	124.84
14	U	1503	CLA	C1-O2A-CGA	2.02	121.75	116.44
14	B	1225	CLA	C1-O2A-CGA	2.02	121.75	116.44
14	U	1501	CLA	C6-C7-C8	-2.02	109.38	115.92
14	G	1117	CLA	C3C-C4C-NC	2.02	112.84	110.57
14	l	1501	CLA	C6-C7-C8	-2.02	109.38	115.92
14	U	1503	CLA	CAC-C3C-C4C	2.02	127.43	124.81
14	a	1104	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
18	B	4004	BCR	C31-C1-C6	-2.02	107.02	110.30
14	L	1501	CLA	CMA-C3A-C4A	2.02	117.21	111.77
14	a	1103	CLA	C4-C3-C2	-2.02	118.49	123.68
14	G	1137	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
14	H	1215	CLA	C11-C10-C8	-2.02	109.38	115.92
14	H	1216	CLA	CHC-C1C-C2C	-2.02	121.13	126.72
14	a	1114	CLA	CMC-C2C-C3C	2.02	131.60	126.12
14	A	1113	CLA	CAC-C3C-C4C	2.02	127.43	124.81
14	A	1128	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
14	b	1226	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
14	H	1231	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
14	G	1115	CLA	CMA-C3A-C4A	2.02	117.20	111.77
14	a	1109	CLA	OBD-CAD-C3D	-2.02	123.66	128.52
14	G	1123	CLA	CHA-C1A-NA	-2.02	121.77	126.40
14	b	1021	CLA	C11-C10-C8	-2.02	109.39	115.92
14	A	1103	CLA	CMC-C2C-C1C	2.02	128.12	125.04
14	a	1113	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
14	H	1223	CLA	CHD-C4C-C3C	-2.02	121.87	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	1223	CLA	CHA-C1A-NA	-2.02	121.77	126.40
14	b	1202	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
14	H	1204	CLA	OBD-CAD-C3D	-2.02	123.66	128.52
14	H	1239	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
14	G	1128	CLA	C3D-C4D-ND	2.02	113.50	110.24
14	G	1140	CLA	C4C-C3C-C2C	-2.02	103.96	106.90
14	B	1231	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
14	H	1226	CLA	CMA-C3A-C4A	2.02	117.19	111.77
14	L	1501	CLA	C6-C7-C8	-2.02	109.40	115.92
14	a	1135	CLA	CHA-C4D-ND	2.02	136.72	132.50
14	b	1226	CLA	CMA-C3A-C4A	2.02	117.19	111.77
14	L	1503	CLA	C1-O2A-CGA	2.01	121.73	116.44
18	V	4021	BCR	C33-C5-C4	2.01	117.49	113.62
14	l	1501	CLA	C1-O2A-CGA	2.01	121.73	116.44
14	H	1021	CLA	C11-C10-C8	-2.01	109.41	115.92
14	a	1104	CLA	CAC-C3C-C2C	2.01	130.97	127.53
14	a	1137	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
14	a	1117	CLA	C3C-C4C-NC	2.01	112.83	110.57
14	B	1216	CLA	CHC-C1C-C2C	-2.01	121.15	126.72
14	H	1023	CLA	C6-C5-C3	-2.01	108.18	113.45
14	B	1023	CLA	C6-C5-C3	-2.01	108.18	113.45
14	a	1128	CLA	C3D-C4D-ND	2.01	113.49	110.24
14	A	1104	CLA	CAC-C3C-C2C	2.01	130.97	127.53
14	l	1503	CLA	C1-O2A-CGA	2.01	121.72	116.44
14	b	1231	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
18	B	4014	BCR	C34-C9-C8	2.01	121.25	118.08
14	A	1123	CLA	CHA-C1A-NA	-2.01	121.79	126.40
14	H	1233	CLA	CAC-C3C-C4C	2.01	127.42	124.81
14	H	1202	CLA	C4C-C3C-C2C	-2.01	103.96	106.90
14	H	1225	CLA	C1-O2A-CGA	2.01	121.72	116.44
18	M	4021	BCR	C33-C5-C4	2.01	117.48	113.62
14	A	1130	CLA	CHA-C1A-NA	-2.01	121.79	126.40
14	a	1115	CLA	CMA-C3A-C4A	2.01	117.18	111.77
14	b	1205	CLA	CMA-C3A-C4A	2.01	117.18	111.77
14	a	1123	CLA	CHA-C1A-NA	-2.01	121.79	126.40
18	A	4008	BCR	C27-C26-C25	-2.01	119.81	122.73
14	H	1214	CLA	CHC-C1C-C2C	-2.01	121.16	126.72
14	b	1216	CLA	CHC-C1C-C2C	-2.01	121.16	126.72
14	b	1202	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
14	B	1202	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
14	A	1137	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
14	G	1103	CLA	C4-C3-C2	-2.01	118.53	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	U	1501	CLA	C1-O2A-CGA	2.01	121.71	116.44
14	b	1206	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
18	a	4001	BCR	C29-C30-C25	2.01	113.57	110.48
14	G	1127	CLA	C4D-C3D-CAD	2.01	110.46	108.10
14	l	1503	CLA	CAC-C3C-C4C	2.01	127.41	124.81
13	a	1011	CL0	C4D-C3D-CAD	2.01	110.46	108.10
14	a	1103	CLA	C4D-C3D-CAD	2.01	110.46	108.10
14	H	1205	CLA	CMA-C3A-C4A	2.01	117.16	111.77
18	m	4021	BCR	C33-C5-C4	2.01	117.47	113.62
14	b	1220	CLA	C4D-C3D-CAD	2.00	110.46	108.10
18	b	4009	BCR	C35-C13-C14	-2.00	120.11	122.92
14	B	1223	CLA	C4C-C3C-C2C	-2.00	103.98	106.90
18	B	4009	BCR	C1-C6-C5	-2.00	119.79	122.61
14	b	1225	CLA	C1-O2A-CGA	2.00	121.70	116.44
14	B	1216	CLA	C4D-C3D-CAD	2.00	110.46	108.10
14	B	1227	CLA	CHA-C4D-ND	2.00	136.69	132.50
18	b	4014	BCR	C34-C9-C8	2.00	121.23	118.08
14	B	1211	CLA	CBC-CAC-C3C	-2.00	106.91	112.43
18	H	4009	BCR	C1-C6-C5	-2.00	119.79	122.61
14	H	1202	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
14	b	1239	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
14	b	1211	CLA	CBC-CAC-C3C	-2.00	106.91	112.43
14	B	1233	CLA	CAC-C3C-C4C	2.00	127.41	124.81
14	a	1140	CLA	C4C-C3C-C2C	-2.00	103.98	106.90
14	B	1233	CLA	CMB-C2B-C3B	2.00	128.42	124.68

All (261) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	G	1011	CL0	NC
13	G	1011	CL0	ND
13	G	1011	CL0	NA
13	a	1011	CL0	NC
13	a	1011	CL0	ND
13	a	1011	CL0	NA
13	A	1011	CL0	NC
13	A	1011	CL0	ND
13	A	1011	CL0	NA
14	G	1012	CLA	ND
14	G	1013	CLA	ND
14	G	1101	CLA	ND
14	G	1102	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
14	G	1103	CLA	ND
14	G	1104	CLA	ND
14	G	1105	CLA	ND
14	G	1106	CLA	ND
14	G	1107	CLA	ND
14	G	1108	CLA	ND
14	G	1109	CLA	ND
14	G	1110	CLA	ND
14	G	1111	CLA	ND
14	G	1112	CLA	ND
14	G	1113	CLA	ND
14	G	1114	CLA	ND
14	G	1115	CLA	ND
14	G	1116	CLA	ND
14	G	1117	CLA	ND
14	G	1118	CLA	ND
14	G	1119	CLA	ND
14	G	1120	CLA	ND
14	G	1122	CLA	ND
14	G	1123	CLA	ND
14	G	1124	CLA	ND
14	G	1125	CLA	ND
14	G	1126	CLA	ND
14	G	1127	CLA	ND
14	G	1128	CLA	ND
14	G	1129	CLA	ND
14	G	1130	CLA	ND
14	G	1131	CLA	ND
14	G	1132	CLA	ND
14	G	1133	CLA	ND
14	G	1134	CLA	ND
14	G	1135	CLA	ND
14	G	1136	CLA	ND
14	G	1137	CLA	ND
14	G	1138	CLA	ND
14	G	1139	CLA	ND
14	G	1140	CLA	ND
14	H	1021	CLA	ND
14	H	1022	CLA	ND
14	H	1023	CLA	ND
14	H	1201	CLA	ND
14	H	1202	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
14	H	1203	CLA	ND
14	H	1204	CLA	ND
14	H	1205	CLA	ND
14	H	1206	CLA	ND
14	H	1208	CLA	ND
14	H	1209	CLA	ND
14	H	1210	CLA	ND
14	H	1211	CLA	ND
14	H	1212	CLA	ND
14	H	1213	CLA	ND
14	H	1214	CLA	ND
14	H	1215	CLA	ND
14	H	1216	CLA	ND
14	H	1217	CLA	ND
14	H	1218	CLA	ND
14	H	1219	CLA	ND
14	H	1220	CLA	ND
14	H	1221	CLA	ND
14	H	1222	CLA	ND
14	H	1223	CLA	ND
14	H	1224	CLA	ND
14	H	1225	CLA	ND
14	H	1226	CLA	ND
14	H	1227	CLA	ND
14	H	1228	CLA	ND
14	H	1229	CLA	ND
14	H	1231	CLA	ND
14	H	1232	CLA	ND
14	H	1233	CLA	ND
14	H	1234	CLA	ND
14	H	1235	CLA	ND
14	H	1236	CLA	ND
14	H	1239	CLA	ND
14	T	1401	CLA	ND
14	U	1501	CLA	ND
14	U	1502	CLA	ND
14	U	1503	CLA	ND
14	W	1701	CLA	ND
14	a	1012	CLA	ND
14	a	1013	CLA	ND
14	a	1101	CLA	ND
14	a	1102	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
14	a	1103	CLA	ND
14	a	1104	CLA	ND
14	a	1105	CLA	ND
14	a	1106	CLA	ND
14	a	1107	CLA	ND
14	a	1108	CLA	ND
14	a	1109	CLA	ND
14	a	1110	CLA	ND
14	a	1111	CLA	ND
14	a	1112	CLA	ND
14	a	1113	CLA	ND
14	a	1114	CLA	ND
14	a	1115	CLA	ND
14	a	1116	CLA	ND
14	a	1117	CLA	ND
14	a	1118	CLA	ND
14	a	1119	CLA	ND
14	a	1120	CLA	ND
14	a	1122	CLA	ND
14	a	1123	CLA	ND
14	a	1124	CLA	ND
14	a	1125	CLA	ND
14	a	1126	CLA	ND
14	a	1127	CLA	ND
14	a	1128	CLA	ND
14	a	1129	CLA	ND
14	a	1130	CLA	ND
14	a	1131	CLA	ND
14	a	1132	CLA	ND
14	a	1133	CLA	ND
14	a	1134	CLA	ND
14	a	1135	CLA	ND
14	a	1136	CLA	ND
14	a	1137	CLA	ND
14	a	1138	CLA	ND
14	a	1139	CLA	ND
14	a	1140	CLA	ND
14	b	1021	CLA	ND
14	b	1022	CLA	ND
14	b	1023	CLA	ND
14	b	1201	CLA	ND
14	b	1202	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
14	b	1203	CLA	ND
14	b	1204	CLA	ND
14	b	1205	CLA	ND
14	b	1206	CLA	ND
14	b	1208	CLA	ND
14	b	1209	CLA	ND
14	b	1210	CLA	ND
14	b	1211	CLA	ND
14	b	1212	CLA	ND
14	b	1213	CLA	ND
14	b	1214	CLA	ND
14	b	1215	CLA	ND
14	b	1216	CLA	ND
14	b	1217	CLA	ND
14	b	1218	CLA	ND
14	b	1219	CLA	ND
14	b	1220	CLA	ND
14	b	1221	CLA	ND
14	b	1222	CLA	ND
14	b	1223	CLA	ND
14	b	1224	CLA	ND
14	b	1225	CLA	ND
14	b	1226	CLA	ND
14	b	1227	CLA	ND
14	b	1228	CLA	ND
14	b	1229	CLA	ND
14	b	1231	CLA	ND
14	b	1232	CLA	ND
14	b	1233	CLA	ND
14	b	1234	CLA	ND
14	b	1235	CLA	ND
14	b	1236	CLA	ND
14	b	1239	CLA	ND
14	k	1401	CLA	ND
14	l	1501	CLA	ND
14	l	1502	CLA	ND
14	l	1503	CLA	ND
14	x	1701	CLA	ND
14	A	1012	CLA	ND
14	A	1013	CLA	ND
14	A	1101	CLA	ND
14	A	1102	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
14	A	1103	CLA	ND
14	A	1104	CLA	ND
14	A	1105	CLA	ND
14	A	1106	CLA	ND
14	A	1107	CLA	ND
14	A	1108	CLA	ND
14	A	1109	CLA	ND
14	A	1110	CLA	ND
14	A	1111	CLA	ND
14	A	1112	CLA	ND
14	A	1113	CLA	ND
14	A	1114	CLA	ND
14	A	1115	CLA	ND
14	A	1116	CLA	ND
14	A	1117	CLA	ND
14	A	1118	CLA	ND
14	A	1119	CLA	ND
14	A	1120	CLA	ND
14	A	1122	CLA	ND
14	A	1123	CLA	ND
14	A	1124	CLA	ND
14	A	1125	CLA	ND
14	A	1126	CLA	ND
14	A	1127	CLA	ND
14	A	1128	CLA	ND
14	A	1129	CLA	ND
14	A	1130	CLA	ND
14	A	1131	CLA	ND
14	A	1132	CLA	ND
14	A	1133	CLA	ND
14	A	1134	CLA	ND
14	A	1135	CLA	ND
14	A	1136	CLA	ND
14	A	1137	CLA	ND
14	A	1138	CLA	ND
14	A	1139	CLA	ND
14	A	1140	CLA	ND
14	B	1021	CLA	ND
14	B	1022	CLA	ND
14	B	1023	CLA	ND
14	B	1201	CLA	ND
14	B	1202	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
14	B	1203	CLA	ND
14	B	1204	CLA	ND
14	B	1205	CLA	ND
14	B	1206	CLA	ND
14	B	1208	CLA	ND
14	B	1209	CLA	ND
14	B	1210	CLA	ND
14	B	1211	CLA	ND
14	B	1212	CLA	ND
14	B	1213	CLA	ND
14	B	1214	CLA	ND
14	B	1215	CLA	ND
14	B	1216	CLA	ND
14	B	1217	CLA	ND
14	B	1218	CLA	ND
14	B	1219	CLA	ND
14	B	1220	CLA	ND
14	B	1221	CLA	ND
14	B	1222	CLA	ND
14	B	1223	CLA	ND
14	B	1224	CLA	ND
14	B	1225	CLA	ND
14	B	1226	CLA	ND
14	B	1227	CLA	ND
14	B	1228	CLA	ND
14	B	1229	CLA	ND
14	B	1231	CLA	ND
14	B	1232	CLA	ND
14	B	1233	CLA	ND
14	B	1234	CLA	ND
14	B	1235	CLA	ND
14	B	1236	CLA	ND
14	B	1239	CLA	ND
14	K	1401	CLA	ND
14	L	1501	CLA	ND
14	L	1502	CLA	ND
14	L	1503	CLA	ND
14	X	1701	CLA	ND

All (4427) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
14	G	1013	CLA	C1A-C2A-CAA-CBA
14	G	1013	CLA	C3A-C2A-CAA-CBA
14	G	1013	CLA	C11-C10-C8-C9
14	G	1101	CLA	CHA-CBD-CGD-O2D
14	G	1102	CLA	C1A-C2A-CAA-CBA
14	G	1102	CLA	CBA-CGA-O2A-C1
14	G	1102	CLA	O1A-CGA-O2A-C1
14	G	1103	CLA	CHA-CBD-CGD-O1D
14	G	1103	CLA	CHA-CBD-CGD-O2D
14	G	1103	CLA	CAD-CBD-CGD-O1D
14	G	1106	CLA	C3A-C2A-CAA-CBA
14	G	1106	CLA	C2A-CAA-CBA-CGA
14	G	1106	CLA	CHA-CBD-CGD-O2D
14	G	1107	CLA	CBD-CGD-O2D-CED
14	G	1108	CLA	CHA-CBD-CGD-O1D
14	G	1108	CLA	CHA-CBD-CGD-O2D
14	G	1108	CLA	CBD-CGD-O2D-CED
14	G	1109	CLA	C1A-C2A-CAA-CBA
14	G	1109	CLA	C3A-C2A-CAA-CBA
14	G	1109	CLA	C2A-CAA-CBA-CGA
14	G	1111	CLA	CBA-CGA-O2A-C1
14	G	1111	CLA	O1A-CGA-O2A-C1
14	G	1112	CLA	C1A-C2A-CAA-CBA
14	G	1112	CLA	C2-C1-O2A-CGA
14	G	1114	CLA	C1A-C2A-CAA-CBA
14	G	1114	CLA	C3A-C2A-CAA-CBA
14	G	1115	CLA	C1A-C2A-CAA-CBA
14	G	1115	CLA	C3A-C2A-CAA-CBA
14	G	1115	CLA	CHA-CBD-CGD-O2D
14	G	1116	CLA	C3A-C2A-CAA-CBA
14	G	1117	CLA	C1A-C2A-CAA-CBA
14	G	1117	CLA	C3A-C2A-CAA-CBA
14	G	1117	CLA	CBD-CGD-O2D-CED
14	G	1118	CLA	C2-C1-O2A-CGA
14	G	1119	CLA	CHA-CBD-CGD-O1D
14	G	1119	CLA	CHA-CBD-CGD-O2D
14	G	1119	CLA	CBD-CGD-O2D-CED
14	G	1120	CLA	C1A-C2A-CAA-CBA
14	G	1120	CLA	C3A-C2A-CAA-CBA
14	G	1122	CLA	C2-C3-C5-C6
14	G	1122	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	G	1123	CLA	C2A-CAA-CBA-CGA
14	G	1124	CLA	C1A-C2A-CAA-CBA
14	G	1125	CLA	C1A-C2A-CAA-CBA
14	G	1126	CLA	CHA-CBD-CGD-O1D
14	G	1126	CLA	CHA-CBD-CGD-O2D
14	G	1127	CLA	C1A-C2A-CAA-CBA
14	G	1127	CLA	C2A-CAA-CBA-CGA
14	G	1128	CLA	CHA-CBD-CGD-O1D
14	G	1128	CLA	CHA-CBD-CGD-O2D
14	G	1128	CLA	C2-C3-C5-C6
14	G	1128	CLA	C4-C3-C5-C6
14	G	1130	CLA	C1A-C2A-CAA-CBA
14	G	1131	CLA	C2-C1-O2A-CGA
14	G	1132	CLA	CBD-CGD-O2D-CED
14	G	1133	CLA	O1A-CGA-O2A-C1
14	G	1135	CLA	C3A-C2A-CAA-CBA
14	G	1137	CLA	C2-C1-O2A-CGA
14	G	1138	CLA	C1A-C2A-CAA-CBA
14	G	1140	CLA	C1A-C2A-CAA-CBA
14	G	1140	CLA	C3A-C2A-CAA-CBA
14	G	1140	CLA	C6-C7-C8-C9
14	H	1021	CLA	CHA-CBD-CGD-O1D
14	H	1021	CLA	CHA-CBD-CGD-O2D
14	H	1201	CLA	C4-C3-C5-C6
14	H	1203	CLA	C1A-C2A-CAA-CBA
14	H	1204	CLA	CHA-CBD-CGD-O1D
14	H	1204	CLA	CHA-CBD-CGD-O2D
14	H	1206	CLA	C1A-C2A-CAA-CBA
14	H	1206	CLA	C3A-C2A-CAA-CBA
14	H	1209	CLA	C1A-C2A-CAA-CBA
14	H	1210	CLA	C1A-C2A-CAA-CBA
14	H	1210	CLA	C2-C1-O2A-CGA
14	H	1210	CLA	CHA-CBD-CGD-O1D
14	H	1211	CLA	C2-C1-O2A-CGA
14	H	1213	CLA	CHA-CBD-CGD-O1D
14	H	1213	CLA	CHA-CBD-CGD-O2D
14	H	1213	CLA	C2-C3-C5-C6
14	H	1213	CLA	C4-C3-C5-C6
14	H	1213	CLA	C6-C7-C8-C9
14	H	1214	CLA	C2A-CAA-CBA-CGA
14	H	1215	CLA	C3A-C2A-CAA-CBA
14	H	1216	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	H	1216	CLA	C3A-C2A-CAA-CBA
14	H	1216	CLA	C2A-CAA-CBA-CGA
14	H	1216	CLA	C2-C3-C5-C6
14	H	1216	CLA	C4-C3-C5-C6
14	H	1217	CLA	C1A-C2A-CAA-CBA
14	H	1217	CLA	C3A-C2A-CAA-CBA
14	H	1217	CLA	CBD-CGD-O2D-CED
14	H	1221	CLA	C1A-C2A-CAA-CBA
14	H	1224	CLA	CHA-CBD-CGD-O1D
14	H	1224	CLA	CHA-CBD-CGD-O2D
14	H	1225	CLA	C1A-C2A-CAA-CBA
14	H	1225	CLA	C3A-C2A-CAA-CBA
14	H	1226	CLA	C2-C1-O2A-CGA
14	H	1227	CLA	C3A-C2A-CAA-CBA
14	H	1228	CLA	C1A-C2A-CAA-CBA
14	H	1228	CLA	CHA-CBD-CGD-O1D
14	H	1229	CLA	C2-C1-O2A-CGA
14	H	1229	CLA	C2-C3-C5-C6
14	H	1229	CLA	C4-C3-C5-C6
14	H	1233	CLA	CHA-CBD-CGD-O1D
14	H	1233	CLA	CHA-CBD-CGD-O2D
14	T	1401	CLA	C1A-C2A-CAA-CBA
14	T	1401	CLA	C3A-C2A-CAA-CBA
14	T	1401	CLA	CHA-CBD-CGD-O1D
14	T	1401	CLA	CHA-CBD-CGD-O2D
14	U	1501	CLA	CHA-CBD-CGD-O1D
14	U	1501	CLA	CHA-CBD-CGD-O2D
14	U	1502	CLA	CHA-CBD-CGD-O1D
14	U	1502	CLA	CHA-CBD-CGD-O2D
14	U	1503	CLA	C1A-C2A-CAA-CBA
14	U	1503	CLA	CBA-CGA-O2A-C1
14	U	1503	CLA	O1A-CGA-O2A-C1
14	U	1503	CLA	C2-C3-C5-C6
14	U	1503	CLA	C4-C3-C5-C6
14	W	1701	CLA	C4-C3-C5-C6
14	a	1013	CLA	C1A-C2A-CAA-CBA
14	a	1013	CLA	C3A-C2A-CAA-CBA
14	a	1013	CLA	C11-C10-C8-C9
14	a	1101	CLA	CHA-CBD-CGD-O2D
14	a	1102	CLA	C1A-C2A-CAA-CBA
14	a	1102	CLA	CBA-CGA-O2A-C1
14	a	1102	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	1103	CLA	CHA-CBD-CGD-O1D
14	a	1103	CLA	CHA-CBD-CGD-O2D
14	a	1103	CLA	CAD-CBD-CGD-O1D
14	a	1106	CLA	C3A-C2A-CAA-CBA
14	a	1106	CLA	C2A-CAA-CBA-CGA
14	a	1106	CLA	CHA-CBD-CGD-O2D
14	a	1107	CLA	CBD-CGD-O2D-CED
14	a	1108	CLA	CHA-CBD-CGD-O1D
14	a	1108	CLA	CHA-CBD-CGD-O2D
14	a	1108	CLA	CBD-CGD-O2D-CED
14	a	1109	CLA	C1A-C2A-CAA-CBA
14	a	1109	CLA	C3A-C2A-CAA-CBA
14	a	1109	CLA	C2A-CAA-CBA-CGA
14	a	1111	CLA	CBA-CGA-O2A-C1
14	a	1111	CLA	O1A-CGA-O2A-C1
14	a	1112	CLA	C1A-C2A-CAA-CBA
14	a	1112	CLA	C2-C1-O2A-CGA
14	a	1114	CLA	C1A-C2A-CAA-CBA
14	a	1114	CLA	C3A-C2A-CAA-CBA
14	a	1115	CLA	C1A-C2A-CAA-CBA
14	a	1115	CLA	C3A-C2A-CAA-CBA
14	a	1115	CLA	CHA-CBD-CGD-O2D
14	a	1116	CLA	C3A-C2A-CAA-CBA
14	a	1117	CLA	C1A-C2A-CAA-CBA
14	a	1117	CLA	C3A-C2A-CAA-CBA
14	a	1117	CLA	CBD-CGD-O2D-CED
14	a	1118	CLA	C2-C1-O2A-CGA
14	a	1119	CLA	CHA-CBD-CGD-O1D
14	a	1119	CLA	CHA-CBD-CGD-O2D
14	a	1119	CLA	CBD-CGD-O2D-CED
14	a	1120	CLA	C1A-C2A-CAA-CBA
14	a	1120	CLA	C3A-C2A-CAA-CBA
14	a	1122	CLA	C2-C3-C5-C6
14	a	1122	CLA	C4-C3-C5-C6
14	a	1123	CLA	C2A-CAA-CBA-CGA
14	a	1124	CLA	C1A-C2A-CAA-CBA
14	a	1125	CLA	C1A-C2A-CAA-CBA
14	a	1126	CLA	CHA-CBD-CGD-O1D
14	a	1126	CLA	CHA-CBD-CGD-O2D
14	a	1127	CLA	C1A-C2A-CAA-CBA
14	a	1127	CLA	C2A-CAA-CBA-CGA
14	a	1128	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	a	1128	CLA	CHA-CBD-CGD-O2D
14	a	1128	CLA	C2-C3-C5-C6
14	a	1128	CLA	C4-C3-C5-C6
14	a	1130	CLA	C1A-C2A-CAA-CBA
14	a	1131	CLA	C2-C1-O2A-CGA
14	a	1132	CLA	CBD-CGD-O2D-CED
14	a	1133	CLA	O1A-CGA-O2A-C1
14	a	1135	CLA	C3A-C2A-CAA-CBA
14	a	1137	CLA	C2-C1-O2A-CGA
14	a	1138	CLA	C1A-C2A-CAA-CBA
14	a	1140	CLA	C1A-C2A-CAA-CBA
14	a	1140	CLA	C3A-C2A-CAA-CBA
14	a	1140	CLA	C6-C7-C8-C9
14	b	1021	CLA	CHA-CBD-CGD-O1D
14	b	1021	CLA	CHA-CBD-CGD-O2D
14	b	1201	CLA	C4-C3-C5-C6
14	b	1203	CLA	C1A-C2A-CAA-CBA
14	b	1204	CLA	CHA-CBD-CGD-O1D
14	b	1204	CLA	CHA-CBD-CGD-O2D
14	b	1206	CLA	C1A-C2A-CAA-CBA
14	b	1206	CLA	C3A-C2A-CAA-CBA
14	b	1209	CLA	C1A-C2A-CAA-CBA
14	b	1210	CLA	C1A-C2A-CAA-CBA
14	b	1210	CLA	C2-C1-O2A-CGA
14	b	1210	CLA	CHA-CBD-CGD-O1D
14	b	1211	CLA	C2-C1-O2A-CGA
14	b	1213	CLA	CHA-CBD-CGD-O1D
14	b	1213	CLA	CHA-CBD-CGD-O2D
14	b	1213	CLA	C2-C3-C5-C6
14	b	1213	CLA	C4-C3-C5-C6
14	b	1213	CLA	C6-C7-C8-C9
14	b	1214	CLA	C2A-CAA-CBA-CGA
14	b	1215	CLA	C3A-C2A-CAA-CBA
14	b	1216	CLA	C1A-C2A-CAA-CBA
14	b	1216	CLA	C3A-C2A-CAA-CBA
14	b	1216	CLA	C2A-CAA-CBA-CGA
14	b	1216	CLA	C2-C3-C5-C6
14	b	1216	CLA	C4-C3-C5-C6
14	b	1217	CLA	C1A-C2A-CAA-CBA
14	b	1217	CLA	C3A-C2A-CAA-CBA
14	b	1217	CLA	CBD-CGD-O2D-CED
14	b	1221	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	b	1224	CLA	CHA-CBD-CGD-O1D
14	b	1224	CLA	CHA-CBD-CGD-O2D
14	b	1225	CLA	C1A-C2A-CAA-CBA
14	b	1225	CLA	C3A-C2A-CAA-CBA
14	b	1226	CLA	C2-C1-O2A-CGA
14	b	1227	CLA	C3A-C2A-CAA-CBA
14	b	1228	CLA	C1A-C2A-CAA-CBA
14	b	1228	CLA	CHA-CBD-CGD-O1D
14	b	1229	CLA	C2-C1-O2A-CGA
14	b	1229	CLA	C2-C3-C5-C6
14	b	1229	CLA	C4-C3-C5-C6
14	b	1233	CLA	CHA-CBD-CGD-O1D
14	b	1233	CLA	CHA-CBD-CGD-O2D
14	k	1401	CLA	C1A-C2A-CAA-CBA
14	k	1401	CLA	C3A-C2A-CAA-CBA
14	k	1401	CLA	CHA-CBD-CGD-O1D
14	k	1401	CLA	CHA-CBD-CGD-O2D
14	l	1501	CLA	CHA-CBD-CGD-O1D
14	l	1501	CLA	CHA-CBD-CGD-O2D
14	l	1502	CLA	CHA-CBD-CGD-O1D
14	l	1502	CLA	CHA-CBD-CGD-O2D
14	l	1503	CLA	C1A-C2A-CAA-CBA
14	l	1503	CLA	CBA-CGA-O2A-C1
14	l	1503	CLA	O1A-CGA-O2A-C1
14	l	1503	CLA	C2-C3-C5-C6
14	l	1503	CLA	C4-C3-C5-C6
14	x	1701	CLA	C4-C3-C5-C6
14	A	1013	CLA	C1A-C2A-CAA-CBA
14	A	1013	CLA	C3A-C2A-CAA-CBA
14	A	1013	CLA	C11-C10-C8-C9
14	A	1101	CLA	CHA-CBD-CGD-O2D
14	A	1102	CLA	C1A-C2A-CAA-CBA
14	A	1102	CLA	CBA-CGA-O2A-C1
14	A	1102	CLA	O1A-CGA-O2A-C1
14	A	1103	CLA	CHA-CBD-CGD-O1D
14	A	1103	CLA	CHA-CBD-CGD-O2D
14	A	1103	CLA	CAD-CBD-CGD-O1D
14	A	1106	CLA	C3A-C2A-CAA-CBA
14	A	1106	CLA	C2A-CAA-CBA-CGA
14	A	1106	CLA	CHA-CBD-CGD-O2D
14	A	1107	CLA	CBD-CGD-O2D-CED
14	A	1108	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	A	1108	CLA	CHA-CBD-CGD-O2D
14	A	1108	CLA	CBD-CGD-O2D-CED
14	A	1109	CLA	C1A-C2A-CAA-CBA
14	A	1109	CLA	C3A-C2A-CAA-CBA
14	A	1109	CLA	C2A-CAA-CBA-CGA
14	A	1111	CLA	CBA-CGA-O2A-C1
14	A	1111	CLA	O1A-CGA-O2A-C1
14	A	1112	CLA	C1A-C2A-CAA-CBA
14	A	1112	CLA	C2-C1-O2A-CGA
14	A	1114	CLA	C1A-C2A-CAA-CBA
14	A	1114	CLA	C3A-C2A-CAA-CBA
14	A	1115	CLA	C1A-C2A-CAA-CBA
14	A	1115	CLA	C3A-C2A-CAA-CBA
14	A	1115	CLA	CHA-CBD-CGD-O2D
14	A	1116	CLA	C3A-C2A-CAA-CBA
14	A	1117	CLA	C1A-C2A-CAA-CBA
14	A	1117	CLA	C3A-C2A-CAA-CBA
14	A	1117	CLA	CBD-CGD-O2D-CED
14	A	1118	CLA	C2-C1-O2A-CGA
14	A	1119	CLA	CHA-CBD-CGD-O1D
14	A	1119	CLA	CHA-CBD-CGD-O2D
14	A	1119	CLA	CBD-CGD-O2D-CED
14	A	1120	CLA	C1A-C2A-CAA-CBA
14	A	1120	CLA	C3A-C2A-CAA-CBA
14	A	1122	CLA	C2-C3-C5-C6
14	A	1122	CLA	C4-C3-C5-C6
14	A	1123	CLA	C2A-CAA-CBA-CGA
14	A	1124	CLA	C1A-C2A-CAA-CBA
14	A	1125	CLA	C1A-C2A-CAA-CBA
14	A	1126	CLA	CHA-CBD-CGD-O1D
14	A	1126	CLA	CHA-CBD-CGD-O2D
14	A	1127	CLA	C1A-C2A-CAA-CBA
14	A	1127	CLA	C2A-CAA-CBA-CGA
14	A	1128	CLA	CHA-CBD-CGD-O1D
14	A	1128	CLA	CHA-CBD-CGD-O2D
14	A	1128	CLA	C2-C3-C5-C6
14	A	1128	CLA	C4-C3-C5-C6
14	A	1130	CLA	C1A-C2A-CAA-CBA
14	A	1131	CLA	C2-C1-O2A-CGA
14	A	1132	CLA	CBD-CGD-O2D-CED
14	A	1133	CLA	O1A-CGA-O2A-C1
14	A	1135	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	A	1137	CLA	C2-C1-O2A-CGA
14	A	1138	CLA	C1A-C2A-CAA-CBA
14	A	1140	CLA	C1A-C2A-CAA-CBA
14	A	1140	CLA	C3A-C2A-CAA-CBA
14	A	1140	CLA	C6-C7-C8-C9
14	B	1021	CLA	CHA-CBD-CGD-O1D
14	B	1021	CLA	CHA-CBD-CGD-O2D
14	B	1201	CLA	C4-C3-C5-C6
14	B	1203	CLA	C1A-C2A-CAA-CBA
14	B	1204	CLA	CHA-CBD-CGD-O1D
14	B	1204	CLA	CHA-CBD-CGD-O2D
14	B	1206	CLA	C1A-C2A-CAA-CBA
14	B	1206	CLA	C3A-C2A-CAA-CBA
14	B	1209	CLA	C1A-C2A-CAA-CBA
14	B	1210	CLA	C1A-C2A-CAA-CBA
14	B	1210	CLA	C2-C1-O2A-CGA
14	B	1210	CLA	CHA-CBD-CGD-O1D
14	B	1211	CLA	C2-C1-O2A-CGA
14	B	1213	CLA	CHA-CBD-CGD-O1D
14	B	1213	CLA	CHA-CBD-CGD-O2D
14	B	1213	CLA	C2-C3-C5-C6
14	B	1213	CLA	C4-C3-C5-C6
14	B	1213	CLA	C6-C7-C8-C9
14	B	1214	CLA	C2A-CAA-CBA-CGA
14	B	1215	CLA	C3A-C2A-CAA-CBA
14	B	1216	CLA	C1A-C2A-CAA-CBA
14	B	1216	CLA	C3A-C2A-CAA-CBA
14	B	1216	CLA	C2A-CAA-CBA-CGA
14	B	1216	CLA	C2-C3-C5-C6
14	B	1216	CLA	C4-C3-C5-C6
14	B	1217	CLA	C1A-C2A-CAA-CBA
14	B	1217	CLA	C3A-C2A-CAA-CBA
14	B	1217	CLA	CBD-CGD-O2D-CED
14	B	1221	CLA	C1A-C2A-CAA-CBA
14	B	1224	CLA	CHA-CBD-CGD-O1D
14	B	1224	CLA	CHA-CBD-CGD-O2D
14	B	1225	CLA	C1A-C2A-CAA-CBA
14	B	1225	CLA	C3A-C2A-CAA-CBA
14	B	1226	CLA	C2-C1-O2A-CGA
14	B	1227	CLA	C3A-C2A-CAA-CBA
14	B	1228	CLA	C1A-C2A-CAA-CBA
14	B	1228	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	B	1229	CLA	C2-C1-O2A-CGA
14	B	1229	CLA	C2-C3-C5-C6
14	B	1229	CLA	C4-C3-C5-C6
14	B	1233	CLA	CHA-CBD-CGD-O1D
14	B	1233	CLA	CHA-CBD-CGD-O2D
14	K	1401	CLA	C1A-C2A-CAA-CBA
14	K	1401	CLA	C3A-C2A-CAA-CBA
14	K	1401	CLA	CHA-CBD-CGD-O1D
14	K	1401	CLA	CHA-CBD-CGD-O2D
14	L	1501	CLA	CHA-CBD-CGD-O1D
14	L	1501	CLA	CHA-CBD-CGD-O2D
14	L	1502	CLA	CHA-CBD-CGD-O1D
14	L	1502	CLA	CHA-CBD-CGD-O2D
14	L	1503	CLA	C1A-C2A-CAA-CBA
14	L	1503	CLA	CBA-CGA-O2A-C1
14	L	1503	CLA	O1A-CGA-O2A-C1
14	L	1503	CLA	C2-C3-C5-C6
14	L	1503	CLA	C4-C3-C5-C6
14	X	1701	CLA	C4-C3-C5-C6
15	G	1121	F6C	C1A-C2A-CAA-CBA
15	G	1121	F6C	C3A-C2A-CAA-CBA
15	G	1121	F6C	C4B-C3B-CAB-CBB
15	G	1121	F6C	CBD-CGD-O2D-CED
15	H	1207	F6C	CAD-CBD-CGD-O1D
15	H	1207	F6C	CAD-CBD-CGD-O2D
15	H	1207	F6C	C1B-C2B-CMB-OMB
15	H	1207	F6C	C3B-C2B-CMB-OMB
15	H	1230	F6C	C1B-C2B-CMB-OMB
15	H	1230	F6C	C3B-C2B-CMB-OMB
15	H	1237	F6C	CHA-CBD-CGD-O1D
15	H	1237	F6C	CHA-CBD-CGD-O2D
15	H	1237	F6C	CBA-CGA-O2A-C1
15	H	1237	F6C	O1A-CGA-O2A-C1
15	H	1237	F6C	C1B-C2B-CMB-OMB
15	H	1237	F6C	C3B-C2B-CMB-OMB
15	H	1237	F6C	C2-C3-C5-C6
15	H	1237	F6C	C4-C3-C5-C6
15	H	1238	F6C	C1B-C2B-CMB-OMB
15	H	1238	F6C	C3B-C2B-CMB-OMB
15	a	1121	F6C	C1A-C2A-CAA-CBA
15	a	1121	F6C	C3A-C2A-CAA-CBA
15	a	1121	F6C	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	a	1121	F6C	CBD-CGD-O2D-CED
15	b	1207	F6C	CAD-CBD-CGD-O1D
15	b	1207	F6C	CAD-CBD-CGD-O2D
15	b	1207	F6C	C1B-C2B-CMB-OMB
15	b	1207	F6C	C3B-C2B-CMB-OMB
15	b	1230	F6C	C1B-C2B-CMB-OMB
15	b	1230	F6C	C3B-C2B-CMB-OMB
15	b	1237	F6C	CHA-CBD-CGD-O1D
15	b	1237	F6C	CHA-CBD-CGD-O2D
15	b	1237	F6C	CBA-CGA-O2A-C1
15	b	1237	F6C	O1A-CGA-O2A-C1
15	b	1237	F6C	C1B-C2B-CMB-OMB
15	b	1237	F6C	C3B-C2B-CMB-OMB
15	b	1237	F6C	C2-C3-C5-C6
15	b	1237	F6C	C4-C3-C5-C6
15	b	1238	F6C	C1B-C2B-CMB-OMB
15	b	1238	F6C	C3B-C2B-CMB-OMB
15	A	1121	F6C	C1A-C2A-CAA-CBA
15	A	1121	F6C	C3A-C2A-CAA-CBA
15	A	1121	F6C	C4B-C3B-CAB-CBB
15	A	1121	F6C	CBD-CGD-O2D-CED
15	B	1207	F6C	CAD-CBD-CGD-O1D
15	B	1207	F6C	CAD-CBD-CGD-O2D
15	B	1207	F6C	C1B-C2B-CMB-OMB
15	B	1207	F6C	C3B-C2B-CMB-OMB
15	B	1230	F6C	C1B-C2B-CMB-OMB
15	B	1230	F6C	C3B-C2B-CMB-OMB
15	B	1237	F6C	CHA-CBD-CGD-O1D
15	B	1237	F6C	CHA-CBD-CGD-O2D
15	B	1237	F6C	CBA-CGA-O2A-C1
15	B	1237	F6C	O1A-CGA-O2A-C1
15	B	1237	F6C	C1B-C2B-CMB-OMB
15	B	1237	F6C	C3B-C2B-CMB-OMB
15	B	1237	F6C	C2-C3-C5-C6
15	B	1237	F6C	C4-C3-C5-C6
15	B	1238	F6C	C1B-C2B-CMB-OMB
15	B	1238	F6C	C3B-C2B-CMB-OMB
16	G	2001	PQN	C19-C18-C20-C21
16	a	2001	PQN	C19-C18-C20-C21
16	A	2001	PQN	C19-C18-C20-C21
18	G	4001	BCR	C11-C10-C9-C8
18	G	4001	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
18	G	4001	BCR	C17-C18-C19-C20
18	G	4001	BCR	C36-C18-C19-C20
18	G	4001	BCR	C21-C22-C23-C24
18	G	4001	BCR	C37-C22-C23-C24
18	G	4001	BCR	C23-C24-C25-C30
18	G	4002	BCR	C1-C6-C7-C8
18	G	4002	BCR	C5-C6-C7-C8
18	G	4003	BCR	C7-C8-C9-C10
18	G	4003	BCR	C7-C8-C9-C34
18	G	4003	BCR	C11-C10-C9-C8
18	G	4003	BCR	C11-C10-C9-C34
18	G	4003	BCR	C10-C11-C12-C13
18	G	4003	BCR	C21-C22-C23-C24
18	G	4003	BCR	C37-C22-C23-C24
18	G	4007	BCR	C11-C10-C9-C8
18	G	4007	BCR	C11-C10-C9-C34
18	G	4007	BCR	C17-C18-C19-C20
18	G	4007	BCR	C36-C18-C19-C20
18	G	4007	BCR	C21-C22-C23-C24
18	G	4007	BCR	C37-C22-C23-C24
18	G	4008	BCR	C7-C8-C9-C10
18	G	4008	BCR	C7-C8-C9-C34
18	G	4008	BCR	C11-C10-C9-C8
18	G	4008	BCR	C11-C10-C9-C34
18	G	4008	BCR	C10-C11-C12-C13
18	G	4008	BCR	C17-C18-C19-C20
18	G	4008	BCR	C36-C18-C19-C20
18	G	4011	BCR	C7-C8-C9-C10
18	G	4011	BCR	C7-C8-C9-C34
18	G	4011	BCR	C10-C11-C12-C13
18	G	4011	BCR	C11-C12-C13-C14
18	G	4011	BCR	C11-C12-C13-C35
18	G	4011	BCR	C23-C24-C25-C26
18	G	4011	BCR	C23-C24-C25-C30
18	H	4004	BCR	C7-C8-C9-C10
18	H	4004	BCR	C7-C8-C9-C34
18	H	4004	BCR	C11-C10-C9-C8
18	H	4004	BCR	C11-C10-C9-C34
18	H	4005	BCR	C11-C10-C9-C8
18	H	4005	BCR	C11-C10-C9-C34
18	H	4006	BCR	C5-C6-C7-C8
18	H	4009	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
18	H	4009	BCR	C11-C10-C9-C8
18	H	4009	BCR	C11-C10-C9-C34
18	H	4009	BCR	C10-C11-C12-C13
18	H	4010	BCR	C11-C10-C9-C8
18	H	4010	BCR	C11-C10-C9-C34
18	H	4010	BCR	C17-C18-C19-C20
18	H	4010	BCR	C36-C18-C19-C20
18	H	4013	BCR	C11-C10-C9-C8
18	H	4013	BCR	C11-C10-C9-C34
18	H	4013	BCR	C11-C12-C13-C14
18	H	4013	BCR	C11-C12-C13-C35
18	H	4013	BCR	C17-C18-C19-C20
18	H	4013	BCR	C36-C18-C19-C20
18	H	4013	BCR	C19-C20-C21-C22
18	H	4013	BCR	C23-C24-C25-C26
18	H	4014	BCR	C7-C8-C9-C10
18	H	4014	BCR	C7-C8-C9-C34
18	H	4014	BCR	C11-C10-C9-C8
18	H	4014	BCR	C11-C10-C9-C34
18	H	4014	BCR	C17-C18-C19-C20
18	H	4014	BCR	C36-C18-C19-C20
18	H	4016	BCR	C7-C8-C9-C34
18	H	4016	BCR	C15-C16-C17-C18
18	H	4016	BCR	C36-C18-C19-C20
18	H	4017	BCR	C7-C8-C9-C10
18	H	4017	BCR	C7-C8-C9-C34
18	H	4017	BCR	C11-C10-C9-C8
18	H	4017	BCR	C11-C10-C9-C34
18	H	4017	BCR	C9-C10-C11-C12
18	H	4017	BCR	C10-C11-C12-C13
18	H	4017	BCR	C18-C19-C20-C21
18	H	4017	BCR	C21-C22-C23-C24
18	H	4017	BCR	C37-C22-C23-C24
18	R	4018	BCR	C7-C8-C9-C10
18	R	4018	BCR	C7-C8-C9-C34
18	R	4018	BCR	C15-C16-C17-C18
18	R	4020	BCR	C10-C11-C12-C13
18	R	4020	BCR	C19-C20-C21-C22
18	U	4019	BCR	C11-C10-C9-C8
18	U	4019	BCR	C11-C10-C9-C34
18	U	4019	BCR	C10-C11-C12-C13
18	U	4019	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
18	U	4019	BCR	C36-C18-C19-C20
18	U	4019	BCR	C21-C22-C23-C24
18	U	4019	BCR	C37-C22-C23-C24
18	U	4022	BCR	C7-C8-C9-C34
18	U	4022	BCR	C11-C10-C9-C8
18	U	4022	BCR	C11-C10-C9-C34
18	U	4022	BCR	C10-C11-C12-C13
18	V	4021	BCR	C1-C6-C7-C8
18	V	4021	BCR	C7-C8-C9-C34
18	V	4021	BCR	C11-C10-C9-C8
18	V	4021	BCR	C11-C10-C9-C34
18	V	4021	BCR	C10-C11-C12-C13
18	V	4021	BCR	C15-C16-C17-C18
18	V	4021	BCR	C17-C18-C19-C20
18	V	4021	BCR	C36-C18-C19-C20
18	V	4021	BCR	C19-C20-C21-C22
18	V	4021	BCR	C23-C24-C25-C30
18	a	4001	BCR	C11-C10-C9-C8
18	a	4001	BCR	C11-C10-C9-C34
18	a	4001	BCR	C17-C18-C19-C20
18	a	4001	BCR	C36-C18-C19-C20
18	a	4001	BCR	C21-C22-C23-C24
18	a	4001	BCR	C37-C22-C23-C24
18	a	4001	BCR	C23-C24-C25-C30
18	a	4002	BCR	C1-C6-C7-C8
18	a	4002	BCR	C5-C6-C7-C8
18	a	4003	BCR	C7-C8-C9-C10
18	a	4003	BCR	C7-C8-C9-C34
18	a	4003	BCR	C11-C10-C9-C8
18	a	4003	BCR	C11-C10-C9-C34
18	a	4003	BCR	C10-C11-C12-C13
18	a	4003	BCR	C21-C22-C23-C24
18	a	4003	BCR	C37-C22-C23-C24
18	a	4007	BCR	C11-C10-C9-C8
18	a	4007	BCR	C11-C10-C9-C34
18	a	4007	BCR	C17-C18-C19-C20
18	a	4007	BCR	C36-C18-C19-C20
18	a	4007	BCR	C21-C22-C23-C24
18	a	4007	BCR	C37-C22-C23-C24
18	a	4008	BCR	C7-C8-C9-C10
18	a	4008	BCR	C7-C8-C9-C34
18	a	4008	BCR	C11-C10-C9-C8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
18	a	4008	BCR	C11-C10-C9-C34
18	a	4008	BCR	C10-C11-C12-C13
18	a	4008	BCR	C17-C18-C19-C20
18	a	4008	BCR	C36-C18-C19-C20
18	a	4011	BCR	C7-C8-C9-C10
18	a	4011	BCR	C7-C8-C9-C34
18	a	4011	BCR	C10-C11-C12-C13
18	a	4011	BCR	C11-C12-C13-C14
18	a	4011	BCR	C11-C12-C13-C35
18	a	4011	BCR	C23-C24-C25-C26
18	a	4011	BCR	C23-C24-C25-C30
18	b	4004	BCR	C7-C8-C9-C10
18	b	4004	BCR	C7-C8-C9-C34
18	b	4004	BCR	C11-C10-C9-C8
18	b	4004	BCR	C11-C10-C9-C34
18	b	4005	BCR	C11-C10-C9-C8
18	b	4005	BCR	C11-C10-C9-C34
18	b	4006	BCR	C5-C6-C7-C8
18	b	4009	BCR	C7-C8-C9-C10
18	b	4009	BCR	C11-C10-C9-C8
18	b	4009	BCR	C11-C10-C9-C34
18	b	4009	BCR	C10-C11-C12-C13
18	b	4010	BCR	C11-C10-C9-C8
18	b	4010	BCR	C11-C10-C9-C34
18	b	4010	BCR	C17-C18-C19-C20
18	b	4010	BCR	C36-C18-C19-C20
18	b	4013	BCR	C11-C10-C9-C8
18	b	4013	BCR	C11-C10-C9-C34
18	b	4013	BCR	C11-C12-C13-C14
18	b	4013	BCR	C11-C12-C13-C35
18	b	4013	BCR	C17-C18-C19-C20
18	b	4013	BCR	C36-C18-C19-C20
18	b	4013	BCR	C19-C20-C21-C22
18	b	4013	BCR	C23-C24-C25-C26
18	b	4014	BCR	C7-C8-C9-C10
18	b	4014	BCR	C7-C8-C9-C34
18	b	4014	BCR	C11-C10-C9-C8
18	b	4014	BCR	C11-C10-C9-C34
18	b	4014	BCR	C17-C18-C19-C20
18	b	4014	BCR	C36-C18-C19-C20
18	b	4016	BCR	C7-C8-C9-C34
18	b	4016	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
18	b	4016	BCR	C36-C18-C19-C20
18	b	4017	BCR	C7-C8-C9-C10
18	b	4017	BCR	C7-C8-C9-C34
18	b	4017	BCR	C11-C10-C9-C8
18	b	4017	BCR	C11-C10-C9-C34
18	b	4017	BCR	C9-C10-C11-C12
18	b	4017	BCR	C10-C11-C12-C13
18	b	4017	BCR	C18-C19-C20-C21
18	b	4017	BCR	C21-C22-C23-C24
18	b	4017	BCR	C37-C22-C23-C24
18	i	4018	BCR	C7-C8-C9-C10
18	i	4018	BCR	C7-C8-C9-C34
18	i	4018	BCR	C15-C16-C17-C18
18	i	4020	BCR	C10-C11-C12-C13
18	i	4020	BCR	C19-C20-C21-C22
18	l	4019	BCR	C11-C10-C9-C8
18	l	4019	BCR	C11-C10-C9-C34
18	l	4019	BCR	C10-C11-C12-C13
18	l	4019	BCR	C17-C18-C19-C20
18	l	4019	BCR	C36-C18-C19-C20
18	l	4019	BCR	C21-C22-C23-C24
18	l	4019	BCR	C37-C22-C23-C24
18	l	4022	BCR	C7-C8-C9-C34
18	l	4022	BCR	C11-C10-C9-C8
18	l	4022	BCR	C11-C10-C9-C34
18	l	4022	BCR	C10-C11-C12-C13
18	m	4021	BCR	C1-C6-C7-C8
18	m	4021	BCR	C7-C8-C9-C34
18	m	4021	BCR	C11-C10-C9-C8
18	m	4021	BCR	C11-C10-C9-C34
18	m	4021	BCR	C10-C11-C12-C13
18	m	4021	BCR	C15-C16-C17-C18
18	m	4021	BCR	C17-C18-C19-C20
18	m	4021	BCR	C36-C18-C19-C20
18	m	4021	BCR	C19-C20-C21-C22
18	m	4021	BCR	C23-C24-C25-C30
18	A	4001	BCR	C11-C10-C9-C8
18	A	4001	BCR	C11-C10-C9-C34
18	A	4001	BCR	C17-C18-C19-C20
18	A	4001	BCR	C36-C18-C19-C20
18	A	4001	BCR	C21-C22-C23-C24
18	A	4001	BCR	C37-C22-C23-C24

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
18	A	4001	BCR	C23-C24-C25-C30
18	A	4002	BCR	C1-C6-C7-C8
18	A	4002	BCR	C5-C6-C7-C8
18	A	4003	BCR	C7-C8-C9-C10
18	A	4003	BCR	C7-C8-C9-C34
18	A	4003	BCR	C11-C10-C9-C8
18	A	4003	BCR	C11-C10-C9-C34
18	A	4003	BCR	C10-C11-C12-C13
18	A	4003	BCR	C21-C22-C23-C24
18	A	4003	BCR	C37-C22-C23-C24
18	A	4007	BCR	C11-C10-C9-C8
18	A	4007	BCR	C11-C10-C9-C34
18	A	4007	BCR	C17-C18-C19-C20
18	A	4007	BCR	C36-C18-C19-C20
18	A	4007	BCR	C21-C22-C23-C24
18	A	4007	BCR	C37-C22-C23-C24
18	A	4008	BCR	C7-C8-C9-C10
18	A	4008	BCR	C7-C8-C9-C34
18	A	4008	BCR	C11-C10-C9-C8
18	A	4008	BCR	C11-C10-C9-C34
18	A	4008	BCR	C10-C11-C12-C13
18	A	4008	BCR	C17-C18-C19-C20
18	A	4008	BCR	C36-C18-C19-C20
18	A	4011	BCR	C7-C8-C9-C10
18	A	4011	BCR	C7-C8-C9-C34
18	A	4011	BCR	C10-C11-C12-C13
18	A	4011	BCR	C11-C12-C13-C14
18	A	4011	BCR	C11-C12-C13-C35
18	A	4011	BCR	C23-C24-C25-C26
18	A	4011	BCR	C23-C24-C25-C30
18	B	4004	BCR	C7-C8-C9-C10
18	B	4004	BCR	C7-C8-C9-C34
18	B	4004	BCR	C11-C10-C9-C8
18	B	4004	BCR	C11-C10-C9-C34
18	B	4005	BCR	C11-C10-C9-C8
18	B	4005	BCR	C11-C10-C9-C34
18	B	4006	BCR	C5-C6-C7-C8
18	B	4009	BCR	C7-C8-C9-C10
18	B	4009	BCR	C11-C10-C9-C8
18	B	4009	BCR	C11-C10-C9-C34
18	B	4009	BCR	C10-C11-C12-C13
18	B	4010	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
18	B	4010	BCR	C11-C10-C9-C34
18	B	4010	BCR	C17-C18-C19-C20
18	B	4010	BCR	C36-C18-C19-C20
18	B	4013	BCR	C11-C10-C9-C8
18	B	4013	BCR	C11-C10-C9-C34
18	B	4013	BCR	C11-C12-C13-C14
18	B	4013	BCR	C11-C12-C13-C35
18	B	4013	BCR	C17-C18-C19-C20
18	B	4013	BCR	C36-C18-C19-C20
18	B	4013	BCR	C19-C20-C21-C22
18	B	4013	BCR	C23-C24-C25-C26
18	B	4014	BCR	C7-C8-C9-C10
18	B	4014	BCR	C7-C8-C9-C34
18	B	4014	BCR	C11-C10-C9-C8
18	B	4014	BCR	C11-C10-C9-C34
18	B	4014	BCR	C17-C18-C19-C20
18	B	4014	BCR	C36-C18-C19-C20
18	B	4016	BCR	C7-C8-C9-C34
18	B	4016	BCR	C15-C16-C17-C18
18	B	4016	BCR	C36-C18-C19-C20
18	B	4017	BCR	C7-C8-C9-C10
18	B	4017	BCR	C7-C8-C9-C34
18	B	4017	BCR	C11-C10-C9-C8
18	B	4017	BCR	C11-C10-C9-C34
18	B	4017	BCR	C9-C10-C11-C12
18	B	4017	BCR	C10-C11-C12-C13
18	B	4017	BCR	C18-C19-C20-C21
18	B	4017	BCR	C21-C22-C23-C24
18	B	4017	BCR	C37-C22-C23-C24
18	I	4018	BCR	C7-C8-C9-C10
18	I	4018	BCR	C7-C8-C9-C34
18	I	4018	BCR	C15-C16-C17-C18
18	I	4020	BCR	C10-C11-C12-C13
18	I	4020	BCR	C19-C20-C21-C22
18	L	4019	BCR	C11-C10-C9-C8
18	L	4019	BCR	C11-C10-C9-C34
18	L	4019	BCR	C10-C11-C12-C13
18	L	4019	BCR	C17-C18-C19-C20
18	L	4019	BCR	C36-C18-C19-C20
18	L	4019	BCR	C21-C22-C23-C24
18	L	4019	BCR	C37-C22-C23-C24
18	L	4022	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
18	L	4022	BCR	C11-C10-C9-C8
18	L	4022	BCR	C11-C10-C9-C34
18	L	4022	BCR	C10-C11-C12-C13
18	M	4021	BCR	C1-C6-C7-C8
18	M	4021	BCR	C7-C8-C9-C34
18	M	4021	BCR	C11-C10-C9-C8
18	M	4021	BCR	C11-C10-C9-C34
18	M	4021	BCR	C10-C11-C12-C13
18	M	4021	BCR	C15-C16-C17-C18
18	M	4021	BCR	C17-C18-C19-C20
18	M	4021	BCR	C36-C18-C19-C20
18	M	4021	BCR	C19-C20-C21-C22
18	M	4021	BCR	C23-C24-C25-C30
19	G	5001	LHG	O1-C1-C2-C3
19	G	5001	LHG	C1-C2-C3-O3
19	G	5001	LHG	C4-O6-P-O3
19	H	5004	LHG	O1-C1-C2-C3
19	a	5001	LHG	O1-C1-C2-C3
19	a	5001	LHG	C1-C2-C3-O3
19	a	5001	LHG	C4-O6-P-O3
19	b	5004	LHG	O1-C1-C2-C3
19	A	5001	LHG	O1-C1-C2-C3
19	A	5001	LHG	C1-C2-C3-O3
19	A	5001	LHG	C4-O6-P-O3
19	B	5004	LHG	O1-C1-C2-C3
20	G	5005	LMG	O6-C1-O1-C7
20	H	5002	LMG	C2-C1-O1-C7
20	H	5002	LMG	O6-C1-O1-C7
20	H	5002	LMG	C11-C10-O7-C8
20	R	5006	LMG	C2-C1-O1-C7
20	R	5006	LMG	O6-C1-O1-C7
20	a	5005	LMG	O6-C1-O1-C7
20	b	5002	LMG	C2-C1-O1-C7
20	b	5002	LMG	O6-C1-O1-C7
20	b	5002	LMG	C11-C10-O7-C8
20	i	5006	LMG	C2-C1-O1-C7
20	i	5006	LMG	O6-C1-O1-C7
20	A	5005	LMG	O6-C1-O1-C7
20	B	5002	LMG	C2-C1-O1-C7
20	B	5002	LMG	O6-C1-O1-C7
20	B	5002	LMG	C11-C10-O7-C8
20	I	5006	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
20	I	5006	LMG	O6-C1-O1-C7
14	G	1138	CLA	O1D-CGD-O2D-CED
14	H	1217	CLA	O1D-CGD-O2D-CED
14	H	1232	CLA	O1D-CGD-O2D-CED
14	a	1138	CLA	O1D-CGD-O2D-CED
14	b	1217	CLA	O1D-CGD-O2D-CED
14	b	1232	CLA	O1D-CGD-O2D-CED
14	A	1138	CLA	O1D-CGD-O2D-CED
14	B	1217	CLA	O1D-CGD-O2D-CED
14	B	1232	CLA	O1D-CGD-O2D-CED
14	H	1239	CLA	C2C-C3C-CAC-CBC
14	b	1239	CLA	C2C-C3C-CAC-CBC
14	B	1239	CLA	C2C-C3C-CAC-CBC
14	H	1021	CLA	O1D-CGD-O2D-CED
14	b	1021	CLA	O1D-CGD-O2D-CED
14	B	1021	CLA	O1D-CGD-O2D-CED
14	G	1012	CLA	CBD-CGD-O2D-CED
14	G	1101	CLA	CBD-CGD-O2D-CED
14	G	1109	CLA	CBD-CGD-O2D-CED
14	G	1112	CLA	CBD-CGD-O2D-CED
14	G	1115	CLA	CBD-CGD-O2D-CED
14	G	1116	CLA	CBD-CGD-O2D-CED
14	G	1122	CLA	CBD-CGD-O2D-CED
14	G	1126	CLA	CBD-CGD-O2D-CED
14	G	1130	CLA	CBD-CGD-O2D-CED
14	G	1131	CLA	CBD-CGD-O2D-CED
14	G	1133	CLA	CBD-CGD-O2D-CED
14	G	1134	CLA	CBD-CGD-O2D-CED
14	G	1138	CLA	CBD-CGD-O2D-CED
14	G	1139	CLA	CBD-CGD-O2D-CED
14	G	1140	CLA	CBD-CGD-O2D-CED
14	H	1021	CLA	CBD-CGD-O2D-CED
14	H	1206	CLA	CBD-CGD-O2D-CED
14	H	1208	CLA	CBD-CGD-O2D-CED
14	H	1211	CLA	CBD-CGD-O2D-CED
14	H	1215	CLA	CBD-CGD-O2D-CED
14	H	1216	CLA	CBD-CGD-O2D-CED
14	H	1218	CLA	CBD-CGD-O2D-CED
14	H	1219	CLA	CBD-CGD-O2D-CED
14	H	1220	CLA	CBD-CGD-O2D-CED
14	H	1224	CLA	CBD-CGD-O2D-CED
14	H	1226	CLA	CBD-CGD-O2D-CED

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
14	H	1227	CLA	CBD-CGD-O2D-CED
14	H	1228	CLA	CBD-CGD-O2D-CED
14	H	1229	CLA	CBD-CGD-O2D-CED
14	H	1232	CLA	CBD-CGD-O2D-CED
14	H	1233	CLA	CBD-CGD-O2D-CED
14	H	1234	CLA	CBD-CGD-O2D-CED
14	H	1239	CLA	CBD-CGD-O2D-CED
14	T	1401	CLA	CBD-CGD-O2D-CED
14	U	1503	CLA	CBD-CGD-O2D-CED
14	W	1701	CLA	CBD-CGD-O2D-CED
14	a	1012	CLA	CBD-CGD-O2D-CED
14	a	1101	CLA	CBD-CGD-O2D-CED
14	a	1109	CLA	CBD-CGD-O2D-CED
14	a	1112	CLA	CBD-CGD-O2D-CED
14	a	1115	CLA	CBD-CGD-O2D-CED
14	a	1116	CLA	CBD-CGD-O2D-CED
14	a	1122	CLA	CBD-CGD-O2D-CED
14	a	1126	CLA	CBD-CGD-O2D-CED
14	a	1130	CLA	CBD-CGD-O2D-CED
14	a	1131	CLA	CBD-CGD-O2D-CED
14	a	1133	CLA	CBD-CGD-O2D-CED
14	a	1134	CLA	CBD-CGD-O2D-CED
14	a	1138	CLA	CBD-CGD-O2D-CED
14	a	1139	CLA	CBD-CGD-O2D-CED
14	a	1140	CLA	CBD-CGD-O2D-CED
14	b	1021	CLA	CBD-CGD-O2D-CED
14	b	1206	CLA	CBD-CGD-O2D-CED
14	b	1208	CLA	CBD-CGD-O2D-CED
14	b	1211	CLA	CBD-CGD-O2D-CED
14	b	1215	CLA	CBD-CGD-O2D-CED
14	b	1216	CLA	CBD-CGD-O2D-CED
14	b	1218	CLA	CBD-CGD-O2D-CED
14	b	1219	CLA	CBD-CGD-O2D-CED
14	b	1220	CLA	CBD-CGD-O2D-CED
14	b	1224	CLA	CBD-CGD-O2D-CED
14	b	1226	CLA	CBD-CGD-O2D-CED
14	b	1227	CLA	CBD-CGD-O2D-CED
14	b	1228	CLA	CBD-CGD-O2D-CED
14	b	1229	CLA	CBD-CGD-O2D-CED
14	b	1232	CLA	CBD-CGD-O2D-CED
14	b	1233	CLA	CBD-CGD-O2D-CED
14	b	1234	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	b	1239	CLA	CBD-CGD-O2D-CED
14	k	1401	CLA	CBD-CGD-O2D-CED
14	l	1503	CLA	CBD-CGD-O2D-CED
14	x	1701	CLA	CBD-CGD-O2D-CED
14	A	1012	CLA	CBD-CGD-O2D-CED
14	A	1101	CLA	CBD-CGD-O2D-CED
14	A	1109	CLA	CBD-CGD-O2D-CED
14	A	1112	CLA	CBD-CGD-O2D-CED
14	A	1115	CLA	CBD-CGD-O2D-CED
14	A	1116	CLA	CBD-CGD-O2D-CED
14	A	1122	CLA	CBD-CGD-O2D-CED
14	A	1126	CLA	CBD-CGD-O2D-CED
14	A	1130	CLA	CBD-CGD-O2D-CED
14	A	1131	CLA	CBD-CGD-O2D-CED
14	A	1133	CLA	CBD-CGD-O2D-CED
14	A	1134	CLA	CBD-CGD-O2D-CED
14	A	1138	CLA	CBD-CGD-O2D-CED
14	A	1139	CLA	CBD-CGD-O2D-CED
14	A	1140	CLA	CBD-CGD-O2D-CED
14	B	1021	CLA	CBD-CGD-O2D-CED
14	B	1206	CLA	CBD-CGD-O2D-CED
14	B	1208	CLA	CBD-CGD-O2D-CED
14	B	1211	CLA	CBD-CGD-O2D-CED
14	B	1215	CLA	CBD-CGD-O2D-CED
14	B	1216	CLA	CBD-CGD-O2D-CED
14	B	1218	CLA	CBD-CGD-O2D-CED
14	B	1219	CLA	CBD-CGD-O2D-CED
14	B	1220	CLA	CBD-CGD-O2D-CED
14	B	1224	CLA	CBD-CGD-O2D-CED
14	B	1226	CLA	CBD-CGD-O2D-CED
14	B	1227	CLA	CBD-CGD-O2D-CED
14	B	1228	CLA	CBD-CGD-O2D-CED
14	B	1229	CLA	CBD-CGD-O2D-CED
14	B	1232	CLA	CBD-CGD-O2D-CED
14	B	1233	CLA	CBD-CGD-O2D-CED
14	B	1234	CLA	CBD-CGD-O2D-CED
14	B	1239	CLA	CBD-CGD-O2D-CED
14	K	1401	CLA	CBD-CGD-O2D-CED
14	L	1503	CLA	CBD-CGD-O2D-CED
14	X	1701	CLA	CBD-CGD-O2D-CED
15	H	1230	F6C	CBD-CGD-O2D-CED
15	H	1237	F6C	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	b	1230	F6C	CBD-CGD-O2D-CED
15	b	1237	F6C	CBD-CGD-O2D-CED
15	B	1230	F6C	CBD-CGD-O2D-CED
15	B	1237	F6C	CBD-CGD-O2D-CED
14	G	1122	CLA	O1A-CGA-O2A-C1
14	H	1235	CLA	O1A-CGA-O2A-C1
14	a	1122	CLA	O1A-CGA-O2A-C1
14	b	1235	CLA	O1A-CGA-O2A-C1
14	A	1122	CLA	O1A-CGA-O2A-C1
14	B	1235	CLA	O1A-CGA-O2A-C1
21	G	6002	LMT	O5B-C1B-O1B-C4'
21	a	6002	LMT	O5B-C1B-O1B-C4'
21	A	6002	LMT	O5B-C1B-O1B-C4'
14	H	1239	CLA	C4C-C3C-CAC-CBC
14	b	1239	CLA	C4C-C3C-CAC-CBC
14	B	1239	CLA	C4C-C3C-CAC-CBC
14	H	1211	CLA	O1D-CGD-O2D-CED
14	H	1216	CLA	O1D-CGD-O2D-CED
14	H	1224	CLA	O1D-CGD-O2D-CED
14	W	1701	CLA	O1D-CGD-O2D-CED
14	b	1211	CLA	O1D-CGD-O2D-CED
14	b	1216	CLA	O1D-CGD-O2D-CED
14	b	1224	CLA	O1D-CGD-O2D-CED
14	x	1701	CLA	O1D-CGD-O2D-CED
14	B	1211	CLA	O1D-CGD-O2D-CED
14	B	1216	CLA	O1D-CGD-O2D-CED
14	B	1224	CLA	O1D-CGD-O2D-CED
14	X	1701	CLA	O1D-CGD-O2D-CED
14	G	1107	CLA	O1D-CGD-O2D-CED
14	G	1108	CLA	O1D-CGD-O2D-CED
14	G	1119	CLA	O1D-CGD-O2D-CED
14	H	1234	CLA	O1D-CGD-O2D-CED
14	a	1107	CLA	O1D-CGD-O2D-CED
14	a	1108	CLA	O1D-CGD-O2D-CED
14	a	1119	CLA	O1D-CGD-O2D-CED
14	b	1234	CLA	O1D-CGD-O2D-CED
14	A	1107	CLA	O1D-CGD-O2D-CED
14	A	1108	CLA	O1D-CGD-O2D-CED
14	A	1119	CLA	O1D-CGD-O2D-CED
14	B	1234	CLA	O1D-CGD-O2D-CED
14	G	1118	CLA	CBA-CGA-O2A-C1
14	G	1133	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	1118	CLA	CBA-CGA-O2A-C1
14	a	1133	CLA	CBA-CGA-O2A-C1
14	A	1118	CLA	CBA-CGA-O2A-C1
14	A	1133	CLA	CBA-CGA-O2A-C1
14	G	1013	CLA	CBD-CGD-O2D-CED
14	G	1102	CLA	CBD-CGD-O2D-CED
14	G	1105	CLA	CBD-CGD-O2D-CED
14	G	1106	CLA	CBD-CGD-O2D-CED
14	G	1111	CLA	CBD-CGD-O2D-CED
14	G	1113	CLA	CBD-CGD-O2D-CED
14	G	1114	CLA	CBD-CGD-O2D-CED
14	G	1123	CLA	CBD-CGD-O2D-CED
14	G	1124	CLA	CBD-CGD-O2D-CED
14	H	1023	CLA	CBD-CGD-O2D-CED
14	H	1204	CLA	CBD-CGD-O2D-CED
14	H	1205	CLA	CBD-CGD-O2D-CED
14	H	1212	CLA	CBD-CGD-O2D-CED
14	H	1213	CLA	CBD-CGD-O2D-CED
14	H	1214	CLA	CBD-CGD-O2D-CED
14	H	1231	CLA	CBD-CGD-O2D-CED
14	U	1501	CLA	CBD-CGD-O2D-CED
14	a	1013	CLA	CBD-CGD-O2D-CED
14	a	1102	CLA	CBD-CGD-O2D-CED
14	a	1105	CLA	CBD-CGD-O2D-CED
14	a	1106	CLA	CBD-CGD-O2D-CED
14	a	1111	CLA	CBD-CGD-O2D-CED
14	a	1113	CLA	CBD-CGD-O2D-CED
14	a	1114	CLA	CBD-CGD-O2D-CED
14	a	1123	CLA	CBD-CGD-O2D-CED
14	a	1124	CLA	CBD-CGD-O2D-CED
14	b	1023	CLA	CBD-CGD-O2D-CED
14	b	1204	CLA	CBD-CGD-O2D-CED
14	b	1205	CLA	CBD-CGD-O2D-CED
14	b	1212	CLA	CBD-CGD-O2D-CED
14	b	1213	CLA	CBD-CGD-O2D-CED
14	b	1214	CLA	CBD-CGD-O2D-CED
14	b	1231	CLA	CBD-CGD-O2D-CED
14	l	1501	CLA	CBD-CGD-O2D-CED
14	A	1013	CLA	CBD-CGD-O2D-CED
14	A	1102	CLA	CBD-CGD-O2D-CED
14	A	1105	CLA	CBD-CGD-O2D-CED
14	A	1106	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	A	1111	CLA	CBD-CGD-O2D-CED
14	A	1113	CLA	CBD-CGD-O2D-CED
14	A	1114	CLA	CBD-CGD-O2D-CED
14	A	1123	CLA	CBD-CGD-O2D-CED
14	A	1124	CLA	CBD-CGD-O2D-CED
14	B	1023	CLA	CBD-CGD-O2D-CED
14	B	1204	CLA	CBD-CGD-O2D-CED
14	B	1205	CLA	CBD-CGD-O2D-CED
14	B	1212	CLA	CBD-CGD-O2D-CED
14	B	1213	CLA	CBD-CGD-O2D-CED
14	B	1214	CLA	CBD-CGD-O2D-CED
14	B	1231	CLA	CBD-CGD-O2D-CED
14	L	1501	CLA	CBD-CGD-O2D-CED
14	G	1106	CLA	O1A-CGA-O2A-C1
14	G	1118	CLA	O1A-CGA-O2A-C1
14	G	1138	CLA	O1A-CGA-O2A-C1
14	H	1203	CLA	O1A-CGA-O2A-C1
14	H	1222	CLA	O1A-CGA-O2A-C1
14	H	1224	CLA	O1A-CGA-O2A-C1
14	a	1106	CLA	O1A-CGA-O2A-C1
14	a	1118	CLA	O1A-CGA-O2A-C1
14	a	1138	CLA	O1A-CGA-O2A-C1
14	b	1203	CLA	O1A-CGA-O2A-C1
14	b	1222	CLA	O1A-CGA-O2A-C1
14	b	1224	CLA	O1A-CGA-O2A-C1
14	A	1106	CLA	O1A-CGA-O2A-C1
14	A	1118	CLA	O1A-CGA-O2A-C1
14	A	1138	CLA	O1A-CGA-O2A-C1
14	B	1203	CLA	O1A-CGA-O2A-C1
14	B	1222	CLA	O1A-CGA-O2A-C1
14	B	1224	CLA	O1A-CGA-O2A-C1
20	G	5005	LMG	O10-C28-O8-C9
20	H	5002	LMG	O10-C28-O8-C9
20	R	5006	LMG	O10-C28-O8-C9
20	a	5005	LMG	O10-C28-O8-C9
20	b	5002	LMG	O10-C28-O8-C9
20	i	5006	LMG	O10-C28-O8-C9
20	A	5005	LMG	O10-C28-O8-C9
20	B	5002	LMG	O10-C28-O8-C9
20	I	5006	LMG	O10-C28-O8-C9
15	G	1121	F6C	O1D-CGD-O2D-CED
15	a	1121	F6C	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	A	1121	F6C	O1D-CGD-O2D-CED
14	G	1117	CLA	O1D-CGD-O2D-CED
14	G	1132	CLA	O1D-CGD-O2D-CED
14	a	1117	CLA	O1D-CGD-O2D-CED
14	a	1132	CLA	O1D-CGD-O2D-CED
14	A	1117	CLA	O1D-CGD-O2D-CED
14	A	1132	CLA	O1D-CGD-O2D-CED
14	G	1125	CLA	CBD-CGD-O2D-CED
14	G	1135	CLA	CBD-CGD-O2D-CED
14	H	1235	CLA	CBD-CGD-O2D-CED
14	a	1125	CLA	CBD-CGD-O2D-CED
14	a	1135	CLA	CBD-CGD-O2D-CED
14	b	1235	CLA	CBD-CGD-O2D-CED
14	A	1125	CLA	CBD-CGD-O2D-CED
14	A	1135	CLA	CBD-CGD-O2D-CED
14	B	1235	CLA	CBD-CGD-O2D-CED
14	G	1131	CLA	O1D-CGD-O2D-CED
14	H	1208	CLA	O1D-CGD-O2D-CED
14	H	1219	CLA	O1D-CGD-O2D-CED
14	a	1131	CLA	O1D-CGD-O2D-CED
14	b	1208	CLA	O1D-CGD-O2D-CED
14	b	1219	CLA	O1D-CGD-O2D-CED
14	A	1131	CLA	O1D-CGD-O2D-CED
14	B	1208	CLA	O1D-CGD-O2D-CED
14	B	1219	CLA	O1D-CGD-O2D-CED
20	H	5002	LMG	O9-C10-O7-C8
20	b	5002	LMG	O9-C10-O7-C8
20	B	5002	LMG	O9-C10-O7-C8
14	G	1109	CLA	O1D-CGD-O2D-CED
14	G	1139	CLA	O1D-CGD-O2D-CED
14	G	1140	CLA	O1D-CGD-O2D-CED
14	a	1139	CLA	O1D-CGD-O2D-CED
14	a	1140	CLA	O1D-CGD-O2D-CED
14	A	1109	CLA	O1D-CGD-O2D-CED
14	A	1139	CLA	O1D-CGD-O2D-CED
14	A	1140	CLA	O1D-CGD-O2D-CED
14	G	1102	CLA	C3-C5-C6-C7
14	H	1202	CLA	C3-C5-C6-C7
14	H	1205	CLA	C3-C5-C6-C7
14	H	1208	CLA	C3-C5-C6-C7
14	H	1214	CLA	C3-C5-C6-C7
14	H	1217	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	H	1223	CLA	C3-C5-C6-C7
14	H	1228	CLA	C3-C5-C6-C7
14	H	1239	CLA	C3-C5-C6-C7
14	a	1102	CLA	C3-C5-C6-C7
14	b	1202	CLA	C3-C5-C6-C7
14	b	1205	CLA	C3-C5-C6-C7
14	b	1208	CLA	C3-C5-C6-C7
14	b	1214	CLA	C3-C5-C6-C7
14	b	1217	CLA	C3-C5-C6-C7
14	b	1223	CLA	C3-C5-C6-C7
14	b	1228	CLA	C3-C5-C6-C7
14	b	1239	CLA	C3-C5-C6-C7
14	A	1102	CLA	C3-C5-C6-C7
14	B	1202	CLA	C3-C5-C6-C7
14	B	1205	CLA	C3-C5-C6-C7
14	B	1208	CLA	C3-C5-C6-C7
14	B	1214	CLA	C3-C5-C6-C7
14	B	1217	CLA	C3-C5-C6-C7
14	B	1223	CLA	C3-C5-C6-C7
14	B	1228	CLA	C3-C5-C6-C7
14	B	1239	CLA	C3-C5-C6-C7
15	H	1238	F6C	C3-C5-C6-C7
15	b	1238	F6C	C3-C5-C6-C7
15	B	1238	F6C	C3-C5-C6-C7
14	G	1106	CLA	CBA-CGA-O2A-C1
14	G	1117	CLA	CBA-CGA-O2A-C1
14	G	1122	CLA	CBA-CGA-O2A-C1
14	G	1137	CLA	CBA-CGA-O2A-C1
14	H	1222	CLA	CBA-CGA-O2A-C1
14	H	1226	CLA	CBA-CGA-O2A-C1
14	H	1235	CLA	CBA-CGA-O2A-C1
14	H	1239	CLA	CBA-CGA-O2A-C1
14	a	1106	CLA	CBA-CGA-O2A-C1
14	a	1117	CLA	CBA-CGA-O2A-C1
14	a	1122	CLA	CBA-CGA-O2A-C1
14	a	1137	CLA	CBA-CGA-O2A-C1
14	b	1222	CLA	CBA-CGA-O2A-C1
14	b	1226	CLA	CBA-CGA-O2A-C1
14	b	1235	CLA	CBA-CGA-O2A-C1
14	b	1239	CLA	CBA-CGA-O2A-C1
14	A	1106	CLA	CBA-CGA-O2A-C1
14	A	1117	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	A	1122	CLA	CBA-CGA-O2A-C1
14	A	1137	CLA	CBA-CGA-O2A-C1
14	B	1222	CLA	CBA-CGA-O2A-C1
14	B	1226	CLA	CBA-CGA-O2A-C1
14	B	1235	CLA	CBA-CGA-O2A-C1
14	B	1239	CLA	CBA-CGA-O2A-C1
20	G	5005	LMG	C29-C28-O8-C9
20	H	5002	LMG	C29-C28-O8-C9
20	R	5006	LMG	C29-C28-O8-C9
20	a	5005	LMG	C29-C28-O8-C9
20	b	5002	LMG	C29-C28-O8-C9
20	i	5006	LMG	C29-C28-O8-C9
20	A	5005	LMG	C29-C28-O8-C9
20	B	5002	LMG	C29-C28-O8-C9
20	I	5006	LMG	C29-C28-O8-C9
14	H	1023	CLA	C2C-C3C-CAC-CBC
14	b	1023	CLA	C2C-C3C-CAC-CBC
14	B	1023	CLA	C2C-C3C-CAC-CBC
14	G	1140	CLA	C8-C10-C11-C12
14	H	1021	CLA	C5-C6-C7-C8
14	a	1140	CLA	C8-C10-C11-C12
14	b	1021	CLA	C5-C6-C7-C8
14	A	1140	CLA	C8-C10-C11-C12
14	B	1021	CLA	C5-C6-C7-C8
14	G	1116	CLA	O1D-CGD-O2D-CED
14	G	1133	CLA	O1D-CGD-O2D-CED
14	H	1206	CLA	O1D-CGD-O2D-CED
14	H	1226	CLA	O1D-CGD-O2D-CED
14	H	1233	CLA	O1D-CGD-O2D-CED
14	a	1109	CLA	O1D-CGD-O2D-CED
14	a	1116	CLA	O1D-CGD-O2D-CED
14	a	1133	CLA	O1D-CGD-O2D-CED
14	b	1206	CLA	O1D-CGD-O2D-CED
14	b	1226	CLA	O1D-CGD-O2D-CED
14	b	1233	CLA	O1D-CGD-O2D-CED
14	A	1116	CLA	O1D-CGD-O2D-CED
14	A	1133	CLA	O1D-CGD-O2D-CED
14	B	1206	CLA	O1D-CGD-O2D-CED
14	B	1226	CLA	O1D-CGD-O2D-CED
14	B	1233	CLA	O1D-CGD-O2D-CED
14	G	1120	CLA	CBD-CGD-O2D-CED
14	H	1222	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	a	1120	CLA	CBD-CGD-O2D-CED
14	b	1222	CLA	CBD-CGD-O2D-CED
14	A	1120	CLA	CBD-CGD-O2D-CED
14	B	1222	CLA	CBD-CGD-O2D-CED
14	H	1217	CLA	O1A-CGA-O2A-C1
14	b	1217	CLA	O1A-CGA-O2A-C1
14	B	1217	CLA	O1A-CGA-O2A-C1
14	G	1103	CLA	C4-C3-C5-C6
14	a	1103	CLA	C4-C3-C5-C6
14	A	1103	CLA	C4-C3-C5-C6
14	H	1201	CLA	C2-C3-C5-C6
14	W	1701	CLA	C2-C3-C5-C6
14	b	1201	CLA	C2-C3-C5-C6
14	x	1701	CLA	C2-C3-C5-C6
14	B	1201	CLA	C2-C3-C5-C6
14	X	1701	CLA	C2-C3-C5-C6
14	G	1104	CLA	CBD-CGD-O2D-CED
14	G	1118	CLA	CBD-CGD-O2D-CED
14	G	1136	CLA	CBD-CGD-O2D-CED
14	a	1104	CLA	CBD-CGD-O2D-CED
14	a	1118	CLA	CBD-CGD-O2D-CED
14	a	1136	CLA	CBD-CGD-O2D-CED
14	A	1104	CLA	CBD-CGD-O2D-CED
14	A	1118	CLA	CBD-CGD-O2D-CED
14	A	1136	CLA	CBD-CGD-O2D-CED
14	G	1131	CLA	C2A-CAA-CBA-CGA
14	G	1139	CLA	C2A-CAA-CBA-CGA
14	G	1140	CLA	C2A-CAA-CBA-CGA
14	H	1022	CLA	C2A-CAA-CBA-CGA
14	H	1212	CLA	C2A-CAA-CBA-CGA
14	H	1223	CLA	C2A-CAA-CBA-CGA
14	H	1225	CLA	C2A-CAA-CBA-CGA
14	H	1227	CLA	C2A-CAA-CBA-CGA
14	H	1228	CLA	C2A-CAA-CBA-CGA
14	a	1131	CLA	C2A-CAA-CBA-CGA
14	a	1139	CLA	C2A-CAA-CBA-CGA
14	a	1140	CLA	C2A-CAA-CBA-CGA
14	b	1022	CLA	C2A-CAA-CBA-CGA
14	b	1212	CLA	C2A-CAA-CBA-CGA
14	b	1223	CLA	C2A-CAA-CBA-CGA
14	b	1225	CLA	C2A-CAA-CBA-CGA
14	b	1227	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	b	1228	CLA	C2A-CAA-CBA-CGA
14	A	1131	CLA	C2A-CAA-CBA-CGA
14	A	1139	CLA	C2A-CAA-CBA-CGA
14	A	1140	CLA	C2A-CAA-CBA-CGA
14	B	1022	CLA	C2A-CAA-CBA-CGA
14	B	1212	CLA	C2A-CAA-CBA-CGA
14	B	1223	CLA	C2A-CAA-CBA-CGA
14	B	1225	CLA	C2A-CAA-CBA-CGA
14	B	1227	CLA	C2A-CAA-CBA-CGA
14	B	1228	CLA	C2A-CAA-CBA-CGA
20	G	5005	LMG	C35-C36-C37-C38
20	H	5002	LMG	C17-C18-C19-C20
20	U	5007	LMG	C35-C36-C37-C38
20	a	5005	LMG	C35-C36-C37-C38
20	b	5002	LMG	C17-C18-C19-C20
20	l	5007	LMG	C35-C36-C37-C38
20	A	5005	LMG	C35-C36-C37-C38
20	B	5002	LMG	C17-C18-C19-C20
20	L	5007	LMG	C35-C36-C37-C38
14	G	1115	CLA	C3-C5-C6-C7
14	H	1204	CLA	C3-C5-C6-C7
14	H	1220	CLA	C3-C5-C6-C7
14	a	1115	CLA	C3-C5-C6-C7
14	b	1204	CLA	C3-C5-C6-C7
14	b	1220	CLA	C3-C5-C6-C7
14	A	1115	CLA	C3-C5-C6-C7
14	B	1204	CLA	C3-C5-C6-C7
14	B	1220	CLA	C3-C5-C6-C7
14	G	1104	CLA	CBA-CGA-O2A-C1
14	G	1130	CLA	CBA-CGA-O2A-C1
14	G	1138	CLA	CBA-CGA-O2A-C1
14	H	1202	CLA	CBA-CGA-O2A-C1
14	H	1203	CLA	CBA-CGA-O2A-C1
14	H	1208	CLA	CBA-CGA-O2A-C1
14	H	1214	CLA	CBA-CGA-O2A-C1
14	H	1224	CLA	CBA-CGA-O2A-C1
14	a	1104	CLA	CBA-CGA-O2A-C1
14	a	1130	CLA	CBA-CGA-O2A-C1
14	a	1138	CLA	CBA-CGA-O2A-C1
14	b	1202	CLA	CBA-CGA-O2A-C1
14	b	1203	CLA	CBA-CGA-O2A-C1
14	b	1208	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	b	1214	CLA	CBA-CGA-O2A-C1
14	b	1224	CLA	CBA-CGA-O2A-C1
14	A	1104	CLA	CBA-CGA-O2A-C1
14	A	1130	CLA	CBA-CGA-O2A-C1
14	A	1138	CLA	CBA-CGA-O2A-C1
14	B	1202	CLA	CBA-CGA-O2A-C1
14	B	1203	CLA	CBA-CGA-O2A-C1
14	B	1208	CLA	CBA-CGA-O2A-C1
14	B	1214	CLA	CBA-CGA-O2A-C1
14	B	1224	CLA	CBA-CGA-O2A-C1
15	H	1230	F6C	C1A-C2A-CAA-CBA
15	b	1230	F6C	C1A-C2A-CAA-CBA
15	B	1230	F6C	C1A-C2A-CAA-CBA
14	G	1134	CLA	O1D-CGD-O2D-CED
14	T	1401	CLA	O1D-CGD-O2D-CED
14	a	1134	CLA	O1D-CGD-O2D-CED
14	k	1401	CLA	O1D-CGD-O2D-CED
14	A	1134	CLA	O1D-CGD-O2D-CED
14	K	1401	CLA	O1D-CGD-O2D-CED
14	G	1122	CLA	O1D-CGD-O2D-CED
14	G	1126	CLA	O1D-CGD-O2D-CED
14	H	1228	CLA	O1D-CGD-O2D-CED
14	a	1122	CLA	O1D-CGD-O2D-CED
14	b	1228	CLA	O1D-CGD-O2D-CED
14	A	1122	CLA	O1D-CGD-O2D-CED
14	B	1220	CLA	O1D-CGD-O2D-CED
14	B	1228	CLA	O1D-CGD-O2D-CED
15	H	1237	F6C	O1D-CGD-O2D-CED
15	b	1237	F6C	O1D-CGD-O2D-CED
15	B	1237	F6C	O1D-CGD-O2D-CED
14	G	1104	CLA	O1A-CGA-O2A-C1
14	G	1128	CLA	O1A-CGA-O2A-C1
14	G	1130	CLA	O1A-CGA-O2A-C1
14	G	1137	CLA	O1A-CGA-O2A-C1
14	H	1202	CLA	O1A-CGA-O2A-C1
14	H	1208	CLA	O1A-CGA-O2A-C1
14	H	1214	CLA	O1A-CGA-O2A-C1
14	H	1226	CLA	O1A-CGA-O2A-C1
14	H	1239	CLA	O1A-CGA-O2A-C1
14	a	1104	CLA	O1A-CGA-O2A-C1
14	a	1128	CLA	O1A-CGA-O2A-C1
14	a	1130	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	1137	CLA	O1A-CGA-O2A-C1
14	b	1202	CLA	O1A-CGA-O2A-C1
14	b	1208	CLA	O1A-CGA-O2A-C1
14	b	1214	CLA	O1A-CGA-O2A-C1
14	b	1226	CLA	O1A-CGA-O2A-C1
14	b	1239	CLA	O1A-CGA-O2A-C1
14	A	1104	CLA	O1A-CGA-O2A-C1
14	A	1128	CLA	O1A-CGA-O2A-C1
14	A	1130	CLA	O1A-CGA-O2A-C1
14	A	1137	CLA	O1A-CGA-O2A-C1
14	B	1202	CLA	O1A-CGA-O2A-C1
14	B	1208	CLA	O1A-CGA-O2A-C1
14	B	1214	CLA	O1A-CGA-O2A-C1
14	B	1226	CLA	O1A-CGA-O2A-C1
14	B	1239	CLA	O1A-CGA-O2A-C1
14	H	1220	CLA	O1D-CGD-O2D-CED
14	a	1126	CLA	O1D-CGD-O2D-CED
14	b	1220	CLA	O1D-CGD-O2D-CED
14	A	1126	CLA	O1D-CGD-O2D-CED
14	G	1130	CLA	O1D-CGD-O2D-CED
14	a	1130	CLA	O1D-CGD-O2D-CED
14	A	1130	CLA	O1D-CGD-O2D-CED
19	G	5001	LHG	O2-C2-C3-O3
19	a	5001	LHG	O2-C2-C3-O3
19	A	5001	LHG	O2-C2-C3-O3
14	G	1135	CLA	C3-C5-C6-C7
14	G	1136	CLA	C3-C5-C6-C7
14	H	1235	CLA	C3-C5-C6-C7
14	a	1135	CLA	C3-C5-C6-C7
14	a	1136	CLA	C3-C5-C6-C7
14	b	1235	CLA	C3-C5-C6-C7
14	A	1135	CLA	C3-C5-C6-C7
14	A	1136	CLA	C3-C5-C6-C7
14	B	1235	CLA	C3-C5-C6-C7
14	G	1131	CLA	CBA-CGA-O2A-C1
14	H	1217	CLA	CBA-CGA-O2A-C1
14	H	1223	CLA	CBA-CGA-O2A-C1
14	a	1131	CLA	CBA-CGA-O2A-C1
14	b	1217	CLA	CBA-CGA-O2A-C1
14	b	1223	CLA	CBA-CGA-O2A-C1
14	A	1131	CLA	CBA-CGA-O2A-C1
14	B	1217	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	1223	CLA	CBA-CGA-O2A-C1
14	G	1117	CLA	O1A-CGA-O2A-C1
14	a	1117	CLA	O1A-CGA-O2A-C1
14	A	1117	CLA	O1A-CGA-O2A-C1
14	H	1215	CLA	O1D-CGD-O2D-CED
14	H	1229	CLA	O1D-CGD-O2D-CED
14	b	1215	CLA	O1D-CGD-O2D-CED
14	b	1229	CLA	O1D-CGD-O2D-CED
14	B	1215	CLA	O1D-CGD-O2D-CED
14	B	1229	CLA	O1D-CGD-O2D-CED
15	H	1230	F6C	O1D-CGD-O2D-CED
15	b	1230	F6C	O1D-CGD-O2D-CED
15	B	1230	F6C	O1D-CGD-O2D-CED
14	b	1218	CLA	O1D-CGD-O2D-CED
15	H	1207	F6C	CBD-CGD-O2D-CED
15	b	1207	F6C	CBD-CGD-O2D-CED
15	B	1207	F6C	CBD-CGD-O2D-CED
21	G	6001	LMT	O5'-C5'-C6'-O6'
21	a	6001	LMT	O5'-C5'-C6'-O6'
21	A	6001	LMT	O5'-C5'-C6'-O6'
14	G	1115	CLA	O1D-CGD-O2D-CED
14	H	1218	CLA	O1D-CGD-O2D-CED
14	a	1115	CLA	O1D-CGD-O2D-CED
14	A	1115	CLA	O1D-CGD-O2D-CED
14	B	1218	CLA	O1D-CGD-O2D-CED
19	H	5004	LHG	C28-C29-C30-C31
19	a	5001	LHG	C11-C12-C13-C14
19	b	5004	LHG	C28-C29-C30-C31
19	A	5001	LHG	C11-C12-C13-C14
19	B	5004	LHG	C28-C29-C30-C31
14	H	1239	CLA	O1D-CGD-O2D-CED
14	b	1239	CLA	O1D-CGD-O2D-CED
14	B	1239	CLA	O1D-CGD-O2D-CED
19	G	5001	LHG	C11-C12-C13-C14
14	G	1138	CLA	C3-C5-C6-C7
14	a	1138	CLA	C3-C5-C6-C7
14	b	1226	CLA	C3-C5-C6-C7
14	A	1138	CLA	C3-C5-C6-C7
14	B	1226	CLA	C3-C5-C6-C7
16	H	2002	PQN	C13-C15-C16-C17
16	b	2002	PQN	C13-C15-C16-C17
16	B	2002	PQN	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	G	1128	CLA	CBA-CGA-O2A-C1
14	a	1128	CLA	CBA-CGA-O2A-C1
14	A	1128	CLA	CBA-CGA-O2A-C1
14	H	1227	CLA	O1D-CGD-O2D-CED
14	U	1503	CLA	O1D-CGD-O2D-CED
14	b	1227	CLA	O1D-CGD-O2D-CED
14	l	1503	CLA	O1D-CGD-O2D-CED
14	B	1227	CLA	O1D-CGD-O2D-CED
14	L	1503	CLA	O1D-CGD-O2D-CED
14	G	1131	CLA	O1A-CGA-O2A-C1
14	a	1131	CLA	O1A-CGA-O2A-C1
14	A	1131	CLA	O1A-CGA-O2A-C1
15	H	1207	F6C	C2A-CAA-CBA-CGA
15	b	1207	F6C	C2A-CAA-CBA-CGA
15	B	1207	F6C	C2A-CAA-CBA-CGA
14	G	1109	CLA	C4-C3-C5-C6
14	G	1116	CLA	C4-C3-C5-C6
14	G	1136	CLA	C4-C3-C5-C6
14	G	1140	CLA	C4-C3-C5-C6
14	H	1022	CLA	C4-C3-C5-C6
14	H	1203	CLA	C4-C3-C5-C6
14	H	1210	CLA	C4-C3-C5-C6
14	a	1109	CLA	C4-C3-C5-C6
14	a	1116	CLA	C4-C3-C5-C6
14	a	1136	CLA	C4-C3-C5-C6
14	a	1140	CLA	C4-C3-C5-C6
14	b	1022	CLA	C4-C3-C5-C6
14	b	1203	CLA	C4-C3-C5-C6
14	b	1210	CLA	C4-C3-C5-C6
14	A	1109	CLA	C4-C3-C5-C6
14	A	1116	CLA	C4-C3-C5-C6
14	A	1136	CLA	C4-C3-C5-C6
14	A	1140	CLA	C4-C3-C5-C6
14	B	1022	CLA	C4-C3-C5-C6
14	B	1203	CLA	C4-C3-C5-C6
14	B	1210	CLA	C4-C3-C5-C6
14	G	1109	CLA	C2-C3-C5-C6
14	G	1116	CLA	C2-C3-C5-C6
14	G	1136	CLA	C2-C3-C5-C6
14	G	1140	CLA	C2-C3-C5-C6
14	H	1022	CLA	C2-C3-C5-C6
14	H	1203	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	H	1210	CLA	C2-C3-C5-C6
14	a	1109	CLA	C2-C3-C5-C6
14	a	1116	CLA	C2-C3-C5-C6
14	a	1136	CLA	C2-C3-C5-C6
14	a	1140	CLA	C2-C3-C5-C6
14	b	1022	CLA	C2-C3-C5-C6
14	b	1203	CLA	C2-C3-C5-C6
14	b	1210	CLA	C2-C3-C5-C6
14	A	1109	CLA	C2-C3-C5-C6
14	A	1116	CLA	C2-C3-C5-C6
14	A	1136	CLA	C2-C3-C5-C6
14	A	1140	CLA	C2-C3-C5-C6
14	B	1022	CLA	C2-C3-C5-C6
14	B	1203	CLA	C2-C3-C5-C6
14	B	1210	CLA	C2-C3-C5-C6
14	G	1111	CLA	C2A-CAA-CBA-CGA
14	a	1111	CLA	C2A-CAA-CBA-CGA
14	A	1111	CLA	C2A-CAA-CBA-CGA
14	G	1112	CLA	O1D-CGD-O2D-CED
14	a	1112	CLA	O1D-CGD-O2D-CED
21	G	6002	LMT	O5'-C1'-O1'-C1
21	a	6002	LMT	O5'-C1'-O1'-C1
21	A	6002	LMT	O5'-C1'-O1'-C1
14	A	1112	CLA	O1D-CGD-O2D-CED
14	H	1226	CLA	C3-C5-C6-C7
14	G	1115	CLA	CBA-CGA-O2A-C1
14	H	1229	CLA	CBA-CGA-O2A-C1
14	a	1115	CLA	CBA-CGA-O2A-C1
14	b	1229	CLA	CBA-CGA-O2A-C1
14	A	1115	CLA	CBA-CGA-O2A-C1
14	B	1229	CLA	CBA-CGA-O2A-C1
14	G	1101	CLA	O1D-CGD-O2D-CED
14	G	1123	CLA	O1D-CGD-O2D-CED
14	U	1501	CLA	O1D-CGD-O2D-CED
14	a	1101	CLA	O1D-CGD-O2D-CED
14	l	1501	CLA	O1D-CGD-O2D-CED
14	A	1101	CLA	O1D-CGD-O2D-CED
14	A	1123	CLA	O1D-CGD-O2D-CED
14	L	1501	CLA	O1D-CGD-O2D-CED
14	H	1223	CLA	O1A-CGA-O2A-C1
14	b	1223	CLA	O1A-CGA-O2A-C1
14	B	1223	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	H	1023	CLA	C4C-C3C-CAC-CBC
14	b	1023	CLA	C4C-C3C-CAC-CBC
14	B	1023	CLA	C4C-C3C-CAC-CBC
14	G	1012	CLA	O1D-CGD-O2D-CED
14	G	1013	CLA	O1D-CGD-O2D-CED
14	H	1214	CLA	O1D-CGD-O2D-CED
14	a	1012	CLA	O1D-CGD-O2D-CED
14	a	1013	CLA	O1D-CGD-O2D-CED
14	a	1123	CLA	O1D-CGD-O2D-CED
14	b	1214	CLA	O1D-CGD-O2D-CED
14	A	1012	CLA	O1D-CGD-O2D-CED
14	A	1013	CLA	O1D-CGD-O2D-CED
14	B	1214	CLA	O1D-CGD-O2D-CED
14	G	1112	CLA	O1A-CGA-O2A-C1
14	a	1112	CLA	O1A-CGA-O2A-C1
14	A	1112	CLA	O1A-CGA-O2A-C1
14	G	1140	CLA	C3-C5-C6-C7
14	a	1140	CLA	C3-C5-C6-C7
14	A	1140	CLA	C3-C5-C6-C7
14	H	1231	CLA	O1D-CGD-O2D-CED
14	b	1231	CLA	O1D-CGD-O2D-CED
14	G	1112	CLA	CBA-CGA-O2A-C1
14	G	1124	CLA	CBA-CGA-O2A-C1
14	H	1021	CLA	CBA-CGA-O2A-C1
14	H	1231	CLA	CBA-CGA-O2A-C1
14	H	1234	CLA	CBA-CGA-O2A-C1
14	a	1112	CLA	CBA-CGA-O2A-C1
14	a	1124	CLA	CBA-CGA-O2A-C1
14	b	1021	CLA	CBA-CGA-O2A-C1
14	b	1231	CLA	CBA-CGA-O2A-C1
14	b	1234	CLA	CBA-CGA-O2A-C1
14	A	1112	CLA	CBA-CGA-O2A-C1
14	A	1124	CLA	CBA-CGA-O2A-C1
14	B	1021	CLA	CBA-CGA-O2A-C1
14	B	1231	CLA	CBA-CGA-O2A-C1
14	B	1234	CLA	CBA-CGA-O2A-C1
15	H	1207	F6C	CBA-CGA-O2A-C1
15	H	1238	F6C	CBA-CGA-O2A-C1
15	b	1207	F6C	CBA-CGA-O2A-C1
15	b	1238	F6C	CBA-CGA-O2A-C1
15	B	1207	F6C	CBA-CGA-O2A-C1
15	B	1238	F6C	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	G	1128	CLA	CBD-CGD-O2D-CED
14	a	1128	CLA	CBD-CGD-O2D-CED
14	A	1128	CLA	CBD-CGD-O2D-CED
14	B	1231	CLA	O1D-CGD-O2D-CED
18	H	4017	BCR	C19-C20-C21-C22
18	b	4017	BCR	C19-C20-C21-C22
18	B	4017	BCR	C19-C20-C21-C22
14	H	1221	CLA	C15-C16-C17-C18
14	b	1221	CLA	C15-C16-C17-C18
14	A	1109	CLA	C8-C10-C11-C12
14	B	1221	CLA	C15-C16-C17-C18
14	G	1109	CLA	C8-C10-C11-C12
14	G	1132	CLA	C5-C6-C7-C8
14	H	1204	CLA	C10-C11-C12-C13
14	H	1205	CLA	C10-C11-C12-C13
14	a	1109	CLA	C8-C10-C11-C12
14	a	1132	CLA	C5-C6-C7-C8
14	b	1204	CLA	C10-C11-C12-C13
14	b	1205	CLA	C10-C11-C12-C13
14	A	1132	CLA	C5-C6-C7-C8
14	B	1204	CLA	C10-C11-C12-C13
14	B	1205	CLA	C10-C11-C12-C13
19	H	5004	LHG	C23-C24-C25-C26
19	b	5004	LHG	C23-C24-C25-C26
19	B	5004	LHG	C23-C24-C25-C26
21	G	6001	LMT	C2'-C1'-O1'-C1
21	a	6001	LMT	C2'-C1'-O1'-C1
21	A	6001	LMT	C2'-C1'-O1'-C1
19	H	5004	LHG	O7-C5-C6-O8
19	b	5004	LHG	O7-C5-C6-O8
19	B	5004	LHG	O7-C5-C6-O8
14	H	1021	CLA	O1A-CGA-O2A-C1
14	H	1234	CLA	O1A-CGA-O2A-C1
14	b	1021	CLA	O1A-CGA-O2A-C1
14	b	1234	CLA	O1A-CGA-O2A-C1
14	B	1021	CLA	O1A-CGA-O2A-C1
14	B	1234	CLA	O1A-CGA-O2A-C1
14	G	1104	CLA	C6-C7-C8-C9
14	G	1109	CLA	C14-C13-C15-C16
14	G	1123	CLA	C6-C7-C8-C9
14	G	1126	CLA	C6-C7-C8-C9
14	G	1138	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
14	H	1021	CLA	C14-C13-C15-C16
14	H	1022	CLA	C11-C10-C8-C9
14	H	1208	CLA	C14-C13-C15-C16
14	H	1213	CLA	C14-C13-C15-C16
14	H	1222	CLA	C6-C7-C8-C9
14	H	1234	CLA	C6-C7-C8-C9
14	U	1501	CLA	C11-C10-C8-C9
14	U	1503	CLA	C14-C13-C15-C16
14	a	1104	CLA	C6-C7-C8-C9
14	a	1109	CLA	C14-C13-C15-C16
14	a	1123	CLA	C6-C7-C8-C9
14	a	1126	CLA	C6-C7-C8-C9
14	a	1138	CLA	C11-C10-C8-C9
14	b	1021	CLA	C14-C13-C15-C16
14	b	1022	CLA	C11-C10-C8-C9
14	b	1208	CLA	C14-C13-C15-C16
14	b	1213	CLA	C14-C13-C15-C16
14	b	1222	CLA	C6-C7-C8-C9
14	b	1234	CLA	C6-C7-C8-C9
14	l	1501	CLA	C11-C10-C8-C9
14	l	1503	CLA	C14-C13-C15-C16
14	A	1104	CLA	C6-C7-C8-C9
14	A	1109	CLA	C14-C13-C15-C16
14	A	1123	CLA	C6-C7-C8-C9
14	A	1126	CLA	C6-C7-C8-C9
14	A	1138	CLA	C11-C10-C8-C9
14	B	1021	CLA	C14-C13-C15-C16
14	B	1022	CLA	C11-C10-C8-C9
14	B	1208	CLA	C14-C13-C15-C16
14	B	1213	CLA	C14-C13-C15-C16
14	B	1222	CLA	C6-C7-C8-C9
14	B	1234	CLA	C6-C7-C8-C9
14	L	1501	CLA	C11-C10-C8-C9
14	L	1503	CLA	C14-C13-C15-C16
15	H	1207	F6C	C14-C13-C15-C16
15	H	1237	F6C	C11-C12-C13-C14
15	b	1207	F6C	C14-C13-C15-C16
15	b	1237	F6C	C11-C12-C13-C14
15	B	1207	F6C	C14-C13-C15-C16
15	B	1237	F6C	C11-C12-C13-C14
14	G	1105	CLA	O1D-CGD-O2D-CED
14	G	1111	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	G	1114	CLA	O1D-CGD-O2D-CED
14	H	1204	CLA	O1D-CGD-O2D-CED
14	a	1105	CLA	O1D-CGD-O2D-CED
14	a	1111	CLA	O1D-CGD-O2D-CED
14	a	1114	CLA	O1D-CGD-O2D-CED
14	b	1204	CLA	O1D-CGD-O2D-CED
14	A	1105	CLA	O1D-CGD-O2D-CED
14	A	1111	CLA	O1D-CGD-O2D-CED
14	A	1114	CLA	O1D-CGD-O2D-CED
14	B	1204	CLA	O1D-CGD-O2D-CED
14	U	1503	CLA	C13-C15-C16-C17
18	G	4001	BCR	C7-C8-C9-C34
18	G	4002	BCR	C7-C8-C9-C34
18	G	4011	BCR	C37-C22-C23-C24
18	H	4004	BCR	C37-C22-C23-C24
18	H	4006	BCR	C37-C22-C23-C24
18	H	4009	BCR	C7-C8-C9-C34
18	a	4001	BCR	C7-C8-C9-C34
18	a	4002	BCR	C7-C8-C9-C34
18	a	4011	BCR	C37-C22-C23-C24
18	b	4004	BCR	C37-C22-C23-C24
18	b	4006	BCR	C37-C22-C23-C24
18	b	4009	BCR	C7-C8-C9-C34
18	A	4001	BCR	C7-C8-C9-C34
18	A	4002	BCR	C7-C8-C9-C34
18	A	4011	BCR	C37-C22-C23-C24
18	B	4004	BCR	C37-C22-C23-C24
18	B	4006	BCR	C37-C22-C23-C24
18	B	4009	BCR	C7-C8-C9-C34
18	G	4001	BCR	C7-C8-C9-C10
18	G	4002	BCR	C7-C8-C9-C10
18	G	4011	BCR	C21-C22-C23-C24
18	H	4004	BCR	C21-C22-C23-C24
18	H	4006	BCR	C21-C22-C23-C24
18	H	4016	BCR	C17-C18-C19-C20
18	U	4022	BCR	C7-C8-C9-C10
18	V	4021	BCR	C7-C8-C9-C10
18	a	4001	BCR	C7-C8-C9-C10
18	a	4002	BCR	C7-C8-C9-C10
18	a	4011	BCR	C21-C22-C23-C24
18	b	4004	BCR	C21-C22-C23-C24
18	b	4006	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
18	b	4016	BCR	C17-C18-C19-C20
18	l	4022	BCR	C7-C8-C9-C10
18	m	4021	BCR	C7-C8-C9-C10
18	A	4001	BCR	C7-C8-C9-C10
18	A	4002	BCR	C7-C8-C9-C10
18	A	4011	BCR	C21-C22-C23-C24
18	B	4004	BCR	C21-C22-C23-C24
18	B	4006	BCR	C21-C22-C23-C24
18	B	4016	BCR	C17-C18-C19-C20
18	L	4022	BCR	C7-C8-C9-C10
18	M	4021	BCR	C7-C8-C9-C10
19	H	5004	LHG	C7-C8-C9-C10
19	b	5004	LHG	C7-C8-C9-C10
19	B	5004	LHG	C7-C8-C9-C10
14	G	1124	CLA	O1A-CGA-O2A-C1
14	a	1124	CLA	O1A-CGA-O2A-C1
14	A	1124	CLA	O1A-CGA-O2A-C1
14	G	1140	CLA	C13-C15-C16-C17
14	H	1211	CLA	C15-C16-C17-C18
14	H	1224	CLA	C13-C15-C16-C17
14	a	1140	CLA	C13-C15-C16-C17
14	b	1211	CLA	C15-C16-C17-C18
14	b	1224	CLA	C13-C15-C16-C17
14	b	1234	CLA	C10-C11-C12-C13
14	l	1503	CLA	C13-C15-C16-C17
14	A	1117	CLA	C15-C16-C17-C18
14	A	1140	CLA	C13-C15-C16-C17
14	B	1211	CLA	C15-C16-C17-C18
14	B	1224	CLA	C13-C15-C16-C17
14	B	1234	CLA	C10-C11-C12-C13
14	L	1503	CLA	C13-C15-C16-C17
14	G	1106	CLA	O1D-CGD-O2D-CED
14	H	1212	CLA	O1D-CGD-O2D-CED
14	a	1106	CLA	O1D-CGD-O2D-CED
14	b	1212	CLA	O1D-CGD-O2D-CED
14	A	1106	CLA	O1D-CGD-O2D-CED
14	B	1212	CLA	O1D-CGD-O2D-CED
14	H	1211	CLA	C3-C5-C6-C7
14	H	1213	CLA	C3-C5-C6-C7
14	b	1211	CLA	C3-C5-C6-C7
14	b	1213	CLA	C3-C5-C6-C7
14	B	1211	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	B	1213	CLA	C3-C5-C6-C7
14	H	1215	CLA	CBA-CGA-O2A-C1
14	b	1215	CLA	CBA-CGA-O2A-C1
14	B	1215	CLA	CBA-CGA-O2A-C1
14	G	1117	CLA	C15-C16-C17-C18
14	G	1119	CLA	C10-C11-C12-C13
14	G	1123	CLA	C8-C10-C11-C12
14	G	1127	CLA	C8-C10-C11-C12
14	G	1140	CLA	C5-C6-C7-C8
14	H	1208	CLA	C15-C16-C17-C18
14	H	1211	CLA	C13-C15-C16-C17
14	H	1216	CLA	C5-C6-C7-C8
14	H	1234	CLA	C10-C11-C12-C13
14	H	1234	CLA	C15-C16-C17-C18
14	U	1503	CLA	C8-C10-C11-C12
14	a	1117	CLA	C15-C16-C17-C18
14	a	1119	CLA	C10-C11-C12-C13
14	a	1123	CLA	C8-C10-C11-C12
14	a	1127	CLA	C8-C10-C11-C12
14	a	1140	CLA	C5-C6-C7-C8
14	b	1208	CLA	C15-C16-C17-C18
14	b	1211	CLA	C13-C15-C16-C17
14	b	1234	CLA	C15-C16-C17-C18
14	l	1503	CLA	C8-C10-C11-C12
14	A	1119	CLA	C10-C11-C12-C13
14	A	1123	CLA	C8-C10-C11-C12
14	A	1127	CLA	C8-C10-C11-C12
14	A	1140	CLA	C5-C6-C7-C8
14	B	1208	CLA	C15-C16-C17-C18
14	B	1211	CLA	C13-C15-C16-C17
14	B	1216	CLA	C5-C6-C7-C8
14	B	1234	CLA	C15-C16-C17-C18
14	L	1503	CLA	C8-C10-C11-C12
14	H	1213	CLA	O1D-CGD-O2D-CED
14	b	1213	CLA	O1D-CGD-O2D-CED
14	B	1213	CLA	O1D-CGD-O2D-CED
14	b	1225	CLA	CBD-CGD-O2D-CED
14	B	1225	CLA	CBD-CGD-O2D-CED
14	G	1013	CLA	C5-C6-C7-C8
14	G	1104	CLA	C10-C11-C12-C13
14	G	1115	CLA	C13-C15-C16-C17
14	G	1117	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	G	1119	CLA	C8-C10-C11-C12
14	G	1125	CLA	C8-C10-C11-C12
14	H	1021	CLA	C15-C16-C17-C18
14	H	1023	CLA	C13-C15-C16-C17
14	H	1215	CLA	C10-C11-C12-C13
14	H	1216	CLA	C13-C15-C16-C17
14	H	1222	CLA	C5-C6-C7-C8
14	H	1222	CLA	C13-C15-C16-C17
14	H	1234	CLA	C8-C10-C11-C12
14	H	1235	CLA	C10-C11-C12-C13
14	a	1013	CLA	C5-C6-C7-C8
14	a	1104	CLA	C10-C11-C12-C13
14	a	1115	CLA	C13-C15-C16-C17
14	a	1117	CLA	C5-C6-C7-C8
14	a	1119	CLA	C8-C10-C11-C12
14	a	1125	CLA	C8-C10-C11-C12
14	b	1021	CLA	C15-C16-C17-C18
14	b	1023	CLA	C13-C15-C16-C17
14	b	1215	CLA	C10-C11-C12-C13
14	b	1216	CLA	C5-C6-C7-C8
14	b	1216	CLA	C13-C15-C16-C17
14	b	1222	CLA	C5-C6-C7-C8
14	b	1222	CLA	C13-C15-C16-C17
14	b	1234	CLA	C8-C10-C11-C12
14	b	1235	CLA	C10-C11-C12-C13
14	A	1013	CLA	C5-C6-C7-C8
14	A	1104	CLA	C10-C11-C12-C13
14	A	1115	CLA	C13-C15-C16-C17
14	A	1117	CLA	C5-C6-C7-C8
14	A	1119	CLA	C8-C10-C11-C12
14	A	1125	CLA	C8-C10-C11-C12
14	B	1021	CLA	C15-C16-C17-C18
14	B	1023	CLA	C13-C15-C16-C17
14	B	1215	CLA	C10-C11-C12-C13
14	B	1216	CLA	C13-C15-C16-C17
14	B	1222	CLA	C5-C6-C7-C8
14	B	1222	CLA	C13-C15-C16-C17
14	B	1234	CLA	C8-C10-C11-C12
14	B	1235	CLA	C10-C11-C12-C13
15	H	1237	F6C	C8-C10-C11-C12
15	b	1237	F6C	C8-C10-C11-C12
15	B	1237	F6C	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	G	1124	CLA	O1D-CGD-O2D-CED
14	a	1124	CLA	O1D-CGD-O2D-CED
14	A	1124	CLA	O1D-CGD-O2D-CED
14	H	1225	CLA	CBD-CGD-O2D-CED
14	H	1205	CLA	O1D-CGD-O2D-CED
14	b	1205	CLA	O1D-CGD-O2D-CED
14	B	1205	CLA	O1D-CGD-O2D-CED
14	G	1122	CLA	C5-C6-C7-C8
14	G	1128	CLA	C10-C11-C12-C13
14	G	1136	CLA	C10-C11-C12-C13
14	G	1138	CLA	C5-C6-C7-C8
14	H	1022	CLA	C5-C6-C7-C8
14	H	1022	CLA	C15-C16-C17-C18
14	H	1222	CLA	C15-C16-C17-C18
14	H	1239	CLA	C15-C16-C17-C18
14	a	1128	CLA	C10-C11-C12-C13
14	a	1136	CLA	C10-C11-C12-C13
14	a	1138	CLA	C5-C6-C7-C8
14	b	1022	CLA	C5-C6-C7-C8
14	b	1022	CLA	C15-C16-C17-C18
14	b	1222	CLA	C15-C16-C17-C18
14	b	1239	CLA	C15-C16-C17-C18
14	A	1128	CLA	C10-C11-C12-C13
14	A	1136	CLA	C10-C11-C12-C13
14	A	1138	CLA	C5-C6-C7-C8
14	B	1022	CLA	C5-C6-C7-C8
14	B	1022	CLA	C15-C16-C17-C18
14	B	1222	CLA	C15-C16-C17-C18
14	B	1239	CLA	C15-C16-C17-C18
16	H	2002	PQN	C18-C20-C21-C22
16	b	2002	PQN	C18-C20-C21-C22
16	B	2002	PQN	C18-C20-C21-C22
14	H	1201	CLA	CBA-CGA-O2A-C1
14	b	1201	CLA	CBA-CGA-O2A-C1
14	B	1201	CLA	CBA-CGA-O2A-C1
14	H	1023	CLA	O1D-CGD-O2D-CED
14	b	1023	CLA	O1D-CGD-O2D-CED
14	B	1023	CLA	O1D-CGD-O2D-CED
14	G	1122	CLA	C2-C1-O2A-CGA
14	G	1128	CLA	C2-C1-O2A-CGA
14	G	1140	CLA	C2-C1-O2A-CGA
14	H	1202	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	H	1214	CLA	C2-C1-O2A-CGA
14	W	1701	CLA	C2-C1-O2A-CGA
14	a	1122	CLA	C2-C1-O2A-CGA
14	a	1128	CLA	C2-C1-O2A-CGA
14	a	1140	CLA	C2-C1-O2A-CGA
14	b	1202	CLA	C2-C1-O2A-CGA
14	b	1214	CLA	C2-C1-O2A-CGA
14	x	1701	CLA	C2-C1-O2A-CGA
14	A	1122	CLA	C2-C1-O2A-CGA
14	A	1128	CLA	C2-C1-O2A-CGA
14	A	1140	CLA	C2-C1-O2A-CGA
14	B	1202	CLA	C2-C1-O2A-CGA
14	B	1214	CLA	C2-C1-O2A-CGA
14	X	1701	CLA	C2-C1-O2A-CGA
15	H	1207	F6C	C2-C1-O2A-CGA
15	b	1207	F6C	C2-C1-O2A-CGA
15	B	1207	F6C	C2-C1-O2A-CGA
14	G	1104	CLA	C15-C16-C17-C18
14	H	1204	CLA	C13-C15-C16-C17
14	H	1225	CLA	C10-C11-C12-C13
14	H	1226	CLA	C13-C15-C16-C17
14	H	1239	CLA	C10-C11-C12-C13
14	a	1104	CLA	C15-C16-C17-C18
14	a	1122	CLA	C5-C6-C7-C8
14	b	1204	CLA	C13-C15-C16-C17
14	b	1225	CLA	C10-C11-C12-C13
14	b	1226	CLA	C13-C15-C16-C17
14	b	1239	CLA	C10-C11-C12-C13
14	A	1104	CLA	C15-C16-C17-C18
14	A	1122	CLA	C5-C6-C7-C8
14	B	1204	CLA	C13-C15-C16-C17
14	B	1225	CLA	C10-C11-C12-C13
14	B	1226	CLA	C13-C15-C16-C17
14	B	1239	CLA	C10-C11-C12-C13
15	H	1237	F6C	C13-C15-C16-C17
15	b	1237	F6C	C13-C15-C16-C17
15	B	1237	F6C	C13-C15-C16-C17
16	H	2002	PQN	C20-C21-C22-C23
16	b	2002	PQN	C20-C21-C22-C23
16	B	2002	PQN	C20-C21-C22-C23
15	H	1238	F6C	C2A-CAA-CBA-CGA
15	b	1238	F6C	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
15	B	1238	F6C	C2A-CAA-CBA-CGA
20	G	5005	LMG	C11-C10-O7-C8
20	a	5005	LMG	C11-C10-O7-C8
20	A	5005	LMG	C11-C10-O7-C8
14	G	1106	CLA	C8-C10-C11-C12
14	G	1128	CLA	C5-C6-C7-C8
14	H	1021	CLA	C13-C15-C16-C17
14	H	1235	CLA	C8-C10-C11-C12
14	a	1106	CLA	C8-C10-C11-C12
14	a	1128	CLA	C5-C6-C7-C8
14	b	1021	CLA	C13-C15-C16-C17
14	A	1106	CLA	C8-C10-C11-C12
14	A	1128	CLA	C5-C6-C7-C8
14	B	1021	CLA	C13-C15-C16-C17
14	B	1235	CLA	C8-C10-C11-C12
14	G	1102	CLA	O1D-CGD-O2D-CED
14	G	1135	CLA	O1D-CGD-O2D-CED
14	a	1135	CLA	O1D-CGD-O2D-CED
14	A	1102	CLA	O1D-CGD-O2D-CED
14	A	1135	CLA	O1D-CGD-O2D-CED
14	G	1125	CLA	C11-C12-C13-C15
14	G	1136	CLA	C6-C7-C8-C10
14	H	1021	CLA	C6-C7-C8-C10
14	H	1021	CLA	C11-C10-C8-C7
14	H	1021	CLA	C11-C12-C13-C15
14	H	1203	CLA	C11-C12-C13-C15
14	H	1216	CLA	C12-C13-C15-C16
14	H	1223	CLA	C11-C10-C8-C7
14	H	1229	CLA	C6-C7-C8-C10
14	a	1125	CLA	C11-C12-C13-C15
14	a	1136	CLA	C6-C7-C8-C10
14	b	1021	CLA	C6-C7-C8-C10
14	b	1021	CLA	C11-C10-C8-C7
14	b	1021	CLA	C11-C12-C13-C15
14	b	1203	CLA	C11-C12-C13-C15
14	b	1216	CLA	C12-C13-C15-C16
14	b	1223	CLA	C11-C10-C8-C7
14	b	1229	CLA	C6-C7-C8-C10
14	A	1125	CLA	C11-C12-C13-C15
14	A	1136	CLA	C6-C7-C8-C10
14	B	1021	CLA	C6-C7-C8-C10
14	B	1021	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
14	B	1021	CLA	C11-C12-C13-C15
14	B	1203	CLA	C11-C12-C13-C15
14	B	1216	CLA	C12-C13-C15-C16
14	B	1223	CLA	C11-C10-C8-C7
14	B	1229	CLA	C6-C7-C8-C10
15	H	1207	F6C	C12-C13-C15-C16
15	b	1207	F6C	C12-C13-C15-C16
15	B	1207	F6C	C12-C13-C15-C16
14	G	1115	CLA	O1A-CGA-O2A-C1
14	H	1231	CLA	O1A-CGA-O2A-C1
14	b	1231	CLA	O1A-CGA-O2A-C1
14	B	1231	CLA	O1A-CGA-O2A-C1
14	G	1132	CLA	C2A-CAA-CBA-CGA
14	G	1134	CLA	C2A-CAA-CBA-CGA
14	H	1209	CLA	C2A-CAA-CBA-CGA
14	H	1211	CLA	C2A-CAA-CBA-CGA
14	H	1213	CLA	C2A-CAA-CBA-CGA
14	a	1132	CLA	C2A-CAA-CBA-CGA
14	a	1134	CLA	C2A-CAA-CBA-CGA
14	b	1209	CLA	C2A-CAA-CBA-CGA
14	b	1211	CLA	C2A-CAA-CBA-CGA
14	b	1213	CLA	C2A-CAA-CBA-CGA
14	A	1132	CLA	C2A-CAA-CBA-CGA
14	A	1134	CLA	C2A-CAA-CBA-CGA
14	B	1209	CLA	C2A-CAA-CBA-CGA
14	B	1211	CLA	C2A-CAA-CBA-CGA
14	B	1213	CLA	C2A-CAA-CBA-CGA
14	G	1113	CLA	O1D-CGD-O2D-CED
14	G	1125	CLA	O1D-CGD-O2D-CED
14	a	1102	CLA	O1D-CGD-O2D-CED
14	a	1113	CLA	O1D-CGD-O2D-CED
14	a	1125	CLA	O1D-CGD-O2D-CED
14	A	1113	CLA	O1D-CGD-O2D-CED
14	A	1125	CLA	O1D-CGD-O2D-CED
14	G	1012	CLA	C15-C16-C17-C18
14	G	1132	CLA	C13-C15-C16-C17
14	a	1012	CLA	C15-C16-C17-C18
14	a	1132	CLA	C13-C15-C16-C17
14	b	1235	CLA	C8-C10-C11-C12
14	A	1012	CLA	C15-C16-C17-C18
14	A	1132	CLA	C13-C15-C16-C17
15	H	1207	F6C	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	b	1207	F6C	C5-C6-C7-C8
15	B	1207	F6C	C5-C6-C7-C8
16	H	2002	PQN	C25-C26-C27-C28
16	b	2002	PQN	C25-C26-C27-C28
16	B	2002	PQN	C25-C26-C27-C28
14	a	1115	CLA	O1A-CGA-O2A-C1
14	A	1115	CLA	O1A-CGA-O2A-C1
21	G	6001	LMT	O5'-C1'-O1'-C1
21	a	6001	LMT	O5'-C1'-O1'-C1
21	A	6001	LMT	O5'-C1'-O1'-C1
14	G	1102	CLA	C8-C10-C11-C12
14	H	1214	CLA	C8-C10-C11-C12
14	H	1223	CLA	C8-C10-C11-C12
14	H	1229	CLA	C8-C10-C11-C12
14	H	1234	CLA	C13-C15-C16-C17
14	b	1214	CLA	C8-C10-C11-C12
14	b	1223	CLA	C8-C10-C11-C12
14	b	1229	CLA	C8-C10-C11-C12
14	b	1234	CLA	C13-C15-C16-C17
14	B	1214	CLA	C8-C10-C11-C12
14	B	1223	CLA	C8-C10-C11-C12
14	B	1229	CLA	C8-C10-C11-C12
14	B	1234	CLA	C13-C15-C16-C17
18	G	4007	BCR	C10-C11-C12-C13
18	H	4004	BCR	C10-C11-C12-C13
18	H	4010	BCR	C10-C11-C12-C13
18	H	4013	BCR	C10-C11-C12-C13
18	R	4018	BCR	C10-C11-C12-C13
18	a	4007	BCR	C10-C11-C12-C13
18	b	4004	BCR	C10-C11-C12-C13
18	b	4010	BCR	C10-C11-C12-C13
18	b	4013	BCR	C10-C11-C12-C13
18	i	4018	BCR	C10-C11-C12-C13
18	A	4007	BCR	C10-C11-C12-C13
18	B	4004	BCR	C10-C11-C12-C13
18	B	4010	BCR	C10-C11-C12-C13
18	B	4013	BCR	C10-C11-C12-C13
18	I	4018	BCR	C10-C11-C12-C13
20	U	5007	LMG	C20-C21-C22-C23
20	L	5007	LMG	C20-C21-C22-C23
14	G	1130	CLA	C3-C5-C6-C7
14	a	1130	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	A	1130	CLA	C3-C5-C6-C7
14	G	1106	CLA	C10-C11-C12-C13
14	H	1203	CLA	C15-C16-C17-C18
14	H	1239	CLA	C5-C6-C7-C8
14	W	1701	CLA	C5-C6-C7-C8
14	a	1102	CLA	C8-C10-C11-C12
14	a	1106	CLA	C10-C11-C12-C13
14	b	1203	CLA	C15-C16-C17-C18
14	b	1239	CLA	C5-C6-C7-C8
14	x	1701	CLA	C5-C6-C7-C8
14	A	1102	CLA	C8-C10-C11-C12
14	A	1106	CLA	C10-C11-C12-C13
14	B	1203	CLA	C15-C16-C17-C18
14	B	1239	CLA	C5-C6-C7-C8
14	X	1701	CLA	C5-C6-C7-C8
20	l	5007	LMG	C20-C21-C22-C23
14	b	1235	CLA	O1D-CGD-O2D-CED
14	H	1229	CLA	O1A-CGA-O2A-C1
14	b	1229	CLA	O1A-CGA-O2A-C1
14	B	1229	CLA	O1A-CGA-O2A-C1
15	H	1207	F6C	O1A-CGA-O2A-C1
15	B	1207	F6C	O1A-CGA-O2A-C1
14	G	1120	CLA	O1D-CGD-O2D-CED
14	G	1133	CLA	C5-C6-C7-C8
14	G	1136	CLA	C5-C6-C7-C8
14	H	1022	CLA	C8-C10-C11-C12
14	H	1224	CLA	C15-C16-C17-C18
14	H	1229	CLA	C10-C11-C12-C13
14	a	1133	CLA	C5-C6-C7-C8
14	a	1136	CLA	C5-C6-C7-C8
14	b	1022	CLA	C8-C10-C11-C12
14	b	1224	CLA	C15-C16-C17-C18
14	b	1229	CLA	C10-C11-C12-C13
14	A	1133	CLA	C5-C6-C7-C8
14	A	1136	CLA	C5-C6-C7-C8
14	B	1022	CLA	C8-C10-C11-C12
14	B	1224	CLA	C15-C16-C17-C18
14	B	1229	CLA	C10-C11-C12-C13
14	H	1235	CLA	O1D-CGD-O2D-CED
14	a	1120	CLA	O1D-CGD-O2D-CED
14	A	1120	CLA	O1D-CGD-O2D-CED
14	B	1235	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	H	1223	CLA	CBD-CGD-O2D-CED
14	b	1223	CLA	CBD-CGD-O2D-CED
14	B	1223	CLA	CBD-CGD-O2D-CED
15	H	1238	F6C	O1A-CGA-O2A-C1
15	b	1207	F6C	O1A-CGA-O2A-C1
15	b	1238	F6C	O1A-CGA-O2A-C1
15	B	1238	F6C	O1A-CGA-O2A-C1
19	G	5001	LHG	C8-C7-O7-C5
19	a	5001	LHG	C8-C7-O7-C5
19	A	5001	LHG	C8-C7-O7-C5
14	G	1115	CLA	C15-C16-C17-C18
14	G	1123	CLA	C5-C6-C7-C8
14	H	1204	CLA	C5-C6-C7-C8
14	H	1211	CLA	C10-C11-C12-C13
14	a	1115	CLA	C15-C16-C17-C18
14	b	1204	CLA	C5-C6-C7-C8
14	b	1211	CLA	C10-C11-C12-C13
14	A	1115	CLA	C15-C16-C17-C18
14	A	1123	CLA	C5-C6-C7-C8
14	B	1204	CLA	C5-C6-C7-C8
14	B	1211	CLA	C10-C11-C12-C13
15	H	1207	F6C	C15-C16-C17-C18
15	b	1207	F6C	C15-C16-C17-C18
15	B	1207	F6C	C15-C16-C17-C18
19	G	5001	LHG	C3-O3-P-O6
19	H	5004	LHG	C4-O6-P-O3
19	a	5001	LHG	C3-O3-P-O6
19	b	5004	LHG	C4-O6-P-O3
19	A	5001	LHG	C3-O3-P-O6
19	B	5004	LHG	C4-O6-P-O3
20	H	5002	LMG	C10-C11-C12-C13
20	b	5002	LMG	C10-C11-C12-C13
20	B	5002	LMG	C10-C11-C12-C13
14	G	1109	CLA	CBA-CGA-O2A-C1
14	a	1109	CLA	CBA-CGA-O2A-C1
14	A	1109	CLA	CBA-CGA-O2A-C1
14	a	1123	CLA	C5-C6-C7-C8
15	H	1207	F6C	C8-C10-C11-C12
15	b	1207	F6C	C8-C10-C11-C12
15	B	1207	F6C	C8-C10-C11-C12
14	H	1222	CLA	O1D-CGD-O2D-CED
14	a	1118	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	b	1222	CLA	O1D-CGD-O2D-CED
14	G	1104	CLA	O1D-CGD-O2D-CED
14	G	1118	CLA	O1D-CGD-O2D-CED
14	a	1104	CLA	O1D-CGD-O2D-CED
14	A	1104	CLA	O1D-CGD-O2D-CED
14	A	1118	CLA	O1D-CGD-O2D-CED
14	B	1222	CLA	O1D-CGD-O2D-CED
20	G	5005	LMG	O9-C10-O7-C8
20	a	5005	LMG	O9-C10-O7-C8
20	A	5005	LMG	O9-C10-O7-C8
14	H	1225	CLA	C15-C16-C17-C18
14	U	1501	CLA	C13-C15-C16-C17
14	b	1225	CLA	C15-C16-C17-C18
14	l	1501	CLA	C13-C15-C16-C17
14	B	1225	CLA	C15-C16-C17-C18
14	L	1501	CLA	C13-C15-C16-C17
14	G	1113	CLA	C2A-CAA-CBA-CGA
14	G	1135	CLA	C2A-CAA-CBA-CGA
14	H	1224	CLA	C2A-CAA-CBA-CGA
14	T	1401	CLA	C2A-CAA-CBA-CGA
14	a	1113	CLA	C2A-CAA-CBA-CGA
14	a	1135	CLA	C2A-CAA-CBA-CGA
14	b	1224	CLA	C2A-CAA-CBA-CGA
14	k	1401	CLA	C2A-CAA-CBA-CGA
14	A	1113	CLA	C2A-CAA-CBA-CGA
14	A	1135	CLA	C2A-CAA-CBA-CGA
14	B	1224	CLA	C2A-CAA-CBA-CGA
14	K	1401	CLA	C2A-CAA-CBA-CGA
14	G	1125	CLA	C16-C17-C18-C20
14	a	1125	CLA	C16-C17-C18-C20
14	A	1125	CLA	C16-C17-C18-C20
20	G	5005	LMG	O6-C5-C6-O5
20	a	5005	LMG	O6-C5-C6-O5
20	A	5005	LMG	O6-C5-C6-O5
14	H	1215	CLA	C3-C5-C6-C7
14	b	1215	CLA	C3-C5-C6-C7
14	B	1215	CLA	C3-C5-C6-C7
14	U	1502	CLA	CBA-CGA-O2A-C1
14	W	1701	CLA	CBA-CGA-O2A-C1
14	l	1502	CLA	CBA-CGA-O2A-C1
14	x	1701	CLA	CBA-CGA-O2A-C1
14	L	1502	CLA	CBA-CGA-O2A-C1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
14	X	1701	CLA	CBA-CGA-O2A-C1
14	b	1223	CLA	C5-C6-C7-C8
14	H	1223	CLA	C5-C6-C7-C8
14	B	1223	CLA	C5-C6-C7-C8
15	b	1237	F6C	C15-C16-C17-C18
18	G	4003	BCR	C9-C10-C11-C12
18	G	4007	BCR	C19-C20-C21-C22
18	R	4018	BCR	C19-C20-C21-C22
18	a	4007	BCR	C19-C20-C21-C22
18	i	4018	BCR	C19-C20-C21-C22
18	A	4007	BCR	C19-C20-C21-C22
18	I	4018	BCR	C19-C20-C21-C22
14	G	1102	CLA	C10-C11-C12-C13
14	a	1102	CLA	C10-C11-C12-C13
14	A	1102	CLA	C10-C11-C12-C13
15	H	1237	F6C	C15-C16-C17-C18
15	B	1237	F6C	C15-C16-C17-C18
18	G	4011	BCR	C11-C10-C9-C34
18	R	4020	BCR	C11-C10-C9-C34
18	a	4011	BCR	C11-C10-C9-C34
18	i	4020	BCR	C11-C10-C9-C34
18	A	4011	BCR	C11-C10-C9-C34
18	I	4020	BCR	C11-C10-C9-C34
19	H	5004	LHG	C11-C10-C9-C8
19	b	5004	LHG	C11-C10-C9-C8
19	B	5004	LHG	C11-C10-C9-C8
14	G	1136	CLA	O1D-CGD-O2D-CED
14	a	1136	CLA	O1D-CGD-O2D-CED
14	A	1136	CLA	O1D-CGD-O2D-CED
14	G	1103	CLA	C11-C12-C13-C15
14	H	1215	CLA	C11-C12-C13-C15
14	H	1223	CLA	C16-C17-C18-C19
14	H	1225	CLA	C16-C17-C18-C19
14	a	1103	CLA	C11-C12-C13-C15
14	b	1215	CLA	C11-C12-C13-C15
14	b	1223	CLA	C16-C17-C18-C19
14	b	1225	CLA	C16-C17-C18-C19
14	A	1103	CLA	C11-C12-C13-C15
14	B	1215	CLA	C11-C12-C13-C15
14	B	1223	CLA	C16-C17-C18-C19
14	B	1225	CLA	C16-C17-C18-C19
19	G	5001	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
19	a	5001	LHG	O9-C7-O7-C5
19	A	5001	LHG	O9-C7-O7-C5
20	G	5005	LMG	C30-C31-C32-C33
14	H	1201	CLA	O1A-CGA-O2A-C1
14	b	1201	CLA	O1A-CGA-O2A-C1
14	B	1201	CLA	O1A-CGA-O2A-C1
20	a	5005	LMG	C30-C31-C32-C33
20	A	5005	LMG	C30-C31-C32-C33
15	G	1121	F6C	C2A-CAA-CBA-CGA
15	a	1121	F6C	C2A-CAA-CBA-CGA
15	A	1121	F6C	C2A-CAA-CBA-CGA
19	b	5004	LHG	C33-C34-C35-C36
19	B	5004	LHG	C33-C34-C35-C36
20	B	5002	LMG	C19-C20-C21-C22
14	G	1131	CLA	C3-C5-C6-C7
14	a	1131	CLA	C3-C5-C6-C7
20	R	5006	LMG	C28-C29-C30-C31
20	i	5006	LMG	C28-C29-C30-C31
20	I	5006	LMG	C28-C29-C30-C31
18	G	4011	BCR	C11-C10-C9-C8
18	R	4020	BCR	C11-C10-C9-C8
18	R	4020	BCR	C20-C21-C22-C23
18	a	4011	BCR	C11-C10-C9-C8
18	i	4020	BCR	C11-C10-C9-C8
18	i	4020	BCR	C20-C21-C22-C23
18	A	4011	BCR	C11-C10-C9-C8
18	I	4020	BCR	C11-C10-C9-C8
18	I	4020	BCR	C20-C21-C22-C23
21	G	6002	LMT	C2'-C1'-O1'-C1
21	a	6002	LMT	C2'-C1'-O1'-C1
21	A	6002	LMT	C2'-C1'-O1'-C1
19	H	5004	LHG	C33-C34-C35-C36
20	H	5002	LMG	C19-C20-C21-C22
20	b	5002	LMG	C19-C20-C21-C22
21	A	6001	LMT	C3-C4-C5-C6
14	H	1234	CLA	C5-C6-C7-C8
14	b	1234	CLA	C5-C6-C7-C8
14	B	1234	CLA	C5-C6-C7-C8
14	G	1109	CLA	O1A-CGA-O2A-C1
14	W	1701	CLA	O1A-CGA-O2A-C1
14	a	1109	CLA	O1A-CGA-O2A-C1
14	x	1701	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	A	1109	CLA	O1A-CGA-O2A-C1
14	X	1701	CLA	O1A-CGA-O2A-C1
14	G	1103	CLA	C11-C12-C13-C14
14	G	1111	CLA	C11-C12-C13-C15
14	G	1112	CLA	C6-C7-C8-C10
14	G	1126	CLA	C11-C12-C13-C14
14	H	1216	CLA	C16-C17-C18-C20
14	H	1221	CLA	C16-C17-C18-C20
14	a	1102	CLA	C11-C12-C13-C15
14	a	1111	CLA	C11-C12-C13-C15
14	a	1112	CLA	C6-C7-C8-C10
14	a	1126	CLA	C11-C12-C13-C14
14	b	1216	CLA	C16-C17-C18-C20
14	b	1221	CLA	C16-C17-C18-C20
14	A	1102	CLA	C11-C12-C13-C15
14	A	1111	CLA	C11-C12-C13-C15
14	A	1112	CLA	C6-C7-C8-C10
14	A	1126	CLA	C11-C12-C13-C14
14	B	1216	CLA	C16-C17-C18-C20
14	B	1221	CLA	C16-C17-C18-C20
14	H	1225	CLA	C4-C3-C5-C6
14	b	1225	CLA	C4-C3-C5-C6
14	B	1225	CLA	C4-C3-C5-C6
20	G	5005	LMG	C13-C14-C15-C16
20	a	5005	LMG	C13-C14-C15-C16
20	A	5005	LMG	C13-C14-C15-C16
21	G	6001	LMT	C3-C4-C5-C6
21	a	6001	LMT	C3-C4-C5-C6
14	H	1021	CLA	C11-C10-C8-C9
14	H	1021	CLA	C11-C12-C13-C14
14	H	1203	CLA	C11-C12-C13-C14
14	b	1021	CLA	C11-C10-C8-C9
14	b	1021	CLA	C11-C12-C13-C14
14	b	1203	CLA	C11-C12-C13-C14
14	B	1021	CLA	C11-C10-C8-C9
14	B	1021	CLA	C11-C12-C13-C14
14	B	1203	CLA	C11-C12-C13-C14
15	H	1237	F6C	C6-C7-C8-C9
15	b	1237	F6C	C6-C7-C8-C9
15	B	1237	F6C	C6-C7-C8-C9
16	H	2002	PQN	C19-C18-C20-C21
16	b	2002	PQN	C19-C18-C20-C21

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Mol	Chain	Res	Type	Atoms
16	B	2002	PQN	C19-C18-C20-C21
14	G	1124	CLA	C5-C6-C7-C8
14	H	1229	CLA	C5-C6-C7-C8
14	a	1124	CLA	C5-C6-C7-C8
14	b	1229	CLA	C5-C6-C7-C8
14	A	1124	CLA	C5-C6-C7-C8
14	B	1229	CLA	C5-C6-C7-C8
14	H	1206	CLA	C2A-CAA-CBA-CGA
14	b	1206	CLA	C2A-CAA-CBA-CGA
14	B	1206	CLA	C2A-CAA-CBA-CGA
14	A	1131	CLA	C3-C5-C6-C7
19	G	5001	LHG	C23-C24-C25-C26
19	a	5001	LHG	C23-C24-C25-C26
19	A	5001	LHG	C23-C24-C25-C26
19	G	5001	LHG	C29-C30-C31-C32
19	H	5004	LHG	C13-C14-C15-C16
19	a	5001	LHG	C29-C30-C31-C32
19	b	5004	LHG	C13-C14-C15-C16
19	A	5001	LHG	C29-C30-C31-C32
19	B	5004	LHG	C13-C14-C15-C16
14	G	1102	CLA	C11-C12-C13-C15
14	G	1125	CLA	C16-C17-C18-C19
14	a	1103	CLA	C11-C12-C13-C14
14	a	1125	CLA	C16-C17-C18-C19
14	A	1103	CLA	C11-C12-C13-C14
14	A	1125	CLA	C16-C17-C18-C19
14	G	1109	CLA	C13-C15-C16-C17
14	G	1115	CLA	C5-C6-C7-C8
14	G	1138	CLA	C8-C10-C11-C12
14	a	1109	CLA	C13-C15-C16-C17
14	a	1115	CLA	C5-C6-C7-C8
14	A	1109	CLA	C13-C15-C16-C17
14	A	1115	CLA	C5-C6-C7-C8
14	A	1138	CLA	C8-C10-C11-C12
15	H	1207	F6C	C3A-C2A-CAA-CBA
15	b	1207	F6C	C3A-C2A-CAA-CBA
15	B	1207	F6C	C3A-C2A-CAA-CBA
14	H	1228	CLA	C5-C6-C7-C8
14	a	1138	CLA	C8-C10-C11-C12
14	b	1228	CLA	C5-C6-C7-C8
14	B	1228	CLA	C5-C6-C7-C8
19	H	5004	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
19	b	5004	LHG	C25-C26-C27-C28
19	B	5004	LHG	C25-C26-C27-C28
14	G	1102	CLA	C3A-C2A-CAA-CBA
14	G	1103	CLA	C3A-C2A-CAA-CBA
14	G	1125	CLA	C3A-C2A-CAA-CBA
14	G	1127	CLA	C3A-C2A-CAA-CBA
14	G	1138	CLA	C3A-C2A-CAA-CBA
14	H	1210	CLA	C3A-C2A-CAA-CBA
14	H	1220	CLA	C3A-C2A-CAA-CBA
14	H	1221	CLA	C3A-C2A-CAA-CBA
14	H	1229	CLA	C3A-C2A-CAA-CBA
14	U	1503	CLA	C3A-C2A-CAA-CBA
14	a	1102	CLA	C3A-C2A-CAA-CBA
14	a	1103	CLA	C3A-C2A-CAA-CBA
14	a	1125	CLA	C3A-C2A-CAA-CBA
14	a	1127	CLA	C3A-C2A-CAA-CBA
14	a	1138	CLA	C3A-C2A-CAA-CBA
14	b	1210	CLA	C3A-C2A-CAA-CBA
14	b	1220	CLA	C3A-C2A-CAA-CBA
14	b	1221	CLA	C3A-C2A-CAA-CBA
14	b	1229	CLA	C3A-C2A-CAA-CBA
14	l	1503	CLA	C3A-C2A-CAA-CBA
14	A	1102	CLA	C3A-C2A-CAA-CBA
14	A	1103	CLA	C3A-C2A-CAA-CBA
14	A	1125	CLA	C3A-C2A-CAA-CBA
14	A	1127	CLA	C3A-C2A-CAA-CBA
14	A	1138	CLA	C3A-C2A-CAA-CBA
14	B	1210	CLA	C3A-C2A-CAA-CBA
14	B	1220	CLA	C3A-C2A-CAA-CBA
14	B	1221	CLA	C3A-C2A-CAA-CBA
14	B	1229	CLA	C3A-C2A-CAA-CBA
14	L	1503	CLA	C3A-C2A-CAA-CBA
14	H	1211	CLA	C8-C10-C11-C12
14	b	1211	CLA	C8-C10-C11-C12
14	B	1211	CLA	C8-C10-C11-C12
16	G	2001	PQN	C23-C25-C26-C27
16	a	2001	PQN	C23-C25-C26-C27
16	A	2001	PQN	C23-C25-C26-C27
14	H	1215	CLA	O1A-CGA-O2A-C1
14	b	1215	CLA	O1A-CGA-O2A-C1
14	B	1215	CLA	O1A-CGA-O2A-C1
14	H	1202	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
14	H	1215	CLA	C11-C12-C13-C14
14	H	1216	CLA	C16-C17-C18-C19
14	H	1225	CLA	C16-C17-C18-C20
14	H	1239	CLA	C16-C17-C18-C19
14	b	1202	CLA	C11-C12-C13-C15
14	b	1215	CLA	C11-C12-C13-C14
14	b	1216	CLA	C16-C17-C18-C19
14	b	1225	CLA	C16-C17-C18-C20
14	b	1239	CLA	C16-C17-C18-C19
14	B	1202	CLA	C11-C12-C13-C15
14	B	1215	CLA	C11-C12-C13-C14
14	B	1216	CLA	C16-C17-C18-C19
14	B	1225	CLA	C16-C17-C18-C20
14	B	1239	CLA	C16-C17-C18-C19
14	G	1125	CLA	C3-C5-C6-C7
14	a	1125	CLA	C3-C5-C6-C7
14	A	1125	CLA	C3-C5-C6-C7
14	b	1210	CLA	C5-C6-C7-C8
14	B	1210	CLA	C5-C6-C7-C8
14	G	1140	CLA	CBA-CGA-O2A-C1
14	a	1140	CLA	CBA-CGA-O2A-C1
14	A	1140	CLA	CBA-CGA-O2A-C1
14	H	1205	CLA	C2-C3-C5-C6
14	b	1205	CLA	C2-C3-C5-C6
14	B	1205	CLA	C2-C3-C5-C6
14	H	1023	CLA	C2A-CAA-CBA-CGA
14	b	1023	CLA	C2A-CAA-CBA-CGA
14	B	1023	CLA	C2A-CAA-CBA-CGA
19	G	5001	LHG	O1-C1-C2-O2
19	a	5001	LHG	O1-C1-C2-O2
19	A	5001	LHG	O1-C1-C2-O2
14	H	1210	CLA	C5-C6-C7-C8
14	G	1112	CLA	C6-C7-C8-C9
14	G	1126	CLA	C11-C12-C13-C15
14	a	1112	CLA	C6-C7-C8-C9
14	a	1126	CLA	C11-C12-C13-C15
14	A	1112	CLA	C6-C7-C8-C9
14	A	1126	CLA	C11-C12-C13-C15
21	G	6002	LMT	C1-C2-C3-C4
21	a	6002	LMT	C1-C2-C3-C4
21	A	6002	LMT	C1-C2-C3-C4
14	G	1012	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	G	1124	CLA	C2-C1-O2A-CGA
14	G	1129	CLA	C2-C1-O2A-CGA
14	G	1136	CLA	C2-C1-O2A-CGA
14	H	1215	CLA	C2-C1-O2A-CGA
14	H	1239	CLA	C2-C1-O2A-CGA
14	a	1012	CLA	C2-C1-O2A-CGA
14	a	1124	CLA	C2-C1-O2A-CGA
14	a	1129	CLA	C2-C1-O2A-CGA
14	a	1136	CLA	C2-C1-O2A-CGA
14	b	1215	CLA	C2-C1-O2A-CGA
14	b	1239	CLA	C2-C1-O2A-CGA
14	A	1012	CLA	C2-C1-O2A-CGA
14	A	1124	CLA	C2-C1-O2A-CGA
14	A	1129	CLA	C2-C1-O2A-CGA
14	A	1136	CLA	C2-C1-O2A-CGA
14	B	1215	CLA	C2-C1-O2A-CGA
14	B	1239	CLA	C2-C1-O2A-CGA
14	G	1115	CLA	C10-C11-C12-C13
14	H	1210	CLA	C10-C11-C12-C13
14	H	1211	CLA	C5-C6-C7-C8
14	a	1115	CLA	C10-C11-C12-C13
14	b	1210	CLA	C10-C11-C12-C13
14	b	1211	CLA	C5-C6-C7-C8
14	A	1115	CLA	C10-C11-C12-C13
14	B	1210	CLA	C10-C11-C12-C13
14	B	1211	CLA	C5-C6-C7-C8
14	U	1502	CLA	O1A-CGA-O2A-C1
14	l	1502	CLA	O1A-CGA-O2A-C1
14	L	1502	CLA	O1A-CGA-O2A-C1
19	a	5001	LHG	C13-C14-C15-C16
19	A	5001	LHG	C13-C14-C15-C16
14	G	1102	CLA	C11-C12-C13-C14
14	H	1223	CLA	C16-C17-C18-C20
14	a	1102	CLA	C11-C12-C13-C14
14	b	1223	CLA	C16-C17-C18-C20
14	A	1102	CLA	C11-C12-C13-C14
14	B	1223	CLA	C16-C17-C18-C20
18	G	4001	BCR	C1-C6-C7-C8
18	G	4001	BCR	C5-C6-C7-C8
18	G	4001	BCR	C23-C24-C25-C26
18	G	4003	BCR	C1-C6-C7-C8
18	G	4003	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	G	4007	BCR	C23-C24-C25-C26
18	G	4007	BCR	C23-C24-C25-C30
18	G	4008	BCR	C1-C6-C7-C8
18	G	4008	BCR	C5-C6-C7-C8
18	G	4008	BCR	C23-C24-C25-C26
18	G	4008	BCR	C23-C24-C25-C30
18	H	4006	BCR	C1-C6-C7-C8
18	H	4006	BCR	C23-C24-C25-C26
18	H	4006	BCR	C23-C24-C25-C30
18	H	4009	BCR	C1-C6-C7-C8
18	H	4009	BCR	C5-C6-C7-C8
18	H	4013	BCR	C23-C24-C25-C30
18	H	4016	BCR	C1-C6-C7-C8
18	H	4016	BCR	C5-C6-C7-C8
18	H	4017	BCR	C23-C24-C25-C26
18	H	4017	BCR	C23-C24-C25-C30
18	R	4020	BCR	C23-C24-C25-C26
18	R	4020	BCR	C23-C24-C25-C30
18	V	4021	BCR	C5-C6-C7-C8
18	V	4021	BCR	C23-C24-C25-C26
18	a	4001	BCR	C1-C6-C7-C8
18	a	4001	BCR	C5-C6-C7-C8
18	a	4001	BCR	C23-C24-C25-C26
18	a	4003	BCR	C1-C6-C7-C8
18	a	4003	BCR	C5-C6-C7-C8
18	a	4007	BCR	C23-C24-C25-C26
18	a	4007	BCR	C23-C24-C25-C30
18	a	4008	BCR	C1-C6-C7-C8
18	a	4008	BCR	C5-C6-C7-C8
18	a	4008	BCR	C23-C24-C25-C26
18	a	4008	BCR	C23-C24-C25-C30
18	b	4006	BCR	C1-C6-C7-C8
18	b	4006	BCR	C23-C24-C25-C26
18	b	4006	BCR	C23-C24-C25-C30
18	b	4009	BCR	C1-C6-C7-C8
18	b	4009	BCR	C5-C6-C7-C8
18	b	4013	BCR	C23-C24-C25-C30
18	b	4016	BCR	C1-C6-C7-C8
18	b	4016	BCR	C5-C6-C7-C8
18	b	4017	BCR	C23-C24-C25-C26
18	b	4017	BCR	C23-C24-C25-C30
18	i	4020	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
18	i	4020	BCR	C23-C24-C25-C30
18	m	4021	BCR	C5-C6-C7-C8
18	m	4021	BCR	C23-C24-C25-C26
18	A	4001	BCR	C1-C6-C7-C8
18	A	4001	BCR	C5-C6-C7-C8
18	A	4001	BCR	C23-C24-C25-C26
18	A	4003	BCR	C1-C6-C7-C8
18	A	4003	BCR	C5-C6-C7-C8
18	A	4007	BCR	C23-C24-C25-C26
18	A	4007	BCR	C23-C24-C25-C30
18	A	4008	BCR	C1-C6-C7-C8
18	A	4008	BCR	C5-C6-C7-C8
18	A	4008	BCR	C23-C24-C25-C26
18	A	4008	BCR	C23-C24-C25-C30
18	B	4006	BCR	C1-C6-C7-C8
18	B	4006	BCR	C23-C24-C25-C26
18	B	4006	BCR	C23-C24-C25-C30
18	B	4009	BCR	C1-C6-C7-C8
18	B	4009	BCR	C5-C6-C7-C8
18	B	4013	BCR	C23-C24-C25-C30
18	B	4016	BCR	C1-C6-C7-C8
18	B	4016	BCR	C5-C6-C7-C8
18	B	4017	BCR	C23-C24-C25-C26
18	B	4017	BCR	C23-C24-C25-C30
18	I	4020	BCR	C23-C24-C25-C26
18	I	4020	BCR	C23-C24-C25-C30
18	L	4019	BCR	C23-C24-C25-C30
18	M	4021	BCR	C5-C6-C7-C8
18	M	4021	BCR	C23-C24-C25-C26
19	G	5001	LHG	C13-C14-C15-C16
14	G	1126	CLA	CBA-CGA-O2A-C1
14	a	1126	CLA	CBA-CGA-O2A-C1
14	A	1126	CLA	CBA-CGA-O2A-C1
14	G	1012	CLA	C10-C11-C12-C13
14	G	1102	CLA	C5-C6-C7-C8
14	G	1126	CLA	C5-C6-C7-C8
14	a	1012	CLA	C10-C11-C12-C13
14	a	1102	CLA	C5-C6-C7-C8
14	a	1126	CLA	C5-C6-C7-C8
14	A	1012	CLA	C10-C11-C12-C13
14	A	1102	CLA	C5-C6-C7-C8
14	A	1126	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	G	1135	CLA	C5-C6-C7-C8
14	U	1501	CLA	C5-C6-C7-C8
14	a	1135	CLA	C5-C6-C7-C8
14	l	1501	CLA	C5-C6-C7-C8
14	A	1135	CLA	C5-C6-C7-C8
14	L	1501	CLA	C5-C6-C7-C8
16	H	2002	PQN	C15-C16-C17-C18
16	b	2002	PQN	C15-C16-C17-C18
16	B	2002	PQN	C15-C16-C17-C18
14	G	1130	CLA	C4-C3-C5-C6
14	a	1130	CLA	C4-C3-C5-C6
14	A	1130	CLA	C4-C3-C5-C6
14	H	1225	CLA	O1D-CGD-O2D-CED
14	b	1225	CLA	O1D-CGD-O2D-CED
14	G	1109	CLA	C11-C12-C13-C15
14	G	1112	CLA	C2-C3-C5-C6
14	G	1140	CLA	C11-C10-C8-C7
14	H	1211	CLA	C12-C13-C15-C16
14	H	1222	CLA	C6-C7-C8-C10
14	H	1225	CLA	C2-C3-C5-C6
14	U	1501	CLA	C11-C10-C8-C7
14	a	1109	CLA	C11-C12-C13-C15
14	a	1112	CLA	C2-C3-C5-C6
14	a	1140	CLA	C11-C10-C8-C7
14	b	1211	CLA	C12-C13-C15-C16
14	b	1222	CLA	C6-C7-C8-C10
14	b	1225	CLA	C2-C3-C5-C6
14	l	1501	CLA	C11-C10-C8-C7
14	A	1109	CLA	C11-C12-C13-C15
14	A	1112	CLA	C2-C3-C5-C6
14	A	1140	CLA	C11-C10-C8-C7
14	B	1211	CLA	C12-C13-C15-C16
14	B	1222	CLA	C6-C7-C8-C10
14	B	1225	CLA	C2-C3-C5-C6
14	L	1501	CLA	C11-C10-C8-C7
16	H	2002	PQN	C17-C18-C20-C21
16	b	2002	PQN	C17-C18-C20-C21
16	B	2002	PQN	C17-C18-C20-C21
15	H	1237	F6C	C3-C5-C6-C7
15	b	1237	F6C	C3-C5-C6-C7
15	B	1237	F6C	C3-C5-C6-C7
14	G	1140	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	1140	CLA	O1A-CGA-O2A-C1
14	A	1140	CLA	O1A-CGA-O2A-C1
14	A	1126	CLA	C10-C11-C12-C13
16	G	2001	PQN	C25-C26-C27-C28
16	a	2001	PQN	C25-C26-C27-C28
16	A	2001	PQN	C25-C26-C27-C28
15	H	1238	F6C	C1A-C2A-CAA-CBA
15	b	1238	F6C	C1A-C2A-CAA-CBA
15	B	1238	F6C	C1A-C2A-CAA-CBA
18	a	4003	BCR	C9-C10-C11-C12
18	A	4003	BCR	C9-C10-C11-C12
14	G	1111	CLA	C11-C12-C13-C14
14	a	1111	CLA	C11-C12-C13-C14
14	A	1111	CLA	C11-C12-C13-C14
14	B	1225	CLA	O1D-CGD-O2D-CED
14	G	1013	CLA	CBA-CGA-O2A-C1
14	G	1127	CLA	CBA-CGA-O2A-C1
14	G	1136	CLA	CBA-CGA-O2A-C1
14	H	1228	CLA	CBA-CGA-O2A-C1
14	U	1501	CLA	CBA-CGA-O2A-C1
14	a	1013	CLA	CBA-CGA-O2A-C1
14	a	1136	CLA	CBA-CGA-O2A-C1
14	b	1228	CLA	CBA-CGA-O2A-C1
14	l	1501	CLA	CBA-CGA-O2A-C1
14	A	1013	CLA	CBA-CGA-O2A-C1
14	A	1136	CLA	CBA-CGA-O2A-C1
14	B	1228	CLA	CBA-CGA-O2A-C1
14	L	1501	CLA	CBA-CGA-O2A-C1
14	G	1012	CLA	C2A-CAA-CBA-CGA
14	G	1126	CLA	C2A-CAA-CBA-CGA
14	a	1012	CLA	C2A-CAA-CBA-CGA
14	a	1126	CLA	C2A-CAA-CBA-CGA
14	A	1012	CLA	C2A-CAA-CBA-CGA
14	A	1126	CLA	C2A-CAA-CBA-CGA
14	G	1126	CLA	C10-C11-C12-C13
14	U	1502	CLA	C8-C10-C11-C12
14	l	1502	CLA	C8-C10-C11-C12
14	L	1502	CLA	C8-C10-C11-C12
15	H	1207	F6C	O1D-CGD-O2D-CED
15	b	1207	F6C	O1D-CGD-O2D-CED
15	B	1207	F6C	O1D-CGD-O2D-CED
14	a	1126	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
15	H	1238	F6C	C8-C10-C11-C12
15	b	1238	F6C	C8-C10-C11-C12
15	B	1238	F6C	C8-C10-C11-C12
20	A	5005	LMG	C29-C30-C31-C32
15	G	1121	F6C	C2B-C3B-CAB-CBB
15	a	1121	F6C	C2B-C3B-CAB-CBB
15	A	1121	F6C	C2B-C3B-CAB-CBB
19	a	5001	LHG	C30-C31-C32-C33
20	G	5005	LMG	C29-C30-C31-C32
20	a	5005	LMG	C29-C30-C31-C32
14	a	1127	CLA	CBA-CGA-O2A-C1
14	A	1127	CLA	CBA-CGA-O2A-C1
14	H	1208	CLA	C16-C17-C18-C19
14	b	1208	CLA	C16-C17-C18-C19
14	B	1208	CLA	C16-C17-C18-C19
19	G	5001	LHG	C30-C31-C32-C33
19	A	5001	LHG	C30-C31-C32-C33
18	V	4021	BCR	C18-C19-C20-C21
18	m	4021	BCR	C18-C19-C20-C21
18	M	4021	BCR	C18-C19-C20-C21
14	G	1111	CLA	C5-C6-C7-C8
14	a	1111	CLA	C5-C6-C7-C8
14	A	1111	CLA	C5-C6-C7-C8
16	G	2001	PQN	C15-C16-C17-C18
16	a	2001	PQN	C15-C16-C17-C18
16	A	2001	PQN	C15-C16-C17-C18
14	G	1110	CLA	CBD-CGD-O2D-CED
14	a	1110	CLA	CBD-CGD-O2D-CED
14	A	1110	CLA	CBD-CGD-O2D-CED
20	l	5007	LMG	C18-C19-C20-C21
14	G	1112	CLA	C4-C3-C5-C6
14	H	1205	CLA	C4-C3-C5-C6
14	a	1112	CLA	C4-C3-C5-C6
14	A	1112	CLA	C4-C3-C5-C6
14	G	1103	CLA	C2-C3-C5-C6
14	a	1103	CLA	C2-C3-C5-C6
14	A	1103	CLA	C2-C3-C5-C6
16	b	2002	PQN	C12-C13-C15-C16
16	B	2002	PQN	C12-C13-C15-C16
20	U	5007	LMG	C18-C19-C20-C21
20	L	5007	LMG	C18-C19-C20-C21
14	G	1111	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	G	1131	CLA	C6-C7-C8-C9
14	G	1140	CLA	C11-C10-C8-C9
14	H	1021	CLA	C6-C7-C8-C9
14	H	1023	CLA	C11-C10-C8-C9
14	H	1214	CLA	C11-C12-C13-C14
14	H	1215	CLA	C6-C7-C8-C9
14	H	1216	CLA	C11-C12-C13-C14
14	H	1229	CLA	C6-C7-C8-C9
14	a	1111	CLA	C6-C7-C8-C9
14	a	1131	CLA	C6-C7-C8-C9
14	a	1140	CLA	C11-C10-C8-C9
14	b	1021	CLA	C6-C7-C8-C9
14	b	1023	CLA	C11-C10-C8-C9
14	b	1214	CLA	C11-C12-C13-C14
14	b	1215	CLA	C6-C7-C8-C9
14	b	1216	CLA	C11-C12-C13-C14
14	b	1229	CLA	C6-C7-C8-C9
14	A	1111	CLA	C6-C7-C8-C9
14	A	1131	CLA	C6-C7-C8-C9
14	A	1140	CLA	C11-C10-C8-C9
14	B	1021	CLA	C6-C7-C8-C9
14	B	1023	CLA	C11-C10-C8-C9
14	B	1214	CLA	C11-C12-C13-C14
14	B	1215	CLA	C6-C7-C8-C9
14	B	1216	CLA	C11-C12-C13-C14
14	B	1229	CLA	C6-C7-C8-C9
14	G	1116	CLA	C2A-CAA-CBA-CGA
14	a	1116	CLA	C2A-CAA-CBA-CGA
14	A	1116	CLA	C2A-CAA-CBA-CGA
15	H	1237	F6C	C1A-C2A-CAA-CBA
15	b	1237	F6C	C1A-C2A-CAA-CBA
15	B	1237	F6C	C1A-C2A-CAA-CBA
14	G	1135	CLA	C8-C10-C11-C12
14	H	1224	CLA	C10-C11-C12-C13
14	a	1135	CLA	C8-C10-C11-C12
14	b	1224	CLA	C10-C11-C12-C13
14	A	1135	CLA	C8-C10-C11-C12
14	B	1224	CLA	C10-C11-C12-C13
18	H	4016	BCR	C7-C8-C9-C10
18	b	4016	BCR	C7-C8-C9-C10
18	B	4016	BCR	C7-C8-C9-C10
14	G	1126	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	1126	CLA	O1A-CGA-O2A-C1
14	A	1126	CLA	O1A-CGA-O2A-C1
14	G	1103	CLA	C1A-C2A-CAA-CBA
14	G	1105	CLA	C1A-C2A-CAA-CBA
14	G	1106	CLA	C1A-C2A-CAA-CBA
14	G	1107	CLA	C1A-C2A-CAA-CBA
14	G	1110	CLA	C1A-C2A-CAA-CBA
14	G	1113	CLA	C1A-C2A-CAA-CBA
14	G	1116	CLA	C1A-C2A-CAA-CBA
14	G	1118	CLA	C1A-C2A-CAA-CBA
14	G	1132	CLA	C1A-C2A-CAA-CBA
14	G	1135	CLA	C1A-C2A-CAA-CBA
14	G	1137	CLA	C1A-C2A-CAA-CBA
14	H	1215	CLA	C1A-C2A-CAA-CBA
14	H	1220	CLA	C1A-C2A-CAA-CBA
14	H	1227	CLA	C1A-C2A-CAA-CBA
14	H	1229	CLA	C1A-C2A-CAA-CBA
14	H	1236	CLA	C1A-C2A-CAA-CBA
14	a	1103	CLA	C1A-C2A-CAA-CBA
14	a	1105	CLA	C1A-C2A-CAA-CBA
14	a	1106	CLA	C1A-C2A-CAA-CBA
14	a	1107	CLA	C1A-C2A-CAA-CBA
14	a	1110	CLA	C1A-C2A-CAA-CBA
14	a	1113	CLA	C1A-C2A-CAA-CBA
14	a	1116	CLA	C1A-C2A-CAA-CBA
14	a	1118	CLA	C1A-C2A-CAA-CBA
14	a	1132	CLA	C1A-C2A-CAA-CBA
14	a	1135	CLA	C1A-C2A-CAA-CBA
14	a	1137	CLA	C1A-C2A-CAA-CBA
14	b	1215	CLA	C1A-C2A-CAA-CBA
14	b	1220	CLA	C1A-C2A-CAA-CBA
14	b	1227	CLA	C1A-C2A-CAA-CBA
14	b	1229	CLA	C1A-C2A-CAA-CBA
14	b	1236	CLA	C1A-C2A-CAA-CBA
14	A	1103	CLA	C1A-C2A-CAA-CBA
14	A	1105	CLA	C1A-C2A-CAA-CBA
14	A	1106	CLA	C1A-C2A-CAA-CBA
14	A	1107	CLA	C1A-C2A-CAA-CBA
14	A	1110	CLA	C1A-C2A-CAA-CBA
14	A	1113	CLA	C1A-C2A-CAA-CBA
14	A	1116	CLA	C1A-C2A-CAA-CBA
14	A	1118	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	A	1132	CLA	C1A-C2A-CAA-CBA
14	A	1135	CLA	C1A-C2A-CAA-CBA
14	A	1137	CLA	C1A-C2A-CAA-CBA
14	B	1215	CLA	C1A-C2A-CAA-CBA
14	B	1220	CLA	C1A-C2A-CAA-CBA
14	B	1227	CLA	C1A-C2A-CAA-CBA
14	B	1229	CLA	C1A-C2A-CAA-CBA
14	B	1236	CLA	C1A-C2A-CAA-CBA
19	H	5004	LHG	C11-C12-C13-C14
19	b	5004	LHG	C11-C12-C13-C14
14	H	1221	CLA	C8-C10-C11-C12
14	b	1221	CLA	C8-C10-C11-C12
14	B	1221	CLA	C8-C10-C11-C12
19	B	5004	LHG	C11-C12-C13-C14
19	H	5004	LHG	C9-C10-C11-C12
19	b	5004	LHG	C9-C10-C11-C12
19	B	5004	LHG	C9-C10-C11-C12
15	H	1207	F6C	C13-C15-C16-C17
15	b	1207	F6C	C13-C15-C16-C17
15	B	1207	F6C	C13-C15-C16-C17
14	G	1118	CLA	C5-C6-C7-C8
14	G	1131	CLA	C5-C6-C7-C8
14	a	1118	CLA	C5-C6-C7-C8
14	a	1131	CLA	C5-C6-C7-C8
14	A	1131	CLA	C5-C6-C7-C8
14	A	1118	CLA	C5-C6-C7-C8
14	H	1215	CLA	C4-C3-C5-C6
14	U	1501	CLA	C4-C3-C5-C6
14	b	1205	CLA	C4-C3-C5-C6
14	b	1215	CLA	C4-C3-C5-C6
14	l	1501	CLA	C4-C3-C5-C6
14	B	1205	CLA	C4-C3-C5-C6
14	B	1215	CLA	C4-C3-C5-C6
14	L	1501	CLA	C4-C3-C5-C6
16	H	2002	PQN	C14-C13-C15-C16
16	b	2002	PQN	C14-C13-C15-C16
16	B	2002	PQN	C14-C13-C15-C16
14	G	1130	CLA	C2-C3-C5-C6
16	H	2002	PQN	C12-C13-C15-C16
14	G	1127	CLA	O1A-CGA-O2A-C1
14	U	1501	CLA	O1A-CGA-O2A-C1
14	a	1127	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	l	1501	CLA	O1A-CGA-O2A-C1
14	A	1127	CLA	O1A-CGA-O2A-C1
14	L	1501	CLA	O1A-CGA-O2A-C1
14	A	1136	CLA	C2A-CAA-CBA-CGA
19	H	5004	LHG	C4-C5-C6-O8
19	b	5004	LHG	C4-C5-C6-O8
19	B	5004	LHG	C4-C5-C6-O8
14	a	1128	CLA	O1D-CGD-O2D-CED
14	H	1208	CLA	CAA-CBA-CGA-O2A
14	b	1208	CLA	CAA-CBA-CGA-O2A
14	B	1208	CLA	CAA-CBA-CGA-O2A
20	R	5006	LMG	O7-C10-C11-C12
20	i	5006	LMG	O7-C10-C11-C12
20	I	5006	LMG	O7-C10-C11-C12
14	A	1128	CLA	O1D-CGD-O2D-CED
14	a	1136	CLA	O1A-CGA-O2A-C1
20	R	5006	LMG	O6-C5-C6-O5
20	i	5006	LMG	O6-C5-C6-O5
20	I	5006	LMG	O6-C5-C6-O5
19	H	5004	LHG	O1-C1-C2-O2
19	b	5004	LHG	O1-C1-C2-O2
19	B	5004	LHG	O1-C1-C2-O2
14	H	1021	CLA	C10-C11-C12-C13
14	b	1021	CLA	C10-C11-C12-C13
14	B	1021	CLA	C10-C11-C12-C13
14	G	1136	CLA	O1A-CGA-O2A-C1
14	A	1136	CLA	O1A-CGA-O2A-C1
14	G	1128	CLA	O1D-CGD-O2D-CED
18	R	4020	BCR	C20-C21-C22-C37
18	i	4020	BCR	C20-C21-C22-C37
18	I	4020	BCR	C20-C21-C22-C37
20	U	5007	LMG	O6-C5-C6-O5
20	l	5007	LMG	O6-C5-C6-O5
20	L	5007	LMG	O6-C5-C6-O5
14	H	1220	CLA	C4-C3-C5-C6
14	b	1220	CLA	C4-C3-C5-C6
14	B	1220	CLA	C4-C3-C5-C6
14	a	1130	CLA	C2-C3-C5-C6
14	b	1215	CLA	C2-C3-C5-C6
14	H	1221	CLA	C16-C17-C18-C19
14	b	1221	CLA	C16-C17-C18-C19
14	B	1221	CLA	C16-C17-C18-C19

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
14	b	1211	CLA	CBA-CGA-O2A-C1
14	B	1211	CLA	CBA-CGA-O2A-C1
14	G	1126	CLA	C8-C10-C11-C12
21	G	6002	LMT	O5B-C5B-C6B-O6B
21	a	6002	LMT	O5B-C5B-C6B-O6B
21	A	6002	LMT	O5B-C5B-C6B-O6B
14	G	1136	CLA	C2A-CAA-CBA-CGA
14	a	1136	CLA	C2A-CAA-CBA-CGA
14	H	1213	CLA	C13-C15-C16-C17
14	a	1126	CLA	C8-C10-C11-C12
14	b	1213	CLA	C13-C15-C16-C17
14	A	1126	CLA	C8-C10-C11-C12
14	B	1213	CLA	C13-C15-C16-C17
14	G	1119	CLA	C2-C1-O2A-CGA
14	G	1123	CLA	C2-C1-O2A-CGA
14	U	1502	CLA	C2-C1-O2A-CGA
14	a	1119	CLA	C2-C1-O2A-CGA
14	a	1123	CLA	C2-C1-O2A-CGA
14	l	1502	CLA	C2-C1-O2A-CGA
14	A	1119	CLA	C2-C1-O2A-CGA
14	A	1123	CLA	C2-C1-O2A-CGA
14	L	1502	CLA	C2-C1-O2A-CGA
14	G	1012	CLA	C13-C15-C16-C17
14	H	1214	CLA	C5-C6-C7-C8
14	a	1012	CLA	C13-C15-C16-C17
14	b	1214	CLA	C5-C6-C7-C8
14	A	1012	CLA	C13-C15-C16-C17
14	B	1214	CLA	C5-C6-C7-C8
14	H	1211	CLA	CBA-CGA-O2A-C1
14	H	1225	CLA	CBA-CGA-O2A-C1
14	b	1225	CLA	CBA-CGA-O2A-C1
14	B	1225	CLA	CBA-CGA-O2A-C1
14	H	1228	CLA	O1A-CGA-O2A-C1
14	b	1228	CLA	O1A-CGA-O2A-C1
14	B	1228	CLA	O1A-CGA-O2A-C1
14	b	1211	CLA	O1A-CGA-O2A-C1
20	a	5005	LMG	C32-C33-C34-C35
20	A	5005	LMG	C32-C33-C34-C35
14	G	1102	CLA	C6-C7-C8-C10
14	G	1115	CLA	C12-C13-C15-C16
14	G	1117	CLA	C6-C7-C8-C10
14	G	1123	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
14	G	1131	CLA	C6-C7-C8-C10
14	H	1021	CLA	C12-C13-C15-C16
14	H	1022	CLA	C6-C7-C8-C10
14	H	1022	CLA	C11-C12-C13-C15
14	H	1023	CLA	C11-C10-C8-C7
14	H	1203	CLA	C12-C13-C15-C16
14	H	1210	CLA	C6-C7-C8-C10
14	H	1213	CLA	C6-C7-C8-C10
14	H	1214	CLA	C11-C12-C13-C15
14	H	1215	CLA	C2-C3-C5-C6
14	H	1215	CLA	C6-C7-C8-C10
14	H	1216	CLA	C11-C12-C13-C15
14	H	1220	CLA	C2-C3-C5-C6
14	H	1221	CLA	C11-C12-C13-C15
14	H	1224	CLA	C12-C13-C15-C16
14	H	1234	CLA	C11-C12-C13-C15
14	H	1239	CLA	C11-C10-C8-C7
14	a	1102	CLA	C6-C7-C8-C10
14	a	1115	CLA	C12-C13-C15-C16
14	a	1117	CLA	C6-C7-C8-C10
14	a	1123	CLA	C6-C7-C8-C10
14	a	1131	CLA	C6-C7-C8-C10
14	b	1021	CLA	C12-C13-C15-C16
14	b	1022	CLA	C6-C7-C8-C10
14	b	1022	CLA	C11-C12-C13-C15
14	b	1023	CLA	C11-C10-C8-C7
14	b	1203	CLA	C12-C13-C15-C16
14	b	1210	CLA	C6-C7-C8-C10
14	b	1213	CLA	C6-C7-C8-C10
14	b	1214	CLA	C11-C12-C13-C15
14	b	1215	CLA	C6-C7-C8-C10
14	b	1216	CLA	C11-C12-C13-C15
14	b	1220	CLA	C2-C3-C5-C6
14	b	1221	CLA	C11-C12-C13-C15
14	b	1224	CLA	C12-C13-C15-C16
14	b	1234	CLA	C11-C12-C13-C15
14	b	1239	CLA	C11-C10-C8-C7
14	A	1102	CLA	C6-C7-C8-C10
14	A	1115	CLA	C12-C13-C15-C16
14	A	1117	CLA	C6-C7-C8-C10
14	A	1123	CLA	C6-C7-C8-C10
14	A	1130	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	A	1131	CLA	C6-C7-C8-C10
14	B	1021	CLA	C12-C13-C15-C16
14	B	1022	CLA	C6-C7-C8-C10
14	B	1022	CLA	C11-C12-C13-C15
14	B	1023	CLA	C11-C10-C8-C7
14	B	1203	CLA	C12-C13-C15-C16
14	B	1210	CLA	C6-C7-C8-C10
14	B	1213	CLA	C6-C7-C8-C10
14	B	1214	CLA	C11-C12-C13-C15
14	B	1215	CLA	C2-C3-C5-C6
14	B	1215	CLA	C6-C7-C8-C10
14	B	1216	CLA	C11-C12-C13-C15
14	B	1220	CLA	C2-C3-C5-C6
14	B	1221	CLA	C11-C12-C13-C15
14	B	1224	CLA	C12-C13-C15-C16
14	B	1234	CLA	C11-C12-C13-C15
14	B	1239	CLA	C11-C10-C8-C7
15	H	1237	F6C	C11-C12-C13-C15
15	H	1238	F6C	C6-C7-C8-C10
15	b	1237	F6C	C11-C12-C13-C15
15	b	1238	F6C	C6-C7-C8-C10
15	B	1237	F6C	C11-C12-C13-C15
15	B	1238	F6C	C6-C7-C8-C10
16	a	2001	PQN	C21-C22-C23-C25
14	H	1211	CLA	O1A-CGA-O2A-C1
20	G	5005	LMG	C32-C33-C34-C35
14	G	1102	CLA	C6-C7-C8-C9
14	G	1109	CLA	C11-C12-C13-C14
14	G	1117	CLA	C6-C7-C8-C9
14	G	1125	CLA	C6-C7-C8-C9
14	G	1136	CLA	C6-C7-C8-C9
14	H	1022	CLA	C11-C12-C13-C14
14	H	1203	CLA	C11-C10-C8-C9
14	H	1210	CLA	C6-C7-C8-C9
14	H	1211	CLA	C14-C13-C15-C16
14	H	1216	CLA	C14-C13-C15-C16
14	H	1221	CLA	C11-C12-C13-C14
14	H	1224	CLA	C14-C13-C15-C16
14	H	1234	CLA	C11-C12-C13-C14
14	H	1239	CLA	C11-C10-C8-C9
14	a	1102	CLA	C6-C7-C8-C9
14	a	1109	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	a	1117	CLA	C6-C7-C8-C9
14	a	1125	CLA	C6-C7-C8-C9
14	a	1136	CLA	C6-C7-C8-C9
14	b	1022	CLA	C11-C12-C13-C14
14	b	1203	CLA	C11-C10-C8-C9
14	b	1210	CLA	C6-C7-C8-C9
14	b	1211	CLA	C14-C13-C15-C16
14	b	1216	CLA	C14-C13-C15-C16
14	b	1221	CLA	C11-C12-C13-C14
14	b	1224	CLA	C14-C13-C15-C16
14	b	1234	CLA	C11-C12-C13-C14
14	b	1239	CLA	C11-C10-C8-C9
14	A	1102	CLA	C6-C7-C8-C9
14	A	1109	CLA	C11-C12-C13-C14
14	A	1117	CLA	C6-C7-C8-C9
14	A	1125	CLA	C6-C7-C8-C9
14	A	1136	CLA	C6-C7-C8-C9
14	B	1022	CLA	C11-C12-C13-C14
14	B	1203	CLA	C11-C10-C8-C9
14	B	1210	CLA	C6-C7-C8-C9
14	B	1211	CLA	C14-C13-C15-C16
14	B	1216	CLA	C14-C13-C15-C16
14	B	1221	CLA	C11-C12-C13-C14
14	B	1224	CLA	C14-C13-C15-C16
14	B	1234	CLA	C11-C12-C13-C14
14	B	1239	CLA	C11-C10-C8-C9
18	U	4019	BCR	C15-C16-C17-C18
18	l	4019	BCR	C15-C16-C17-C18
18	L	4019	BCR	C15-C16-C17-C18
18	V	4021	BCR	C14-C15-C16-C17
18	m	4021	BCR	C14-C15-C16-C17
18	M	4021	BCR	C14-C15-C16-C17
14	H	1213	CLA	CBA-CGA-O2A-C1
14	a	1119	CLA	CBA-CGA-O2A-C1
14	b	1213	CLA	CBA-CGA-O2A-C1
14	A	1119	CLA	CBA-CGA-O2A-C1
14	B	1213	CLA	CBA-CGA-O2A-C1
14	B	1211	CLA	O1A-CGA-O2A-C1
18	V	4021	BCR	C37-C22-C23-C24
18	m	4021	BCR	C37-C22-C23-C24
18	M	4021	BCR	C37-C22-C23-C24
13	G	1011	CL0	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
13	a	1011	CL0	C16-C17-C18-C20
13	A	1011	CL0	C16-C17-C18-C20
15	H	1207	F6C	C16-C17-C18-C19
15	b	1207	F6C	C16-C17-C18-C19
15	B	1207	F6C	C16-C17-C18-C19
14	H	1202	CLA	C8-C10-C11-C12
14	H	1208	CLA	C5-C6-C7-C8
14	b	1202	CLA	C8-C10-C11-C12
14	B	1202	CLA	C8-C10-C11-C12
14	B	1208	CLA	C5-C6-C7-C8
19	H	5004	LHG	C32-C33-C34-C35
19	b	5004	LHG	C32-C33-C34-C35
19	B	5004	LHG	C32-C33-C34-C35
14	G	1119	CLA	CBA-CGA-O2A-C1
14	H	1203	CLA	C10-C11-C12-C13
14	b	1203	CLA	C10-C11-C12-C13
14	b	1208	CLA	C5-C6-C7-C8
14	B	1203	CLA	C10-C11-C12-C13
14	b	1202	CLA	CAA-CBA-CGA-O2A
16	a	2001	PQN	C18-C20-C21-C22
16	A	2001	PQN	C18-C20-C21-C22
14	G	1013	CLA	C8-C10-C11-C12
14	A	1013	CLA	C8-C10-C11-C12
16	G	2001	PQN	C18-C20-C21-C22
14	H	1021	CLA	CAA-CBA-CGA-O2A
14	H	1202	CLA	CAA-CBA-CGA-O2A
14	b	1021	CLA	CAA-CBA-CGA-O2A
14	B	1021	CLA	CAA-CBA-CGA-O2A
14	B	1202	CLA	CAA-CBA-CGA-O2A
20	U	5007	LMG	C39-C40-C41-C42
14	G	1111	CLA	C4-C3-C5-C6
14	G	1138	CLA	C4-C3-C5-C6
14	H	1235	CLA	C4-C3-C5-C6
14	a	1111	CLA	C4-C3-C5-C6
14	a	1138	CLA	C4-C3-C5-C6
14	b	1235	CLA	C4-C3-C5-C6
14	A	1111	CLA	C4-C3-C5-C6
14	A	1138	CLA	C4-C3-C5-C6
14	B	1235	CLA	C4-C3-C5-C6
20	I	5007	LMG	C39-C40-C41-C42
20	L	5007	LMG	C39-C40-C41-C42
14	H	1224	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	a	1013	CLA	C8-C10-C11-C12
14	b	1224	CLA	C5-C6-C7-C8
14	B	1224	CLA	C5-C6-C7-C8
14	G	1109	CLA	C16-C17-C18-C20
14	a	1109	CLA	C16-C17-C18-C20
14	A	1109	CLA	C16-C17-C18-C20
15	B	1238	F6C	C13-C15-C16-C17
14	G	1112	CLA	C3A-C2A-CAA-CBA
14	G	1124	CLA	C3A-C2A-CAA-CBA
14	H	1203	CLA	C3A-C2A-CAA-CBA
14	a	1112	CLA	C3A-C2A-CAA-CBA
14	a	1124	CLA	C3A-C2A-CAA-CBA
14	b	1203	CLA	C3A-C2A-CAA-CBA
14	A	1112	CLA	C3A-C2A-CAA-CBA
14	A	1124	CLA	C3A-C2A-CAA-CBA
14	B	1203	CLA	C3A-C2A-CAA-CBA
15	H	1238	F6C	C13-C15-C16-C17
15	b	1238	F6C	C13-C15-C16-C17
18	G	4011	BCR	C19-C20-C21-C22
18	a	4011	BCR	C19-C20-C21-C22
18	A	4011	BCR	C19-C20-C21-C22
21	G	6001	LMT	C2-C1-O1'-C1'
21	a	6001	LMT	C2-C1-O1'-C1'
21	A	6001	LMT	C2-C1-O1'-C1'
14	a	1133	CLA	C11-C12-C13-C14
14	A	1133	CLA	C11-C12-C13-C14
14	H	1210	CLA	CBA-CGA-O2A-C1
14	b	1210	CLA	CBA-CGA-O2A-C1
14	B	1210	CLA	CBA-CGA-O2A-C1
14	H	1217	CLA	C5-C6-C7-C8
14	b	1217	CLA	C5-C6-C7-C8
14	B	1217	CLA	C5-C6-C7-C8
20	G	5005	LMG	C7-C8-C9-O8
20	a	5005	LMG	C7-C8-C9-O8
20	A	5005	LMG	C7-C8-C9-O8
14	H	1226	CLA	C5-C6-C7-C8
14	b	1226	CLA	C5-C6-C7-C8
14	B	1226	CLA	C5-C6-C7-C8
14	H	1214	CLA	C15-C16-C17-C18
14	b	1214	CLA	C15-C16-C17-C18
14	B	1214	CLA	C15-C16-C17-C18
14	G	1126	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	a	1126	CLA	C4-C3-C5-C6
14	A	1126	CLA	C4-C3-C5-C6
13	G	1011	CL0	C16-C17-C18-C19
13	a	1011	CL0	C16-C17-C18-C19
13	A	1011	CL0	C16-C17-C18-C19
14	G	1133	CLA	C11-C12-C13-C14
14	H	1202	CLA	C11-C12-C13-C14
14	b	1202	CLA	C11-C12-C13-C14
14	A	1133	CLA	C11-C12-C13-C15
14	B	1202	CLA	C11-C12-C13-C14
14	A	1136	CLA	C13-C15-C16-C17
19	H	5004	LHG	C3-O3-P-O6
19	b	5004	LHG	C3-O3-P-O6
19	B	5004	LHG	C3-O3-P-O6
14	G	1013	CLA	O1A-CGA-O2A-C1
14	A	1013	CLA	O1A-CGA-O2A-C1
14	H	1201	CLA	C3-C5-C6-C7
14	b	1201	CLA	C3-C5-C6-C7
14	B	1201	CLA	C3-C5-C6-C7
14	H	1217	CLA	C2A-CAA-CBA-CGA
14	b	1217	CLA	C2A-CAA-CBA-CGA
14	B	1217	CLA	C2A-CAA-CBA-CGA
14	G	1136	CLA	C13-C15-C16-C17
14	a	1136	CLA	C13-C15-C16-C17
19	H	5004	LHG	O6-C4-C5-O7
19	b	5004	LHG	O6-C4-C5-O7
19	B	5004	LHG	O6-C4-C5-O7
14	H	1225	CLA	O1A-CGA-O2A-C1
14	a	1013	CLA	O1A-CGA-O2A-C1
14	b	1225	CLA	O1A-CGA-O2A-C1
14	B	1225	CLA	O1A-CGA-O2A-C1
14	G	1133	CLA	C11-C12-C13-C15
14	H	1239	CLA	C16-C17-C18-C20
14	a	1133	CLA	C11-C12-C13-C15
14	b	1239	CLA	C16-C17-C18-C20
14	B	1239	CLA	C16-C17-C18-C20
14	A	1140	CLA	CAA-CBA-CGA-O2A
14	G	1119	CLA	O1A-CGA-O2A-C1
14	a	1119	CLA	O1A-CGA-O2A-C1
14	B	1223	CLA	O1D-CGD-O2D-CED
20	G	5005	LMG	O7-C8-C9-O8
20	a	5005	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
20	A	5005	LMG	O7-C8-C9-O8
14	b	1223	CLA	O1D-CGD-O2D-CED
14	G	1140	CLA	CAA-CBA-CGA-O2A
14	a	1140	CLA	CAA-CBA-CGA-O2A
18	G	4001	BCR	C15-C16-C17-C18
18	a	4001	BCR	C15-C16-C17-C18
18	A	4001	BCR	C15-C16-C17-C18
15	H	1237	F6C	C3A-C2A-CAA-CBA
15	b	1237	F6C	C3A-C2A-CAA-CBA
15	B	1237	F6C	C3A-C2A-CAA-CBA
14	b	1208	CLA	C16-C17-C18-C20
14	H	1214	CLA	C10-C11-C12-C13
14	b	1214	CLA	C10-C11-C12-C13
14	B	1214	CLA	C10-C11-C12-C13
14	a	1111	CLA	C3-C5-C6-C7
14	H	1223	CLA	O1D-CGD-O2D-CED
14	G	1138	CLA	C2-C3-C5-C6
14	a	1138	CLA	C2-C3-C5-C6
14	A	1138	CLA	C2-C3-C5-C6
14	A	1119	CLA	O1A-CGA-O2A-C1
14	G	1109	CLA	C11-C10-C8-C9
14	G	1115	CLA	C14-C13-C15-C16
14	G	1117	CLA	C11-C12-C13-C14
14	G	1117	CLA	C14-C13-C15-C16
14	G	1127	CLA	C14-C13-C15-C16
14	G	1128	CLA	C6-C7-C8-C9
14	G	1135	CLA	C11-C10-C8-C9
14	G	1140	CLA	C14-C13-C15-C16
14	H	1204	CLA	C14-C13-C15-C16
14	H	1211	CLA	C11-C12-C13-C14
14	H	1224	CLA	C11-C12-C13-C14
14	a	1109	CLA	C11-C10-C8-C9
14	a	1115	CLA	C14-C13-C15-C16
14	a	1117	CLA	C11-C12-C13-C14
14	a	1117	CLA	C14-C13-C15-C16
14	a	1127	CLA	C14-C13-C15-C16
14	a	1128	CLA	C6-C7-C8-C9
14	a	1135	CLA	C11-C10-C8-C9
14	a	1140	CLA	C14-C13-C15-C16
14	b	1204	CLA	C14-C13-C15-C16
14	b	1211	CLA	C11-C12-C13-C14
14	b	1224	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	b	1225	CLA	C11-C10-C8-C9
14	A	1109	CLA	C11-C10-C8-C9
14	A	1115	CLA	C14-C13-C15-C16
14	A	1117	CLA	C11-C12-C13-C14
14	A	1117	CLA	C14-C13-C15-C16
14	A	1127	CLA	C14-C13-C15-C16
14	A	1128	CLA	C6-C7-C8-C9
14	A	1135	CLA	C11-C10-C8-C9
14	A	1140	CLA	C14-C13-C15-C16
14	B	1204	CLA	C14-C13-C15-C16
14	B	1211	CLA	C11-C12-C13-C14
14	B	1224	CLA	C11-C12-C13-C14
15	H	1238	F6C	C6-C7-C8-C9
15	b	1238	F6C	C6-C7-C8-C9
15	B	1238	F6C	C6-C7-C8-C9
14	G	1117	CLA	C10-C11-C12-C13
14	G	1125	CLA	C15-C16-C17-C18
14	a	1117	CLA	C10-C11-C12-C13
14	a	1125	CLA	C15-C16-C17-C18
14	A	1117	CLA	C10-C11-C12-C13
14	A	1125	CLA	C15-C16-C17-C18
19	H	5004	LHG	C2-C3-O3-P
19	b	5004	LHG	C2-C3-O3-P
19	B	5004	LHG	C2-C3-O3-P
14	G	1137	CLA	C2A-CAA-CBA-CGA
14	a	1137	CLA	C2A-CAA-CBA-CGA
14	A	1137	CLA	C2A-CAA-CBA-CGA
14	H	1208	CLA	C16-C17-C18-C20
14	a	1118	CLA	C6-C7-C8-C10
14	B	1208	CLA	C16-C17-C18-C20
14	G	1111	CLA	C3-C5-C6-C7
14	G	1124	CLA	C3-C5-C6-C7
14	a	1124	CLA	C3-C5-C6-C7
14	A	1111	CLA	C3-C5-C6-C7
14	A	1124	CLA	C3-C5-C6-C7
18	G	4002	BCR	C23-C24-C25-C26
18	G	4003	BCR	C23-C24-C25-C26
18	G	4003	BCR	C23-C24-C25-C30
18	G	4011	BCR	C5-C6-C7-C8
18	H	4010	BCR	C23-C24-C25-C26
18	H	4010	BCR	C23-C24-C25-C30
18	H	4017	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	R	4018	BCR	C1-C6-C7-C8
18	R	4018	BCR	C5-C6-C7-C8
18	R	4020	BCR	C5-C6-C7-C8
18	U	4019	BCR	C23-C24-C25-C30
18	a	4002	BCR	C23-C24-C25-C26
18	a	4003	BCR	C23-C24-C25-C26
18	a	4003	BCR	C23-C24-C25-C30
18	a	4011	BCR	C1-C6-C7-C8
18	a	4011	BCR	C5-C6-C7-C8
18	b	4010	BCR	C23-C24-C25-C26
18	b	4010	BCR	C23-C24-C25-C30
18	b	4017	BCR	C5-C6-C7-C8
18	i	4018	BCR	C1-C6-C7-C8
18	i	4018	BCR	C5-C6-C7-C8
18	i	4020	BCR	C5-C6-C7-C8
18	l	4019	BCR	C23-C24-C25-C30
18	A	4002	BCR	C23-C24-C25-C26
18	A	4003	BCR	C23-C24-C25-C26
18	A	4003	BCR	C23-C24-C25-C30
18	A	4011	BCR	C1-C6-C7-C8
18	A	4011	BCR	C5-C6-C7-C8
18	B	4010	BCR	C23-C24-C25-C26
18	B	4010	BCR	C23-C24-C25-C30
18	B	4017	BCR	C5-C6-C7-C8
18	I	4018	BCR	C1-C6-C7-C8
18	I	4018	BCR	C5-C6-C7-C8
18	I	4020	BCR	C5-C6-C7-C8
13	G	1011	CL0	C10-C11-C12-C13
13	a	1011	CL0	C10-C11-C12-C13
14	G	1116	CLA	CAA-CBA-CGA-O2A
14	a	1116	CLA	CAA-CBA-CGA-O2A
14	A	1116	CLA	CAA-CBA-CGA-O2A
13	A	1011	CL0	C10-C11-C12-C13
14	G	1110	CLA	O1D-CGD-O2D-CED
14	G	1118	CLA	C6-C7-C8-C10
14	A	1118	CLA	C6-C7-C8-C10
14	H	1022	CLA	C3-C5-C6-C7
14	b	1022	CLA	C3-C5-C6-C7
14	B	1022	CLA	C3-C5-C6-C7
15	H	1238	F6C	C3A-C2A-CAA-CBA
15	b	1238	F6C	C3A-C2A-CAA-CBA
15	B	1238	F6C	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	G	5005	LMG	C42-C43-C44-C45
20	a	5005	LMG	C42-C43-C44-C45
14	G	1125	CLA	C5-C6-C7-C8
14	a	1110	CLA	O1D-CGD-O2D-CED
20	A	5005	LMG	C42-C43-C44-C45
14	A	1110	CLA	O1D-CGD-O2D-CED
14	a	1125	CLA	C5-C6-C7-C8
14	G	1132	CLA	C4-C3-C5-C6
14	a	1132	CLA	C4-C3-C5-C6
14	A	1132	CLA	C4-C3-C5-C6
14	G	1109	CLA	C12-C13-C15-C16
14	G	1117	CLA	C11-C12-C13-C15
14	G	1117	CLA	C12-C13-C15-C16
14	G	1125	CLA	C6-C7-C8-C10
14	G	1126	CLA	C11-C10-C8-C7
14	G	1127	CLA	C12-C13-C15-C16
14	G	1128	CLA	C6-C7-C8-C10
14	G	1135	CLA	C11-C10-C8-C7
14	G	1138	CLA	C11-C10-C8-C7
14	G	1140	CLA	C6-C7-C8-C10
14	H	1022	CLA	C11-C10-C8-C7
14	H	1208	CLA	C6-C7-C8-C10
14	H	1208	CLA	C12-C13-C15-C16
14	H	1224	CLA	C11-C12-C13-C15
14	a	1109	CLA	C12-C13-C15-C16
14	a	1117	CLA	C11-C12-C13-C15
14	a	1117	CLA	C12-C13-C15-C16
14	a	1125	CLA	C6-C7-C8-C10
14	a	1126	CLA	C11-C10-C8-C7
14	a	1128	CLA	C6-C7-C8-C10
14	a	1135	CLA	C11-C10-C8-C7
14	a	1138	CLA	C11-C10-C8-C7
14	b	1022	CLA	C11-C10-C8-C7
14	b	1208	CLA	C6-C7-C8-C10
14	b	1208	CLA	C12-C13-C15-C16
14	b	1224	CLA	C11-C12-C13-C15
14	l	1501	CLA	C2-C3-C5-C6
14	A	1109	CLA	C12-C13-C15-C16
14	A	1117	CLA	C11-C12-C13-C15
14	A	1117	CLA	C12-C13-C15-C16
14	A	1125	CLA	C6-C7-C8-C10
14	A	1126	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
14	A	1128	CLA	C6-C7-C8-C10
14	A	1135	CLA	C11-C10-C8-C7
14	A	1138	CLA	C11-C10-C8-C7
14	B	1022	CLA	C11-C10-C8-C7
14	B	1208	CLA	C6-C7-C8-C10
14	B	1208	CLA	C12-C13-C15-C16
14	B	1224	CLA	C11-C12-C13-C15
16	G	2001	PQN	C21-C22-C23-C25
16	A	2001	PQN	C21-C22-C23-C25
14	H	1213	CLA	O1A-CGA-O2A-C1
14	b	1213	CLA	O1A-CGA-O2A-C1
14	B	1213	CLA	O1A-CGA-O2A-C1
14	H	1023	CLA	C10-C11-C12-C13
14	b	1023	CLA	C10-C11-C12-C13
14	A	1125	CLA	C5-C6-C7-C8
14	B	1023	CLA	C10-C11-C12-C13
18	G	4003	BCR	C19-C20-C21-C22
18	G	4008	BCR	C9-C10-C11-C12
18	G	4011	BCR	C9-C10-C11-C12
18	H	4014	BCR	C19-C20-C21-C22
18	a	4003	BCR	C19-C20-C21-C22
18	a	4008	BCR	C9-C10-C11-C12
18	a	4011	BCR	C9-C10-C11-C12
18	b	4014	BCR	C19-C20-C21-C22
18	A	4003	BCR	C19-C20-C21-C22
18	A	4008	BCR	C9-C10-C11-C12
18	A	4011	BCR	C9-C10-C11-C12
18	B	4014	BCR	C19-C20-C21-C22
15	H	1207	F6C	C16-C17-C18-C20
15	b	1207	F6C	C16-C17-C18-C20
15	B	1207	F6C	C16-C17-C18-C20
14	H	1023	CLA	CBA-CGA-O2A-C1
14	b	1023	CLA	CBA-CGA-O2A-C1
14	B	1023	CLA	CBA-CGA-O2A-C1
20	U	5007	LMG	C29-C28-O8-C9
20	l	5007	LMG	C29-C28-O8-C9
20	L	5007	LMG	C29-C28-O8-C9
19	b	5004	LHG	C34-C35-C36-C37
14	U	1502	CLA	C10-C11-C12-C13
14	l	1502	CLA	C10-C11-C12-C13
14	L	1502	CLA	C10-C11-C12-C13
19	H	5004	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
19	B	5004	LHG	C34-C35-C36-C37
14	G	1103	CLA	CAD-CBD-CGD-O2D
14	H	1221	CLA	CAD-CBD-CGD-O2D
14	a	1103	CLA	CAD-CBD-CGD-O2D
14	b	1221	CLA	CAD-CBD-CGD-O2D
14	A	1103	CLA	CAD-CBD-CGD-O2D
14	B	1221	CLA	CAD-CBD-CGD-O2D
15	H	1238	F6C	C15-C16-C17-C18
15	b	1238	F6C	C15-C16-C17-C18
15	B	1238	F6C	C15-C16-C17-C18
14	G	1103	CLA	CBD-CGD-O2D-CED
14	A	1103	CLA	CBD-CGD-O2D-CED
14	G	1125	CLA	CBA-CGA-O2A-C1
14	a	1125	CLA	CBA-CGA-O2A-C1
14	A	1125	CLA	CBA-CGA-O2A-C1
14	G	1132	CLA	C2-C3-C5-C6
14	U	1501	CLA	C2-C3-C5-C6
14	a	1132	CLA	C2-C3-C5-C6
14	A	1132	CLA	C2-C3-C5-C6
14	L	1501	CLA	C2-C3-C5-C6
14	a	1103	CLA	CBD-CGD-O2D-CED
14	a	1013	CLA	C3-C5-C6-C7
14	a	1109	CLA	C3-C5-C6-C7
14	A	1013	CLA	C3-C5-C6-C7
14	A	1109	CLA	C3-C5-C6-C7
14	H	1210	CLA	C2A-CAA-CBA-CGA
14	b	1210	CLA	C2A-CAA-CBA-CGA
14	B	1210	CLA	C2A-CAA-CBA-CGA
14	G	1132	CLA	C16-C17-C18-C20
14	a	1132	CLA	C16-C17-C18-C20
14	A	1132	CLA	C16-C17-C18-C20
14	G	1101	CLA	CHA-CBD-CGD-O1D
14	G	1106	CLA	CHA-CBD-CGD-O1D
14	G	1111	CLA	CHA-CBD-CGD-O1D
14	G	1111	CLA	CHA-CBD-CGD-O2D
14	G	1113	CLA	CHA-CBD-CGD-O1D
14	G	1113	CLA	CHA-CBD-CGD-O2D
14	G	1114	CLA	CHA-CBD-CGD-O1D
14	G	1114	CLA	CHA-CBD-CGD-O2D
14	G	1115	CLA	CHA-CBD-CGD-O1D
14	G	1120	CLA	CHA-CBD-CGD-O1D
14	G	1120	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	G	1123	CLA	CHA-CBD-CGD-O1D
14	G	1123	CLA	CHA-CBD-CGD-O2D
14	G	1132	CLA	CHA-CBD-CGD-O1D
14	G	1132	CLA	CHA-CBD-CGD-O2D
14	G	1134	CLA	CHA-CBD-CGD-O1D
14	G	1134	CLA	CHA-CBD-CGD-O2D
14	G	1138	CLA	CHA-CBD-CGD-O1D
14	H	1022	CLA	CHA-CBD-CGD-O1D
14	H	1205	CLA	CHA-CBD-CGD-O1D
14	H	1205	CLA	CHA-CBD-CGD-O2D
14	H	1210	CLA	CHA-CBD-CGD-O2D
14	H	1216	CLA	CHA-CBD-CGD-O1D
14	H	1216	CLA	CHA-CBD-CGD-O2D
14	H	1218	CLA	CHA-CBD-CGD-O1D
14	H	1218	CLA	CHA-CBD-CGD-O2D
14	H	1220	CLA	CHA-CBD-CGD-O1D
14	H	1220	CLA	CHA-CBD-CGD-O2D
14	H	1222	CLA	CHA-CBD-CGD-O1D
14	H	1222	CLA	CHA-CBD-CGD-O2D
14	H	1223	CLA	CHA-CBD-CGD-O1D
14	H	1228	CLA	CHA-CBD-CGD-O2D
14	H	1234	CLA	CHA-CBD-CGD-O1D
14	a	1101	CLA	CHA-CBD-CGD-O1D
14	a	1106	CLA	CHA-CBD-CGD-O1D
14	a	1111	CLA	CHA-CBD-CGD-O1D
14	a	1111	CLA	CHA-CBD-CGD-O2D
14	a	1113	CLA	CHA-CBD-CGD-O1D
14	a	1113	CLA	CHA-CBD-CGD-O2D
14	a	1114	CLA	CHA-CBD-CGD-O1D
14	a	1114	CLA	CHA-CBD-CGD-O2D
14	a	1115	CLA	CHA-CBD-CGD-O1D
14	a	1120	CLA	CHA-CBD-CGD-O1D
14	a	1120	CLA	CHA-CBD-CGD-O2D
14	a	1123	CLA	CHA-CBD-CGD-O1D
14	a	1123	CLA	CHA-CBD-CGD-O2D
14	a	1132	CLA	CHA-CBD-CGD-O1D
14	a	1132	CLA	CHA-CBD-CGD-O2D
14	a	1134	CLA	CHA-CBD-CGD-O1D
14	a	1134	CLA	CHA-CBD-CGD-O2D
14	a	1138	CLA	CHA-CBD-CGD-O1D
14	b	1022	CLA	CHA-CBD-CGD-O1D
14	b	1205	CLA	CHA-CBD-CGD-O1D

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
14	b	1205	CLA	CHA-CBD-CGD-O2D
14	b	1210	CLA	CHA-CBD-CGD-O2D
14	b	1216	CLA	CHA-CBD-CGD-O1D
14	b	1216	CLA	CHA-CBD-CGD-O2D
14	b	1218	CLA	CHA-CBD-CGD-O1D
14	b	1218	CLA	CHA-CBD-CGD-O2D
14	b	1220	CLA	CHA-CBD-CGD-O1D
14	b	1220	CLA	CHA-CBD-CGD-O2D
14	b	1222	CLA	CHA-CBD-CGD-O1D
14	b	1222	CLA	CHA-CBD-CGD-O2D
14	b	1223	CLA	CHA-CBD-CGD-O1D
14	b	1228	CLA	CHA-CBD-CGD-O2D
14	b	1234	CLA	CHA-CBD-CGD-O1D
14	A	1101	CLA	CHA-CBD-CGD-O1D
14	A	1106	CLA	CHA-CBD-CGD-O1D
14	A	1111	CLA	CHA-CBD-CGD-O1D
14	A	1111	CLA	CHA-CBD-CGD-O2D
14	A	1113	CLA	CHA-CBD-CGD-O1D
14	A	1113	CLA	CHA-CBD-CGD-O2D
14	A	1114	CLA	CHA-CBD-CGD-O1D
14	A	1114	CLA	CHA-CBD-CGD-O2D
14	A	1115	CLA	CHA-CBD-CGD-O1D
14	A	1120	CLA	CHA-CBD-CGD-O1D
14	A	1120	CLA	CHA-CBD-CGD-O2D
14	A	1123	CLA	CHA-CBD-CGD-O1D
14	A	1123	CLA	CHA-CBD-CGD-O2D
14	A	1132	CLA	CHA-CBD-CGD-O1D
14	A	1132	CLA	CHA-CBD-CGD-O2D
14	A	1134	CLA	CHA-CBD-CGD-O1D
14	A	1134	CLA	CHA-CBD-CGD-O2D
14	A	1138	CLA	CHA-CBD-CGD-O1D
14	B	1022	CLA	CHA-CBD-CGD-O1D
14	B	1205	CLA	CHA-CBD-CGD-O1D
14	B	1205	CLA	CHA-CBD-CGD-O2D
14	B	1210	CLA	CHA-CBD-CGD-O2D
14	B	1216	CLA	CHA-CBD-CGD-O1D
14	B	1216	CLA	CHA-CBD-CGD-O2D
14	B	1218	CLA	CHA-CBD-CGD-O1D
14	B	1218	CLA	CHA-CBD-CGD-O2D
14	B	1220	CLA	CHA-CBD-CGD-O1D
14	B	1220	CLA	CHA-CBD-CGD-O2D
14	B	1222	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	B	1222	CLA	CHA-CBD-CGD-O2D
14	B	1223	CLA	CHA-CBD-CGD-O1D
14	B	1228	CLA	CHA-CBD-CGD-O2D
14	B	1234	CLA	CHA-CBD-CGD-O1D
14	a	1136	CLA	C15-C16-C17-C18
14	A	1136	CLA	C15-C16-C17-C18
14	G	1013	CLA	C3-C5-C6-C7
14	G	1109	CLA	C3-C5-C6-C7
14	H	1210	CLA	O1A-CGA-O2A-C1
14	G	1136	CLA	C15-C16-C17-C18
14	A	1127	CLA	C13-C15-C16-C17
14	b	1210	CLA	O1A-CGA-O2A-C1
14	B	1210	CLA	O1A-CGA-O2A-C1
14	G	1109	CLA	C16-C17-C18-C19
14	a	1109	CLA	C16-C17-C18-C19
14	A	1109	CLA	C16-C17-C18-C19
14	H	1203	CLA	C3-C5-C6-C7
14	b	1203	CLA	C3-C5-C6-C7
14	B	1203	CLA	C3-C5-C6-C7
14	G	1127	CLA	C13-C15-C16-C17
14	a	1127	CLA	C13-C15-C16-C17
19	G	5001	LHG	C31-C32-C33-C34
19	a	5001	LHG	C31-C32-C33-C34
20	R	5006	LMG	C29-C30-C31-C32
19	A	5001	LHG	C31-C32-C33-C34
20	i	5006	LMG	C29-C30-C31-C32
20	I	5006	LMG	C29-C30-C31-C32
14	G	1125	CLA	C11-C12-C13-C14
14	G	1126	CLA	C11-C10-C8-C9
14	H	1225	CLA	C11-C10-C8-C9
14	a	1125	CLA	C11-C12-C13-C14
14	a	1126	CLA	C11-C10-C8-C9
14	A	1125	CLA	C11-C12-C13-C14
14	A	1126	CLA	C11-C10-C8-C9
14	B	1225	CLA	C11-C10-C8-C9
20	L	5007	LMG	O10-C28-O8-C9
20	U	5007	LMG	O10-C28-O8-C9
20	l	5007	LMG	O10-C28-O8-C9
20	a	5005	LMG	C36-C37-C38-C39
20	A	5005	LMG	C36-C37-C38-C39
14	G	1129	CLA	C1A-C2A-CAA-CBA
14	H	1202	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	a	1129	CLA	C1A-C2A-CAA-CBA
14	b	1202	CLA	C1A-C2A-CAA-CBA
14	A	1129	CLA	C1A-C2A-CAA-CBA
14	B	1202	CLA	C1A-C2A-CAA-CBA
14	b	1023	CLA	C16-C17-C18-C20
14	G	1103	CLA	C2-C1-O2A-CGA
14	H	1228	CLA	C2-C1-O2A-CGA
14	a	1103	CLA	C2-C1-O2A-CGA
14	b	1228	CLA	C2-C1-O2A-CGA
14	A	1103	CLA	C2-C1-O2A-CGA
14	B	1228	CLA	C2-C1-O2A-CGA
14	G	1129	CLA	CBA-CGA-O2A-C1
14	a	1129	CLA	CBA-CGA-O2A-C1
14	A	1129	CLA	CBA-CGA-O2A-C1
20	G	5005	LMG	C36-C37-C38-C39
18	U	4019	BCR	C19-C20-C21-C22
18	l	4019	BCR	C19-C20-C21-C22
18	L	4019	BCR	C19-C20-C21-C22
14	B	1204	CLA	O1A-CGA-O2A-C1
18	R	4018	BCR	C14-C15-C16-C17
19	G	5001	LHG	C3-O3-P-O5
19	G	5001	LHG	C4-O6-P-O5
19	H	5004	LHG	C4-O6-P-O5
19	a	5001	LHG	C3-O3-P-O5
19	a	5001	LHG	C4-O6-P-O5
19	b	5004	LHG	C4-O6-P-O5
19	A	5001	LHG	C3-O3-P-O5
19	A	5001	LHG	C4-O6-P-O5
19	B	5004	LHG	C4-O6-P-O5
14	G	1118	CLA	C6-C7-C8-C9
14	H	1023	CLA	C16-C17-C18-C20
14	U	1503	CLA	C16-C17-C18-C20
14	a	1118	CLA	C6-C7-C8-C9
14	l	1503	CLA	C16-C17-C18-C20
14	A	1118	CLA	C6-C7-C8-C9
14	B	1023	CLA	C16-C17-C18-C20
19	G	5001	LHG	O6-C4-C5-C6
19	H	5004	LHG	O6-C4-C5-C6
19	a	5001	LHG	O6-C4-C5-C6
19	b	5004	LHG	O6-C4-C5-C6
19	A	5001	LHG	O6-C4-C5-C6
19	B	5004	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
14	a	1103	CLA	O1D-CGD-O2D-CED
14	A	1103	CLA	O1D-CGD-O2D-CED
14	H	1204	CLA	O1A-CGA-O2A-C1
14	b	1204	CLA	O1A-CGA-O2A-C1
14	L	1503	CLA	C16-C17-C18-C20
14	G	1111	CLA	CAD-CBD-CGD-O1D
14	G	1113	CLA	CAD-CBD-CGD-O1D
14	G	1123	CLA	CAD-CBD-CGD-O1D
14	H	1022	CLA	CAD-CBD-CGD-O1D
14	H	1223	CLA	CAD-CBD-CGD-O1D
14	H	1234	CLA	CAD-CBD-CGD-O1D
14	a	1111	CLA	CAD-CBD-CGD-O1D
14	a	1113	CLA	CAD-CBD-CGD-O1D
14	a	1123	CLA	CAD-CBD-CGD-O1D
14	b	1022	CLA	CAD-CBD-CGD-O1D
14	b	1223	CLA	CAD-CBD-CGD-O1D
14	b	1234	CLA	CAD-CBD-CGD-O1D
14	A	1111	CLA	CAD-CBD-CGD-O1D
14	A	1113	CLA	CAD-CBD-CGD-O1D
14	A	1123	CLA	CAD-CBD-CGD-O1D
14	B	1022	CLA	CAD-CBD-CGD-O1D
14	B	1223	CLA	CAD-CBD-CGD-O1D
14	B	1234	CLA	CAD-CBD-CGD-O1D
14	G	1103	CLA	O1D-CGD-O2D-CED
14	G	1115	CLA	C16-C17-C18-C19
14	a	1115	CLA	C16-C17-C18-C19
14	A	1115	CLA	C16-C17-C18-C19
13	G	1011	CL0	C12-C13-C15-C16
13	a	1011	CL0	C12-C13-C15-C16
13	A	1011	CL0	C12-C13-C15-C16
14	G	1115	CLA	C11-C12-C13-C15
14	G	1126	CLA	C6-C7-C8-C10
14	G	1128	CLA	C11-C10-C8-C7
14	G	1135	CLA	C6-C7-C8-C10
14	H	1204	CLA	C12-C13-C15-C16
14	H	1223	CLA	C6-C7-C8-C10
14	H	1234	CLA	C6-C7-C8-C10
14	H	1239	CLA	C11-C12-C13-C15
14	a	1115	CLA	C11-C12-C13-C15
14	a	1126	CLA	C6-C7-C8-C10
14	a	1127	CLA	C12-C13-C15-C16
14	a	1128	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
14	a	1135	CLA	C6-C7-C8-C10
14	a	1140	CLA	C6-C7-C8-C10
14	b	1204	CLA	C12-C13-C15-C16
14	b	1223	CLA	C6-C7-C8-C10
14	b	1234	CLA	C6-C7-C8-C10
14	b	1239	CLA	C11-C12-C13-C15
14	A	1115	CLA	C11-C12-C13-C15
14	A	1126	CLA	C6-C7-C8-C10
14	A	1127	CLA	C12-C13-C15-C16
14	A	1128	CLA	C11-C10-C8-C7
14	A	1135	CLA	C6-C7-C8-C10
14	A	1140	CLA	C6-C7-C8-C10
14	B	1204	CLA	C12-C13-C15-C16
14	B	1223	CLA	C6-C7-C8-C10
14	B	1234	CLA	C6-C7-C8-C10
14	B	1239	CLA	C11-C12-C13-C15
16	H	2002	PQN	C21-C22-C23-C25
16	b	2002	PQN	C21-C22-C23-C25
16	B	2002	PQN	C21-C22-C23-C25
14	G	1125	CLA	O1A-CGA-O2A-C1
14	a	1125	CLA	O1A-CGA-O2A-C1
14	A	1125	CLA	O1A-CGA-O2A-C1
18	l	4019	BCR	C9-C10-C11-C12
14	G	1125	CLA	CAA-CBA-CGA-O2A
14	H	1220	CLA	CAA-CBA-CGA-O2A
14	b	1220	CLA	CAA-CBA-CGA-O2A
14	A	1125	CLA	CAA-CBA-CGA-O2A
14	B	1220	CLA	CAA-CBA-CGA-O2A
19	a	5001	LHG	C24-C25-C26-C27
19	G	5001	LHG	C24-C25-C26-C27
19	A	5001	LHG	C24-C25-C26-C27
14	H	1203	CLA	C5-C6-C7-C8
14	b	1203	CLA	C5-C6-C7-C8
14	G	1120	CLA	C2A-CAA-CBA-CGA
14	a	1120	CLA	C2A-CAA-CBA-CGA
14	A	1120	CLA	C2A-CAA-CBA-CGA
14	G	1132	CLA	C16-C17-C18-C19
14	H	1228	CLA	C6-C7-C8-C9
14	b	1228	CLA	C6-C7-C8-C9
14	A	1132	CLA	C16-C17-C18-C19
14	B	1228	CLA	C6-C7-C8-C9
14	a	1125	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	a	1132	CLA	C16-C17-C18-C19
14	B	1203	CLA	C5-C6-C7-C8
13	G	1011	CL0	O1A-CGA-O2A-C1
13	a	1011	CL0	O1A-CGA-O2A-C1
13	A	1011	CL0	O1A-CGA-O2A-C1
14	H	1023	CLA	O1A-CGA-O2A-C1
14	b	1023	CLA	O1A-CGA-O2A-C1
14	B	1023	CLA	O1A-CGA-O2A-C1
13	G	1011	CL0	C14-C13-C15-C16
13	a	1011	CL0	C14-C13-C15-C16
13	A	1011	CL0	C14-C13-C15-C16
14	H	1022	CLA	C6-C7-C8-C9
14	H	1208	CLA	C6-C7-C8-C9
14	H	1214	CLA	C6-C7-C8-C9
14	H	1216	CLA	C6-C7-C8-C9
14	H	1223	CLA	C11-C10-C8-C9
14	b	1022	CLA	C6-C7-C8-C9
14	b	1208	CLA	C6-C7-C8-C9
14	b	1214	CLA	C6-C7-C8-C9
14	b	1216	CLA	C6-C7-C8-C9
14	b	1223	CLA	C11-C10-C8-C9
14	B	1022	CLA	C6-C7-C8-C9
14	B	1208	CLA	C6-C7-C8-C9
14	B	1214	CLA	C6-C7-C8-C9
14	B	1216	CLA	C6-C7-C8-C9
14	B	1223	CLA	C11-C10-C8-C9
14	G	1129	CLA	O1A-CGA-O2A-C1
14	a	1129	CLA	O1A-CGA-O2A-C1
14	A	1129	CLA	O1A-CGA-O2A-C1
14	G	1112	CLA	C3-C5-C6-C7
14	a	1112	CLA	C3-C5-C6-C7
14	A	1112	CLA	C3-C5-C6-C7
14	G	1123	CLA	O1A-CGA-O2A-C1
14	a	1123	CLA	O1A-CGA-O2A-C1
14	A	1123	CLA	O1A-CGA-O2A-C1
18	G	4003	BCR	C18-C19-C20-C21
18	H	4006	BCR	C18-C19-C20-C21
18	H	4013	BCR	C18-C19-C20-C21
18	R	4020	BCR	C18-C19-C20-C21
18	a	4003	BCR	C18-C19-C20-C21
18	b	4006	BCR	C18-C19-C20-C21
18	b	4013	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
18	i	4020	BCR	C18-C19-C20-C21
18	A	4003	BCR	C18-C19-C20-C21
18	B	4006	BCR	C18-C19-C20-C21
18	B	4013	BCR	C18-C19-C20-C21
18	I	4020	BCR	C18-C19-C20-C21
14	A	1130	CLA	C6-C7-C8-C10
14	G	1133	CLA	C3-C5-C6-C7
14	a	1133	CLA	C3-C5-C6-C7
14	A	1133	CLA	C3-C5-C6-C7
14	H	1204	CLA	C4-C3-C5-C6
14	B	1204	CLA	C4-C3-C5-C6
14	G	1130	CLA	C6-C7-C8-C10
14	H	1021	CLA	C16-C17-C18-C20
14	a	1130	CLA	C6-C7-C8-C10
14	b	1021	CLA	C16-C17-C18-C20
14	B	1021	CLA	C16-C17-C18-C20
14	G	1127	CLA	CAA-CBA-CGA-O2A
14	H	1213	CLA	CAA-CBA-CGA-O2A
14	a	1127	CLA	CAA-CBA-CGA-O2A
14	b	1213	CLA	CAA-CBA-CGA-O2A
14	A	1127	CLA	CAA-CBA-CGA-O2A
14	B	1213	CLA	CAA-CBA-CGA-O2A
14	H	1216	CLA	C15-C16-C17-C18
14	b	1216	CLA	C15-C16-C17-C18
14	B	1216	CLA	C15-C16-C17-C18
14	H	1216	CLA	O1A-CGA-O2A-C1
14	B	1216	CLA	O1A-CGA-O2A-C1
14	H	1022	CLA	C2-C1-O2A-CGA
14	H	1221	CLA	C2-C1-O2A-CGA
14	H	1234	CLA	C2-C1-O2A-CGA
14	H	1235	CLA	C2-C1-O2A-CGA
14	b	1022	CLA	C2-C1-O2A-CGA
14	b	1221	CLA	C2-C1-O2A-CGA
14	b	1234	CLA	C2-C1-O2A-CGA
14	b	1235	CLA	C2-C1-O2A-CGA
14	B	1022	CLA	C2-C1-O2A-CGA
14	B	1221	CLA	C2-C1-O2A-CGA
14	B	1234	CLA	C2-C1-O2A-CGA
14	B	1235	CLA	C2-C1-O2A-CGA
18	i	4018	BCR	C14-C15-C16-C17
18	I	4018	BCR	C14-C15-C16-C17
20	U	5007	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
20	l	5007	LMG	C32-C33-C34-C35
14	b	1210	CLA	C15-C16-C17-C18
14	b	1216	CLA	O1A-CGA-O2A-C1
20	L	5007	LMG	C32-C33-C34-C35
21	G	6002	LMT	C5'-C4'-O1B-C1B
14	B	1210	CLA	C15-C16-C17-C18
19	G	5001	LHG	C15-C16-C17-C18
19	a	5001	LHG	C15-C16-C17-C18
19	A	5001	LHG	C15-C16-C17-C18
21	a	6002	LMT	C5'-C4'-O1B-C1B
21	A	6002	LMT	C5'-C4'-O1B-C1B
19	G	5001	LHG	O6-C4-C5-O7
19	a	5001	LHG	O6-C4-C5-O7
19	A	5001	LHG	O6-C4-C5-O7
14	b	1204	CLA	C4-C3-C5-C6
18	G	4002	BCR	C23-C24-C25-C30
18	G	4011	BCR	C1-C6-C7-C8
18	U	4019	BCR	C23-C24-C25-C26
18	a	4002	BCR	C23-C24-C25-C30
18	l	4019	BCR	C23-C24-C25-C26
18	A	4002	BCR	C23-C24-C25-C30
18	L	4019	BCR	C23-C24-C25-C26
14	H	1210	CLA	C15-C16-C17-C18
20	G	5005	LMG	C2-C1-O1-C7
20	a	5005	LMG	C2-C1-O1-C7
20	A	5005	LMG	C2-C1-O1-C7
14	a	1123	CLA	CBA-CGA-O2A-C1
14	G	1106	CLA	C11-C12-C13-C14
14	A	1106	CLA	C11-C12-C13-C14
14	G	1123	CLA	CBA-CGA-O2A-C1
14	b	1204	CLA	CBA-CGA-O2A-C1
14	A	1123	CLA	CBA-CGA-O2A-C1
14	G	1125	CLA	C4-C3-C5-C6
14	a	1125	CLA	C4-C3-C5-C6
14	A	1125	CLA	C4-C3-C5-C6
14	H	1225	CLA	C11-C10-C8-C7
14	b	1225	CLA	C11-C10-C8-C7
14	B	1225	CLA	C11-C10-C8-C7
14	G	1115	CLA	C11-C12-C13-C14
14	G	1128	CLA	C11-C10-C8-C9
14	G	1138	CLA	C6-C7-C8-C9
14	H	1203	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	a	1115	CLA	C11-C12-C13-C14
14	a	1128	CLA	C11-C10-C8-C9
14	a	1138	CLA	C6-C7-C8-C9
14	b	1203	CLA	C14-C13-C15-C16
14	A	1115	CLA	C11-C12-C13-C14
14	A	1128	CLA	C11-C10-C8-C9
14	A	1138	CLA	C6-C7-C8-C9
14	B	1203	CLA	C14-C13-C15-C16
16	G	2001	PQN	C21-C22-C23-C24
16	a	2001	PQN	C21-C22-C23-C24
16	A	2001	PQN	C21-C22-C23-C24
18	H	4016	BCR	C9-C10-C11-C12
18	U	4019	BCR	C9-C10-C11-C12
18	U	4022	BCR	C9-C10-C11-C12
18	V	4021	BCR	C9-C10-C11-C12
18	b	4016	BCR	C9-C10-C11-C12
18	m	4021	BCR	C9-C10-C11-C12
18	B	4016	BCR	C9-C10-C11-C12
18	L	4019	BCR	C9-C10-C11-C12
18	M	4021	BCR	C9-C10-C11-C12
14	U	1503	CLA	C16-C17-C18-C19
14	a	1106	CLA	C11-C12-C13-C14
14	l	1503	CLA	C16-C17-C18-C19
14	H	1204	CLA	CBA-CGA-O2A-C1
14	B	1204	CLA	CBA-CGA-O2A-C1
14	L	1503	CLA	C16-C17-C18-C19
13	G	1011	CL0	CBA-CGA-O2A-C1
13	a	1011	CL0	CBA-CGA-O2A-C1
13	A	1011	CL0	CBA-CGA-O2A-C1
14	b	1216	CLA	CBA-CGA-O2A-C1
14	G	1127	CLA	C5-C6-C7-C8
14	a	1127	CLA	C5-C6-C7-C8
14	A	1127	CLA	C5-C6-C7-C8
21	A	6002	LMT	O5'-C5'-C6'-O6'
14	H	1235	CLA	C2-C3-C5-C6
14	b	1235	CLA	C2-C3-C5-C6
14	B	1235	CLA	C2-C3-C5-C6
14	H	1021	CLA	C16-C17-C18-C19
14	H	1228	CLA	C6-C7-C8-C10
14	b	1021	CLA	C16-C17-C18-C19
14	B	1021	CLA	C16-C17-C18-C19
14	B	1228	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
14	H	1216	CLA	CBA-CGA-O2A-C1
14	B	1216	CLA	CBA-CGA-O2A-C1
21	G	6002	LMT	O5'-C5'-C6'-O6'
21	a	6002	LMT	O5'-C5'-C6'-O6'
15	H	1237	F6C	C2A-CAA-CBA-CGA
15	b	1237	F6C	C2A-CAA-CBA-CGA
15	B	1237	F6C	C2A-CAA-CBA-CGA
20	i	5006	LMG	O9-C10-C11-C12
14	G	1104	CLA	C2A-CAA-CBA-CGA
14	b	1228	CLA	C6-C7-C8-C10
14	H	1208	CLA	CAA-CBA-CGA-O1A
14	b	1208	CLA	CAA-CBA-CGA-O1A
14	B	1208	CLA	CAA-CBA-CGA-O1A
20	R	5006	LMG	O9-C10-C11-C12
20	I	5006	LMG	O9-C10-C11-C12
14	H	1226	CLA	C15-C16-C17-C18
18	R	4020	BCR	C9-C10-C11-C12
18	l	4022	BCR	C9-C10-C11-C12
18	I	4020	BCR	C9-C10-C11-C12
18	L	4022	BCR	C9-C10-C11-C12
20	I	5006	LMG	C33-C34-C35-C36
14	b	1226	CLA	C15-C16-C17-C18
14	B	1226	CLA	C15-C16-C17-C18
20	R	5006	LMG	C33-C34-C35-C36
20	i	5006	LMG	C33-C34-C35-C36
14	H	1217	CLA	C4-C3-C5-C6
14	b	1217	CLA	C4-C3-C5-C6
14	B	1217	CLA	C4-C3-C5-C6
14	H	1205	CLA	C5-C6-C7-C8
14	b	1205	CLA	C5-C6-C7-C8
14	B	1205	CLA	C5-C6-C7-C8
14	G	1115	CLA	C2-C1-O2A-CGA
14	a	1115	CLA	C2-C1-O2A-CGA
14	A	1115	CLA	C2-C1-O2A-CGA
14	H	1222	CLA	C16-C17-C18-C20
14	b	1222	CLA	C16-C17-C18-C20
14	B	1222	CLA	C16-C17-C18-C20
14	a	1104	CLA	C2A-CAA-CBA-CGA
14	A	1104	CLA	C2A-CAA-CBA-CGA
20	U	5007	LMG	O1-C7-C8-O7
20	l	5007	LMG	O1-C7-C8-O7
20	L	5007	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
14	b	1208	CLA	C13-C15-C16-C17
14	H	1202	CLA	C3A-C2A-CAA-CBA
14	H	1209	CLA	C3A-C2A-CAA-CBA
14	H	1219	CLA	C3A-C2A-CAA-CBA
14	H	1233	CLA	C3A-C2A-CAA-CBA
14	b	1202	CLA	C3A-C2A-CAA-CBA
14	b	1209	CLA	C3A-C2A-CAA-CBA
14	b	1219	CLA	C3A-C2A-CAA-CBA
14	b	1233	CLA	C3A-C2A-CAA-CBA
14	B	1202	CLA	C3A-C2A-CAA-CBA
14	B	1209	CLA	C3A-C2A-CAA-CBA
14	B	1219	CLA	C3A-C2A-CAA-CBA
14	B	1233	CLA	C3A-C2A-CAA-CBA
14	B	1208	CLA	C13-C15-C16-C17
18	i	4020	BCR	C9-C10-C11-C12
14	H	1208	CLA	C13-C15-C16-C17
14	G	1115	CLA	C6-C7-C8-C9
14	G	1117	CLA	C11-C10-C8-C9
14	H	1214	CLA	C14-C13-C15-C16
14	H	1239	CLA	C14-C13-C15-C16
14	U	1501	CLA	C11-C12-C13-C14
14	a	1115	CLA	C6-C7-C8-C9
14	a	1117	CLA	C11-C10-C8-C9
14	b	1214	CLA	C14-C13-C15-C16
14	b	1239	CLA	C14-C13-C15-C16
14	l	1501	CLA	C11-C12-C13-C14
14	A	1115	CLA	C6-C7-C8-C9
14	A	1117	CLA	C11-C10-C8-C9
14	B	1214	CLA	C14-C13-C15-C16
14	B	1239	CLA	C14-C13-C15-C16
14	L	1501	CLA	C11-C12-C13-C14
16	G	2001	PQN	C24-C23-C25-C26
16	a	2001	PQN	C24-C23-C25-C26
16	A	2001	PQN	C24-C23-C25-C26
18	G	4007	BCR	C16-C17-C18-C36
18	G	4011	BCR	C16-C17-C18-C36
18	H	4006	BCR	C11-C10-C9-C34
18	H	4010	BCR	C16-C17-C18-C36
18	H	4016	BCR	C35-C13-C14-C15
18	a	4007	BCR	C16-C17-C18-C36
18	a	4011	BCR	C16-C17-C18-C36
18	b	4006	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
18	b	4010	BCR	C16-C17-C18-C36
18	b	4016	BCR	C35-C13-C14-C15
18	A	4007	BCR	C16-C17-C18-C36
18	A	4011	BCR	C16-C17-C18-C36
18	B	4006	BCR	C11-C10-C9-C34
18	B	4010	BCR	C16-C17-C18-C36
18	B	4016	BCR	C35-C13-C14-C15
13	G	1011	CL0	C5-C6-C7-C8
18	H	4005	BCR	C36-C18-C19-C20
18	B	4005	BCR	C36-C18-C19-C20
18	B	4006	BCR	C7-C8-C9-C34
14	a	1122	CLA	C3-C5-C6-C7
14	A	1122	CLA	C3-C5-C6-C7
13	a	1011	CL0	C5-C6-C7-C8
13	A	1011	CL0	C5-C6-C7-C8
14	G	1122	CLA	C1A-C2A-CAA-CBA
14	H	1212	CLA	C1A-C2A-CAA-CBA
14	a	1122	CLA	C1A-C2A-CAA-CBA
14	b	1212	CLA	C1A-C2A-CAA-CBA
14	A	1122	CLA	C1A-C2A-CAA-CBA
14	B	1212	CLA	C1A-C2A-CAA-CBA
14	G	1104	CLA	C6-C7-C8-C10
14	G	1111	CLA	C6-C7-C8-C10
14	G	1119	CLA	C11-C10-C8-C7
14	G	1119	CLA	C12-C13-C15-C16
14	G	1127	CLA	C11-C10-C8-C7
14	H	1211	CLA	C11-C10-C8-C7
14	a	1104	CLA	C6-C7-C8-C10
14	a	1111	CLA	C6-C7-C8-C10
14	a	1119	CLA	C11-C10-C8-C7
14	a	1119	CLA	C12-C13-C15-C16
14	a	1127	CLA	C11-C10-C8-C7
14	b	1211	CLA	C11-C10-C8-C7
14	A	1104	CLA	C6-C7-C8-C10
14	A	1111	CLA	C6-C7-C8-C10
14	A	1119	CLA	C11-C10-C8-C7
14	A	1119	CLA	C12-C13-C15-C16
14	A	1127	CLA	C11-C10-C8-C7
14	B	1211	CLA	C11-C10-C8-C7
15	H	1237	F6C	C6-C7-C8-C10
15	b	1237	F6C	C6-C7-C8-C10
15	B	1237	F6C	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
16	G	2001	PQN	C17-C18-C20-C21
16	a	2001	PQN	C17-C18-C20-C21
16	A	2001	PQN	C17-C18-C20-C21
14	G	1122	CLA	C3-C5-C6-C7
18	B	4010	BCR	C19-C20-C21-C22
14	G	1108	CLA	CAA-CBA-CGA-O2A
14	a	1108	CLA	CAA-CBA-CGA-O2A
14	A	1108	CLA	CAA-CBA-CGA-O2A
14	G	1117	CLA	C3-C5-C6-C7
14	H	1225	CLA	C3-C5-C6-C7
14	a	1117	CLA	C3-C5-C6-C7
14	A	1117	CLA	C3-C5-C6-C7
14	G	1129	CLA	C2A-CAA-CBA-CGA
14	a	1129	CLA	C2A-CAA-CBA-CGA
14	A	1129	CLA	C2A-CAA-CBA-CGA
14	H	1023	CLA	C8-C10-C11-C12
14	b	1023	CLA	C8-C10-C11-C12
14	B	1023	CLA	C8-C10-C11-C12
14	b	1220	CLA	CBA-CGA-O2A-C1
14	B	1220	CLA	CBA-CGA-O2A-C1
14	B	1225	CLA	C3-C5-C6-C7
19	a	5001	LHG	C25-C26-C27-C28
14	H	1204	CLA	C2-C3-C5-C6
14	b	1204	CLA	C2-C3-C5-C6
14	B	1204	CLA	C2-C3-C5-C6
19	G	5001	LHG	C25-C26-C27-C28
14	H	1220	CLA	CBA-CGA-O2A-C1
19	A	5001	LHG	C25-C26-C27-C28
16	H	2002	PQN	C23-C25-C26-C27
16	b	2002	PQN	C23-C25-C26-C27
16	B	2002	PQN	C23-C25-C26-C27
14	b	1225	CLA	C3-C5-C6-C7
18	G	4007	BCR	C16-C17-C18-C19
18	G	4011	BCR	C16-C17-C18-C19
18	H	4006	BCR	C11-C10-C9-C8
18	H	4016	BCR	C12-C13-C14-C15
18	a	4007	BCR	C16-C17-C18-C19
18	a	4011	BCR	C16-C17-C18-C19
18	b	4006	BCR	C11-C10-C9-C8
18	b	4016	BCR	C12-C13-C14-C15
18	A	4007	BCR	C16-C17-C18-C19
18	A	4011	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	B	4006	BCR	C11-C10-C9-C8
18	B	4016	BCR	C12-C13-C14-C15
18	H	4010	BCR	C19-C20-C21-C22
18	R	4020	BCR	C15-C16-C17-C18
18	b	4010	BCR	C19-C20-C21-C22
18	i	4020	BCR	C15-C16-C17-C18
18	I	4020	BCR	C15-C16-C17-C18
14	H	1220	CLA	O1A-CGA-O2A-C1
14	b	1220	CLA	O1A-CGA-O2A-C1
14	B	1220	CLA	O1A-CGA-O2A-C1
15	G	1121	F6C	CAA-CBA-CGA-O1A
15	a	1121	F6C	CAA-CBA-CGA-O1A
20	a	5005	LMG	C33-C34-C35-C36
14	G	1125	CLA	C2-C3-C5-C6
14	a	1125	CLA	C2-C3-C5-C6
14	A	1125	CLA	C2-C3-C5-C6
15	A	1121	F6C	CAA-CBA-CGA-O1A
20	A	5005	LMG	C33-C34-C35-C36
20	G	5005	LMG	C33-C34-C35-C36
15	G	1121	F6C	CAA-CBA-CGA-O2A
15	a	1121	F6C	CAA-CBA-CGA-O2A
15	A	1121	F6C	CAA-CBA-CGA-O2A
20	A	5005	LMG	C14-C15-C16-C17
20	G	5005	LMG	C14-C15-C16-C17
20	a	5005	LMG	C14-C15-C16-C17
18	H	4005	BCR	C1-C6-C7-C8
18	H	4005	BCR	C5-C6-C7-C8
18	H	4009	BCR	C23-C24-C25-C30
18	H	4016	BCR	C23-C24-C25-C30
18	H	4017	BCR	C1-C6-C7-C8
18	R	4020	BCR	C1-C6-C7-C8
18	b	4005	BCR	C5-C6-C7-C8
18	b	4009	BCR	C23-C24-C25-C30
18	b	4016	BCR	C23-C24-C25-C30
18	b	4017	BCR	C1-C6-C7-C8
18	i	4020	BCR	C1-C6-C7-C8
18	B	4005	BCR	C1-C6-C7-C8
18	B	4005	BCR	C5-C6-C7-C8
18	B	4009	BCR	C23-C24-C25-C30
18	B	4016	BCR	C23-C24-C25-C30
18	B	4017	BCR	C1-C6-C7-C8
18	I	4020	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
18	b	4005	BCR	C36-C18-C19-C20
14	G	1108	CLA	CAA-CBA-CGA-O1A
14	a	1108	CLA	CAA-CBA-CGA-O1A
14	A	1108	CLA	CAA-CBA-CGA-O1A
14	l	1503	CLA	C15-C16-C17-C18
14	L	1503	CLA	C15-C16-C17-C18
14	H	1228	CLA	C4-C3-C5-C6
14	b	1228	CLA	C4-C3-C5-C6
14	B	1228	CLA	C4-C3-C5-C6
15	H	1238	F6C	C4-C3-C5-C6
15	b	1238	F6C	C4-C3-C5-C6
15	B	1238	F6C	C4-C3-C5-C6
14	U	1503	CLA	C15-C16-C17-C18
14	H	1236	CLA	CAA-CBA-CGA-O2A
14	b	1233	CLA	CAA-CBA-CGA-O1A
14	b	1236	CLA	CAA-CBA-CGA-O2A
14	B	1236	CLA	CAA-CBA-CGA-O2A
14	H	1233	CLA	CAA-CBA-CGA-O1A
14	B	1233	CLA	CAA-CBA-CGA-O1A
14	H	1226	CLA	C2A-CAA-CBA-CGA
14	b	1226	CLA	C2A-CAA-CBA-CGA
14	B	1226	CLA	C2A-CAA-CBA-CGA
14	b	1221	CLA	C10-C11-C12-C13
14	H	1221	CLA	C10-C11-C12-C13
14	B	1221	CLA	C10-C11-C12-C13
14	H	1202	CLA	CAA-CBA-CGA-O1A
14	B	1202	CLA	CAA-CBA-CGA-O1A
14	G	1123	CLA	C11-C10-C8-C7
14	G	1126	CLA	C2-C3-C5-C6
14	G	1138	CLA	C6-C7-C8-C10
14	H	1210	CLA	C11-C10-C8-C7
14	U	1502	CLA	C6-C7-C8-C10
14	a	1123	CLA	C11-C10-C8-C7
14	a	1126	CLA	C2-C3-C5-C6
14	b	1210	CLA	C11-C10-C8-C7
14	l	1502	CLA	C6-C7-C8-C10
14	A	1123	CLA	C11-C10-C8-C7
14	A	1126	CLA	C2-C3-C5-C6
14	A	1138	CLA	C6-C7-C8-C10
14	B	1210	CLA	C11-C10-C8-C7
14	L	1502	CLA	C6-C7-C8-C10
15	H	1238	F6C	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	b	1238	F6C	C2-C3-C5-C6
15	B	1238	F6C	C2-C3-C5-C6
14	b	1202	CLA	CAA-CBA-CGA-O1A
14	H	1236	CLA	CAA-CBA-CGA-O1A
14	b	1236	CLA	CAA-CBA-CGA-O1A
14	B	1236	CLA	CAA-CBA-CGA-O1A
14	G	1012	CLA	C4-C3-C5-C6
14	a	1012	CLA	C4-C3-C5-C6
14	A	1012	CLA	C4-C3-C5-C6
14	G	1136	CLA	CAA-CBA-CGA-O2A
14	a	1136	CLA	CAA-CBA-CGA-O2A
14	A	1136	CLA	CAA-CBA-CGA-O2A
14	G	1106	CLA	C6-C7-C8-C9
14	G	1127	CLA	C11-C10-C8-C9
14	G	1135	CLA	C6-C7-C8-C9
14	H	1223	CLA	C6-C7-C8-C9
14	H	1224	CLA	C6-C7-C8-C9
14	H	1239	CLA	C11-C12-C13-C14
14	U	1502	CLA	C11-C10-C8-C9
14	a	1106	CLA	C6-C7-C8-C9
14	a	1127	CLA	C11-C10-C8-C9
14	a	1135	CLA	C6-C7-C8-C9
14	b	1223	CLA	C6-C7-C8-C9
14	b	1224	CLA	C6-C7-C8-C9
14	b	1239	CLA	C11-C12-C13-C14
14	l	1502	CLA	C11-C10-C8-C9
14	A	1106	CLA	C6-C7-C8-C9
14	A	1127	CLA	C11-C10-C8-C9
14	A	1135	CLA	C6-C7-C8-C9
14	B	1223	CLA	C6-C7-C8-C9
14	B	1224	CLA	C6-C7-C8-C9
14	B	1239	CLA	C11-C12-C13-C14
14	L	1502	CLA	C11-C10-C8-C9
16	H	2002	PQN	C21-C22-C23-C24
16	b	2002	PQN	C21-C22-C23-C24
16	B	2002	PQN	C21-C22-C23-C24
14	G	1012	CLA	C3A-C2A-CAA-CBA
14	G	1136	CLA	C3A-C2A-CAA-CBA
14	H	1231	CLA	C3A-C2A-CAA-CBA
14	a	1012	CLA	C3A-C2A-CAA-CBA
14	a	1136	CLA	C3A-C2A-CAA-CBA
14	b	1231	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	A	1012	CLA	C3A-C2A-CAA-CBA
14	A	1136	CLA	C3A-C2A-CAA-CBA
14	B	1231	CLA	C3A-C2A-CAA-CBA
14	G	1104	CLA	CAD-CBD-CGD-O2D
14	G	1118	CLA	CAD-CBD-CGD-O2D
14	G	1134	CLA	CAD-CBD-CGD-O2D
14	G	1138	CLA	CAD-CBD-CGD-O2D
14	H	1211	CLA	CAD-CBD-CGD-O2D
14	a	1104	CLA	CAD-CBD-CGD-O2D
14	a	1118	CLA	CAD-CBD-CGD-O2D
14	a	1134	CLA	CAD-CBD-CGD-O2D
14	a	1138	CLA	CAD-CBD-CGD-O2D
14	b	1211	CLA	CAD-CBD-CGD-O2D
14	A	1104	CLA	CAD-CBD-CGD-O2D
14	A	1118	CLA	CAD-CBD-CGD-O2D
14	A	1134	CLA	CAD-CBD-CGD-O2D
14	A	1138	CLA	CAD-CBD-CGD-O2D
14	B	1211	CLA	CAD-CBD-CGD-O2D
14	a	1134	CLA	CAA-CBA-CGA-O2A
14	A	1134	CLA	CAA-CBA-CGA-O2A
14	G	1138	CLA	CAA-CBA-CGA-O2A
14	H	1239	CLA	CAA-CBA-CGA-O2A
14	a	1138	CLA	CAA-CBA-CGA-O2A
14	b	1239	CLA	CAA-CBA-CGA-O2A
14	A	1138	CLA	CAA-CBA-CGA-O2A
14	B	1239	CLA	CAA-CBA-CGA-O2A
19	G	5001	LHG	O7-C7-C8-C9
14	H	1021	CLA	CAA-CBA-CGA-O1A
14	b	1021	CLA	CAA-CBA-CGA-O1A
14	B	1021	CLA	CAA-CBA-CGA-O1A
20	B	5002	LMG	C21-C22-C23-C24
14	G	1131	CLA	C4-C3-C5-C6
14	U	1502	CLA	C4-C3-C5-C6
14	a	1131	CLA	C4-C3-C5-C6
14	l	1502	CLA	C4-C3-C5-C6
14	A	1131	CLA	C4-C3-C5-C6
14	L	1502	CLA	C4-C3-C5-C6
14	G	1101	CLA	CAA-CBA-CGA-O2A
14	G	1134	CLA	CAA-CBA-CGA-O2A
14	a	1101	CLA	CAA-CBA-CGA-O2A
14	A	1101	CLA	CAA-CBA-CGA-O2A
20	H	5002	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
14	H	1228	CLA	C2-C3-C5-C6
14	b	1228	CLA	C2-C3-C5-C6
14	B	1228	CLA	C2-C3-C5-C6
19	a	5001	LHG	O7-C7-C8-C9
20	b	5002	LMG	C21-C22-C23-C24
18	H	4005	BCR	C17-C18-C19-C20
18	b	4005	BCR	C17-C18-C19-C20
18	m	4021	BCR	C21-C22-C23-C24
18	B	4005	BCR	C17-C18-C19-C20
20	U	5007	LMG	O1-C7-C8-C9
20	l	5007	LMG	O1-C7-C8-C9
20	L	5007	LMG	O1-C7-C8-C9
14	G	1114	CLA	CAA-CBA-CGA-O2A
14	a	1101	CLA	CAA-CBA-CGA-O1A
14	a	1114	CLA	CAA-CBA-CGA-O2A
14	A	1101	CLA	CAA-CBA-CGA-O1A
14	A	1114	CLA	CAA-CBA-CGA-O2A
20	a	5005	LMG	C31-C32-C33-C34
14	H	1235	CLA	CAA-CBA-CGA-O2A
14	b	1235	CLA	CAA-CBA-CGA-O2A
14	B	1235	CLA	CAA-CBA-CGA-O2A
19	A	5001	LHG	O7-C7-C8-C9
14	G	1101	CLA	CAA-CBA-CGA-O1A
14	G	1114	CLA	CAA-CBA-CGA-O1A
14	a	1114	CLA	CAA-CBA-CGA-O1A
14	A	1114	CLA	CAA-CBA-CGA-O1A
20	A	5005	LMG	C31-C32-C33-C34
14	G	1013	CLA	O2A-C1-C2-C3
14	H	1022	CLA	O2A-C1-C2-C3
14	H	1213	CLA	O2A-C1-C2-C3
14	a	1013	CLA	O2A-C1-C2-C3
14	b	1022	CLA	O2A-C1-C2-C3
14	b	1213	CLA	O2A-C1-C2-C3
14	A	1013	CLA	O2A-C1-C2-C3
14	B	1022	CLA	O2A-C1-C2-C3
14	B	1213	CLA	O2A-C1-C2-C3
20	G	5005	LMG	C31-C32-C33-C34
19	H	5004	LHG	O9-C7-O7-C5
19	b	5004	LHG	O9-C7-O7-C5
19	B	5004	LHG	O9-C7-O7-C5
14	G	1102	CLA	CHA-CBD-CGD-O1D
14	G	1102	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	G	1112	CLA	CHA-CBD-CGD-O2D
14	G	1117	CLA	CHA-CBD-CGD-O1D
14	G	1117	CLA	CHA-CBD-CGD-O2D
14	G	1122	CLA	CHA-CBD-CGD-O2D
14	G	1127	CLA	CHA-CBD-CGD-O1D
14	G	1127	CLA	CHA-CBD-CGD-O2D
14	G	1129	CLA	CHA-CBD-CGD-O2D
14	G	1135	CLA	CHA-CBD-CGD-O1D
14	G	1138	CLA	CHA-CBD-CGD-O2D
14	H	1022	CLA	CHA-CBD-CGD-O2D
14	H	1023	CLA	CHA-CBD-CGD-O1D
14	H	1023	CLA	CHA-CBD-CGD-O2D
14	H	1201	CLA	CHA-CBD-CGD-O1D
14	H	1201	CLA	CHA-CBD-CGD-O2D
14	H	1202	CLA	CHA-CBD-CGD-O1D
14	H	1202	CLA	CHA-CBD-CGD-O2D
14	H	1203	CLA	CHA-CBD-CGD-O1D
14	H	1206	CLA	CHA-CBD-CGD-O1D
14	H	1206	CLA	CHA-CBD-CGD-O2D
14	H	1215	CLA	CHA-CBD-CGD-O1D
14	H	1215	CLA	CHA-CBD-CGD-O2D
14	H	1217	CLA	CHA-CBD-CGD-O1D
14	H	1217	CLA	CHA-CBD-CGD-O2D
14	H	1223	CLA	CHA-CBD-CGD-O2D
14	H	1225	CLA	CHA-CBD-CGD-O1D
14	H	1225	CLA	CHA-CBD-CGD-O2D
14	H	1235	CLA	CHA-CBD-CGD-O1D
14	H	1235	CLA	CHA-CBD-CGD-O2D
14	a	1102	CLA	CHA-CBD-CGD-O1D
14	a	1102	CLA	CHA-CBD-CGD-O2D
14	a	1112	CLA	CHA-CBD-CGD-O2D
14	a	1117	CLA	CHA-CBD-CGD-O1D
14	a	1117	CLA	CHA-CBD-CGD-O2D
14	a	1122	CLA	CHA-CBD-CGD-O2D
14	a	1127	CLA	CHA-CBD-CGD-O1D
14	a	1127	CLA	CHA-CBD-CGD-O2D
14	a	1129	CLA	CHA-CBD-CGD-O2D
14	a	1138	CLA	CHA-CBD-CGD-O2D
14	b	1022	CLA	CHA-CBD-CGD-O2D
14	b	1023	CLA	CHA-CBD-CGD-O1D
14	b	1023	CLA	CHA-CBD-CGD-O2D
14	b	1201	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	b	1201	CLA	CHA-CBD-CGD-O2D
14	b	1202	CLA	CHA-CBD-CGD-O1D
14	b	1202	CLA	CHA-CBD-CGD-O2D
14	b	1203	CLA	CHA-CBD-CGD-O1D
14	b	1206	CLA	CHA-CBD-CGD-O1D
14	b	1206	CLA	CHA-CBD-CGD-O2D
14	b	1215	CLA	CHA-CBD-CGD-O1D
14	b	1215	CLA	CHA-CBD-CGD-O2D
14	b	1217	CLA	CHA-CBD-CGD-O1D
14	b	1217	CLA	CHA-CBD-CGD-O2D
14	b	1223	CLA	CHA-CBD-CGD-O2D
14	b	1225	CLA	CHA-CBD-CGD-O1D
14	b	1225	CLA	CHA-CBD-CGD-O2D
14	b	1235	CLA	CHA-CBD-CGD-O1D
14	b	1235	CLA	CHA-CBD-CGD-O2D
14	A	1102	CLA	CHA-CBD-CGD-O1D
14	A	1102	CLA	CHA-CBD-CGD-O2D
14	A	1112	CLA	CHA-CBD-CGD-O2D
14	A	1117	CLA	CHA-CBD-CGD-O1D
14	A	1117	CLA	CHA-CBD-CGD-O2D
14	A	1122	CLA	CHA-CBD-CGD-O2D
14	A	1127	CLA	CHA-CBD-CGD-O1D
14	A	1127	CLA	CHA-CBD-CGD-O2D
14	A	1129	CLA	CHA-CBD-CGD-O2D
14	A	1138	CLA	CHA-CBD-CGD-O2D
14	B	1022	CLA	CHA-CBD-CGD-O2D
14	B	1023	CLA	CHA-CBD-CGD-O1D
14	B	1023	CLA	CHA-CBD-CGD-O2D
14	B	1201	CLA	CHA-CBD-CGD-O1D
14	B	1201	CLA	CHA-CBD-CGD-O2D
14	B	1202	CLA	CHA-CBD-CGD-O1D
14	B	1202	CLA	CHA-CBD-CGD-O2D
14	B	1203	CLA	CHA-CBD-CGD-O1D
14	B	1206	CLA	CHA-CBD-CGD-O1D
14	B	1206	CLA	CHA-CBD-CGD-O2D
14	B	1215	CLA	CHA-CBD-CGD-O1D
14	B	1215	CLA	CHA-CBD-CGD-O2D
14	B	1217	CLA	CHA-CBD-CGD-O1D
14	B	1217	CLA	CHA-CBD-CGD-O2D
14	B	1223	CLA	CHA-CBD-CGD-O2D
14	B	1225	CLA	CHA-CBD-CGD-O1D
14	B	1225	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	B	1235	CLA	CHA-CBD-CGD-O1D
14	B	1235	CLA	CHA-CBD-CGD-O2D
15	H	1230	F6C	CHA-CBD-CGD-O1D
15	H	1230	F6C	CHA-CBD-CGD-O2D
15	b	1230	F6C	CHA-CBD-CGD-O1D
15	b	1230	F6C	CHA-CBD-CGD-O2D
15	B	1230	F6C	CHA-CBD-CGD-O1D
15	B	1230	F6C	CHA-CBD-CGD-O2D
14	G	1126	CLA	CAA-CBA-CGA-O2A
14	a	1126	CLA	CAA-CBA-CGA-O2A
14	A	1126	CLA	CAA-CBA-CGA-O2A
18	H	4010	BCR	C16-C17-C18-C19
18	b	4010	BCR	C16-C17-C18-C19
18	B	4010	BCR	C16-C17-C18-C19
14	G	1110	CLA	CAA-CBA-CGA-O2A
14	a	1110	CLA	CAA-CBA-CGA-O2A
14	A	1110	CLA	CAA-CBA-CGA-O2A
14	b	1204	CLA	CAA-CBA-CGA-O2A
14	H	1204	CLA	CAA-CBA-CGA-O2A
14	B	1204	CLA	CAA-CBA-CGA-O2A
20	l	5007	LMG	O8-C28-C29-C30
20	L	5007	LMG	O8-C28-C29-C30
14	b	1218	CLA	CAA-CBA-CGA-O2A
14	B	1218	CLA	CAA-CBA-CGA-O2A
14	G	1140	CLA	CAA-CBA-CGA-O1A
14	a	1140	CLA	CAA-CBA-CGA-O1A
14	A	1140	CLA	CAA-CBA-CGA-O1A
20	U	5007	LMG	O8-C28-C29-C30
14	G	1013	CLA	C11-C10-C8-C7
14	G	1131	CLA	C2-C3-C5-C6
14	U	1502	CLA	C2-C3-C5-C6
14	a	1013	CLA	C11-C10-C8-C7
14	a	1131	CLA	C2-C3-C5-C6
14	a	1138	CLA	C6-C7-C8-C10
14	l	1502	CLA	C2-C3-C5-C6
14	A	1013	CLA	C11-C10-C8-C7
14	A	1131	CLA	C2-C3-C5-C6
14	L	1502	CLA	C2-C3-C5-C6
14	H	1222	CLA	C16-C17-C18-C19
14	W	1701	CLA	CAA-CBA-CGA-O2A
14	x	1701	CLA	CAA-CBA-CGA-O2A
14	X	1701	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	G	1134	CLA	CAA-CBA-CGA-O1A
14	H	1218	CLA	CAA-CBA-CGA-O2A
14	a	1134	CLA	CAA-CBA-CGA-O1A
14	G	1126	CLA	C3-C5-C6-C7
14	A	1126	CLA	C3-C5-C6-C7
14	H	1211	CLA	C11-C10-C8-C9
14	H	1222	CLA	C11-C12-C13-C14
14	b	1211	CLA	C11-C10-C8-C9
14	b	1222	CLA	C11-C12-C13-C14
14	B	1211	CLA	C11-C10-C8-C9
14	B	1222	CLA	C11-C12-C13-C14
18	G	4001	BCR	C19-C20-C21-C22
18	a	4001	BCR	C19-C20-C21-C22
18	A	4001	BCR	C19-C20-C21-C22
13	G	1011	CL0	C15-C16-C17-C18
13	a	1011	CL0	C15-C16-C17-C18
13	A	1011	CL0	C15-C16-C17-C18
21	G	6001	LMT	O5B-C1B-O1B-C4'
14	H	1210	CLA	C13-C15-C16-C17
14	B	1210	CLA	C13-C15-C16-C17
14	b	1222	CLA	C16-C17-C18-C19
14	B	1222	CLA	C16-C17-C18-C19
14	a	1126	CLA	C3-C5-C6-C7
14	b	1210	CLA	C13-C15-C16-C17
14	H	1233	CLA	CAA-CBA-CGA-O2A
14	A	1134	CLA	CAA-CBA-CGA-O1A
14	B	1233	CLA	CAA-CBA-CGA-O2A
14	H	1215	CLA	C2A-CAA-CBA-CGA
14	b	1215	CLA	C2A-CAA-CBA-CGA
14	B	1215	CLA	C2A-CAA-CBA-CGA
21	a	6001	LMT	O5B-C1B-O1B-C4'
14	b	1233	CLA	CAA-CBA-CGA-O2A
18	H	4006	BCR	C7-C8-C9-C34
18	b	4006	BCR	C7-C8-C9-C34
21	A	6001	LMT	O5B-C1B-O1B-C4'
18	V	4021	BCR	C21-C22-C23-C24
18	M	4021	BCR	C21-C22-C23-C24
13	G	1011	CL0	C1A-C2A-CAA-CBA
13	a	1011	CL0	C1A-C2A-CAA-CBA
13	A	1011	CL0	C1A-C2A-CAA-CBA
14	G	1012	CLA	C1A-C2A-CAA-CBA
14	H	1022	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	H	1219	CLA	C1A-C2A-CAA-CBA
14	H	1222	CLA	C1A-C2A-CAA-CBA
14	H	1223	CLA	C1A-C2A-CAA-CBA
14	W	1701	CLA	C1A-C2A-CAA-CBA
14	a	1012	CLA	C1A-C2A-CAA-CBA
14	b	1022	CLA	C1A-C2A-CAA-CBA
14	b	1219	CLA	C1A-C2A-CAA-CBA
14	b	1222	CLA	C1A-C2A-CAA-CBA
14	b	1223	CLA	C1A-C2A-CAA-CBA
14	x	1701	CLA	C1A-C2A-CAA-CBA
14	A	1012	CLA	C1A-C2A-CAA-CBA
14	B	1022	CLA	C1A-C2A-CAA-CBA
14	B	1219	CLA	C1A-C2A-CAA-CBA
14	B	1222	CLA	C1A-C2A-CAA-CBA
14	B	1223	CLA	C1A-C2A-CAA-CBA
14	X	1701	CLA	C1A-C2A-CAA-CBA
14	a	1110	CLA	CAA-CBA-CGA-O1A
14	A	1110	CLA	CAA-CBA-CGA-O1A
15	b	1230	F6C	CAA-CBA-CGA-O2A
20	l	5007	LMG	C28-C29-C30-C31
14	G	1126	CLA	CAA-CBA-CGA-O1A
14	a	1126	CLA	CAA-CBA-CGA-O1A
14	A	1126	CLA	CAA-CBA-CGA-O1A
14	B	1235	CLA	CAA-CBA-CGA-O1A
14	G	1110	CLA	CAA-CBA-CGA-O1A
15	H	1230	F6C	CAA-CBA-CGA-O2A
15	B	1230	F6C	CAA-CBA-CGA-O2A
14	U	1501	CLA	C2A-CAA-CBA-CGA
14	l	1501	CLA	C2A-CAA-CBA-CGA
14	L	1501	CLA	C2A-CAA-CBA-CGA
20	U	5007	LMG	C28-C29-C30-C31
20	L	5007	LMG	C28-C29-C30-C31
14	H	1235	CLA	CAA-CBA-CGA-O1A
14	b	1235	CLA	CAA-CBA-CGA-O1A
14	W	1701	CLA	CAA-CBA-CGA-O1A
14	X	1701	CLA	CAA-CBA-CGA-O1A
19	G	5001	LHG	O9-C7-C8-C9
19	a	5001	LHG	O9-C7-C8-C9
19	A	5001	LHG	O9-C7-C8-C9
19	H	5004	LHG	C3-O3-P-O5
19	b	5004	LHG	C3-O3-P-O5
19	B	5004	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
14	G	1116	CLA	CAA-CBA-CGA-O1A
14	G	1138	CLA	CAA-CBA-CGA-O1A
14	a	1116	CLA	CAA-CBA-CGA-O1A
14	a	1138	CLA	CAA-CBA-CGA-O1A
14	x	1701	CLA	CAA-CBA-CGA-O1A
14	A	1116	CLA	CAA-CBA-CGA-O1A
14	A	1138	CLA	CAA-CBA-CGA-O1A
20	U	5007	LMG	O10-C28-C29-C30
14	a	1116	CLA	C3-C5-C6-C7
18	H	4016	BCR	C23-C24-C25-C26
18	b	4005	BCR	C1-C6-C7-C8
18	b	4016	BCR	C23-C24-C25-C26
18	B	4016	BCR	C23-C24-C25-C26
14	H	1221	CLA	CAA-CBA-CGA-O2A
19	H	5004	LHG	O7-C7-C8-C9
19	b	5004	LHG	O7-C7-C8-C9
19	B	5004	LHG	O7-C7-C8-C9
14	G	1013	CLA	C2A-CAA-CBA-CGA
14	a	1013	CLA	C2A-CAA-CBA-CGA
14	A	1013	CLA	C2A-CAA-CBA-CGA
20	l	5007	LMG	O10-C28-C29-C30
20	L	5007	LMG	O10-C28-C29-C30
14	H	1218	CLA	CAA-CBA-CGA-O1A
14	b	1218	CLA	CAA-CBA-CGA-O1A
14	B	1218	CLA	CAA-CBA-CGA-O1A
15	H	1207	F6C	CAA-CBA-CGA-O2A
15	b	1207	F6C	CAA-CBA-CGA-O2A
15	B	1207	F6C	CAA-CBA-CGA-O2A
14	b	1222	CLA	C8-C10-C11-C12
14	b	1239	CLA	CAA-CBA-CGA-O1A
14	B	1239	CLA	CAA-CBA-CGA-O1A
19	H	5004	LHG	C8-C7-O7-C5
14	G	1116	CLA	C3-C5-C6-C7
14	H	1215	CLA	CAD-CBD-CGD-O1D
14	A	1116	CLA	C3-C5-C6-C7
14	H	1239	CLA	CAA-CBA-CGA-O1A
14	H	1222	CLA	C8-C10-C11-C12
14	B	1222	CLA	C8-C10-C11-C12
14	H	1210	CLA	C11-C10-C8-C9
14	b	1210	CLA	C11-C10-C8-C9
14	B	1210	CLA	C11-C10-C8-C9
14	b	1221	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	B	1221	CLA	CAA-CBA-CGA-O2A
20	U	5007	LMG	O7-C10-C11-C12
20	l	5007	LMG	O7-C10-C11-C12
20	L	5007	LMG	O7-C10-C11-C12
15	H	1238	F6C	C5-C6-C7-C8
15	b	1238	F6C	C5-C6-C7-C8
15	B	1238	F6C	C5-C6-C7-C8
20	H	5002	LMG	C29-C30-C31-C32
20	B	5002	LMG	C29-C30-C31-C32
14	H	1211	CLA	CAA-CBA-CGA-O2A
14	H	1224	CLA	CAA-CBA-CGA-O2A
14	b	1211	CLA	CAA-CBA-CGA-O2A
14	b	1224	CLA	CAA-CBA-CGA-O2A
14	l	1502	CLA	CAA-CBA-CGA-O2A
14	B	1211	CLA	CAA-CBA-CGA-O2A
14	B	1224	CLA	CAA-CBA-CGA-O2A
14	L	1502	CLA	CAA-CBA-CGA-O2A
20	b	5002	LMG	O7-C10-C11-C12
20	B	5002	LMG	O7-C10-C11-C12
14	G	1103	CLA	C3-C5-C6-C7
14	a	1103	CLA	C3-C5-C6-C7
20	b	5002	LMG	C29-C30-C31-C32
14	a	1118	CLA	C4-C3-C5-C6
14	A	1118	CLA	C4-C3-C5-C6
14	G	1133	CLA	C11-C10-C8-C7
14	H	1213	CLA	C12-C13-C15-C16
14	H	1217	CLA	C2-C3-C5-C6
14	H	1222	CLA	C11-C12-C13-C15
14	H	1226	CLA	C6-C7-C8-C10
14	H	1228	CLA	C3A-C2A-CAA-CBA
14	a	1133	CLA	C11-C10-C8-C7
14	b	1213	CLA	C12-C13-C15-C16
14	b	1217	CLA	C2-C3-C5-C6
14	b	1222	CLA	C11-C12-C13-C15
14	b	1226	CLA	C6-C7-C8-C10
14	b	1228	CLA	C3A-C2A-CAA-CBA
14	A	1133	CLA	C11-C10-C8-C7
14	B	1213	CLA	C12-C13-C15-C16
14	B	1217	CLA	C2-C3-C5-C6
14	B	1222	CLA	C11-C12-C13-C15
14	B	1226	CLA	C6-C7-C8-C10
14	B	1228	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	H	1204	CLA	CAA-CBA-CGA-O1A
14	b	1204	CLA	CAA-CBA-CGA-O1A
20	L	5007	LMG	O9-C10-C11-C12
14	U	1502	CLA	CAA-CBA-CGA-O2A
14	a	1122	CLA	CAA-CBA-CGA-O2A
14	b	1210	CLA	CAA-CBA-CGA-O2A
14	A	1122	CLA	CAA-CBA-CGA-O2A
20	H	5002	LMG	O7-C10-C11-C12
21	a	6001	LMT	C4B-C5B-C6B-O6B
14	A	1103	CLA	C3-C5-C6-C7
14	A	1103	CLA	O1A-CGA-O2A-C1
18	H	4017	BCR	C11-C12-C13-C14
18	b	4017	BCR	C11-C12-C13-C14
18	B	4017	BCR	C11-C12-C13-C14
14	G	1122	CLA	CAA-CBA-CGA-O1A
14	H	1211	CLA	CAA-CBA-CGA-O1A
14	a	1122	CLA	CAA-CBA-CGA-O1A
14	b	1211	CLA	CAA-CBA-CGA-O1A
14	A	1122	CLA	CAA-CBA-CGA-O1A
14	B	1204	CLA	CAA-CBA-CGA-O1A
14	B	1211	CLA	CAA-CBA-CGA-O1A
20	U	5007	LMG	O9-C10-C11-C12
18	H	4009	BCR	C19-C20-C21-C22
18	b	4009	BCR	C19-C20-C21-C22
18	B	4009	BCR	C19-C20-C21-C22
13	a	1011	CL0	CAA-CBA-CGA-O2A
13	A	1011	CL0	CAA-CBA-CGA-O2A
14	G	1122	CLA	CAA-CBA-CGA-O2A
14	H	1210	CLA	CAA-CBA-CGA-O2A
14	B	1210	CLA	CAA-CBA-CGA-O2A
21	A	6001	LMT	C4B-C5B-C6B-O6B
14	a	1103	CLA	O1A-CGA-O2A-C1
20	l	5007	LMG	O9-C10-C11-C12
21	G	6001	LMT	C4B-C5B-C6B-O6B
14	G	1105	CLA	CAA-CBA-CGA-O2A
14	G	1113	CLA	CAA-CBA-CGA-O2A
14	a	1105	CLA	CAA-CBA-CGA-O2A
14	a	1113	CLA	CAA-CBA-CGA-O2A
14	A	1105	CLA	CAA-CBA-CGA-O2A
14	A	1113	CLA	CAA-CBA-CGA-O2A
19	b	5004	LHG	C8-C7-O7-C5
14	a	1114	CLA	C2C-C3C-CAC-CBC

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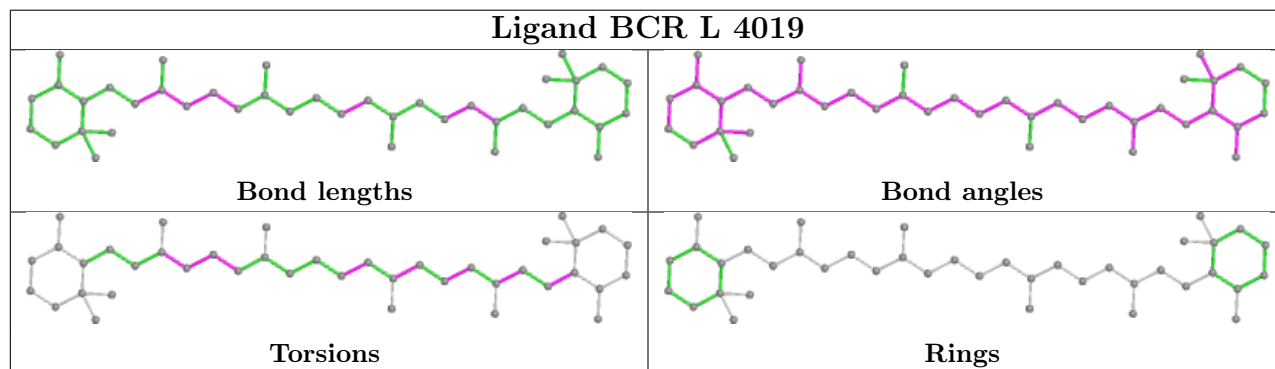
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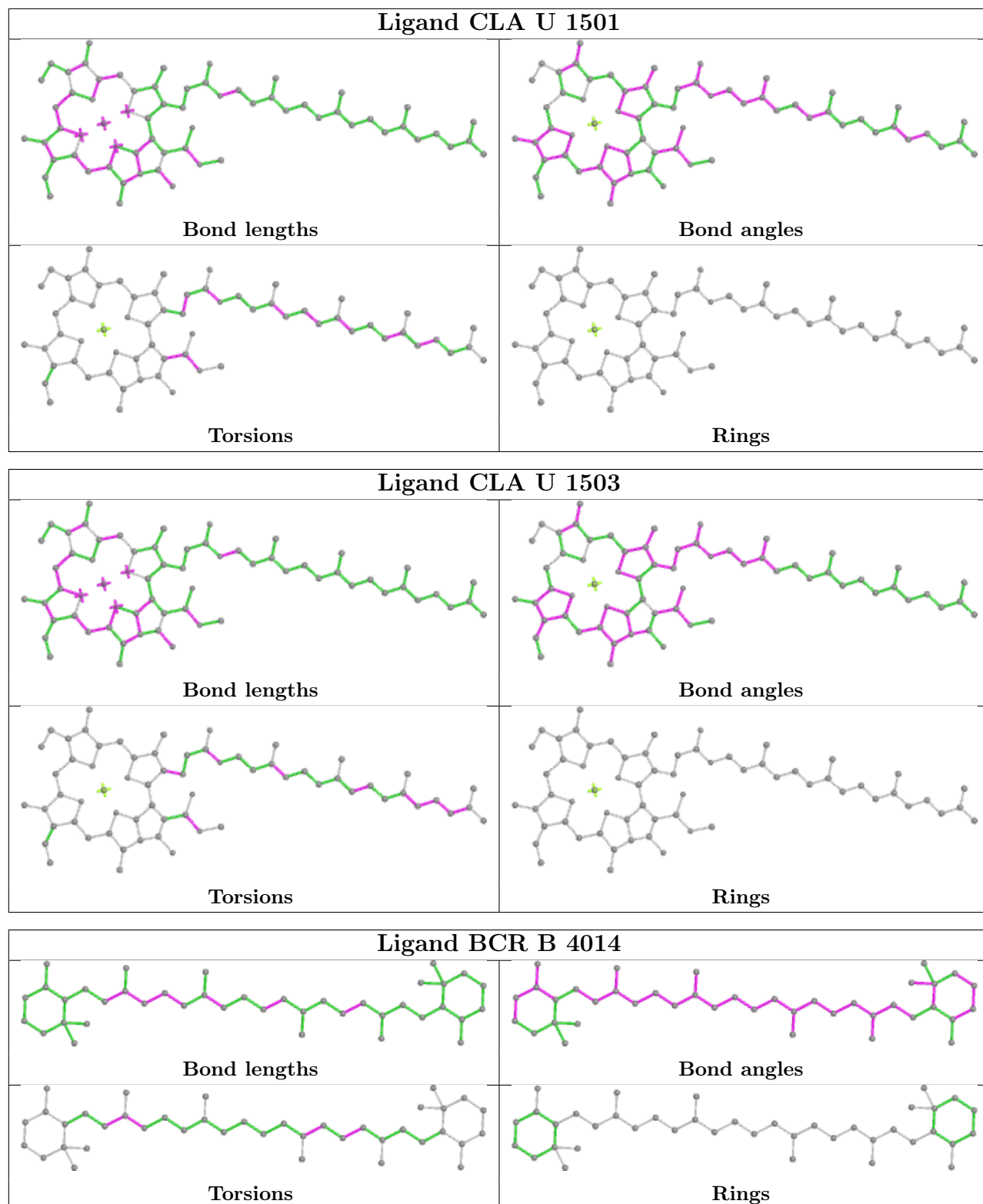
Mol	Chain	Res	Type	Atoms
13	G	1011	CL0	CAA-CBA-CGA-O2A
14	H	1226	CLA	CAA-CBA-CGA-O2A
14	b	1226	CLA	CAA-CBA-CGA-O2A
19	B	5004	LHG	O9-C7-C8-C9
20	H	5002	LMG	O9-C10-C11-C12
14	G	1103	CLA	O1A-CGA-O2A-C1
14	H	1205	CLA	C13-C15-C16-C17
14	b	1205	CLA	C13-C15-C16-C17
14	B	1205	CLA	C13-C15-C16-C17
14	G	1114	CLA	C2C-C3C-CAC-CBC
14	A	1114	CLA	C2C-C3C-CAC-CBC
14	U	1502	CLA	CAA-CBA-CGA-O1A
14	l	1502	CLA	CAA-CBA-CGA-O1A
14	L	1502	CLA	CAA-CBA-CGA-O1A
20	b	5002	LMG	O9-C10-C11-C12
20	B	5002	LMG	O9-C10-C11-C12
14	G	1118	CLA	C4-C3-C5-C6
14	B	1226	CLA	CAA-CBA-CGA-O2A

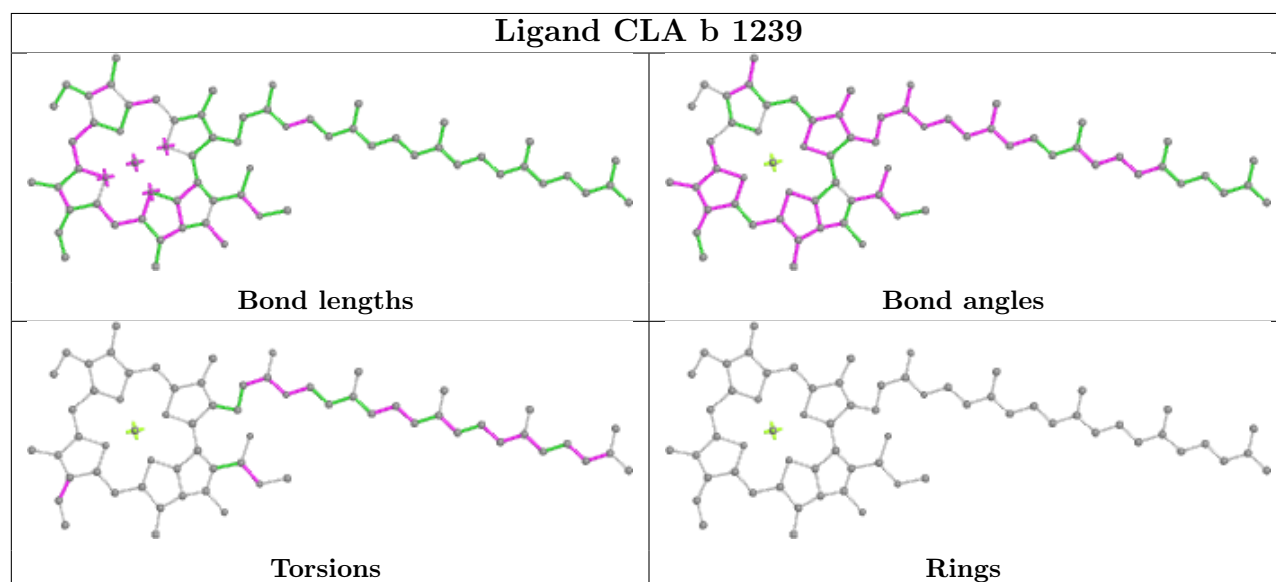
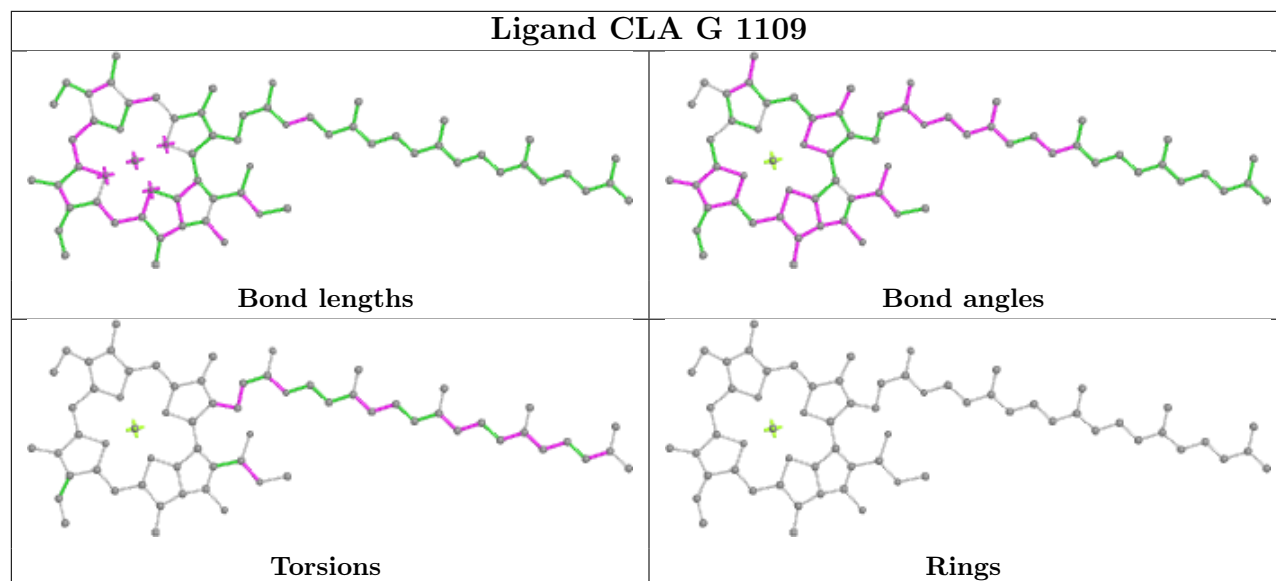
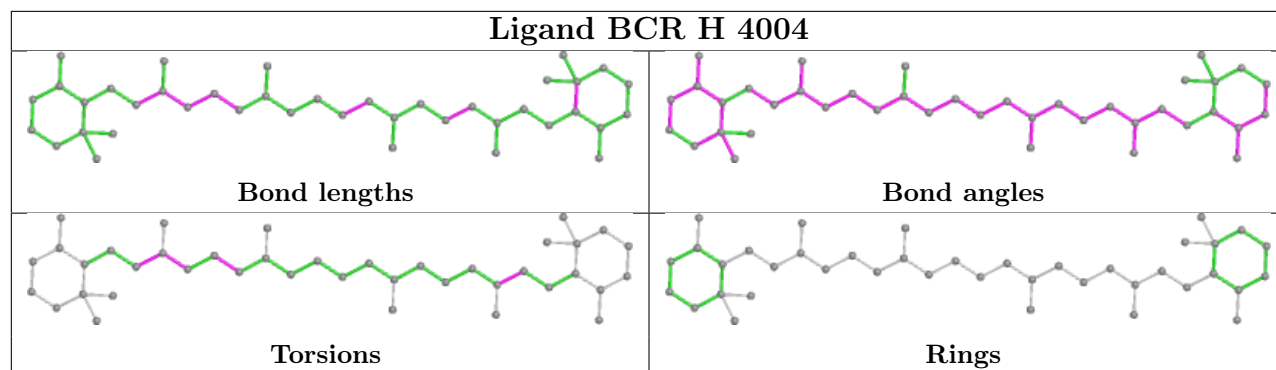
There are no ring outliers.

No monomer is involved in short contacts.

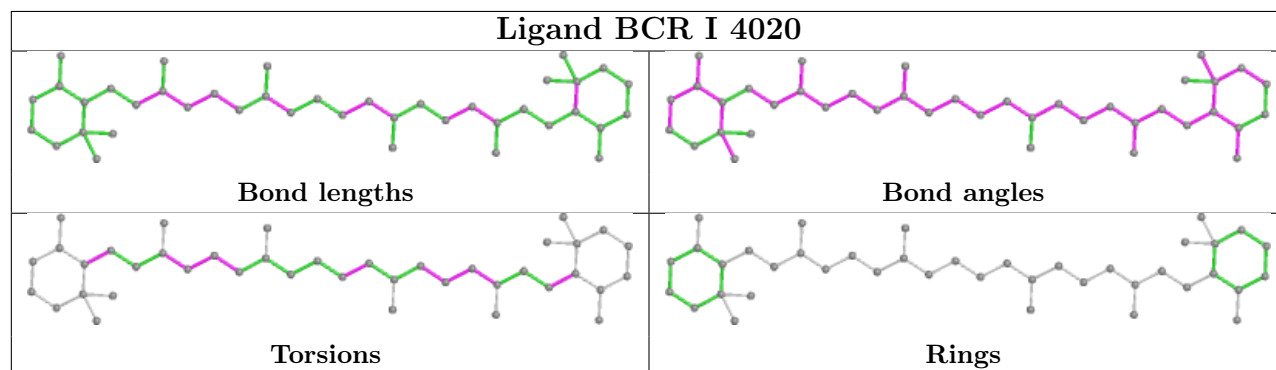
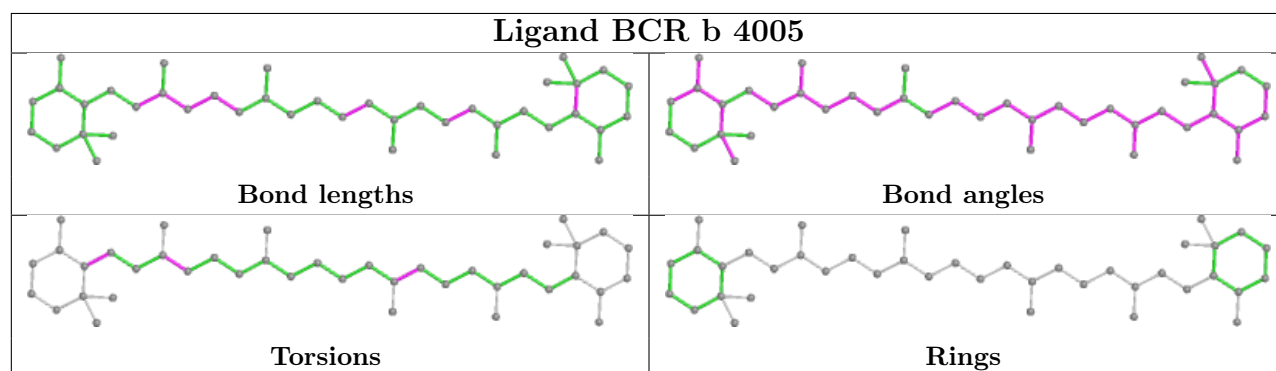
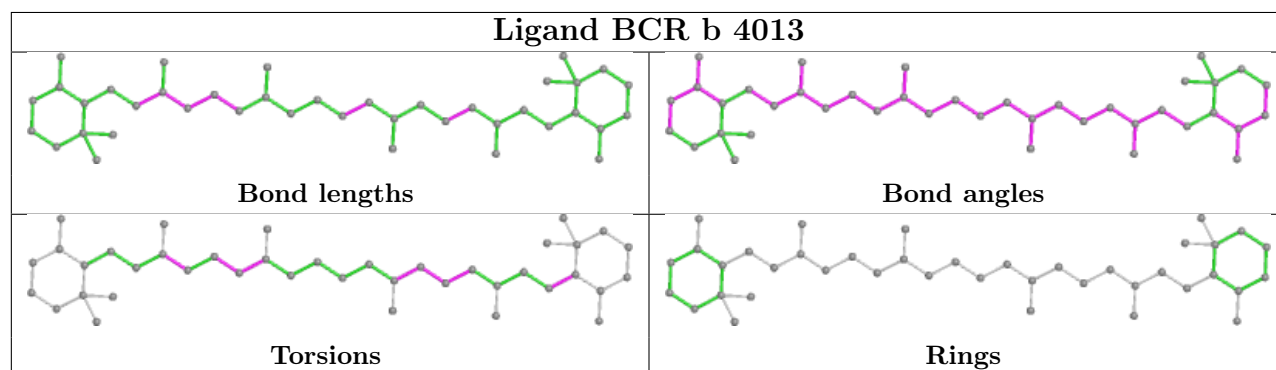
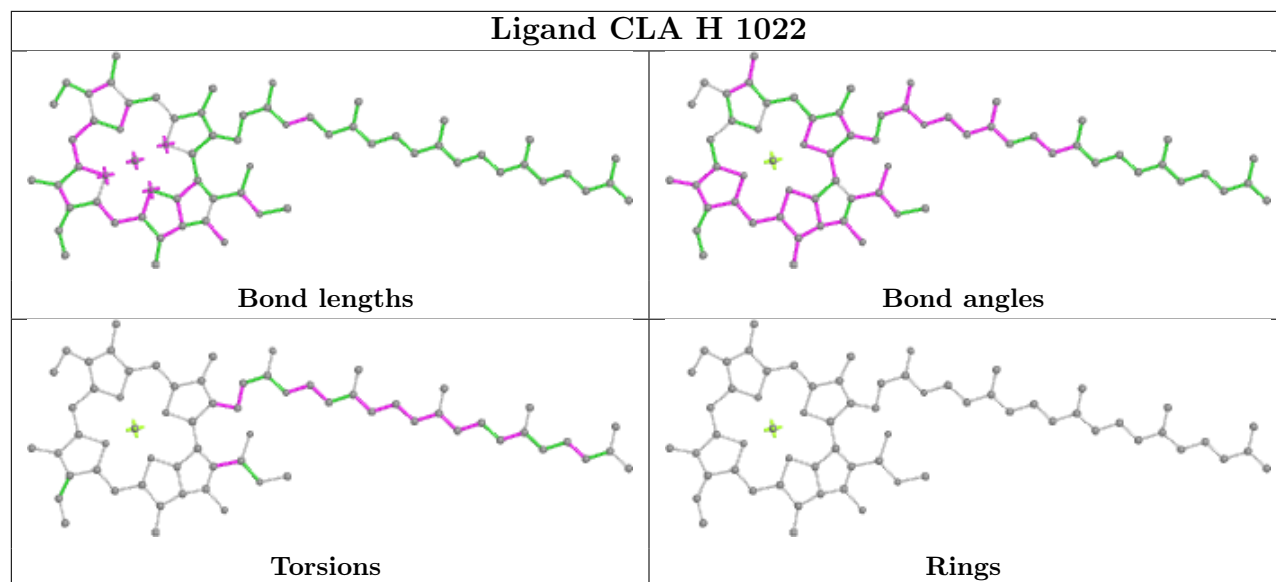
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

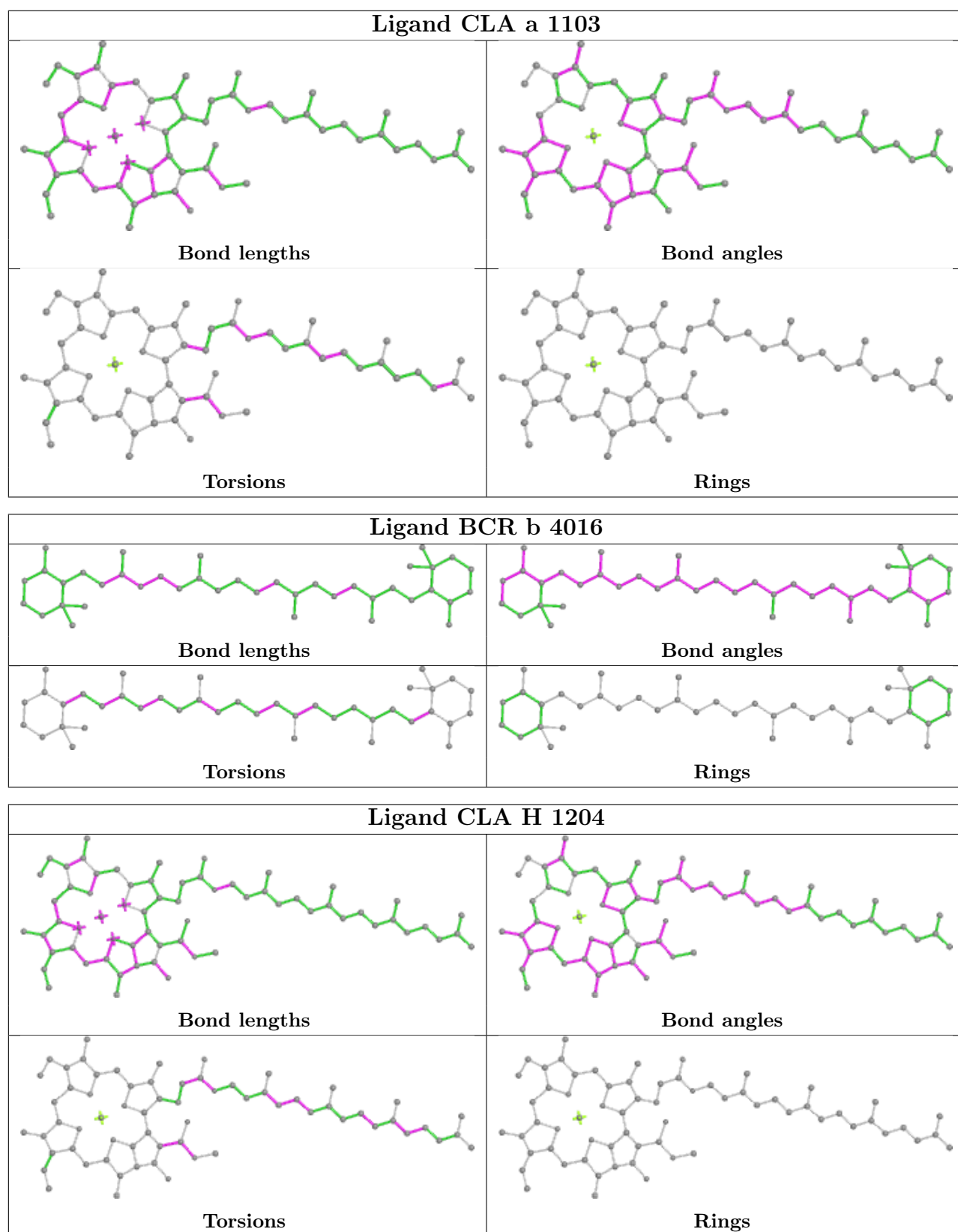


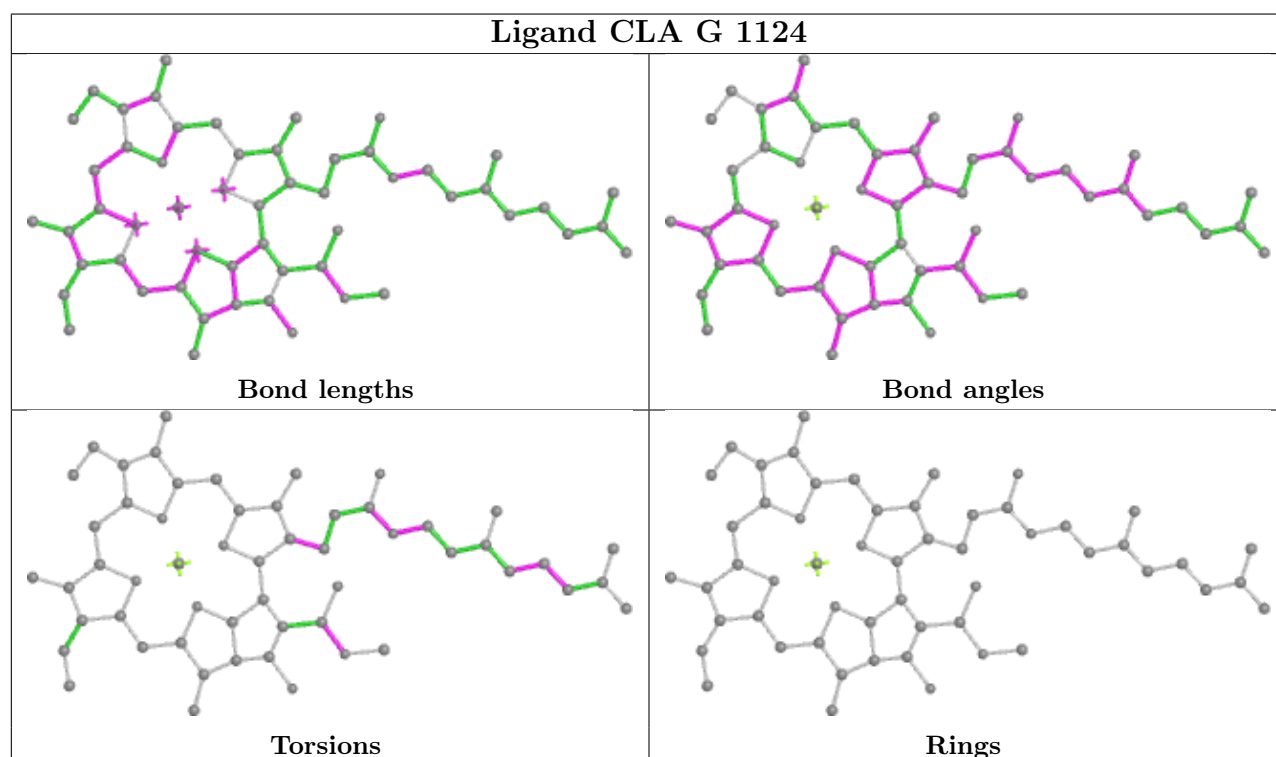
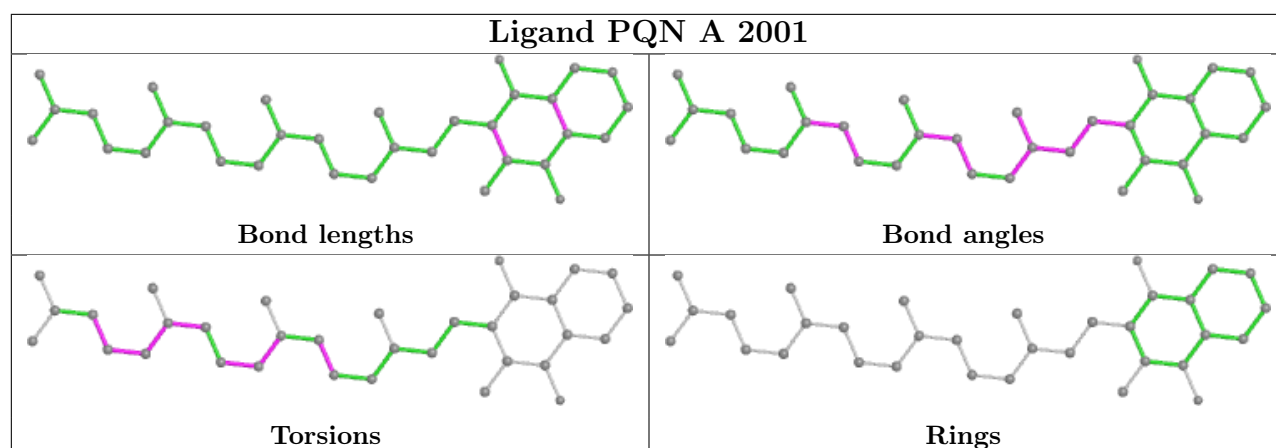


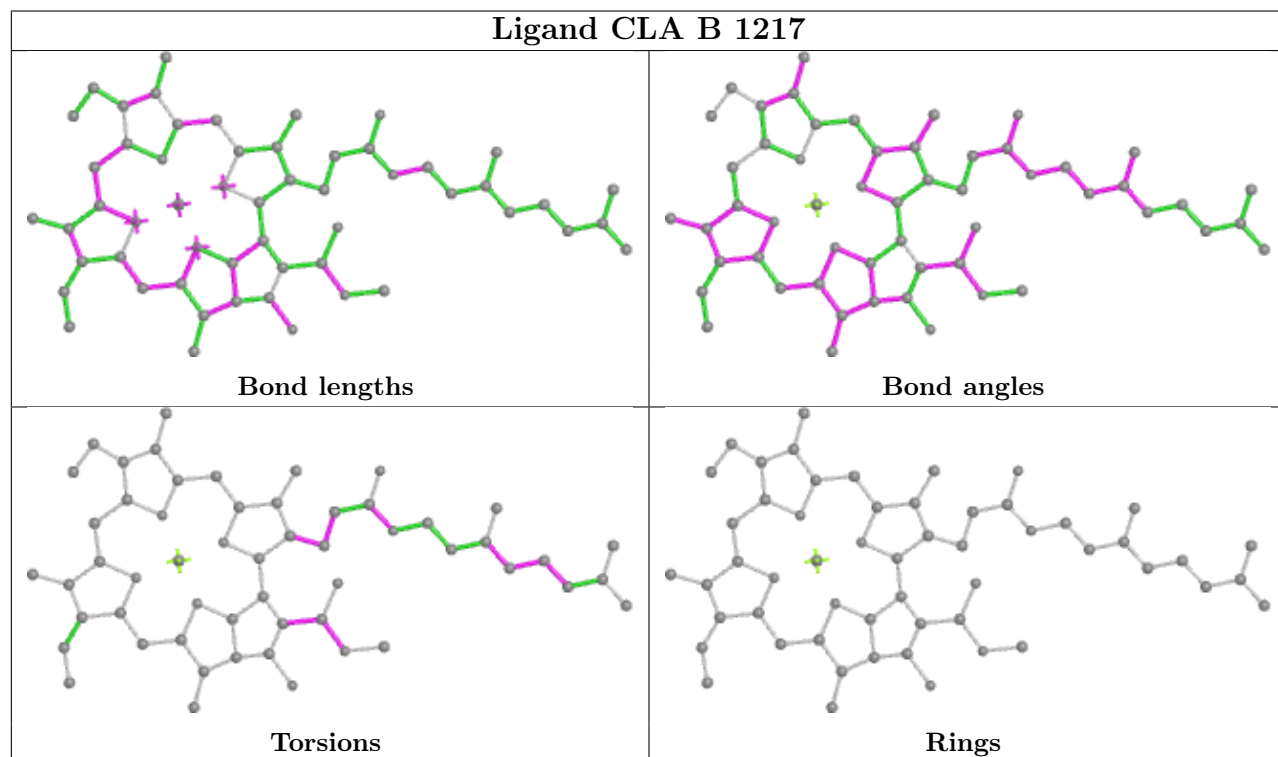
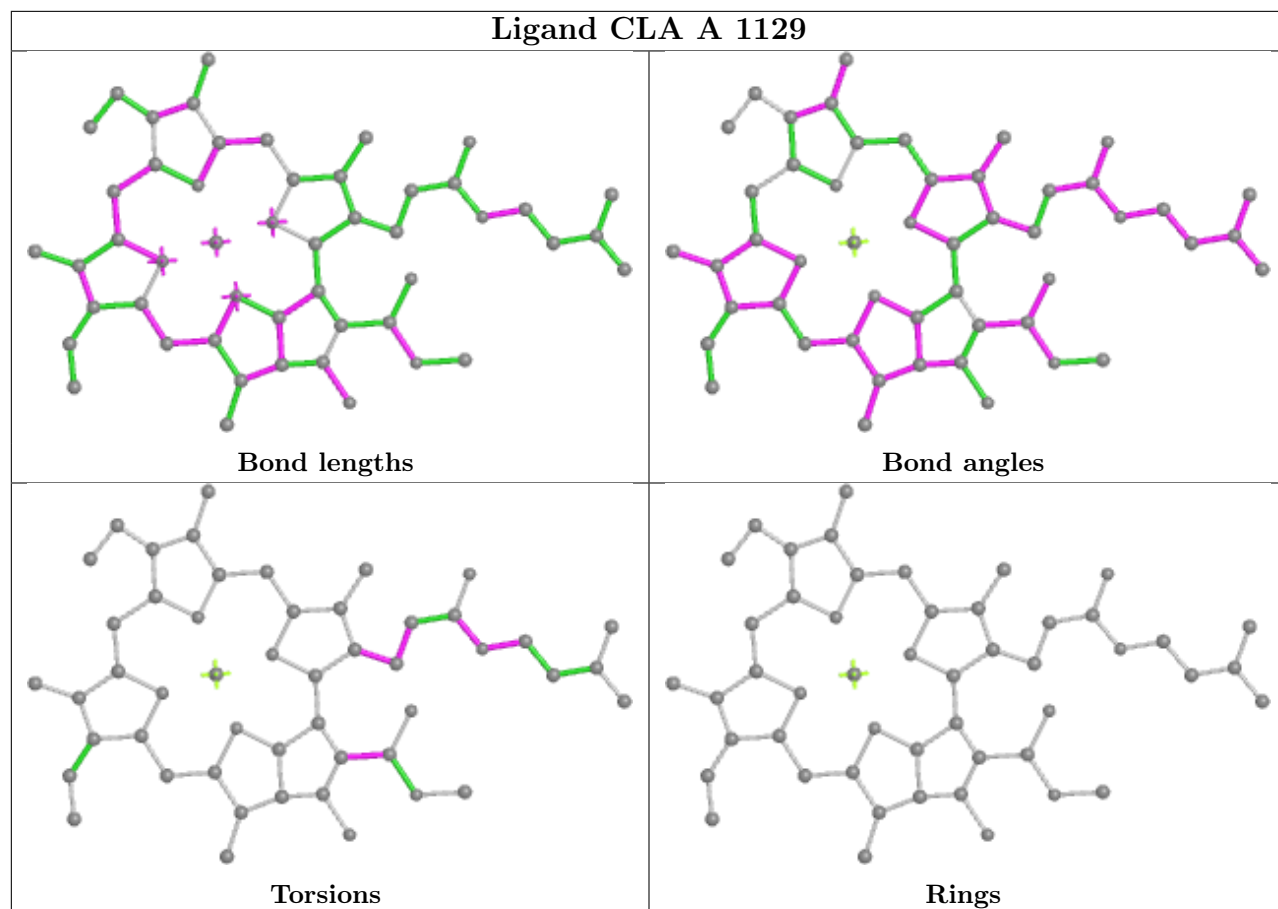


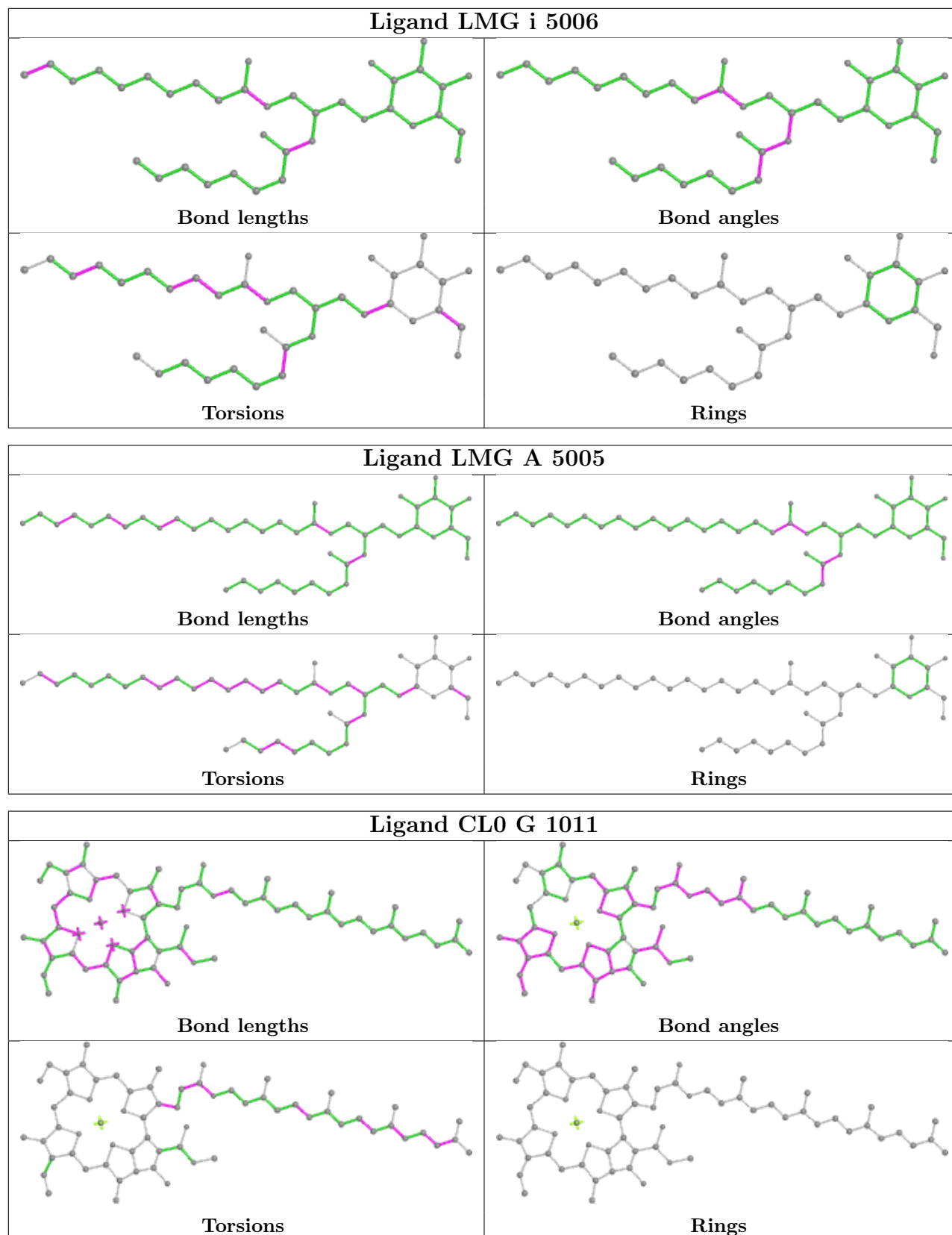


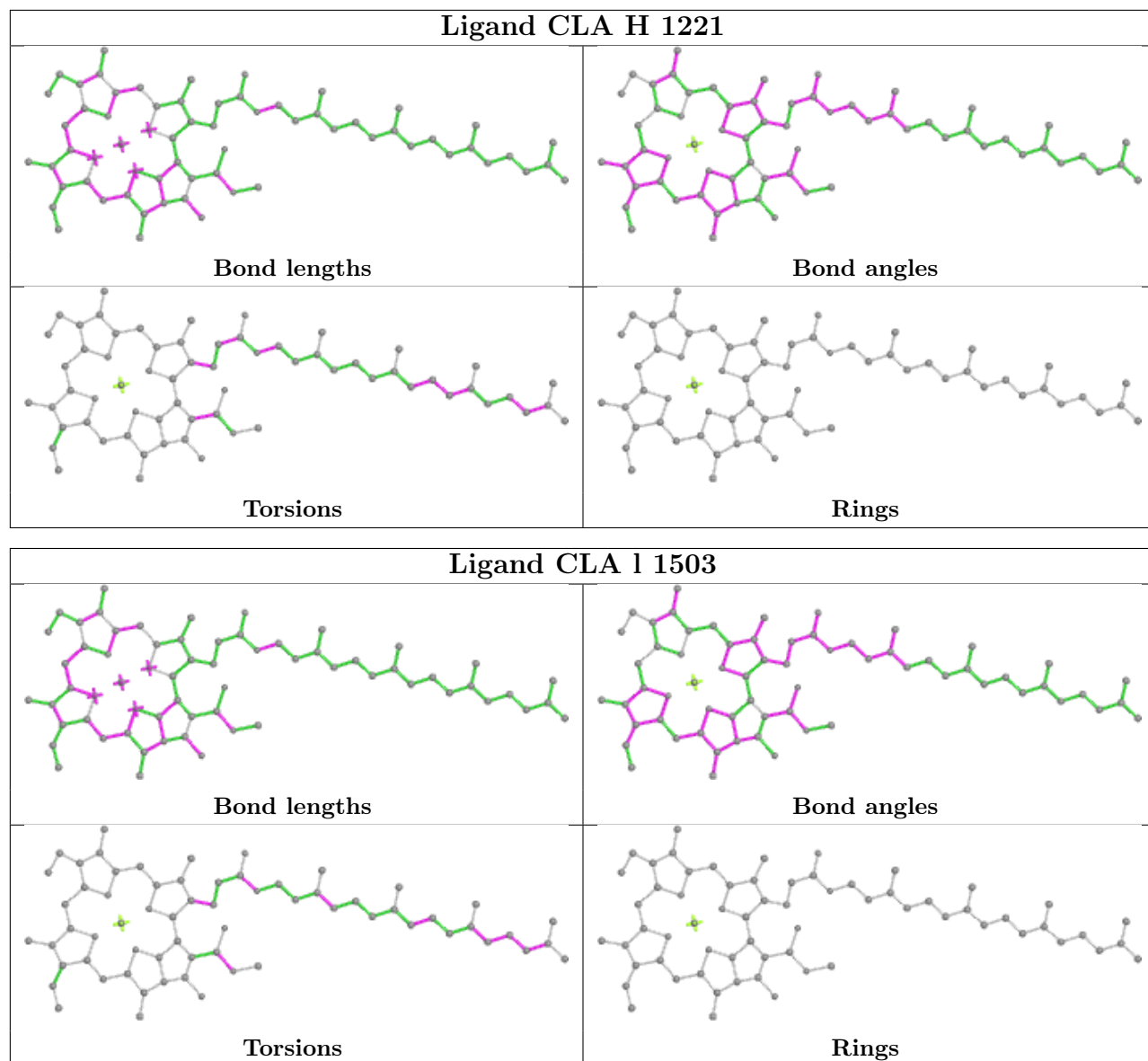


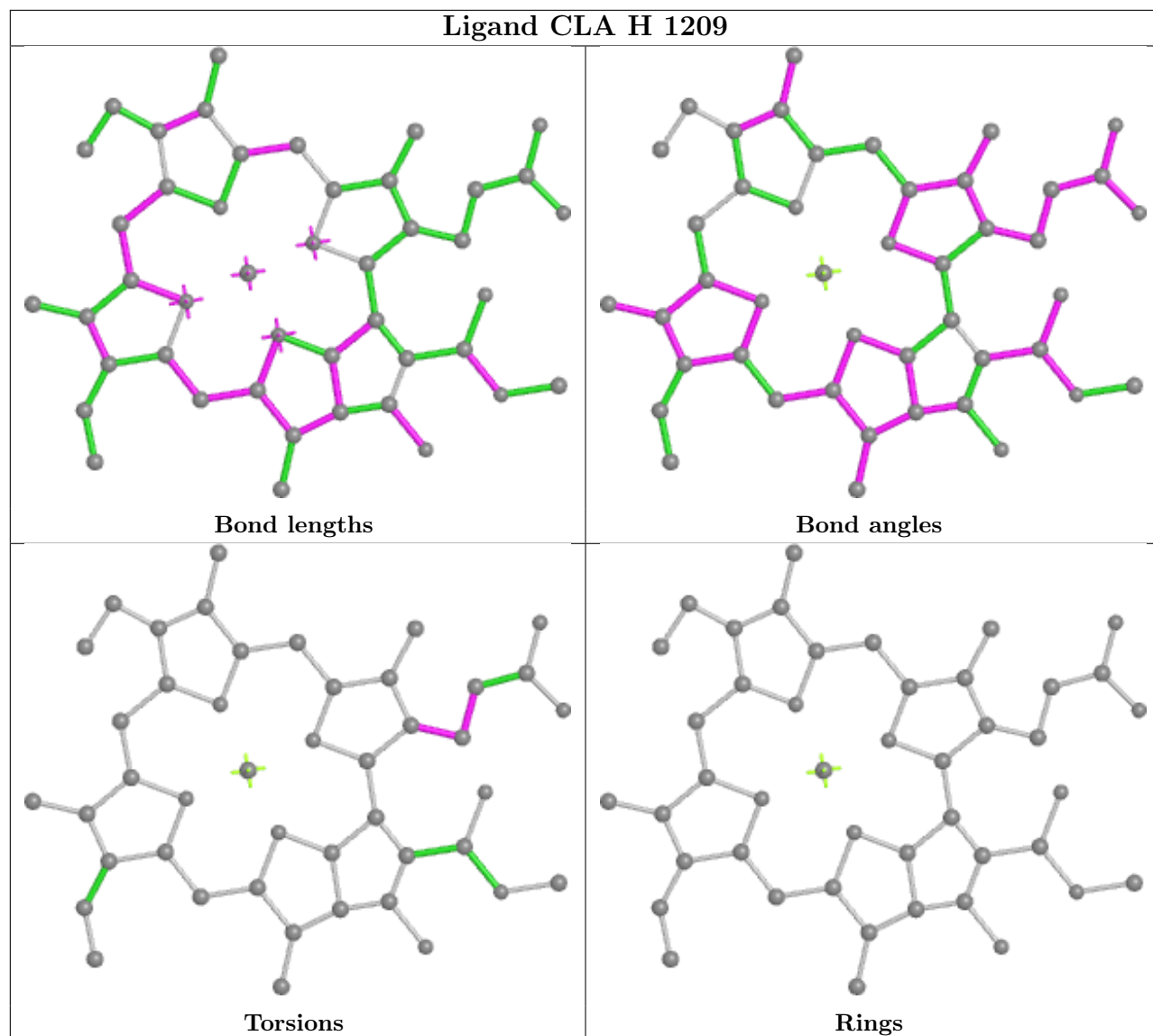


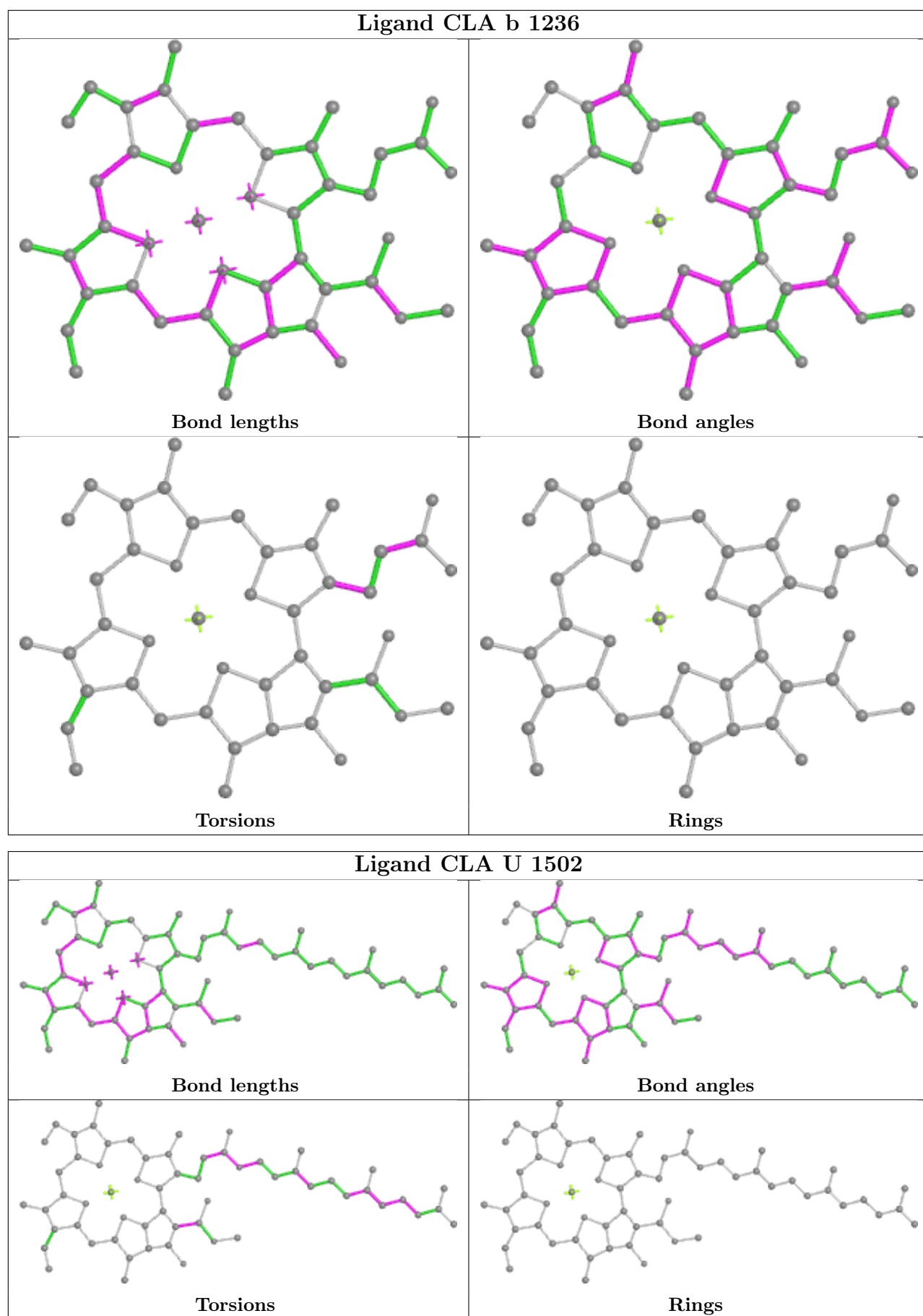




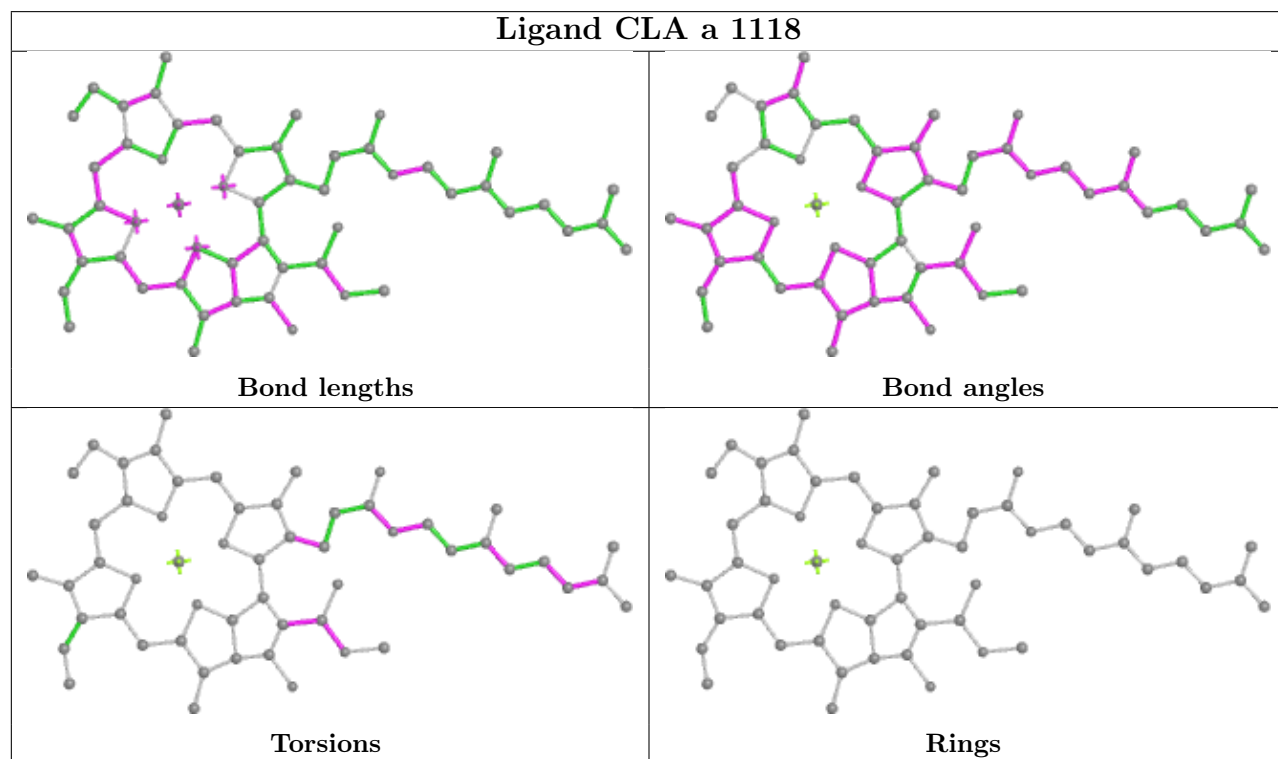
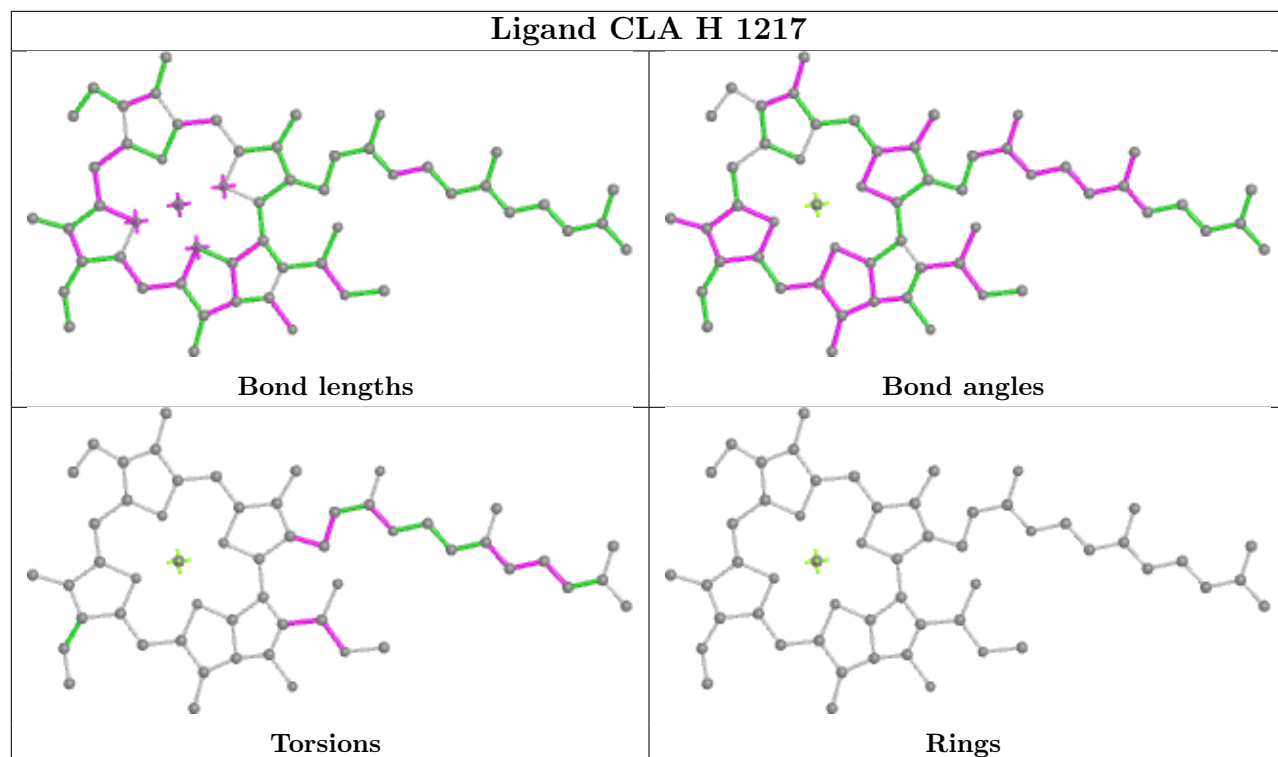


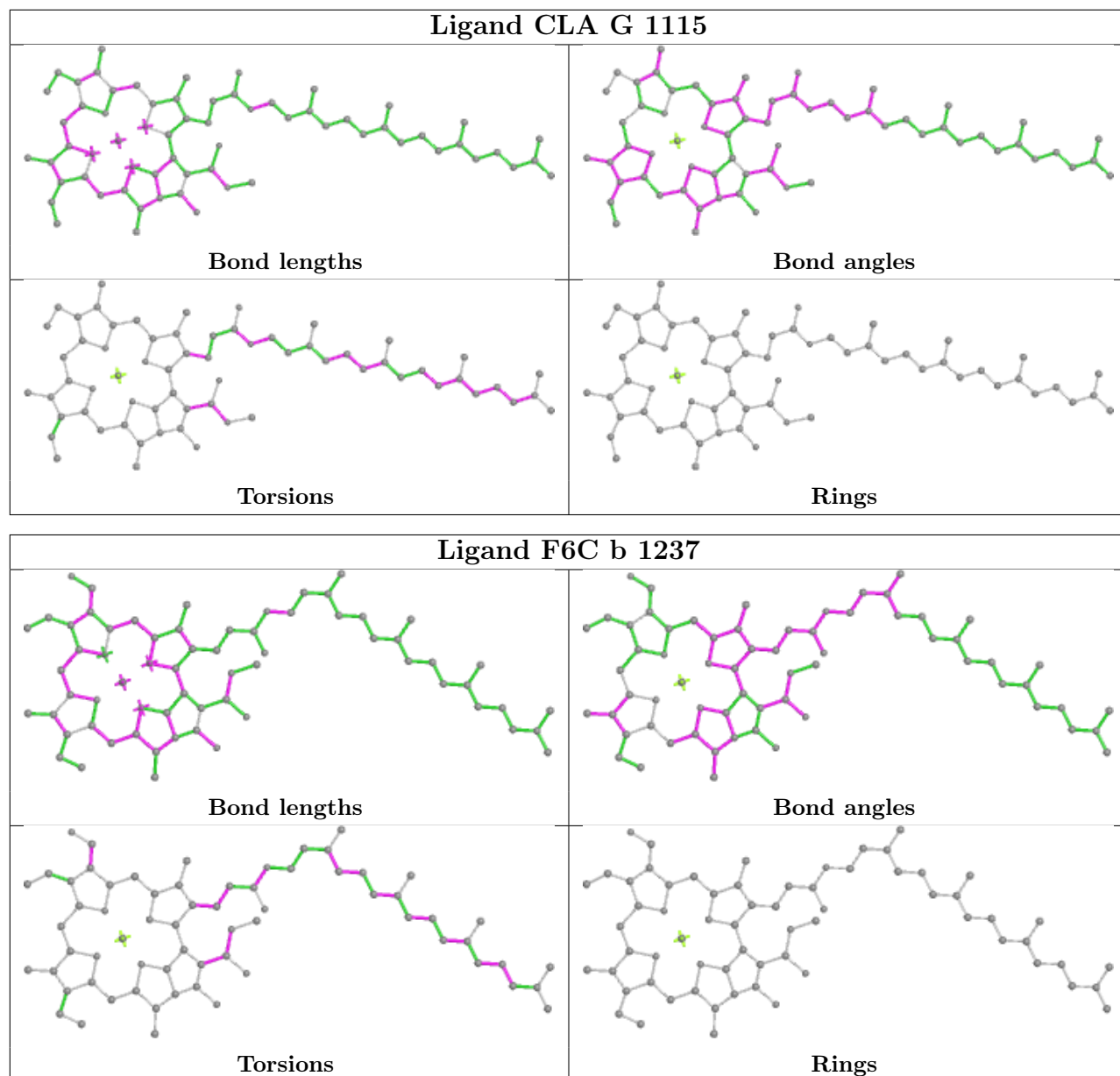


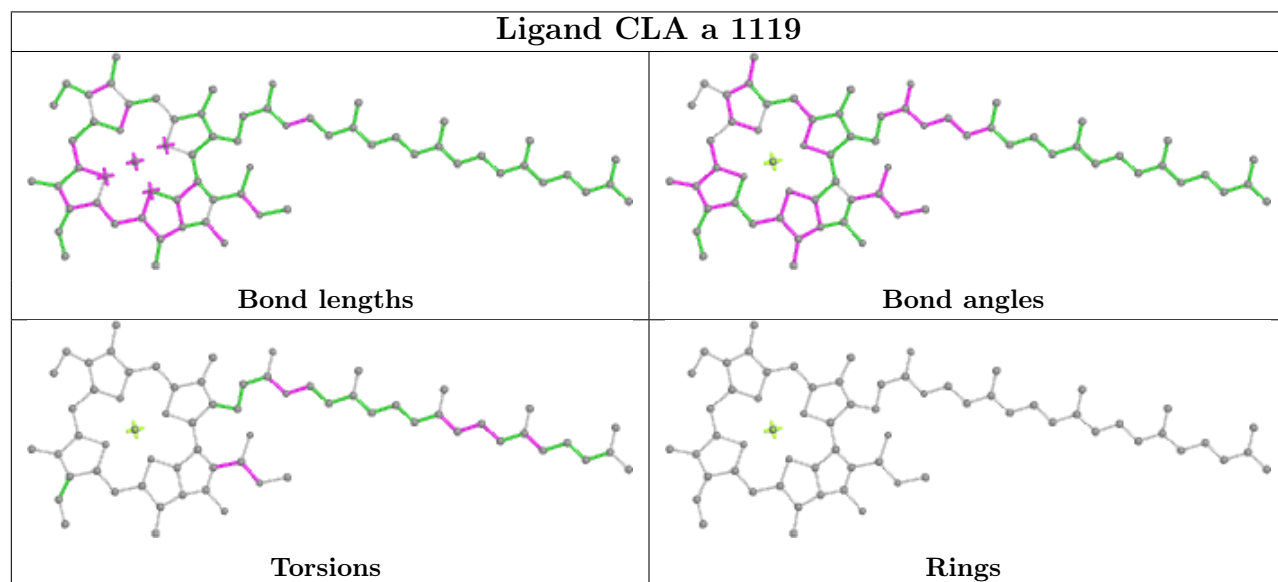
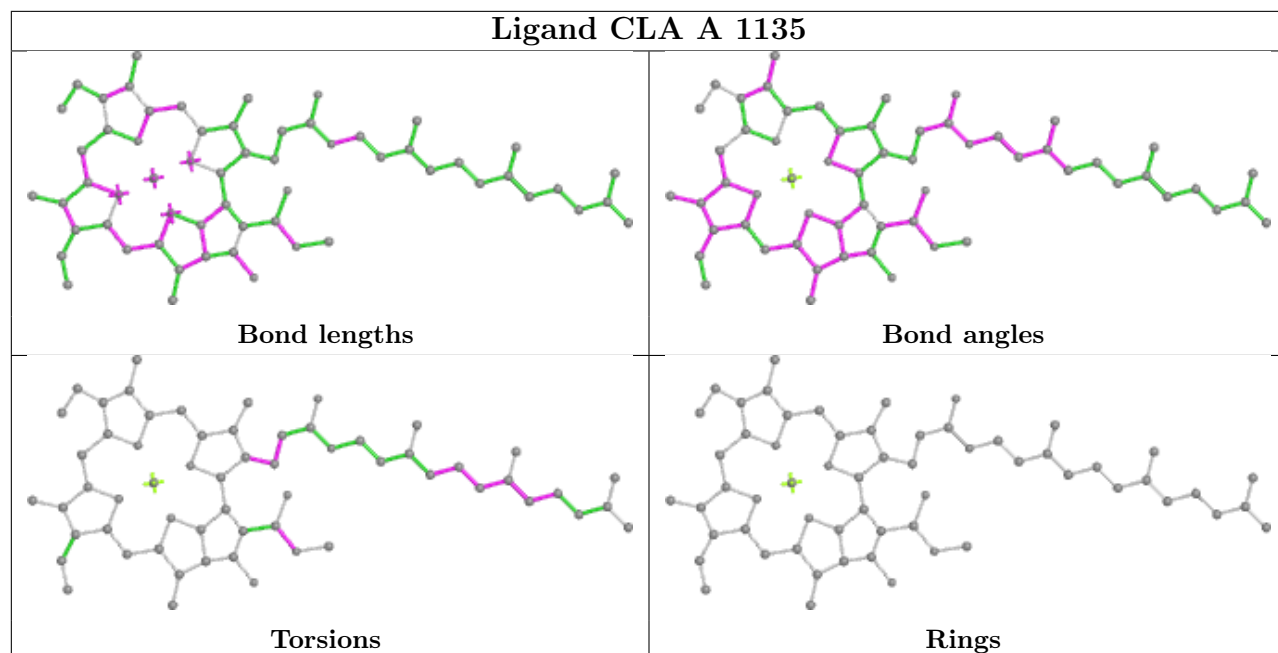


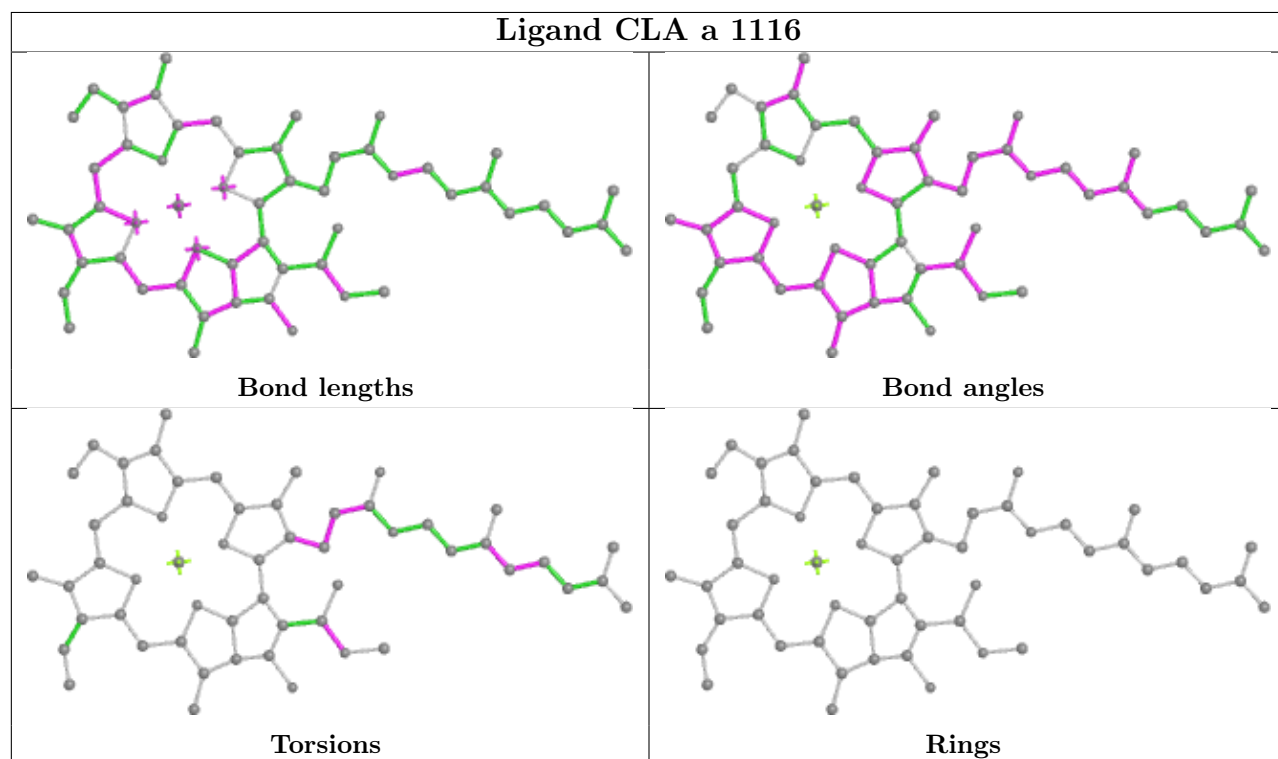
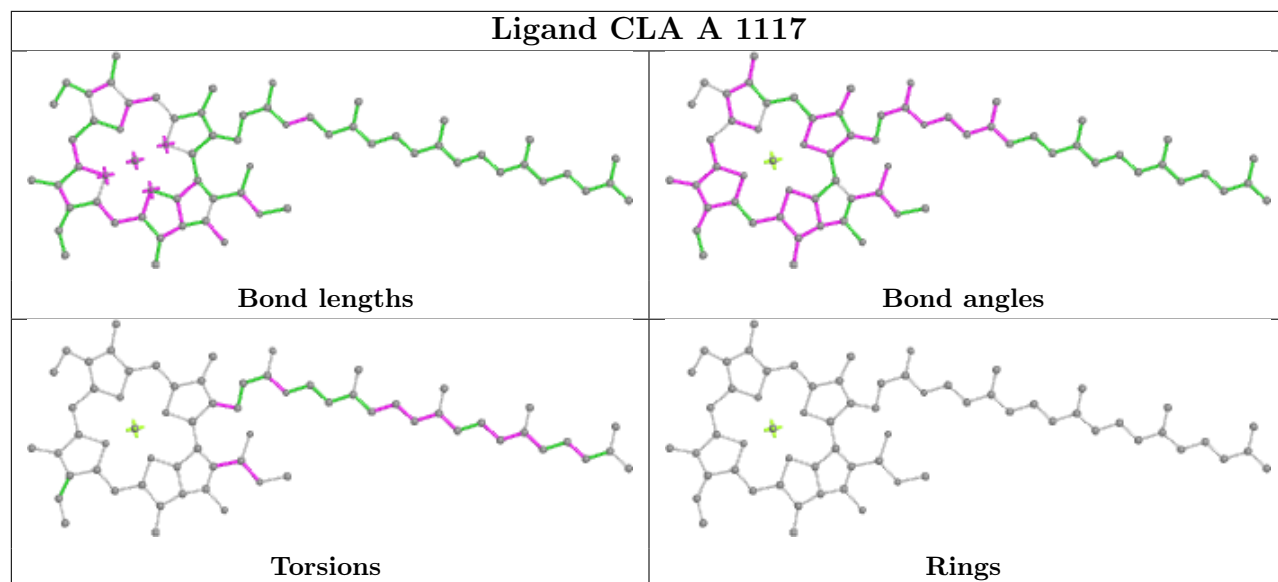


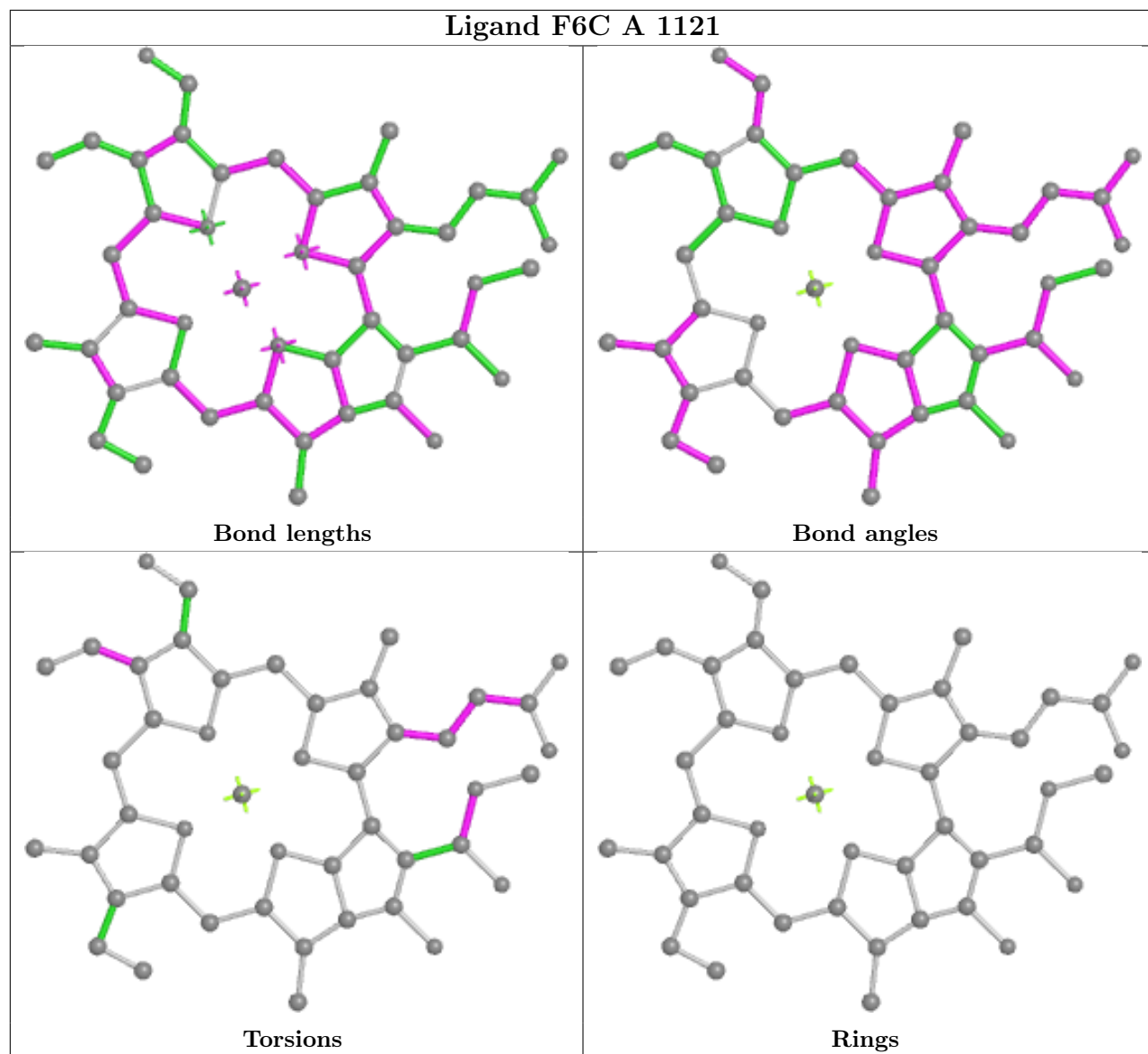


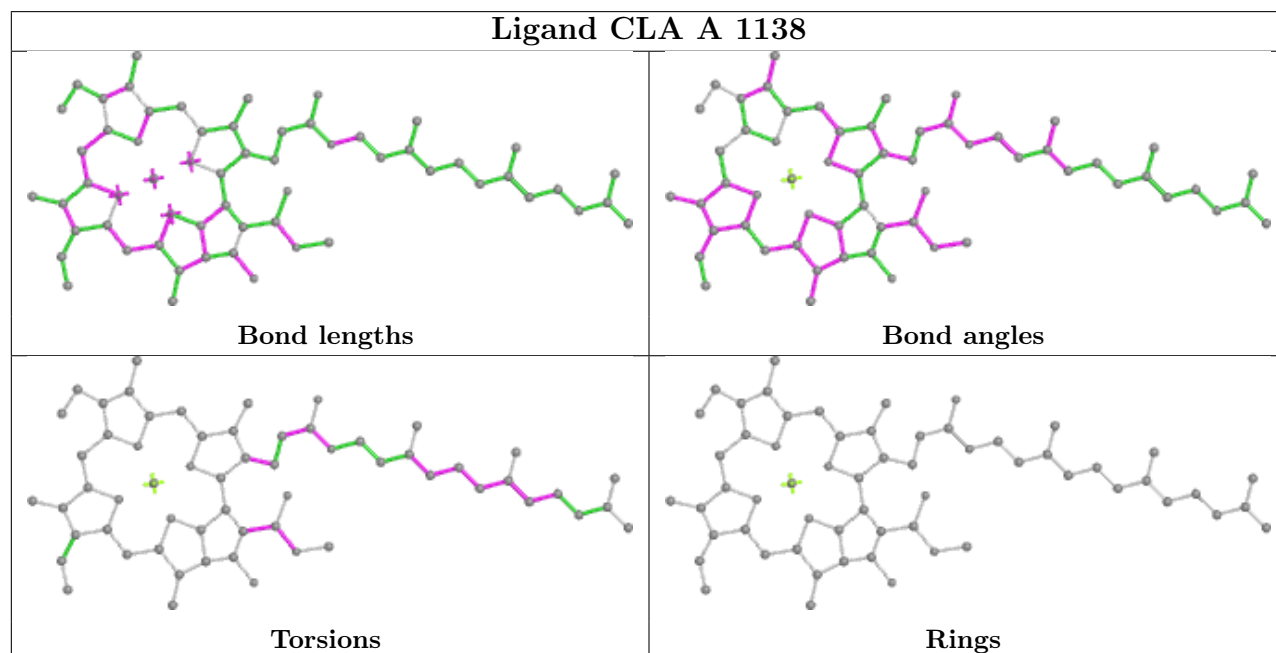
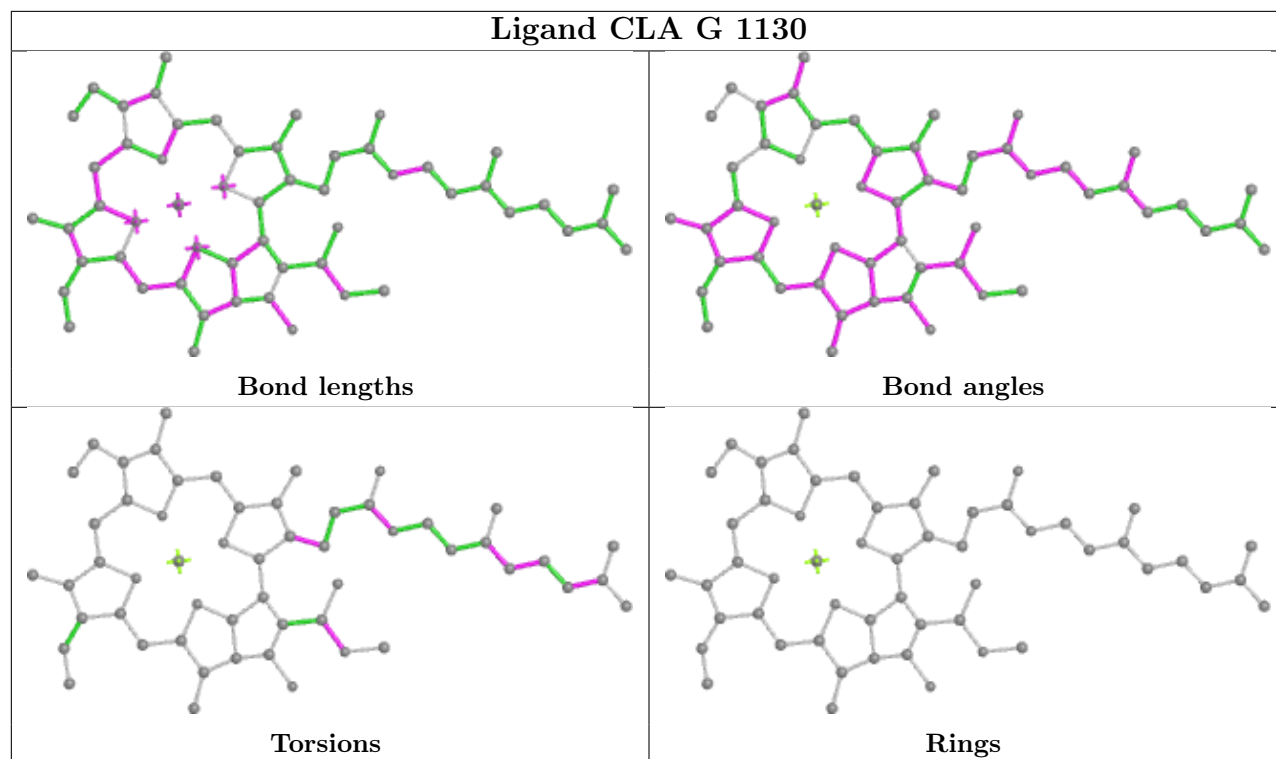


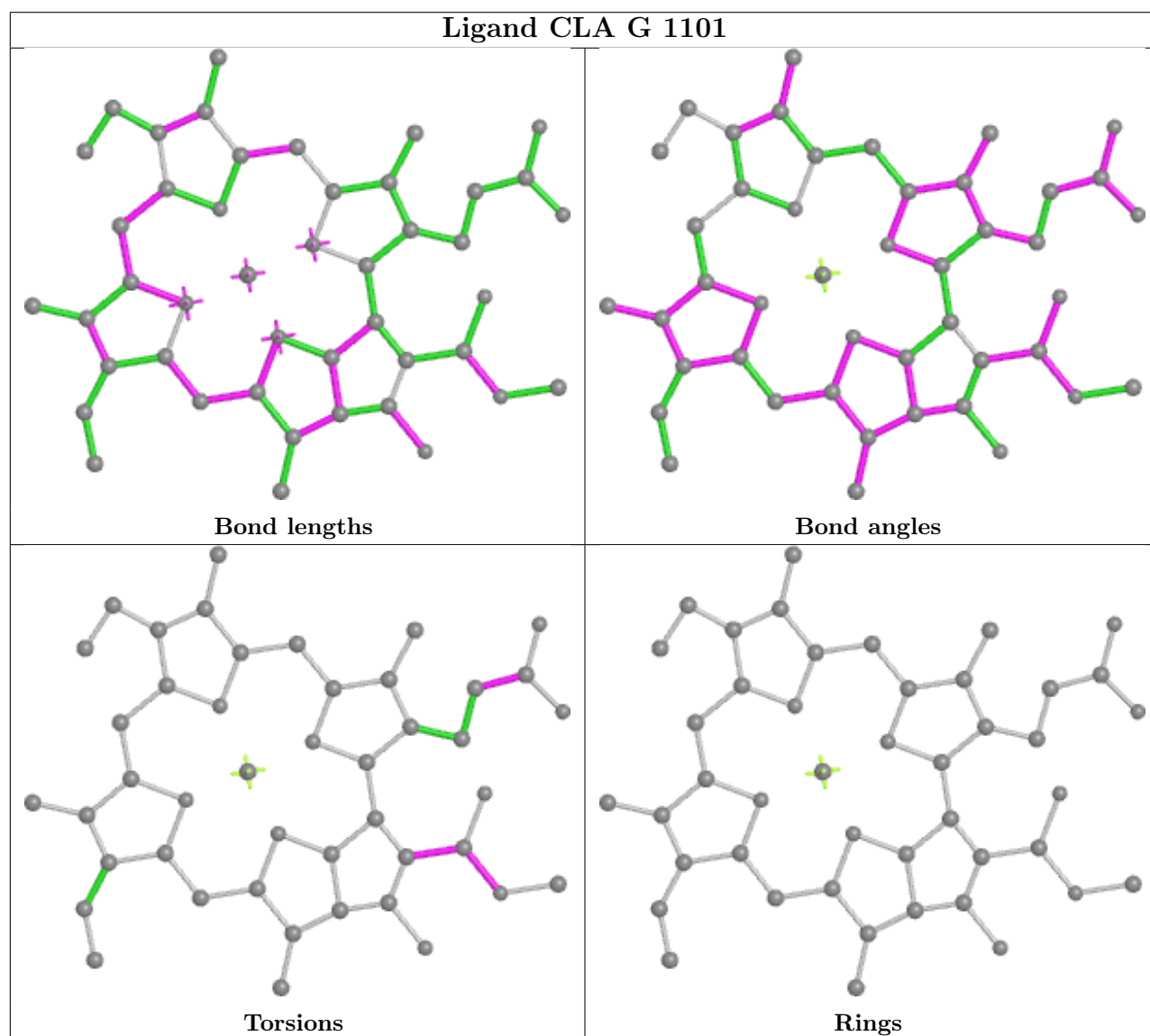
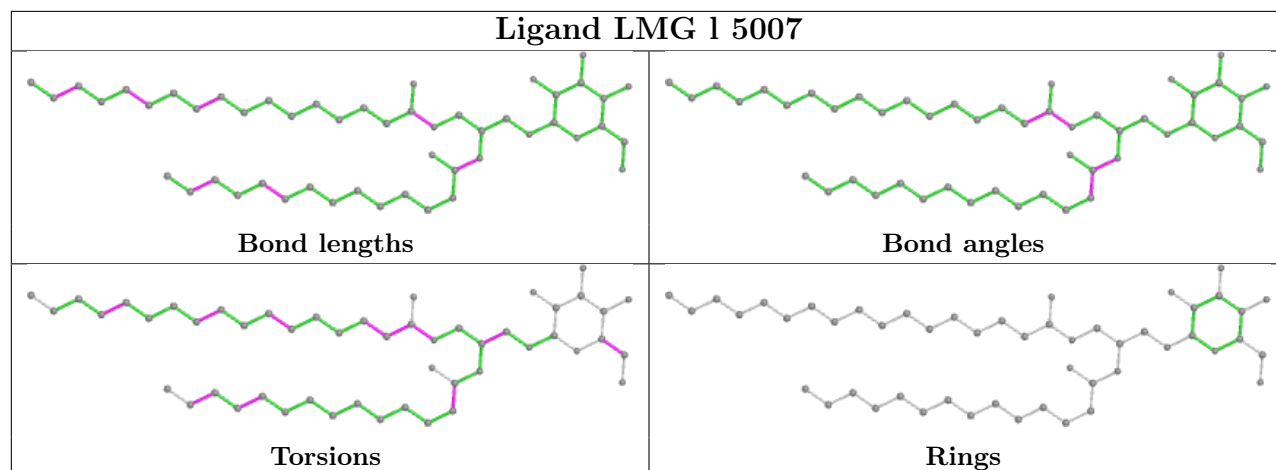


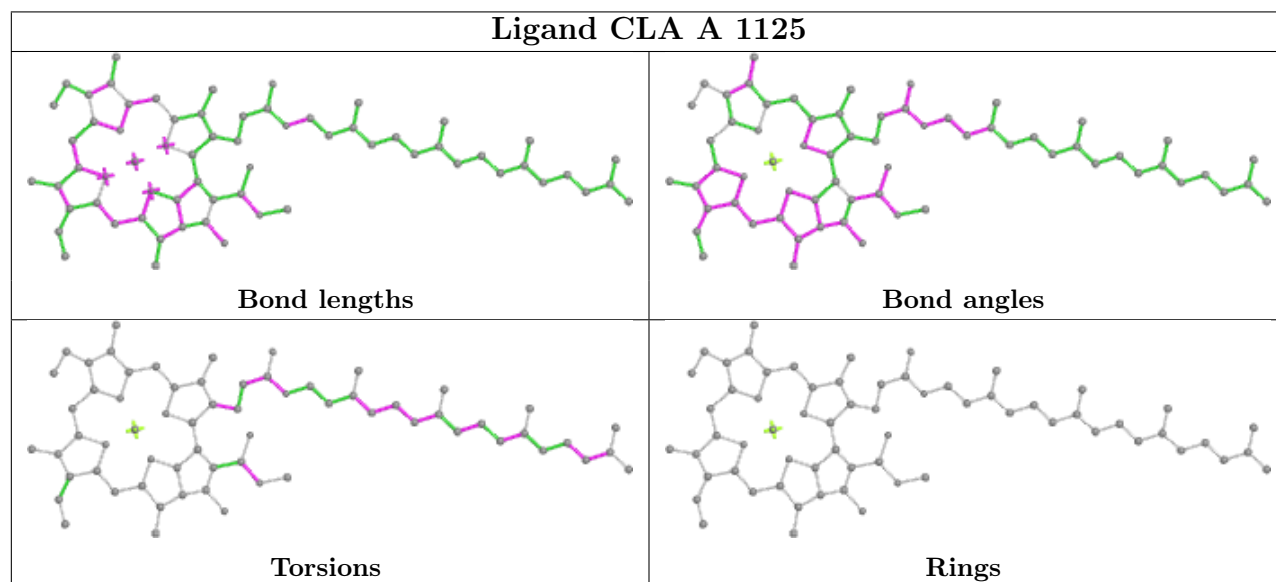
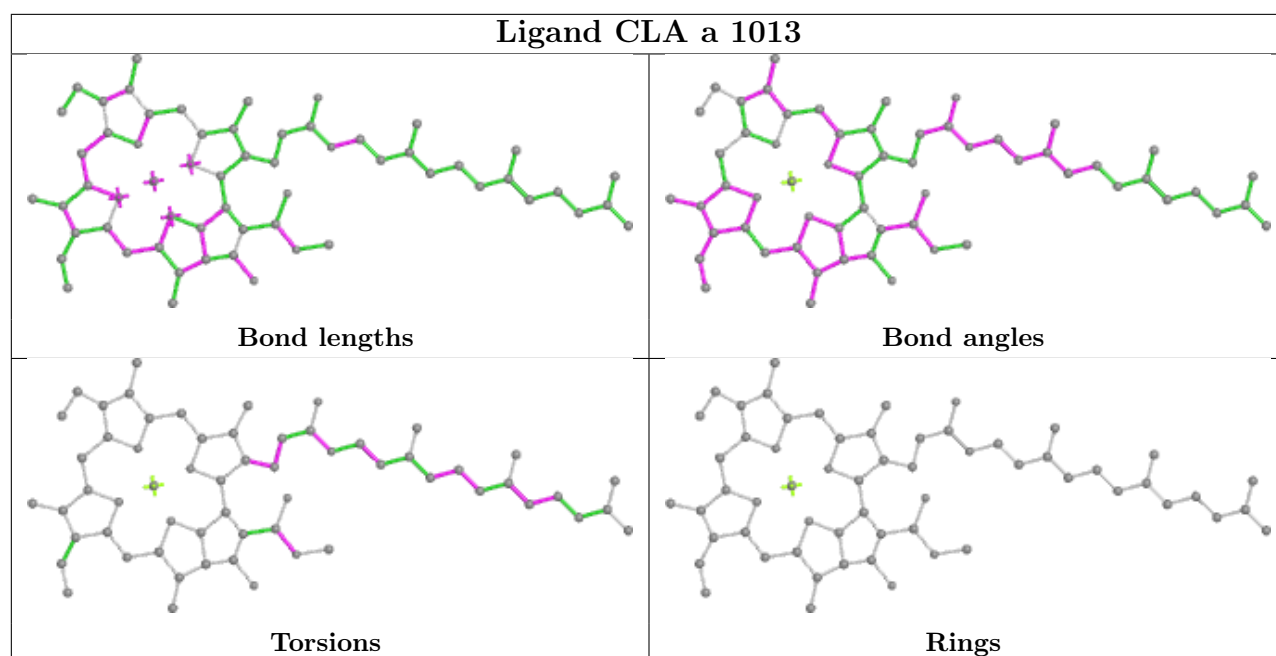




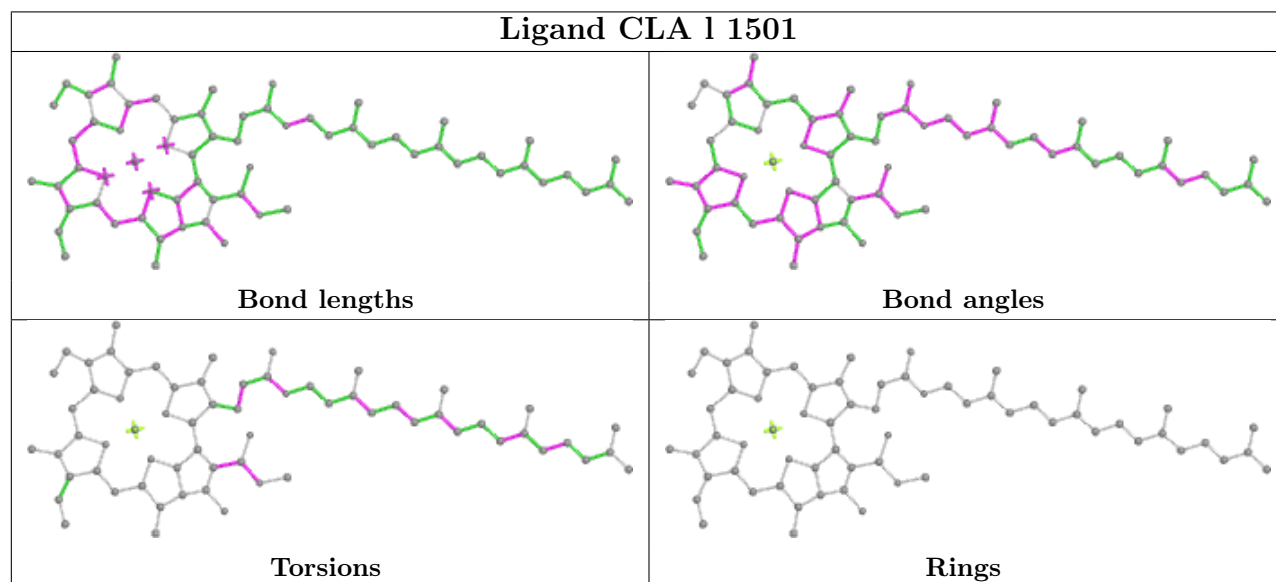
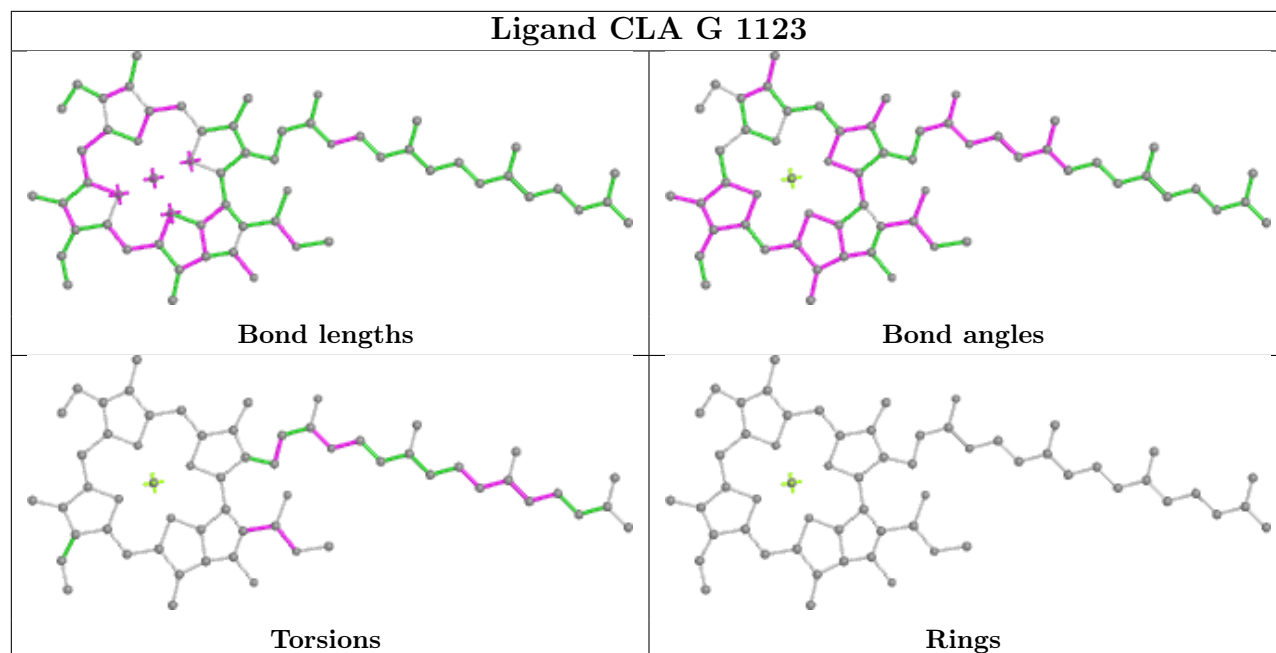


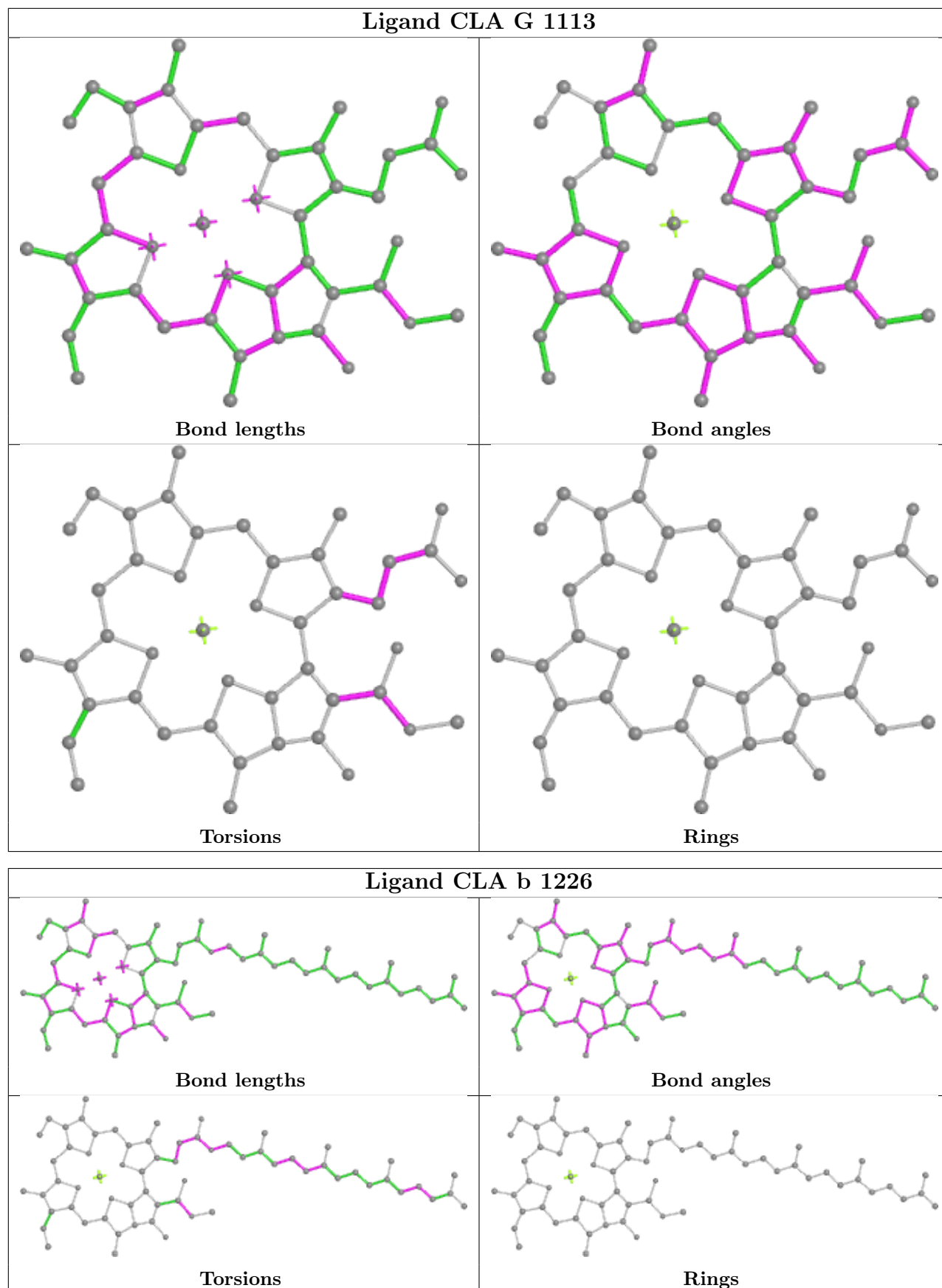


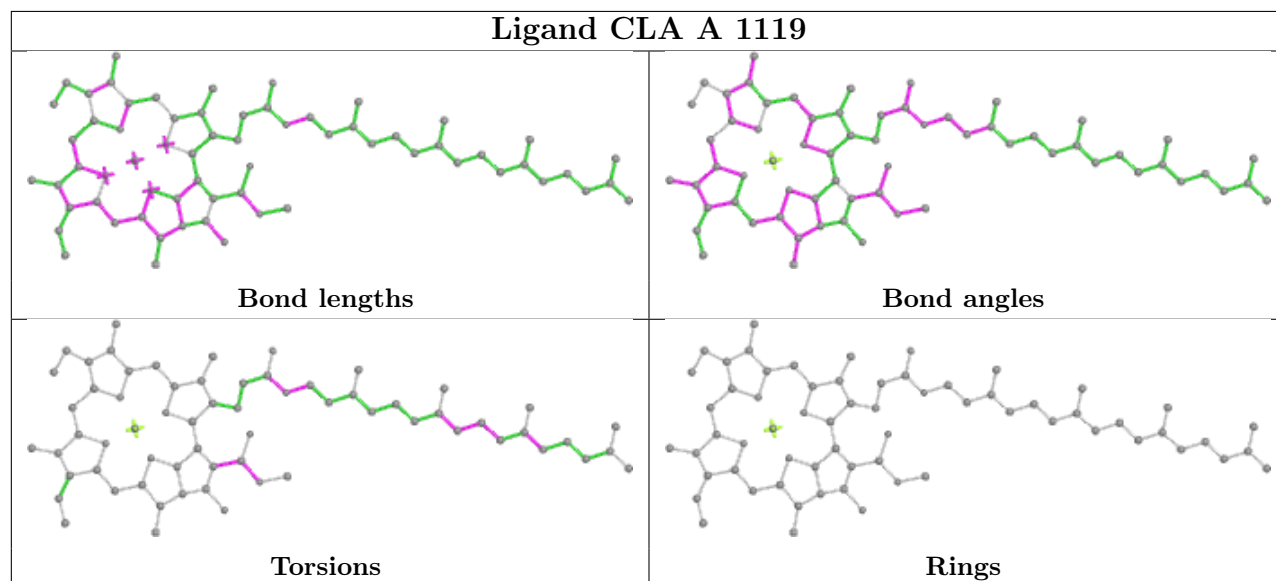
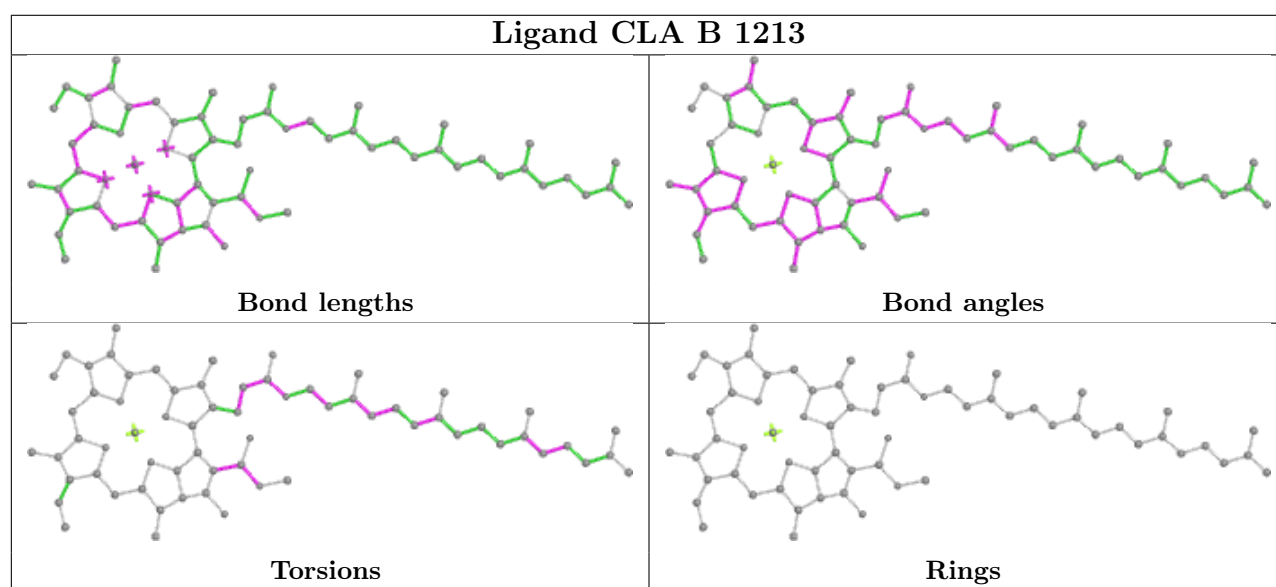
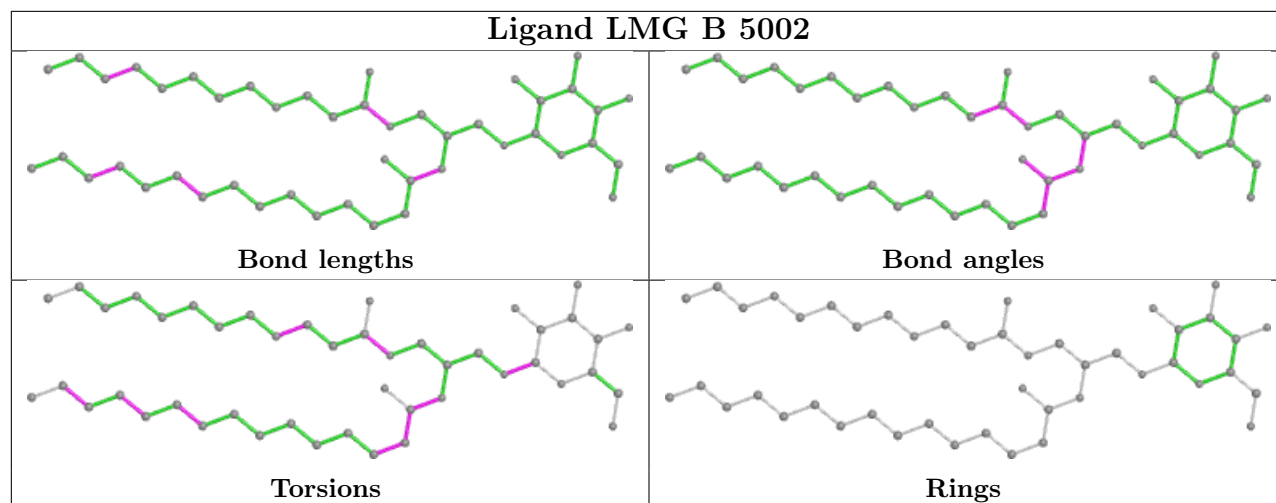


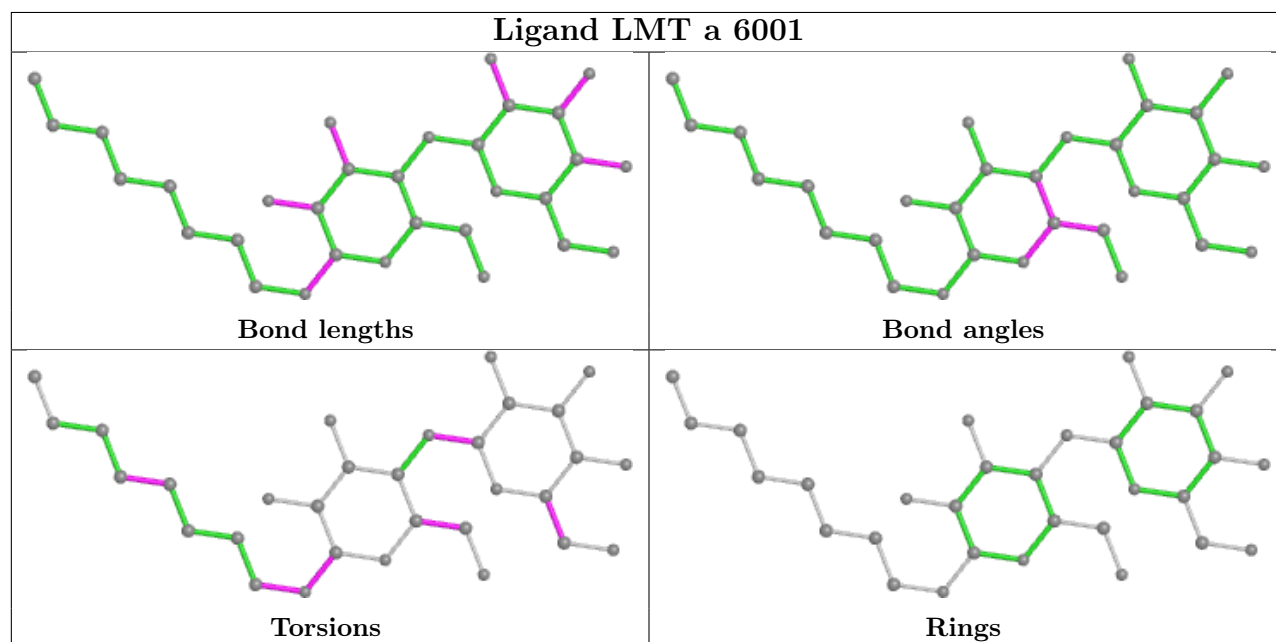
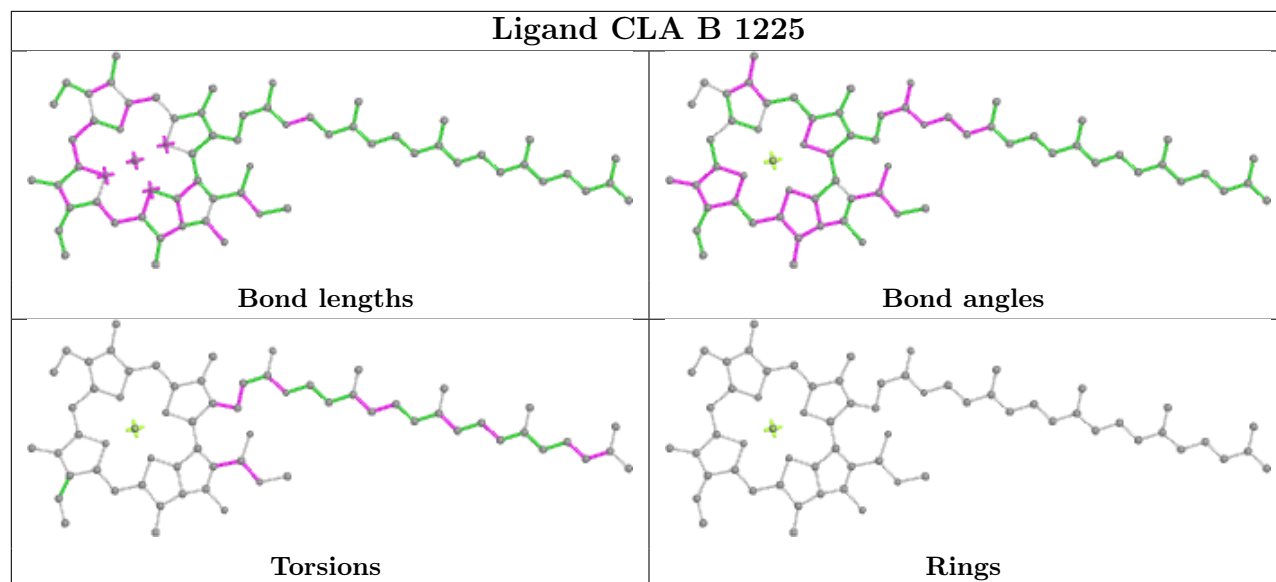


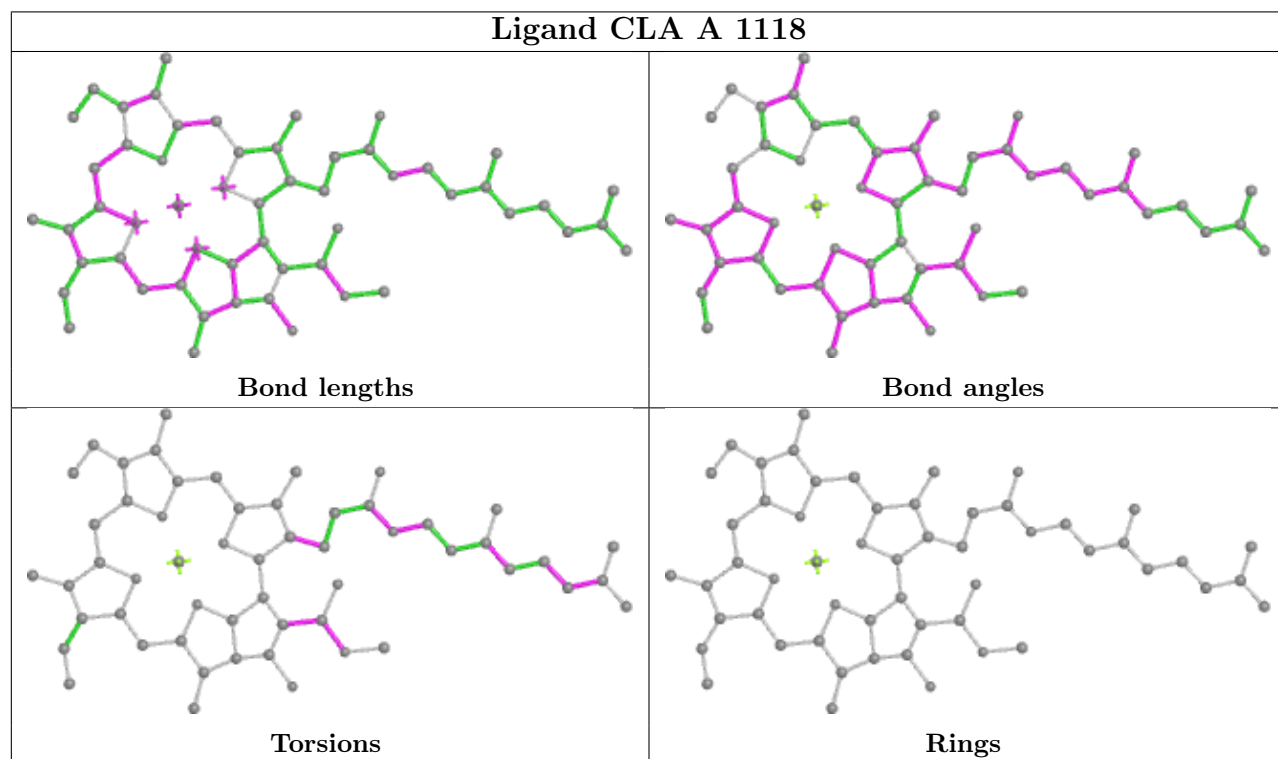
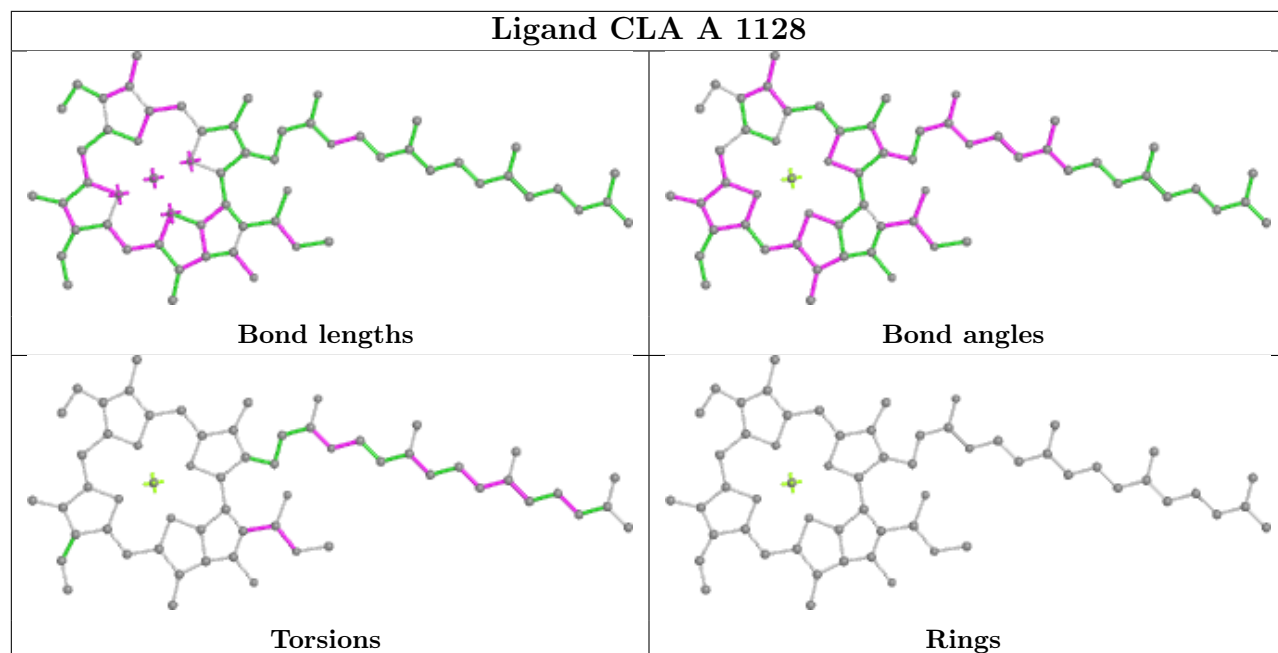


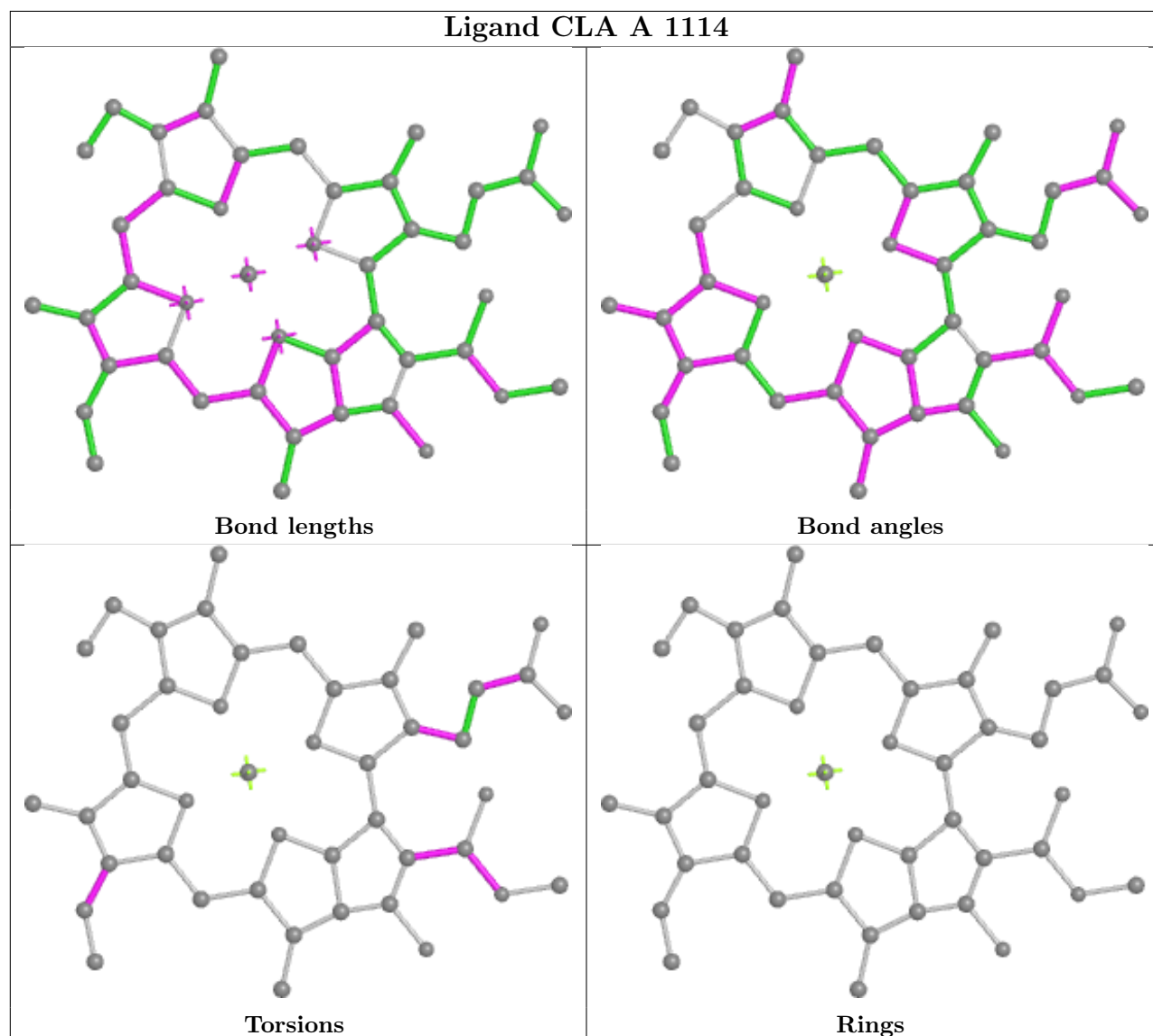
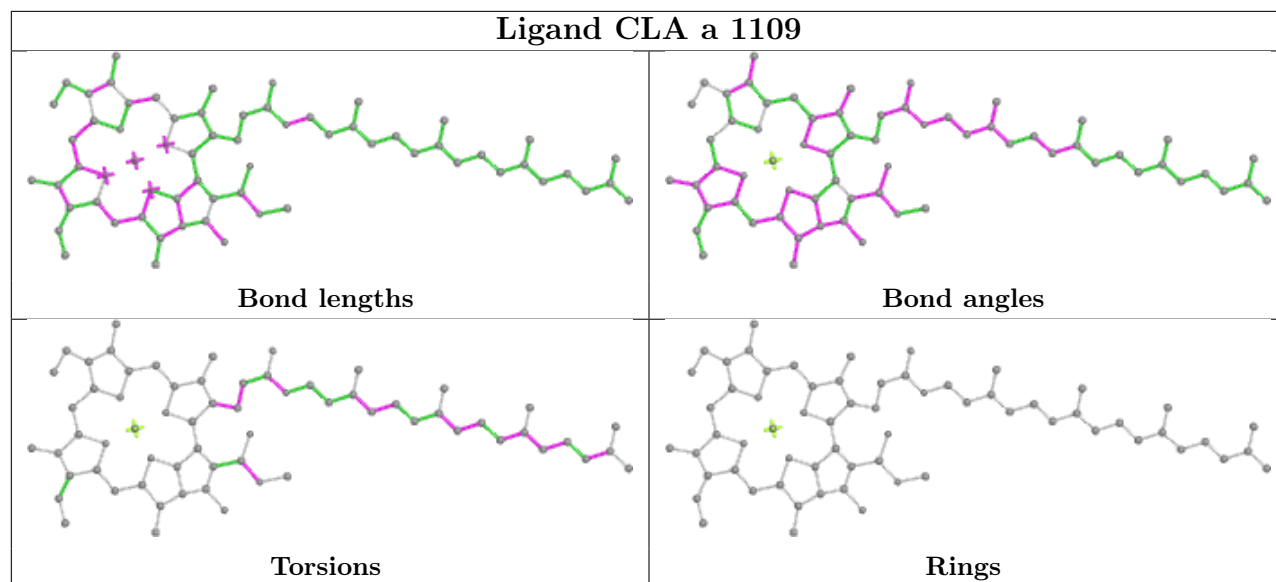


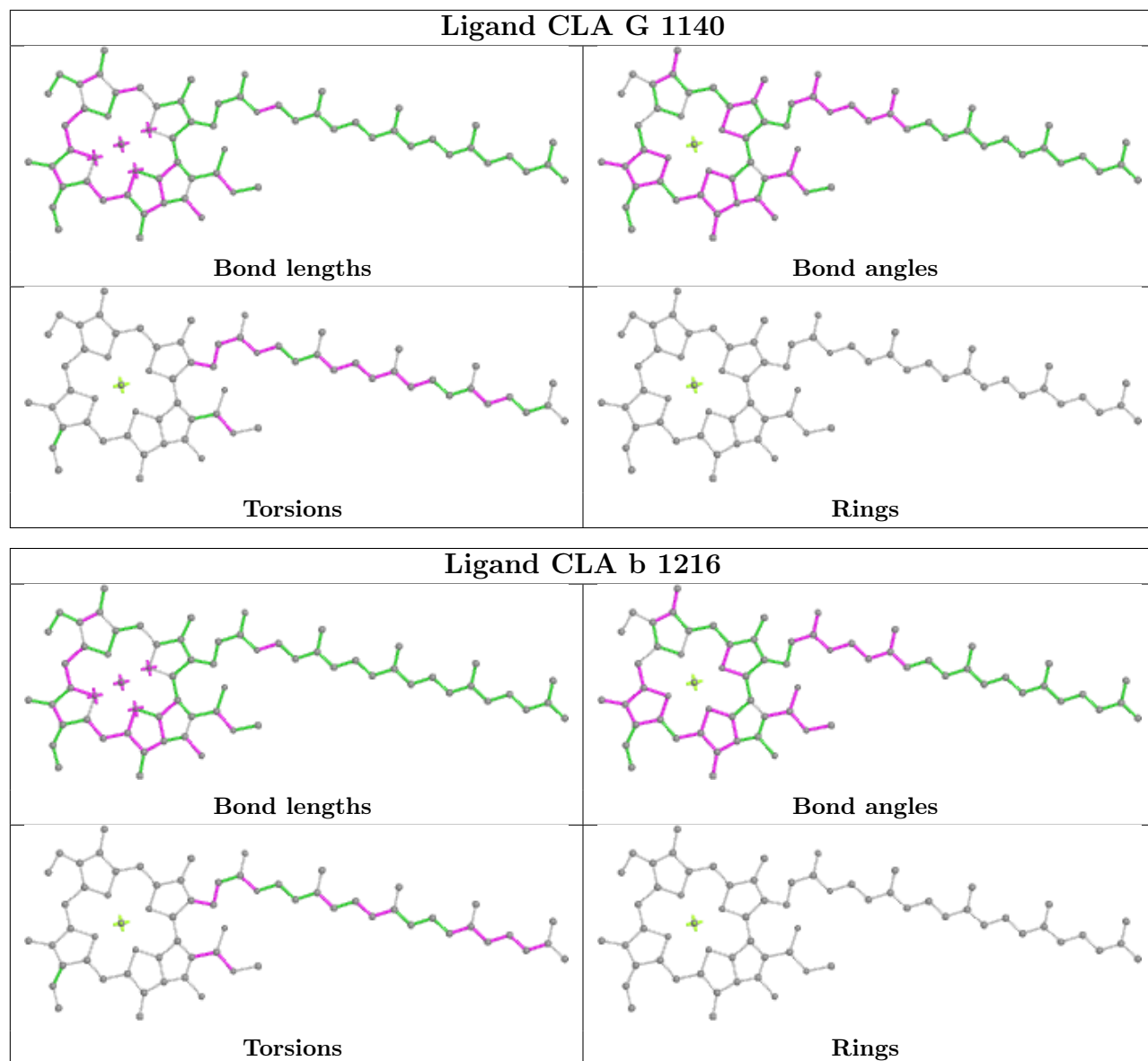


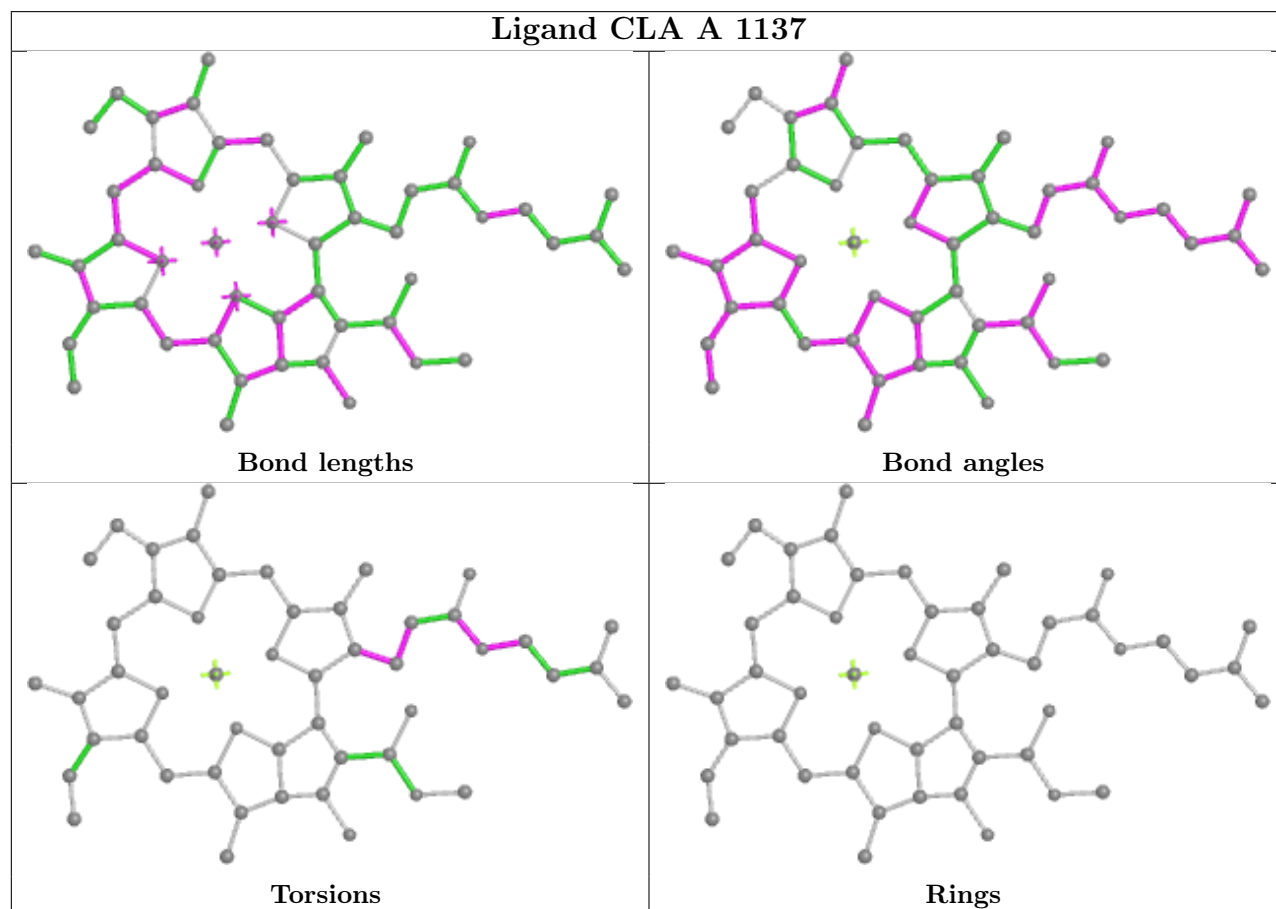
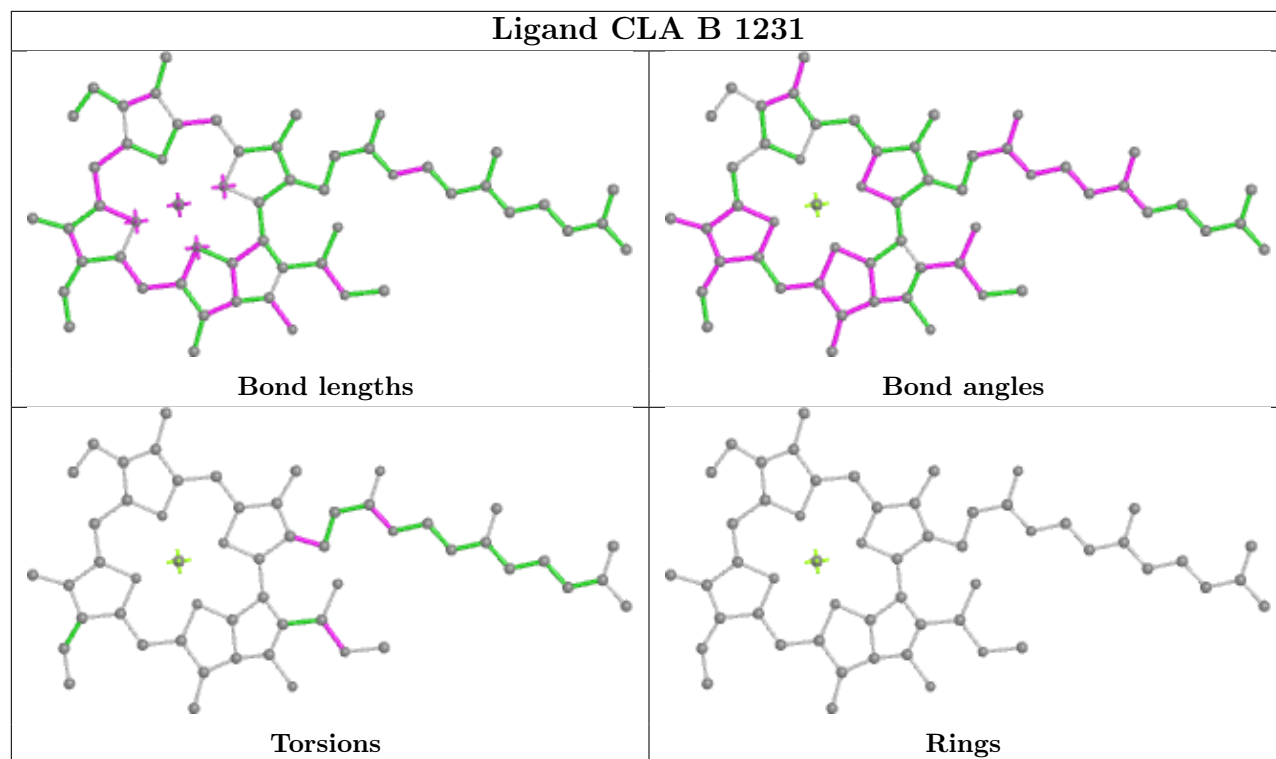




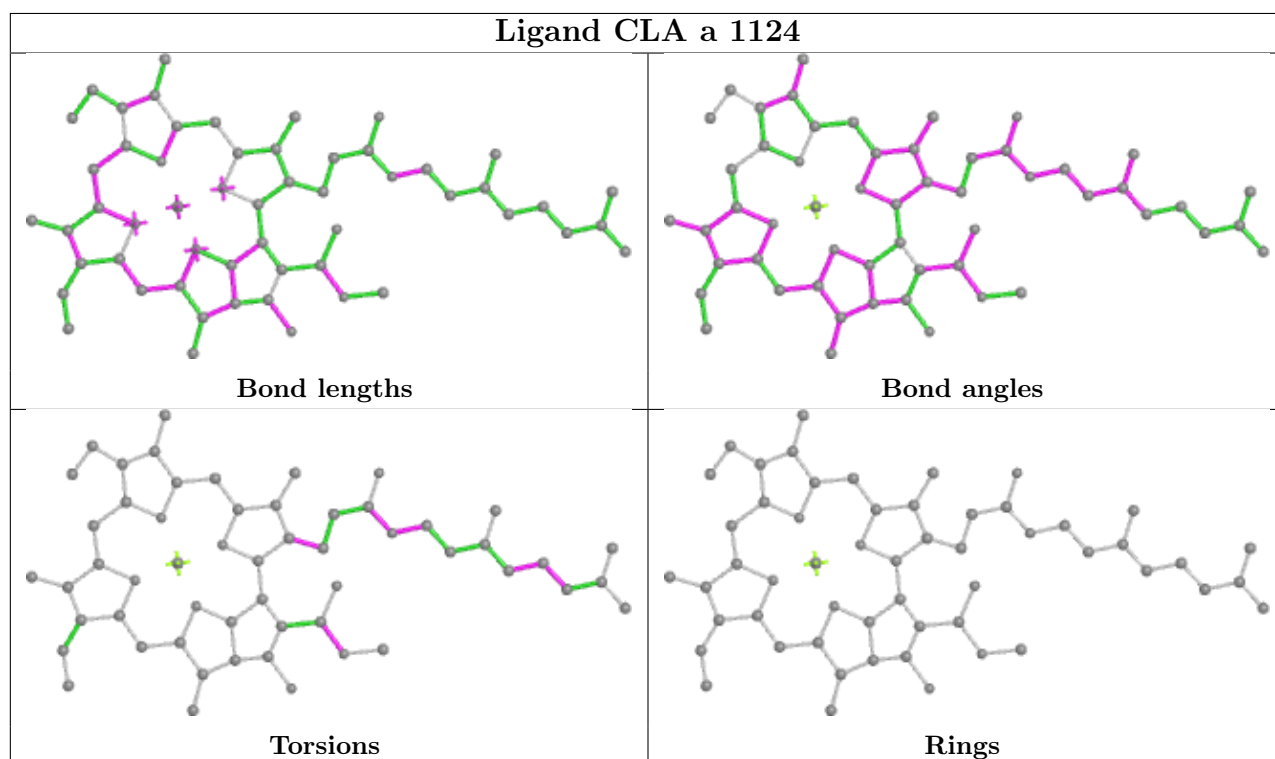
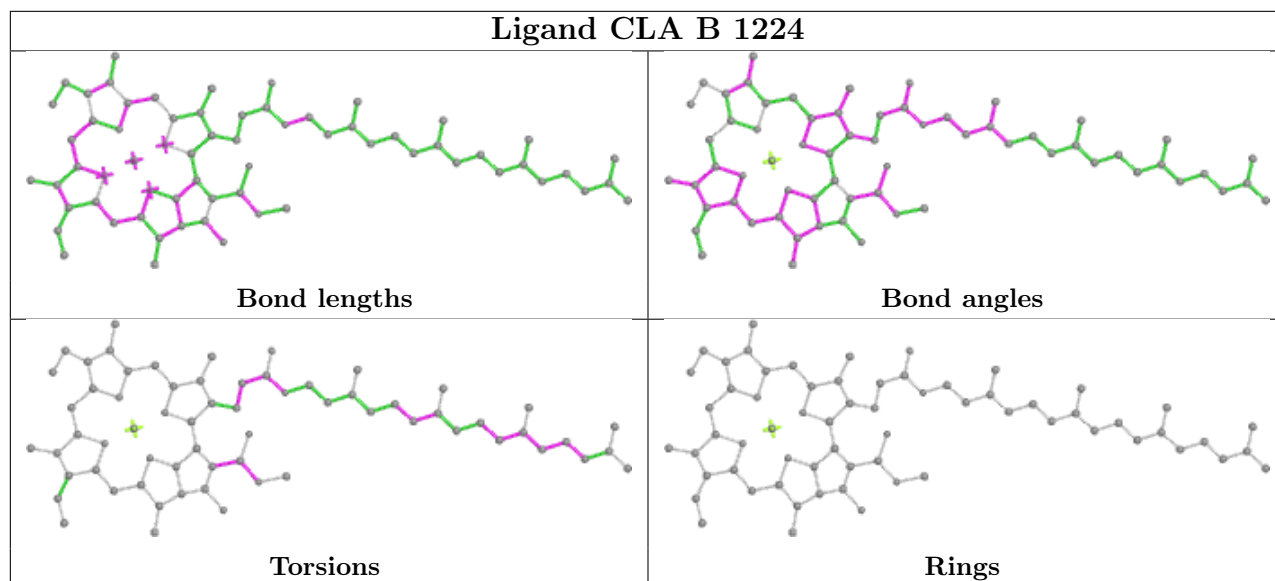
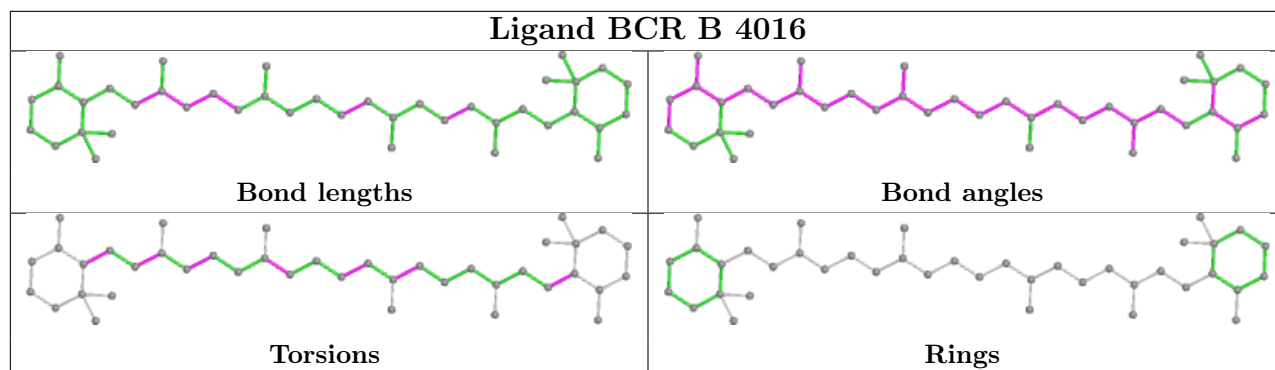


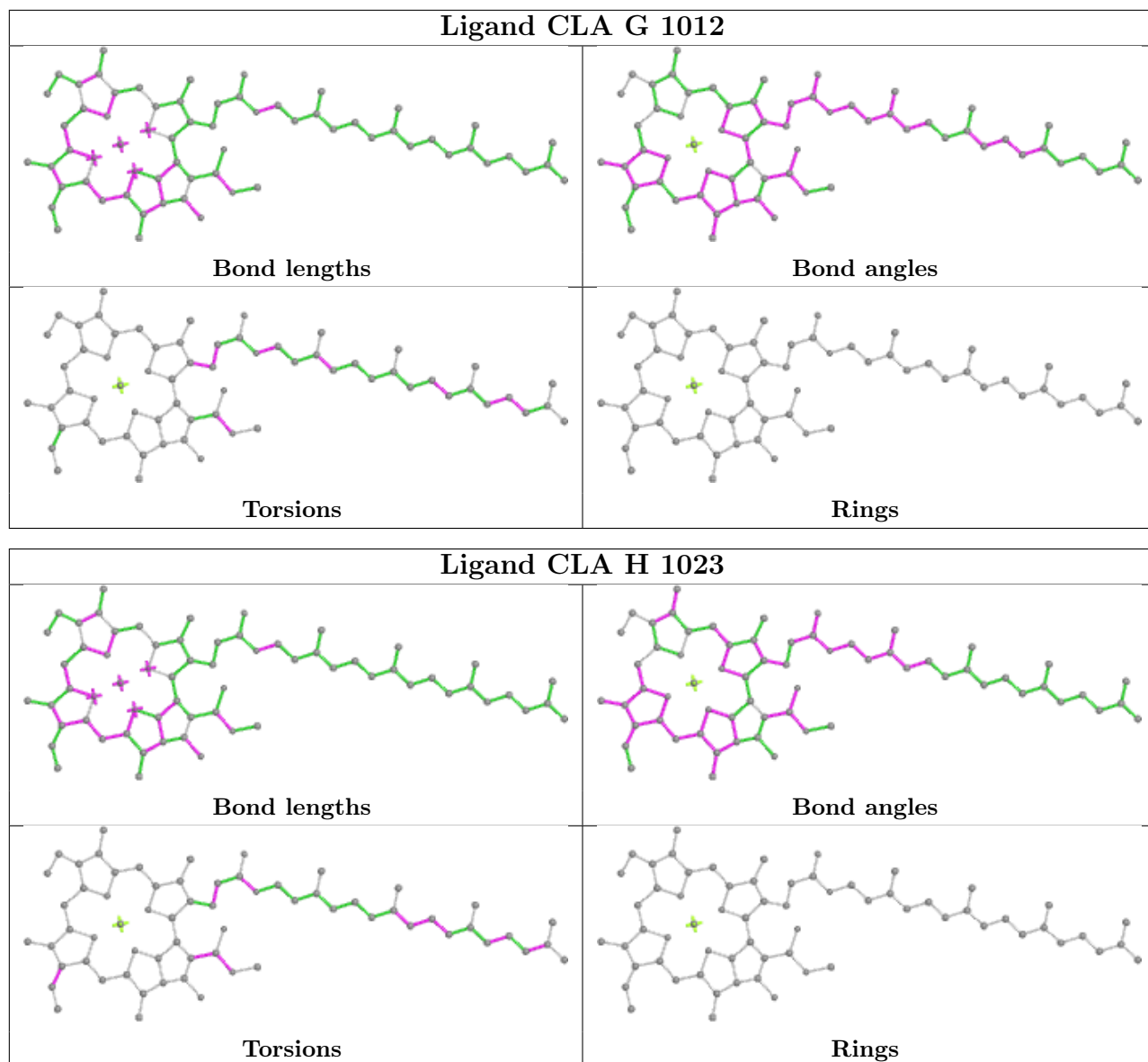


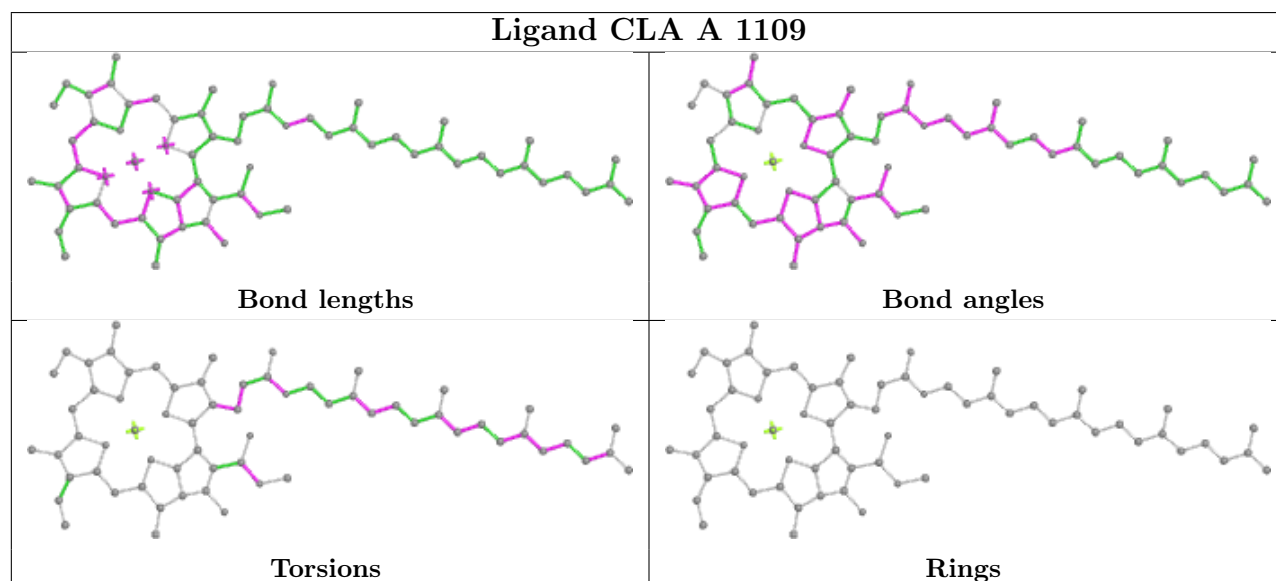
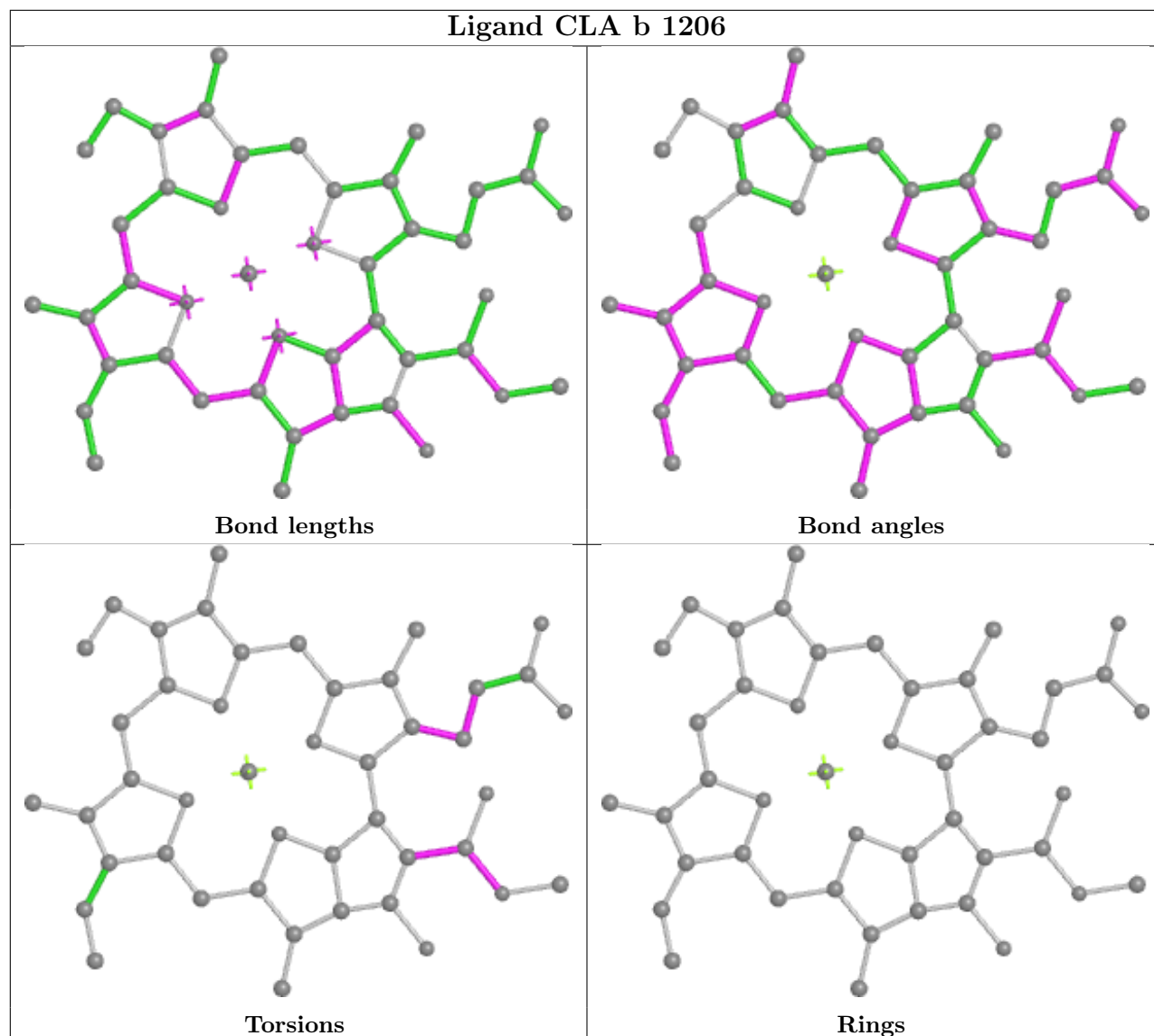


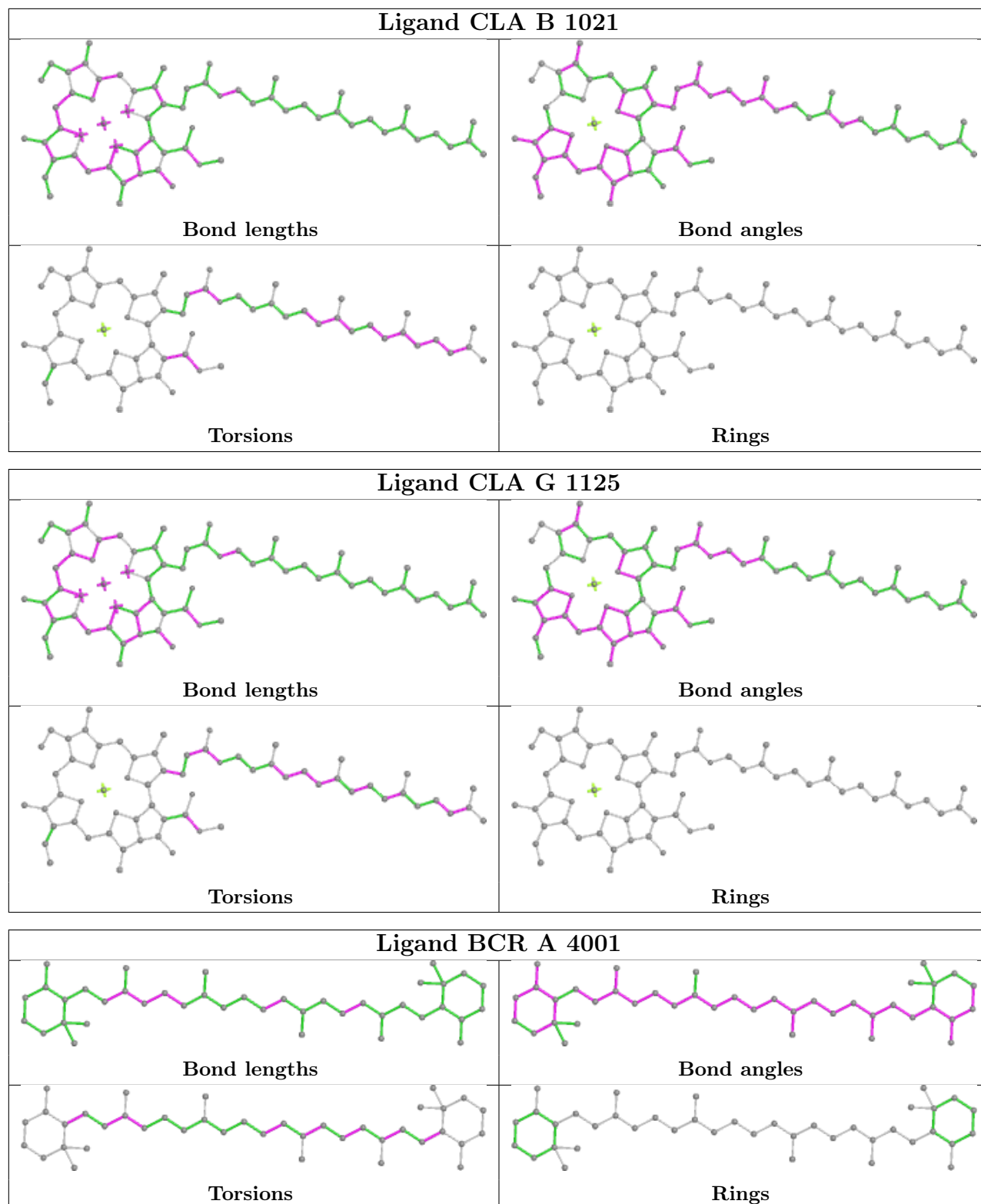


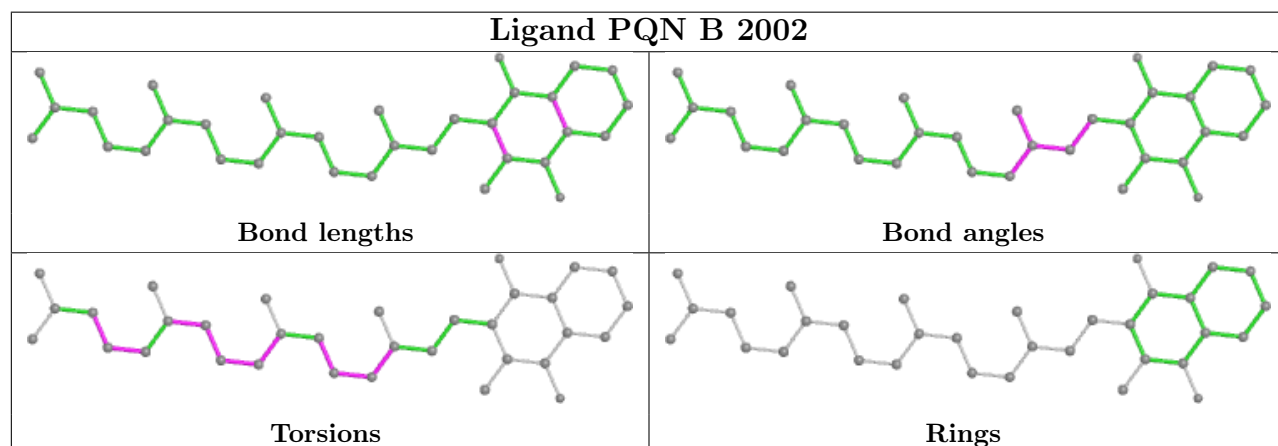
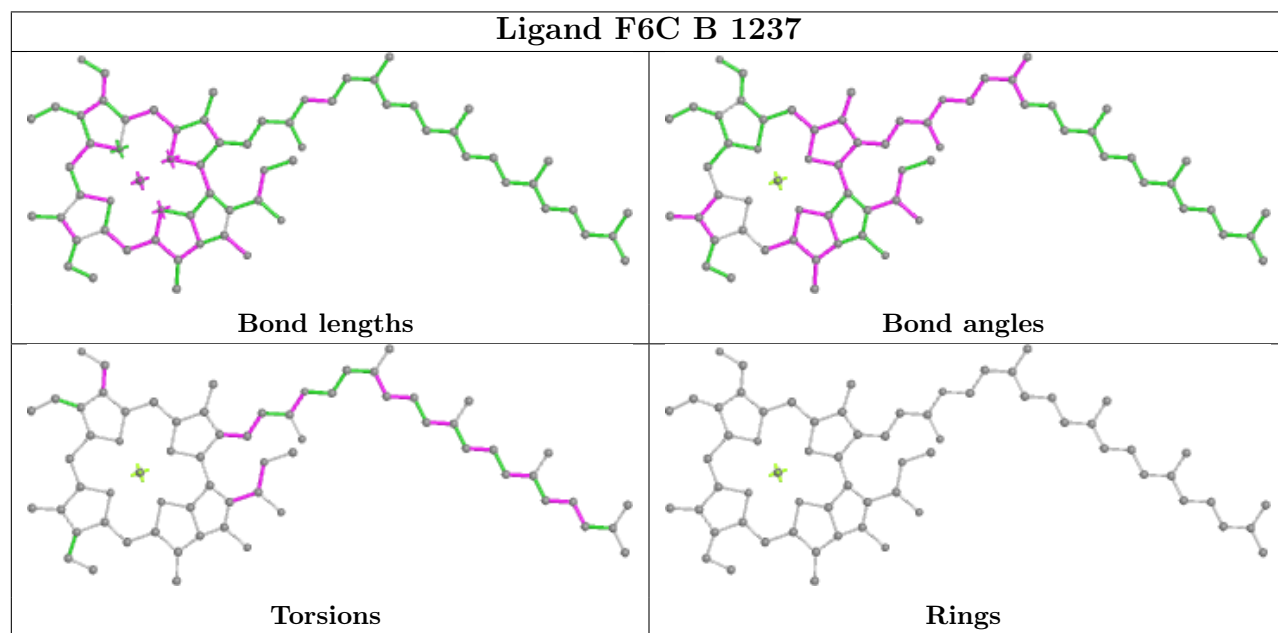
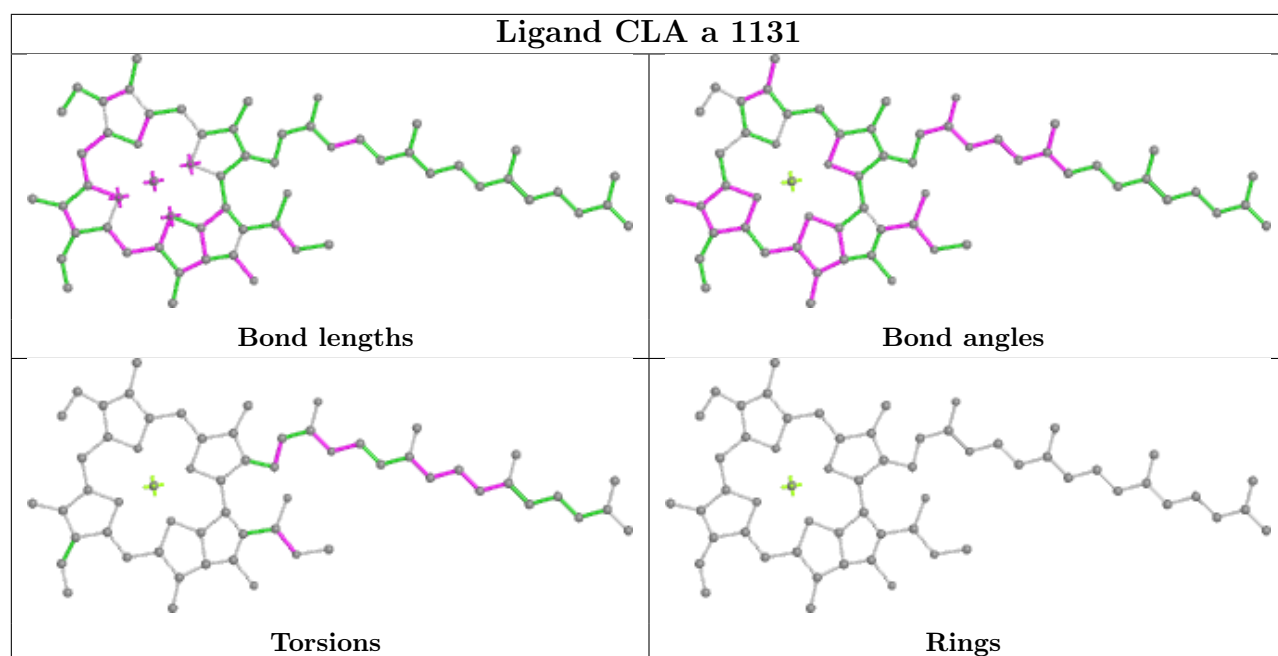


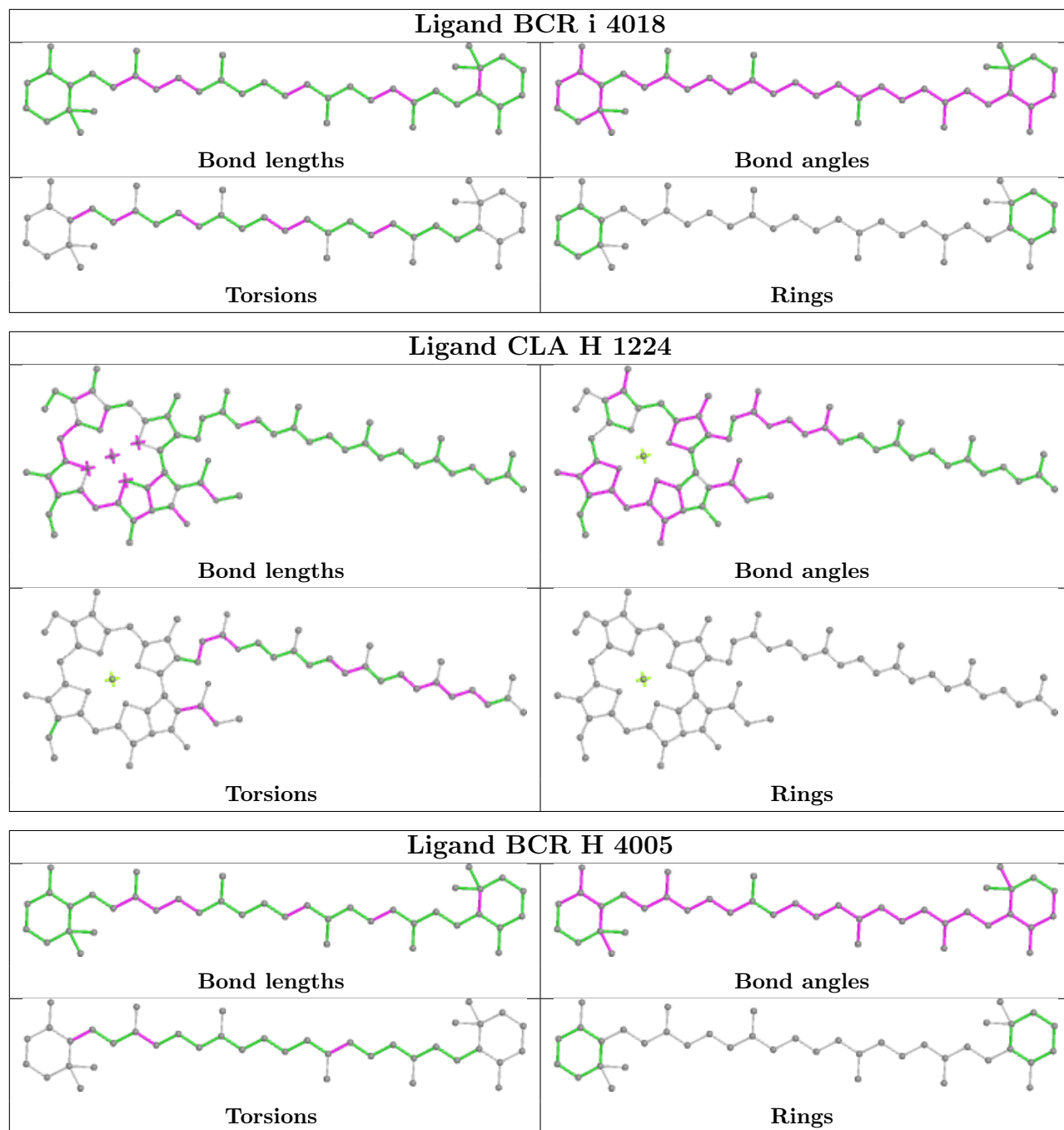


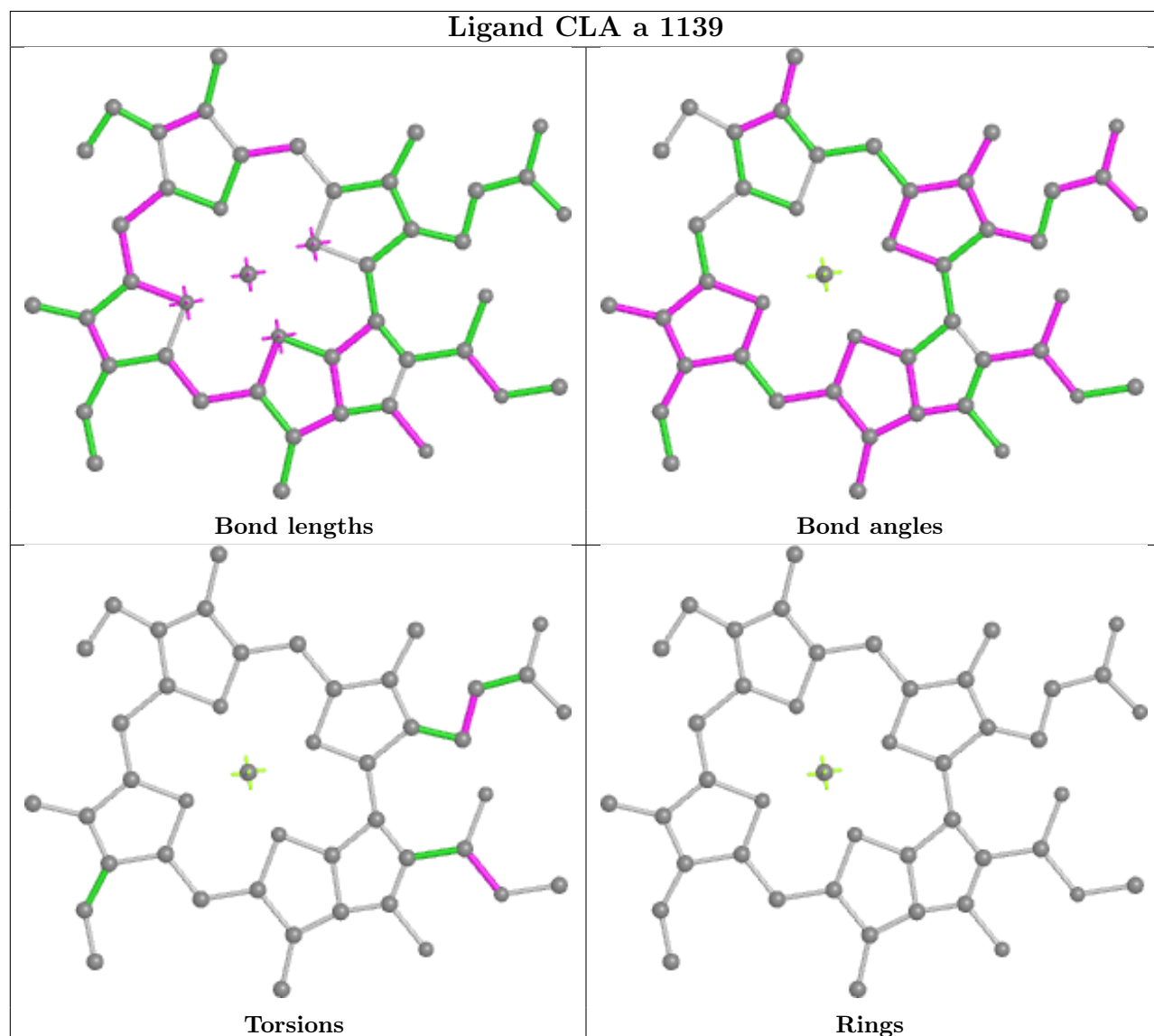
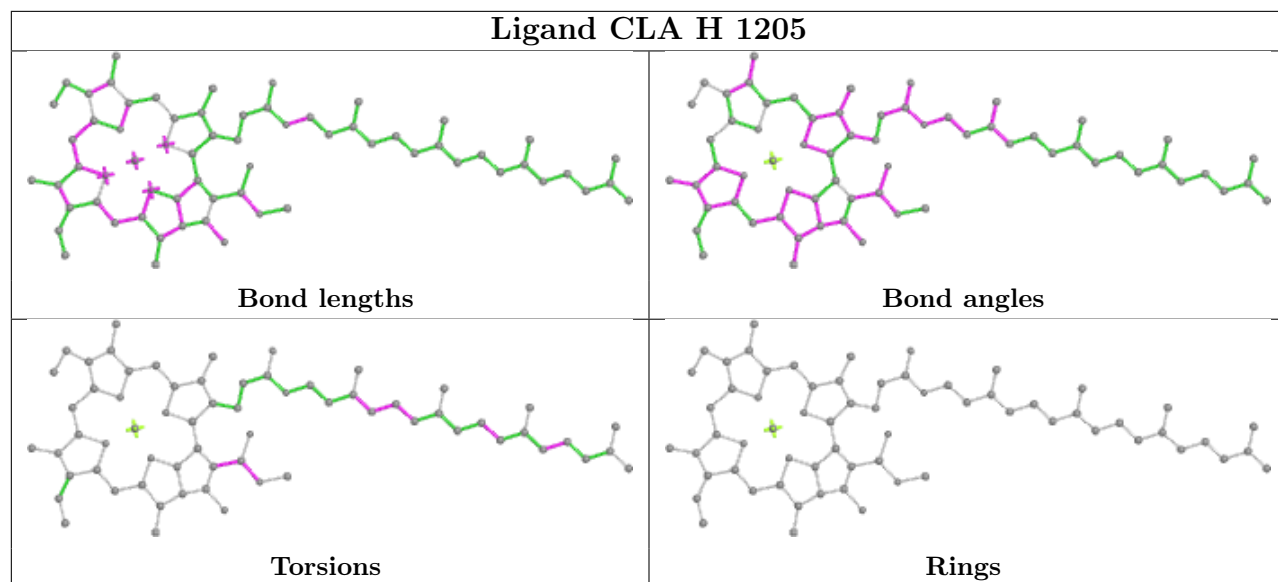


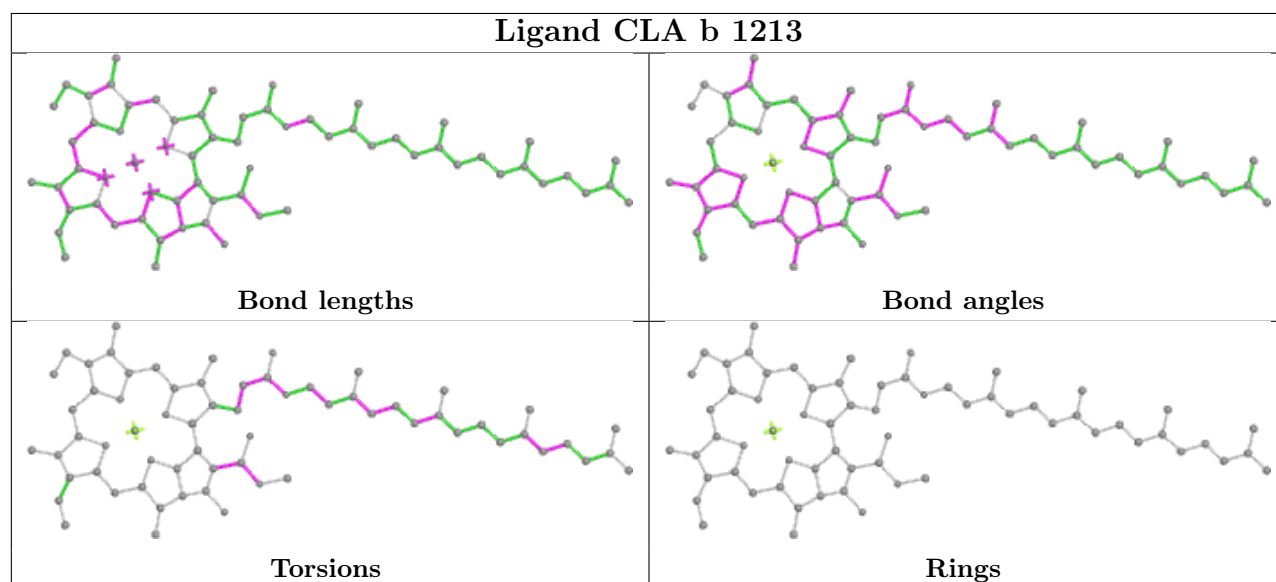
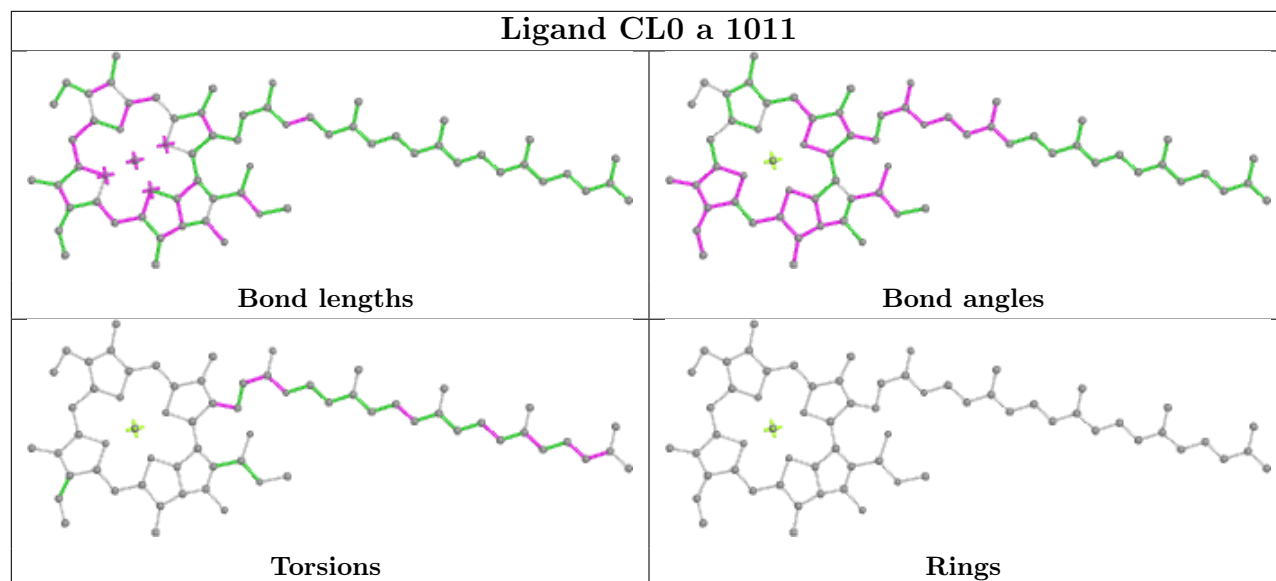
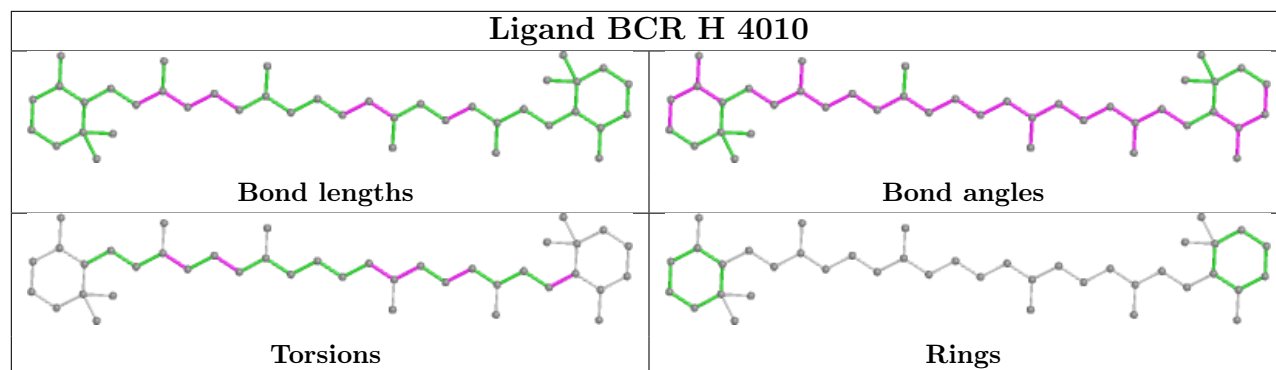




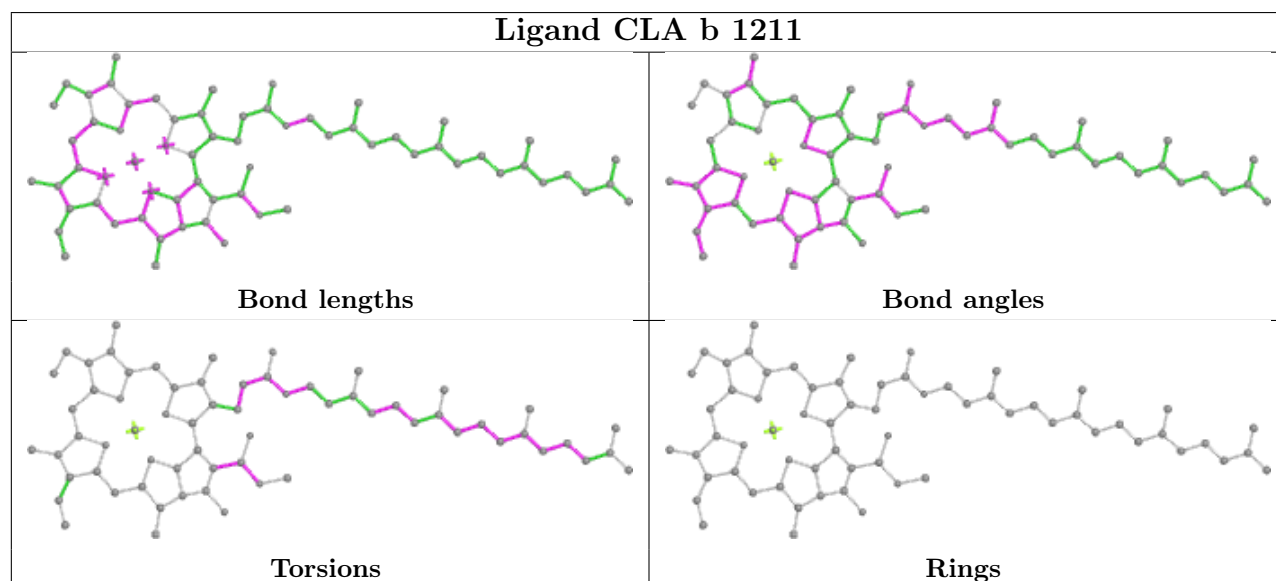
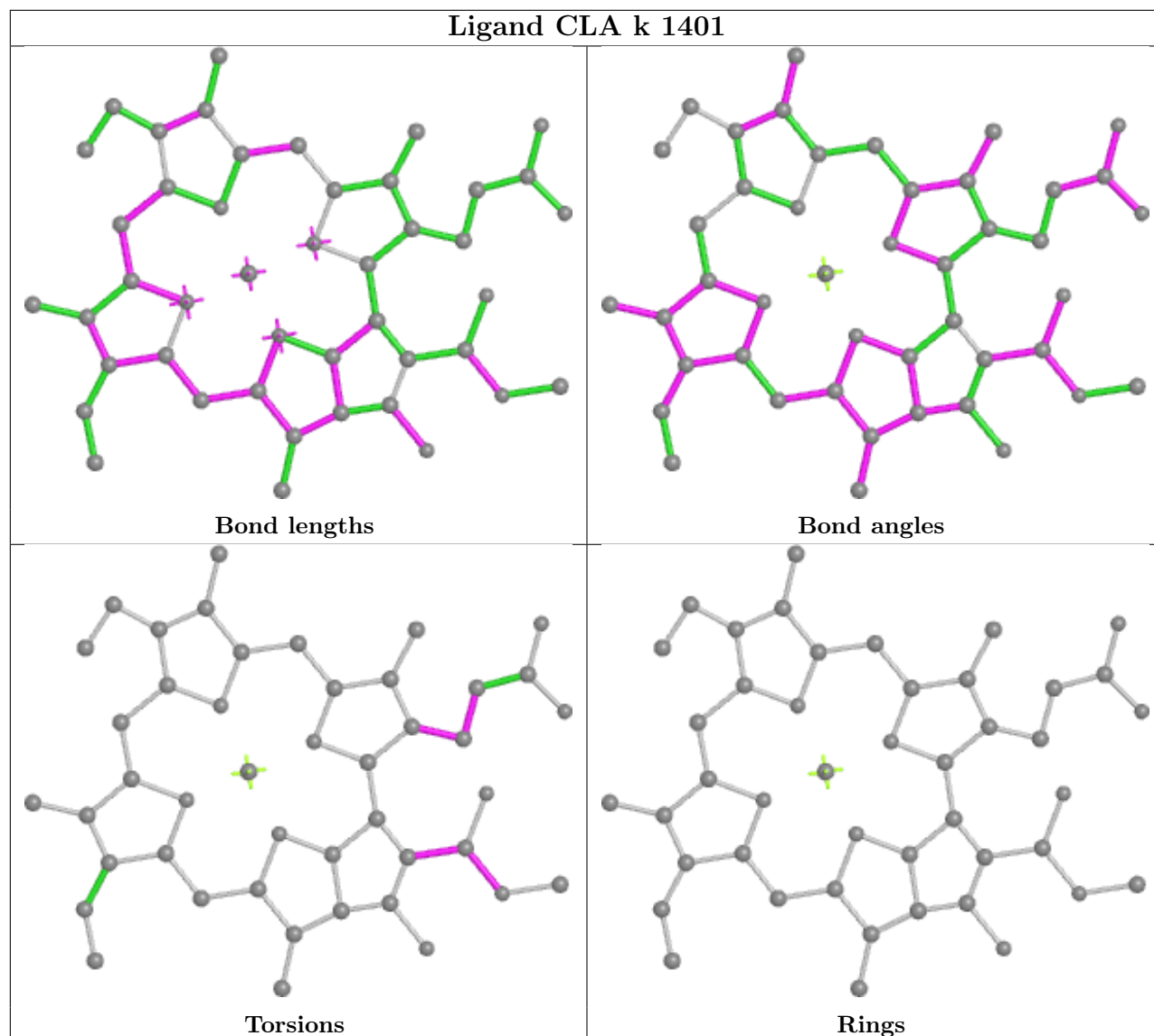


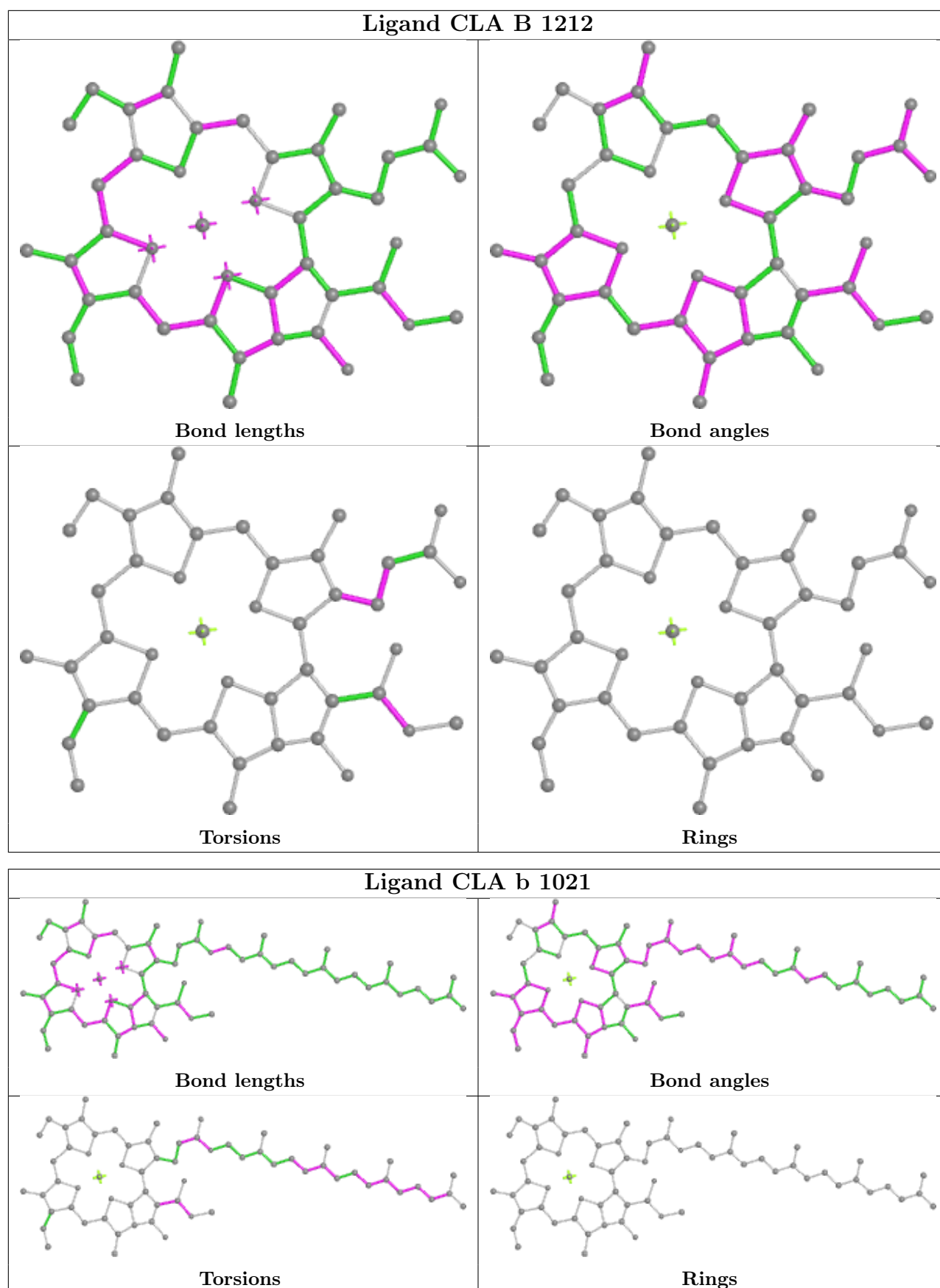


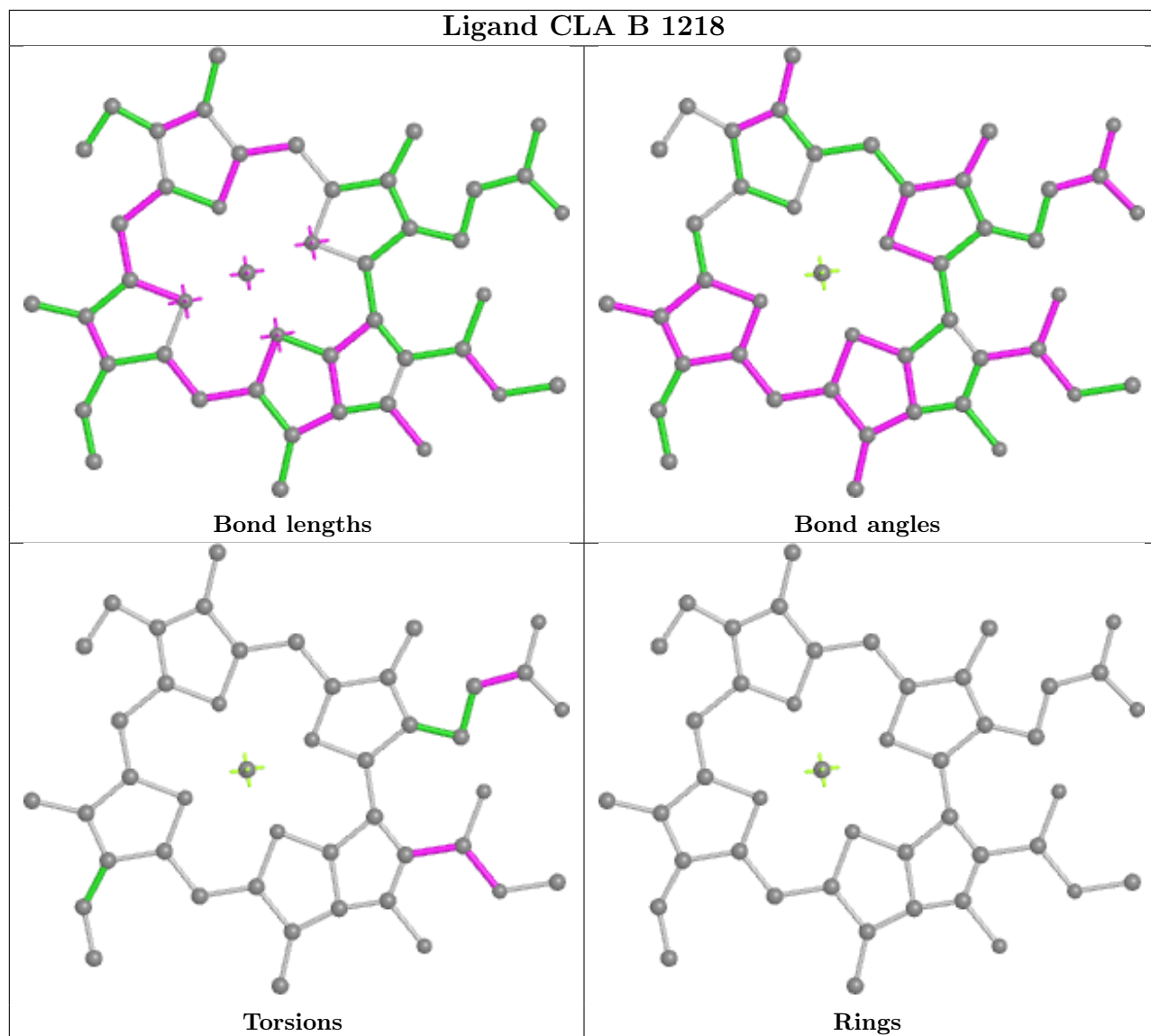
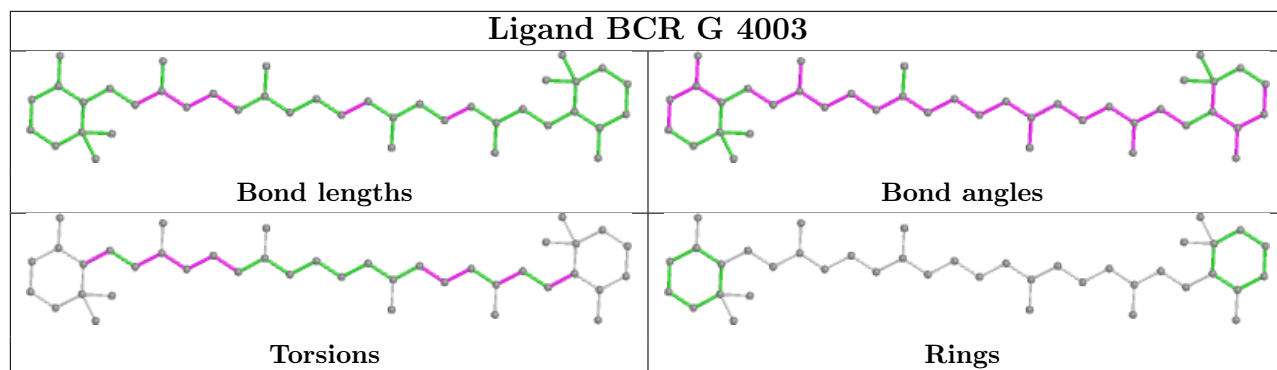


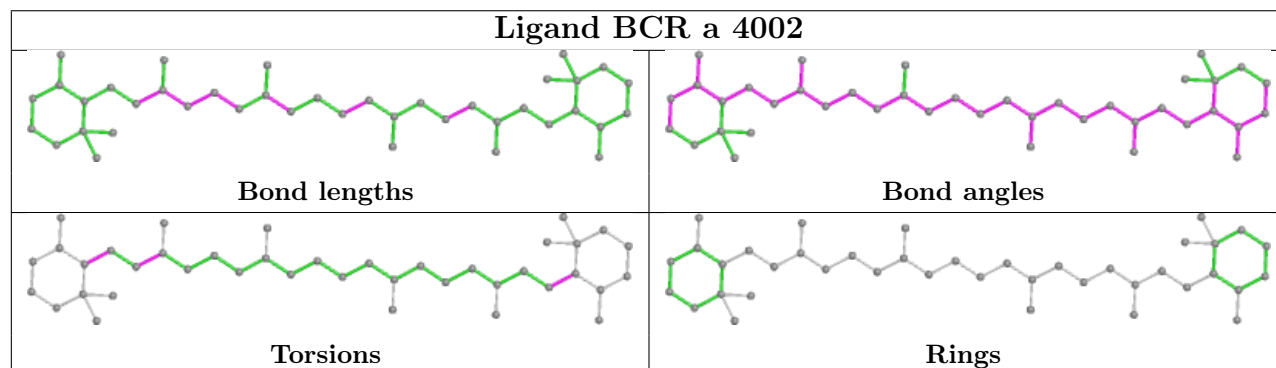
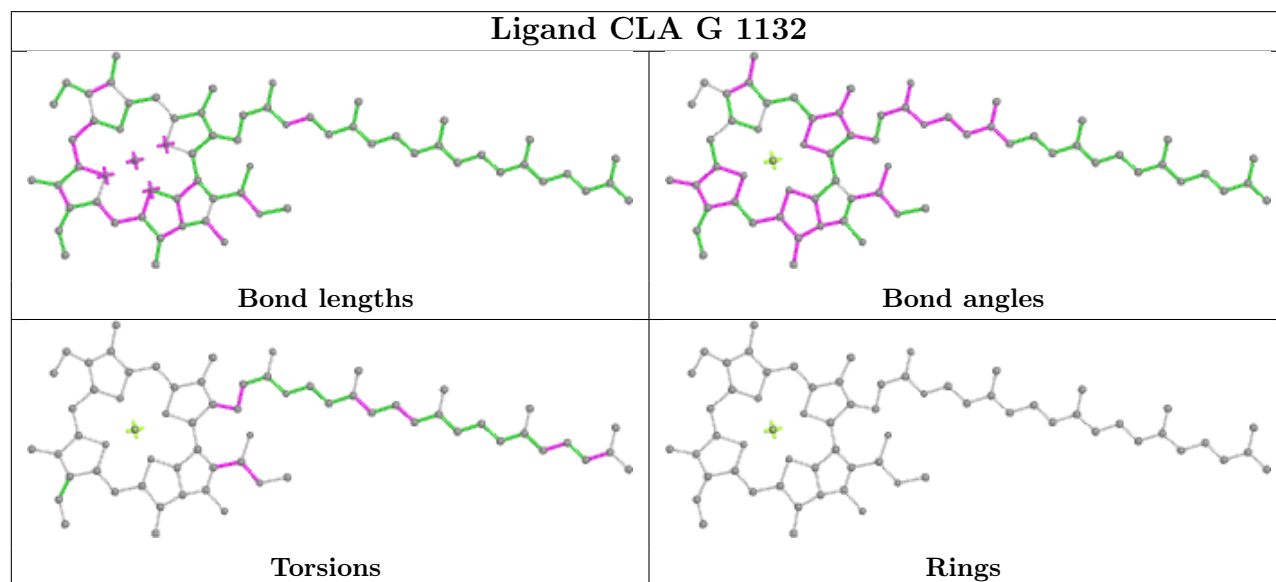
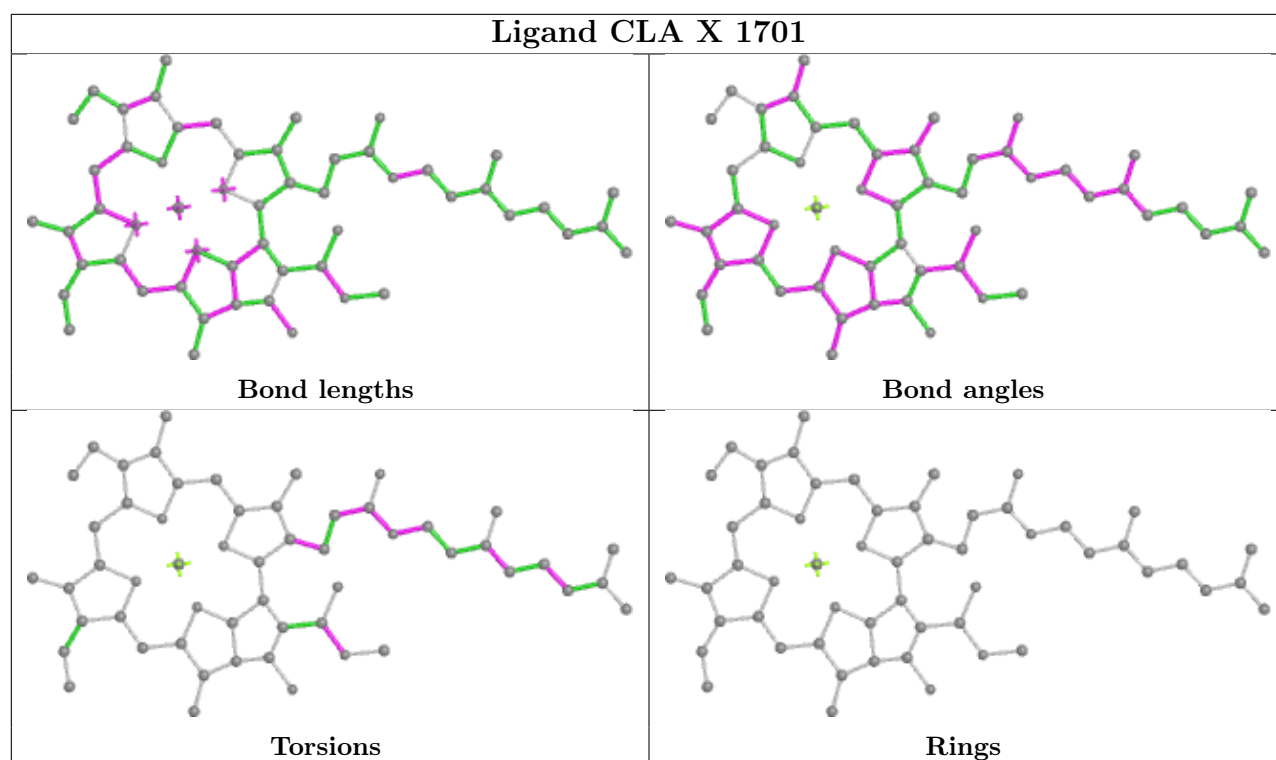


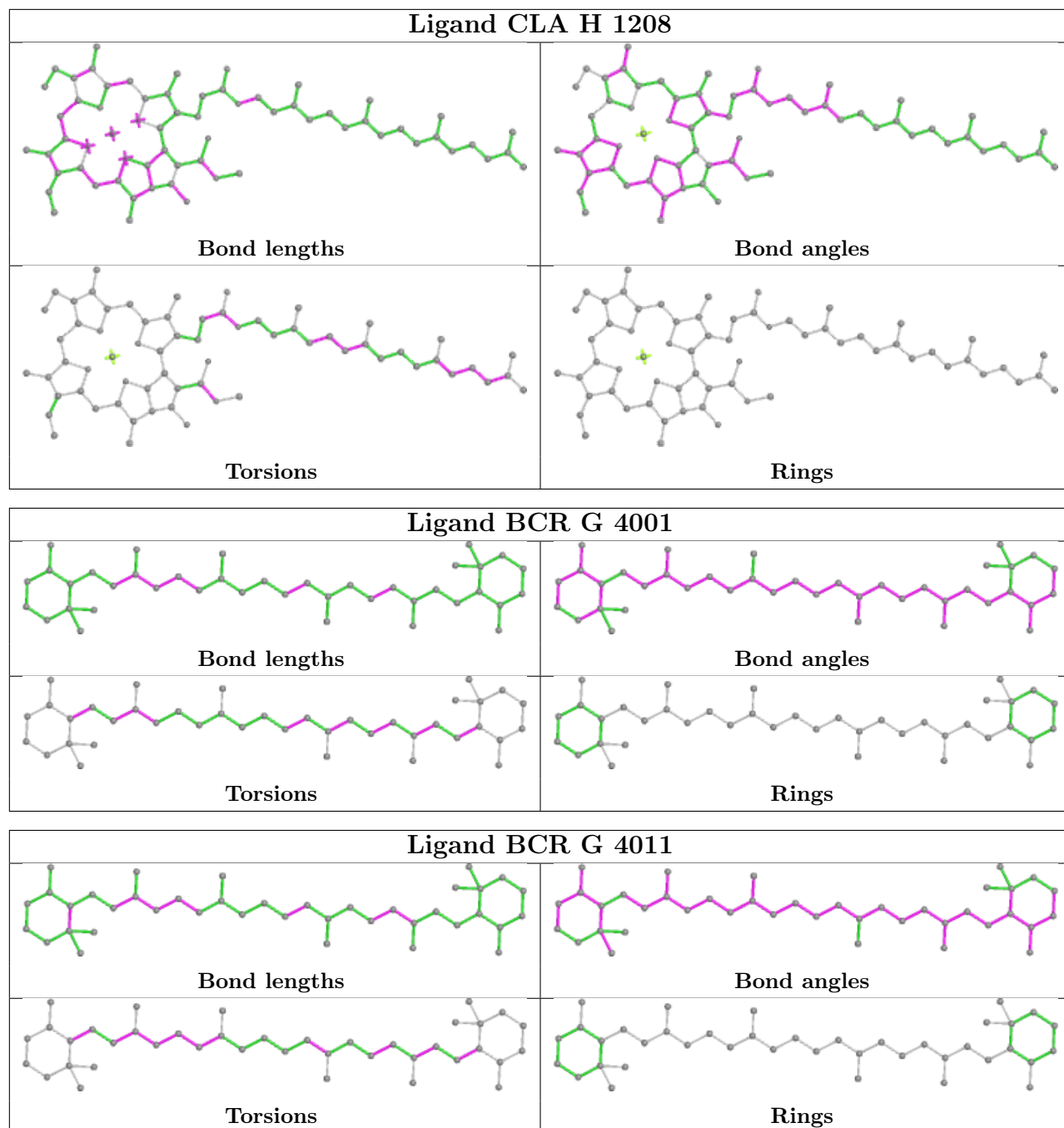


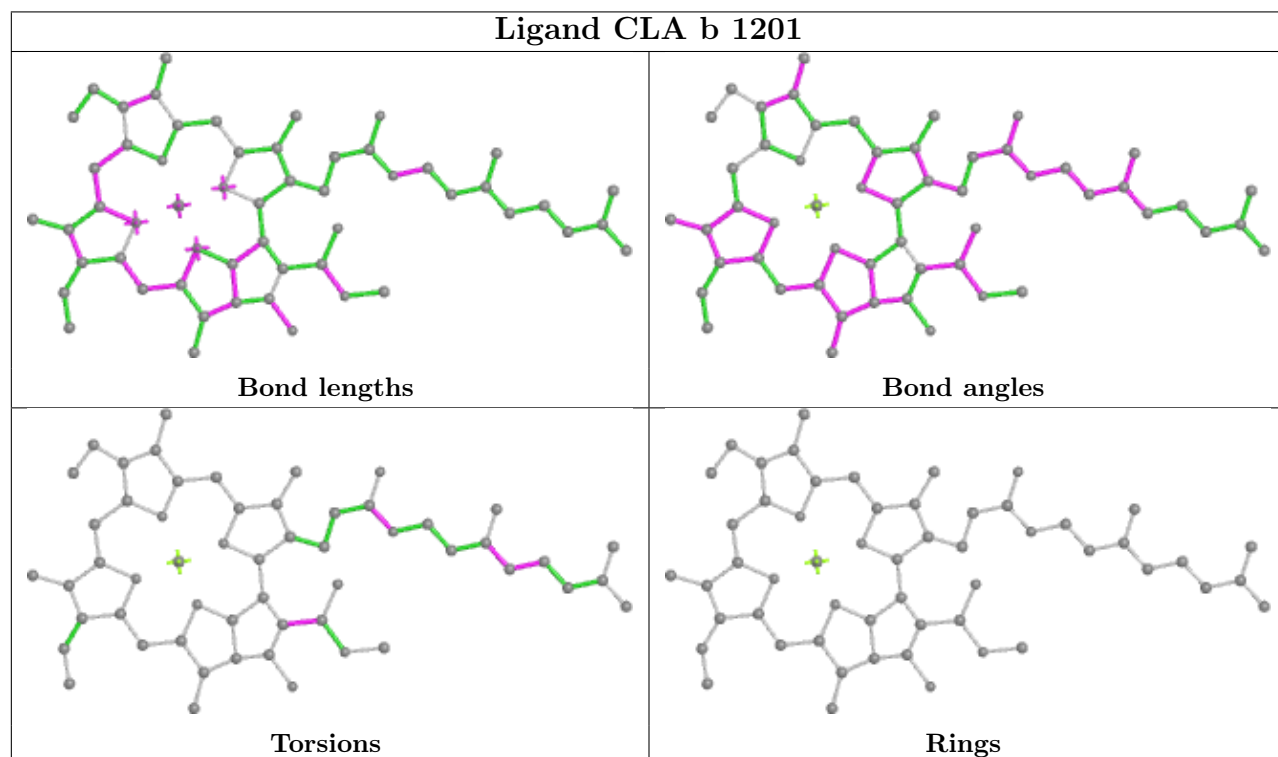
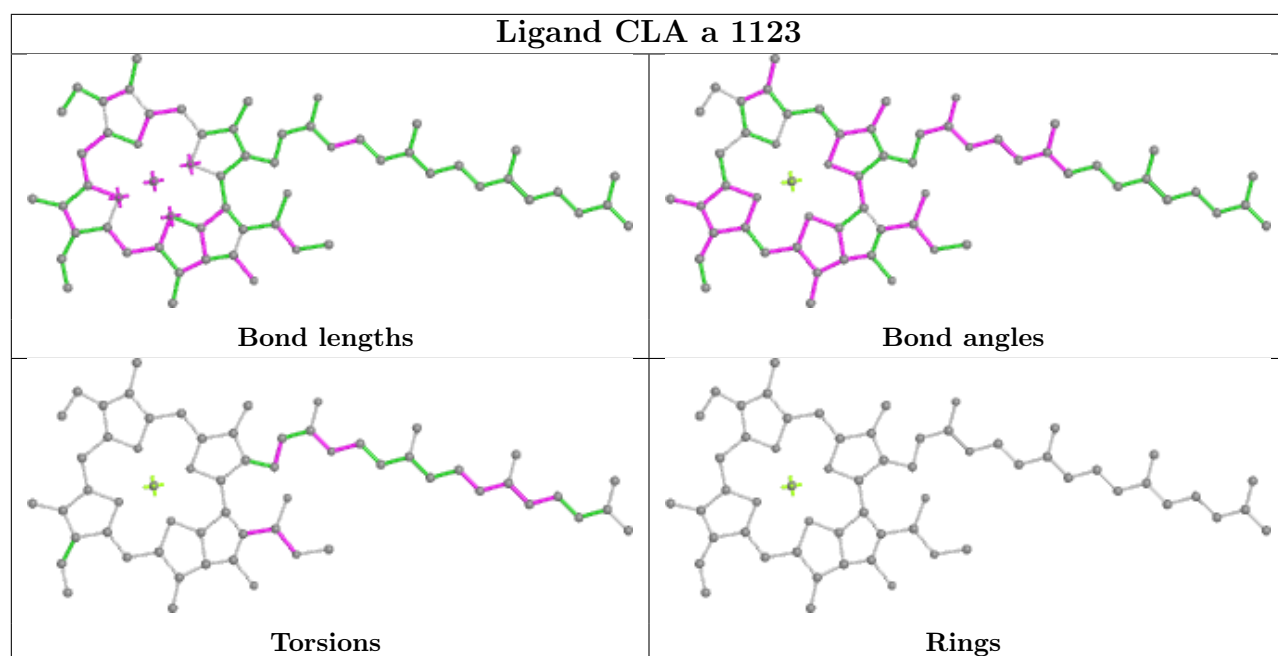


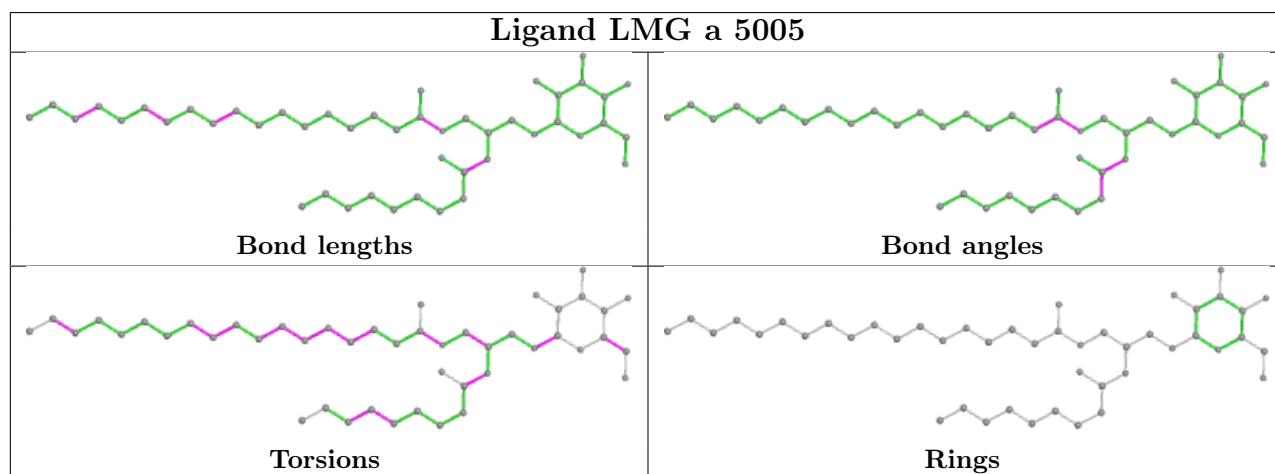
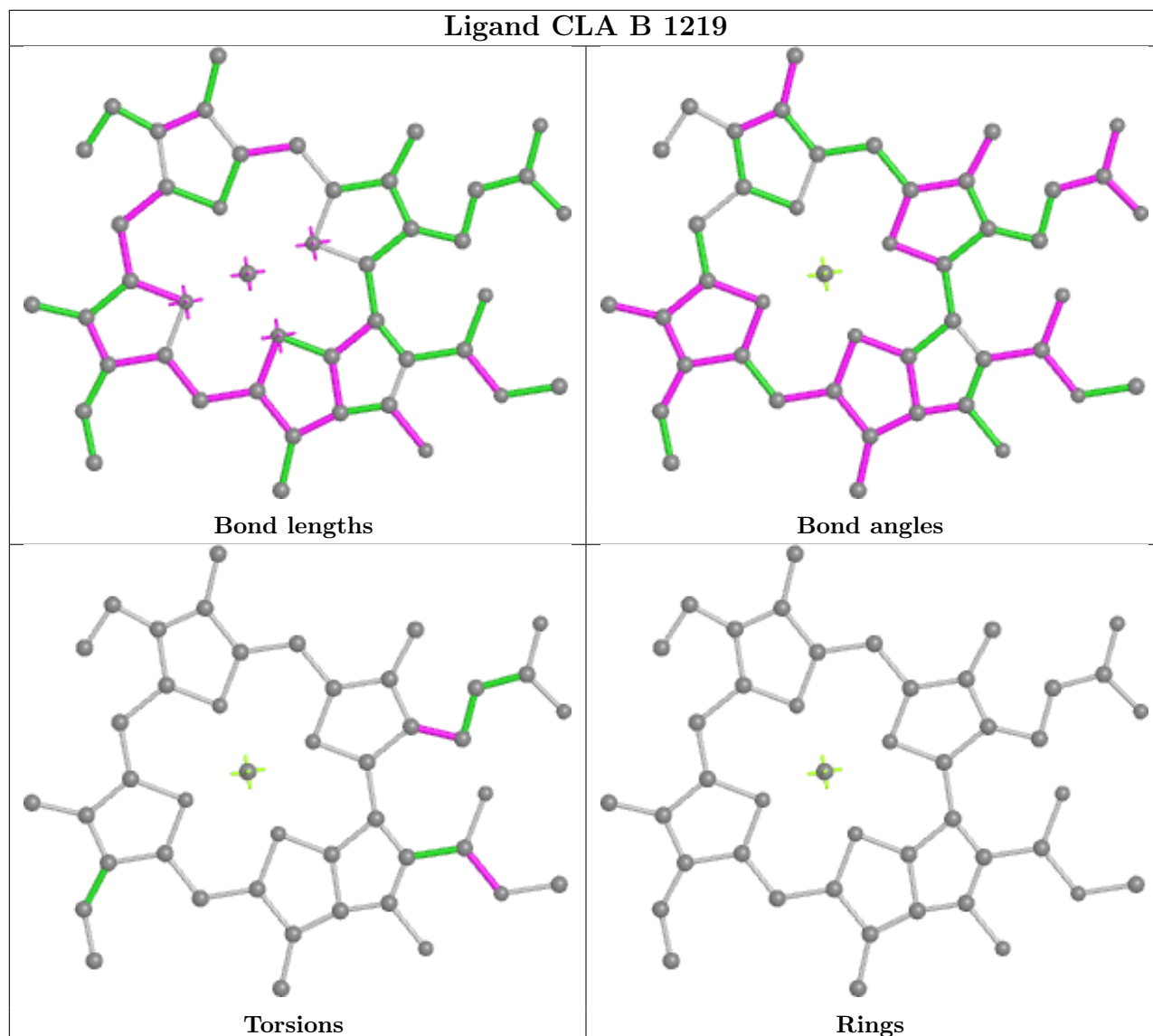


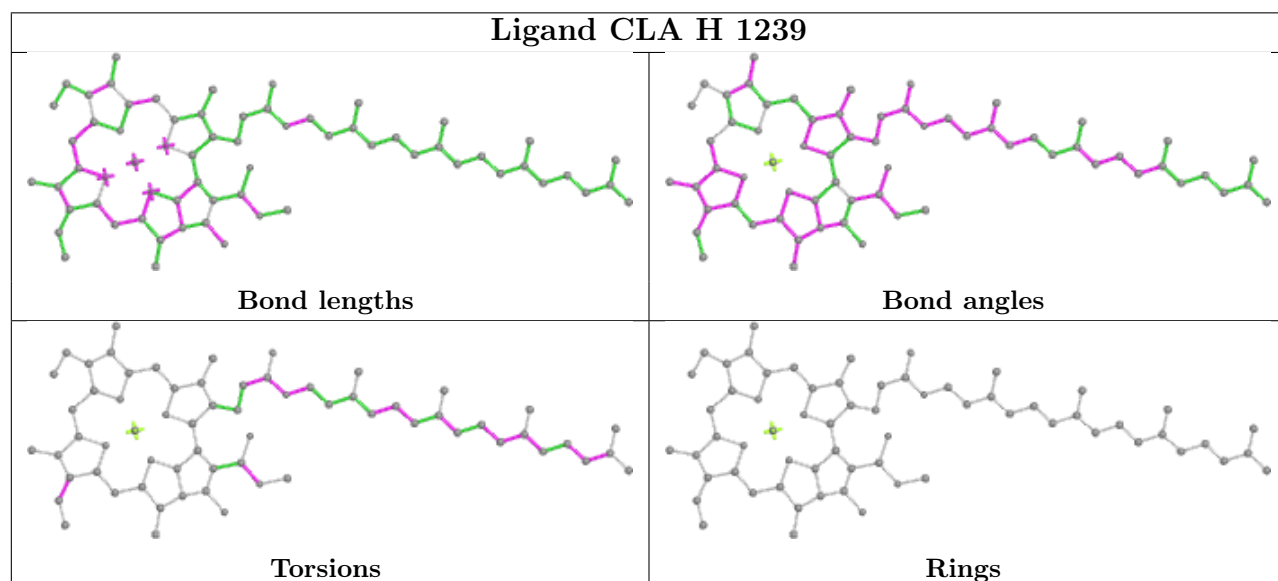
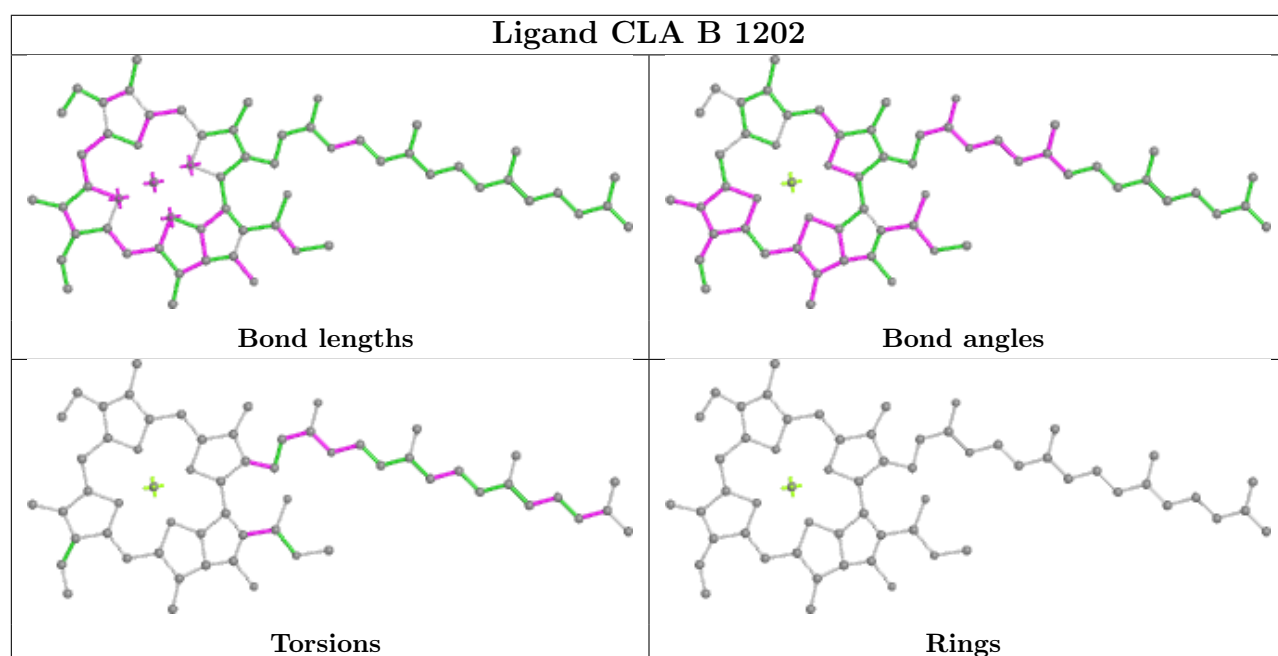
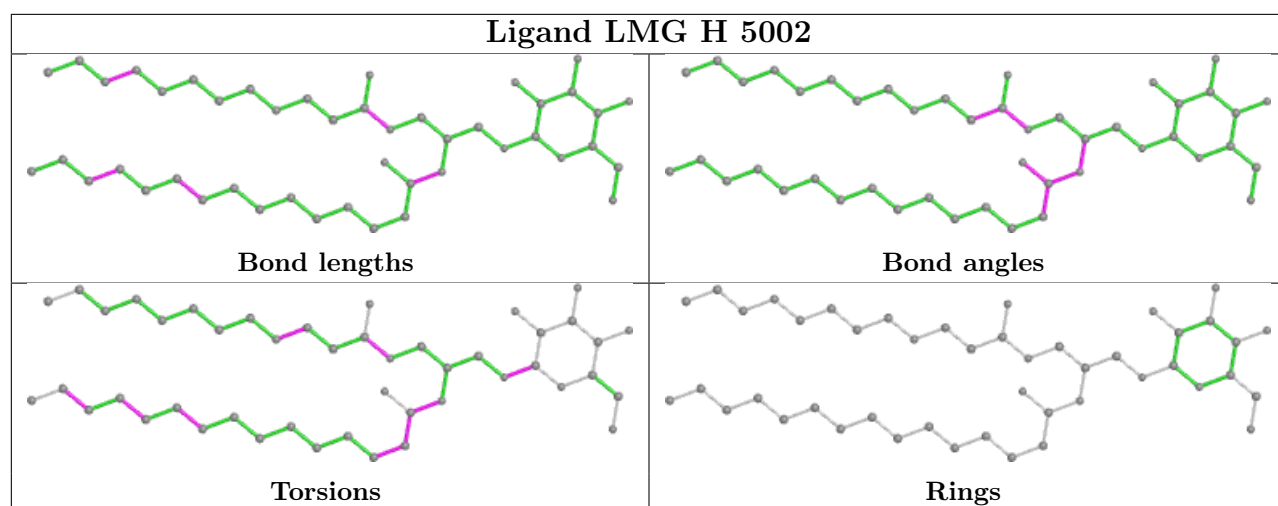




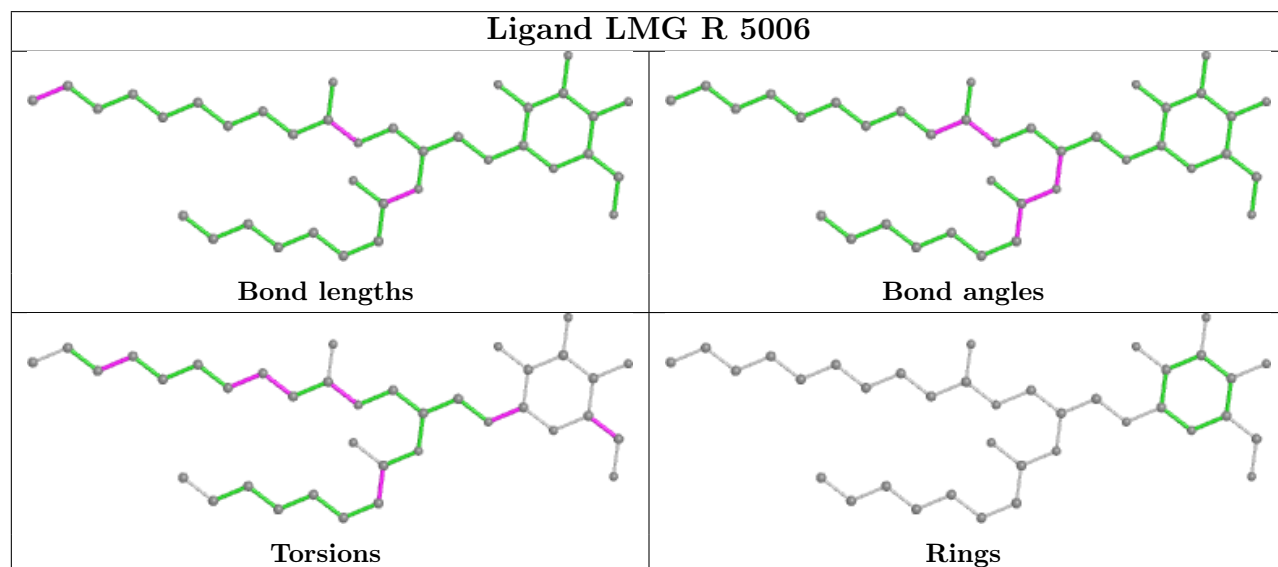
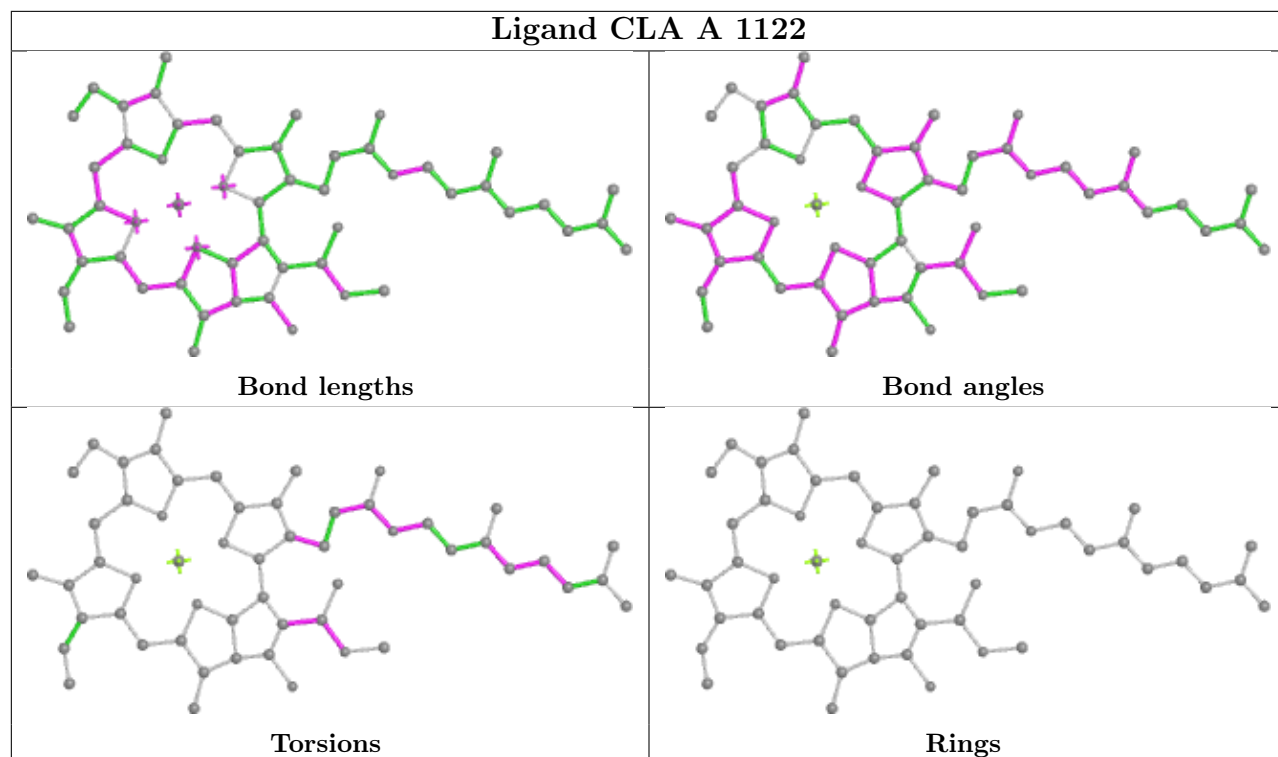


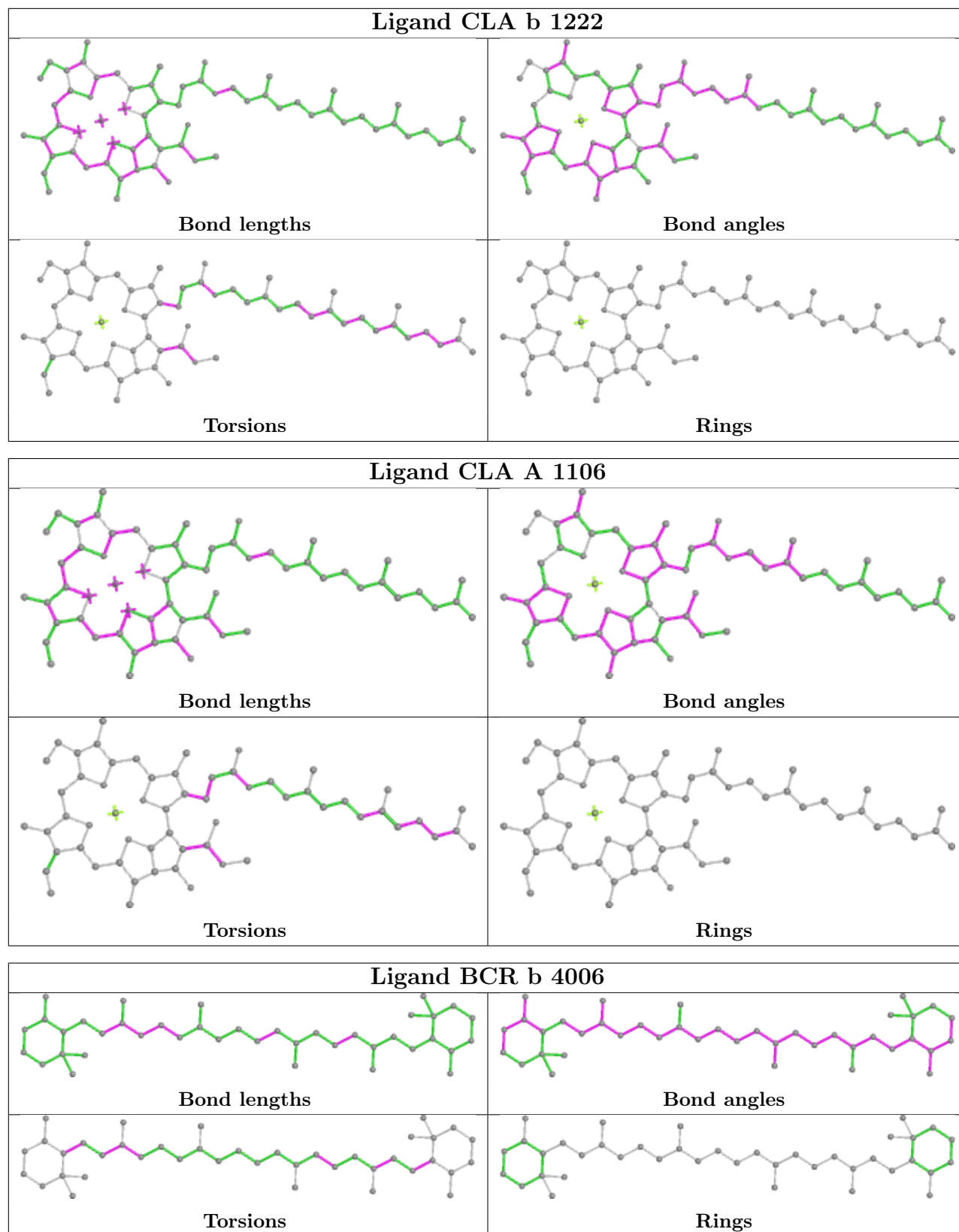


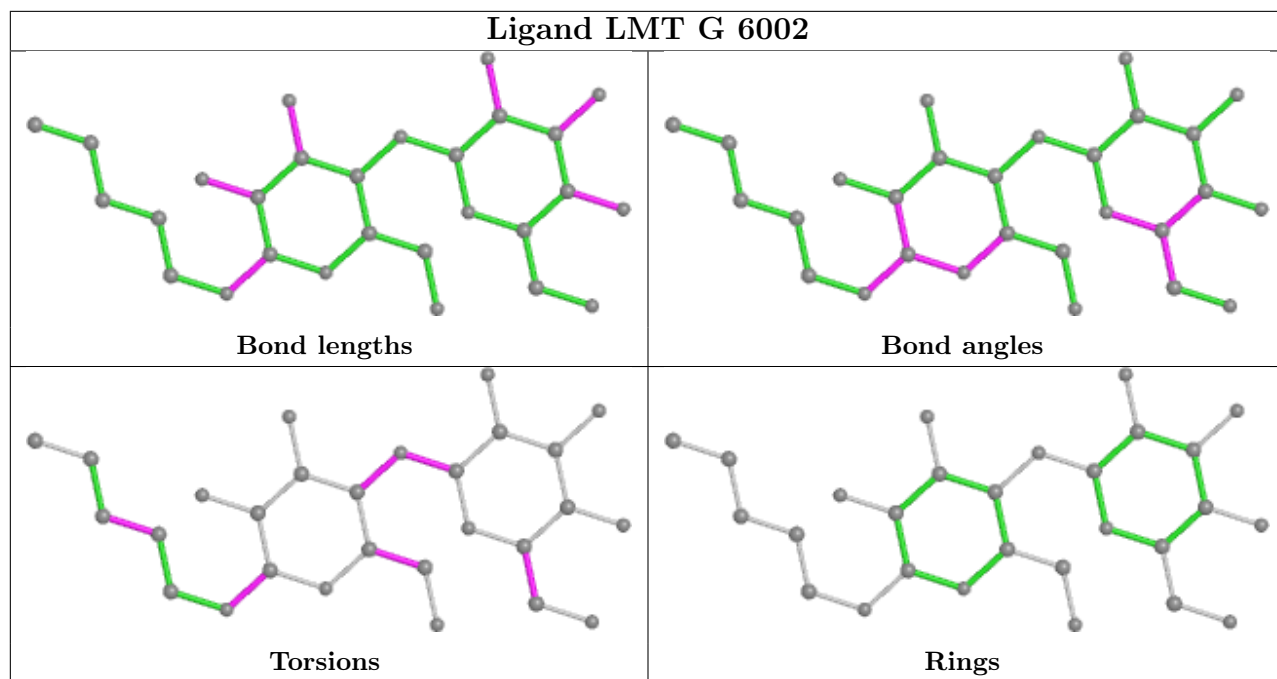


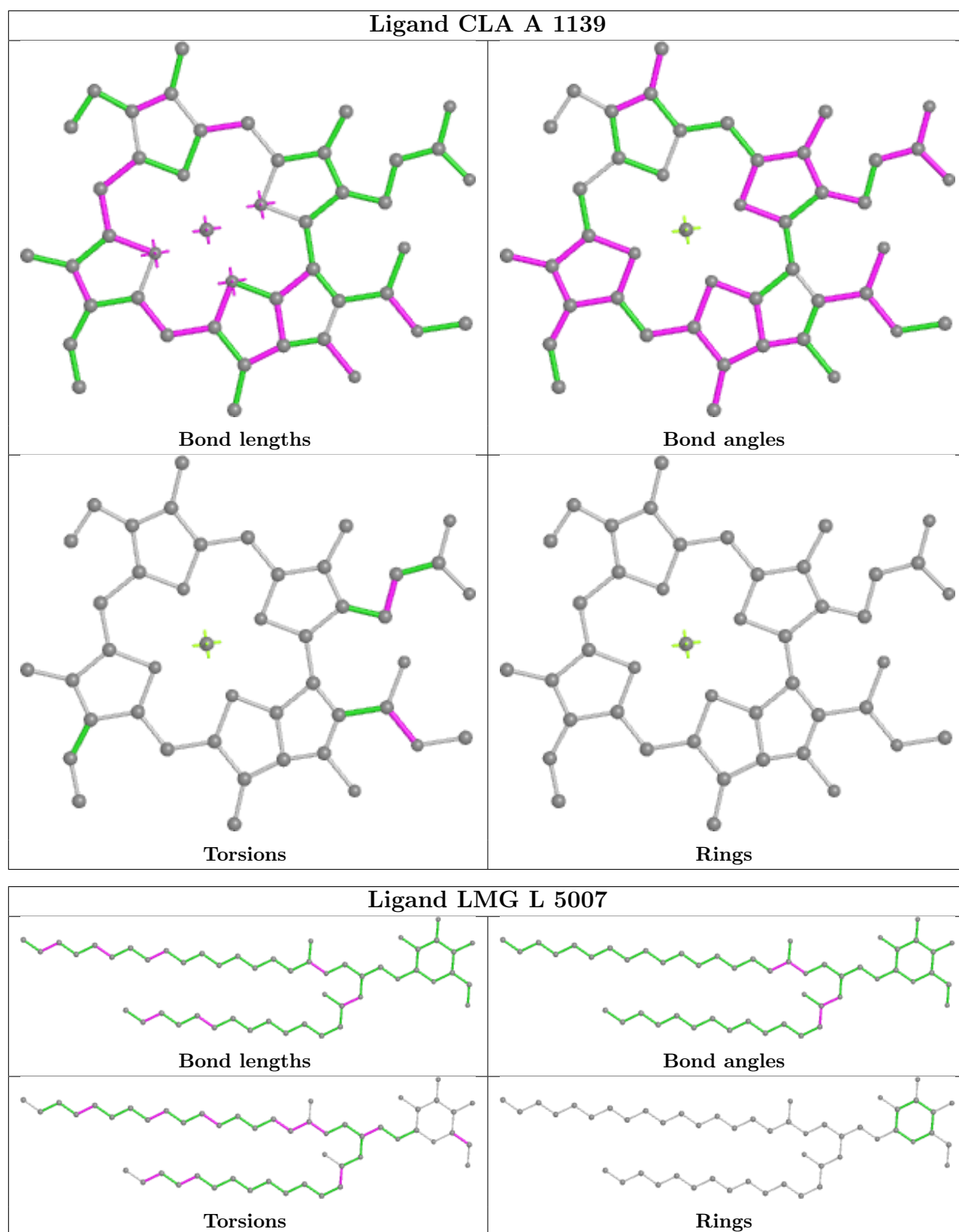


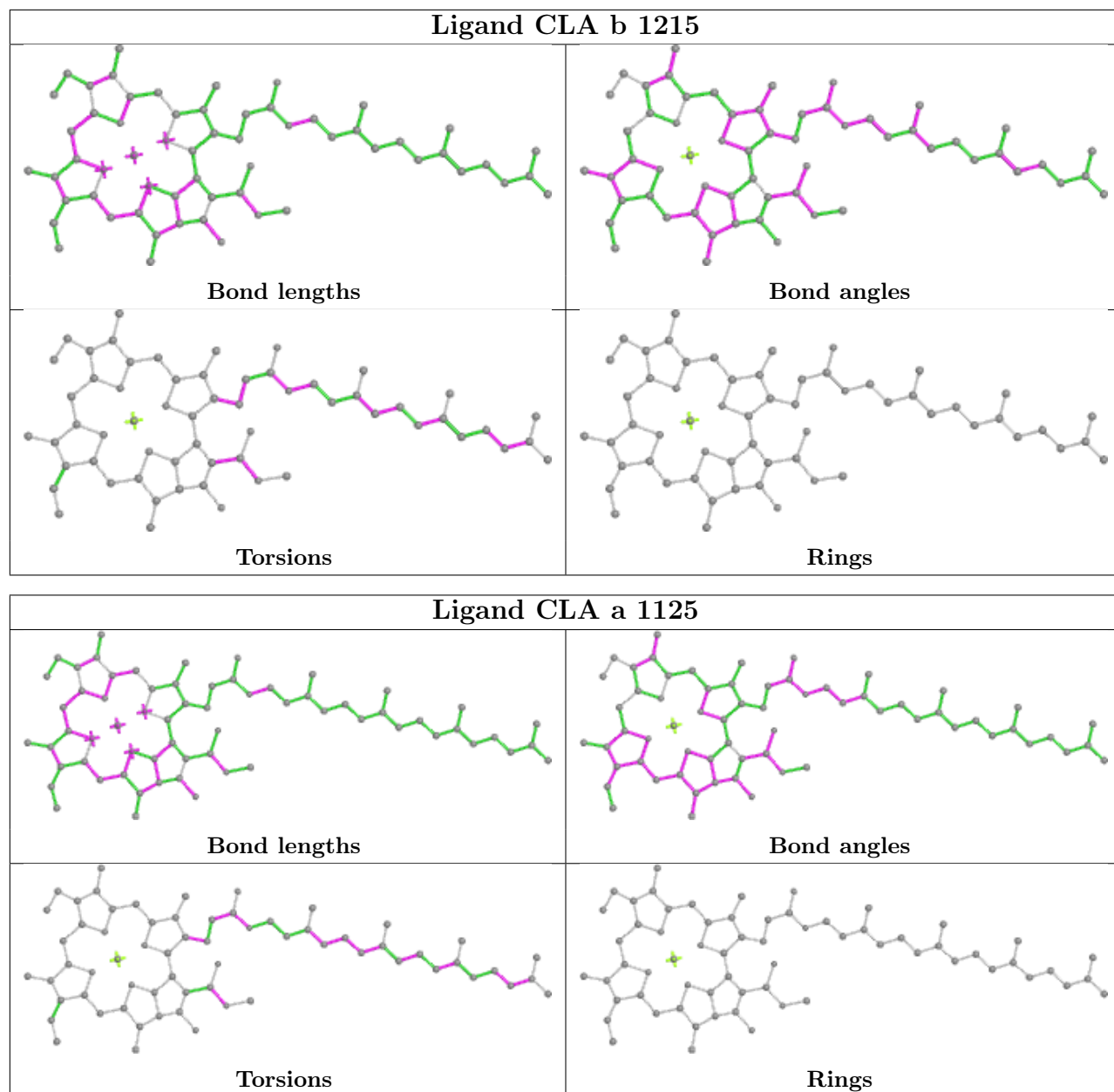


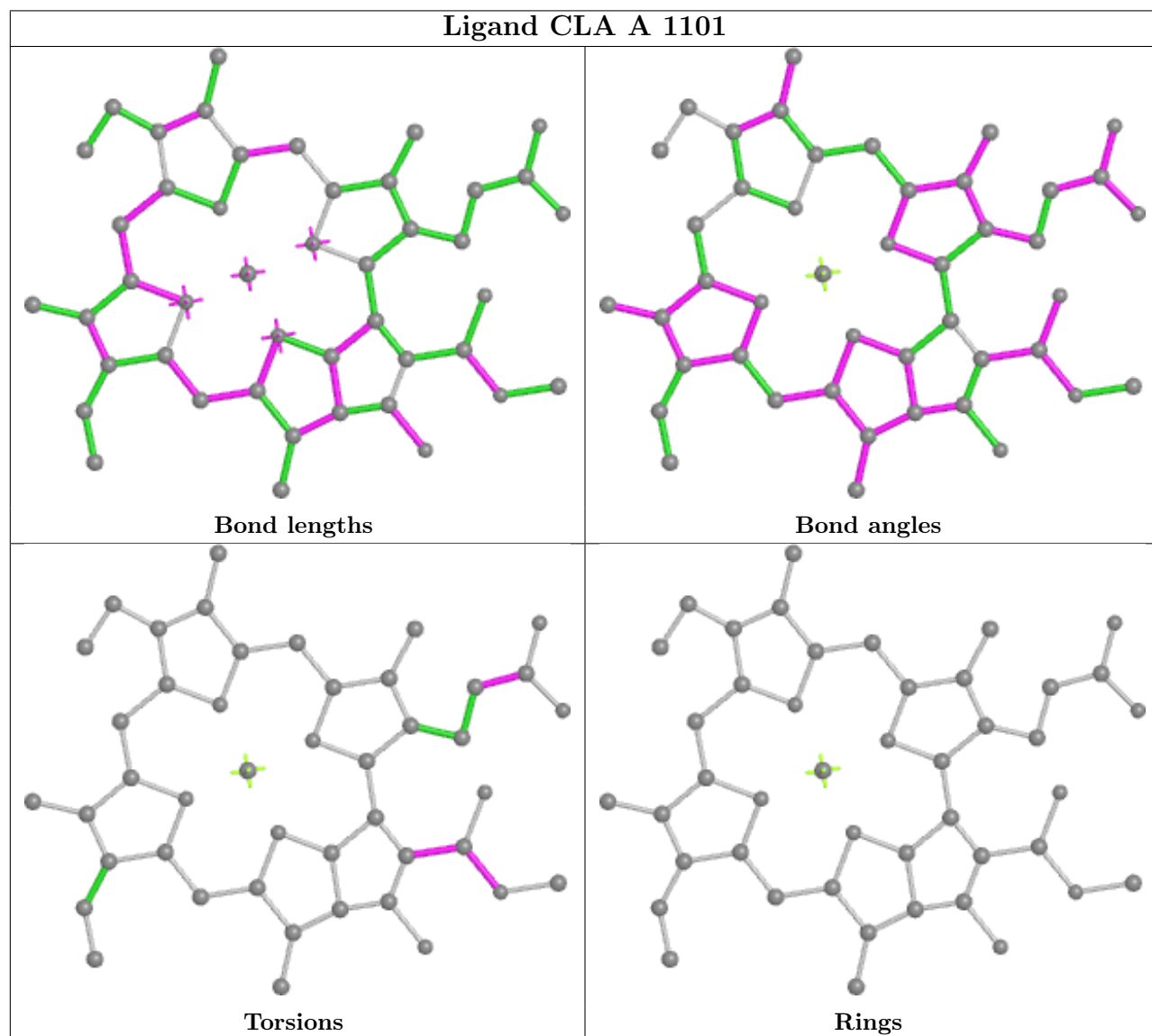
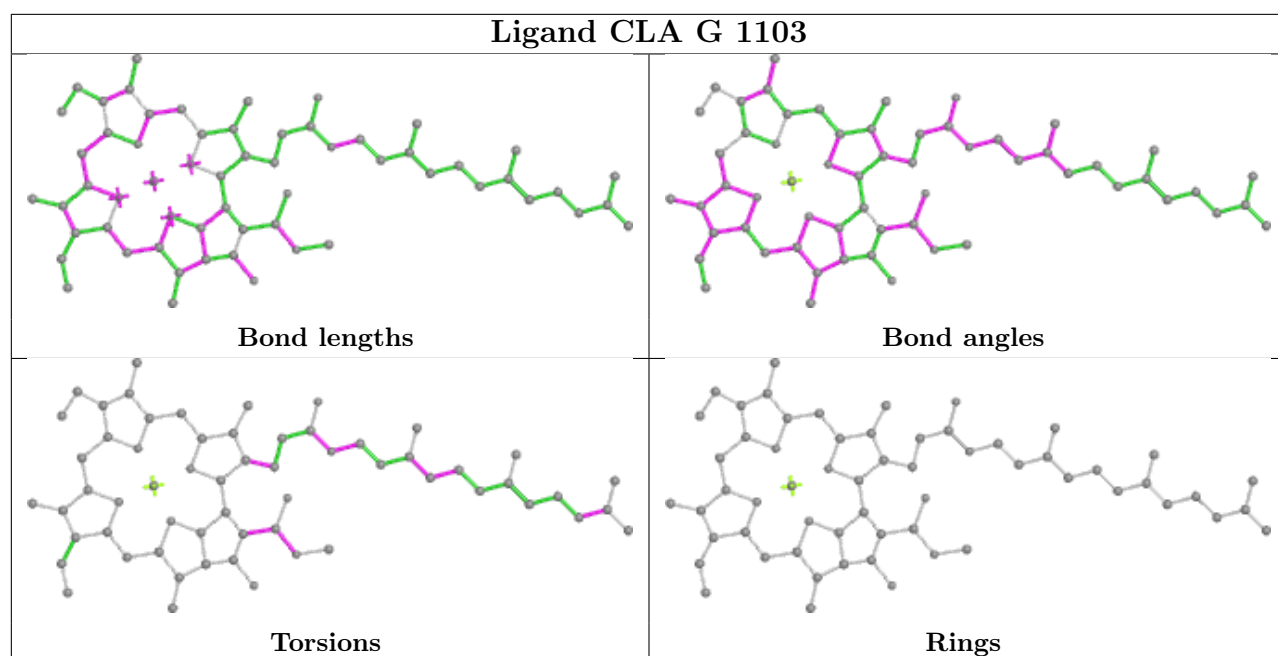


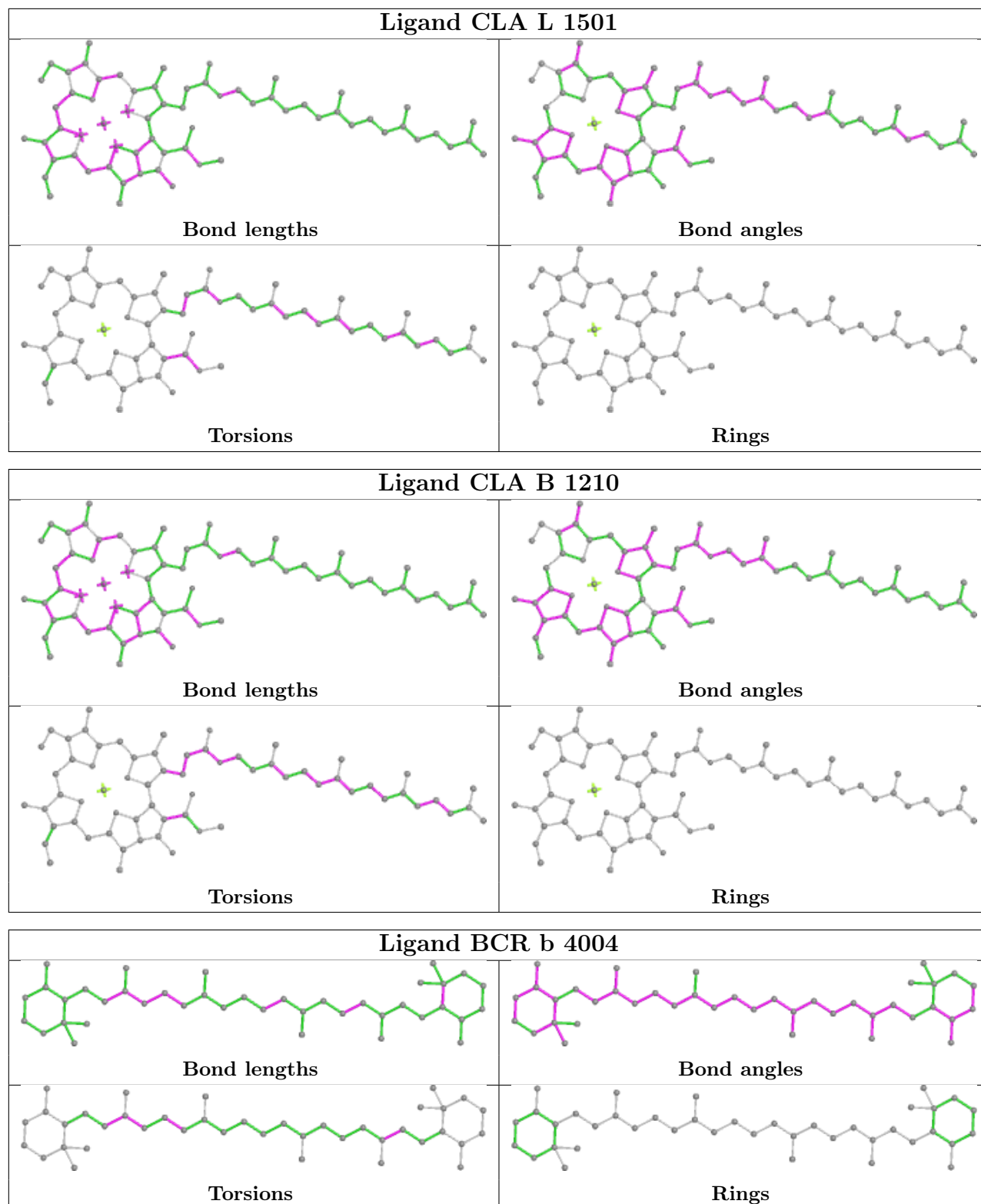


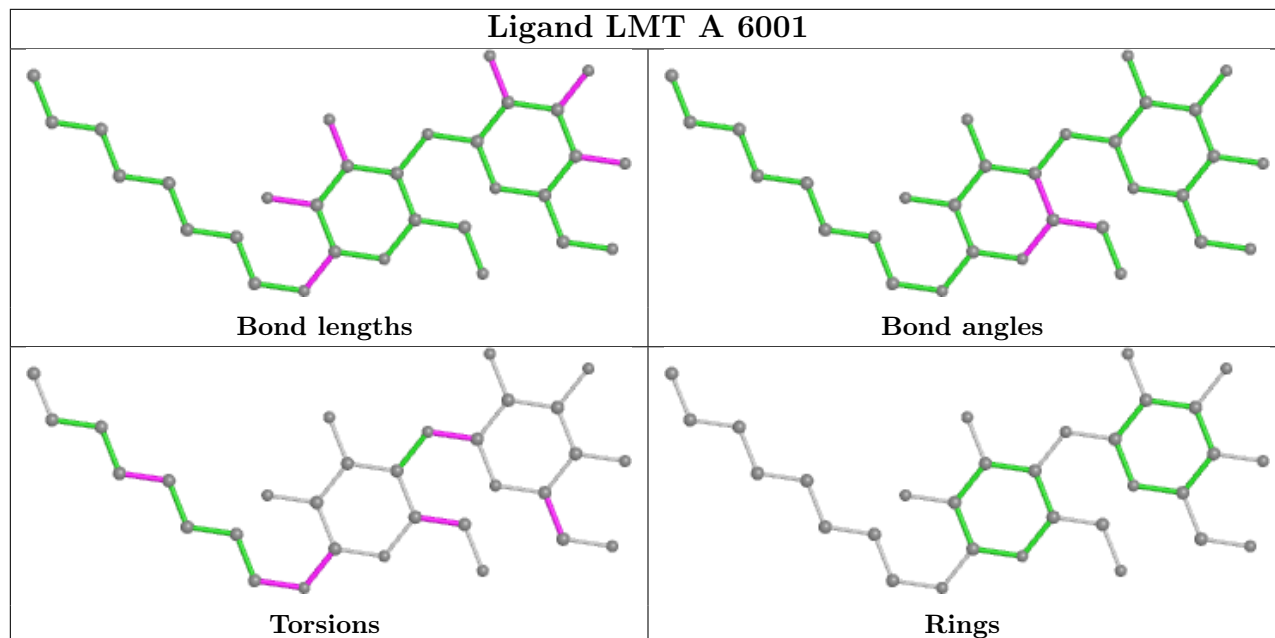
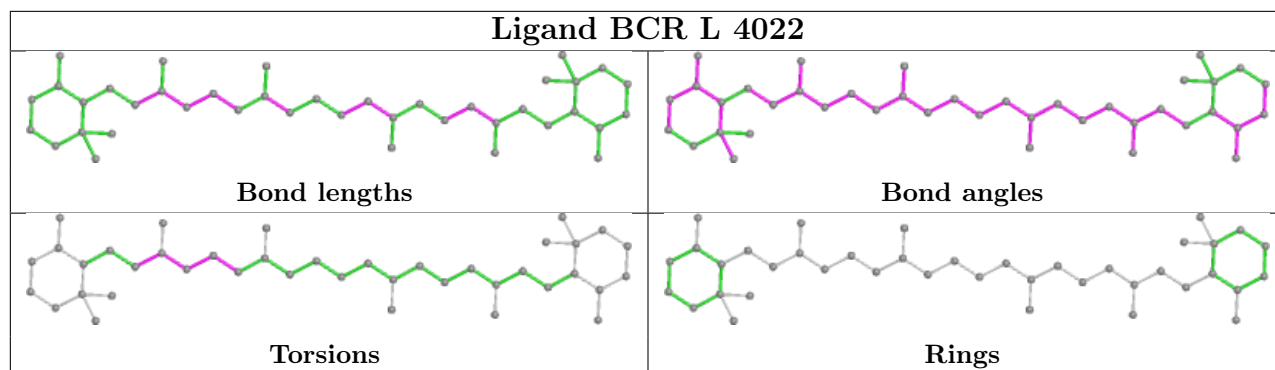




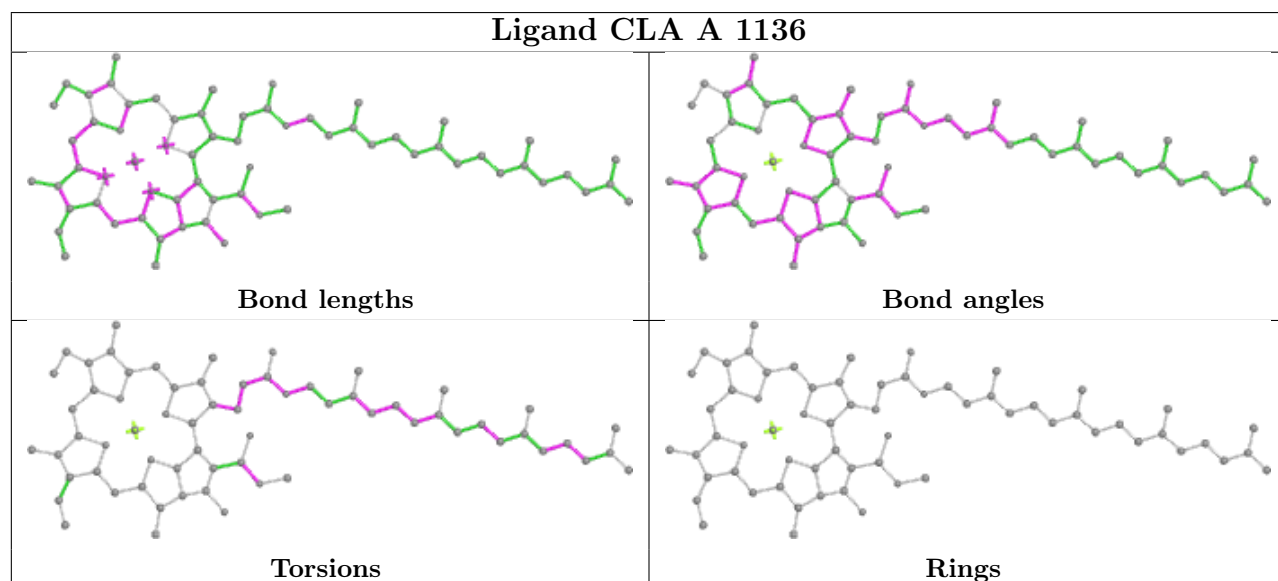
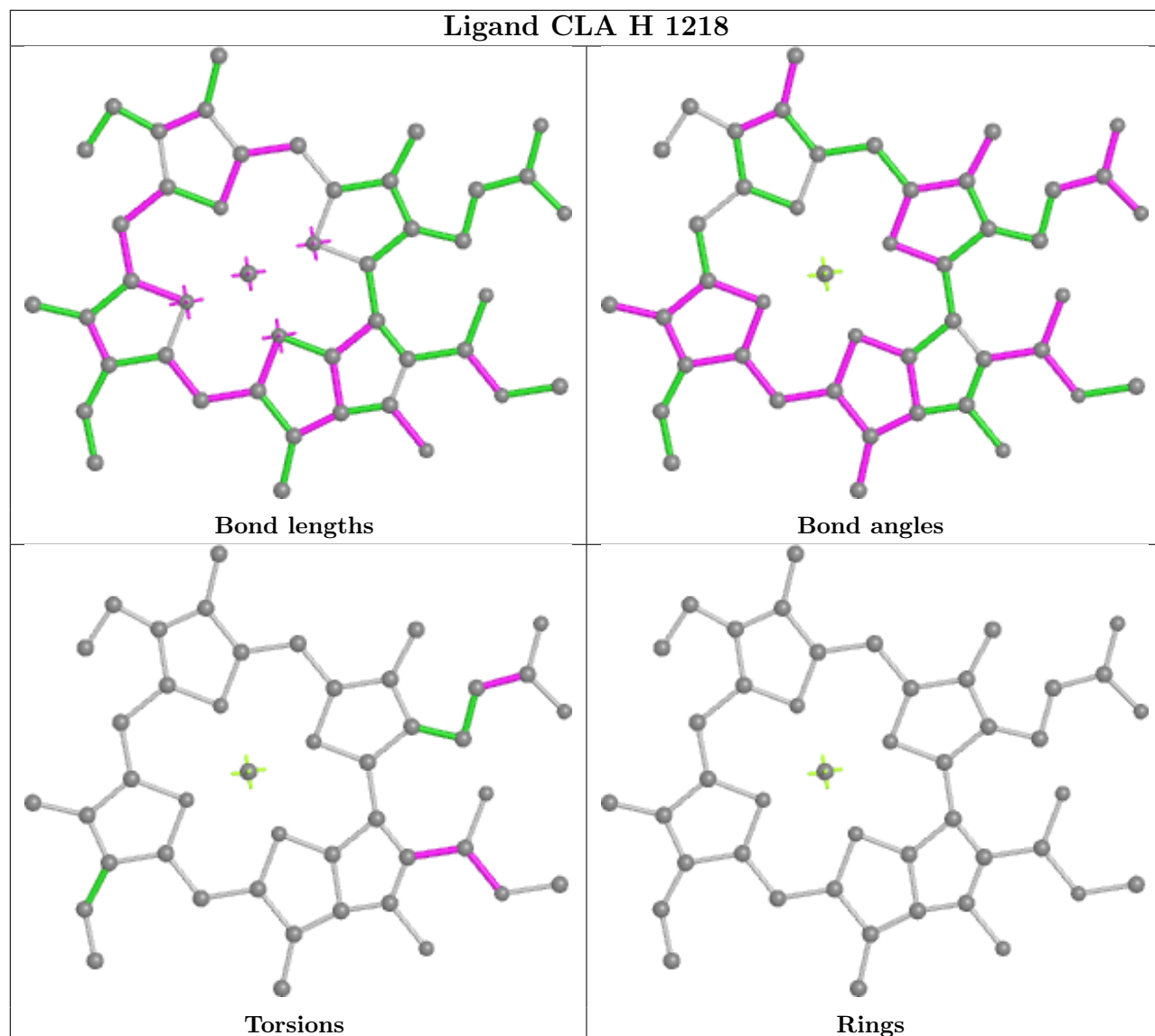


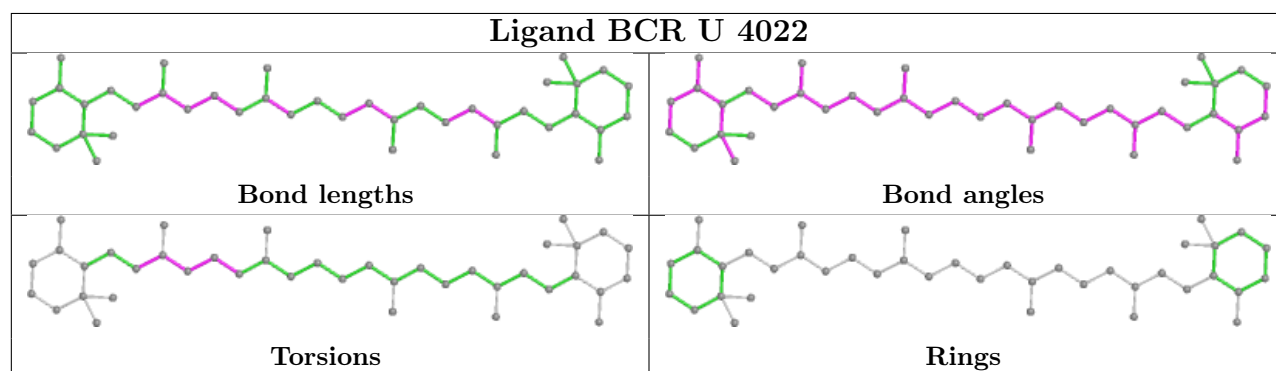
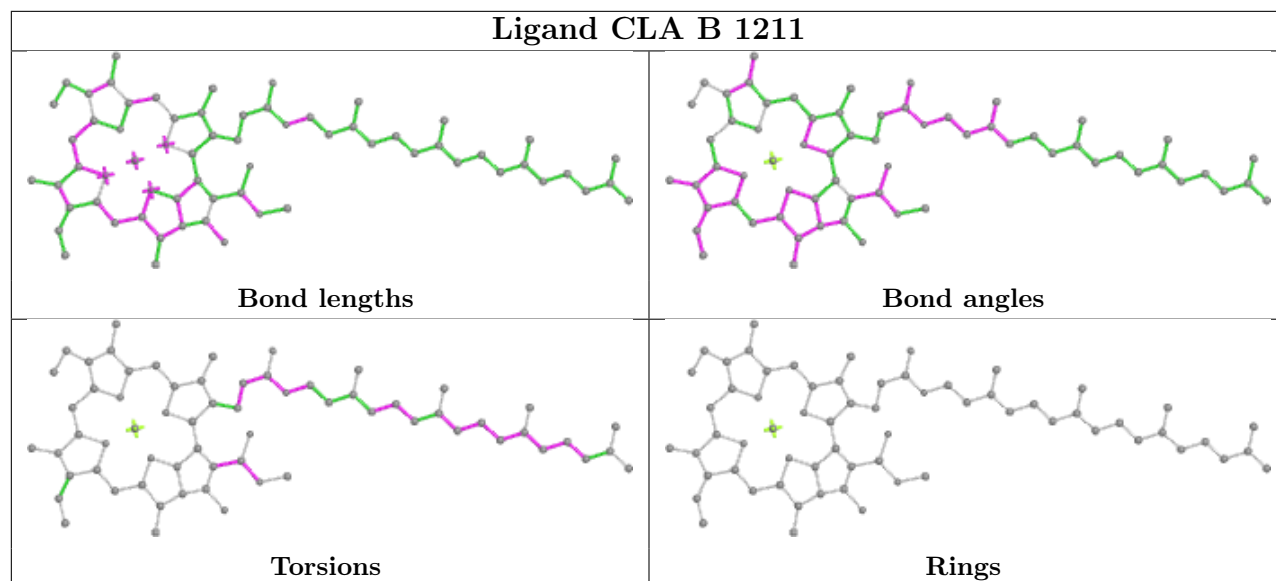
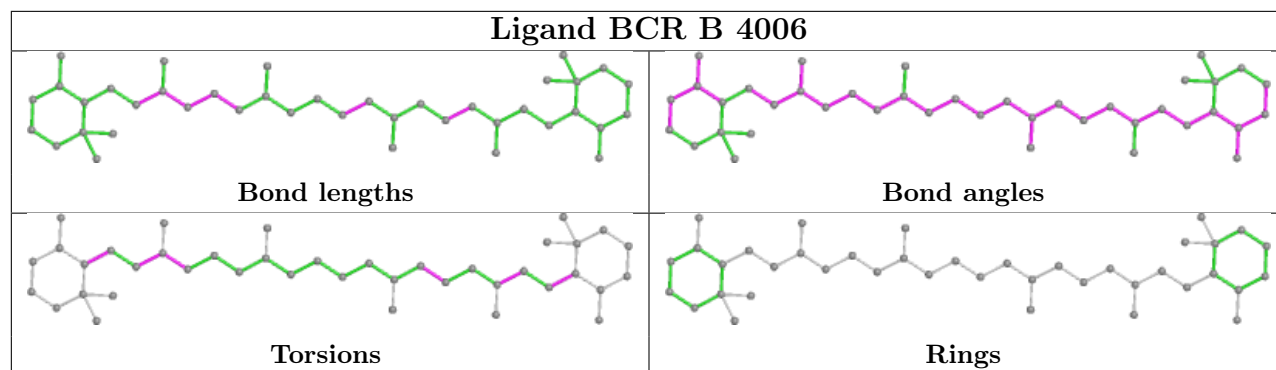


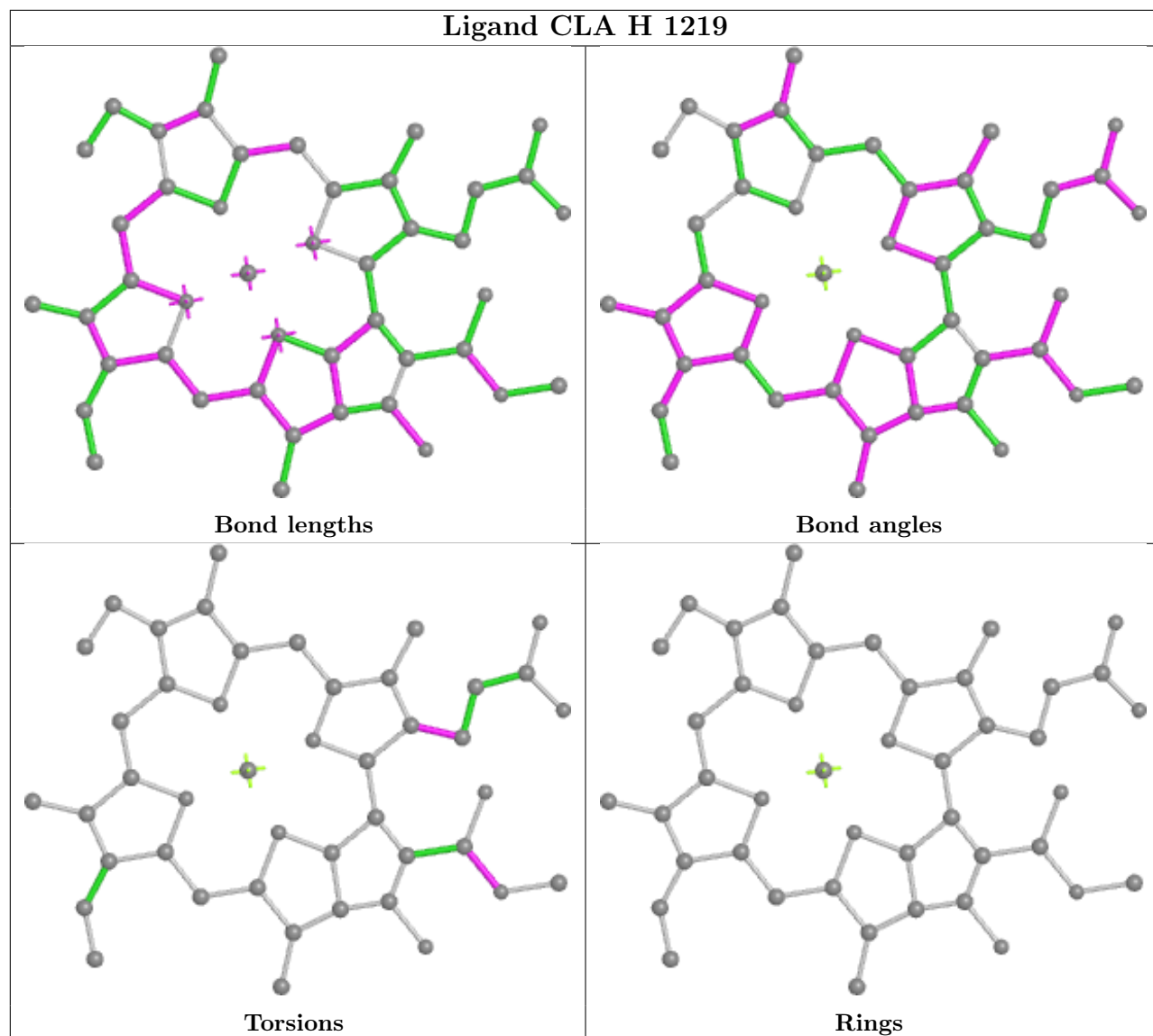


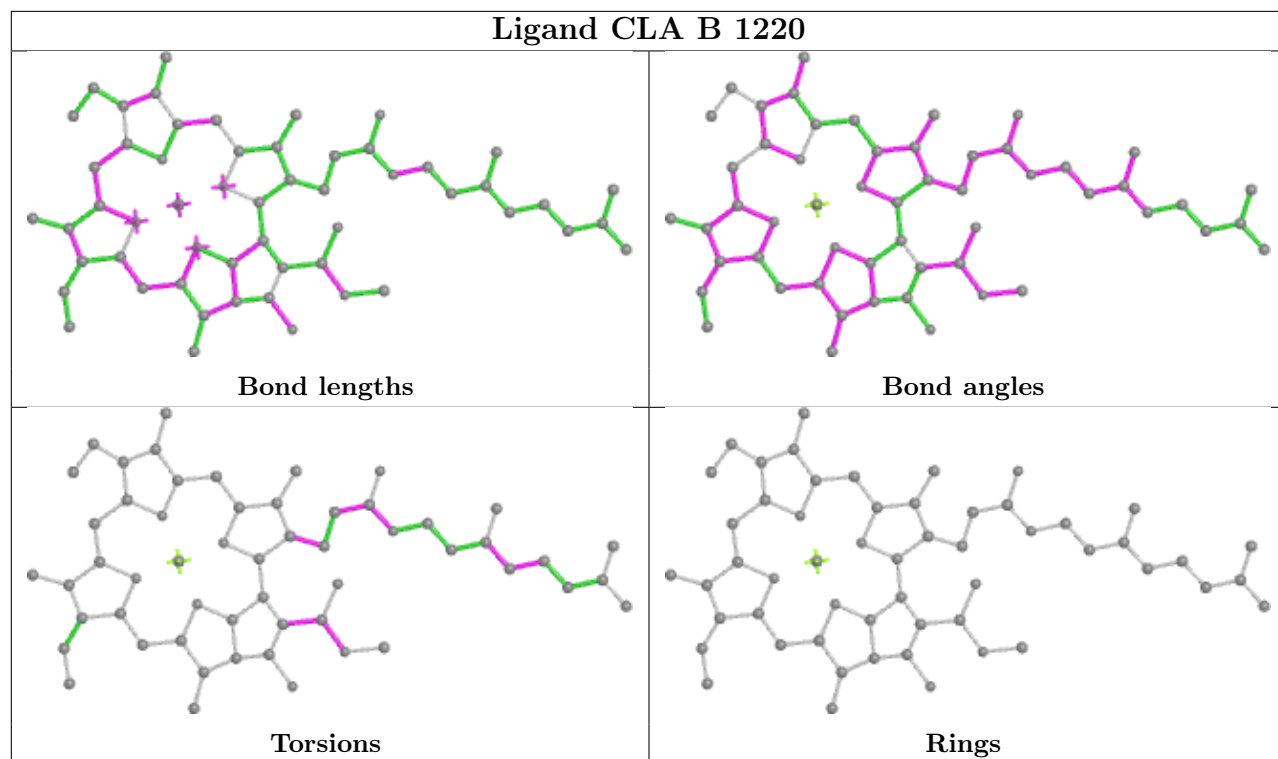


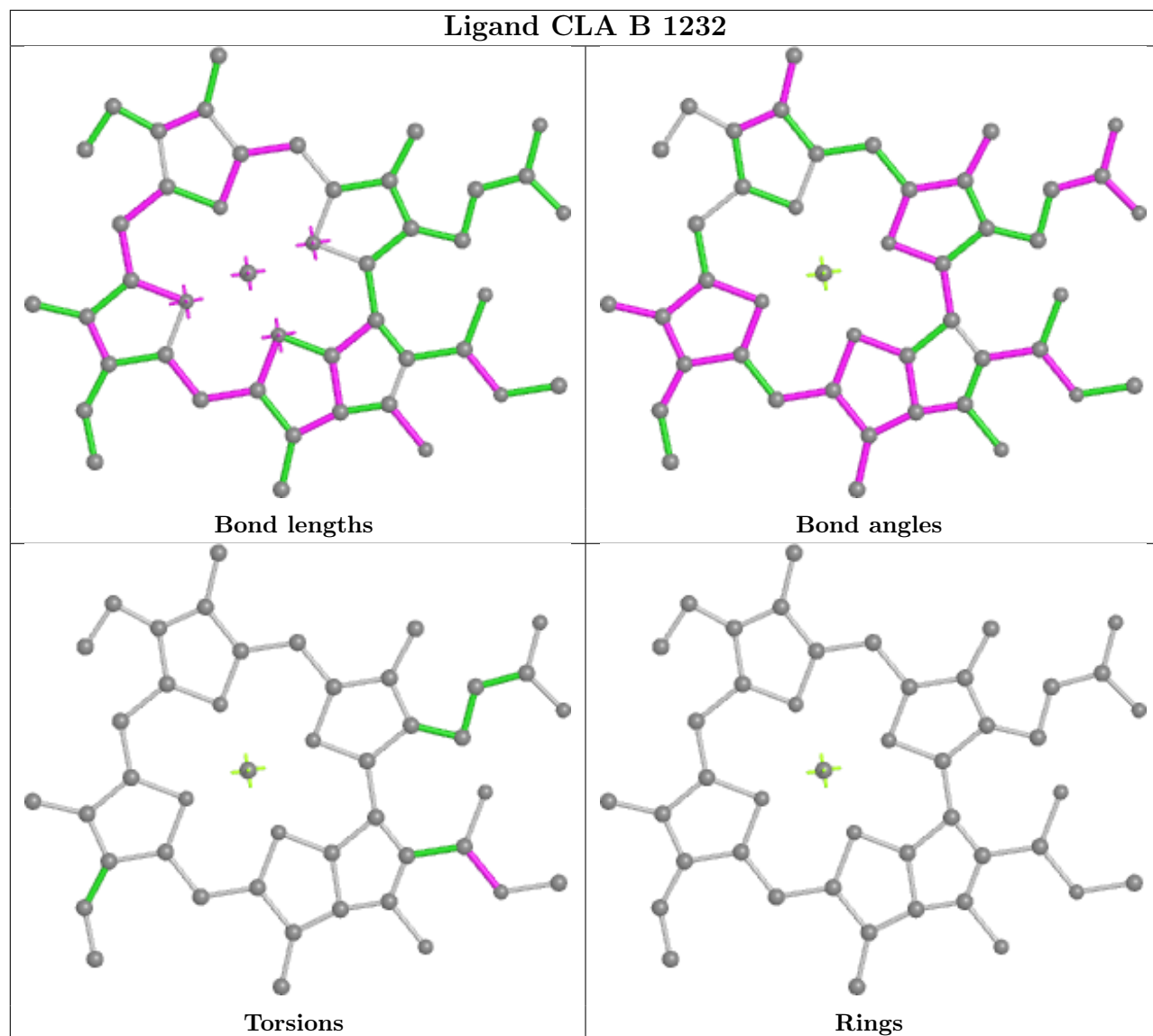


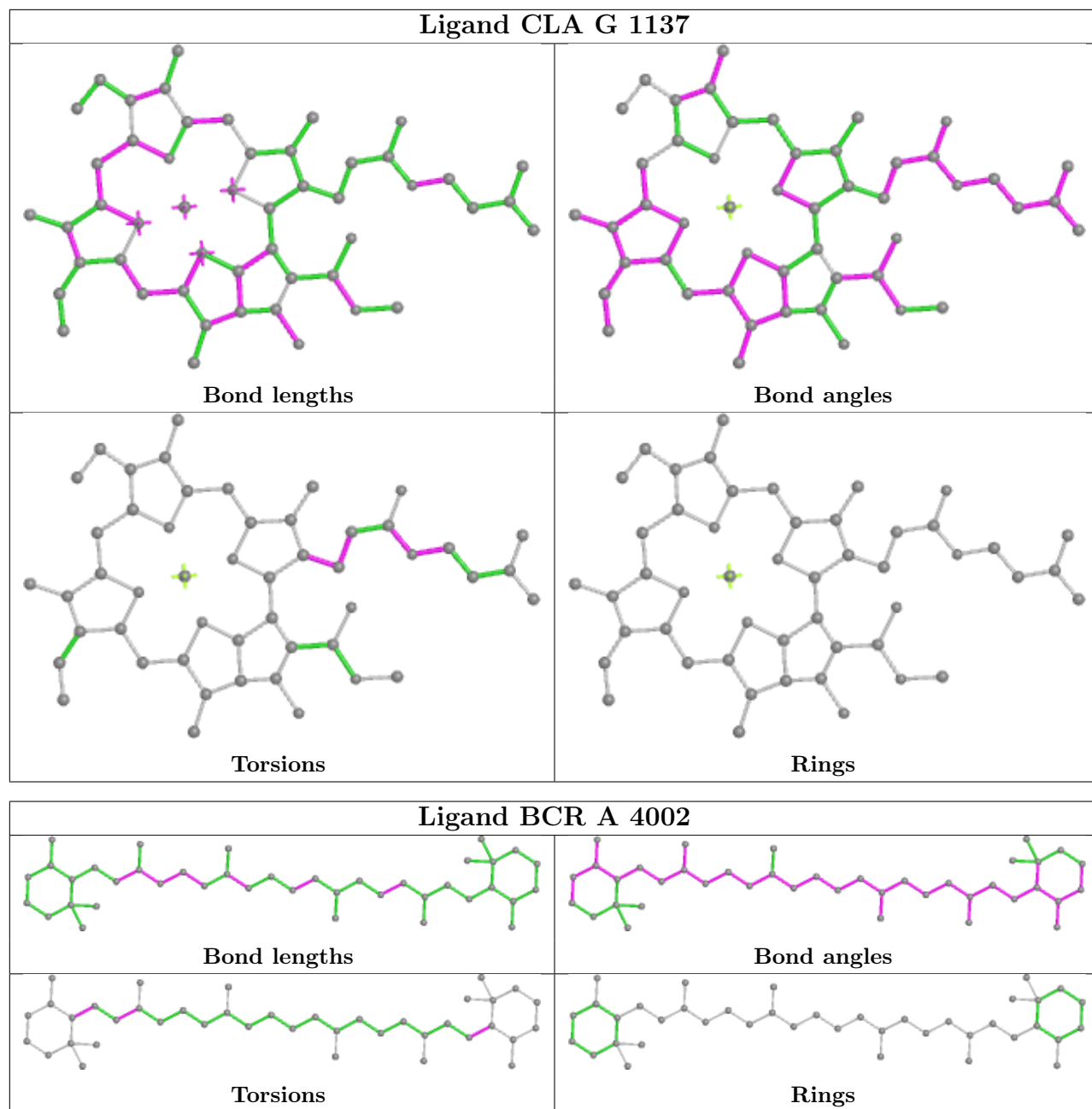


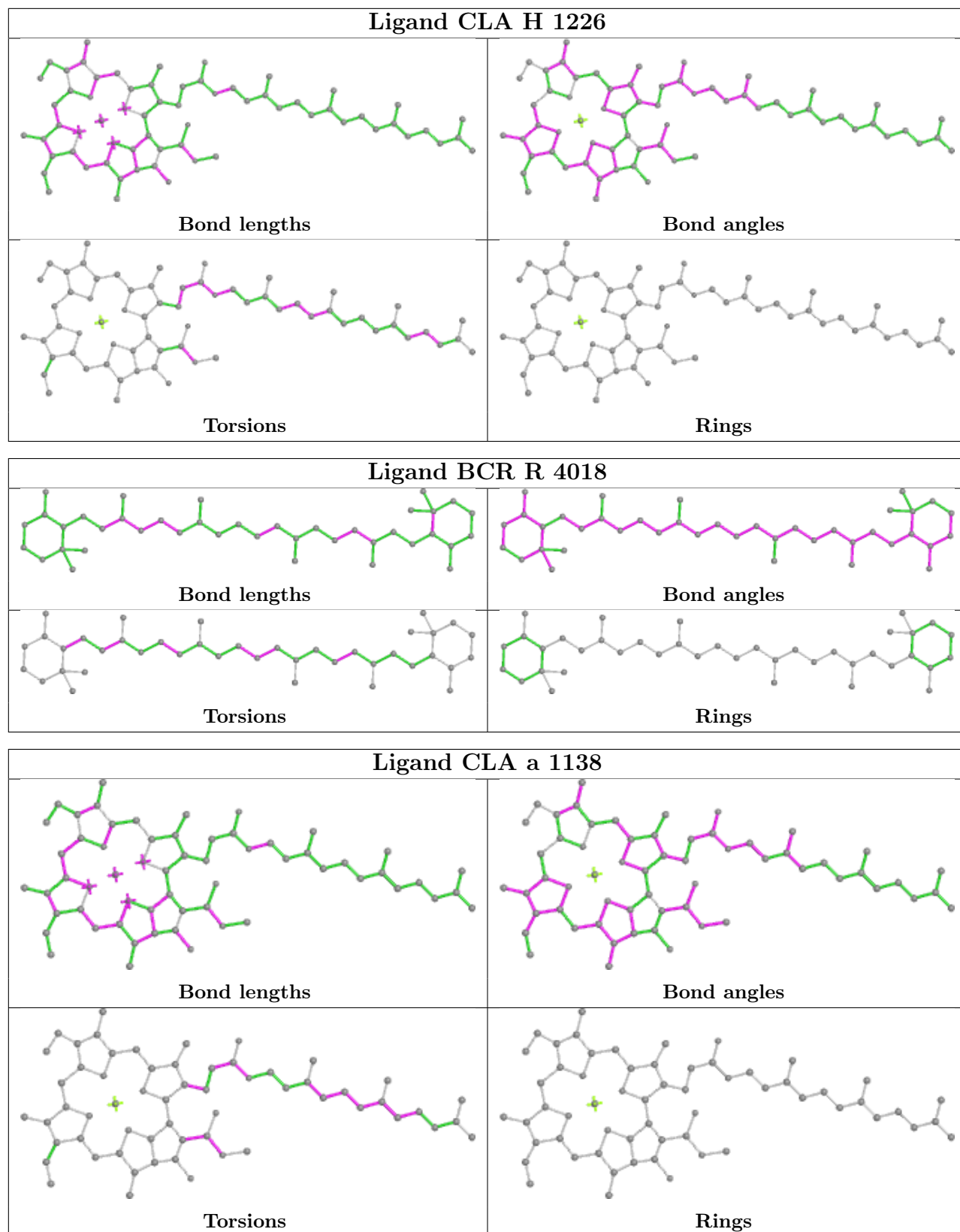


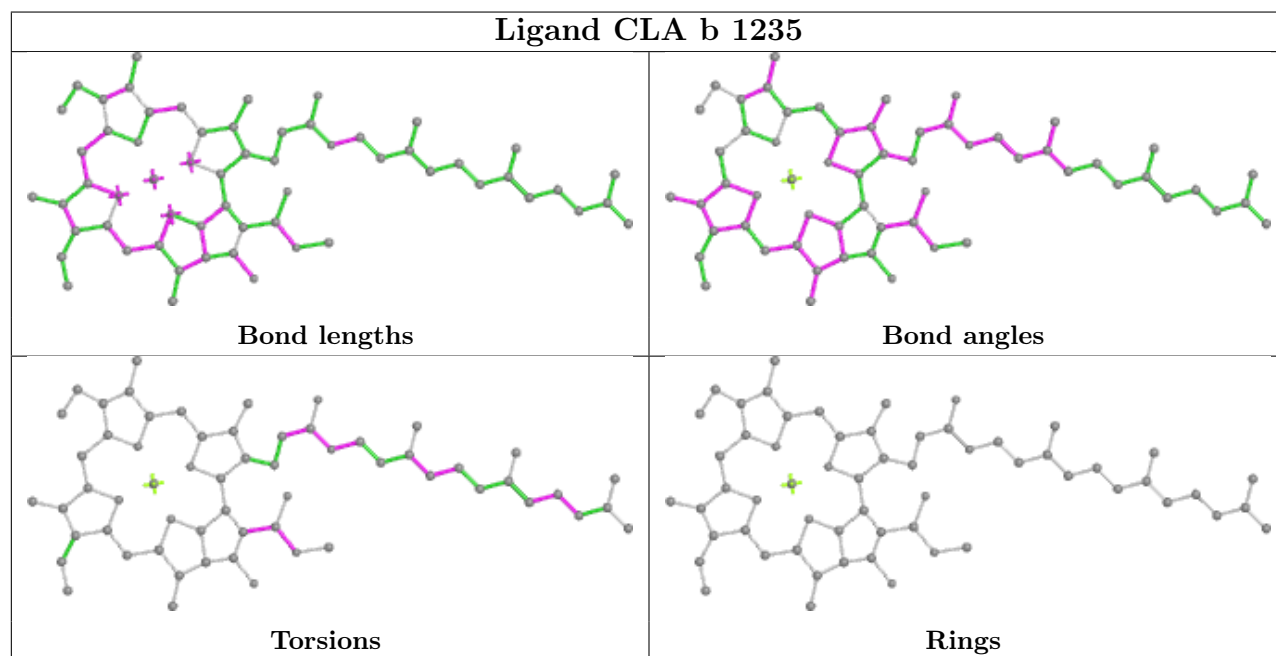
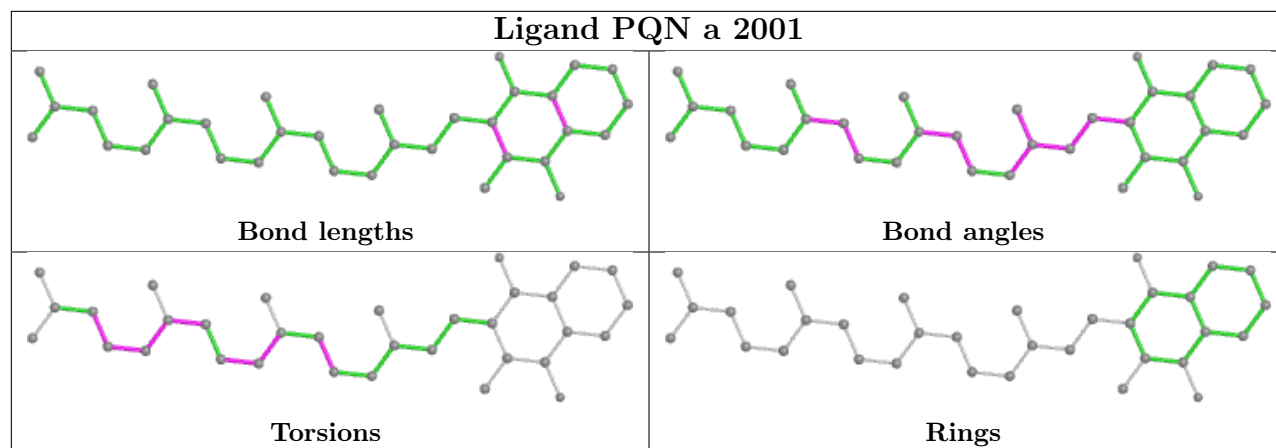
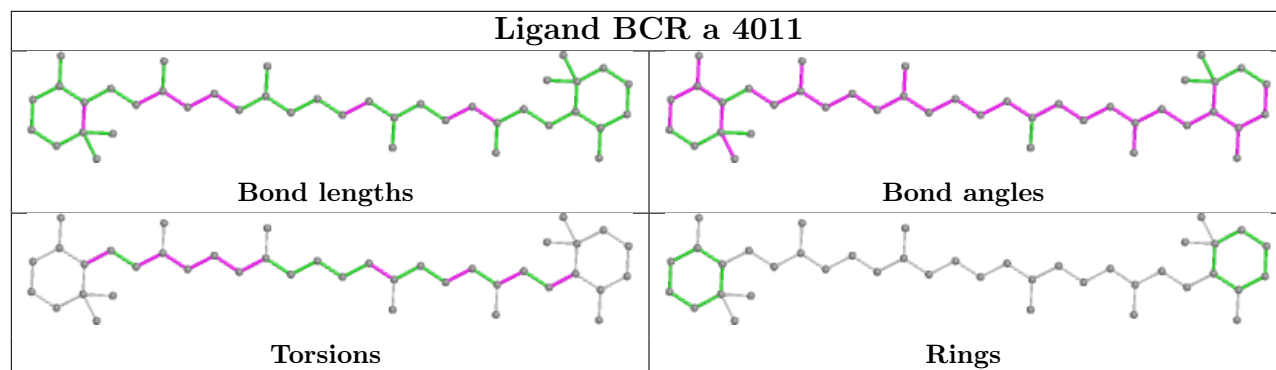




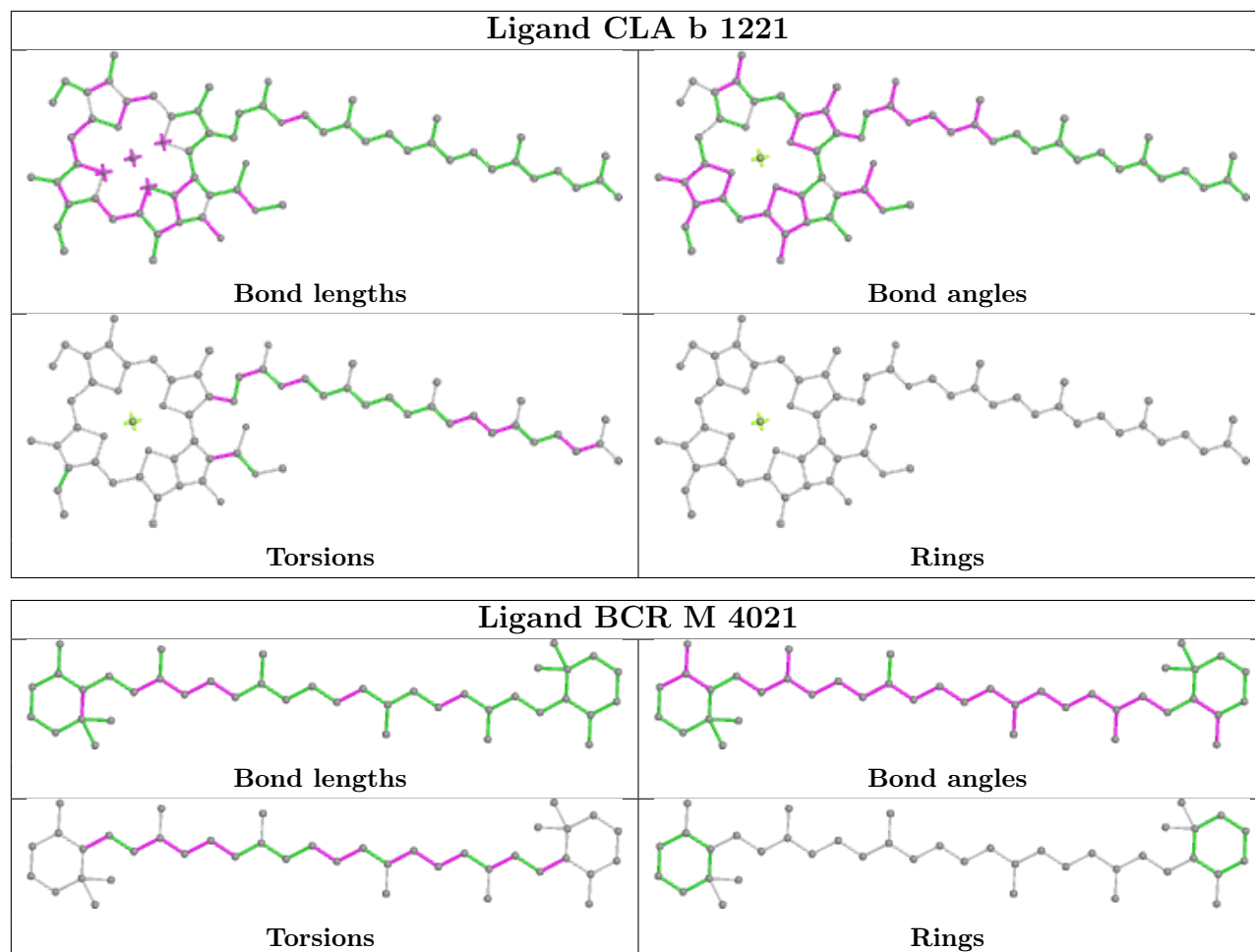


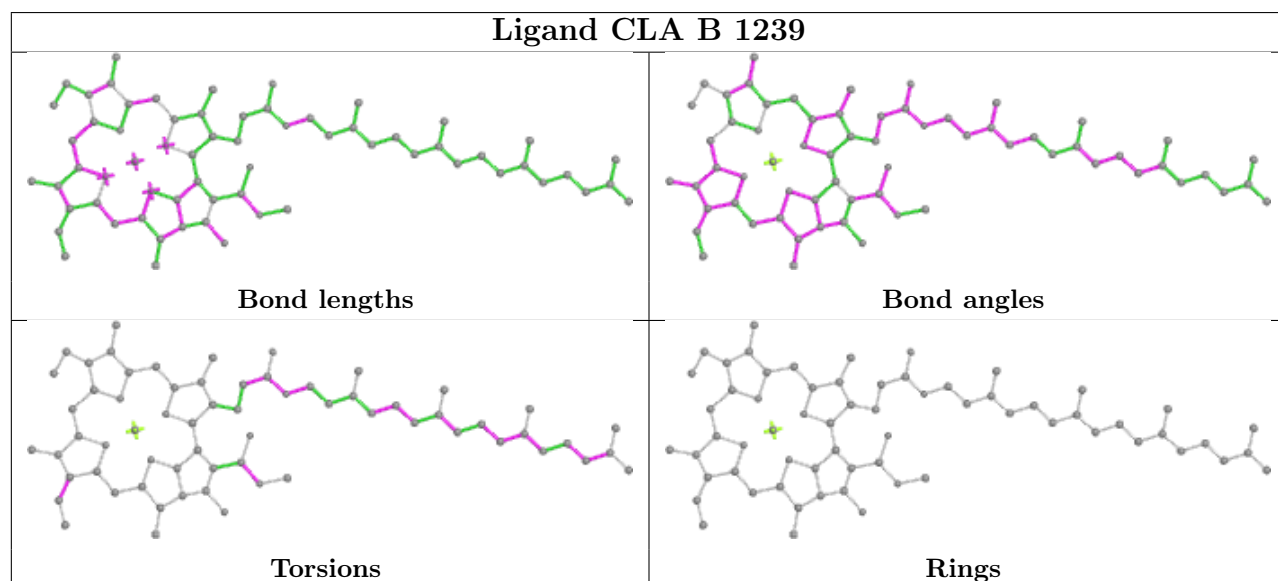
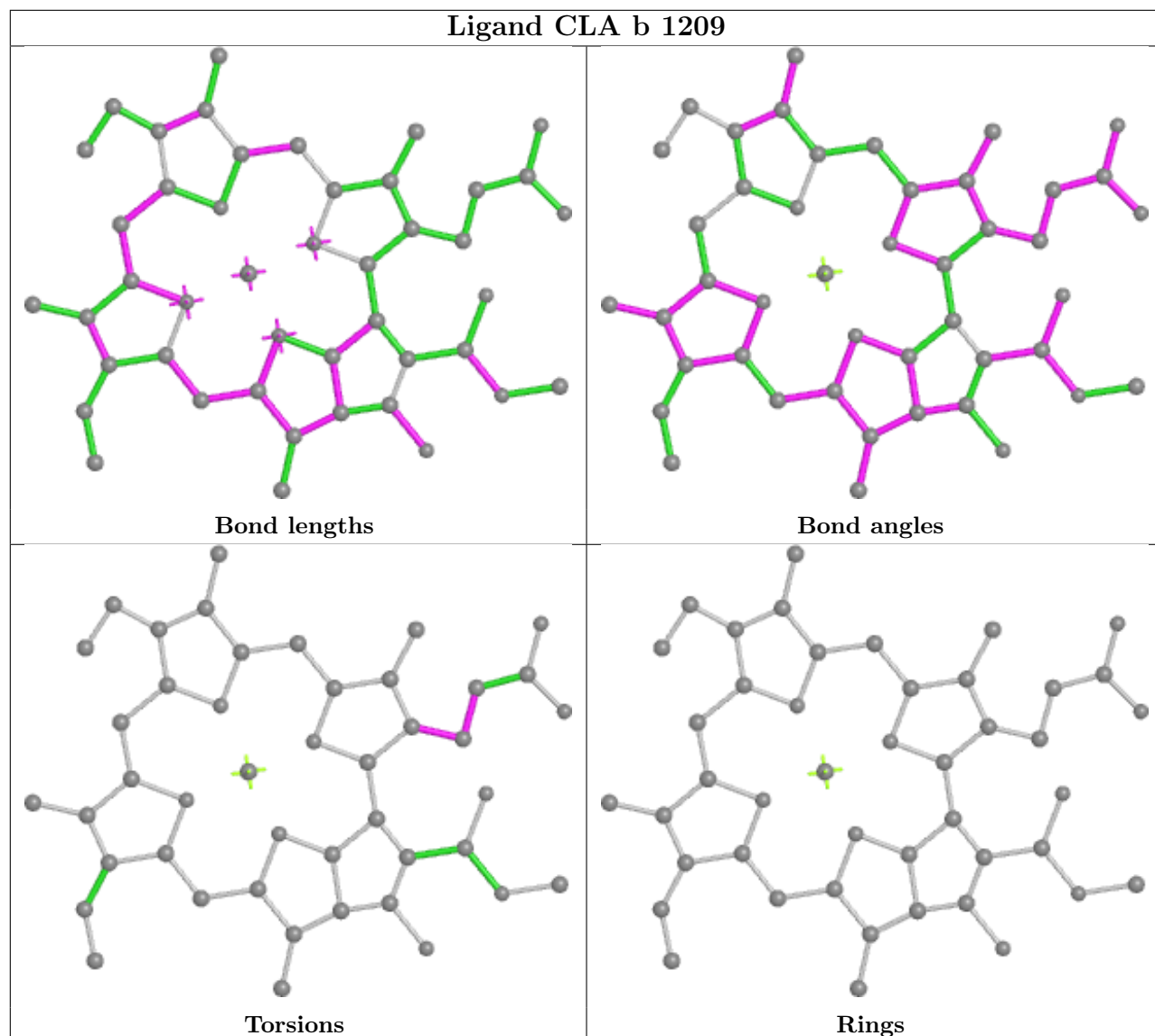


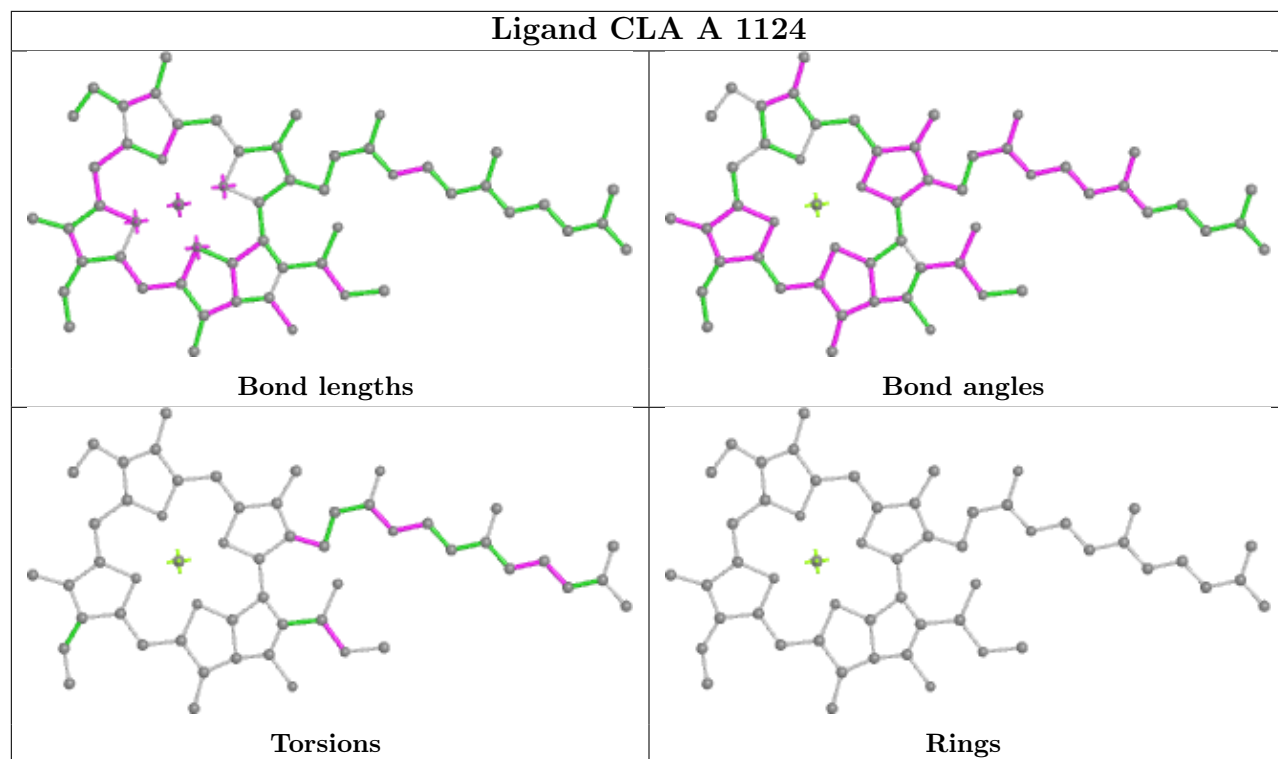


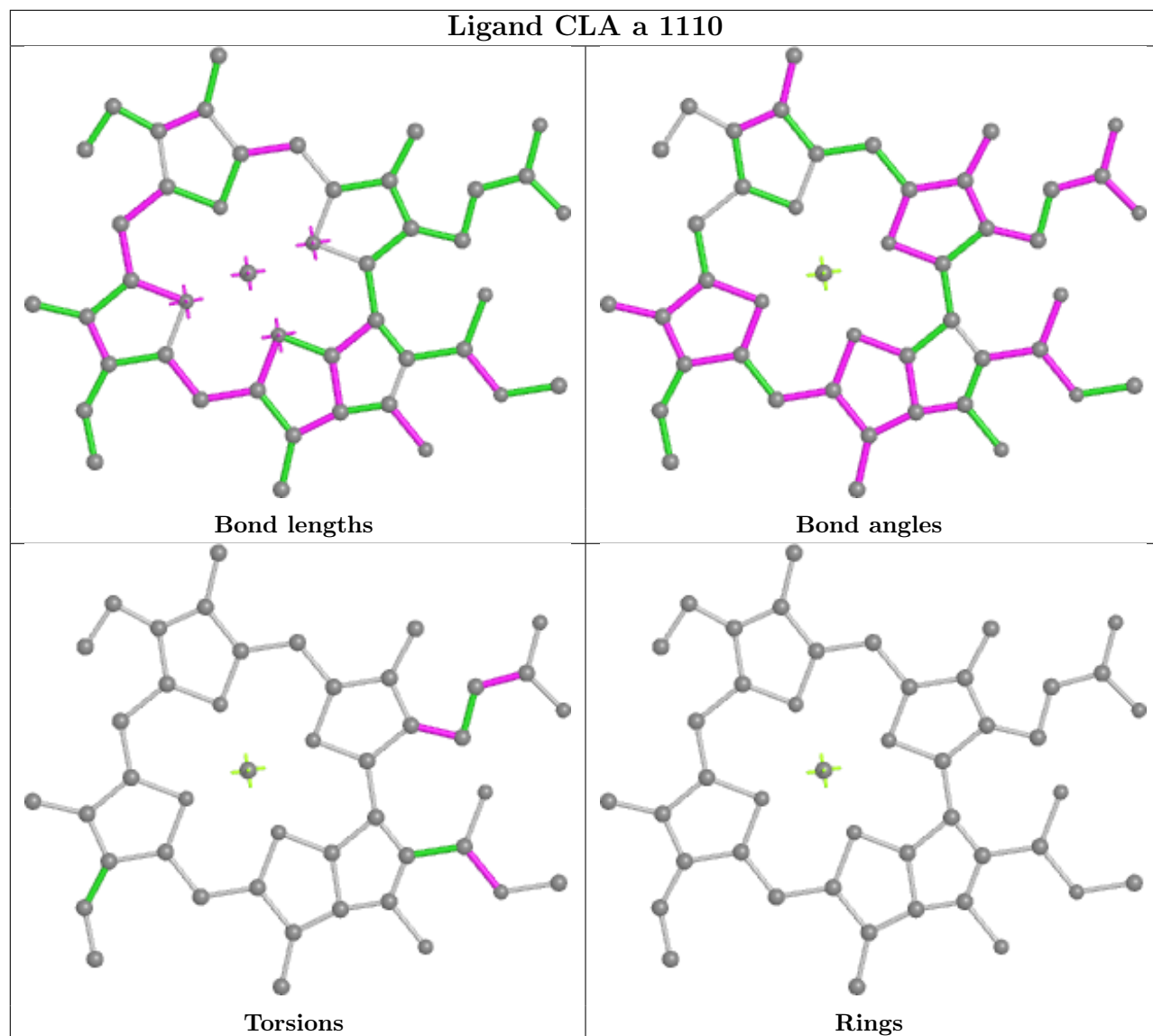


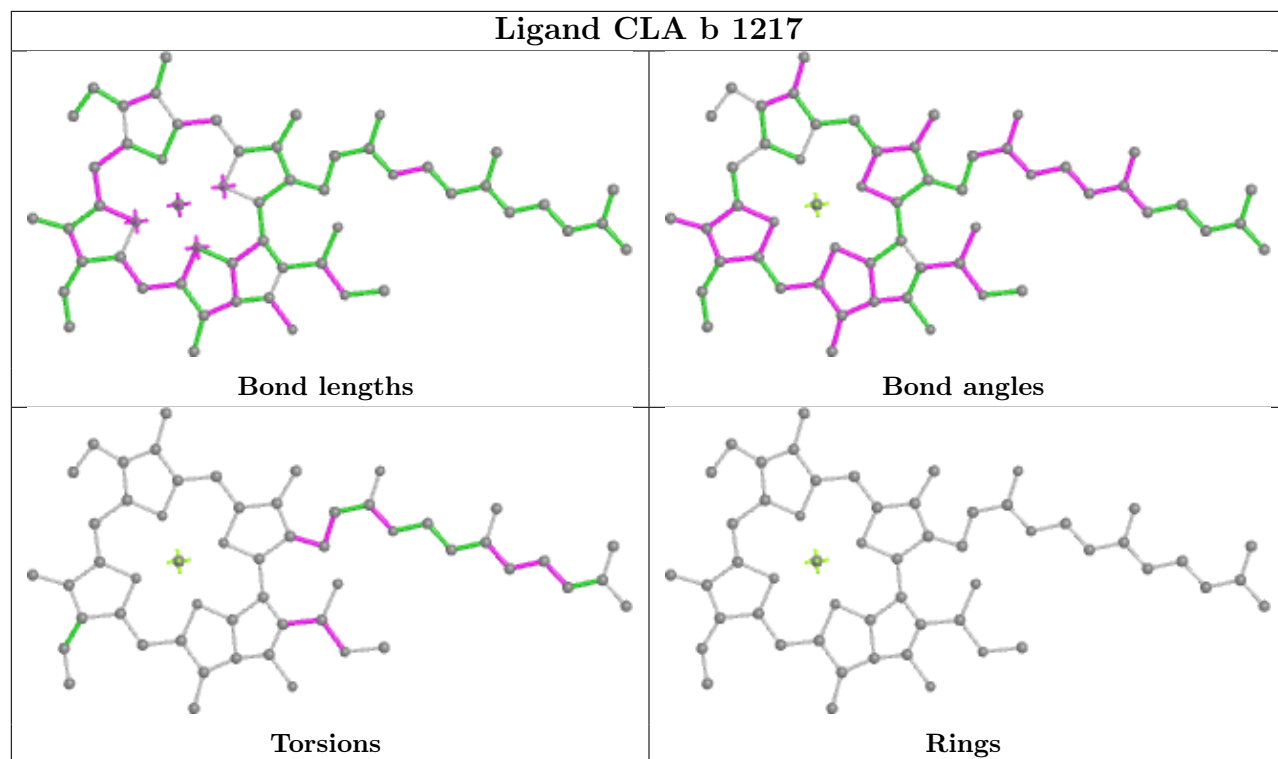


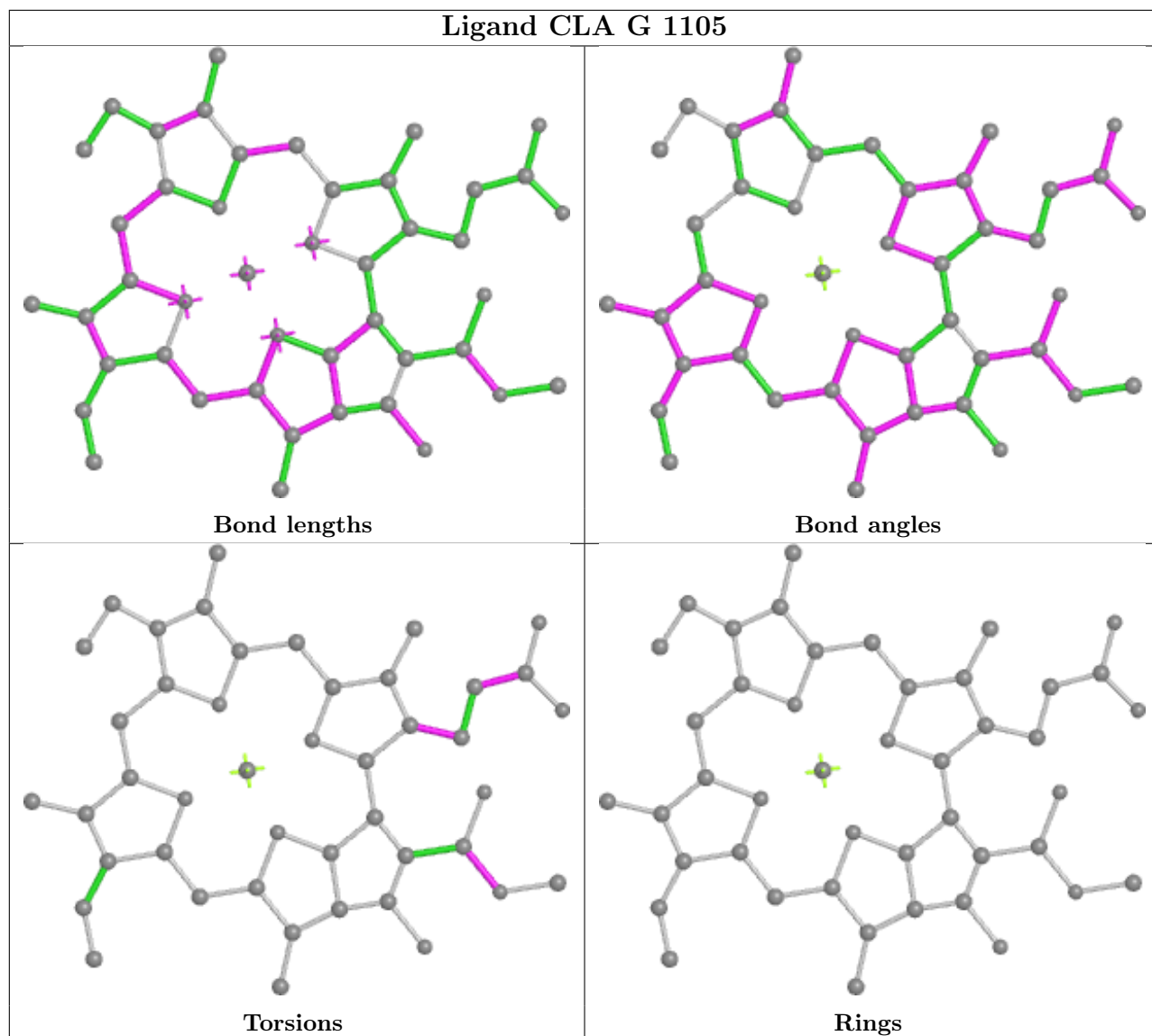


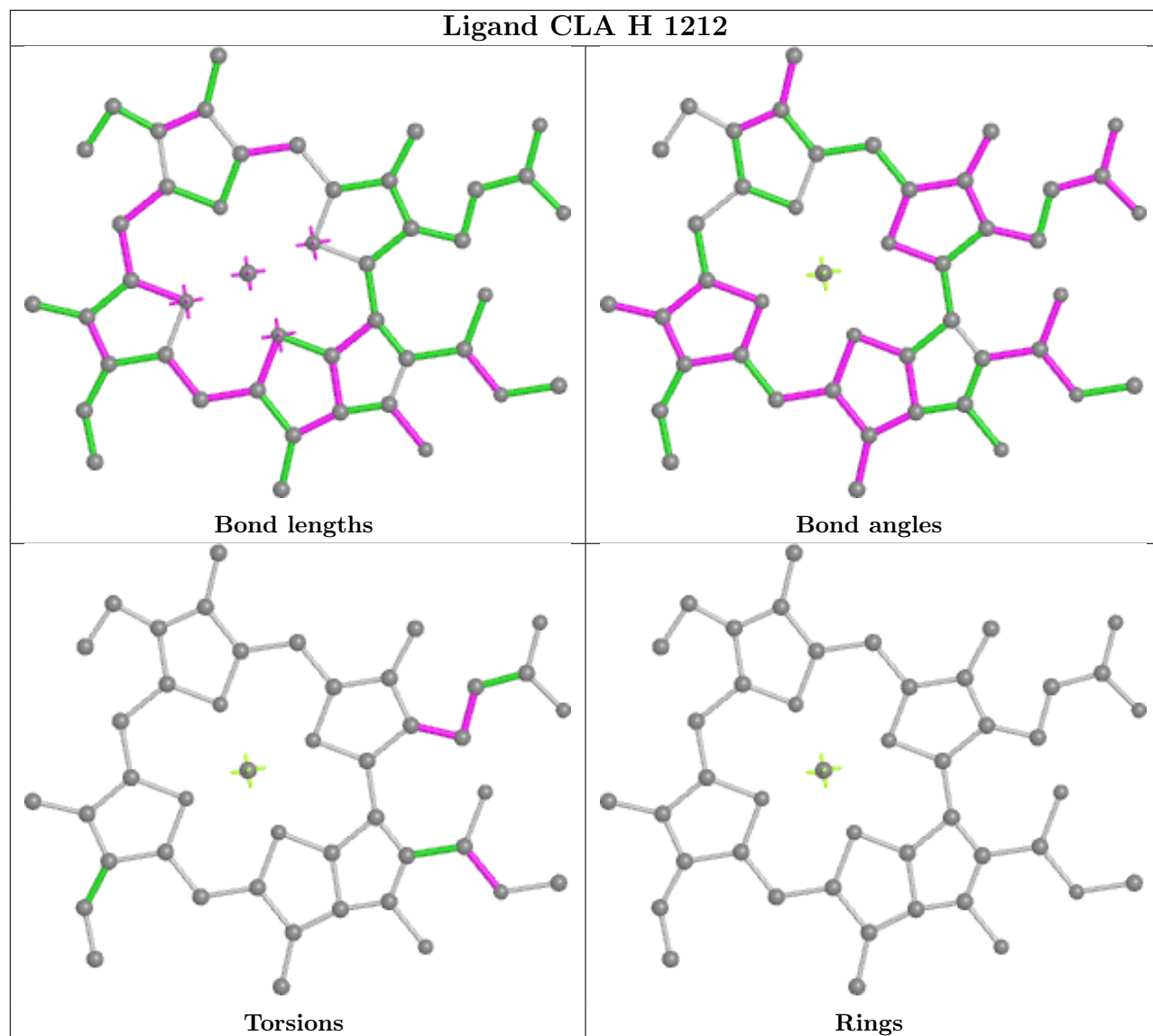


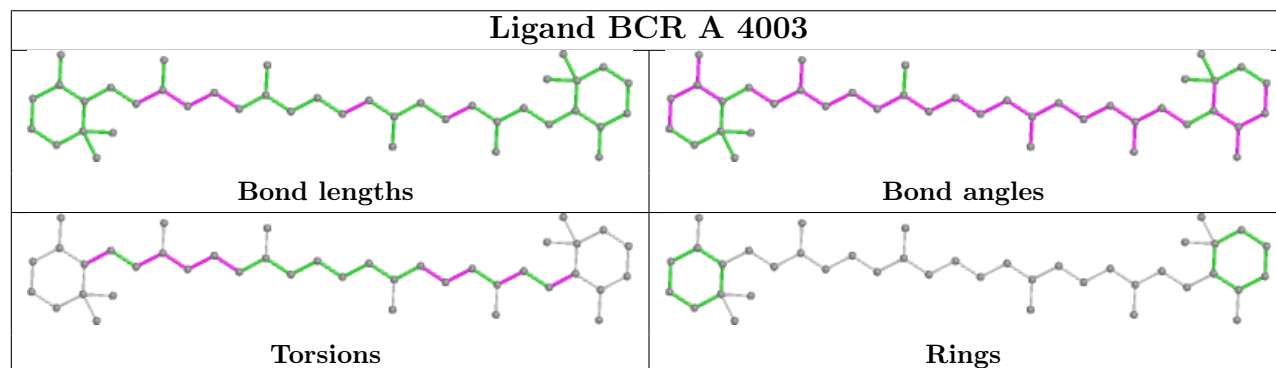
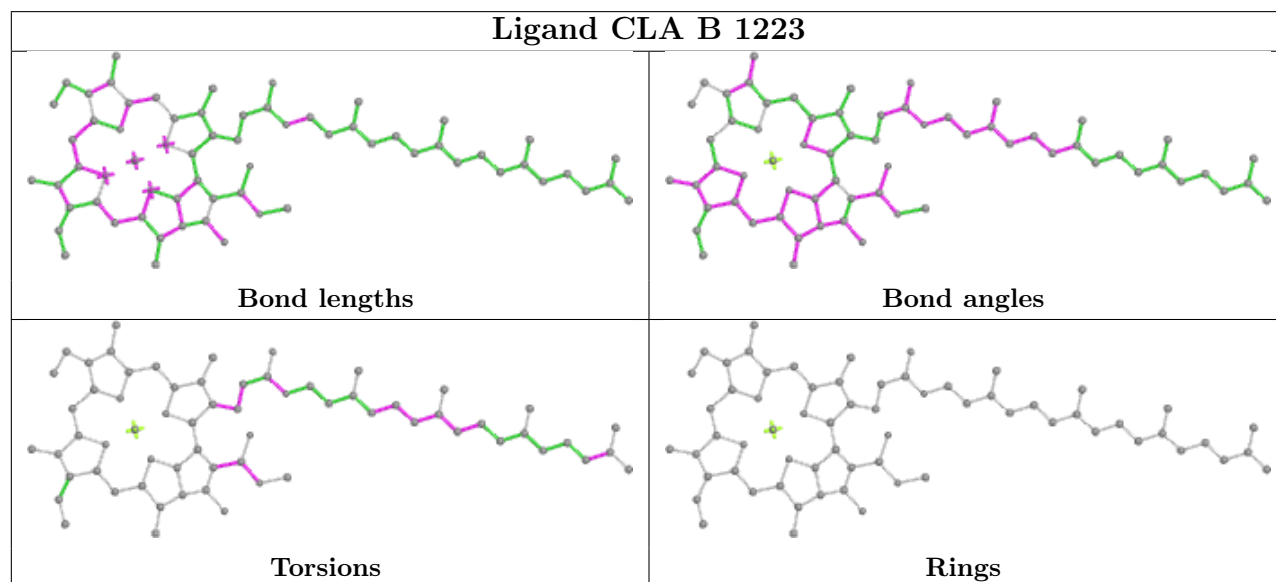
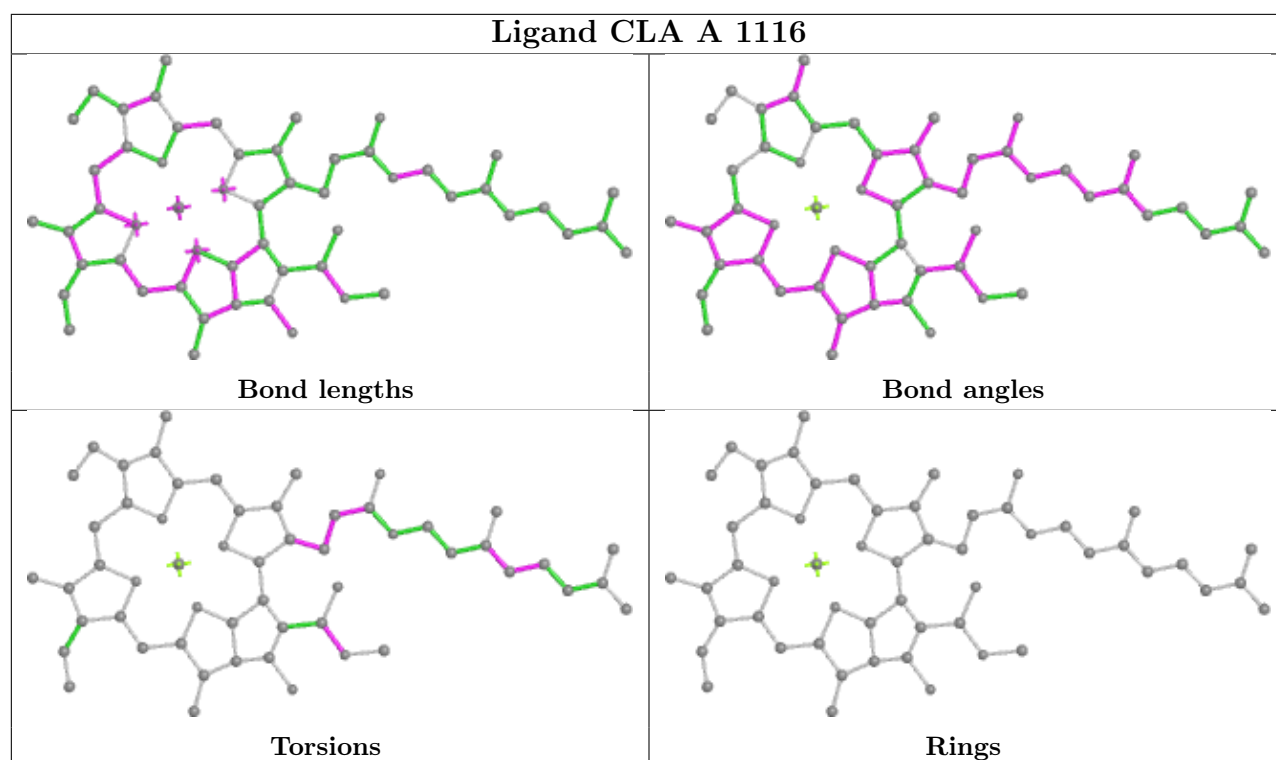




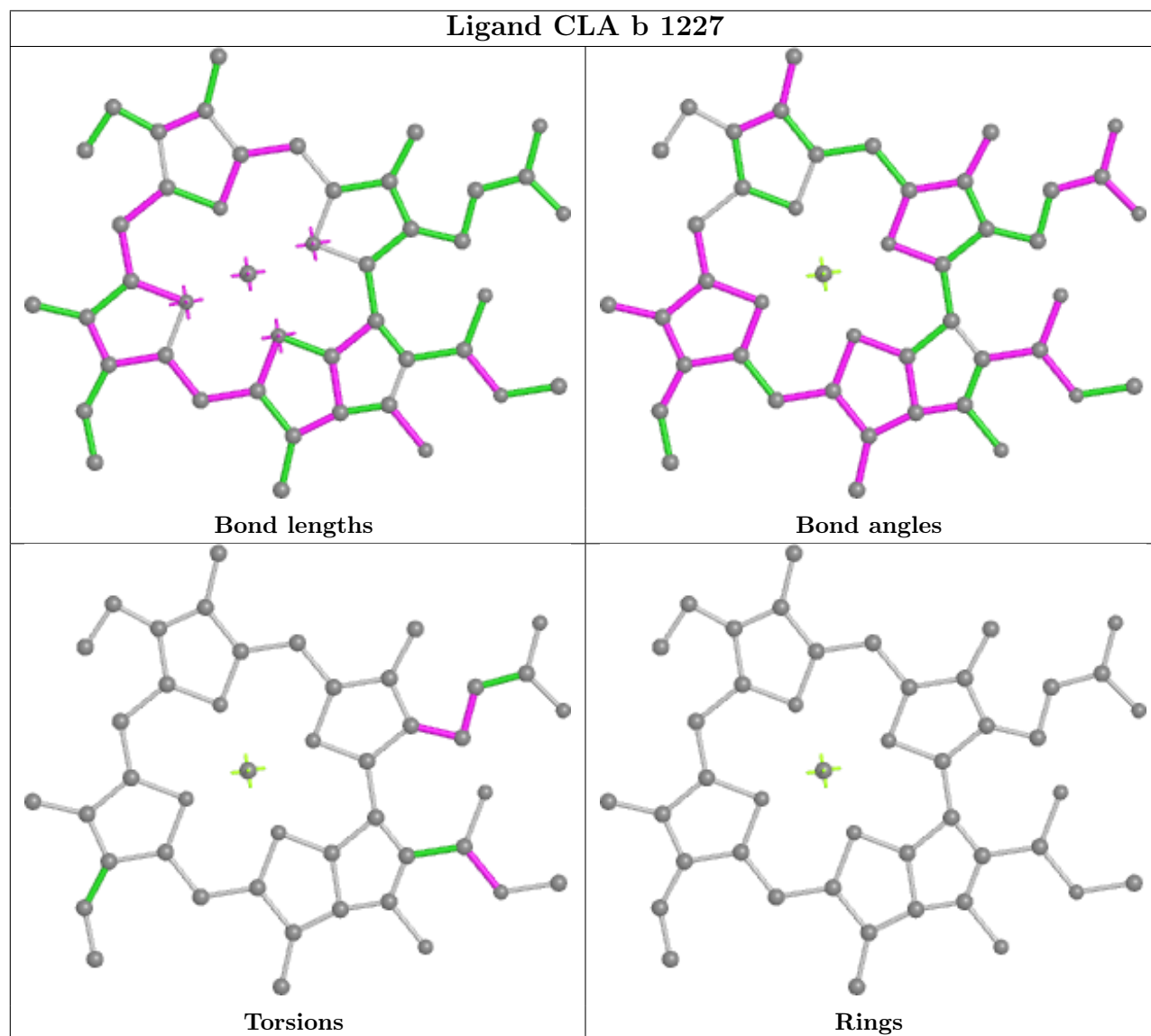
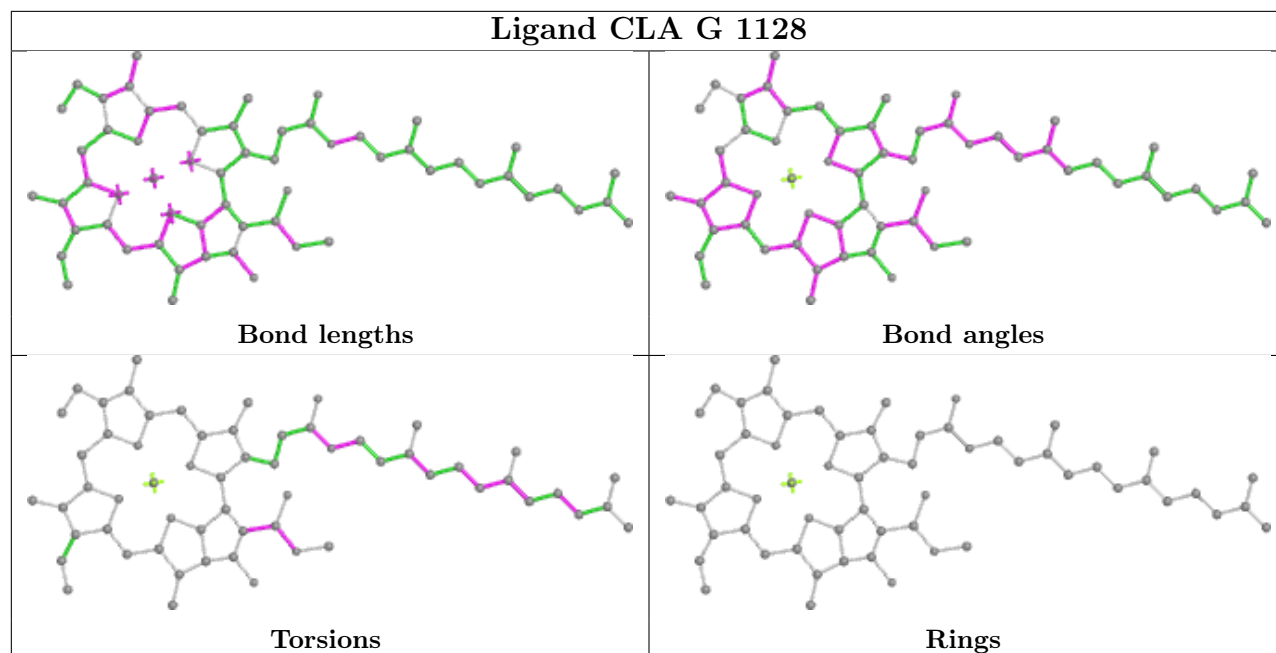


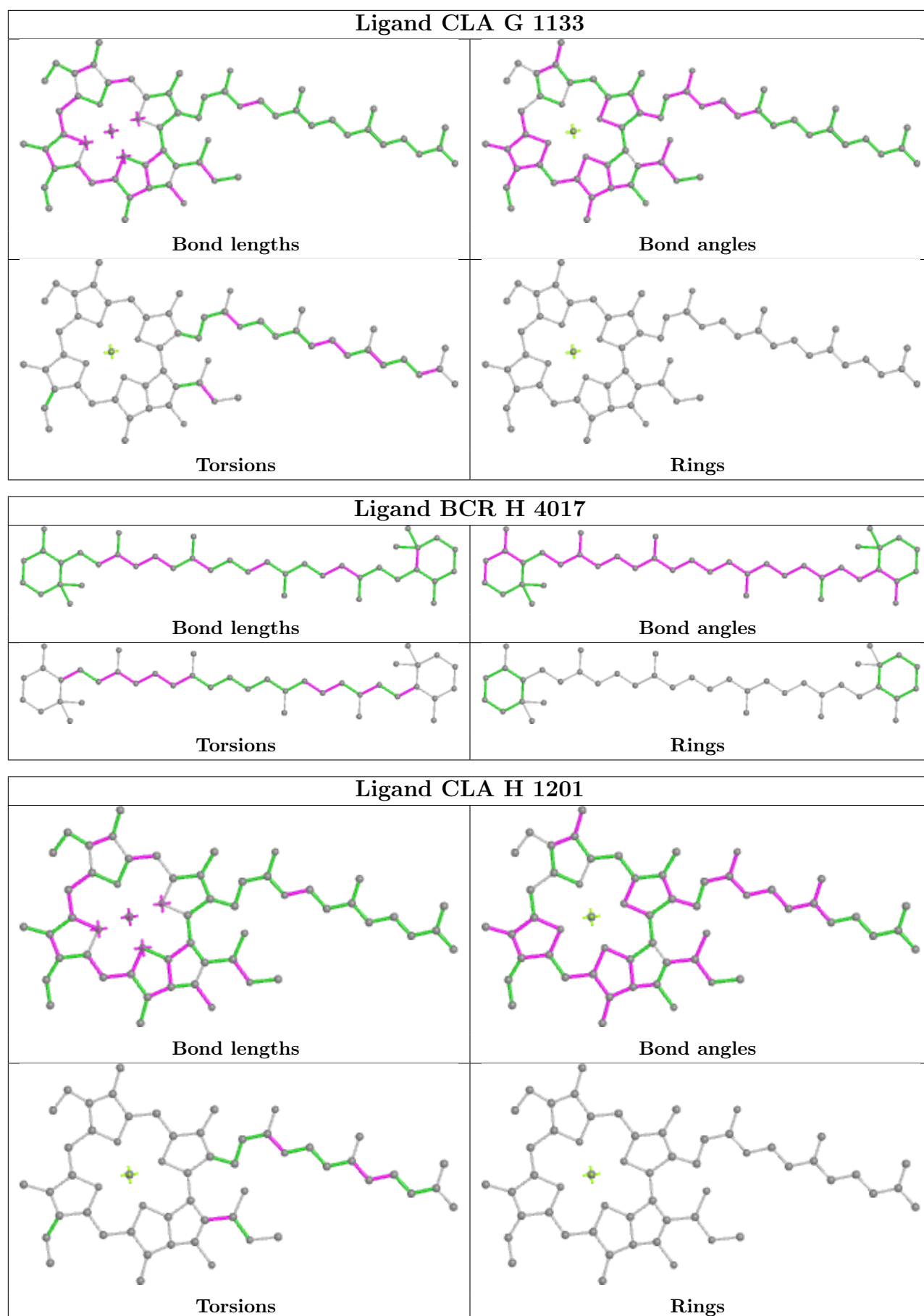


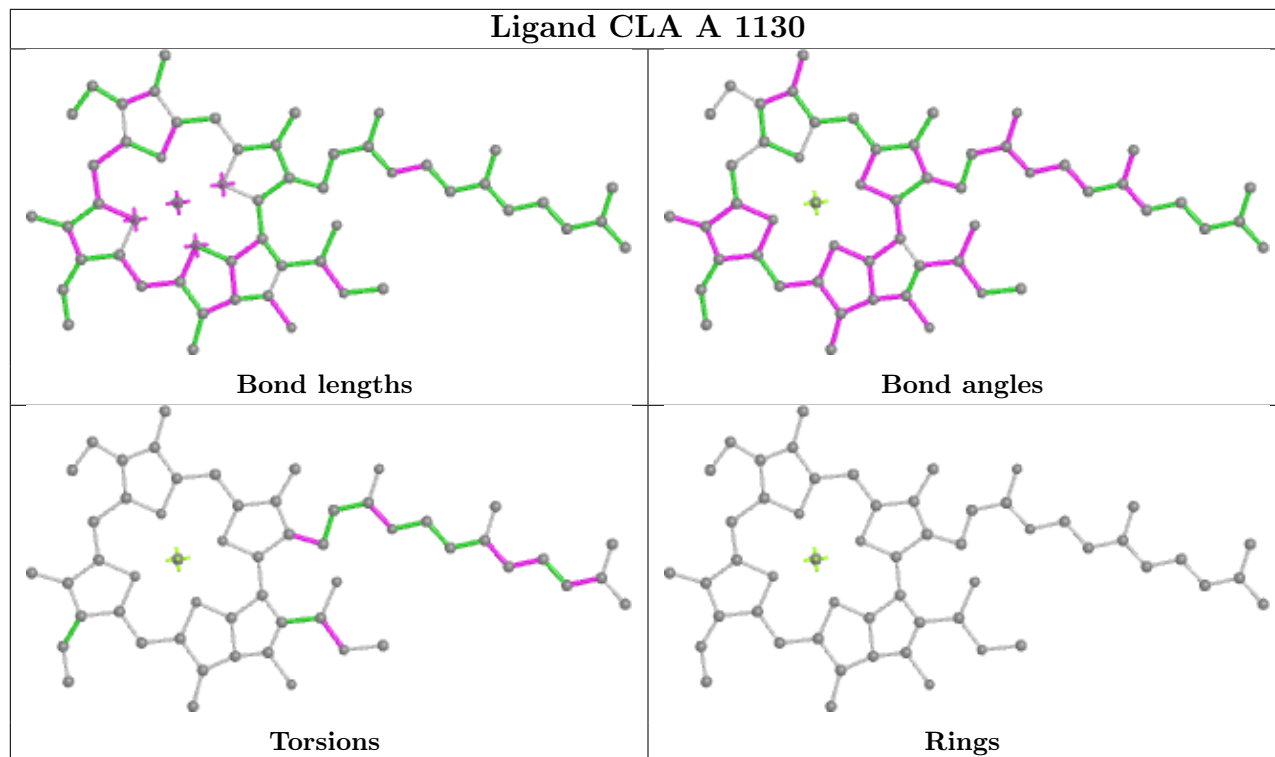
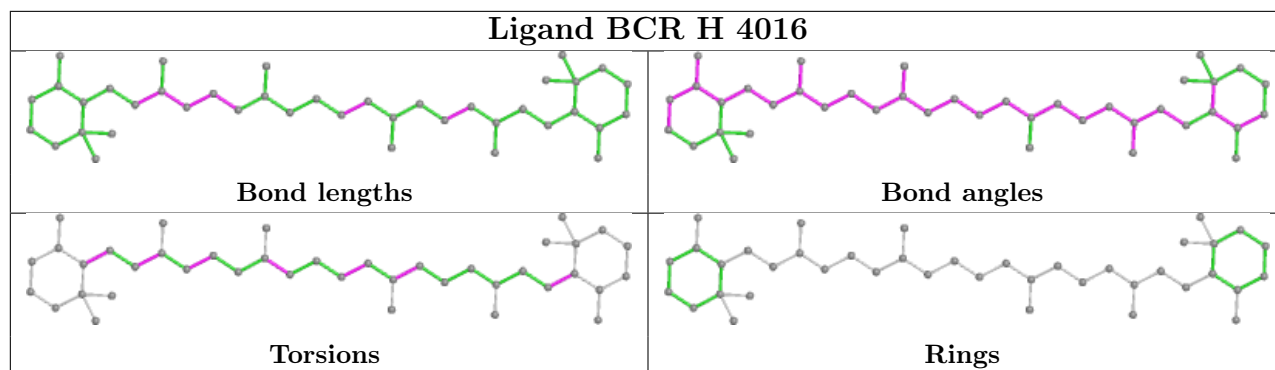


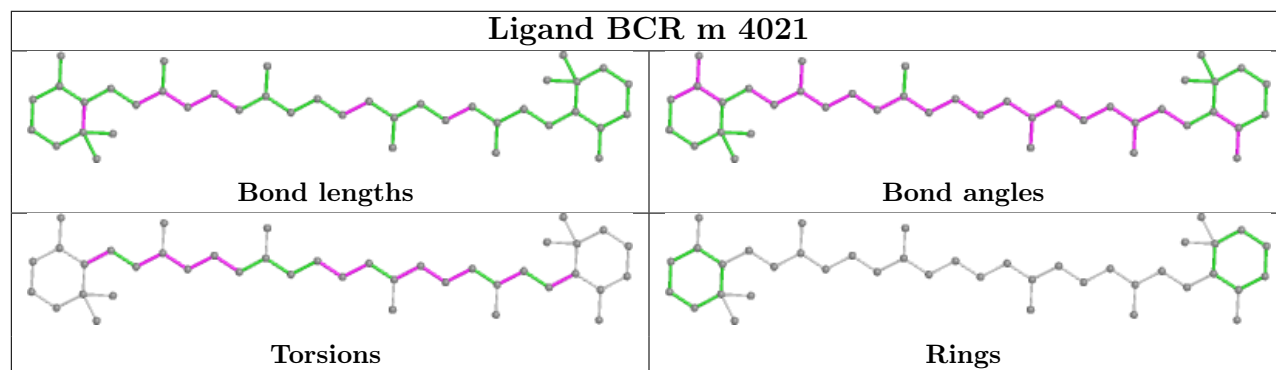
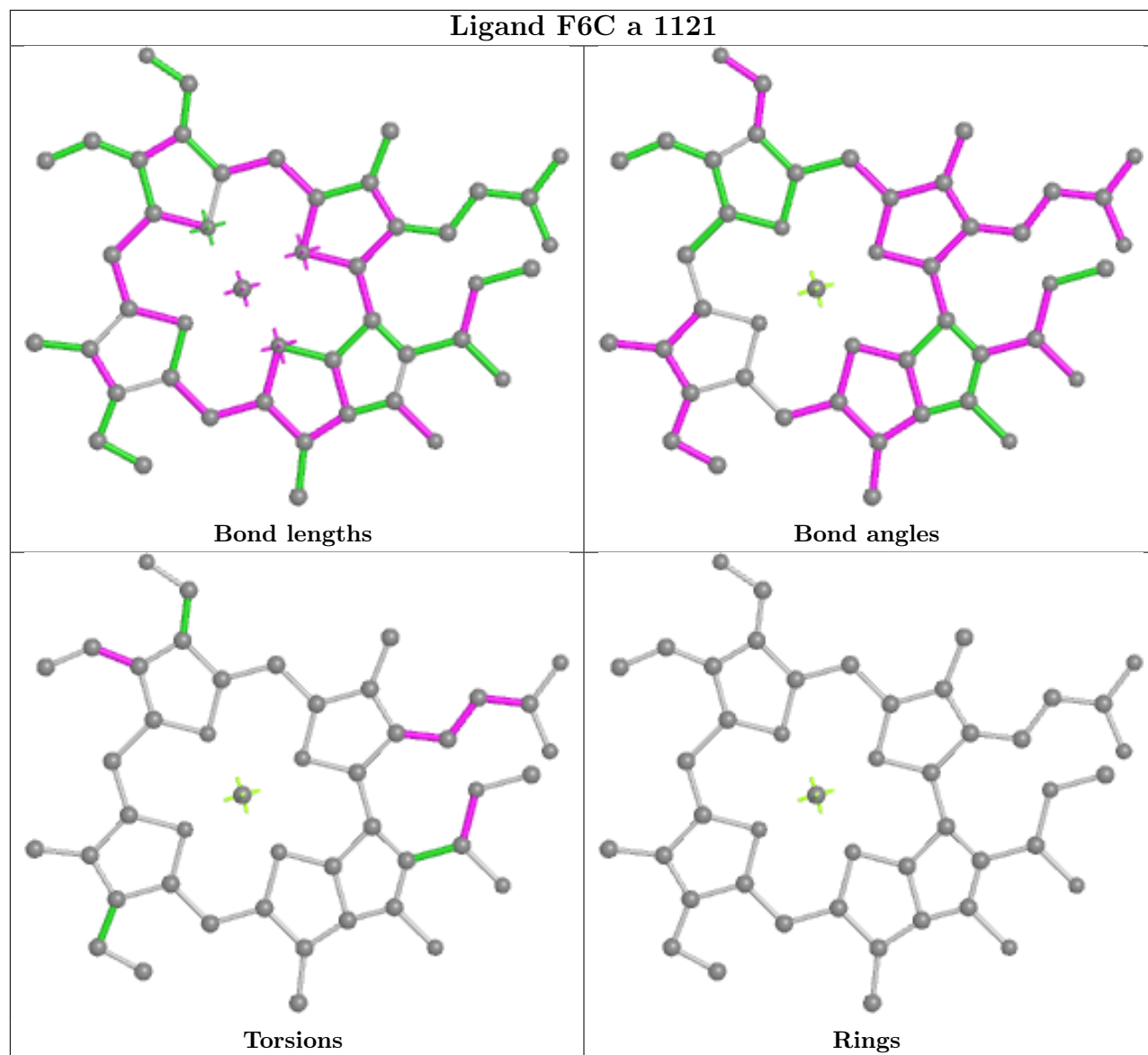


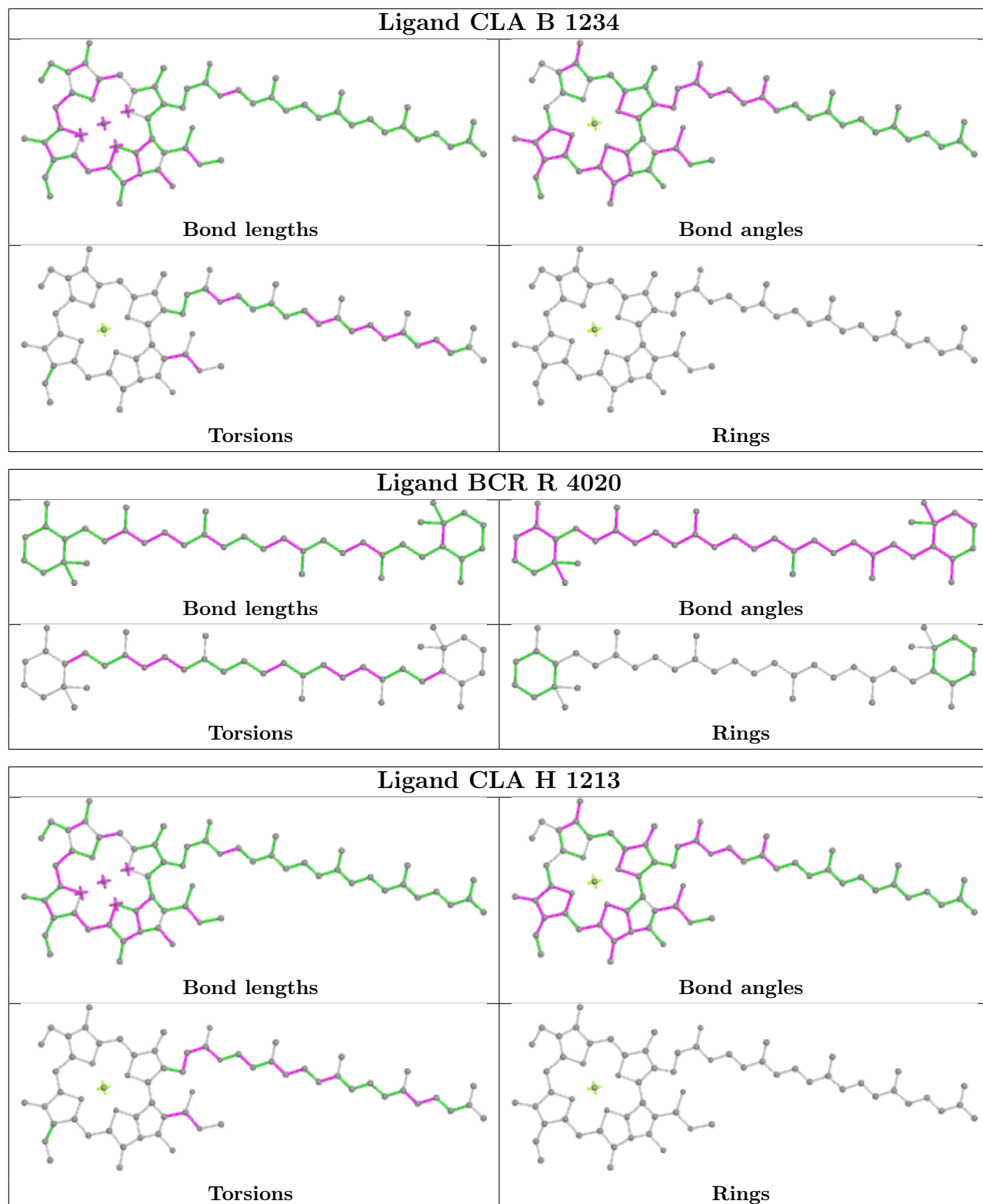


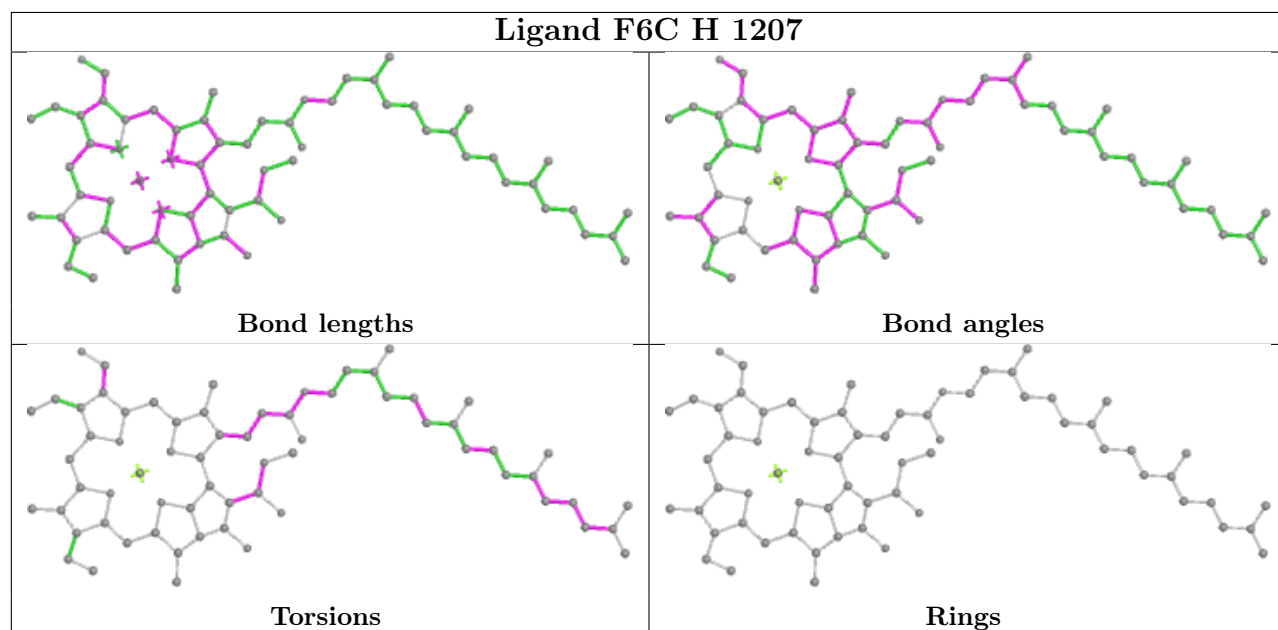
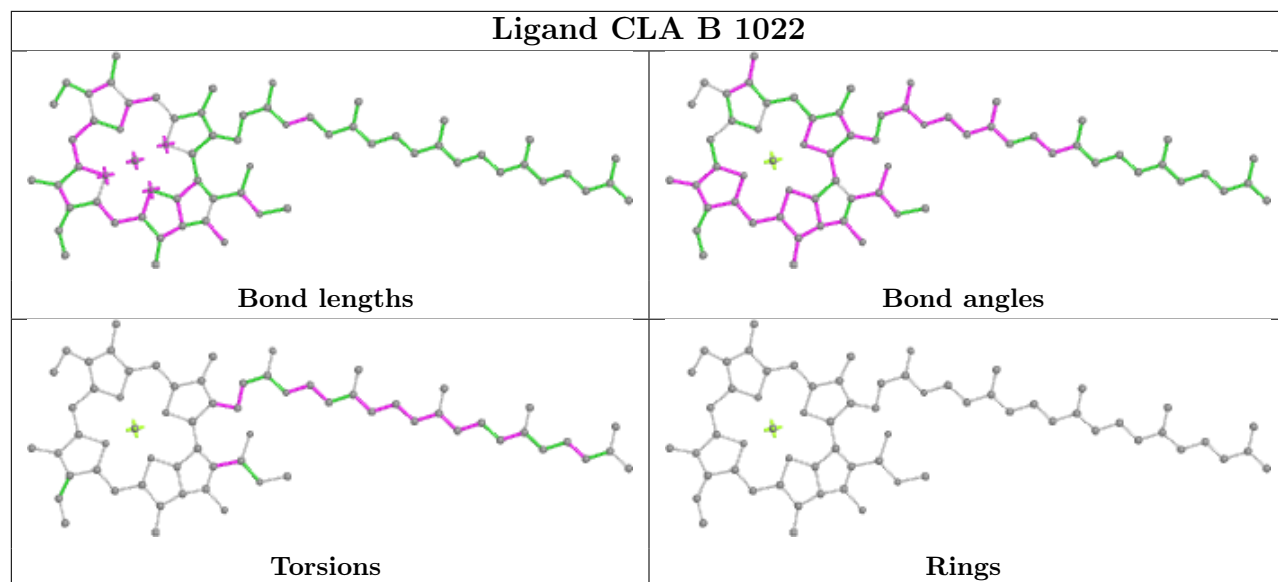


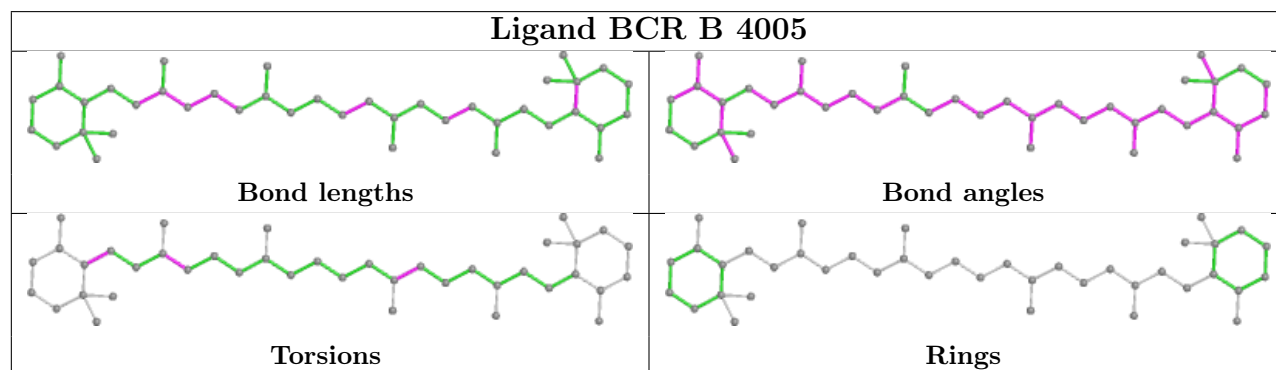
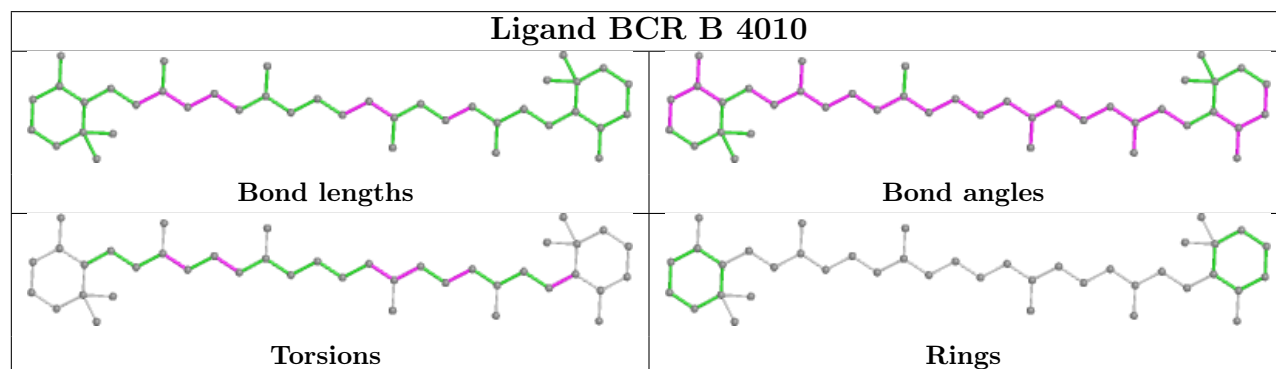
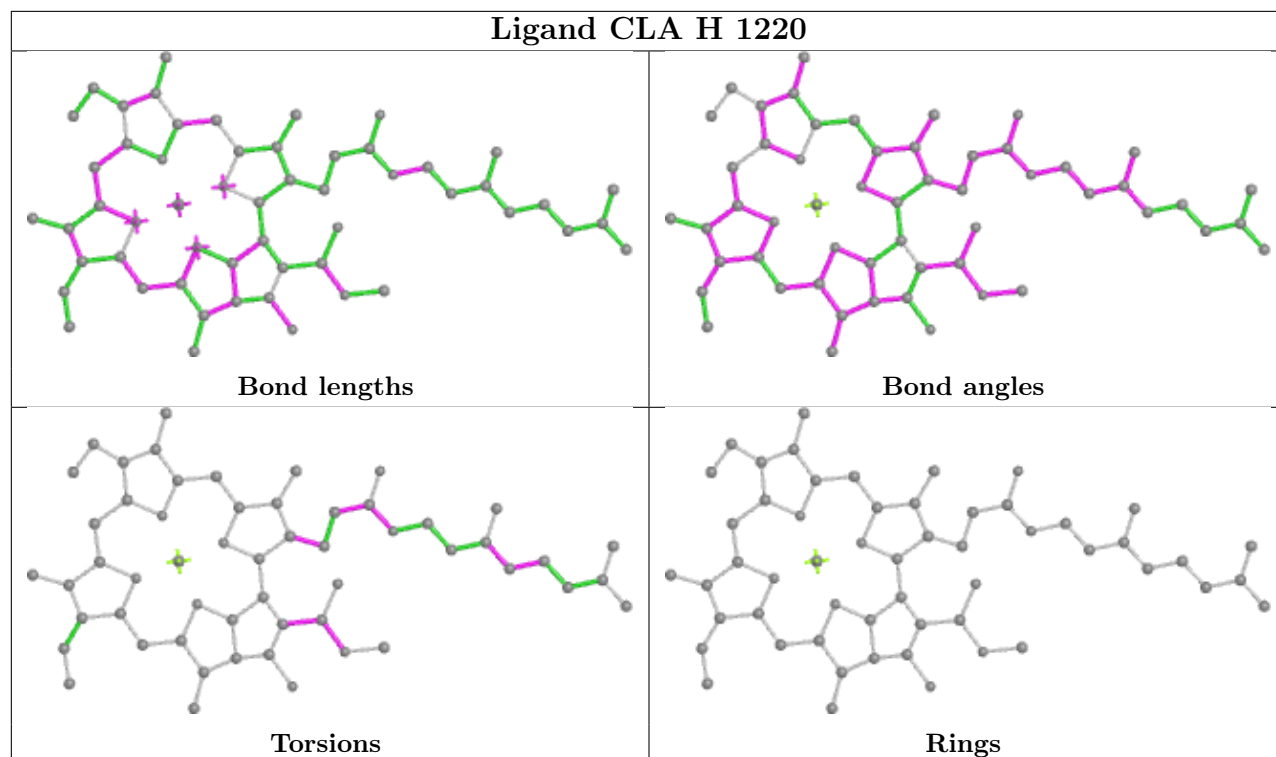


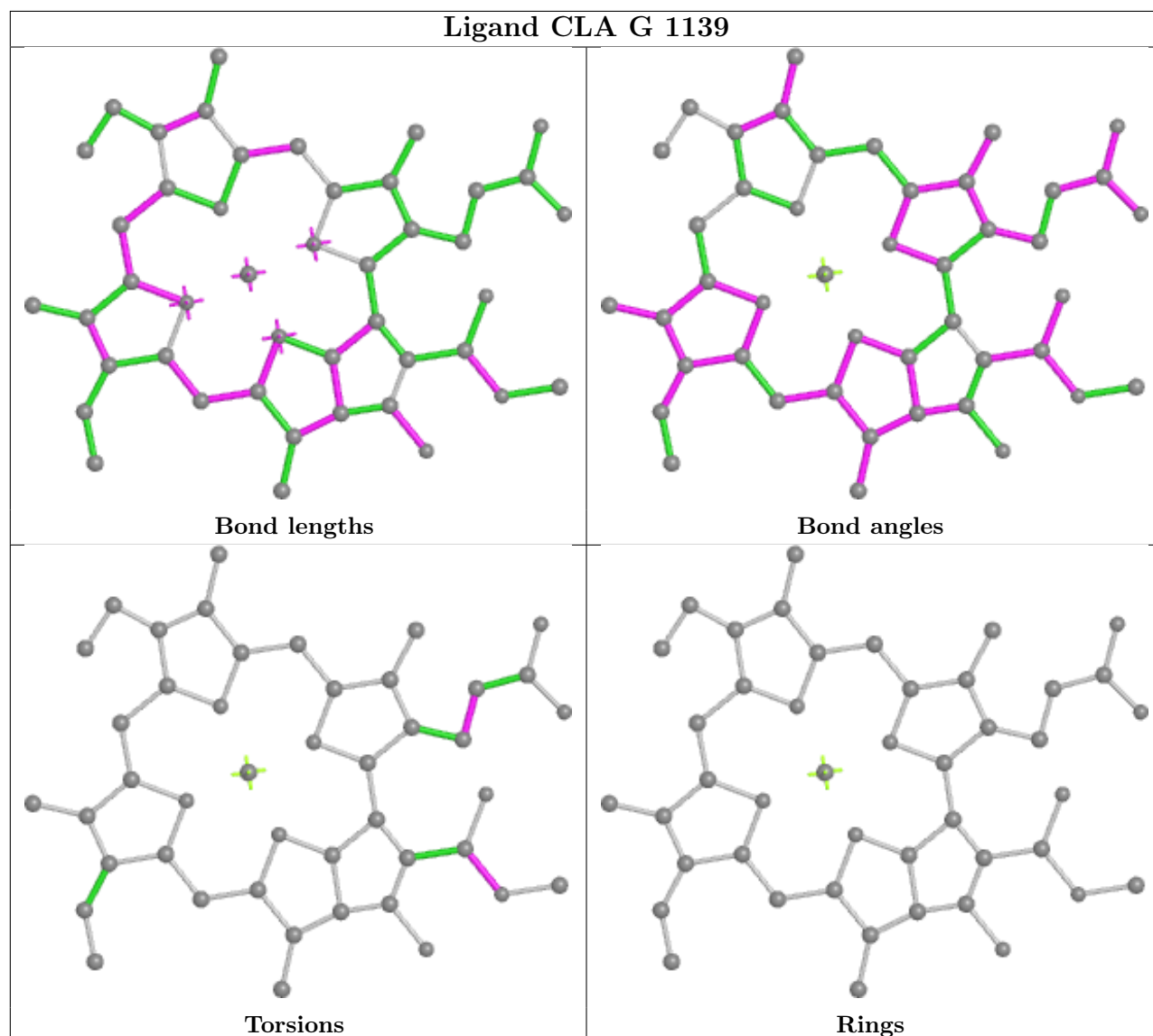
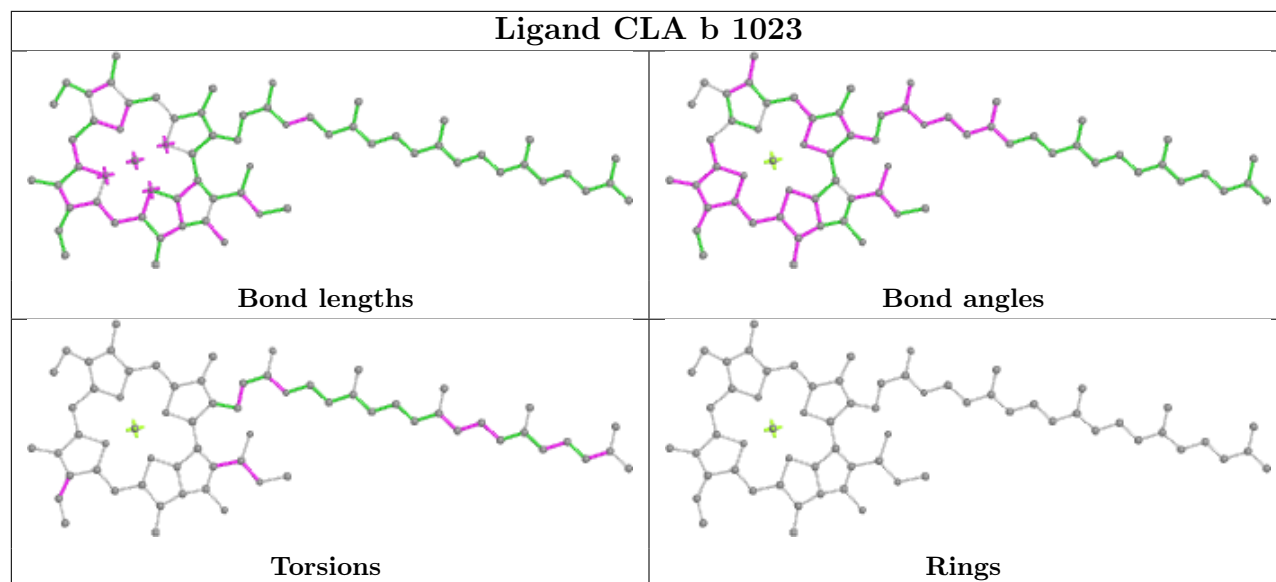




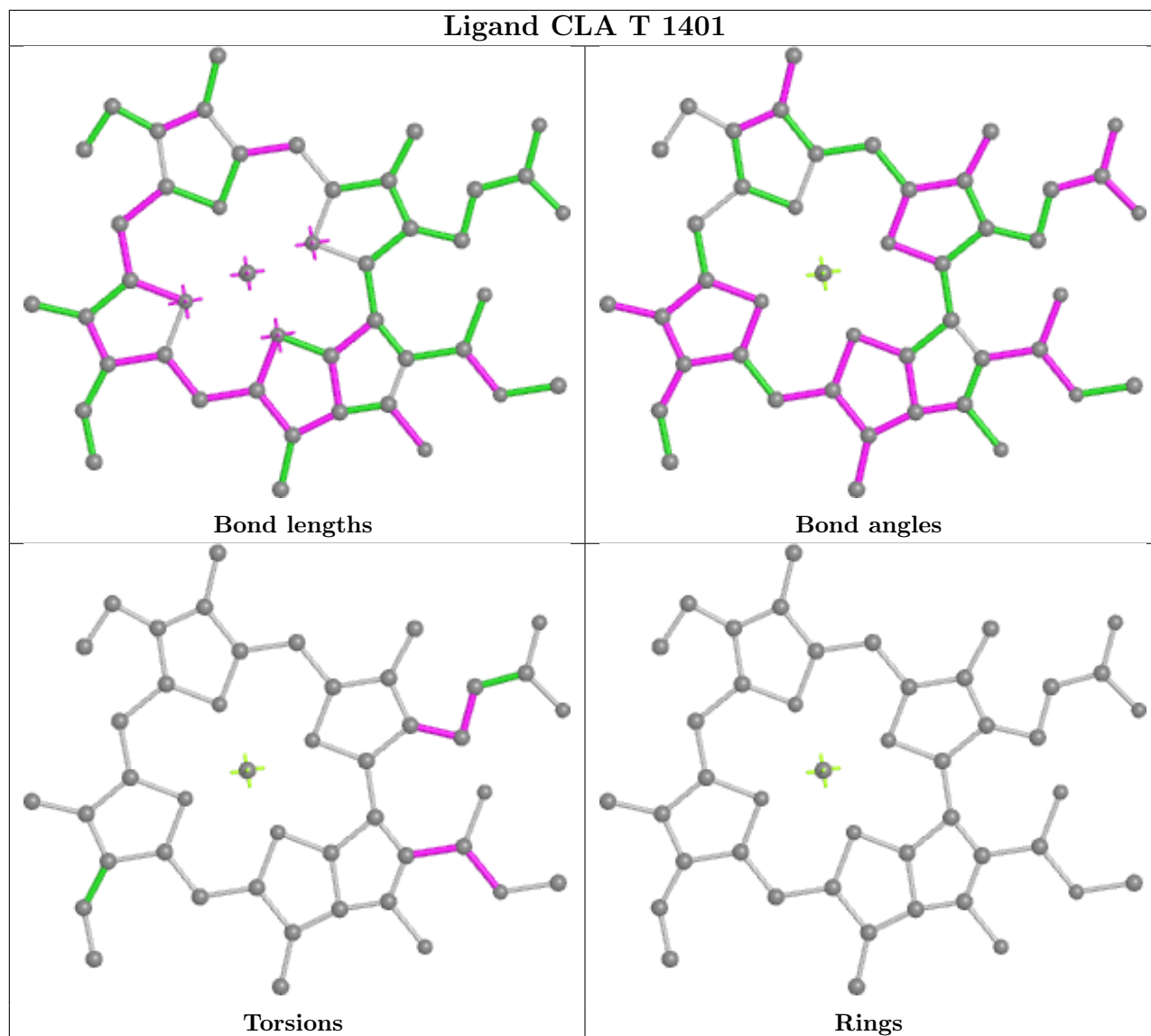


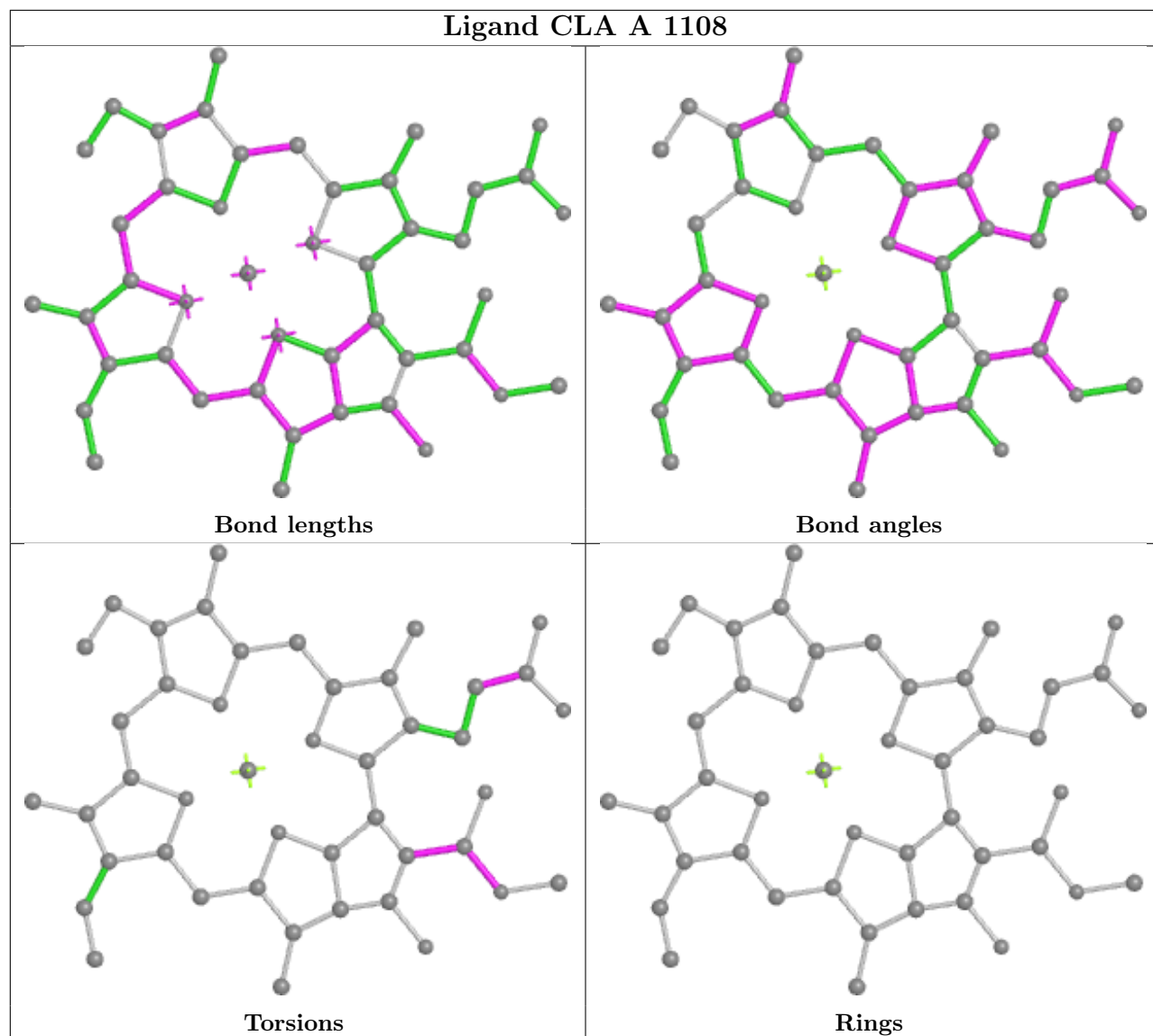


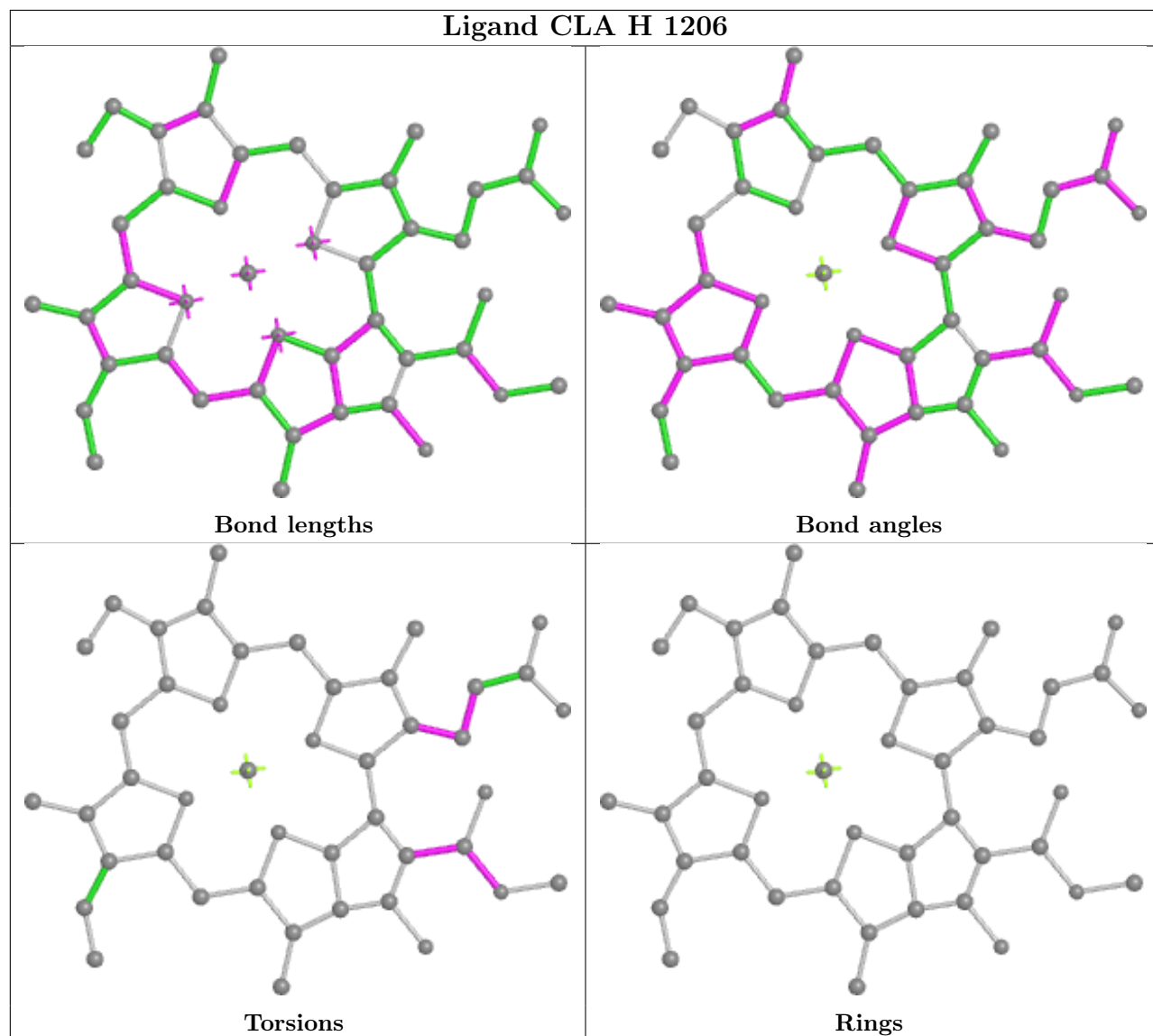


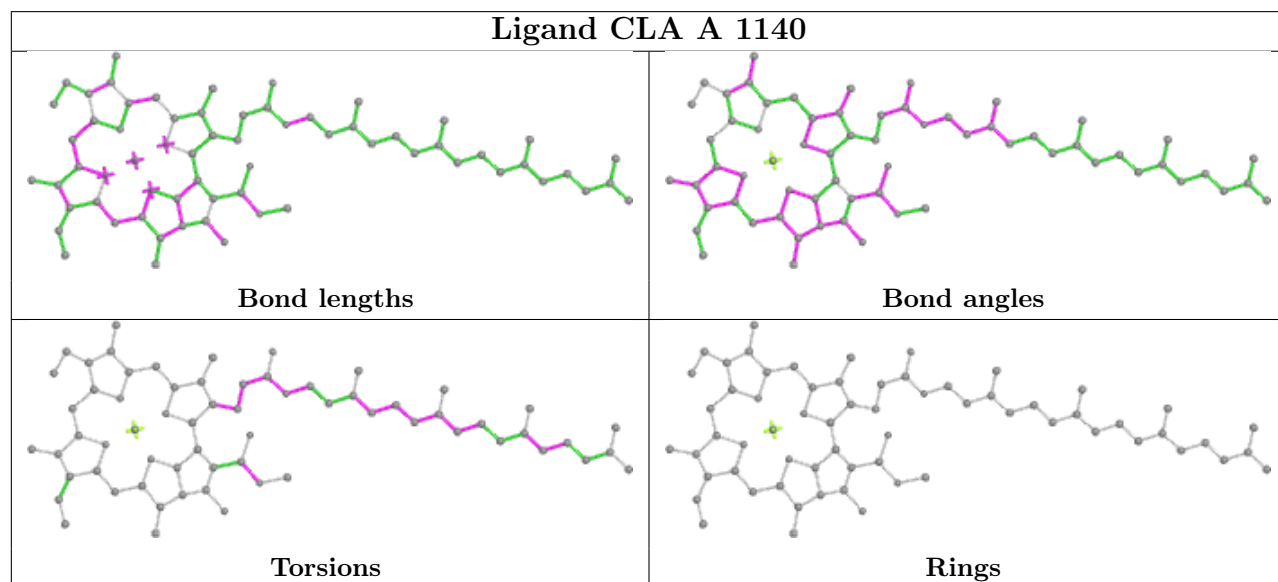
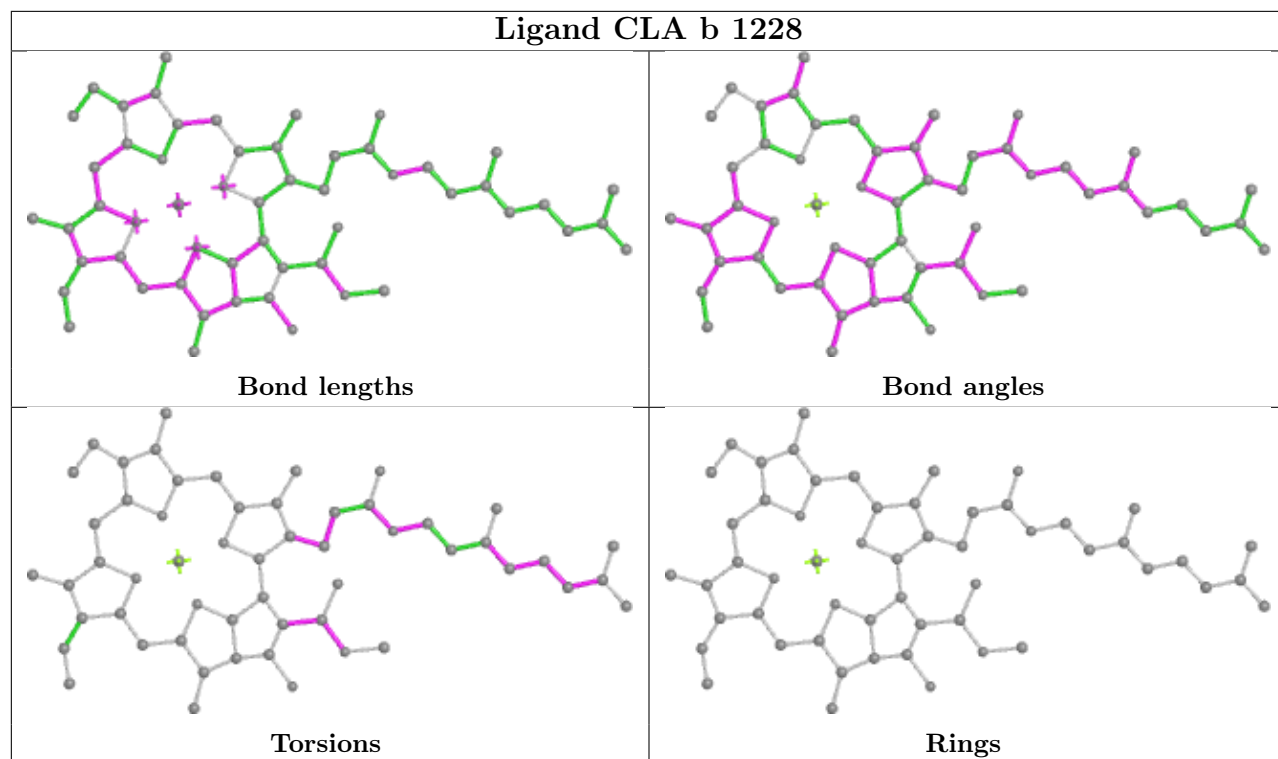


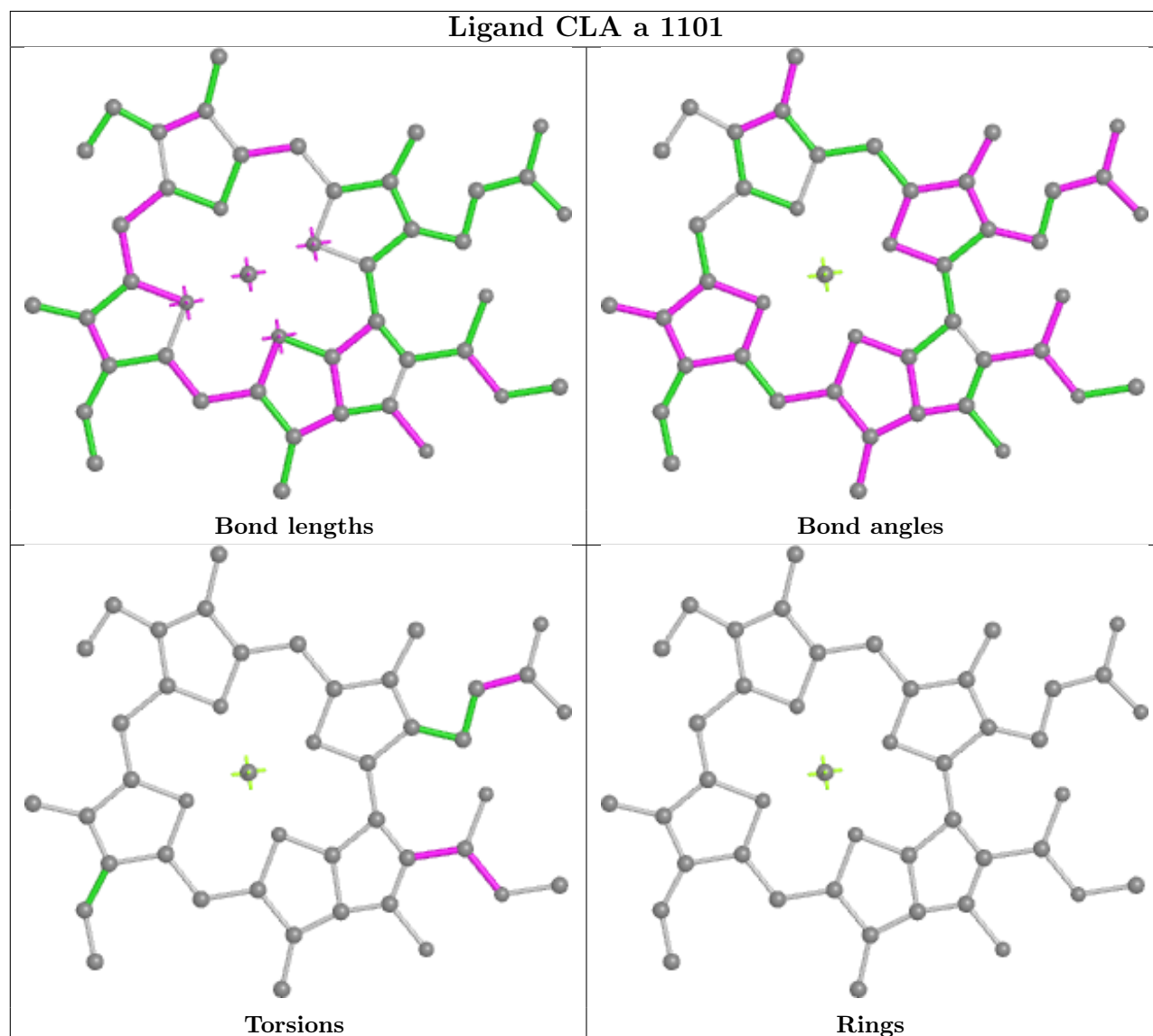
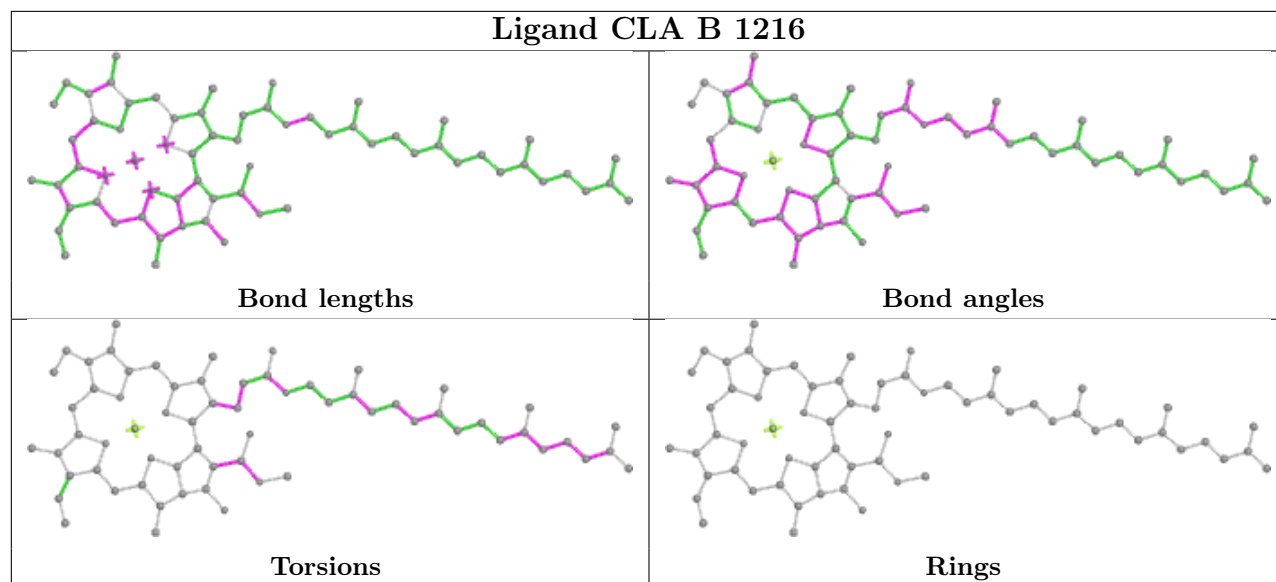


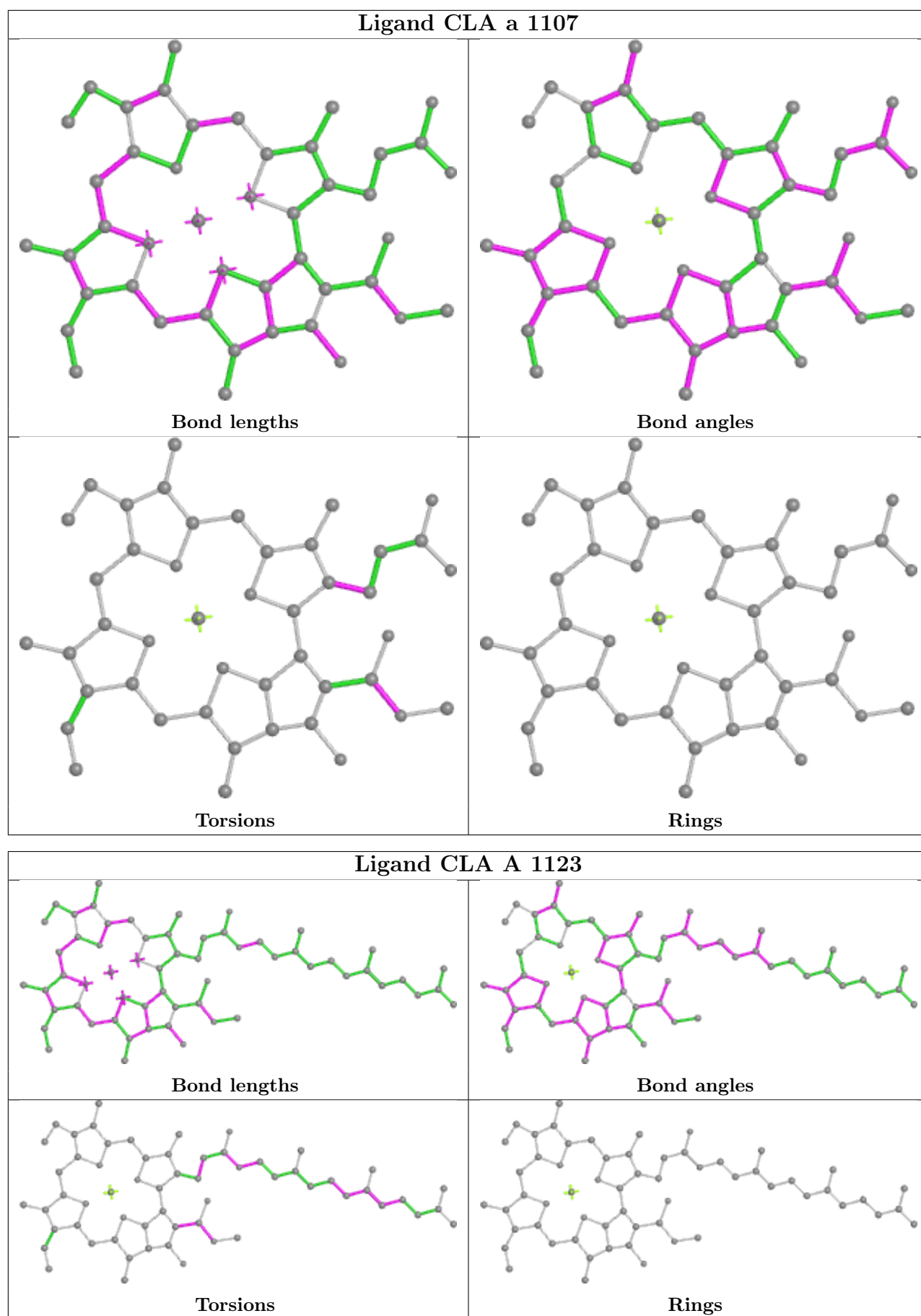


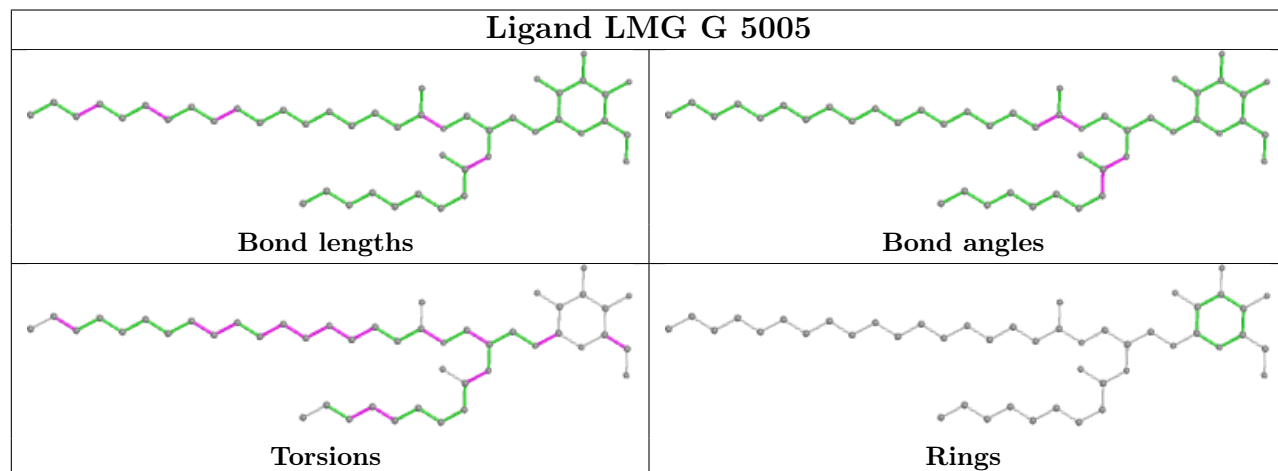
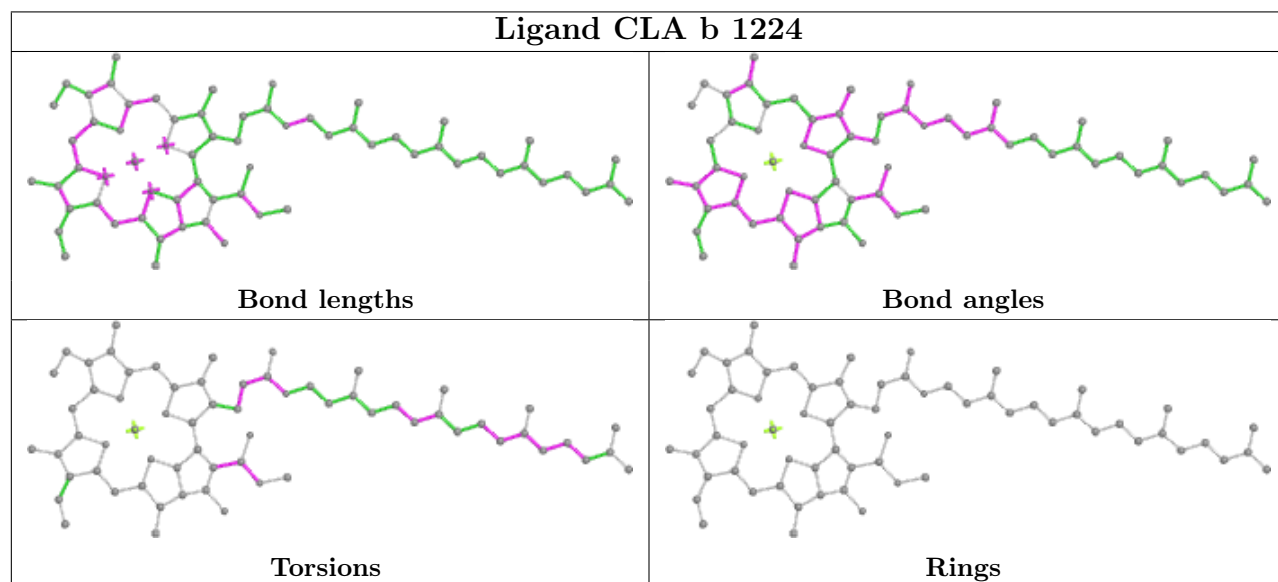
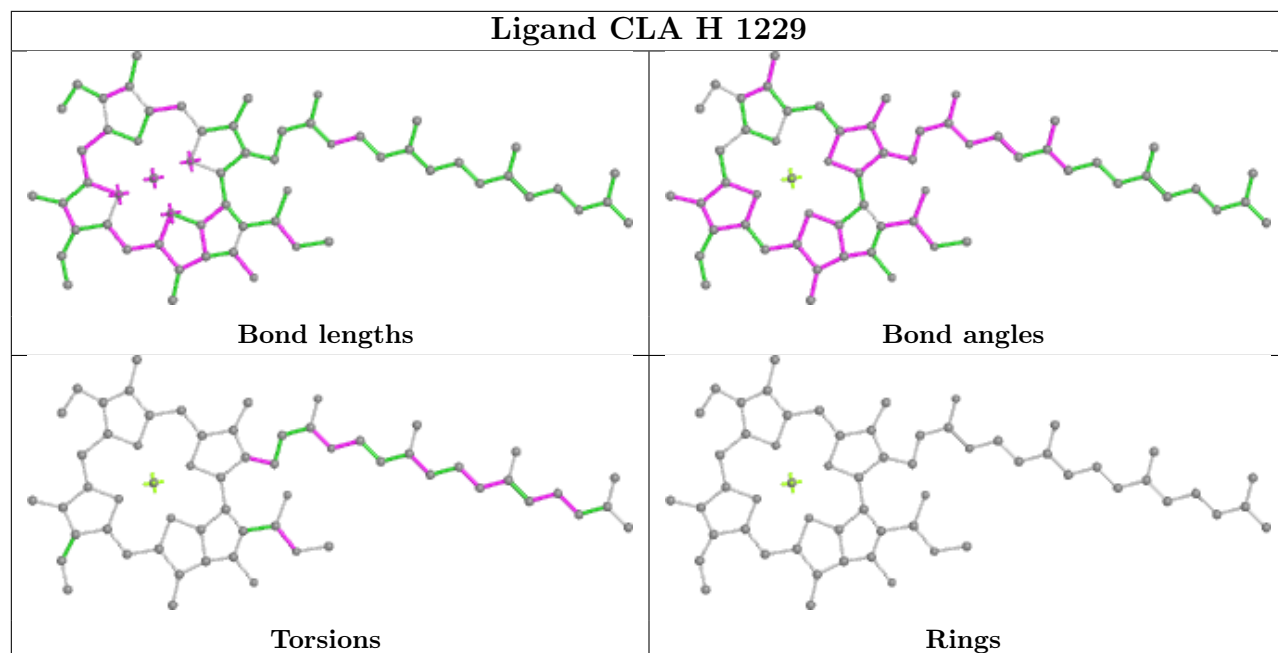


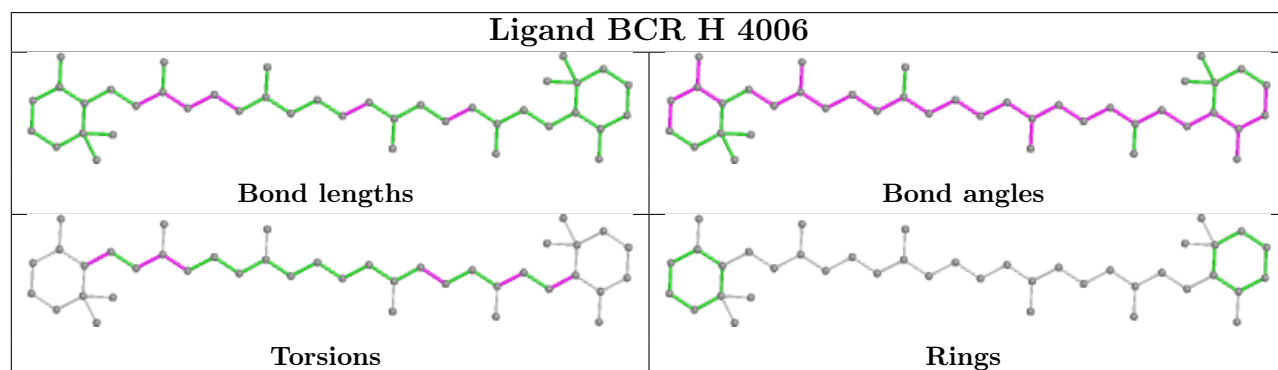
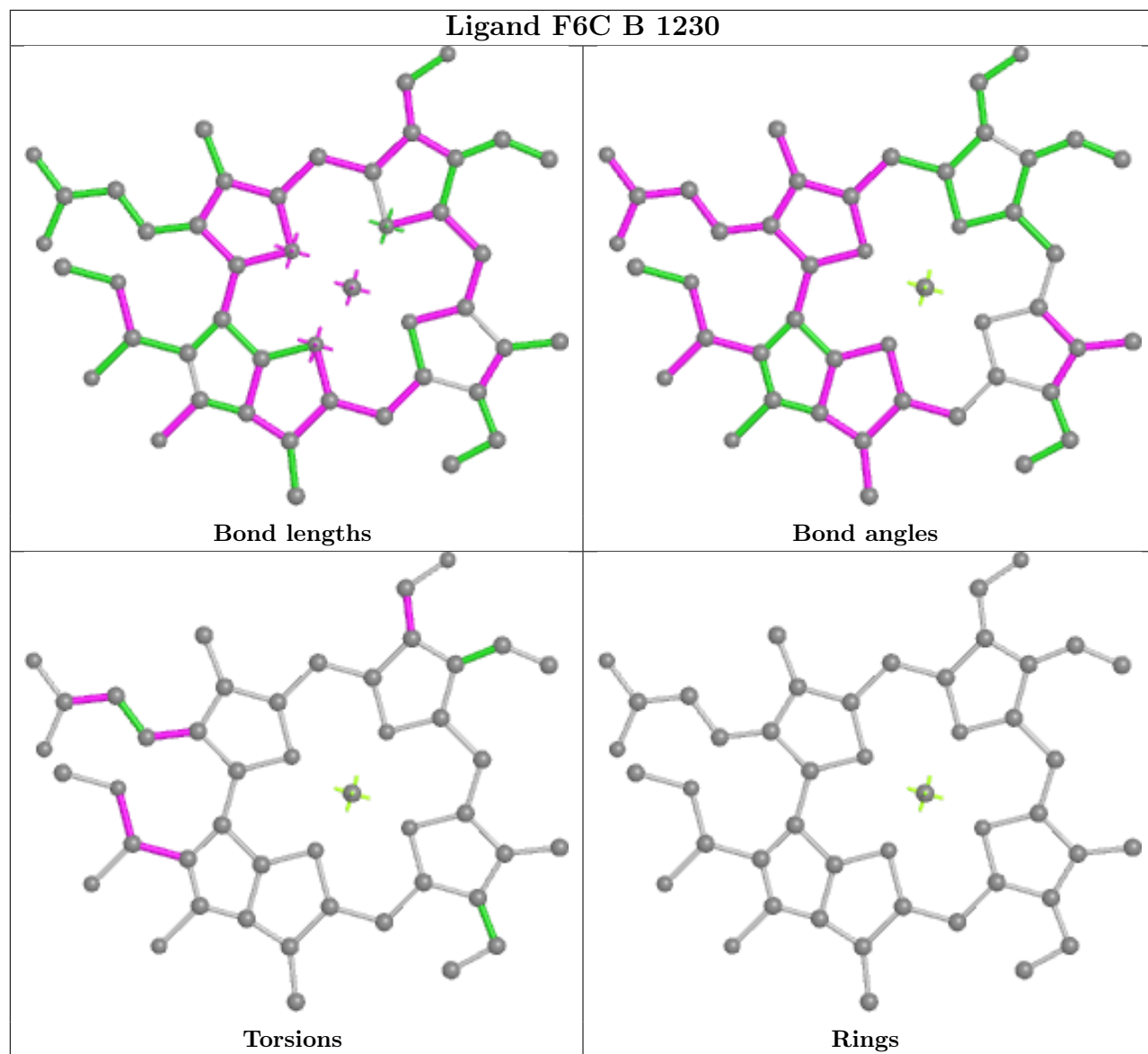




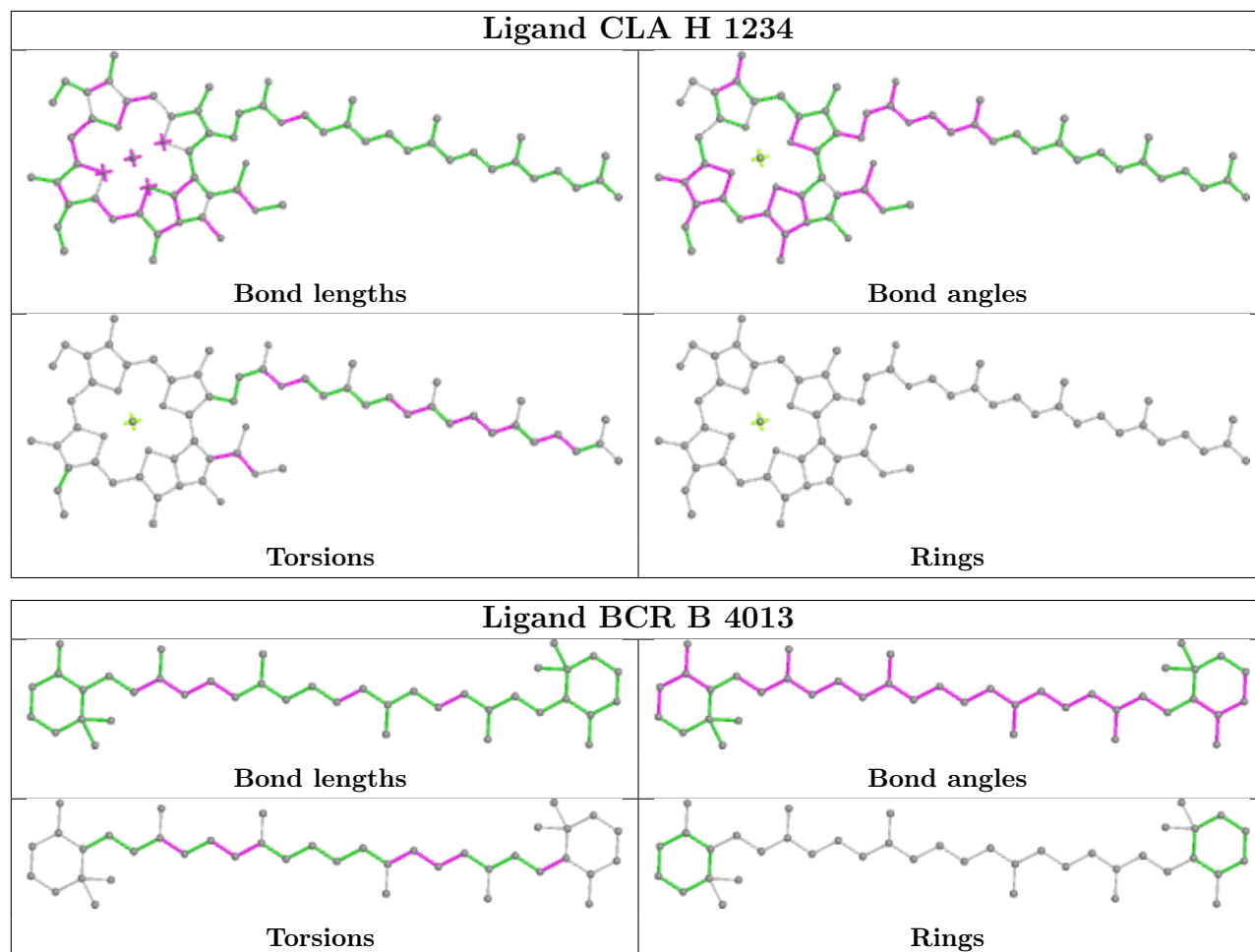


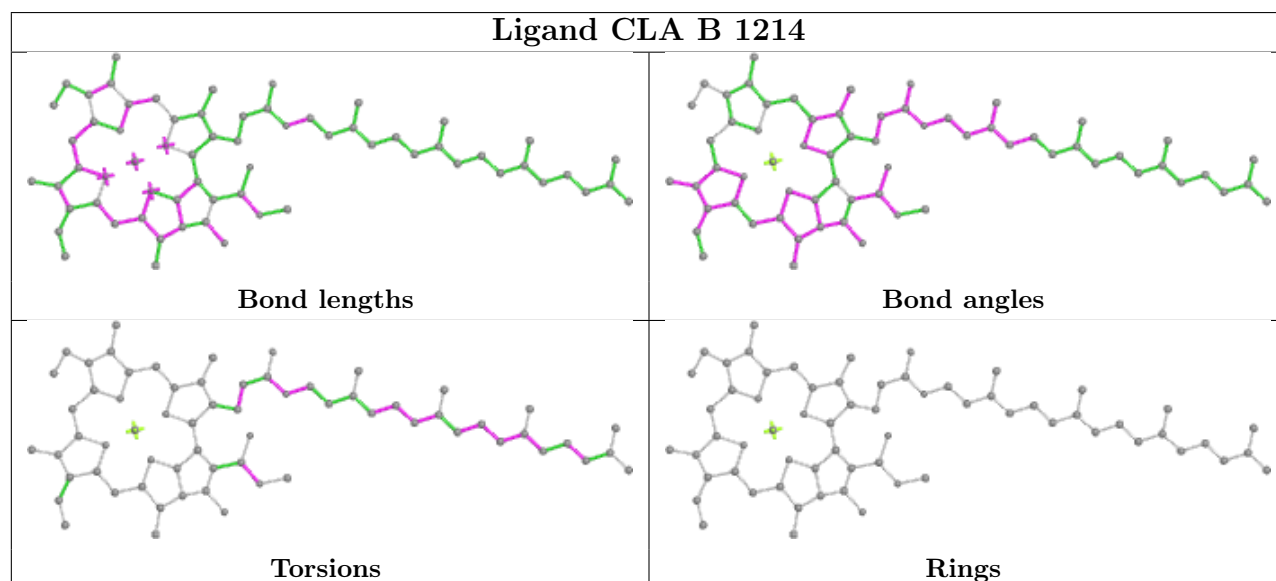
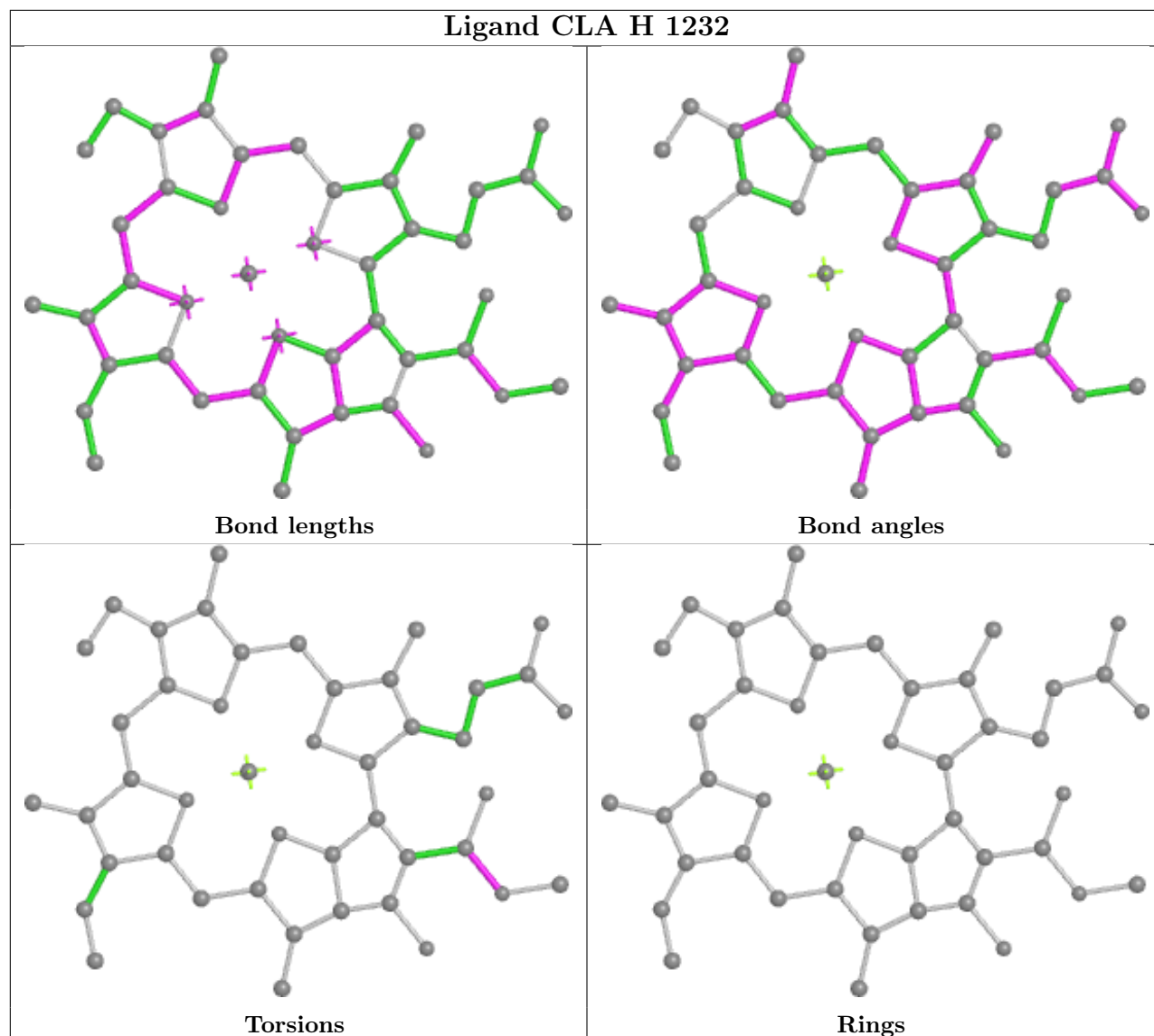


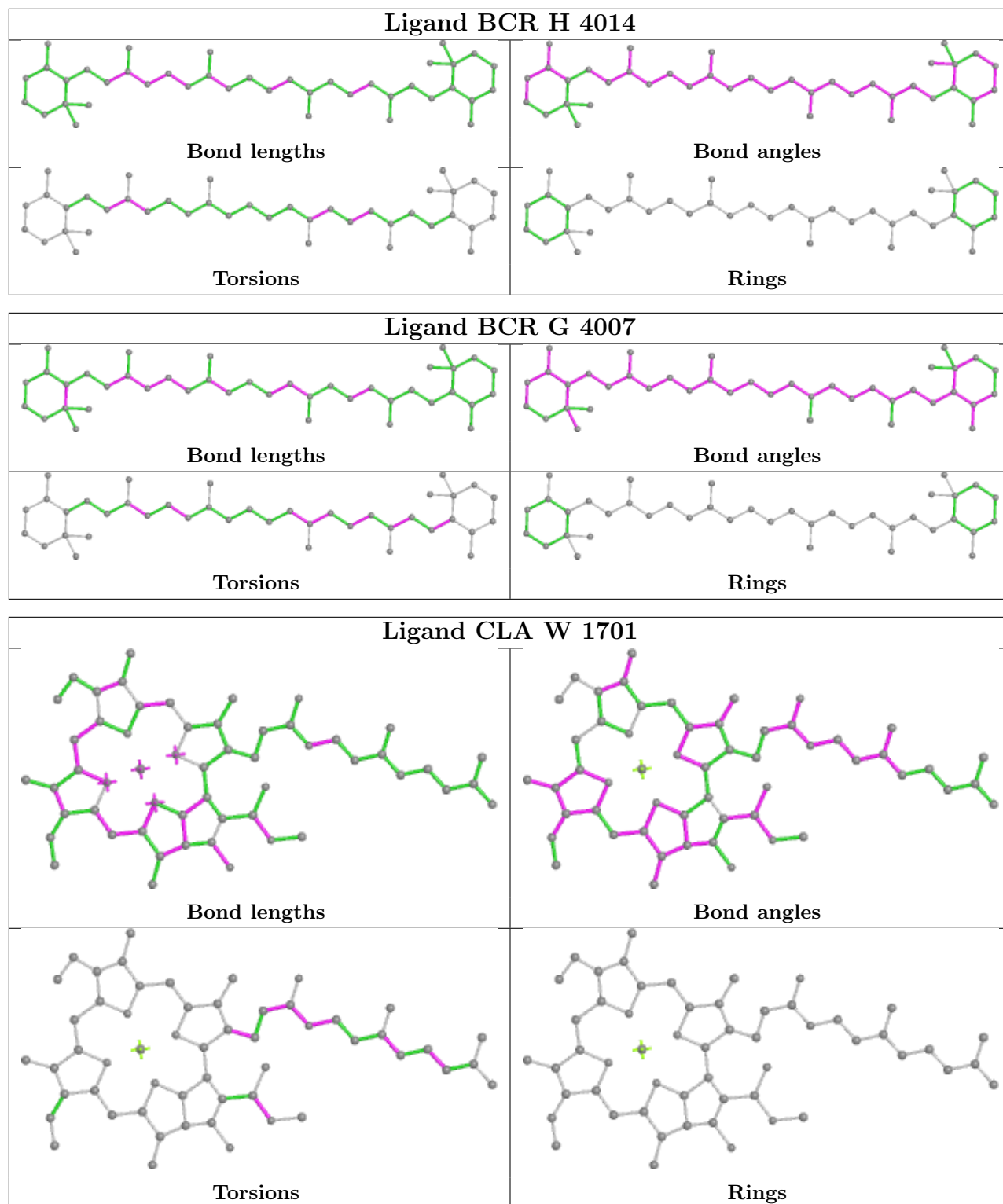


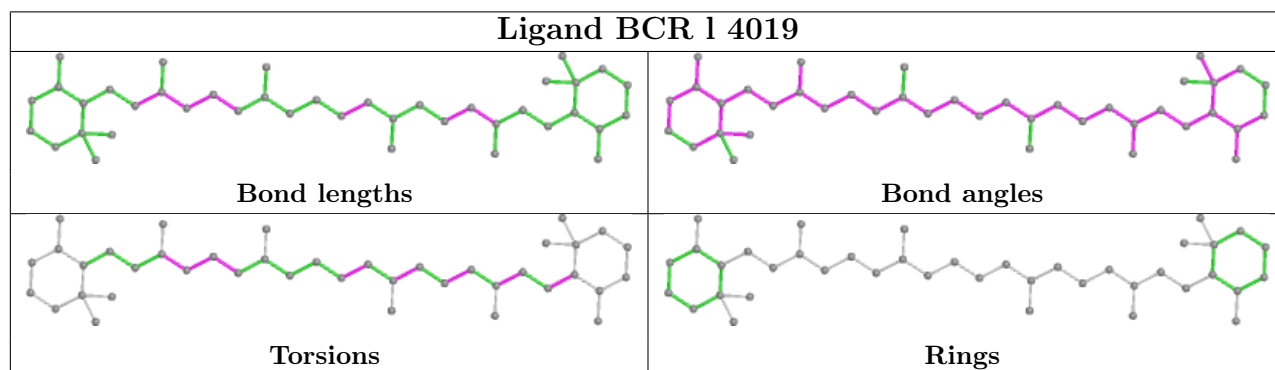
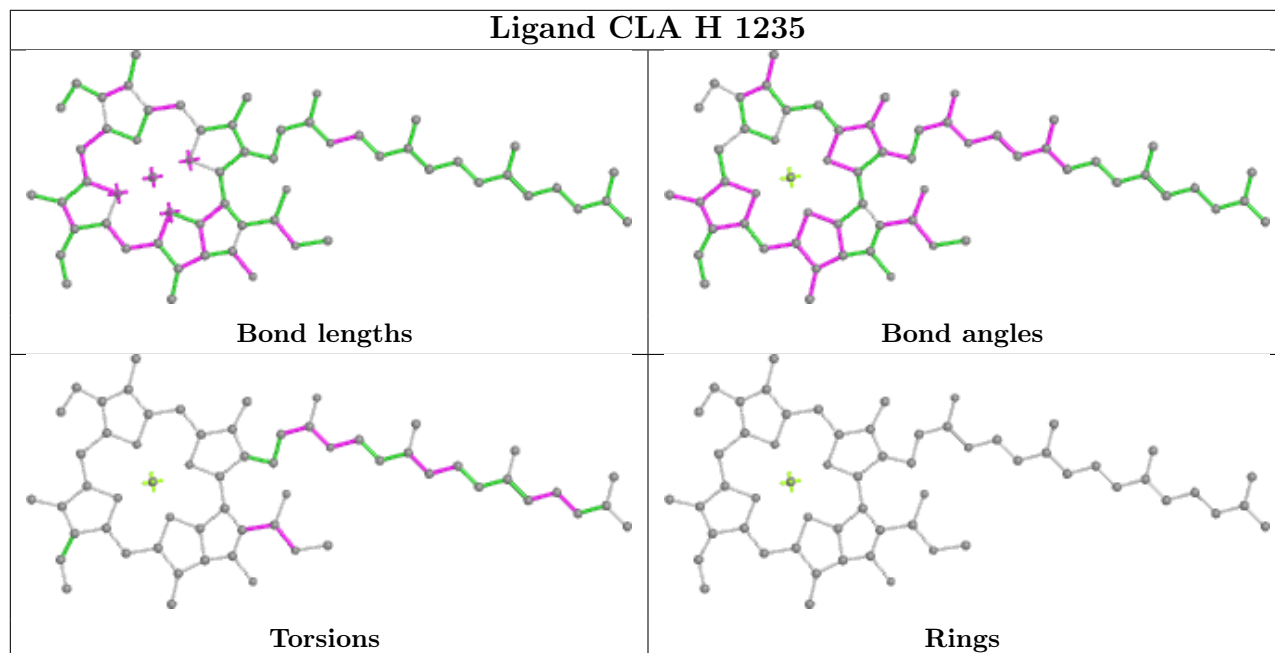
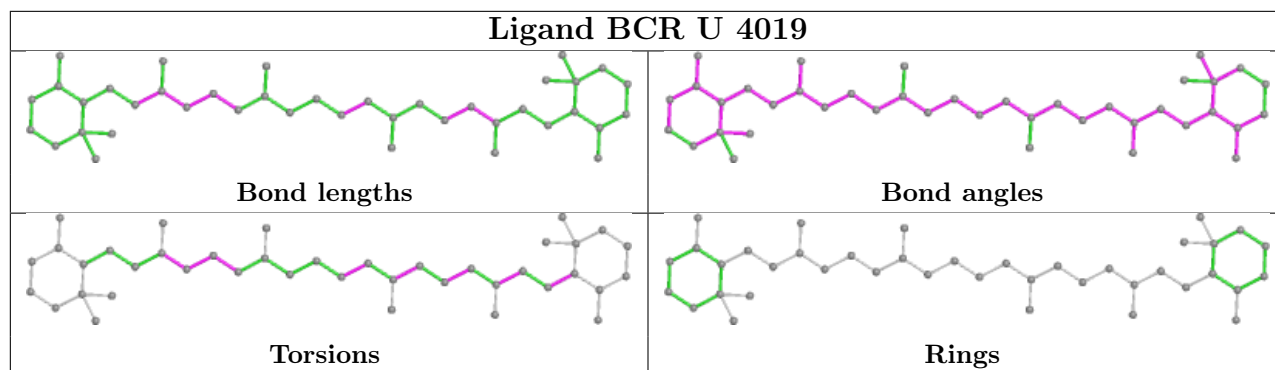
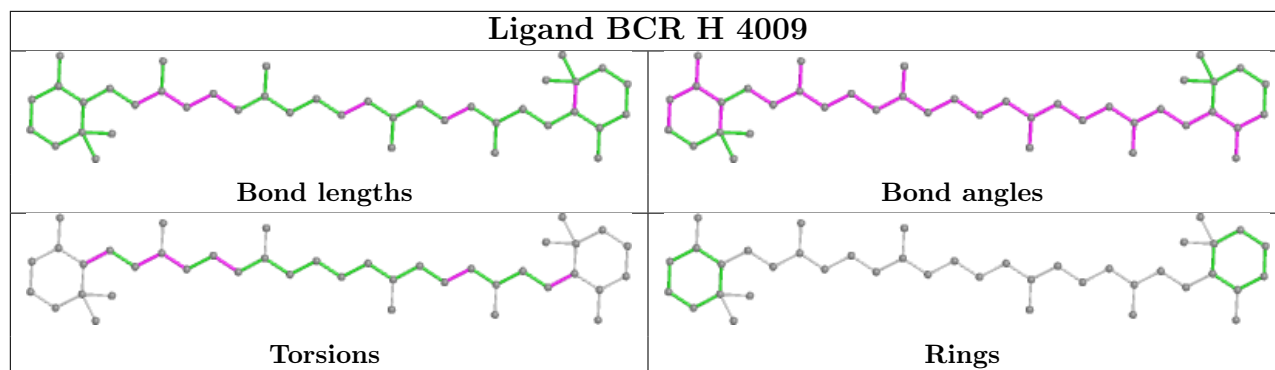


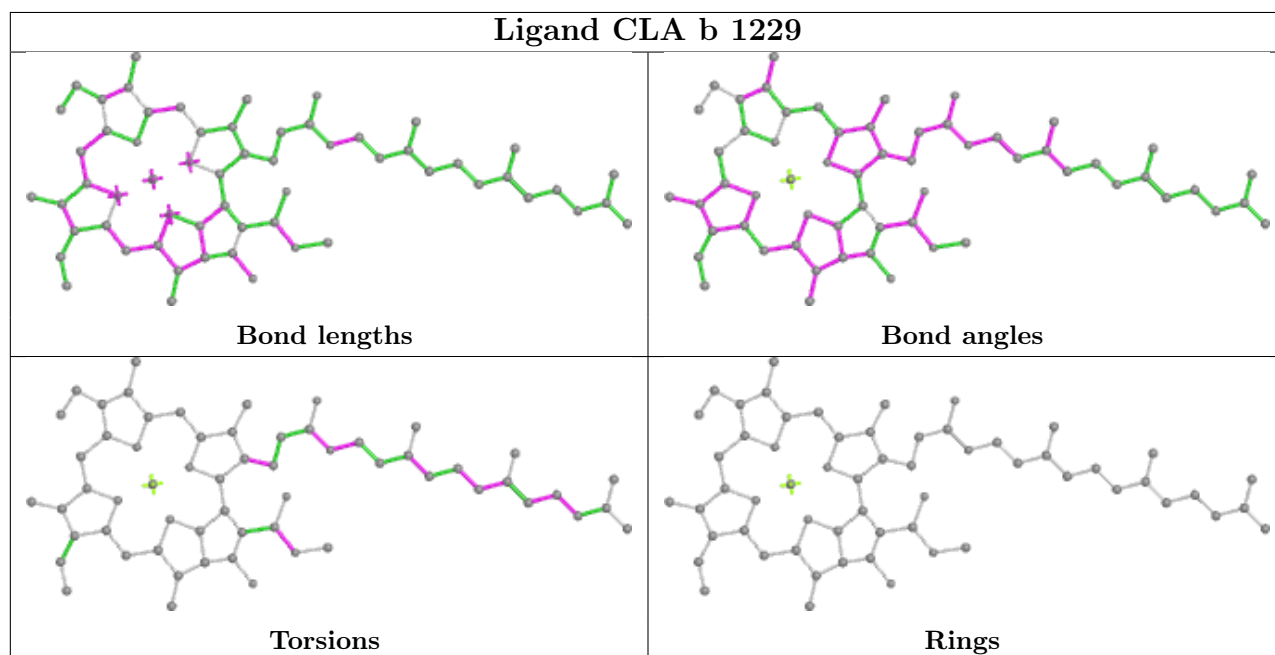
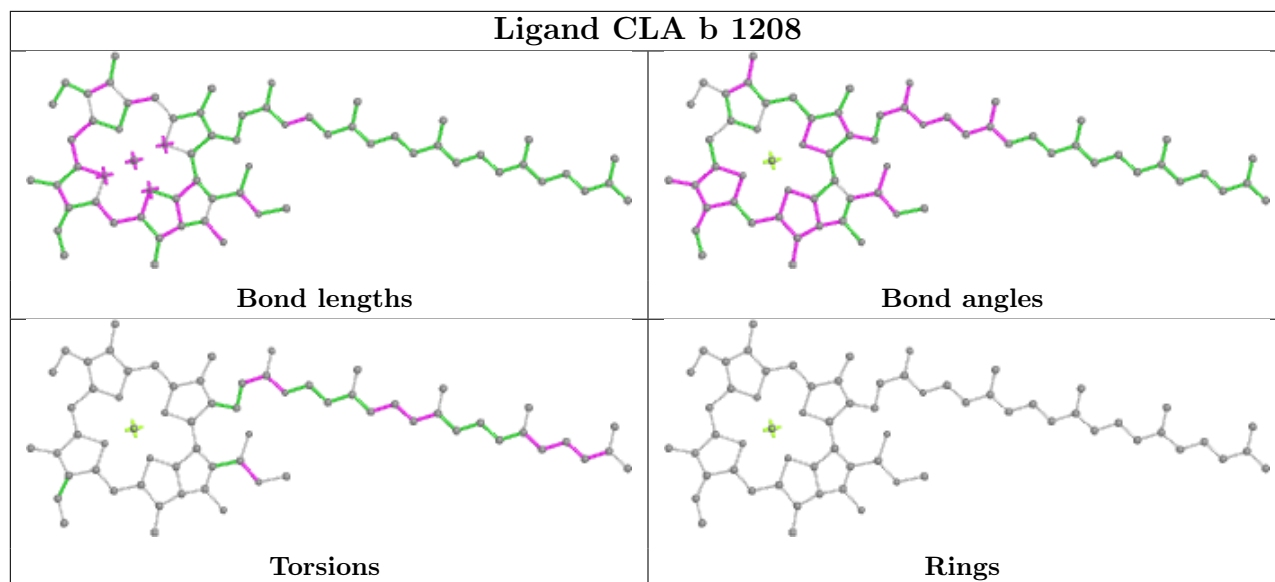


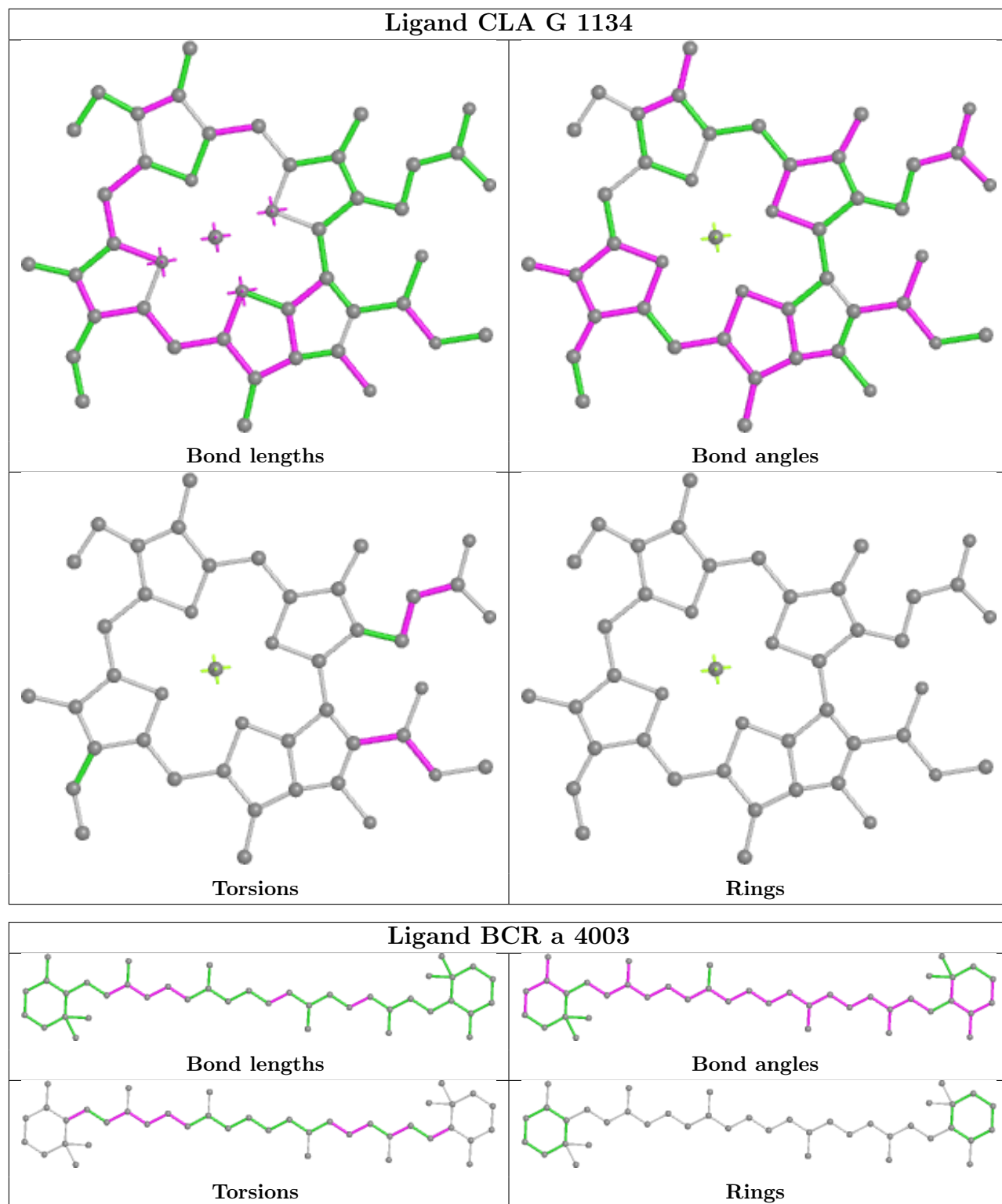


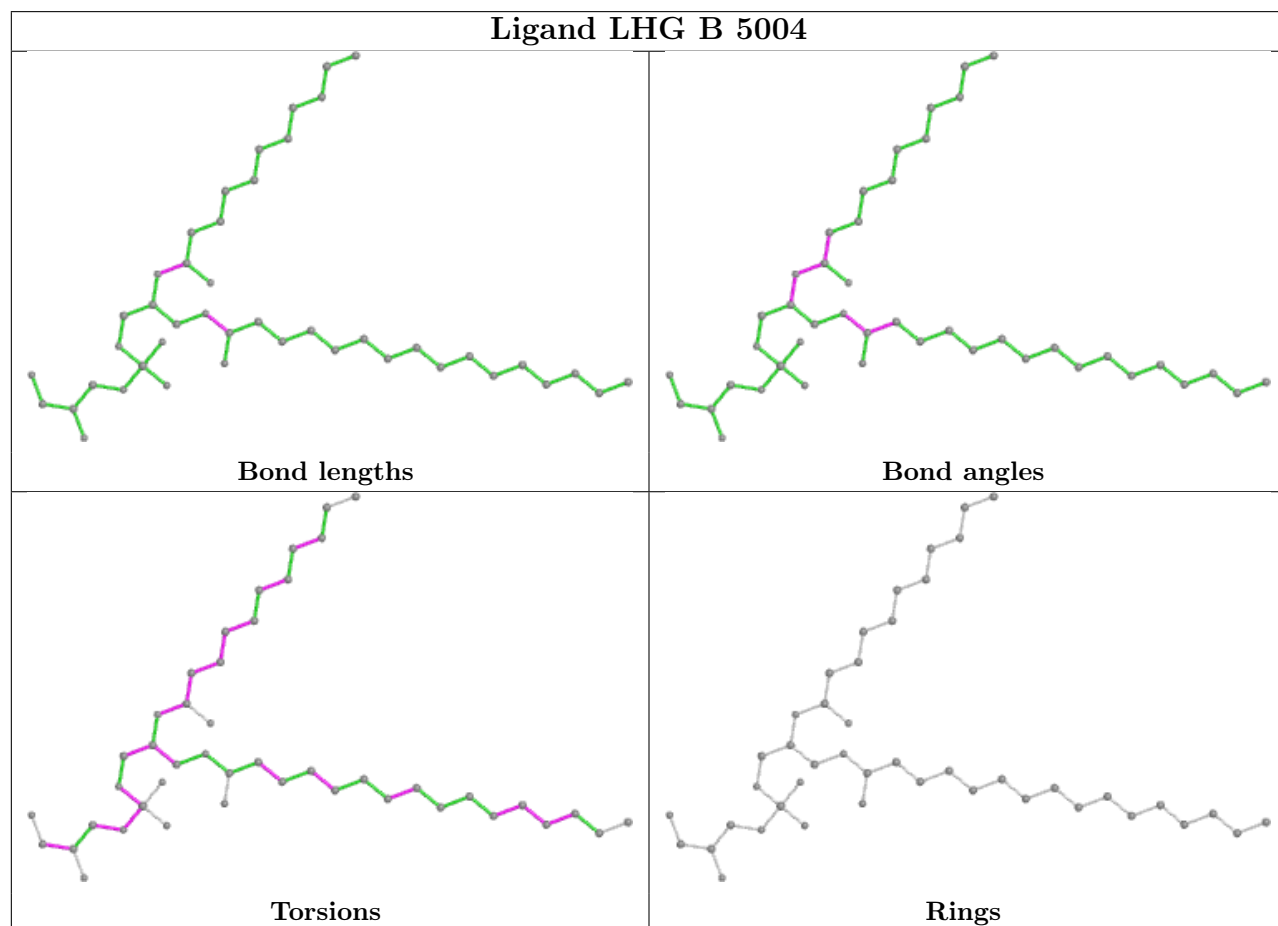
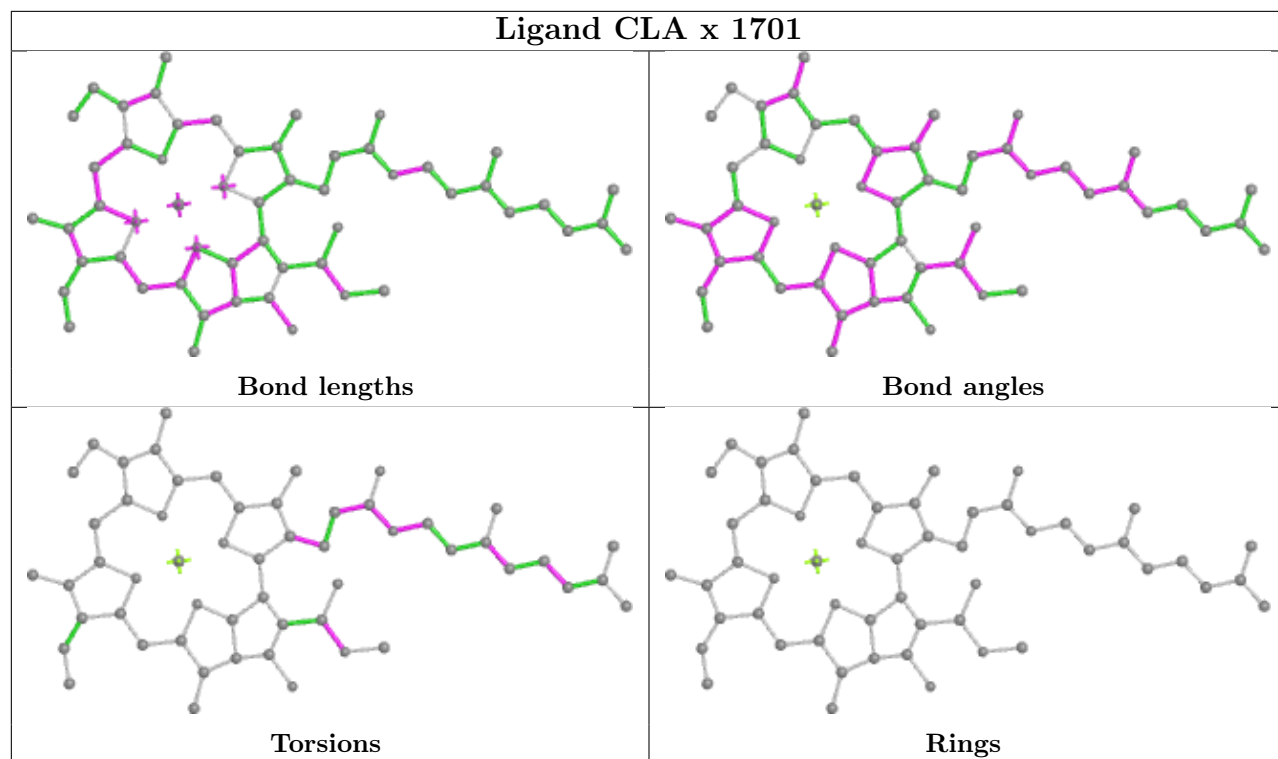


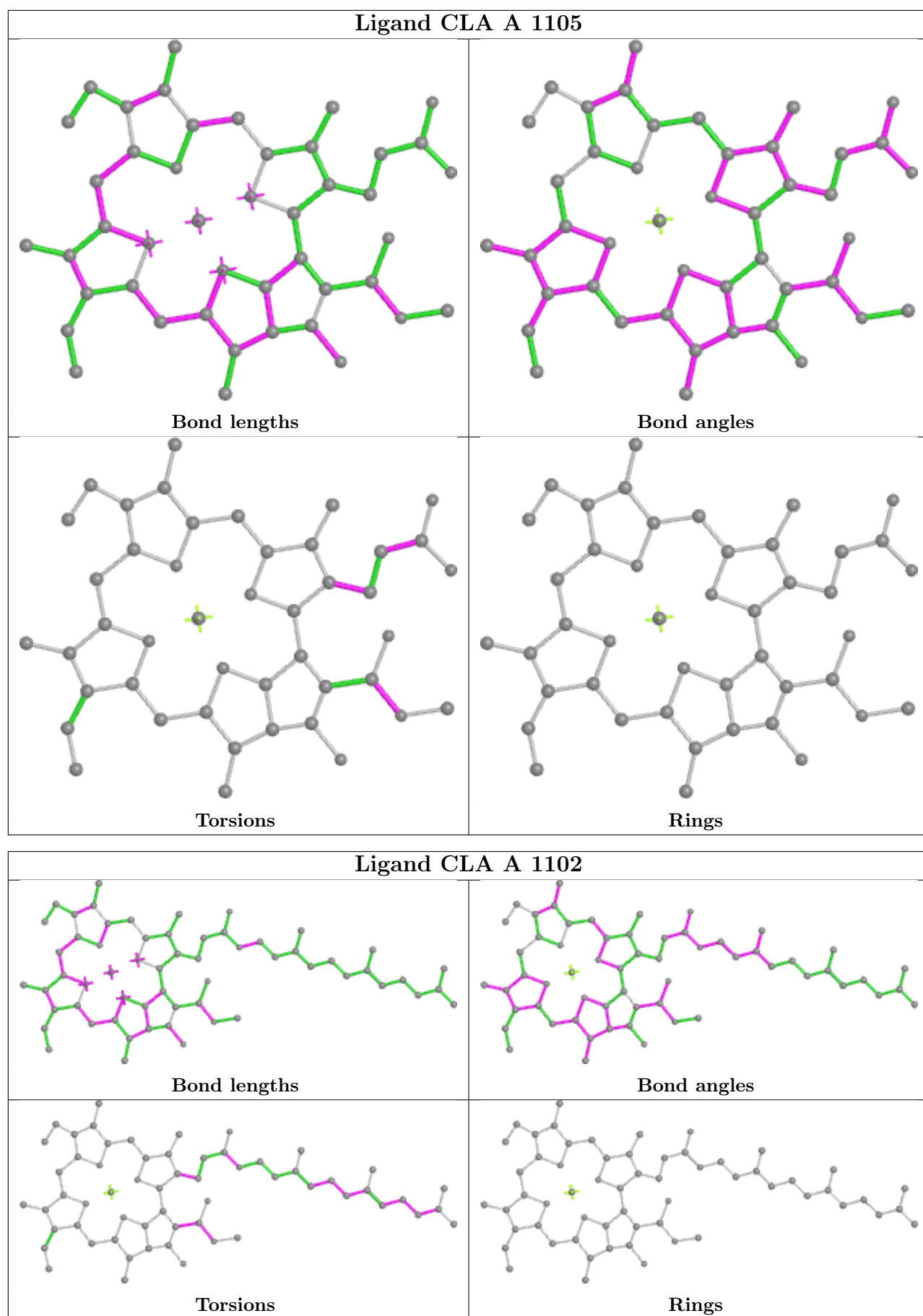




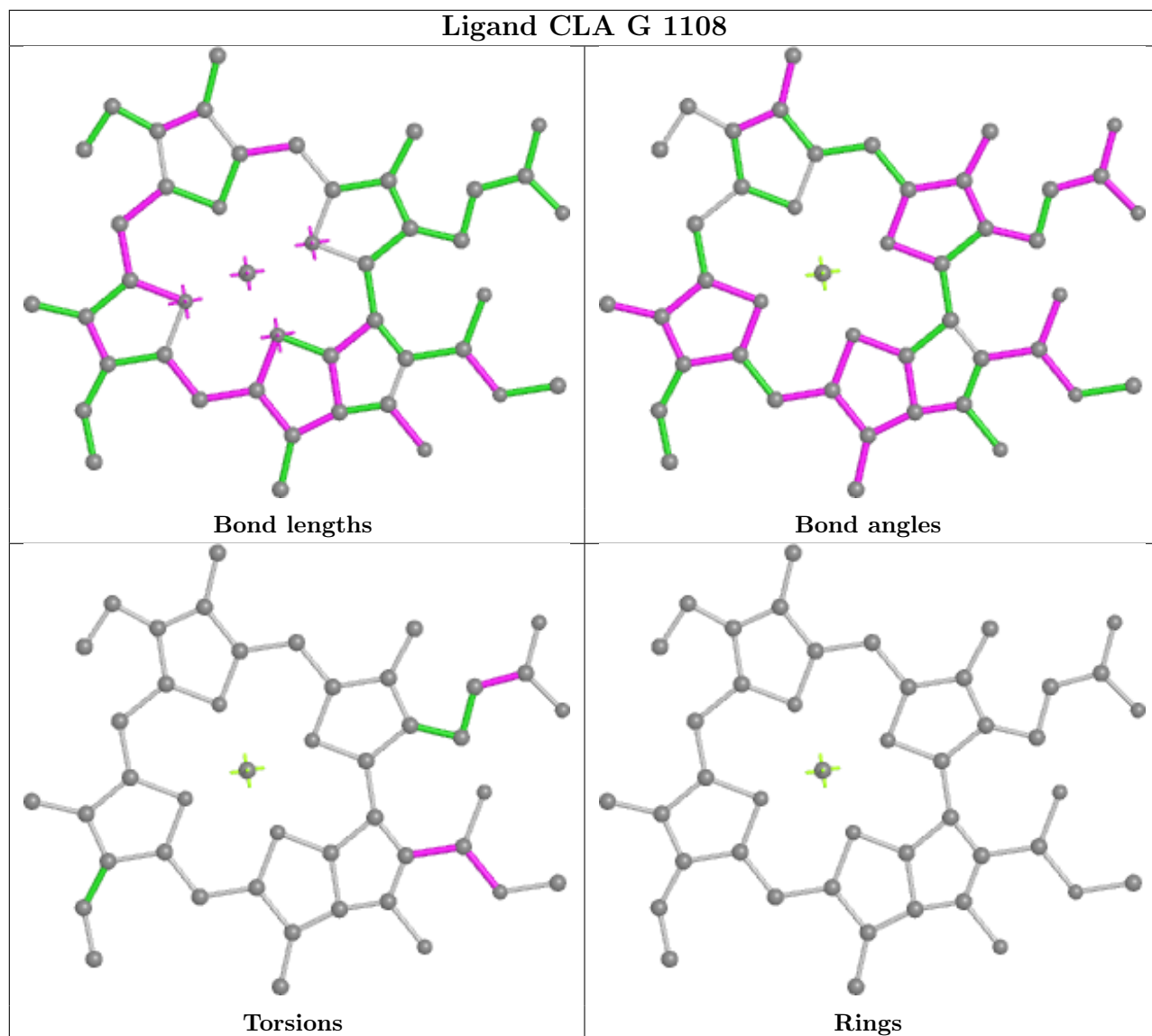


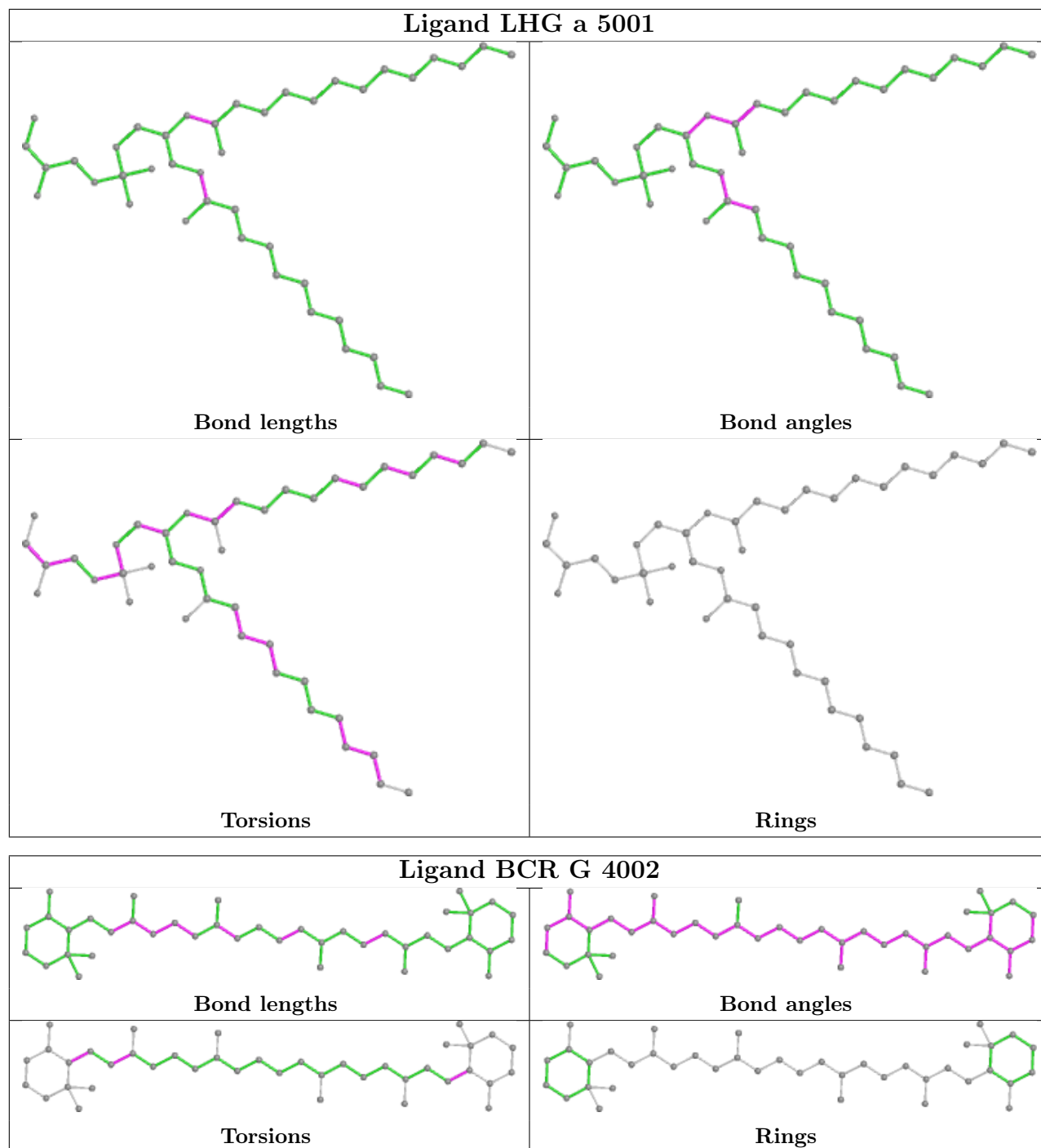


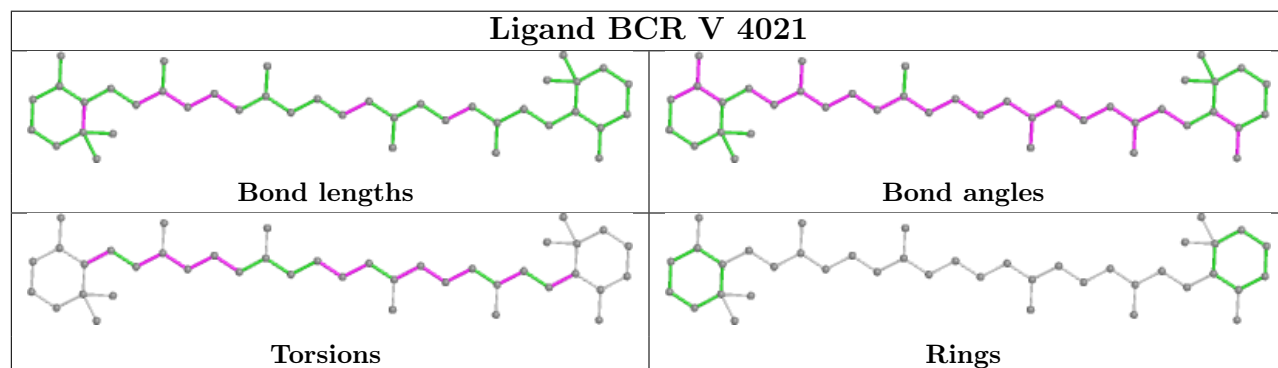
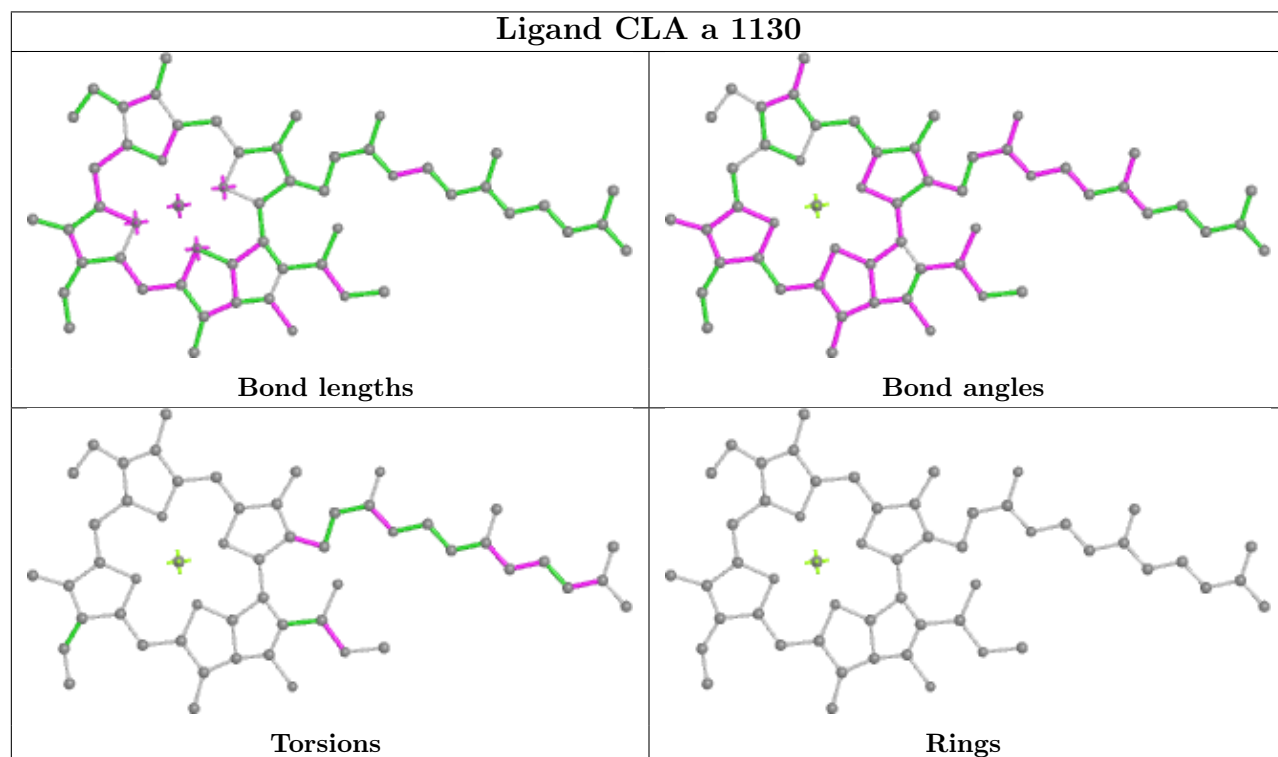
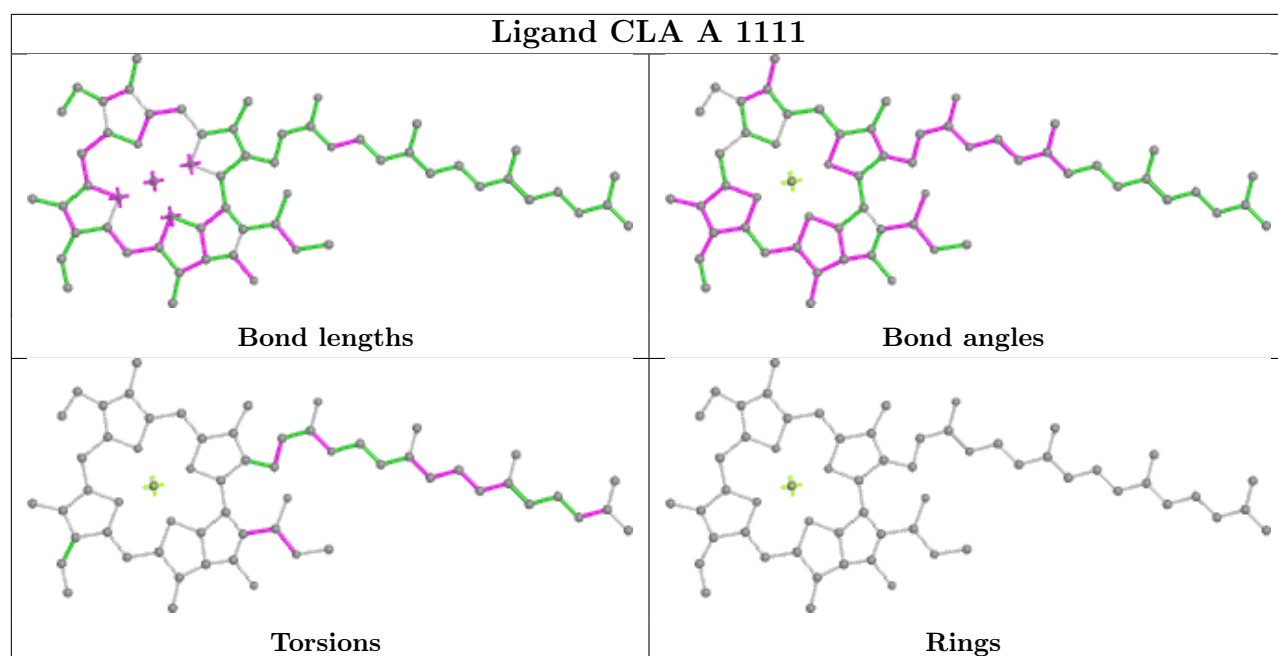


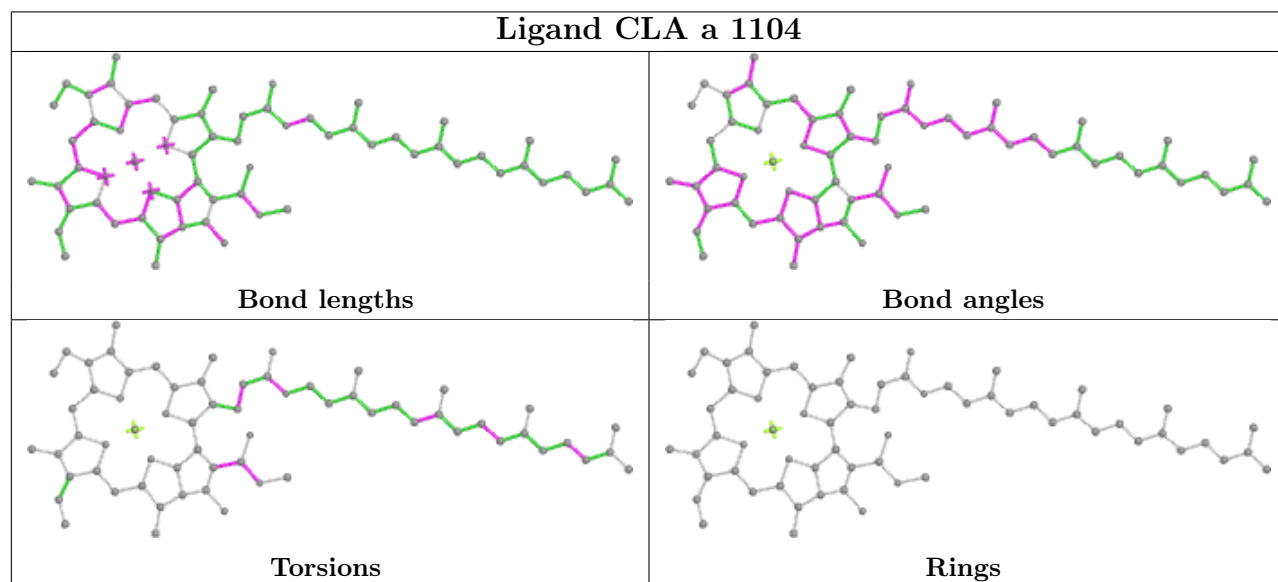
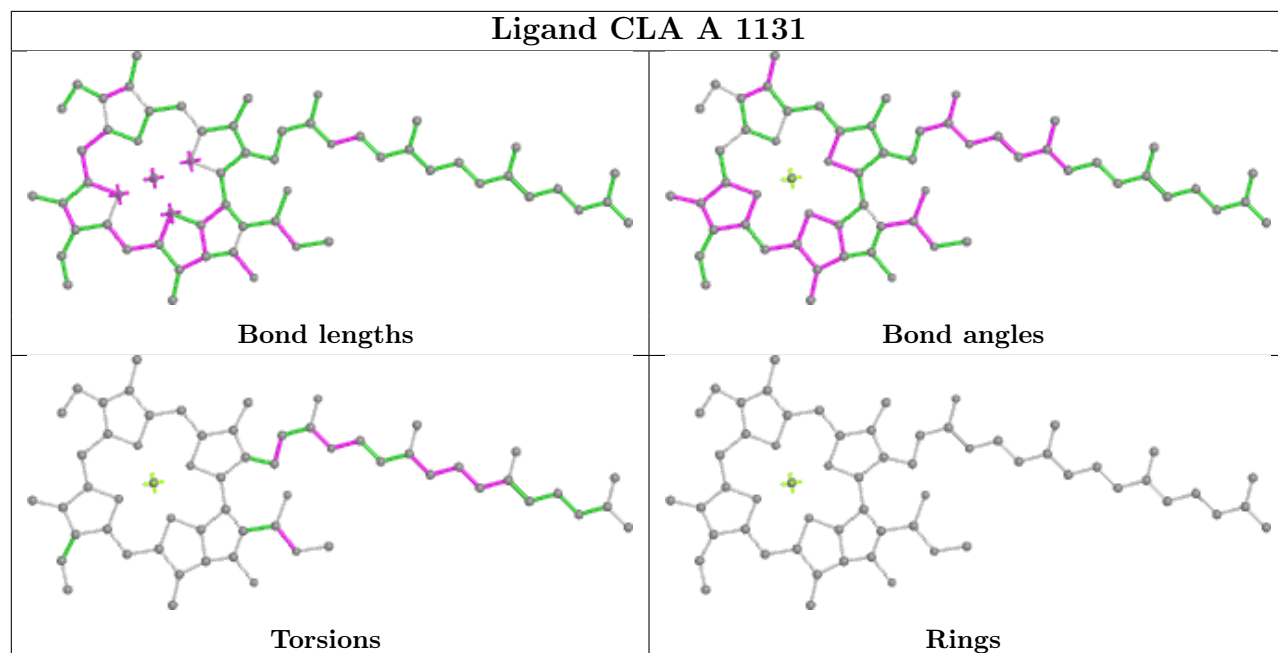


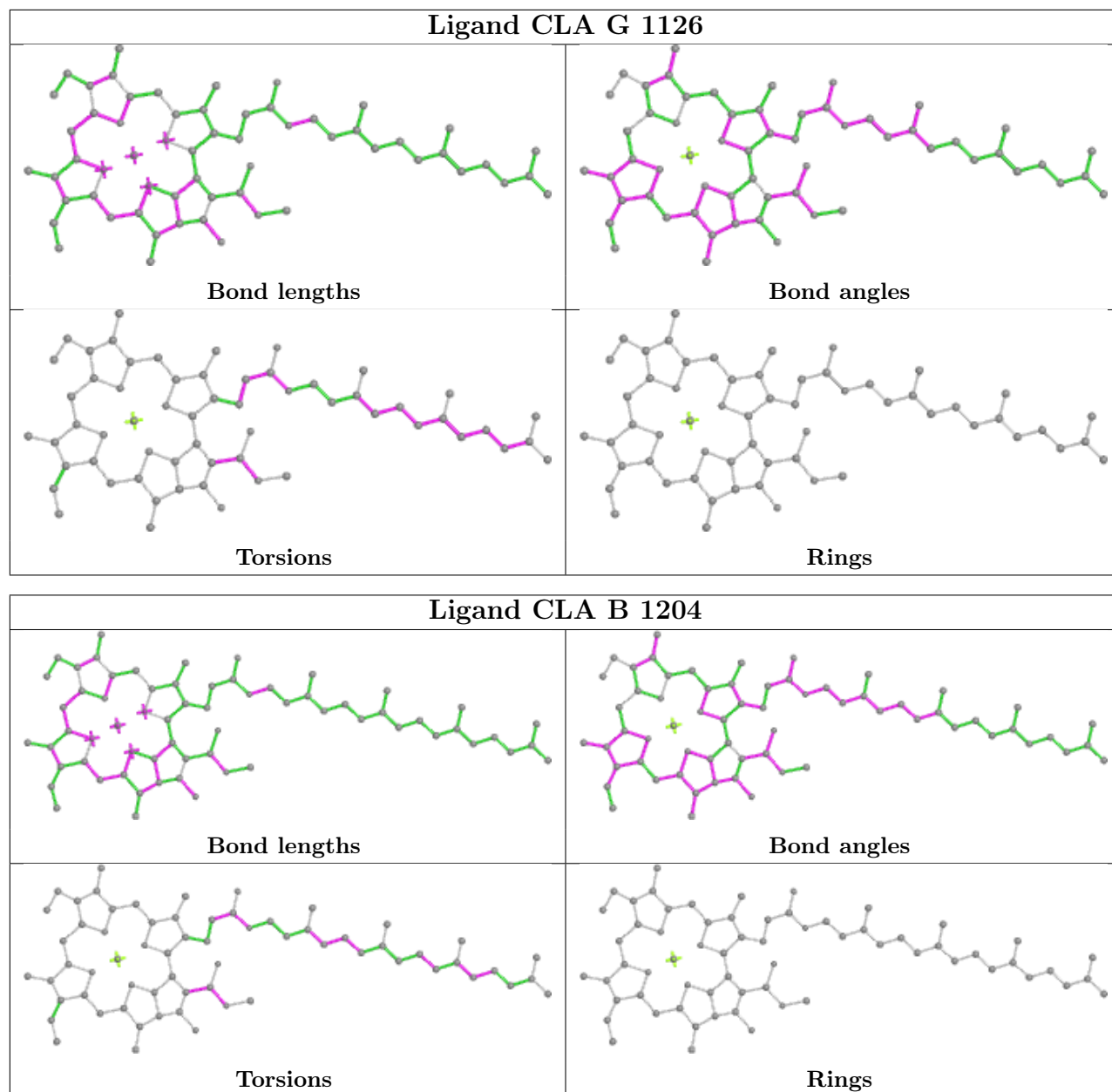


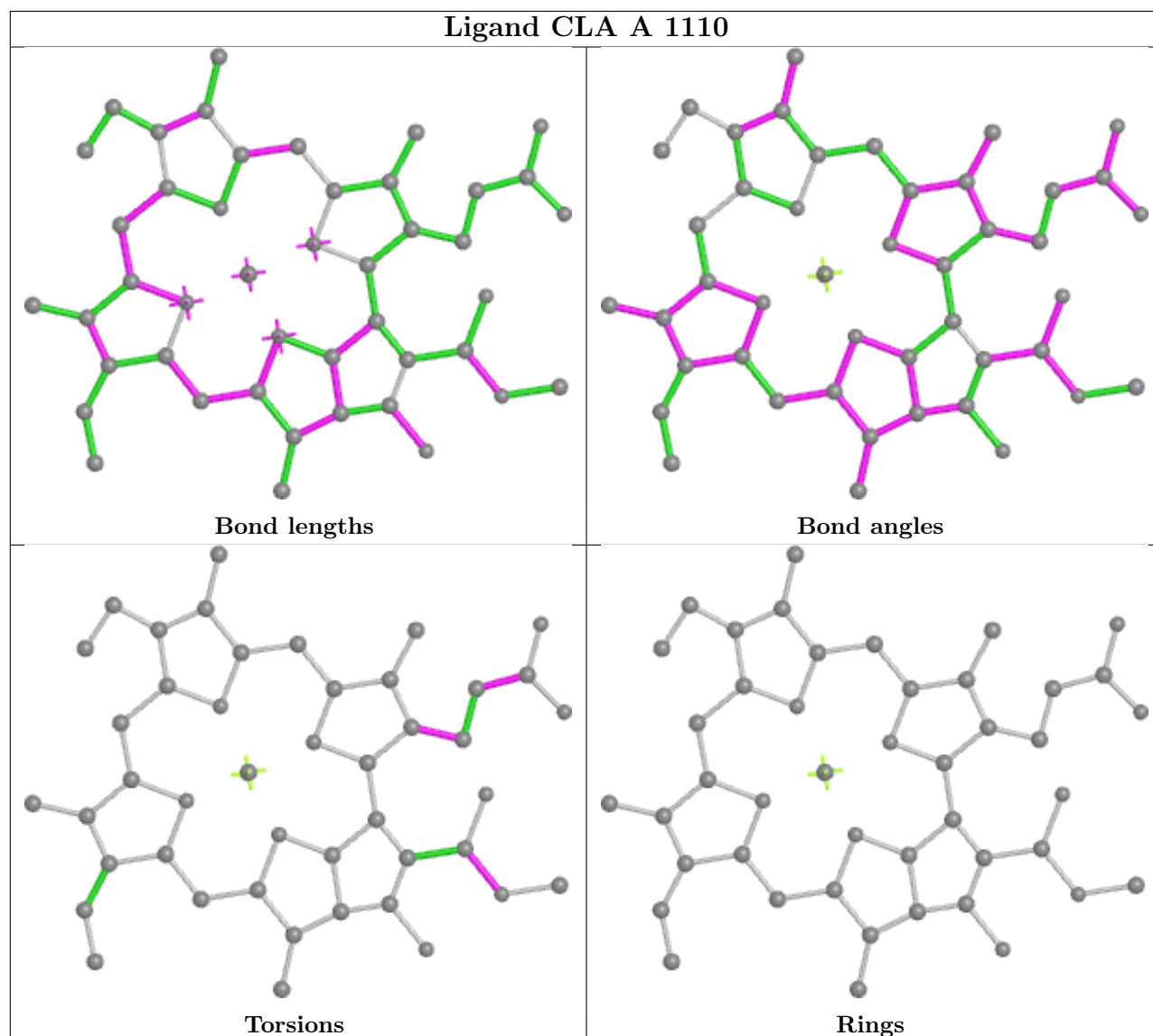
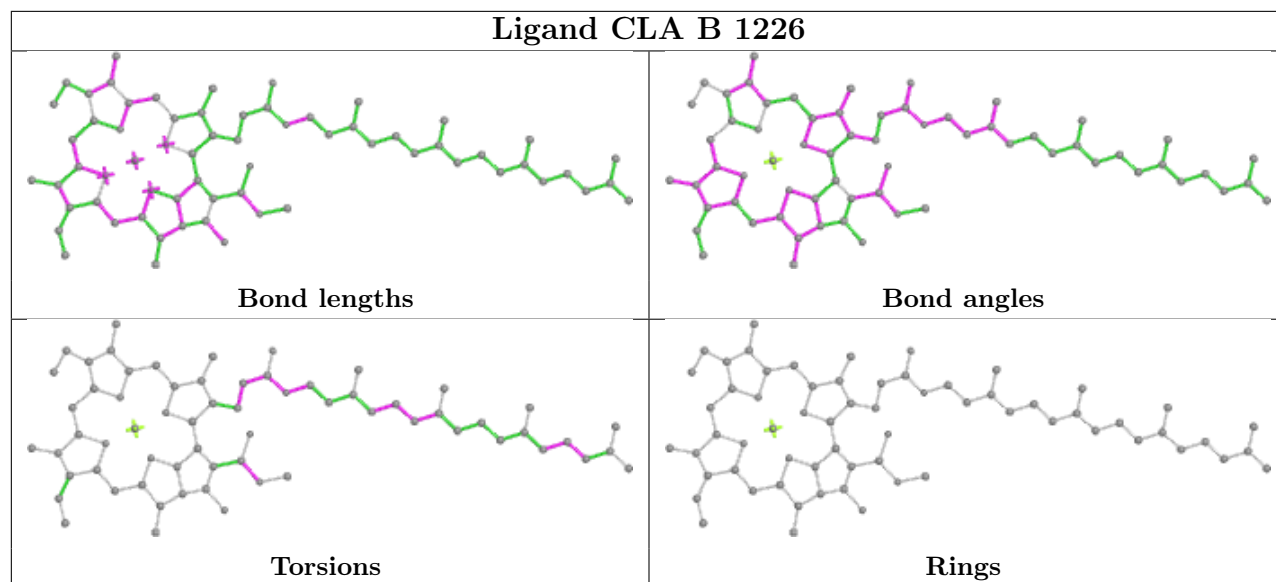


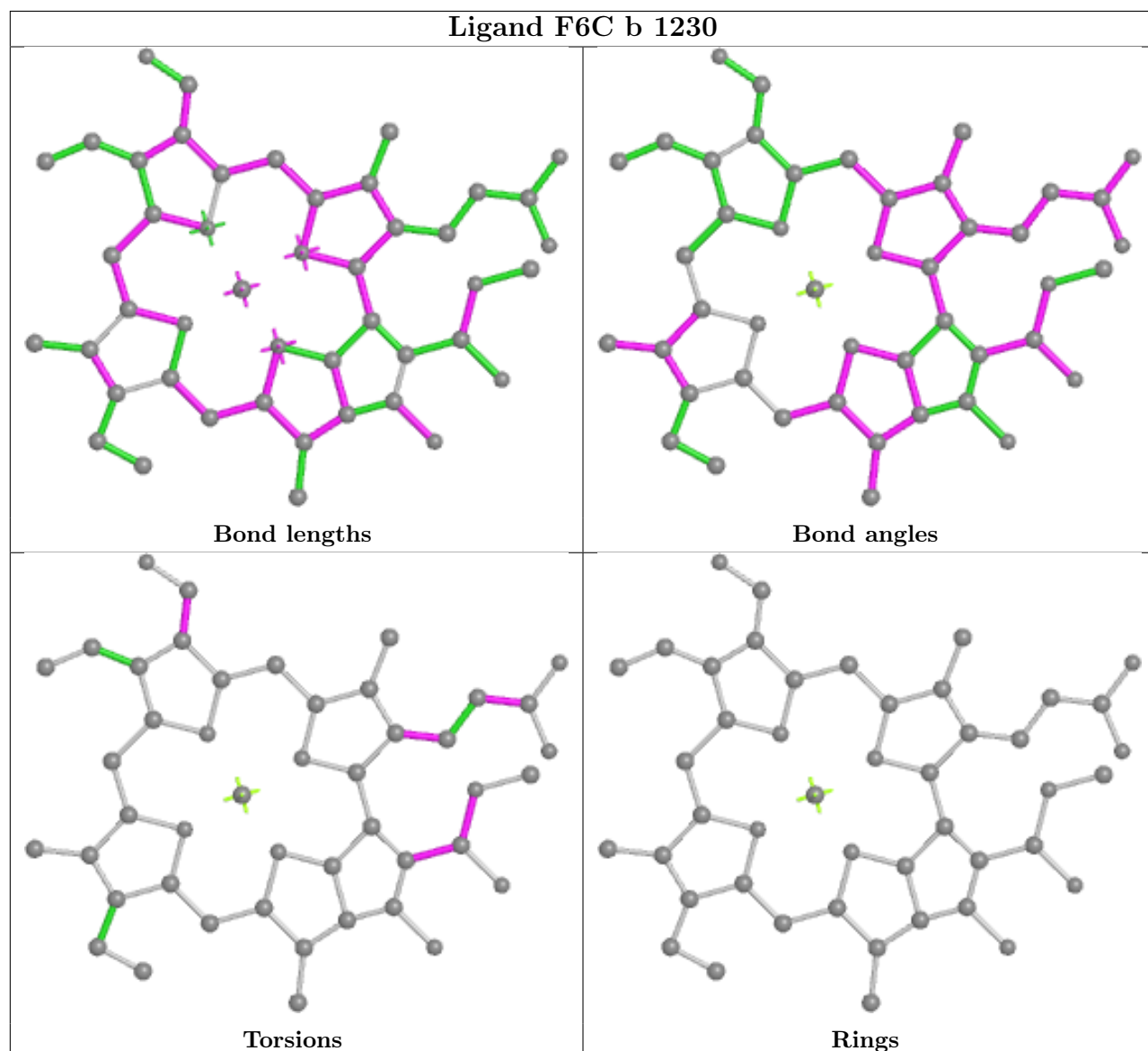
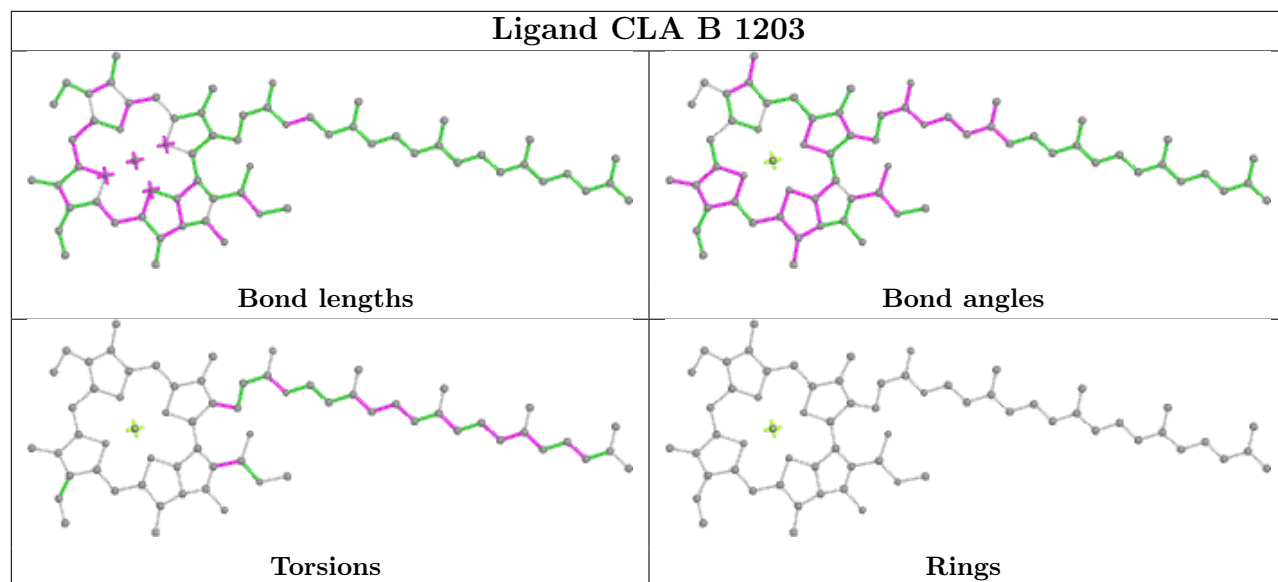


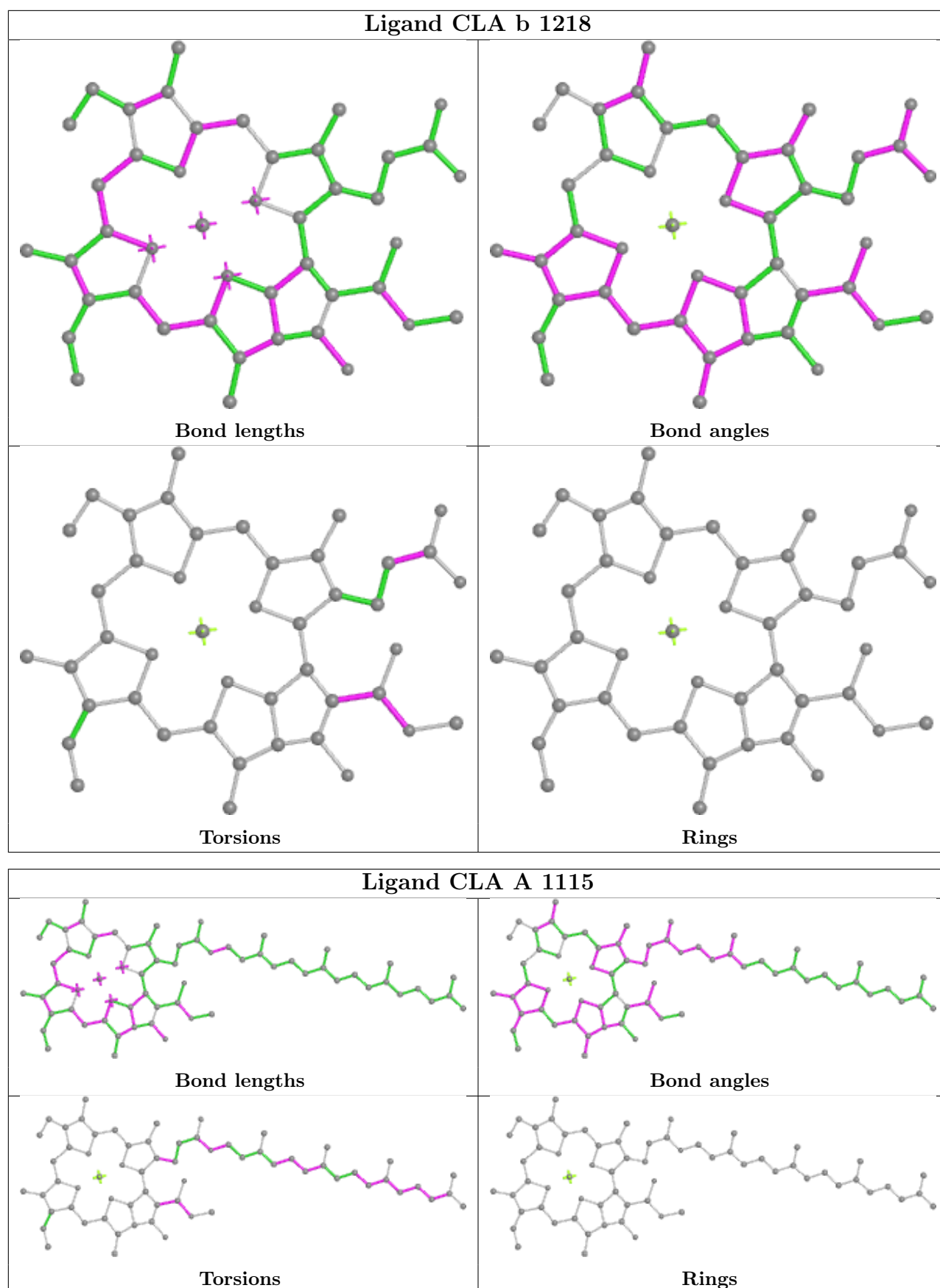




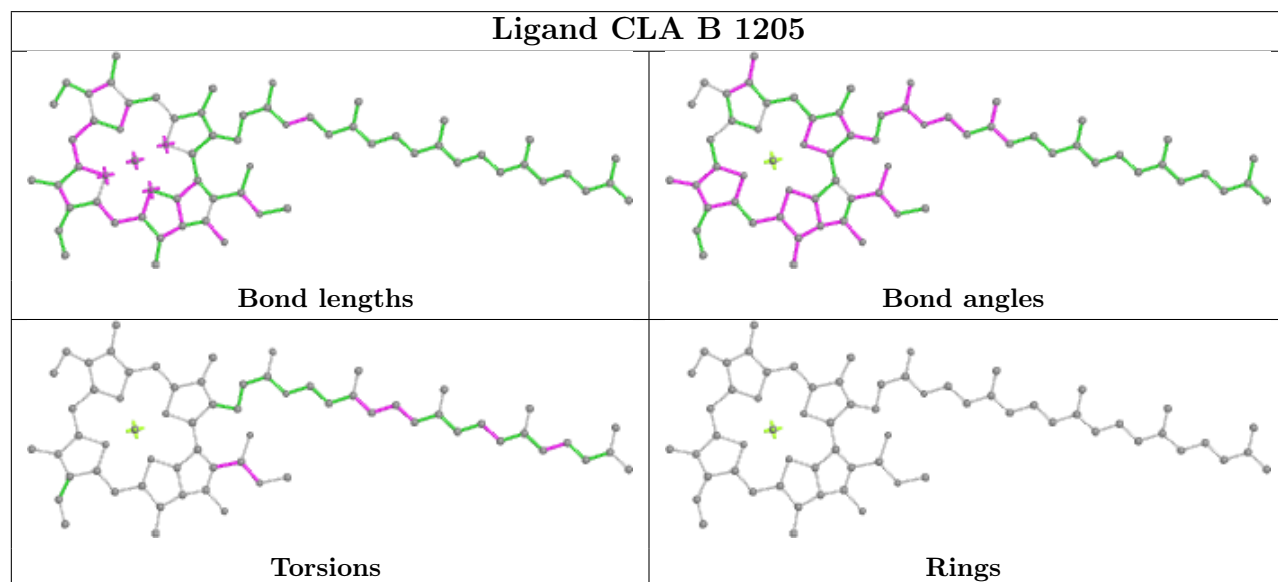
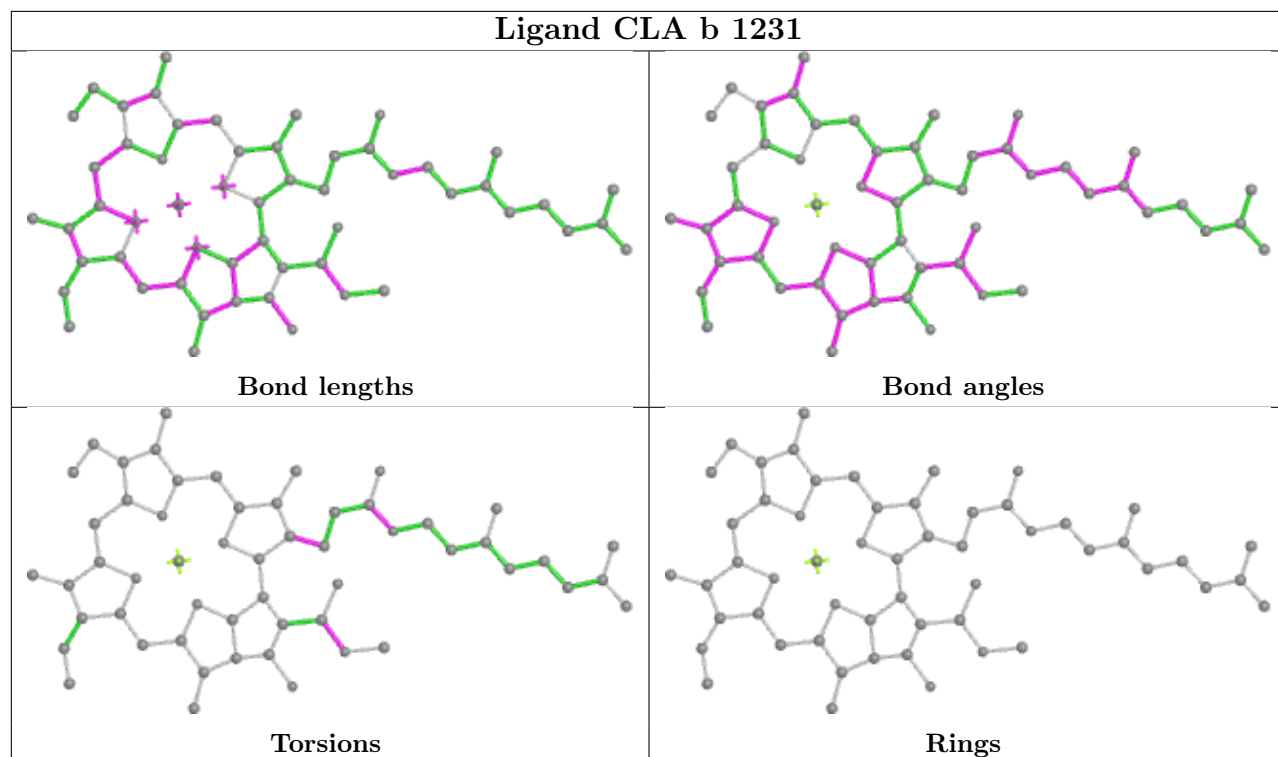


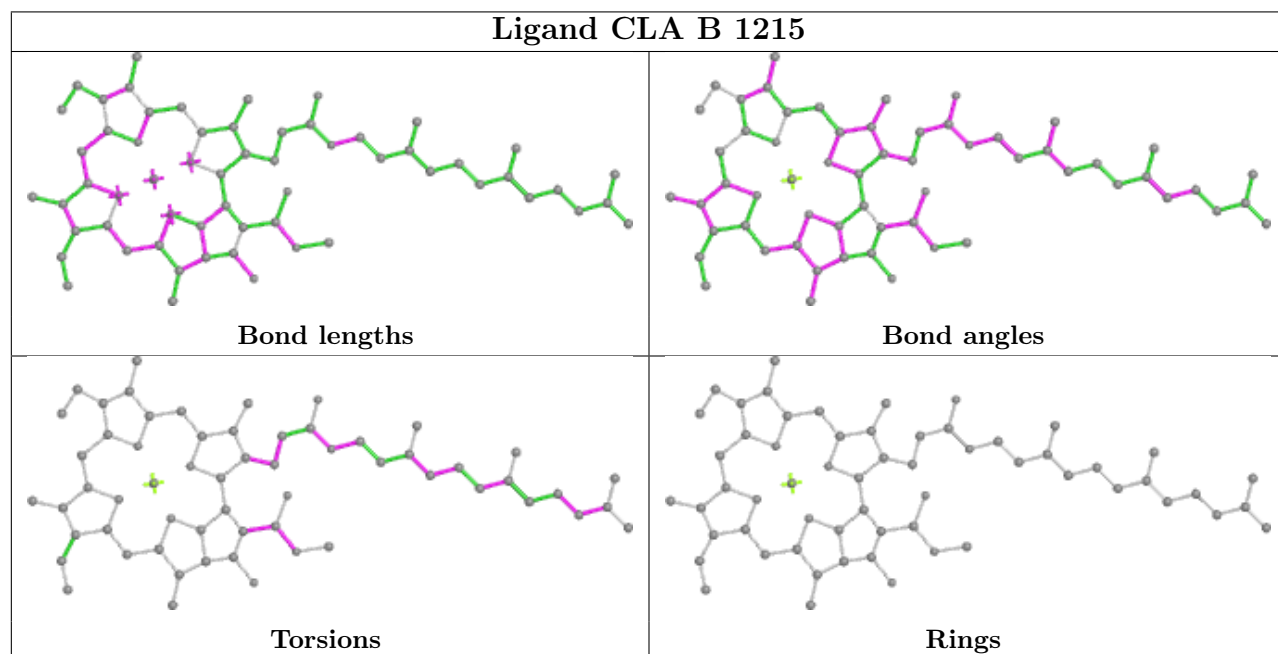
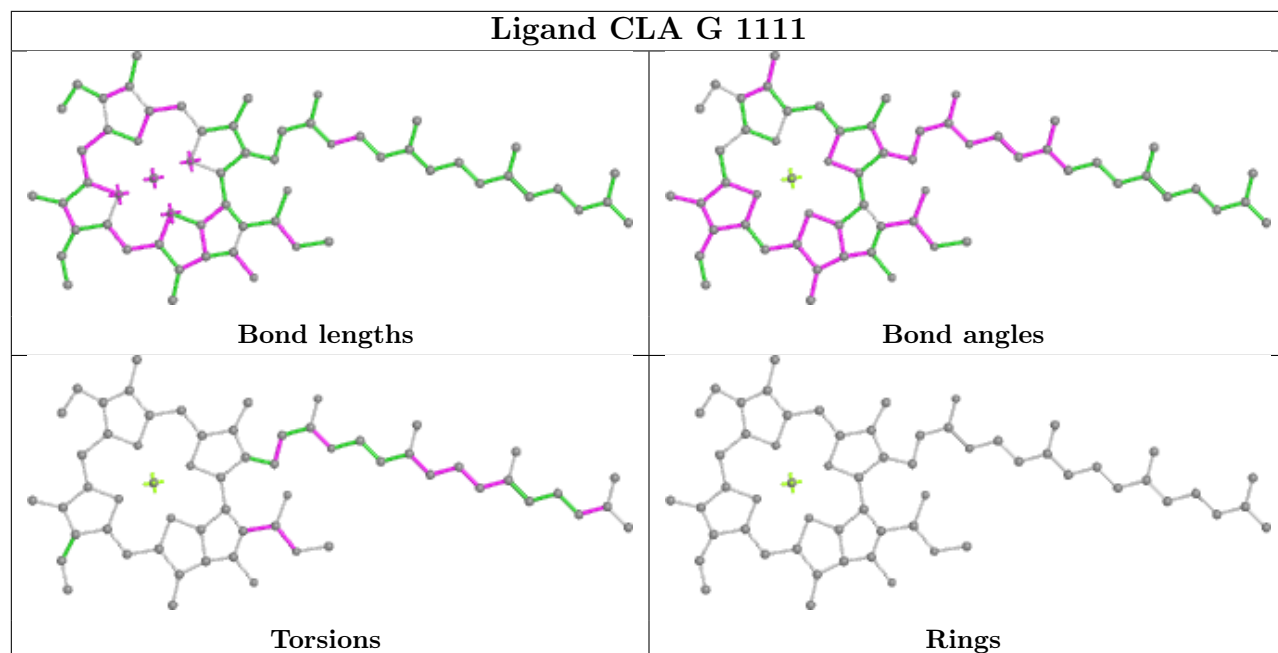


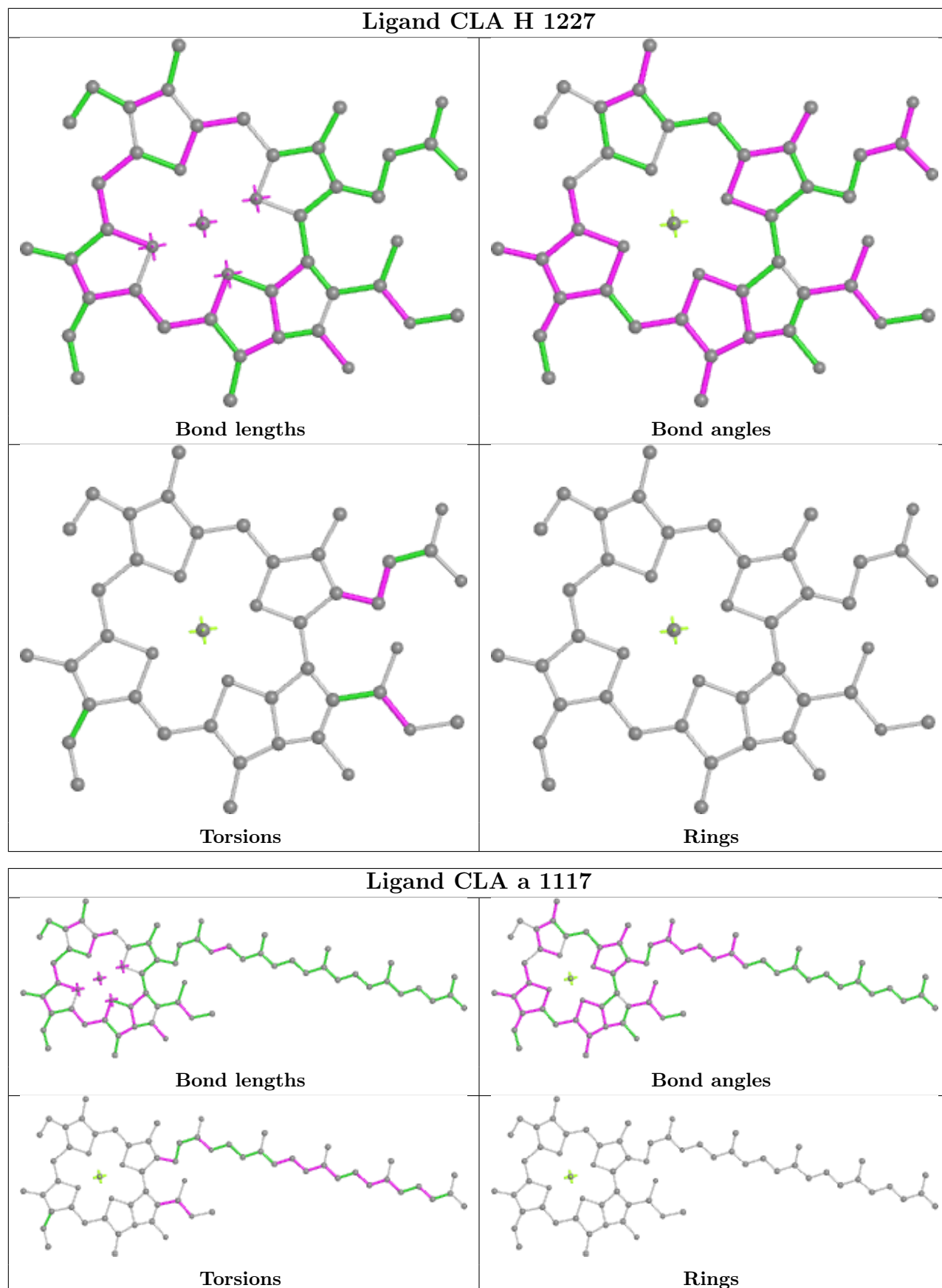


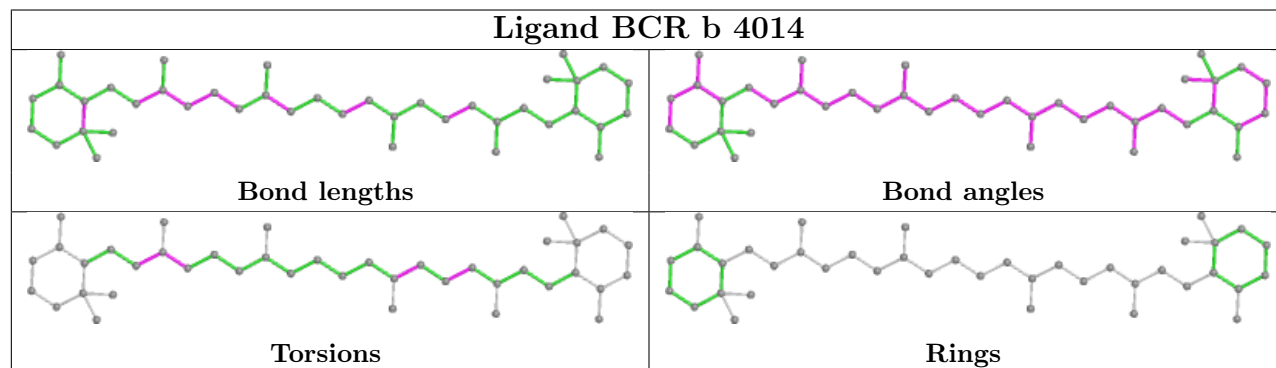
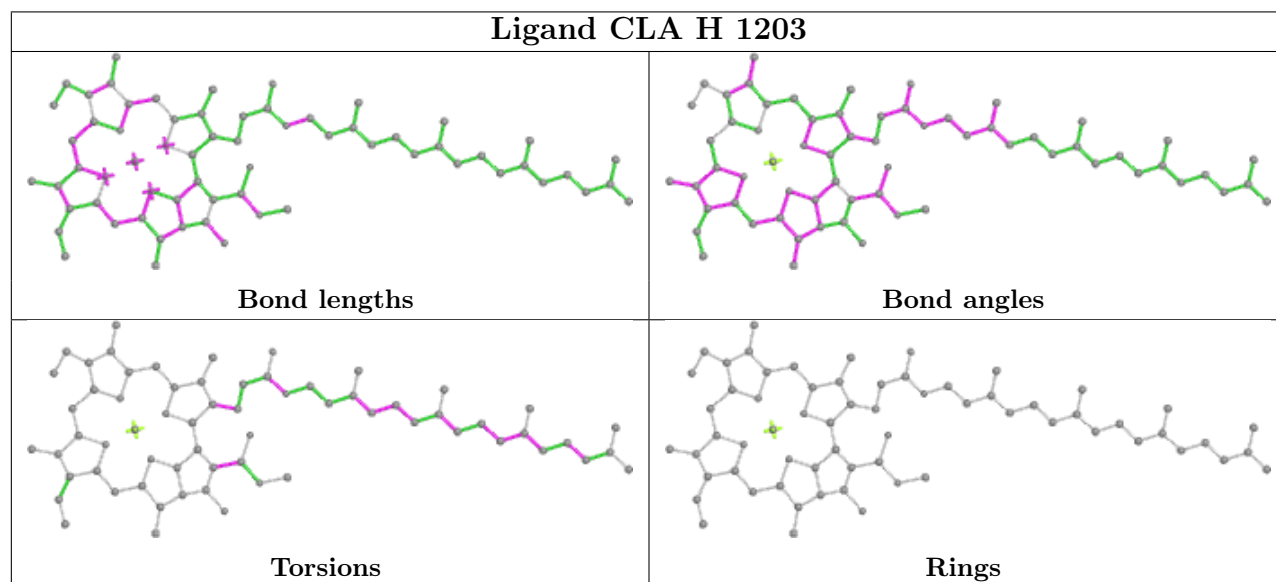
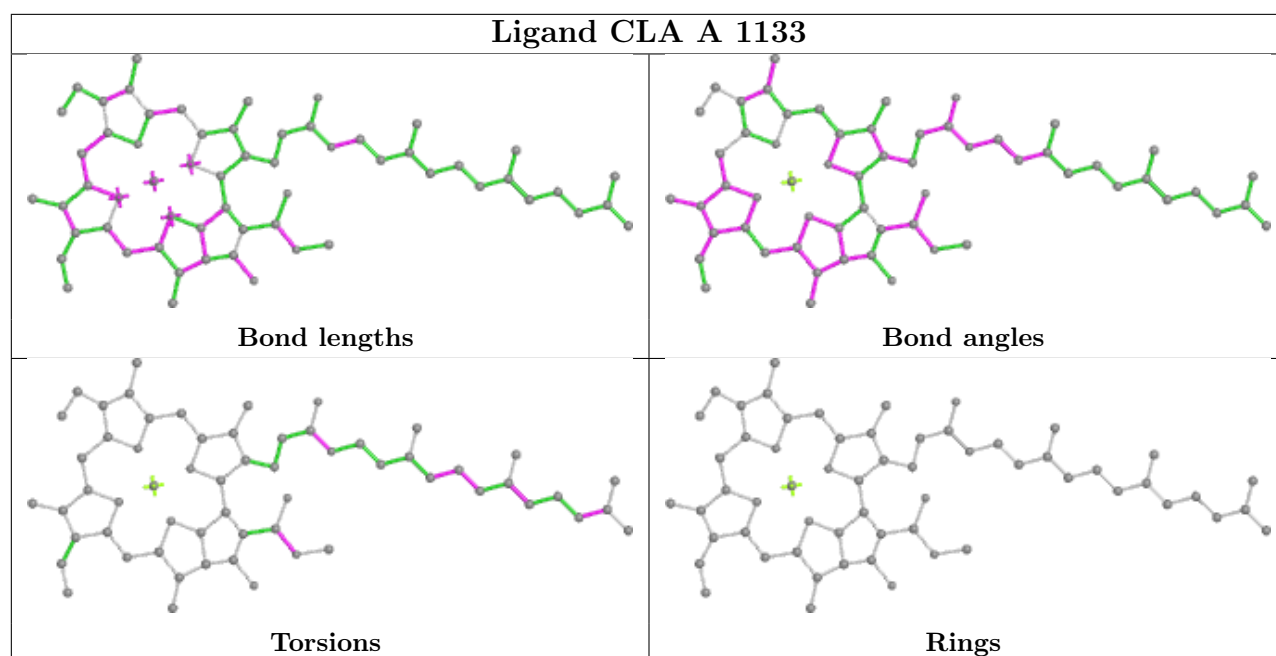


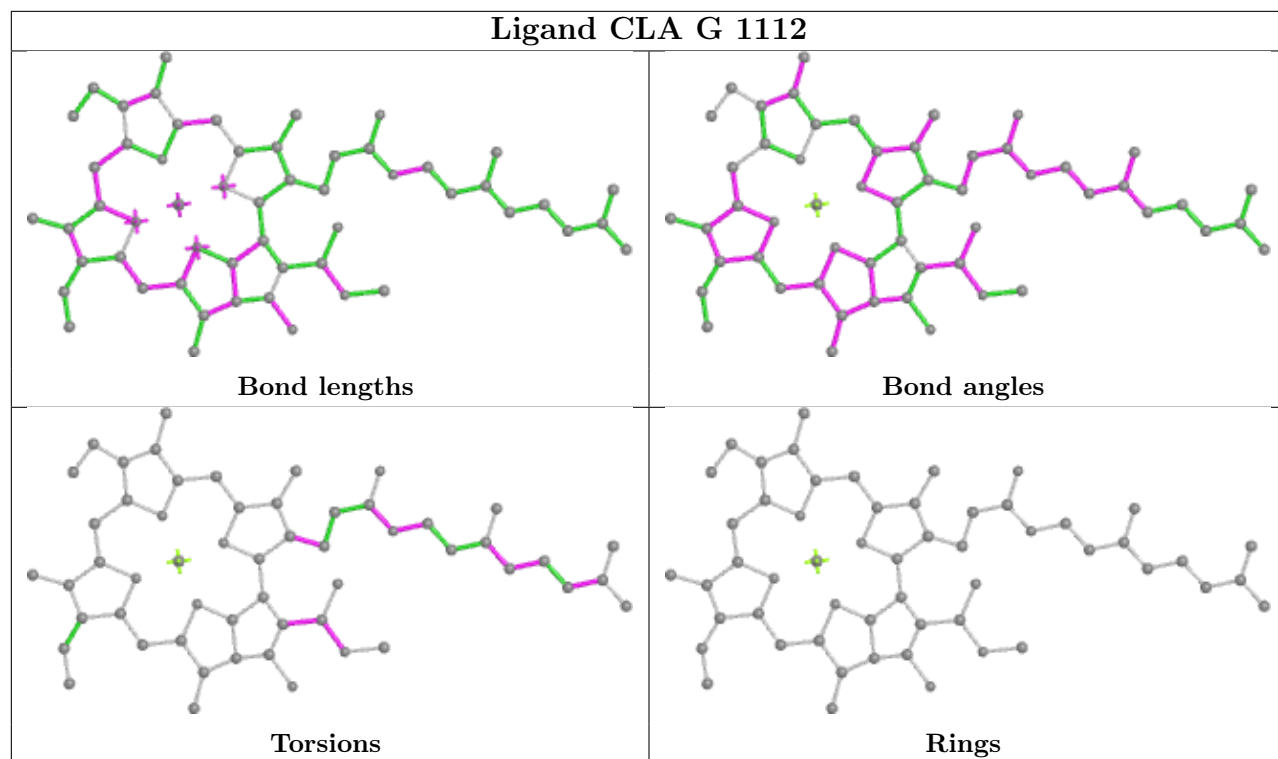


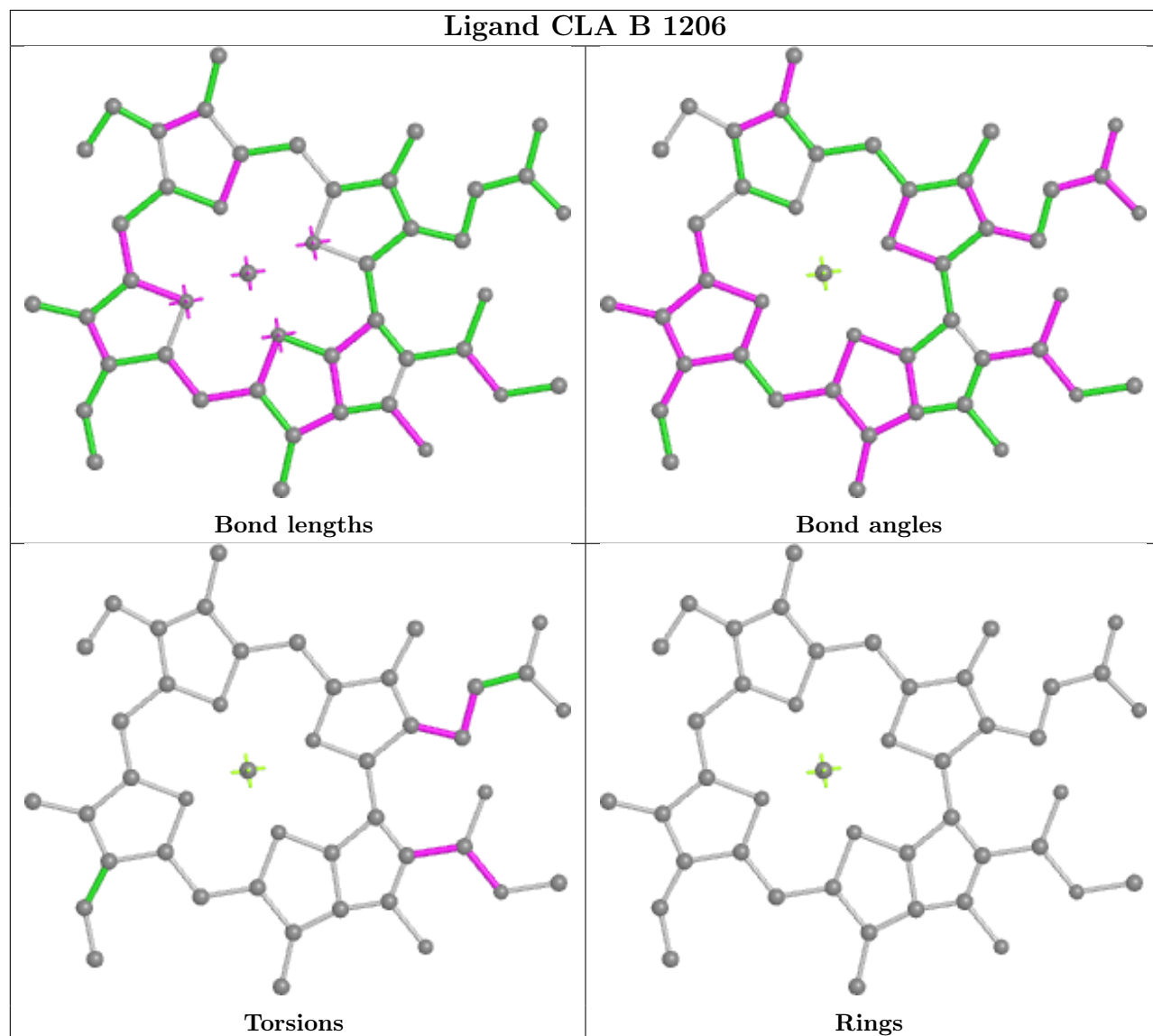


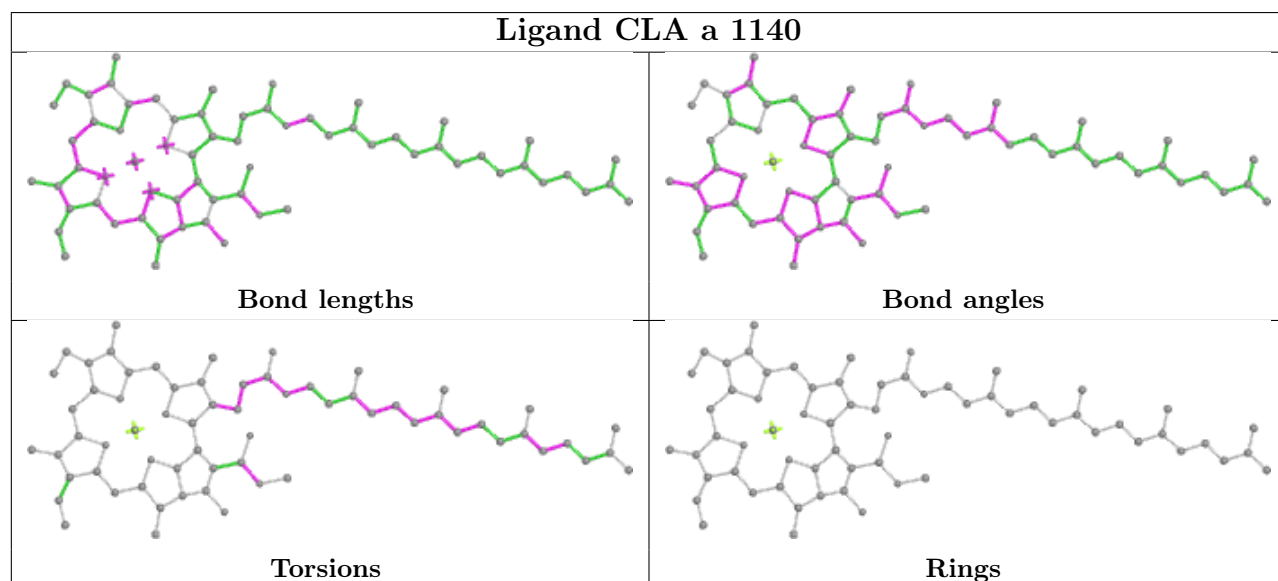
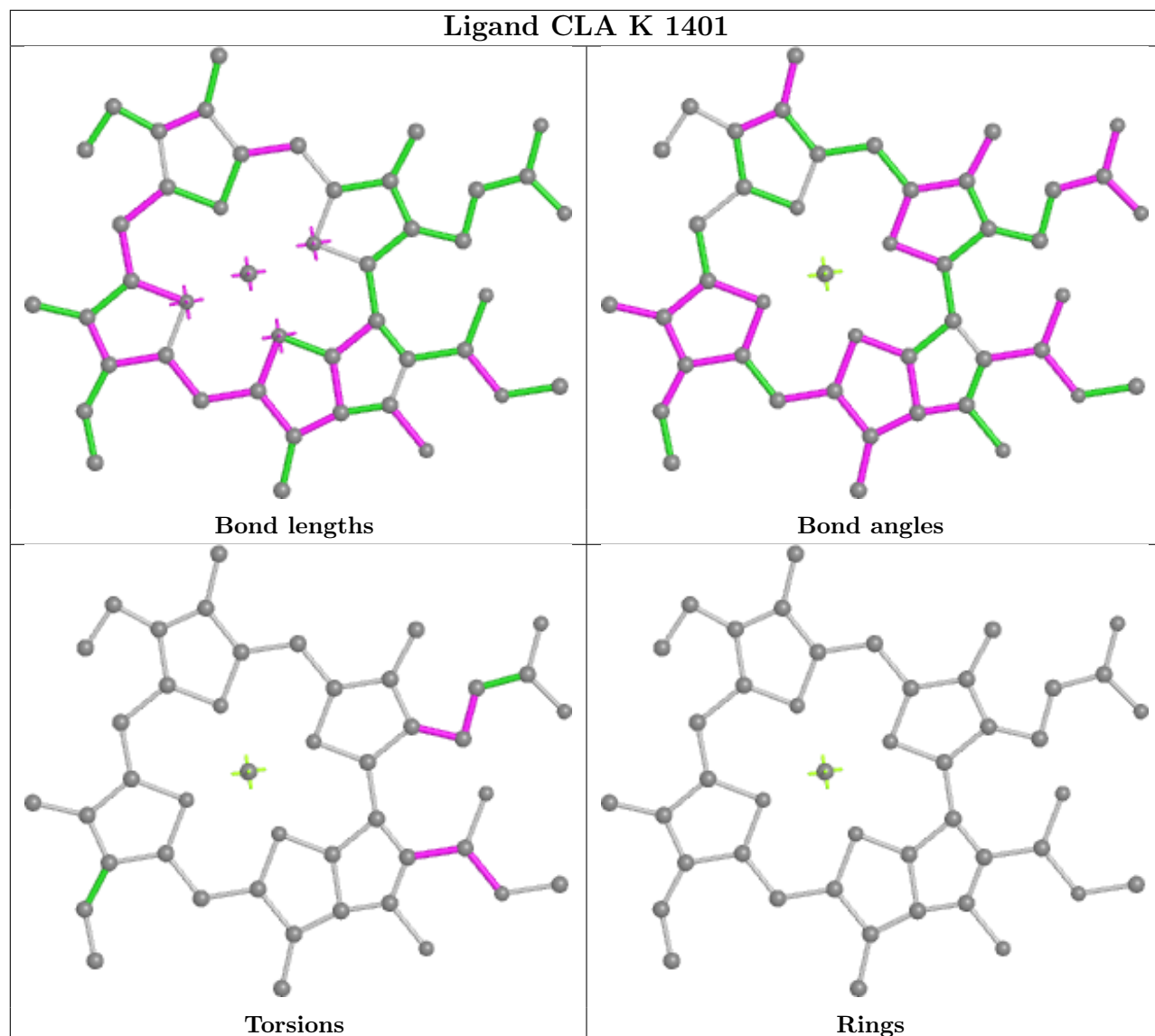


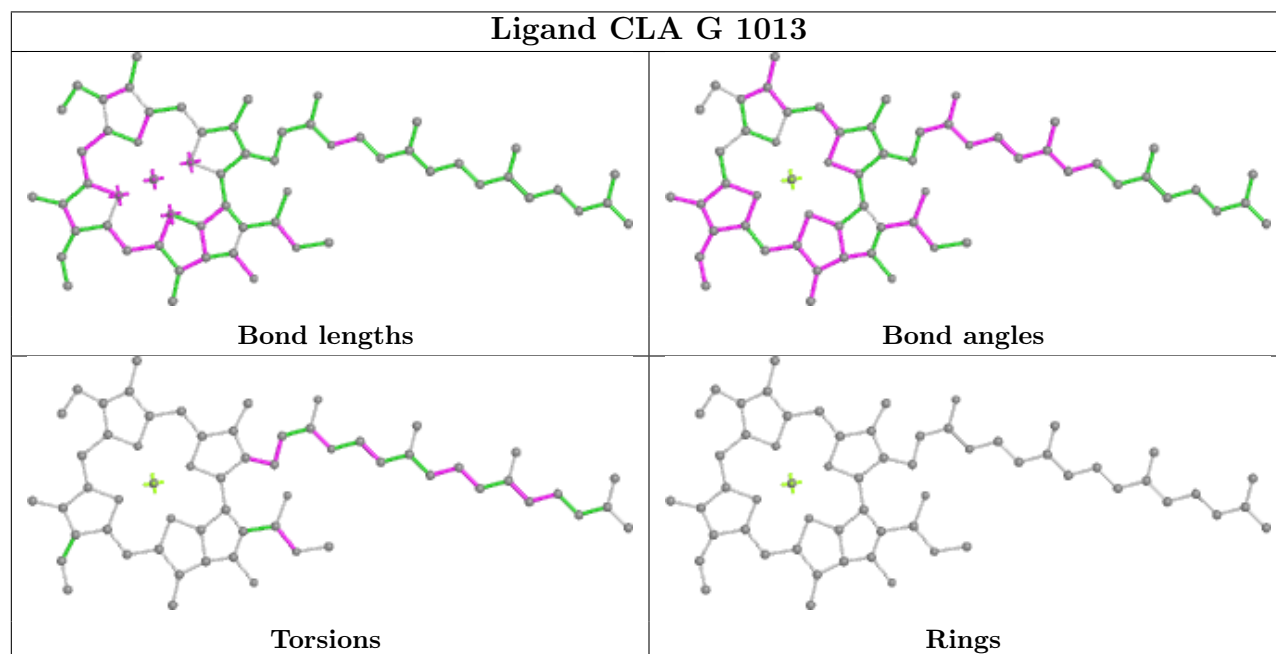
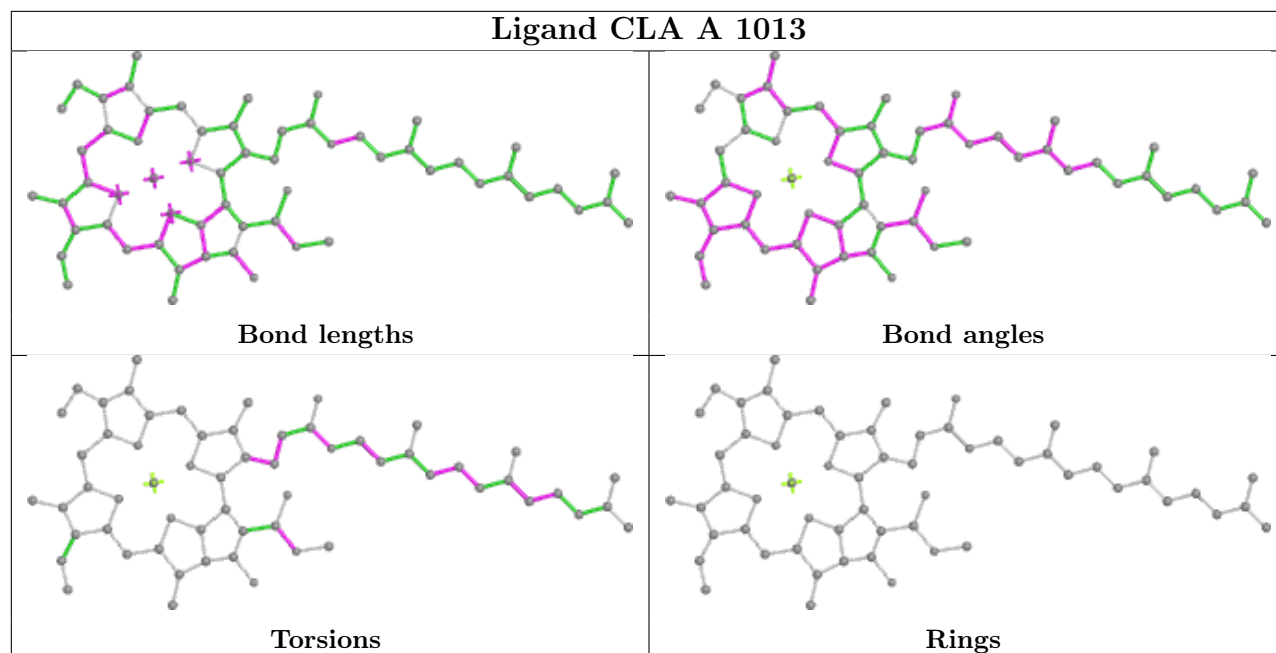




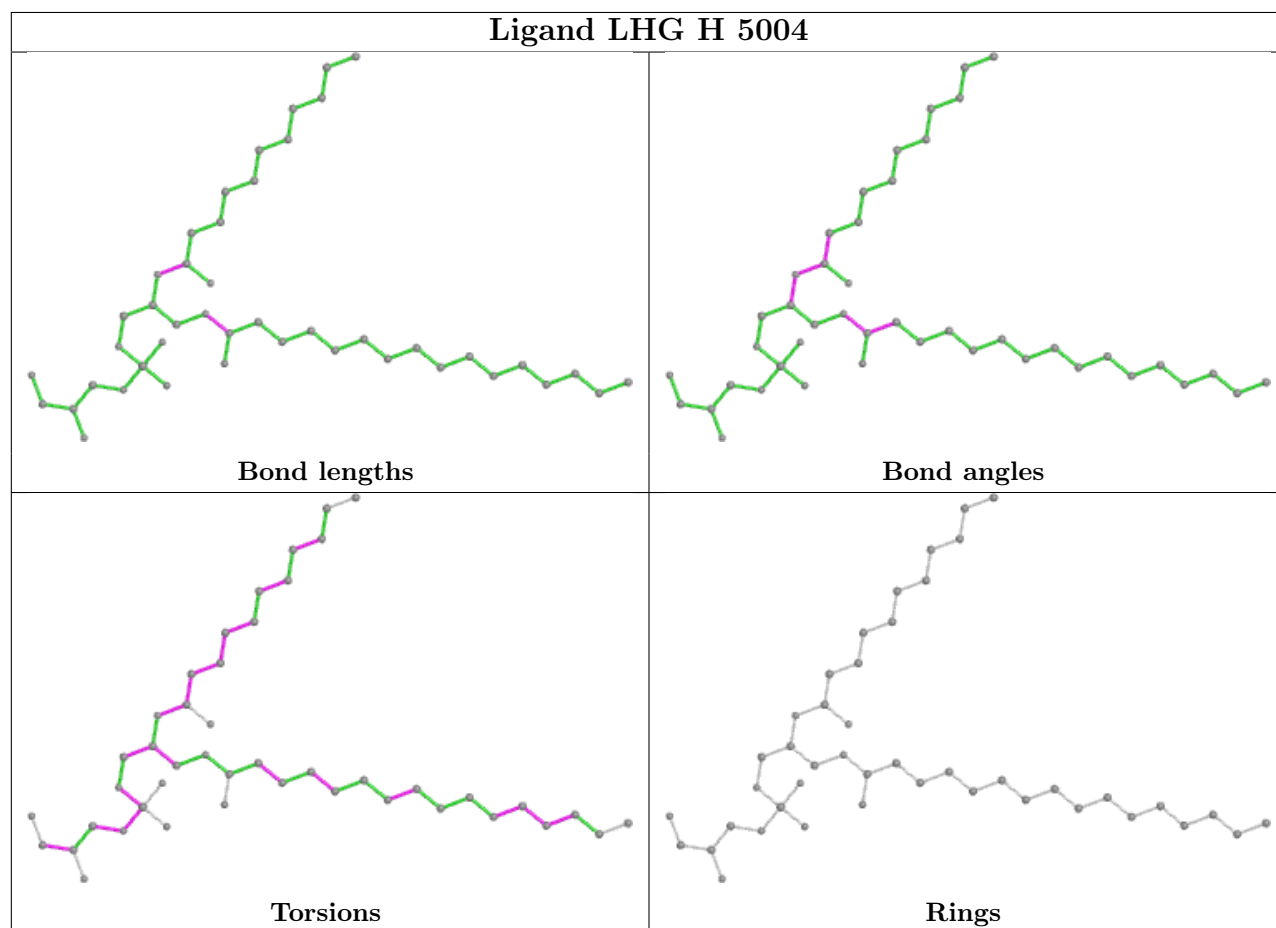
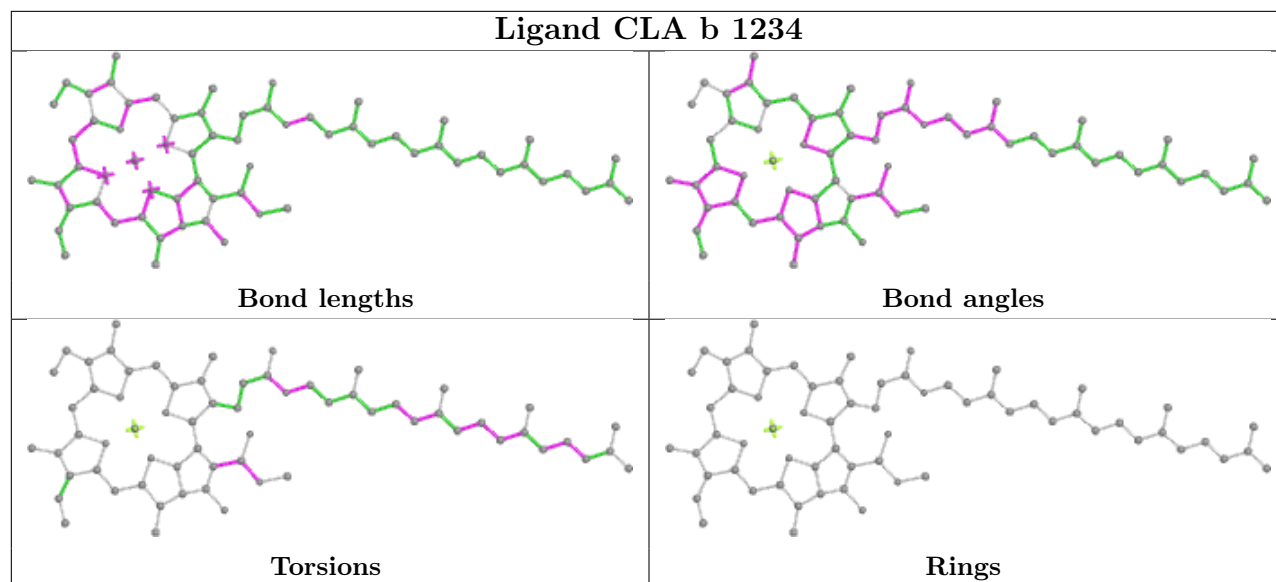


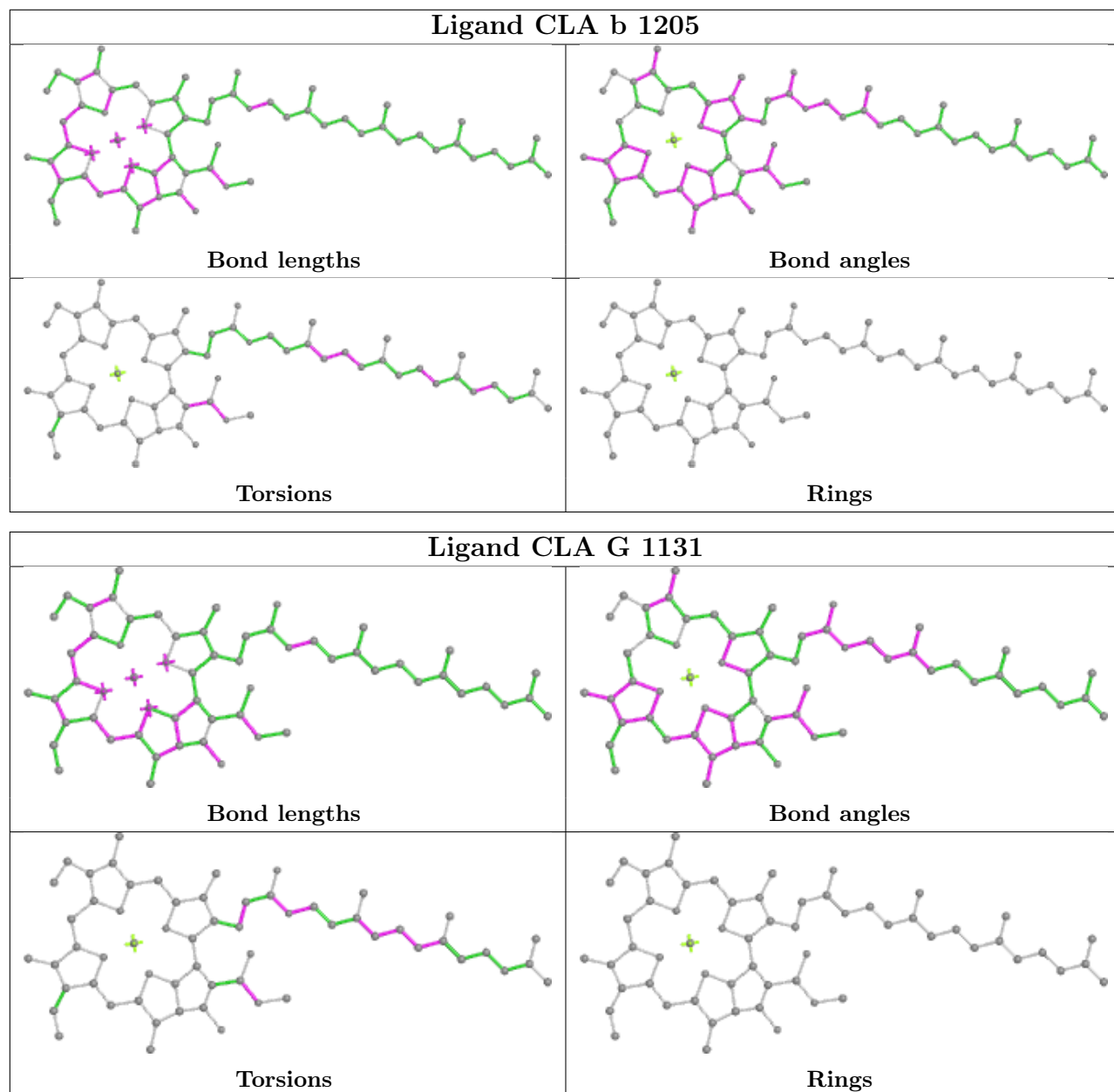


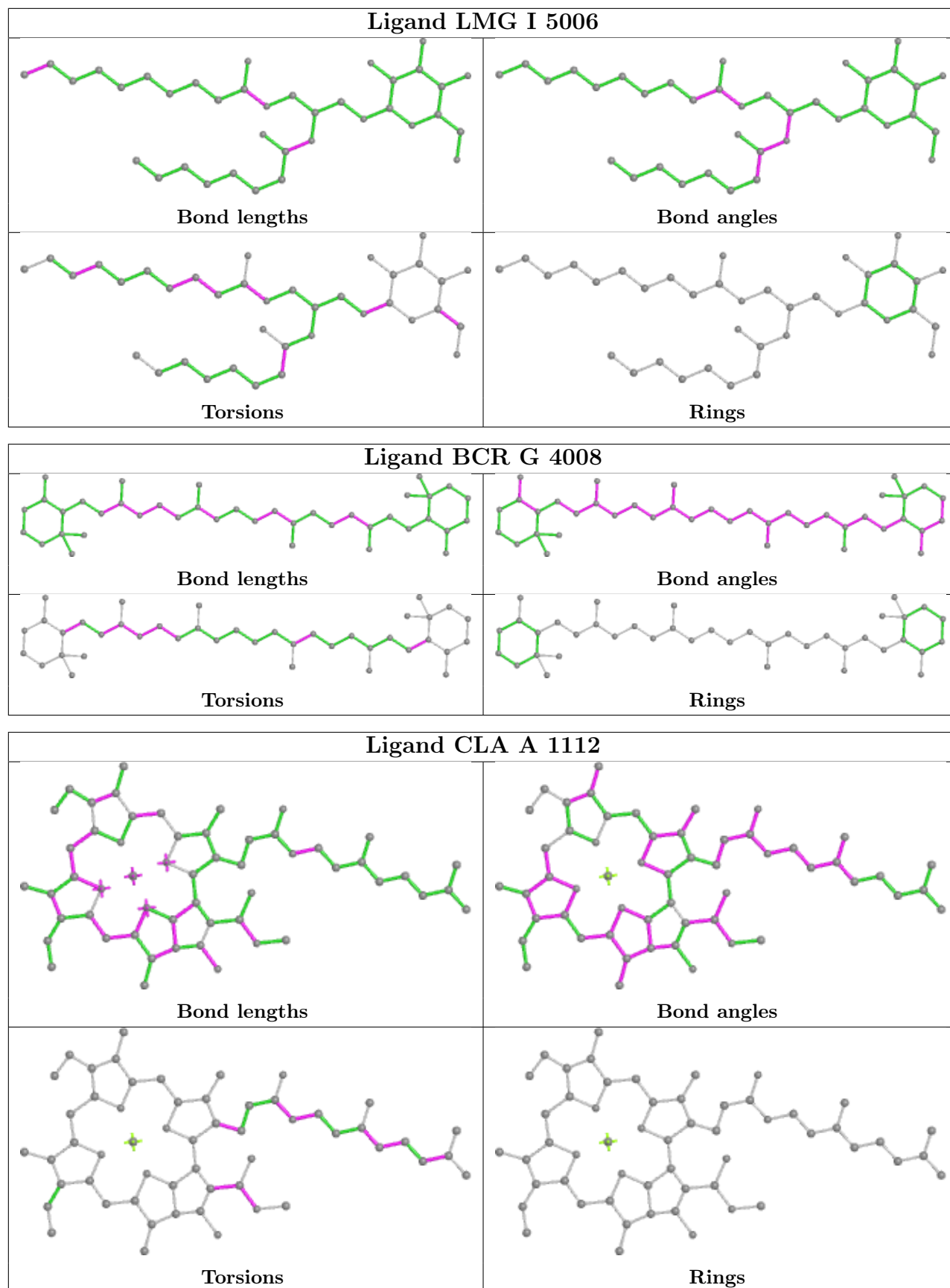


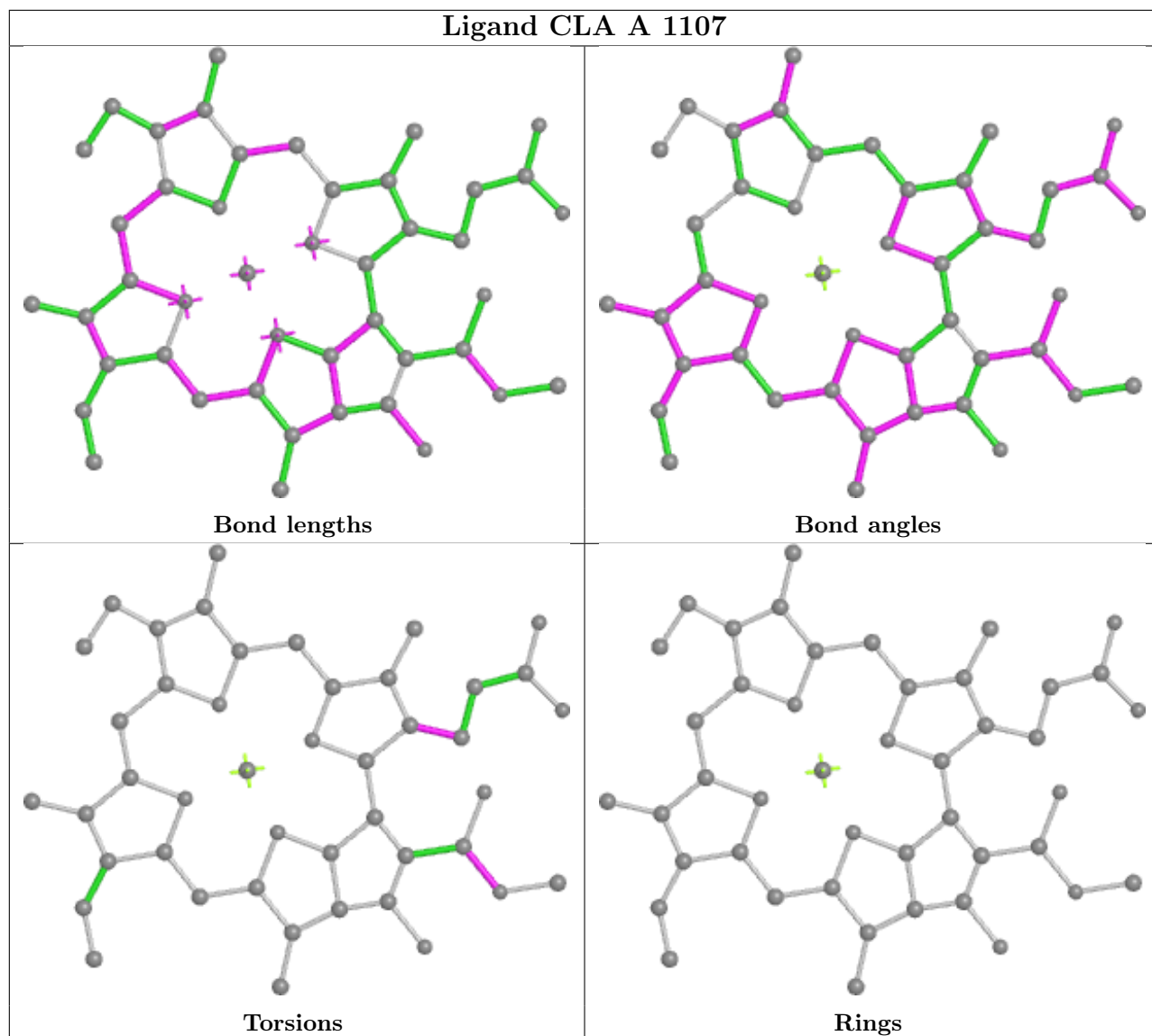


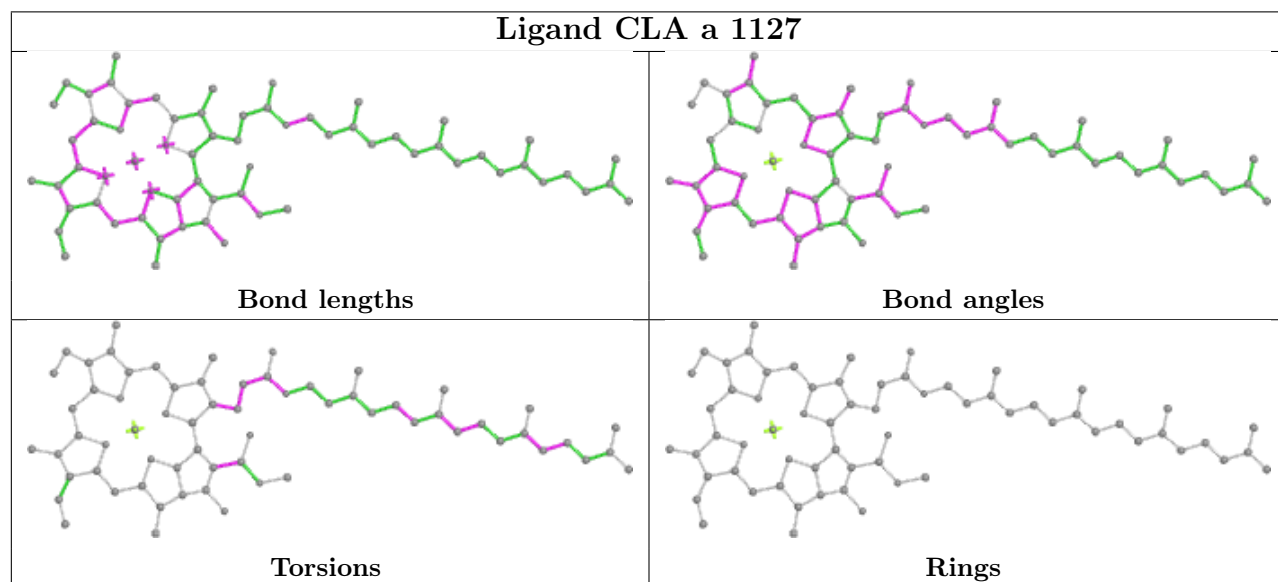
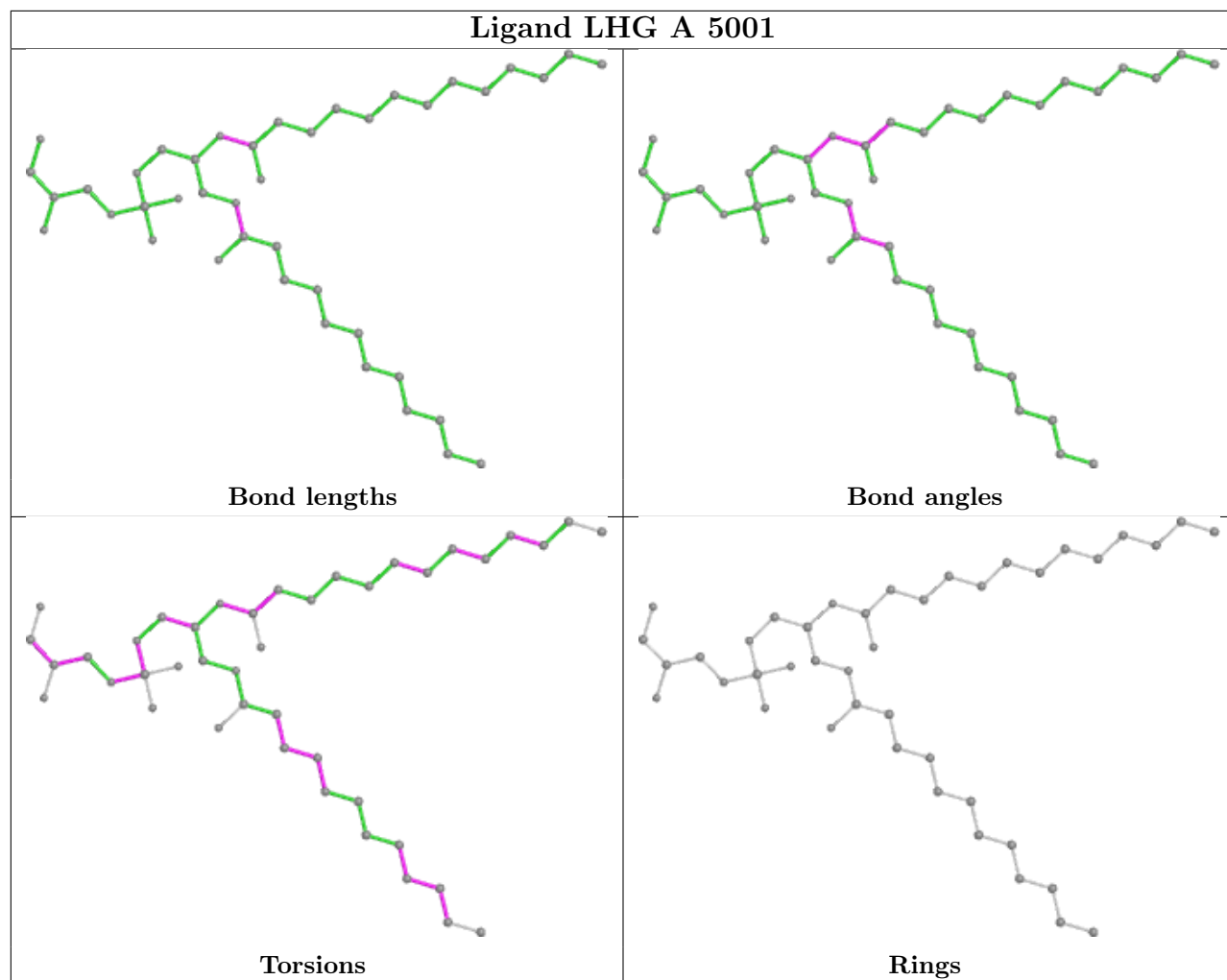


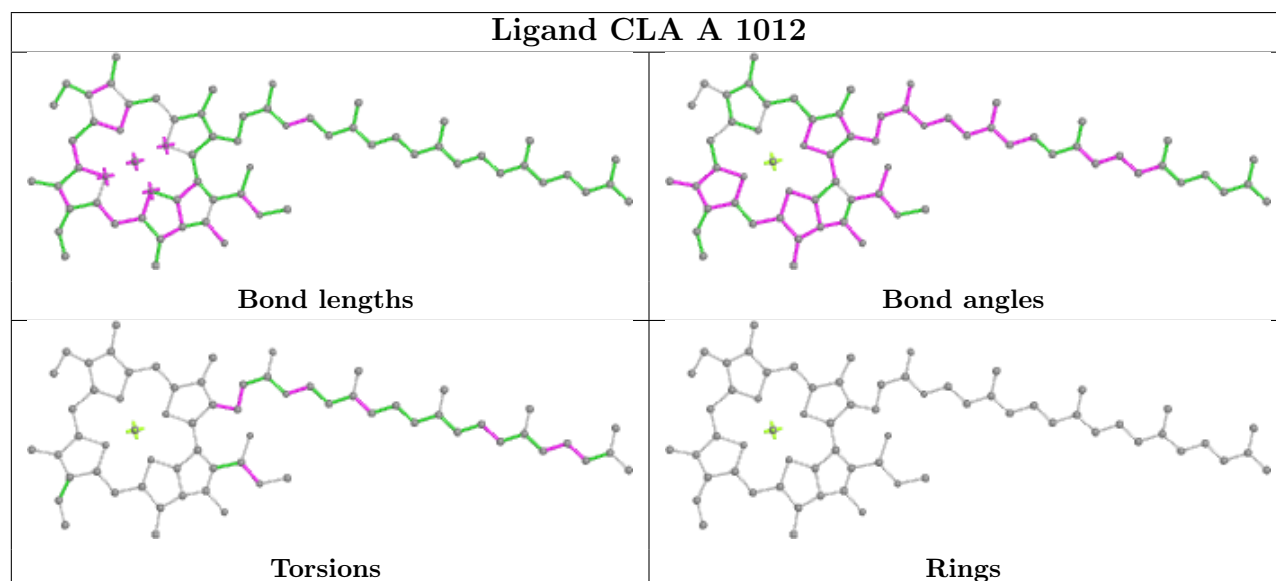
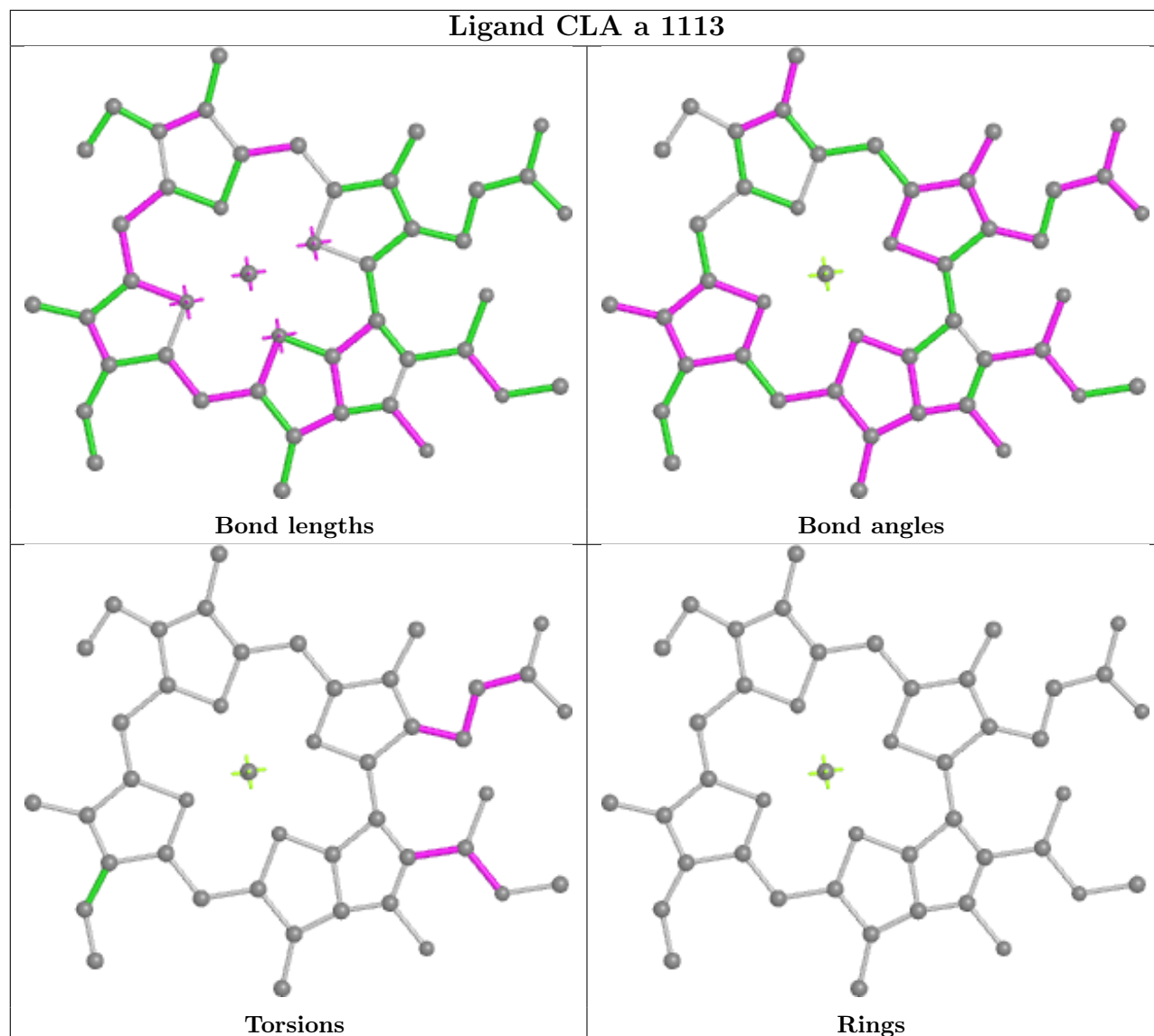


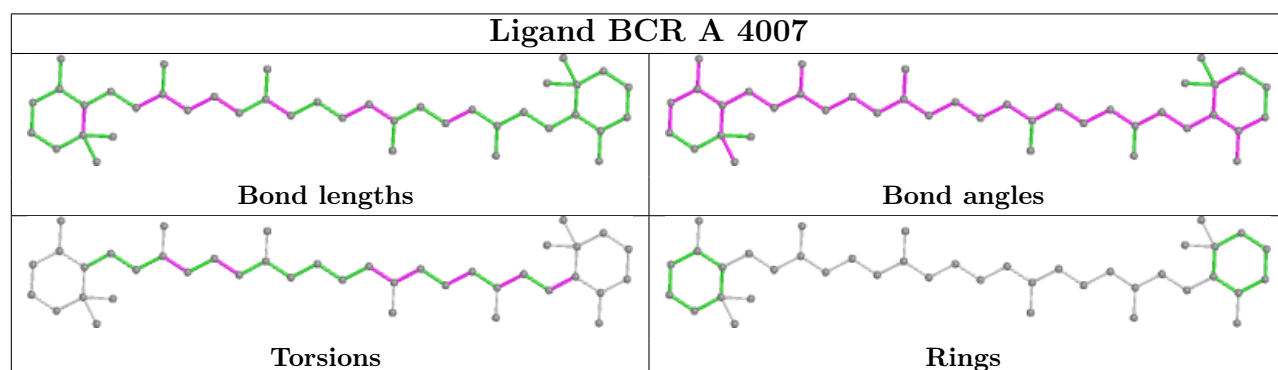
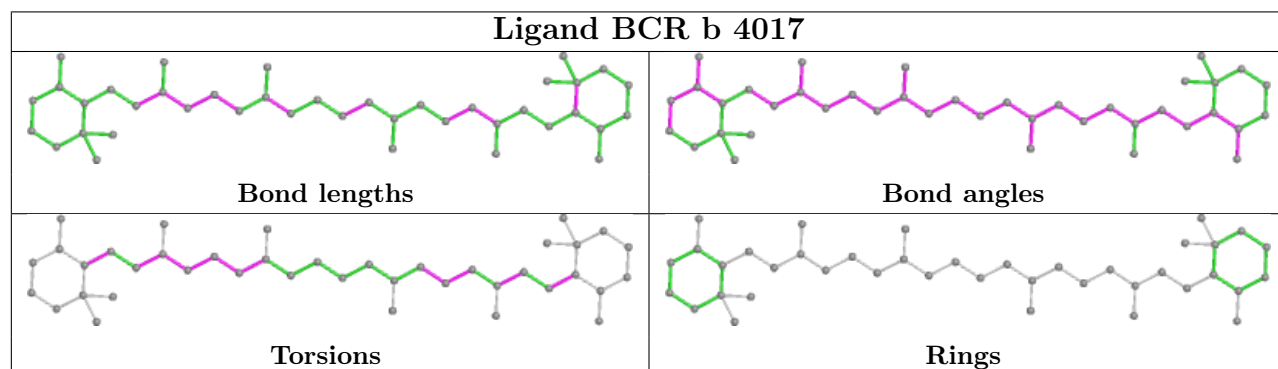
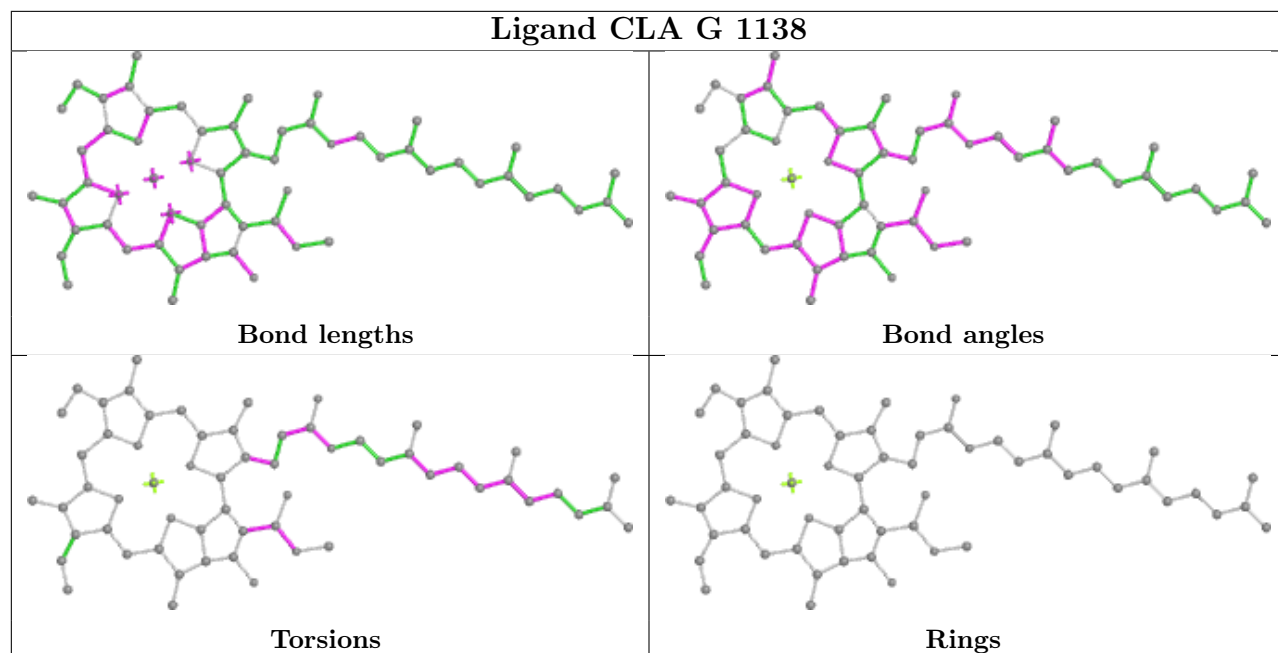


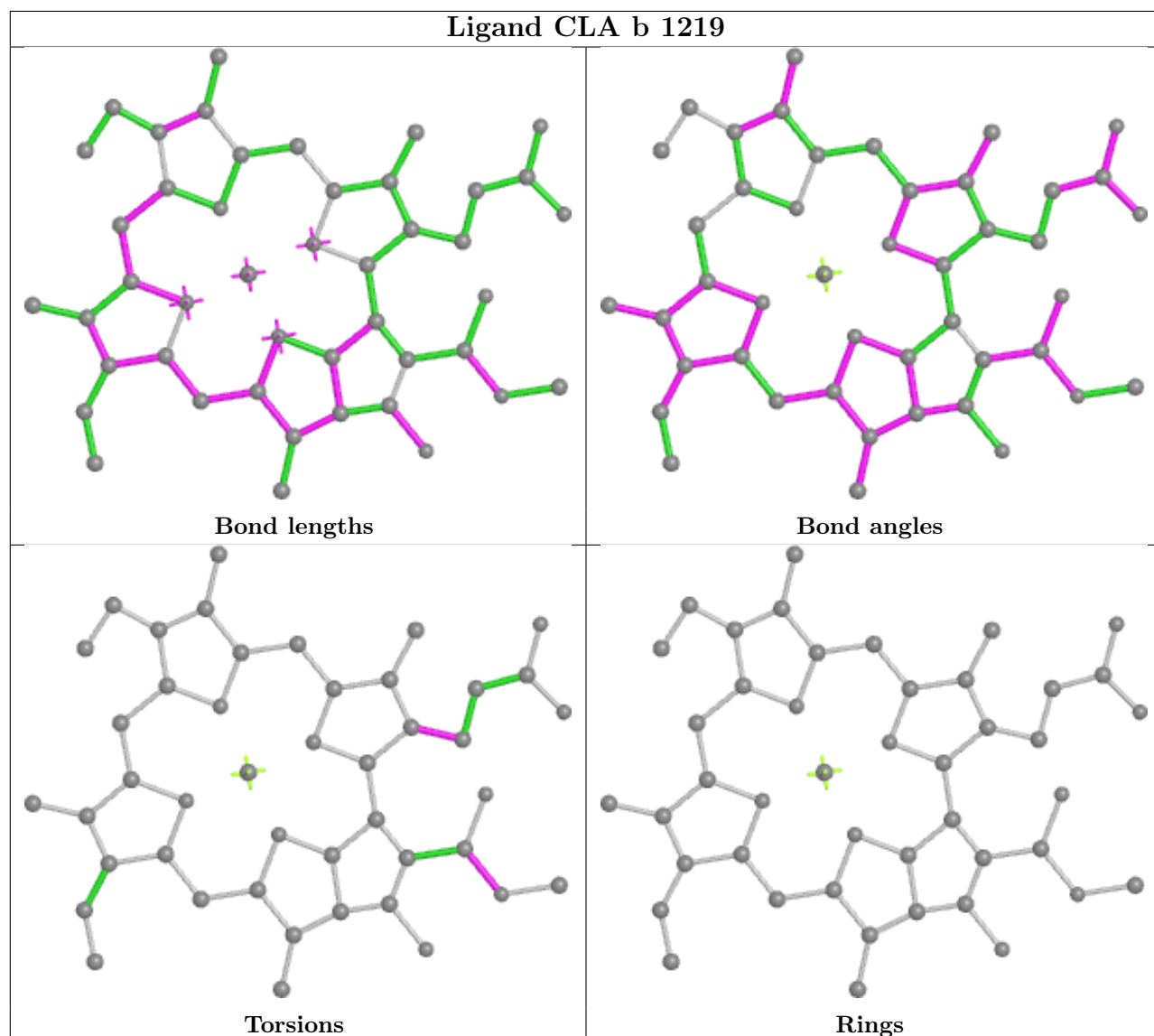
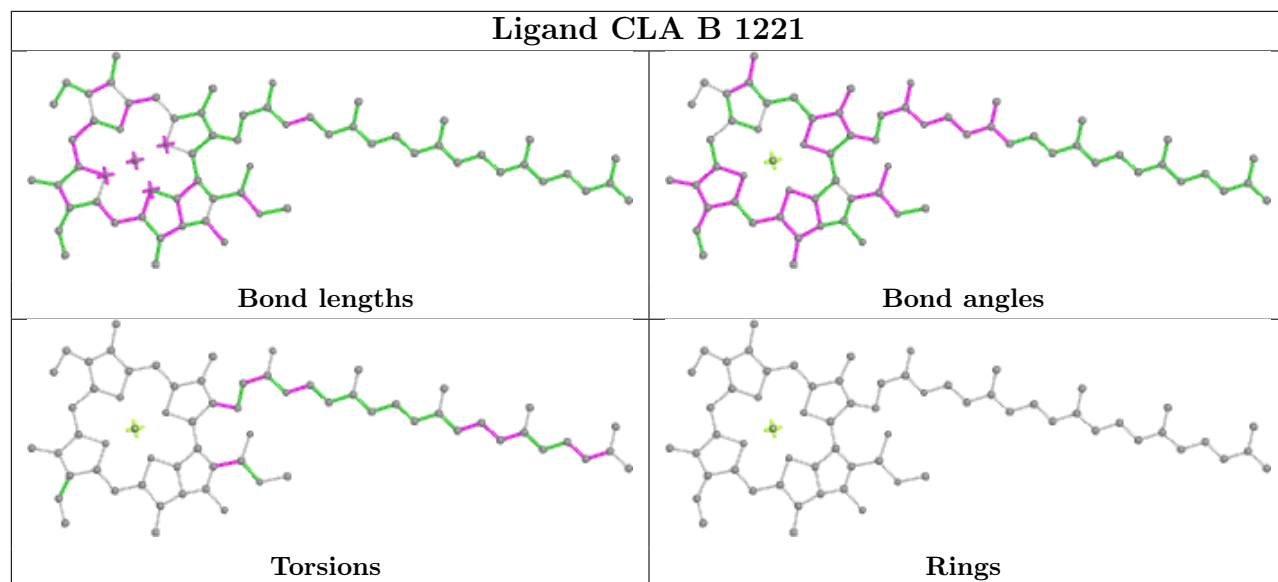




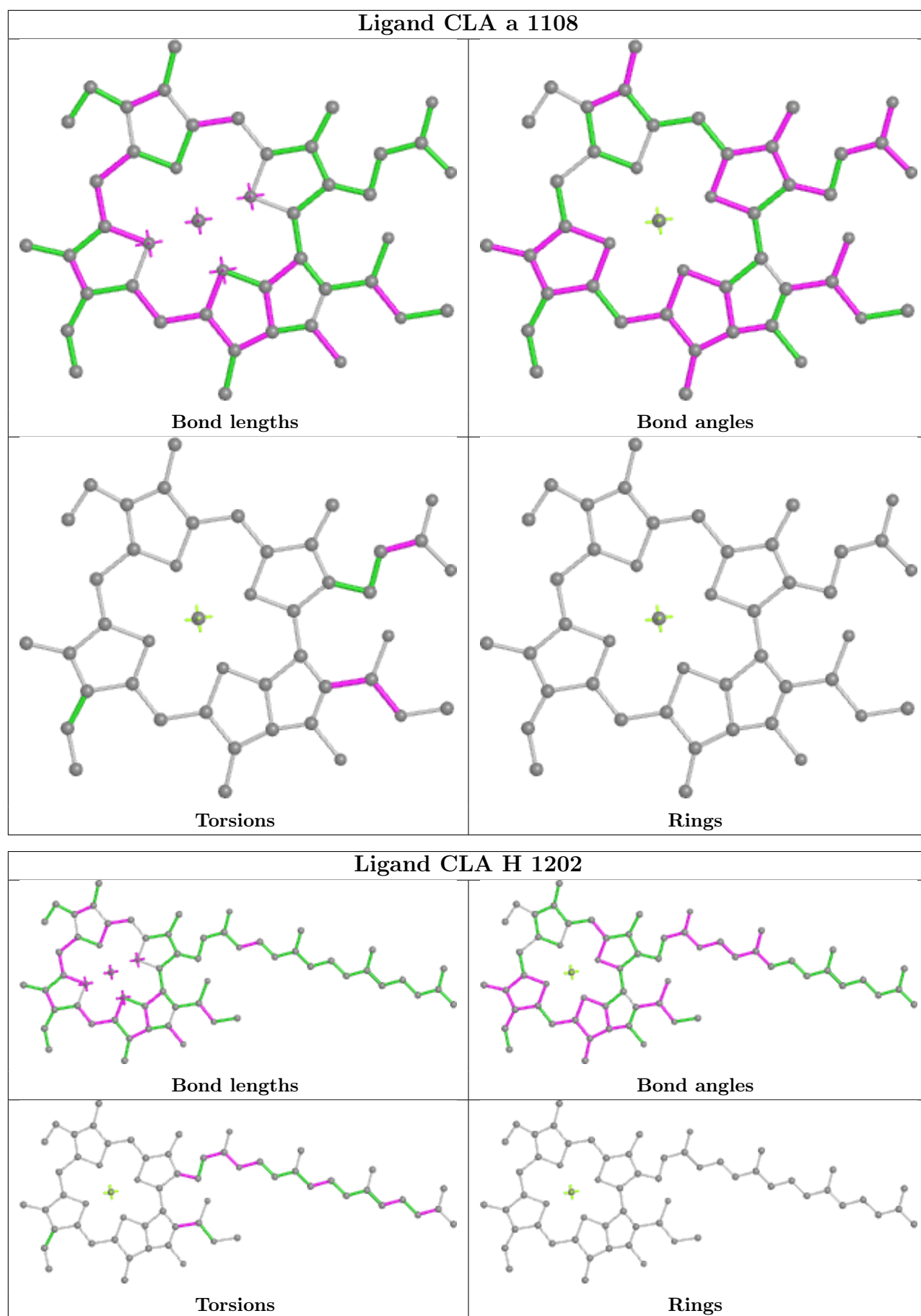


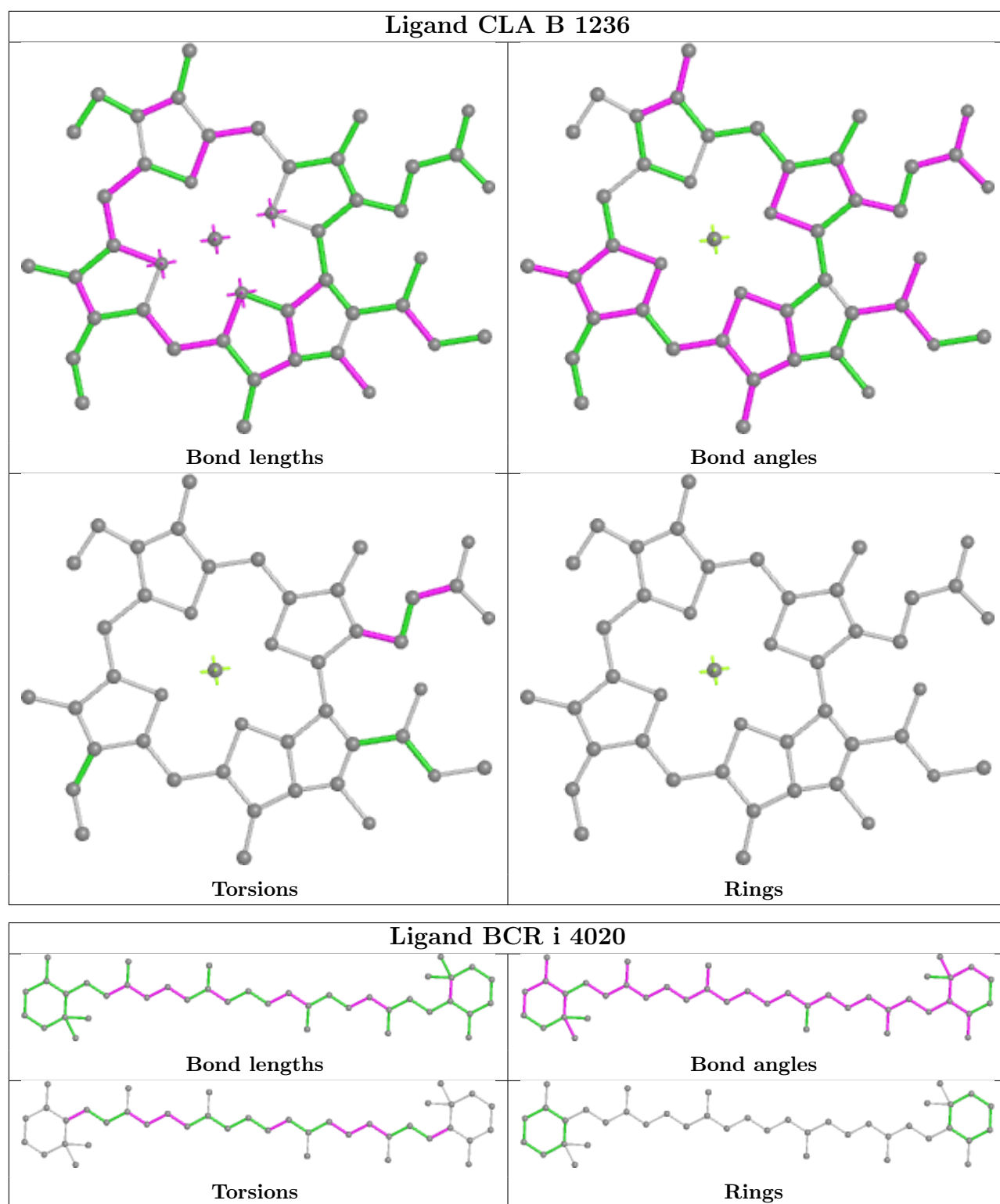


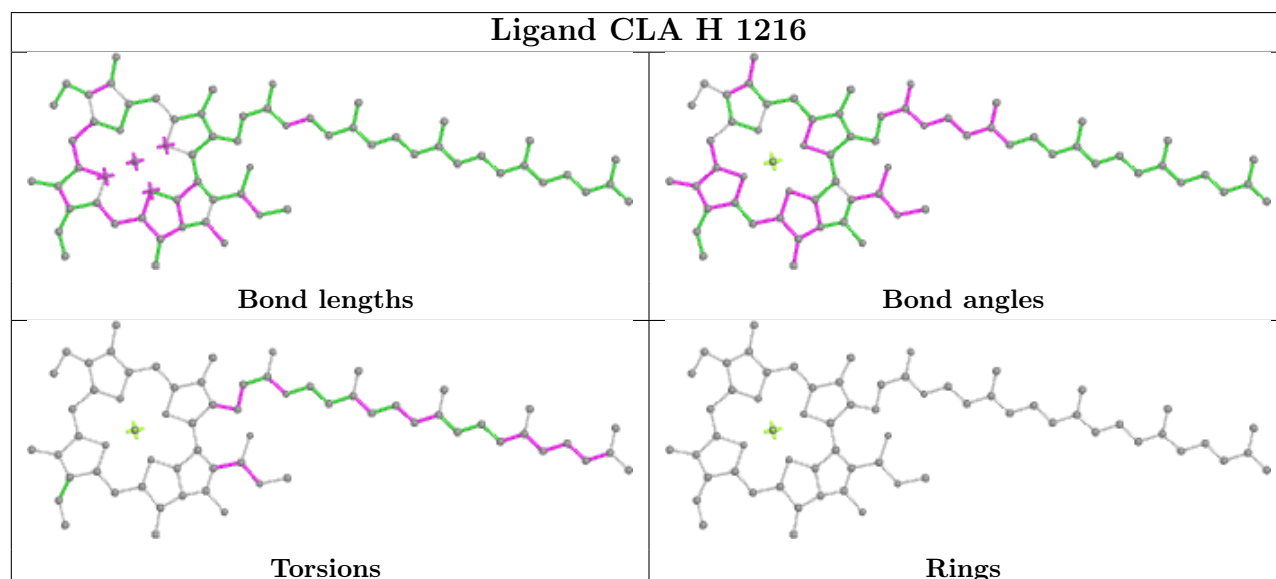
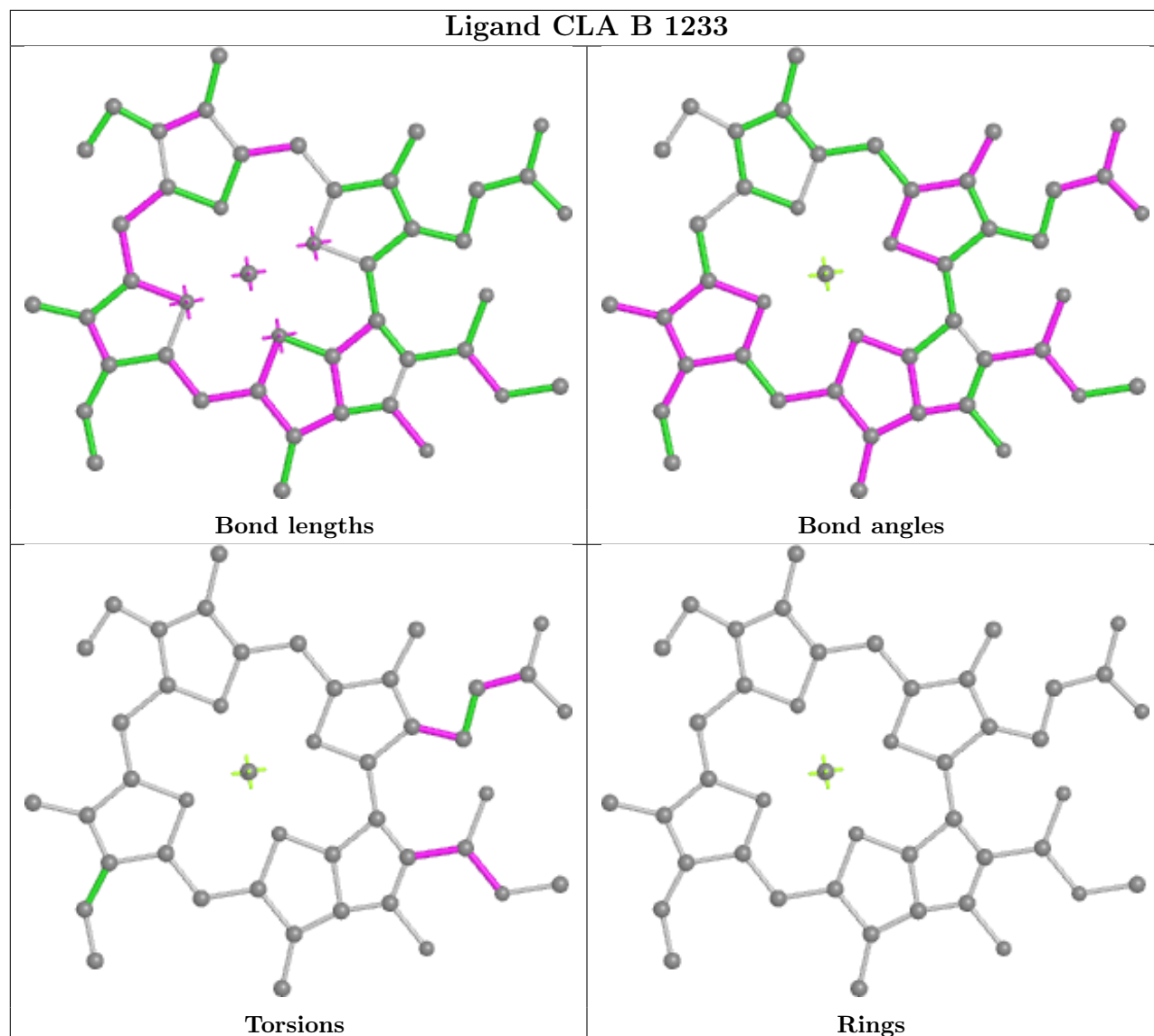


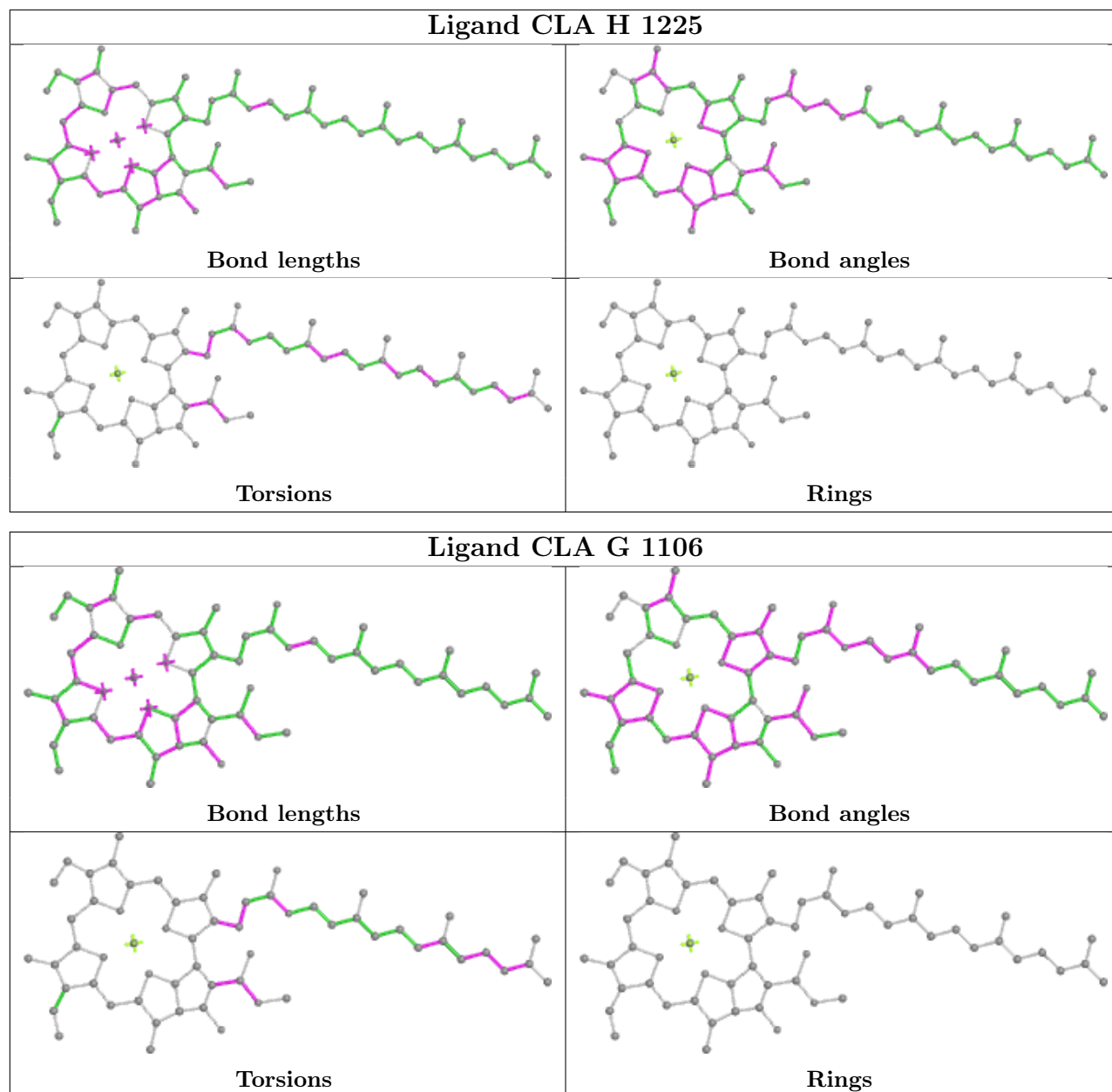


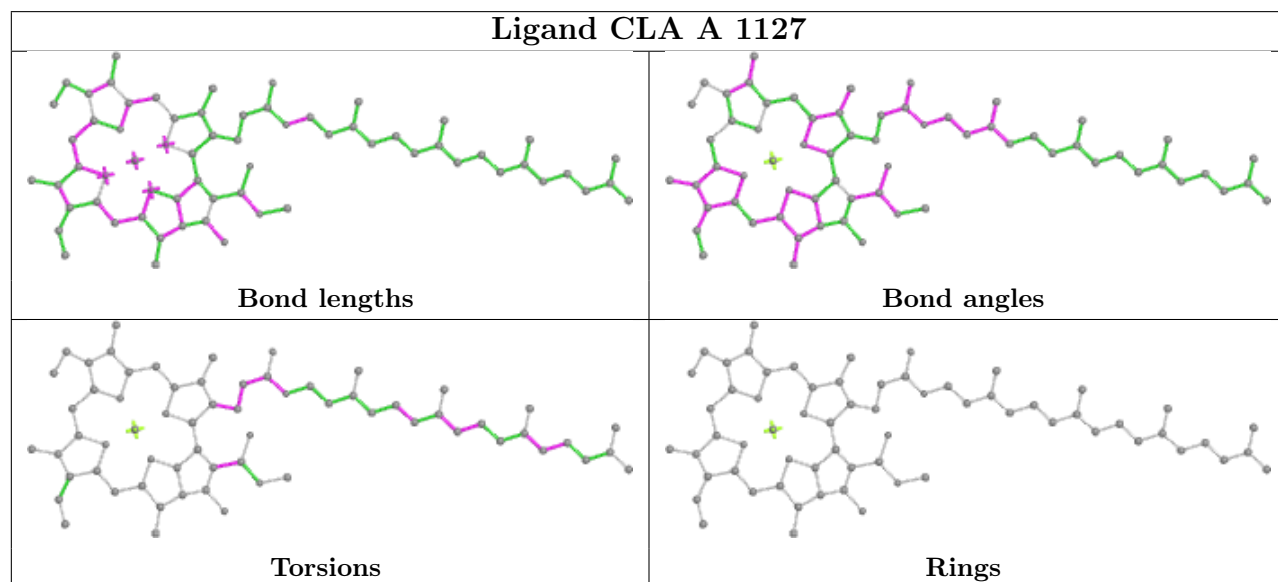
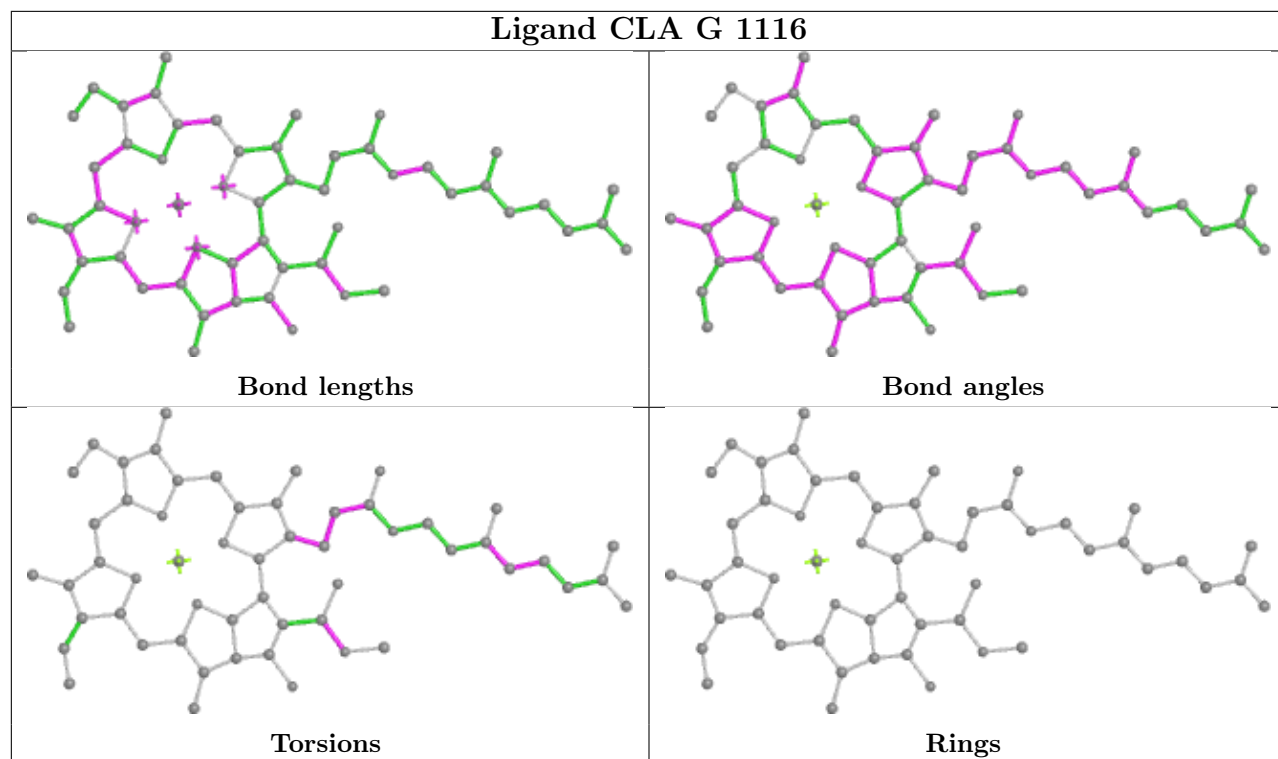


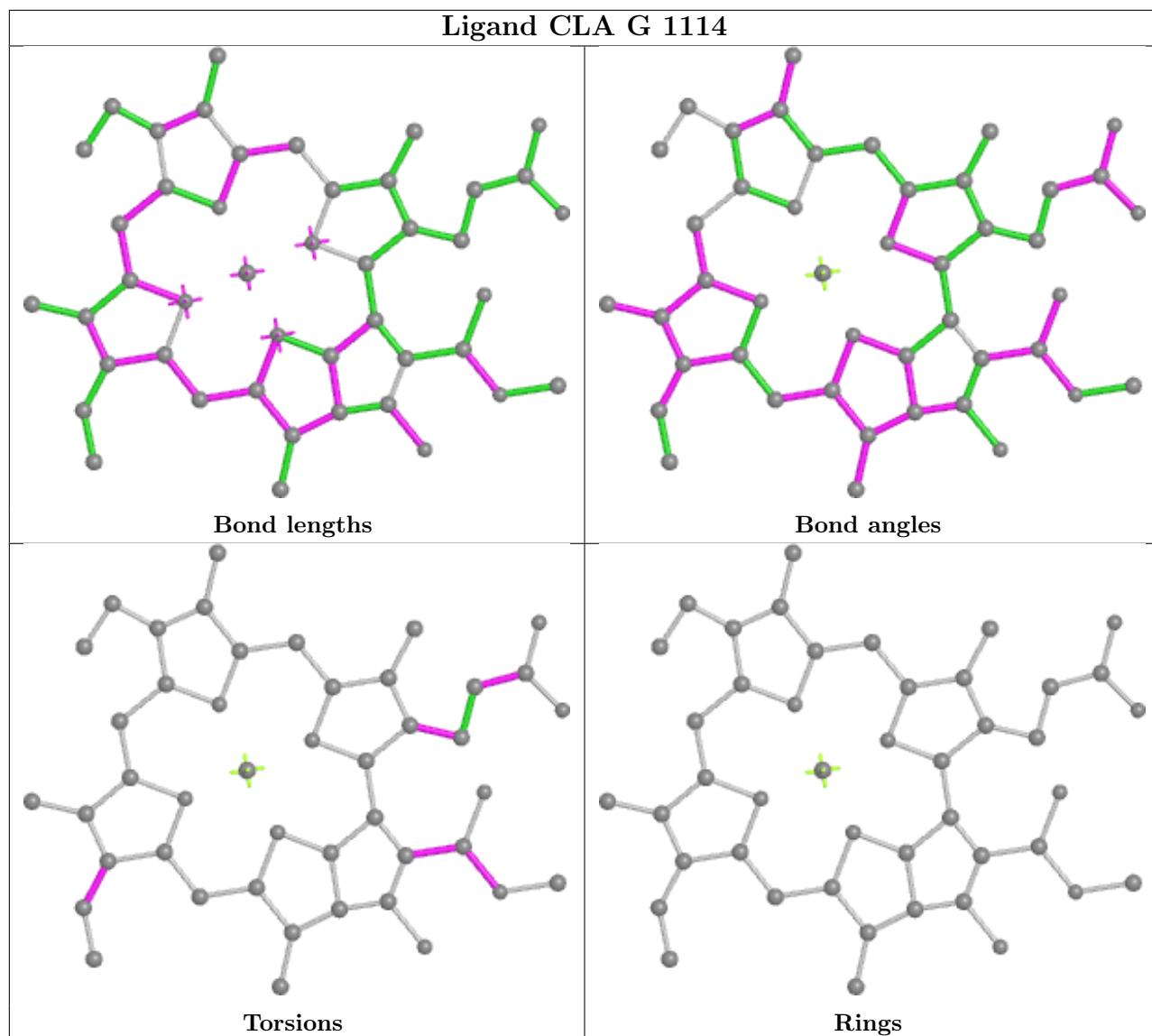


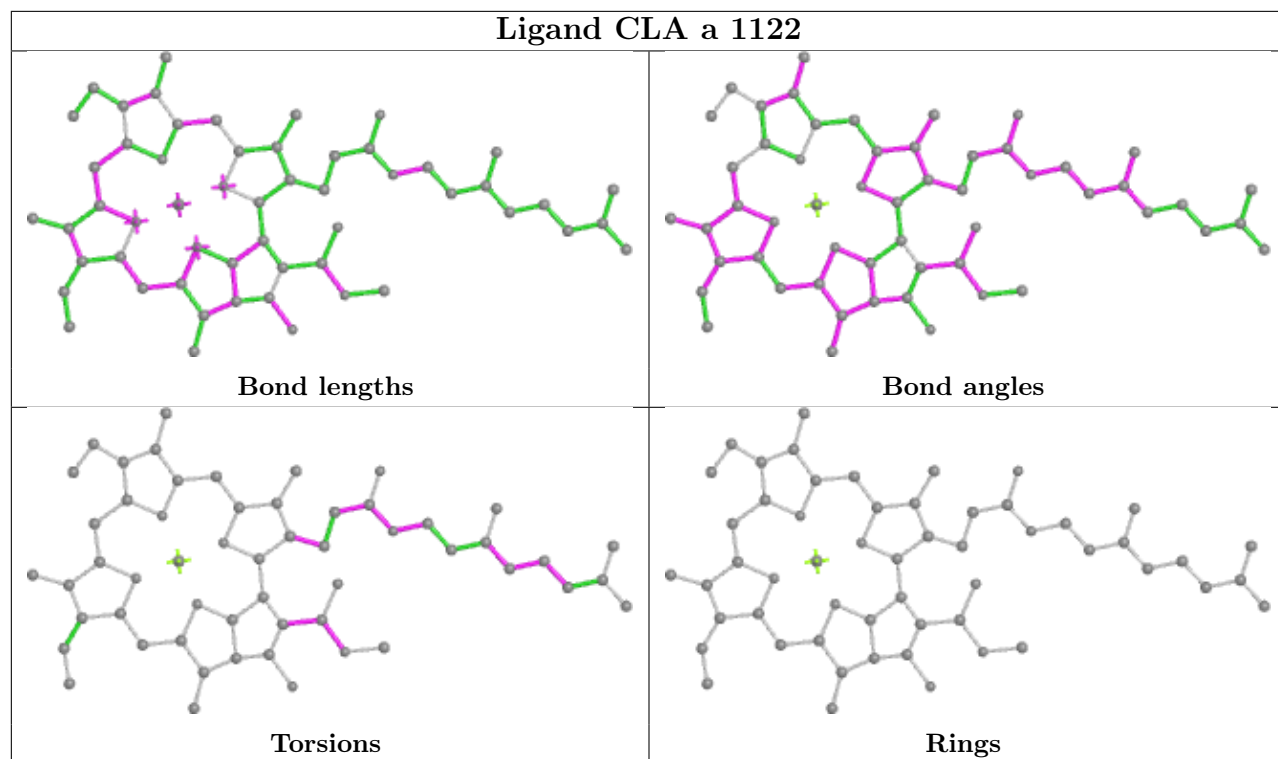


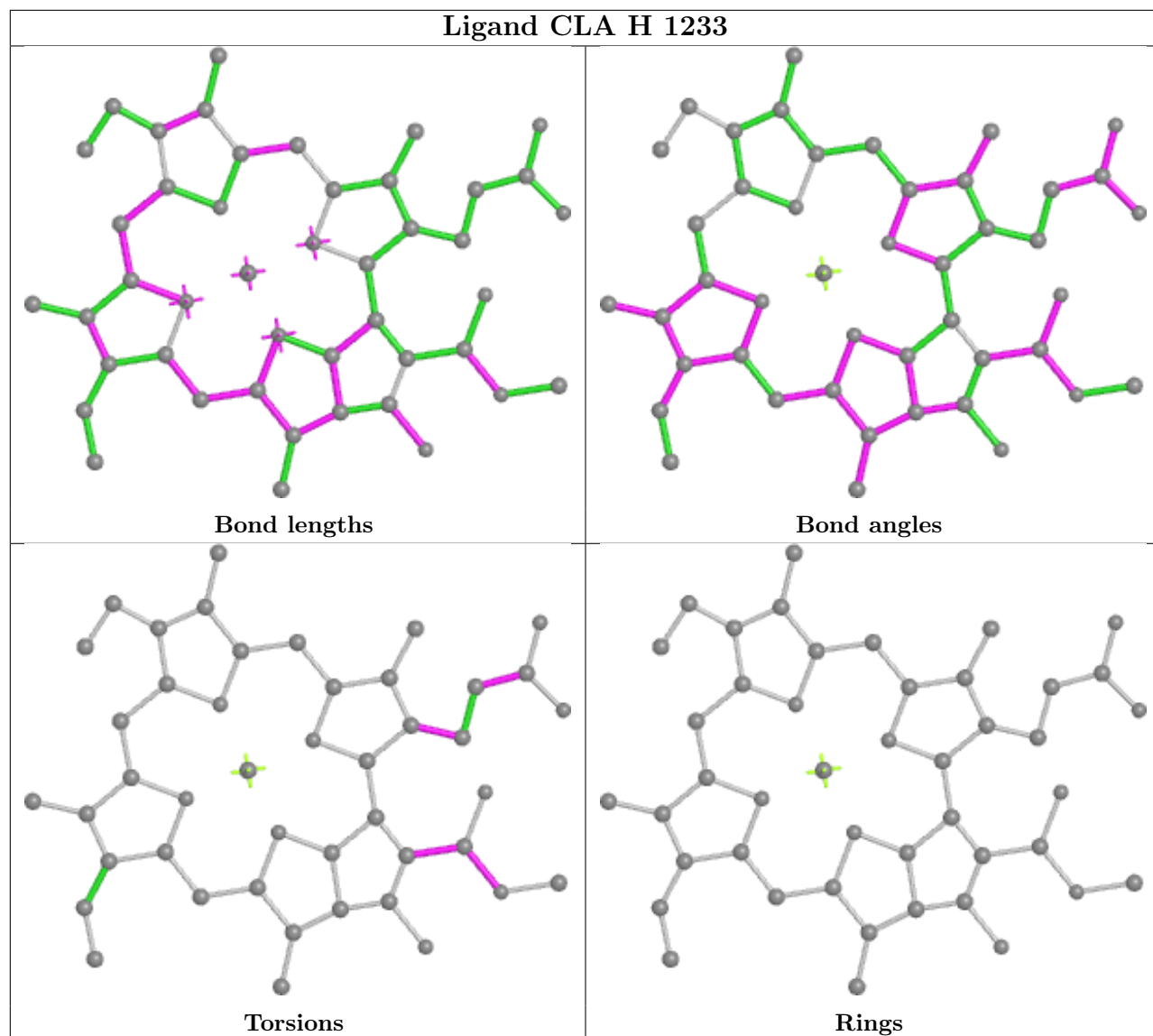




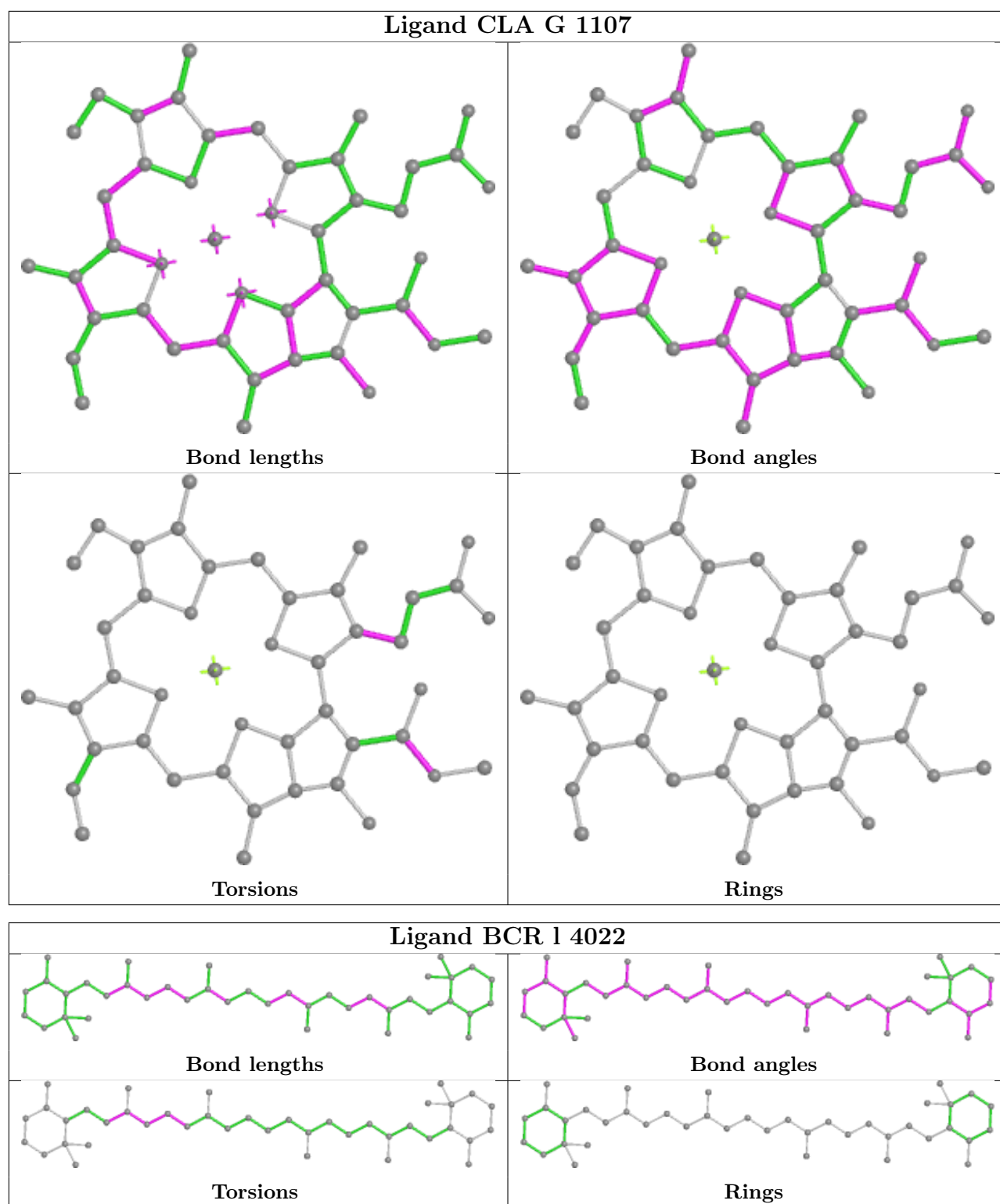


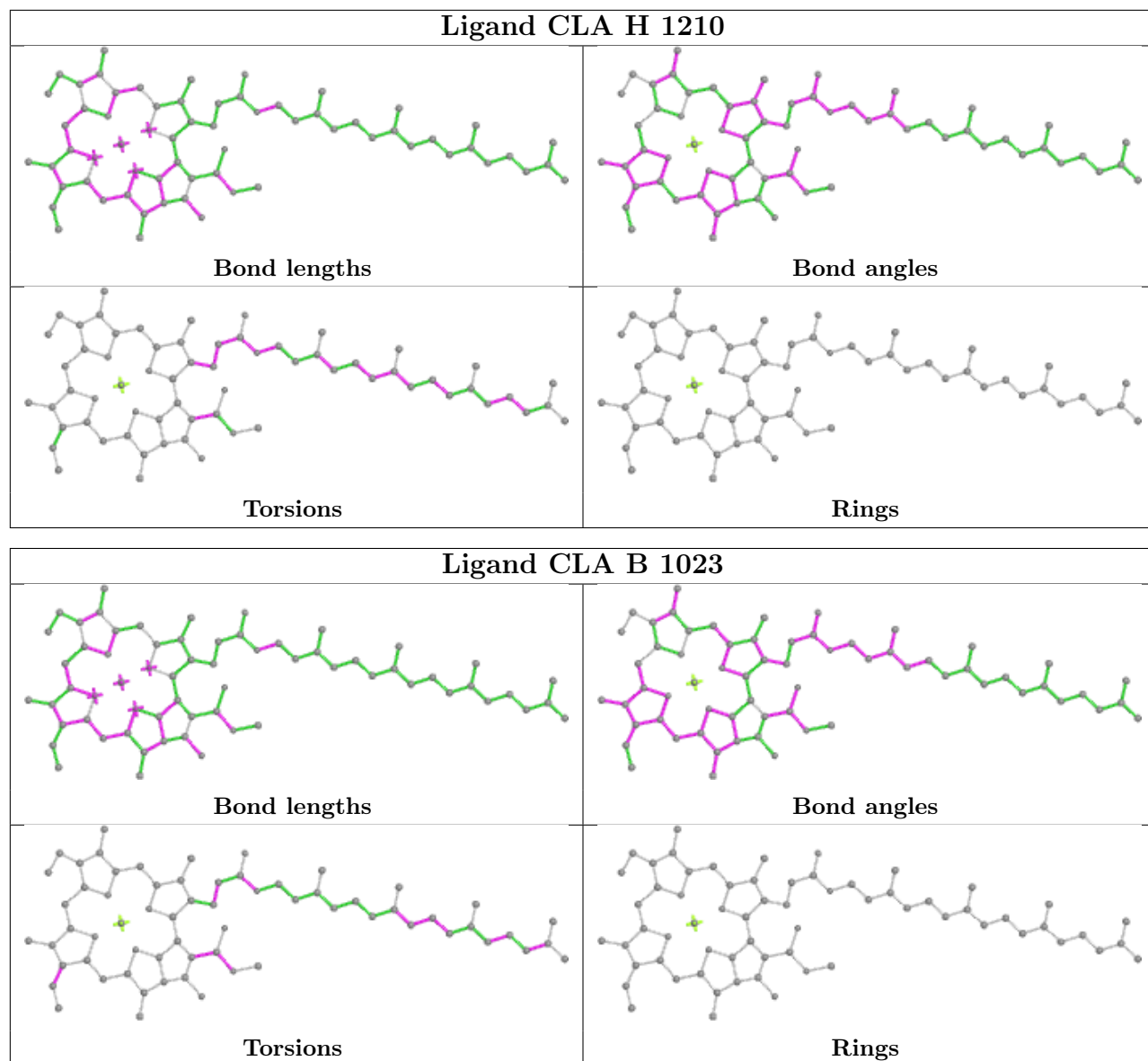


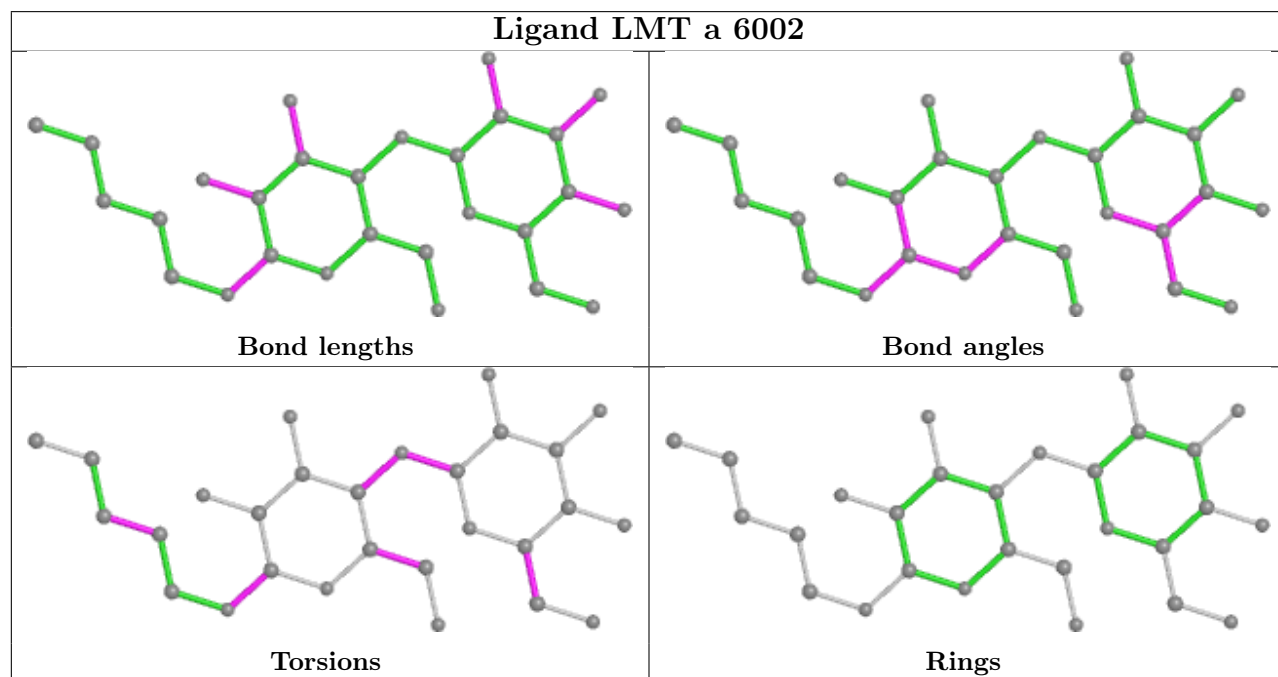
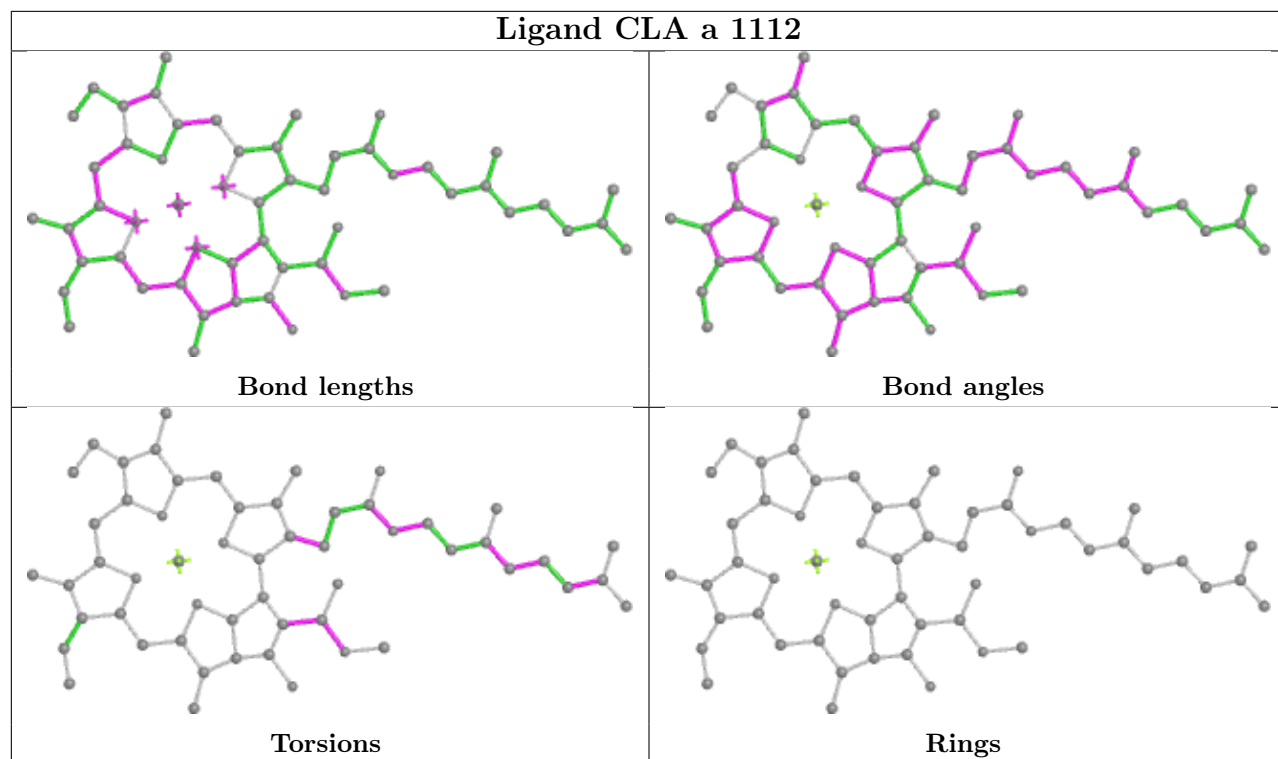


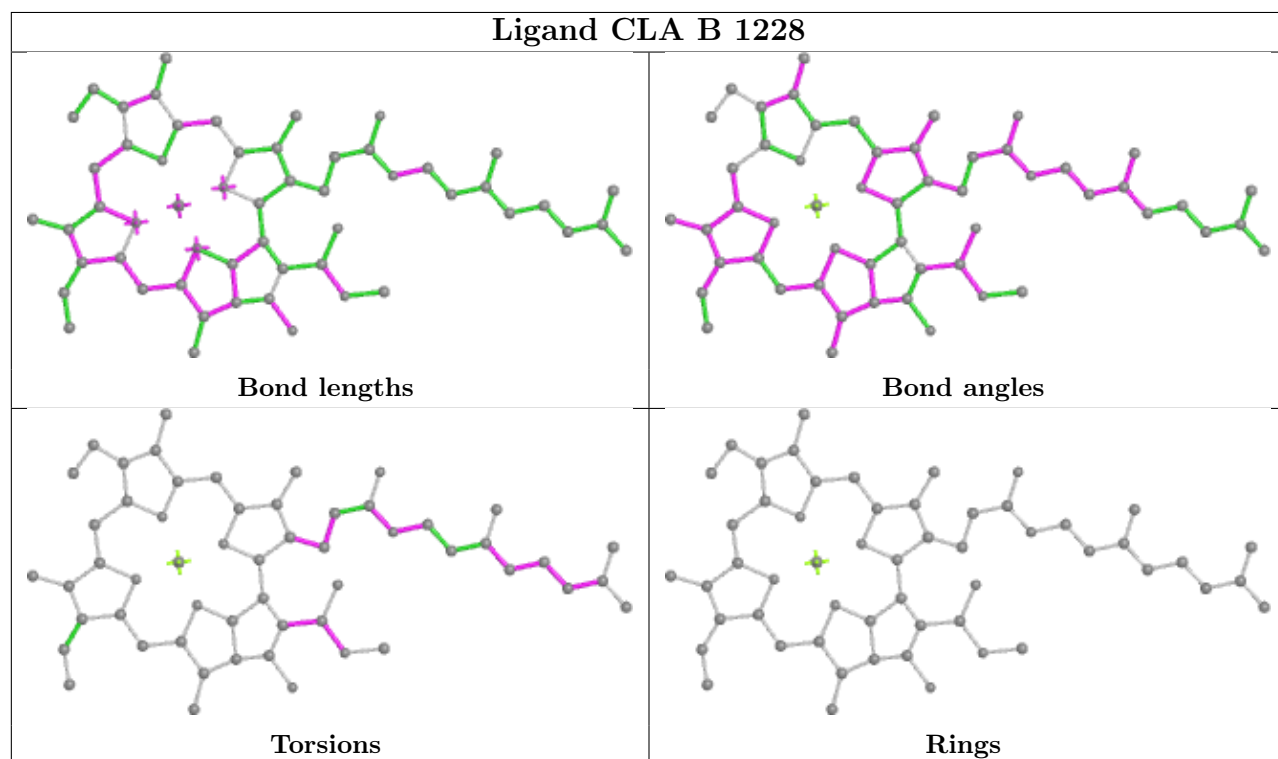
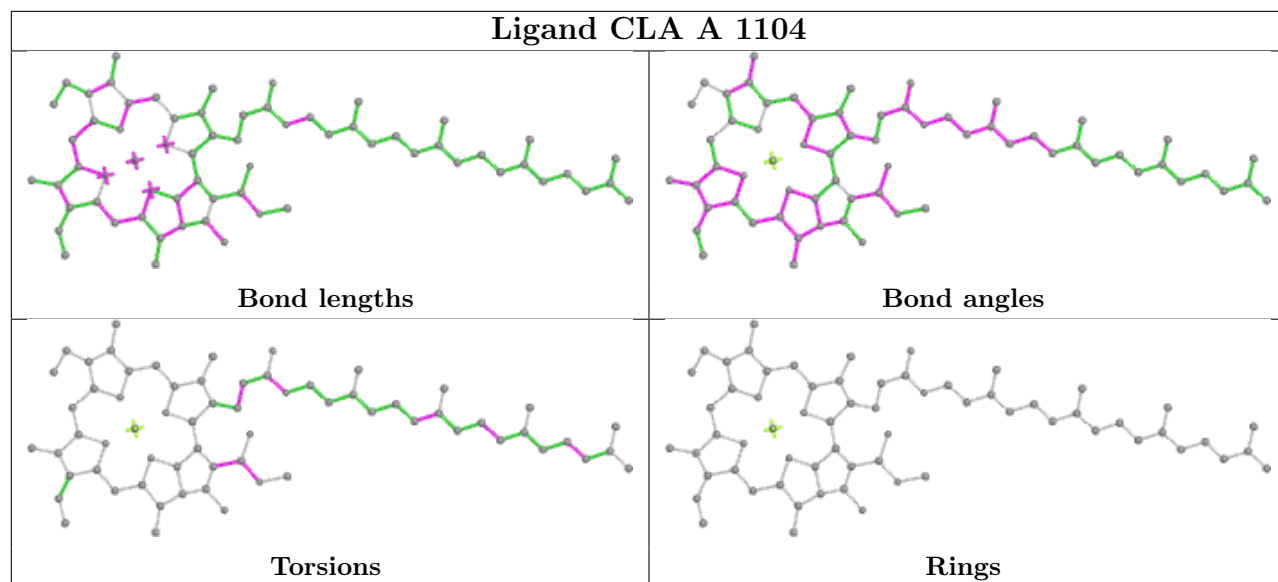


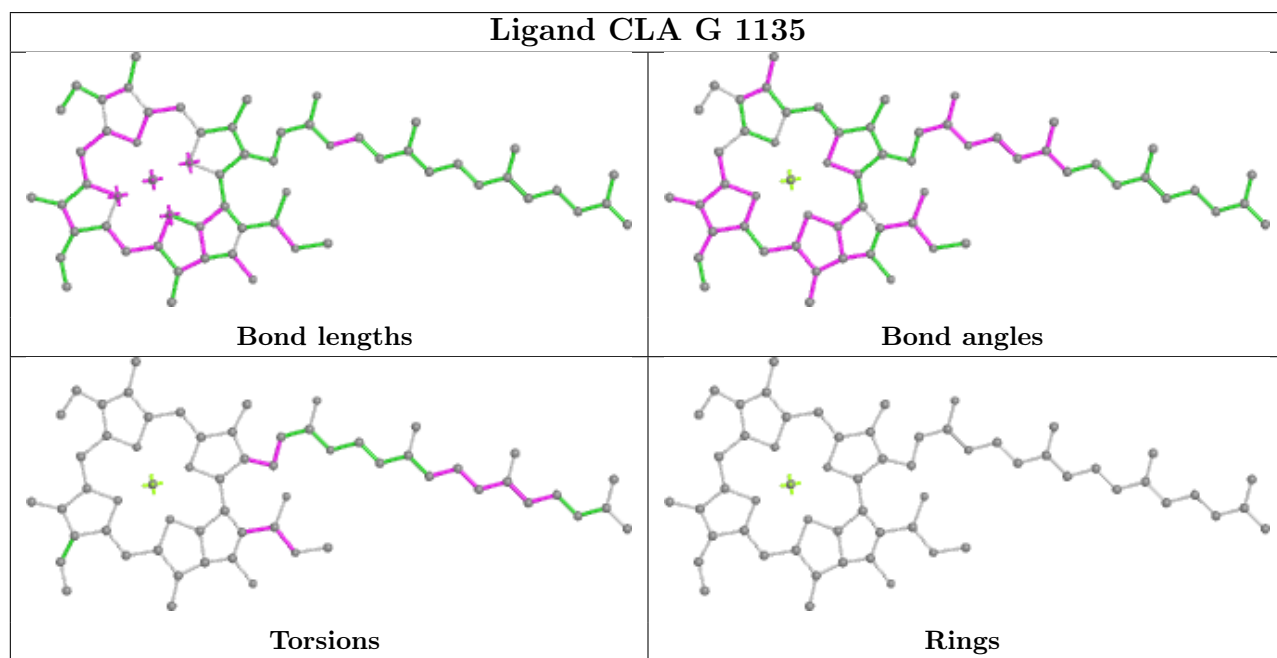
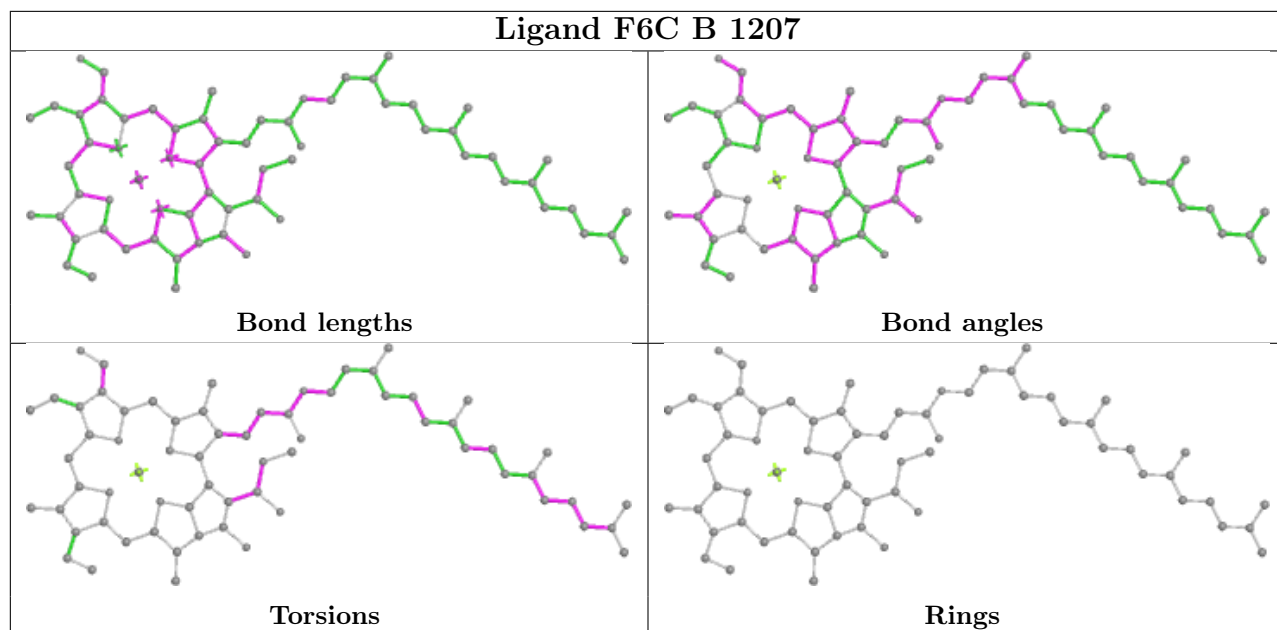


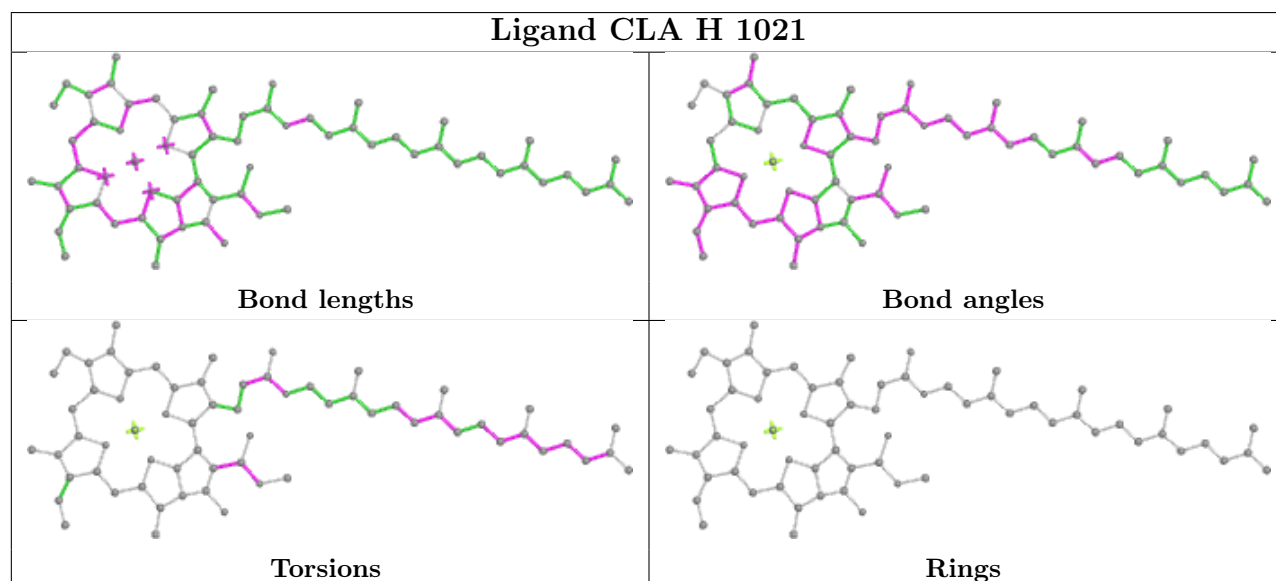
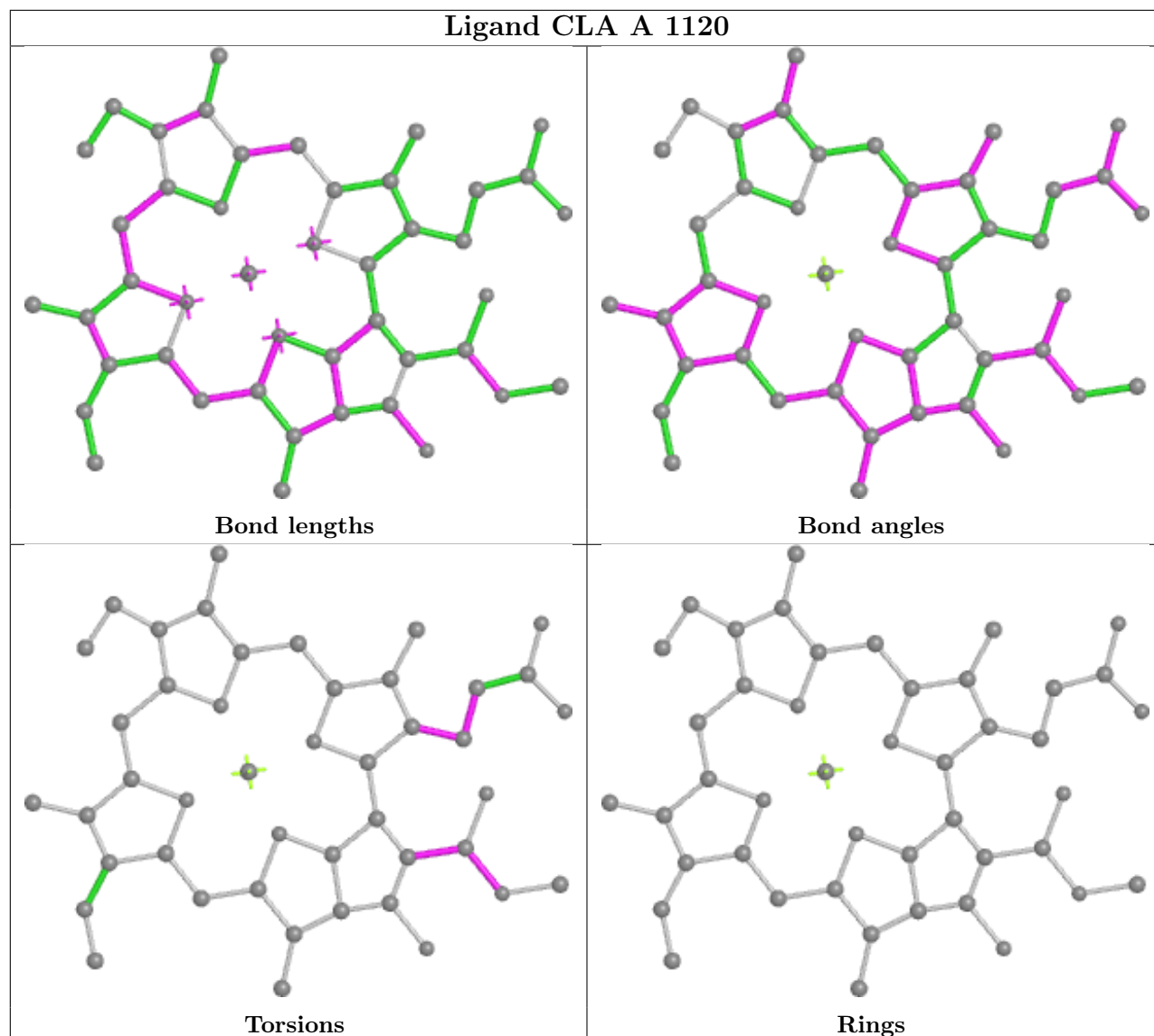


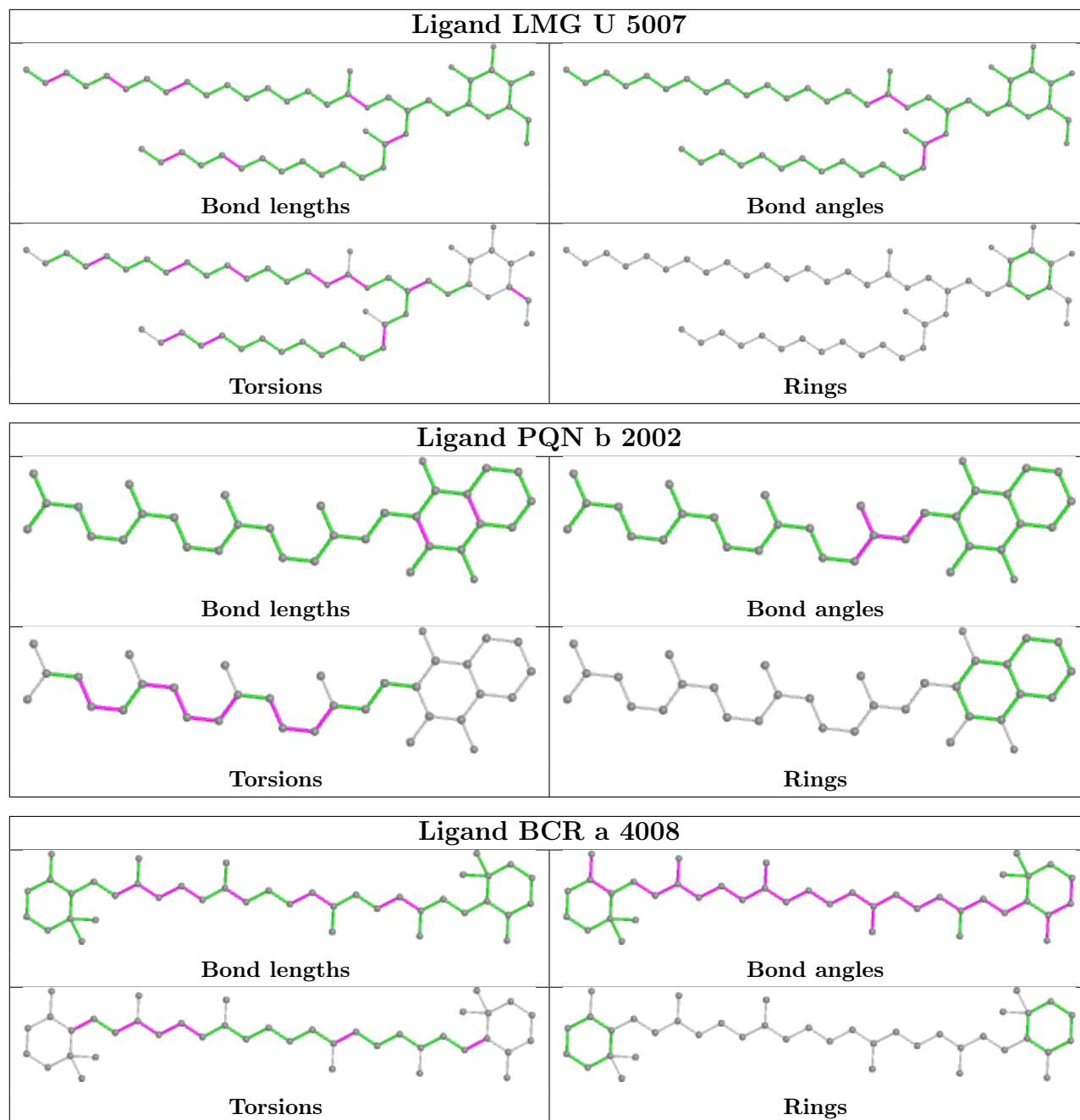


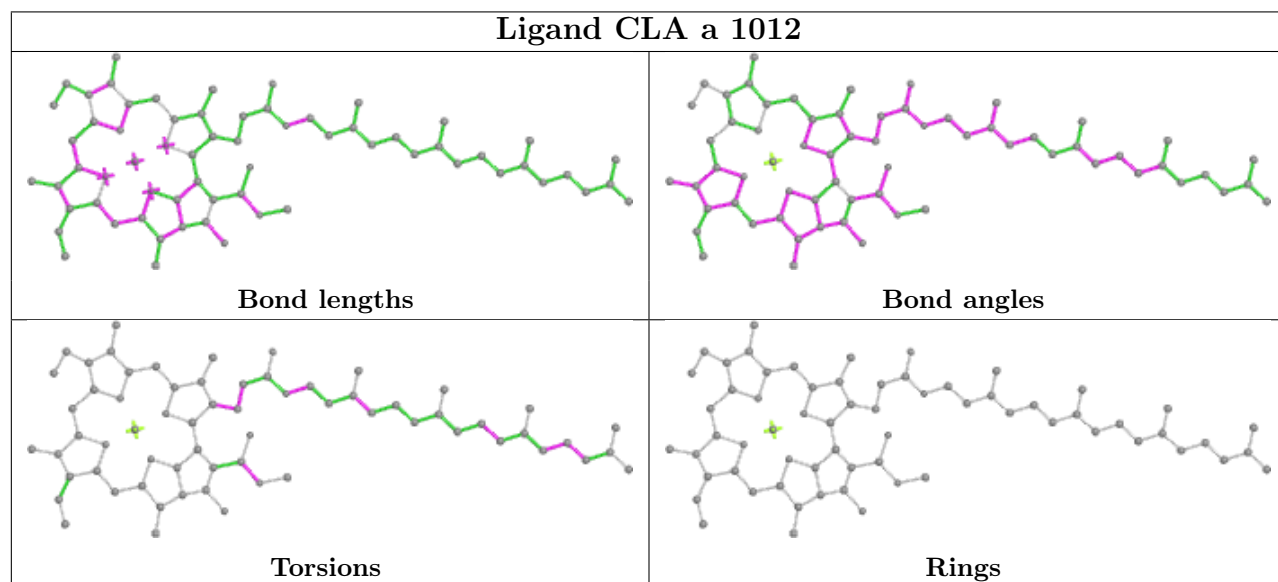
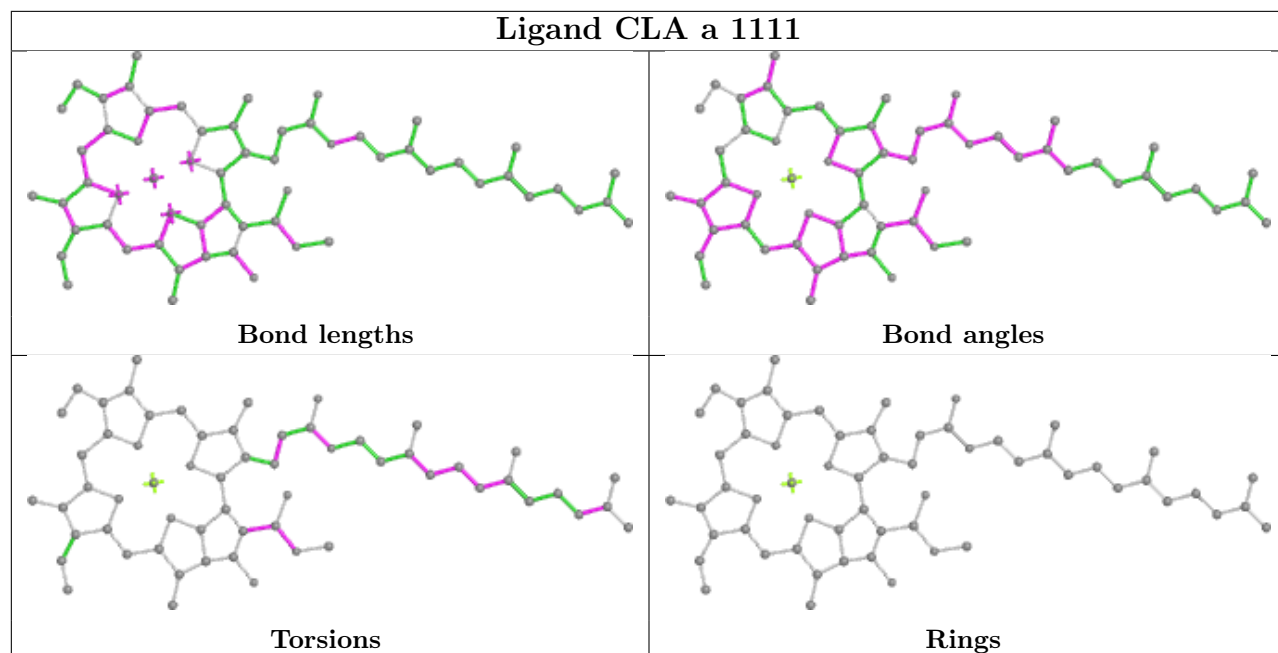




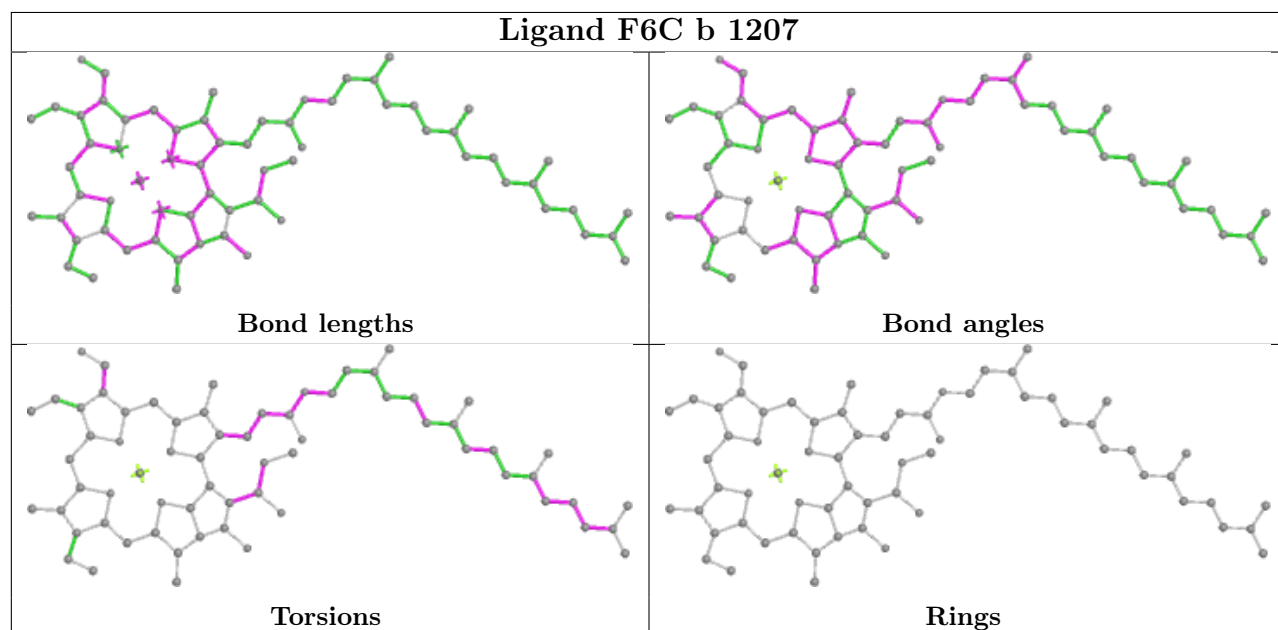
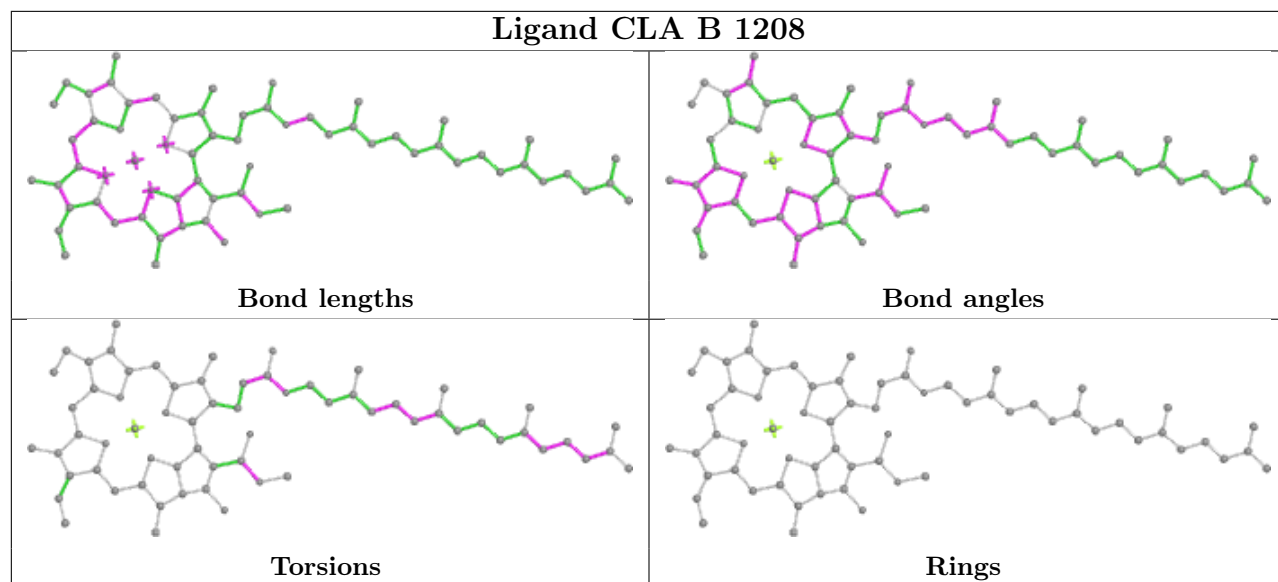


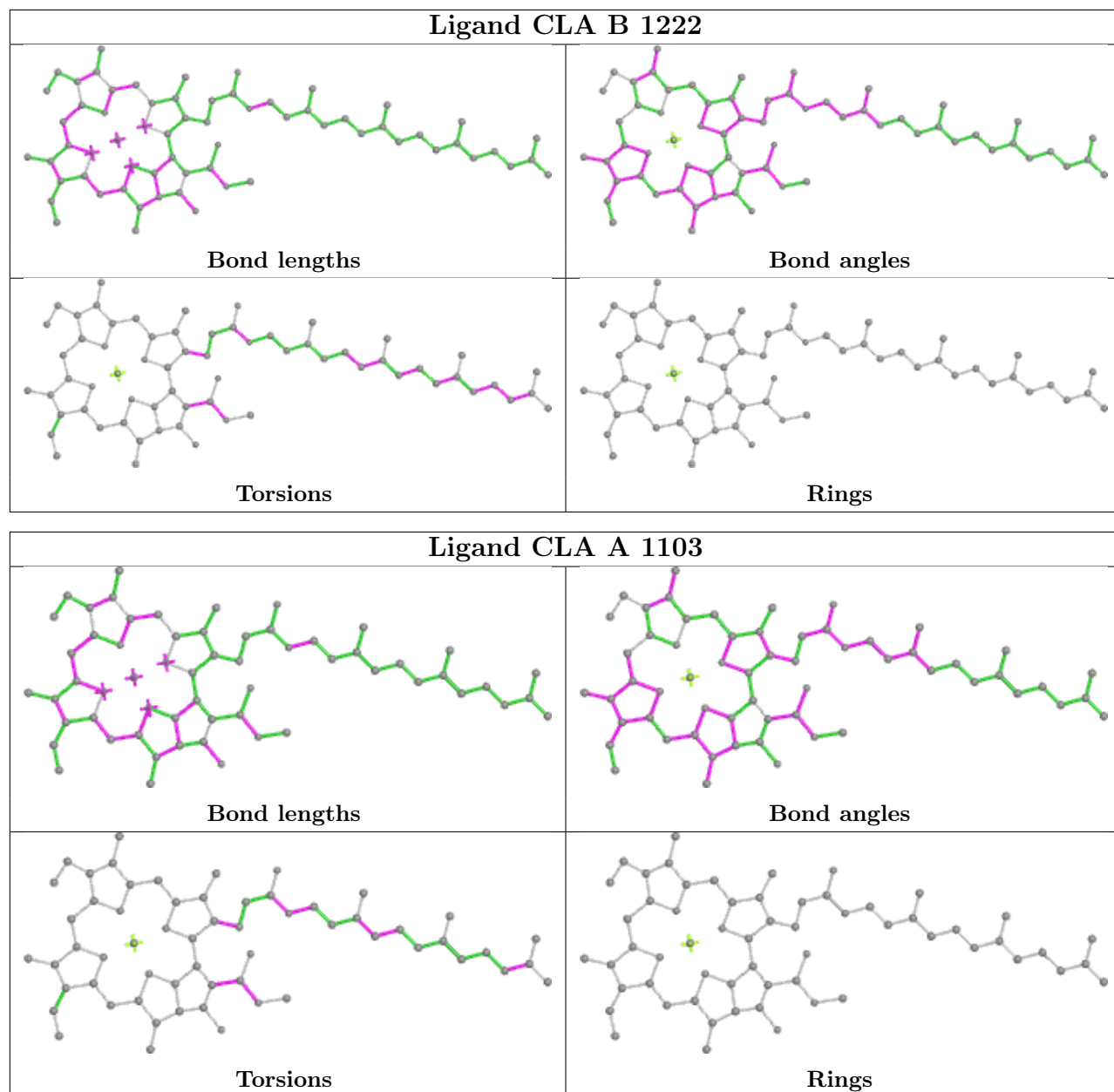


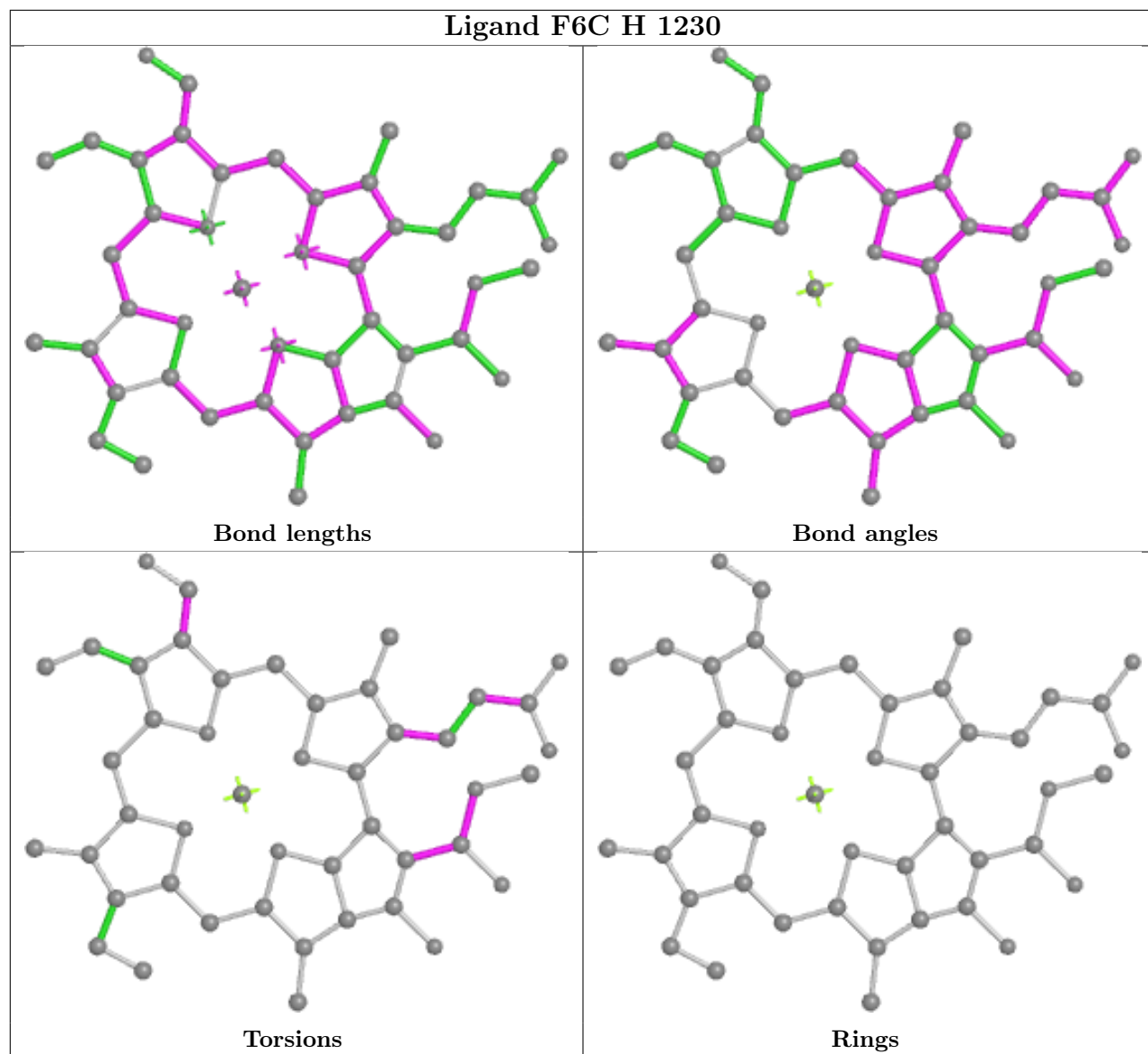


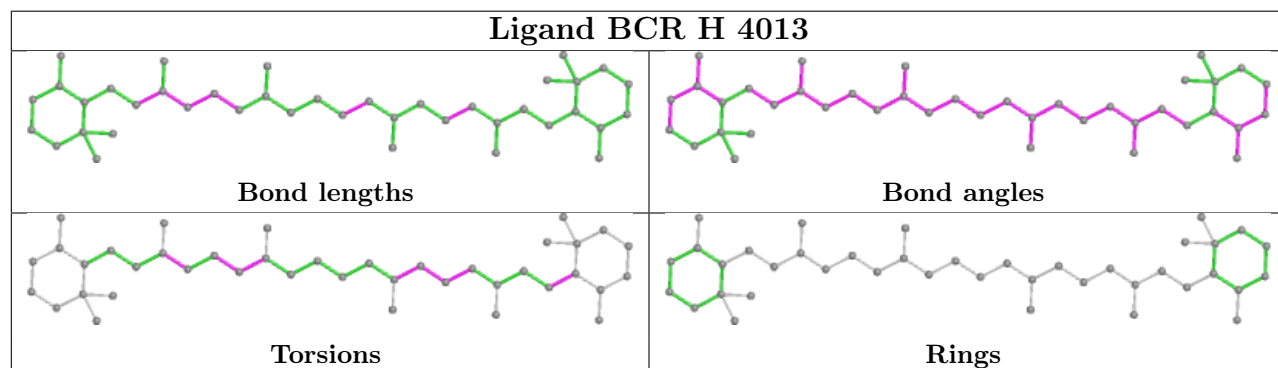
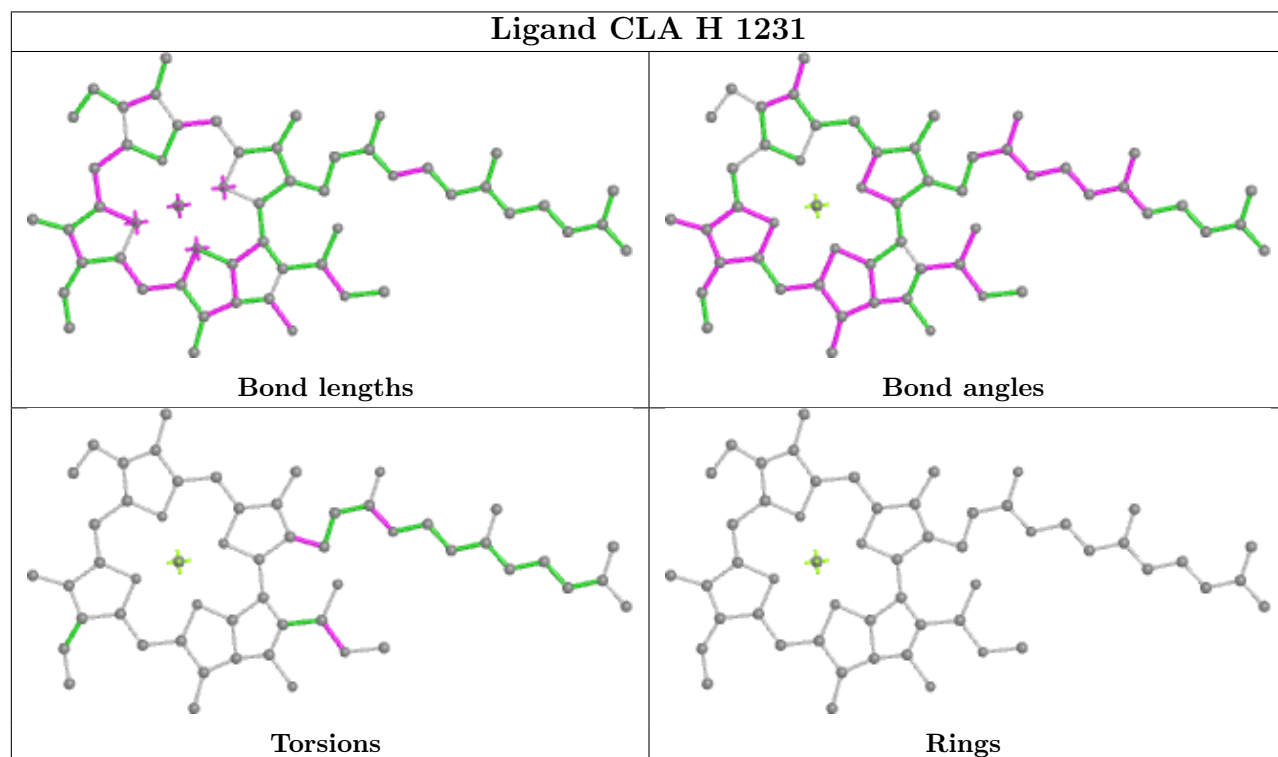
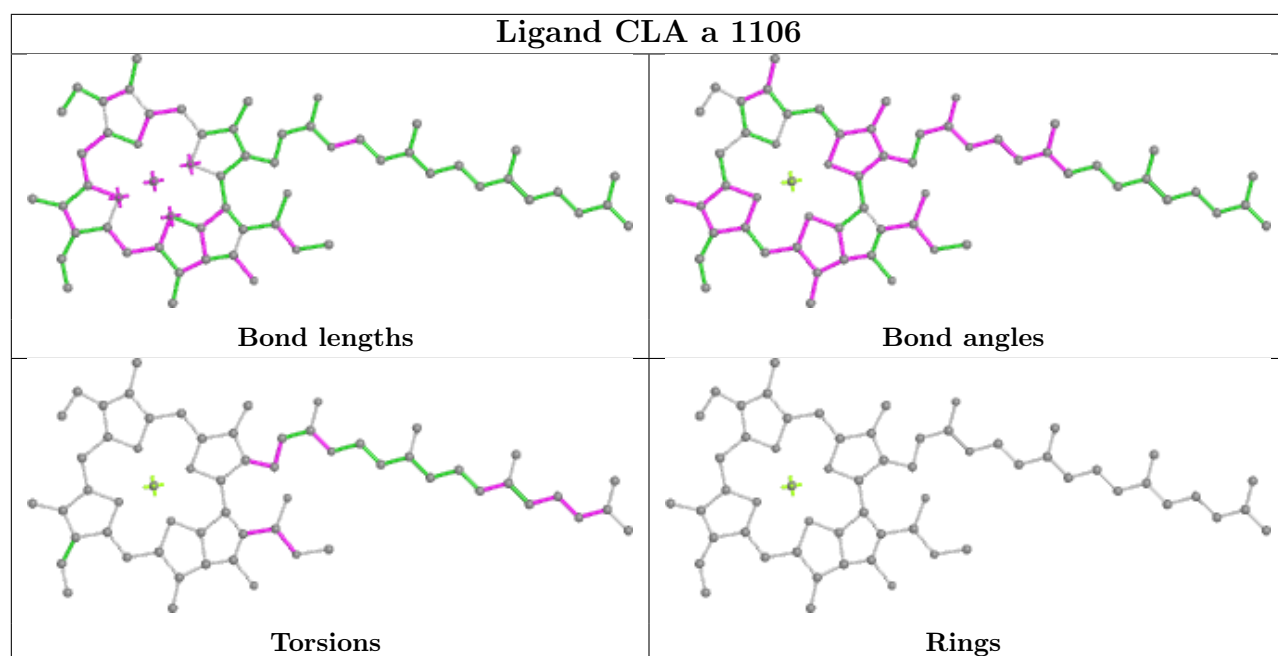


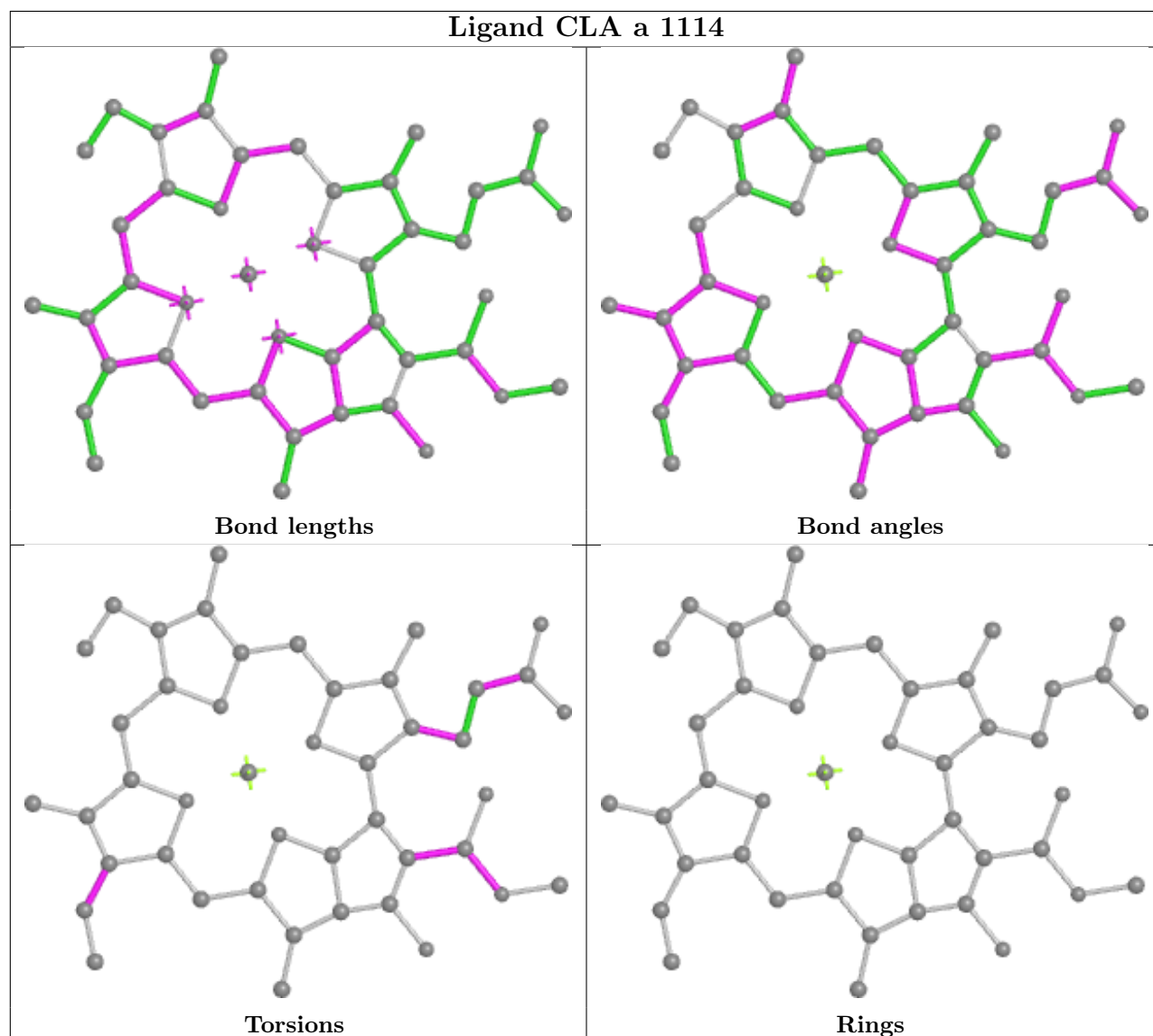
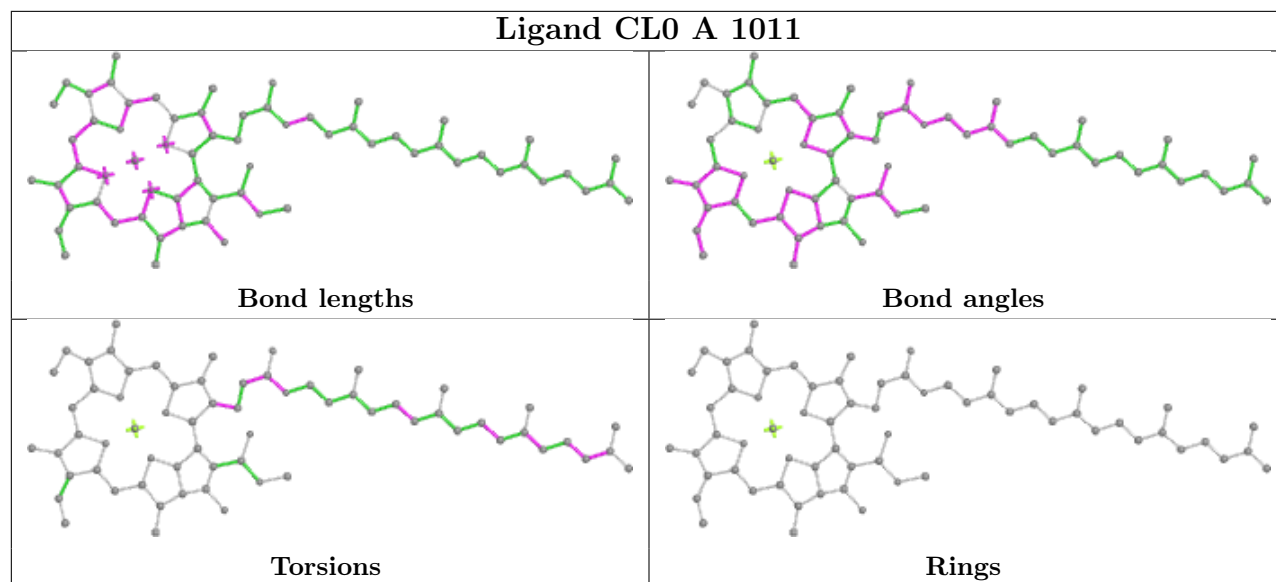


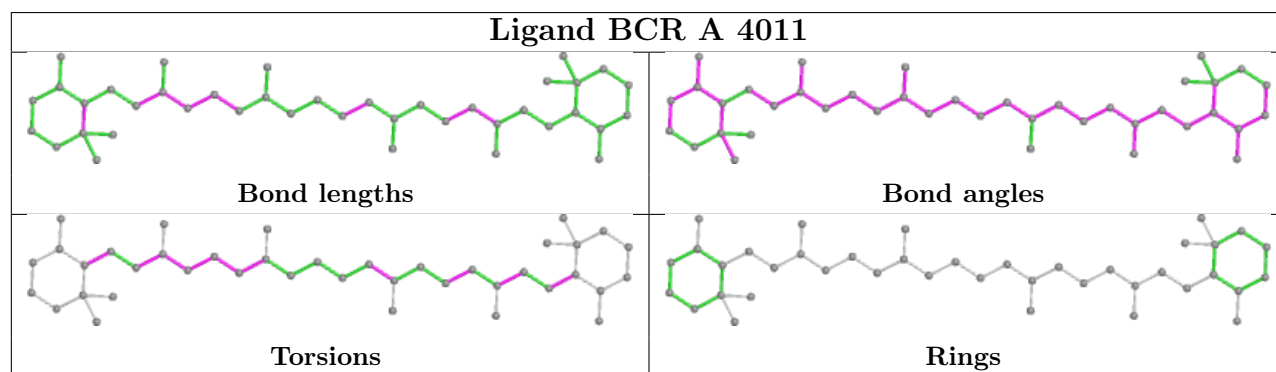
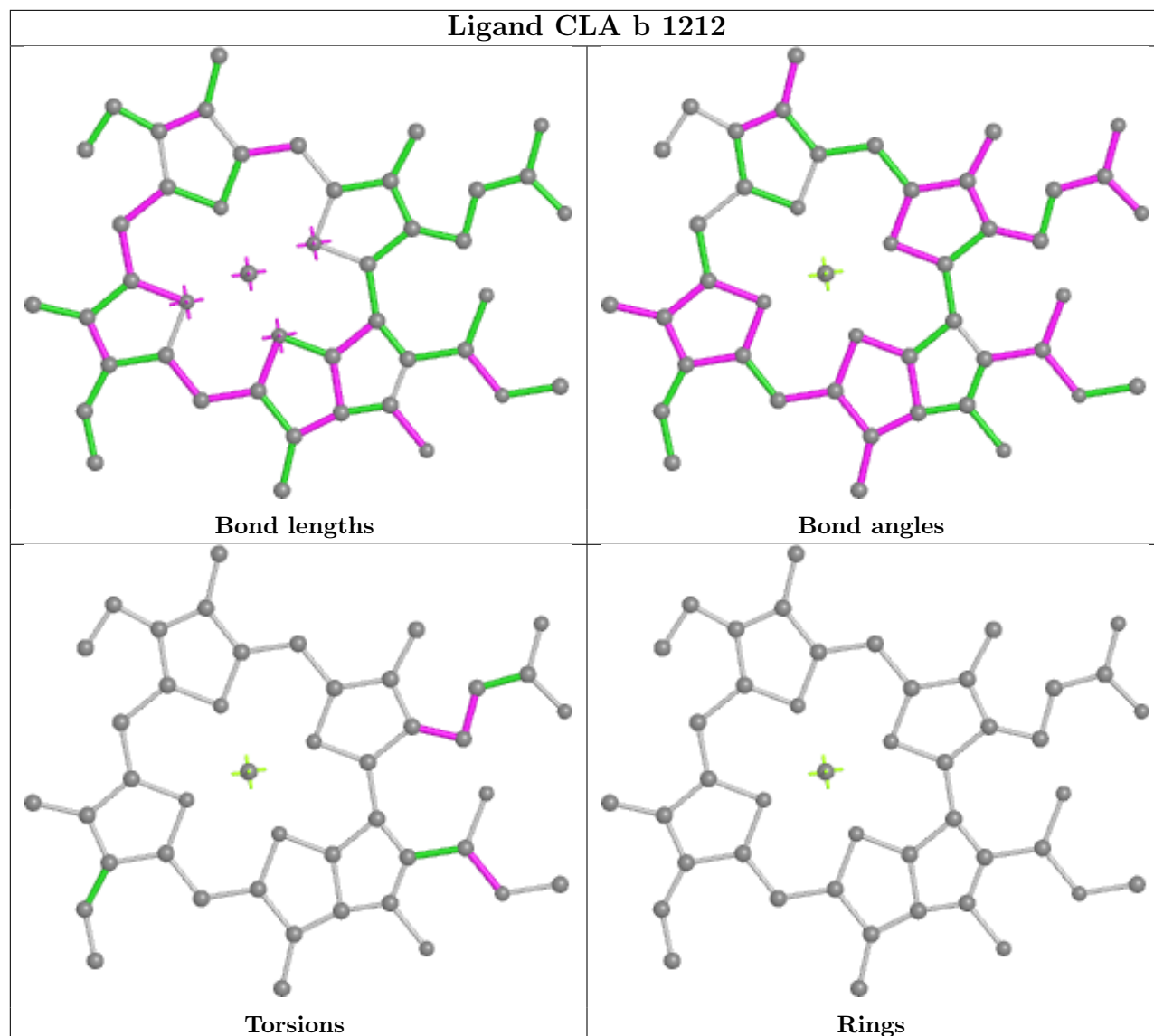


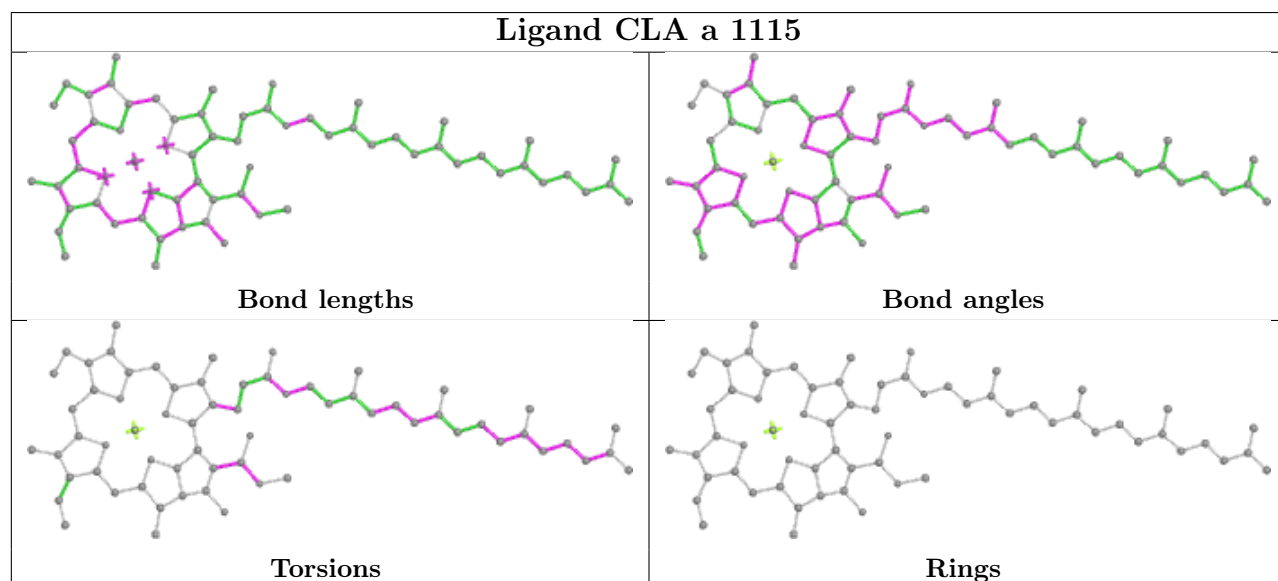
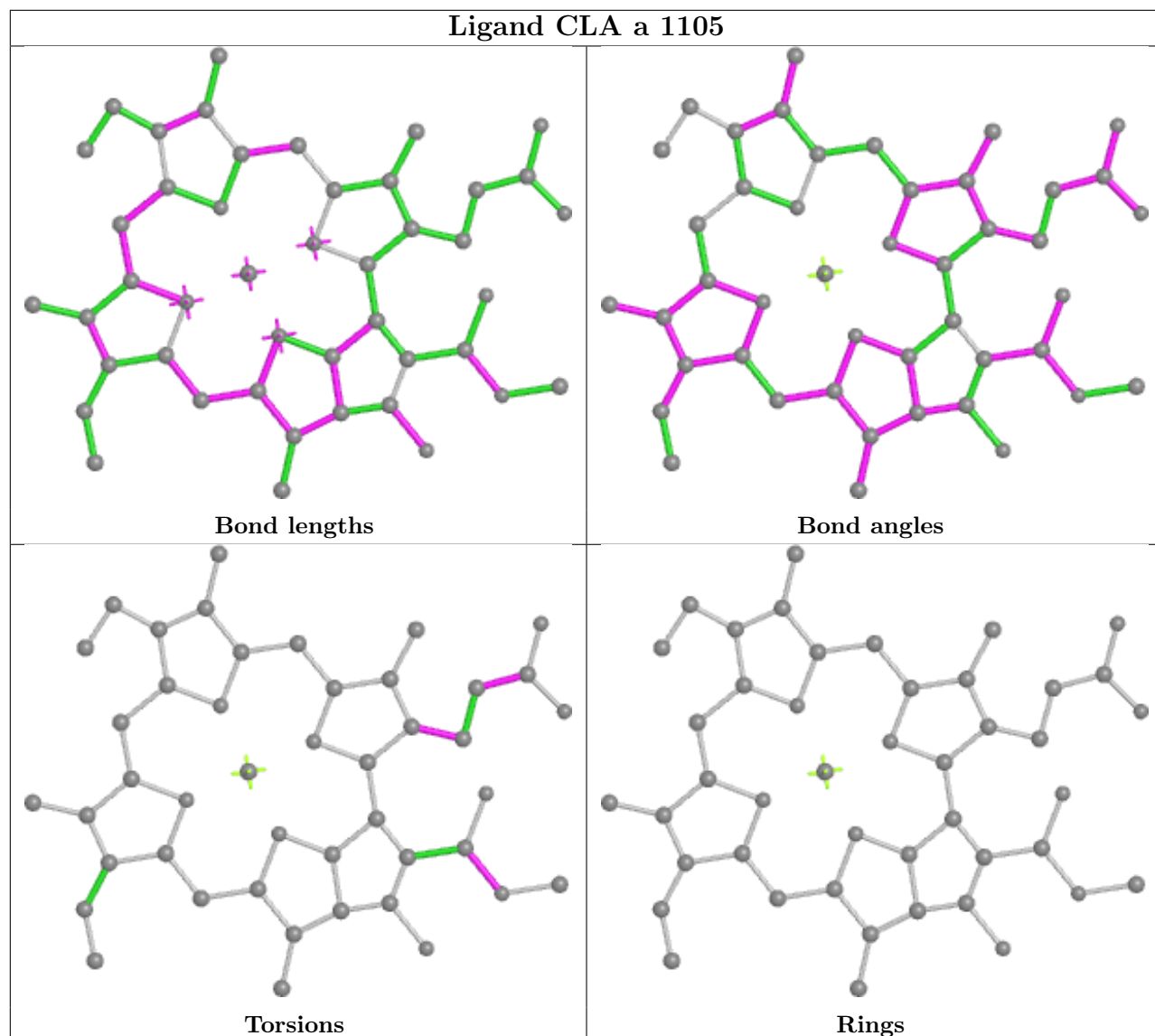


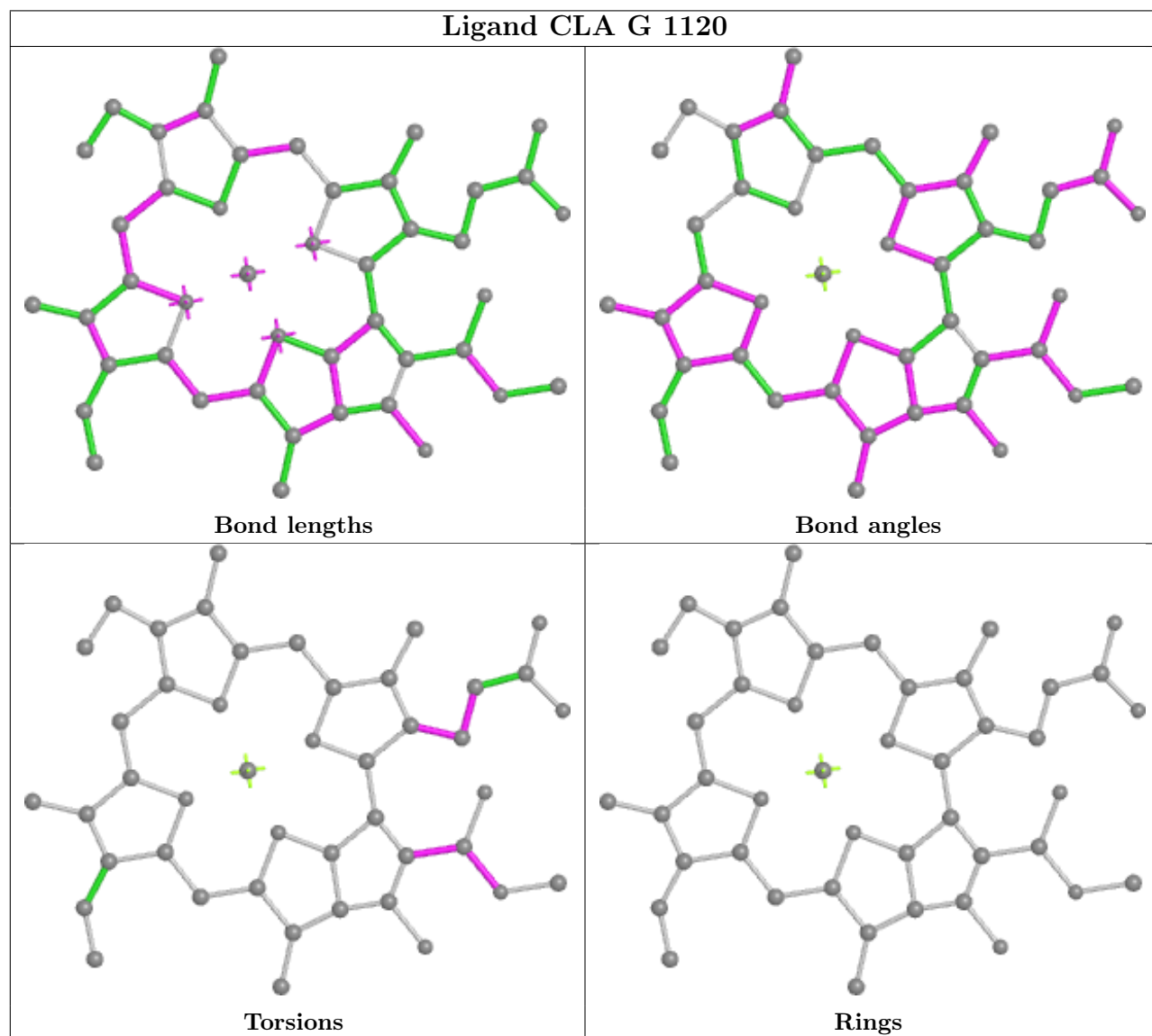
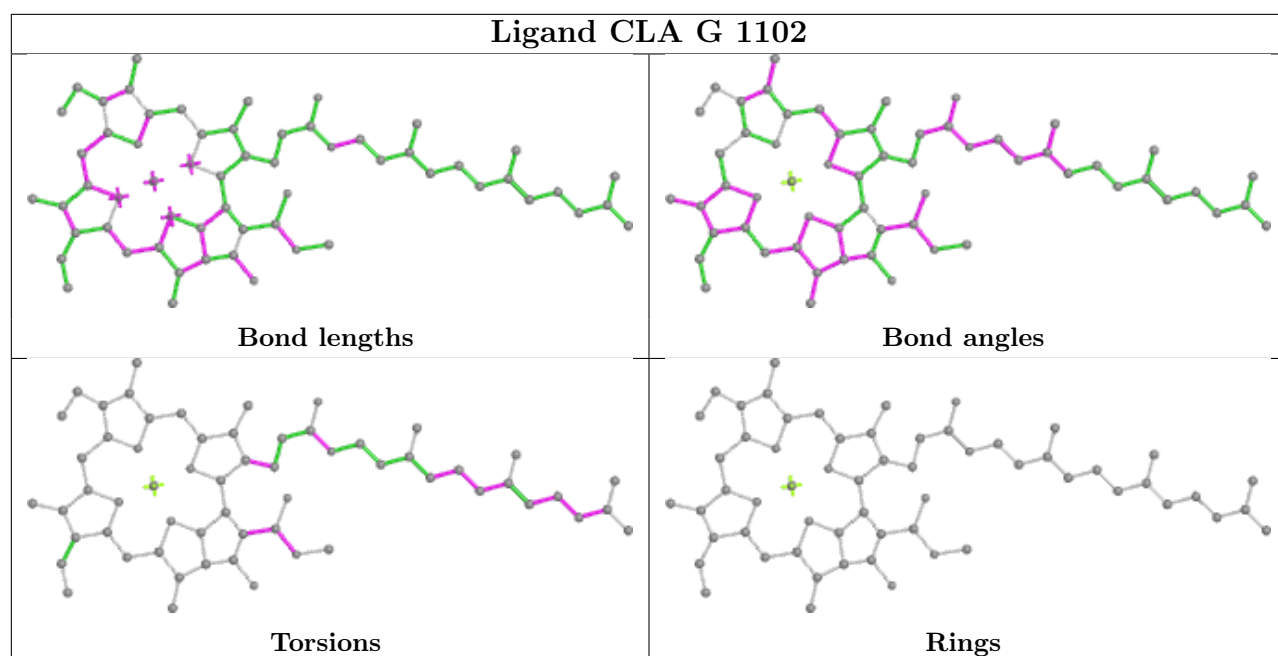




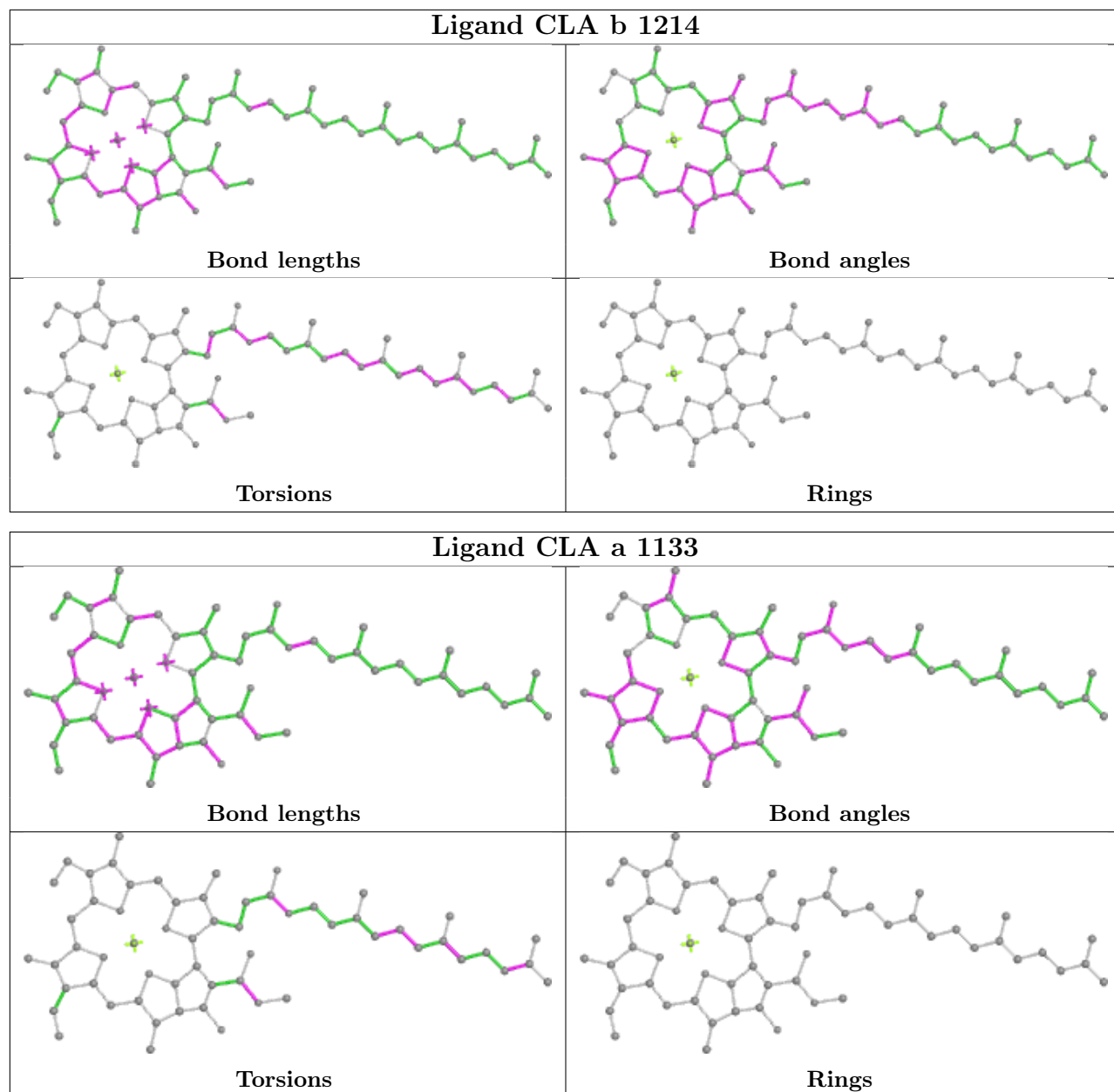


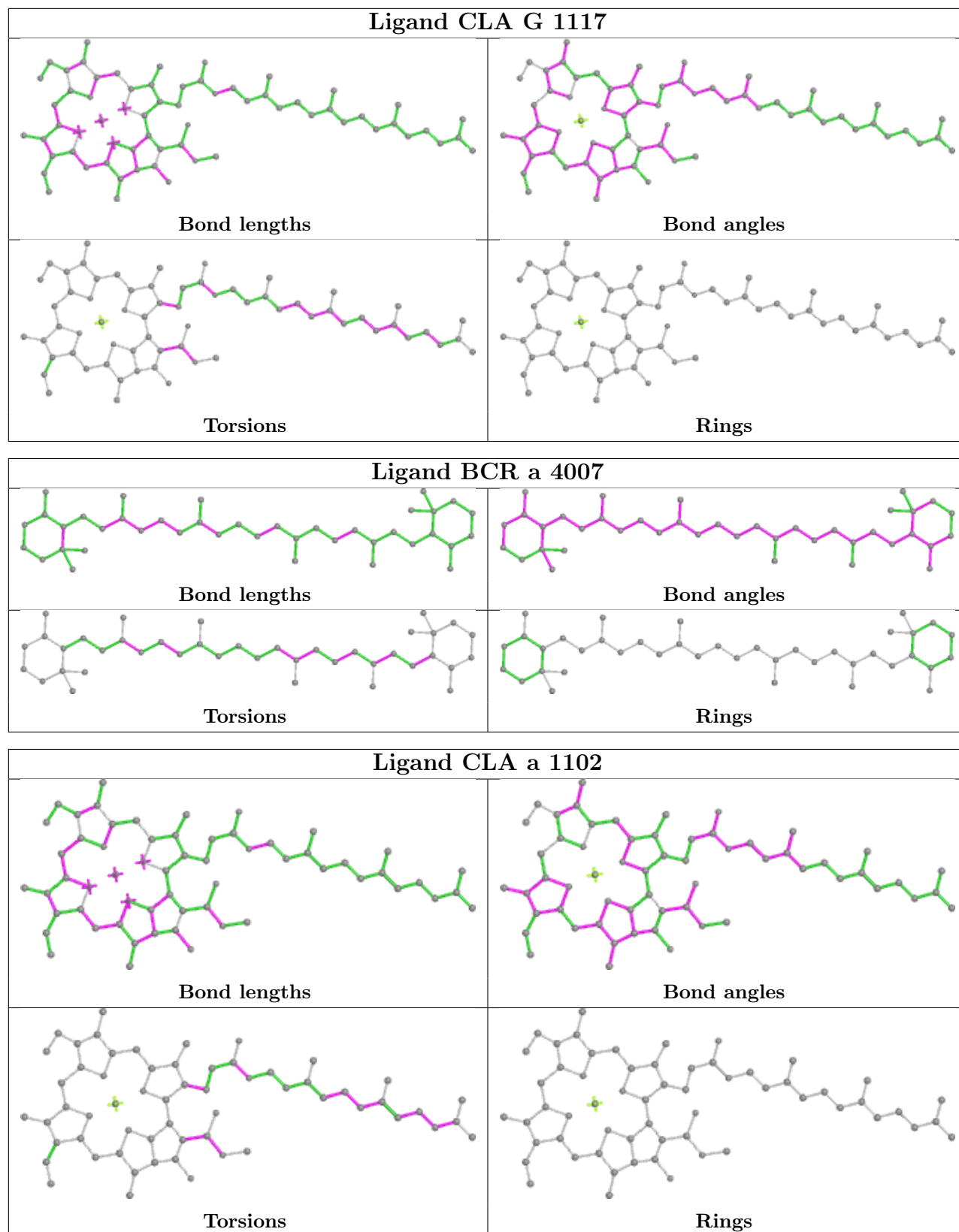


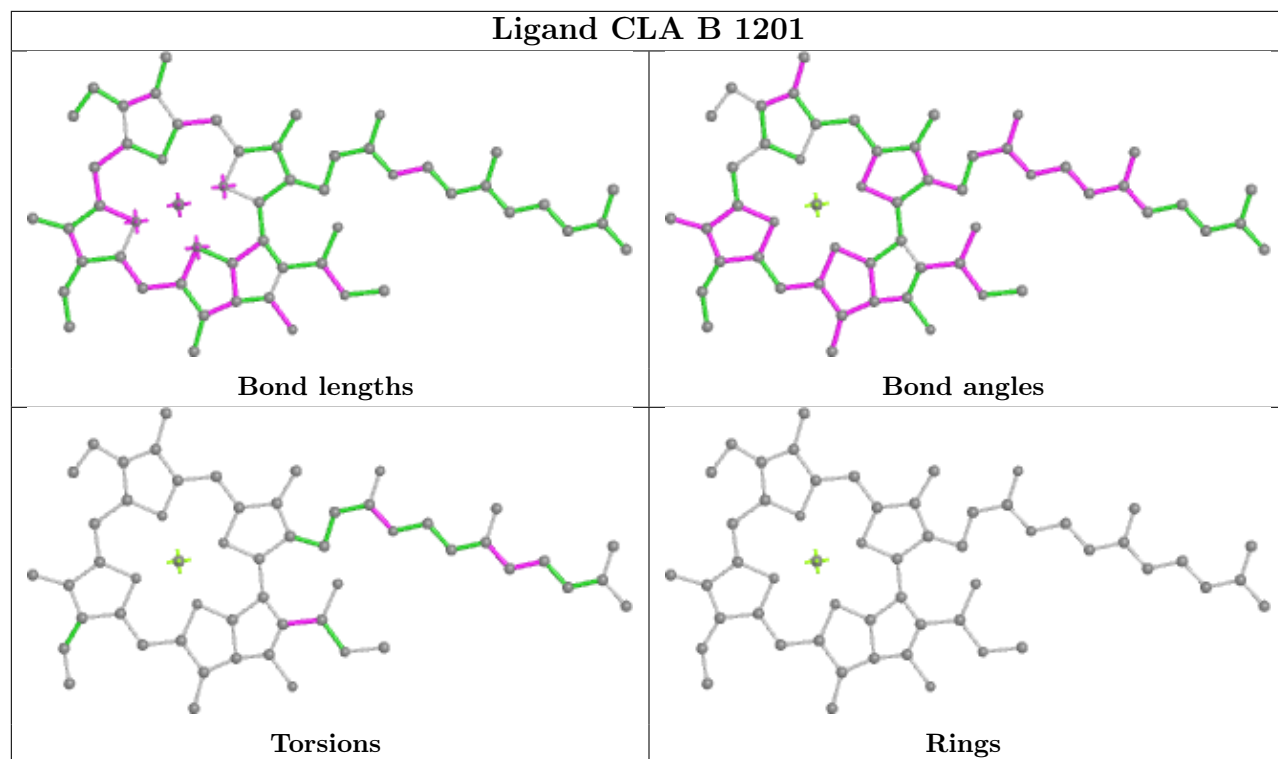


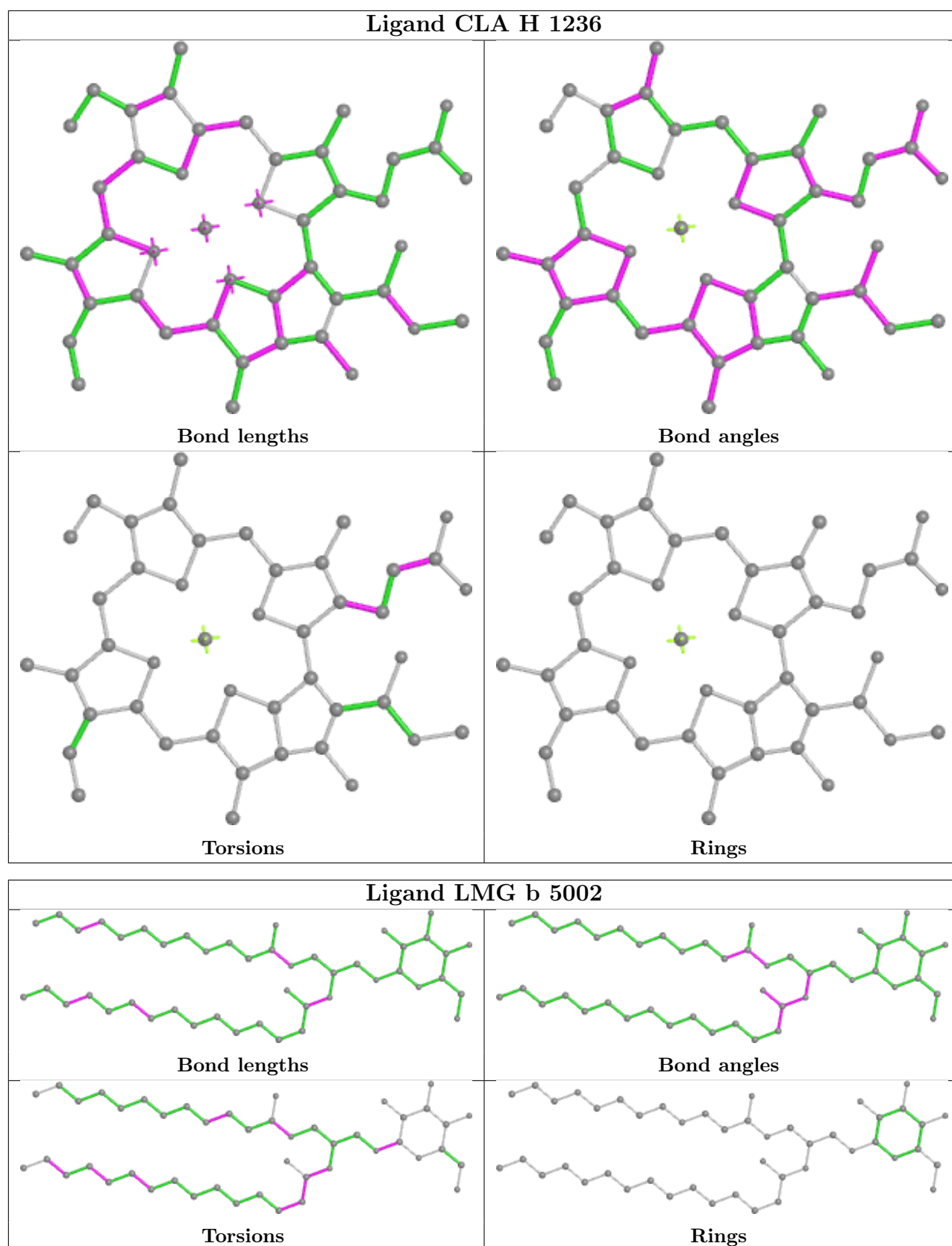


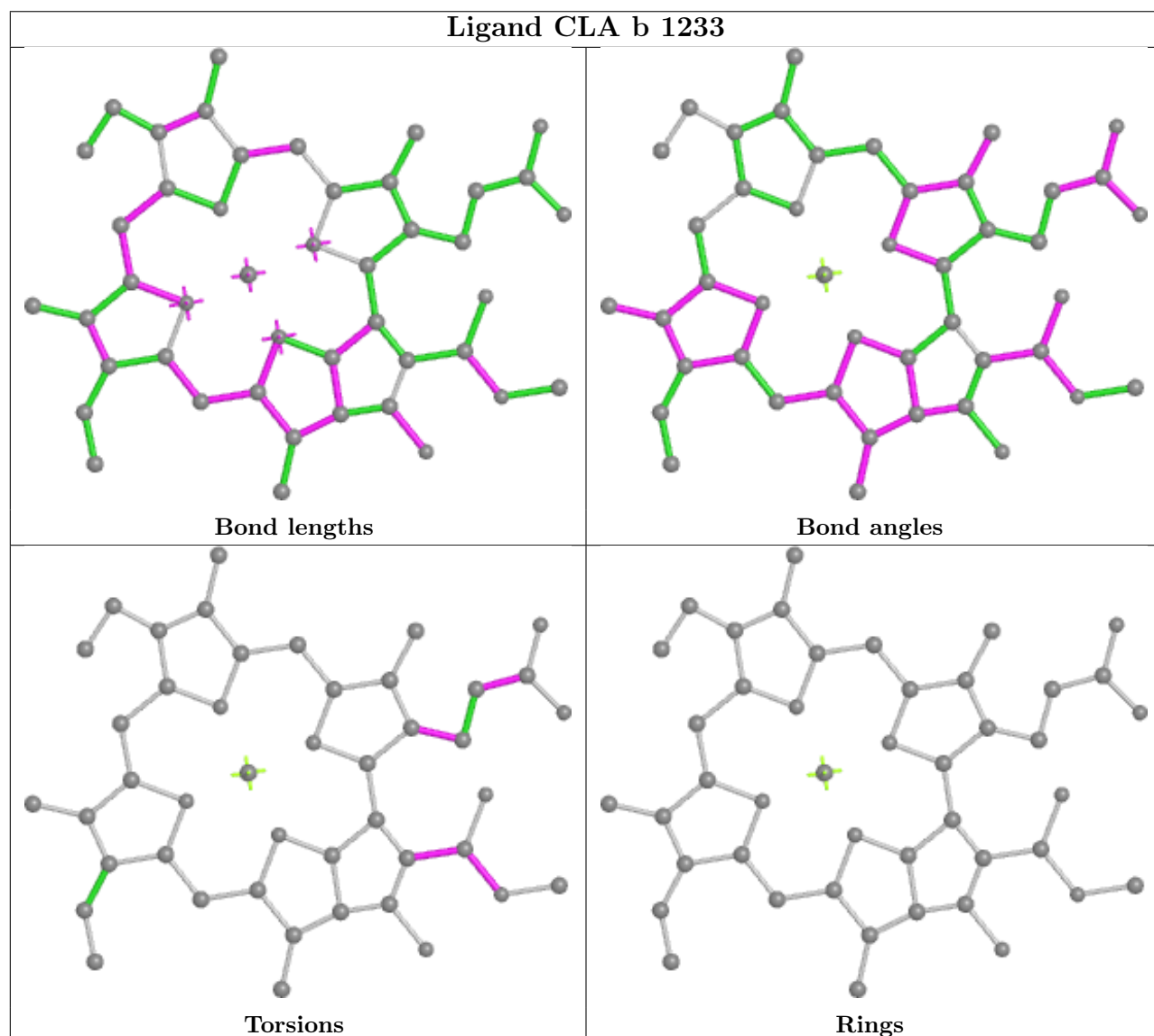
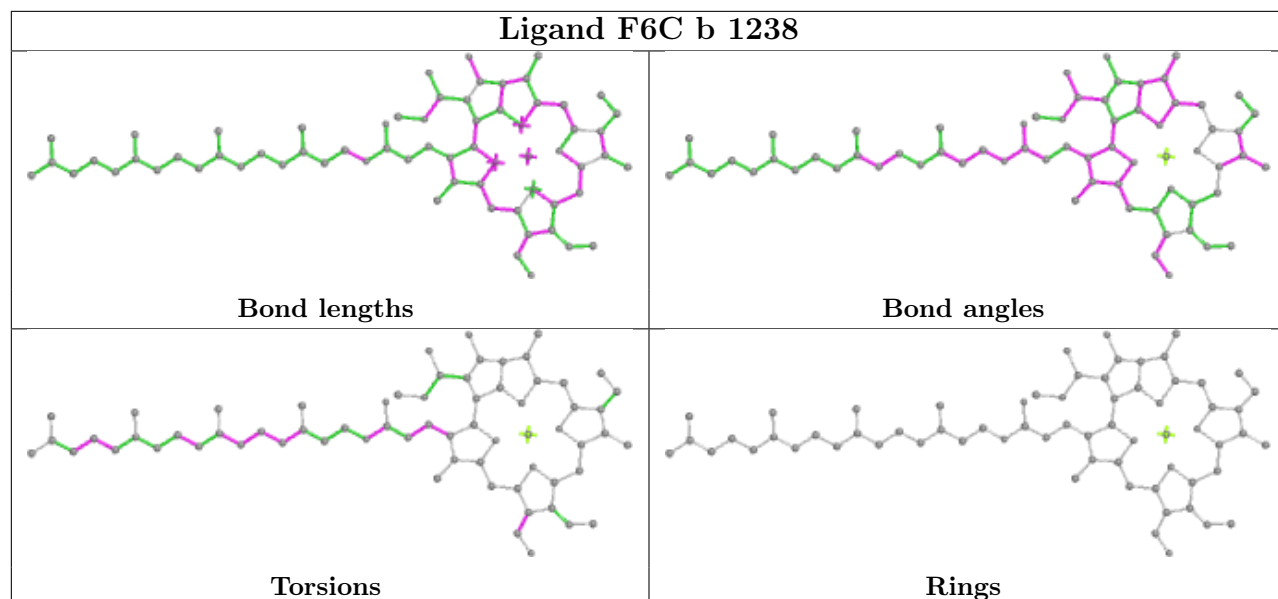


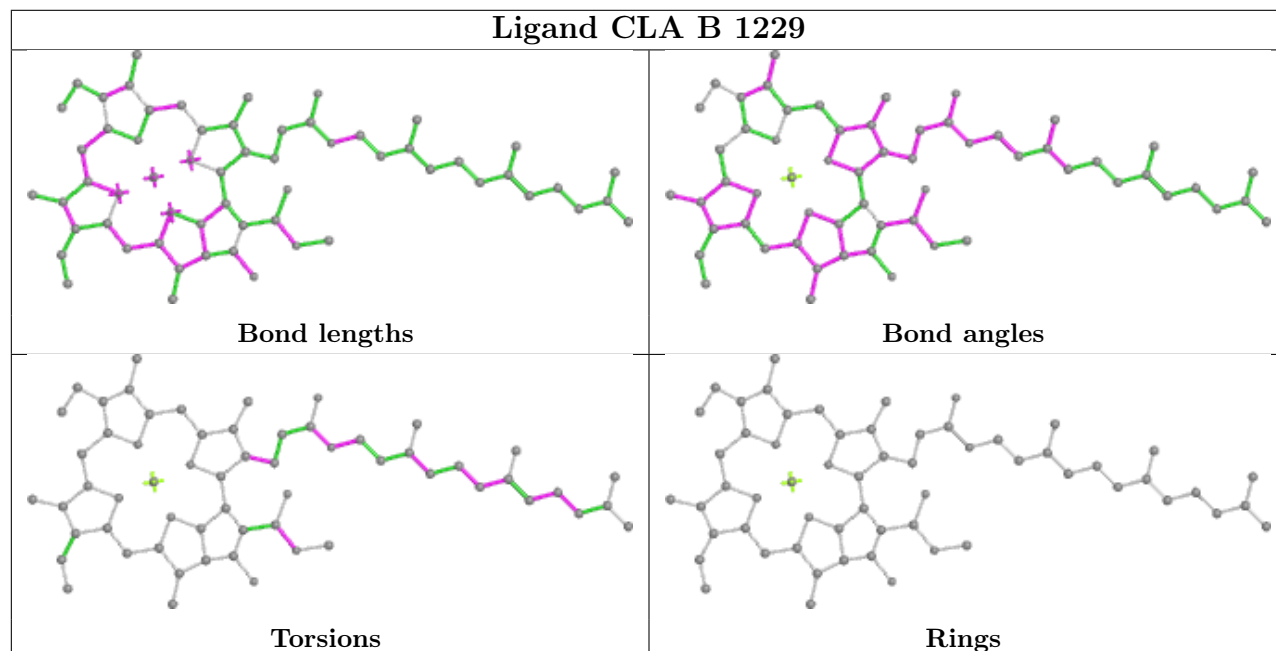
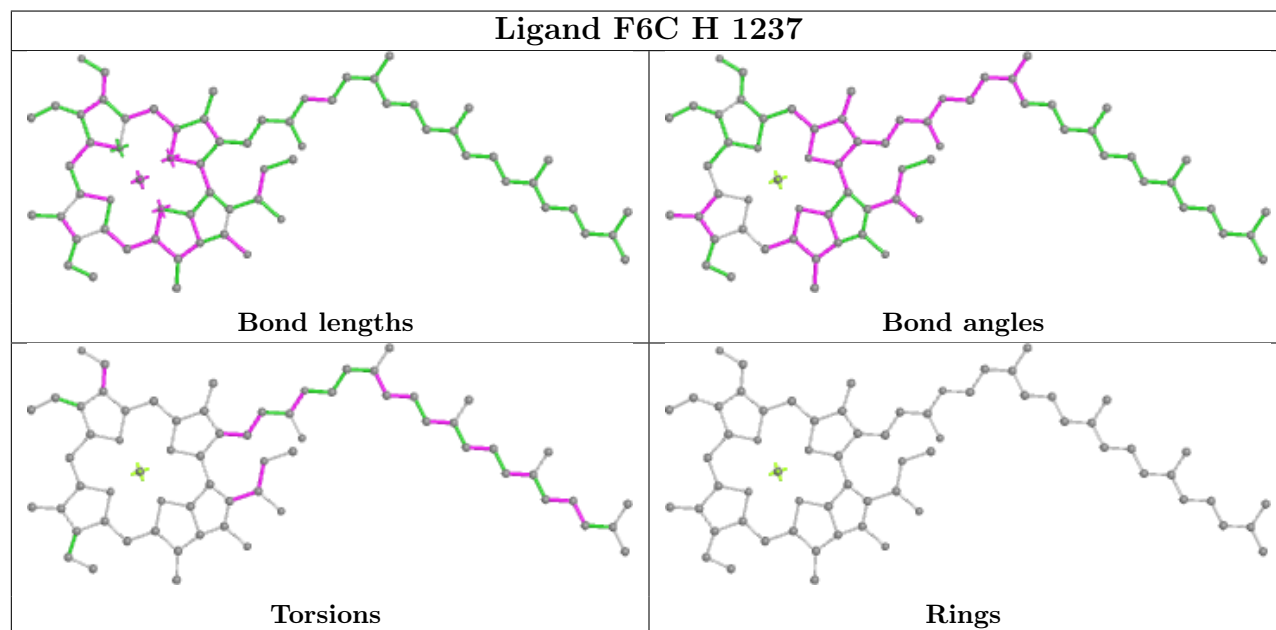
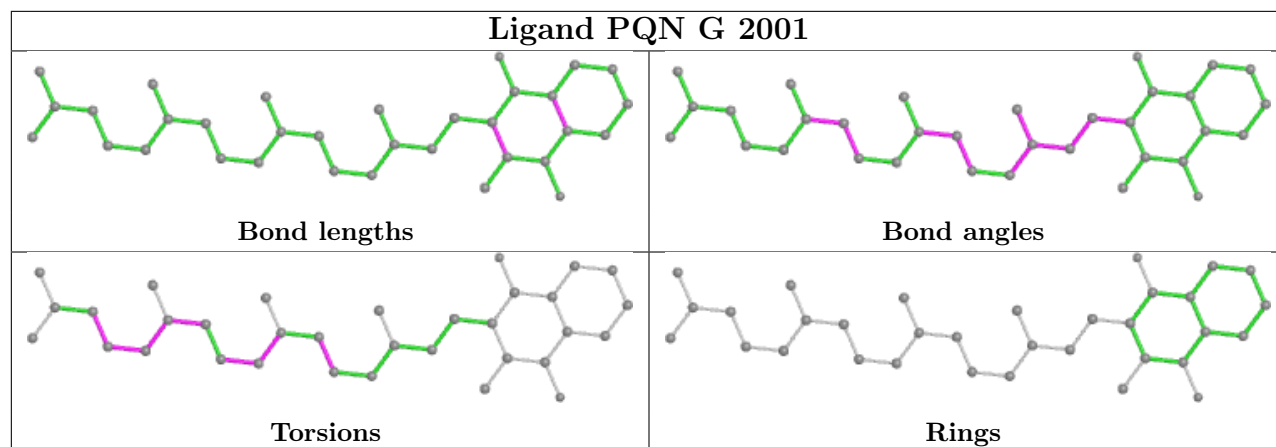


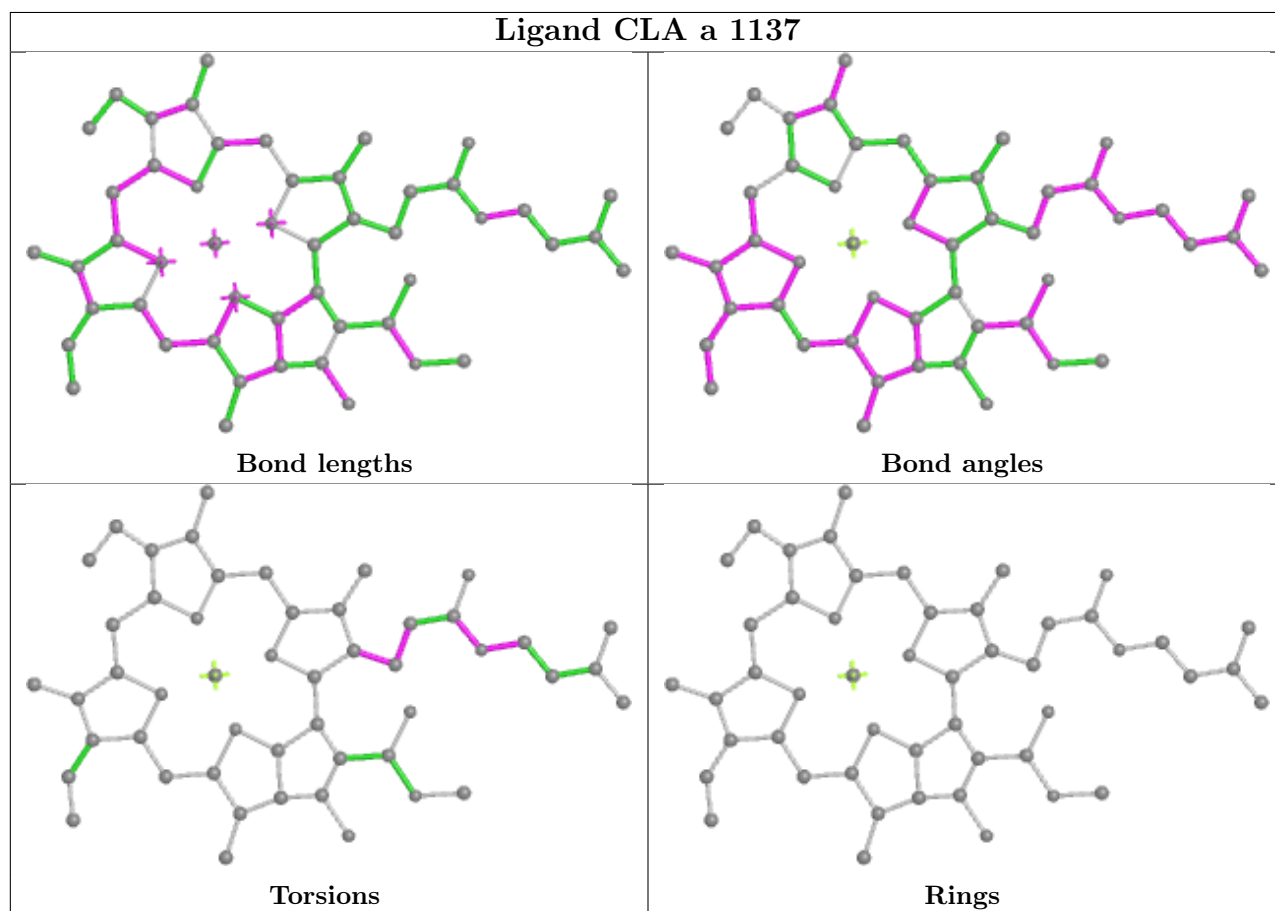
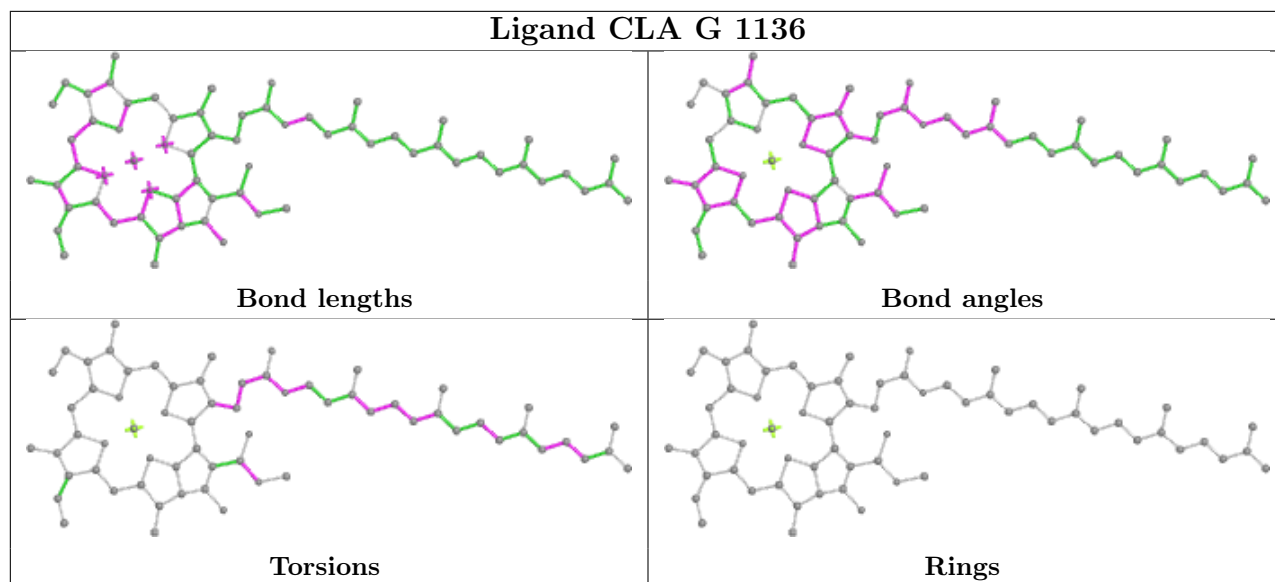


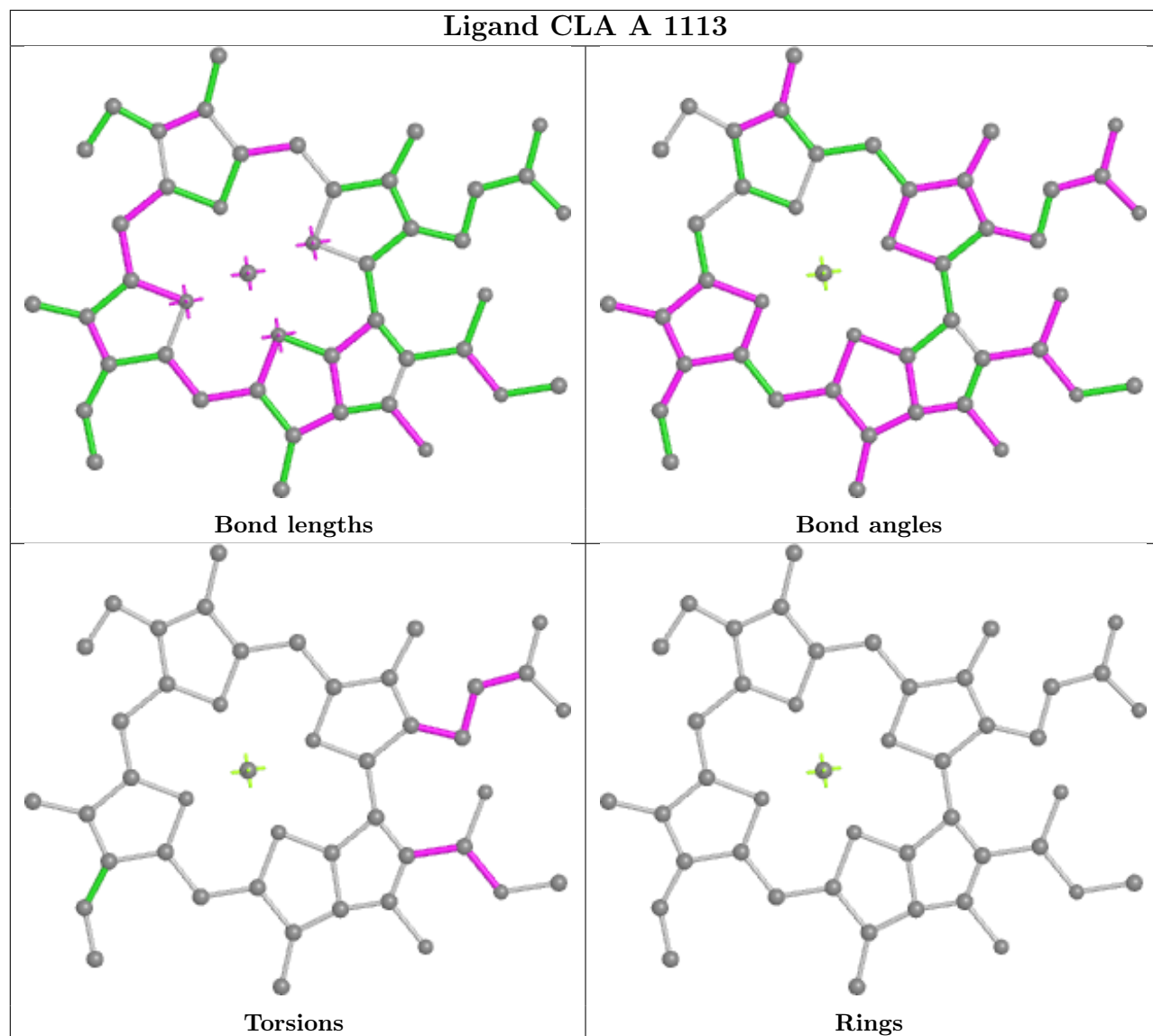




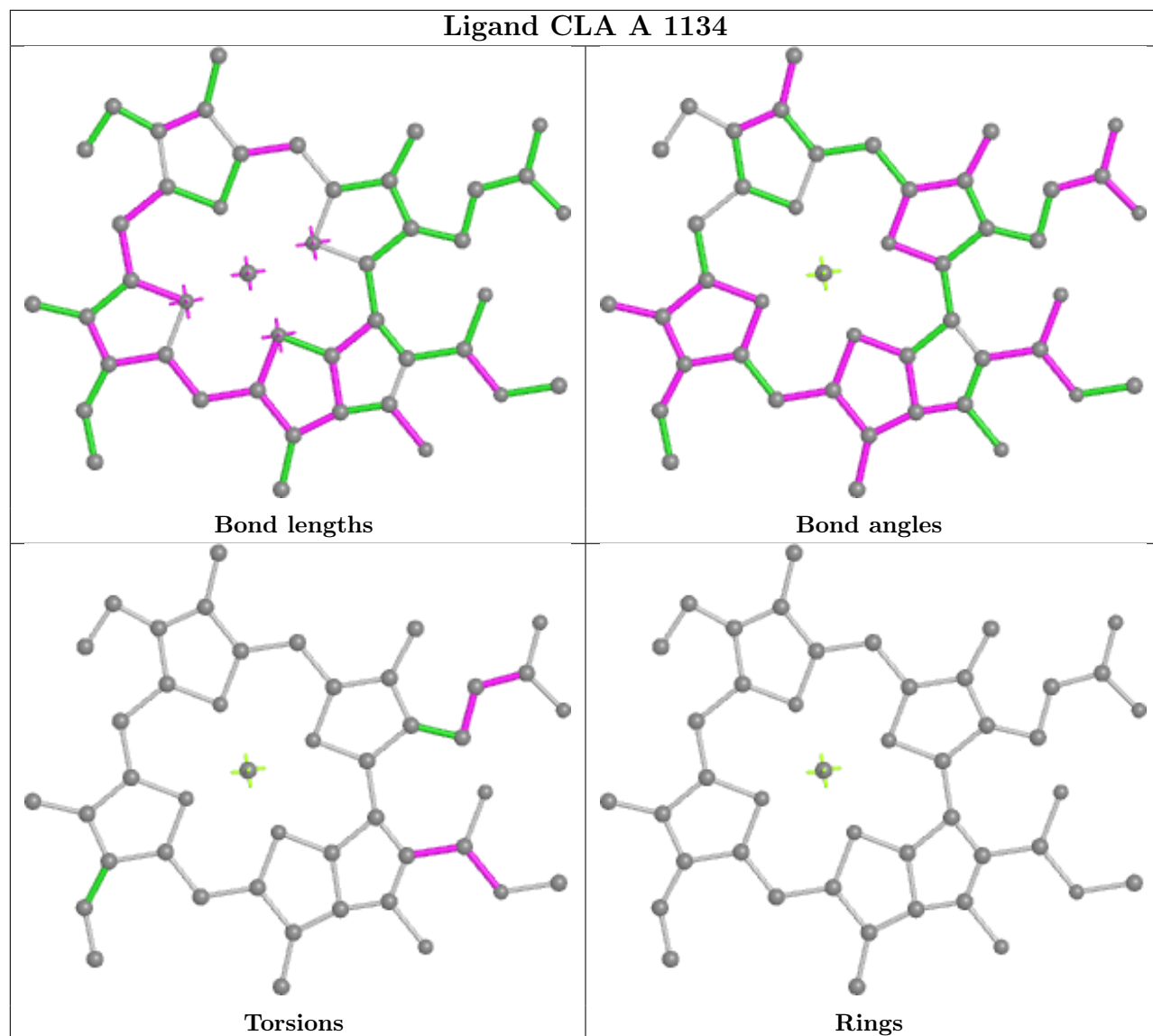


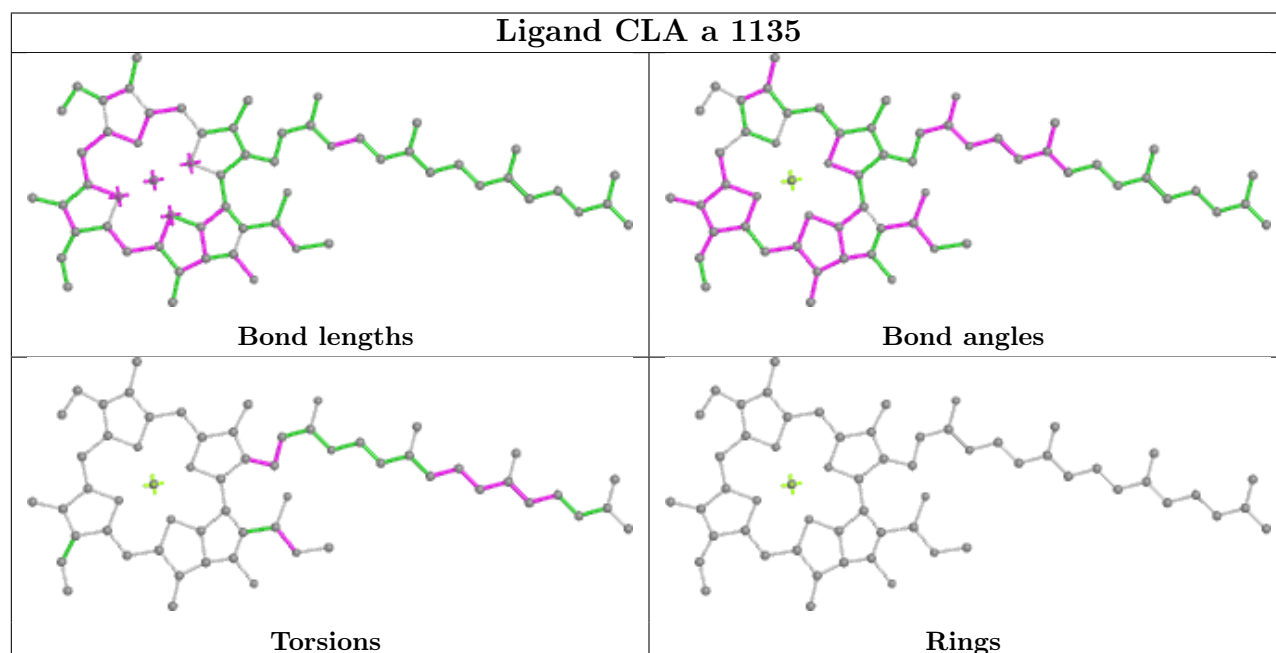
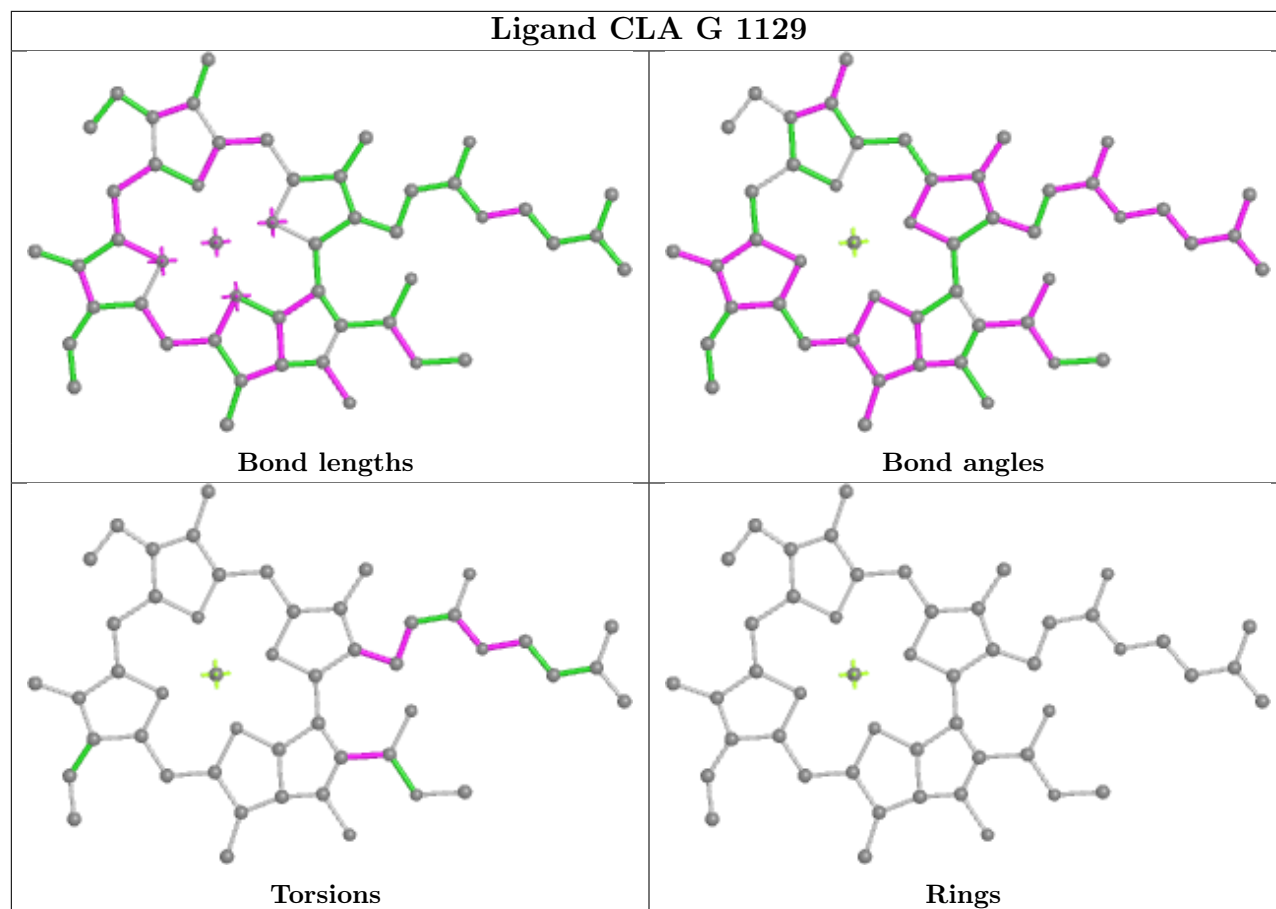


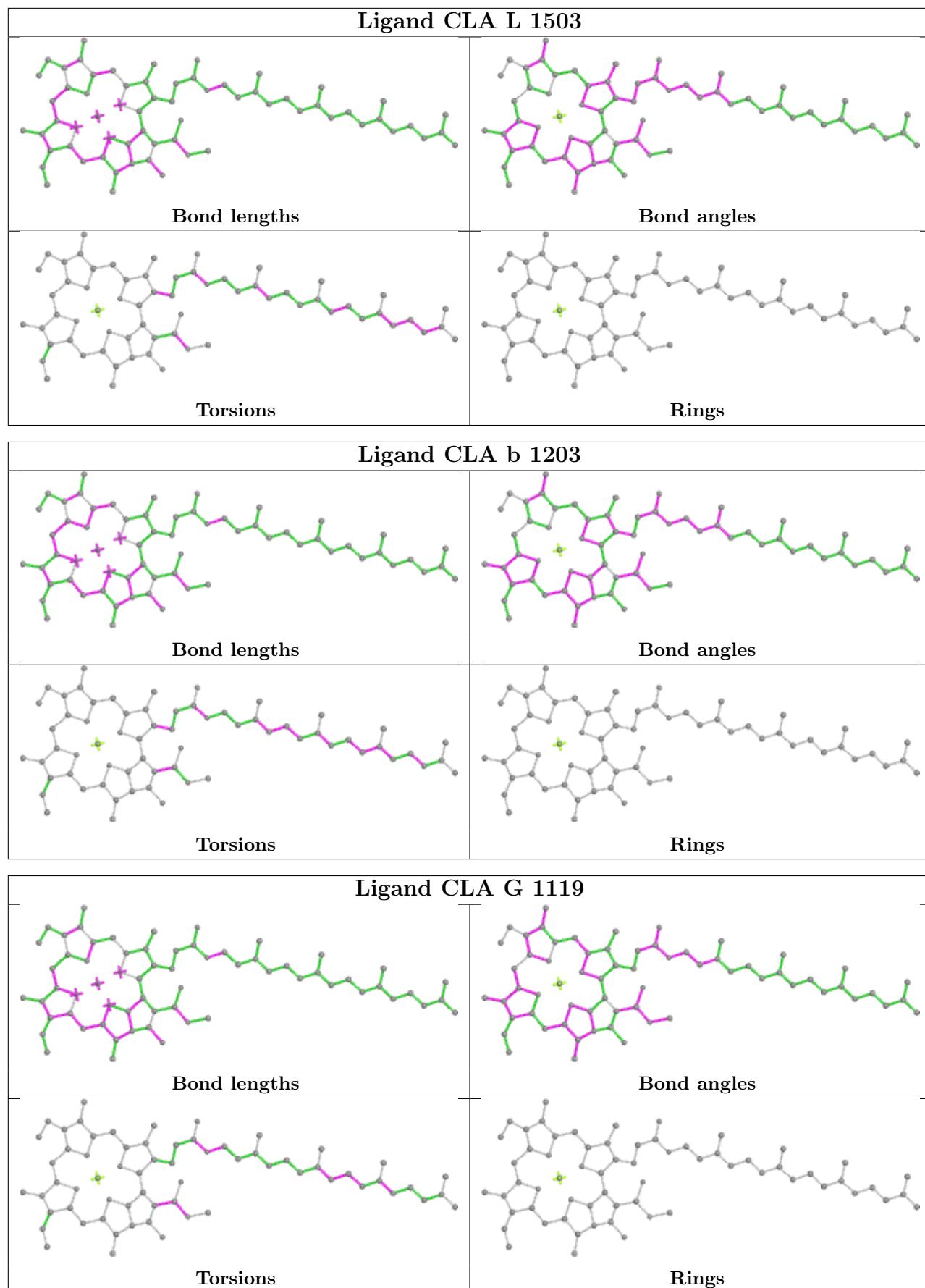


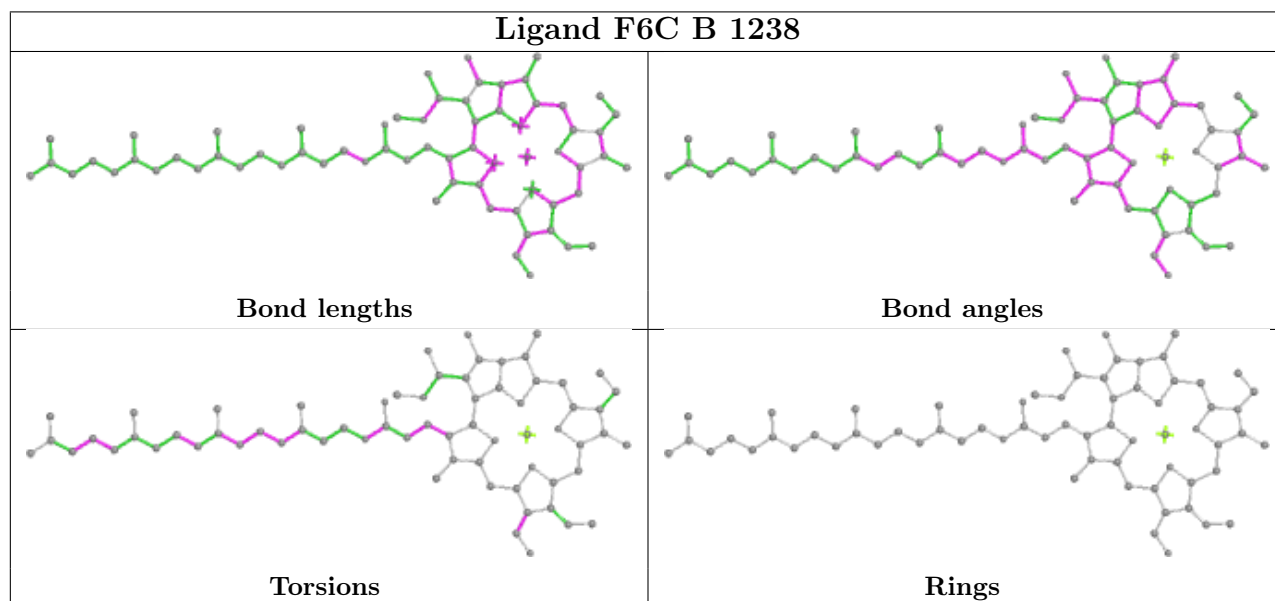
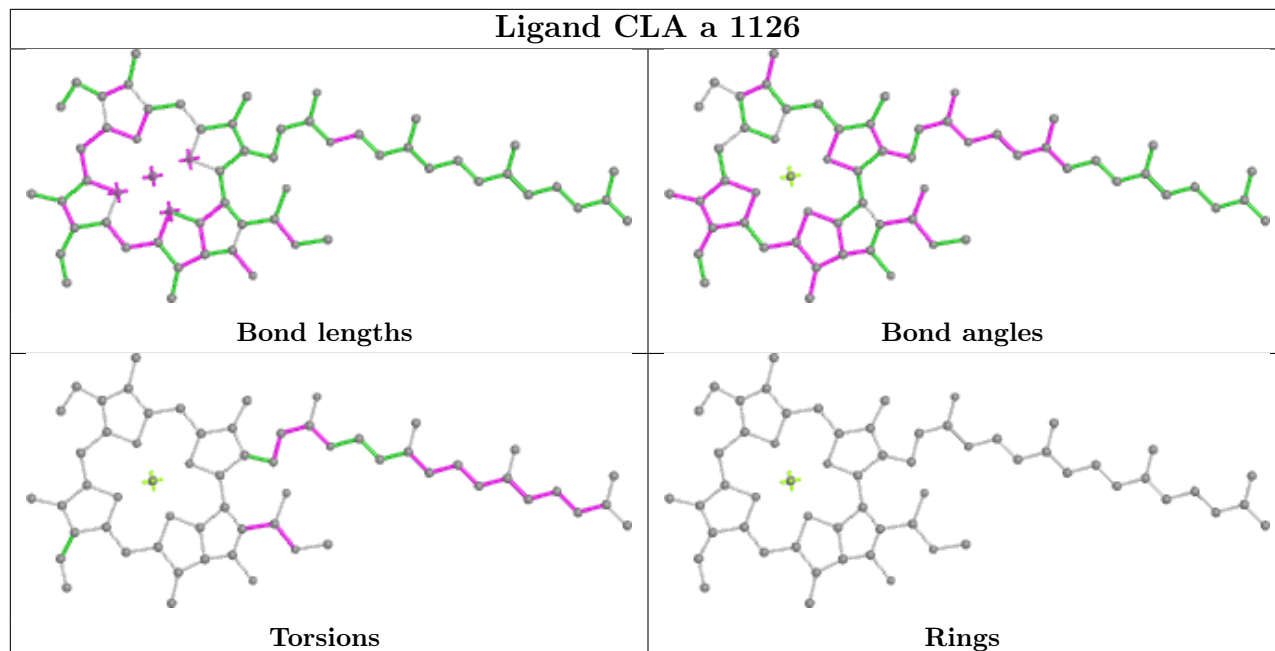
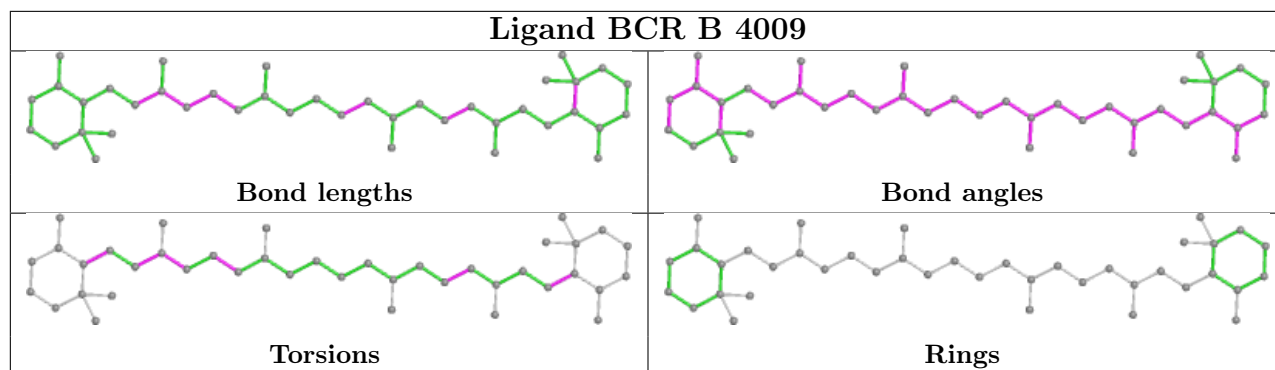


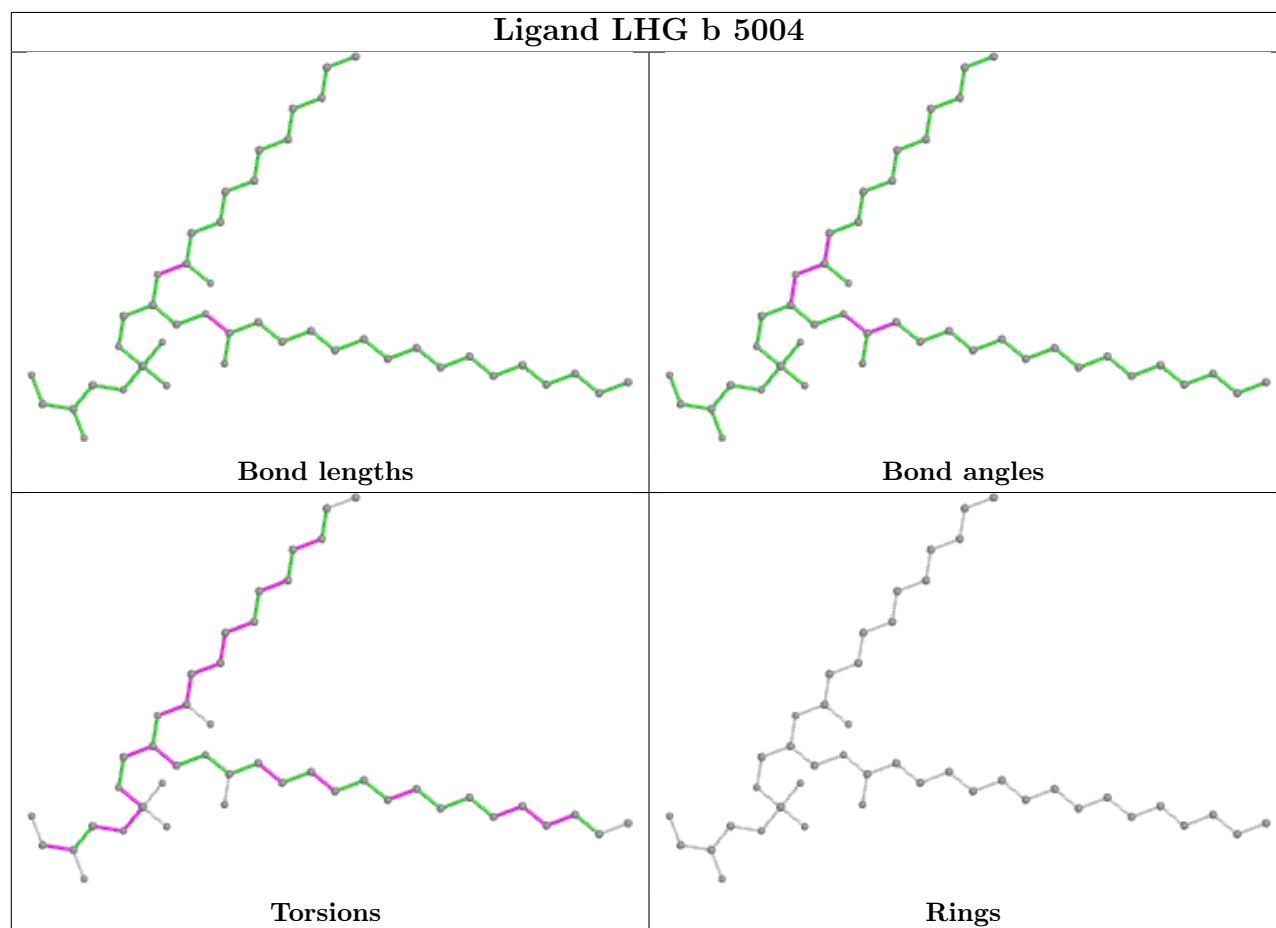
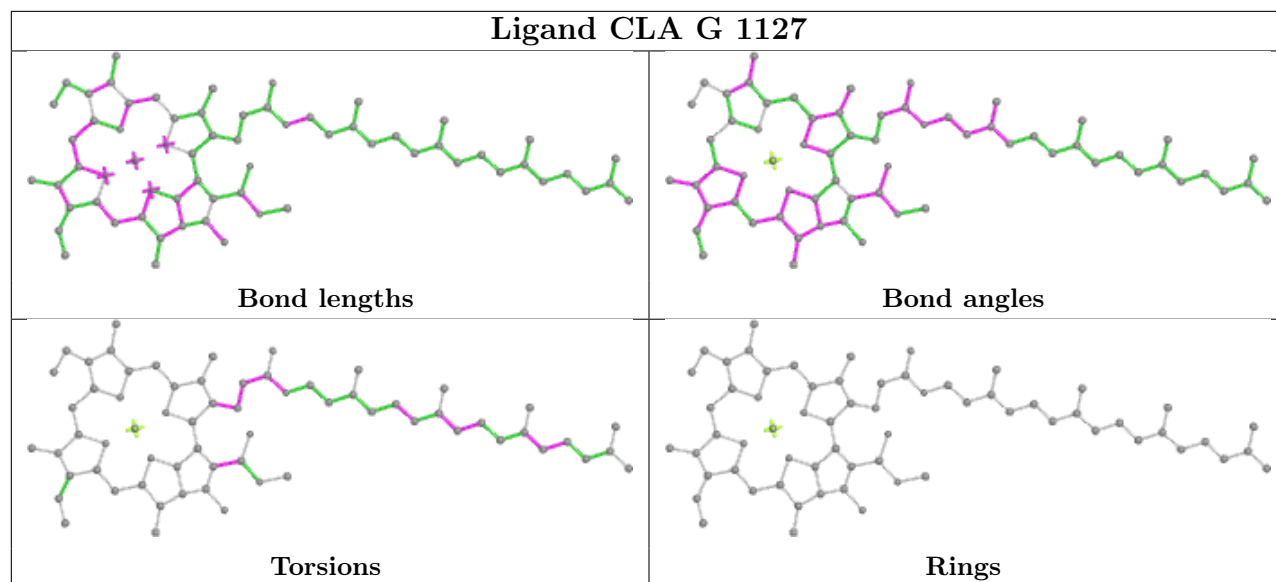


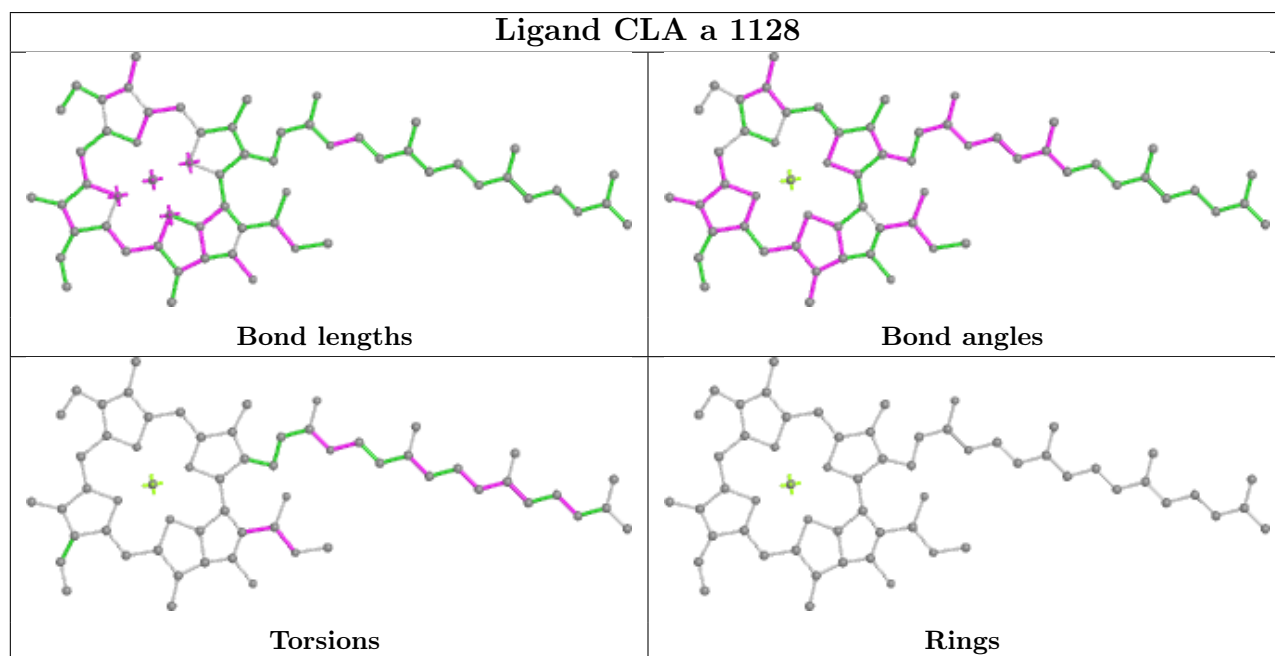
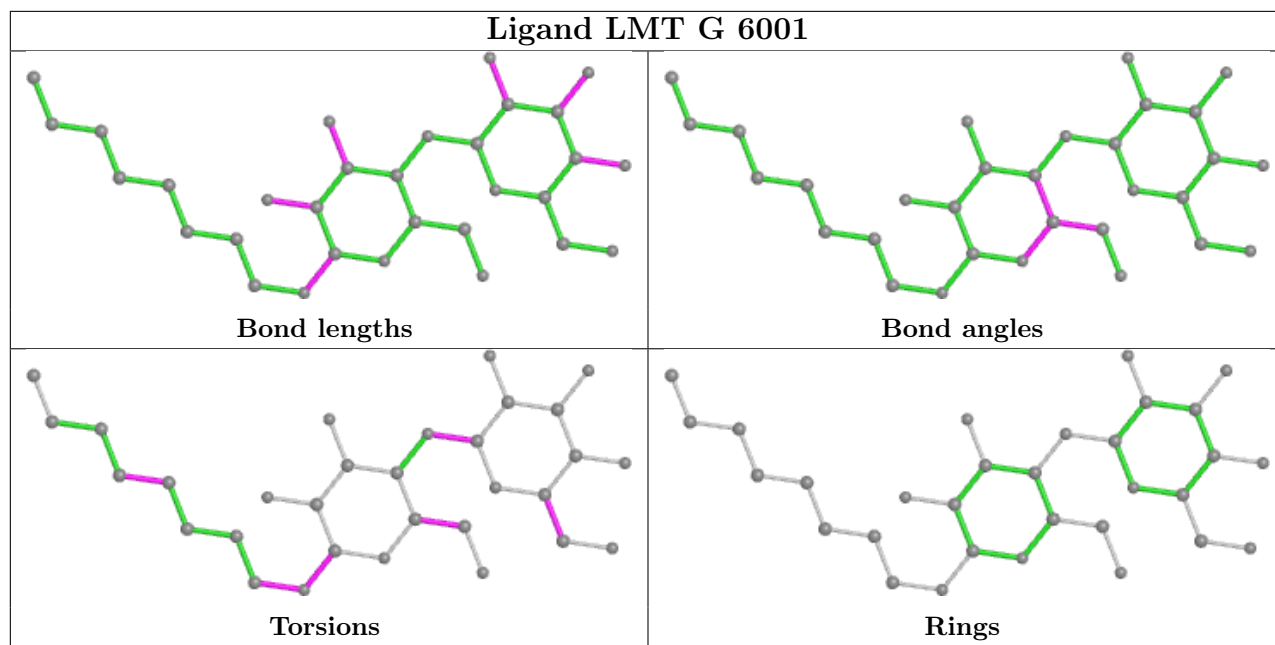


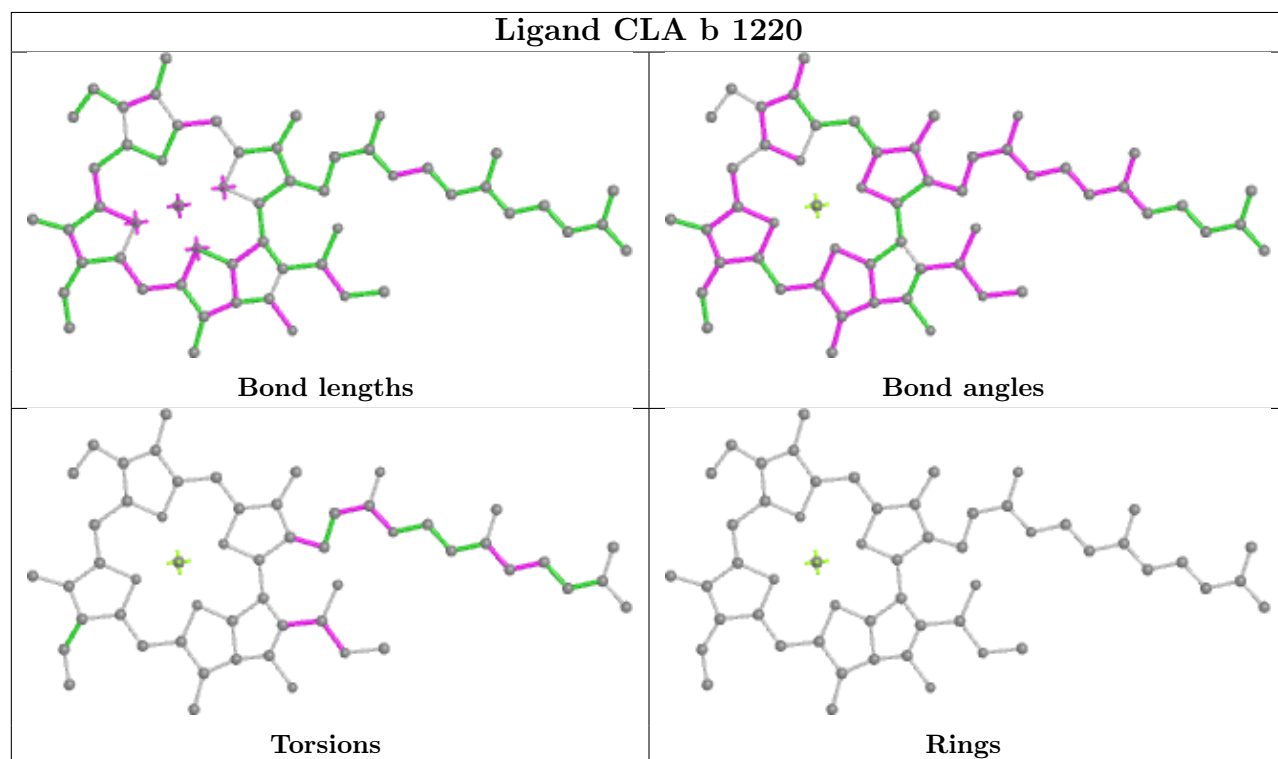
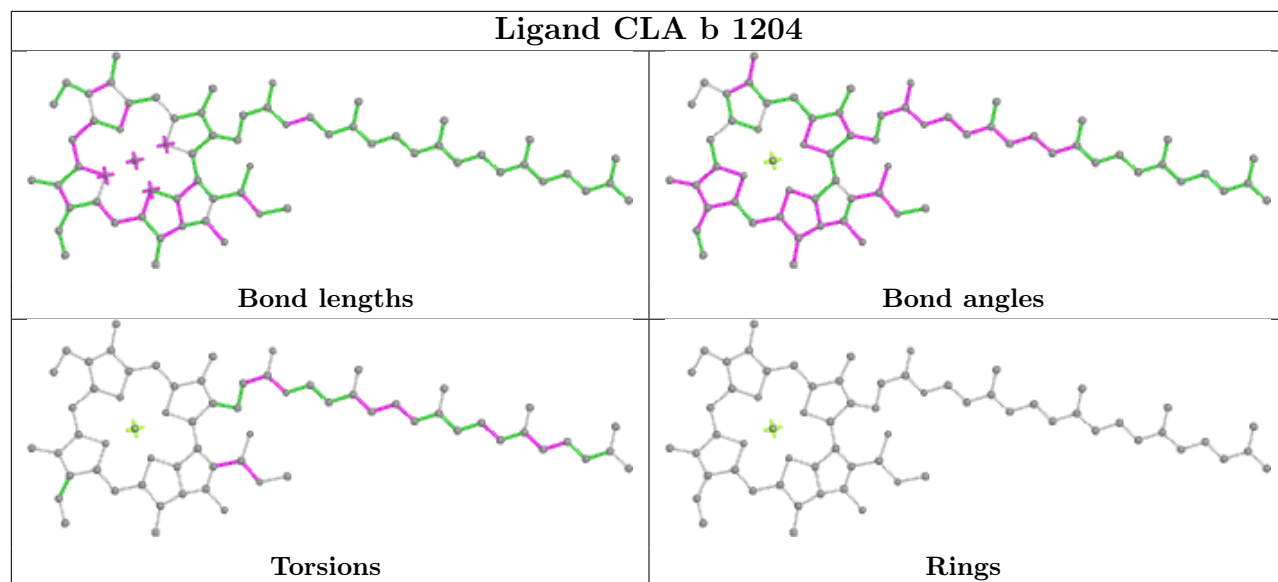


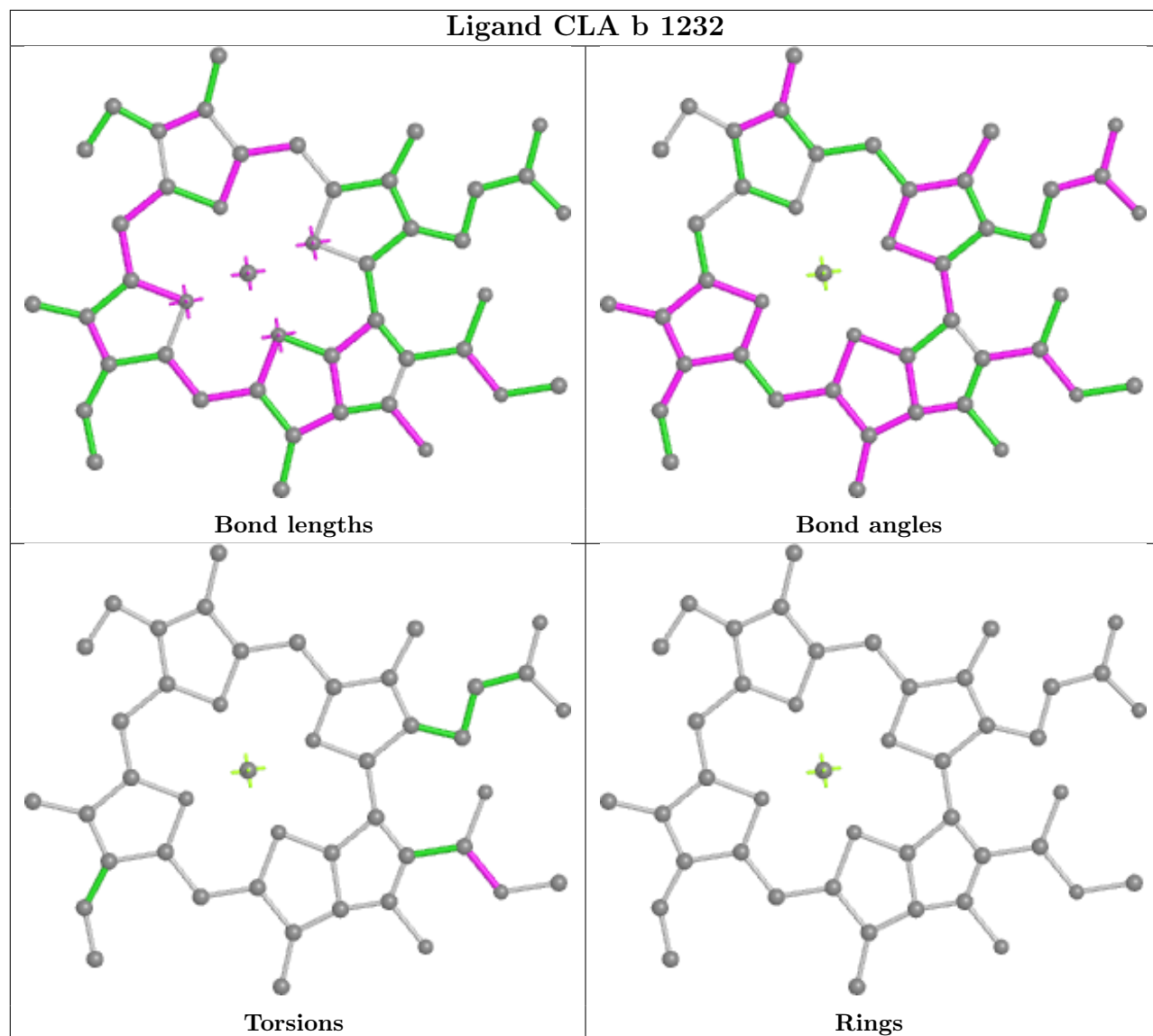




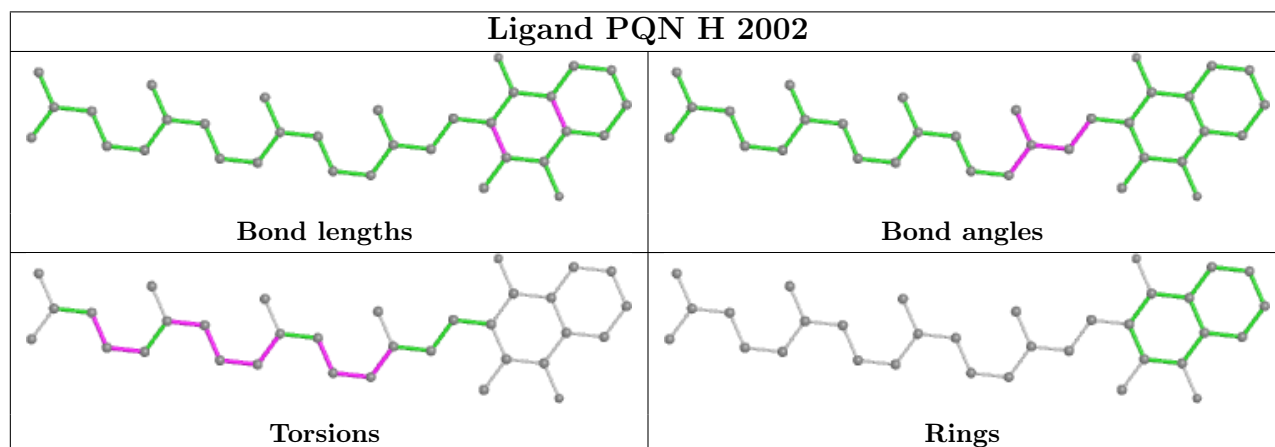
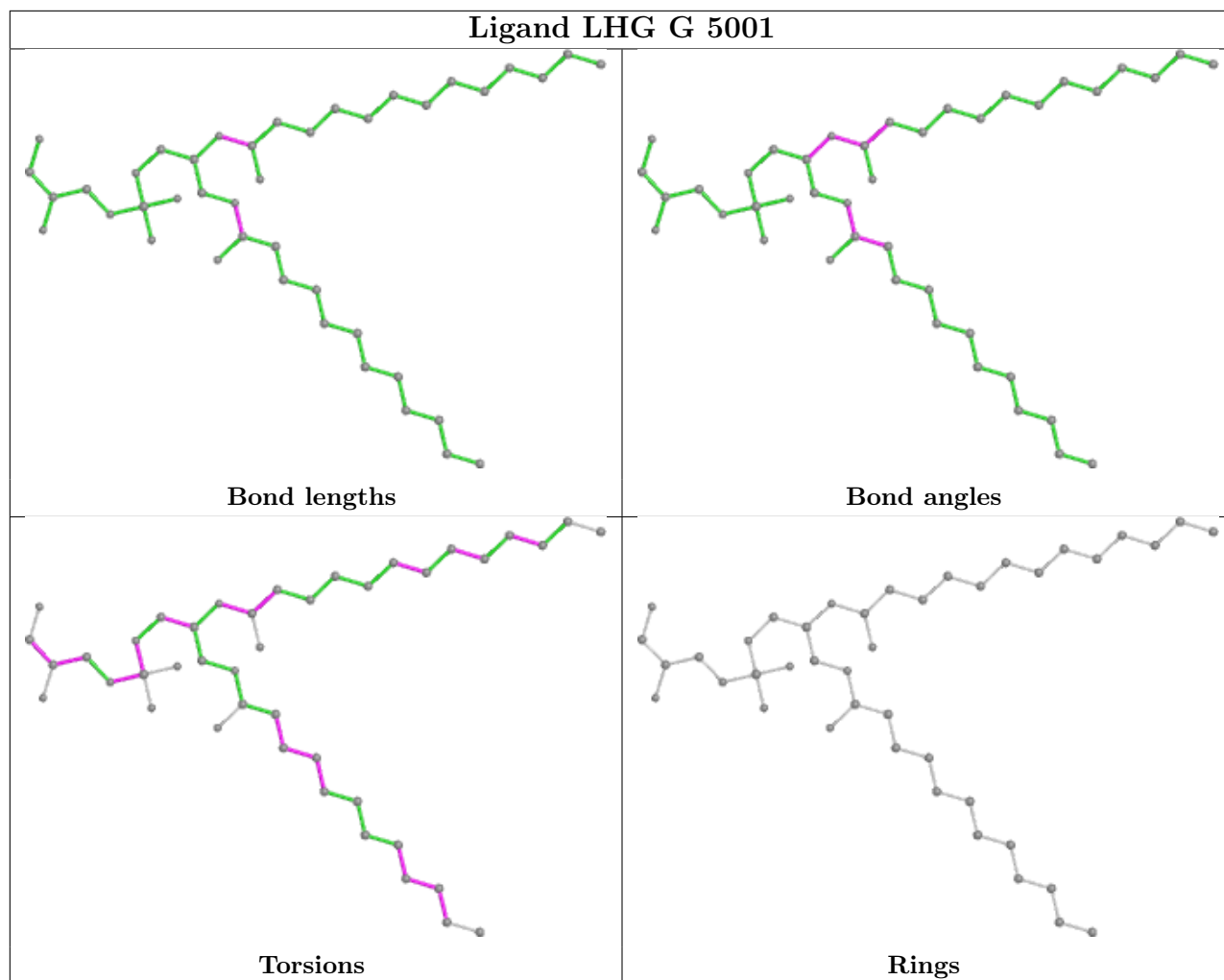


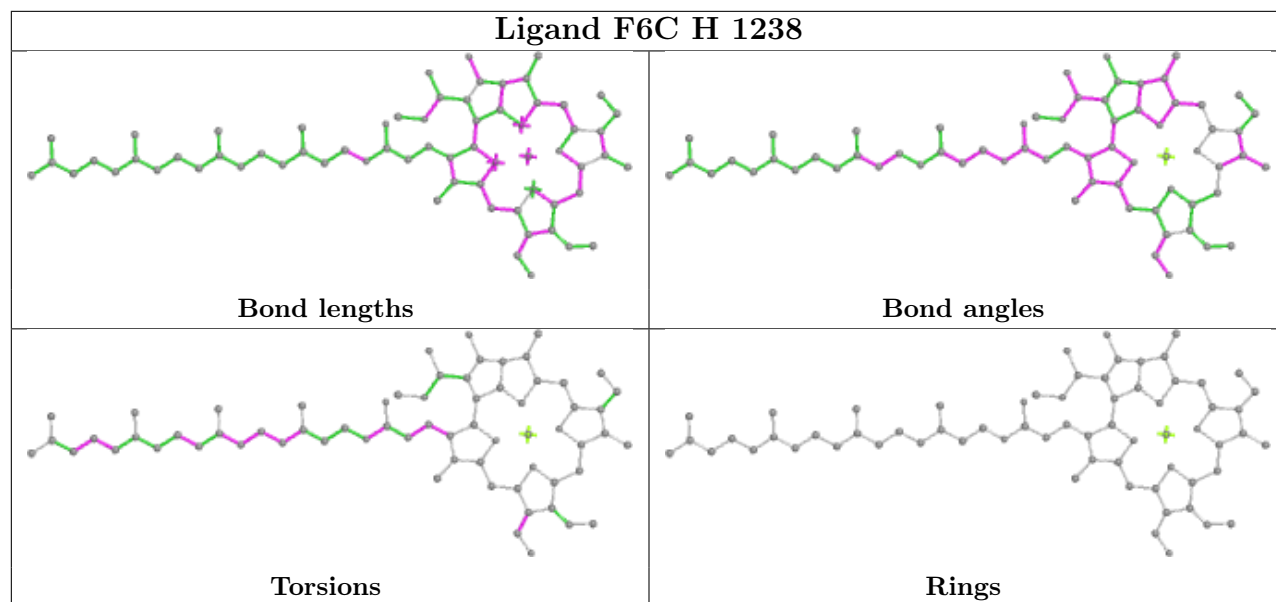
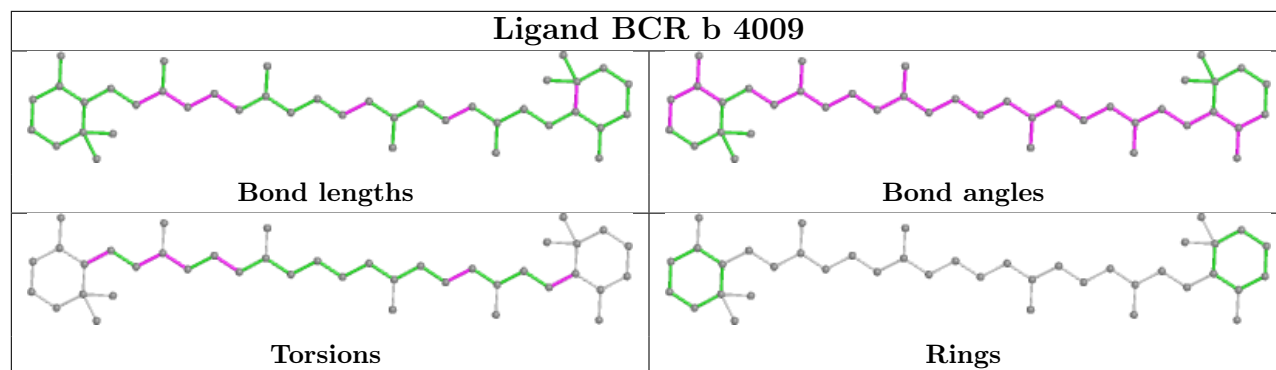


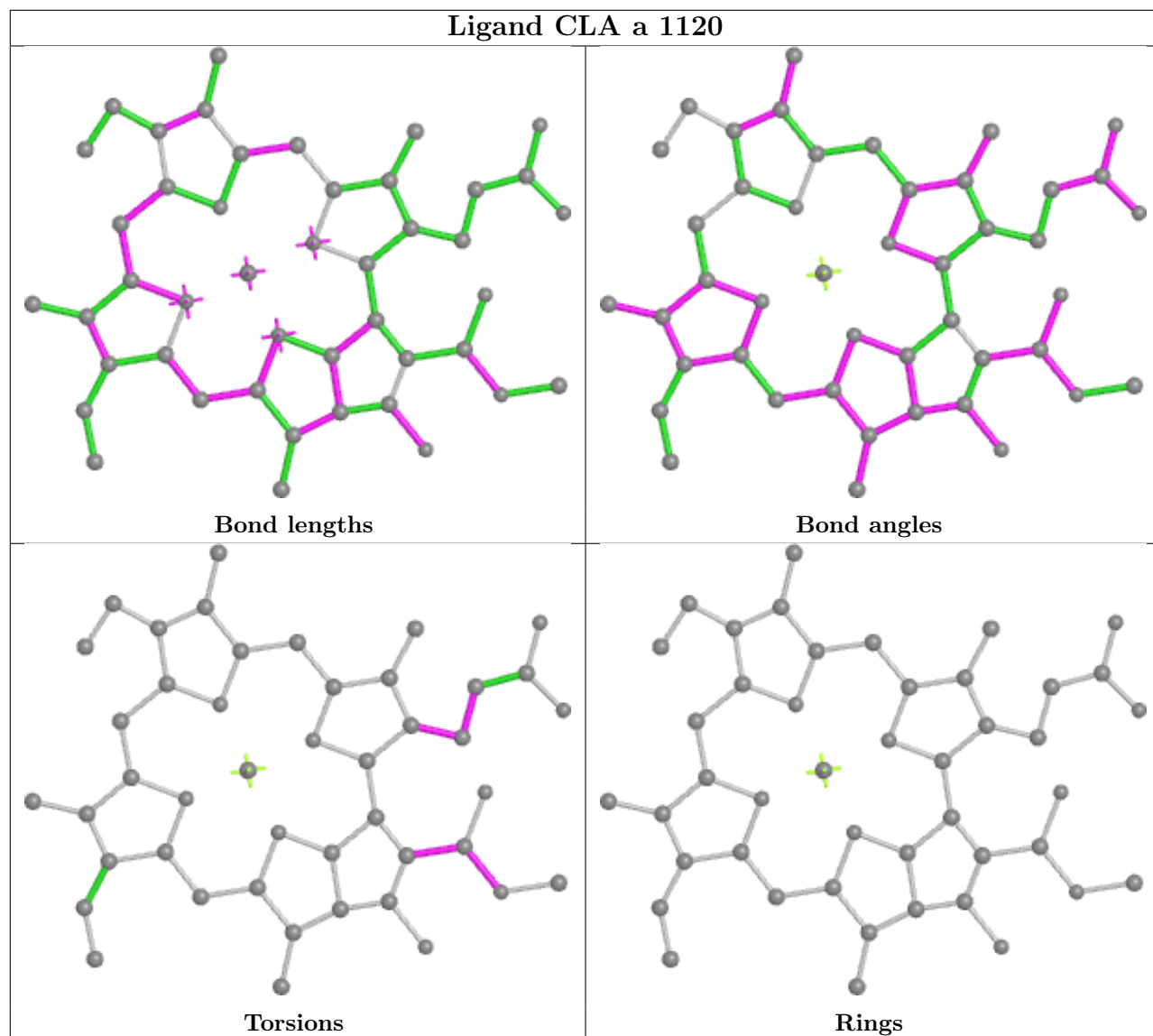


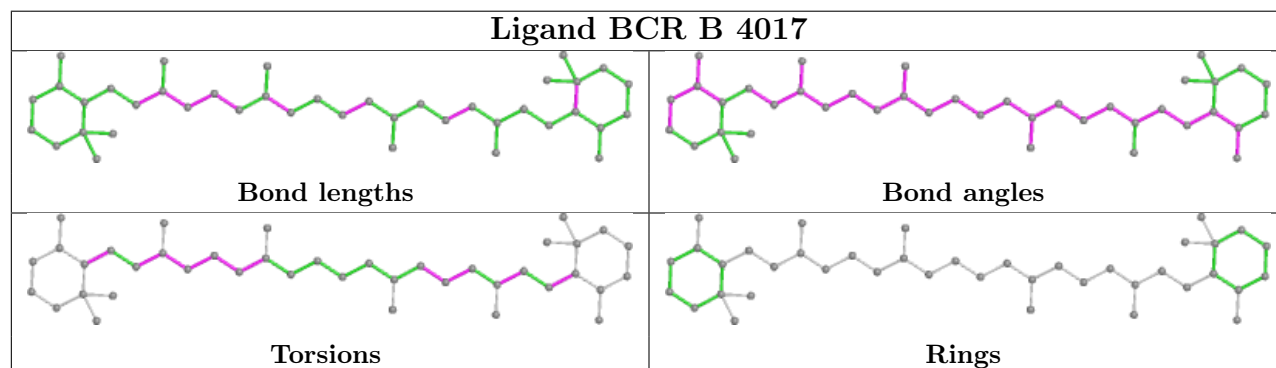
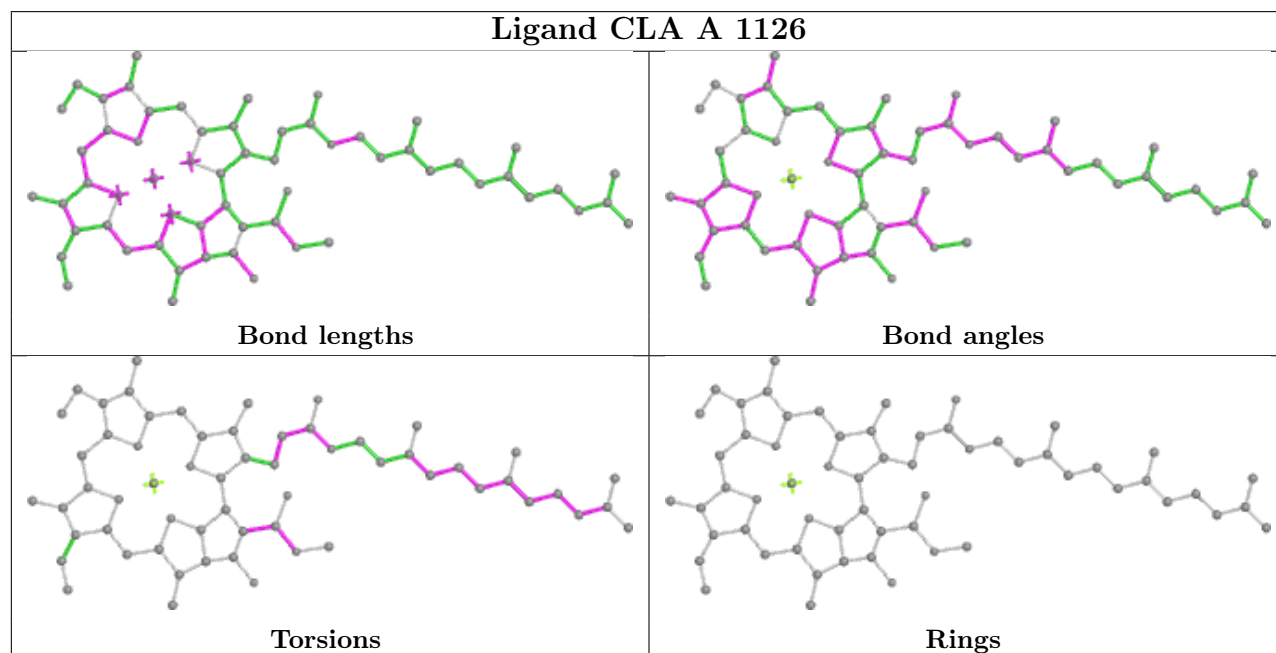
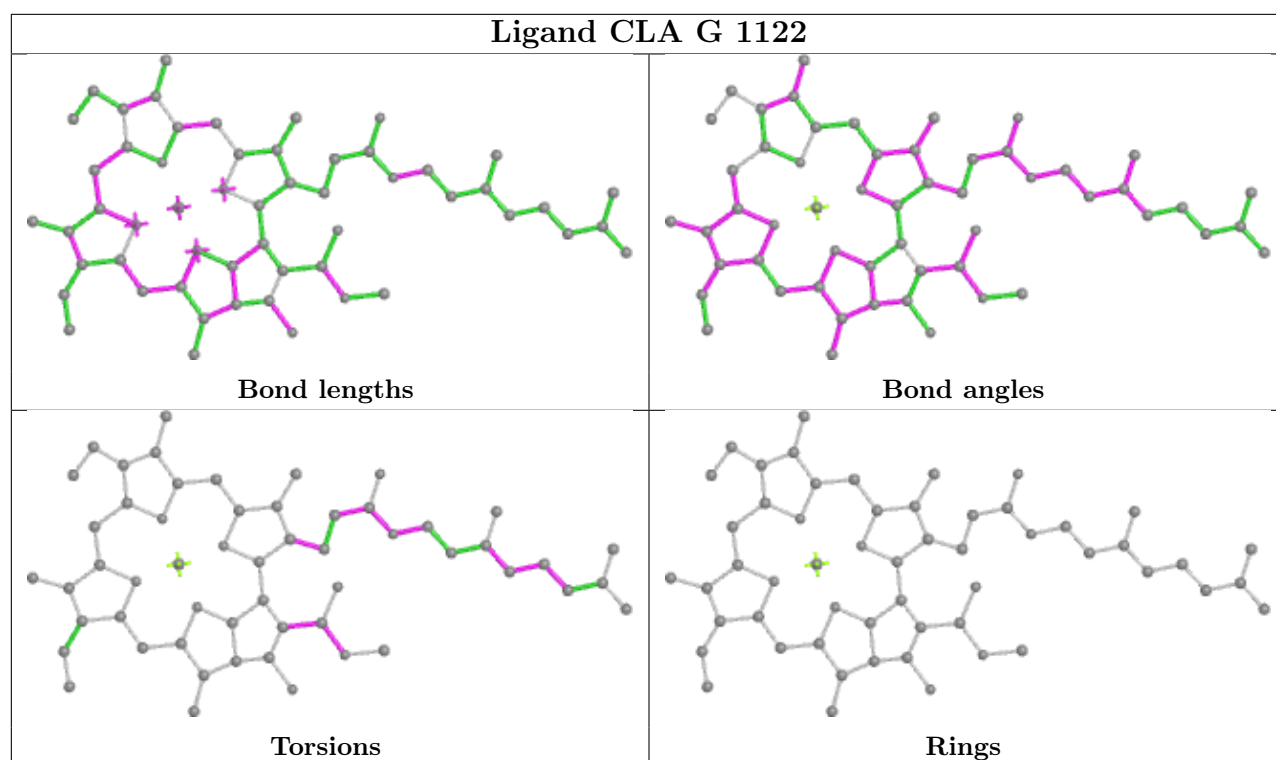


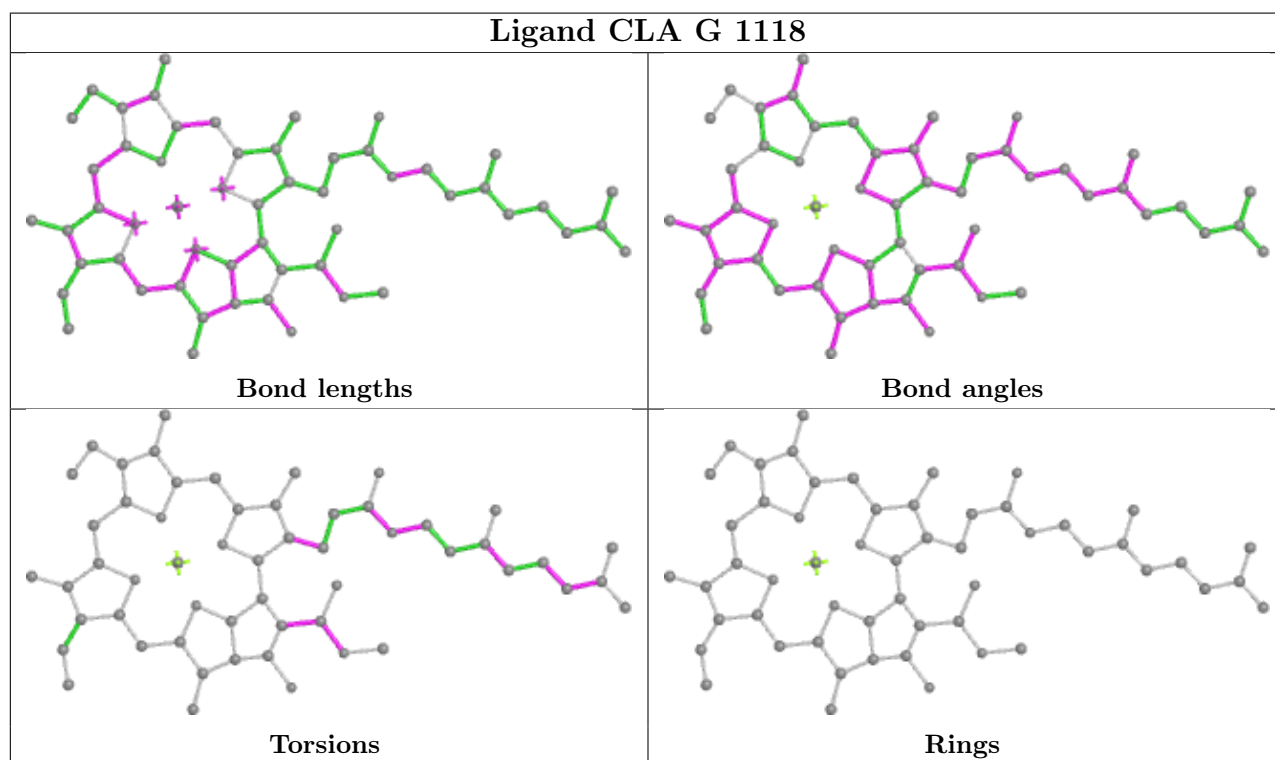
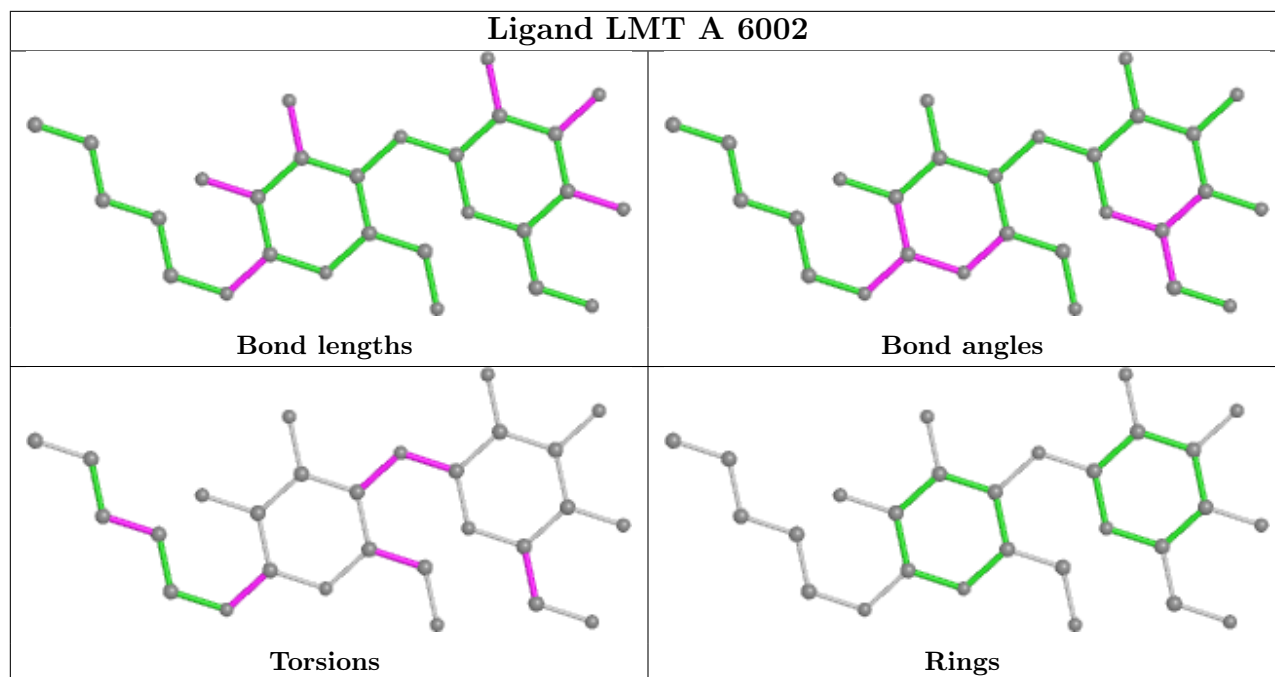


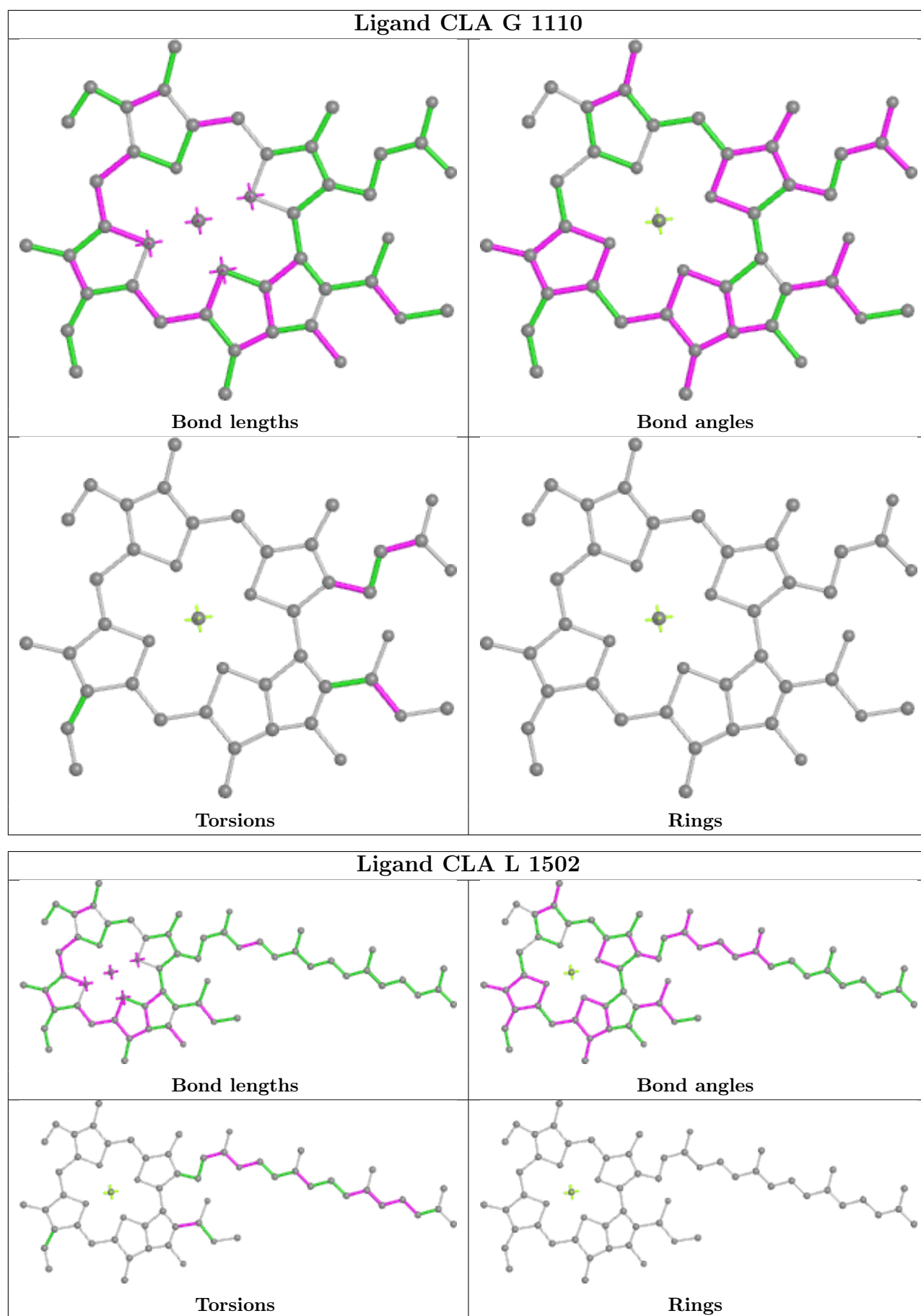


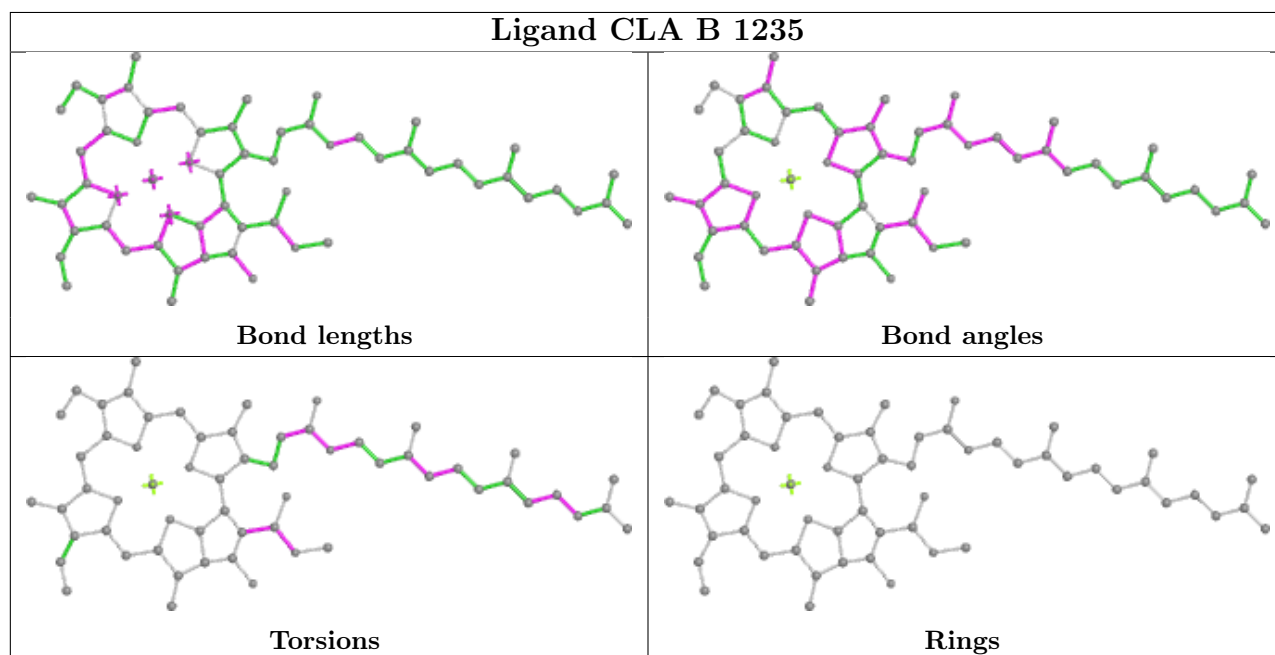
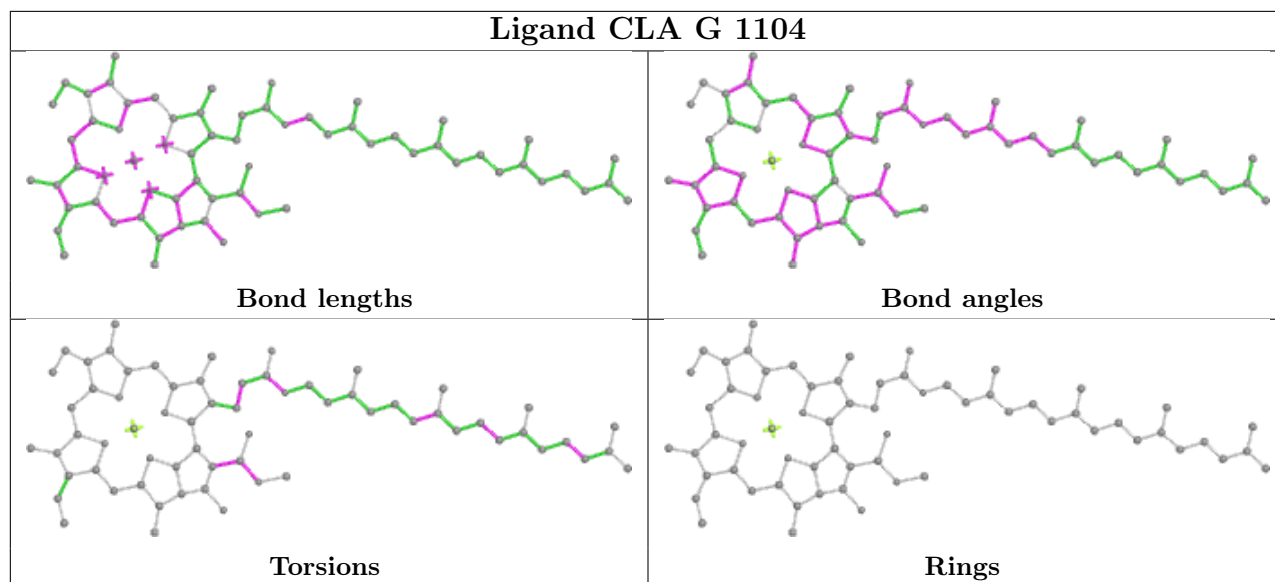


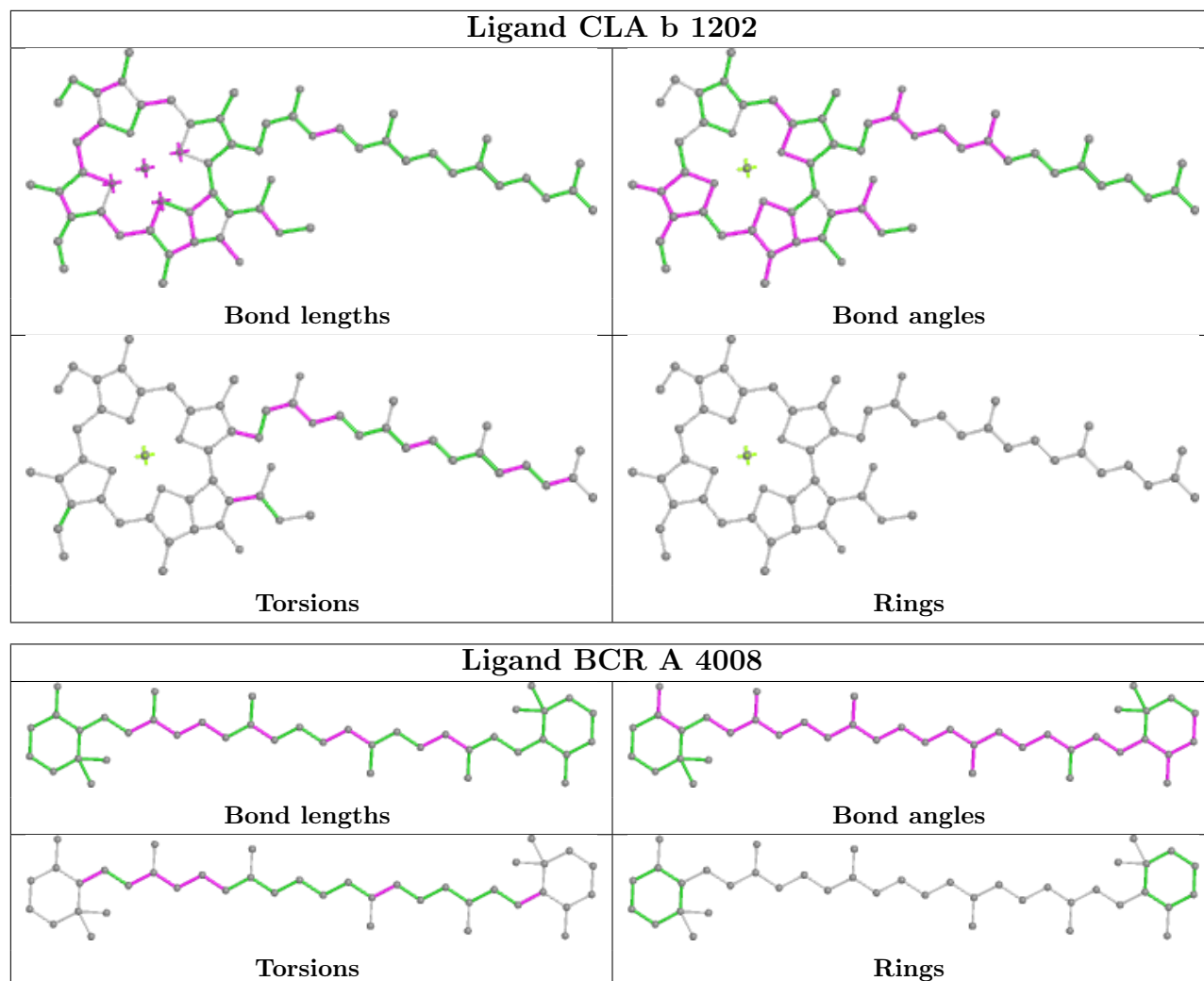




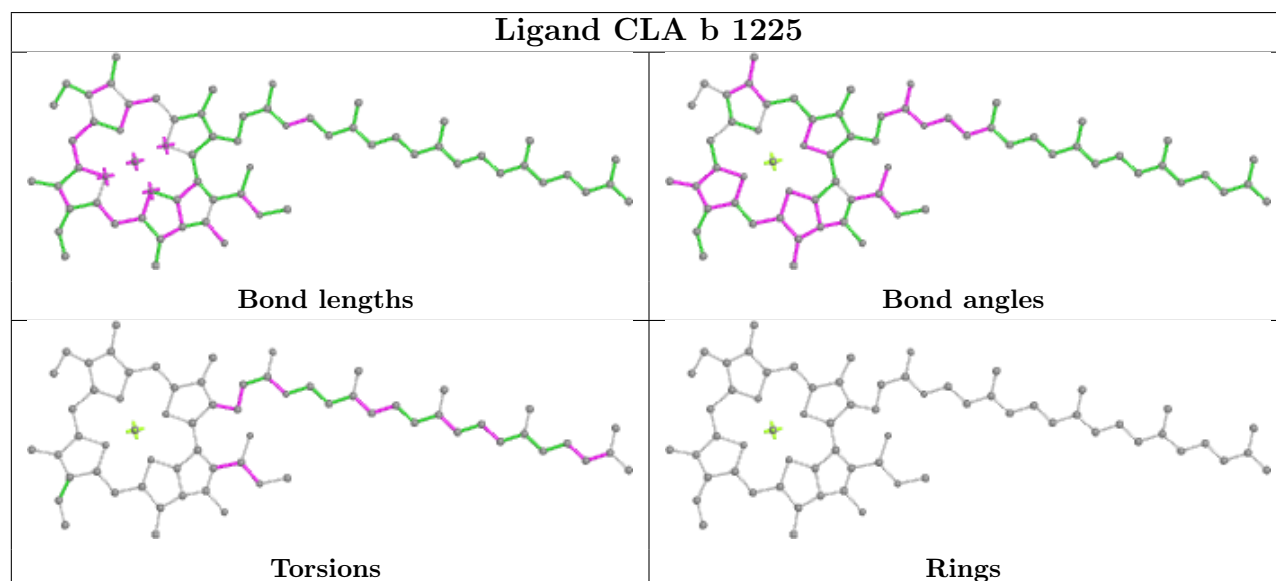
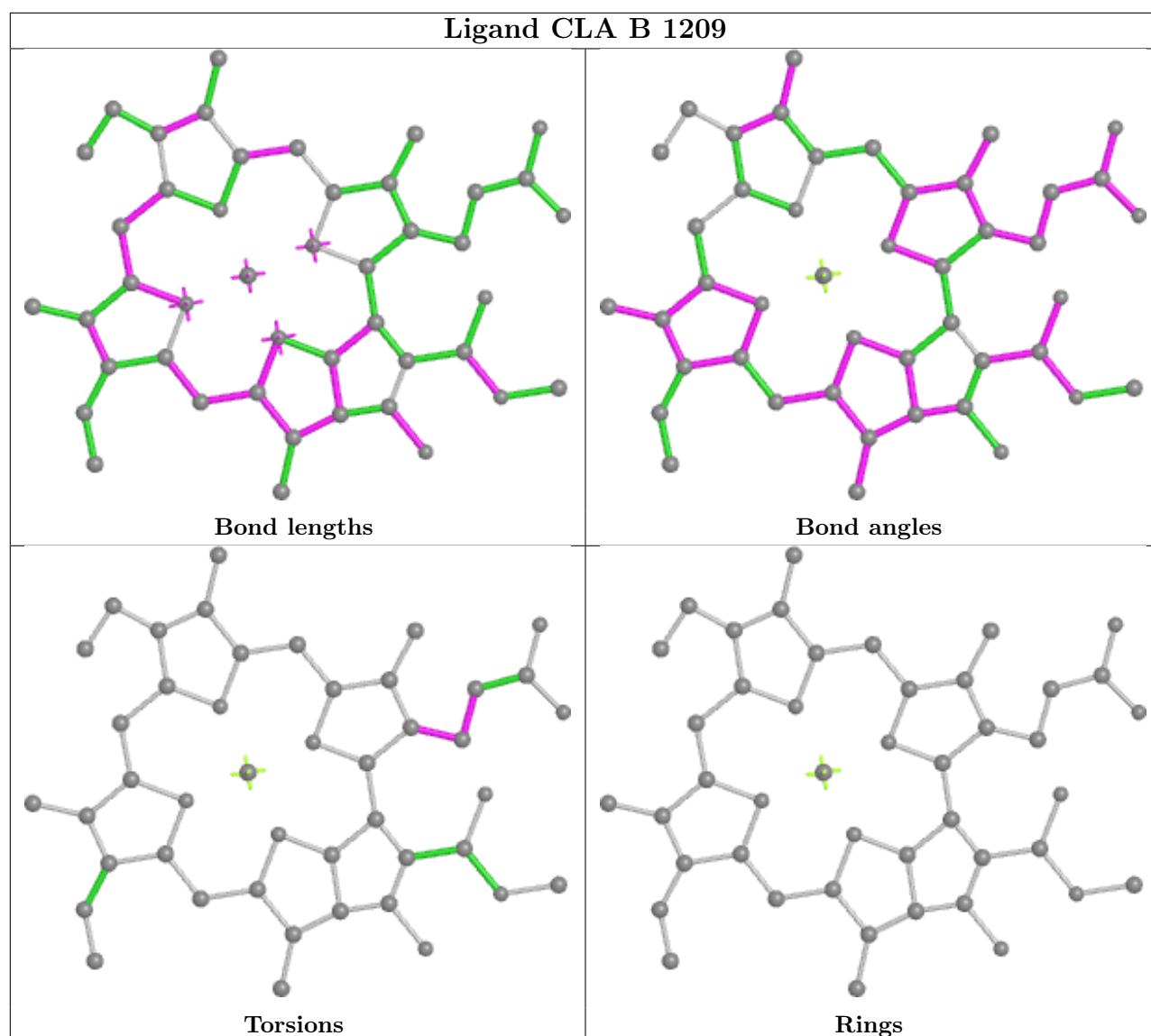


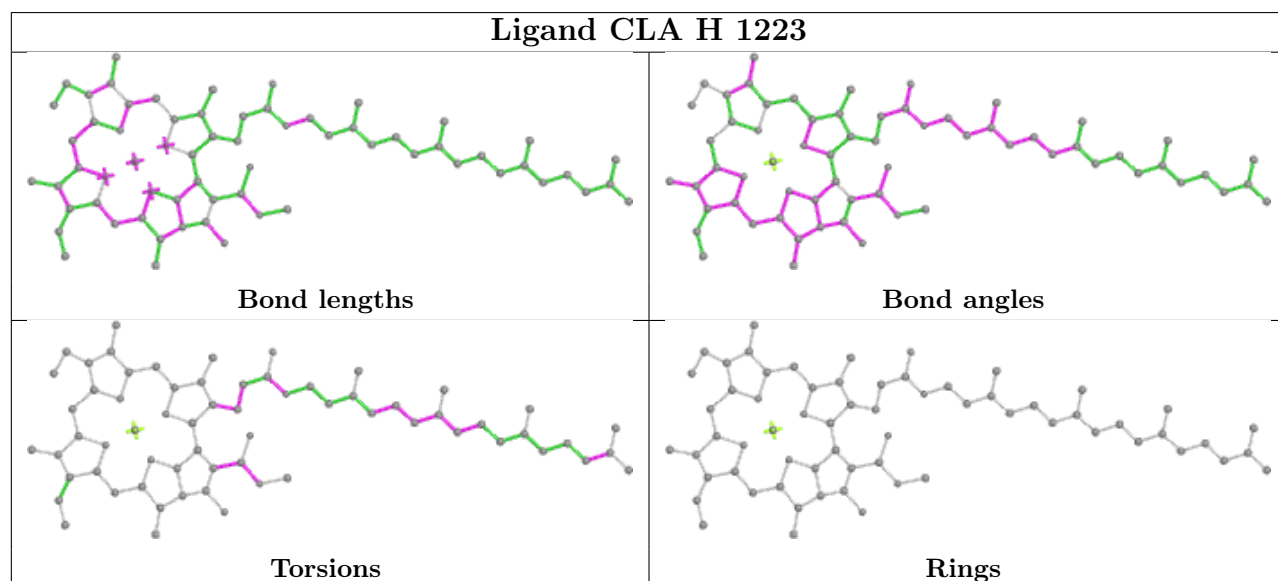
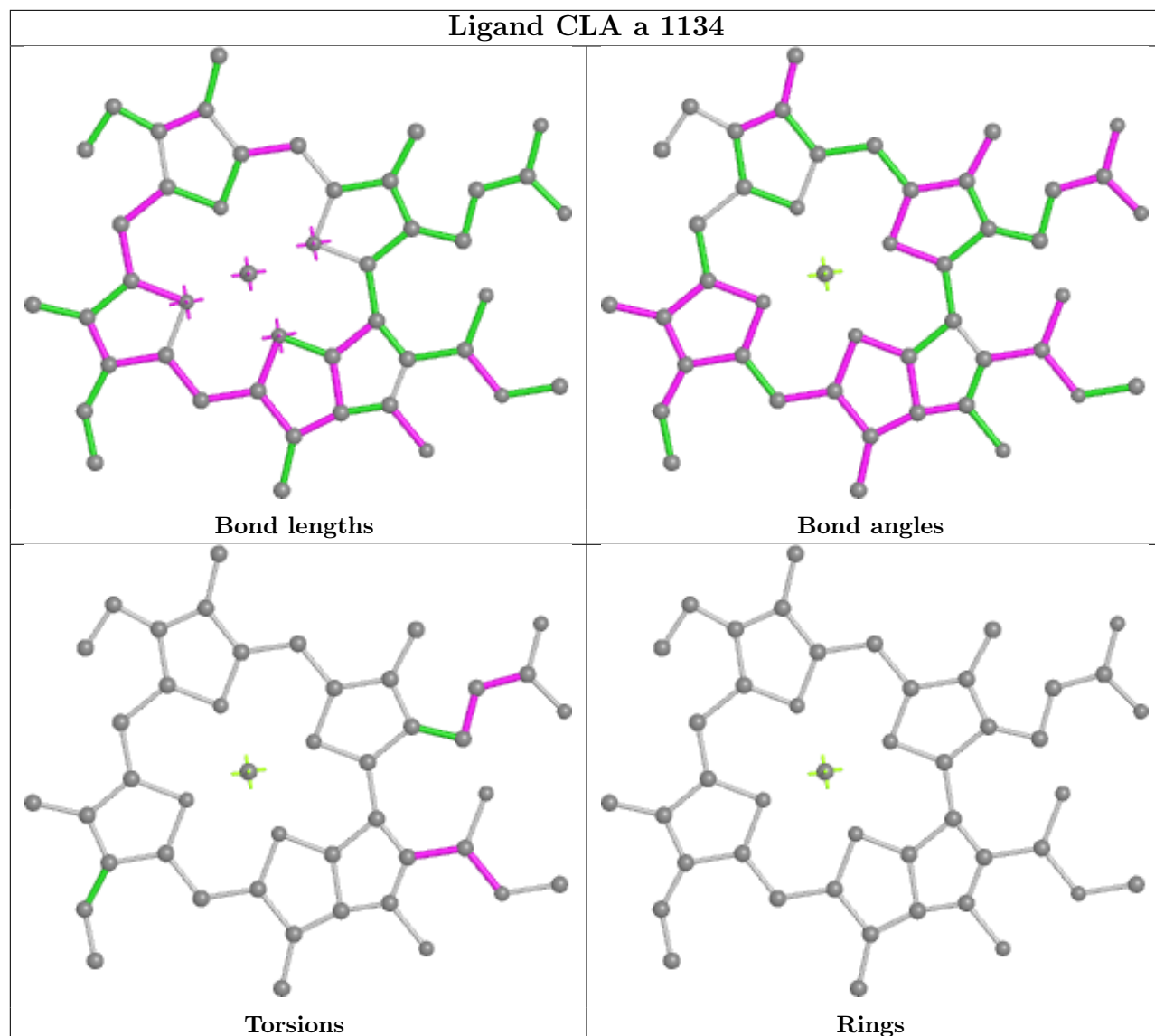


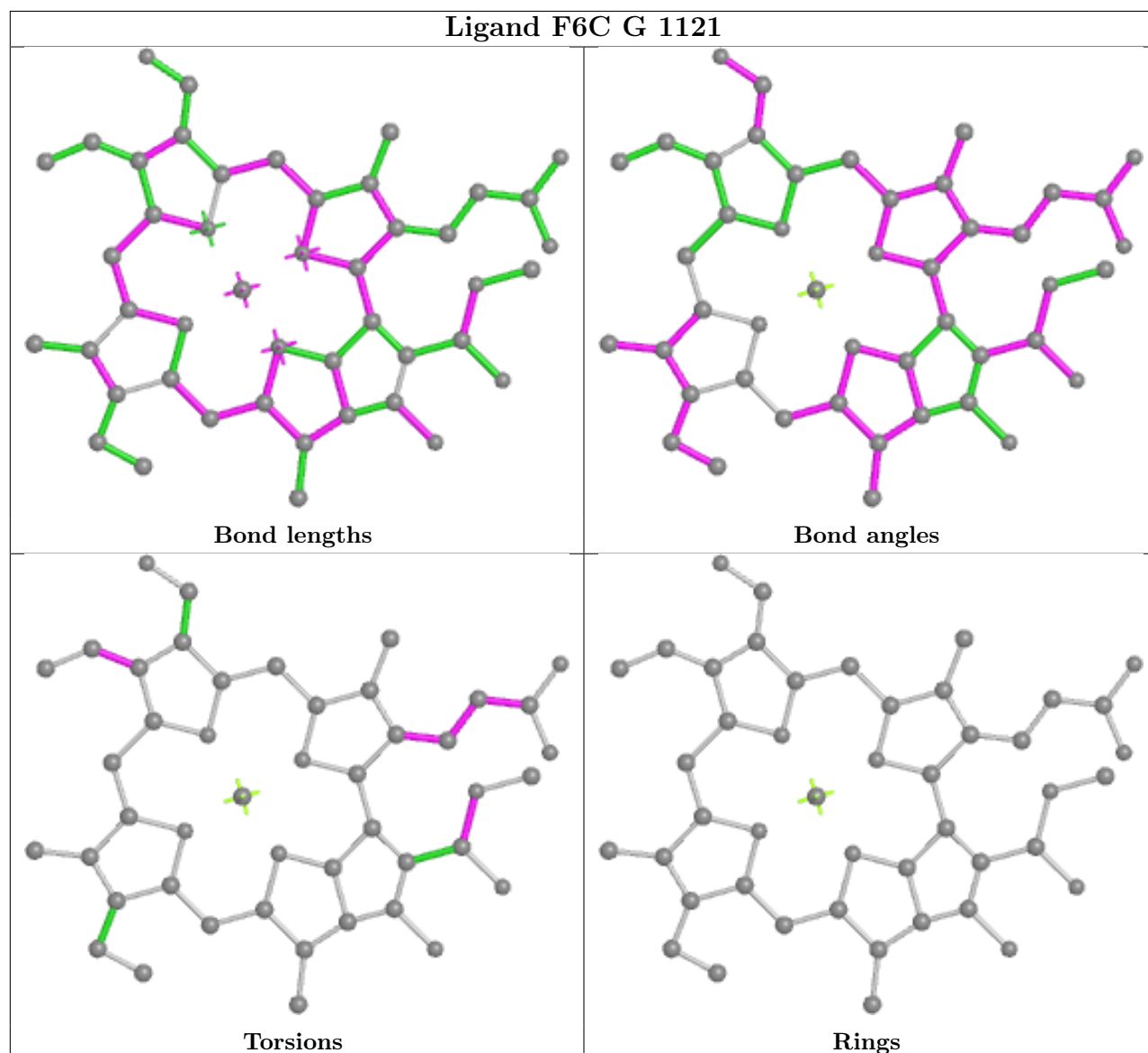
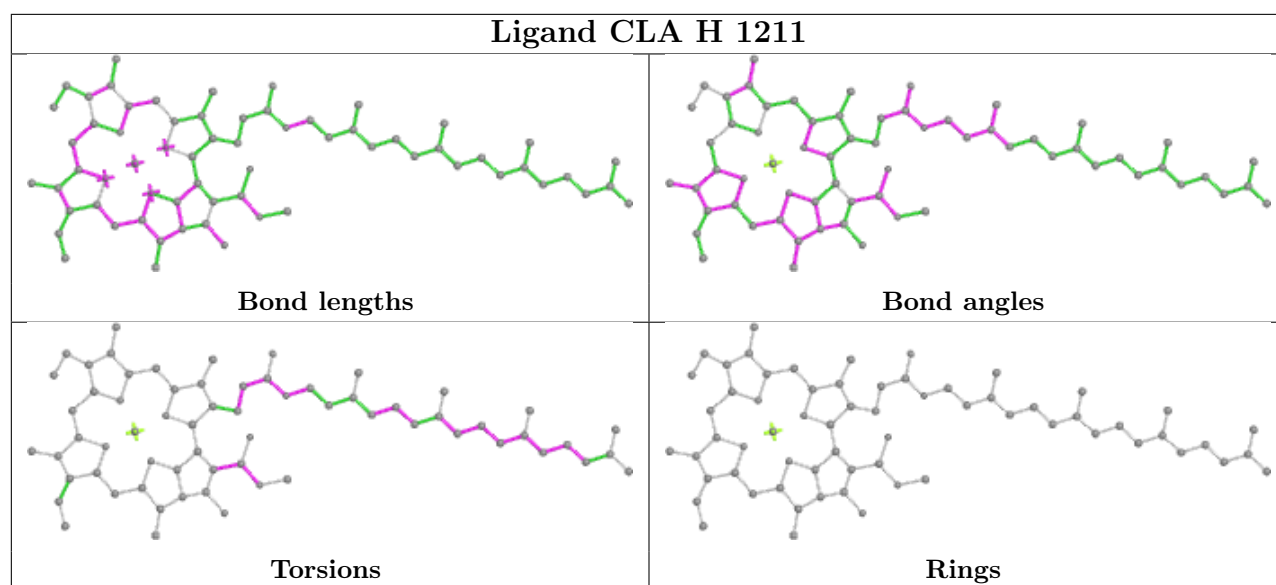


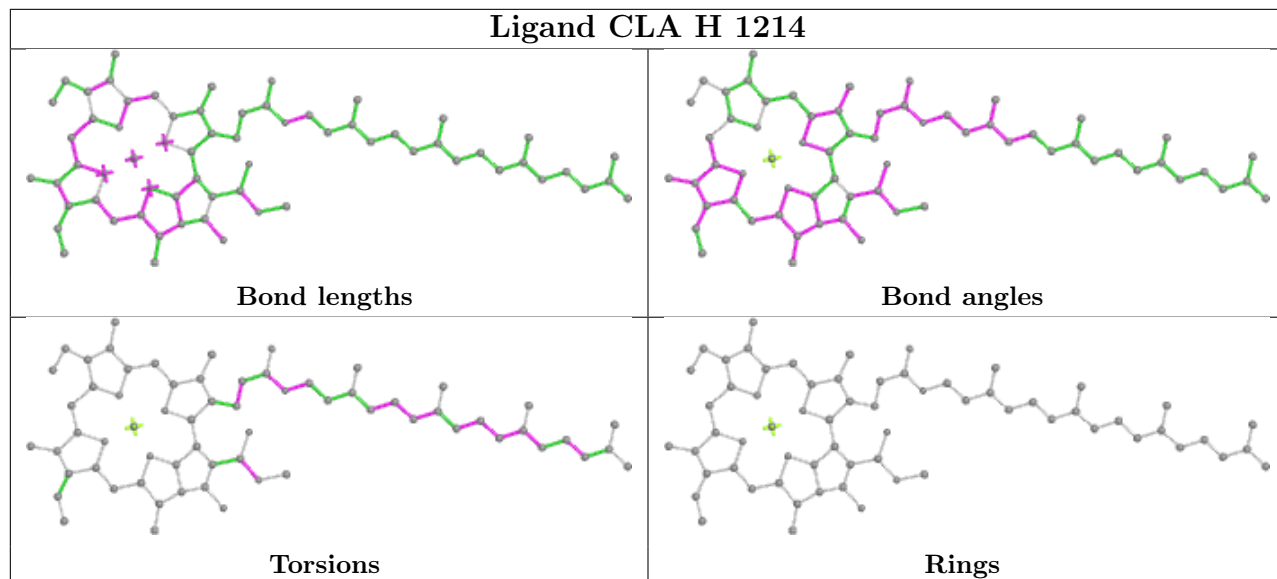
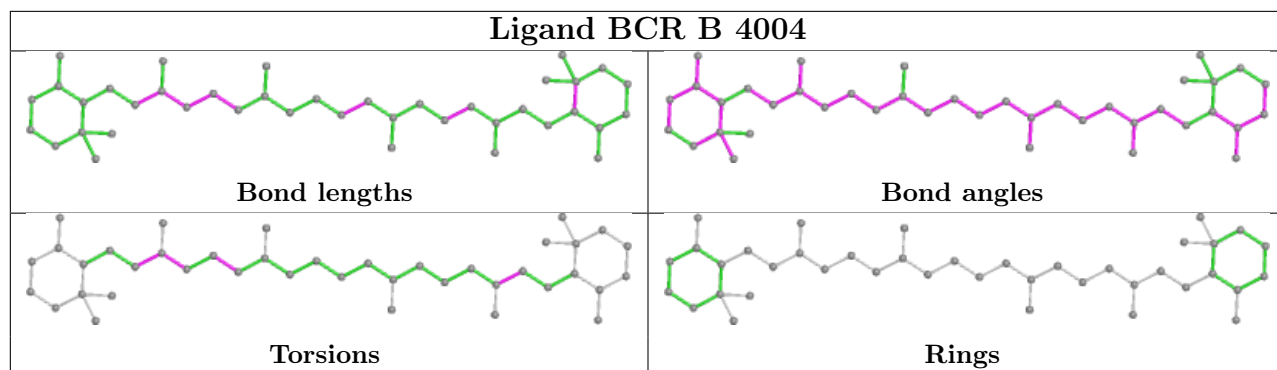


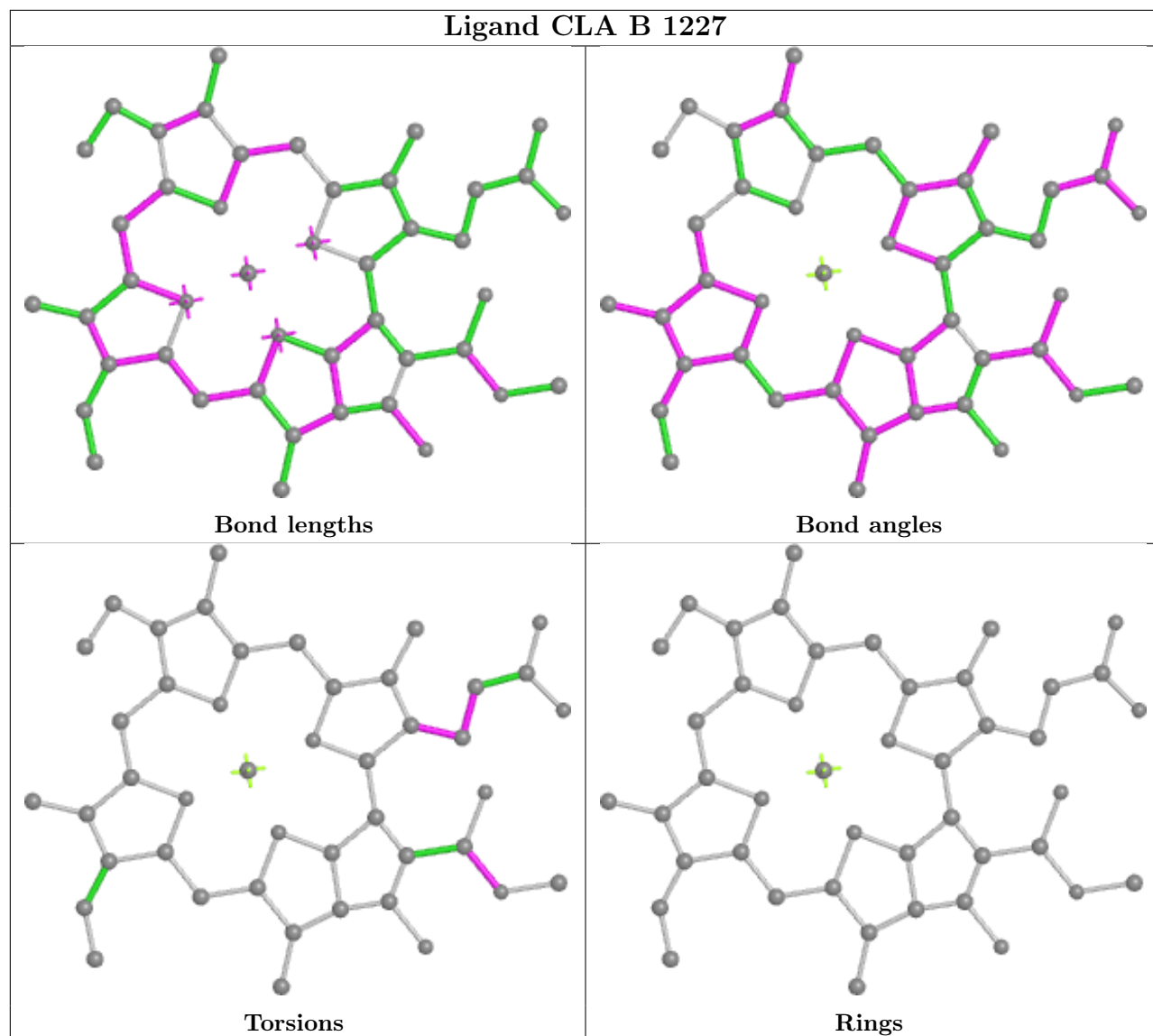


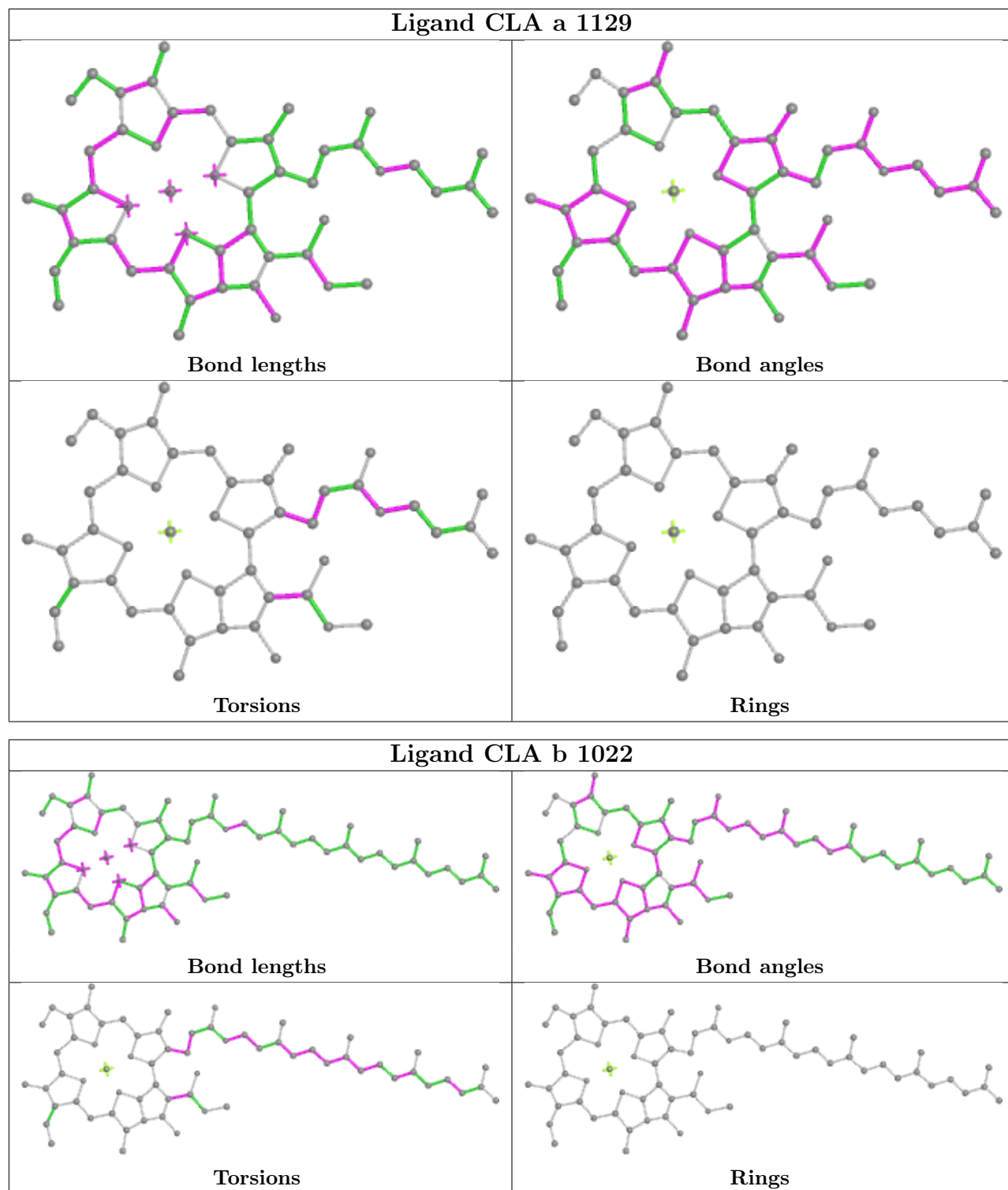


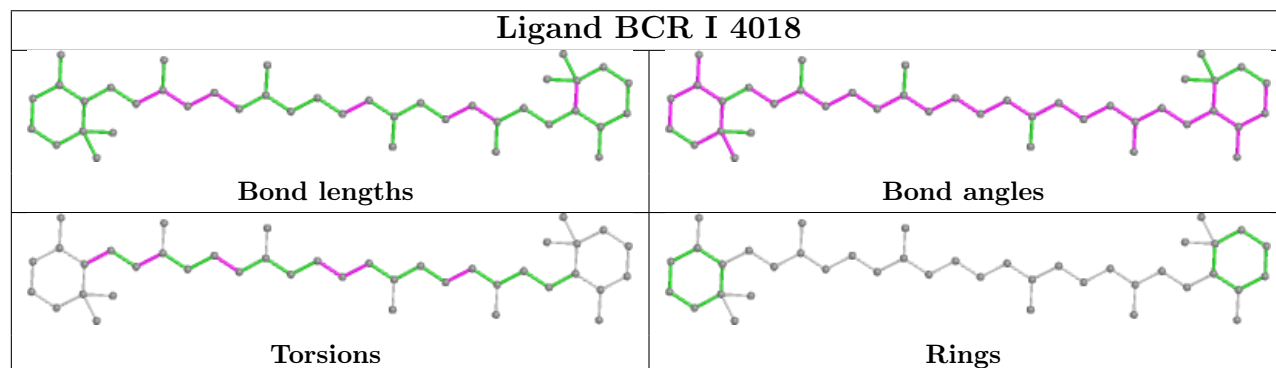
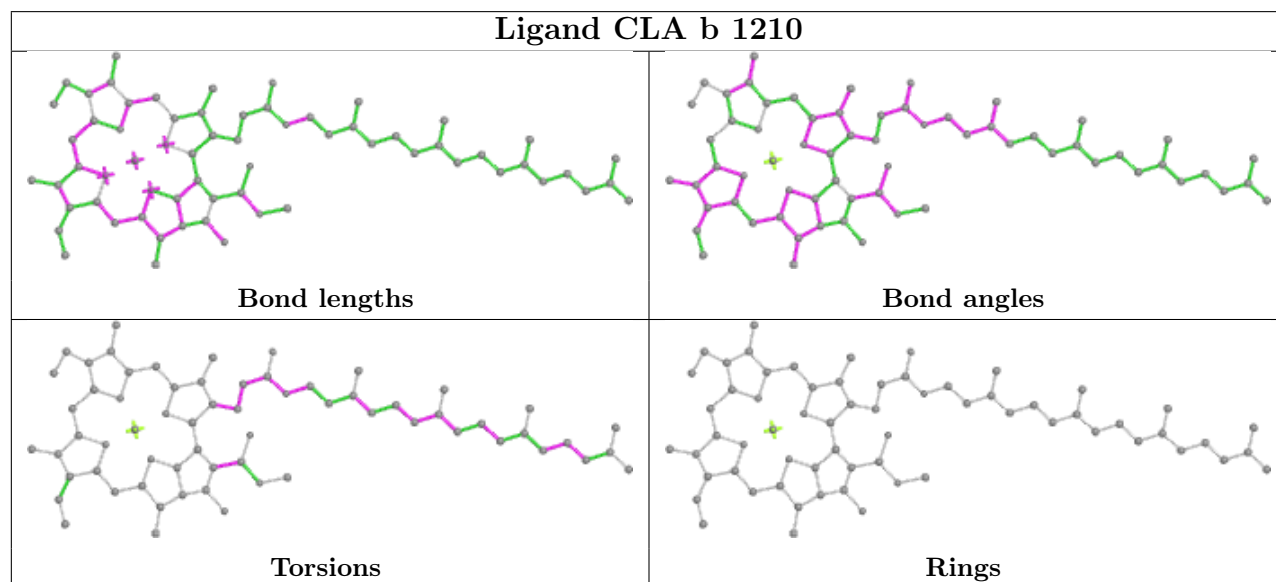
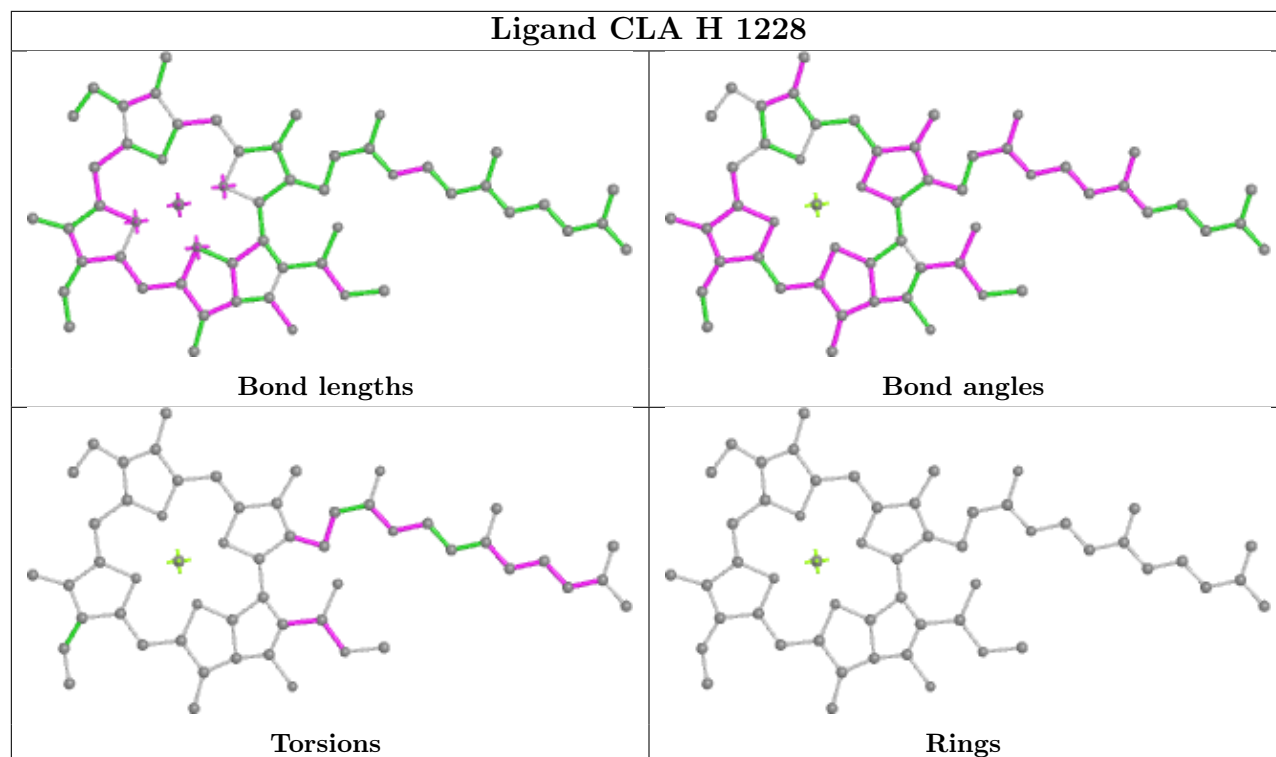


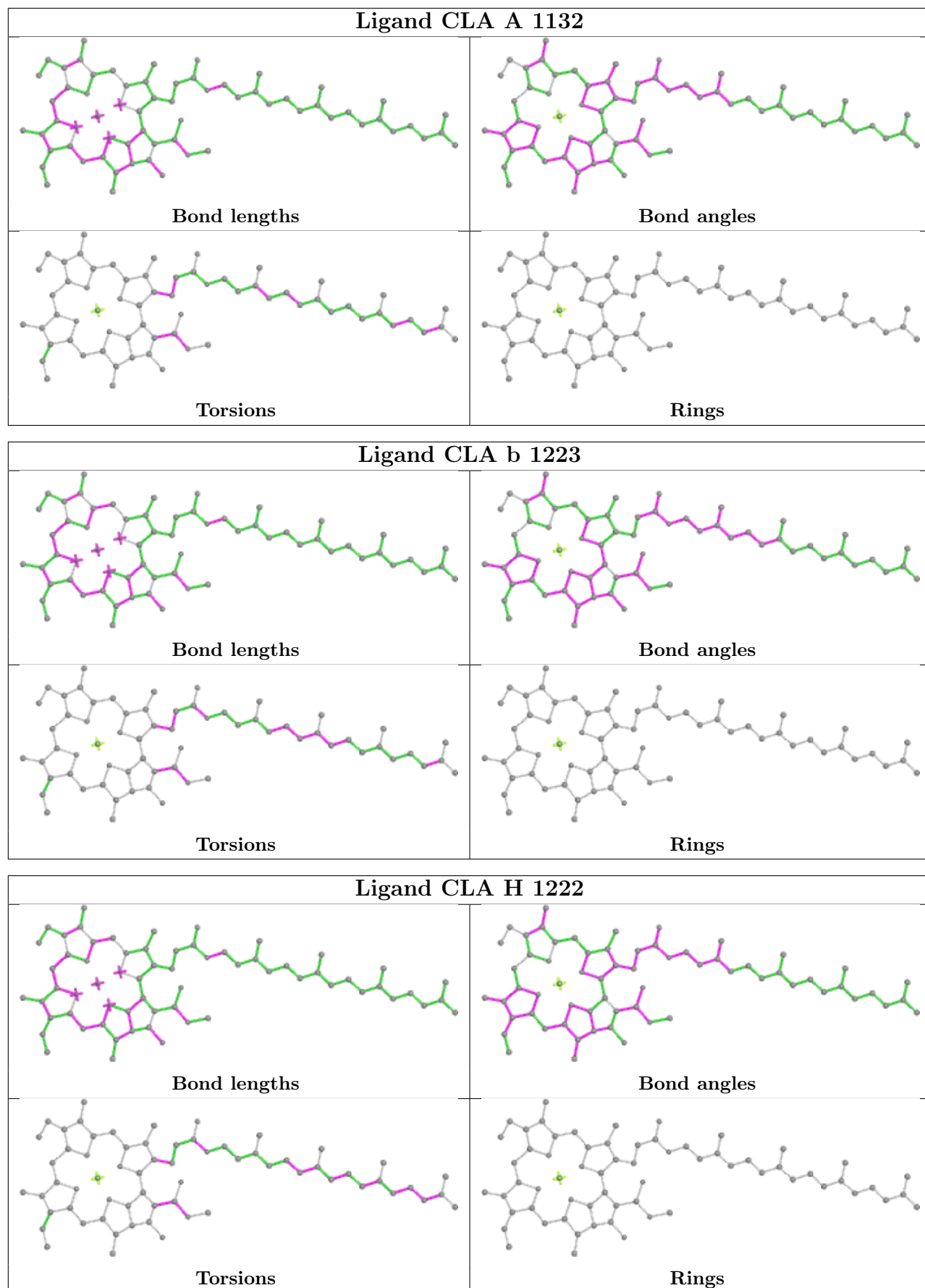




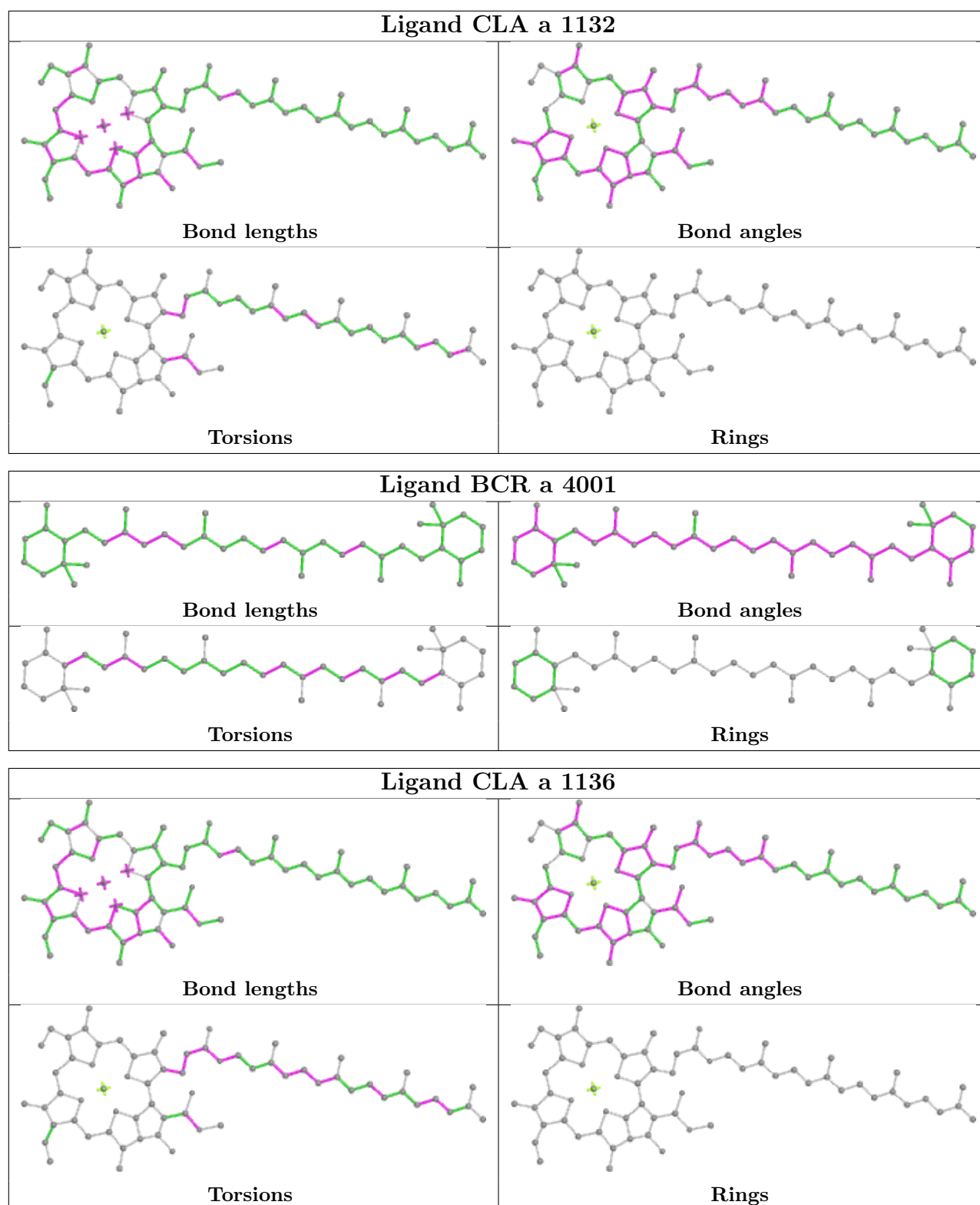


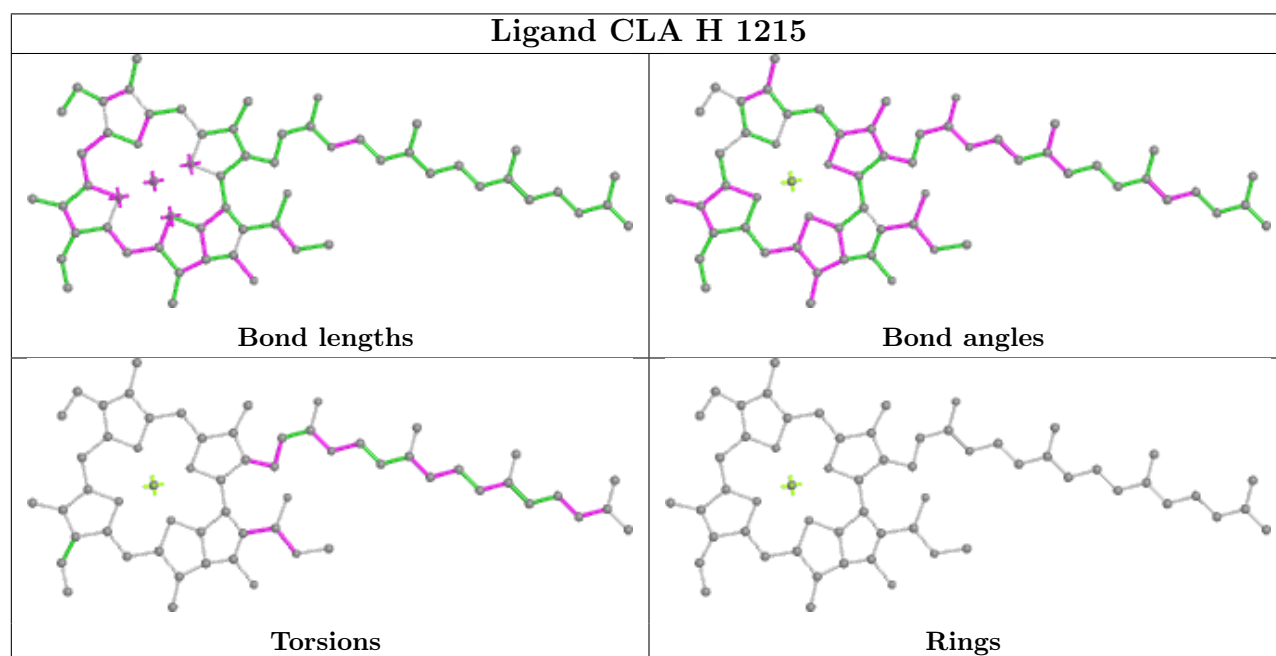
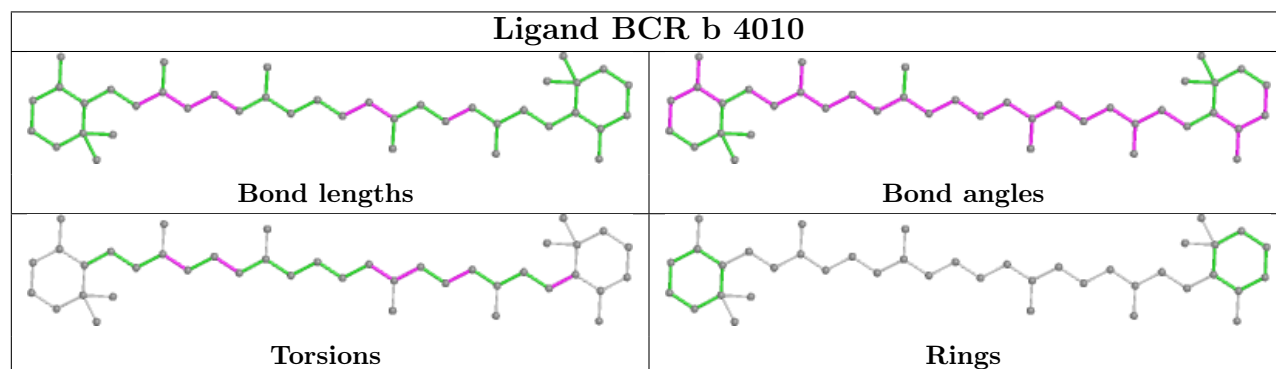
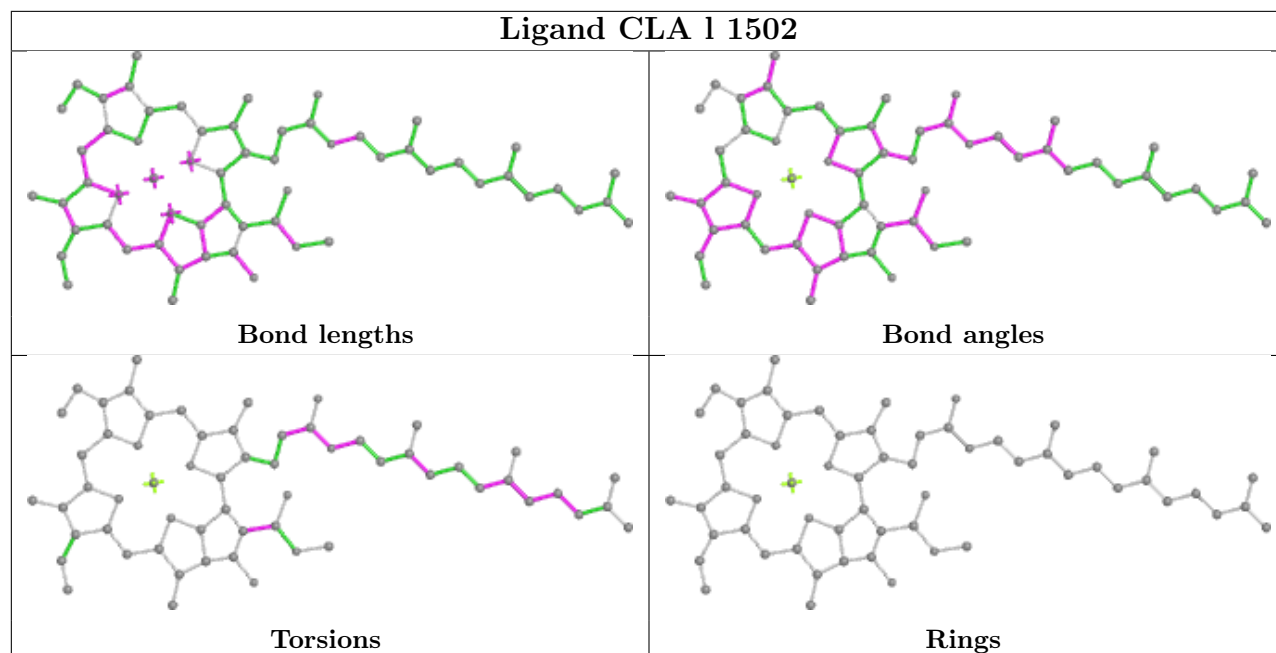












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	T	1
9	k	1
9	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	49:UNK	C	69:VAL	N	9.76
1	k	49:UNK	C	69:VAL	N	9.75
1	K	49:UNK	C	69:VAL	N	9.75

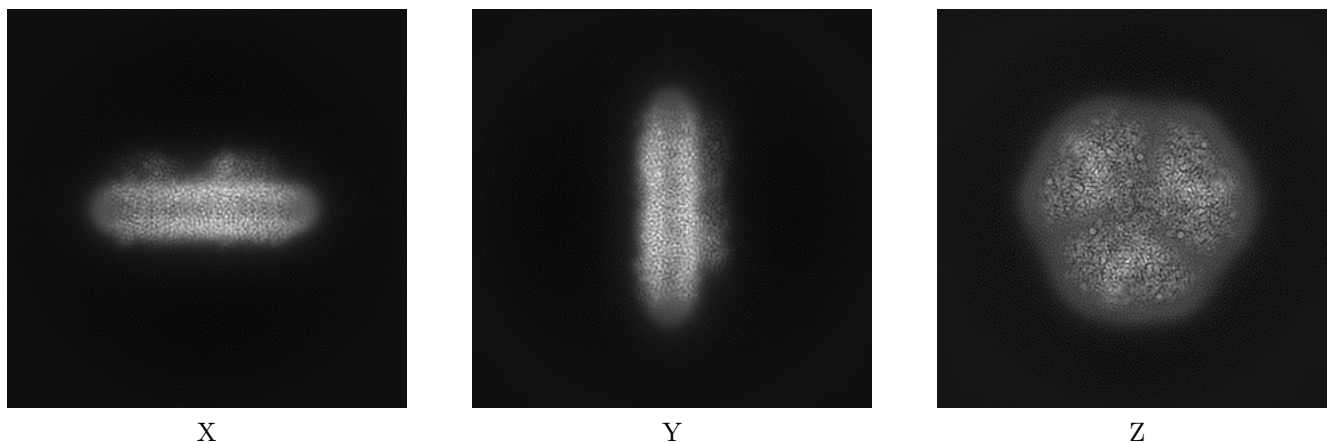
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23563. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

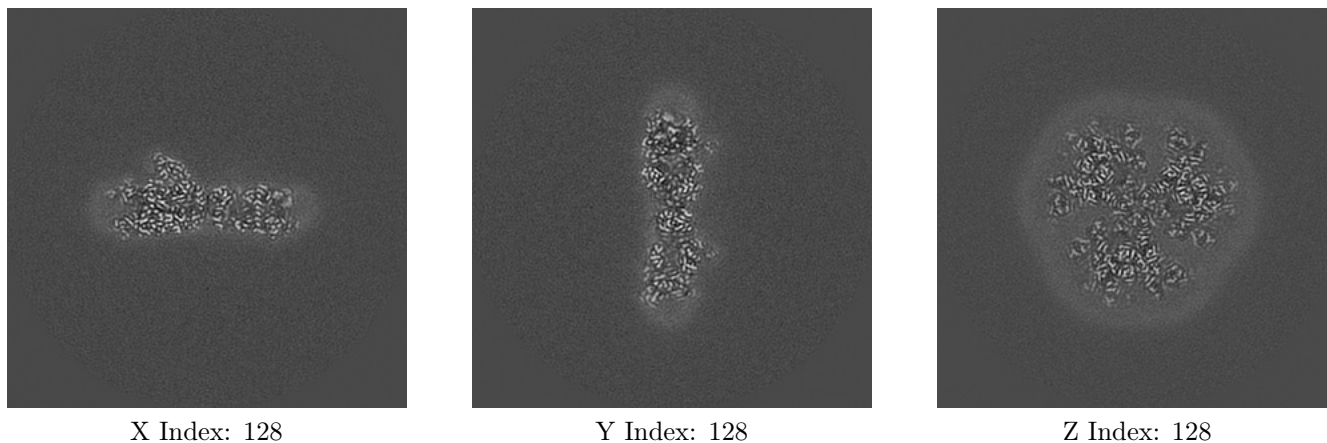
#### 6.1.1 Primary map



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

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

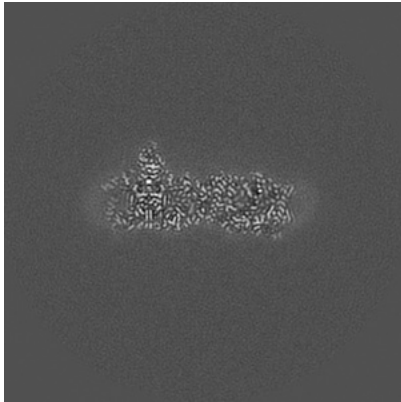
#### 6.2.1 Primary map



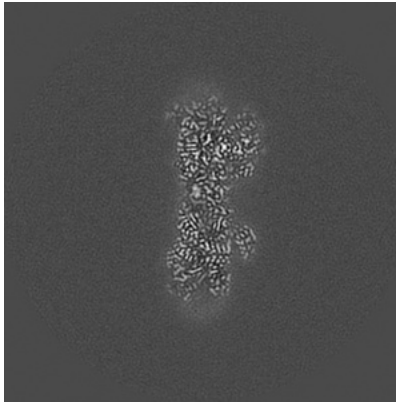
The images above show central slices of the map in three orthogonal directions.

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

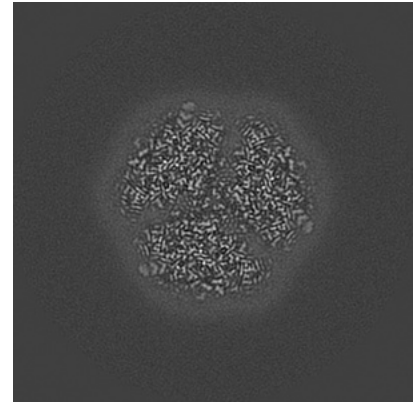
### 6.3.1 Primary map



X Index: 121



Y Index: 140

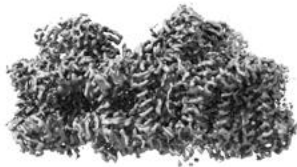


Z Index: 120

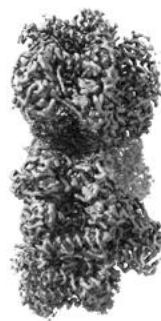
The images above show the largest variance slices of the map in three orthogonal directions.

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

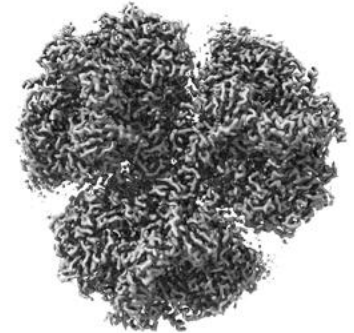
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

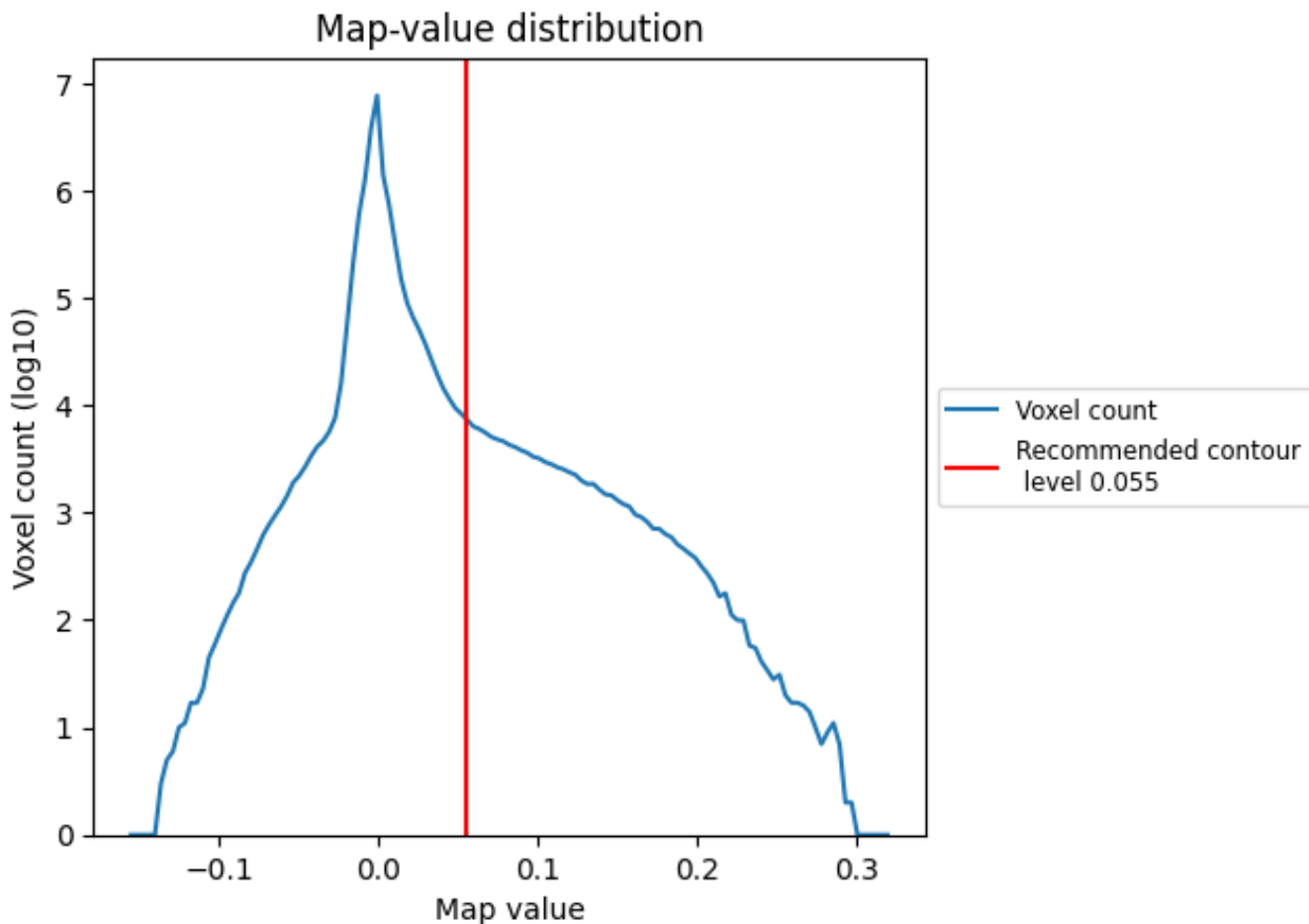
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

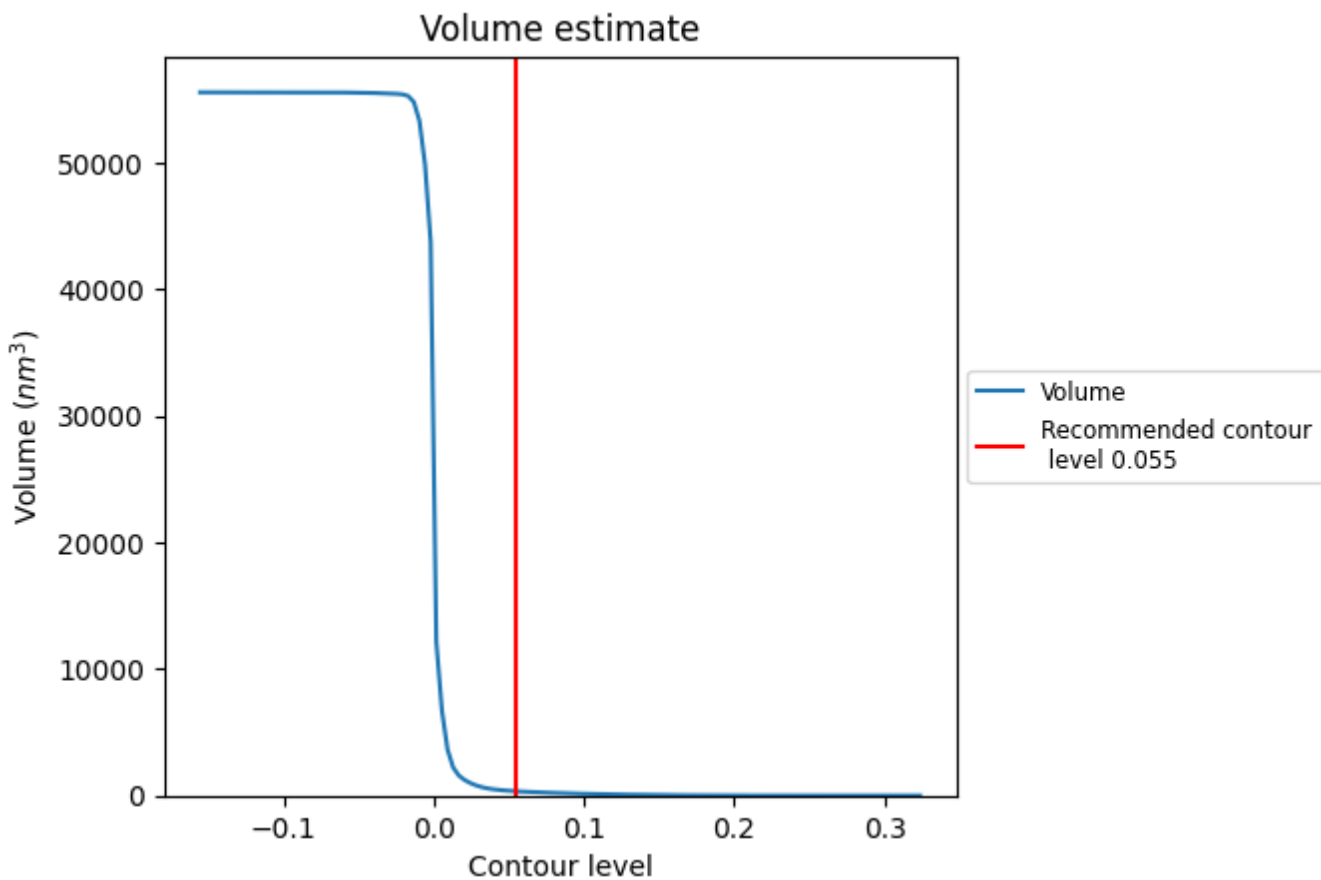
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

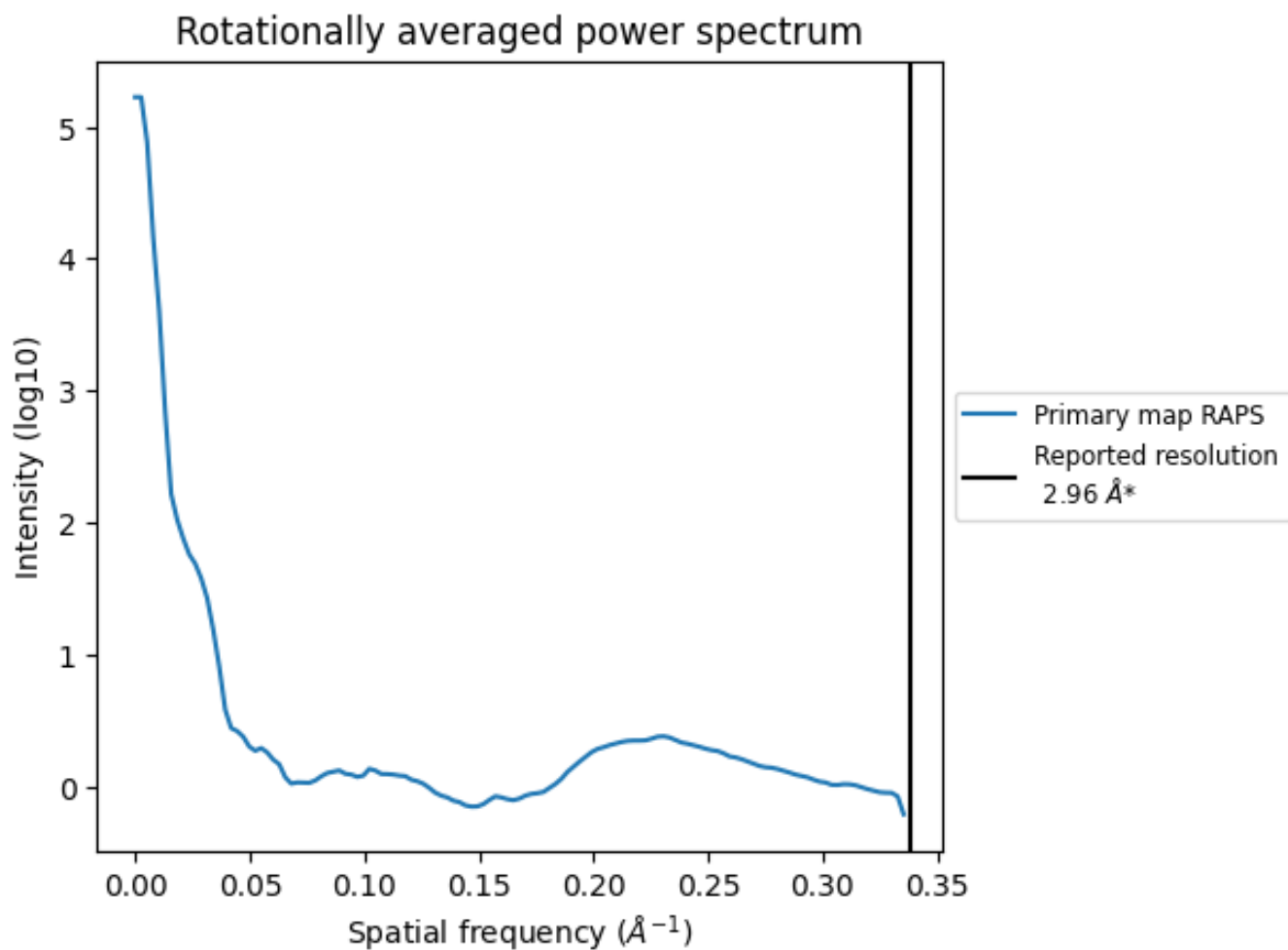


The volume at the recommended contour level is 339  $\text{nm}^3$ ; this corresponds to an approximate mass of 306 kDa.

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



### 7.3 Rotationally averaged power spectrum i

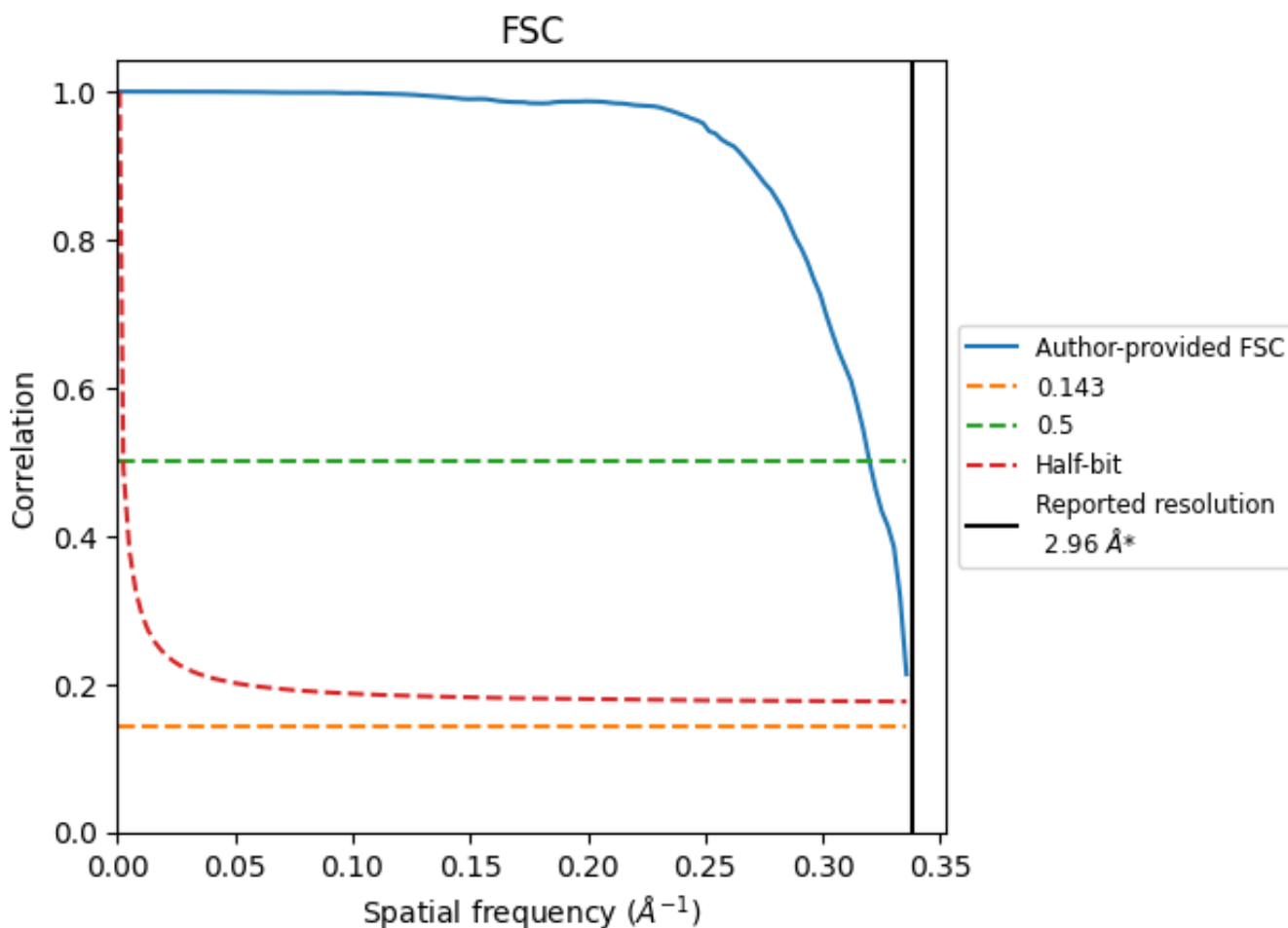


\*Reported resolution corresponds to spatial frequency of 0.338 Å<sup>-1</sup>

## 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 0.338 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

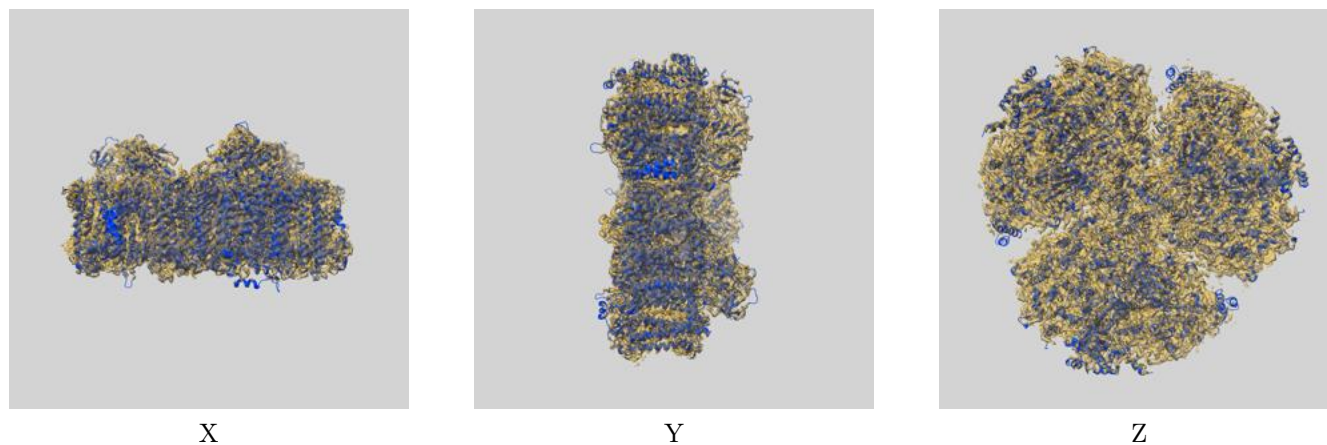
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	-	3.13	-
Unmasked-calculated*	-	-	-

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

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

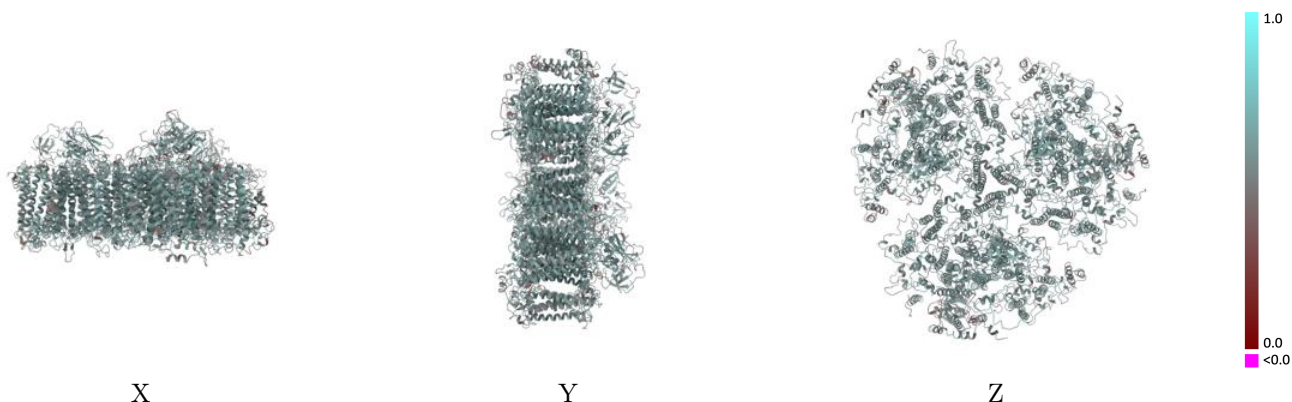
This section contains information regarding the fit between EMDB map EMD-23563 and PDB model 7LX0. Per-residue inclusion information can be found in section 3 on page 37.

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



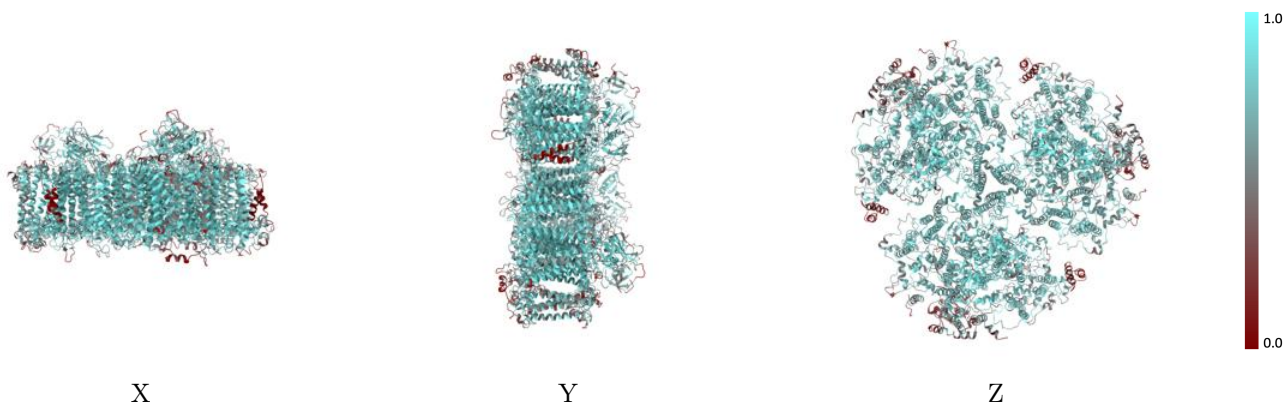
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



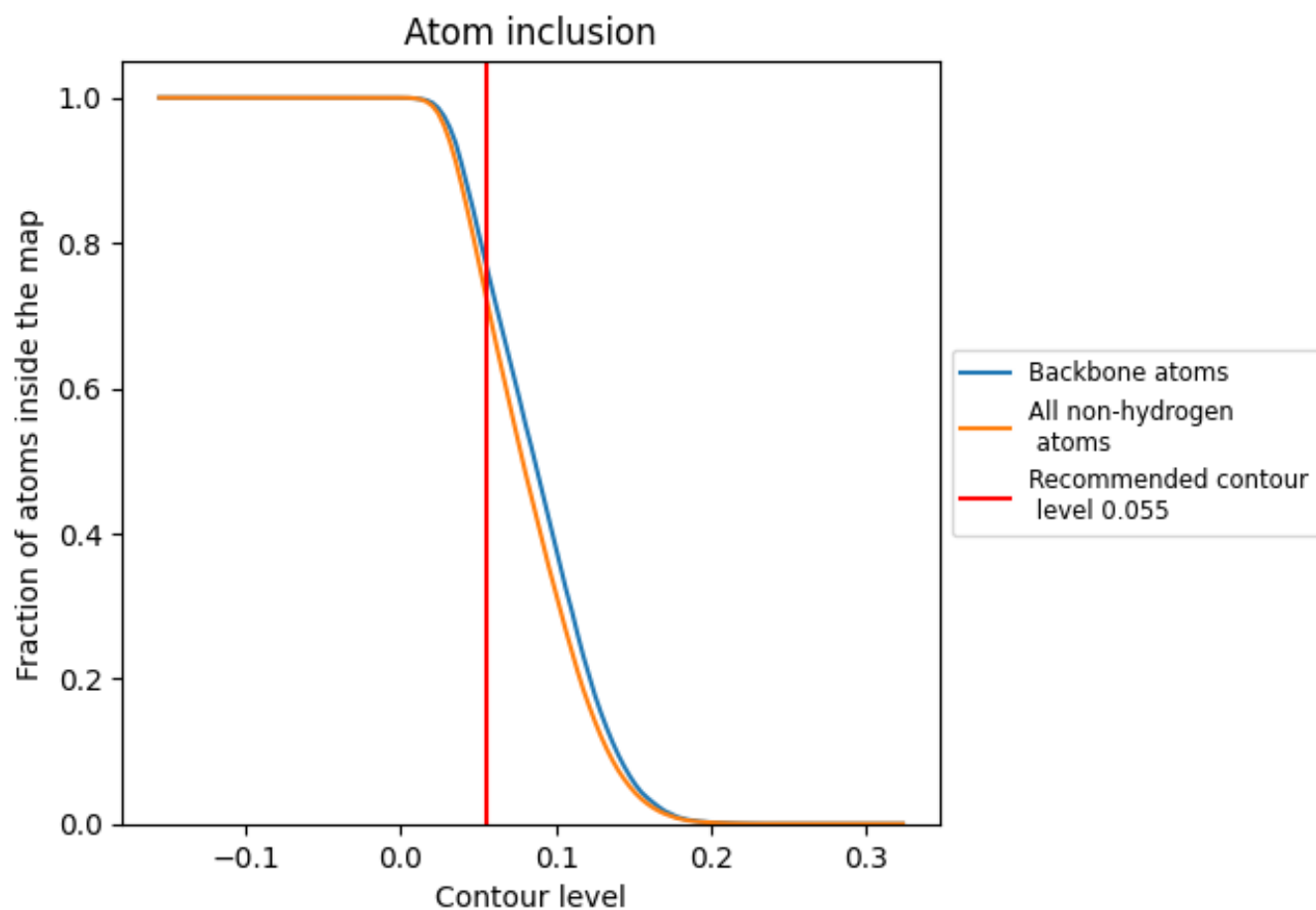
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.055).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 73% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7260	 0.5650
A	 0.7678	 0.5740
B	 0.7701	 0.5740
C	 0.7787	 0.5640
D	 0.6532	 0.5490
E	 0.5631	 0.5200
F	 0.3944	 0.4990
G	 0.7697	 0.5750
H	 0.7684	 0.5770
I	 0.7965	 0.5720
J	 0.4494	 0.4770
K	 0.0918	 0.4640
L	 0.7762	 0.5720
M	 0.7000	 0.5480
N	 0.7854	 0.5550
O	 0.6523	 0.5470
P	 0.5611	 0.5160
Q	 0.3973	 0.5010
R	 0.7835	 0.5670
S	 0.4583	 0.4730
T	 0.0714	 0.4560
U	 0.7795	 0.5690
V	 0.7107	 0.5530
W	 0.4914	 0.4970
X	 0.4811	 0.4960
a	 0.7691	 0.5770
b	 0.7654	 0.5770
c	 0.7870	 0.5610
d	 0.6448	 0.5480
e	 0.5404	 0.5100
f	 0.3964	 0.4930
i	 0.7922	 0.5750
j	 0.4405	 0.4730
k	 0.1054	 0.4620
l	 0.7703	 0.5720



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Chain	Atom inclusion	Q-score
m	 0.7000	 0.5570
x	 0.4777	 0.4930